HIDDEN IN THE LAYERS
Interpretation of Neural Networks for Natural Language Processing

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Contents

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Preface

In recent years, deep neural networks dominated the area of Natural Language Processing (NLP). For a while, it might almost seem that all tasks became purely machine learning problems, and the language itself became secondary. The primary problems are technical: getting more and more data and making the learning algorithms more efficient. Deep learning methods allow us to do machine translation, automatic text summarization, sentiment analysis, question answering, and many other tasks in a quality that was hardly imaginable ten years ago. This unprecedented progress in our ability to solve NLP tasks has its downsides too. End-to-end-trained models are black boxes that are very hard to interpret, and the model can manifest unintended behavior that can range from seemingly stupid and unexplainable errors to hidden gender or racial bias.

One of the main concerns of linguistics is to conceptualize language in such a way that allows us to name and discuss complex language phenomena that would otherwise be difficult to grasp or to teach a non-native speaker. Traditionally, NLP took over these conceptualizations and used them to represent language for solving practical tasks. Over time, it appeared that not all concepts from linguistics are necessarily useful for NLP. With deep neural networks, almost all linguistic assumptions were discarded. Sentences are treated merely as sequences of words that get split into smaller subword units based on simple statistical heuristics. Dozens of hidden layers of neural networks learn presumably a more and more abstract and more informative representation of the input until they ultimately provide the output without telling us what the representations in between mean.

This situation in NLP puts us into a unique situation. We have machine learning models that can do tasks as skillfully as never before and develop their own language representation. This calls for an inspection to what extent the linguistic conceptualizations are consistent with what the models learn. Do neural networks use morphology and syntax the way people do when they talk about language? Or do they develop their own better way? What is hidden in the layers?

Introduction

In this book, we try to peek into the black box of trained neural models, and to see how the emergent representations correspond to traditional linguistic abstractions. We mostly deal with large pre-trained language models and machine translation models.

In Chapter 1, we introduce the reader into the world of deep learning and its applications in Natural Language Processing (NLP). Readers who are experts in deep learning can skip this chapter. We hope others will find the introductory chapter useful even beyond the scope of this book.

In Chapter 2, we show how the deep learning concepts are used in several notable models, including Word2Vec, Transformer and BERT. The subsequent chapters deal with analyzing the models introduced in this chapter.

In Chapter 3, we look at the problem of interpreting trained neural network models in general. We also outline the two approaches that we focus on in this book: supervised probing, and unsupervised clustering and visualisation.

In Chapter 4, we discuss the interpretation of Word2Vec and other word embeddings. We show various methods for embedding space visualisation, component analysis and embedding space transformations for interpretation.

In Chapter 5, we analyze attention and self-attention mechanisms, in which we can observe weighted links between representations of individual tokens. We particularly focus on syntax, summarizing the amount of syntax in the attentions across the layers of several NLP models.

In Chapter 6, we look at contextual word embeddings and the linguistically interpretable features they capture. We try to link the linguistic features to various levels of linguistic abstraction, going from morphology over syntax to semantics.

1

Deep Learning

Before talking about the interpretation of neural networks in Natural Language Processing (NLP), we should explain what deep learning is and how it is used in NLP. In this chapter, we summarize the basic concepts of deep learning, briefly sketch the history, and discuss details of neural architectures that we talk about in the later chapters of the book.

1.1 Fundamentals of Deep Learning

Deep learning is a branch of Machine Learning (ML), and like many scientific concepts, it does not have an exact definition everyone would agree upon. By deep learning, we usually mean ML with neural networks that have many layers (Goodfellow et al., 2016). By 'many,' people usually mean more than experts before 2006 used to believe was numerically feasible (Hinton and Salakhutdinov, 2006; Bengio et al., 2007). In practice, the networks have dozens of layers.

The first method that allowed using multiple layers was unsupervised layer-wise pre-training (Bengio et al., 2007) that demonstrated the potential of deeper neural networks. These methods were followed by innovations allowing training the models end-to-end by error back-propagation only (Srivastava et al., 2014; Nair and Hinton, 2010; Ioffe and Szegedy, 2015; Ba et al., 2016; He et al., 2016) without any pre-training, which started the boom of deep learning methods after 2014.

1.1.1 What is Machine Learning?

Neural networks and other ML models are trained to fit training data, while still generalizing for unseen data, i.e., instances that were not in the training set. For example, we train a machine translation system on pairs of sentences that are translations of each other, but of course, the goal is to have a model that can reliably translate any sentence, not only examples from the training data.

During training, we try to minimize the error the model makes on the training data. However, minimizing the training error does not guarantee that the model works well for data that are not in the training set. In other words, even with a low training error, the model can *overfit*, i.e., perform well on the training data without generalizing for data instances not encountered during training. To ensure that the model can make correct predictions on data instances that were not used for training, we use

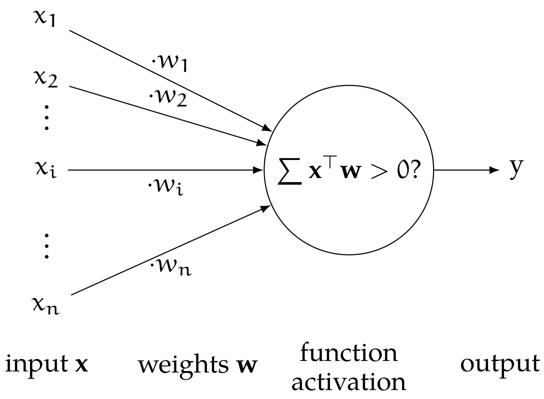


Figure 1.1: Illustration of a single artificial neuron with inputs $\mathbf{x} = (x_1, \dots, x_n)$ and weights $\mathbf{w} = (w_1, \dots, w_n)$.

another dataset, usually called the *validation set* that is only used for estimating the performance of the model on unseen data.

Deep learning models are particularly prone to overfitting. With millions of trainable parameters, they can easily memorize entire training sets. We already insinuated that the crucial part of the deep learning story is techniques that allow training bigger models with many layers. Bigger models have a bigger capacity to learn more complicated tasks. Large models are, on the other hand, more prone to overfitting. The History of deep learning is a somewhat story of innovations that allow training larger models and innovations that prevent large models from overfitting.

1.1.2 Perceptron Algorithm

Deep learning originates in studying artificial neural networks (Goodfellow et al., 2016, p. 12). Artificial neural networks are inspired by a simplistic model of a biological neuron (McCulloch and Pitts, 1943; Rosenblatt, 1958; Widrow, 1960). In the model, the neuron collects information on its dendrites. Based on that, it sends a signal on the axon, its single output. Formally, we say that the artificial neuron has an input, a vector $\mathbf{x} = (x_1, \dots, x_n) \in \mathbb{R}^n$ of real numbers. For each input component x_i, there is a weight $w_i \in \mathbb{R}$ corresponding to the importance of the input component. The weighted sum of the input is called the *activation*. We get the neuron *output* by applying the *activation function* on the activation. In the simplest case, the activation function is the signum function. More activation functions are discussed in Section 1.2. The model is illustrated in Figure 1.1.

The first successful experiments with such a model date back to the 1950s when the geometrically motivated perceptron algorithm (Rosenblatt, 1958) for learning the model weights was first introduced. The model is used for the classification of the inputs into two distinct classes. The inputs are interpreted as points in a multi-dimensional vector space. The learning algorithm searches for a hyperplane separating one class of the inputs from the other. The trained weights are interpreted as a normal vector of the hyperplane. The algorithm iterates over the training examples: If an example is misclassified, it rotates the hyperplane towards the misclassified example by subtracting the input from the weight vector. This simple algorithm is guaranteed to converge to a separating hyperplane if it exists (Novikoff, 1962). The linear-algebraic intuition developed for the perceptron algorithm is also important for the current neural networks where inputs of network layers are also interpreted as points in multi-dimensional space.

During the following 60 years of ML and Artificial Intelligence (AI) development, neural networks fell out of the main research interest, especially during the so-called AI winters in the 1970s and 1990s (Crevier, 1993, p. 203).

In the rest of the chapter, we do not closely follow the history of neural networks but only discuss the innovations that seem to be the most important from the current perspective. Techniques that are particularly useful for NLP are then discussed in Section 1.3. For a comprehensive overview of the history of neural network research, we refer the reader to a survey by Schmidhuber (2014).

1.1.3 Multi-Layer Networks

The geometrically motivated perceptron learning algorithm cannot be efficiently generalized to networks with a more complicated structure of interconnected neurons. With more a complex network structure, we no longer interpret the learning as a geometric problem of finding a separating hyperplane. Instead, we view the network as a parameterized continuous function. The goal of the learning is to optimize the parameter values with respect to a continuous error function, usually called the *loss function*. The loss function is usually some kind of continuous dissimilarity measure between the network output from the desired output.

During training, we treat the network as a function of its parameters, given a training dataset that is considered constant at one training step. This allows computing gradients of the network parameters with respect to the loss function and updating the parameters accordingly. The training uses a simple property of derivative that it determines the direction in which a continuous function increases or decreases. This information can be used to shift the parameters in such a way that the loss function decreases. Note that each gradient is computed independently, and we only compute the derivatives at a particular point, so we can only shift the parameters by a small step in the direction of the derivatives. Furthermore, with a large training set, we are able to process only small batches of training data, which introduces stochasticity in the

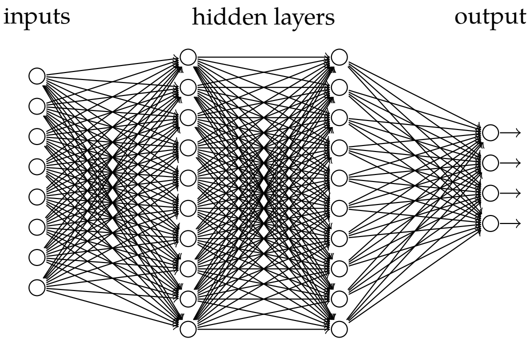


Figure 1.2: Multi-layer perceptron with two fully connected hidden layers.

training process, i.e., add random noise that increases the robustness of the training. The training algorithm is called *stochastic gradient descent*.

At inference time, the parameters are fixed, and the network is treated as a function of its inputs with constant parameters.

The original perceptron used the signum function as the activation function. In order to make the function defined by the network differentiable, the signum function was often replaced by sigmoid function or hyperbolic tangent, yielding values between -1 and 1.

For the sake of efficiency, the neurons in artificial neural networks are almost always organized in layers. This allows us to re-formulate the computation as a matrix multiplication (Fahlman and Hinton, 1987). Layers implemented by matrix multiplication are called *fully connected* or *dense* layers. Let $\mathbf{h}_i = (h_i^0, \ldots, h_i^n) \in \mathbb{R}^n$ be the output of the i-th layer of the network and the input of the $(i+1)$-th layer. Let $A : \mathbb{R} \to \mathbb{R}$ be the activation function. The value of the k-th neuron in the $(i+1)$-th layer of dimension m is

$$h_{i+1}^k = A\left(\sum_{l=0}^{n} h_i^l \cdot w_i^{(l,k)} + b_i^{(k)}\right) \tag{1.1}$$

which is, in fact, the definition of matrix multiplication. It thus holds:

$$\mathbf{h}_{i+1} = A\left(\mathbf{h}_i \mathbf{W}_i + \mathbf{b}_i\right) \tag{1.2}$$

where $\mathbf{W}_i \in \mathbb{R}^{n \times m}$ is a parameter matrix, and $\mathbf{b}_i \in \mathbb{R}^m$ is a bias vector.

Not only did this make the computation efficient, but it also led to a reconceptualization of the network architectures. Current literature no longer talks about single neurons, but almost always about network layers. This reconceptualization then allows innovations like attention mechanism (Bahdanau et al., 2014), residual connec-

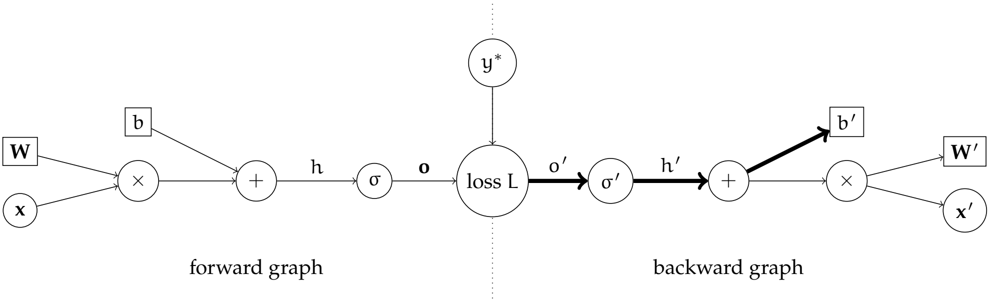


Figure 1.3: Computation graph for back-propagation algorithm for logistic regression $o = \sigma(\mathbf{W}\mathbf{x} + b)$. The highlighted path corresponds to the computation of $\frac{\partial L}{\partial b}$, which is, according to the algorithm, equal to $\frac{\partial L}{\partial o} \cdot \frac{\partial o}{\partial h} \cdot \frac{\partial h}{\partial b}$.

tions (He et al., 2016), or layer normalization (Ba et al., 2016) which conceptually, not only for the sake of computational efficiency, treat the neuron outputs as elements of vectors and matrices.

A network with feed-forward fully connected layers is illustrated in Figure 1.2. This architecture is usually called a *multi-layer perceptron*, even though it is not trained with the perceptron algorithm but using the error back-propagation algorithm.

1.1.4 Error Back-Propagation

We already mentioned how a neural network is trained when the parameter gradients are known. For simple networks, it was possible to infer the equations for the gradients using pen and paper. For more complicated networks, an algorithmic solution poses a great advantage.

The *Error Back-Propagation* Algorithm (Werbos, 1990) is a simple graph algorithm that can infer equations for parameter gradients for an arbitrarily complicated network. This invention opened a path for training large networks.

While using the back-propagation algorithm, we represent the computation as a directed acyclic graph where each node corresponds to an input, trainable parameter, or an operation. This graph is called the *forward computation graph*. To compute the derivative of a parameter with respect to the function, we build a *backward graph* with reversed edges and operations replaced by their derivatives. The derivative of a parameter with respect to the loss is then computed by multiplying the values on a path from the loss to a copy of the parameter in the backward graph. The algorithm is illustrated in Figure 1.3.

The back-propagation algorithm, together with techniques ensuring a smooth gradient flow within the network and regularization techniques, allows training models end-to-end from raw input. During the training process, neural networks develop an input representation such that the task that we train the model for becomes easy to solve (Bengio et al., 2003; LeCun et al., 2015). However, it took more than ten years before this remarkable property of the learning algorithm attracted the attention of the researchers.

1.1.5 Representation Learning

Deep learning dramatically changes how data is represented. In NLP, the text used to be tokenized and enriched by automatic annotations that include part-of-speech tags, syntactic relations between words or entity detection. This representation was usually used to get meaningful features for a ML model. In statistical Machine Translation (MT), words are represented by monolingual and bilingual co-occurrence tables, which are used for probability estimations within the models. In deep learning models, the text is represented with tensors of continuous values that are not explicitly hand-designed but implicitly inferred during model optimization.

This is often considered to be one of the most important properties of neural networks. Goodfellow et al. (2016, p. 5) even consider the representation learning ability to be the feature that distinguishes deep learning from the previous ML techniques. In both Computer Vision (CV) and NLP models, consecutive layers learn more contextualized and presumably more abstract representation of the input. As we will discuss in the following sections, the representations learned by the networks are often general and can often be reused for solving different tasks than they were trained for.

1.2 Deep Learning Techniques in Computer Vision

Although this book is primarily about neural networks in NLP, the story of deep learning would not be complete if we did not mention innovations that come from CV. The success of deep neural networks in CV tasks started the increased interest in neural networks, and it is likely that without the progress made in CV, deep learning would not be as successful in NLP either.

Images are usually represented as a table of three-channel (RGB: red, green, blue) pixels, i.e., a three-dimensional tensor. Note that if we disregard the exact number of channels, this is the same form as the input and output of most network layers. This allows us to treat the input in the same way as all other layers in the network.

1.2.1 Convolutional Networks

The main tool used in CV are convolutional networks (LeCun et al., 1998). The main components used in Convolutional Neural Networks (CNNs) are convolutional and max-pooling layers.

Two-dimensional convolutions can be explained as applying a sliding window projection over a 3D input tensor and measuring the similarity between the input

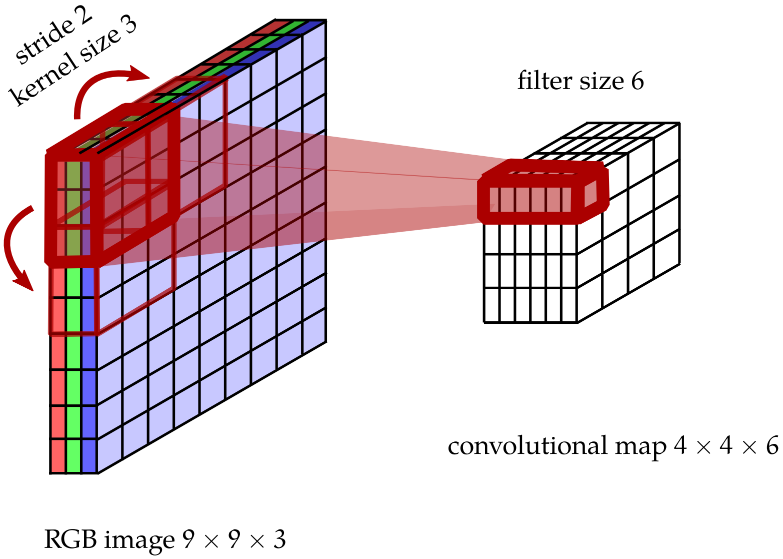

stride 2
kernel size 3
filter size 6
convolutional map $4 \times 4 \times 6$
RGB image $9 \times 9 \times 3$

Figure 1.4: Illustration of a 2D convolution over a 9×9 RGB image with stride 2, kernel size 3 and number of filters 6.

window and filters that are the learned parameters of the models. The two main hyperparameters of a convolutional layer are the number of filters and the window size. Another attribute of the convolution is the *stride* which is the size of the step by which the window moves. The resulting feature map is roughly stride-times smaller in the first two dimensions (weight and height). A 2D convolution over an RGB image is illustrated in Figure 1.4.

Max-pooling is a dimensionality reduction technique that is used to decrease information redundancy during image processing. Similarly to convolutions, it proceeds as a sliding window and reduces each window into a single vector by taking the maximum values from the window. Alternatively, average-pooling can be used that yields the average of the window instead of the maximum.

Convolution is usually interpreted as a latent feature extraction over the input tensor where the filters correspond to the latent features. Max-pooling can be interpreted as a soft existential quantifier applied over the window, i.e., the result of max-pooling says whether and how much the latent features are present in the given region of the image.

Visualizations of trained convolution filters show that the representation in the network is often similar to features used in classical CV methods such as edge detection (Erhan et al., 2009). It also appears that with the growing number of layers, more

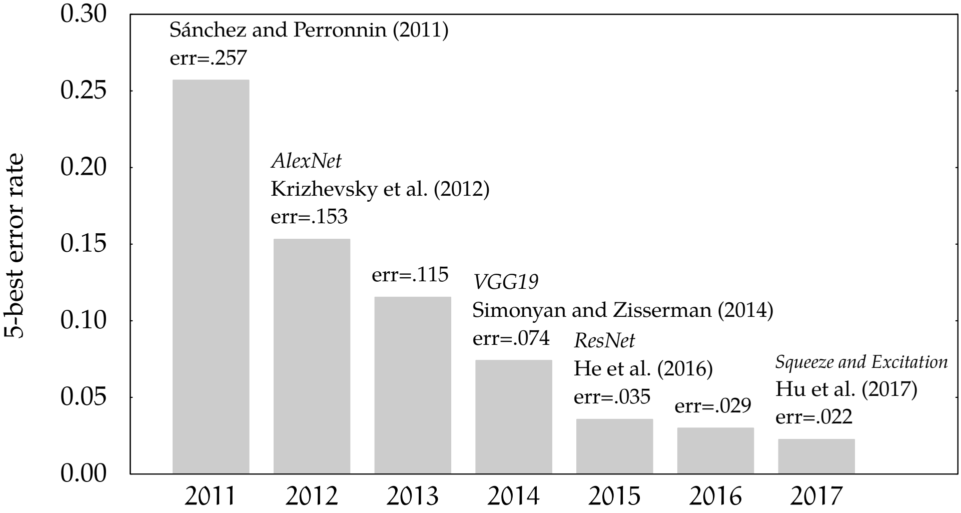


Figure 1.5: Development of performance in ImageNet image classification task between 2011 and 2017. The figures are taken from the official website of the challenge. Columns without citations correspond to submissions that did not provide a citation.

abstract representations are learned (Mahendran and Vedaldi, 2015; Olah et al., 2017). Although, in theory, shallow networks with a single hidden layer have the same capabilities (Hornik, 1991), in practice, well-trained deeper networks usually perform better (Goodfellow et al., 2016, p. 192–194).

CNNs operating in only one dimension are also used in NLP. Deep one-dimensional CNNs got a lot of attention in 2017 because they offered a significant speedup compared to methods that were popular at that time (e.g., in machine translation: Gehring et al., 2017; or question answering: Wu et al., 2017). However, soon the NLP community shifted to Self-Attentive Networks (SANs) that allow the same speedup by parallelization and better performance.

1.2.2 AlexNet and Image Classification on the ImageNet Challenge

The mechanism of convolutional and max-pooling layers in CNNs is known since 1998 when LeCun et al. (1998) used them for hand-written digit recognition, but they reached mainstream popularity after Krizhevsky et al. (2012) used them in the ImageNet challenge (Deng et al., 2009). For a long time, the ImageNet challenge was the main venue where researchers in CV compared their methods, and many of the crucial innovations in deep learning were introduced in the context of this challenge.

The challenge uses a large dataset of manually annotated images. Every image is a real-world photograph focused on one object of 1,000 classes. The classes are objects from every-day life, excluding persons. The labels of the objects are manually linked with WordNet synsets (Miller, 1995). The training part of the dataset consists of 150 million labeled images. The test set contains another 150 thousand images, an order of magnitude bigger than all previously used datasets. Note that the word 'net' in the dataset name does not refer to neural networks but WordNet, which was an inspiration for creating the ImageNet dataset.

During the last years, CNNs and other deep learning techniques helped to decrease the 5-best error more than ten times (see Figure 1.5 for more details). The 5-best error is the proportion of cases when the correct label is not present in the 5 best-scoring labels, the primary evaluation measure on this task.

AlexNet (Krizhevsky et al., 2012) was the first model that succeeded in the challenge, and it is often said that its success started the new interest in deep learning. The model combines many recent innovations in neural networks at the same time and used an efficient GPU implementation, which was not common at that time. The network outperformed all previous approaches by a large margin. Moreover, the image representation learned by the network (activations in its penultimate layer) showed interesting semantic properties, allowing the network to be used to estimate image similarity based on its content.

AlexNet consists of five convolutional layers interleaved by three max-pooling layers and followed by two fully connected layers. CNNs were well-known at that time; however, AlexNet was deeper than previously used CNNs and took advantage of several recent innovations.

One important innovation was the use of Rectified Linear Units (ReLUs) (Hahnloser et al., 2000; Nair and Hinton, 2010) instead of the smooth activation functions mentioned in the previous section (1.1).

This activation function allows better propagation of the loss gradient to deeper layers of the network by reducing the effect of the vanishing gradient problem. The derivative of hyperbolic tangent has an upper bound of one and has values close to zero on most of its domain. Therefore, training networks with more than one or two hidden layers (AlexNet had seven layers; Krizhevsky et al., 2012) is hardly possible with the traditional smooth activation functions. During the computation of the loss gradient with the chain rule, the gradient gets repeatedly multiplied by values smaller than one and eventually vanishes. ReLU reduces this effect, although it does not entirely solve this problem. However, the gradient is still zero on half of the domain, which means that the probability that the gradient is zero grows exponentially with the network depth. See Figure 1.6 for visualization of the activation function course and their derivatives.

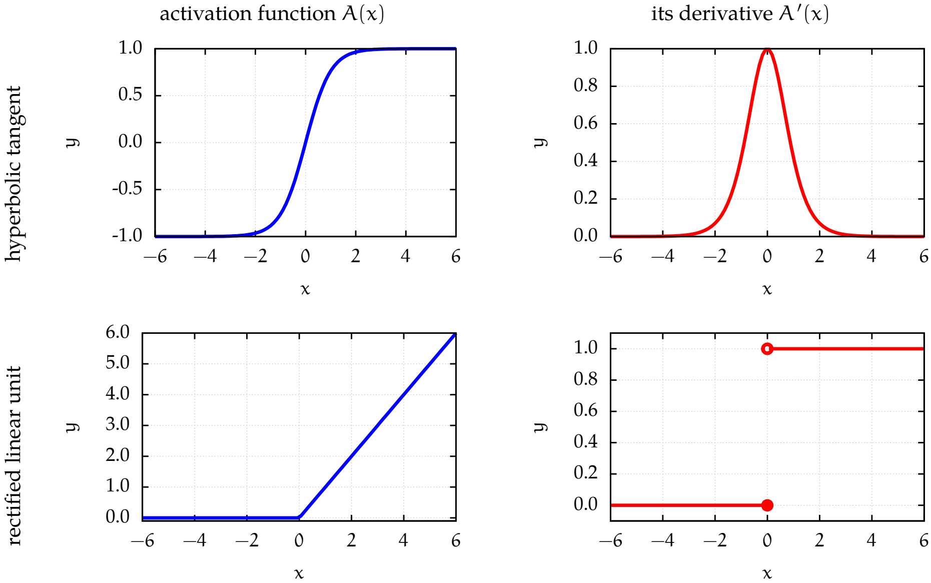


Figure 1.6: Activation functions and their derivatives.

The AlexNet network has 208 million parameters, making it prone to overfitting because it has a capacity to memorize the training set with only little generalization. AlexNet used *dropout* (Srivastava et al., 2014)[1] to reduce overfitting. It is a technique that introduces random noise in the network during training and thus forces the model to be more robust to variance in the data. With dropout, neuron outputs are randomly set to zero with a probability that is a hyperparameter of model training. In practice, dropout is implemented as multiplication by a random binary matrix after applying the activation function. Dropout can also be interpreted as ensembling exponentially many networks with a subset of currently active neurons that share all their weights (Hara et al., 2016).

Both dropout and ReLU are now one of the key techniques used both in CV and NLP.

1.2.3 Convolutional Networks after AlexNet

The development of neural networks for CV did not stop with AlexNet. Except for vision-specific best-practices (Simonyan and Zisserman, 2014), two major innovations

[1] The paper was published in a journal in 2014, however its preprint was available already in 2012 before the ImageNet competition.

come from image recognition, and that now play a crucial role in deep Recurrent Neural Networks (RNNs) and Transformers in NLP.

As we discussed in the previous section, one of the major problems of the deep neural network architectures is the vanishing gradient problem, which makes training of deeper models difficult. The ReLU activation function partially solved the problem because the gradients are always either ones or zeros. Dropout can help by forcing updates in neurons that would otherwise never change. Other techniques also help to improve the gradient flow in the network during training.

One of them is the normalization of the network activation. These are regularization techniques that ensure that the neuron activations have almost zero mean and almost unit variance. It makes propagation of the gradient easier by keeping the neuron activations near the values where the derivatives of the activation functions vary the most.

Batch normalization (Ioffe and Szegedy, 2015) and layer normalization (Ioffe and Szegedy, 2015) are the most frequently used. Batch normalization attempts to ensure that activation values for each neuron are normally distributed over the training examples. Layer normalization, on the other hand, normalizes the activations on each layer.

The normalization tricks allowed the development of another technique that makes training of networks with many layers easier, *residual connections* (He et al., 2016). In residual networks, outputs of later layers are summed with outputs of previous layers (see Figure 1.7).

Residual connections improve the gradient flow during the loss back-propagation because the loss does not need to propagate via the non-linearities causing the vanishing gradient problem. It can flow directly via the summation operator, which is linear with respect to the derivative. Note also that applying the residual connection requires that the dimensionality of the layers must not change during the convolution.

Before introducing residual connections, the state-of-the-art image classification networks had around 20 layers (Simonyan and Zisserman, 2014; Szegedy et al., 2015), ResNet (He et al., 2016), the first network with residual connections, used up to 150 layers while decreasing the classification error to only 3.5%.

Image classification into 1,000 classes is not the only task that the CV community attempts to solve. CV tasks include object localization (Girshick, 2015; Ren et al., 2015), face recognition (Parkhi et al., 2015; Schroff et al., 2015), traffic sign recognition (Zhu et al., 2016), scene text recognition (Jaderberg et al., 2014) and many others. Although there are many task-specific techniques, in all current approaches, images are first processed using a stack of convolutional layers with max-pooling and other techniques also used in image classification.

Representations learned by networks trained on the ImageNet dataset generalize beyond the scope of the task and seem to be aware of abstract concepts (Mahendran and Vedaldi, 2015; Zeiler and Fergus, 2014; Olah et al., 2017). The ImageNet dataset is also one of the biggest CV datasets available, often orders of magnitude bigger than

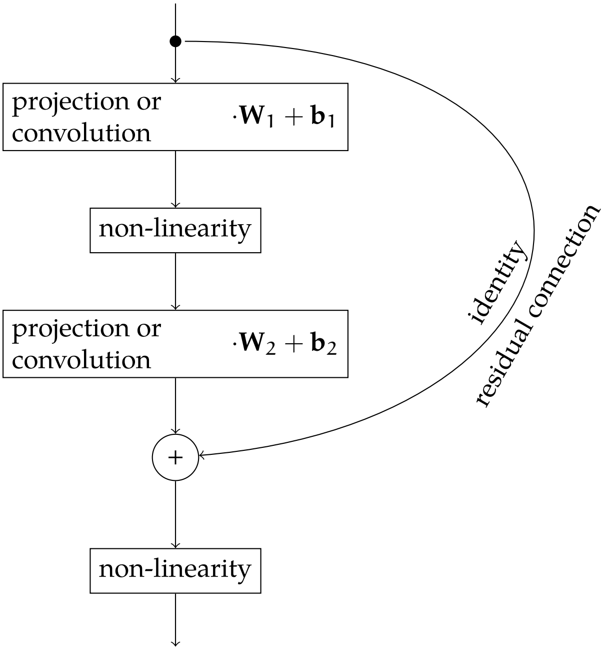

projection or convolution
$\cdot\mathbf{W}_1 + \mathbf{b}_1$
non-linearity
projection or convolution
$\cdot\mathbf{W}_2 + \mathbf{b}_2$
+
non-linearity
identity
residual connection

Figure 1.7: Network with a residual connection skipping one layer.

datasets for more specific tasks (Huh et al., 2016). This makes the representations learned by the image classification networks suitable to use in other CV tasks (such as object detection Girshick, 2015; animal species classification Branson et al., 2014; or satellite image Marmanis et al., 2016) as well as tasks combining vision with other modalities (such as visual question answering, Antol et al., 2015; or image captioning Vinyals et al., 2015). After 2018 (Peters et al., 2018a; Devlin et al., 2019), the reuse of pretrained representations from networks trained for different tasks became standard in NLP as well.

1.3 Deep Learning Techniques in Natural Language Processing

Unlike CV that processes continuous signals that can be directly provided to a Neural Network (NN), in NLP, we need to deal with the fact that language is written using discrete symbols. The use of the symbols, how the symbols group into words, or larger units, the amount of information carried by a single symbol; this all varies dramatically across languages. Nevertheless, the symbols are always discrete. Deep learning models for NLP thus need to convert the discrete input into a continuous representation that is processed by the network before it eventually generates a discrete output.

In all NLP tasks, we can thus distinguish three phases of the computation:

- Obtaining a continuous representation of the discrete input (often called word or symbol *embedding*) by replacing the discrete symbols with continuous vectors;
- Processing of the continuous representation (*encoding*) using various architectures;
- Generating discrete (or rarely continuous) output, sometimes called *decoding*.

Approaches to the phases may vary in complexity. This is most apparent in the case of generating an output which can be done either using simple classification, sequence labeling techniques such as conditional random fields (Lafferty et al., 2001) or connectionist temporal classification (Graves et al., 2006) or using relatively complex autoregressive decoders (Sutskever et al., 2014).

The rest of the section discusses these three phases in more detail. First (Section 1.3.1), we discuss embedding of discrete symbols into a continuous space. In the following section (1.3.2), we discuss three main architectures that can be used for processing an embedded sequence: RNNs, CNNs, and SANs. The following section (1.3.3) summarizes classification and sequence labeling techniques as a means of generating discrete output. Finally, we discuss autoregressive decoding which is a technique that allows generating arbitrarily long sequences.

1.3.1 Word Embeddings

Neural networks rely on continuous mathematics. When using neural networks for NLP, we need to bridge the gap between the symbolic nature of the written language and the continuous quantities processed by neural networks. The most intuitive way of doing so is using a predefined finite indexed set of symbols called a vocabulary (those are typically words, characters, or sub-word units) and represent the input as one-hot vectors.

We denote a *one-hot vector* having one on the i-th position and zeros elsewhere as $\mathbf{1}_i$ (see Figure 1.8). If the one-hot vector is used as the input of a layer, it gets multiplied by a weight matrix. The multiplication then corresponds to selecting one column from the weight matrix. The vectors that form the weight matrix are called symbol *embeddings*.

The embeddings are sometimes also called the *distributed representation* of the input tokens to stress out that the information about the word is no longer present in a single dimension of the input vector, but distributed in all dimensions of the embeddings. However, following this principle, all hidden layers of a NN can be considered a distributed representation of the input. To avoid this confusion and confusion with distributional semantics, we avoid using this term.

Note also that in this setup, the only information that the networks have available about the input words is that they belong to certain classes of equivalence (usually we

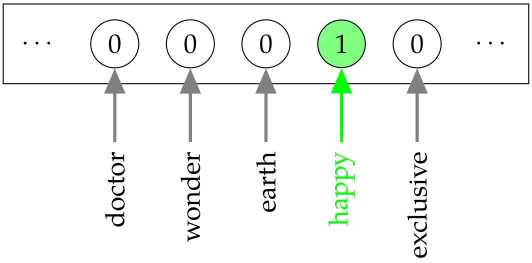


Figure 1.8: Illustration of a one-hot vector.

consider words with the same spelling to be the equivalent) indicated by the one-hot vector. The only information that the network can later work with is the co-occurrence of these classes of equivalence and their co-occurrence with target labels. The models thus heavily rely on the distributional hypothesis (Harris, 1954). The hypothesis says that the meaning of the words can be inferred from the contexts in which they are used. The success of neural networks for NLP shows that the hypothesis holds at least to some extent.

Now, consider we are going to train a neural network that predicts a probability of a word in a sentence given a window of its three predecessors, i.e., acts like a four-gram Language Model (LM). The network has three input words represented by one-hot vectors with vocabulary V, and one output, a distribution over the same vocabulary. For simplicity, we further assume the network has one hidden layer $\mathbf{h} \in \mathbb{R}^m$ of dimension m before the classification layer. Formally, we can write:

$$\mathbf{h} = \tanh\left(\mathbf{1}_{w_{n-3}}\mathbf{W}_3 + \mathbf{1}_{w_{n-2}}\mathbf{W}_2 + \mathbf{1}_{w_{n-1}}\mathbf{W}_1 + \mathbf{b}_h\right) \tag{1.3}$$

$$\mathsf{P}(w_n) = \operatorname{softmax}(\mathbf{Wh} + \mathbf{b}) \tag{1.4}$$

where $\mathbf{W}_i \in \mathbb{R}^{|V| \times m}$ are the embedding matrices for the words in the window of predecessors and $\mathbf{W} \in \mathbb{R}^{m \times |V|}$ a projection matrix from the hidden state $\mathbf{h}$ to the output distribution, $\mathbf{b}_h$ and $\mathbf{b}$ are corresponding biases, tanh is an arbitrarily chosen activation function.

All four projection matrices have $|V| \cdot m$ parameters. With the vocabulary size of ten thousand words and the hidden layer with hundreds of hidden units, this means millions of parameters. All three embedding matrices have a similar function in the model. They project the one-hot vectors to a common representation used in the hidden layer, also reflecting the position in the window of the predecessors. The target representation space used by the hidden layer should be the same because the output classifier cannot distinguish where the values came from unless the weight matrices learn this during model training.

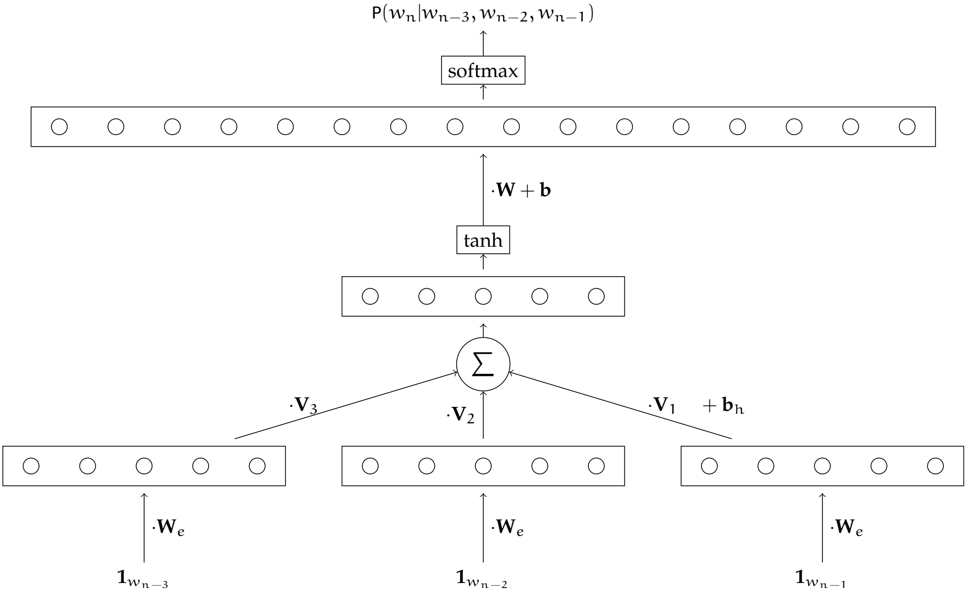


Figure 1.9: Architecture of a feed-forward language model with window size 3 with shared word embeddings $\mathbf{W}_e$.

