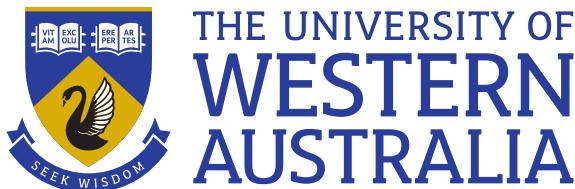


On the surprising capacity of linear combinations of embeddings for natural language processing

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BCM in Computation and Pure Mathematics;
BE in Electrical and Electronic Engineering
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This thesis is presented for the degree of
Doctor of Philosophy
of The University of Western Australia

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Date: September 3, 2018

In memoriam of
Laurie White
1927–2018

Abstract

As Webber's classic 1929 text *English Composition and Literature* states: "A sentence is a group of words expressing a complete thought." Human's use natural language is used to represent thoughts. Thus the representation of natural language, in turn, is of fundamental importance in the field of artificial intelligences. Natural language understanding is an area which fundamentally revolves around how to represent text in a form that an algorithm can manipulate in such a way as to mimic the ability of a human to truly understand the text's meaning. In this dissertation, we aim to extend the practical reach of this area, by exploring a commonly overlooked method for natural language representation: linear combinations (i.e. weighted sums) of embedded representations. This dissertation is organised as a collection of research publications: with the novel contributions published as in conference proceedings or journals; and with the literature review having been published as part of a book.

When considering how to represent English input into a natural language processing system, a common response is to consider modelling it as a sequential modelling problem: time-series of words. A more complex alternative is to base the input model the grammatical tree structures used by linguists. But there are also simpler models: systems based on just summing the word embeddings. On a variety of tasks, these work very well – often better than the more complex models. This dissertation examines these linear combinations of embeddings for natural language understanding tasks.

In brief, it is found that a sum of embeddings is a particularly effective dimensionality-reduced representation of a bag of words. The dimensionality reduction is carried out at the word level via the implicit matrix factorization on the collocation probability matrix. It thus captures into the dense word embeddings the key features of lexical semantics: words that occur in similar contexts have similar meanings. We find that summing these representations of words gives us a very useful representation of structures built upon words.

A limitation of the sum of embedding representation is that it is unable to represent word order. This representation does not capture any order related information; unlike for example a recurrent neural network. Recurrent neural networks, and other more complex models, are out performed by sums of embeddings in tasks where word order is not highly significant. It is found that even in tasks were word order does matter to an extent, the improved training capacity of the simpler model still can mean that it performs better than more complex models. This limitation thus hurt surprisingly little.

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Lorem Ipsum

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Date: [insert date]

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to sign

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Part I

Introduction

Chapter 1

Introduction

It has been a continual surprise, that simple combinations of embeddings performs so well for a variety of tasks in natural language processing. At first glance, such simple methods capturing only unordered word use should have little capacity in the rich and highly structured nature of human language. However at a second glance, similar surface information has been used in information retrieval with great success since the inception of the field (Maron 1961). Linear combinations of embeddings can be considered as a dimensionality reduction of a bag of words, with a particular weighting scheme. Dimensionality reduction can be characterised as finding the best low dimensional representation of a high dimensional input according to some quality criterion. In the case of word embeddings, that quality criterion is generally along the lines the ability to predict the co-occurring words – an salient quality of lexical semantics. As such, linear combinations of embeddings take as input a very sparse high dimensional bag of words (which is itself a strong surface form representation), take reduce it to a dense representation that captures lexical semantics.

Throughout over the last three years that we have been considering this problem, others also have also found, often to their own surprise, the strength of simple linear combinations of embeddings.

Arora, Liang, and Ma (2017)’s work describes a ““A simple but tough-to-beat baseline for sentence embeddings””, which is a linear combination of word embeddings. There proposed model is a more complicated combination than considered here. But never the least, is primarily a weighted sum of embeddings, with small adjustment based on linear dimensionality reduction methods. In particular when using the word embeddings of Wieting et al. (2016), they find this to be very competitive with more complex models which take into account word order.

Cifka and Bojar (2018) found that taking a mean of word embeddings outperformed almost all their more sophisticated machine-translation-based sentence representations when used on classification and paraphrase detection tasks. This is not to say that linear combinations of embeddings are ideal models for all tasks. They clearly can not truly handle all the complexities of language. But rather that the occurrence of the complexities they can not handle is rarer in practice in many tasks than is often expected.

Conneau et al. (2018) constructed 10 probing tasks to isolate the some of the information captured by sentence representations. They found the strong performance of averaged word embeddings on sentence level tasks to be striking. They attribute it to the sentence level information being redundantly encoded in the word-forms: the surface level information is surprisingly useful for what at first looks like a sophisticated tasks. With the exception of their word-content task, they did find more sophisticated models able to perform better the the averaged word embeddings. However, when correlating the performance of their probing task against real world tasks, they found that the word-content probing task was by far the most positively correlated with the real word tasks. This makes it clear how valuable this surface information is in practical tasks.

In the work presented this dissertation, we find that that even in tasks where it would seem that non-surface information incorporating word-order is required, in practice other issues cause the more powerful models that are (theoretically) able to handle these situations correctly may them to be never-the-less outperformed. This is particularly the case where the theoretical improvement from incorporating this information is small, relative to the practical complexity of the techniques required to leverage it. Such a case where where word order matters but the error from ignoring it is small, is particular illustrated in ??.

At a high-level the success of these techniques comes down to most human language being easy to understand and simple. This expectation of language being easily understood is highlight by

(Grice 1975), which brings the *expectation* the communication is conducted following the cooperative principle. The overall supermaxim for Grice's cooperative principle is the speakers should "be perspicuous" or more perspicuously, should use speech that is clearly expressed and easily understood. The particular relevant maxims within the principle are: the *maxim of quantity*, that one should make contributions no more nor less informative than required; and the *maxim of manner*: to avoid ambiguity and obscurity of expression, and to make contributions that are brief and orderly. While Grice originally proposed these are exceptions upon conversation, the general principle applies more broadly to natural language communication. This general principle being that language used is normally expected to be understood easily – thus fulfilling the goal of communicating.

Adversarial examples are reasonably easy to construct. An adversarial example to a linear combination of word embeddings is any text where the word order significantly effects that meaning; and where multiple possible word orders exist. For such an adversary to be significant, both word orders must be reasonably likely to occur. However; such cases are rarer than one might expect is demonstrated in ???. Particularly when punctuation is included, which it reasonably can be as a token embedding. As such, while these cases certainly exist, we find that for real applications they are sufficiently rare that the simplicity of the linear combinations of embeddings approach can work very well.

This when applied in sentence or phrase representation contexts, such as discussed in ??, and ?? this gives support to the notion that word order is often not a very significant feature in determining meaning. While it seems clear that word order, and other factors of linguistic structure must contribute significantly to the meaning of the phrase. However, our result suggest that it is often in a minor way, and that for many tasks these linear combinations are superior due to their simplicity and effectiveness. While taking into account greater linguistic structure may be the key to bridging the between "almost perfect" and "true perfection", the current state of the field for many tasks has not reached "almost perfect", and as such simpler methods still form an important part. The successes of the sums of word embeddings discussed in ??, and ?? leads us to consider other uses of linear combinations for representation. ?? and ?? consider tasks well outside of phrase representation where the order clearly does not matter.

To further understand the relationship between SOWE and BOW, and the extent to which word order matters the capacity to reverse the conversion from phrase to SOWE in investigated in ?? and ???. The results in ?? show that it is indeed largely possible to reconstruct bags of words from SOWE, suggesting that when considered as a dimensionality reduction technique SOWE does not lose much information. This is extended in ?? to order those bags of words back to sentences via a simple tri-gram language model. This had some success at outright reconstructing the sentences. This highlights the idea that for many bags of words (which can be reconstructed from a sum of word embeddings) there may truly be only one reasonable sentence from which they might have come. This would explain why SOWE, and BOW, ignorance of word order does not prevent them from being useful representation of sentence.

On the complexity of models. One of the attractive features of these linear combinations is there simplicity. This is true both in an implementation sense, and in the sense of gradient descent. For example, the vanishing gradient problem in deep networks, especially RNNs and RvNNs simply does not exist for a sum of word embeddings due to it not being as an input structure. This in contrast to RNNs which are deep in time, and RvNNs which are deep in structure. Deep networks can be placed upon the input processing as represented by a RNN, RvNN or linear combination of embeddings, but for the RNN, and RvNN the network is already depth even with only one hidden layer on top.

1.1 Thesis Overview

This thesis tackles a number of natural language understanding problems, and in the solutions draws conclusions on the capacity of linear combinations of embeddings.

The representation of *sentences* is investigated in ??, through a paraphrase grouping tasks. Similarly, the representation of *phrases* is investigated in ?? through a color understanding (estimation) task. Given the observed properties found by sums of word embeddings, this leads to the investigation of if weighted sums of word sense embeddings might better resplendent a particular usage of a word in ???. The capacity also lends to the investigation of using a sum of word embeddings to represent the contexts of all usages of a named entity, for the point of view character detection task investigated in ???. We conclude with a complementary pair of works in ????, which investigate the ability to recover bags of words and sentences, from sums of word embeddings rep-

There are a few papers which show RNNs are only as powerful as Regex, or that they don't have much memory

Chapter	Structure	Task	Embeddings
??	Sentences	Paraphrase grouping	Word2Vec (Mikolov et al. 2013)
??	Short Phrases	Color understanding	FastText (Bojanowski et al. 2017)
??	Word Senses	Similarity with context & Word sense disambiguation	AdaGram (Bartunov et al. 2015) & Bespoke greedy sense embeddings
??	Adj. Contexts	POV character detection	FastText (Bojanowski et al. 2017)
??	Sentences	Recovering bags of words	GLoVE (Pennington, Socher, and Manning 2014)
??	Sentences	Recovering sentences	GLoVE (Pennington, Socher, and Manning 2014)

Table 1.1: Summary of the investigations published within this dissertation.

resenting sentences. These final works illustrate some of the reasons why the linear combinations work so well.

1.1.1 ?? “How Well Sentence Embeddings Capture Meaning” (Lyndon White et al. 2015)

We begin by examining methods for representing sentences. Sentences are a fundamental unit of communication – a sentence is a single complete idea.

The core goal is to determine if an sentence embedding clearly separated the different ideas. Paraphrases are defined by a bidirectional entailment relationship between two sentences. This is a equivalence relationship, it thus gives rise to a partitioning of all sentences in natural language space. If a sentence embedding is of high quality, it will be easy to define a corresponding partitioning of the embedding space. One way to determine how easy it is to define the corresponding partitioning it to attempt to do just that as a supervised classification task using a weak classifier. A weak classifier, such as the linear SVM we used, is required as a more powerful classifier (such as a deep neural network) could learn arbitrary transforms. The classification task is to take in a sentence embedding and predict which group of paraphrases it belongs to. Where the target paraphrase group is defined using other paraphrases with the same meaning as the candidate.

Under this course of evaluation it was found that the sum and mean of word embeddings performed very well as a sentence representation. These LCOWEs were the best performing models under evaluation. They were closely followed by the bag of words, which is advantaged by being much higher dimensionality than other models. The LCOWEs outperform the bag of words as they also capture synonyms and other features of lexical relatedness. Slightly worse than the bag of words was the bag of words with PCA dimensionality reduction to 300 dimensions. This confirms our expectation that LCOWEs are a better form of dimensionality reduction for preserving meaning from a bag of words than PCA.

The poor results of the paragraph vector models (Le and Mikolov 2014) is in line with the observation in the footnotes of the less well-known follow up work Mesnil et al. (2014). That the performance reported Le and Mikolov (2014) can not be reliably repeated on other tasks, or even the same takes with a slightly different implementation.

A limitation of this work is that it does not include the examination of any encoder-decoder based methods, such as Skip-Thought (Kiros et al. 2015), or machine translation models. Another limitation of the work is that the URAE use a pretrained model with only 200 dimensions, rather than 300 dimensions as was used in the other evaluations.

Paraphrases provide one source of grounding for evaluation of sentences. Color names are a subset of short phrases which also have a ground truth for meaning – the color. They are thus useful for evaluating the performance of LICOWE on short phrases.

1.1.2 ?? “Learning of Colors from Color Names: Distribution and Point Estimation” (Lyndon. White et al. 2018)

To evaluated the performance of input representations for short phrases, we considered a color understanding task. Color understanding is considered as grounded microcosm of natural language

understanding (Monroe, Goodman, and Potts 2016). It appears as a complicated sub-domain, with many of the same issues that plague natural language understanding in general: it features a lot of ambiguity, substantial morphological and syntax structure, and depends significantly on context that is not made available to the natural language understanding algorithms. Unlike natural language more generally, it has a comparatively small vocabulary, and it has grounded meaning. The meaning of a particular utterance, say **bluish green**, can be grounded to a point in color space, say in HSV (192°, 93%, 72%), based on the questioning the speaker. The general meaning of the a color phrase can be grounded to a distribution over color space, based on surveying the population of speakers.

Models were thus created to learn a mapping from natural language space, to points or distributions in color space. Three input representations were considered: a sum of word embeddings (SOWE), a convolutional neural network (CNN), and a recurrent neural network (RNN). The SOWE corresponds to a bag of words – no knowledge of order. The CNN corresponds to a bag of ngrams – it includes features of all length, thus can encode order. The RNN is a fully sequential model – all inputs are processed in order and it must remember previous inputs.

It was expected that this task would benefit significantly from a knowledge of word order. For example, **bluish green** and **greenish blue** are visibly different colors. The former being greener than the later. However, it was found that the SOWE was the best performing input representation, followed closely by the CNN , with the RNN performing much worse. This was even the case when the test set was restricted to only contain colors names for which multiple different word orders (representing different colors) were found in the training set. This can be attributed to the difficulty in training the more complicated models. In contrast to a simple feed-forward SOWE, in a RNN the gradient must propagate further from the output, and there is more weights to be learned in the gates. This difficulty dominated over the limitation in being able to model the color names correctly. We note that while **bluish green** and **greenish blue** are different colors, but they are never the less similar colors. As such, the error from treating them as the same, is less than the error caused by training difficulties.

The solving problem of color estimation from natural language color name, has pragmatic uses. Color estimation from description has utility as a tool for improving human-computer interaction. For example allowing free(-er) text for specifying colors in plotting software, using point estimation. It also has utility as an education tool: people from different cultures, especially non-native English speakers, may not know exactly what color range is described by **dark salmon**, and our model allows for tools to be created to answer such queries using distribution estimation.

A limitation of this study is the metrics used. For distribution estimation, the perplexity of the discretized distributions in color space is reported. It would be preferable to uses Kullback–Leibler divergence, which would allow comparisons to future works that output truly continuous distributions. Kullback–Leibler divergence is monotonically related the to discretized perplexity, however. For point estimation, using an evaluation metric such as a Delta-E, which is controlled for the varying sensitivity of human perception for different hues. Neither limitation has direct bearing on the assessment of the input representations.

1.1.3 ?? “Finding Word Sense Embeddings Of Known Meaning” (Lyndon White et al. 2018a)

With the demonstrated utility of linear combinations of embeddings for representing the meanings of larger structures made from words, it is worth investigating their utility for representing the possible different meanings of words. When it comes to representing word senses, it may be desirable to find a representation for the exact sense of a word being used in a particular example. A very fine grained word sense for just that one use. If one has a collection of induced word senses, it seems reasonable to believe that the ideal word sense for a particular use, must lay somewhere between them in embedding space. Further more, if one knows the probably of each of the coarse induced senses being the correct sense for this use, then it makes sense that the location of the fine grained sense embedding would be closer to the more likely coarse sense, and further from the less likely coarse sense. As such we propose a method to define these specific case word senses based on a probability weighted sum of coarser word sense embeddings. We say that we *refit* the original sense embeddings, using the single example sentence to induce the fine grained sense embedding.

Using this we define a similarity measure which we call RefittedSim, which we find to work better than AvgSimC (Reisinger and Mooney 2010). AvgSimC is a probability-weighted average of all the pairwise similarity scores for each sense embedding. In contrast RefittedSim is a single similarity score as measured between the two refitted vectors – which are the probability weighted

averages of the coarser sense vectors. On the embeddings used in our evaluations this gave a solid improvement over AvgSimC. It is also asymptotically faster to evaluate.

We also evaluated using refitting for word sense disambiguation (WSD). Normally, induced senses can not be used for word sense disambiguation, as they do not correspond to standard dictionary word senses. By using the WordNet gloss (definition) as an example sentence, we are able to use refitting to create a new set of sense embeddings suitable for WSD. Using this we can use the skip-gram formulation for probability of the context given the refitted sense, and so apply Baye’s theorem to find the most-likely sense. However, we found that the results were only marginally better than the baseline. Nearly unsupervised WSD is a very difficult problem; with a strong baseline of simply reporting the most-common sense. Our results do suggest that our refitting method does not learn features that are antithetical to WSD. However, they do incorporate the most frequent sense as a prior and seem to provide little benefit beyond that.

A limitation of this study was that it did not perform the evaluation on state-of-the-art word-sense embeddings. As such, while it’s comparisons between these embeddings are valid they can not be readily compared to the current state-of-the-art on the tasks.

1.1.4 ?? “NovelPerspective: Identifying Point of View Characters” (Lynden White et al. 2018b)

Given the success of LCOWEs for representing meaningful linguistic structures (sentences and phrases), a natural follow up question is on its capacity to represent combinations of words that do not feature this natural kind of structure. These would be more arbitrary bags of words; that never the less may be useful features for a particular task. The task investigated in this work was about identifying point of view characters in a novel.

Given some literary text written in third person limited point of view, such as Robert Jordan’s popular “*Wheel of Time*” series of novels, it is useful to a reader (or person analysing the text), to identify which sections are from the perspective of which character. That is to say, we would like to classify the chapters of a book according to which character they are from the perspective of. This at first looks like a multiclass classification problem; however it is in-fact an information extraction problem. The set of possible classes for any given chapter is the set of all named entities in the book. Different books have different characters, thus the set of named entities in the training data will not match that of an arbitrary book selected by a user. As such, the named entity tokens themselves can not be used in training for this task. Instead, it must be determined whether or not a named entity is the point of view character, based on how the named entity token is used. To do this, an representation of the context of use is needed.

The task can be treated as a binary classification problem. Given some feature vector representing how a particular named entity token was used throughout a chapter, find the probability of that named entity being the point of view character. We considered two possible feature sets to use to generate the feature vectors for named entity token use. Both feature sets consider the context primarily in terms of the token (word) immediately prior to, and the token (word) immediately after the named entity. We define a 200 dimensional hand-crafted *classical feature set* in terms of the counts of adjacent part of speech tags, position in the text, and token frequency. We define a *mean of word embedding based feature set* as the concatenation of the mean of the word embedding for the words occurring immediately prior, to the mean of the word occurring immediately after. As this was using 300 dimensional embeddings, this gives a 600 dimensional feature vector.

It was found that the two feature sets performed similarly, with both working very well. It seems like the primary difficulty was with the high dimensionality of the word embedding based feature set. Without sufficient training data, it over-fit quiet easily. It’s performance dropped sharply on the testset, compared to it’s oracle performance if trained on the testset, when the largest book series was removed. This likely could have been ameliorated by using lower dimensional embeddings.

The good performance of the word embedding based feature set is surprising here as it does not include any frequency information. We used a mean, rather than a sum, of word embeddings to represent the context of named entity token use. In the classical feature set, we found that by far the most important feature was how often that named entity token was used. Indeed just reporting the most frequently mentioned named entity gave a very strong baseline. The lexical information captured by the MOWE is clearly similarly useful to the part of speech tag counts, and almost certainly makes more fine grained information available to the classifier. Thus allowing it to define good decisions boundaries for if the feature vector represents a point of view character or not.

A limitation of this study is that different binary classifiers were used for the two feature sets. Ideally, the performance using a range of classifiers for both would have been reported. Our

preliminary results suggested that the classifier choice was not significant. With logistic regression, SVM, and decision trees giving similarly high results for both feature sets.

1.1.5 ?? “Generating Bags of Words from the Sums of their Word Embeddings” (Lyndon White et al. 2016a)

Given the consideration of a sum of word embeddings as dimensionality reduced form of a bag of words a important question is to how recoverable the bag of words is from the sum. A practical way to lower bound the loss of information is to demonstrate a deterministic method that can recover a portion of the bag of words.

We propose as method to extract the original bag of words from a sum of word embeddings. Thus placing a bound on the information lost in the transformation of BOW to SOWE. This is done via a simple greedy algorithm with a correction step. The core of this method functions by iteratively searching the vocabulary of word embeddings for the nearest embedding to the sum, adding it's word to the bag of words and subtracting its embedding from the sum. It is thus only computationally viable with reasonably small vocabularies. This method works as each component word in the sum has a unique directional contribution in the high dimensional space. As one would expect, the works better the higher dimensional the embeddings are, and with fewer words. Even with relatively low dimensions it works quiet well. This shows use that embeddings are not for example constantly cancelling each other in the sum.

Can I comment that "This method would not work as well on a mean of word embeddings", is there something interesting to say about that?

An interesting alternative to this deterministic method would be to train a supervised model to project from SOWE to a fuzzy bag of words. This is similar to the word-content task considered by Adi et al. (2017). In that task a binary classifier was trained to take a sentence representation and a word embedding for a single word that may or may not appear in the sentence.

1.1.6 ?? “Modelling Sentence Generation from Sum of Word Embedding Vectors as a Mixed Integer Programming Problem” (Lyndon White et al. 2016b)

Given that it was demonstrated that the bag of word can be recovered, the obvious follow up question is if we can recover the the sentence. This ?? is a small supplement to ??.

The word ordering problem tackled is given a bag of words, and a trigram language model determine the most-likely order for words. This allows bags of words to be turned into the most likely sentences. We define a deterministic algorithm to solve this using linear mixed integer programming. Using this algorithm we can use the partially recovered bags of words from ?? and determine how frequently they can be correctly ordered to find the original sentence.

We find that surprisingly often they can. The majority of sentences of length up to 18 can be successfully recovered from a SOWE. With, as expected, the longer the sentence the more difficult the recovery. This suggests that the number of likely possible orderings for the words in a sentence is much lower than it may at first seem. Particularly since this method based on a simple trigram language does so well. It no doubt a more sophisticated neural network based language model would be significantly better.

The algorithm used in our method is a minor extension of that of Horvat and Byrne (2014). We take advantage of the slight differences between the word ordering problem and the generalised asymmetric travelling sales man problem. We can eliminate some branches that would not be possibly for a travelling salesman solver; by directly defining it as a mixed integer linear programming problem.

The use of the methods of ?? and ??, together with a system trained to output a approximation to a SOWE, is an interesting, though not really practical, method for natural language generation.

1.2 Some Math

Should I just delete this section? What is it adding?

1.2.1 Word Embeddings

Given a word represented by an integer w , from a vocabulary $\mathbb{V} \subset \mathbb{Z}$, and a matrix of embeddings, represented as C : its embedding can be found by slicing out the w th column: $C_{:,w}$. For \tilde{e}_w the

elementary unit vector, i.e. the one-hot vector representation of w it can be seen that the word embedding can be represented as the product of the embedding matrix with the one-hot vector.

$$C_{:,w} = C \tilde{e}_w$$

1.2.2 Sum of Word Embeddings

For some sequence of (not necessarily unique words) words $\mathcal{W} \in \mathbb{V}^{\mathbb{Z}_0}$ represented $\mathcal{W} = (w^1, w^2, \dots, w^n)$, where w^i is an integer representing which word the i th word is.

The sum of word embeddings (SOWE) representation is written as:

$$\sum_{i=1}^{i=n} C_{:,w^i}$$

The bag of word (BOW) representation is written as a vector from $\mathbb{Z}^{|\mathbb{V}|}$.

$$\tilde{x} = \sum_{i=1}^{i=n} \tilde{e}_{w^i}$$

Using this the sum of word embeddings can be seen to be the product of the embedding matrix with a BOW vector.

$$\sum_{i=1}^{i=n} C_{:,w^i} = \sum_{i=1}^{i=n} C \tilde{e}_{w^i} = C \sum_{i=1}^{i=n} \tilde{e}_{w^i} = C \tilde{x}$$

1.2.3 Mean of Word Embeddings

The mean of word embeddings representation is written as:

$$\frac{1}{n} \sum_{i=1}^{i=n} C_{:,w^i}$$

Note that n is equal to the element-wise sum of the BOW vector (x), i.e. to its l1-norm:

$$n = \|\tilde{x}\|_1 = \sum_{\forall j \in \mathbb{V}} \tilde{x}_j$$

Thus the mean of word embeddings can be seen as the product of the embedding matrix with the l1-normalized BOW vector.

$$\frac{1}{n} \sum_{i=1}^{i=n} C_{:,w^i} = \frac{1}{n} \sum_{i=1}^{i=n} C \tilde{e}_{w^i} = \frac{1}{n} C \sum_{i=1}^{i=n} x = C \frac{\tilde{x}}{\|\tilde{x}\|_1}$$

1.2.4 Linear Combination of Embeddings

The full generalisation of this is that any linear combination of embeddings can be seen as product of the embedding matrix, the a weighted bag of words.

A weighting function for linear combination scheme can be defined, mapping from a given bag of words, and a word, to the weighting of that word. $\alpha : \mathbb{Z}^{|\mathbb{V}|} \times \mathbb{V} \rightarrow \mathbb{R}$.

(For example for the mean of word embeddings $\alpha(\tilde{x}, w) = \frac{1}{\|\tilde{x}\|_1}$.)

From the weighting function, we can evaluated it for a given BOW, for each word in the vocabulary to define a weighting vector $\tilde{\alpha}^{\tilde{x}}$:

$$\tilde{\alpha}^{\tilde{x}} = [\alpha(\tilde{x}, w)]_{w \in \mathbb{V}}$$

Using \odot as the Hadamard (i.e. element-wise) product, we can thus write:

$$\sum_{i=1}^{i=n} \alpha(\tilde{x}, w^i) C_{:,w^i} = C \sum_{i=1}^{i=n} \alpha(\tilde{x}, w^i) \tilde{e}_{w^i} = C (\tilde{\alpha}^{\tilde{x}} \odot \tilde{x})$$

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Part II

Literature Review

Neural Representations of Natural Language

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4 Word Representations

You shall know a word by the company it keeps.

— J.R. Firth, 1957

Word embeddings are the core innovation that has brought machine learning to the forefront of natural language processing. This chapter discusses how one can create a numerical vector that captures the salient features (e.g. semantic meaning) of a word. Discussion begins with the classic language modelling problem. By solving this, using a neural network-based approach, word-embeddings are created. Techniques such as CBOW and skip-gram models (word2vec), and more recent advances in relating this to common linear algebraic reductions on co-locations as discussed. The chapter also includes a detailed discussion of the often confusing hierarchical softmax, and negative sampling techniques. It concludes with a brief look at some other applications and related techniques.

We begin the consideration of the representation of words using neural networks with the work on language modeling. This is not the only place one could begin the consideration: the information retrieval models, such as LSI (Dumais et al. 1988) and LDA (Blei, Ng, and Jordan 2003), based on word co-location with documents would be the other obvious starting point. However, these models are closer to the end point, than they are to the beginning, both chronologically, and in this chapter’s layout. From the language modeling work, comes the contextual (or acausal) language model works such as skip-gram, which in turn lead to the post-neural network co-occurrence based works. These co-occurrence works are more similar to the information retrieval co-location based methods than the probabilis-

The epigraph at the beginning of this section is overused. However, it is obligatory to include it in a work such as this, as it so perfectly sums up why representations useful for language modelling are representations that capture semantics (as well as syntax).

Word Vector or Word Embedding?

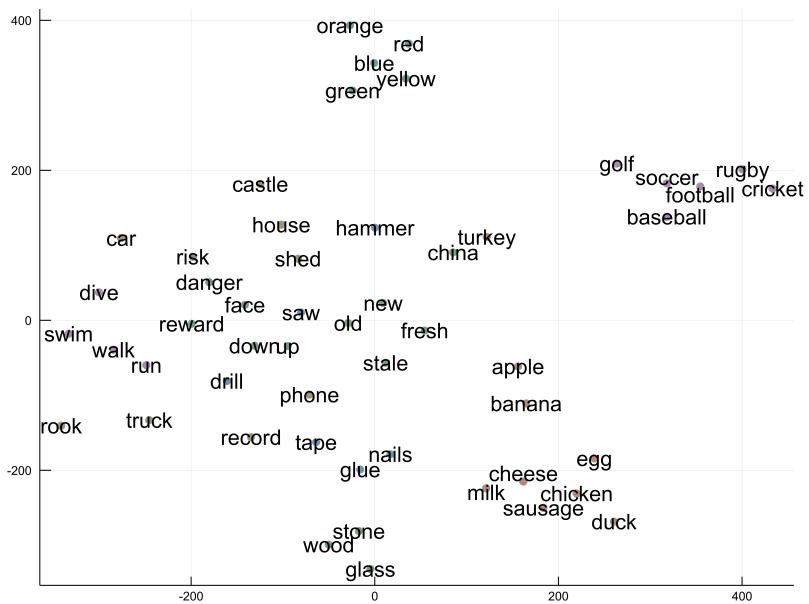
Some literature uses the term *word vector*, or *vector-space model* to refer to representations from LDA and LSA etc. Other works use the terms are used synonymously with *word embedding*. Word embeddings are vectors, in any case.