Given this observation, we can factorize the matrices into two parts: the first one performing the projection to a common representation space of dimension m that can be shared among the window of predecessors, and the second projection adapting the vector to the specific role in the network based on the word position. Formally:

$$\mathbf{h} = \tanh\left(\mathbf{1}_{w_{n-3}}\mathbf{W}_e V_3 + \mathbf{1}_{w_{n-2}}\mathbf{W}_e\mathbf{V}_2 + \mathbf{1}_{w_{n-1}}\mathbf{W}_e\mathbf{V}_1 + \mathbf{b}_h\right) \tag{1.5}$$

where $\mathbf{W}_e \in \mathbb{R}^{|V| \times m}$ is the shared word embedding matrix and $\mathbf{V}_i$ are smaller projection matrices of size $m \times m$. This step approximately halves the number of network parameters. This is also the way that word embeddings are currently used in most NLP tasks. The architecture of the described trigram LM is illustrated in Figure 1.9.

The previous thoughts led us exactly to the architecture of the first successful neural LM (Bengio et al., 2003). The feed-forward architecture not only achieved decent quantitative results in terms of corpus perplexity, but it also developed word representations with interesting properties. Words with similar meaning tend to have similar vector representations in terms of Euclidean or cosine distance. Moreover, the learned representations appear to be useful features for other NLP tasks (Collobert et al., 2011).

Mikolov et al. (2010) trained an RNN-based LM for speech recognition where the word representations manifest another interesting property. The vectors seemed to behave linearly with respect to some semantic shifts, e.g., words that differ only in gender tend to have a constant difference vector. Mikolov et al. (2013c) further examined this property of the word vectors and developed a simple feed-forward architecture that was no longer a good LM but still produced word embeddings with all the interesting properties, i.e., being useful machine-learning features for NLP tasks, clustering words with similar meaning and behaving linearly with respect to some semantic shifts.

Pre-trained embeddings using one of the above-mentioned methods are an important building block in NLP tasks with limited training data (dependency parsing: Chen and Manning, 2014, Straka and Straková, 2017; question answering: Seo et al., 2016) when the model is supposed to generalize for words which were not seen in the training data, but for which we have good pre-trained embeddings. In tasks with a large amount of training data such as MT, we usually train the word embeddings together with the rest of the model (Qi et al., 2018).

The development of universally usable word vector representations became an independent subfield of NLP research. The research community mostly focuses on studying theoretical properties of the embeddings (Levy and Goldberg, 2014; Agirre et al., 2016) and multilingual embeddings either with or without the use of parallel data (Luong et al., 2015; Conneau et al., 2017).

Word embeddings and their interpretations are discussed in detail in Chapter 4.

1.3.2 Architectures for Sequence Processing

In NLP, we usually treat the text as a sequence of tokens that correspond to words, subwords, or characters. Deep learning architectures for sequence processing thus must be able to process sequential data of different lengths. The length of sentences processed by the MT systems typically varies from a few words to tens of words. In the CzEng parallel (Bojar et al., 2016b) 90% of sentences have between 20 and 350 tokens.

The architectures are used to produce an intermediate representation, so-called *hidden states* which the network uses further for generating outputs. The intermediate representation can be trained either end-to-end when learning an NLP task, or it can be a pre-trained one. In this section, we describe how these architectures work when treating them as a black box. We open the box and discuss possible interpretations in Chapter 6.

Currently, there are two main types of architectures used: RNNs, and SANs. The architectures are explained in detail in the following sections.

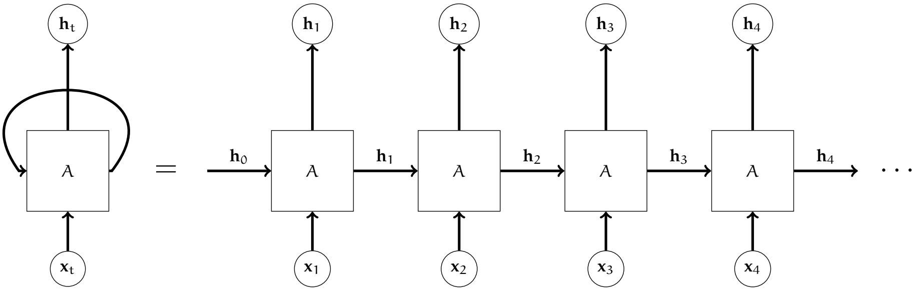


Figure 1.10: States of an RNN unrolled in time.

Recurrent Networks

RNNs are historically the oldest and probably still frequently used architecture for sequence processing in a variety of tasks including speech recognition (Graves et al., 2013; Chan et al., 2016), handwriting recognition (Graves and Schmidhuber, 2009; Keysers et al., 2017), or neural machine translation (Bahdanau et al., 2014; Chen et al., 2018). It was the architecture of the first choice partially because of its theoretical strengths—RNNs are proved to be Turing complete (Siegelmann and Sontag, 1995)—and because an efficient way for training them has been known since 1997 (Hochreiter and Schmidhuber, 1997).

Unlike the feed-forward networks which are stateless, a recurrent network can be best described as applying the same function A sequentially on the previous network state and current input (Elman, 1990). Computation of a new state $\mathbf{h}_t \in \mathbb{R}^d$ from the previous state $\mathbf{h}_{t-1} \in \mathbb{R}^d$ and current input $\mathbf{x}_t \in \mathbb{R}^n$ can be described using a recurrent equation

$$\mathbf{h}_t = A(\mathbf{h}_{t-1}, \mathbf{x}_t) \tag{1.6}$$

where the initial state $\mathbf{h}_0$ is either fixed or a result of the previous computation. Depending on the output of the task, either the final state of the RNN $\mathbf{h}_{T_x}$ where T_x is the length of the input sequence or the whole matrix $\mathbf{H} = (\mathbf{h}_1, \mathbf{h}_2, \dots, \mathbf{h}_{T_x}) \in \mathbb{R}^{T_x \times d}$ is used for further processing.

For inference, only the current state of the network is required. However, to learn its parameters via back-propagation in time (Werbos, 1990), we need to unroll all its steps. In this sense, even a simple RNN is a deep network because the back-propagation must be conducted through many unrolled layers. From the training perspective, RNNs in NLP tasks can easily have tens or hundreds of layers. Unrolling the network is illustrated in Figure 1.10.

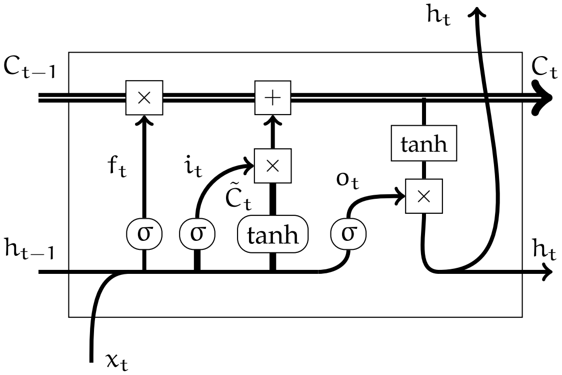


Figure 1.11: Scheme of an LSTM cell with the information highway (double line) at the top. Non-linear projections are in rounded boxes, element-wise operations in angular boxes, variables denoted at the arrows correspond to Equations 1.8 to 1.13.

The depth of the unrolled network is the factor that makes training of such architectures difficult. With a simple non-linear activation function (so-called Elman cell, Elman, 1990):

$$\mathbf{h}_t = \tanh\left(\mathbf{W}[\mathbf{h}_{t-1};\mathbf{x}_t] + \mathbf{b}\right), \tag{1.7}$$

it would be impossible for the network to learn to also consider longer dependencies in the sequence due to the *vanishing gradient problem* (already discussed in Section 1.2).

When we compute the parameter derivatives during the error back-propagation, the gradients get multiplied by the derivative of tanh every time we go one step back in time. Because the derivative is between zero and one, the training signal weakens in every time step, until it eventually vanishes. It effectively prevents the network from learning to consider also longer dependencies.

ReLU activation is claimed to reduce the issue in the context of CV (see Section 1.2). Its derivative is zero for $x < 0$ and one otherwise, so the gradient can eventually vanish in case of longer sequences too.

A solution to the instability problems came with introducing the mechanism of Long Short-Term Memory (LSTM) networks, which ensures that during the error back-propagation, there is always a path through which the gradient can flow via operations that are linear with respect to the derivative. The path, sometimes called information highway (Srivastava et al., 2015), is illustrated as the double straight line on the top of Figure 1.11.

This configuration is achieved by using two distinct hidden states, private state **C** and public state **h** where the state **C** is updated using the linear operations only. A gating mechanism explicitly decides what information from the input can enter the information highway (*input gate*), which part of the state should be deleted (*forget gate*) and what part of the private hidden state should be published (*output gate*).

Formally, an LSTM network of dimension d updates its two hidden states $\mathbf{h}_{t-1} \in \mathbb{R}^d$ and $\mathbf{C}_{t-1} \in \mathbb{R}^d$ based on the input $\mathbf{x}_t$ in time step t in the following way:

$$\begin{aligned}
\mathbf{f}_t &= \sigma\left(\mathbf{W}_f \cdot [\mathbf{h}_{t-1}; \mathbf{x}_t] + \mathbf{b}_f\right) && (1.8)\\
\mathbf{i}_t &= \sigma\left(\mathbf{W}_i \cdot [\mathbf{h}_{t-1}; \mathbf{x}_t] + \mathbf{b}_i\right) && (1.9)\\
\mathbf{o}_t &= \sigma\left(\mathbf{W}_o \cdot [\mathbf{h}_{t-1}; \mathbf{x}_t] + \mathbf{b}_o\right) && (1.10)\\
\tilde{\mathbf{C}}_t &= \tanh\left(\mathbf{W}_c \cdot [h_{t-1}; \mathbf{x}_t] + \mathbf{b}_C\right) && (1.11)\\
\mathbf{C}_t &= \mathbf{f}_t \odot \mathbf{C}_{t-1} + i_t \odot \tilde{\mathbf{C}}_t && (1.12)\\
\mathbf{h}_t &= \mathbf{o}_t \odot \tanh \mathbf{C}_t. && (1.13)
\end{aligned}$$

where $\odot$ denotes point-wise multiplication. The cell is shown in Figure 1.11.

The values of the forget gate $\mathbf{f}_t \in (0,1)^d$ control how much information is kept in the memory cell by point-wise multiplication. In the next step, we compute the candidate state $\tilde{\mathbf{C}} \in \mathbb{R}^d$ in the same way as the new state is computed in the Elman RNN cells. Values of this candidate state are not combined directly with the memory. First, they are weighted using the input gate $\mathbf{i}_t \in (0,1)^d$ and added to the memory already pruned by the forget gate. The new output state $\mathbf{h}_t$ is computed by applying tanh non-linearity on the memory state $\mathbf{C}_t$ and weighting it by the output gate $\mathbf{o}_t \in (0,1)^d$.

As previously mentioned, LSTM networks have two separate states $\mathbf{C}_t$ and $\mathbf{h}_t$. The private hidden state $\mathbf{C}_t$ is only updated using addition and point-wise multiplication. The tanh non-linearity is only applied while computing the output state $\mathbf{h}_t$. The gradient from the output passes through only one non-linearity before entering the information highway.

Later, other numerically stable versions of RNNs appeared. They all have the property that there is a path on which the gradient can propagate without vanishing (Balduzzi and Ghifary, 2016; Lee et al., 2017). The most frequently used variant is Gated Recurrent Units (GRUs) (Cho et al. 2014, Figure 1.12):

$$\begin{aligned}
\mathbf{z}_t &= \sigma\left(\mathbf{W}_z[\mathbf{h}_{t-1}; \mathbf{x}_t] + \mathbf{b}_z\right) && (1.14)\\
\mathbf{r}_t &= \sigma\left(\mathbf{W}_r[\mathbf{h}_{t-1}; \mathbf{x}_t] + \mathbf{b}_r\right) && (1.15)\\
\tilde{\mathbf{h}}_t &= \tanh\left(\mathbf{W}[\mathbf{r}_t \odot \mathbf{h}_{t-1}; \mathbf{x}_t] + \mathbf{b}\right) && (1.16)\\
\mathbf{h}_t &= (1 - \mathbf{z}_t) \odot \mathbf{h}_{t-1} + \mathbf{z}_t \odot \tilde{\mathbf{h}}_t. && (1.17)
\end{aligned}$$

The GRU networks have fewer parameters than LSTM networks which may speed up training under some circumstances. The performance of both network types is comparable and is task-dependent (Chung et al., 2014).

A commonly used method for improving RNN performance is building a bidirectional network (Schuster and Paliwal, 1997; Graves and Schmidhuber, 2005). Two in-

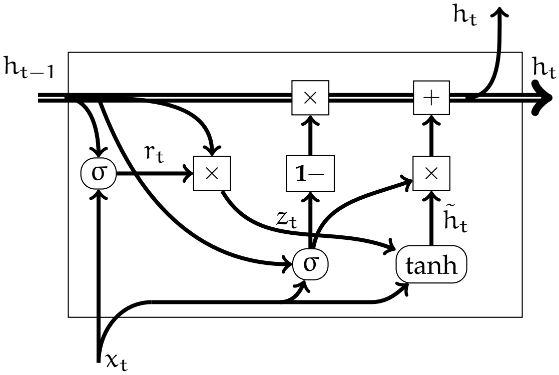


Figure 1.12: Scheme of an GRU cell following the same conventions as Figure 1.11.

dependent RNN networks are used in parallel, each of them processing the sequence from one end. The output states are then concatenated. In this way, the network can better capture dependencies in both directions in the input sequence. Bidirectional RNNs became a standard in many NLP tasks (Bahdanau et al., 2014; Ling et al., 2015; Seo et al., 2016; Kiperwasser and Goldberg, 2016; Lample et al., 2016). Note that in this setup, every network state may contain information about the complete sequence.

Self-Attentive Networks

SANs are neural networks where at least for some layers, the states of the next layer are computed as a linear combination of the states on the previous layer. It is called self-attention because states from a network layer are used to "attend", collect information from themself to create a new layer. The intuition that is often used to explain the SANs is that in every layer, every word collects relevant pieces of information from other words and thus gets more informed about in what context it is used. Although we will see in Chapter 5 that this intuition is often not entirely true, in this section, it will help us to better understand the technicalities of the architecture.

There exist several variants of SANs (Parikh et al., 2016; Lin et al., 2017). In this section, we discuss in detail the encoder part of the architecture introduced by Vaswani et al. (2017), called *Transformer*, that achieves state-of-the-art results in MT.

A *Transformer layer* for sequence encoding consists of *two sub-layers*[2].

The first sub-layer is self-attentive, the second one is a non-linear projection to a larger dimension followed by a linear projection back to the original dimension. All

[2] Note that even the sub-layer consists of several network layers. A better term would probably be *block* as in ResNet (He et al., 2016), however, we follow the terminology introduced by Vaswani et al. (2017).

sub-layers contain dropout, layer normalization, and are connected using residual connections. The scheme of the architecture is displayed in Figure 1.14.

The self-attentive sub-layer first computes the similarity between all states using the scaled dot-product attention. One possible interpretation of attention is probabilistic retrieving of values $\mathbf{V} = (\mathbf{v}_1, \dots, \mathbf{v}_n) \in \mathbb{R}^{n \times d}$ which are associated with some keys $\mathbf{K} = (\mathbf{k}_1, \dots, \mathbf{k}_n) \in \mathbb{R}^{n \times d}$ for each of m query vectors $\mathbf{Q} = (\mathbf{q}_1, \dots, \mathbf{q}_m) \in \mathbb{R}^{m \times d}$. Because all queries, keys, and values are sets of vectors, we can for the sake of computational efficiency write them as matrices. The scaled dot-product attention can be then written as a matrix multiplication:

$$\operatorname{Attn}(\mathbf{Q}, \mathbf{K}, \mathbf{V}) = \operatorname{softmax}\left(\frac{\mathbf{Q}\mathbf{K}^\top}{\sqrt{d}}\right)\mathbf{V} \tag{1.18}$$

where d is the model dimension, i.e., the second dimension of all three matrices involved in the equation, which is the Transformer model constant across the layers. The matrix-multiplication formulation is important because it allows fast parallelization when computing on GPUs.

By normalizing the similarity over the keys using the softmax function, we get a probability distribution which is then applied over the value matrix $\mathbf{V}$ in a weighted sum. In case of the self-attentive encoder, all three matrices $\mathbf{Q}$, $\mathbf{K}$, $\mathbf{V}$ are the same, i.e., the states on the next layer $\mathbf{H}^{(i)} = (\mathbf{h}_1^i, \dots, \mathbf{h}_n^{(i)})$ are computed as:

$$\mathbf{H}^{(i)} = \sum \operatorname{softmax}\left(\frac{\mathbf{H}^{(i-1)}\mathbf{H}^{(i-1)\top}}{\sqrt{d}}\right)\mathbf{H}^{(i-1)}. \tag{1.19}$$

To allow collecting different pieces of information from different words, Vaswani et al. (2017) also introduced another innovation to the attention mechanism, *multi-headed attention*. In the multi-head setup, all the query, key, and value matrices are first linearly projected as illustrated in Figure 1.13. Note that even though the inputs to the attention are the same, the projections do not share parameters. The projected states are then split into multiple sub-matrices, so-called heads. The attention is computed for each of the heads independently according to Equation 1.18. Outputs of the attention are then concatenated and linearly projected to the original model dimension, forming a sequence of context vectors. In the Transformer model, the keys and values are always the same. In case the attention is used as self-attention, the queries are identical as well.

The multi-head setup uses two independent projections for keys and values. The keys and values are thus different in the individual heads. Formally for h heads,

$$\begin{aligned} \operatorname{Multihead}(\mathbf{Q}, \mathbf{V}) &= (\mathbf{H}_1 \oplus \cdots \oplus \mathbf{H}_h)\mathbf{W}^O & (1.20) \\ \mathbf{H}_i &= \operatorname{Attn}(\mathbf{Q}\mathbf{W}_i^Q, \mathbf{V}\mathbf{W}_i^K, \mathbf{V}\mathbf{W}_i^V) & (1.21) \end{aligned}$$

where $\mathbf{W}^O \in \mathbb{R}^{hd \times d}$, and $\mathbf{W}_i^Q$, $\mathbf{W}_i^K$, $\mathbf{W}_i^V \in \mathbb{R}^{d \times d}$ are trainable parameters.

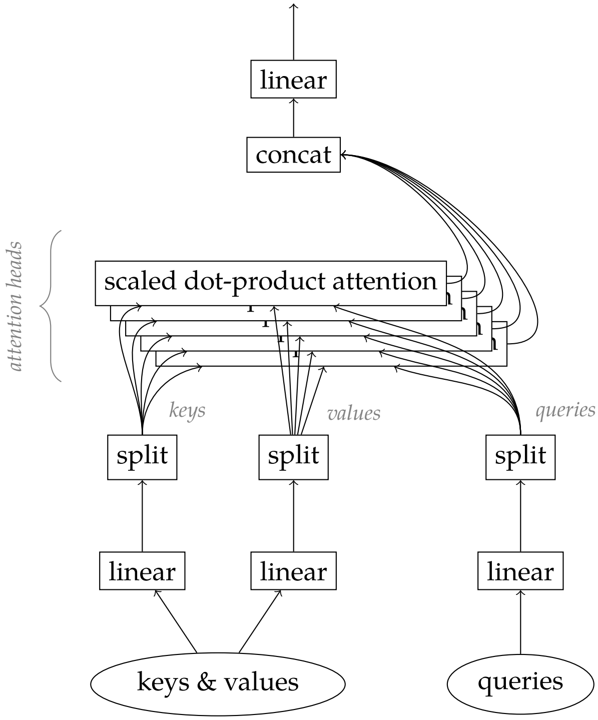


Figure 1.13: Scheme of the multi-headed scaled dot-product attention.

SANs do not have any means to capture the order of the symbols and thus require using additional positional encoding to distinguish the positions within the sequence. The Transformer model uses analytically computed *positional encoding*. The positional encoding for model dimension 60 is plotted in Figure 1.15. Note that for different dimensions, the encoding values change with a different frequency which allows estimating the relative position of the inputs.

Computationally, SANs are as fast as CNNs because the self-attention can be computed in a single matrix multiplication which can be highly parallelized when computed on GPU. On the other hand, we need to store a matrix with the similarity of all pairs of the input states in the GPU memory for each layer of the network. Due to this, the memory demands grow quadratically with the length of the input sequence. A summary of the computational complexity of the discussed networks for sequence processing is given in Table 1.1.

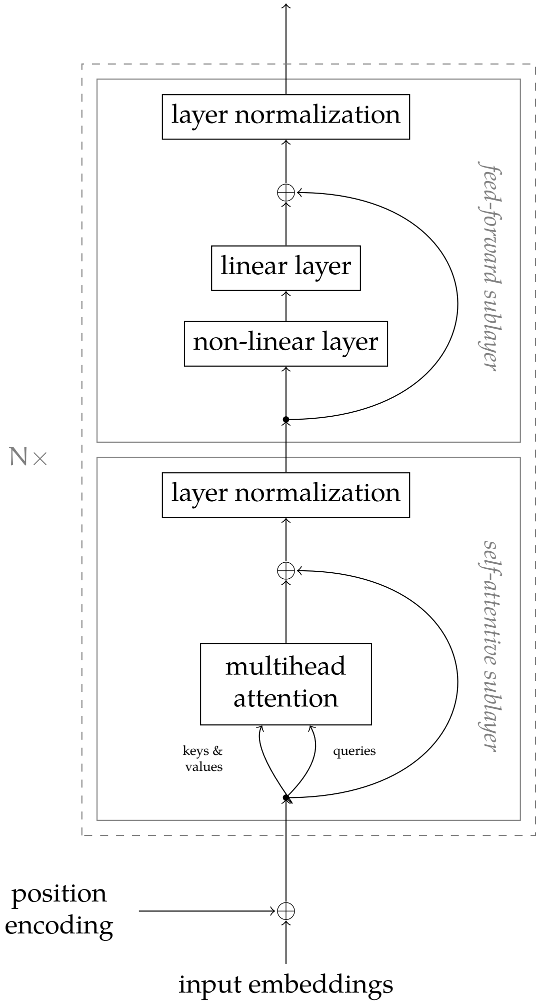


Figure 1.14: Scheme of a self-attentive encoder network from the Transformer model with N layers.

1.3.3 Generating Output

So far, we have only discussed how the neural networks process symbolic input into an intermediate representation. In the following sections, we discuss what architectures are used to generate output from neural networks.

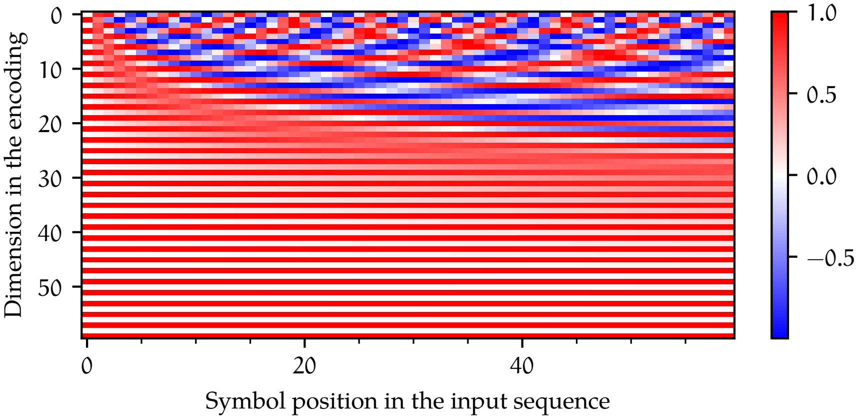


Figure 1.15: Visualization of the position encoding used in the Transformer model with embedding dimension 60 and input length up to 8.

We discuss in detail three special cases:

- The output is a symbol from a closed set of possible answers—*classification*;
- The output is a sequence of symbols of the same length as the input—*sequence labeling*;
- The output is a sequence of symbols of an arbitrary length—*autoregressive decoding*.

Classification

In the simplest case, the network produces only one discrete output, i.e., we want to classify the input into a fixed set of previously known classes. An example of such an NLP task is sentiment analysis (Pang et al., 2002; Pak and Paroubek, 2010) where the goal is to classify whether a text carries a positive or negative sentiment. Another example can be classification of text into a set of genres (Kessler et al., 1997; Lee and Myaeng, 2002).

The most common approach to these tasks is applying a multi-layer perceptron over a fixed-size representation of the input. The fixed-size vector can be for instance the final state of an RNN or a result of a pooling function applied over states produced by one of the architectures mentioned in Section 1.3.2. The most frequently used methods are max-pooling and mean-pooling, computing the maximum or average of the states in time, respectively.

	computation	sequential operations	memory
Recurrent	$O(n \cdot d^2)$	$O(n)$	$O(n \cdot d)$
Convolutional	$O(k \cdot n \cdot d^2)$	$O(1)$	$O(n \cdot d)$
Self-attentive	$O(n^2 \cdot d)$	$O(1)$	$O(n^2 \cdot d)$

Table 1.1: Comparison of the asymptotic computational, sequential and memory complexities of the architectures processing a sequence of length n, and state dimensionality d. CNN has kernel size k. The first column contains complexity in case of sequential computation, the second column shows the asymptotic number of sequential operation during parallel computation, and the third column shows the memory complexity.

The classification network can then consist of multiple non-linear layers before the actual classification, which is usually done by taking the maximum or sampling from a distribution estimated by the softmax function.

The softmax function over a vector $\mathbf{l}$ is defined as:

$$\operatorname{softmax}(\mathbf{l})_i = \frac{\exp l_i}{\sum_{l_j \in \mathbf{l}} \exp l_j}. \tag{1.22}$$

Note that the softmax function is monotonic, so if we are interested only in the best-scoring prediction, at inference time, we can take the maximum value of vector $\mathbf{l}$ before the softmax function. The values of $\mathbf{l}$ are often called *logits*.

When the output of the network is estimated using the softmax function, we can measure the error that the network makes as a cross entropy between the estimated probability distribution P_y and the true output distribution, given such distribution exists. In practice, the true distribution is unknown. However, we usually assume that the true distribution exists and assigns all the probability mass to the target value y^* in the training data. This assumption might be problematic, e.g., when estimating the probability of the next word in a text. It is, in fact, never the case that there is only one possible follow-up word. Nevertheless, the assumption simplifies the computation of cross-entropy loss which can be then expressed as

$$L(\mathsf{P}_y, y^*) = -\log \mathsf{P}_y(y^*). \tag{1.23}$$

In this way, the derivative of the loss function with respect to the logits is

$$\frac{\partial L(\mathsf{P}_y, y^*)}{\partial \mathbf{l}} = \mathsf{P}_y - \mathbf{1}_{y^*} \tag{1.24}$$

where $\mathbf{1}_{y^*}$ is a one-hot vector for value y^*.

The loss gradient with respect to the logits is back-propagated to the network using the chain rule. The softmax function with cross-entropy loss is used not only in the case of single-output classification but also in sequence labeling and autoregressive decoding discussed in the following sections.

For completeness, we should also mention that when the output of the network is supposed to be a continuous value, we can perform a linear regression over the input representation and optimize the estimation using a mean squared error

$$L(y, y^*) = (y - y^*)^2, \tag{1.25}$$

which is differentiable and thus the error can be back-propagated to the network.

Sequence Labeling

When the desired output of a network is a sequence of discrete symbols having the same length as the input and monotonically aligned with the input, we can apply a multi-layer perceptron over each state of the network. In this case, the labels assigned to every state are conditionally independent given the network states. The loss function used to train the network is a sum of cross entropy over the network output distributions.

In NLP, many tasks can be formulated as sequence labeling. Besides the more theoretically motivated tasks such as part-of-speech tagging or semantic role labeling, we can mention information extraction where the goal is marking entities in a text or named entity recognition.

The labels assigned to the input symbols often have their own, usually simple grammar rules. When we label the beginnings and ends of sequences, we need to make sure the end symbol never comes before the start symbol. In these cases, conditional random fields can be applied over the state sequence (Lafferty et al., 2001; Do and Artieres, 2010).

Autoregressive Decoding

In some tasks such as MT or abstractive text summarization, the output cannot be monotonically aligned with the input and the number of output symbols differs from the number of the input symbols. In such cases, we need a mechanism that is able to generate output symbols in a general while loop and is conditioned on the entire input. Such a while loop is sometimes called *autoregressive decoder* because the computation in every time step depends on the previous state of the loop and previous outputs and generates the output symbols left-to-right.

Historically, autoregressive decoding has developed from discriminative language modeling using RNNs. We will thus first explain this principle on the RNN LMs and later generalize the principle for CNNs and SANs.

LMs are probabilistic models estimating the probability of sentences in a language represented by a corpus that the model is trained on. The probability is factorized over the words or smaller units. Within the statistical paradigm, word probabilities were usually estimated based on a finite window of previous words using n-gram statistics computed on a training corpus (Manning and Schütze, 1999). When approached as a sequence labeling problem, it can be done using an RNN which can, in theory, handle unlimited history (Mikolov et al., 2010; Sundermeyer et al., 2012). In both cases, the probability of a sentence is estimated using the chain rule:

$$\mathrm{P}(w_1, \dots, w_n) = \mathrm{P}(w_1 | \texttt{<s>}) \cdot \dots \cdot \mathrm{P}(w_n | w_{n-1}, \dots, w_1, \texttt{<s>}) \tag{1.26}$$

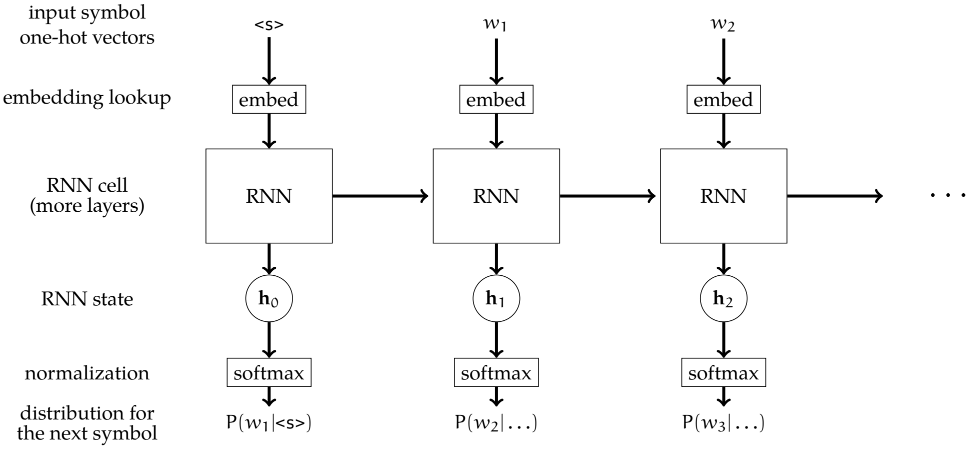


Figure 1.16: Illustration of LM formulated as a sequence labeling problem.

The inputs to the neural LM are word embeddings. In every time step, the model estimates a probability distribution over the vocabulary. Formally we let

$$\mathrm{P}(w_{n+1} | w_n, \dots, w_1, \texttt{<s>}), \mathbf{s}_n = \mathrm{RNN}(w_n, \mathbf{s}_{n-1}) \tag{1.27}$$

where $\mathbf{s}_n$ is the state of the model in the n-th step. The distribution expresses how likely the following word w_{n+1} is to appear in a sentence with a prefix of words $w_1, \dots, w_n$. The model is optimized towards cross entropy as a standard sequence labeling task. An RNN LM formulated as sequence labeling is illustrated in Figure 1.16.

Autoregressive decoding is based on sampling from such a model. In every time step, we can sample from a distribution over the output words. In the next step, the sampled word is provided as the model input as if it were a word in a sentence that

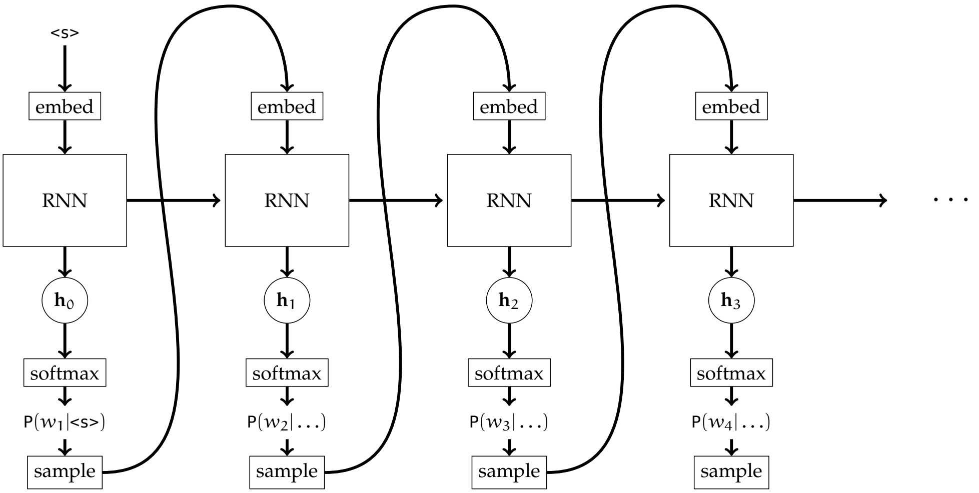


Figure 1.17: RNN LM used as an autoregressive decoder.

the LM is supposed to score. The words are sampled from the model in a while loop until a special end symbol is generated. The sampling is illustrated in Figure 1.17.

The missing part that distinguishes an LM from an autoregressive decoder is conditioning the LM on other inputs than the previously decoded symbols. In case of MT, it would be the source sentence. In the simplest case, this can be done by explicitly assigning the initial state of the RNN with a result of a previous computation.

In the early work, these were max-pooled CNN states (Kalchbrenner and Blunsom, 2013), however, more promising results are achieved with LSTM networks (Sutskever et al., 2014). A disadvantage of this approach is that the input needs to be represented as a fixed-sized vector (max-pooled CNN states, the final state of an RNN) regardless of what the input length is. The performance of such models quickly decreases with the size of the input (Sutskever et al., 2014).

Bahdanau et al. (2014) introduced a technique overcoming this drawback of autoregressive decoding, called *attention mechanism*. In every decoding step, the model computes a distribution over the variable-length input representation and uses it to compute the *context vector*, a weighted average over the input representation. Having been originally introduced in the context of Neural Turing Machines (Graves et al., 2014), the distribution is usually interpreted as addressing the input representation analogically to addressing memory cells in random-access memory.

For input sequence of length T_x, encoder states $\mathbf{H} = (\mathbf{h}_1, \dots, \mathbf{h}_{T_x}) \in \mathbb{R}^{T_x \times d_n}$ of dimension d_h, and decoder state $\mathbf{s}_i$ of dimension d_s, the attention model with intermediate dimension d_a defines the attention energies $e_{ij} \in \mathbb{R}$, attention distribution

$\alpha_i \in \mathbb{R}^{T_x}$, and the context vector $\mathbf{c}_i \in \mathbb{R}^{d_h}$ in the i-th decoder step as:

$$e_{ij} = \mathbf{v}_a^\top \tanh(\mathbf{W}_a \mathbf{s}_i + \mathbf{U}_a \mathbf{h}_j + \mathbf{b}_a) + b_e, \tag{1.28}$$

$$\alpha_{ij} = \frac{\exp(e_{ij})}{\sum_{k=1}^{T_x} \exp(e_{ik})}, \tag{1.29}$$

$$\mathbf{c}_i = \sum_{j=1}^{T_x} \alpha_{ij} \mathbf{h}_j. \tag{1.30}$$

The trainable parameters $\mathbf{W}_a \in \mathbb{R}^{d_s \times d_a}$ and $\mathbf{U}_a \in \mathbb{R}^{d_h \times d_a}$ are projection matrices that transform the decoder and encoder states $\mathbf{s}_i$ and $\mathbf{h}_j$ into a common vector space and $\mathbf{v}_a \in \mathbb{R}^{d_a}$ is a weight vector over the dimensions of this space, $\mathbf{b}_a \in \mathbb{R}^{d_a}$ and $b_e \in \mathbb{R}$ are biases for the respective projections. The context vector $\mathbf{c}_i$ is then concatenated with the decoder state $\mathbf{s}_i$ and used for classification of the following output symbol.

Together with techniques for data preprocessing (Sennrich et al., 2016b,c), the attention model was the crucial innovation that helped to improve neural MT quality over the statistical MT and set a new state of the art in the field of MT.

SANs can be used similarly to CNNs. In the Transformer model (Vaswani et al., 2017), a stack of self-attentive and feed-forward sub-layers is applied on the already decoded sequence and the result is used to produce the next output symbol. Similar to the CNN decoder, the self-attentive layers are interleaved with cross-attentive layers attending the encoder states.

At training time, the computation can be parallelized as in the case of the CNN decoder. In the self-attentive layers, we need to limit the attention distribution only to the words that have already been decoded. This is in practice implemented by multiplying the matrix of attention energies with a triangle matrix, as shown in Figure 1.18.

Self-attentive sequence-to-sequence models currently provide the best results in sequence generation tasks (Bojar et al., 2018). Nevertheless, they suffer from the low decoding speed and quadratic memory demands, limiting the practical application to sequences of at most hundreds of tokens.

So far, we have only discussed how the output sequence probability is modeled using the autoregressive decoder. Finding the sequence that receives the highest probability by the decoder is, however, a difficult problem. The number of possible output sequences grows exponentially with its length, which makes an exhaustive search intractable.

The most straightforward heuristics is greedily choosing the most probable output symbol in every step. Another commonly used heuristic is the *beam search* algorithm that approximates the exhaustive search over all possible target strings while keeping only a few best-scoring hypotheses in every time step (Sutskever et al., 2014). The algorithm trades off the efficiency of greedy decoding (when the output symbol with maximum probability is selected at each time step) while maintaining a relatively wide search space.

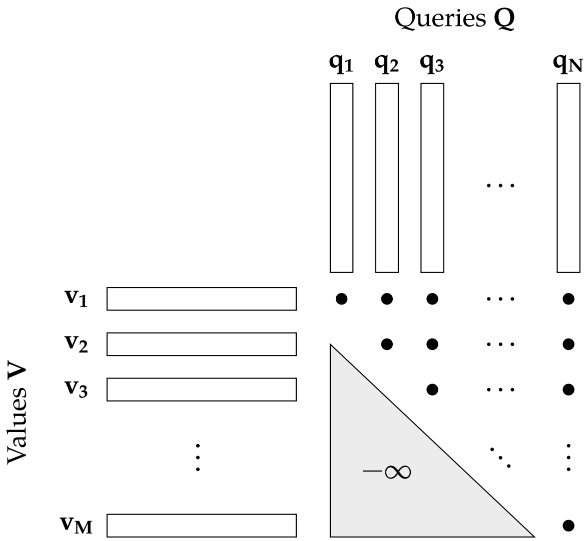


Figure 1.18: Masking while computing energy values in the self-attention layer in the Transformer decoder. Masking prevents the self-attention to attend to symbols to the right from the previously decoded symbol.

The algorithm keeps track of k hypotheses (*beam*). A hypothesis is either a partially generated sequence (*unfinished*), or a sequence that ends with a special end symbol (*finished*). In each step, all hypotheses are expanded with all possible tokens from the vocabulary. The expanded hypotheses are scored and k best of them are kept for the next step.

1.4 Conclusion

After major success in CV in 2012 and 2013, deep learning attracted the attention of the NLP research community. Soon after that, deep learning methods reached state-of-the-art results in most NLP tasks and became the first choice method. The standard deep learning architecture design consists of discrete symbol embedding, contextualizing the embeddings using an encoder, and using the representations to generate discrete output.

In practice, the embeddings or the encoder are pre-trained on large corpora and only the output layers are trained. This is discussed in more detail in the next chapter, together with NLP modeling breakthroughs from 2013 to 2020.

2

Notable Models

In the previous chapter, we described what are the main building blocks of deep neural networks used for Natural Language Processing (NLP). In this chapter, we will discuss the deep learning methods on examples of several notable models from recent history. Rather than trying to exhaustively enumerate neural NLP models, we focus on a few models that brought important innovations into the field which we broadly discuss in the rest of the book.

2.1 Word2Vec and the Others

When solving NLP tasks, we need to convert a discrete input into continuous values the neural networks can work with. This is done by learning a vector for each discrete input symbol and storing the learned vectors in a lookup table. These vectors are called word embeddings and were discussed in Section 1.3.1.

The pioneering work of Bengio et al. (2003) and Collobert et al. (2008) noticed that word embeddings learned during language modeling has interesting spatial properties (similar words get similar representations in terms of Euclidean and cosine distance) and most importantly, they can be used as very informative input features for machine learning models.

Pre-trained word embeddings reached mainstream popularity with the Word2Vec model (Mikolov et al., 2013c). Unlike its predecessors, the model is very simple. It was also published together with an efficient implementation which caused that the model can be easily trained on a large amount of data when using a very large vocabulary.

Word2Vec can be viewed as a simple Language Model (LM), however, when training the model, we are not interested in the LM performance at all. Language modeling only provides a training signal to train the embeddings. Word2Vec can be trained in two setups: Continuous Bag of Words (CBOW) and Skip-gram. The difference between these two models is how they treat the context (see Figure 2.1).

The CBOW model first averages the embeddings of words in a small context window (typically, windows of size 3–7 are used) and use it to predict what the word in the middle is using a linear classifier. The Skip-gram model is conditioned the other way round: given an embedding of a word, a linear classifier predicts what words are in the window of surrounding words. These two models have a similar performance in downstream tasks, however, the Skip-gram model demonstrates further interesting properties that are discussed in greater detail in Chapter 4.

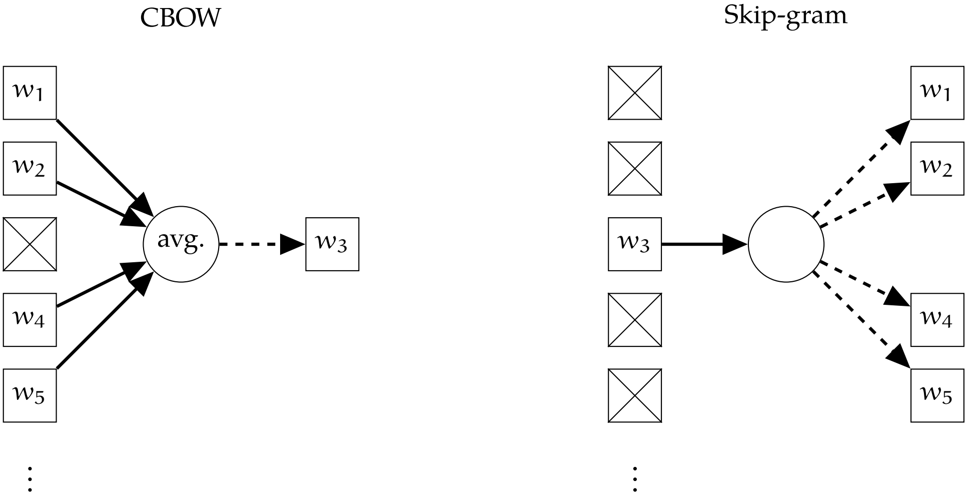


Figure 2.1: Scheme of the CBOW and Skip-gram training.

Pre-trained word embeddings from Word2Vec found use in many machine-learning approaches to NLP which triggered further research in pre-trained word embeddings.

In the GloVe model, Pennington et al. (2014a) managed to include document-level information in the embeddings. In FastText models, Bojanowski et al. (2017), on the other hand, managed to include subword information in the word embeddings. Unlike Word2Vec and GloVe, that store a single embedding for each word, FastText computes the embeddings as an average of embeddings of character n-grams the word consists of. FastText currently poses the state of the art in word embeddings pretraining.

2.2 Attention and Machine Translation with Recurrent Neural Networks

In the second half of 2014, Bahdanau et al. (2014) introduced a Recurrent Neural Network (RNN)-based model that meant a paradigm change in Machine Translation (MT). The model introduced the attention mechanism within the autoregressive decoding framework that we discussed in Section 1.3.3. It was the first neural model that attacked the translation quality of by that time state-of-the-art phrase-based models.

MT quality is annually evaluated in competitions at Workshop of Machine Translation (WMT). Research teams from both academia and industry are invited to use their MT systems to translate test sets provided by the organizers. The translations are then rated by bilingual speakers. The findings of the competition provide a nice

tokenized	Strawberry ice cream is the best .
32k vocabulary	Stra@@ w@@ berry ice cream is the best .
16k vocabulary	Stra@@ w@@ ber@@ ry ice cre@@ am is the best .

Table 2.1: Examples of subword segmentation with byte-pair-encoding (Sennrich et al., 2016c). Subwords were estimated on the WMT14 training set for English-German translation.

overview of what the state of the art in MT is. In the WMT 2015 competition (Bojar et al., 2015), the phrase-based statistical MT systems still outperformed the neural ones (Jean et al., 2015).

Two major innovations in 2016 have allowed the clear dominance of neural models in machine translation since then. Not only did neural systems from the University of Edinburgh (Sennrich et al., 2016a) won the WMT competition (Bojar et al., 2016a), but also Google announced the deployment of neural MT system in Google Translate (Wu et al., 2016).

The first innovation was using sub-word segmentation (Sennrich et al., 2016c) that to a large extent eliminates the problem of having a limited vocabulary. Instead of using word-like tokens, the sentences are segmented using statistical heuristics that keep frequent words together and split the less frequent ones into smaller units. This allows the model learning to generalize towards morphology, but most importantly helps with translating named entities which are often partially translated and partially transliterated. Examples of subword segmentation are provided in Table 2.1.

The second crucial innovation was synthetic data generation using *back-translation* (Sennrich et al., 2016b). In the previous MT paradigm, statistical MT, the translation process was decomposed into two main components: a translation model for model translation adequacy and a target language model for modeling target sentence fluency. One of the advantages of this decomposition was that the language model can leverage monolingual data in the target language. When using back-translation, the monolingual data in the target language are machine-translated in the source language, resulting in parallel data with synthetic source side and authentic target side. The synthetic data are combined with the authentic parallel data and used to train the next iteration of the models.

2.3 Transformer for Machine Translation

In a paper with the catchy name *Attention is All You Need*, Vaswani et al. (2017) introduced a new architecture that significantly pushed the state of the art in translation quality. The architecture is called Transformer and it is a fully self-attentive architecture (as we described in Section 1.3.2) that uses an autoregressive decoder.

Transformer-based models show better modeling capabilities, but still heavily depend on the innovations invented for RNN-based models, i.e., sub-word text segmentation and back-translation. Models based on the Transformer were the best-scoring models in all tasks in recent WMT competitions (Bojar et al., 2018; Barrault et al., 2019).

From today's view, the invention of the Transformer architecture was the crucial innovation that found use in almost all areas of NLP. Because it can be heavily parallelized, it allows non-autoregressive text generation (Gu et al., 2018; Libovický and Helcl, 2018). Moreover, it is the basis of the current pre-trained representation models (Devlin et al., 2019; Liu et al., 2019b) that significantly pushed the state of the art in many NLP tasks and that we also discuss later in the chapter.

In 2017, research teams competing in the annual WMT competition did not manage to take advantage of the recent invention, the best-performing systems in the competition were based on RNNs (Sennrich et al., 2017; Bojar et al., 2017). However, in 2018 and 2019, all the best-performing systems were already based on Transformers (Junczys-Dowmunt, 2018; Bojar et al., 2018; Barrault et al., 2019).

2.4 CoVe: Contextual Embeddings are Born

The first experiments with model probing (discussed in detail in Chapter 6) discovered that hidden states of the sequence processing network carry a lot of information about the input sentence. This was especially pronounced in the case of the MT encoder that needs to capture the source meaning in such a way that the decoder can generate a full sentence in the target language (Hill et al., 2017; Adi et al., 2017).

McCann et al. (2017) leveraged this observation and used a trained encoder from an MT model for transfer learning. They were also the first ones to explicitly introduce the concept of contextual word vectors. In their approach, called CoVe Context Vectors (CoVe), they train a Neural Machine Translation (NMT) system with a 2-layer bidirectional Long Short-Term Memory (LSTM) encoder with Global Vectors for Word Representation (GloVe) word vectors on input, and then explicitly denote the resulting hidden states as context vectors:

$$\text{CoVe}(w) = \text{MT-LSTM}(\text{GloVe}(w)) \tag{2.1}$$

where w is the input word, GloVe is its pre-trained embedding vector, and MT-LSTM is the trained MT encoder state corresponding to the word; the equation is reproduced from (McCann et al., 2017).

Since CoVe, the term *contextual word embeddings* is often used to refer to hidden states of a model when these are used outside of the model as vector word representations. In this book, we often do not strictly differentiate between hidden states and contextual word embeddings, as these are just different names for principally the same thing; the terminology mostly reflects how the representations are *used*, not how they are *obtained*.

Unlike standard NMT models that work with a relatively small vocabulary of tens of thousands of subword units, CoVe works on word level and uses *GloVe* embeddings. These design decisions decrease the performance of the MT itself, on the other hand, it allows using a large embedding table covering 2.2M word forms which would otherwise be impossible with an MT trained from random initialization.

CoVe was tested on a wide range of NLP tasks: sentiment analysis (Maas et al., 2011), question classification (Voorhees and Tice, 1999), entailment classification (Bowman et al., 2015), and answer span selection (Rajpurkar et al., 2016) and reached state-of-the-art in all of them.

2.5 ELMo: Sesame Street Begins

Another pre-trained contextual representation model that attracted the attention of the NLP community is called Embeddings using Language Models (ELMo). A preprint announcing CoVe was published in August 2017 on arXiv, and the first preprint of a paper announcing ELMo appeared only two months later on OpenReview. ELMo is a part of the AllenNLP software package (Gardner et al., 2018) which also contributed to the popularity of the model before CoVe found wider use. Also, the paper introducing ELMo was awarded as the best paper at the NAACL 2018 conference.

Unlike CoVe that uses the encoder from an NMT model, ELMo is pre-trained as a language model and thus only requires monolingual data for pre-training. This is a large advantage because parallel data in a sufficient amount are only available for relatively few languages.

The architecture of ELMo (Peters et al., 2018a) is, in principle, similar to CoVe: it consists of 2 two-layer unidirectional LSTMs. (It was preceded by a 1-layer variant called Language-Model-Augmented Sequence Tagger (TagLM) (Peters et al., 2017) which did not perform so well and did not receive such attention.) Instead of using static word embeddings, ELMo uses a character-level Convolutional Neural Network (CNN) and a stack of feed-forward layers to obtain word representations that are passed to the LSTMs, so the model can to some extent considered open-vocabulary. The scheme of the architecture is shown in Figure 2.2.

ELMo is trained as two LMs: one in the forward and one in the backward direction while sharing the input representation and the output layer. The standard bidirectional network cannot be used here. In bidirectional RNNs, every output state contains information about the entire input sequence. The sequence-labeling component of the LM would only learn to copy the input tokens to the output without any generalization. As a result, 4 LSTM states correspond to each input word after running the model.

The model was trained on the 1 billion word benchmark for language modeling (Chelba et al., 2014). Surprisingly, the forward and backward LM reach approximately the same perplexity. The evaluation using similar tasks as CoVe and several more

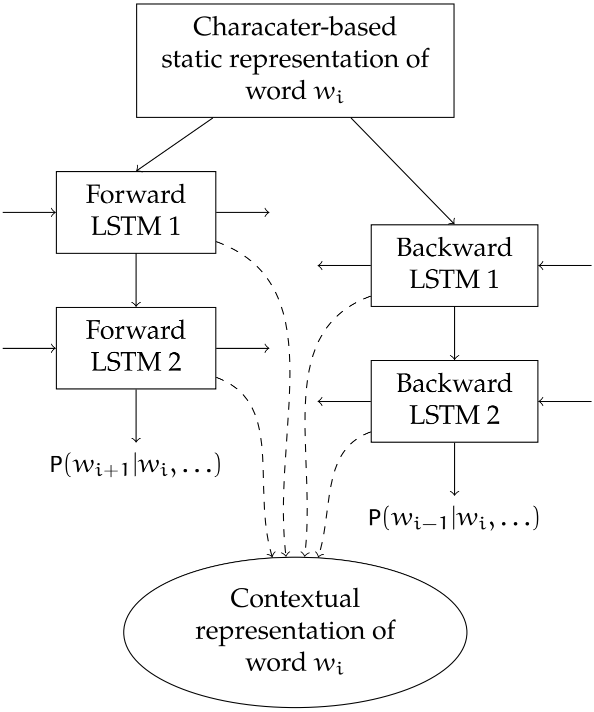


Figure 2.2: Architecture of ELMo.

tasks such as semantic role labeling and coreference resolution and set up the new state of the art in all of them.

2.6 BERT: Pre-trained Transformers

One year after ELMo was published, another pre-trained model called Bidirectional Encoder Representations from Transformers (BERT) appeared. Unlike the previous general-purpose contextual representation, BERT is based on the Transformer architecture. The model was developed and published by Google, which as a company had previously invented Transformers, and used the know-how it already had in this area. Similar to ELMo, the acronym chosen for the model is the name of a character from Sesame Street, an American educational children's television series. Also, the paper introducing BERT received the same award as ELMo one year later.

It was the third type of a pre-trained representation model in a short time that significantly pushed state of the art in many NLP tasks. Now, two years later, pre-trained Transformers are still the major tool used in NLP.

Already at the time when ELMo was developed, it was well-known for more than a year that Transformer-based models outperform RNNs in MT. Replacing RNNs by Transformers might seem like a natural step forward. However, classical LM training with the Transformer model requires masking future tokens in the self-attentive layers (see Section 1.3.3 and Figure 1.18 for more details). That would make such a model very memory-inefficient.

Instead, BERT is trained using the so-called *masked language model* objective. At training time, 15% of the input tokens are selected for masking (i.e., either replaced by a special [MASK] token, replaced by a random word, and kept unchanged). A sequence labeler applied after the Transformer encoder predicts what were the tokens that were masked out. The masked LM objective is illustrated in Figure 2.3.

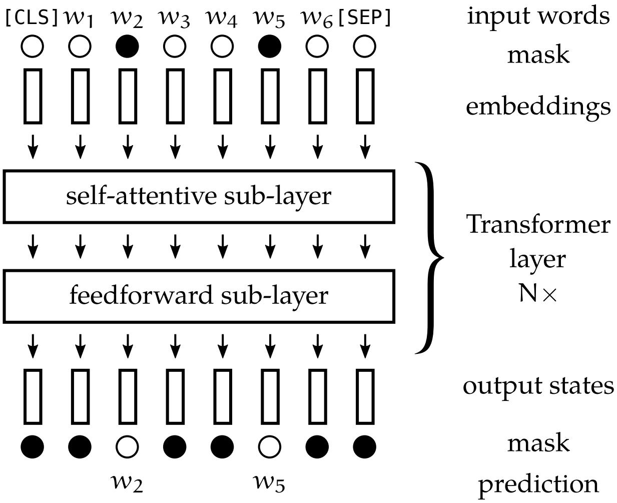


Figure 2.3: Illustration of training BERT-like models with masked LM objective.

The original BERT also uses an auxiliary sentence-adjacency training objective. It is trained using pairs of sentences. The two input sentences are separated using a special [SEP] token and there is a special [CLS] token at the beginning. A vector corresponding to the [CLS] token is then used to predict whether the two sentences follow each other in a coherent text. The vector is thus supposed to be a constant-size representation of the entire input.

With BERT, it was for the third time in a short time when new state-of-the-art results on a large variety of tasks were announced. Meanwhile, Wang et al. (2018) introduced GLUE (General Language Understanding Evaluation), a standardized benchmark for sentence representation evaluation. It aggregates a collection of NLP tasks

WordPiece	A tiger is a (big) cat
SentencePiece	A _tiger _is _a _(big) _cat .

Table 2.2: An example of tokenization when using WordPiece and SentencePiece.

that can be formulated as classification problems. BERT replaced ELMo on top of the GLUE leaderboard.

Liu et al. (2019b) at Facebook revisited training of BERT and introduced a new model called RoBERTa. They noticed that BERT was significantly undertrained. They further noticed that the sentence adjacency objective does hot have a large effect on transfer learning performance when the model is trained on sufficiently large data. The original BERT was trained on 3.3 billion English words. Liu et al. (2019b) did not report the exact number of words only say that they used 160 GB of raw text, which is approximately 10 times bigger corpus.

One further difference between BERT and RoBERTa is in input tokenization. BERT uses WordPiece (Wu et al., 2016) tokenization that separates words from punctuation, whereas RoBERTa uses SentencePiece (Kudo and Richardson, 2018). SentencePiece keeps spaces as parts of the tokens which makes the tokenization fully reversible. It makes production deployment easier, on the other hand, the segmentation often contradicts our linguistic intuition, especially when using punctuation. For instance, in the example in Table 2.2, the word "big" is a different token when used in brackets when using SentencePiece.

RoBERTa outperformed BERT in all tasks when having the same number of parameters. On the other hand, these results show that sufficient computation resources to train models that reach state-of-the-art results on a wide range of tasks are only available to large companies such as Google or Facebook. Nevertheless, it is important to note the companies publicly released their models and made their code freely available both for the research community and other enterprises.

The computation demands of training and using a BERT-like model, led to further research on computationally cheaper variants of the models. DistillBERT (Sanh et al., 2020) improves efficiency by introducing a smaller model derived from already trained BERT using knowledge distillation (Hinton et al., 2015). Better efficiency at training time can be achieved by a more clever sampling of masked words. In the standard setup, only the 15% masked words provide training signal to the network. Clark et al. (2020) address this issue by splitting the model into two parts: a generator suggesting tokens and a discriminator predicting if those suggestions are part of the original sentence.

Originally, Google released BERT for English and Chinese. Currently, BERT-like models are available in many languages among other French (Martin et al., 2019; Le et al., 2020), Italian (Polignano et al., 2019), Russian (Kuratov and Arkhipov, 2019), Spanish (Cañete et al., 2020), Finish (Yang et al., 2020) or Turkish (Schweter, 2020), mostly developed either by local academic institutions or rarely by local enterprises.

In addition to that, the original release of BERT included a multilingual version of BERT that was trained for 104 languages. During training, the model is not informed about the language identity and only works with plain text. Facebook later applied the methodology used for RoBERTa to a multilingual model and developed XLM-R (Conneau et al., 2020) covering 100 languages and significantly outperforming multilingual BERT. The multilingual model is used mostly for zero-shot learning with languages for which we do not have training data (Pires et al., 2019) or when training a single model for multiple languages using the shared representation (Kondratyuk and Straka, 2019).

2.7 GPT and GPT-2

At around the same as BERT, Radford et al. (2019a) from Open AI, a US-based non-profit private research laboratory published a pre-trained Transformer-based language model which they called Generative Pre-Trained Transformer (GPT). Similar to BERT and ELMo, they used the hidden state of the model as input features in a wide range of downstream tasks, and for a time before BERT was published they set a new state of the art in few NLP tasks.

The following version of the model from February 2019, GPT-2 (Radford et al., 2019b) attracted much more attention. It was trained on 40 GB of web text, approximately 5 times more than BERT. The biggest version of the model has around 1.5 billion parameters, which is 18 times more than the standard version of BERT and 5 times more than BERT Large.

GPT-2 showed an excellent performance in a so-called zero-shot setup in tasks like question answering or text summarization. In the zero-shot setup, the model is not finetuned on task-specific training data but used in the generative setup. For question answering it means: the model is given the question on the input followed with a natural language command that an answer should follow (typically something like "Answer:") and we let the model continue in the same way as when we generate a target sentence in machine translation models. In most of the tasks, the performance is significantly below the state of the art, however, the zero-shot performance was still a large surprise for the community.

The authors of the model were reluctant to publish the model because of potential misuse of the model (Solaiman et al., 2019), e.g., for better automation of fraudulent email management, generating abusive content on social networks, or fake news. Although it might be difficult for humans to distinguish a genuine and machine-generated text, it can be relatively easily automatically detected (Gehrmann et al., 2019). Also because of that, the authors decided that the benefits for the research community of having access to the model outweigh potential risks and released the model in November 2019.

2.8 Conclusion

In this chapter, we have described several models that from today's perspective pose milestones for developing models for NLP. With the exception of MT, which is an important task itself, all the other models only provide vector representation of language input that is later used in particular NLP tasks. The pre-trained word embeddings combined with light-weight recurrent architectures are still an important choice in practical applications under limited resource conditions and when model speed is an issue. However, nowadays, the pre-trained Transformers reach the state of the art in almost all NLP tasks.

3
Interpretation of Neural Networks

Neural Networks (NNs) are state-of-the-art models in many Machine Learning (ML) tasks. These NNs are usually trained end-to-end and treated as a *black box*[1] after training. With rising capabilities and deployment of these models, the demand grows in the last few years for understanding the inner workings, or interpretation, of these models. Interpretability may be important for trusting the model in a real-world setting, general human curiosity, detecting bias in the models, or increasing social acceptance of modern technologies (Molnar, 2020).

Interpretation as a source of trust is most important when ML models' potential errors have serious consequences, such as in medical applications or self-driving cars. In Natural Language Processing (NLP), applications such as machine translation may benefit from this approach to interpretation. Bias detection is vital in applications such as automatic CV (*curriculum vitae*) analysis.

Human curiosity is also a strong motivation for posing questions concerning which linguistic concepts manifest in NNs and if NNs approach language differently from humans.

Just as there is not only a single reason to be interested in interpretation, there is no single definition of the concept of interpretation itself. There is no mathematical definition of interpretation (Molnar, 2020). Lipton (2018) notes that "the task of *interpretation* appears underspecified," and the "concept of interpretability appears simultaneously important and slippery". Miller (2019) defines interpretability as "the degree to which a human can understand the cause of a decision," which leaves us with a similarly vague notion of *understanding*.

One way to avoid this issue in the context of a specific research question is to state in the beginning what does the presented view of interpretation entail (see Montavon et al. (2018) for an example[2] of this practice). However, this approach is rarely used in research papers, and it will not help us with a general overview. The use of the

[1] "A Black Box Model is a system that does not reveal its internal mechanisms. In machine learning, "black box" describes models that cannot be understood by looking at their parameters (e.g., a neural network)." (Molnar, 2020, Section 1.3)

[2] They proceed by giving a sequence of definitions that are progressively more specific and delimit the range of methods that they are concerned with: "An interpretation is the mapping of an abstract concept (e.g., a predicted class) into a domain that the human can make sense of.", "An explanation is the collection of features of the interpretable domain, that have contributed for a given example to produce a decision (e.g., classification or regression)." (Montavon et al., 2018)

concept of interpretation of NNs varies significantly in the literature and is rarely made explicit.

Since we cannot produce a unified concept, we may at least try to sort the various ways in which researchers use the term. Lipton (2018) distinguishes between two main groups of properties of interpretable models: *transparency* and *post-hoc interpretability*.

Transparency consists of understanding the mechanism by which the model works. The understanding is achieved by selecting a model architecture and a training algorithm that is sufficiently simple (or decomposable) to be understandable. Restricting the complexity of the machine learning model to achieve interpretability is also called *intrinsic interpretability* (Molnar, 2020). Linear regression, logistic regression, and the decision tree are often considered interpretable (Molnar, 2020). However, as Lipton (2018) points out, "neither linear models, rule-based systems, nor decision trees are intrinsically interpretable. Sufficiently high-dimensional models, unwieldy rule lists, and deep decision trees could all be considered less transparent than comparatively compact neural networks." Building transparent ML models is also sometimes called *explainable* Artificial Intelligence (AI). Due to the complexity of NLP tasks, models that are simple enough to be interpretable in this sense cannot produce good results and therefore are rarely used.

Post-hoc (or extrinsic) interpretability is a way of extracting information from models that are already trained. The "advantage of this concept of interpretability is that we can interpret opaque models after-the-fact, without sacrificing predictive performance" (Lipton, 2018).

With the current deep NNs used in NLP, we can only talk about the extrinsic interpretability, which is also what we are interested in the rest of the book. Rather than developing intrinsically interpretable algorithms, we present empirical post-hoc interpretation of state-of-the-art NLP models in the last five years.

We can divide the methods of post-hoc interpretability into two categories, *structural* and *behavioral* analysis; we can also distinguish visualization as a third separate method.

Structural analysis, with which we deal in this book, analyzes and interprets the internal parameters of trained models, such as emergent word representations (embeddings) or attentions. In linguistical structural interpretation, we try to find correspondences of the internal representations to existing linguistic abstractions, such as part of speech labels or syntactic structures; this may involve (and typically involves) searching for linguistic abstractions which the model was not explicitly trained to learn (e.g., searching for morphological features in a machine translation model). Structural analysis can be performed both in a supervised way (probing) as well as in unsupervised ways. We describe these two approaches in this section.

Behavioral analysis observes the behavior of the trained model on the task for which it was trained, typically using specially constructed inputs to investigate the behavior of the model in specific situations to see what the model can or cannot do.

Behavioral analysis treats the model as a black box, not directly analyzing its learned parameters. We do not deal with behavioral analysis in this book; please refer, e.g., to Section 4 of (Belinkov and Glass, 2019) for an overview.

Visualization methods are usually qualitative, and they can be used to present a large amount of information.

Further information can also be found in the overview of methods for analyzing deep learning models for NLP (Belinkov and Glass, 2019).

3.1 Supervised Methods: Probing

According to Belinkov and Glass (2019), the most common approach for examining linguistic properties in neural network components is using a classifier to predict these properties from activations of the neural network. We refer to this approach as *probing*. Probing models are also sometimes called auxiliary or diagnostic classifiers Liu et al. (2019a). At first, the term *probing* was used in general to refer to any post-hoc interpretations of neural networks. However, gradually the term shifted and is now almost exclusively used for training supervised classifiers (see, e.g., Hewitt and Manning (2019)), which is how we use the term in this book.

Probing requires data annotated for the studied property. This means that with probing, we can only reveal the kind of information that we have previously decided to look for in the representations and for which we have an annotated dataset.

This introduces a systemic bias into the research. It is easier to probe for properties that are already described in formal linguistic frameworks with large annotated datasets. The results that find these properties in the representations then retroactively affirm the correctness of the conceptualization and design decisions made for the annotation. There have been recent efforts for probing to standardize test data (Gül Şahin et al., 2019).

Peters et al. (2018a) use a linear classifier to probe for Part of Speech (PoS) in Embeddings using Language Models (ELMo) and CoVe Context Vectors (CoVe), asserting that "[a]s the linear classifier adds only a small amount of model capacity, this is a direct test of the [contextual] representation". We (Rosa et al., 2020) show that such an assertion may be problematic without careful evaluation of the memorization effect, which can occur even with a linear classifier, but in the setting used by authors, the risk of memorization is not large.

Hewitt and Liang (2019) measured probe's selectivity, i.e., the difference of accuracy for linguistic and control tasks. For instance, one linguistic task was PoS tagging, and the corresponding control task was retrieving randomly assigned tags to words.

3.2 Unsupervised Methods: Clustering and Component Analysis

Unsupervised methods go in the other direction than supervised methods. Supervised methods start from the abstraction that we want to find and try to train a classifier to extract it from the representation. With unsupervised methods, we first analyze the features that emerge in the representations and only then do we try to map them to existing linguistic abstractions. A prototypical example of an unsupervised structural analysis method is clustering. We first cluster the representations, then observe the clusters and search for an existing set of labels that can be assigned to them.

Unsupervised methods reduce the bias inherent in the choice of the information to classify in probing. On the other hand, the results are usually harder to quantify.

We can illustrate this with an example. In (Musil, 2019), we show that it is possible to train a probing classifier that labels PoS based on the Czech word embeddings from a Neural Machine Translation (NMT) encoder. However, this merely shows that it may be possible to divide the high dimensional space by criteria that are mostly arbitrary but do not by themselves prove that this division is important for the NMT system. The unsupervised approach shows that in the first few dimensions of Principal Component Analysis (PCA), the embeddings form clusters that correspond to PoS, suggesting that PoS is indeed important for the encoder. However, probing enabled us to easily compare embeddings from different sources in a quantitative way, by comparing the accuracy of the probing classifier. That is not possible with the unsupervised approach.

There is a number of unsupervised approaches that can be used to analyze various components of the neural models, either analyzing the models directly or after applying various transformations. We review here two groups of transformation methods: clustering and component analysis.

Clustering is a method of grouping datapoints together based on their similarity. The resulting groups (clusters) can then be assigned with labels. A shortcoming of clustering is that it is "hard" by default, i.e., each data point belongs to exactly one cluster. This problem can be partially alleviated by hierarchical clustering, which provides more fine-grained information about similarities of the clusters and thus indirectly about the similarity of the data points in different clusters.

Component Analysis Component analysis is a process of transforming a multidimensional space (e.g., word embeddings) with the goal of obtaining interpretable features as the components of the transformed space. We describe two methods in detail, PCA in Section 4.6 and Independent Component Analysis (ICA) in Section 4.7.

3.3 Network Layers and Linguistic Units

In analyzing and interpreting internal NN representations of language input, we often take the representations and investigate how they correspond to some existing linguistic abstractions. For this, we obviously need to be able to map the representations to individual language units, such as words and sentences.

As most of the models we deal with in this book take a single sentence as their input, it is relatively straightforward to map their internal representations to the sentences.[3]

However, for analyzing words, we are facing two crucial problems. One is based on the fact that in most NN models used in NLP, only the input-layer embeddings directly correspond to words, while the hidden states[4] in the subsequent processing layer cannot be easily mapped directly to words; one hidden state might encode various kinds of information about various words. Moreover, current NLP models typically do not operate on words but rather on subwords, making the mapping of the representations to words even harder.

In this section, we review the problems and discuss available ways of dealing with them.

3.3.1 Words versus States

NLP models employ various mechanisms of passing information between individual layers of the model. However, be it Convolutional Neural Networks (CNNs), Recurrent Neural Networks (RNNs) or Self-Attentive Networks (SANs), what they all have in common is that the mechanism enables information about individual input words to be mixed, strengthened, weakened, shifted forward and backward, etc. In the initial layer, the word representations (static embeddings) are context-independent, and thus the representation at a given position corresponds to and only to the input word at the same position (i.e., the ith embedding corresponds to the ith input word). In subsequent layers, however, the representations (hidden states) at any position may, in theory, correspond to any and all input words.[5] It may thus be that a given ith state corresponds mostly to the ith word, but it may also be that it mostly represents the $i+1$th word, it may combine under various weights some information about the $i-1$th word with some other information about the ith word, etc.[6] Most NLP models are not explicitly forced during training to keep the correspondence of the input words and hidden states at the same positions.[7] On a related note, it has been shown that the neural network models are apt at storing information useful for them at any

[3] However, we do not largely deal with analyzing sentence-level representations in this book.

[4] As explained in Section 2.4, in our text, we often do not strictly differentiate between hidden states and contextual word embeddings.

[5] The architecture may limit this to some extent, e.g., by using residual connections that explicitly pass through the state from the previous layer, or CNNs which have a finite kernel size.

[6] Technically, as weights within a neural model are rarely exactly zero, a given state typically contains some information about *all* of the input words to some extent. However, the distributions of the weights are often quite peaked rather than flat, which means that a given hidden state is typically mostly determined by only a few aspects of a few input words.

[7] Residual connections may partially encourage this correspondence. Some models are also forced to represent the input words by the *output* states at the corresponding positions, which may encourage them (but not force them) to keep this correspondence even in internal hidden states.

available place, especially if storing the information at the default place is disabled, as we will discuss later in Section 5.3.

However, multiple studies found that typically, the hidden states tend to be centered on the input words, i.e., that the i-th hidden state typically mostly contains information about the i-th input word.

Already the work of Bahdanau et al. (2014) states that "Each (hidden state) h_i contains information about the whole input sequence with a strong focus on the parts surrounding the i-th word of the input sequence.", and "Due to the tendency of RNNs to better represent recent inputs, the (hidden state) h_j will be focused on the words around x_j." However, it is not clear from the work whether the authors have some solid arguments for these claims or whether these are rather intuitive expectations.

Some indirect evidence is provided by Koehn and Knowles (2017), who find that in an attention-based NMT system, there is typically a 75% match between the source word most attended to while producing a given target word, and the source word aligned to the target word by standard word-aligner. Supposing that the information about the aligned source word is the most important, we can deduce that the corresponding hidden state mostly contains information about that word. However, the authors also found that for one of their examined setups, the attention is typically off by one, mostly attending to the word *following* the aligned word, which may either be caused by the decoder operating with the information about the word to translate in the next step, and/or by the hidden state representations to be shifted by one with respect to the input words (see Section 5.1).

Ethayarajh (2019) provides some further evidence, showing that for ELMo, Bidirectional Encoder Representations from Transformers (BERT) and Generative Pre-Trained Transformer (GPT) models, the cosine self-similarity of contextual representations of a word (the similarity of contextual representations of occurrences of the same word in different contexts) is practically always greater than the cosine similarity to contextual embeddings of other words.[8] The context-specific information within the contextual embedding can become quite strong, but the signal corresponding to the identity of the word at the given position seems to stay stronger than the signals corresponding to any other word.

Thus, even though this is not perfectly accurate, it is common to refer to the i-th hidden state as a state *corresponding* to the i-th input word, implying that the i-th hidden state somehow represents the i-th input word, in the context of the input sentence (as well as in the context of the task which the NN system is trained to perform).

[8] The self-similarity is lowest for stopwords (such as common determiners, prepositions, and conjunctions), which are rather semantically vacuous and mostly fulfill a syntactic function within their immediate context.

3.3.2 Words versus Subwords

As discussed in Sections 2.5 and 2.6, current NLP models typically do not operate directly on words, but their input is first tokenized into *subwords*, which has many important benefits. Therefore, in the network, there are usually no explicit representations of words, as all embeddings and hidden states are only computed for the subwords.

While subwords are a very useful concept for most NLP end tasks, they pose a problem for linguistic interpretations of the trained models, as many linguistic formalisms, such as PoS or syntax, are based on words. A notable exception is the notion of morphs and morphemes, which correspond to parts of words and are thus similar to NN subwords in principle; however, multiple studies have found that morphemes and subwords seem to be very different and cannot be easily mapped to each other (Sennrich et al., 2016c; Banerjee and Bhattacharyya, 2018; Bostrom and Durrett, 2020). Therefore, the base unit on which most NN models operate, a subword, is hard to map to any linguistic abstraction, which poses important challenges for linguistic interpretation of such models.

There are three common workarounds to this problem.

From Words to Subwords

The first option is modifying the linguistic abstraction to apply to subwords. For example, for PoS tagging, we might assign the same PoS tag to all subwords (so, e.g., "hell ic opter" would be labelled "NOUN NOUN NOUN"). Alternatively we might label the first subword with the tag of the original word and the subsequent subwords with a special continuation tag (so "hell ic opter" would be labeled for example "NOUN –NOUN –NOUN" or "NOUN – –"). This is especially natural when dealing with linguistic abstractions that span multiple words, such as named entities or syntactic phrases, where it makes little difference whether the span is composed of several words or a slightly larger number of subwords (Mareček and Rosa, 2019). However, for strictly word-based concepts, such as PoS tags, morphological labels, or dependency syntax, this approach does not seem adequate, as it is not straightforward to see which linguistic feature should be captured in which subword or subwords of the original word and thus how the individual subwords should be labeled. This approach thus may be useful for *training* NLP models to solve such tasks, but not for linguistically *interpreting* such models.