Dumais et al. (1988), “Using latent semantic analysis to improve access to textual information”

Blei, Ng, and Jordan (2003), “Latent dirichlet allocation”

4 Word Representations

Figure 4.1: Some word embeddings from the FastText project (Bojanowski et al. 2017). They were originally 300 dimensions but have been reduced to 2 using t-SNE (Maaten and Hinton 2008) algorithm. The colors are from 5 manually annotated categories done before this visualisation was produced: foods, sports, colors, tools, other objects, other. Note that many of these words have multiple meanings (see ??), and could fit into multiple categories. Also notice that the information captioned by the unsupervised word embeddings is far finer grained than the manual categorisation. Notice, for example, the separation of ball-sports, from words like run and walk. Not also that china and turkey are together; this no doubt represents that they are both also countries.



tic language modeling methods for word embeddings from which we begin this discussion.

Word embeddings are vector representations of words. An dimensionality reduced scatter plot example of some word embeddings is shown in Figure 4.1.

4.1 Representations for Language Modeling

Probability writing convention

We follow convention that capitalised W^i is a random variable, and w^i is a particular value which W^i may take. The probability of it taking that value would normally be written $P(W^i=w^i)$. We simply write $P(w^i)$ to mean the same thing. This is a common abridged (abuse-of) notation. The random variable in question is implicitly given by the name of its value.

Rosenfeld (2000), "Two decades of statistical

The language modeling task is to predict the next word given the prior words (Rosenfeld 2000). For example, if a sentence begins For lunch I will have a hot, then there is a high probability that the next word will be dog or meal, and lower probabilities of words such as day or are. Mathematically it is formulated as:

$$P(W^i=w^i | W^{i-1}=w^{i-1}, \dots, W^1=w^1) \quad (4.1)$$

or to use the compact notation

$$P(w^i | w^{i-1}, \dots, w^1) \quad (4.2)$$

where W^i is a random variable for the i th word, and w^i is a value (a word) it could, (or does) take. For exam-

4.1 Representations for Language Modeling

ple:

$$P(\text{dog} \mid \text{hot}, \text{a}, \text{want}, \text{I}, \text{lunch}, \text{For})$$

The task is to find the probabilities for the various words that w^i could represent.

The classical approach is trigram statistical language modeling. In this, the number of occurrences of word triples in a corpus is counted. From this joint probability of triples, one can condition upon the first two words, to get a conditional probability of the third. This makes the Markov assumption that the next state depends only on the current state, and that that state can be described by the previous two words. Under this assumption Equation (4.2) becomes:

$$P(w^i \mid w^{i-1}, \dots, w^1) = P(w^i \mid w^{i-1}, w^{i-2}) \quad (4.3)$$

More generally, one can use an n -gram language model where for any value of n , this is simply a matter of defining the Markov state to contain different numbers of words.

This Markov assumption is, of-course, an approximation. In the previous example, a trigram language model finds $P(w^i \mid \text{hot}, \text{a})$. It can be seen that the approximation has lost key information. Based only on the previous 2 words the next word w^i could now reasonably be day, but the sentence: For lunch I will have a hot day makes no sense. However, the Markov assumption in using n -grams is required in order to make the problem tractable – otherwise an unbounded amount of information would need to be stored.

A key issue with n -gram language models is that there exists a data-sparsity problem which causes issues in training them. Particularly for larger values of n . Most combinations of words occur very rarely (Ha et al. 2009). It is thus hard to estimate their occurrence probability. Combinations of words that do not occur in the corpus are naturally given a probability of zero. This is unlikely to be true though – it is simply a matter of rare phrases never occurring in a finite corpus. Several approaches

language modeling: Where do we go from here?"

Maaten and Hinton (2008), "Visualizing data using t-SNE"

Google n-gram corpora

Google has created a very large scale corpora of 1,2,3,4, and 5-grams from over 10^{12} words from the Google Books project. It has been made freely available at <https://books.google.com/ngrams/datasets> (Lin et al. 2012). Large scale n-gram corpora are also used outside of statistical language modeling by corpus linguists investigating the use of language.

Ha et al. (2009), "Extending Zipf's law to n-grams for large corpora"

4 Word Representations

Katz (1987) and Kneser and Ney (1995), “Estimation of probabilities from sparse data for the language model component of a speech recognizer”; “Improved back-off for m-gram language modeling”

An extended look at classical techniques in statistical language modelling can be found in Goodman (2001)

Brown et al. (1992), “Class-based n-gram models of natural language”

have been taken to handle this. The simplest is add-one smoothing which adds an extra “fake” observation to every combination of terms. In common use are various back-off methods (Katz 1987; Kneser and Ney 1995) which use the bigram probabilities to estimate the probabilities of unseen trigrams (and so forth for other n-grams.). However, these methods are merely clever statistical tricks – ways to reassign probability mass to leave some left-over for unseen cases. Back-off is smarter than add-one smoothing, as it portions the probability fairly based on the $(n-1)$ -gram probability. Better still would be a method which can learn to see the common-role of words (Brown et al. 1992). By looking at the fragment: For lunch I want a hot, any reader knows that the next word is most likely going to be a food. We know this for the same reason we know the next word in For elevenses I had a cold . . . is also going to be a food. Even though elevenses is a very rare word, we know from the context that it is a meal (more on this later), and we know it shares other traits with meals, and similarly have / had, and hot / cold. These traits influence the words that can occur after them. Hard-clustering words into groups is nontrivial, particularly given words having multiple meanings, and subtle differences in use. Thus the motivation is for a language modeling method which makes use of these shared properties of the words, but considers them in a flexible soft way. This motivates the need for representations which hold such linguistic information. Such representations must be discoverable from the corpus, as it is beyond reasonable to effectively hard-code suitable feature extractors. This is exactly the kind of task which a neural network achieves implicitly in its internal representations.

4.1.1 The Neural Probabilistic Language Model

Bengio et al. (2003), “A Neural Probabilistic Language Model”

Bengio et al. (2003) present a method that uses a neural network to create a language model. In doing so

4.1 Representations for Language Modeling

it implicitly learns the crucial traits of words, during training. The core mechanism that allowed this was using an embedding or loop-up layer for the input.

4.1.1.1 Simplified Model considered with Input Embeddings

To understand the neural probabilistic language model, let's first consider a simplified neural trigram language model. This model is a simplification of the model introduced by Bengio et al. (2003). It follows the same principles, and highlights the most important idea in neural language representations. This is that of training a vector representation of a word using a lookup table to map a discrete scalar word to a continuous-space vector which becomes the first layer of the network.

The neural trigram probabilistic network is defined by:

$$P(w^i | w^{i-1}, w^{i-2}) = \text{smax} \left(V \varphi \left(U [C_{:,w^{i-1}}; C_{:,w^{i-2}}] + \tilde{b} \right) + \tilde{k} \right) \quad (4.4)$$

where U , V , \tilde{b} , \tilde{k} are the weight matrices and biases of the network. The matrix C defines the embedding table, from which the word embeddings, $C_{:,w^{i-1}}$ and $C_{:,w^{i-2}}$, representing the previous two words (w^{i-1} and w^{i-2}) are retrieved. The network is shown in Figure 4.2

In the neural trigram language model, each of the previous two words is used to look-up a vector from the embedding matrix. These are then concatenated to give a dense, continuous-space input to the above hidden layer. The output layer is a softmax layer, it gives the probabilities for each word in the vocabulary, such that $\hat{y}_{w^i} = P(w^i | w^{i-1}, w^{i-2})$. Thus producing a useful language model.

The word embeddings are trained, just like any other parameter of the network (i.e. the other weights and

Lookup word embeddings: Hashmap or Array?
The question is purely one of implementation. For purposes of the theory, it does not matter if the implementation is using a String to Vector dictionary (e.g. a hashmap), or a 2D array from which a column is indexed-out (sliced-from) via an integer index representing the word. In the tokenization of the source text, it is common to transform all the words into integers, so as to save memory, especially if string interning is not in use. At that point it makes sense to work with an array. For our notational purposes in this book, we will treat the word w^i as if it were an integer index, though thinking of it as a string index into a hashmap changes little in the logic.

$C_{:,w^i}$ not $C_{:,i}$

Note that here we use the word w^i as the index to lookup the word embeddings. i is the index of the word index in the corpus. That is to say that if the i th word, and the j th word are the same: i.e $w^i = w^j$, then they will index out the same vector from C . $w^i = w^j \Rightarrow C_{:,w^i} = C_{:,w^j}$.

One-hot product or Indexed-lookup

4 Word Representations

In some works you may see the process of retrieving the word vector from a matrix of word vectors described as a one-hot multiplication. For a word represented by the index w , where \tilde{e}^w the one-hot vector with a 1 in the w th position, and for C , the table of word embeddings, one can write $C\tilde{e}^w$ to find the embedding for w . We will write $C_{:,w}$ and refer to this as looking up the word vector from the w th column. Of course $C_{:,w} = C\tilde{e}^w$, however in practical implementation the performance ramifications are huge. Matrix column indexing is effectively an $O(1)$ operation (in a column major language), whereas a dense matrix-vector product is $O(n^2)$. The one-hot product can be used in a pinch to support using embeddings in neural network toolkits that do not support lookup/embedding layers. However, we strongly suggest that if your toolkit does not support lookup/embedding layers then it is unsuitable for use in NLP applications. Some tool-kits, e.g. Flux.jl (<https://github.com/FluxML/Flux.jl>), explicitly handle sparse one-hot types, and automatically make this transformation. In that case, it is outright equivalent.

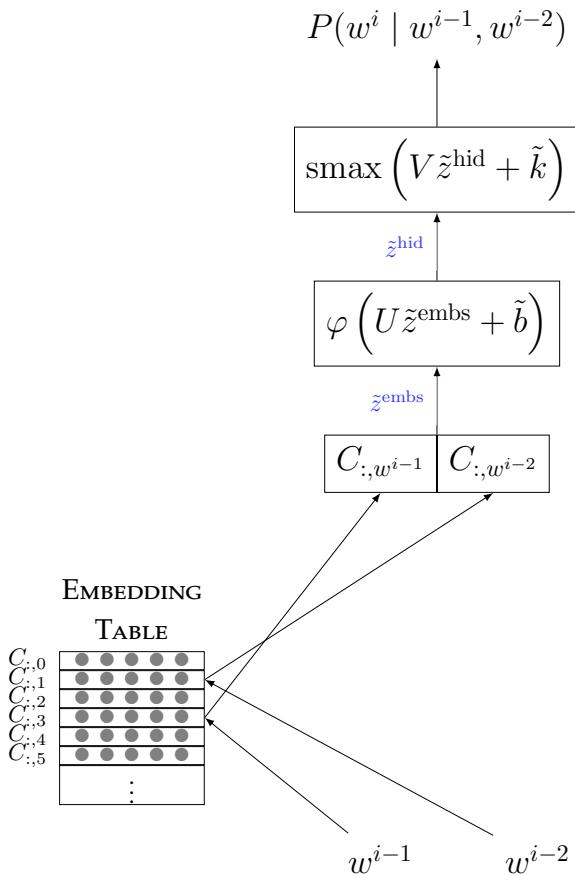


Figure 4.2: The Neural Trigram Language Model

4.1 Representations for Language Modeling

biases) via gradient descent. An effect of this is that the embeddings of words which predict the same future word will be adjusted to be nearer to each other in the vector space. The hidden layer learns to associate information with regions of the embedding space, as the whole network (and every layer) is a continuous function. This effectively allows for information sharing between words. If two word's vectors are close together because they mostly predict the same future words, then that area of the embedding space is associated with predicting those words. If words a and b often occur as the word prior to some similar set of words (w, x, y, \dots) in the training set and word b also often occurs in the training set before word z , but (by chance) a never does, then this neural language model will predict that z is likely to occur after a . Where-as an n-gram language model would not. This is because a and b have similar embeddings, due to predicting a similar set of words. The model has learnt common features about these words implicitly from how they are used, and can use those to make better predictions. These features are stored in the embeddings which are looked up during the input.

4.1.1.2 Simplified Model considered with input and output embeddings

We can actually reinterpret the softmax output layer as also having embeddings. An alternative but equivalent diagram is shown in Figure 4.3.

The final layer of the neural trigram language model can be rewritten per each index corresponding to a possible next word (w^i):

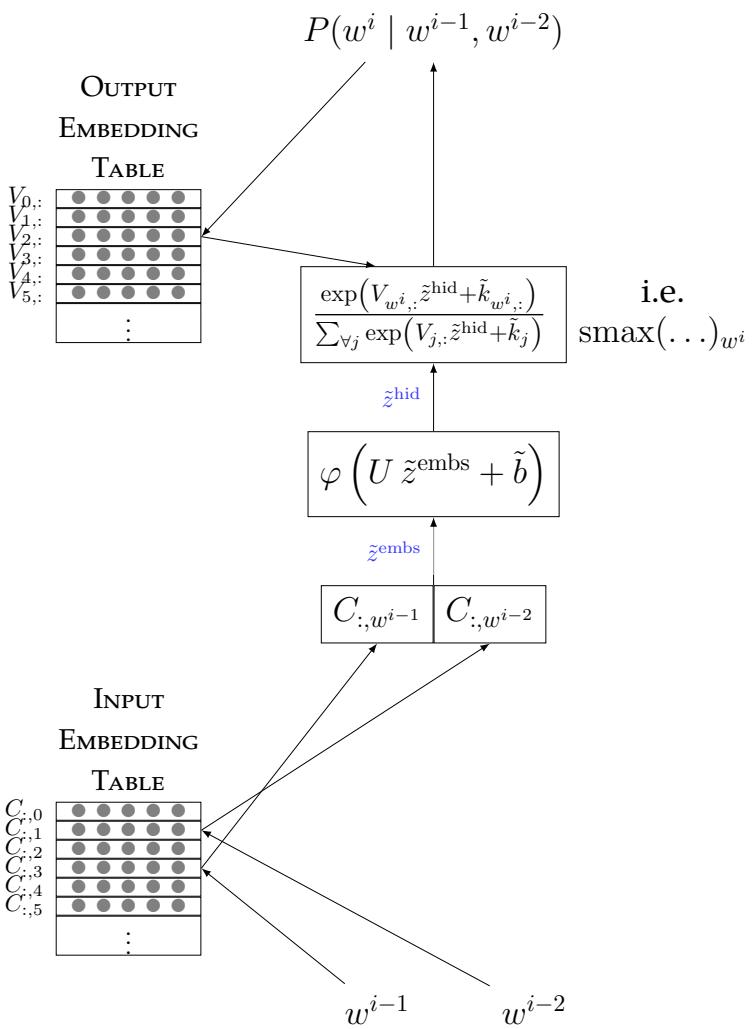
$$\text{smax}(V\tilde{z}^{\text{hid}} + \tilde{k})_{w^i} = \frac{\exp(V_{w^i,:}\tilde{z}^{\text{hid}} + \tilde{k}_{w^i})}{\sum_{\forall j} \exp(V_{j,:}\tilde{z}^{\text{hid}} + \tilde{k}_j)} \quad (4.5)$$

Consider, that the matrix product of a row vector with a column vector is the dot product $V_{w_i,:}\tilde{z}^{\text{hid}}$ can be seen as computing the dot product between the output embedding for w_i and the hidden layer representation of the prior words/context (w^{i-1} and w^{i-2} in this case)

4 Word Representations

in the form of \tilde{z}^{hid} . This leads to an alternate interpretation of the whole process as minimising the dot-product distance between the output embedding and the context representation. This is particularly relevant for the skip-gram model discussed in Section 4.2.2 (with just one input word and no hidden layer).

Figure 4.3: Neural Trigram Language Model as considered with output embeddings. This is mathematically identical to Figure 4.2



4.1 Representations for Language Modeling

In this formulation, we have $V_{w_i,:}$ as the output embedding for w^i . As we considered $C_{:,w_i}$ as its input embedding.

4.1.1.3 Bayes-like Reformulation

When we consider the model with output embeddings, it is natural to also consider it under the light of the Bayes-like reformulation from Section 2.5.1.1:

$$P(Y=i \mid Z=\tilde{z}) = \frac{R(Z=\tilde{z} \mid Y=i) R(Y=i)}{\sum_{\forall j} R(Z=\tilde{z} \mid Y=j) R(Y=j)} \quad (4.6)$$

which in this case is:

$$P(w^i \mid w^{i-1}, w^{i-2}) = \frac{R(Z=\tilde{z}^{\text{hid}} \mid W^i=w^i) R(W^i=w^i)}{\sum_{\forall v \in \mathbb{V}} R(Z=\tilde{z}^{\text{hid}} \mid W^i=v) R(W^i=v)} \quad (4.7)$$

where $\sum_{\forall v \in \mathbb{V}}$ is summing over every possible word v from the vocabulary \mathbb{V} , which does include the case $v = w^i$.

Notice the term:

$$\frac{R(W^i=w^i)}{\sum_{\forall v \in \mathbb{V}} R(W^i=v)} = \frac{\exp(\tilde{k}_{w^i})}{\sum_{\forall v \in \mathbb{V}} \exp(\tilde{k}_v)} \quad (4.8)$$

$$= \frac{1}{\sum_{\forall v \in \mathbb{V}} \exp(\tilde{k}_v - \tilde{k}_{w^i})} \quad (4.9)$$

The term $R(W^i=w^i) = \exp(\tilde{k}_{w^i})$ is linked to the unigram word probabilities: $P(Y=y)$. If $\mathbb{E}(R(Z \mid W_i)) = 1$ then the optimal value for \tilde{k} would be given by the log unigram probabilities: $k_{w^i} = \log P(W^i=w^i)$. This condition is equivalent to if $\mathbb{E}(V\tilde{z}^{\text{hid}}) = 0$. Given that V is normally¹ initialized as a zero mean Gaussian, this

¹no pun intended

4 Word Representations

condition is at least initially true. This suggests, interestingly, that we can predetermine good initial values for the output bias \tilde{k} using the log of the unigram probabilities. In practice this is not required, as it is learnt rapidly by the network during training.

4.1.1.4 The Neural Probabilistic Language Model

Bengio et al. (2003), “A Neural Probabilistic Language Model”

Input vocabulary and output vocabulary do not have to be the same
 Schwenk (2004) suggests using only a subset of the vocabulary as options for the output, while allowing the full vocabulary in the input space – with a fall-back to classical language models for the missed words. This decreases the size of the softmax output layer, which substantially decreases the time taken to train or evaluate the network. As a speed-up technique this is now eclipsed by hierarchical softmax and negative sampling discussed in Section 4.4. The notion of a different input and output vocabulary though remains important for word-sense embeddings as will be discussed in ??.

Schwenk (2004), “Efficient training of large neural networks for language modeling”

Bengio et al. (2003) derived a more advanced version of the neural language model discussed above. Rather than being a trigram language model, it is an n -gram language model, where n is a hyper-parameter of the model. The knowledge sharing allows the data-sparsity issues to be ameliorated, thus allowing for a larger n than in traditional n-gram language models. Bengio et al. (2003) investigated values for 2, 4 and 5 prior words (i.e. a trigram, 5-gram and 6-gram model). The network used in their work was marginally more complex than the trigram neural language model. As shown in Figure 4.4, it features a layer-bypass connection. For n prior words, the model is described by:

$$\begin{aligned} P(w^i | w^{i-1}, \dots, w^{i-n}) = & \text{smax}(\\ & + V \varphi \left(U^{\text{hid}} [C_{:,w^{i-1}}; \dots; C_{:,w^{i-n}}] + \tilde{b} \right) \\ & + U^{\text{bypass}} [C_{:,w^{i-1}}; \dots; C_{:,w^{i-n}}] \\ & + \tilde{k})_{w^i} \end{aligned} \quad (4.10)$$

The layer-bypass is a connivance to aid in the learning. It allows the input to directly affect the output without being mediated by the shared hidden layer. This layer-bypass is an unusual feature, not present in future works deriving from this, such as Schwenk (2004). Though in general it is not an unheard of technique in neural network machine learning.

This is the network which begins the notions of using neural networks with vector representations of words. Bengio et al. focused on the use of the of sliding window of previous words – much like the traditional

4.1 Representations for Language Modeling

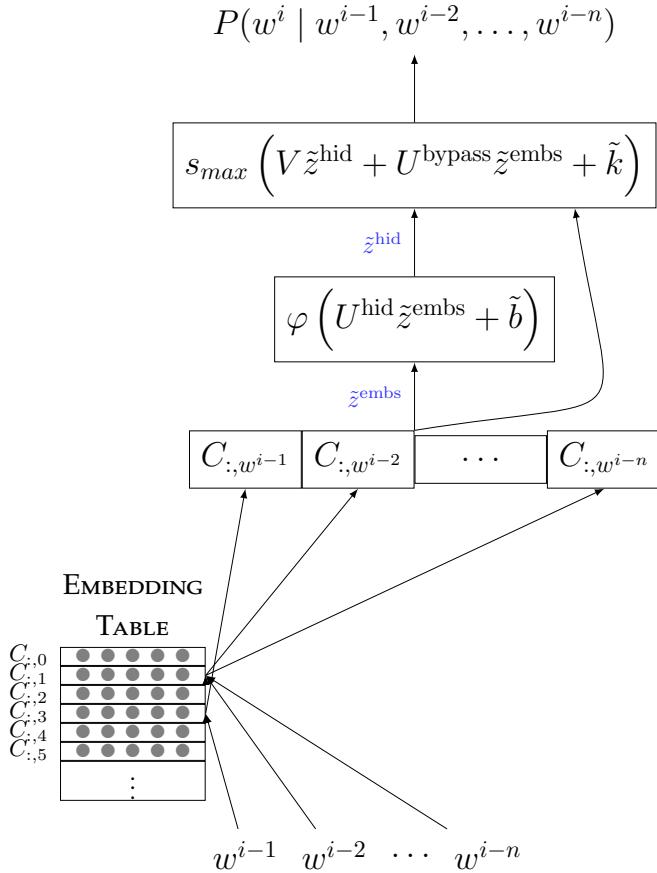


Figure 4.4: Neural Probabilistic Language Model

n-grams. At each time-step the window is advanced forward and the next is word predicted based on the shifted context of prior words. This is of-course exactly identical to extracting all n-grams from the corpus and using those as the training data. They very briefly mention that an RNN could be used in its place.

4.1.2 RNN Language Models

In Mikolov, Karafiat, et al. (2010) an RNN is used for language modelling, as shown in Figure 4.5. Using the terminology of Chapter 3, this is an encoder RNN, made using Basic Recurrent Units. Using an RNN eliminates the Markov assumption of a finite window of prior words forming the state. Instead, the state is learned, and stored in the state component of the RUs.

Mikolov, Karafiat, et al. (2010), "Recurrent neural network based language model."

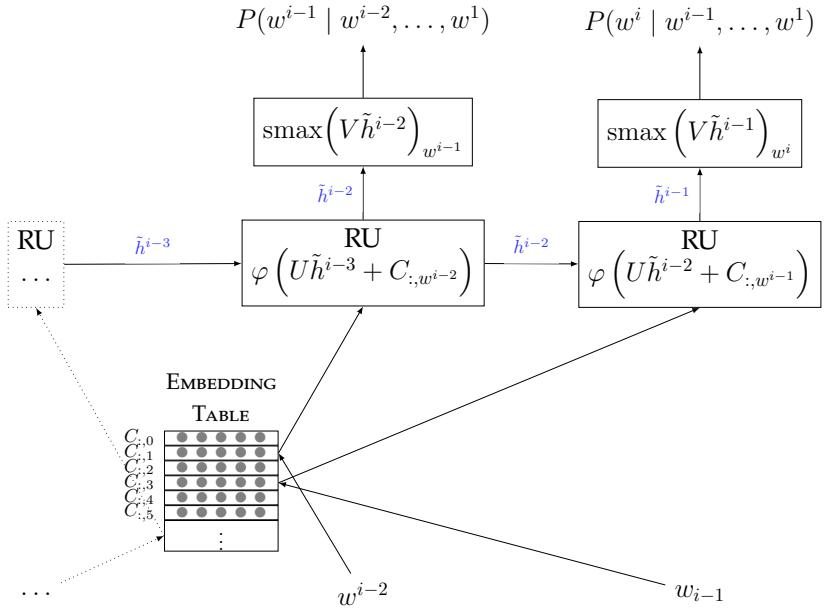
No Bias?

4 Word Representations

It should be noticed that Equations (4.11) and (4.12) are missing the bias terms. This is not commented on in Mikolov, Karafiat, et al. (2010). But in the corresponding chapter of Mikolov’s thesis (Tomas 2012), it is explicitly noted that biases were not used in the network as it was not found that they gave a significant improvement to the result. This is perhaps surprising, particularly in the output softmax layer given the very unbalanced class (unigram) frequencies.

In the papers for several of Mikolov’s other works, including those for skip-gram and CBOW discussed in Section 4.2, the bias terms are also excluded. We have matched those equations here. We do note though, that it is likely that many publicly available implementations of these algorithms would include the bias term: due either to a less close reading of the papers, or to the assumption that the equations are given in *design matrix* form: where the bias is not treated as a separate term to the weights, and the input is padded with an extra 1. We do not think this is at all problematic.

We discuss this further for the case of hierarchical softmax in Section 4.4.1, where the level is a proxy for the unigram frequency – and thus for the bias.



This state \tilde{h}_i being the hidden state (and output as this is a basic RU) from the i time-step. The i th time-step takes as its input the i th word. As usual this hidden layer was an input to the hidden-layer at the next time-step, as well as to the output softmax.

$$\tilde{h}^i = \varphi(U\tilde{h}^{i-1} + C_{:,w_i}) \quad (4.11)$$

$$P(w^i | w^{i-1}, \dots, w^1) = \text{smax}(V\tilde{h}^{i-1})_{w^i} \quad (4.12)$$

Rather than using a basic RU, a more advanced RNN such as a LSTM or GRU-based network can be used. This was done by Sundermeyer, Schlüter, and Ney (2012) and Jozefowicz, Zaremba, and Sutskever (2015), both of whom found that the more advanced networks gave significantly better results.

4.2 Acausal Language Modeling

Figure 4.5: RNN Language Model. The RU equation

The step beyond a normal language model, which uses the prior words to predict the next word, is what we

4.2 Acausal Language Modeling

will term acausal language modelling. Here we use the word acausal in the signal processing sense. It is also sometimes called contextual language modelling, as the whole context is used, not just the prior context. The task here is to predict a missing word, using the words that precede it, as well as the words that come after it.

As it is acausal it cannot be implemented in a real-time system, and for many tasks this renders it less, directly, useful than a normal language model. However, it is very useful as a task to learn a good representation for words.

The several of the works discussed in this section also feature hierarchical softmax and negative sampling methods as alternative output methods. As these are complicated and easily misunderstood topics they are discussed in a more tutorial fashion in Section 4.4. This section will focus just on the language model logic; and assume the output is a normal softmax layer.

4.2.1 Continuous Bag of Words

The continuous bag of words (CBOW) method was introduced by Mikolov, Chen, et al. (2013). In truth, this is not particularly similar to bag of words at all. No more so than any other word representation that does not have regard for order of the context words (e.g. skip-gram, and GloVe).

The CBOW model takes as its input a context window surrounding a central skipped word, and tries to predict the word that it skipped over. It is very similar to earlier discussed neural language models, except that the window is on both sides. It also does not have any non-linearities; and the only hidden layer is the embedding layer.

shown is the basic RU used in Mikolov, Karafiat, et al. (2010). It can be substituted for a LSTM RU or an GRU as was done in Sundermeyer, Schluter, and Ney (2012) and Jozefowicz, Zaremba, and Sutskever (2015), with appropriate changes.

Sundermeyer, Schluter, and Ney (2012), “LSTM neural networks for language modeling”

Jozefowicz, Zaremba, and Sutskever (2015), “An empirical exploration of recurrent network architectures”

Are CBOW & Skip-Gram Neural Networks?

It is sometimes asserted that these models are not in fact neural networks at all. This assertion is often based on their lack of a traditional hidden-layer, and similarities in form to several other mathematical models (discussed in Section 4.3). This distinction is purely academic though. Any toolkit that can handle the prior discussed neural network models can be used to implement CBOW and Skip-Gram, more simply than using a non-neural network focused optimiser.