From Subwords to Words

A second option is to reconstruct word representations from the subword representations *ex post*. This is usually done by taking the average of the subword representations (i.e., mean-pooling), although other options are also possible, such as taking the sum of the representations,[9] max-pooling the representations, or training and applying a small NN to perform a non-linear combination of the subword representations (Libovický et al., 2020). This makes it then straightforward to analyze the word representations for word-level linguistic features. However, it should be kept in mind that in this case, we are not directly analyzing the representations in the network, but only their transformation, which we performed ourselves, which makes the analysis partially indirect, and any findings obtained via this method should be carefully assessed on the possible influences of the used word embedding reconstruction onto the analysis (for example, if we find that PoS is seemingly more strongly encoded in representations of short words than long words, it is quite possible that in fact, it is strongly encoded only in some subwords of the long words and therefore seems weaker in the average of the subword representations).

Fully Word-Based Approach

The third workaround is to train the model for analysis in a word-based manner, without using the subword tokenization (Rosa et al., 2020). While this gets rid of the problem completely, making the interpretation straightforward, this also means that we are, in fact, analyzing different models than the ones that are actually used in practice (typically, word-based models are significantly weaker than subword-based models). If our goal is to understand a particular model or set of models used in practice, it is quite unclear how an analysis of a slightly different model relates to this, as the difference of using words instead of subwords may have a large impact on how the models work internally. These kinds of analyses are thus highly trustworthy in interpreting the analyzed word-based models – arguably more trustworthy than any similar analyses of the subword-based models, as they operate directly on words in all steps without the need of the somewhat *ad hoc* word-to-subword or subword-to-word mappings which may introduce some noise into the analyses. However, we should be very wary about any interpretative claims about the subword-based models based on analyses of word-based models, as there is no clear reason why the findings made for one class of the models should also hold for the other class.

3.4 Conclusion

Although the concept of interpretation is somewhat vague and lacking a proper theory, we can distinguish a few important directions in the expanding field of interpreting neural networks in NLP. Training probing classifiers, transforming and visualizing the variable space, and constructing challenge sets for behavioral analysis seem

[9] Summation and mean-pooling are very similar operations and can often be used interchangeably. However, since words are split into variable-length sequences of subwords, using summation instead of mean-pooling leads to the resulting vectors varying in their norm, which is irrelevant if they are only compared using, e.g., cosine distance, but may be important in other usages.

to be the most important areas of research. In further chapters, we deal with the first two.

However, any interpretation approach is potentially problematic. We discussed some of the problems in this chapter, including the threat of mistaking probing classifier memorization for model abstraction (especially with strong probing classifiers) or the difficulties involved in mapping network states to input words.

4
Emblems of the Embeddings

In this chapter, we discuss the interpretation of continuous space representations of words, the so-called *word embeddings*. As explained in Section 1.3.1, word embeddings are vectors. Either they can be trained as part of a Neural Network (NN) for a specific task, or they can be obtained by a method that is intended specifically for generating word embeddings. We call these embeddings *pre-trained*.

Because the embeddings are randomly initiated before the training and all the dimensions of the vector are connected to the same inputs in the next layer of the network, individual dimensions of word embeddings usually do not have a direct interpretation. Any feature that would be represented in the embeddings corresponds to a linear combination of dimensions. The embedding vector of a single word does not have any significance by itself. It is only its relations to the other words (embeddings) that make the vector meaningful (in this respect, word embeddings are a realization of the structuralist view of language).

In the following sections we will go through a few examples of interpretation of word embeddings. We have chosen examples that we find interesting without striving for a complete survey. The reader may find a broader survey in (Belinkov and Glass, 2019).

In Section 4.1 we look at word analogies in various models for pre-trained word representations. Sections 4.2–4.4 are concerned with visualizing the embedding space. In Section 4.5 we mention embeddings of emoticons. In Sections 4.6 and 4.7 we talk about component analysis. We discuss word derivations in Section 4.8. Mapping of embedding spaces is discussed in Section 4.9. In Section 4.10, we talk about debiasing word representations, as an example of a feedback loop, where interpretation influences the representation itself.

4.1 Word Analogies

In this section we talk about three different models for pre-trained representations that show interesting linguistic regularities.

4.1.1 Word2Vec and Semantic Arithmetic

Word embeddings often have properties that do not directly follow from the training task. The most well-known example was found by Mikolov et al. (2013a,c), who developed the Word2Vec model (see Section 2.1). The Skip-gram variant of this model

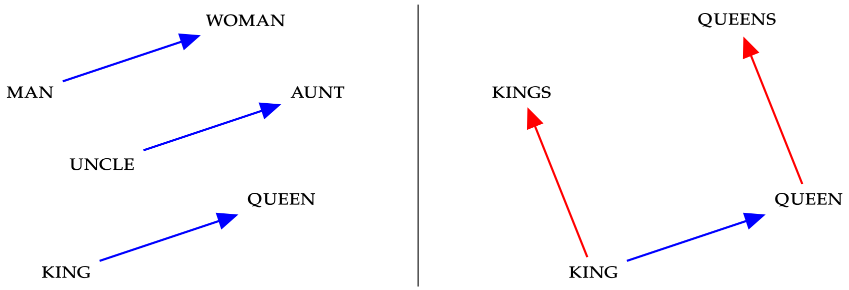


Figure 4.1: Examples of semantic vector arithmetic according to Mikolov et al. (2013c).

was trained to predict the words that form the context of a given word. Surprisingly, representations from this model frequently obey the vector arithmetic of meanings illustrated by Figure 4.1 and by the following equation:

$$v_{\text{king}} - v_{\text{man}} + v_{\text{woman}} \approx v_{\text{queen}},$$

meaning that if we start with the word "king", by subtracting the vector for the word "man" and adding the vector for the word "woman" we arrive at a vector that is nearest in the vector space to the one that corresponds to the word "queen". We can interpret this as the word *queen* being to *woman* as *king* is to *man*. Amongst the types of relationships that this model captures, they name country–capital (e.g. *Italy–Rome*), adjective–comparative (e.g. *cold–colder*), city–state (e.g. *Dallas–Texas*), and person–job (e.g. *Picasso–painter*).

The problem of finding word $b*$, such that the relation $b : b*$ is the same as $a : a*$ for given words a, $a*$, and b, is in Natural Language Processing (NLP) called an *analogy task*.

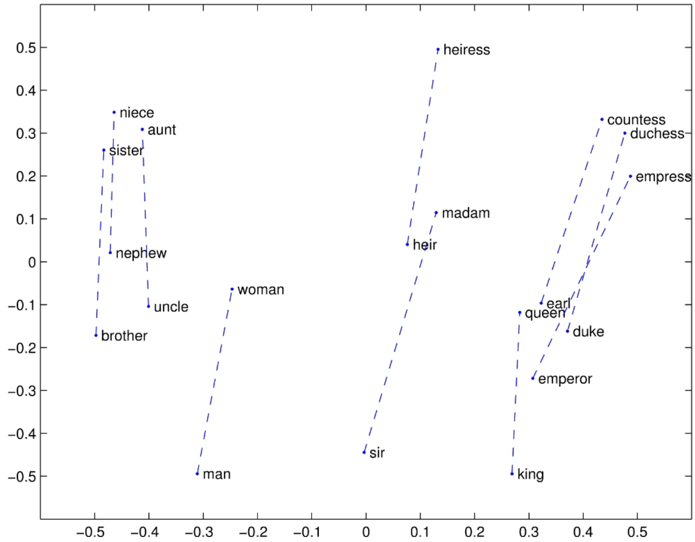
Mikolov et al. (2013b) also trained the same model with phrases instead of words, producing vectors that exhibit additive compositionality. For example:

$$v_{\text{Germany}} + v_{\text{capital}} \approx v_{\text{Berlin}}.$$

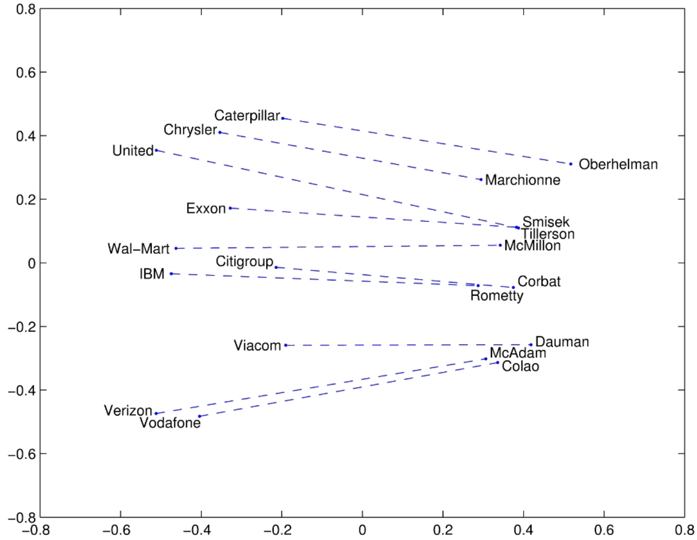
The Word2Vec models show us that meaning can be (at least to some extent) organized in a geometrically interpretable way.

4.1.2 Glove Word Analogies

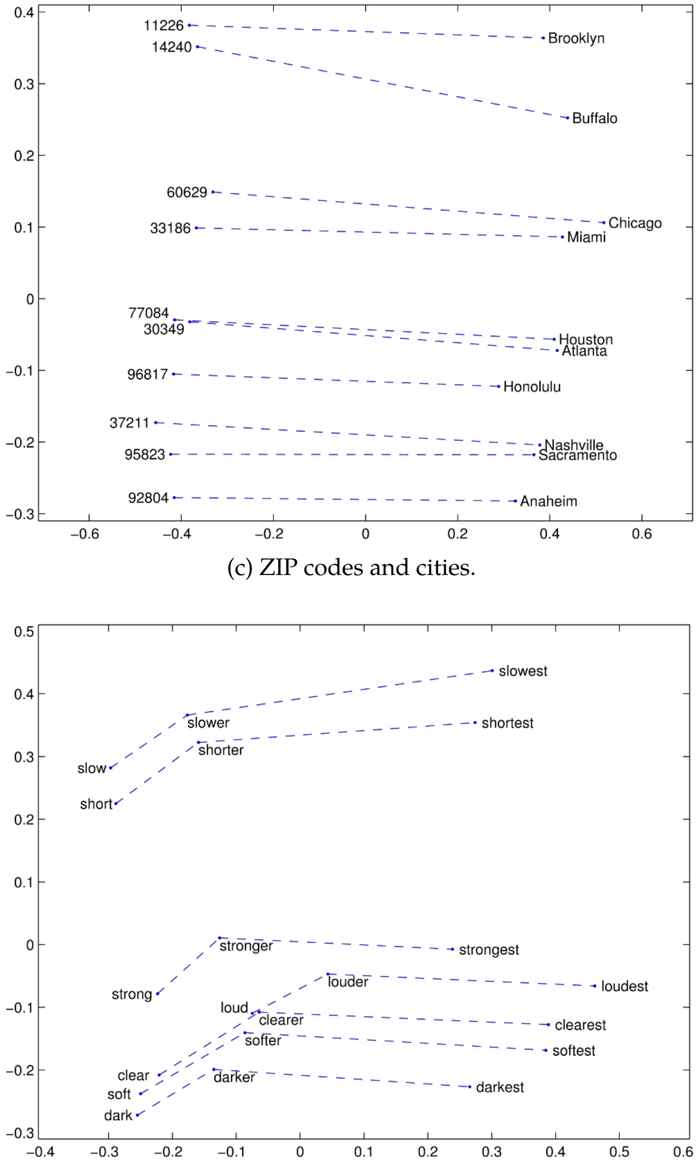
The predictive methods of training word embeddings use *local* context in each training step, and the resulting representation is a generalization of that. This is in contrast with the older statistical, count-based methods for creating distributed word representations, which are using the *global* co-occurrence matrix or its decomposition.



(a) Analogies to *man–woman* relation.



(b) Company and CEO.



(c) ZIP codes and cities.

(d) Comparison of adjectives.

Figure 4.2: Word analogies in the Glove embeddings. Reprinted from (Pennington et al., 2014b).

Following the success of the predictive methods, Global Vectors for Word Representation (GloVe) (Pennington et al., 2014a) combined the two paradigms. The vectors are learned in such a way that the dot product of two word vectors equals the logarithm of the words' probability of co-occurrence.

GloVe performs well on word analogy tasks. Similarly to Word2Vec, the vector space of GloVe shows linear substructures (see Figure 4.2) where similar relations between the words are represented by a similar direction of vector difference in the embedding space. The authors explain this by "the fact that the logarithm of a ratio equals the difference of logarithms, this objective associates (the logarithm of) ratios of co-occurrence probabilities with vector differences in the word vector space. Because these ratios can encode some form of meaning, this information gets encoded as vector differences as well." (Pennington et al., 2014b)

Another interesting property of the model is that nearest neighbors in the embedding space (by Euclidean distance or cosine similarity) may "reveal rare but relevant words that lie outside an average human's vocabulary." (Pennington et al., 2014b) The authors give the following example with the closest words to the target word "frog": *frog*, *frogs*, *toad*, *litoria*, *leptodactylidae*, *rana*, *lizard*, and *eleutherodactylus*.

4.1.3 FastText Subword Correspondence

In morphologically rich languages, each word has many forms that share the same meaning. The difference in the form expresses various syntactic properties. Assigning a vector to each word-form prevents the representations of the forms of the same word to share information. Bojanowski et al. (2017) proposed a method of obtaining vector representations from unsupervised data that makes sharing information across word-forms possible. The FastText method is based on Skip-gram (see Section 2.1). It assigns embeddings to character n-grams. Then it treats words as bags of character n-grams.

Figure 4.3 illustrates that character n-grams with similar meaning have similar embeddings. It shows that parts of words with similar meaning, e.g., *-ness* and *-ncy* have similar embeddings.

4.2 Positioning Words

In Figure 4.4, we see a method of word embeddings visualization, which aims at illustrating relations between specifically chosen words. In this case, we regard the embeddings as points in a multidimensional space. For both the horizontal and the vertical axis in the figure, we selected a pair of words. The pair determines a line in the embedding space. Other selected words are then mapped onto the axes by geometrically projecting their embedding vectors onto the line defined by the axis words.

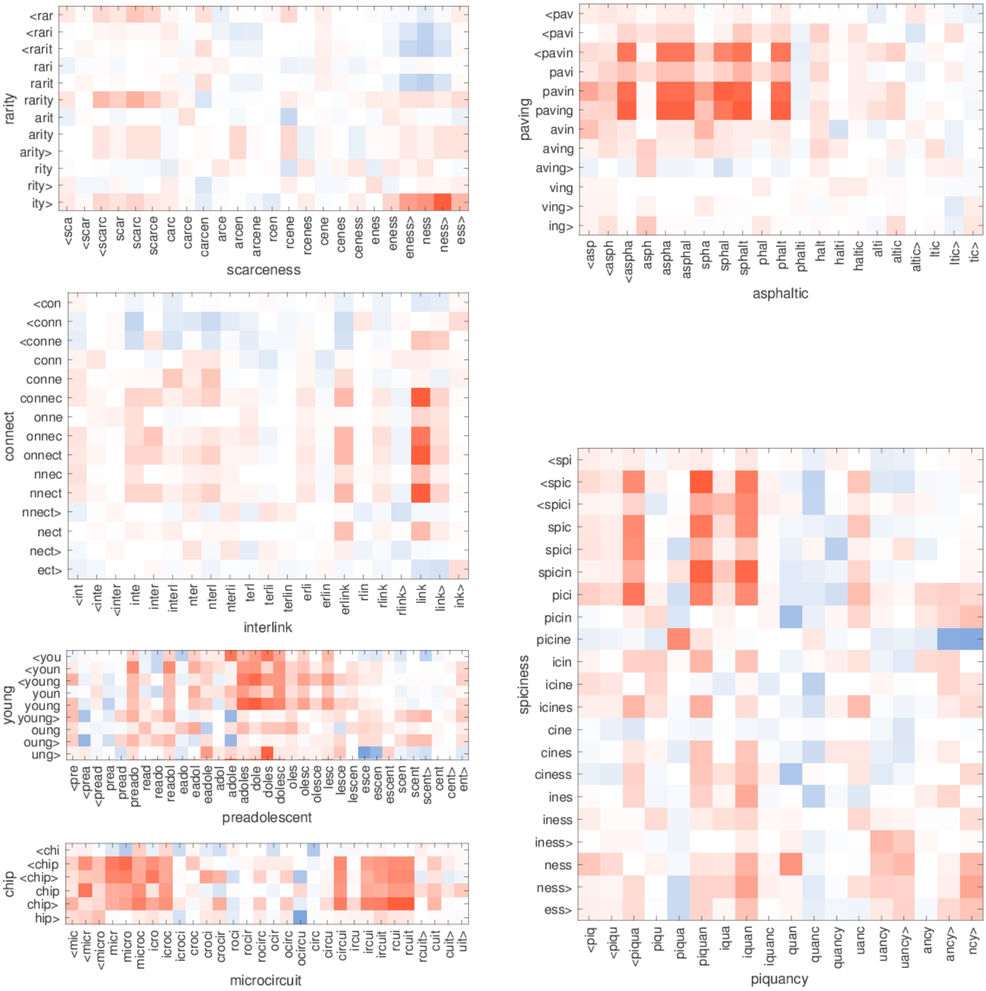


Figure 4.3: Similarity between character n-grams in FastText embeddings. Red indicates positive cosine, blue indicates negative. Reprinted from (Bojanowski et al., 2017).

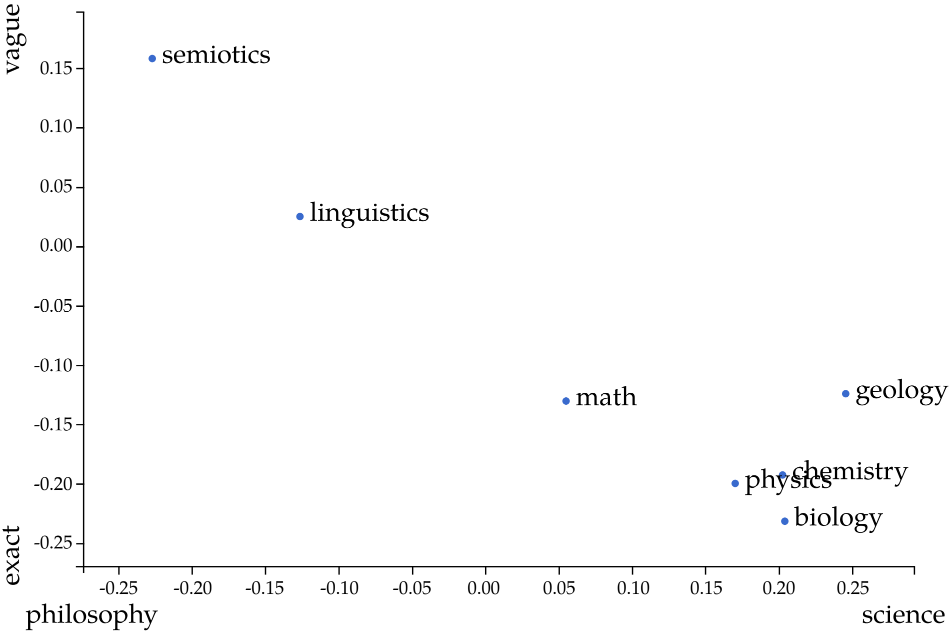


Figure 4.4: Word vectors for names of selected scientific disciplines ploted relative to the axis formed by the vectors for the vector differences between the words *philosophy–science* and *exact–vague*. This image was generated by a web service that we are no longer able to find.

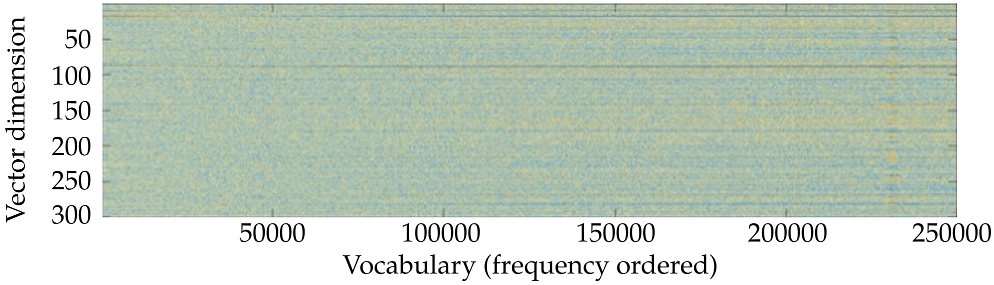
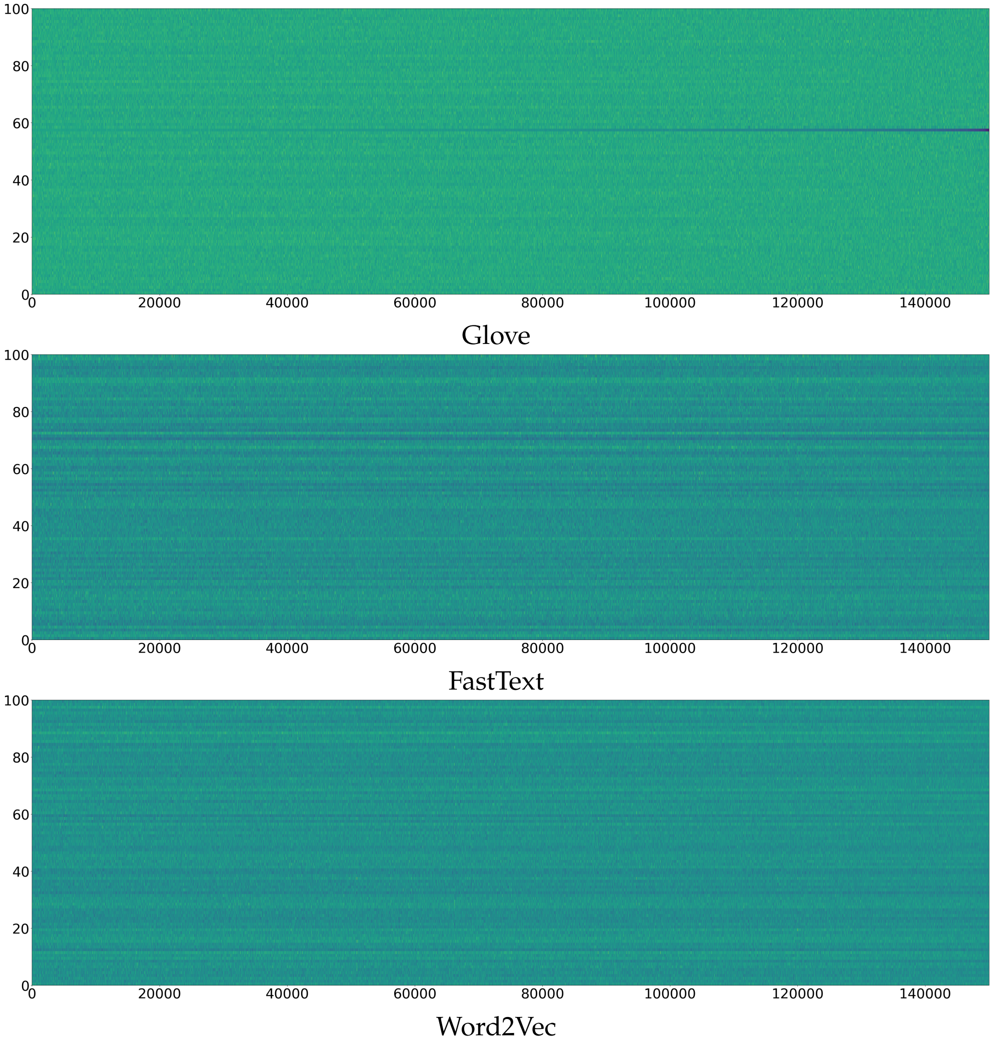


Figure 4.5: Horizontal bands in the Glove word embeddings. Each column represents one embedding vector. The columns are sorted by the frequency of the words they represent, with the most frequent on the right. Reprinted from (Pennington et al., 2014b).



Glove

FastText

Word2Vec

Figure 4.6: Horizontal bands in Glove, FastText and Word2Vec embeddings. The vertical axis represents embedding dimensions, the horizontal axis is the vocabulary. Thefore each column of the colormap is a single embedding vector, with similar colors representing similar values. The embeddings were trained on the Czech National Corpus (version SYN4, Hnátková et al., 2014)

4.3 Embedding Bands

An interesting way to visualize embeddings is a colormap where the color of each pixel represents one numeric value, and each column represents an embedding for a particular word (Pennington et al., 2014b). In Figure 4.5, we see that there are horizontal bands that are more pronounced for more frequent words. The vertical bands are caused by clusters of similar words with similar frequencies (such as numbers). The horizontal bands may result from the fact that the cost function of the model contains a dot product of the embeddings. The vectors are multiplied component-wise in the dot product, and this has a greater impact than additive interactions. According to Pennington et al. (2014b), the bands are unlikely to have a linguistic origin, and this feature is not unique to GloVe. Figure 4.6 shows that other word vector models have this property as well.

4.4 Visualising Word Embeddings with T-SNE

Word embeddings typically have hundreds of dimensions. There are various ways to project embeddings from the high-dimensional vector space to two or three dimensions to visualize them. One popular method is t-SNE (Maaten and Hinton, 2008). It is a stochastic method that aims to project vectors close to each other if they were close in the original vector space. You can see an example of t-SNE mapping in Figure 4.7. The word embeddings in this figure are taken from a neural Language Model (LM), trained on the Czech part of the CzEng corpus (Bojar et al., 2016b). With Czech word embeddings, we can identify larger clusters organized by Part of Speech (PoS), divided into smaller clusters organized by meaning similarities.

4.5 Emoji Embeddings

An increasing volume of online communication contains emojis. Since they can be represented in Unicode, it is possible to treat them the same way as standard text.

Illendula and Yedulla (2018) have successfully induced emoji embeddings based on co-occurrence of emojis in tweets. The resulting embeddings helped them achieve state-of-the-art results in sentiment analysis, suggesting that the sentiment expressed by the emojis can be identified in this way.

A different approach was chosen by Eisner et al. (2016), who trained emoji embeddings based on their Unicode descriptions. This also leads to better sentiment analysis. The resulting embeddings visualized by t-SNE are shown in Figure 4.8. We see that emojis with similar meaning (e.g., state flags, astrological signs, animals) tend to form clusters.

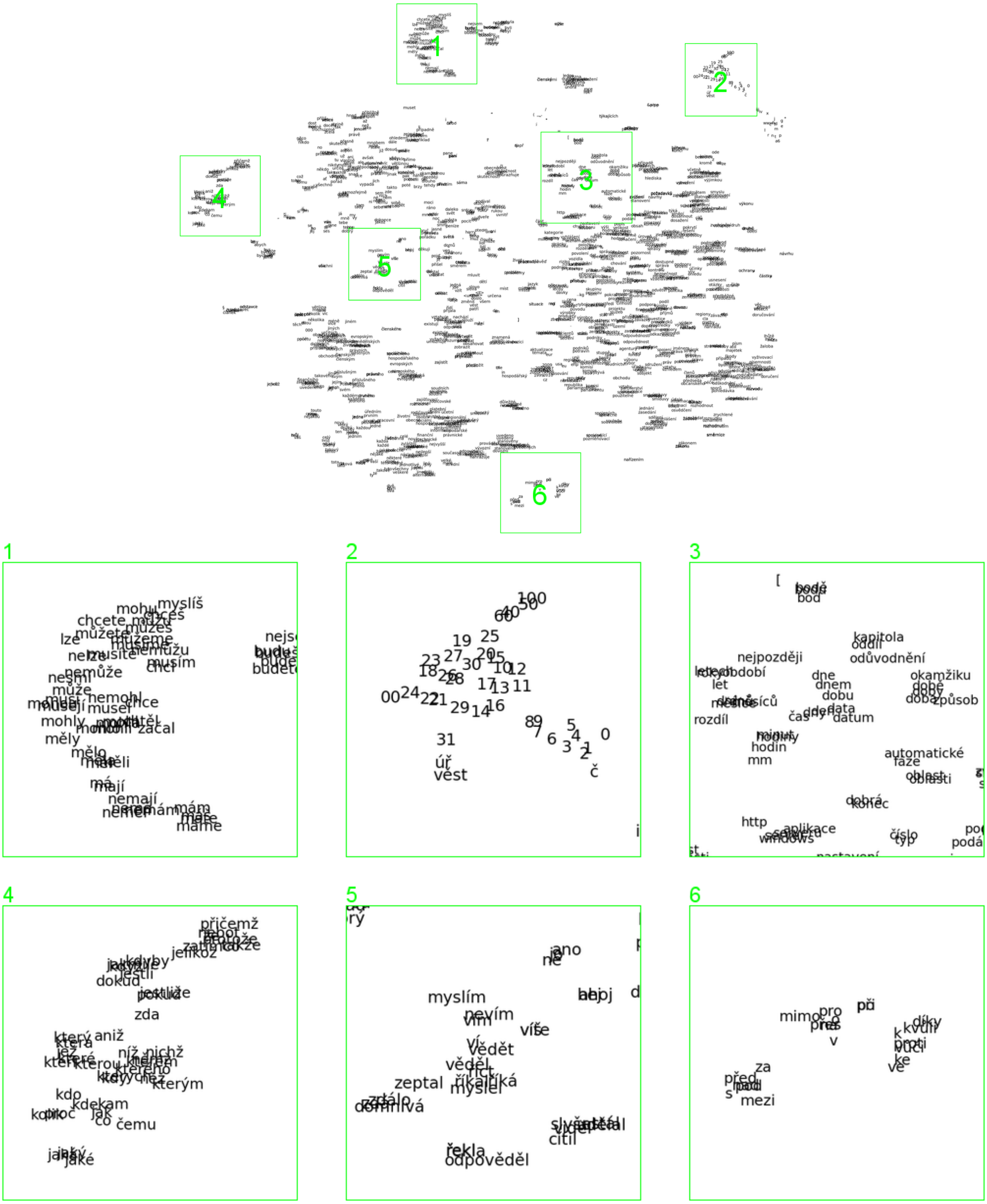


Figure 4.7: A t-SNE projection of 300 dimensional word embeddings from a neural language model trained on the Czech side of the CzEng corpus. Clusters of modal verbs (1), numbers (2), words related to time (3), pronouns (4), verbs related to knowledge (5), and prepositions (6) are clearly visible. Reprinted from (Musil, 2017).

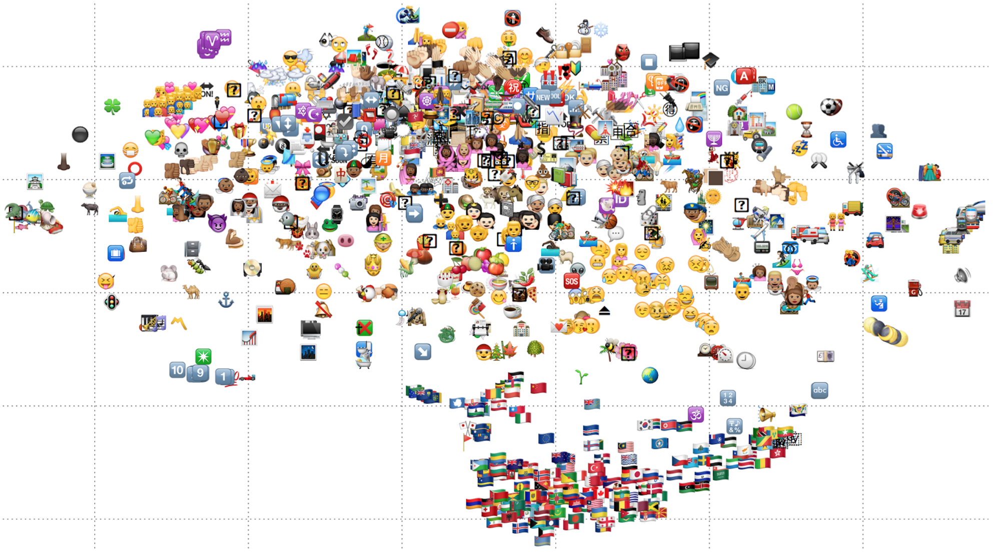


Figure 4.8: The space of emoji embeddings visualised by t-SNE. Reprinted from (Eisner et al., 2016).

4.6 Principal Component Analysis

Principal Component Analysis (PCA) is a process that decomposes multidimensional data into *principal components*. Each component is a linear combination of the individual dimensions. The PCA algorithm (Pearson, 1901; Hotelling, 1936) iteratively finds components that best characterize the data by maximizing the components' variance. PCA is commonly used to decorrelate data or project data into a lower-dimension space, e.g., to visualize it.

The input of the PCA algorithm is a dataset consisting of n samples, each represented by a d-dimensional vector. The output is a linear projection of the dataset, such that the first dimension of the output vectors explains the most of the possible variance. The next dimension explains the most of the remaining variance, etc.

4.6.1 Visualisation

PCA is commonly used as a tool for dimensionality reduction. It fits this purpose because it is a linear transformation that explains the most variance for a given number of dimensions. It can be used to reduce the multidimensional embeddings down to 2 or 3 dimensions for visualization.

In Figure 4.9, we see an example of this practice. We (Musil, 2019) examined Czech word embeddings from a Recurrent Neural Network (RNN) based Neural Machine Translation (NMT) system. Each point in the plot corresponds to one word, and the color represents PoS of that word. We see that the PoS form clusters in the embedding space.

4.6.2 Correlations with Principal Components

We know that individual dimensions of word embeddings usually do not have a conceptual interpretation. What about principal components? Hollis and Westbury (2016) have found that principal components from Word2Vec embeddings correlate with psycholinguistic qualities such as *concreteness*, *meaning specificity*, *valence*, or *dominance*. Inspired by their approach, we compared the structure of Czech word embeddings for English-Czech NMT and Word2Vec (Musil, 2019). Our method is based on correlating PCA dimensions with categorical linguistic data. Figure 4.10 shows correlations of PoS information with PCA components for NMT encoder, NMT decoder, and Word2Vec embeddings. We show that although it is possible to successfully predict the PoS tags from word embeddings of Word2Vec and various translation models, not all of the embedding spaces show the same structure. The information about PoS is present in Word2Vec embeddings. Still, the high degree of organization by PoS in the NMT decoder suggests that this information is more important for machine translation; therefore, the NMT model represents it more directly.

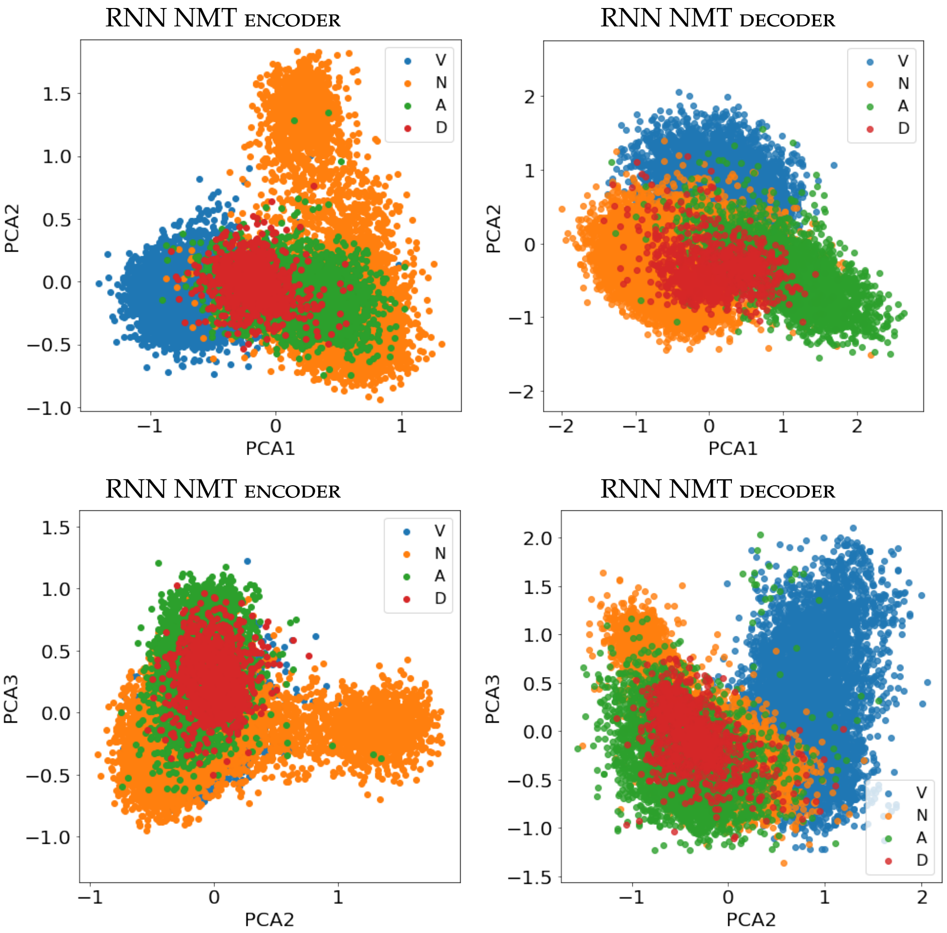
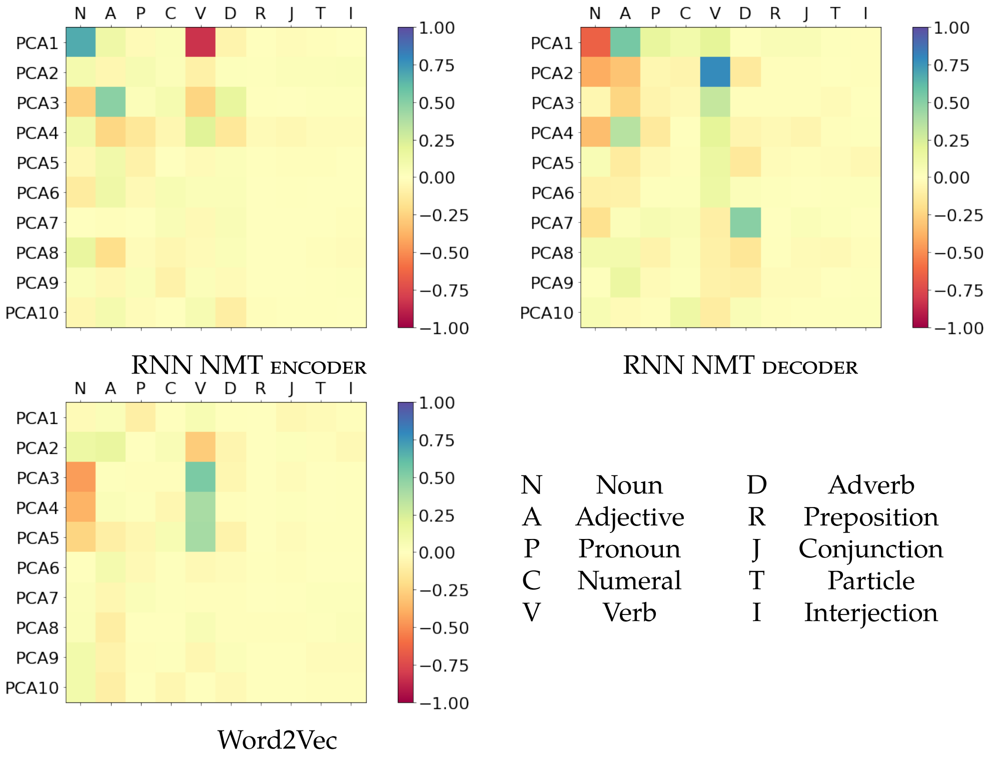


Figure 4.9: Distribution of the four largest PoS classes for Czech word embeddings along the first/second and second/third PCA dimensions of the embeddings from a NMT RNN model. The Czech-English RNN NMT ENCODER is on the left and the English-Czech RNN NMT DECODER on the right. V = verbs, N = nouns, A = adjectives, D = adverbs.



RNN NMT ENCODER

RNN NMT DECODER

Word2Vec

N	Noun	D	Adverb
A	Adjective	R	Preposition
P	Pronoun	J	Conjunction
C	Numeral	T	Particle
V	Verb	I	Interjection

Figure 4.10: Correlations of PoS and PCA dimensions from the encoder of the Czech-English RNN NMT model (top left), the decoder of the English-Czech RNN NMT model (top right) and the Word2Vec model (bottom). The direction of the PCA dimensions is arbitrary, so the sign of the correlation is not important in itself, only if there are values with opposite signs in the same row we know that they are negatively correlated. Reprinted from (Musil, 2019).

4.6.3 Histograms of Principal Components

We also show that further examining histograms of classes along the principal component is important to understand the structure of representation of information in embeddings (Musil, 2019):

Look at the histograms of the four most important PoS classes along the dimensions of the PCA of the embeddings in Figure 4.11. The histogram for the first dimension of the RNN NMT ENCODER embeddings (Fig. 4.11, bottom left) demonstrates that in this dimension, verbs are separated from the rest of the PoS categories.

For the first PCA dimension of the RNN NMT DECODER embeddings, nouns are concentrated on one side, adjectives on the other side, and verbs with adverbs are in the middle.

For the second PCA dimension of the RNN NMT DECODER embeddings, verbs are concentrated on one side, and all other categories are on the other side.

The second PCA dimension shows an interesting distribution of nouns. There is a separate cluster of nouns, which is even more apparent if we plot the distribution along two PCA dimensions in a planar graph in Figure 4.9. When we take a sample of words from this cluster, it contains almost exclusively named entities: *Fang, Eliáši, Još, Aenea, Bush, Eddie, Zlatoluna, Gordon, Bellondová, and Hermiona*.

There is a similar distribution of nouns in the third PCA dimension of the RNN NMT DECODER embeddings. The smaller group again consists of named entities.

This is a stronger result than just being able to predict these categories with a classifier: not only can the PoS (named entities, verb forms, and possibly other categories) be inferred from the embeddings, but the embeddings space is structured according to these categories.

4.6.4 Sentiment Analysis

Sentiment analysis is the task of deciding whether the given text is positive or negative, how much, and what makes it so.

We have found (Musil, 2019) that the shape of the space of word embeddings for a model trained for sentiment analysis is triangular. We examined a Convolutional Neural Network (CNN) trained to predict the sentiment of comments in a Czech film database. In Figure 4.12, we see a sample of the words plotted along the first two principal components. The first component represents the polarity of the words (good/bad); the second component represents intensity (strong/neutral). The triangular shape may be explained by the fact that words that are far from the center on the polarity axis are never of low intensity. This is an example of a neural network adapting to a specific task.

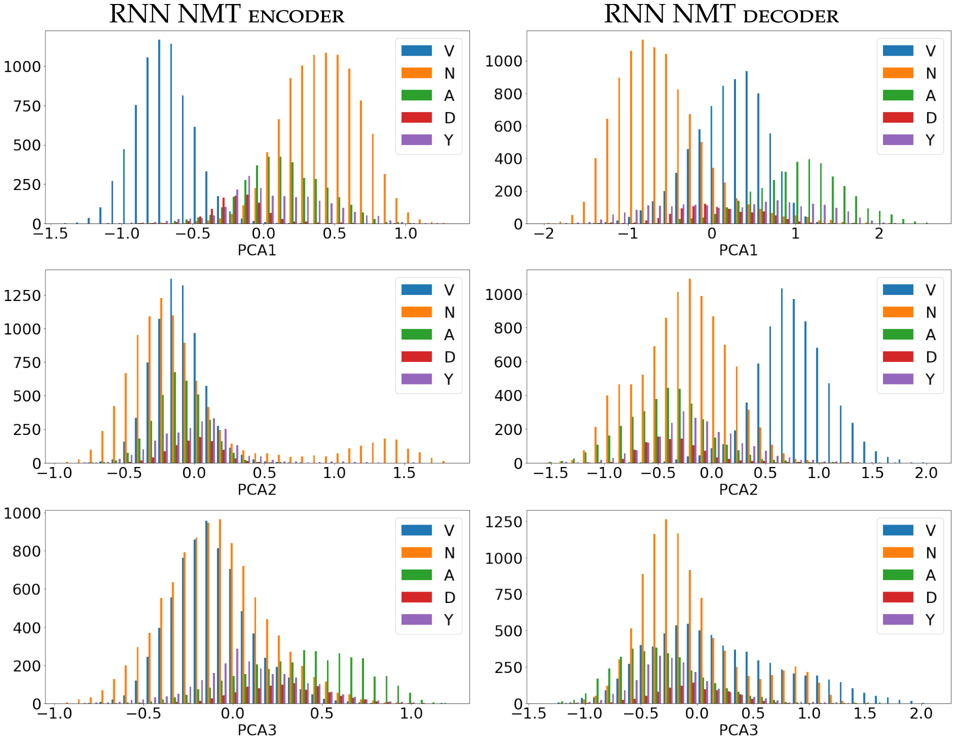


Figure 4.11: Histograms of the four largest PoS classes along the first three PCA dimensions of the embeddings from the NMT RNN model. The Czech-English RNN NMT ENCODER is on the left and the English-Czech RNN NMT DECODER on the right. V = verbs, N = nouns, A = adjectives, D = adverbs, Y = other. Reprinted from (Musil, 2019).

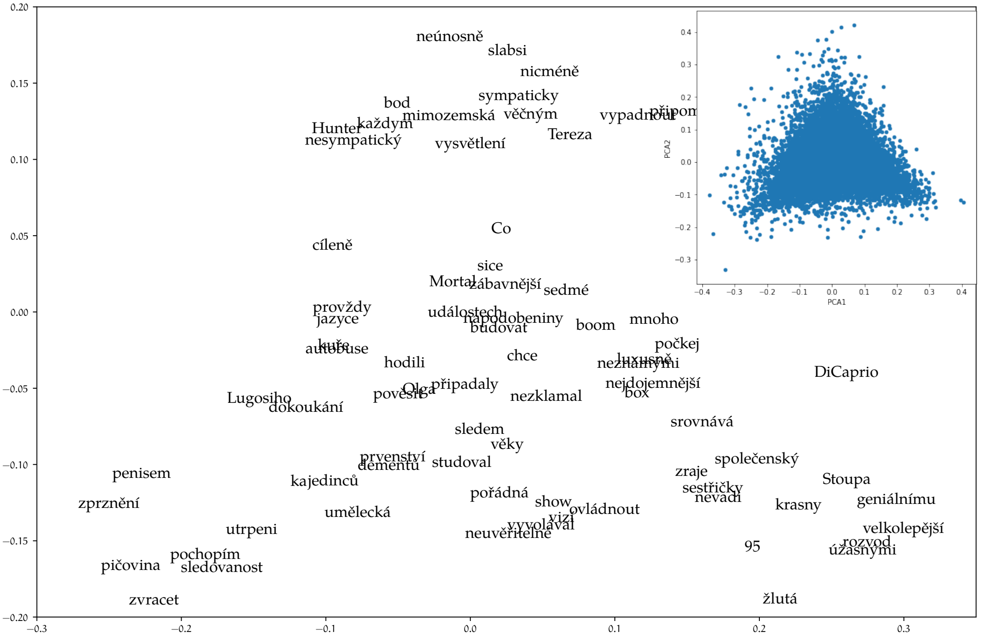


Figure 4.12: A random sample of words from the distribution of the embeddings from the sentiment analysis CNN model along the first (horizontal) and second (vertical) PCA dimension. The top right subplot shows the complete distribution.

4.7 Independent Component Analysis

Independent Component Analysis (ICA) (Jutten and Herault, 1991; Comon, 1994; Hyvärinen and Oja, 2000) is a method similar to PCA that decomposes multidimensional data into components along which the data are distributed as non-Gaussianly as possible. It can be used, e.g., to extract features from distributed representations of words (Honkela et al., 2010).

In this section, we present preliminary findings of our ongoing research into Independent Component Analysis (ICA). We have used NMT and Word2Vec embeddings from models trained on the *fiction* part of the Czech side of the Czeng corpus (Bojar et al., 2016b).

We look at the words that are closest to the extremes in each ICA component. We have found that the components represent various types of categories. In the following examples, each list contains 20 words associated with one component, having either the 20 highest or 20 lowest values for that component. We show that the components represent various types of categories:

Semantic category: words with similar semantic content (e.g., law and justice) from various syntactic categories (in this case predominantly nouns in nominative and genitive morphological case):
zákona, Unie, členských, zákon, stanoví, Komise, zákony, soud, zákonů, zákonem, Evropské, práva, práv, ustanovení, nařízení, porušení, soudu, tj, souladu, podmínek
Glosses: *law*$_{\text{noun gen. sg.}}$, *union*$_{\text{noun nom. sg.}}$, *member*$_{\text{adj. gen. masc.}}$, *law*$_{\text{noun nom. sg.}}$, *determines*$_{\text{verb}}$, *comittee*$_{\text{noun nom. sg.}}$, *laws*$_{\text{noun nom. pl.}}$, *court*$_{\text{noun nom. sg.}}$, *laws*$_{\text{noun gen. pl.}}$, *law*$_{\text{noun inst. sg.}}$, *european*$_{\text{adj. gen. fem. sg.}}$, *rights*$_{\text{noun nom. pl.}}$, *rights*$_{\text{noun gen. pl.}}$, *provision*$_{\text{noun sg.}}$, *regulation*$_{\text{noun sg.}}$, *violation*$_{\text{noun sg.}}$, *court*$_{\text{noun gen. sg.}}$, *ie*$_{\text{shortcut}}$, *compliance*$_{\text{noun gen. sg.}}$, *conditions*$_{\text{noun gen. pl.}}$

Semantic and syntactic category: words that are defined both semantically and syntactically, in this case, predominantly verbs associated with *going somewhere* in the past tense masculine:
šel, zašel, zajít, jít, spěchal, šla, zavedl, vešel, dopravit, nešel, vrátil, poslal, vydal, šli, poslat, přišel, odjel, přijel, jel, dorazil
Glosses: *went*$_{\text{verb masc.}}$, *went down*$_{\text{verb masc.}}$, *go down*$_{\text{verb inf.}}$, *go*$_{\text{verb inf.}}$, *hurried*$_{\text{verb masc.}}$, *went*$_{\text{verb fem.}}$, *led*$_{\text{verb masc.}}$, *entered*$_{\text{verb masc.}}$, *transport*$_{\text{verb inf.}}$, *didn't go*$_{\text{verb masc.}}$, *returned*$_{\text{verb masc.}}$, *sent*$_{\text{verb masc.}}$, *issued*$_{\text{verb masc.}}$, *went*$_{\text{verb masc. pl.}}$, *send*$_{\text{verb inf.}}$, *came*$_{\text{verb masc.}}$, *left*$_{\text{verb masc.}}$, *came*$_{\text{verb masc.}}$, *went*$_{\text{verb masc.}}$, *arrived*$_{\text{verb masc.}}$

Syntactic subcategory: words with specific syntactic features, but semantically diverse (in this case, adjectives in feminine singular form):
Velká, moudrá, občanská, dlouhá, slabá, čestná, železná, překrásná, hladká, určitá, marná,

tmavá, hrubá, příjemná, bezpečná, měkká, svatá, nutná, volná, zajímavá
Glosses: *big*$_{\text{adj. fem.}}$, *wise*$_{\text{adj. fem.}}$, *citizen*$_{\text{adj. fem.}}$, *long*$_{\text{adj. fem.}}$, *weak*$_{\text{adj. fem.}}$, *honest*$_{\text{adj. fem.}}$, *iron*$_{\text{adj. fem.}}$, *beautiful*$_{\text{adj. fem.}}$, *smooth*$_{\text{adj. fem.}}$, *certain*$_{\text{adj. fem.}}$, *in vain*$_{\text{adj. fem.}}$, *dark*$_{\text{adj. fem.}}$, *gross*$_{\text{adj. fem.}}$, *pleasant*$_{\text{adj. fem.}}$, *safe*$_{\text{adj. fem.}}$, *soft*$_{\text{adj. fem.}}$, *holy*$_{\text{adj. fem.}}$, *necessary*$_{\text{adj. fem.}}$, *free*$_{\text{adj. fem.}}$, *interesting*$_{\text{adj. fem.}}$

Feature across POS categories: e.g., feminine plural form for adjectives, pronouns and verbs:
tyto, tyhle, neměly, byly, mohly, začaly, vynořily, zmizely, měly, objevily, všechny, vypadaly, nebyly, zdály, změnily, staly, takové, podobné, jiné, tytéž
Glosses: *these*$_{\text{pron. fem. pl.}}$, *those*$_{\text{pron. fem. pl.}}$, *didn't have*$_{\text{verb fem. pl.}}$, *were*$_{\text{verb fem. pl.}}$, *could*$_{\text{verb fem. pl.}}$, *began*$_{\text{verb fem. pl.}}$, *emerged*$_{\text{verb fem. pl.}}$, *disappeared*$_{\text{verb fem. pl.}}$, *had*$_{\text{verb fem. pl.}}$, *discovered*$_{\text{verb fem. pl.}}$, *all*$_{\text{pron. fem. pl.}}$, *looked*$_{\text{verb fem. pl.}}$, *weren't*$_{\text{verb fem. pl.}}$, *seemed*$_{\text{verb fem. pl.}}$, *changed*$_{\text{verb fem. pl.}}$, *happened*$_{\text{verb fem. pl.}}$, *such*$_{\text{pron. fem. pl.}}$, *similar*$_{\text{adj. fem. pl.}}$, *other*$_{\text{adj. fem. pl.}}$, *same*$_{\text{pron. fem. pl.}}$

Stylistic: in this case, words that often appear in informal spoken language (often second person verbs and colloquial forms):
máš, bys, tý, nemáš, seš, ses, víš, Hele, kterej, sis, jseš, bejt, vo, svýho, celej, děláš, chceš, teda, každej, velkej
Glosses: *have*$_{\text{verb 2nd}}$, *would*$_{\text{verb 2nd}}$, *the*$_{\text{pron. fem. gen. coll.}}$, *don't have*$_{\text{verb 2nd}}$, *are*$_{\text{verb 2nd coll.}}$, *have*$_{\text{verb 2nd refl.}}$, *know*$_{\text{verb 2nd}}$, *Hey*$_{\text{intj. coll.}}$, *which*$_{\text{pron. masc. coll.}}$, *have*$_{\text{verb 2nd refl.}}$, *are*$_{\text{verb 2nd coll.}}$, *be*$_{\text{verb inf. coll.}}$, *about*$_{\text{prep. coll.}}$, *your*$_{\text{pron. masc. gen. coll.}}$, *whole*$_{\text{adj. masc. coll.}}$, *do*$_{\text{verb 2nd}}$, *want*$_{\text{verb 2nd}}$, *well*$_{\text{part. coll.}}$, *each*$_{\text{pron. masc. coll.}}$, *big*$_{\text{adj. masc. coll.}}$

We are finding that many ICA components represent various features of words. It seems to classify not only morphology and syntax but also semantics, so it is a promising research direction for inquiries about representations of meaning.

4.8 Word Derivations

Word derivation is a type of word formation, where new words are created by adding or changing affixes of existing words. We studied word embeddings from an English-Czech NMT system and found that they contain interesting information about morphological derivation (Musil et al., 2019).

In Figure 4.13, each data point represents a pair of Czech words, one of which is derived from the other, usually by a prefix or a suffix. We have identified several classes of word derivations, corresponding to the semantic change associated with them, such as creating a diminutive or making an adjective into a corresponding adverb. The figure shows a plot where each point corresponds to the difference of the two vectors that represent the pair of words in a derivational relation. The vector dif-

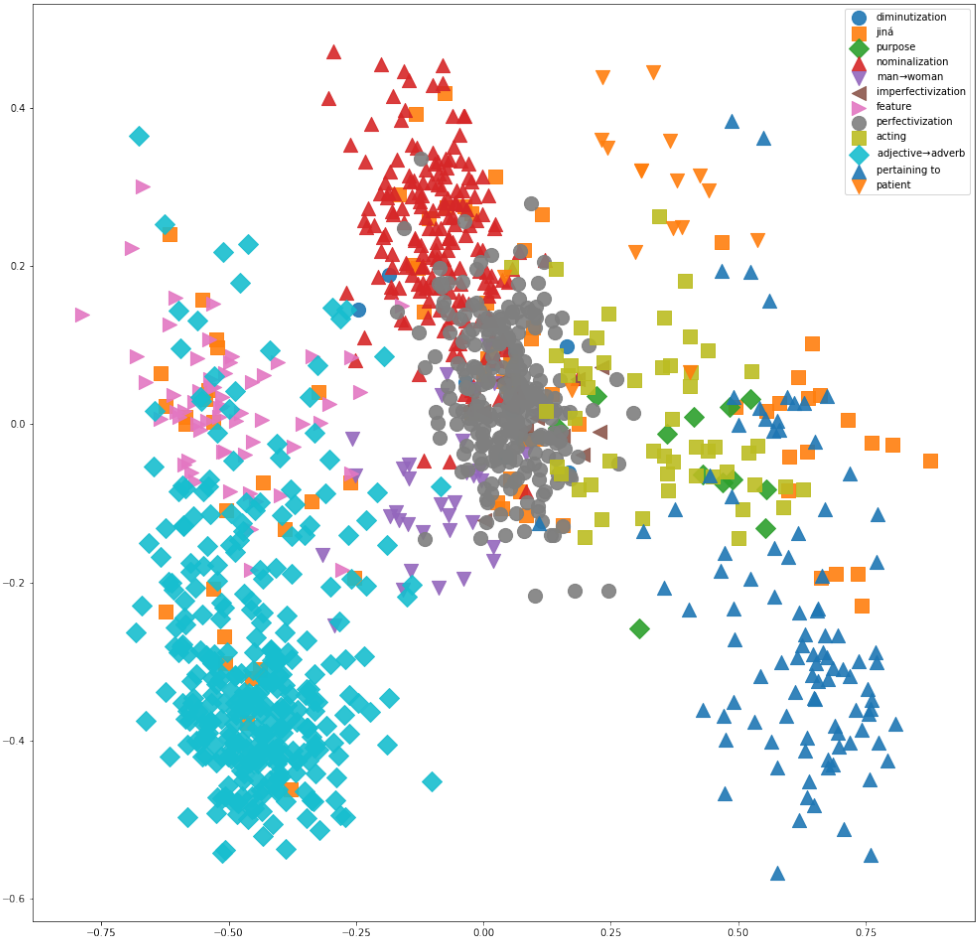


Figure 4.13: Clusters of the derivation types. Each point represents a pair of words, e.g. ▲ kompenzovat – kompenzace (compensate – compensation), ◆ luxus – luxusní (luxury – luxurious), ▲ filosofie – filosofický (philosophy – philosophical).

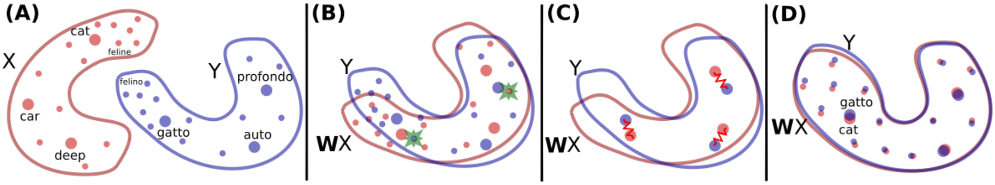


Figure 4.14: Unsupervised mapping of embedding spaces. (A) English – Italian, (B) adversarial learning, (C) Procrustes, (D) expanding dense regions. Reprinted from (Conneau et al., 2018a).

ferences were projected into the first two dimensions by PCA. It is evident that the derivational pairs form clusters corresponding to the classes of the semantic derivational type.

4.9 Mapping Embedding Spaces

It is sometimes possible to map vectors from one embedding space into another in an unsupervised manner. This mapping can then serve as a starting point for an unsupervised NMT system. Unsupervised NMT is a recent technique that allows training translation models without parallel corpora. One of the first methods for unsupervised NMT (Lample et al., 2018) starts by mapping the word embedding spaces of the two languages on each other. Then it creates a simple word-for-word translation model for each translation direction and creates a training corpus by translating monolingual data with these models. It iteratively improves the models and training corpus by training one of the systems on the data produced as translations by the other system. Each system is learning to translate from the synthetic data (translations) to the natural data (original monolingual corpus). As it is getting better, it produces better translations and, therefore, better training data for the other model, which translates in the opposite direction.

The first step of this method, the mapping of the embedding spaces, can be done in an unsupervised manner (Conneau et al., 2018a). The method is illustrated in Figure 4.14. It finds a linear mapping between two sets of embeddings that were trained on monolingual data for two different languages. The initial mapping is found with adversarial learning. The discriminator part of the model is learning to predict whether two randomly selected word embeddings come from the same distribution (from the same language). The other part of the model is learning a rotation matrix to fool the discriminator. When the discriminator cannot effectivelly distinguish the languages, the embedding spaces have been roughly aligned. This is possible because the embedding spaces have similar shapes, even for different languages. This is an interesting property of word embeddings, given that unless the two languages are very

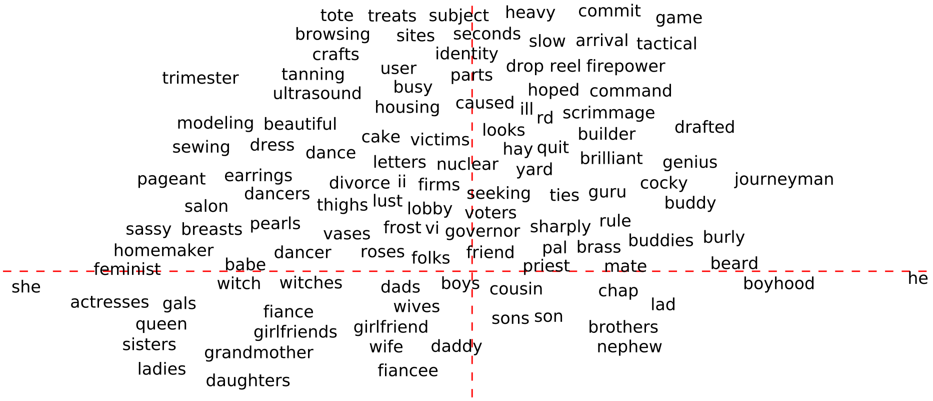


Figure 4.15: A sample of words from the Word2Vec model. The horizontal line represent the *she–he* axis. The vertical axis denotes whether the corresponding word should be gendered according to the classifier. Reprinted from (Bolukbasi et al., 2016).

closely related, the words cannot be mapped between them one-on-one. Because the embeddings are randomly initialized at the beginning of the training, they are not the same even for two instances of the same model trained on the same data. The fact that despite all this, the embedding spaces can be linearly mapped on each other with enough precision to serve as a base for a translation system, based only on the shape of the embedding spaces, means that there is a structure that is common to (at least Indoeuropean) languages and it is captured in the shape of the embedding space.

4.10 Debiasing: Interpretation as Manipulation

Real-world datasets reflect the biases of the society that produced them. Computers may seem impartial, but machine learning can turn biased datasets into biased models that can even amplify the biases from the training data (Zhao et al., 2017). NLP models can be deployed in various contexts where preserving or amplifying biases can be potentially harmful to specific social groups. The discussion of necessity and particular techniques for mitigating bias is beyond the scope of this book. Regardless of that, biases in word embeddings pose a problem that can be diminished with the help of interpretation of the learned representations.

Bolukbasi et al. (2016) have found that Word2Vec embeddings tend to contain biases implicit to the data that the model has been trained on. One way to show the bias is to use the vector analogy method. For example, the model they have been inspecting says that *man* is to *programmer* as *woman* is to *homemaker*.

They trained a classifier to determine the words that should be gendered. Figure 4.15 shows a sample of words from the model. The horizontal axis represents the *she-he* direction in the embedding space. The vertical axis represents the score from a model that predicts whether the word should be gendered. The horizontal line separates the gendered words (below), such as *brother*, or *queen* and words that should not be inherently gendered, such as *genius* or *tanning*. The words above the line that are far from the center on the horizontal axis show gender bias. The debiasing process consists of finding these words and removing the gender dimension from their embeddings.

4.11 Conclusion

There are two main techniques of interpretation for word embeddings: probing and component analysis. With probing, we can show that various linguistic features are represented in the embeddings, depending on the task that the model is trained for. With component analysis, we can show what features are important for a given task. However, for more complex tasks, such as language modeling or machine translation, we do not yet understand the structure of the embedding space completely.

Pretrained word embeddings contain information about both morphology and lexical semantics. When the embeddings are trained for a specific task, the embeddings tend to be organized by the information that is important for the given task (e.g., emotional polarity for sentiment analysis).

5

May I Have Your Attention?

With the advent of neural networks in Natural Language Processing (NLP), traditional linguistics-based methods such as parsing or word-alignment are no longer a part of modern NLP solutions. Instead, new mechanisms were introduced that are capable of generating these linguistic abstractions latently, but of course, only if they are needed and in the form most suitable for the particular task. The attention mechanism (described in Sections 1.3.2 and 2.2) allows the network to consider each component individually (typically words or subwords) of the input (typically sentences) and to decide how much this component will contribute to currently computed input representation. It provides weighted links between the language units that can be interpreted as a sentence structure relevant to the particular task. These emergent structures may be compared to explicit discrete linguistically motivated structures such as dependency trees, constituency trees, word alignment, coreference links, or semantic relations.

For example, consider syntactic trees, which have been widely used in the past as a preprocessing step for various NLP tasks and provided the systems with information about relations between words. The syntactic trees were learned from manually annotated treebanks. Such annotations required many design decisions on how to capture specific language phenomena in the tree structure. Moreover, various NLP tasks might benefit from differently annotated trees. The main limitation of using the treebanks is that the tree structures are discrete and include only a limited number of relations between words.

In the current neural architectures, the attention mechanism learns the relations between tokens in an unsupervised way. With the current complex architectures, models can capture many different weighted relations between the same tokens over different layers and attention-heads. Therefore, the structures generated by the attention mechanism overcome the drawbacks of using explicit syntactic structures. They consist of multiple complete graphs with weighted edges optimized for the target NLP task.

However, the price paid for using the attention mechanism is very difficult interpretability. The number of relations the current neural architectures consider is enormous and makes the attention hard to interpret even when it is fully trained. For example, for one 10-words-long sentence, instead of 10 discrete labelled edges in a dependency tree, we have 20,736 real numbers in the attention mechanism.[1]

Our goal is to organize these vast amounts of numbers, find the underlying structure of the attention mechanism, and visualize it. We want to find out to what extent the self-attentions resemble syntactic relations, and cross-lingual attentions resemble word alignment as we know them from the original non-neural systems. We also want to investigate whether these structures differ across NLP tasks.

5.1 Cross-Lingual Attentions and Word Alignment

The term *attention* was first introduced by Bahdanau et al. (2014) for modelling word alignments in neural machine translation, and its generalization then became a universal approximation of NLP structures. This work was a breakthrough for the Neural Machine Translation (NMT) systems since it brought the translation quality to the level of previously widely used phrase-based systems (see Section 2.2). Each time the translation model generates a word, it attends to ("looks at") all the positions (tokens) in the source sentence representation and chooses the ones that are most relevant for the current translation. The weighted average of the attended representations is then used as input into a classifier predicting the target word to be generated. It is important that the search itself is "soft"; non-negative weights are assigned to all the positions. In practice, however, a trained model assigns typically only a small number of positions with weights significantly greater than zero. Therefore, the concept of word-alignment was preserved in the modern NMT systems; it was only transformed into a softer and more flexible shape.

In the previously used phrase-based systems (Koehn et al., 2007), the word alignment was used as a preprocessing step for developing phrase dictionaries. The connections between tokens were discrete. Each connection either was there or was not. Even though the algorithms for unsupervised word alignment (Och and Ney, 2000) were based on Expectation-Maximization algorithm and used probability distributions, the resulting alignments were discrete. A specific symmetrization approaches were needed to get the final word-alignment from the two one-directional 1-to-many alignments.

In the early NMT architectures using a fixed-size transition vector (Sutskever et al., 2014), the word alignment disappeared entirely since the only transition between encoder and decoder was one fixed-sized vector.

The connections between individual positions in source and target sentences returned with the attention mechanism, but with the following essential differences. First, the attention mechanism is soft and may be represented as a complete bipartite graph with weighted edges. Second, the attention mechanism connects only the

[1] We consider BERT's base model using the initial `[CLS]` and final `[SEP]` tokens. The number is computed for ten subword units.

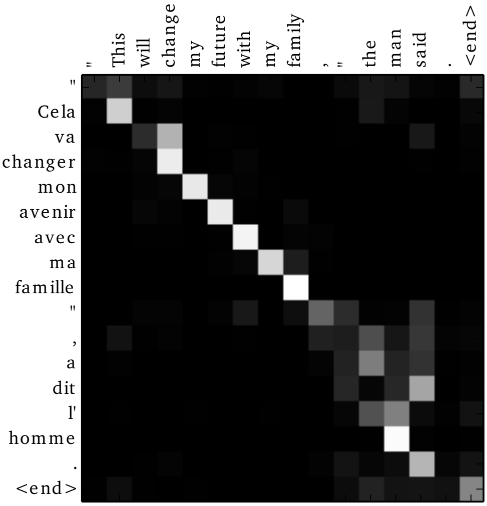


Figure 5.1: Example of cross-lingual attention distributions. Soft alignment of "the man". Reprinted from (Bahdanau et al., 2014, Figure 3d).

contextual embeddings on respective positions,[2] not the words themselves, as it was in the original word-alignment. It is difficult to find what information a contextual embedding stores or to what extent it represents the word at its position. Moreover, we cannot know what information from the attended contextual embeddings, if any, is eventually used by the classifier. Even though it is very often simplified into an assumption that a given contextual embedding mostly represents the word on that position, it may not be true (see Section 3.3.1). Therefore, we deliberately talk about attention to source sentence *positions* instead of attention to particular words.

The soft word-alignment used by the attention mechanism is much more adequate. To translate a word correctly, one needs to know not only its counterpart in the source language but also many other words from its context. Even though the necessary context might be present in the contextual embedding, the visualisations of attention weights show that the attentions are indeed more spread across different positions in the source sentence than the traditional word-alignment was. In the attention visualisation in Figure 5.1, we can see that the source phrase *'the man'* was translated into *'l' homme'*. Traditional word-alignment would map *'the'* to *'l''* and *'man'* to *'homme'*. However, such alignment is not sufficient for translation, as one must consider also

[2] In the NMT architecture proposed by Bahdanau et al. (2014), the contextual embeddings are concatenations of forward and backward Recurrent Neural Networks (RNNs) and therefore may contain any information from the whole sentence.

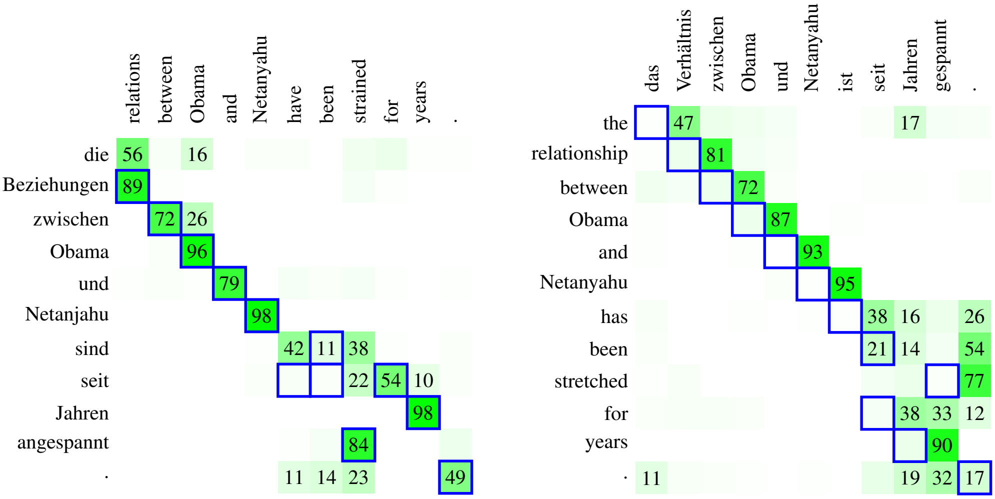


Figure 5.2: Word alignment (marked by blue squares) compared to attention weights (green squares). Reprinted from Koehn and Knowles (2017, Figures 8 and 9) under CC-BY-4.0 licence.

he word following *'the'* to determine whether it should be translated as *'le'*, *'la'*, *'les'* or *'l''*. The attention mechanism solves it naturally letting the model look at the context vector of the word *'man'* as well and translate the word *'the'* correctly into *'l''*.

The translation model has two possibilities on how to deal with the context. Some information is stored in the contextual embeddings themselves, and the attention mechanism controls everything else needed for the translation. The contextual embeddings must contain information about how much they are important for translating different words; such information is passed to the attention mechanism.

Koehn and Knowles (2017) compared the attention weights to the word-alignment, which was automatically created by fast-align alignment tool[3] (Dyer et al., 2013). The results are illustrated in Figure 5.2 and show that translation of some words requires information from more source contextual embeddings when compared to the word-alignment.

However, they also showed that training an NMT system can lead to very non-intuitive attentions. In Figure 5.2, we can see an example of attentions in German-English translation. The model learned that in order to generate the English word, it is best not to attend to its counterpart in German but to the following token. Despite

[3] `https://github.com/clab/fast_align`

such shifted attentions, this translation system had comparable results with other systems, in which the attentions roughly matched the alignments.

The explanation of such a non-intuitive behaviour is probably a side effect of the end-to-end training setup. Although the architecture is designed to learn particular words at particular places, it may sometimes be more convenient for the network to learn the problem differently. Here the forward part of the encoder might put a strong emphasis on the previous word in its contextual representations. The attention mechanism then prefers to attend to the following positions, which also represent the previous words well.

The mismatch between the attention mechanism and the word-alignment led some researchers to develop systems that would increase the correspondence with word-alignments using some kind of supervision. For example, Liu et al. (2016) came with an additional loss function that penalized the disagreement between attention weights and the conventional word-alignment models. In this way, they treated the attention variables as observable variables. The training objective then resembled that in the multi task-learning. However, all of these attempts gained no or only tiny improvements in translation quality.

Ghader and Monz (2017) published a more detailed analysis answering the question of what the attention-mechanism really models and how similar are attentions to alignments in different syntactic phenomena. They show that attention follows different patterns depending on the type of the word being generated.

For example, the attention model matches with word alignment to a high degree in the case of nouns. The attention distribution of nouns also has one of the lowest entropies meaning that on average, the attention of nouns tends to be concentrated.

A different situation was observed when translating verbs. The low correlation with word-alignment confirms that attention to other parts of source sentence rather than the aligned word is necessary for translating verbs and that attention does not necessarily have to follow alignments. The attention entropy of verbs is high and shows that the attention is more distributed compared to nouns. It also confirms that the correct translation of verbs requires the systems to pay attention to different parts of the source sentence. This may be the reason why the approaches pushing the attention mechanism to be more similar to alignments did not succeed.

In Table 5.1, Ghader and Monz (2017) show what types of tokens the translation model attends to when generating different parts-of-speech. When generating nouns, the most attended roles (besides their noun counetrparts) are adjectives and determiners. When generating verbs, the attention model covers auxiliary verbs, adverbs, negation particles, subjects, and objects.

These analyses were performed on German-English translation. We suppose that the observations may be different for other language pairs.

POS tag	roles (attention %)	description
NOUN	punc (16%)	Punctuations
	pn (12%)	Prepositional complements
	attr (10%)	Attributive adjectives or numbers
	det (10%)	Determiners
VERB	adv (16%)	Adverbial functions including negation
	punc (14%)	Punctuations
	aux (9%)	Auxiliary verbs
	obj (9%)	Objects
	subj (9%)	Subjects
CONJ	punc (28%)	Punctuations
	adv (11%)	Adverbial functions including negation
	conj (10%)	All members in a coordination

Table 5.1: Statistics of syntactic labels at positions attended by nouns, verbs, and conjunctions. Reprinted from Ghader and Monz (2017, Table 7) under CC-BY-4.0 licence.