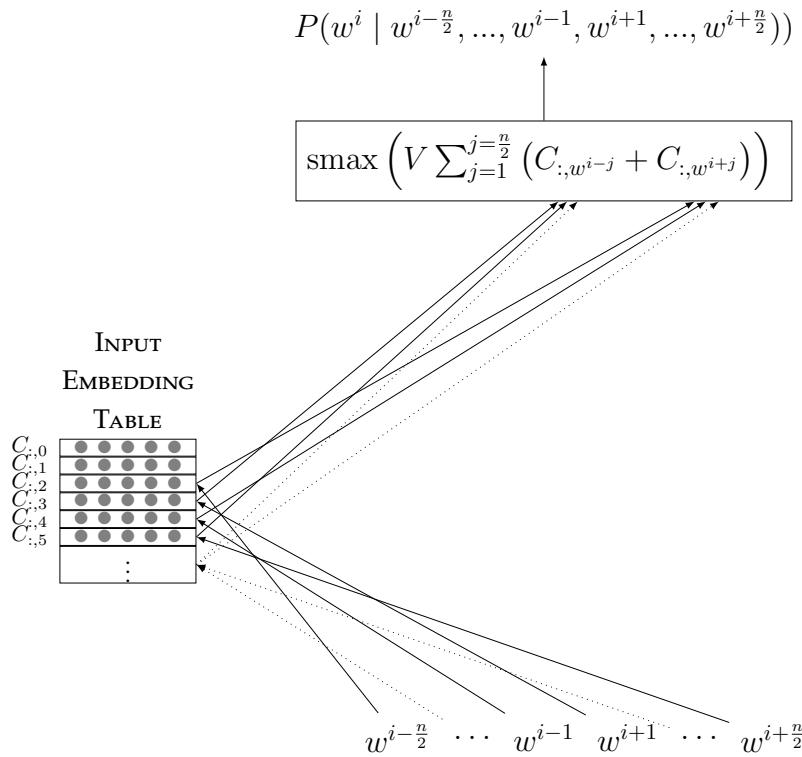
It also should be noted that embedding lookup is functionally an unusual hidden layer – this becomes obvious when considering the lookup as an one-hot product. Though it does lack a non-linear activation function.

Mikolov, Chen, et al. (2013), “Efficient estimation of word

4 Word Representations

representations in vector space”

Figure 4.6: CBOW Language Model



For a context window of width n words – i.e. $\frac{n}{2}$ words to either side, of the target word w^i , the CBOW model is defined by:

$$\begin{aligned} P(w^i | w^{i-\frac{n}{2}}, \dots, w^{i-1}, w^{i+1}, \dots, w^{i+\frac{n}{2}}) \\ = \text{smax} \left(V \sum_{j=i+1}^{j=\frac{n}{2}} (C_{:,w^{i-j}} + C_{:,w^{i+j}}) \right) \end{aligned} \quad (4.13)$$

This is shown in diagrammatic form in Figure 4.6. By optimising across a training dataset, useful word embeddings are found, just like in the normal language model approaches.

4.2.2 Skip-gram

Skip-gram naming

In different publications this model may be called skipgram, skip-gram, skip-gram, skip gram etc. Further, it may be called

The converse of CBOW is the skip-grams model Mikolov, Chen, et al. (2013). In this model, the central word is used to predict the words in the context.

4.2 Acausal Language Modeling

word2vec after the publicly released implementation of the algorithm. Though the word2vec software can also be used for CBOW, so sometimes it can refer to CBOW.

Mikolov, Chen, et al. (2013), “Efficient estimation of word representations in vector space”

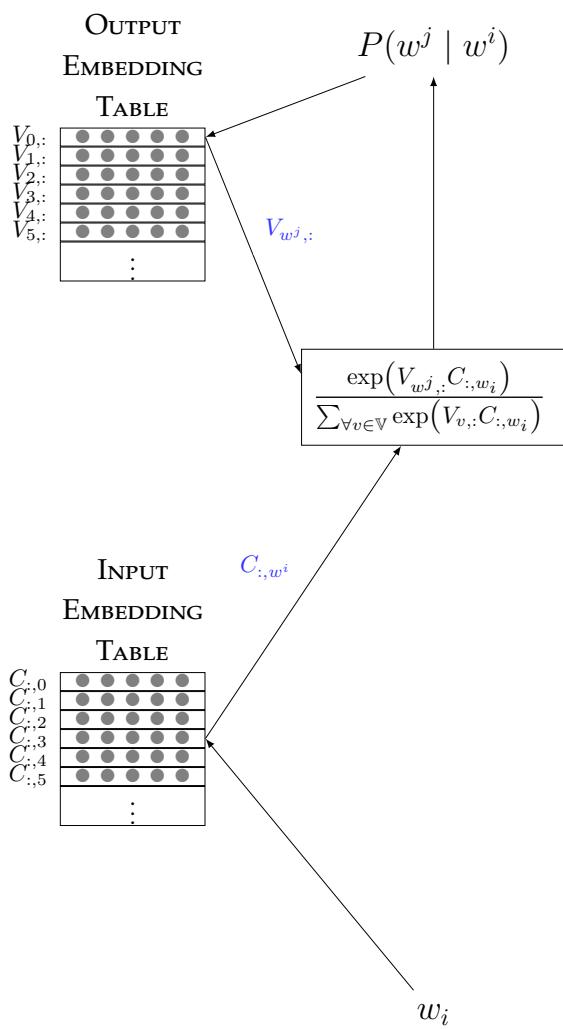


Figure 4.7: Skip-gram language Language Model. Note that the probability $P(w^j | w^i)$ is optimised during training for every w^j in a window around the central word w^i . Note that the final layer in this diagram is just a softmax layer, written in in output embedding form.

4 Word Representations

The model itself is single word input, and its output is a softmax for the probability of each word in the vocabulary occurring in the context of the input word. This can be indexed to get the individual probability of a given word occurring as usual for a language model. So for input word w^i the probability of w^j occurring in its context is given by:

$$P(w^j | w^i) = \text{smax} (V C_{:,w^i})_{w^j} \quad (4.14)$$

The goal, is to maximise the probabilities of all the observed outputs that actually *do* occur in its context. This is done, as in CBOW by defining a window for the context of a word in the training corpus, $(i - \frac{n}{2}, \dots, i - 1, i + 1, \dots, i + \frac{n}{2})$. It should be understood that while this is presented similarly to a classification task, there is no expectation that the model will actually predict the correct result, given that even during training there are multiple correct results. It is a regression to an accurate estimate of the probabilities of co-occurrence (this is true for probabilistic language models more generally, but is particularly obvious in the skip-gram case).

Note that in skip-gram, like CBOW, the only hidden layer is the embedding layer. Rewriting Equation (4.14) in output embedding form:

$$P(w^j | w^i) = \text{smax} (V C_{:,w^i})_{w^j} \quad (4.15)$$

$$P(w^j | w^i) = \frac{\exp(V_{w^j,:} C_{:,w^i})}{\sum_{v \in \mathbb{V}} \exp(V_{v,:} C_{:,v})} \quad (4.16)$$

The key term here is the product $V_{w^j,:} C_{:,w^i}$. The remainder of Equation (4.16) is to normalise this into a probability. Maximising the probability $P(w^j | w^i)$ is equivalent to maximising the dot produce between $V_{w^j,:}$, the output embedding for w^j and $C_{:,w^i}$ the input embedding for w^i . This is to say that the skip-gram probability is maximised when the angular difference between the input embedding for a word, and the output embeddings for its co-occurring words is minimised. The

4.2 Acausal Language Modeling

dot-product is a measure of vector similarity – closely related to the cosine similarity.

Skip-gram is much more commonly used than CBOW.

4.2.3 Analogy Tasks

One of the most notable features of word embeddings is their ability to be used to express analogies using linear algebra. These tasks are keyed around answering the question: b is to a , as what is to c ? For example, a semantic analogy would be answering that Aunt is to Uncle as King is to Queen. A syntactic analogy would be answering that King is to Kings as Queen is to Queens. The latest and largest analogy test set is presented by Gladkova, Drozd, and Matsuoka (2016), which evaluates embeddings on 40 subcategories of knowledge. Analogy completion is not a practical task, but rather serves to illustrate the kinds of information being captured, and the way in which it is represented (in this case linearly).

The analogies work by relating similarities of differences between the word vectors. When evaluating word similarity using word embeddings a number of measures can be employed. By far the cosine similarity is the most common. This is given by

$$\text{sim}(\tilde{u}, \tilde{v}) = \frac{\tilde{u} \cdot \tilde{v}}{\|\tilde{u}\| \|\tilde{v}\|} \quad (4.17)$$

This value becomes higher the closer the word embedding \tilde{u} and \tilde{v} are to each other, ignoring vector magnitude. For word embeddings that are working well, then words with closer embeddings should have correspondingly greater similarity. This similarity could be syntactic, semantic or other. The analogy tasks can help identify what kinds of similarities the embeddings are capturing.

Using the similarity scores, a ranking of words to complete the analogy is found. To find the correct word for

Analogy Tasks uncover prejudice in corpora

Bolukbasi et al. (2016) and Caliskan, Bryson, and Narayanan (2017) use analogy tasks, and related variant formulations to find troubling associations between words, such as Bolukbasi et. al's titular Man is to Computer Programmer, as Woman is to Homemaker. Finding these relationships in the embedding space, indicated that they are present in the training corpus, which in turn shows their prevalence in society at large. It has been observed that machine learning can be a very good mirror upon society.

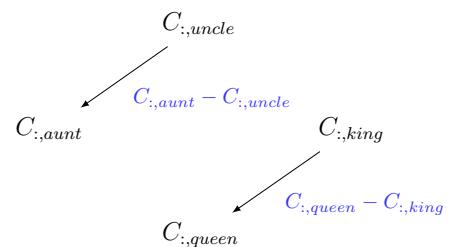
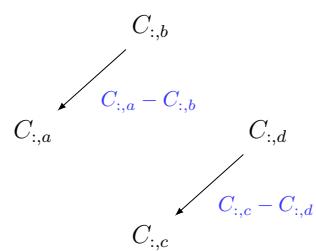


Figure 4.8: Example of analogy algebra



4 Word Representations

Figure 4.9: Vectors involved in analogy ranking tasks, this may help to understand the math in Equation (4.19)

Gladkova, Drozd, and Matsuoka (2016), "Analogy-based detection of morphological and semantic relations with word embeddings: what works and what doesn't."

Pennington, Socher, and Manning (2014), "GloVe: Global Vectors for Word Representation"

d in: d is to c as b is to a the following is computed using the table of embeddings C over the vocabulary \mathbb{V} :

$$\operatorname{argmax}_{\forall d \in \mathbb{V}} \operatorname{sim}(C_{:,d} - C_{:,c}, C_{:,a} - C_{:,b}) \quad (4.18)$$

$$\text{i.e } \operatorname{argmax}_{\forall d \in \mathbb{V}} \operatorname{sim}(C_{:,d}, C_{:,a} - C_{:,b} + C_{:,c}) \quad (4.19)$$

This is shown diagrammatically in Figures 4.8 and 4.9. Sets of embeddings where the vector displacement between analogy terms are more consistent score better.

Initial results in Mikolov, Yih, and Zweig (2013) were relatively poor, but the surprising finding was that this worked at all. Mikolov, Chen, et al. (2013) found that CBOW performed poorly for semantic tasks, but comparatively well for syntactic tasks; skip-gram performed comparatively well for both, though not quite as good in the syntactic tasks as CBOW. Subsequent results found in Pennington, Socher, and Manning (2014) were significantly better again for both.

4.3 Co-location Factorisation

4.3.1 GloVe

Distance weighted co-occurrence and dynamic window sizing

When training skip-gram and CBOW, Mikolov et al. used dynamic window sizing. This meant that if the specified window size was n , in any given training case being considered the actual window size was determined as a random number between 0 and n . Pennington et al. achieve a similar effect by weighting co-occurrences within a window with inverse proportion to the distance between the word. That is to

Skip-gram, like all probabilistic language models, is a intrinsically prediction-based method. It is effectively optimising a neural network to predict which words will co-occur in the with in the range of given by the context window width. That optimisation is carried out per-context window, that is to say the network is updated based on the local co-occurrences. In Pennington, Socher, and Manning (2014) the authors show that if one were to change that optimisation to be global over all co-occurrences, then the optimisation criteria becomes minimising the cross-entropy between the true co-occurrence probabilities, and the value of the embedding product, with the cross entropy measure being weighted by the frequency of the occurrence of

4.3 Co-location Factorisation

the word. That is to say if skip-gram were optimised globally it would be equivalent to minimising:

$$\text{Loss} = - \sum_{\forall w^i \in \mathbb{V}} \sum_{\forall w^j \in \mathbb{V}} X_{w^i, w^j} P(w^j | w^i) \log(V_{w^j, :} C_{:, w^i}) \quad (4.20)$$

for \mathbb{V} being the vocabulary and for X being the a matrix of the true co-occurrence counts, (such that X_{w^i, w^j} is the number of times words w^i and w^j co-occur), and for P being the predicted probability output by the skip-gram.

Minimising this cross-entropy efficiently means factorising the true co-occurrence matrix X , into the input and output embedding matrices C and V , under a particular set of weightings given by the cross entropy measure.

Pennington, Socher, and Manning (2014) propose an approach based on this idea. For each word co-occurrence of w^i and w^j in the vocabulary: they attempt to find optimal values for the embedding tables C , V and the per word biases \tilde{b}, \tilde{k} such that the function $s(w^i, w^j)$ (below) expresses an approximate log-likelihood of w^i and w^j .

$$\text{optimise } s(w^i, w^j) = V_{w^j, :} C_{:, w^i} + \tilde{b}_{w^i} + \tilde{k}_{w^j} \quad (4.21)$$

$$\text{such that } s(w^i, w^j) \approx \log(X_{w^i, w^j}) \quad (4.22)$$

This is done via the minimisation of

$$\text{Loss} = - \sum_{\forall w^i} \sum_{\forall w^j} f(X_{w^i, w^j}) (s(w^i, w^j) - \log(X_{w^i, w^j})) \quad (4.23)$$

Where $f(x)$ is a weighing between 0 and 1 given by:

$$f(x) = \begin{cases} \left(\frac{x}{100}\right)^{0.75} & x < 100 \\ 1 & \text{otherwise} \end{cases} \quad (4.24)$$

This can be considered as a saturating variant of the effective weighing of skip-gram being X_{w^i, w^j} .

While GloVe out-performed skip-gram in initial tests subsequent more extensive testing in Levy, Goldberg,

say if w^i and w^j occur in the same window (i.e. $|i - j| < n$), then rather than contributing 1 to the entry in the co-occurrence count X_{w^i, w^j} , they contribute $\frac{1}{|i - j|}$.

Subsampling, and weight saturation

Skip-gram and CBOW models use a method called subsampling to decrease the effect of common words. The subsampling method is to randomly discard words from training windows based on their unigram frequency. This is closely related to the saturation of the co-occurrence weights as calculated by $f(X)$ used by GloVe. Averaged over all training cases the effect is nearly the same.

Key Factors

Mentioned as Asides

There is an interesting pattern of factors being considered as not part of the core algorithm. We have continued this in the side-notes of this section; with the preceding notes on Distance weighting and subsampling. While the original papers consider these as unimportant to the main thrust of the algorithms Levy, Goldberg, and Dagan (2015) found them to be crucial hyperparameters.

Pennington, Socher, and Manning (2014), "GloVe: Global Vectors for Word Representation"

4 Word Representations

Levy, Goldberg, and Dagan (2015), “Improving Distributional Similarity with Lessons Learned from Word Embeddings”

Implementing GloVe

To implement GloVe in any technical programming language with good support for optimisation is quiet easy, as it is formed into a pure optimization problem. It is also easy to do in a neural network framework, as these always include an optimiser. Though unlike in normal neural network training there are no discrete training cases, just the global co-occurrence statistics.

Levy and Goldberg (2014), “Neural word embedding as implicit matrix factorization”

Li et al. (2015), “Word Embedding Revisited: A New Representation Learning and Explicit Matrix Factorization Perspective.”

Cotterell et al. (2017), “Explaining and Generalizing Skip-Gram through Exponential Family Principal Component Analysis”

Landgraf and Bellay (2017), “word2vec Skip-Gram with Negative Sampling is a Weighted Logistic PCA”

and Dagan (2015) with more tuned parameters, found that skip-gram marginally out-performed GloVe on all tasks.

4.3.2 Further equivalence of Co-location Prediction to Factorisation

GloVe highlights the relationship between the co-located word prediction neural network models, and the more traditional non-negative matrix factorization of co-location counts used in topic modeling. Very similar properties were also explored for skip-grams with negative sampling in Levy and Goldberg (2014) and in Li et al. (2015) with more direct mathematical equivalence to weighed co-occurrence matrix factorisation; Later, Cotterell et al. (2017) showed the equivalence to exponential principal component analysis (PCA). Landgraf and Bellay (2017) goes on to extend this to show that it is a weighted logistic PCA, which is a special case of the exponential PCA. Many works exist in this area now.

4.3.3 Conclusion

We have now concluded that neural predictive co-location models are functionally very similar to matrix factorisation of co-location counts with suitable weightings, and suitable similarity metrics. One might now suggest a variety of word embeddings to be created from a variety of different matrix factorisations with different weightings and constraints. Traditionally large matrix factorisations have significant problems in terms of computational time and memory usage. A common solution to this, in applied mathematics, is to handle the factorisation using an iterative optimisation procedure. Training a neural network, such as skip-gram, is indeed just such an iterative optimisation procedure.

4.4 Hierarchical Softmax and Negative Sampling

4.4 Hierarchical Softmax and Negative Sampling

Hierarchical softmax, and negative sampling are effectively alternative output layers which are computationally cheaper to evaluate than regular softmax. They are powerful methods which pragmatically allow for large speed-up in any task which involves outputting very large classification probabilities – such as language modelling.

4.4.1 Hierarchical Softmax

Hierarchical softmax was first presented in Morin and Bengio (2005). Its recent use was popularised by Mikolov, Chen, et al. (2013), where words are placed as leaves in a Huffman tree, with their depth determined by their frequency.

One of the most expensive parts of training and using a neural language model is to calculate the final softmax layer output. This is because the softmax denominator includes terms for each word in the vocabulary. Even if only one word's probability is to be calculated, one denominator term per word in the vocabulary must be evaluated. In hierarchical softmax, each word (output choice), is considered as a leaf on a binary tree. Each level of the tree roughly halves the space of the output words to be considered. The final level to be evaluated for a given word contains the word's leaf-node and another branch, which may be a leaf-node for another word, or a deeper sub-tree

The tree is normally a Huffman tree (Huffman 1952), as was found to be effective by Mikolov, Chen, et al. (2013). This means that for each word w^i , the word's depth (i.e its code's length) $l(w^i)$ is such that over all words: $\sum_{w^j \in \mathbb{V}} P(w^j) \times l(w^j)$ is minimised. Where $P(w^i)$ is word w^i 's unigram probability, and \mathbb{V} is the

Morin and Bengio (2005),
“Hierarchical probabilistic neural network language model”

Mikolov, Chen, et al. (2013),
“Efficient estimation of word representations in vector space”

SemHuff

It can be noted that the Huffman encoding scheme specifies only the depth of a given word in the tree. It does not specify the order. Yang et al. (2016) make use of the BlossomV algorithm (Kolmogorov 2009) to pair the nodes on each layer according to their similarity. They found that on the language modelling task this improved performance, in the way one would expect. They used a lexical resource to determine similarity, however noted that a prior trained word-embedding model could

4 Word Representations

be used to define similarity instead – the new encoding can then be used to define a new model which will find new (hopefully better) embeddings. This is similar to the original method used by (Morin and Bengio 2005), but only using the similarity measure for re-ordering nodes at the same depth, after the depth is decided by Huffman encoding. In our own experimentation, when applying it to other tasks, we did not see large improvements. It is nevertheless a very interesting idea, and quite fun to implement and observe the results.

Huffman (1952), "A method for the construction of minimum-redundancy codes"

vocabulary. The approximate solution to this is that $l(w^i) \approx -\log_2(P(w^i))$. From the tree, each word can be assigned a code in the usual way, with 0 for example representing taking one branch, and 1 representing the other. Each point in the code corresponds to a node in the binary tree, which has a decision tied to it. This code is used to transform the large multinomial softmax classification into a series of binary logistic classifications. It is important to understand that the layers in the tree are not layers of the neural network in the normal sense – the layers of the tree do not have an output that is used as the input to another. The layers of the tree are rather subsets of the neurons on the output layer, with a relationship imparted on them.

It was noted by Mikolov, Chen, et al. (2013), that for vocabulary \mathbb{V} :

- Using normal softmax would require each evaluation to perform $|\mathbb{V}|$ operations.
- Using hierarchical softmax with a balanced tree, would mean the expected number of operations across all words would be $\log_2(|\mathbb{V}|)$.
- Using a Huffman tree gives the expected number of operations $\sum_{w^j \in \mathbb{V}} -P(w^j) \log_2(P(w^j)) = H(\mathbb{V})$, where $H(\mathbb{V})$ is the unigram entropy of words in the training corpus.

The worse case value for the entropy is $\log_2(|\mathbb{V}|)$. In-fact Huffman encoding is provably optimal in this way. As such this is the minimal number of operations required in the average case.

4.4.1.1 An incredibly gentle introduction to hierarchical softmax

In this section, for brevity, we will ignore the bias component of each decision at each node. It can either be handled nearly identically to the weight; or the matrix

4.4 Hierarchical Softmax and Negative Sampling

can be written in *design matrix form* with an implicitly appended column of ones; or it can even be ignored in the implementation (as was done in Mikolov, Chen, et al. (2013)). The reasoning for being able to ignore it is that the bias in normal softmax encodes unigram probability information; in hierarchical softmax, when used with the common Huffman encoding, its the tree's depth in tree encodes its unigram probability. In this case, not using a bias would at most cause an error proportionate to 2^{-k} , where k is the smallest integer such that $2^{-k} > P(w^i)$.

4.4.1.1 First consider a binary tree with just 1 layer and 2 leaves

and 2 leaves The leaves are n^{00} and n^{01} , each of these leaf nodes corresponds to a word from the vocabulary, which has size two, for this toy example.

From the initial root which we call n^0 , we can go to either node n^{00} or node n^{01} , based on the input from the layer below which we will call \tilde{z} .

Here we write n^{01} to represent the event of the first non-root node being the branch given by following left branch, while n^{01} being to follow the right branch. (The order within the same level is arbitrary in any case, but for our visualisation purposes we'll used this convention.)

We are naming the root node as a notation convenience so we can talk about the decision made at n^0 . Note that $P(n^0) = 1$, as all words include the root-node on their path.

We wish to know the probability of the next node being the left node (i.e. $P(n^{00} | \tilde{z})$) or the right-node (i.e. $P(n^{01} | \tilde{z})$). As these are leaf nodes, the prediction either equivalent to the prediction of one or the other of the two words in our vocabulary.

We could represent the decision with a softmax with two outputs. However, since it is a binary decision, we

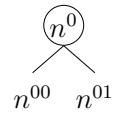


Figure 4.10: Tree for 2 words

4 Word Representations

do not need a softmax, we can just use a sigmoid.

$$P(n^{01} | \tilde{z}) = 1 - P(n^{00} | \tilde{z}) \quad (4.25)$$

The weight matrix for a sigmoid layer has a number of columns governed by the number of outputs. As there is only one output, it is just a row vector. We are going to index it out of a matrix V . For the notation, we will use index 0 as it is associated with the decision at node n^0 . Thus we call it $V_{0,:}$.

$V_{0,:}\tilde{z}$ is a dot product

We mentioned in the marginalia earlier, but just as an extra reminder: the matrix product of a row vector like $V_{0,:}$ with a (column) vector like \tilde{z} is their vector dot product.

$$P(n^{00} | \tilde{z}) = \sigma(V_{0,:}\tilde{z}) \quad (4.26)$$

$$P(n^{01} | \tilde{z}) = 1 - \sigma(V_{0,:}\tilde{z}) \quad (4.27)$$

Note that for the sigmoid function: $1 - \sigma(x) = \sigma(-x)$. Allowing the formulation to be written:

$$P(n^{01} | \tilde{z}) = \sigma(-V_{0,:}\tilde{z}) \quad (4.28)$$

thus

$$P(n^{0i} | \tilde{z}) = \sigma((-1)^i V_{0,:}\tilde{z}) \quad (4.29)$$

Noting that in Equation (4.29), i is either 0 (with $-1^0 = 1$) or 1 (with $-1^1 = -1$).

4.4.1.1.2 Now consider 2 layers with 3 leaves Consider a tree with nodes: $n^0, n^{00}, n^{000}, n^{001}, n^{01}$. The leaves are n^{000}, n^{001} , and n^{01} , each of which represents one of the 3 words from the vocabulary.

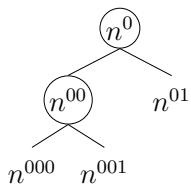


Figure 4.11: Tree for 3 words

$$P(n^{00} | \tilde{z}) = \sigma(V_{0,:}\tilde{z}) \quad (4.30)$$

$$P(n^{01} | \tilde{z}) = \sigma(-V_{0,:}\tilde{z}) \quad (4.31)$$

We must now calculate $P(n^{000} | \tilde{z})$. Another binary decision must be made at node n^{00} . The decision at n^{00} is to find out if the predicted next node is n^{000} or

4.4 Hierarchical Softmax and Negative Sampling

n^{001} . This decision is made, with the assumption that we have reached n^{00} already.

So the decision is defined by $P(n^{000} \mid z, n^{00})$ is given by:

$$P(n^{000} \mid \tilde{z}) = P(n^{000} \mid \tilde{z}, n^{00}) P(n^{00} \mid \tilde{z}) \quad (4.32)$$

$$P(n^{000} \mid \tilde{z}, n^{00}) = \sigma(V_{00,:}\tilde{z}) \quad (4.33)$$

$$P(n^{001} \mid \tilde{z}, n^{00}) = \sigma(-V_{00,:}\tilde{z}) \quad (4.34)$$

We can use the conditional probability chain rule to recombine to compute the three leaf nodes final probabilities.

$$P(n^{01} \mid \tilde{z}) = \sigma(-V_{0,:}\tilde{z}) \quad (4.35)$$

$$P(n^{000} \mid \tilde{z}) = \sigma(V_{00,:}\tilde{z})\sigma(V_{0,:}\tilde{z}) \quad (4.36)$$

$$P(n^{001} \mid \tilde{z}) = \sigma(-V_{00,:}\tilde{z})\sigma(V_{0,:}\tilde{z}) \quad (4.37)$$

4.4.1.1.3 Continuing this logic Using this system, we know that for a node encoded at position $[0t^1t^2t^3 \dots t^L]$, e.g. $[010 \dots 1]$, its probability can be found recursively as:

$$\begin{aligned} P(n^{0t^1 \dots t^L} \mid \tilde{z}) &= \\ P(n^{0t^1 \dots t^L} \mid \tilde{z}, n^{0t^1 \dots t^{L-1}}) P(n^{0t^1 \dots t^{L-1}} \mid \tilde{z}) \end{aligned} \quad (4.38)$$

Thus:

$$P(n^{0t^1} \mid \tilde{z}) = \sigma\left((-1)^{t^1} V_{0,:}\tilde{z}\right) \quad (4.39)$$

$$P(n^{0t^1,t^2} \mid \tilde{z}, n^{0t^1}) = \sigma\left((-1)^{t^2} V_{0t^1,:}\tilde{z}\right) \quad (4.40)$$

$$P(n^{0t^1 \dots t^i} \mid \tilde{z}, n^{0t^1 \dots t^{i-1}}) = \sigma\left((-1)^{t^i} V_{0t^1 \dots t^{i-1},:}\tilde{z}\right) \quad (4.41)$$

The conditional probability chain rule, is applied to get:

$$P(n^{0t^1 \dots t^L} \mid \tilde{z}) = \prod_{i=1}^{i=L} \sigma\left((-1)^{t^i} V_{0t^1 \dots t^{i-1},:}\tilde{z}\right) \quad (4.42)$$

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Combining multiplications

If one wants to find both $V_{00,:}\tilde{z}$ and $V_{0,:}\tilde{z}$, then this can be done using matrices simultaneously, thus potentially taking advantage of optimized matrix multiplication routines.

$$\begin{bmatrix} V_{0,:} \\ V_{00,:} \end{bmatrix} z = \begin{bmatrix} V_{0,:}\tilde{z} \\ V_{00,:}\tilde{z} \end{bmatrix}$$

Thus the whole product for all of the decisions can be written as $V\tilde{z}$. The problem then becomes indexing the relevant node rows.

However computing every single decision is beyond what is required for most uses: hierarchical softmax lets us only compute the decisions that are on the path to the word-leaf we which we wish to query. Computing all of them is beyond what is required.

Packing tree node elements into a matrix with fast indexing is a non-trivial problem. The details on optimising such multiplications and tree packing are beyond the scope of this book.

In general there may be very little scope here for optimisation, as on most hardware (and BLAS systems) matrix products with n columns, takes a similar amount of time to n vector dot products. As such storing the row vectors of V in a hashmap indexed by node-path, and looping over them as required may be more practical.