5.2 Self-Attentions and Syntactic Relations

Another breakthrough in machine translation architecture occurred with the publication of the article by Vaswani et al. (2017). The authors introduced a new architecture called Transformer (see Section 1.3.2) using the attention mechanism as the main building block. Later, the Transformer proved to be a universal encoder for many NLP task, mainly thanks to the Bidirectional Encoder Representations from Transformers (BERT) model (see Section 2.6). Transformer's self-attentive encoder consists of several (6 to 24) layers. Each layer produces contextual embeddings that correspond to sub-words of the source sentence, and each one can possibly attend to any of the contextual embeddings from the previous layer using the self-attention mechanism (see Figure 5.3). In each layer, the contextual representation of the whole sentence is updated and passed to the next layer. The information stored at the contextual embeddings may also diverge from the sub-words at the respective positions in the source sentence (see Section 3.3.1). However, due to residual connections skipping the attention layers, which are mixed with the attention outputs in 1:1 ratio, we can probably safely assume that each attention head at each layer corresponds to the sub-word at the respective position.

While the cross-lingual attention may be seen as a parallel to the word alignment in statistical Machine Translation (MT), the self-attention mechanism may be seen as a parallel to structural relations between words. The original paper by Vaswani et al. (2017) already mentioned that many attention heads exhibit behaviour that seems re-

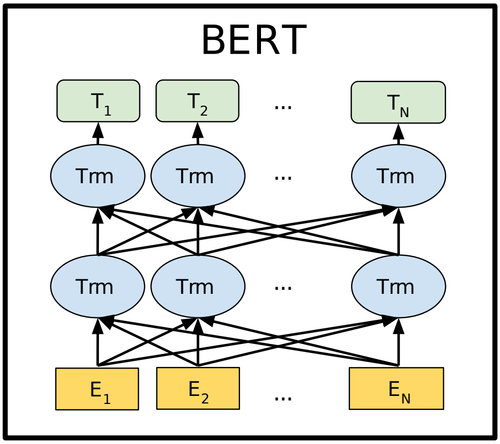


Figure 5.3: Self-attention mechanism in Transformer (BERT). Reprinted from Devlin et al. (2019, Figure 3 left) under CC-BY-4.0 licence.

lated to the structure of the sentence, such as dependency syntax or coreference links. Note that the models are trained end-to-end for MT or language modelling, and there is no explicit supervision that would direct the models towards specific attention patterns. They are emergent and only formed using the training signal that comes from the errors the Neural Network (NN) makes when generating words. Each attention head forms a complete bipartite weighted graph expressing the connections between individual pairs of sub-word units (or more precisely, between their contextual representations of two consecutive layers).

In the following sections, we try to categorize different types of attention heads and discuss what structural phenomena can be identified within the attention patterns.

5.2.1 Categorization of Self-Attention Heads

One way of analyzing the self-attention mechanism is to inspect individual attention heads visually and describe frequently occurring patterns.

Many related papers attempt to classify patterns in self-attention heads. They analyzed different model variants and tasks (Raganato and Tiedemann, 2018; Mareček and Rosa, 2019; Vig and Belinkov, 2019; Kovaleva et al., 2019; Voita et al., 2019; Clark et al., 2019; Kim et al., 2020). Based on the literature and our own qualitative exploration, we put together all the self-attention patterns that were observed. For each pattern, we show an example of a self-attention heatmap, comment in what models and how often it occurs, and speculate what might be its function in the model. Even

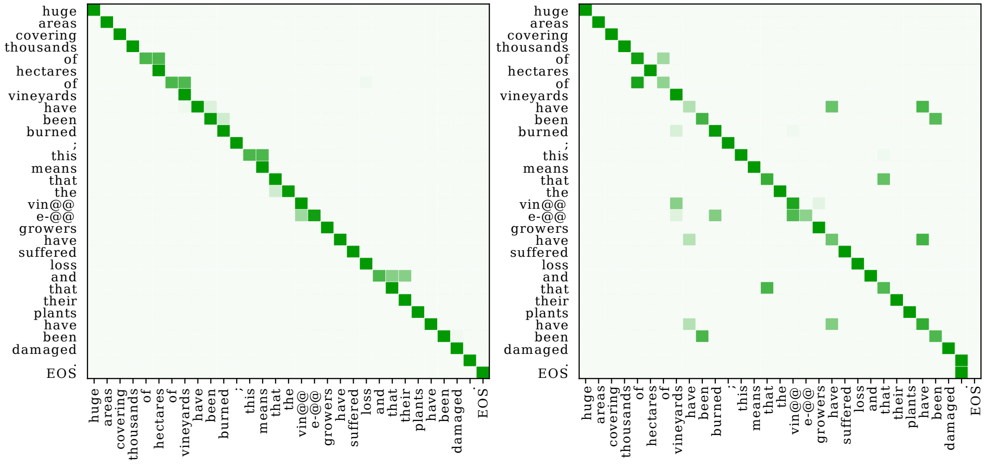


Figure 5.4: Two examples of self-attention heads mostly attending to the same position. The head on the left also captures some types of function words. The head on the right attends to all equal tokens in the sentence.

though the self-attention patterns may differ across Transformers trained for different tasks, many of the basic patterns were reported by all the cited papers.

Main diagonal – Attending to the same position. One of the most trivial head patterns is the attention to the same position. We observe such heads appearing for almost all tasks. In BERT, they are more frequently in the lower layers. Clark et al. (2019) note that, even though attention to the same position is generally very scarce, these specialized heads do the opposite and they, in fact, double the residual connections and allow the network to copy the whole information to the next layer. In NMT, such heads occur typically in the first layer (Mareček and Rosa, 2019). In some cases, most states attend to the same positions, but some of them attend elsewhere. The role of such partially diagonal head may be processing a specific phenomenon that only occurs for some of the states.[4]

Two examples of this kind of heads are given in Figure 5.4.

Diagonal – Attending to the adjacent position. Another pattern, similar to the first one, is attending to the previous or the next position. We suppose that such heads are essential for Transformers since the keys and values in the self-attention are treated as

[4] For example, consider a head attending to subjects when processing verbs. In this case, all the verbs attend to their subjects, whereas all the other words attend to the same position.

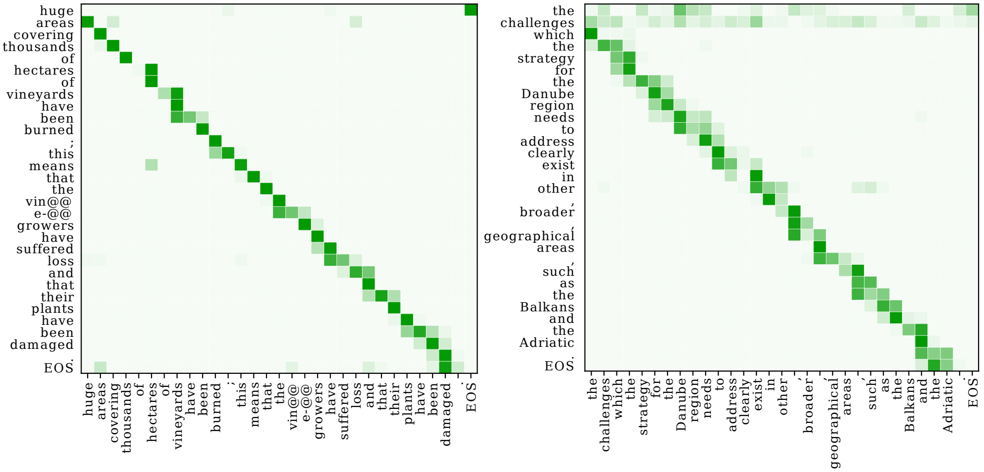


Figure 5.5: Two examples of self-attention heads mostly attending to the previous and pre-previous position.

unordered sets, so the model must learn the token adjacency. Some attention heads attend to more distant positions, e.g., the pre-previous one, and there are also heads dividing their attention into more adjacent tokens. Two examples are given in Figure 5.5. As for the *main diagonal* pattern, such heads occurs in NMT mainly in the first layer. In BERT, they appear mostly in earlier layers of the network. Therefore, Raganato and Tiedemann (2018) speculate the transformer tries to find long dependencies between words on higher layers, whereas it tends to focus on local dependencies in lower layers.

Vertical – All positions attend to one particular position. Almost all relevant literature discusses the pattern where all positions attend to one particular position in the previous layer. One example is given in Figure 5.6 (left). Such positions often correspond to technical or functional tokens. Kovaleva et al. (2019) and Clark et al. (2019) show that in BERT, there exist attention-heads focusing mainly on the separator `[SEP]` or class `[CLS]` position. We (Mareček and Rosa, 2019) and Raganato and Tiedemann (2018) show that NMT transformer also includes heads focusing on punctuation marks, especially on the final period. One possible explanation is that these positions are used for aggregating sentence-level information. The `[CLS]` token is deed designed for this purpose. It is forced to aggregate the information about the whole sentence by one of the BERT's training objective. This pattern is a special case of the following *Heterogenous* pattern. We provide some observations related to this pattern in the following paragraph.

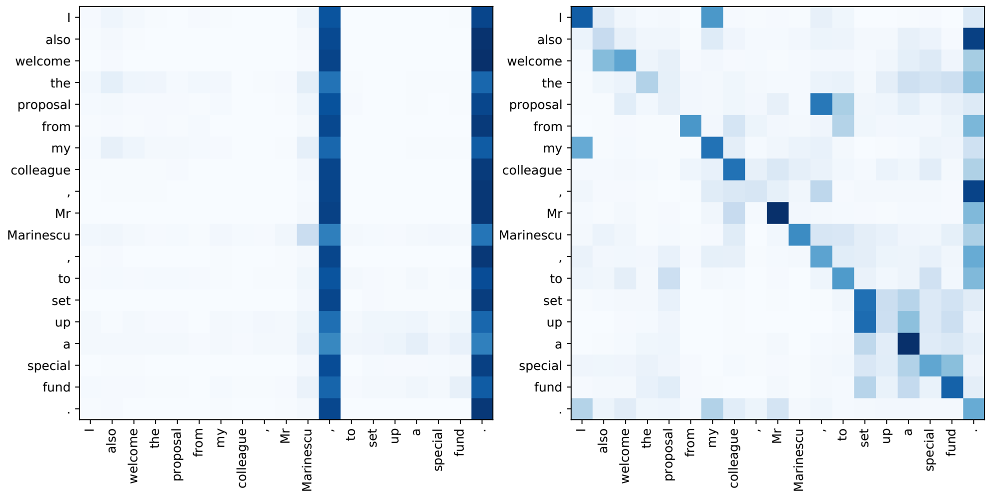


Figure 5.6: Self-attention heads representing the vertical pattern (on the left) and the heterogeneous pattern (on the right).

Heterogenous. Some of the heads typically combine several of the previously defined patterns. An example is given in Figure 5.6 (right). Kovaleva et al. (2019) mention that they are highly variable depending on the specific input and cannot be characterized by a distinct structure.

Many attention heads found both in BERT and NMT encoders combine attention to one particular position (typically `[CLS]` or `[SEP]` in BERT and punctuation marks in NMT) with another function. Clark et al. (2019) report that over half of BERT's attention in layers 6–10 focuses on `[SEP]`. The specific role of `[SEP]` and `[CLS]` may be caused by the fact that they are guaranteed to be present and are never masked out, whereas the most common tokens as punctuation marks are not. They found attention heads where the direct objects attend to respective verbs or where the possessive pronouns attend to respective nouns. All tokens for which the attention head's function was not applicable attended to `[SEP]`. They conducted additional experiments using gradient-based measures (Sundararajan et al., 2017) showing that gradients for attentions to `[SEP]` are very low. Therefore they conclude that attending to `[SEP]` can be understood as a "no-op" function. In NMT, we found many heterogenous heads combining two of the previous functions. For example, the first half of the positions attends to the previous tokens and the second half attends to the final punctuation.

Balustrades. In our experiments with NMT (Mareček and Rosa, 2019) we observe that the most frequent pattern, appearing in about two-thirds of the attention heads, is

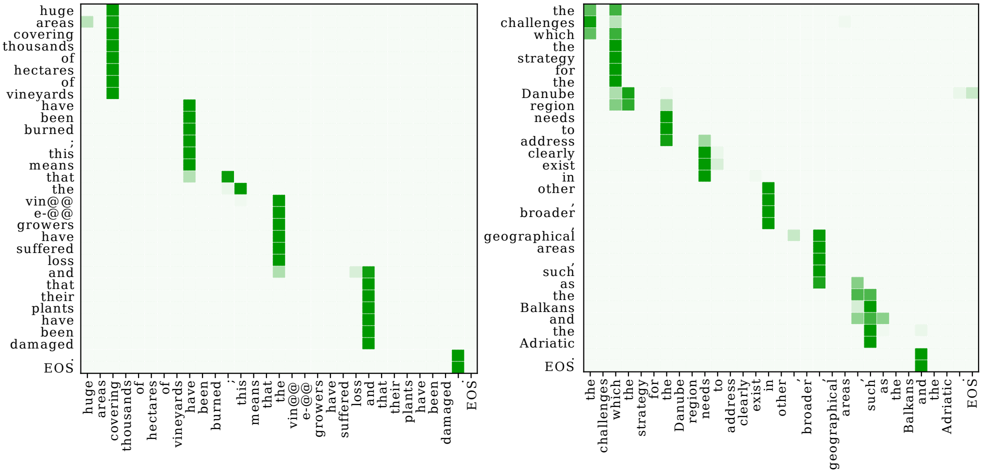


Figure 5.7: Two examples of self-attention heads representing the balustrades pattern.

a series of vertical bars, typically placed at the diagonal, which resemble the balusters of a staircase railing. We show a couple of examples in Figure 5.7. In such attention heads, sequences of consecutive tokens attend to one position in the previous layer. The lengths of the sequences differ; some heads include a higher number of rather short, e.g. 3- to 5-token long sequences; other heads include only a couple of long sequences. A typical sequence attends to a position inside it, very often to its first or the last token. Longer sequences often attend to positions that correspond to punctuation marks or conjunctions. Some heads attend almost exclusively to the sentence-final punctuation. This pattern, therefore, combines the *Diagonal* and the *Vertical* patterns and fills the transition between them. The balustrades were observed in NMT models across different languages. The individual vertical bars may be treated as linguistic phrases and may be used to infer syntactic trees (see more in Section 5.2.5).

Attending to the equal word-pieces. In NMT, there is typically one or two heads where each output state attends to all instances of the same subword, usually with a more or less uniform distribution (see the subwords “of”, “have” and “that” in Figure 5.4 (right). We have also seen these heads to sometimes attend to very similar but not identical subwords (e.g. singular and plural).

Attending to everything. Clark et al. (2019) noticed that some attention heads, especially those in the lower layers of BERT, attend broadly across many positions in the previous layer. These high-entropy attention heads typically spend at most 10%

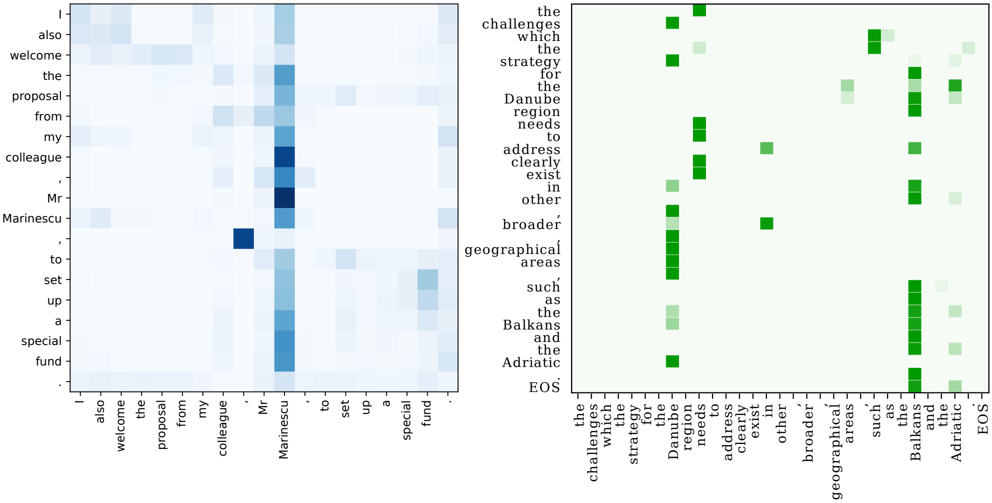


Figure 5.8: Examples of self-attention heads attending to the rare tokens from the BERT model (in blue) and NMT model (in green).

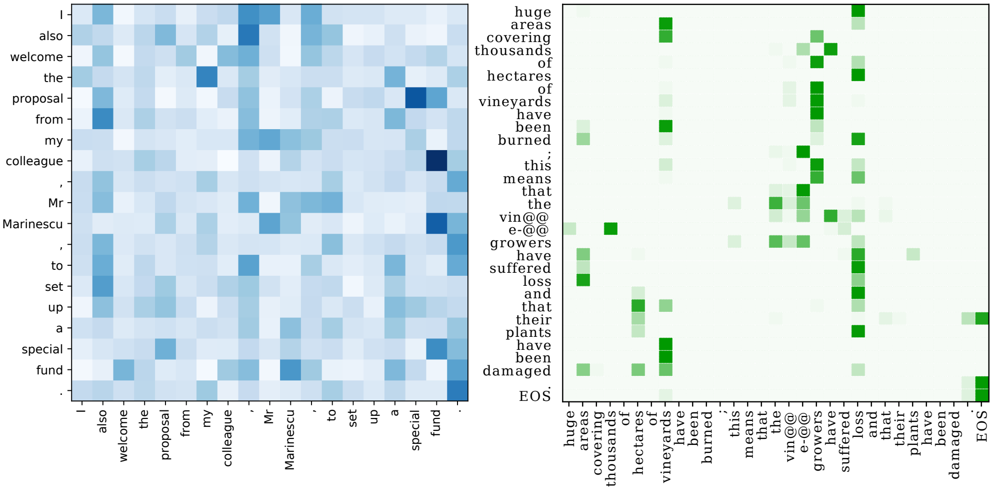


Figure 5.9: Examples of self-attention heads with scattered attentions from the BERT model (in blue) and NMT model (in green).

of their attention mass on each of the positions and their output is then roughly the representation of the whole sentence.

Block. For tasks with two distinct sentences at the input, Kovaleva et al. (2019) identified heads doing only the intra-sentence attention (e.g. in BERT finetuned for Textual Entailment or Paraphrase Detection). Similarly, as in the *Attending-to-everything* pattern, these heads spread the attention across many positions. However, in this pattern, all the attention goes into the other sentence, forming a shape of two square blocks.

Attending to rare words. Voita et al. (2019) mention that some of the BERT's heads, all the positions attend to some least frequent tokens in the sentence. Two examples are given in Figure 5.8.

Scattered. The rest of the heads do not resemble any of the patterns mentioned above. We cannot exactly say what they do. Their entropy is rather low, and therefore, they look more like random points scattered within the matrix. Examples are given in Figure 5.9.

We identified eight patterns of self-attention heads in total. The distinction between individual types of patterns is often somewhat fuzzy. Moreover, their distributions vary across different trained models. The main aim was to describe the heads and try to outline what is their function in the model. In Table 5.2, we present rough counts of types of heads for each layer of Transformer NMT[5] and pre-trained BERT, respectively. The first layer of NMT systems contains many diagonal patterns and differs from all the other layers containing many balustrade patterns and scattered heads. The situation is different in the BERT model. The whole first half of its heads contains diagonal and scattered patterns. After that, the heterogeneous patterns prevail, and in the last two layers, there are mainly vertical patterns.

5.2.2 Highly Redundant Attention Heads

When examining the patterns of self-attention heads, we observe a high level of redundancy. We can find heads in the same layer performing almost the same function. Many similar heads can be found across layers. However, their roles may differ since different layers encode different information.

[5] The numbers were computed manually on a sample of source sentence processed by English-to-German NMT system. However, the other language pairs from experiments by Mareček and Rosa (2019) exhibit similar proportions.

	main diagonal	diagonal	vertical	balustrades	rare words	heterogenous	scattered	equal
L0	6	3	1	0	0	4	2	1
L1	0	0	0	9	0	0	7	0
L2	0	0	0	7	1	0	8	0
L3	0	0	0	6	0	2	8	0
L4	0	0	1	3	0	3	7	0
L5	0	1	0	8	0	1	5	0

	main diagonal	diagonal	vertical	balustrades	rare words	heterogenous	scattered	equal
L0	0	3	0	0	0	0	9	0
L1	0	2	0	0	0	1	9	0
L2	0	2	0	0	0	0	9	1
L3	0	2	1	0	0	1	8	0
L4	1	2	1	1	0	1	6	0
L5	0	2	0	2	0	3	5	0
L6	0	0	0	1	1	6	4	0
L7	0	0	0	1	0	7	4	0
L8	0	0	2	0	0	4	6	0
L9	0	0	3	2	0	3	4	0
L10	0	0	9	0	0	3	0	0
L11	0	0	10	0	0	2	0	0

Table 5.2: Proportions of the self-attentions patterns over layers in NMT (left) and BERT (right).

We show some studies that were examining whether such a large number of self-attention heads is really needed. Recall that the standard Transformer model's encoder for neural machine translation consists of 6 layers, each includes 16 self-attention heads, which is 96 heads in total. The large model of BERT uses 24 layers with 16 heads, i.e. 384 heads in total.

Michel et al. (2019) experimented with Transformer NMT and BERT models. They made an interesting observation that most attention heads can be individually removed at the inference time (i.e. without retraining the model) without any significant degradation of the model's performance. In the Transformer NMT Encoder, they found only eight heads out of 96 whose elimination significantly changed the translation quality. Interestingly, four of them improved the translations, and four of them worsened it. They also experimented with iterative pruning of more heads at once (in order from the least important ones) and concluded that about 20% of the NMT heads and about 40% of the BERT's heads can be removed at once without any significant negative impact of the model's performance without any retraining of the model. They also notice that the attention-heads in the Encoder-Decoder part of NMT are much less redundant that the self-attention heads used in the Encoder and the Decoder.

Voita et al. (2019) performed more elaborated experiments for head pruning using fine-tuning of the encoder's parameters and therefore were able to prune even more heads. However, their approach required changes in the original architecture. They introduced a gating mechanism to individual attention heads and a relaxation of L_0 regularization that converges to head-gates being either almost open or almost closed. During the fine-tuning, they fix the decoder's parameters and fine-tune only the encoder so that the functions of the pruned encoder cannot move to the decoder. They performed their experiments on English to Russian NMT and showed that their method is able to prune 44 out of 48 heads with the BLEU drooped only by 0.25 points. If there are ten heads left (and 38 of them are pruned), the BLEU score decreases only by 0.15 points. Further, they examined which heads are being pruned and concluded that the diagonal heads, the heads having some clear syntactic functions, and the one head attending to rare words are mostly retained, whereas the heads with rather unclear functions are mostly removed.

To conclude, experiments showed that many of the attention heads in the Transformer architectures are redundant and may be removed without strongly affecting the output quality. Interestingly, the redundancy cannot be avoided simply by training a model with fewer attention heads. Voita et al. (2019) showed that if a model with the same head-counts as resulted from their experiments is trained from scratch, it does not reach as good results as the one acquired by pruning the heads from the fully equipped base model.

5.2.3 Syntactic Features of Self-Attention Heads

In the Transformer's self-attention mechanism, each position (corresponding to one token) may attend to any of the positions on the previous layer. These inter-token relations may be seen as internal, latently learned structures of sentences. Many works are aiming to compare these latently learned relations to dependency or constituency syntactic structures proposed by linguists (see the overview Table 5.3). Three issues make such comparison difficult:

- There are usually many attention heads along the layers working in parallel. It is possible to infer the structure of a sentence from one head only (Raganato and Tiedemann, 2018), but it is more likely that many more heads perform some kind of syntactic function, and therefore we need to use them all or better to somehow choose only the syntactic ones (Voita et al., 2019; Clark et al., 2019; Limisiewicz et al., 2020).
- Even though the vectors that are attended do not represent the words themselves but rather some kind of contextual representations that may be very distant from the original input words at respective positions, many papers simplify

Research	Transformer model	Tree type	Syntactic evaluation	Evaluation data	Syntactic heads
Raganato and Tiedemann (2018)	NMT encoder (6 layers 8 heads)	dep.	tree induction	PUD treebank	0% – 8%
Vig and Belinkov (2019)	GPT-2	dep.	dep. alignment	Wikipedia	—
Clark et al. (2019)	BERT	dep.	dep. accuracy, tree induction	WSJ PennTB	—
Voita et al. (2019)	NMT Encoder (6 layers 8 heads)	dep.	dep. accuracy	WMT, OpenSubtitles	15% – 19%
Limisiewicz et al. (2020)	BERT, mBERT	dep.	dep. accuracy, tree induction	PUD, EuroParl	46%
Mareček and Rosa (2019)	NMT encoder (6 layers 16 heads)	const.	tree induction	EuroParl	19% – 33%
Kim et al. (2020)	BERT, GPT-2, RoBERTa, XLNet	const.	tree induction	WSJ PennTB, MNLI	—

Table 5.3: Summary of syntactic properties observed in self-attention heads of various Transformer models. The evaluation methods used are: (a) dependency (dep.) or constituency (const.) tree induction, (b) dependency alignment, (c) dependency accuracy.

this problem and treat the attentions as relations between words. See Section 3.3 for details.

- Traditional linguistic structures are trees, whereas the attention mechanism is generally a complete graph. It could be possible to adapt the Transformer architecture to work with more tree-like-shaped attentions (Wang et al., 2019a). However, it would then diverged from the original network we want to analyse.

The questions we would like to answer in this section are the following: How much syntax is hidden in the self-attention weight-matrices? Which attention heads match known syntactic features? Is it possible to infer complete syntactic trees form self-attentions weight-matrices without any supervision?

We divide the analysis into three parts: searching for dependency syntax, searching for constituency syntax, and searching for other sentence relations, such as coreference links.

5.2.4 Dependency Trees

The first observations that some of the self-attention heads exhibit behaviour related to a syntactic structure were provided in the original paper introducing Transformer (Vaswani et al., 2017).

Raganato and Tiedemann (2018) induce dependency trees from self-attention matrices of NMT encoder. Their experiments were done for translations from English to 7 different languages. Their approach assumes that the whole syntactic tree can be induced from just one attention head. For each head, they use the maximum spanning tree algorithm (Edmonds, 1967) to add edges for pairs of tokens with high attention weights and assure that the obtained graph is a tree. They use the tree root from the annotated gold data to find the direction of the edges. The trees extracted in this way are generally worse than the right-branching baseline[6] and outperform it slightly for a few heads. Nevertheless, their experiments showed that the syntactic behaviour of individual heads changes along the layers and the most syntactic heads in NMT appear at the top layers of the encoder. The results are visualized in the overview in Figure 5.11 under letter F.

Following articles focused on the analysis of individual features and classification of Transformer's self-attention heads.

Vig and Belinkov (2019) apply multiple metrics to examine properties of attention matrices computed in GPT-2 language model. They showed that in some heads, the attentions concentrate on tokens representing specific POS tags, and the pairs of tokens are more often attended one to another if they are connected by an edge in dependency tree. They observe that the strongest dependency alignment occurs in the middle layers of the model (4th and 5th counting from the input out of 12 layers in total). They also point that different dependency types (relation labels) are captured in different places of the model. Attentions in upper layers align more with subject relations whereas in the lower layer with modifying relations, such as auxiliaries, determiners, conjunctions, and expletives. This is also related to the fact that the higher the layer, the more distant the attention connections are. See letter D in Figure 5.11.

Voita et al. (2019) analyzed NMT encoders of translation systems from English to three European languages and also observed an alignment with dependency relations. They picked four types of dependency labels (noun subject, direct object, adjective modifier, and adverbial modifier) and measured how t extent they are captured by individual self-attention heads. -They separately address the cases where a verb attends to its dependent subject, and a subject attends to its governor verb. The heads with more than 10% improvement over positional baseline[7] were identified as syntactic. Such heads were found in all encoder's layers except from the first one.

[6] The right-branching baseline is a tree where each token is governed by its left neighbour.

[7] In the positional baseline, the most frequent offset is added to the index of relation's dependent/governor to find its governor/dependent, e.g., for the adjective-to-noun relations in English, the most frequent offset is +1.

In the head-pruning experiments, which we described in Section 5.2.2, the authors showed that the share of syntactic heads rises from 17% in the original model to 40% when 75% heads are cut out, while a change in BLEU is negligible. These results support the claim that the model's ability to capture syntax is essential to its performance in not syntactic tasks.

A similar evaluation of dependency accuracy, but for BERT pre-trained model, was conducted by (Clark et al., 2019). They identify syntactic heads that significantly outperform positional baseline for syntactic labels: prepositional object, determiner, direct object, possession modifier, auxiliary passive, clausal component, marker, phrasal verb particle. Most of the syntactic heads were found in the middle layers (4th to 8th out of 12). However, there exist no single heads that would capture all the relations of one type.

In another experiment, Clark et al. (2019) induce dependency tree from attentions. Instead of extracting structure from each head (Raganato and Tiedemann, 2018) they use probing to learn the weights of individual attention heads and then use maximum spanning tree on the weighted-average of the attention matrices. This approach produces trees with 61% Unlabeled Attachment Score (UAS) and can be improved to 77% by making weights dependent on the static word representation (fixed GloVe vectors). Both the numbers are significantly higher than the right-branching baseline (27%).

We conduct a related analysis for English (BERT) and multilingual model (Multilingual BERT (mBERT)) in (Limisiewicz et al., 2020). We observe that the information about one dependency type can be split across many self-attention heads. In other cases, the opposite may happen: many heads perform the same syntactic function. Examples of two heads aligned with dependency relations are shown in Figure 5.10. We introduce algorithms for averaging self-attention matrices to obtain better dependency accuracy than in a single matrix. Furthermore, we extract labelled dependency trees from the averaged heads and achieves 52% UAS and show that in the multilingual model (mBERT) specific relation (noun subject, determines) are found in the same heads across typologically similar languages.

5.2.5 Constituency Trees

Less effort was devoted to analysing attention heads in terms of syntactic phrases and deriving constituency tree structures.

In Mareček and Rosa (2019), we examine the encoder of Transformer NMT system for translation between English, French, and German. We observe that in many heads, continuous sequences of words attend to the same token, forming shapes similar to balusters (Figure 5.7). Furthermore, these continuous sequences often overlap with syntactic phrases. This notion is employed in our method for constituency tree induction. We compute weights for all such continuous sequences of tokens across all heads by summing the respective attentions. Then we induce constituency trees using the CKY algorithm (Ney, 1991). As a result, we produce trees that achieve up to

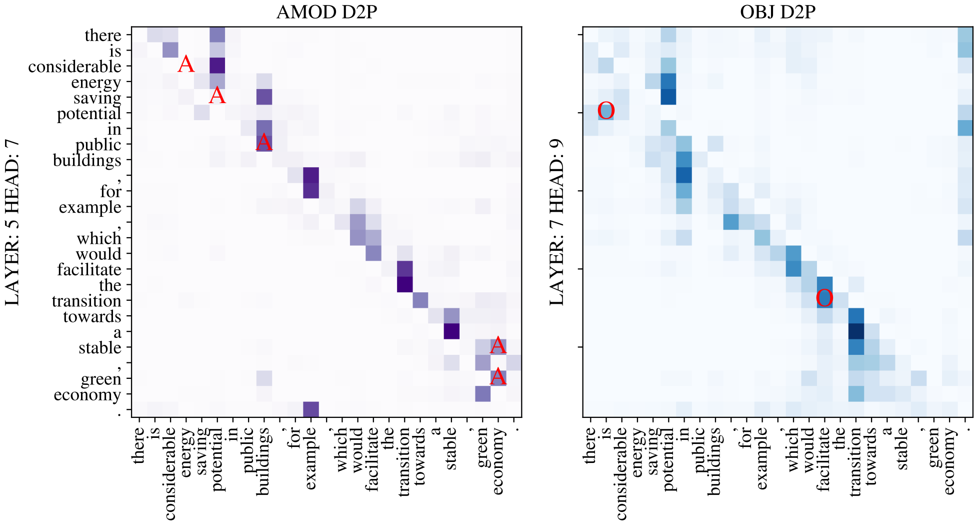


Figure 5.10: Self-attentions in particular heads of a Language Model (BERT) aligns with dependency relation *adjective modifier* and *object*. The gold relations are marked with red crosses.

32.8% F1 score for English sentences, 43.6% for German and 44.2% for French.[8] The results can be improved by selecting syntactic heads and using only them in the algorithm. This approach requires a sample of 100 annotated sentences for head selection and raise F1 by up to 8% in English.

The extraction of constituency trees from several Transformer-based Language Models was described by Kim et al. (2020). They present a comprehensive study that covers many different pre-trained networks, including BERT and Generative Pre-Trained Transformer (GPT)-2. Their approach is based on computing distances between each pair of subsequent words. In each step, they perform tree branching in the place where the distance is the highest. The authors propose three distance measures for pairs of contextual embeddings in a given layer: cosine, L1, and L2 distances; and two measures for comparing attention distributions of the subsequent words in each self-attention head: Jensen-Shannon and Hellinger distances. The best parse trees, which were extracted from XLNet-base model using Helinger distance on averaged attentions in the 7th layer, achieved 40.1% F1 score on WSJ Penn Treebank. Generally, attention distribution distances perform better than contextual vector ones. Authors also observe that models trained on common language modelling objective (i.e., next-word prediction in GPT) captured syntax better than masked language models (e.g., BERT). In line with the previous research, the middle layers of analyzed networks tend to be more syntactic.

5.2.6 Syntactic Information across Layers

Figure 5.11 summarizes the evaluation of syntactic information across layers for different models and approaches. The values are normalized so that the best layer for each method has 1.0. The methods A), B), C), and G) show undirected UAS trees extracted by probing the n-th layer (Hewitt and Manning, 2019; Chi et al., 2020). The method D) shows the Dependency alignment averaged across all heads in the n-th layer (Vig and Belinkov, 2019). The methods E) and F) show UAS of trees induced from attention heads by maximum spanning tree algorithm (Raganato and Tiedemann, 2018; Limisiewicz et al., 2020).

In Transformer-based language models (BERT, mBERT, and GPT-2), middle layers are the most syntactic. In the NMT models, the top layers of the encoder are the most syntactic. However, it is important to note that the NMT Transformer encoder is only the first half of the whole translation architecture. Therefore the most syntactic layer is, in fact, in the middle of the process. In RNN Language Model (ELMo) the first layer is more syntactic than the second one.

[8] The evaluation was done on 1000 sentences for each language parsed with supervised Stanford Parser.

[9] The results for the best layer (corresponding to value 1.0 in the plot) are: A) 82.5; B) 79.8; C) 80.1; D) 22.3; E) 24.3; F) en2cs: 23.9, en2de: 20.9, en2et: 22.1, en2fi: 24.0, en2ru: 22.4, en2tr: 17.5, en2zh: 21.6; G) 77.0.

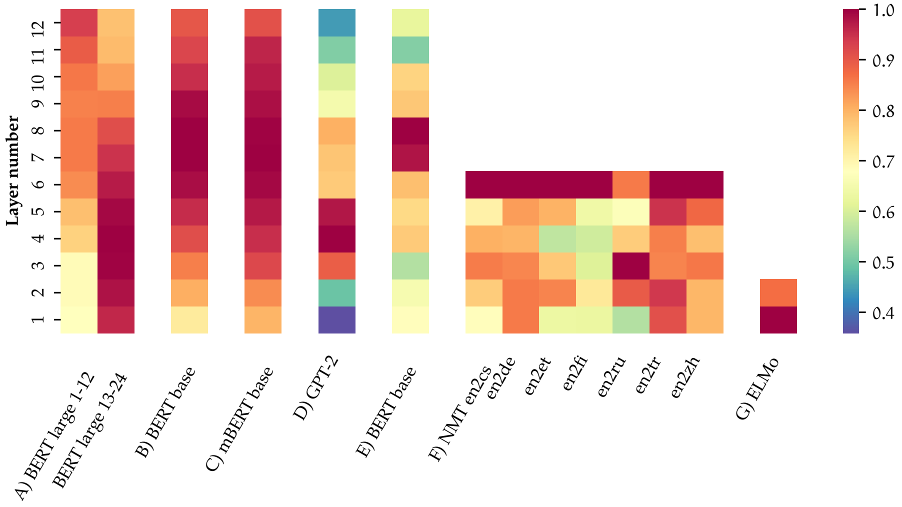


Figure 5.11: Relative syntactic information across attention models and layers.[9]

We conjecture that the initial Transformer's layers capture simple relations (e.g., attending to next or previous tokens) and the last layers mostly capture task-specific information. Therefore, they are less syntactic.

We also observe that in supervised probing (Hewitt and Manning, 2019; Chi et al., 2020), relatively better results are obtained from initial and top layers than in unsupervised structure induction (Raganato and Tiedemann, 2018; Limisiewicz et al., 2020), i.e., the distribution across layers is smoother. It suggests that the syntactic structure could be memorized to a more considerable extent in the probe instead of being captured by non-syntactic layers.

5.2.7 Other Relations between Words

Self-attention heads do not capture only syntactic relations. Besides the trivial ones, which were overviewed in Section 5.2.1, there are heads that exhibit rather semantic or discourse functions. Vaswani et al. (2017) claim that some of the attention heads in the Transformer NMT encoder are apparently involved in anaphora resolution (coreference). Clark et al. (2019) found a similar head performing coreference in the BERT model. This head achieved 65% accuracy at linking the coreferent to its antecedent, which is comparable to rule-based coreference resolvers. This is a very good result;

note that the learning is fully unsupervised. The attention head is particularly capable of fuzzy matching between synonyms.