In languages/libraries with slow looping constructs (numpy, R, octave), where calling into suitable library routines is much faster, this may give some speed-up;

4.4.1.2 Formulation

The formulation above is not the same as in other works. This subsection shows the final steps to reach the conventional form used in Mikolov, Sutskever, et al. (2013).

Here we have determined that the 0th/left branch represents the positive choice, and the other probability is defined in terms of this. It is equivalent to have the 1th/right branch representing the positive choice:

$$P(n^{0t^1\dots t^L} | \tilde{z}) = \prod_{i=1}^{i=L} \sigma((-1)^{t^i+1} V_{0t^1\dots t^{i-1},:}\tilde{z}) \quad (4.43)$$

or to allow it to vary per node: as in the formulation of Mikolov, Sutskever, et al. (2013). In that work they use $ch(n)$ to represent an arbitrary child node of the node

n and use an indicator function $\llbracket a = b \rrbracket = \begin{cases} 1 & a = b \\ -1 & a \neq b \end{cases}$

such that they can write $\llbracket n^b = ch(n^a) \rrbracket$ which will be 1 if n^a is an arbitrary (but consistent) child of n^b , and 0 otherwise.

$$P(n^{0t^1\dots t^L} | \tilde{z}) = \prod_{i=1}^{i=L} \sigma(\llbracket n^{0t^1\dots t^i} = ch(n^{0t^1\dots t^{i-1}}) \rrbracket V_{0t^1\dots t^{i-1},:}\tilde{z}) \quad (4.44)$$

There is no functional difference between the three formulations. Though the final one is perhaps a key reason for the difficulties in understanding the hierarchical softmax algorithm.

4.4.1.3 Loss Function

Using normal softmax, during the training, the cross-entropy between the model's predictions and the ground

4.4 Hierarchical Softmax and Negative Sampling

truth as given in the training set is minimised. Cross entropy is given by

$$CE(P^*, P) = \sum_{\forall w^i \in \mathbb{V}} \sum_{\forall z^j \in \mathbb{Z}} -P^*(w^i | z^j) \log P(w^i | z^j) \quad (4.45)$$

Where P^* is the true distribution, and P is the approximate distribution given by our model (in other sections we have abused notation to use P for both). \mathbb{Z} is the set of values that are input into the model, (or equivalently the values derived from them from lower layers) – the context words in language modelling. \mathbb{V} is the set of outputs, the vocabulary in language modeling. The training dataset \mathcal{X} consists of pairs from $\mathbb{V} \times \mathbb{Z}$.

The true probabilities (from P^*) are implicitly given by the frequency of the training pairs in the training dataset \mathcal{X} .

$$Loss = CE(P^*, P) = \frac{1}{|\mathcal{X}|} \sum_{\forall (w^i, z^i) \in \mathcal{X}} -\log P(w^i | z^i) \quad (4.46)$$

The intuitive understanding of this, is that we are maximising the probability estimate of all pairings which actually occur in the training set, proportionate to how often they occur. Note that the \mathbb{Z} can be non-discrete values, as was the whole benefit of using embeddings, as discussed in Section 4.1.1.

This works identically for hierarchical softmax as for normal softmax. It is simply a matter of substituting in the (different) equations for P . Then applying back-propagation as usual.

4.4.2 Negative Sampling

Negative sampling was introduced in Mikolov, Sutskever, et al. (2013) as another method to speed up this problem.

but even here it is likely to be minor. The time may be better spent writing a C extension library to do this part of the program. Or learning to use a language with fast for loops (e.g. Julia (Bezanson et al. 2014)).

Mikolov, Sutskever, et al. (2013), “Distributed representations of words and phrases and their compositionality”

How does this relate to word vectors?

After the length of this section, one may have forgotten why we are doing this in the first place. Recall that CBOW, skip-gram and all other language modelling based word embedding methods are based around predicting $P(w^o | w^i, \dots, w^j)$ for some words. For skip-gram that is just $P(w^o | w^i)$. The term $n^{0t^1\dots t^L}$ in $P(n^{0t^1\dots t^L} | z)$, just represents as a path through the tree to the leaf node which represents the word w^o . i.e $P(n^{0t^1\dots t^L} | z) = P(w^o | z)$. The output of the final hidden layer is z (i.e. the z is the input to the output layer) In normal language models z encodes all the information about what the model knows of predictions based on w^i, \dots, w^j . z is thus a proxy term in the conditional probability for those words. In skip-gram there is no hidden layer, and it is just $z = C_{:, w^i}$ proxying only for w_i , and the model defines its probability output by $P(w^o | w^i) = P(w^o | C_{:, w^i})$.

The gradient calculations

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They are not fun. They never are for back-propagation. We recommend using a framework with automated differentiation, and/or performing gradient checks against a numerical differentiation tool (simple finite-differencing will do in a pinch).

Mikolov, Sutskever, et al. (2013), "Distributed representations of words and phrases and their compositionality"

Gutmann and Hyvärinen (2012), "Noise-contrastive estimation of unnormalized statistical models, with applications to natural image statistics"

Much like hierarchical softmax in its purpose. However, negative sampling does not modify the network's output, but rather the loss function.

Negative Sampling is a simplification of Noise Contrast Estimation (Gutmann and Hyvärinen 2012). Unlike Noise Contrast Estimation (and unlike softmax), it does not in fact result in the model converging to the same output as if it were trained with softmax and cross-entropy loss. However the goal with these word embeddings is not to actually perform the language modelling task, but only to capture a high-quality vector representation of the words involved.

4.4.2.1 A Motivation of Negative Sampling

Recall from Section 4.2.2 that the (supposed) goal, is to estimate $P(w^j | w^i)$. In truth, the goal is just to get a good representation, but that is achieved via optimising the model to predict the words. In Section 4.2.2 we considered the representation of $P(w^j | w^i)$ as the w^j th element of the softmax output.

$$P(w^j | w^i) = \text{smax}(V C_{:,w^i})_{w^j} \quad (4.47)$$

$$P(w^j | w^i) = \frac{\exp(V_{w^j,:} C_{:,w^i})}{\sum_{k=1}^N \exp(V_{k,:} C_{:,k})} \quad (4.48)$$

Why is not using softmax wrong?

The notation abuse may be hiding just how bad it is to not use softmax. Recall that the true meaning of $P(w^j | w^i)$ is actually $P(W^j=w^j | W^i=w^i)$. By not using softmax, with its normalising denominator this means that: $\sum_{\forall w^j \in \mathcal{V}} P(w^j | w^i) \neq 1$ (except by coincidence).

This is not the only valid representation. One could use a sigmoid neuron for a direct answer to the co-location probability of w^j occurring near w^i . Though this would throw away the promise of the probability distribution to sum to one across all possible words that could be co-located with w^i . That promise could be enforced by other constraints during training, but in this case it will not be. It is a valid probability if one does not consider it as a single categorical prediction, but rather as independent predictions.

4.4 Hierarchical Softmax and Negative Sampling

$$P(w^j | w^i) = \sigma(V C_{:,w^i})_{w^j} \quad (4.49)$$

$$\text{i.e. } P(w^j | w^i) = \sigma(V_{w^j,:} C_{:,w^i}) \quad (4.50)$$

Lets start from the cross-entropy loss. In training word w^j does occur near w^i , we know this because they are a training pair presented from the training dataset \mathcal{X} . Therefore, since it occurs, we could make a loss function based on minimising the negative log-likelihood of all observations.

$$\text{Loss} = \sum_{\forall (w^i, w^j) \in \mathcal{X}} -\log P(w^j | w^i) \quad (4.51)$$

This is the cross-entropy loss, excluding the scaling factor for how often it occurs.

However, we are not using softmax in the model output, which means that there is no trade off for increasing (for example) $P(w^1 | w^i)$ vs $P(w^2 | w^i)$. This thus admits the trivially optimal solution $\forall w^j \in \mathbb{V} P(w^j | w^i) = 1$. This is obviously wrong – even beyond not being a proper distribution – some words are more commonly co-occurring than others.

So from this we can improve the statement. What is desired from the loss function is to reward models that predict the probability of words that *do* co-occur as being higher, than the probability of words that *do not*. We know that w^j does occur near w^i as it is in the training set. Now, let us select via some arbitrary means a w^k that does not – a negative sample. We want the loss function to be such that $P(w^k | w^i) < P(w^j | w^i)$. So for this single term in the loss we would have:

$$\text{loss}(w^j, w^i) = \log P(w^k | w^i) - \log P(w^j | w^i) \quad (4.52)$$

The question is then: how is the negative sample w^k to be found? One option would be to deterministically search the corpus for these negative samples, making sure to never select words that actually do co-occur. However that would require enumerating the entire

Loss Function

Readers may want to reread Section 4.4.1.3 to brush up on how we use the training dataset as a ground truth probability estimate implicitly when using cross-entropy loss. When doing so one should remember that that the conditioning term, z , for skip-grams is the co-located words as there is no hidden layer.

Most words

do not co-occur

Some simple reasoning can account for this as a reasonable consequence of Zipf's law (Zipf 1949) and a prior of

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the principle of indifference, but there is a further depth to it as explained by Ha et al. (2009).

Is Equation (4.53) a function?

No, at the point at which the Loss started including randomly selected samples, it ceased to be a function in the usual mathematical sense. It is still a function in the common computer programming sense though – it is just not deterministic.

corpus. We can instead just pick them randomly, we can sample from the unigram distribution. As statistically, in any given corpus most words do not co-occur, a randomly selected word in all likelihood will not be one that truly does co-occur – and if it is, then that small mistake will vanish as noise in the training, overcome by all the correct truly negative samples.

At this point, we can question, why limit ourselves to one negative sample? We could take many, and do several at a time, and get more confidence that $P(w^j | w^i)$ is indeed greater than other (non-existent) co-occurrence probabilities. This gives the improved loss function of

$$\text{loss}(w^j, w^i) = \left(\sum_{\forall w^k \in \text{samples}(D^{1g})} \log P(w^k | w^i) \right) - \log P(w^j | w^i) \quad (4.53)$$

where D^{1g} stands for the unigram distribution of the vocabulary and $\text{samples}(D^{1g})$ is a function that returns some number of samples from it.

Consider, though is this fair to the samples? We are taking them as representatives of all words that do not co-occur. Should a word that is unlikely to occur at all, *but was unlucky enough to be sampled*, contribute the same to the loss as a word that was very likely to occur? More reasonable is that the loss contribution should be in proportion to how likely the samples were to occur. Otherwise it will add unexpected changes and result in noisy training. Adding a weighting based on the unigram probability ($P^{1g}(w^k)$) gives:

$$\text{loss}(w^j, w^i) = \left(\sum_{\forall w^k \in \text{samples}(D^{1g})} P^{1g}(w^k) \log P(w^k | w^i) \right) - \log P(w^j | w^i) \quad (4.54)$$

4.4 Hierarchical Softmax and Negative Sampling

The expected value is defined by

$$\mathbb{E}_{X \sim D} [f(x)] = \sum_{\forall x \text{ values for } X} P^d f(x) \quad (4.55)$$

In an abuse of notation, we apply this to the samples, as a sample expected value and write:

$$\sum_{k=1}^{k=n} \mathbb{E}_{w^k \sim D^{1g}} [\log P(w^k | w^i)] \quad (4.56)$$

to be the sum of the n samples expected values. This notation (abuse) is as used in Mikolov, Sutskever, et al. (2013). It gives the form:

$$\text{loss}(w^j, w^i) = \left(\sum_{k=1}^{k=n} \mathbb{E}_{w^k \sim D^{1g}} [\log P(w^k | w^i)] \right) - \log P(w^j | w^i) \quad (4.57)$$

Mikolov, Sutskever, et al. (2013), "Distributed representations of words and phrases and their compositionality"

Consider that the choice of unigram distribution for the negative samples is not the only choice. For example, we might wish to increase the relative occurrence of rare words in the negative samples, to help them fit better from limited training data. This is commonly done via subsampling in the positive samples (i.e. the training cases)). So we replace D^{1g} with D^{ns} being the distribution of negative samples from the vocabulary, to be specified as a hyper-parameter of training.

Mikolov, Sutskever, et al. (2013) uses a distribution such that

$$P^{D^{ns}}(w^k) = \frac{P^{D^{1g}}(w^k)^{\frac{2}{3}}}{\sum_{\forall w^o \in \mathbb{V}} P^{D^{1g}}(w^o)^{\frac{2}{3}}} \quad (4.58)$$

which they find to give better performance than the unigram or uniform distributions.

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Using this, and substituting in the sigmoid for the probabilities, this becomes:

$$\begin{aligned} \text{loss}(w^j, w^i) = & \\ & \left(\sum_{k=1}^{k=n} \mathbb{E}_{w^k \sim D^{\text{ns}}} [\log \sigma(V_{w^k,:} C_{:,w^i})] \right) - \log \sigma(V_{w^j,:} C_{:,w^i}) \end{aligned} \quad (4.59)$$

By adding a constant we do not change the optimal value. If we add the constant $-K$, we can subtract 1 in each sample term.

$$\begin{aligned} \text{loss}(w^j, w^i) = & \\ & \left(\sum_{k=1}^{k=n} \mathbb{E}_{w^k \sim D^{\text{ns}}} [-1 + \log \sigma(V_{w^k,:} C_{:,w^i})] \right) - \log \sigma(V_{w^j,:} C_{:,w^i}) \end{aligned} \quad (4.60)$$

Finally we make use of the identity $1 - \sigma(\tilde{z}) = \sigma(-\tilde{z})$ giving:

$$\begin{aligned} \text{loss}(w^j, w^i) = & \\ & - \log \sigma(V_{w^j,:} C_{:,w^i}) - \sum_{k=1}^{k=n} \mathbb{E}_{w^k \sim D^{\text{ns}}} [\log \sigma(-V_{w^k,:} C_{:,w^i})] \end{aligned} \quad (4.61)$$

Calculating the total loss over the training set \mathcal{X} :

$$\begin{aligned} \text{Loss} = & - \sum_{\forall (w^i, w^j) \in \mathcal{X}} \\ & \left(\log \sigma(V_{w^j,:} C_{:,w^i}) + \sum_{k=1}^{k=n} \mathbb{E}_{w^k \sim D^{\text{ns}}} [\log \sigma(-V_{w^k,:} C_{:,w^i})] \right) \end{aligned} \quad (4.62)$$

This is the negative sampling loss function used in Mikolov, Sutskever, et al. (2013). Perhaps the most confusing part of this is the notation. Without the abuses

4.5 Natural Language Applications – beyond language modeling

around expected value, this is written:

$$\begin{aligned} Loss = & - \sum_{\forall (w^i, w^j) \in \mathcal{X}} \\ & \left(\log \sigma(V_{w^j,:} C_{:,w^i}) + \sum_{\forall w^k \in \text{samples}(D^{\text{ns}})} P^{\text{D}^{\text{ns}}}(w^k) \log \sigma(-V_{w^k,:} C_{:,w^i}) \right) \end{aligned} \quad (4.63)$$

4.5 Natural Language Applications – beyond language modeling

While statistical language models are useful, they are of-course in no way the be-all and end-all of natural language processing. Simultaneously with the developments around representations for the language modelling tasks, work was being done on solving other NLP problems using similar techniques (Collobert and Weston 2008).

Collobert and Weston (2008), "A unified architecture for natural language processing: Deep neural networks with multitask learning"

4.5.1 Using Word Embeddings as Features

Turian, Ratinov, and Bengio (2010) discuss what is now perhaps the most important use of word embeddings. The use of the embeddings as features, in unrelated feature driven models. One can find word embeddings using any of the methods discussed above. These embeddings can be then used as features instead of, for example bag of words or hand-crafted feature sets. Turian, Ratinov, and Bengio (2010) found improvements on the state of the art for chunking and Named Entity Recognition (NER), using the word embedding methods of that time. Since then, these results have been superseded again using newer methods.

Pretrained

Word-Embeddings

Pretrained Word Embeddings are available for most models discussed here. They are trained on a lot more data than most people have reasonable access to. It can be useful to substitute word embeddings as a representation in most systems, or to use them as initial value for neural network systems that will learn them as they train the system as a whole. There are many many

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online pretrained word embeddings. One of the more recent and comprehensive set is that of Bojanowski et al. (2017) (based on a skip-gram extension), <https://fasttext.cc/docs/en/pretrained-vectors.html>. They provide embeddings for 294 languages, trained on Wikipedia based on the work of which is an extension to skip-grams.

Turian, Ratinov, and Bengio (2010), "Word representations: a simple and general method for semi-supervised learning"

Fu et al. (2016), "Efficient and Distributed Algorithms for Large-Scale Generalized Canonical Correlations Analysis"

Bojanowski et al. (2017), "Enriching Word Vectors with Subword Information"

4.6 Aligning Vector Spaces Across Languages

Given two vocabulary vector spaces, for example one for German and one for English, a natural and common question is if they can be aligned such that one has a single vector space for both. Using canonical correlation analysis (CCA) one can do exactly that. There also exists generalised CCA for any number of vector spaces (Fu et al. 2016), as well as kernel CCA for a non-linear alignment.

The inputs to CCA, are two sets of vectors, normally expressed as matrices. We will call these: $C \in \mathbb{R}^{n^C \times m^C}$ and $V \in \mathbb{R}^{n^V \times m^V}$. They are both sets of vector representations, not necessarily of the same dimensionality. They could be the output of any of the embedding models discussed earlier, or even a sparse (non-embedding) representations such as the point-wise mutual information of the co-occurrence counts. The other input is series pairs of elements from within those sets that are to be aligned. We will call the elements from that series of pairs from the original sets C^* and V^* respectively. C^* and V^* are subsets of the original sets, with the same number of representations. In the example of applying this to translation, if each vector was a word embedding: C^* and V^* would contain only words with a single known best translation, and this does not have to be the whole vocabulary of either language.

By performing CCA one solves to find a series of vectors (also expressed as a matrix), $S = [\tilde{s}^1 \dots \tilde{s}^d]$ and $T = [\tilde{t}^1 \dots \tilde{t}^d]$, such that the correlation between $C^* \tilde{s}^i$ and $V^* \tilde{t}^i$ is maximised, with the constraint that for all $j < i$ that $C^* \tilde{s}^i$ is uncorrelated with $C^* \tilde{s}^j$ and that $V^* \tilde{t}^i$ is uncorrelated with $V^* \tilde{t}^j$. This is very similar to principal component analysis (PCA), and like PCA the number of components to use (d) is a variable which can be decreased to achieve dimensionality reduction. When complete, taking S and T as matrices gives pro-

4.6 Aligning Vector Spaces Across Languages

jection matrices which project C and V to a space where aligned elements are as correlated as possible. The new common vector space embeddings are given by: CS and VT . Even for sparse inputs the outputs will be dense embeddings.

Faruqui and Dyer (2014) investigated this primarily as a means to use additional data to improve performance on monolingual tasks. In this, they found a small and inconsistent improvement. However, we suggest it is much more interesting as a multi-lingual tool. It allows similarity measures to be made between words of different languages. Gujral, Khayrallah, and Koehn (2016) use this as part of a hybrid system to translate out of vocabulary words. Klein et al. (2015) use it to link word-embeddings with image embeddings.

Dhillon, Foster, and Ungar (2011) investigated using this to create word-embeddings. We noted in Equation (4.16), that skip-gram maximise the similarity of the output and input embeddings according to the dot-product. CCA also maximises similarity (according the correlation), between the vectors from one set, and the vectors for another. As such given representations for two words from the same context, initialised randomly, CCA could be used repeatedly to optimise towards good word embedding capturing shared meaning from contexts. This principle was used by Dhillon, Foster, and Ungar (2011), though their final process more complex than described here. It is perhaps one of the more unusual ways to create word embeddings as compared to any of the methods discussed earlier.

Aligning embeddings using linear algebra after they are fully trained is not the only means to end up with a common vector space. One can also directly train embeddings on multiple languages concurrently as was done in Shi et al. (2015), amongst others. Similarly, on the sentence embedding side Zou et al. (2013), and Socher et al. (2014) train embeddings from different languages and modalities (respectively) directly to be near to their partners (these are discussed in Chapter 6). A

Gujral, Khayrallah, and Koehn (2016), "Translation of Unknown Words in Low Resource Languages"

Klein et al. (2015), "Associating neural word embeddings with deep image representations using fisher vectors"

Dhillon, Foster, and Ungar (2011), "Multi-view learning of word embeddings via cca"

Dhillon, Foster, and Ungar (2011), "Multi-view learning of word embeddings via cca"

Shi et al. (2015), "Learning Cross-lingual Word Embeddings via Matrix Co-factorization."

Socher et al. (2014), "Grounded compositional

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semantics for finding and
describing images with
sentences”

Ruder (2017), “A survey
of cross-lingual embedding
models”

survey paper on such methods was recently published by Ruder (2017).

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5 Word Sense Representations

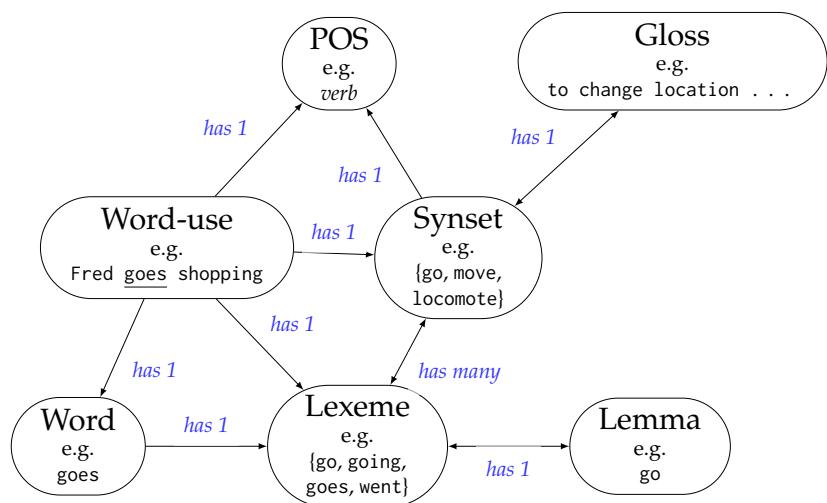
- 1a.** *In a literal, exact, or actual sense; not figuratively, allegorically, etc.*
- 1b.** *Used to indicate that the following word or phrase must be taken in its literal sense, usually to add emphasis.*
- 1c.** *colloq. Used to indicate that some (frequently conventional) metaphorical or hyperbolical expression is to be taken in the strongest admissible sense: 'virtually, as good as'; (also) 'completely, utterly, absolutely' ...*
- 2a** *With reference to a version of something, as a transcription, translation, etc.: in the very words, word for word.*
- 2b.** *In extended use. With exact fidelity of representation; faithfully.*
- 3a.** *With or by the letters (of a word). Obs. rare.*
- 3b.** *In or with regard to letters or literature. Obs. rare.*

— the seven senses of literally, *Oxford English Dictionary*, 3rd ed., 2011

In this chapter, techniques for representing the multiple meanings of a single word are discussed. This is a growing area, and is particularly important in languages where polysemous and homonymous words are common. This includes English, but it is even more prevalent in Mandarin for example. The techniques discussed can broadly be classified as lexical word sense representation, and as word sense induction. The inductive techniques can be sub-classified as clustering-based or as prediction-based.

5 Word Sense Representations

Figure 5.1: The relationship between terms used to discuss various word sense problems. The lemma is used as the representation for the lexeme, for WordNet's purposes when indexing. For many tasks each the word-use is pre-tagged with its lemma and POS tag, as these can be found with high reliability using standard tools. Note that the arrows in this diagram are *directional*. That is to say, for example, each Synset has 1 POS, but each POS has many Synsets.



5.1 Word Senses

Words have multiple meanings. A single representation for a word cannot truly describe the correct meaning in all contexts. It may have some features that are applicable to some uses but not to others, it may be an average of all features for all uses, or it may only represent the most common sense. For most word-embeddings it will be an unclear combination of all of the above. Word sense embeddings attempt to find representations not of words, but of particular senses of words.

Polysemous/Homonymous
A word with multiple meanings i.e. senses. For NLP representational purposes polysemous and homonymous are synonymous.

Part of Speech/POS
The syntactic category a word belongs to. Different POS tags come from different tag sets. Can be simple as the WordNet tag set: noun, adjective, verb, etc. or complex as in the Brown tag set: VBG-verb,

The standard way to assign word senses is via some lexicographical resource, such as a dictionary, or a thesaurus. There is not a canonical list of word senses that are consistently defined in English. Every dictionary is unique, with different definitions and numbers of word senses. The most commonly used lexicographical resource is WordNet (Miller 1995), and the multi-lingual BabelNet (Navigli and Ponzetto 2010). The relationship between the terminology used in word sense problems is shown in Figure 5.1

5.1 Word Senses

5.1.1 Word Sense Disambiguation

Word sense disambiguation is one of the hardest problems in NLP. Very few systems significantly outperform the baseline, i.e. the most frequent sense (MFS) technique.

Progress on the problem is made difficult by several factors.

The sense is hard to identify from the context. Determining the sense may require very long range information: for example the information on context may not even be in the same sentence. It may require knowing the domain of the text, because word sense uses vary between domains. Such information is external to the text itself. It may in-fact be intentionally unclear, with multiple correct interpretations, as in a pun. It maybe unintentionally unknowable, due to a poor writing style, such that it would confuse any human reader. These difficulties are compounded by the limited amount of data available.

There is only a relatively small amount of labelled data for word sense problems. It is the general virtue of machine learning that given enough data, almost any input-output mapping problem (i.e. function approximation) can be solved. Such an amount of word sense annotated data is not available. This is in contrast to finding unsupervised word embeddings, which can be trained on any text that has ever been written. The lack of very large scale training corpora renders fully supervised methods difficult. It also results in small sized testing corpora; which leads to systems that may appear to perform well (on those small test corpora), but do not generalise to real world uses. In addition, the lack of human agreement on the correct sense, resulting in weak ground truth, further makes creating new resources harder. This limited amount of data compounds the problem's inherent difficulties.

*gerund/present participle,
NN- noun, singular or mass.*

Word-use

An occurrence of a word in a text, such as a training corpus. Each word will have multiple uses in a text. Each word-use will only have one particular meaning and will thus belong to one synset.

Lemma

The base form of the word as defined by a lexicographical resource. It is normally closely related to (often identical to) the stem which is the word's root form with all morphological inflections (e.g. tenses) removed.

Lexeme

The set of words that share a common lemma: go, going, goes, and went all belong to the lexeme headed by the lemma go

Synset

A synset is a set of synonymous words: that is words that have the same meaning. In lexicographic terms the synset is the core unit of meaning. Identifying the synset of a word-use is the same as identifying the word sense. Every word sense corresponds to one synset.

Gloss

A gloss is the dictionary entry for a word sense, it normally includes both the definition and an example of use. In WordNet each synset shares a common gloss.

Lemmatization

5 Word Sense Representations

Lemmatization is the method of converting a word into its lemma. Due to the similarity of the lemma to the stem, this in essence means removing the tense and plurality information (stemming), with some additional special-cases. WordNet is indexed by lemmas, and comes with a lemmatizer called `morphy` allowing any word to be looked up by lemmatizing it to its lemma.

Unlemmatization

Given a lemma (as one can extract from WordNet) and a full POS tag (such as a Brown-style tag) for a word, it is possible to undo the lemmatization with a high degree of reliability using relatively simple rules (again due to the similarity of the lemma to the stem). The POS tag encodes the key inflectional features that are lost. `Patten.en` (De Smedt and Daelemans 2012) is a python library encoding such rules (pluralisation, verb conjugation, etc.); though combining them with the POS tag to drive them is a task left for the reader. This can be used to find substitute words using WordNet's features, for finding synonyms, antonyms and other lemmas from lexically related categories.

Miller (1995), "WordNet: a lexical database for English"

Navigli and Ponzetto (2010), "BabelNet: Building a very large multilingual semantic network"

It can also be said that word senses are highly artificial and do not adequately represent meaning. However, WSD is required to interface with lexicographical resources, such as translation dictionaries (e.g. BabelNet), ontologies (e.g. OpenCyc), and other datasets (e.g. ImageNet (Deng et al. 2009)).

It may be interesting to note, that the number of meanings that a word has is approximately inversely proportional related to its frequency of use rank (G. K. Zipf 1945). That is to say the most common words have far more meanings than rarer words. It is related to (and compounds with) the more well-known Zipf's Law on word use (G. Zipf 1949), and can similarly be explained-based on Zipf's core premise of the principle of least effort. This aligns well with our notion that precise (e.g. technical) words exist but are used only infrequently – since they are only explaining a single situation. This also means that by most word-uses are potentially very ambiguous.

The most commonly used word sense (for a given word) is also overwhelmingly more frequent than its less common brethren – word sense usage also being roughly Zipfian distributed (Kilgarriff 2004). For this reason the Most Frequent Sense (MFS) is a surprisingly hard baseline to beat in any WSD task.

5.1.1.1 Most Frequent Sense

Given a sense annotated corpus, it is easy to count how often each sense of a word occurs. Due to the overwhelming frequency of the most frequent sense, it is unlikely for even a small training corpus to have the most frequent sense differing from the use in the language as a whole.