5.3 Interpretability of Attentions Not as Easy as Expected

There has been a substantial amount of work done on interpreting attention mechanisms across different tasks and architectures. Many papers suggested reasonable explanations of the behaviour of the attention models, and it was generally assumed that each attention mechanism could be explained. For example, Bahdanau et al. (2014) consider the attention is the explanation and does not dispute its validity in any way. However, in 2019 several papers appeared (Jain and Wallace, 2019; Serrano and Smith, 2019; Pruthi et al., 2019) showing that some of the interpretations may be useless. Serrano and Smith (2019) suggest that an interpretable attention model must "not only suggest explanations that make sense to people, but also ensure that those explanations accurately represent the true reasons for the model's decisions." This is sometimes called a *faithful* explanation (Ross et al., 2017).

The basic questions that these articles raised are:

- How do the model predictions change if we change the distributions of attention weights?
- Would alternative (or even contra-factual) attention weights necessarily yield different results?
- How much do the attention weights correlate with the importances of input representations?

Earlier studies (Serrano and Smith, 2019; Pruthi et al., 2019) focused mainly on the text classification tasks, i.e., the tasks where a single sequence is classified into a small number of classes and concluded that these tasks do not satisfy their definition of being interpretable. Vashishth et al. (2019) extended the analysis to more complex tasks and showed that attention weights are interpretable in the architectures, in which attentions are essential for models predictions. In simple architectures, where the function of the attention mechanism may be equally performed by RNN gating units, the interpretability is questionable.

In the following text, we show three methods addressing the questions about interpretability of different types of neural architectures. This section aims to show that we cannot blindly interpret the attention weights as importances of individual inputs for the network decisions. We always have to bear in mind that the information flow in the network may be different than expected.

5.3.1 Eliminate the Highest Attention Weight

One of the experiments that attempt to disprove the direct interpretability of attentions was proposed by Serrano and Smith (2019). It is based on zeroing out the highest attention weight from the attention distribution and measuring how it affects the model's output distributions. All the experiments were done at test time; training of the model remained unchanged.

Consider a trained model which is applied to a test data and consider one attention layer inside the model which is going to be examined. For each instance of the test data, select the most attended input component i^* (the one with the highest attention weight), leave it out by setting the weight to 0, and renormalize all the other weights so that they sum to 1. How does it affect the model? The impact of such change can be measured using Jensen-Shannon (JS) divergence of the output distributions over labels[10] or by examining how many final decisions of the model were flipped.

Serrano and Smith (2019) performed experiments on single sequence tasks of topic classification and sentiment analysis. Not surprisingly, when α_{i^*} was small, it caused almost no changes in the output distribution. However, even for larger attention weights as 0.4, the JS divergences were still close to zero. The number of model decisions that were flipped (changed from 0 to 1 or from 1 to 0) was also relatively small. Only slightly more than 10% of decisions has changed. These results suggested that the interpretation of such single-sequence tasks is at least questionable.

Vashishth et al. (2019) categorize NLP tasks into the three groups according to their inputs and outputs:

- *Single sequence tasks*, e.g., sentiment analysis, topic classification,
- *Pair sequence tasks*, e.g., natural language inference, question answering,
- *Generation tasks*, e.g., machine translation, text summarization.

Unlike Serrano and Smith (2019), who tested their method only on the single sequence tasks, they applied the same method also on the pair-sequence and generation tasks and reported much more apparent correlations on them. Figure 5.12 shows that in the machine translation task, the components which are important according to the attention weights really have an impact on the results and zeroing the attentions harms the model predictions. They conclude that attention weights are interpretable in the architectures where attentions are essential for models predictions and do not only behave as gating units.

Serrano and Smith (2019) also showed results for different model architectures. They compared

- RNN architecture with an attention layer on top
- Convolutional Neural Network (CNN) with an attention layer on top
- no encoder, only one attention layer looking at the input word embeddings

and showed that zeroing out the attentions in the architecture without encoder proved to have a higher effect on the number of decision flips. This is probably caused by the fact that zeroing out an attention weight really eliminates the word from computations. In contrast, RNN may propagate information about the important words to the

[10] To be able to assess the magnitudes of the JS divergence, the authors compare it with the JS divergence after erasure of a random component r from the attention input. The difference between these two JS divergences should then correlate with the differences of the zeroed-out attention weights $\alpha_{i^*} - \alpha_r$.

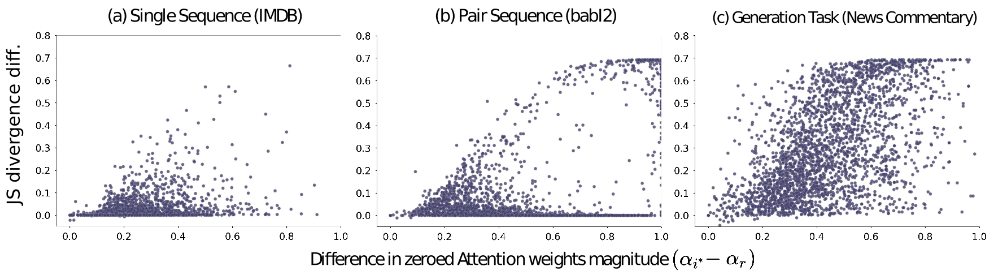


Figure 5.12: Eliminating the highest attention weights affects the output distributions. Comparison for different types of NLP tasks. Reprinted from (Vashishth et al., 2019, Figure 3).

following representations. In CNN, information about the word can be present in as many components as the window size is. The results are shown in Figure 5.13.

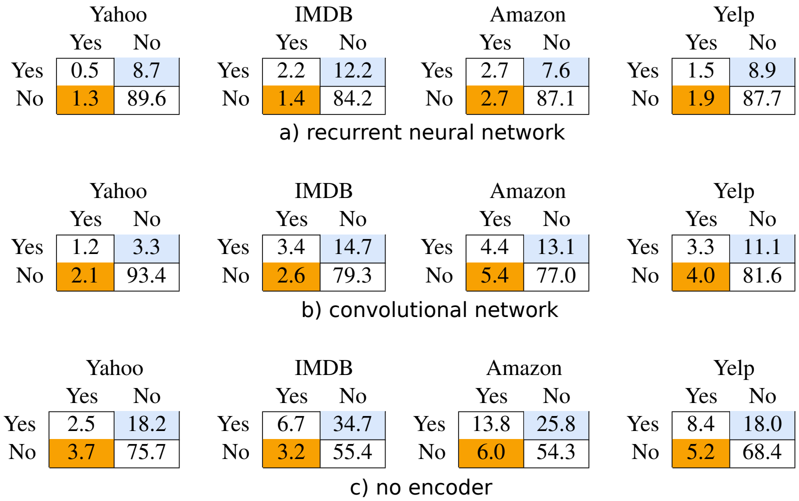
5.3.2 Change the Whole Attention Distribution

Another approach was suggested by Jain and Wallace (2019). Instead of zeroing out one attention weight, they propose to change the whole distribution of weights at once and measure their impact on predictions. Putting together the works by Jain and Wallace (2019), Vashishth et al. (2019), and Wiegreffe and Pinter (2019), we found four tested variants for changing the attention weights:

- *uniform* – distribute the weights uniformly,
- *random* – randomly sample weights from the uniform distribution $U(0, 1)$ and normalize,
- *random permutation* – scramble the original weights, reassigning each value to an arbitrary, randomly sampled index,
- **adversarial attention** - search for such attention distribution that differs as much as possible from the original attentions, but at the same time, does not substantially change the predictions.

Moreover, there are two possibilities when to apply the changes. We can either use the original trained model and apply the changes of attention weights at inference time or manipulate with attention weights during training so that the other parameters of the model could adapt to these different conditions.

First, it is necessary to answer an important question: Is the attention mechanism needed for a given task at all? Wiegreffe and Pinter (2019) argue that "if attention models are not useful compared to very simple baselines, i.e. their parameter capacity is not being used, there is no point in using their outcomes for any type of explanation." They performed a simple baseline experiment in which all attention weights



	Yahoo		IMDB		Amazon		Yelp	
	Yes	No	Yes	No	Yes	No	Yes	No
Yes	0.5	8.7	2.2	12.2	2.7	7.6	1.5	8.9
No	1.3	89.6	1.4	84.2	2.7	87.1	1.9	87.7

a) recurrent neural network

	Yahoo		IMDB		Amazon		Yelp	
	Yes	No	Yes	No	Yes	No	Yes	No
Yes	1.2	3.3	3.4	14.7	4.4	13.1	3.3	11.1
No	2.1	93.4	2.6	79.3	5.4	77.0	4.0	81.6

b) convolutional network

	Yahoo		IMDB		Amazon		Yelp	
	Yes	No	Yes	No	Yes	No	Yes	No
Yes	2.5	18.2	6.7	34.7	13.8	25.8	8.4	18.0
No	3.7	75.7	3.2	55.4	6.0	54.3	5.2	68.4

c) no encoder

Figure 5.13: How eliminating the highest attentions affects the model's decisions. Comparison of different architectures. Reprinted from Serrano and Smith (2019, Figure 9) under CC-BY-4.0 licence.

were frozen and uniformly distributed over the input states, both during training and testing. The idea is that if the results of such a network with fixed attentions are comparable to the results of the original network with trained attentions, we can say that the attention mechanism is unnecessarily complex and useless for that task. However, we cannot say that the attention weights of the original network are not interpretable. They might be, since it may be convenient for the network to use the attention mechanism, but at the same time, the weights may be very random, and there may be a high variance between two independently trained models. The irrelevance of trained attentions may be partially confirmed by an experiment in which a network is trained normally, but the attention weights are frozen to uniform only during the inference time. Then, if the results are still similar, we can say that the attention model is really not interpretable, since the weights do not matter at all. Similar experiments can be done with the *random* and *random permutation* baselines.

The results across a variety of different tasks were reported by Vashishth et al. (2019), and we show their results in Figure 5.14.

The differences between the results for the single sequence tasks (SST, IMDB) are very small. If the attention weights were fixed already in the training phase, the rela-

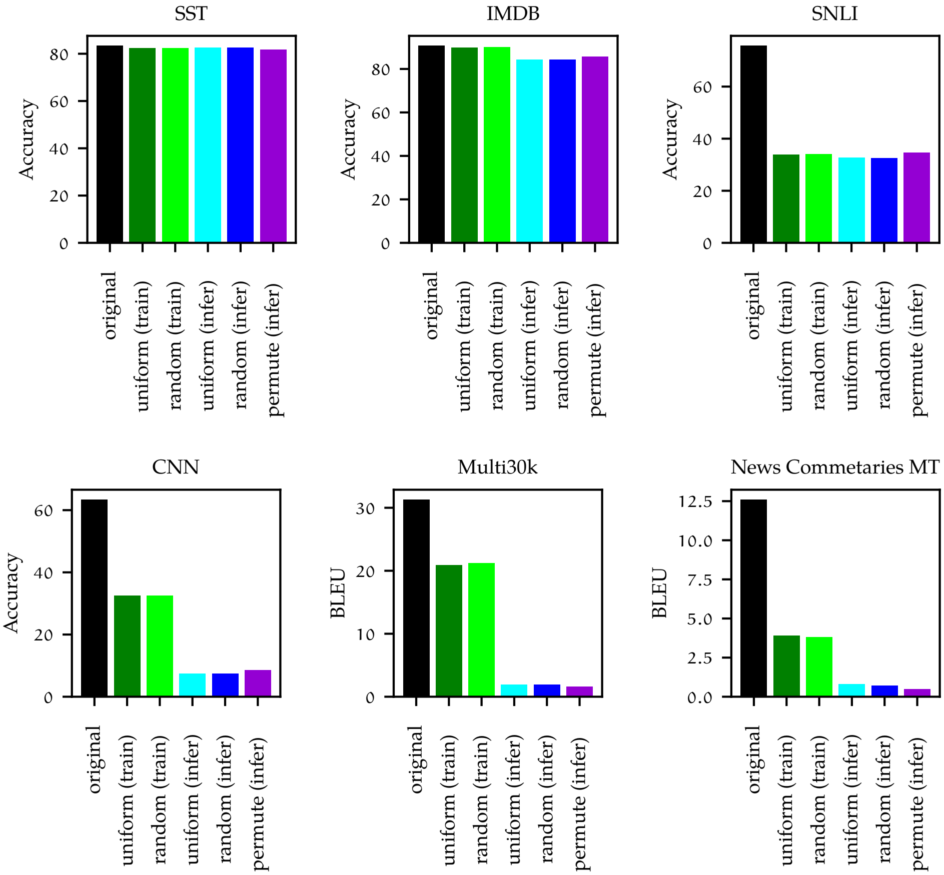


Figure 5.14: Performance comparison between the original models and the baseline models using uniform, random, or permuted attention weights. The results are taken from Vashishth et al. (2019).

tive drop in performance is about 1% compared to the original model. Therefore, the attention mechanism is not necessary for this type of tasks. [11]

If the originally trained model was used instead, but the attention weights remained fixed to uniform/random/permuted during the inference, the performance drops are higher. It is still quite small for the SST task, which means that the attention weights of the original models cannot be interpreted since they are irrelevant for the predictions. The performance drop on the IMDB dataset is higher, so the attention weights are sometimes needed, but they bring only at most 7% improvement.

The performance drops on the pair sequence tasks (SNLI, CNN) and generation tasks (Multi30k, NC) are far more substantial, which proves the importance of the attention model in these tasks.

All the three baseline approaches of changing the attention distribution showed to have a similar impact on the models.

Jain and Wallace (2019) introduced a method called *adversarial attention* with the aim of "explicitly seek out attention weights that differ as much as possible from the observed attention distribution and yet leave the prediction effectively unchanged." They want to examine whether the attention models provide *transparency* (Lipton, 2018), i.e. whether the attention weights explain why the model generated a particular output. They claim that if such adversarial attention distributions are found, they may be viewed as an alternative and equally plausible explanation for the same output and, therefore, violate the property of *transparency*. Their approach aims to find k adversarial attention distributions $\alpha^(i)$ by maximizing their Jensen-Shannon divergence from the original attention distribution α and keeping the new output distributions similar to the original distributions. They show that for the single-sequence and pair-sequence tasks, they can find many mutually different attention weight distributions with Jensen-Shanon Divergence about 0.5[12] and conclude that the explainability of attention weights in such tasks is thus questionable.

However, Wiegreffe and Pinter (2019) pointed out that the adversarial distributions proposed by (Jain and Wallace, 2019) do not confirm non-explainability of the attention model, because the attentions were not assigned arbitrarily by the model, but were computed separately on top of the originally trained parameters. Moreover, the adversarial distributions were computed independently for each instance, which increased the degree of freedom and therefore, the adversarial attentions were easy to find.

[11] We would need to investigate further what are the 1% of cases for which the original model is better; these may be the hard cases that cannot be solved by the baseline models. However, it may also be possible that increasing the number of parameters by enlarging the vector sizes of the baseline models would also bring such improvement.

[12] Note that the Jensen-Shannon divergence between two categorical distributions is bounded from above by 0.69.

Model	Objective function	Gender identification		Sentiment analysis	
		Acc.	Attn.mass	Acc.	Attn.mass
Embeddings + Attention	orig.	100.0	99.2	70.7	48.4
	penal.	99.2	0.8	48.4	8.7
	unused	66.8	–	48.9	–
BiLSTM + Attention	orig.	100.0	96.8	76.9	77.7
	penal.	100.0	$< 10^{-6}$	61.0	0.07
	unused	63.3	–	49.1	–
BERT + Mean pooling	orig.	100.0	80.8	90.8	59.0
	penal.	99.9	$< 10^{-3}$	90.6	$< 10^{-3}$
	unused	72.8	–	50.4	–

Table 5.4: Accuracy of various attention models and their attention mass on the impermissible tokens. A comparison between the original models (orig.), models with penalized impermissible tokens (penal.) and models not using these tokens at all (unused). These results were taken from Table 3 of the original paper Pruthi et al. (2019).

5.3.3 Do Not Attend to Useful Tokens

Unlike Jain and Wallace (2019) and Serrano and Smith (2019), who modified the attention distributions of a trained model post-hoc, Pruthi et al. (2019) proposed a fully trained method interfering the model only with a different training objective. They construct a set of simple tasks. Each task has a known set of tokens that are needed for that task. They mark these tokens as impermissible and penalize them in the objective function. They perform experiments on three architectures:

- Static embeddings + Attention mechanism
- Recurrent network + Attention mechanism
- BERT + Mean pooling

In Table 5.4, we show the results of the following two of their tasks:

- *Gender Identification* – labelling Wikipedia biographies with gender (female or male). Impermissible tokens here are all gender pronouns (he, she, himself, herself etc.)
- *Sentiment Analysis with Distractor Sentences* – labelling movie reviews with a sentiment (positive or negative). A distractor sentence was added to each movie, and all original movie-review sentences were treated as impermissible.

In the Gender identification task, we can see that even though when the gender pronouns are omitted from the data, the accuracy is at most 72.8%, with only minimal attention paid to the pronouns (less than 1% of attention mass) the accuracies are almost perfect (at least 99.2%). This shows that even though the attention may be diminished, the models are still able to rely on them. In the Sentiment analysis task, we can see that reducing attention mass to impermissible tokens sometimes reduces overall accuracy. The drop in accuracy depends on the complexity of the model. Whereas we observe more than 20% drop for the simple Embeddings+Attention model, the drop for BERT model is only 0.2%, even though the attention mass to impermissible tokes was lower than 0.001%. This can be explained by the fact that both RNN and BERT can transfer the needed information from one token to the contextual representations of other tokens.

5.4 Conclusion

The attention mechanism is currently a central and important component of neural networks used for solving NLP tasks. Naively, individual attention weights may be interpreted as importances of individual tokens or dependencies between them. Many studies appeared showing that attention mechanism resembles some linguistic relations. For example, cross-lingual attentions in machine translations align counterpart words, some of the self-attentions heads capture specific syntactic functions between words, some of the heads resemble coreferential links.

We categorized the self-attention heads into eight patterns and showed their different distributions in the BERT and NMT models. We also summarized the distributions of syntactic heads across layers and different models.

However, we must realize that the attentions might be sometimes misleading and may carry very different information from which we would think based on the attended tokens.

- Even the attention with only a minimal weight may be significant, and, conversely, the information from the most attended token may be discarded by the model.
- The more complex models as RNNs or Transformers may easily transfer any information between individual contextual representations of words. Therefore, attention to a contextual representation of one token may obtain properties of a different token.
- The attentions may be misleading mainly when a too strong neural network with many parameters is used on a very simple and effortless task.

6

Contextual Embeddings as Un-hidden States

In this chapter, we deal with contextual word embeddings. We start by briefly looking at how they emerged as reinterpretations of hidden states of neural models trained for various tasks in Section 6.1. The main section of this chapter, 6.2, summarizes the current state of knowledge about various kinds of linguistically interpretable features that can (or cannot) be found in contextual embeddings, going from morphology and syntax to semantics, world knowledge and common sense. Section 6.3 takes a different point of view, investigating to what extent these linguistic features can be found in individual models and model layers. We also touch on the multilingual aspects of contextual embeddings in Section 6.4.

By contextual word embeddings, we understand word representations taken from neural models trained for a Natural Language Processing (NLP) task, such as language modeling. As the model typically only needs unannotated plaintext data for training, which are available in large quantities, very strong contextual word embeddings can be obtained in this way. These can then be directly used in many end tasks, where training even a very simple classifier on top of the contextual word embeddings often reaches or outperforms previous state-of-the-art. Those previous approaches are typically sophisticated models designed and tuned specifically for the end task but severely limited by only being trained on the end task dataset, not making full use of the general language knowledge learnable from the available vast plaintext data.

The general understanding is that this power of contextual word embeddings comes from the fact that a wide range of general features emerge in the representations through training, capturing various important properties of the input words and sentences. While one might expect the model to learn only features necessary to solve the task for which the model is trained, it seems that with a sufficiently challenging and general training task, the model cannot easily “cheat” the task by learning only a handful of features and ignoring most of the information on the input. Rather, it seems that it becomes economical for the model to latently develop some general language understanding and use this to solve the task eventually. Thus, it is of great interest to investigate this phenomenon, analyzing the contextual word embeddings to see whether the emergent features somehow correspond to the traditional ways and abstractions in which linguists think about language understanding, such as morphology, syntax, and semantics.

6 CONTEXTUAL EMBEDDINGS AS UN-HIDDEN STATES

6.1 How Contextual Embeddings Came to Be

Static word embeddings were a key invention that made it possible to efficiently use Neural Networks (NNs) for processing textual language data. Much has been said about the words' properties captured by the word embeddings (see Chapter 4). However, they are unable to capture information about the immediate context of the word; they are type-based, not token-based representations, fixed for the model's vocabulary of words (or subwords).[1] Static word embeddings are thus somewhat impractical for handling homonymous or polysemous words, where the word needs to be understood differently based on its context.[2]

Instead, what has been the mainstream approach practically since the boom of deep neural NLP are NN architectures which look at input words together with their immediate context, using Convolutional Neural Networks (CNNs), Recurrent Neural Networks (RNNs), and attentive meachanisms. In CNNs, filters look at short spans of words at once. In RNNs, the internal state when processing a word is influenced by the previous words; or also following words in case of Bidirectional Recurrent Neural Networks (biRNNs). Attentive and self-attentive mechanisms allow the network to attend selectively to multiple words at once, or, while processing a word, to attend to other words that provide important context.

As an RNN iterates over the sequence of input words, the RNN cell passes through a series of *hidden states* until reaching a *final state* at the end of the sequence. One way of looking at that, especially if the individual input words are of no further interest to us, is that the hidden states are only temporary intermediate states, and only the final state is of interest and represents the whole sentence.

In many cases, however, we are still interested in the individual words, e.g., in the case of Part of Speech (PoS) tagging or Named Entity Recognition (NER).[3] In such cases, we are thus mostly interested in the hidden states – which might also be called *output states* in such case, but the term hidden states is much more common – as these may serve as representations of the words in the context of the sentence and the end task. Indeed, already the seminal work by Bahdanau et al. (2014) did choose to use the hidden states as representations of the input words for Neural Machine Translation (NMT) with great success, even though Machine Translation (MT) is, in principle, a

[1] In this chapter, we will mostly talk about words, even if this can often mean subwords. The main reason is that it is much more complicated to assign linguistic categories to subwords than to words. Therefore, all of the analyses of word representations that operate on subword representations need to deal with this issue, typically by deriving word representations by averaging the subword representations, as has been discussed in Section 3.3.2.

[2] While there have been attempts at disambiguating individual word senses and assigning them different word embeddings, such as the work of Neelakantan et al. (2015), such methods are somewhat limited, never became the mainstream in NLP, and eventually mostly fell out of use.

[3] Leaving aside the fact that the RNN final state usually turns out not to be a very good representation of the sentence (Graves, 2014; Hochreiter et al., 2001).

sentence-to-sentence mapping task and so using the RNN final state as input representation might theoretically make more sense.

In this way, hidden states of recurrent neural encoders started to be used as contextual word representations, at first only as intermediate representations within a model trained for a given task.[4] Gradually, however, researchers have realised that these representations are often more general and can be used as pre-trained word representations even for other tasks than the one they were originally trained for, within the concept of transfer learning. To understand why this is possible, many studies investigated the representations using probing and other methods, showing that, while containing some end-task-specific information, the representations often capture some linguistically interpretable features to some extent. For example, a linear projection of the representations can often be found which quite accurately maps onto some traditional PoS labels.

Once hidden states started to be used as word representations independently of the models within which they were trained, they started to be referred to as *contextual word embeddings* (see Section 2.4); since then, we could also metaphorically say that the *hidden states stopped being hidden*.[5] The neural model which is trained and used to provide the hidden states is typically referred to as a *contextualizer*, as it enriches static word embeddings with information based on the immediate context of the words.

While nearly any model with a word-level encoder trained for any NLP task can be used as a contextualizer, it has been found that some models work better than others. At first, NMT models were typically used, with CoVe Context Vectors (CoVe) being a typical representative. Later, it has been found that the Language Model (LM) task seems to lead to better, more general and more expressive contextual word embeddings, with Embeddings using Language Models (ELMo) being the first widely successful contextualizer. Further research then led to even more advanced and specialized architectures and training methods. Currently, the most well-known and most successful contextualizer is Bidirectional Encoder Representations from Transformers (BERT) and its subsequent derivates.

6.2 What do Hidden States Hide?

In the next sections, we try to summarize the current state of knowledge about features that tend to emerge in contextual word embeddings and can be mapped to various linguistic abstractions.

Generally, as explained, e.g., by Liu et al. (2019a), basic linguistically interpretable features can be easily extracted from the representations, even with a linear classifier

[4] It is usually assumed that the recurrent encoder's ith hidden state can be thought of as a representation corresponding to the ith input word. While this is by no means theoretically guaranteed, it has been found that, in practice, this mostly holds, as we discussed in Section 3.3.

[5] As explained in Section 2.4, in our text, we often do not strictly differentiate between hidden states and contextual word embeddings.

(i.e., they are linearly encoded in the representations). For more fine-grained abstractions, such as higher-order syntactic relations or semantics, it might be necessary to train a more powerful Multi-Layer Perceptron (MLP) extractor; and still, some information simply seems not to be captured at all (e.g., third-order syntactic relations).

We would like to note that several surveys on this topic have already been published, which we have partially used as inspiration and which we can recommend to a reader interested in a more extensive list of existing work on the topic; in our book, we rather focus on summarizing the existing knowledge than on providing an exhaustive overview of all existing studies.

- Belinkov and Glass (2019) review analysis and visualization methods, challenge sets (probing datasets), and include a table of works categorized by the component they analyze, the linguistic property they look for, and the method they use.[6]
- Rogers et al. (2020) review studies that analyze and interpret the representations from BERT.

6.2.1 Morphology

In the last years, multiple researchers demonstrated that hidden states of trained NLP models usually encode various morphological information to some degree. They mostly focused on PoS, but also investigated various other more fine-grained morphological features. They mostly utilized probing with linear models or MLPs (see Section 3.1).

The general finding is that all models trained for any NLP task, such as MT or LM, seem to capture morphological information to some extent (Belinkov et al., 2017a; Peters et al., 2018a; Tenney et al., 2018). All contextual embeddings seem to capture morphology to a greater extent than static embeddings, such as Skip-Gram (SG) or Global Vectors for Word Representation (GloVe) (Belinkov et al., 2017b; Blevins et al., 2018; Tenney et al., 2018). This is demonstrated by the probing models being able to predict PoS from the contextual embeddings with higher accuracies than from static embeddings.

In multilayer contextualizers, we have the option to extract hidden states to use as contextual embeddings from various layers. As we will discuss in Section 6.3.2, it has been found that linguistic features tend to be mostly captured at different layers based on the architecture of the contextualizer. For RNN-based contextualizers, such as ELMo, all linguistic features tend to be most strongly captured in the first layer. However, for Transformer-based contextualizers, different linguistic features are spread across the layers differently; morphology tends to be captured most strongly in the hidden states of the initial and middle layers of the model.

[6] https://boknilev.github.io/nlp-analysis-methods/table1.html

As we will discuss in more detail in Section 6.3.3, contextual embeddings obtained from models trained for the LM task tend to capture morphological features more strongly than models trained for other tasks (such as MT or autoencoding). This does not hold if the task itself contains strong morphological signals (such as PoS tagging, syntactic parsing or Semantic Role Labelling (SRL)), in which case PoS can be often predicted from the hidden states with an accuracy approaching 100% (Blevins et al., 2018). A comparison of the PoS probing accuracies for several pre-training tasks can be seen in Figure 6.4 on page 128.

There is also evidence that models which apply a character-level CNN to the inputs tend to capture morphological features to a greater extent (Belinkov et al., 2017a).

6.2.2 Syntax

We have already discussed the possibility of looking for syntactic features in self-attentions (see Chapter 5). Probably an even wider range of works have successfully looked for syntactic features in contextual word embeddings.

As even static embeddings have been shown to capture *morphology* to a considerable extent, it came as no surprise that it is also captured by contextual embeddings. However, as static embeddings cannot in principle capture the syntactic structure of a sentence, probing contextual embeddings for syntactic abstractions is of great interest.

Constituency Syntax

Various authors have shown that most deep NN models trained for NLP tasks do encode features which can be mapped to constituency syntax.

Most works focus on predicting *syntactic constituent labels*,[7] showing that these can be predicted from contextual embeddings with much higher accuracy than from static embeddings, suggesting that such syntactic features emerge in the model. This has been shown already for simple MT and LM models (Shi et al., 2016; Blevins et al., 2018), and later confirmed also for more complex contextualizers (Tenney et al., 2018; Peters et al., 2018b). The authors used classical probing, as well as other methods, such as *edge probing* of Tenney et al. (2018), probing gold node pairs for the constituent labels, or indirect evidence provided by improvements observed when contextual embeddings are used as input for training a syntactic parser (Peters et al., 2018b). These results suggest that capturing the language's syntax helps the models in understanding the language.

[7] E.g., *VP* (verb phrase), *NP* (noun phrase), or *SINV* (inverted declarative sentence, using the VSO word order).

The trained models have been also shown to capture features relevant for other linguistic abstractions, such as chunking boundaries[8] or Combinatory Categorial Grammar (CCG) supertags[9] (Liu et al., 2019a).

Dependency Syntax

The first studies aimed at looking for dependency syntax in trained neural network models looked at activations of individual neurons. For example, Karpathy et al. (2015) found some patterns in gate activation statistics of individual neurons in Long Short-Term Memory (LSTM) cells in character-level LMs that correspond to various long-range dependencies in the sentence, concluding that such a neuron can capture, e.g., the correspondence relation of quotes or brackets.

Blevins et al. (2018) train a binary classifier on contextual representations of pairs of words, predicting whether there is a dependency edge between the two words. All of the probed models showed a considerable amount of syntactic features.[10]

Tenney et al. (2018, 2019) use *edge probing* to probe contextual embeddings for dependency syntax. They use gold information about the dependency tree structure, taking gold syntactic edges as input and trying to predict the dependency edge relation label from the contextual representations of the two words. They find that information about the edge label is rather easy to extract from the representations, suggesting that they do capture features that correspond to the syntactic relations abstractions.

Hewitt and Manning (2019) take an unusual approach, designing *structural probes* and probing for various numeric structural descriptors rather than training binary or multiclass classifiers. In this way, they are able to find linear transformations from ELMo and BERT contextual embeddings to node tree distance and to node tree depth, which achieve sufficiently high performance for the authors to claim that "entire syntax trees are embedded implicitly in deep models' vector geometry".[11]

[8] In the syntactic sense, a *chunk* is a constituent phrase; the task of *chunking*, which is a simplification of the task of full syntactic parsing, typically consists of splitting the sentence into a flat sequence of unlabeled chunks, instead of a hierarchy of labeled constituents.

[9] CCG (Steedman and Baldridge, 2011) supertags encode partial constituent labels using forward and backward slashes; e.g., "the" could be labeled as *NP/N* as it must be completed by a noun (*N*) from the right to form a noun phrase (*NP*).

[10] Hidden states from an MT model led to a 73% accuracy, and hidden states from an LM model led to an 80% accuracy in probing, compared to 95% accuracy achieved by using hidden states from a syntactic parser model; the random baseline is 50%.

[11] We see these claims as probably inadequately strong, as the authors do not convincingly show that the syntactic features are indeed embedded in the representations and not just, to some extent, memorized by the strong probing classifier.

More Complex Syntactic Relations

Liu et al. (2019a) investigate ELMo, finding that the contextual representations do *not* capture information about third-order syntactic relations (great-grandparent prediction task) or conjuncts (identification of conjunct tokens in a coordination construction), which is manifested by the fact that a linear probe is unable to extract such information from the representations.

A stronger MLP probe is able to perform these predictions, which Liu et al. (2019a) interpret as the representations capturing information necessary to solve the task, but not directly capturing features that would correspond to these more complex syntactic abstractions. As, obviously, the task is solvable even from plain text (even though a stronger classifier would be needed), this only means that ELMo does not forget the necessary features from the input and stores them in such a way that they can be easily extracted and utilized by a strong-enough classifier.

Grammatical Correctness

One of the classical views of a Language Model is that of an LM being a tool which decides whether a given sentence is or is not valid in the given language. It is thus quite natural to ask whether LM representations capture features that would distinguish between grammatical and agrammatical sentences; and whether these features are general, or whether they are rather limited to certain structures or phenomena.

Probably the first work that looked for evidence of trained NN models capturing syntax was the work of Linzen et al. (2016). The authors designed a task of predicting the grammatical correctness of a sentence, with a number of hard cases presumably requiring the model to understand morphological number agreement between subject and predicate.[12] They then probed a simple single-layer unidirectional LSTM-based LM with a logistic regression probe. Based on the negative results on the hard cases, the authors concluded that the model does not capture this syntactic phenomenon. However, they only used the final state of the LSTM, assuming that it would capture information about the whole sentence. With the current state of knowledge, we can see the flaw in the experiment, as the final state typically mostly captures information about the corresponding word (i.e., sentence-final punctuation) and, to some extent, neighboring words; e.g., the mean of all hidden states should have been probed instead. Nevertheless, the authors also tried training the model directly for the end task, this time obtaining positive results, and thus concluding that even a simple LSTM-based model is *capable* of learning syntax if trained to do so.

The task of predicting grammatical correctness was revisited by Liu et al. (2019a), who trained a probe to predict token-level grammatical errors, i.e., for each token, the

[12] The hard cases require a deeper syntactic understanding of language than only checking a small local context by containing intervening nouns or phrases between the agreement participants, as in "Alluvial **soils** *carried in the floodwaters* **add** nutrients to the floodplains.".

task is to say whether the token needs to be edited to make the sentence grammatically correct; the authors posit that solving this task requires understanding of syntax and grammar of the language. They probe ELMo representations, finding a similar situation as with harder syntactic relations: the model captures some information necessary for solving the task (as shown by a successful MLP probe), but does not capture the information about the grammatical correctness itself (attested by an unsuccessful linear probe). Moreover, even the stronger probe reaches rather low accuracies in absolute terms, even though it outperforms previous state-of-the-art (which is also rather low), suggesting that this is a rather hard task, still beyond the capabilities of current models.

6.2.3 Coreference

In coreference, we deal with the phenomenon of several entities (typically pronouns or noun phrases) referring to the same real-world entity.[13] While based on the performance of neural models on various tasks, we may assume that they have a way of understanding this notion, we may ask how they capture this, and whether their grasp of the phenomenon is general or limited.

The contextual embeddings seem to understand coreference in easier cases where it can be determined from morphosyntactic cues, as shown, for example, by Peters et al. (2018b), who find that the similarity of the embeddings of the referential pronoun and the antecedent noun is often high enough for correct coreference resolution.

However, in harder coreference cases which require deeper semantic understanding, as represented by the Winograd coreference resolution dataset (Levesque et al., 2012),[14] the contextual embeddings typically perform poorly, only slightly outperforming static embeddings baselines (Tenney et al., 2018).

6.2.4 Semantics

In Chapter 4, we have seen that neural models can learn lexical semantics to a great extent. In this section, we thus go beyond lexical semantics, particularly focusing on semantic labels that are context-dependent, such as semantic roles or word senses.

A grave issue with any probing for semantic information is the strong threat of falsely positive results, as many semantic ambiguities can be resolved solely based on morphosyntactic cues. As we already know that morphosyntactic features are well captured by the contextual embeddings, a semantic probe can easily learn to perform

[13] E.g., "John told Mary he liked her, and she let him kiss her on her cheek.", where "John", "he" and "him" refer to one entity (John) and "Mary", "her" and "she" to another entity (Mary).

[14] The Winograd scheme focuses on cases of coreference which are morphologically and syntactically ambiguous and irresolvable, such as "*Characters* entertain *audiences* because **they** want people to be happy." where resolving whether "they" refers to characters or audiences requires semantic understanding or even real-world knowledge.

the semantic labeling based on these morphosyntactic cues, failing to reveal whether the semantic distinction is captured in the contextual representation explicitly.

When the analyses are properly executed and carefully examined, we typically find only mildly positive results for various specific semantic labels, showing that some semantics is captured. It is rare to find a semantic feature which would be captured very strongly in the representations; and if so, it is often the case that the seemingly semantic feature can actually be very well predicted based solely on morphosyntactic cues, and thus the probe does not prove that, beyond morphology and syntax, semantics would also be captured.

Semantic Tagging

Various authors have probed contextual embeddings for various semantic labels, such as semantic roles (Palmer et al., 2005),[15] semantic proto-roles (Teichert et al., 2017; Rudinger et al., 2018),[16] or sem-tagging (Bjerva et al., 2016).[17] The general finding seems to be that the models do *not* capture deeper semantic features to a great extent, only lightly outperforming the static embeddings baselines (Belinkov et al., 2017b; Tenney et al., 2018).

We can also understand named entity labels[18] as a kind of semantic labels. Here, contextual embeddings seem to capture information about named entity types to some extent, strongly outperforming a static embeddings baseline but still being far from comparable state-of-the-art results (Liu et al., 2019a).

The good performance of some semantic label probes can usually be explained by inspecting the results more thoroughly, revealing that the good results are obtained, especially for the cases where the correct label can be easily determined solely from morphosyntactic cues (Tenney et al., 2018). Thus, the experiments mostly only reconfirm the interpretation that the representations capture morphological and syntactic features, but do not seem to exhibit a deeper understanding of the meaning of the sentence.

However, any negative result in interpreting neural networks must be taken with a grain of salt. The aforementioned results clearly show that the probed neural models do not seem to capture semantic features similar to various classical semantic labels. While a plausible explanation is that the models do not capture any semantic features at all, an alternative explanation is also possible: that the models do have a deeper understanding of language than we have been able to show, but that the way in which they encode the semantics of the language is so different from the labels we use that we just have not been able to recognize it yet.

[15] E.g., *agent*, *location*, *purpose*, *direction*.

[16] This is a more fine-grained variant of semantic roles.

[17] This is a semantic extension of PoS tagging, distinguishing, e.g., determiners into categories such as *proximal* (e.g. "this") and *distal* (e.g. "that").

[18] E.g., *person*, *organization*, *geographical entity*.

Noun Gender

It has been already discussed in Chapter 4 that even static embeddings do typically capture features which correspond to the *morphological* gender of nouns in languages where nouns are gendered, as in Czech. However, in this section, we are rather interested in capturing the *semantic* gender of nouns, even and especially when this is *not* morphologically marked, as in English.