The Most Frequent Sense (MFS) method of word sense disambiguation is defined by counting the frequency of a particular word sense for a particular POS tagged word. For the i th word use being the word w^i , hav-

5.2 Word Sense Representation

ing some sense s^j then without any further context the probability of that sense being the correct sense is $P(s^j | w^i)$. One can use the part of speech tag p_i (for the i th word use) as an additional condition, and thus find $P(s^j | w^i, p_i)$. WordNet encodes this information for each lemma-synset pair (i.e. each word sense) using the SemCor corpus counts. This is also used for sense ordering, which is why most frequent sense is sometimes called first sense. This is a readily available and practical method for getting a baseline probability of each sense. Most frequent sense can be applied for word sense disambiguation using this frequency-based probability estimate: $\text{argmax}_{\forall s^j} P(s^j | w^i, p_i)$.

In the most recent SemEval WSD task (Moro andNavigli 2015), MFS beat all submitted entries for English, both overall, and on almost all cuts of the data. The results for other languages were not as good, however in other languages the true corpus-derived sense counts were not used.

5.2 Word Sense Representation

It is desirable to create a vector representation of a word sense much like in Chapter 4 representations were created for words. We desire to an embedding to represent each word sense, as normally represented by a word-synset pair. This section considers the representations for the lexical word senses as given from a dictionary. We consider a direct method of using a labelled corpus, and an indirect method makes use of simpler sense-embeddings to partially label a corpus before retraining. These methods create representations corresponding to senses from WordNet. Section 5.3 considers the case when the senses are to also be discovered, as well as represented.

Deng et al. (2009), “ImageNet: A Large-Scale Hierarchical Image Database”

G. K. Zipf (1945), “The meaning-frequency relationship of words”

G. Zipf (1949), *Human behavior and the principle of least effort: an introduction to human ecology*

Kilgarriff (2004), “How Dominant Is the Commonest Sense of a Word?”

Semantic Syllepsis

(Also known as pathological sentences that kill almost all WSD systems.) Consider the sentence: John used to work for the newspaper that you are carrying.. In this sentence the word-use newspaper simultaneously have two different meanings: it is both the company, and the object. This violates our earlier statement that every word-use belongs to exactly one synset. WSD systems are unable to handle these sentences as they attempt to assign a single sense to each word-use. Most word sense induction systems cannot do much better: at best a new sense could be allocated for the joint use, which does not correspond to the linguistic notion of the word having two senses for different parts of the sentence. Most works on word sense disambiguation outright ignore these sentences, or consider them to be ungrammatical, or incorrect. However, they are readily

5 Word Sense Representations

understood and used without thought by most native speakers. These constructions are also known as *zeugma*, although *zeugma* is itself a highly polysemous word, so its usage varies.

De Smedt and Daelemans (2012), "Pattern for python"

Moro and Navigli (2015), "SemEval-2015 Task 13: Multilingual All-Words Sense Disambiguation and Entity Linking"

WordNet is not a strong moral baseline

WordNet, as a resource-based partly on the work of Princeton undergraduate students in the early 1990's, and on the literature of 1961, is not the kind of resource one might hope for from an AI information perspective. The glosses include a number of biases. These biases are reflective of the language use, but are not necessarily ideal to be encoded into a system. For example:

S: (v) nag, peck, hen-peck (bother persistently with trivial complaints) 'She nags her husband all day long's. Other dictionaries regularly show up in the News for similar content.

Another problem is the source of the word sense counts. As discussed in the main text, sense counts are important in WSD systems. The counts come from SemCor, a sense annotated subset of the Brown Corpus. The Brown Corpus is a sampling of American texts from 1961. The cultural norms of 1961 were not

5.2.1 Directly supervised method

The simple and direct method is to take a dataset that is annotated with word senses, and then treat each sense-word pair as if it were a single word, then apply any of the methods for word representation discussed in Chapter 4. Iacobacci, Pilehvar, and Navigli (2015) use a CBOW language model (Mikolov et al. 2013) to do this. This does, however, run into the aforementioned problem, that there is relatively little training data that has been manually sense annotated. Iacobacci, Pilehvar, and Navigli (2015) use a third-party WSD tool, namely BabelFly (Moro, Raganato, and Navigli 2014), to annotate the corpus with senses. This allows for existing word representation techniques to be applied.

Chen, Liu, and Sun (2014) applies a similar technique, but using a word-embedding-based partial WSD system of their own devising, rather than an external WSD tool.

5.2.2 Word embedding-based disambiguation method

Chen, Liu, and Sun (2014) uses an almost semi-supervised approach to train sense vectors. They partially disambiguate their training corpus, using initial word sense vectors and WordNet. They then completely replace these original (phase one) sense-vectors, by using the partially disambiguated corpus to train new (phase two) sense-vectors via a skip-gram variant. This process is shown in Figure 5.2.

The **first phase** of this method is in essence a word-embedding-based WSD system. When assessed as such, they report that it only marginally exceeds the MFS baseline, though that is not at all unusual for WSD algorithms as discussed above.

5.2 Word Sense Representation

They assign a sense vector to every word sense in WordNet. This sense vector is the average of word-embeddings of a subset of words in the gloss, as determined using pretrained skip-grams (Mikolov et al. 2013). For the word w with word sense w^{s^i} , a set of candidate words, $cands(w^{s^i})$, is selected from the gloss based on the following set of requirements. First, the word must be a content word: that is a verb, noun, adverb or adjective; secondly, its cosine distance to w must be below some threshold δ ; finally, it must not be the word itself. When these requirements are followed $cands(w^{s^i})$ is a set of significant closely related words from the gloss.

The phase one sense vector for w^{s^i} is the mean of the word vectors for all the words in $cands(w^{s^i})$. The effect of this is that we expect that the phase one sense vectors for most words in the same synset will be similar but not necessarily identical. This expectation is not guaranteed however. As an example, consider the use of the word *china* as a synonym for *porcelain*: the single sense vector for *china* will likely be dominated by its more significant use referring to the country, which would cause very few words in the gloss for the *porcelain* synset to be included in $cands$. Resulting in the phase one sense vectors for the synonymous senses of *porcelain* and *china* actually being very different.

The phase one sense vectors are used to disambiguate the words in their unlabelled training corpus. For each sentence in the corpus, an initial *content vector* is defined by taking the mean of the skip-gram word embedding (not word sense) for all content words in the sentence. For each word in the sentence, each possible sense-embedding is compared to the context vector. If one or more sense vectors are found to be closer than a given threshold, then that word is tagged with the closest of those senses, and the context vector is updated to use the sense-vector instead of the word vector. Words that do not come within the threshold are not tagged, and the context vector is not updated. This is an important part of their algorithm, as it ensures that words without clear senses do not get a sense ascribed to them. This

the norms of today. (For context, note that the US did not pass the Civil Rights act to end segregation until 1964). As such, one should not trust WordNet (or SemCor) to reflect current sense counts, for words which have undergone usage change since 1961. Furthermore, when creating downstream resources based on WordNet, one should not use these sense counts to determine how important it is to include a concept. If ImageNet (Deng et al. 2009) for example, had used SemCor counts to determine which synsets of images would be included, then items rarely discussed in 1961 literature, like wheelchairs, and prosthesis would be excluded. Which would in turn make many image processing systems systematically unhelpful in processing images relating to the disabled. (Do not fear: even the initial release of ImageNet contains hundreds of images of wheelchairs, and prosthesis) Unintentional biasing of data can have on-going effects on the behaviour of machine learning-based systems far beyond the original conception.

Iacobacci, Pilehvar, and Navigli (2015), "SensEmbed: learning sense embeddings for word and relational similarity"

Chen, Liu, and Sun (2014), "A Unified Model for Word

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Sense Representation and Disambiguation.”

WSD with embeddings

It is beyond the scope of this work to fully discuss WSD systems. However, we will remark that (single sense) word embeddings are a generally useful feature as an input to any NLP ML system. As such they can be used as features in a fully supervised WSD system. The idea of using them in this way is similar to the LSI enhanced Lesk WSD system of Basile, Caputo, and Semeraro (2014).

Cosine distance

Here we talk of cosine distance, where a smaller distance implies more similar (and 0.0 identical). Contrasting this with the cosine similarity, where higher value implies more similar (and 1.0 identical).

Cosine distance is still not a true metric as $d^{\cos}(v, kv) = 0$ for all $k \in \mathbb{R}_+$. Other times you may see cosine similarity, ranging between -1 (most different) and 1 (most similar). Cosine similarity is given by $\text{sim}(a, b) = \frac{\tilde{a} \cdot \tilde{b}}{\|\tilde{a}\|_2 \|\tilde{b}\|_2} = \cos(\angle \tilde{a} \tilde{b})$ i.e. the unit-length normalised dot product of the vectors. Cosine distance is usually defined as $d^{\cos}(\tilde{a}, \tilde{b}) = \frac{1 - \text{sim}(\tilde{a}, \tilde{b})}{2}$. Ranging between 0 (most similar) and 1 (most different).

Can we go from induced senses to lexical senses

A natural question given the existence of many WSI systems, and the existing

thus avoids any dubious sense tags for the next training step.

In **phase two** of training Chen, Liu, and Sun (2014) employ the skip-gram word-embedding method, with a variation, to predict the word senses. They train it on the partially disambiguated corpus produced in phase one. The original sense vectors are discarded. Rather than the model being tasked only to predict the surrounding words, it is tasked to predict surrounding words and their sense-tags (where present). In the loss function the prediction of tags and words is weighted equally.

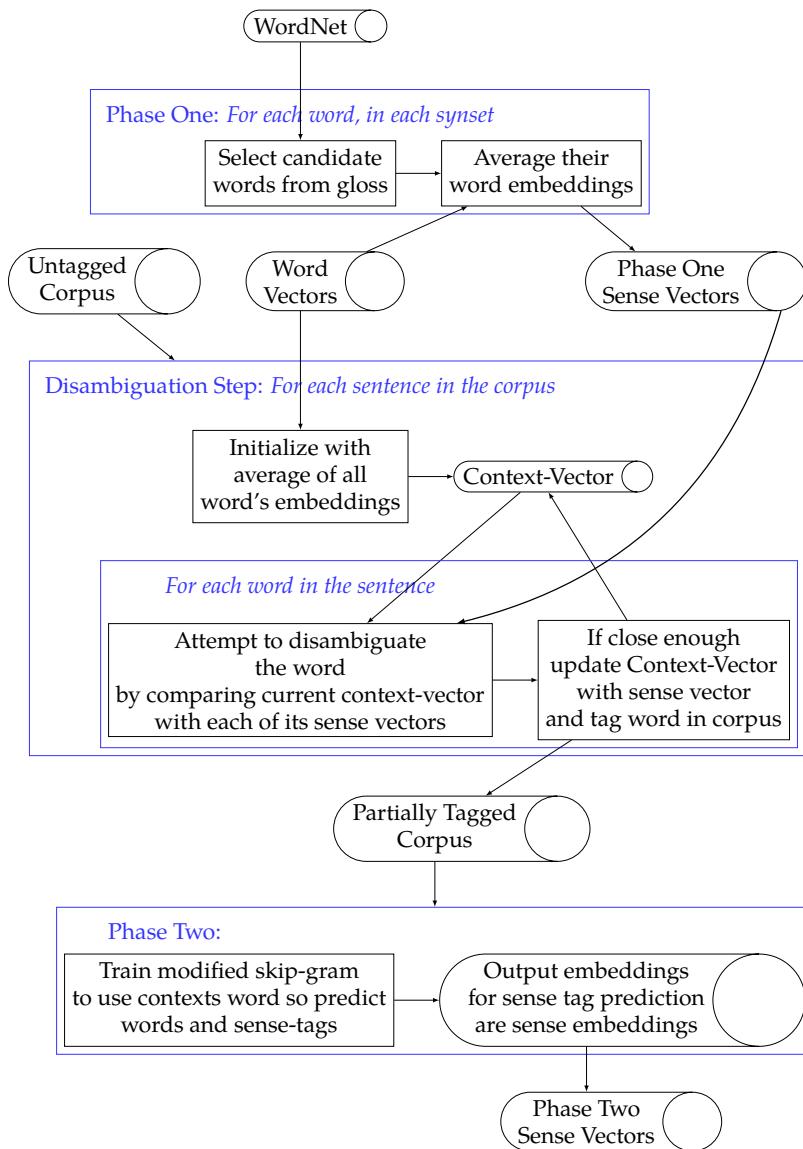
Note that the input of the skip-gram is the just central word, not the pair of central word with sense-tag. In this method, the word sense embeddings are output embeddings; though it would not be unreasonable to reverse it to use input embeddings with sense tags, or even to do both. The option to have input embeddings and output embeddings be from different sets, is reminiscent of Schwenk (2004) for word embeddings.

The phase one sense vectors have not been assessed on their representational quality. It could be assumed that because the results for these were not reported, they were worse than those found in phase two. The phase two sense vectors were not assessed for their capacity to be used for word sense disambiguation. It would be desirable to extend the method of Chen, Liu, and Sun (2014), to use the phase two vectors for WSD. This would allow this method to be used to disambiguate its own training data, thus enabling the method to become self-supervised.

5.3 Word Sense Induction (WSI)

In this section we will discuss methods for finding a word sense without reference to a standard set of senses. Such systems must discover the word senses at the same

5.3 Word Sense Induction (WSI)



wealth of lexically indexed resources, is if we can align induced senses to a set of lexically defined senses. Agirre, Martínez, et al. (2006) proposed a method for doing this using a weighted mapping-based on the probabilities found using induced sense WSD on a labelled “mapping” corpus. This has only been used on relatively small datasets with only hundreds of words (SenseEval 3 (Mihalcea, Chklovski, and Kilgarriff 2004) and SemEval-2007 Task 02 (Agirre and Soroa 2007)). Our own investigations in White et al. (2018) with the larger SemEval 2007 Task 7 (Navigli, Litkowski, and Hargraves 2007) suggest that it may not scale very well to real-word WSD tasks. That work proposed an alternative method that worked better, though still not as well as could be hoped. Finding suitable methods to link unsupervised representations, to human defined senses remains a topic worthy of research.

Figure 5.2: The process used by Chen, Liu, and Sun (2014) to create word sense embeddings.

5 Word Sense Representations

time as they find their representations. One strong advantage of these methods is that they do not require a labelled dataset. As discussed there are relatively few high-quality word sense labelled datasets. The other key advantage of these systems is that they do not rely on fixed senses determined by a lexicographer. This is particularly useful if the word senses are highly domain specific; or in a language without strong lexicographical resources. This allows the data to inform on what word senses exist.

Why do skip-grams perform so well on SCWS?

SCWS is a corpus designed for evaluating word sense embeddings. Single sense embeddings (e.g. skip-grams) cannot take advantage of the context information in the SCWS. However, they do often perform comparably to the word sense embeddings. Sometimes even outperforming them. It is unclear if this highlights the difficulty of the task (i.e. that the impact of context is hard to gauge), or it might be due to the (implicit) most frequent sense dominating both the use in the tasks, and the representation in a single sense. Alternatively, it may just be the result of the fine tuning of the more mature single-sense embedding methods (and that with more time and tuning multiple sense methods could do proportionally better).

Most vector word sense induction and representation approaches are evaluated on similarity tests. Such tests include WordSim-353 (Finkelstein et al. 2001) for context-less, or Stanford’s Contextual Word Similarities (SCWS) for similarity with context information (Huang et al. 2012). This evaluation is also suitable for evaluating single sense word-embeddings, e.g. skip-grams.

We can divide the WSI systems into context clustering-based approaches, and co-location prediction-based approaches. This division is similar to the separation of co-location matrix factorisation, and co-location prediction-based approaches discussed in Chapter 4. It can be assumed thus that at the core, like for word embeddings, they are fundamentally very similar. One could think of prediction of collocated words as a soft indirect clustering of contexts that can have those words.

5.3.1 Context Clustering-based Approaches

As the meaning of a word, according to word embedding principles, is determined by the contexts in which it occurs, we expect that different meanings (senses) of the same words should occur in different contexts. If we cluster the contexts that a word occurs in, one would expect to find distinct clusters for each sense of the word. It is on this principle that the context clustering-based approaches function.

5.3 Word Sense Induction (WSI)

5.3.1.1 Offline clustering

The fundamental method for most clustering-based approaches is as per Schütze (1998). That original work is not a neural word sense embedding, however the approach remains the same. Pantel and Lin (2002) and Reisinger and Mooney (2010) are also not strictly neural word embedding approaches (being more classical vector representations), however the overall method is also very similar.

The clustering process is done by considering all word uses, with their contexts. The contexts can be a fixed-sized window of words (as is done with many word-embedding models), the sentence, or defined using some other rule. Given a pair of contexts, some method of measuring their similarity must be defined. In vector representational works, this is ubiquitously done by assigning each context a vector, and then using the cosine similarity between those vectors.

The **first step** in all the offline clustering methods is thus to define the representations of the contexts. Different methods define the context vectors differently:

- Schütze (1998) uses variations of inverse-document-frequency (idf) weighted bags of words, including applying dimensionality reduction to find a dense representation.
- Pantel and Lin (2002) use the mutual information vectors between words and their contexts.
- Reisinger and Mooney (2010), use td-idf or χ^2 weighted bag of words.
- Huang et al. (2012) uses td-idf weighted averages of (their own) single sense word embeddings for all words in the context.
- Kågebäck et al. (2015) also uses a weighted average of single sense word skip-gram embeddings,

Schütze (1998), "Automatic Word Sense Discrimination"

Pantel and Lin (2002), "Discovering word senses from text"

Reisinger and Mooney (2010), "Multi-prototype vector-space models of word meaning"

On context representations

These co-location clustering methods require finding a representation for the context (from this a similarity metric is applied, and the clustering is then done). More generally, this can be related to the next chapter: Chapter 6, as any of these methods could be used to derive a vector representation of a context. In most works (including all the works discussed here) comparatively simple representations of the contexts are used. It would be interesting to extend the sentence representation methods, and apply them to this use.

Huang et al. (2012), "Improving word representations via global context and multiple word prototypes"

Kågebäck et al. (2015), "Neural context embed-

5 Word Sense Representations

dings for automatic discovery of word senses”

On clustering

Clustering can be defined as a (mixed integer) optimisation task, of assigning points to clusters so as to satisfy some loss function-based around minimising intra-cluster variance while maximising inter-cluster variance (or a similar measure). As this is NP-hard, most clustering methods are approximate. K-means is very popular because of its simplicity, however it easily falls into local minima, and so normally it is run dozens of times (at least) to obtain more optimal results. K-means also has the issue of having to select the number of clusters (k). It should be remembered that there exist many other clustering methods than k-means (and its variants). These other methods use different loss functions, and different strategies to overcome the NP-hard nature of the problem. In particular their mixture model methods, hierarchical methods, spectral methods, and others. We personally favour affinity propagation (Frey and Dueck 2007), though there is provably no ideal clustering algorithm even in the non-heuristic case (Kleinberg 2003). On

with the weighting based on two factors. One based on how close the words were, and the other on how likely the co-occurrence was according to the skip-gram model.

It is interesting to note that idf, td-idf, mutual information, skip-gram co-occurrence probabilities (being a proxy for point-wise mutual information (Levy and Goldberg 2014)), are all closely related measures.

The **second step** in off-line clustering is to apply a clustering method to cluster the word-uses. This clustering is done based on the calculated similarity of the context representation where the words are used. Again, different WSI methods use different clustering algorithms.

- Schütze (1998) uses a group average agglomerative clustering method.
- Pantel and Lin (2002) use a custom hierarchical clustering method.
- Reisinger and Mooney (2010) use mixtures of von-Mises-Fisher distributions.
- Huang et al. (2012) use spherical k-means.
- Kågebäck et al. (2015) use k-means.

The **final step** is to find a vector representation of each cluster. For non-neural embedding methods this step is not always done, as defining a representation is not the goal, though in general it can be derived from most clustering techniques. Schütze (1998) and Kågebäck et al. (2015) use the centroids of their clusters. Huang et al. (2012) use a method of relabelling the word uses with a cluster identifier, then train a (single-sense) word embedding method on cluster identifiers rather than words. This relabelling technique is similar to the method later used by Chen, Liu, and Sun (2014) for learning lexical sense representations, as discussed in Section 5.2.2. As each cluster of contexts represents a sense, those

5.3 Word Sense Induction (WSI)

cluster embeddings are thus also considered as suitable word sense embeddings.

To summarize, all the methods for inducing word sense embeddings via off-line clustering follow the same process. **First:** represent the contexts of word use, so as to be able to measure their similarity. **Second:** use the context's similarity to cluster them. **Finally:** find a vector representation of each cluster. This cluster representation is the induced sense embedding.

5.3.1.2 Online clustering

The methods discussed above all use off-line clustering. That is to say the clustering is performed after the embedding is trained. Neelakantan et al. (2015) perform the clustering during training. To do this they use a modified skip-gram-based method. They start with a fixed number of randomly initialised sense vectors for each context. These sense vectors are used as input embeddings for the skip-gram context prediction task, over single sense output embeddings. Each sense also has, linked to it, a context cluster centroid, which is the average of all output embeddings for the contexts that the sense is assigned to. Each time a training instance is presented, the average of the context output embeddings is compared to each sense's context cluster centroid. The context is assigned to the cluster with the closest centroid, updating the centroid value. This can be seen as similar to performing a single k-means update step for each training instance. Optionally, if the closest centroid is further from the context vector than some threshold, a new sense can be created using that context vector as the initial centroid. After the assignment of the context to a cluster, the corresponding sense vector is selected for use as the input vector in the skip-gram context prediction task.

Kågebäck et al. (2015) investigated using their weighting function (as discussed in Section 5.3.1.1) with the online clustering used by Neelakantan et al. (2015).

any clustering task (word sense or otherwise) it is worth investigating several clustering algorithms, and not just settling for k-means (particularly not settling for k-means run once.). A series of interesting and easy reading articles on clustering can be found at: <http://alexhwilliams.info/itsneuronalblog/2015/09/11/clustering1/>, <http://alexhwilliams.info/itsneuronalblog/2015/10/01/clustering2/>, and <http://alexhwilliams.info/itsneuronalblog/2015/11/18/clustering-is-easy/>

Neelakantan et al. (2015), "Efficient non-parametric estimation of multiple embeddings per word in vector space"

5 Word Sense Representations

They found that this improved the quality of the representations. More generally any such weighting function could be used. This online clustering approach is loosely similar to the co-location prediction-based approaches.

5.3.2 Co-location Prediction-based Approaches

Probability

One may wish to brush up on basic probability notions for this section. In particular joint, conditional and marginal probabilities definitions; as well as Bayes Theorem and the probability chain-rule which come from those. In brief these are as follows.

Conditional Probability:

$$P(A | B) = \frac{P(A, B)}{P(B)}$$

Marginal Probability:

$$P(A) = \sum_{\forall b} P(A, B = b)$$

Bayes Theorem:

$$P(A | B) = \frac{P(B | A)P(A)}{P(B)}$$

Probability Chain-rule:

$$\begin{aligned} P(A^n, \dots, A^1) \\ = P(A^n | A^{n-1}, \dots, A^1)P(A^{n-1}, \dots, A^1) \end{aligned}$$

e.g.

$$\begin{aligned} P(A, B, C) \\ = P(A | B, C)P(B | C)P(C) \end{aligned}$$

The latter three rules are consequences of the first.

Tian et al. (2014), "A Probabilistic Model for Learning Multi-Prototype Word Embeddings."

Rather than clustering the contexts, and using those clusters to determine embeddings for different senses, one could consider the sense as a latent variable in the task used to find word embeddings – normally a language modelling task. The principle is that it is not the word that determines its collocated context words, but rather the word sense. So the word sense can be modelled as a hidden variable, where the word, and the context words are being observed.

Tian et al. (2014) used this to define a skip-gram-based method for word sense embeddings. For input word w^i with senses $\mathcal{S}(w^i)$, the probability of output word w^o occurring near w^i can be given as:

$$P(w^o | w^i) = \sum_{\forall s^k \in \mathcal{S}(w^i)} P(w^o | s^k, w^i)P(s^k | w^i) \quad (5.1)$$

Given that a sense s^k only belongs to one word w^i , we know that k th sense of the i th word only occurs when the i th word occurs. We have that the joint probability $P(w^i, s^k) = P(s^k)$.

We can thus rewrite Equation (5.1) as:

$$P(w^o | w^i) = \sum_{\forall s^k \in \mathcal{S}(w^i)} P(w^o | s^k)P(s^k | w^i) \quad (5.2)$$

A softmax classifier can be used to define $P(w^o | s^k)$, just like in normal language modelling. With output

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embeddings for the words w^o , and input embeddings for the word senses s^k . This softmax can be sped-up using negative sampling or hierarchical softmax. The later was done by Tian et al. (2014).

Equation (5.2) is in the form of a mixture model with a latent variable. Such a class of problems are often solved using the Expectation Maximisation (EM) method. In short, the EM procedure functions by performing two alternating steps. The **E-step** calculates the expected chance of assigning word sense for each training case ($\hat{P}(s^l | w^o)$) in the training set \mathcal{X} . Where a training case is a pairing of a word use w^i , and context word w^o , with $s^l \in \mathcal{S}(w^i)$, formally we have:

$$\hat{P}(s^l | w^o) = \frac{\hat{P}(s^l | w^i)P(w^o | s^l)}{\sum_{\forall s^k \in \mathcal{S}(w^i)} \hat{P}(w^o | s^k)P(s^k | w^i)} \quad (5.3)$$

The **M-step** updates the prior likelihood of each sense (that is without context) using the expected assignments from the E-step.

$$\hat{P}(s^l | w^i) = \frac{1}{|\mathcal{X}|} \sum_{\forall (w^o, w^i) \in \mathcal{X}} \hat{P}(s^l | w^o) \quad (5.4)$$

During this step the likelihood of the $P(w^o | w^i)$ can be optimised to maximise the likelihood of the observations. This is done via gradient descent on the neural network parameters of the softmax component: $P(w^o | s^k)$. By using this EM optimisation the network can fit values for the embeddings in that softmax component.

A limitation of the method used by Tian et al. (2014), is that the number of each sense must be known in advance. One could attempt to solve this by using, for example, the number of senses assigned by a lexicographical resource (e.g. WordNet). However, situations where such resources are not available or not suitable are one of the main circumstances in which

5 Word Sense Representations

WSI is desirable (for example in work using domain specific terminology, or under-resourced languages). In these cases one could apply a heuristic-based on the distribution of senses-based on the distribution of words (G. K. Zipf 1945). An attractive alternative would be to allow senses to be determined-based on how the words are used. If they are used in two different ways, then they should have two different senses. How a word is being used can be determined by the contexts in which it appears.

Bartunov et al. (2015), “Breaking Sticks and Ambiguities with Adaptive Skip-gram”

WordNet and BabelNet

As mentioned in the previous sections, WordNet and BabelNet are the predominant lexicons used for word senses. It is not directly relevant to this section, but we have space here to remark upon them. WordNet (Tengi 1998) as a very well established tool has a binding in practically every modern programming language suitable for NLP. WordNet.jl (<https://github.com/JuliaText/WordNet.jl>) is the Julia binding. NLTK (Bird, Klein, and Loper 2009) includes one for Python.

BabelNet (Navigli and Ponzetto 2010) is intended to be accessed as an online resource, via a RESTful API. Users receive 1000 free queries per day. Academic users can request an upgrade to 50,000 queries per day, or to download a copy of the database. From personal experience we found those requests to be handled easily and rapidly.

Bartunov et al. (2015) extend on this work by making the number of senses for each word itself a fit-able parameter of the model. This is a rather Bayesian modelling approach, where one considers the distribution of the prior.

Considering again the form of Equation (5.2)

$$P(w^o | w^i) = \sum_{\forall s^k \in \mathcal{S}(w^i)} P(w^o | s^k) P(s^k | w^i) \quad (5.5)$$

The prior probability of a sense given a word, but no context, is $P(s^k | w^i)$. This is Dirichlet distributed. This comes from the definition of the Dirichlet distribution as the prior probability of any categorical classification task. When considering that the sense may be one from an unlimited collection of possible senses, then that prior becomes a Dirichlet process.

In essence, this prior over a potentially unlimited number of possible senses becomes another parameter of the model (along with the input sense embeddings and output word embeddings). The fitting of the parameters of such a model is beyond the scope of this book; it is not entirely dissimilar to the fitting via expectation maximisation incorporating gradient descent used by Tian et al. (2014). The final output of Bartunov et al. (2015) is as desired: a set of induced sense embeddings, and a language model that is able to predict how likely a word is to occur near that word sense ($P(w^o | s^k)$).

5.4 Conclusion

By application of Bayes' theorem, the sense language model can be inverted to take a word's context, and predict the probability of each word sense.

$$P(s^l | w^o) = \frac{P(w^o | s^l)P(s^l | w^i)}{\sum_{\forall s^k \in \mathcal{S}(w^i)} P(w^o | s^k)P(s^k | w^i)} \quad (5.6)$$

with the common (but technically incorrect) assumption that all words in the context are independent.

Given a context window:

$\mathcal{W}^i = (w^{i-\frac{n}{2}}, \dots, w^{i-1}, w^{i+1}, \dots, w^{i+\frac{n}{2}})$, we have:

$$P(s^l | \mathcal{W}^i) = \frac{\prod_{\forall w^j \in \mathcal{W}^i} P(w^j | s^l)P(s^l | w^i)}{\sum_{s^k \in \mathcal{S}(w^i)} \prod_{\forall w^j \in \mathcal{W}^i} P(w^j | s^k)P(s^k | w^i)} \quad (5.7)$$

Independence Assumption

Technically, Equation (5.6) does not require the independence of the probabilities of the context words. Rather it only requires that the context words be conditionally independent on the word in question w^i . Nevertheless, even the conditional independence assumption is incorrect, except for a theoretical perfect embedding capturing perfect information. The conditional independence assumption remains useful as an approximation.

Finding the nearest neighbours (Nearest Neighbour Trees)

A common evaluation task with any representation is to find its nearest neighbours. The naïve solution is to check the distance to all points. For n points this is $O(n)$ operations. For word embeddings n is the size of the vocabulary, perhaps 100,000 words. Performing 100,000 operations per check, is not entirely unreasonable on modern computers (even when the operations are on 300 dimensional representations). However, for word sense embeddings, which have many senses per word in the vocabulary, this means many more points to check. 30 senses per word is not unusual for fine-grained word sense induction. Having a total $n = 3,000,000$ representations to check causes a noticeable delay. To

5.4 Conclusion

Word sense representations allow the representations of the senses of words when one word has multiple meanings. This increases the expressiveness of the representation. These representations can in general be applied anywhere word embeddings can. They are particularly useful for translation, and in languages with large numbers of homonyms.

The word representation discussions in this chapter naturally lead to the next section on phrase representation. Rather than a single word having many meanings, the next chapter will discuss how a single meaning may take multiple words to express. In such longer structure's representations, the sense embeddings discussed here are often unnecessary, as the ambiguity may be resolved by the longer structure. Indeed, the methods discussed in this chapter have relied on that fact to distinguish the senses using the contexts.

5 Word Sense Representations

solve this we can use data structures designed for fast nearest neighbour querying. A k-d tree takes at worst $O(n \log_2(n))$ time to construct. Once constructed on average it takes $O(\log(n))$ to find the nearest neighbour to any point. This makes checking the nearest neighbour nearly instantaneous for even the largest vocabularies.

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6 Sentence Representations and Beyond

A sentence is a group of words expressing a complete thought.

— *English Composition and Literature*,
Webster, 1923

This chapter discusses representations for larger structures in natural language. The primary focus is on the sentence level. However, many of the techniques also apply to sub-sentence structures (phrases), and super-sentence structures (documents). The three main types of representations discussed here are: unordered models, such as sum of word embeddings; sequential models, such as recurrent neural networks; and structured models, such as recursive autoencoders.

It can be argued that the core of true AI, is in capturing and manipulating the representation of an idea. In natural language a sentence (as defined by Webster in the quote above), is such a representation of an idea, but it is not machine manipulatable. As such the conversion of sentences to a machine manipulatable representation is an important task in AI research.

All techniques which can represent documents (or paragraphs) by necessity represent sentences as well. A document (or a paragraph), can consist only of a single sentence. Many of these models always work for sub-sentence structures also, like key-phrases. When considering representing larger documents, neural network embedding models directly compete with vector information retrieval models, such as LSI (Dumais et al. 1988), probabilistic LSI (Hofmann 2000) and LDA (Blei, Ng, and Jordan 2003).

Word Embeddings as a by-product

Many sentence representation methods produce word embeddings as a by-product. These word embeddings are either output embeddings, from the softmax, or input embeddings from a lookup layer.

Initialising input embeddings

It is common (but not ubiquitous) to initialise the input embeddings using pre-trained embeddings from one of the methods discussed in Chapter 4, then allow them to be fine-tuned while training the sentence representation method.

Dumais et al. (1988), “Using latent semantic analysis to

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improve access to textual information”

Hofmann (2000), “Learning the similarity of documents: An information-geometric approach to document retrieval and categorization”

Blei, Ng, and Jordan (2003), “Latent dirichlet allocation”

Word Sense Embeddings in Sentence Embeddings

While ?? was all about sense embeddings, they are unmentioned here. One might think that they would be very useful for sentence embeddings. However, they are not as needful as one might expect. The sense of a word being used is determined by the context. Ideally, it is determined by what the context means. As a sentence embedding is a direct attempt to represent the meaning of such a context, determining the sense of each word within it is not required. Using sense embeddings instead of word embeddings is a valid extension to many of these methods. However it requires performing word sense disambiguation, which as discussed is very difficult.

Mitchell and Lapata (2008), “Vector-based Models of Semantic Composition.”

SOWE is the product of the BOW with an embedding matrix

The reader may recall from Chapter 4, that a word-embedding lookup is the same as a one-hot vector product: $C_{:,w^i} = C \hat{e}_{w^i}$. Similar can be said for sum of

6.1 Unordered and Weakly Ordered Representations

A model that does not take into account word order cannot perfectly capture the meaning of a sentence. Mitchell and Lapata (2008) give the poignant examples of:

- It was not the sales manager who hit the bottle that day, but the office worker with the serious drinking problem.
- That day the office manager, who was drinking, hit the problem sales worker with a bottle, but it was not serious.

These two sentences have the same words, but in a different structure, resulting in their very different meanings. In practice, however, representations which discard word order can be quite effective.

6.1.1 Sums of Word Embeddings

Classically, in information retrieval, documents have been represented as bags of words (BOW). That is to say a vector with length equal to the size of the vocabulary, with each position representing the count of the number of occurrences of a single word. This is much the same as a *one-hot vector* representing a word, but with every word in the sentence/document counted. The word embedding equivalent is sums of word embeddings (SOWE), and mean of word embeddings (MOWE). These methods, like BOW, lose all order information in the representation. In many cases it is possible to recover a BOW from a much lower dimensional SOWE (Lyndon White et al. 2016a).

Surprisingly, these unordered methods have been found on many tasks to be extremely well performing, bet-

6.1 Unordered and Weakly Ordered Representations

ter than several of the more advanced techniques discussed later in this chapter. This has been noted in several works including: Lyndon White et al. (2015), Ritter et al. (2015) and R. Wang, Liu, and McDonald (2017). It has been suggested that this is because in English there are only a few likely ways to order any given bag of words. It has been noted that given a simple n-gram language model the original sentences can often be recovered from BOW (Horvat and Byrne 2014) and thus also from a SOWE (Lyndon White et al. 2016b). Thus word-order may not in-fact be as important as one would expect in many natural language tasks, as it is in practice more proscribed than one would expect. That is to say very few sentences with the same word content, will in-practice be able to have it rearranged for a very different meaning. However, this is unsatisfying, and certainly cannot capture fine grained meaning.

The step beyond this is to encode the n-grams into a bag of words like structure. This is a bag of n-grams (BON), e.g. bag of trigrams. Each index in the vector thus represents the occurrence of an n-gram in the text. So It is a good day today, has the trigrams: (It is a),(is a good),(a good day),(good day today). As is obvious for all but the most pathological sentences, recovering the full sentence order from a bag of n-grams is possible even without a language model.

The natural analogy to this with word embeddings might seem to be to find n-gram embeddings by the concatenation of n word embeddings; and then to sum these. However, such a sum is less informative than it might seem. As the sum in each concatenated section is equal to the others, minus the edge words.

Instead one should train an n-gram embedding model directly. The method discussed in Chapter 4, can be adapted to use n-grams rather than words as the basic token. This was explored in detail by (Li et al. 2017). Their model is based on the skip-gram word embedding method. They take as input an n-gram embedding, and attempt to predict the surrounding n-grams. This reduces to the original skip-gram method for the case

word embeddings (SOWE) and bag of words (BOW). For some set of words $\mathcal{W} = \{w_1, \dots, w_n\}$: the BOW representation is $B_{\mathcal{W}} = \sum_{w^i \in \mathcal{W}} \hat{e}_{w^i}$; the SOWE representation is $\sum_{w^i \in \mathcal{W}} C_{w^i} = CB_{\mathcal{W}}$. As with word-embeddings, it is immensely cheaper to calculate this via lookup and sum, rather than via matrix product; except on systems with suitable sparse matrix product tricks.

Lyndon White et al. (2016a), “Generating Bags of Words from the Sums of their Word Embeddings”

Lyndon White et al. (2015), “How Well Sentence Embeddings Capture Meaning”

Ritter et al. (2015), “Leveraging Preposition Ambiguity to Assess Compositional Distributional Models of Semantics”

R. Wang, Liu, and McDonald (2017), “A Matrix-Vector Recurrent Unit Model for Capturing Compositional Semantics in Phrase Embeddings”

Horvat and Byrne (2014), “A Graph-Based Approach to String Regeneration.”

Lyndon White et al. (2016b), “Modelling Sentence Generation from Sum of Word Embedding Vectors as a Mixed Integer Programming Problem”

Li et al. (2017), “Neural Bag-of-Ngrams.”

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of unigrams. Note that the surrounding n-grams will overlap in words (for $n > 1$) with the input n-gram. As the overlap is not complete, this task remains difficult enough to encourage useful information to be represented in the embeddings. Li et al. (2017) also consider training n-gram embeddings as a bi-product of text classification tasks.

6.1.2 Paragraph Vector Models (Defunct)

Window vs Context

It is important to be clear in this section on the difference between the window and the context. The window is the words near the target word. The context (in this context) refers to the larger structure (sentence, paragraph, document) that a representation is attempting to be found for. The window is always a subset of the context. In modelling the context many windows within it will be considered (one per target word). Some works say sentence vector, document vector or paragraph vector. We say context vector as it could be any of the above. In theory it could even be a whole collection of documents.

Le and Mikolov (2014), “Distributed Representations of Sentences and Documents”

PV Model Implementations

There is a popular third-party implementation of both the paragraph vector models, under the name doc2vec in the python gensim library (Rehůrek and Sojka 2010).

Le and Mikolov (2014) introduced two models for representing documents of any length by using augmented word-embedding models. The models are called Paragraph Vector Distributed Memory (PV-DM) model, and the Paragraph Vector Distributed Bag of Words model (PV-DBOW). The name Paragraph Vector is a misnomer, it function on texts of any length and has most often (to our knowledge) been applied to documents and sentences rather than any in-between structures. The CBOW and skip-gram models are extended with an additional context vector that represents the current document (or other super-word structure, such as sentence or paragraph). This, like the word embeddings, is initialised randomly, then trained during the task. Le and Mikolov (2014) considered that the context vector itself must contain useful information about the context. The effect in both cases of adding a context vector is to allow the network to learn a mildly different accusal language model depending on the context. To do this, the context vector would have to learn a representation for the context.

PV-DBOW is an extension of CBOW. The inputs to the model are not only the word-embedding $C_{:,w_j}$ for the words w^j from the window, but also a context-embedding $D_{:,d^k}$ for its current context (sentence, paragraph or document) d^k . The task remains to predict which word was the missing word from the center of

6.2 Sequential Models

the context w^i .

along with many information retrieval vector models such as LDA.

$$\begin{aligned} P(w^i \mid d^k, w^{i-\frac{n}{2}}, \dots, w^{i-1}, w^{i+1}, \dots, w^{i+\frac{n}{2}}) \\ = \text{smax}(WD_{:,d^k} + U \sum_{j=i+1}^{j=\frac{n}{2}} (C_{:,w^{i-j}} + C_{:,w^{i+j}})) \end{aligned} \quad (6.1)$$

PV-DM is the equivalent extension for skip-grams. Here the input to the model is not only the central word, but also the context vector. Again, the task remains to predict the other words from the window.

$$P(w^j \mid d^k, w^i) = [\text{smax}(WD_{:,d^k} + V C_{:,w^i})]_{w_j} \quad (6.2)$$

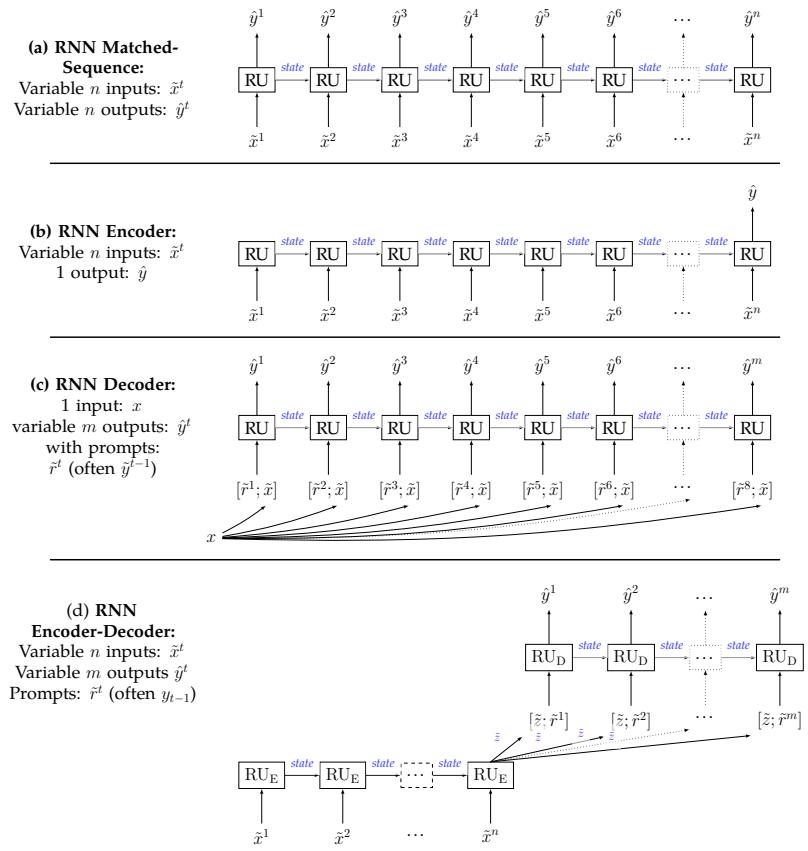
The results of this work are now considered of limited validity. There were failures to reproduce the reported results in the original evaluations which were on sentiment analysis tasks. These were documented online by several users, including by the second author.¹ A follow up paper, Mesnil et al. (2014) found that reweighed bags of n-grams (S. Wang and Christopher D Manning 2012) out performed the paragraph vector models. Conversely, Lau and Baldwin (2016) found that on short text-similarity problems, with the right tuning, the paragraph vector models could perform well; however they did not consider the reweighed n-grams of (S. Wang and Christopher D Manning 2012). On a different short text task, Lyndon White et al. (2015) found the paragraph vector models to significantly be out-performed by SOWE, MOWE, BOW, and BOW with dimensionality reduction. This highlights the importance of rigorous testing against a suitable baseline, on the task in question.

Mesnil et al. (2014), “Ensemble of generative and discriminative techniques for sentiment analysis of movie reviews”

S. Wang and Christopher D Manning (2012), “Baselines and bigrams: Simple, good sentiment and topic classification”

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Figure 6.1: The unrolled structure of an RNN for use in (a) Matched-sequence (b) Encoding, (c) Decoding and (d) Encoding-Decoding (sequence-to-sequence) problems. RU is the recurrent unit – the neural network which reoccurs at each time step. (Repeated from Figure 3.1)



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The majority of this section draws on the recurrent neural networks (RNN) as discussed in Chapter 3. Every RNN learns a representation of all its input and output in its state. We can use RNN encoders and decoders (as shown in Figure 6.1) to generate representations of sequences by extracting a coding layer. One can take any RNN encoder, and select one of the hidden state layers after the final recurrent unit (RU) that has processed the last word in the sentence. Similarly for any RNN decoder, one can select any hidden state layer before the first recurrent unit that begins to produce words. For an RNN encoder-decoder, this means selecting the hidden layer from between. This was originally considered in Cho et al. (2014), when using a machine translation

Cho et al. (2014), "Learning Phrase Representations using RNN Encoder-Decoder

¹<https://groups.google.com/forum/\#!msg/word2vec-toolkit/Q49F1rN0QRo/DoRuBoVNFb0J>

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RNN, to create embeddings for the translated phrases. Several other RNNs have been used in this way since.

[for Statistical Machine Translation](#)

6.2.1 VAE and encoder-decoder

Bowman, Vilnis, et al. (2016) presents an extension on this notion, where in-between the encode and the decode stages there is a variational autoencoder (VAE). This is shown in Figure 6.2. The variational autoencoder (Kingma and Welling 2014) has been demonstrated to have very good properties in a number of machine learning applications: they are able to work to find continuous latent variable distributions over arbitrary likelihood functions (such as in the neural network); and are very fast to train. Using the VAE, it is hoped that a better representation can be found for the sequence of words in the input and output.

[Bowman, Vilnis, et al. \(2016\), "Generating Sentences from a Continuous Space"](#)

[Kingma and Welling \(2014\), "Auto-Encoding Variational Bayes"](#)

Bowman, Vilnis, et al. (2016) trained the network as encoder-decoder reproducing its exact input. They found that short syntactically similar sentences were located near to each other according to this space, further to that, because it has a decoder, it can generate these nearby sentences, which is not possible for most sentence embedding methods.

Interestingly, they use the VAE output, i.e. the *code*, only as the state input to the decoder. This is in-contrast to the encoder-decoders of Cho et al. (2014), where the *code* was concatenated to the input at every timestep of the decoder. Bowman, Vilnis, et al. (2016) investigated such a configuration, and found that it did not yield an improvement in performance.

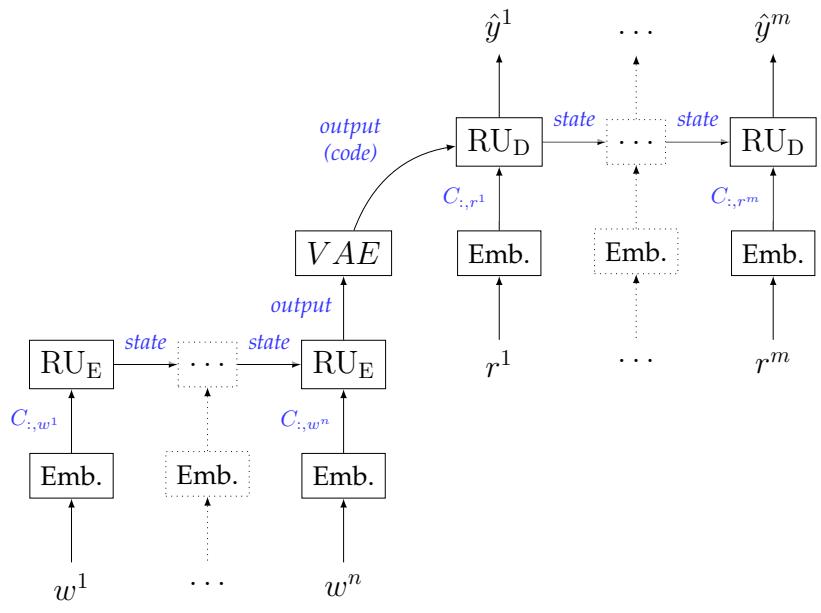
6.2.2 Skip-thought

Kiros et al. (2015) draws inspiration from the works on acausal language modelling, to attempt to predict

[Kiros et al. \(2015\), "Skip-Thought Vectors"](#)

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Figure 6.2: The VAE plus encoder-decoder of Bowman, Vilnis, et al. (2016). Note that during training, $\hat{y}^i = w^i$, as it is an autoencoder model. As is normal for encoder-decoders the prompts are the previous output (target during training, predicted during testing): $r^i = \hat{y}^{i-1}$, with $r^1 = \hat{y}^0 = <\text{EOS}>$ being a pseudo-token marker for the end of the string. The Emb. step represents the embedding table lookup. In the diagrams for Chapter 4 we showed this as a table but just as a block here for conciseness.



the previous and next sentence. Like in the acausal language modelling methods, this task is not the true goal. Their true goal is to capture a good representation of the current sentence. As shown in Figure 6.3 they use an encoder-decoder RNN, with two decoder parts. One decoder is to produce the previous sentence. The encoder part takes as its input is the current sentence, and produces as its output the code, which is input to the decoders. The other decoder is to produce the next sentence. As described in Section 3.2.3, the prompt used for the decoders includes the previous word, concatenated to the code (from the encoder output).

That output code is the representation of the sentence.

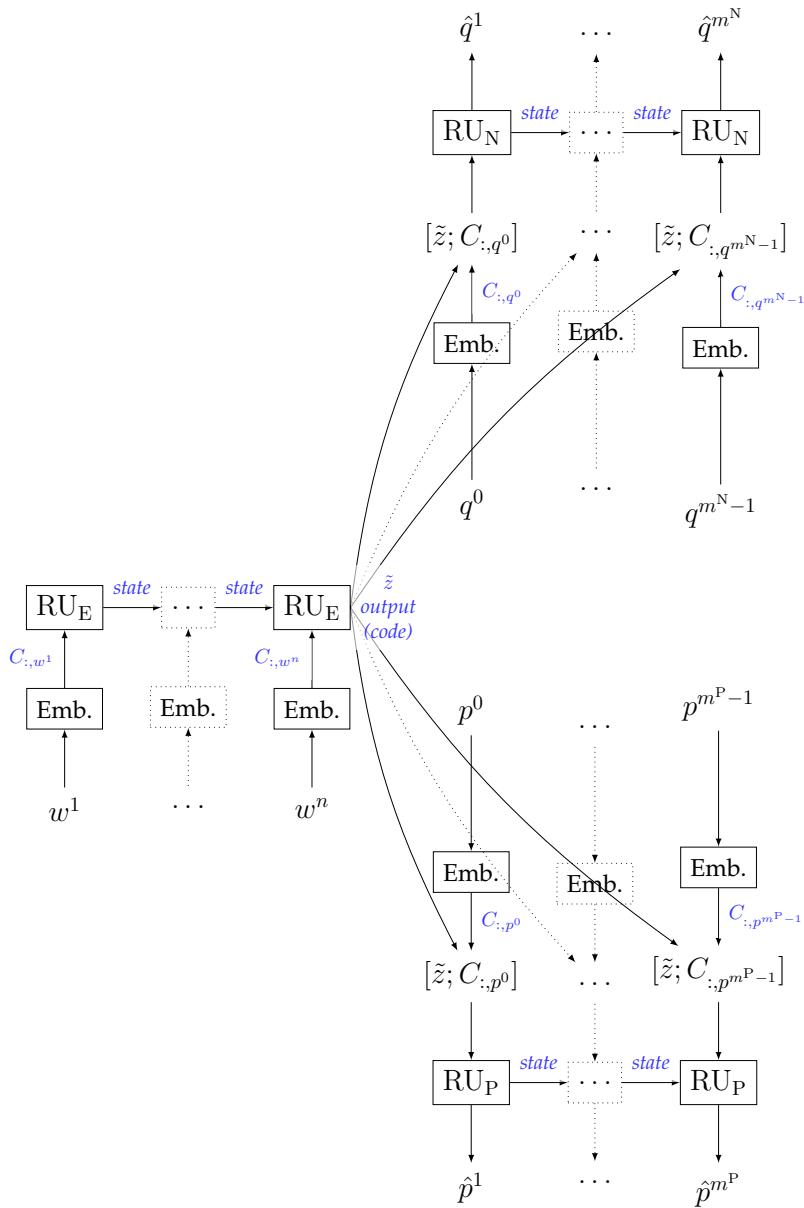
6.3 Structured Models

Parsers

There are many high-quality parsing libraries available. The most well known is the Stanford CoreNLP library (Christopher D. Manning et al. 2014) for java. It has an interactive web-demo at <http://corenlp.run/>, which was used to produce Figures 6.4 and 6.5.

The sequential models are limited to process the information as a series of time-steps one after the other. They processes sentences as ordered lists of words. However, the actual structure of a natural language is not so simple. Linguists tend to break sentences down into a tree structure. This is referred to as parsing. The two most common forms are constituency parse trees,

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NLTK (Bird, Klein, and Loper 2009) contains several different parsers, including a binding to CoreNLP parsers. The newer spaCy library (Honnibal and Johnson 2015) for python, presently only features a dependency parser.

Figure 6.3: The skip-thought model (Kiros et al. 2015). Note that for the next and previous sentences respectively the outputs are \hat{q}^i and \hat{p}^i , and the prompts are q^{i-1} and p^{i-1} . As there is no intent to use the decoders after training, there is no need to worry about providing an evaluation-time prompt, so the prompt is always the previous word. $p^0 = p^{m^P} = q^0 = q^{m^N} = <\text{EOS}>$ being a pseudo-token marker for the end of the string. The input words are w^i , which come from the current sentence. The Emb. steps represents the look-up of the embedding for the word.

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and dependency parse trees. Examples of each are shown in Figures 6.4 and 6.5. It is beyond the scope of this book to explain the precise meaning of these trees, and how to find them. The essence is that these trees represent the structure of the sentence, according to how linguists believe sentences are processed by humans.

The constituency parse breaks the sentence down into parts such as noun phrase (NP) and verb phrase (VP), which are in turn broken down into phrases, or (POS tagged) words. The constituency parse is well thought-of as a hierarchical breakdown of a sentence into its parts. Conversely, a dependency parse is better thought of as a set of binary relations between head-terms and their dependent terms. These structures are well linguistically motivated, so it makes sense to use them in the processing of natural language.

We refer here to models incorporating tree (or graph) structures as structural models. Particular variations have their own names, such as recursive neural networks (RvNN), and recursive autoencoders (RAE). We use the term structural model as an all encompassing term, and minimise the use of the easily misread terms: recursive vs recurrent neural networks. A sequential model (an RNN) is a particular case of a structural model, just as a linked list is a particular type of tree. However, we will exclude sequential models from this discussion except where marked.

[Socher \(2014\), "Recursive Deep Learning for Natural Language Processing and Computer Vision"](#)

[Goller and Kuchler \(1996\), "Learning task-dependent distributed representations by backpropagation through structure"](#)

[Pollack \(1990\), "Recursive distributed representations"](#)

The initial work on structural models was done in the thesis of Socher (2014). It builds on the work of Goller and Kuchler (1996) and Pollack (1990), which present back-propagation through structure. Back-propagation can be applied to networks of any structure, as the chain-rule can be applied to any differentiable equation to find its derivative. Structured networks, like all other networks, are formed by the composition of differentiable functions, so are differentiable. In a normal network the same composition of functions is used for all input cases, whereas in a structured network it is allowed to vary based on the inputs. This means

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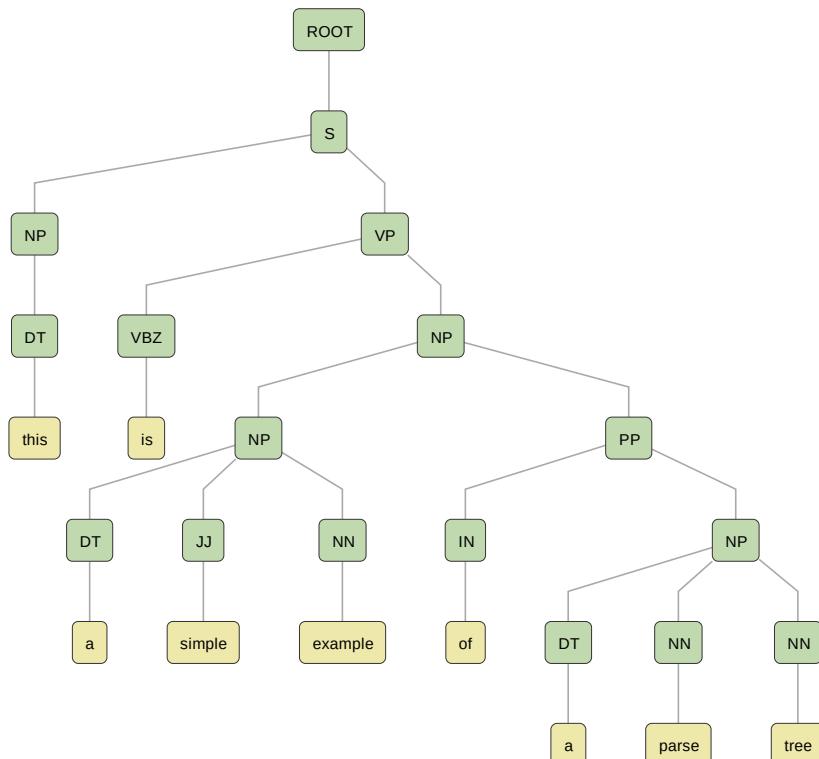


Figure 6.4: A constituency parse tree for the sentence: This is a simple example of a parse tree. In this diagram the leaf nodes are the input words, their immediate parents are their POS tags, and the other nodes with multiple children represent sub-phrases of the sentence, for example NP is a Noun Phrase.