Zhao et al. (2019) find that ELMo captures gender in nouns. The authors identify two gender-related principal components of the representations using Principal Component Analysis (PCA):

- *contextual gender*, based, e.g., on the occurrence of a "he" or "she" pronoun in the sentence (so, e.g., a "librarian" is disambiguated as being male or female in the given sentence),
- *occupational gender*, which is the gender embedded in the word itself, either explicitly marked (e.g. "actress") or stereotypical (e.g. a female "nurse" versus a male "developer").

The authors interpret this as the contextual representations being gender-biased, which happens because of the inherent gender bias of the text corpora used to induce the representations; the authors also present an effective way of debiasing the representations by augmenting the training data with gender-swapped sentences. This is related to the findings of static word embeddings capturing gender, as discussed in Section 4.10.

6.2.5 Context

It is logical to expect contextual word embeddings to encode the context of the word to some extent. But is it only limited local immediate context, so that we could obtain competitive contextual embeddings just by mixing the static embeddings of several neighboring words? Or are the embeddings also influenced by more distant words in more intricate ways? Research shows that the strongest component of a contextual word embedding still is the word identity, especially in shallow layers of the contextualizers. However, as we go to deeper layers of the contextualizers, the contextual embeddings capture wider and wider context, starting with immediate surroundings but eventually being able to capture information about other words from anywhere in the sentence.

Tenney et al. (2018) compare the ELMo embeddings both to classical non-contextual embeddings, as well as to locally contextualized embeddings, obtained by applying a word-level CNN with a kernel size of either 3 or 5 over the static word embeddings, i.e., integrating information about 1 or 2 neighboring words at each side of the word. They find that for morphological and syntactic probing tasks, not much is gained by full contextual embeddings over the locally contextualized embeddings (0–2 percentage points); this might mean that little non-local information is encoded in the contextual embeddings or that non-local information is of little relevance for the probing tasks. The latter actually seems more likely, as the situation is quite different for the semantic tasks; these seem to require more non-local information for the probe to perform well, and, accordingly, the full ELMo embeddings outperform the locally contextualized embeddings more clearly (1-5 percentage points). Thus, the conclusion seems to be that ELMo embeddings are much more than just static embeddings enriched with information about neighboring words, and do actually also capture important non-local features from the sentence.

Ethayarajh (2019) investigated how contextual the contextual embeddings really are. They found that the base of a contextual word embedding still seems to be a static component shared by all occurrences of the same word. However, especially for higher layers of multilayer contextualizers, the static component is rather weak, with the cosine self-similarity of different occurrences of the same word getting weaker in the higher layers, i.e., the representations are getting more context-specific.

Peters et al. (2018b) note that local syntax seems to be the dominant signal in the contextual embeddings, encoding syntactic phrase pertinence and boundaries; i.e., the contextualizer does not simply combine neighboring words weighted by their distance, it does also take syntax into account.

6.2.6 Word Senses

A concept closely related to context are word senses, i.e., discriminating between multiple senses of a single polysemous word (such as "train" in "I came on a train." versus "I train young children."). Trivially, static word embeddings are incapable of that distinction since the same vector is used for the word in any context. As contextual word embeddings do take context into account and represent the word with a different vector in each context, we may expect that the word sense distinction could be made based on the contextual embeddings. This turns out to be true, even to the extent that the contextual embeddings pertaining to various occurrences of an individual polysemous word often tend to form multiple clusters or clouds corresponding to its individual senses.

We might also be interested in the distinction between simply encoding context and encoding features more directly corresponding to a word sense abstraction. As a word sense is predominantly determined by the immediate context in which the word is used, such a distinction is not trivial to make. However, there seems to be evidence that the contextual representations do indeed go beyond simply encoding context and actually distinguish the individual senses.

Peters et al. (2018a) use a k-nearest neighbours (k-NN)-based approach to investigate the relation of contextual word embeddings to word senses. They first compute CoVe and ELMo representations of words in sentences from SemCor 3.0 (Miller et al., 1994), a corpus with annotations of word senses. Then, for each sense of each polysemous word, they compute a representation of the sense as the average of the contextual embeddings of these senses of the word which occur in the training part

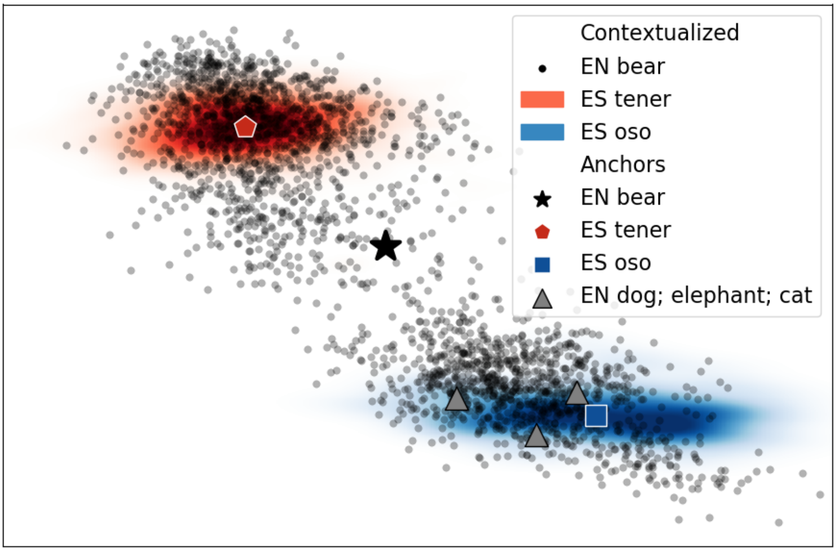


Figure 6.1: Clustering of the English word "bear" according to its verb sense (corresponding to Spanish "tener") and its animal sense (corresponding to Spanish "oso"). Reprinted from Schuster et al. (2019, Figure 2) under CC-BY-4.0 licence.

of the corpus. Then, they assign each word in the test sentences with the sense corresponding to the sense vector closest to the contextual vector of the word. This can be seen as k-NN with $k = 1$, i.e., checking whether, given an oracle clustering of the contextual embeddings according to word senses, the tested word would fall into the correct cluster.

The authors find that ELMo contextual embeddings do surpass the most-common-sense baseline (F_1 65.9%) by several percentage points, showing that *word senses are captured by ELMo embeddings to some extent*. This is *not true for CoVe*, which does not surpass the baseline.

As the approach used does not involve training a probing classifier but rather uses a non-parametric method, there is no risk of the sense disambiguation information to be hidden elsewhere than in the representations themselves. Nevertheless, Peters et al. (2018a) do not investigate how the sense information is encoded. Therefore, it is unclear whether what the representations capture can be mapped to an actual abstraction over senses or whether the sense disambiguation information only consists of information about several neighboring words.

Schuster et al. (2019) demonstrate that, for a fixed word form, ELMo contextual embeddings cluster according to the various senses of the word. In their example, reprinted in Figure 6.1, they show how the contextual embeddings for the English word "bear" cluster into two clouds, one corresponding to the verb meaning, and the other corresponding to the animal meaning; the image also shows that the representation for the animal "bear" is closer, e.g., to "elephant" or "cat" than to the representation for the verb "bear". They further claim that the word sense is the strongest signal in the contextual embeddings, as they show that the representations of a given word with an identical sense in different contexts are more similar to each other than representations of the same word in similar contexts but with different senses. Interestingly, all of these are just side-results for the authors, as their main goal is cross-lingual alignment of contextual word embeddings.

6.2.7 World Knowledge and Common Sense

Da and Kasai (2019) show that BERT captures some world knowledge or common-sense information to some extent, such as how large something is or whether something is an animal. They show that using BERT for this kind of common sense reasoning outperforms previous approaches, but that the model still often fails, suggesting that BERT is unable to get sufficient world knowledge from its training data.

Rogers et al. (2020) review some works in this area, concluding that BERT can perform well in some tasks focusing on world knowledge, reaching competitive performance to state-of-the-art question-answering systems (Petroni et al., 2019). However, BERT's apparent world knowledge is rather of a stereotypical factoid nature, mostly based on frequent cooccurrences but not able to infer more complex relations and interactions (Poerner et al., 2019). The BERT model thus seems to contain some world knowledge but is not able to use for reasoning.

6.3 What is Hidden Where?

In the previous section, we looked at what kinds of linguistic features are captured by contextual word embeddings, disregarding where the contextual embeddings come from. We now fill this gap by reviewing how the contextualizers differ in the number of linguistic features captured and looking at how the linguistic features are distributed among various layers of the contextualizer models.

6.3.1 Comparison of Architectures and Models

All of the contextual word embeddings, including hidden states taken from models trained for another purpose (such as NMT models), seem to capture morphology and syntax rather well and even a little of semantics, typically to a greater extent than static embeddings (Tenney et al., 2018).

In this section, we focus mostly on the effect of the architecture of the contextualizer; we will focus on the effect of the pre-training task in Section 6.3.3.

In general, the representations from simpler models, such as CoVe, typically seem to be weaker than representations from the more recent and complex contextualizers, as demonstrated by their lower probing accuracies; nevertheless, CoVe representations still typically capture the linguistic features to a significantly higher degree than static word embeddings (Tenney et al., 2018).

Tenney et al. (2018) find that ELMo seems to capture syntax better than CoVe.[19] However, this difference can be mostly explained by the underlying character-CNN static word embeddings being more informative in this sense – i.e., already the character-based static embeddings used in ELMo seem to be significantly more syntactic than classical word-based embeddings, and the further layers seem to add a similar amount of contextual and syntactic information as in CoVe. It should also be noted that these experiments did not control for the different data sizes of the contextualizer pre-training data, with CoVe being pre-trained on a several times smaller dataset.[20]

Even though BERT typically outperforms ELMo on practical tasks, it does not seem to capture the linguistic features to a considerably greater extent; it can be used to predict various linguistic accuracies with higher accuracy than ELMo (typically by 2 to 3 percentage points), but only if the weights of the layer mix are trained on a task-specific dataset (Tenney et al., 2018). It is possible that a considerable portion of this difference is caused by tokenization, where ELMo uses rather standard tokenization which matches the tokenization in the probing datasets to a great extent, while BERT uses a purely technical splitting into subwords and may thus operate on very different tokens than what is used in the benchmarks.

A large improvement of BERT over ELMo can be observed for Winograd coreference (see Section 6.2.3), where all previous models failed to significantly outperform the static embeddings baseline. BERT is the first model to outperform the baseline by 6 percentage points, suggesting that it does capture some more elaborate semantic information.

Generative Pre-Trained Transformer (GPT) usually seems to be similar to ELMo or slightly weaker, but still way above CoVe (Tenney et al., 2018). I.e., although performing better than BERT as an LM, it seems to be slightly weaker in capturing linguistic features.

An exception to this general trend may be found in the work of Kim et al. (2020), who focused on extracting constituency trees from pre-trained LMs, finding that GPT-2 actually outperforms BERT on this task. The authors hypothesize that this may be

[19] Probe accuracies consistently seem to be about 10% higher for ELMo than CoVe, regardless of whether we probe for, e.g., constituent labels or dependency relations.

[20] As CoVe is an MT model, it requires parallel data, while monolingual data are sufficient for ELMo. In the work of Tenney et al. (2018), the particular probed models used 7 million sentences versus 30 million sentences, respectively.

due to the training objective, with a standard auto-recursive LM being better suited for constituency phrases than a masked auto-decoding LM.

6.3.2 Distribution of Linguistic Features across Layers

In multilayer contextualizers, contextual representations can be taken from any layer, or multiple layers can be concatenated or mixed.[21] We now investigate into which layers to look for what kind of linguistic features.

RNN-based models capture linguistic features in the first layer

We first look at the RNN-based models, such as CoVe and ELMo. These models prototypically contain two layers of hidden states, but some authors also investigated deeper multilayer variants of these models.

Many authors show that, especially for morphological and syntactic annotation, the linguistic features can be best extracted by probes or projections applied to the first layer of the model, no matter whether the network has two or more layers (Zhang and Bowman, 2018; Liu et al., 2019a; Peters et al., 2018b). It is further claimed that the second layer (as well as potential subsequent layers) are already more task-specific and do not capture easily interpretable linguistic features very well (Liu et al., 2019a).

However, Peters et al. (2018a) show that for word sense disambiguation, using the second layer of a two-layer CoVe or ELMo model for prediction of the sense class actually leads to better results than using the first layer. This suggests that even in the simpler models, some deeper linguistic information (such as some semantic aspects) is better captured in deeper layers. Nevertheless, this may also be explained as the word senses actually being crucial for the training task (machine translation or language modeling). This would corroborate the hypothesis of other authors that the subsequent layers are more task-specific but go against their implication of the deeper layers thus being less useful for extracting linguistic features.

Figure 6.2, reprinted from (Tenney et al., 2019, figure A.1), provides yet another view on this issue. The authors show that morphological, syntactic as well as some shallow semantic features are mostly captured in the first layer of ELMo; while noting that the shallow semantic tasks – semantic role labeling and coreference – can be mostly solved using syntactic cues. For deeper semantic tasks (semantic proto-roles and semantic relations), the information seems to be rather equally distributed among the first and second layer of ELMo; however, as ELMo is shown not to capture these semantic features to a great extent, this probably does not mean that semantic features are *also* captured in the second layer, but rather that they are *not even* captured in the first layer.

[21] E.g., for ELMo, it is a standard approach to take a weighted combination of the individual layers to utilize for transfer learning.

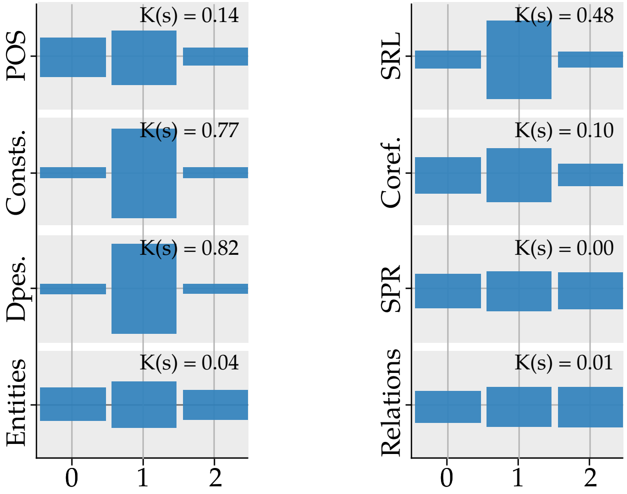


Figure 6.2: Scalar mixing weights for the ELMo encoder. Layer 0 is the character CNN that produces per-word representations, and layers 1 and 2 are the LSTM layers. Reprinted from Tenney et al. (2019, Figure A.1) under CC-BY-4.0 licence.

Transformers encode more complex linguistic features in later layers

With the more complex multilayer Transformer-based contextualizers, the situation is quite different, as linguistic features seem to be more spread out across the layers.

Multiple authors have found and repeatedly confirmed that generally speaking:

- the initial layers learn morphological features (Belinkov et al., 2017a)
- the intermediate layers capture syntax (Peters et al., 2018b); different levels of syntax are captured at different layers (Blevins et al., 2018), e.g., with constituency syntax being more local and captured at lower layers than dependency syntax (Tenney et al., 2018)
- the later layers tend to encode more semantic features and coreference-related features (Peters et al., 2018b)
- the final layers do not capture many linguistic features as they already seem to be overly specialized for the language modeling training task, i.e., typically for next word prediction (Peters et al., 2018b)
- the linguistics features generally tend to be concentrated in the intermediate layers (Liu et al., 2019a)
- features pertaining to a given linguistic abstraction are typically not contained to only one layer, but are spread over multiple layers (Tenney et al., 2019); therefore, the linguistic information is best extracted by using a specifically trained scalar mix of all the layers (Liu et al., 2019a)

Most weight over layers	Gravity center of layer attention	Linguistic features	Layer attention distribution shape
11–13	11.7	Part of speech	peaked
11–17	13.1	Constituency syntax	very peaked
12–17	13.8	Dependency syntax	very peaked
13–18	13.6	Semantic roles	peaked
14–20	13.2	Named entities	flat
13–22	12.7	Semantic proto-roles	very flat
15–22	12.8	Semantic relations	very flat
16–20	15.8	Coreference	peaked

Table 6.1: Distribution of linguistic features in the 24-layer BERT-large, intepreted from Tenney et al. (2019). For each feature type, we list an estimate of the range of layers on which it is captured significantly more than on other layers, together with the "center of gravity" of the layer attention, and a note how peaked or flat the distribution of the layer attention weights is.

It is easy to note that the depth of the layers capturing the linguistic features seems to roughly correspond to the depth traditionally assigned to the respective linguistic abstractions;[22] i.e., as we go deeper in the Transformer layers, we find deeper linguistic features. Tenney et al. (2019) go as far as to claim that BERT rediscovered the classical NLP pipeline. They demonstrate that, similarly to classical pipelines, BERT first determines the PoS of the words, continuing with syntax and named entities, and moving on to semantics. The division of the analyses is not hard, the individual "steps" actually overlap and gradually develop across layers, but the authors argue that the analysis steps still seem to depend on each other similarly as in the classical pipelines. However, some aspects of these claims have been disputed, e.g., by Elazar et al. (2020).

Similar claims are made by Jawahar et al. (2019), who particularly focus on syntax. They show that BERT captures short-range syntactic phenomena, such as syntactic phrases, in lower layers than long-range dependencies. They also explicitly analyze the compositional structure of BERT representations and draw parallels to traditional syntactic analysis.

However, the findings of Kim et al. (2020) are partially in conflict with the other authors, showing that the syntacticity of BERT layers indeed seems to increase as we move to further layers, but the trend seems to be opposite for GPT-2, observing higher syntacticity in the initial layers.

[22] When understanding the surface forms as the shallow abstractions, taking the analytical approach which goes in the direction from the surface to meaning, not the other way round.

We try to interpret the findings of Tenney et al. (2019) in Table 6.1. The authors use probes to extract the linguistic features from the layers employing *layer attention*, i.e., a trained task-specific linear combination of the model representations from the model layers. This provides them with a set of layer weights for each of the tasks (i.e., for each of the linguistic features which they probe for). The authors then interpret these layer weights as a measure of the degree to which the given linguistic feature is encoded within the given layer.

For each linguistic feature type examined by the authors, we also report its "center of gravity" (the authors' term) of the layer attention from (Tenney et al., 2019, Figure 1); please refer to the original paper for the full figure. The center of gravity is the weighted average of the layer numbers weighted by the layer attention weights, i.e., it is the average layer capturing the given linguistic feature.

Figure 6.3, reprinted from (Tenney et al., 2019, figure 2), shows the distribution of the layer weights for the individual tasks. In Table 6.1, we estimate how peaked or flat the distribution of these weights is. Some features seem to be mostly captured on only a few layers (the layer attention is rather peaked), while others seem to be more spread out (the layer attention is rather flat).

Thus, based on the graphs in Figure 6.3, we can estimate the layers on which the features are mostly captured. Unfortunately, the authors present the data in the form of graphs, but the exact numbers are not listed. Therefore, the layers which seem to capture the features significantly more than other layers were only approximately estimated from the graphs. In this way, we attempt to approximately answer the question of on which layers the respective linguistic features are captured. However, please note that this is all rather approximate, as there is no clear way of answering that question; refer to (Tenney et al., 2019) for the original data and interpretations.

The table confirms the rough notion of the layer depth corresponding to the depth of the linguistic features, going from morphology over syntax and semantics, with coreference being the deepest. However, the distribution of some features across layers is actually quite flat, especially for the semantic ones; i.e., some features seem to be spread quite evenly across most or all of the layers. We thus should be careful with any strong claims based on the observations.

6.3.3 Effect of Pre-training Task

Technically, any NLP task can be used to pre-trained a contextualizer to provide contextual embeddings. However, not all pre-training tasks are equally good for this purpose, as shown by several studies (Belinkov et al., 2017a,b; Peters et al., 2018b; Blevins et al., 2018; Zhang and Bowman, 2018; Liu et al., 2019a).

In general, many authors have found that using the LM task for pre-training is the best choice in most cases, as such contextual embeddings seem to best transfer to other tasks. Relatedly, such contextual embeddings are also usually found to most strongly

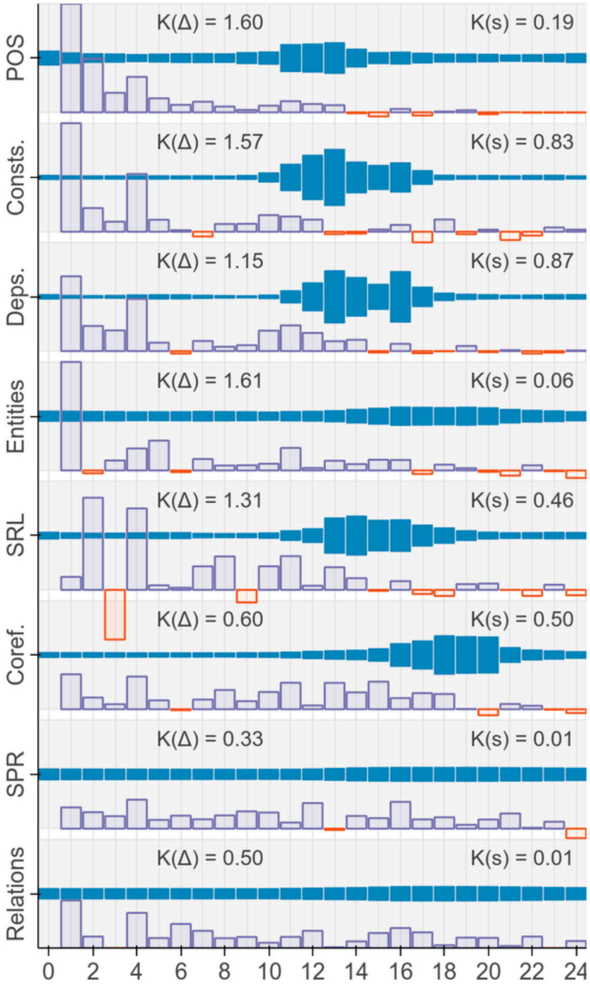
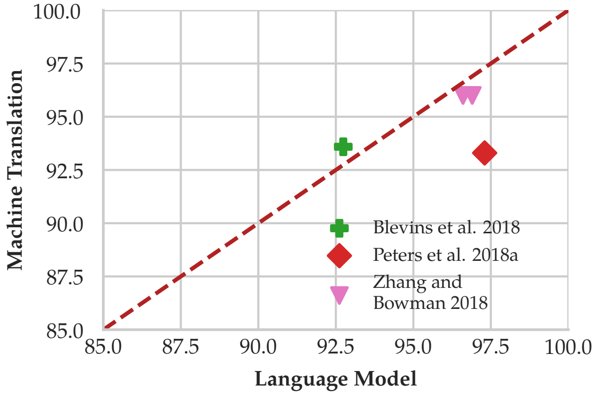
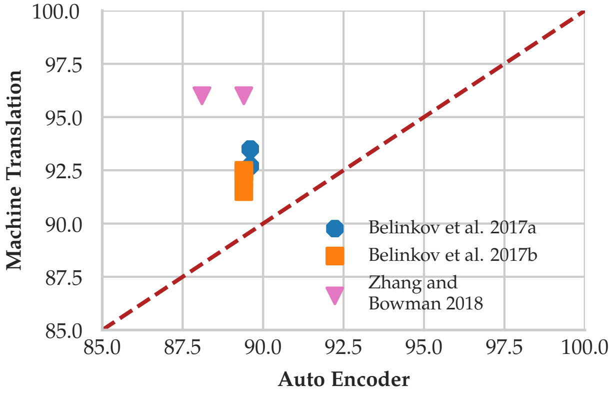


Figure 6.3: Mixing weights for layer attention (solid blue) for BERT-large. The horizontal axis is the encoded layer. Reprinted from Tenney et al. (2019, Figure 2) under CC-BY-4.0 licence.



(a) Machine Translation compared with Language Model pre-training.



(b) Machine Translation compared with Auto Encoder pre-training.

Figure 6.4: Accuracy of PoS tag probing from RNN representation divided by the pre-training objective.

capture linguistically interpretable features, compared, e.g., to hidden states from an MT model (even if training data of comparable sizes are used to pre-train the models).

Nevertheless, quite logically, if the contextualizer is directly trained for a linguistic feature, then this feature is typically captured more strongly in its hidden states than in a general LM; e.g., when a model is trained for PoS tagging, it will capture PoS features more strongly than an LM. This also generalizes to models trained for a different but strongly related task; e.g., a parsing model will also capture PoS very strongly. Still, this provides task-specific contextual embeddings, which are *stronger* in capturing task-specific features but *weaker* in capturing other features. In this sense, the LM task seems to be the most general language-related task, as it seems to provide the most general contextual embeddings.

However, LM as a pre-training task has an additional benefit of typically having much larger training data available than any other task. Thus, in practice, contextual embeddings from an LM typically outperform even task-specific contextual embeddings unless task-specific training data of considerable size are available.

A detailed study of the effects of the pre-training task, as well as effects of the size of the training data, was conducted, e.g., by Zhang and Bowman (2018), investigating CoVe and ELMo contextual embeddings obtained using various pre-training tasks (LM, MT, skip-thought[23] and autoencoding[24]) and probing them on several morphosyntactic tasks (PoS prediction and CCG supertag prediction).

In Figure 6.4, we present a comparison of the effects of different pre-training tasks for contextual embeddings probed for PoS tags. Each point denotes a pair of results obtained in the same paper and for the same dataset, but with different types of embeddings or pre-training objective (but with a similar amount of training data used for the pre-training). Therefore, we can observe that the setting plotted on the y-axis is better than the x-axis setting if the points are above the plotted identity function (red dashed line).[25] We can see that MT models capture PoS features much better than auto-encoders, which can be interpreted as translation from and to the same language. It is likely that the latter task is straightforward and therefore, does not require the model so strongly to encode morphosyntactic features in the latent space. However, we can see that when using same-sized pre-training data, the difference between the results of Machine Translation and Language Model pre-training is small; still, much larger data are typically available for LM than for MT pre-training.

[23] For a sentence in a longer text, predict it's preceding and its following sentence.

[24] Using a classical denoising autoencoder, where the input is corrupted to some extent and the autoencoder is trained to predict the original uncorrupted input.

[25] We cannot say whether a method represented by another point performs better, as the evaluation settings differ.

6.4 Multilinguality

So far, we have only talked about pre-trained representation models for a single language evaluated on English. However, pre-trained Transformers show remarkable ability to work with multiple languages within a single model.

Multilingual BERT (mBERT) (Devlin et al., 2019), which was followed by XLM-RoBERTa (XLM-R) (Conneau et al., 2020) and DistilBERT (Sanh et al., 2020), gained popularity as a contextual representation for many multilingual tasks.

mBERT is a deep Transformer encoder that is trained in a multi-task learning setup, first, to be able to guess what words were masked-out in the input and, second, to decide whether two sentences follow each other in a coherent text.

It was trained using the same procedure as English BERT: a combination of a masked language model (MLM) objective and sentence-adjacency objective using plain text in over 100 languages without making any difference among the languages.

Conneau et al. (2020) claim that the original mBERT is under-trained and train a similar model on a larger dataset that consists of two terabytes of plain text extracted from CommonCrawl (Wenzek et al., 2020). Unlike mBERT, XLM-R uses a SentencePiece-based vocabulary (Kudo and Richardson, 2018) of 250k tokens, the rest of the architecture remains the same as in the case of mBERT. The model is trained using the MLM objective, only without the sentence adjacency prediction.

Kondratyuk and Straka (2019) managed to achieve very strong results in dependency parsing in 75 languages by training a single model that used mBERT as an input representation without telling the model what the input language was. In this way, the model reached very good results even for languages where only test data and no training data are available.

Often, the success of zero-shot transfer is implicitly considered to be the main measure of language neutrality of a representation. Despite many positive results, some findings in the literature are rather mixed, indicating limited language neutrality.

Zero-shot learning abilities were examined by Pires et al. (2019) on NER and PoS tagging, showing that the success strongly depends on how typologically similar the languages are. Similarly, Wu and Dredze (2019) trained good multilingual models but struggled to achieve good results in the zero-shot setup for POS tagging, NER, and XLNI. Rönnqvist et al. (2019) draw similar conclusions for language-generation tasks.

Wang et al. (2019b) succeeded in zero-shot dependency parsing, but required supervised projection trained on word-aligned parallel data. The results of Chi et al. (2020) on dependency parsing suggest that methods like structural probing (Hewitt and Manning, 2019) might be more suitable for zero-shot transfer.

Pires et al. (2019) also assessed mBERT on cross-lingual sentence retrieval between three language pairs. They observed that if they subtract the average difference between the embeddings from the target language representation, the retrieval accuracy significantly increases.

XTREME (Hu et al., 2020) and XGLUE (Liang et al., 2020), two recently introduced benchmarks for multilingual representation evaluation, assess representations on a wider range of zero-shot transfer tasks that include natural language inference (Conneau et al., 2018b) and question answering (Artetxe et al., 2019; Lewis et al., 2019). Their results show a clearly superior performance of XLM-R compared to mBERT.

Many works clearly show that downstream task models can extract relevant features from the multilingual representations (Wu and Dredze, 2019; Kudugunta et al., 2019; Kondratyuk and Straka, 2019). But they do not directly show language-neutrality, i.e., to what extent similar phenomena are represented similarly across languages. It is thus impossible to say whether the representations are language-agnostic or if they contain some implicit language identification.

We (Libovický et al., 2019) argue that in zero-shot transfer from the source language to the target language, there is a risk of "overfitting" the source language – validation data in the source language are typically used to stop the training once the performance on the data stops increasing, but this might mean that the model is already too specialized to the source language, while a less specialized model might be more transferable, i.e., the training should probably be stopped earlier.

We (Libovický et al., 2019) circumvent the identified problem by analyzing the representations on tasks of cross-lingual word-alignment, cross-lingual sentence retrieval, and machine translation quality estimation, which directly utilize the pretrained multilingual contextual embeddings with no further training; the embeddings are simply averaged and compared using cosine distance to measure word or sentence similarity, which for each of the tasks should be maximized. We find that the multilingual contextual embeddings outperform bilingual static word embeddings which were explicitly trained to be cross-lingual, whereas the cross-linguality of the contextual embeddings is an emergent property not explicitly imposed during training. We observe high accuracies for sentence retrieval and state-of-the-art performance for word alignment. For quality estimation, the results are very poor, suggesting that a deeper understanding of the meaning of the sentences is required than what is captured by the representations.

Following Pires et al. (2019), we (Libovický et al., 2019) also show that, while the representations are already quite language-neutral, they in fact strongly encode the language identity, actually leading to state-of-the-art results in language prediction. However, the language-neutral component and the language-specific component are easy to separate: a language centroid can be computed as an average of representations of sentences in the given language and subtracted from the contextual embedding to obtain a mostly language-neutral embedding. These language-neutral embeddings perform even better in the cross-lingual tasks, while the language centroids cluster nicely according to traditional typological language families (see Figure 6.5).

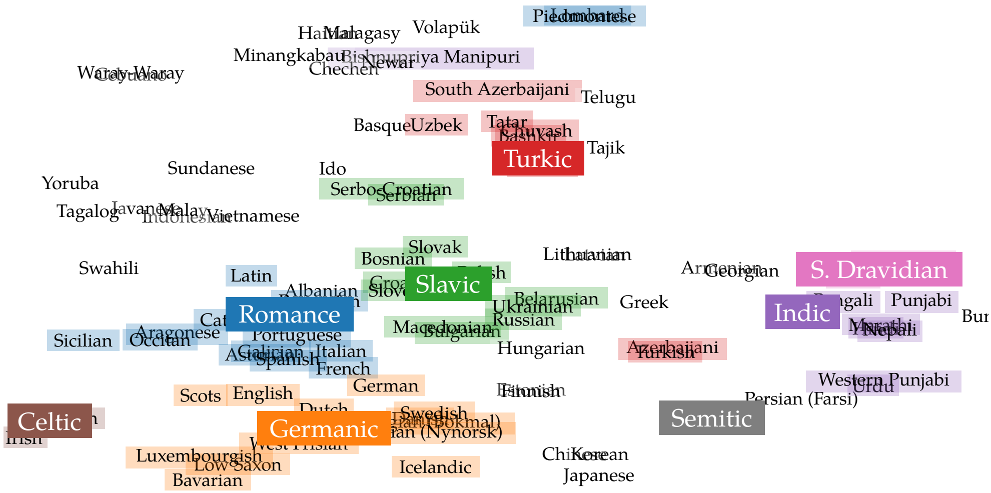


Figure 6.5: Language centroids of the mean-pooled representations from the 8th layer of cased mBERT on a tSNE plot with highlighted language families. Reprinted from Libovický et al. (2019).

6.5 Conclusion

In this chapter, we looked at contextual word embeddings, which emerged as "unhidden" states and turned out to be a further improvement over static word embeddings, taking into account not only the word identities (type-level information) but also the context of the sentence (token-level information).

The contextual embeddings seem to capture morphological and syntactic features quite well. However, they typically perform rather poorly on tasks requiring a deeper understanding of the meaning of the sentence, suggesting that semantic features are mostly not captured by the contextual embeddings.

Contextual embeddings thus constitute a clear improvement over static embeddings as well as over many classical symbolic approaches based on explicit linguistic knowledge, but only for a certain range of shallow and medium-depth linguistic abstractions, such as morphology and syntax. However, for deeper linguistic abstractions, such as semantics and pragmatics, the current contextual embeddings still fail to demonstrate a sufficient level of capturing the relevant features; in these areas, we are probably still far from outperforming and replacing the classical approaches.

Contextual embeddings are obtained as hidden states of neural models, trained for NLP tasks. In the past, representations from MT models were often used, but eventually, it was established that training the network for the language modeling task on a large dataset leads to very versatile high-quality contextual embeddings, transferrable to many other tasks. If transferability is not required, better contextual embeddings can be obtained by training directly on the target task, but usually only if a large-enough dataset is available; for tasks with small datasets, the LM-pre-trained embeddings are a better choice.

As new and better NN models are introduced, often thanks to research in MT, better contextual embeddings can be obtained by training these new models for the LM task. However, even the simplest models usually lead to contextual embeddings which capture linguistic features way better than static word embeddings, and switching to better models often brings only slight further improvements.

Afterword

The representations and structures that emerge in neural models have been shown to often have some similarity to classical linguistic abstractions. However, this only answers the first and simplest of a sequence of logical questions. There are some similarities to classical linguistic structures, but what are the differences? Can we e.g. define a new syntactic formalism that would closely correspond to the features we observe in the models? The latent linguistic features emergent in neural models have proven themselves to be far more useful for solving various language processing tasks than any abstractions previously defined by linguists; should we thus rethink the way we describe and understand language to reflect this fact? And can we, in turn, further improve the models we now use for processing language based on these new ways of viewing language?

Still, all of these questions are only further steps on a path to the ultimate goal of linguistics: Can a complex interpretation and understanding of what is really going on in the state-of-the-art neural models bring us closer to actually understanding how language works?

Summary

In this book, we explore neural-network architectures and models that are used for Natural Language Processing (NLP). We analyze their internal representations (word-embeddings, hidden states, attention mechanism, and contextual embeddings) and review what properties these representations have and what kinds of linguistically interpretable features emerge in them. We use our own experimental results, as well as the results published by other research teams to present an overview of models and representations and their linguistic properties.

In the beginning, we explain the basic concepts of deep learning and its usage in NLP and discuss details of the most prominent neural architectures and models. Then, we outline the concept of interpretability, different views on it, and introduce basic supervised and unsupervised methods that are used for interpreting trained neural-network models.

The next part is devoted to static word embeddings. We show various methods for embeddings space visualization, component analysis and embedding space transformations for interpretation. Pretrained word embbedings contain information about both morphology and lexical semantics. When the embbedings are trained for a specific task, the embeddings tend to be organised by the information that is important for the given task (e.g. emotional polarity for sentiment analysis).

We also analyze attention mechanisms, in which we can observe weighted links between representations of individual tokens. We show that the cross-lingual attentions mostly connect mutually corresponding tokens; however, in some cases, they may be very different from the traditional word-alignments. We mainly focus on self-attentions in Transformers. Some heads connect tokens with certain syntactic relations. This motivated researchers to infer syntactic trees from the self-attentions and compare them to the linguistic annotations. We summarize the amount of syntax in the attentions across the layers of several NLP models. We also point out the fact that attentions might sometimes be very misleading and may carry very different information from which we would think based on the attended tokens.

In the last part, we look at contextual word embeddings and the linguistic features they capture. They constitute a clear improvement over static word embeddings, especially in terms of capturing morphological and syntactic features. However, some higher linguistic abstractions, such as semantics, seem to be reflected in the current contextual embeddings only very weakly or not at all.

List of Figures

List of Tables

List of Abbreviations

AI Artificial Intelligence

BERT Bidirectional Encoder Representations from Transformers
biRNN Bidirectional Recurrent Neural Network
BLEU BiLingual Evaluation Understudy

CBOW Continuous Bag of Words
CCG Combinatory Categorial Grammar
CNN Convolutional Neural Network
CoVe CoVe Context Vectors
CV Computer Vision

ELMo Embeddings using Language Models

GloVe Global Vectors for Word Representation
GPT Generative Pre-Trained Transformer
GRU Gated Recurrent Unit

ICA Independent Component Analysis

k-NN k-nearest neighbours

LM Language Model
LSTM Long Short-Term Memory

mBERT Multilingual BERT
ML Machine Learning
MLP Multi-Layer Perceptron
MT Machine Translation

NER Named Entity Recognition
NLP Natural Language Processing
NMT Neural Machine Translation
NN Neural Network

PCA Principal Component Analysis

PoS	Part of Speech
ReLU	Rectified Linear Unit
RNN	Recurrent Neural Network
SAN	Self-Attentive Network
SG	Skip-Gram
SRL	Semantic Role Labelling
TagLM	Language-Model-Augmented Sequence Tagger
UAS	Unlabeled Attachment Score
WMT	Workshop of Machine Translation
XLM-R	XLM-RoBERTa

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Index