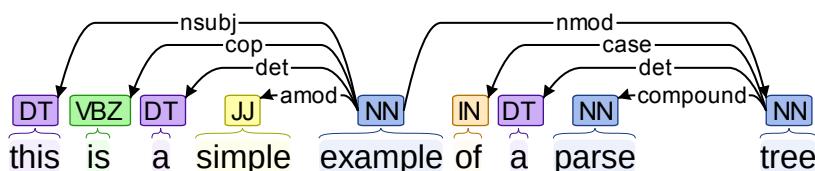


Figure 6.5: A dependency parse tree for the sentence This is a simple example of a parse tree. This is a simple example of a parse tree, This flattened view may be misleading. example is at the peak of the tree, with direct children being: this, is, a, simple, and tree. tree has direct children being: of, a, and parse.

that structuring a network according to its parse tree is possible.

6.3.1 Constituency Parse Tree (Binary)

Tree structured networks work by applying a recursive unit (which we will call RV) function across pairs (or other groups) of the representations of the lower levels, to produce a combined representation. The network structure for an input of binary tree structured text is itself a binary tree of RVs. Each RV (i.e. node in the

Machine learning frameworks for structural models
 Structural networks cannot be easily defined in most static neural network libraries, such as TensorFlow. These implementations function by defining a single computational graph that is used to process each training/test case. The same graph is used for each input. By definition, the structure of the network differs from training/test

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case to training/test case. Technically the same problems apply to RNNs, as each case can have a different number of inputs. This is normally worked around by defining the network graph for the longest input to be considered, then padding all the inputs to this length, and ensuring that the padding does not interfere with the gradient updates. The equivalent tricks for structured networks are significantly more complex. The exception to this is of-course via dynamic components to the static frameworks (which TensorFlow and other such frameworks certainly do have). Even in a dynamic framework it remains a non-trivial task to implement these networks.

Implementing Back-propagation through structure

Conceptually, back-propagation through structure is not significantly more complex than back-propagation through time. However, in practice it is a very difficult algorithm to get right. It is very important to test for correctness using gradient checks, as it is easy to make a mistake and end-up with models that seem to work ok, but are actually crippled due to some mistake in the coding. Unfolding recursive autoencoders are particularly difficult, as the gradient must be propagated from all leaves. And output interior nodes cannot have their gradients calculated

graph) can be defined by the composition function:

$$f^{\text{RV}}(\tilde{u}, \tilde{v}) = \varphi \left([S \ R] \begin{bmatrix} \tilde{u} \\ \tilde{v} \end{bmatrix} + \tilde{b} \right) \quad (6.3)$$

$$= \varphi(S\tilde{u} + R\tilde{v} + \tilde{b}) \quad (6.4)$$

where \tilde{u} and \tilde{v} are the left and right substructures embeddings (word embeddings at the leaf node level), and S and R are the matrices defining how the left and right children's representations are to be combined.

This is a useful form as all constituency parse trees can be converted into binary parse trees, via left-factoring or right factoring (adding new nodes to the left or right to take some of the children). This is sometimes called binarization, or putting them into Chomsky normal form. This form of structured network has been used in many words, including Socher, Christopher D Manning, and Ng (2010), Socher, Pennington, et al. (2011), Socher, Huang, et al. (2011), Socher, Lin, et al. (2011) and Zhang et al. (2014). Notice that S and R matrices are shared for all RVs, so all substructures are composed in the same way, based only on whether they are on the left, or the right.

6.3.2 Dependency Tree

The dependency tree is the other commonly considered parse-tree. Structured networks based upon the dependency tree have been used by Socher, Karpathy, et al. (2014), Iyyer, Boyd-Graber, Claudino, et al. (2014), and Iyyer, Boyd-Graber, and Daumé III (2014). In these works rather than a using composition matrix for left-child and right-child, the composition matrix varies depending on the type of relationship of between the head word and its child. Each dependency relationship type has its own composition matrix. That is to say there are distinct composition matrices for each of nsub, det, nmod, case etc. This allows for multiple inputs to a single head node to be distinguished by their relationship, rather than their order. This is important for

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networks using a dependency parse tree structure as the relationship is significant, and the structure allows a node to have any number of inputs.

Consider a function $\pi(i, j)$ which returns the relationship between the head word at position i and the child word at position j . For example, using the tree shown in Figure 6.5, which has $w^8 = \text{parse}$ and $w^9 = \text{tree}$ then $\pi(8, 9) = \text{compound}$. This is used to define the composed representation for each RV:

$$f^{RV}(i) = \varphi \left(W^{\text{head}} C_{:, w^i} + \sum_{j \in \text{children}(i)} W^{\pi(i, j)} f_{RV}(j) + \tilde{b} \right) \quad (6.5)$$

Here $C_{:, w^i}$ is the word embedding for w^i , and W^{head} encodes the contribution of the headword to the composed representation. Similarly, $W^{\pi(i, j)}$ encodes the contribution of the child words. Note that the terminal case is just $f_{RV}(i) = \varphi(W^{\text{head}} C_{:, w^i} + \tilde{b})$ when a node i has no children. This use of the relationship to determine the composition matrix, increases both the networks expressiveness, and also handles the non-binary nature of dependency trees.

A similar technique could be applied to constituency parse trees. This would be using the part of speech (e.g. VBZ, NN) and phrase tags (e.g. NP, VP) for the sub-structures to choose the weight matrix. This would, however, lose the word-order information when multiple inputs have the same tag. This would be the case, for example, in the right-most branch shown in Figure 6.4, where both parse and tree have the NN POS tag, and thus using only the tags, rather than the order would leave parse tree indistinguishable from tree parse. This is not a problem for the dependency parse, as word relationships unambiguously correspond to the role in the phrase's meaning. As such, allowing the dependency relationship to define the mathematical relationship, as encoded in the composition matrix, only enhances expressibility.

until the gradients of their children are calculated. The solution to this is to process the node gradient calculation using a priority queue, where the priority is set by the depth of the node. Thus ensuring that all children are processed before their parents.

Socher, Christopher D Manning, and Ng (2010), "Learning continuous phrase representations and syntactic parsing with recursive neural networks"

Socher, Karpathy, et al. (2014), "Grounded compositional semantics for finding and describing images with sentences"

Iyyer, Boyd-Graber, Claudino, et al. (2014), "A neural network for factoid question answering over paragraphs"

Iyyer, Boyd-Graber, and Daumé III (2014), "Generating Sentences from Semantic Vector Space Representations"

Extended example

The full example for the $f^{RV}(9)$ from Equation (6.5) is:

$$\begin{aligned} f^{RV}(9) &= \varphi(W^{\text{head}} C_{:, \text{tree}} \\ &+ W^{\text{compound}}(W^{\text{head}} C_{:, \text{parse}} + \tilde{b}) \\ &+ W^{\text{det}}(W^{\text{head}} C_{:, \text{a}} + \tilde{b}) \\ &+ W^{\text{case}}(W^{\text{head}} C_{:, \text{of}} + \tilde{b}) \\ &+ \tilde{b}) \end{aligned}$$

This in turn would be composed as part of $f^{RV}(5)$ for the whole tree headed by $w^5 = \text{example}$. The output of each RV is a representation of that substructure.

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No gates

No long-term memory

We note that a limitation of most structural models, compared to the sequential RNNs, is their lack of explicit gating on memory (e.g. as in GRU and LSTM). Any given path down a tree can be looked at as a simple RNN comprised only of basic recurrent units. However, these paths are much shorter (being the logarithm of) than the full sequential length of the sentence, which offsets the need for such gating. Recall that the gating is to provide the longer short term memory.

Stenetorp (2013), "Transition-based Dependency Parsing Using Recursive Neural Networks"

The finer detail of parsing

Parsing is one of the most well studied problems in computational linguistics. Presented here is only the highest level overview. For more details on this, we recommend consulting the source materials. Ideally, with reference to a good traditional (that is to say non-neural network based) NLP textbook, such as: C. Manning and Schütze (1999).

For even greater capacity for the inputs to control the composition, would be to allow every word be composed in a different way. This can be done by giving the child nodes their own composition matrices, to go with their embedding vectors. The composition matrices encode the relationship, and the operation done in the composition. So not only is the representation of the (sub)phrase determined by a relationship between its constituents (as represented by their embeddings), but the nature of that relationship (as represented by the matrix) is also determined by those same constituents. In this approach at the leaf-nodes, every word not only has a word vector, but also a word matrix. This is discussed in Section 6.4.

6.3.3 Parsing

The initial work for both contingency tree structured networks (Socher, Christopher D Manning, and Ng 2010) and for dependency tree structured networks (Stenetorp 2013) was on the creation of parsers. This is actually rather different to the works that followed. In other works the structure is provided as part of the input (and is found during preprocessing). Whereas a parser must induce the structure of the network, from the unstructured input text. This is simpler for contingency parsing, than for dependency parsing.

When creating a binary contingency parse tree, any pair of nodes can only be merged if they are adjacent. The process described by Socher, Christopher D Manning, and Ng (2010), is to consider which nodes are to be composed into a higher level structure each in turn. For each pair of adjacent nodes, an RV can be applied to get a merged representation. A linear scoring function is also learned, that takes a merged representation and determines how good it was. This is trained such that correct merges score highly. Hinge loss is employed for this purpose. The Hinge loss function works on similar principles to negative sampling (see the motivation

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given in Section 4.4.2). Hinge loss is used to cause the merges that occur in the training set to score higher than those that do not. To perform the parse, nodes are merged; replacing them with their composed representation; and the new adjacent pairing score is then recomputed. Socher, Christopher D Manning, and Ng (2010) considered both greedy, and dynamic programming search to determine the order of composition, as well as a number of variants to add additional information to the process. The dependency tree parser extends beyond this method.

Dependency trees can have child-nodes that do not correspond to adjacent words (non-projective language). This means that the parser must consider that any (un-linked) node be linked to any other node. Traditional transition-based dependency parsers function by iteratively predicting links (transitions) to add to the structure based on its current state. Stenetorp (2013) observed that a composed representation similar to Equation (6.4), was an ideal input to a softmax classifier that would predict the next link to make. Conversely, the representation that is suitable for predicting the next link to make, is itself a composed representation. Note, that Stenetorp (2013) uses the same matrices for all relationships (unlike the works discussed in Section 6.3.2). This is required, as the relationships must be determined from the links made, and thus are not available before the parse. Bowman, Gauthier, et al. (2016), presents a work an an extension of the same principles, which combines the parsing step with the processing of the data to accomplish some task, in their case detecting entailment.

Getting the Embeddings out of the Parser

The implementation of Socher, Christopher D Manning, and Ng (2010), is publicly available. However, it does not export embeddings. It is nested deep inside the Stanford Parser, and thus accessing the embeddings is not at all trivial.

Bowman, Gauthier, et al. (2016), “A fast unified model for parsing and sentence understanding”

6.3.4 Recursive Autoencoders

Recursive autoencoders are autoencoders, just as the autoencoder discussed in Section 2.5.2, they reproduce their input. It should be noted that unlike the encoder-decoder RNN discussed in Section 6.2.1, they cannot

Application to image retrieval

An interesting application of structured networks was shown in Socher, Karpathy, et al. (2014). A dependency tree structured network was

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trained on a language modelling task (not as a recursive autoencoder, although that would also have been a valid option). Then, separately a convolutional neural network was trained to produce a vector output of the same dimensionality – an image embedding – such that its distance to its caption’s composed vector representation was minimised. The effect of this was that images and their captions are projected to a common vector space. This allowed for smart image retrieval, from descriptions, by having a set of all images, and storing their embedding representations. Then for any query, the sentence embedding can be found and the vector space of images can be searched for the nearest. The reverse is not generally as useful, as one can’t reasonably store all possible captions describing an image, so as to be able to search for the best one for a user provided image. This process of linking a sequence representation to an image embedding is not restricted to structured networks, and can be done with any of the representation methods discussed in this chapter. Further, as discussed in Section 4.6 it can also be done using pre-trained embedding on both sides through (kernel) CCA.

Unfolding RAE implementation

The implementation, and a pretrained model, of the unfolding recursive autoencoder of Socher, Huang, et

be trivially used to generate natural language from an arbitrary embeddings, as they require the knowledge of the tree structure to unfold into. Solving this would be the inverse problem of parsing (discussed in Section 6.3.3).

The models presented in Socher, Huang, et al. (2011) and Iyyer, Boyd-Graber, and Daumé III (2014) are unfolding recursive autoencoders. In these models an identical inverse tree is defined above the highest node. The loss function is the sum of the errors at the leaves, i.e. the distance in vector space between the reconstructed words embeddings and the input word-embeddings. This was based on a simpler earlier model: the normal (that is to say, not unfolding) recursive autoencoder.

The normal recursive autoencoder, as used in Socher, Pennington, et al. (2011) and Zhang et al. (2014) only performs the unfolding for a single node at a time during training. That means that it assesses how well each merge can individually be reconstructed, not the success of the overall reconstruction. This per merge reconstruction has a loss function based on the difference between the reconstructed embeddings and the inputs embeddings. Note that those inputs/reconstructions are not word embeddings: they are the learned merged representations, except when the inputs happen to be leaf node. This single unfold loss covers the auto-encoding nature of each merge; but does not give any direct assurances of the auto-encoding nature of the whole structure. However, it should be noted that while it is not trained for, the reconstruction components (that during training are applied only at nodes) can nevertheless be applied recursively from the top layer, to allow for full reconstruction.

6.3.4.1 Semi-supervised

In the case of all these autoencoders, except Iyyer, Boyd-Graber, and Daumé III (2014), a second source of information is also used to calculate the loss during train-

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ing. The networks are being simultaneously trained to perform a task, and to regenerate their input. This is often considered as semi-supervised learning, as unlabelled data can be used to train the auto-encoding part (unsupervised) gaining a good representation, and the labelled data can be used to train the task output part (supervised) making that representation useful for the task. This is done by imposing an additional loss function onto the output of the central/top node.

- In Socher, Pennington, et al. (2011) this was for sentiment analysis.
- In Socher, Huang, et al. (2011) this was for paraphrase detection.
- In Zhang et al. (2014) this was the distance between embeddings of equivalent translated phrases of two RAEs for different languages.

The reconstruction loss and the supervised loss can be summed, optimised in alternating sequences, or the reconstructed loss can be optimised first, then the labelled data used for fine-tuning.

al. (2011) is available online at <https://tinyurl.com/URAE2011>. It is easy to use as a command-line Matlab script to generate embeddings.

Socher, Christopher D Manning, and Ng (2010), “Learning continuous phrase representations and syntactic parsing with recursive neural networks”

6.4 Matrix Vector Models

6.4.1 Structured Matrix Vector Model

Socher, Huval, et al. (2012) proposed that each node in the graph should define not only a vector embedding, but a matrix defining how it was to be combined with other nodes. That is to say, each word and each phrase has both an embedding, and a composition matrix.

Sequential models are often preferred to structural models

Sequential (RNN) models are much more heavily researched than structural models. They have better software libraries, are easier to implement, and have more known “tricks” (like gates and attention). In theory it is possible for a sequential model (with sufficiently deep and wide RUs) to internalise the connections that a structural model would possess. While structural models are theoretically nicer from a linguistics standpoint, pragmatically they are the last resort in modelling. When at-

6 Sentence Representations and Beyond

tempting to find a useful representation of a sentence for a task, one should first try a sum of word embeddings with a simple network on-top, then a sequential model (based on LSTM or GRU), and only if these fail then try a structured model. Arguably before using any neural network approach at all, one should eliminate bag of words, bag of n-grams, the dimensionality reduced version of those bags, and also eliminate LSI and LDA as inputs for the task.

Socher, Huval, et al. (2012), "Semantic compositionality through recursive matrix-vector spaces"

Consider this for binary constituency parse trees. The composition function is as follows:

$$f^{\text{RV}}(\tilde{u}, \tilde{v}, U, V) = \varphi([S \ R][U\tilde{v}; V\tilde{u}] + \tilde{b}) \quad (6.6)$$

$$= \varphi(SU\tilde{v} + RV\tilde{u} + \tilde{b}) \quad (6.7)$$

$$F^{\text{RV}}(U, V) = W[U; V] = W^1U + W^rV \quad (6.8)$$

f^{RV} gives the composed embedding, and F^{RV} gives the composing matrix. The S and R represent the left and right composition matrix components that are the same for all nodes (regardless of content). The U and V represent the per word/node child composition matrix components. We note that S and R could, in theory, be rolled in to U and R as part of the learning. The \tilde{u} and \tilde{v} represent the per word/node children embeddings, and W represents the method for merging two composition matrices.

We note that one can define increasingly complex and powerful structured networks along these lines; though one does run the risk of very long training times and of over-fitting.

6.4.2 Sequential Matrix Vector Model

R. Wang, Liu, and McDonald (2017), "A Matrix-Vector Recurrent Unit Model for Capturing Compositional Semantics in Phrase Embeddings"

A similar approach, of capturing a per word matrix, was used on a sequential model by R. Wang, Liu, and McDonald (2017). While sequential models are a special case of structured models, it should be noted that unlike the structured models discussed prior, this matrix vector RNN features a gated memory. This matrix-vector RNN is an extension of the GRU discussed in Chapter 3, but without a reset gate.

In this sequential model, advancing a time step, is to perform a composition. This composition is for between the input word and the (previous) state. Rather than directly between two nodes in the network as in the structural case. It should be understood that composing

6.4 Matrix Vector Models

with the state is not the same as composing the current input with the previous input. But rather as composing the current input with all previous inputs (though not equally).

As depicted in Figure 6.6 each word, w^t is represented by a word embedding \tilde{x}^t and matrix: \tilde{X}^{w^t} , these are the inputs at each time step. The network outputs and states are the composed embedding \hat{y}^t and matrix Y^t .

Remember:

The product of a matrix with a concatenated vector, is the same as the sum of the two blocks of that matrix each multiplied by the blocks of that vector.

$$h^t = \tanh(W^h[x^t; \hat{y}^{t-1}] + \tilde{b}^h) \quad (6.9)$$

$$z^t = \sigma(Y^{t-1}x^t + X^t\hat{y}^{t-1} + \tilde{b}^z) \quad (6.10)$$

$$\hat{y}^t = z^t \odot h^t + (1 - z^t) \odot \hat{y}^{t-1} \quad (6.11)$$

$$Y^t = \tanh(W^Y[Y^{t-1}; X^t] + \tilde{b}^Y) \quad (6.12)$$

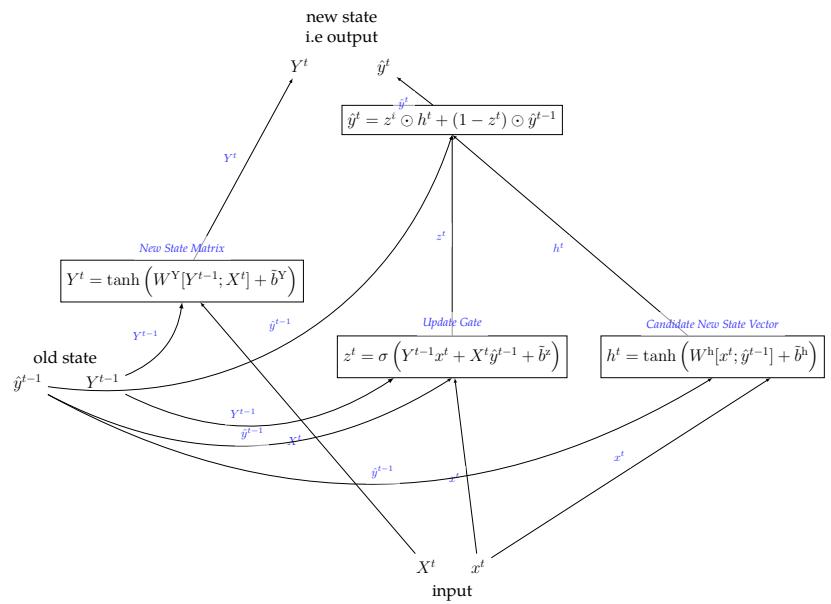
The matrices W^h , W^Y and the biases \tilde{b}^h , \tilde{b}^z , \tilde{b}^Y are shared across all time steps/compositions. W^Y controls how the next state-composition Y^t matrix is generated from its previous value and the input composition matrix, X^t ; W^h similarly controls the value of the candidate state-embedding h^t .

h^t is the candidate composed embedding (to be output/used as state). z_t is the update gate, it controls how much of the actual composed embedding (\hat{y}^t) comes from the candidate h^t and how much comes from the previous value (\hat{y}^{t-1}). The composition matrix Y^t (which is also part of the state/output) is not gated.

Notice, that the state composition matrix Y^{t-1} is only used to control the gate z^t , not to directly affect the candidate composed embedding h^t . Indeed, in fact one can note that all similarity to the structural method of Socher, Huval, et al. (2012) is applied in the gate z^t . The method for calculating h^t is similar to that of a normal RU.

6 Sentence Representations and Beyond

Figure 6.6: A Matrix Vector recurrent unit



The work of R. Wang, Liu, and McDonald (2017), was targeting short phrases. This likely explains the reason for not needing a forget gates. The extension is obvious, and may be beneficial when applying this method to sentences

6.5 Conclusion, on compositionality

It is tempting to think of the structured models as compositional, and the sequential models as non-compositional. However, this is incorrect.

The compositional nature of the structured models is obvious: the vector for a phrase is composed from the vectors of the words that the phrase is formed from.

Sequential models are able to learn the structures. For example, learning that a word from n time steps ago is to be remembered in the RNN state, to then be optimally combined with the current word, in the determination of the next state. This indirectly allows the same compositionality as the structured models. It

6.5 Conclusion, on compositionality

has been shown that sequential models are indeed in-practice able to learn such relationships between words (L. White et al. 2017). More generally as almost all aspects of language have some degree of compositionality, and sequential models work very well on most language tasks, this implicitly shows that they have sufficient representational capacity to learn sufficient degrees of compositional processing to accomplish these tasks.

L. White et al. (2017), "Learning Distributions of Meant Color"

In fact, it has been suggested that even some unordered models such as sum of word embeddings are able to capture some of what would be thought of as compositional information. Ritter et al. (2015) devised a small corpus of short sentences describing containing relationships between the locations of objects. The task and dataset was constructed such that a model must understand some compositionality, to be able to classify which relationships were described. Ritter et al. (2015) tested several sentence representations as the input to a naïve Bayes classifier being trained to predict the relationship. They found that when using sums of high-quality word embeddings as the input, the accuracy not only exceeded the baseline, but even exceeded that from using representation from a structural model. This suggests that a surprising amount of compositional information is being captured into the embeddings; which allows simple addition to be used as a composition rule. Though it being ignorant of word order does mean it certainly couldn't be doing so perfectly, however the presence of other words may be surprisingly effective hinting at the word order (Lyndon White et al. 2016b), thus allow for more apparently compositional knowledge to be encoded than is expected.

To conclude, the compositionality capacity of many models is not as clear cut as it may initially seem. Further to that the requirement for a particular task to actually handle compositional reasoning is also not always present, or at least not always a significant factor in practical applications. We have discussed many models in this section, and their complexity varies sig-

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nificantly. They range from the very simple sum of word embeddings all the way to the the structured matrix models, which are some of the more complicated neural networks ever proposed.

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Part III

Publications

How Well Sentence Embeddings Capture Meaning

This paper was presented at the 20th Australasian Document Computing Symposium, in 2015.

Chapter 6

How Well Sentence Embeddings Capture Meaning

Abstract

Several approaches for embedding a sentence into a vector space have been developed. However, it is unclear to what extent the sentence’s position in the vector space reflects its semantic meaning, rather than other factors such as syntactic structure. Depending on the model used for the embeddings this will vary – different models are suited for different down-stream applications. For applications such as machine translation and automated summarization, it is highly desirable to have semantic meaning encoded in the embedding. We consider this to be the quality of *semantic localization* for the model – how well the sentences’ meanings coincides with their embedding’s position in vector space. Currently the semantic localization is assessed indirectly through practical benchmarks for specific applications.

In this paper, we ground the semantic localization problem through a *semantic classification* task. The task is to classify sentences according to their meaning. A SVM with a linear kernel is used to perform the classification using the sentence vectors as its input. The sentences from subsets of two corpora, the Microsoft Research Paraphrase corpus and the Opinosis corpus, were partitioned according to their semantic equivalence. These partitions give the target classes for the classification task. Several existing models, including URAE, PV-DM and PV-DBOW, were assessed against a bag of words benchmark.

6.1 Introduction

Sentence embeddings are often referred to as semantic vector space representations **iyyer2014generating**. Embedding the meaning of a sentence into a vector space is expected to be very useful for natural language tasks. Vector representation of natural languages enables discourse analysis to take advantage of the array of tools available for computation in vector spaces. However, the embeddings of a sentence may encode a number of factors including semantic meaning, syntactic structure and topic. Since many of these embeddings are learned unsupervised on textual corpora using various models with different training objectives, it is not entirely clear the emphasis placed on each factor in the encoding. For applications where encoding semantic meaning is particularly desirable, such as machine translation and automatic summarization, it is crucial to be able to assess how well the embeddings capture the sentence’s semantics. In other words, for successful application to these areas it is required that the embeddings generated by the models correctly encode meaning such that sentences with the same meaning are co-located in the vector space, and sentences with differing meanings are further away. However, few current models are directly trained to optimize for this criteria.

Currently sentence embeddings are often generated as a byproduct of unsupervised, or semi-supervised, tasks. These tasks include: word prediction **le2014distributed**; recreation of input, as in the auto-encoders of **SocherEtAl2011:RAE**; **SocherEtAl2011:PoolRAE** and **iyyer2014generating**; and syntactic structural classification **SocherEtAl2013:CVG**; **socher2010PhraseEmbedding**. As a result the vector representations of the input sentences learned by these models are tuned towards the chosen optimization task. When employing the embeddings produced as features for other tasks, the information captured by the embeddings often proved to be very useful: e.g. approaching or exceeding previous state-of-the-art results, in sentiment analysis **SocherEtAl2011:RAE**;

SocherMVRNN; le2014distributed and paraphrase detection **SocherEtAl2011:PoolRAE**. However these practical applications do not directly show how well meaning is captured by the embeddings.

This paper provides a new method to assess how well the models are capturing semantic information. A strict definition for the semantic equivalence of sentences is: that each sentence shall entail the other. Such mutually entailing sentences are called *paraphrases*. In this paper we propose to use paraphrases to assess how well the true semantic space aligns with the vector space the models embed into. It thus assesses whether projecting a sentence via the models in to the vector space preserves meaning.

The evaluation corpora were prepared by grouping paraphrases from the Microsoft Research Paraphrase (MSRP) **msrParapharaCorpus** and Opinosis **ganesan2010opinosis** corpora. A semantic classification task was defined which assesses if the model's embeddings could be used to correctly classify sentences as belonging to the paraphrase group with semantically equivalent sentences. Ensuring that sentences of common meaning, but differing form are located in vector space together, is a challenging task and shows a model's semantic encoding strength. This assessment, together with out recent work in the area, allows for a better understanding of how these models work, and suggest new directions for the development in this area.

The assessment proposed in this paper adds to the recent work on semantic evaluation methods, such as the work of Gershman and Tenenbaum **gershmanphrase** and of Ritter et. al. **RitterPosition**. In particular, the real-world corpus based assessment in this paper is highly complementary to the structured artificial corpus based assessment of Ritter et. al. These methods are discussed in more detail in the next section.

The rest of the paper is organized into the following sections. ?? discusses the existing models being assessed, the traditional assessment methods, and the aforementioned more recent semantic correctness based assessments. ?? describes the processes by which the models are evaluated using our new method, and the parameters used in the evaluation. ?? continues into more details on the development of the evaluation corpora for the semantic classification evaluation task. ?? details the results from evaluating the models and discusses the implications for their semantic consistency. ?? closes the paper and suggests new directions for development.

6.2 Background

6.2.1 Models

Three well known sentence embedding methods are evaluated in this work. The compositional distributed model of the Unfolding Recursive Autoencoder (URAE) by Socher et. al. **SocherEtAl2011:PoolRAE**; and the two word content predictive models, Distributed Memory (PV-DM) and Distributed Bag of Words by Le and Mikolov **le2014distributed**. In addition to these advanced sentence embedding models, a simple average of word embeddings, from Mikolov et. al. **mikolovSkip**, is also assessed. These models and their variant forms have been applied to a number of natural language processing tasks in the past, as detailed in the subsequent sections, but not to a real-sentence semantic classification task as described here.

Unfolding Recursive Auto-Encoder (URAE)

The Unfolding Recursive Autoencoder (URAE) **SocherEtAl2011:PoolRAE** is an autoencoder based method. It functions by recursively using a single layer feedforward neural-network to combine embedded representations, following the parse tree. Its optimization target is to be able to reverse (unfold) the merges and produce the original sentence. The central folding layer – where the whole sentence is collapsed to a single embedding vector – is the sentence representation.

PV-DM

The Distributed Memory Paragraph Vectors (PV-DM) **le2014distributed** method is based on an extension of the Continuous Bag-of-Words word-embedding model **mikolov2013efficient**. It is trained using a sliding window of words to predict the next word. The softmax predictor network is fed a word-embedding for each word in the window, plus an additional sentence embedding vector which is reused for all words in the sentence – called the paragraph vector in **le2014distributed**. These input embeddings can be concatenated or averaged; in the results below they were concatenated. During training both word and sentence vectors are allowed to vary, in evaluation (i.e.

inference), the word vectors are locked and the sentence vector is trained until convergence on the prediction task occurs.

PV-DBOW

Distributed Bag of Words Paragraph Vectors (PV-DBOW) **le2014distributed**, is based on the Skip-gram model for word-embeddings, also from **mikolov2013efficient**. In PV-DBOW a sentence vector is used as the sole input to a neural net. That network is tasked with predicting the words in the sentence. At each training iteration, the network is tasked to predict a number of words from the sentence, selected with a specified window size, using the sentence vector being trained as the input. As with PV-DM to infer embedding the rest of the network is locked, and only the sentence vector input allowed to vary, it is then trained to convergence.

Sum and Mean of Word Embeddings (SOWE and MOWE)

Taking the element-wise sum or mean of the word embeddings over all words in the sentence also produces a vector with the potential to encode meaning. Like traditional bag of words no order information is encoded, but the model can take into consideration word relations such as synonymity as encoded by the word vectors. The mean was used as baseline in **le2014distributed**. The sum of word embeddings first considered in **mikolovSkip** for short phrases, it was found to be an effective model for summarization in **KaagebExtractiveSummaristation**. The cosine distance, as is commonly used when comparing distances between embeddings, is invariant between sum and mean of word embeddings. Both sum and mean of word embeddings are computationally cheap models, particularly given pretrained word embeddings are available.

6.2.2 General Evaluation Methods

As discussed in the introduction, current methods of evaluating the quality of embedding are on direct practical applications designed down-stream.

Evaluation on a Paraphrase Detection task takes the form of being presented with pairs of sentences and tasked with determining if the sentences are paraphrases or not. The MSRP Corpus, **msrParapharaCorpus** which we used in the semantic classification task, is intended for such use. This pairwise check is valuable, and does indicate to a certain extent if the embeddings are capturing meaning, or not. However, by considering groups of paraphrases, a deeper intuition can be gained on the arrangement of meaning within the vector space.

Sentiment Analysis is very commonly used task for evaluating embeddings. It was used both for the recursive autoencoder in **SocherEtAl2011:RAE** and for the paragraph vector models in **le2014distributed**. Sentiment Analysis is classifying a text as positive or negative, or assigning a score as in the Sentiment Treebank **RvNTN**. Determining the sentiment of a sentence is partially a semantic task, but it is lacking in several areas that would be required for meaning. For example, there is only an indirect requirement for the model to process the subject at all. Sentiment Analysis is a key task in natural language processing, but it is distinct from semantic meaning.

Document Classification is a classic natural language processing task. A particular case of this is topic categorization. Early work in the area goes back to **maron1961automatic** and **borko1963automatic**. Much more recently it has been used to assess the convolution neural networks of **DBLP:journals/corr/ZhangL15**, where the articles of several news corpora were classified into categories such as “Sports”, “Business” and “Entertainment”. A huge spectrum of different sentences are assigned to the same topic. It is thus too broad and insufficiently specific to evaluate the consistency of meanings. Information retrieval can be seen as the inverse of the document classification task.

Information Retrieval is the task of identifying the documents which most match a query. Such document selection depends almost entirely on topic matching. Suitable results for information retrieval have no requirement to agree on meaning, though text with the same meaning are more likely to match the same queries.

The evaluation of semantic consistency requires a task which is fine grained, and preserving meaning. Document Classification and Information Retrieval are insufficiently fine-grained. Sentiment Analysis does not preserve meaning, only semantic orientation. Paraphrase Detection is directly relevant to evaluating semantic constancy, however it is a binary choice based on a pairwise comparison – a more spatial application is desirable for evaluating these vector spaces. Thus the current down-stream application tasks are not sufficient for assessing semantic consistency – more specialized methods are required.

6.2.3 Evaluations of Semantic Consistency

Semantic consistency for word embeddings is often measured using the analogy task. In an analogy the meta-relation: *A is to B as C is to D*. Mikolov et. al. **mikolov2013linguisticsubstructures** demonstrated that the word-embedding models are semantically consistent by showing that the semantic relations between words were reflected as a linear offset in the vector space. That is to say, for embeddings $\tilde{x}_a, \tilde{x}_b, \tilde{x}_c, \tilde{x}_d$ corresponding to words A, B, C and D, respectively; it was tested that if for a strong relationship matching between A/B and C/D, then the offset vector would be approximately equal: $\tilde{x}_b - \tilde{x}_a \approx \tilde{x}_d - \tilde{x}_c$. Rearranging this in word space gets the often quoted example of *King – Man + Woman ≈ Queen*, As man is to woman, king is to queen. In the rating task as described by **jurgens2012semeval**, the goal is to rank such analogous word pairs based on the degree the relation matches. Thus to evaluate the word-embedding model using this task, it was a matter of sorting closeness of the corresponding offset vectors. Surprisingly strong results were found on this task **mikolov2013linguisticsubstructures**. It was thus demonstrated that word embeddings were not simply semantically consistent, but more so that this consistency was displayed as local linearity. This result gives confidence in the semantic quality of the word embeddings. However, this relationship analogy test cannot be performed for sentence embeddings.

Gershman et. al. **gershmanphrase**, compares the distances of modified sentences in vector space, to the semantic distances ascribed to them by human raters. Like the analogy task for word vectors, this task requires ranking the targets based on the vector distance, however instead of rating on the strength of relationships it measures simply the similarities of the sentences to an original base sentence for each group. In that evaluation 30 simple base sentences of the form *A [adjective1] [noun1] [prepositional phrase] [adjective2] [noun2]* were modified to produce 4 difference derived sentences. The derived sentences were produced by swapping the nouns, swapping the adjectives, reversing the positional phrase (so *behind* becomes *in front of*), and a paraphrase by doing all of the aforementioned changes. Human raters were tasked with sorting the transformed sentences in similarity to the base sentence. This evaluation found that the embedding models considered did not agree with the semantic similarity rankings placed by humans. While the sentence embedding models performed poorly on the distance ranking measure, it is also worth considering how they perform on a meaning classification task.

A meaning classification task was recently proposed by Ritter et. al. **RitterPosition**, to classify sentences based on which spatial relationship was described. The task was to classify the sentence as describing: *Adhesion to Vertical Surface*, *Support by Horizontal Surface*, *Full Containment*, *Partial Containment*, or *Support from Above*. In this evaluation also, the sentences took a very structured form: *There is a [noun1] [on/in] the [noun2]*. These highly structured sentences take advantage of the disconnection between word content and the positional relationship described to form a task that must be solved by a compositional understanding combining the understanding of the words. “*The apple is on the refrigerator*” and “*The magnet is on the refrigerator*” belong to two separate spatial categories, even though the word content is very similar. Surprisingly, the simple model of adding word vectors outperformed compositional models such as the recursive autoencoder. The result does have some limitation due to the highly artificial nature of the sentences, and the restriction to categorizing into a small number of classes based only on the meaning in terms of positional relationship. To generalize this task, in this paper we consider real world sentences being classed into groups according to their full semantic meaning.

6.3 Methodology

To evaluate how well a model’s vectors capture the meaning of a sentence, a semantic classification task was defined. The task is to classify sentences into classes where each shares the same meaning. Each class is thus defined as a paraphrase groups. This is a far finer-grained task than topic classification. It is a multiclass classification problem, rather than the binary decision problem of paraphrase detection. Such multiclass classification requires the paraphrase groups to be projected into compact and distinct groups in the vector space. A model which produces such embeddings which are thus easily classifiable according to their meaning can be seen to have good semantic localization.

This semantic classification does not have direct practical application – it is rare that the need will be to quantify sentences into groups with the same prior known meaning. Rather it serves as a measure to assess the models general suitability for other tasks requiring a model with consistency between meaning and embedding.

To evaluate the success at the task three main processes are involved, as shown in ??: Corpus Preparation, Model Preparation, and the Semantic Classification task itself.

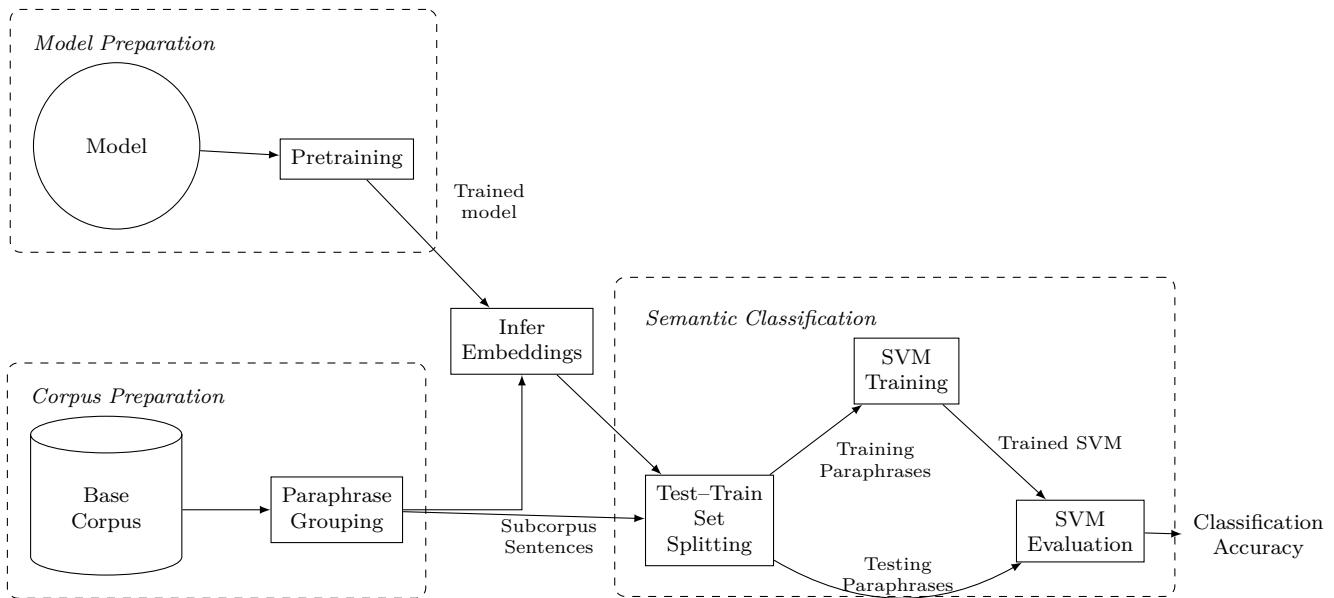


Figure 6.1: Process Diagram for the Evaluation of Semantic Consistency via our method

6.3.1 Corpus Preparation

The construction of each of the corpora is detailed more fully in the next section. In brief: Two corpora were constructed by selecting subsets of the Microsoft Research Paraphrase (MSRP) **msrParapharaCorpus** and of the Opinosis **ganesan2010opinosis** corpora. The corpora were partitioned into groups of paraphrases – sentences with the same meaning. Any paraphrase groups with less than three sentences were discarded. The paraphrase grouping was carried out manually for Opinosis, and automatically for the MSRP corpus using the existing paraphrase pairings. The paraphrase groups divide the total semantic space of the corpora into discrete classes, where each class contains sentences sharing the same meaning.

It is by comparing the ability of the models to produce embeddings which can be classified back into these classes, that we can compare the real semantic space partitions to their corresponding vector embedding space regions.

6.3.2 Model Preparation and Inferring Vectors

Prior to application to semantic classification, as with any task the models had to be pretrained. Here we use the term *pretraining* to differentiate the model training from the classifier training. The pretraining is not done using the evaluation corpora as they are both very small. Instead other data are used, and the inference/evaluation procedure given for each method was then used to produce the vectors for each sentence. The model parameters used are detailed below.

Unfolding Recursive Auto-Encoder (URAE)

In this evaluation we make use of the pretrained network that Socher et. al. have graciously made available¹, full information is available in the paper **SocherEtAl2011:PoolRAE**. It is initialized on the unsupervised Collobert and Weston word embeddings **collobert2008unified**, and training on a subset of 150,000 sentences from the gigaword corpus. It produces embeddings with 200 dimensions. This pretrained model when used with dynamic pooling and other word based features performed very well on the MSRP corpus paraphrase detection. However in the evaluation below the dynamic pooling techniques are not used as they are only directly suitable for enhancing pairwise comparisons between sentences.

¹<http://www.socher.org/index.php/Main/DynamicPoolingAndUnfoldingRecursiveAutoencodersForParaphraseDetection>

Paragraph Vector Methods (PV-DM and PV-DBOW)

Both PV-DM and PV-DBOW, were evaluated using the GenSim implementation **rehurek_lrec** from the current *develop* branch². Both were trained on approximately 1.2 million sentences from randomly selected Wikipedia articles, and the window size was set to 8 words, and the vectors were of 300 dimensions.

Sum and Mean of Word Embeddings (SOWE and MOWE)

The word embeddings used for MOWE were taken from the Google News pretrained model³ based on the method described in **mikolovSkip**. This has been trained on 100 million sentences from Google News. A small portion of the evaluation corpus did not have embeddings in the Google News model. These tokens were largely numerals, punctuation symbols, proper nouns and unusual spellings, as well as the stop-words: “and”, “a” and “of”. These words were simply skipped. The resulting embeddings have 300 dimensions, like the word embeddings they were based on.

²<https://github.com/piskvorky/gensim/tree/develop/>

³<https://code.google.com/p/word2vec/>

Bag of Words (BOW and PCA BOW)

A bag of words (BOW) model is also presented as a baseline. There is a dimension in each vector embedding for the count of each token, including punctuation, in the sentence. In the Opinosis and MSRP subcorpora there were a total of 1,085 and 2,976 unique tokens respectively, leading to BOW embeddings of corresponding dimensionality. As it is a distributional rather than distributed representation, the BOW model does not need any pretraining step. For comparison to the lower dimensional models Principle Component Analysis (PCA) was applied to the BOW embeddings to produce an additional baseline set of embeddings of 300 dimensions – in line with PV-DM, PV-DBOW, SOWE, and MOWE models. It does not quite follow the steps shown in ??, as the PCA pretraining step is performed on the training embeddings only during the SVM classification process, and it is used to infer the PCA BOW embeddings during the testing step. This avoids unfair information transfer where the PCA would otherwise be about to choose representations optimized for the whole set, including the test data. It was found that when the PCA model was allowed to cheat in this way it performed a few percentage points better. The bag of words models do not have any outside knowledge.

6.3.3 Semantic Classification

The core of this evaluation procedure is in the semantic classification step. A support vector machine (SVM), with a linear kernel, and class weighting was applied to the task of predicting which paraphrase group each sentence belongs to. Classification was verified using 3-fold cross-validation across different splits of the testing/training data, the average results are shown in this section. The splits were in proportion to the class size. For the smallest groups this means there were two training cases and one test case to classify.

In this paper, only a linear kernel was used, because a more powerful kernel such as RBF may be able to compensate for irregularities in the vector space, which makes model comparison more difficult. Scikit-learn **scikit-learn** was used to orchestrate the cross-validation and to interface with the LibLinear SVM implementation **LIBLINEAR**. As the linear SVM's classification success depends on how linearly separable the input data is, thus this assessed the quality of the localization of the paraphrase groupings embeddings.

6.4 Corpus Construction

6.4.1 Microsoft Research Paraphrased Grouped Subcorpus

The MSRP corpus is a very well established data set for the paraphrase detection task **msrParapharaCorpus**. Sentences are presented as pairs which are either paraphrases, or not. A significant number of paraphrases appear in multiple different pairings. Using this information, groups of paraphrases can be formed.

The corpus was partitioned according to sentence meaning by taking the symmetric and transitive closures the set of paraphrase pairs. For example if sentences A , B , C and D were present in the original corpus as paraphrase pairs: A, B, D, A and B, C then the paraphrase group $\{A, B, C, D\}$ is found. Any paraphrase groups containing less than 3 phrases were discarded. The resulting sub-corpus has the breakdown as shown in ??.

6.4.2 Opinosis Paraphrase Grouped Subcorpus

The Opinosis Corpus **ganesan2010opinosis** was used as secondary source of original real-world text. It is sourced from several online review sites: TripAdvisor, Edmunds.com, and Amazon.com, and contains single sentence statements about hotels, cars and electronics. The advantage of this as a source for texts is that comments on the quality of services and products tend to be along similar lines. The review sentences are syntactically simpler than sentences from a news-wire corpus, and also contain less named entities. However, as they are from more casual communications, the adherence to grammar and spelling may be less formal.

Paraphrases were identified using the standard criterion: bidirectional entailment. For a paraphrase group S of sentences: $\forall s_1, s_2 \in S, s_1 \models s_2 \wedge s_2 \models s_1$, every sentence in the group entails the every other sentence in the group. A stricter interpretation of bidirectional entailment was used, as compared to the “mostly bidirectional entailment” used in the MSRP corpus. The grouping was carried out manually. Where it was unclear as to the group a particular phrase should belong to it was left out of the corpus entirely. The general guidelines were as follows.

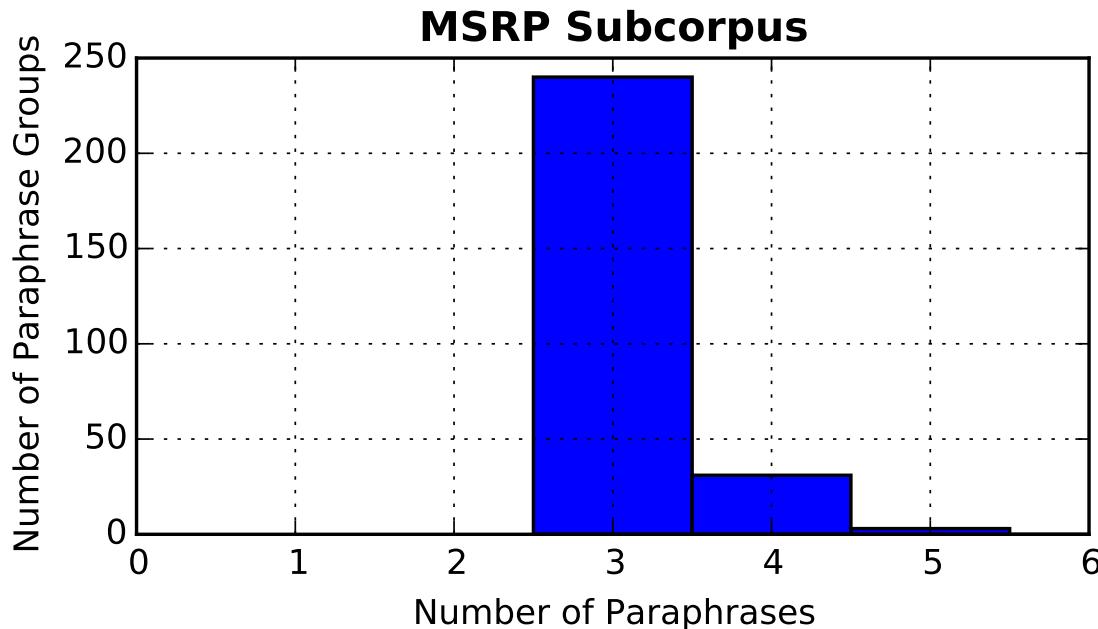


Figure 6.2: Break down of how many paraphrases groups are present in the MSRP subcorpus of which sizes. It contains a total of 859 unique sentences, broken up into 273 paraphrase groups.

- Tense, Transitional Phrases, and Discourse and Pragmatic Markers were ignored.
- Statement intensity was coarsely quantized.
- Approximately equal quantitative and qualitative values were treated as synonymous.
- Sentences with entities mentioned explicitly were grouped separately from similar statements where they were implied.
- Sentences with additional information were grouped separately from those without that information.

The final point is the most significant change from the practices apparent in the construction of the MSRP corpus. Sentences with differing or additional information were classified as non-paraphrases. This requirement comes from the definition of bidirectional entailment. For example, “*The staff were friendly and polite.*”, “*The staff were polite.*” and “*The staff were friendly.*” are in three separate paraphrase groups. The creators of the MSRP corpus, however, note “...the majority of the equivalent pairs in this dataset exhibit ‘mostly bidirectional entailments’, with one sentence containing information ‘that differs’ from or is not contained in the other.” **msrParapharaCorpus**. While this does lead to more varied paraphrases; it strays from the strict linguistic definition of a paraphrase, which complicates the evaluation of the semantic space attempted here. This stricter adherence to bidirectional entailment resulted in finer separation of groups, which makes this a more challenging corpus.

After the corpus had been broken into paraphrase groups some simple post-processing was done. Several artifacts present in the original corpus were removed, such as substituting the ampersand symbol for &. Any paraphrase groups containing identical sentences were merged, and duplicates removed. Finally, any group with less than three phrases was discarded. With this complete the breakdown is as in ??.

Further information on the construction of the corpora in this section, and download links are available online.⁴

6.5 Results and Discussion

6.5.1 Classification Results and Discussion

The results of performing the evaluation method described in ?? are shown in ??.

⁴http://white.ucc.asn.au/resources/paraphrase_grouped_corpora/

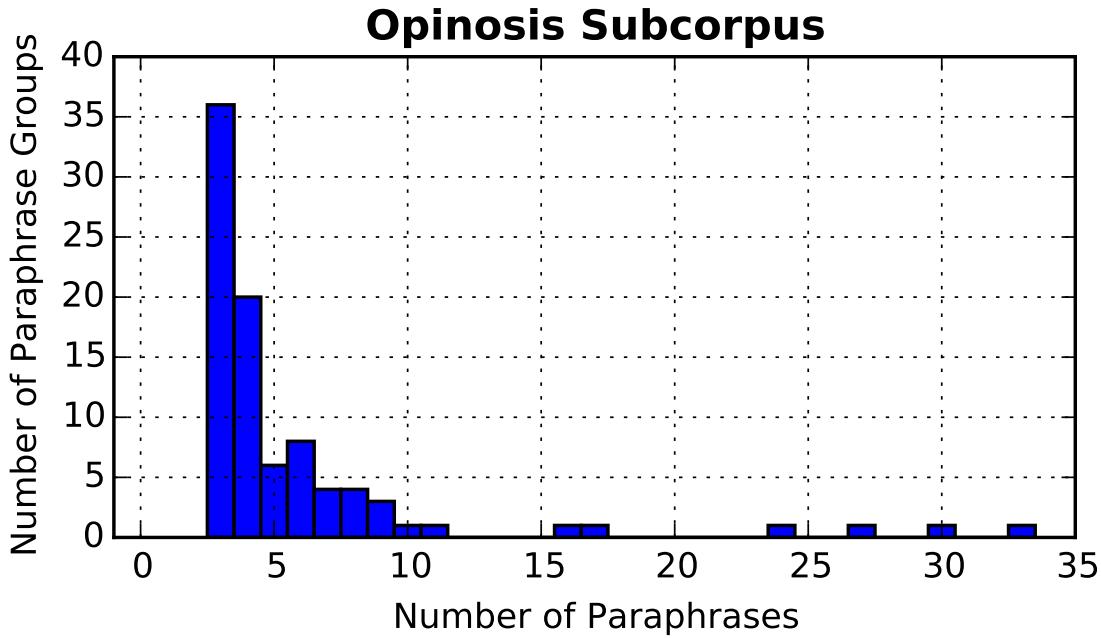


Figure 6.3: Break down of how many paraphrases groups are present in the Opinosis subcorpus of which sizes. It contains a total of 521 unique sentences, broken up into 89 paraphrase groups.

	MSRP Subcorpus	Opinosis Subcorpus
PV-DM	78.00%	38.26%
PV-DBOW	89.93%	32.19%
URAE	51.14%	20.86%
MOWE	97.91%	69.30%
SOWE	98.02%	68.75%
BOW	98.37%	65.23%
PCA BOW	97.96%	54.43%

Table 6.1: The semantic classification accuracy of the various models across the two evaluation corpora.

While the relative performance of the models is similar between the corpora, the absolute performance differs. On the absolute scale, all the models perform much better on the MSRP subcorpus than on the Opinosis subcorpus. This can be attributed to the significantly more distinct classes in the MSRP subcorpus. The Opinosis subcorpus draws a finer line between sentences with similar meanings. As discussed earlier, for example there is a paraphrase group for “*The staff were polite.*”, another for “*The staff were friendly.*”, and a third for “*The staff were friendly and polite.*”. Under the guidelines used for paraphrases in MSRP, these would all have been considered the same group. Secondly, there is a much wider range of topics in the MSRP. Thus the paraphrase groups with different meanings in MSRP corpus are also more likely to have different topic entirely than those from Opinosis. Thus the the ground truth of the semantics separability of phrases from the MSRP corpus is higher than for Opinosis, making the semantic classification of the Opinosis subcorpus is a more challenging task.

The URAE model performs the worst of all models evaluated. In **KaagebExtractiveSummaristation** it was suggested that the URAE’s poor performance at summarizing the Opinosis corpus could potentially be attributed to the less formally structured product reviews – the URAE being a highly structured compositional model. However, here it also performed poorly on the MSRP – which it was created for **SocherEtAl2011:PoolRAE**. The exact same model from **SocherEtAl2011:PoolRAE** was used here – though this did put it at a dimensional disadvantage over the other models having 200 dimensions to the other’s 300. The key difference from **SocherEtAl2011:PoolRAE**, beyond the changing to a multiclass classification problem, was the lack of the complementary word-level features as used in the dynamic pooling layer. This suggests the model could benefit from such world level features – as the very strong performance of the word-based model indicates.

The word based models, MOWE, SOWE, BOW and PCA BOW, performed very well. This

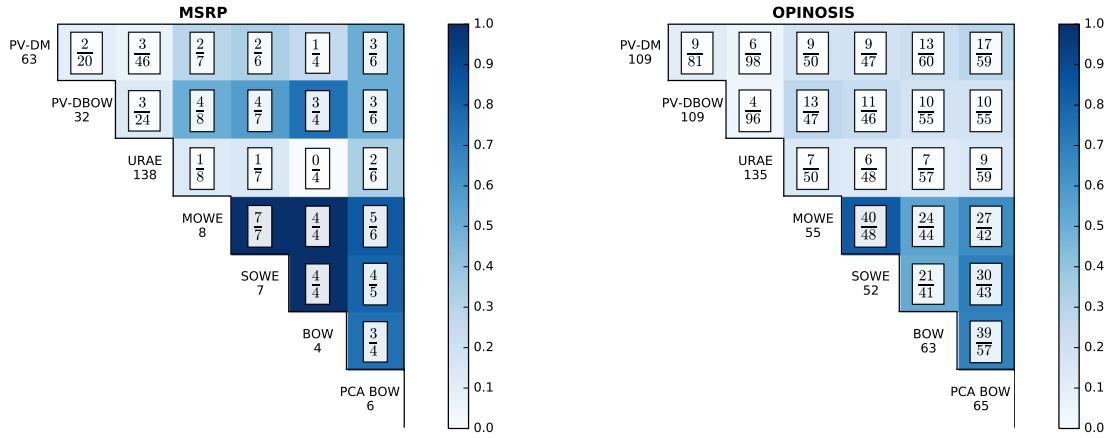


Figure 6.4: The misclassification agreement between each of the models for the MSRP (left) and Opinosis (right) subcorpora. Below each model name is the total mistakes made. The denominator of each fraction is the number of test cases incorrectly classified by both models. The numerator is the portion of those misclassifications which were classified in the same (incorrect) way by both models. The shading is in-proportion to that fraction.

suggests that word choice is a very significant factor in determining meaning; so much so that the models which can make use of word order information, URAE and PV-DM, were significantly outperformed by methods which made more direct use of the word content.

The very high performance of the BOW maybe attributed to its very high dimensionality, though the MOWE and SOWE performed similarly. The PCA step can be considered as being similar to choosing an optimal set of words to keep so as to maximum variability in the bag of words. It loses little performance, even though decreasing vector size by an order of magnitude – particularly on the easier MSRP dataset.

6.5.2 Model Agreement

The misclassifications of the models can be compared. By selecting one of the test/train folds from the classification task above, and comparing the predicted classifications for each test-set sentence, the similarities of the models were assessed. The heatmaps in ?? show the agreement in errors. Here misclassification agreement is given as an approximation to $P(m_1(x) = m_2(x) | m_1(x) \neq y \wedge m_2(x) \neq y)$, for a randomly selected sentence x , with ground truth classification y , where the models m_1 and m_2 are used to produce classifications. Only considering the cases where both models were incorrect, rather than simple agreement, avoids the analysis being entirely dominated by the agreement of the models with the ground truth.

The word based models showed significant agreement. Unsurprisingly MOWE and SOWE have almost complete agreement in both evaluations. The other models showed less agreement – while they got many of the same cases wrong the models produced different misclassifications. This overall suggests that the various full sentence models are producing substantially dissimilar maps from meaning to vector space. Thus it seems reasonable that using a ensemble approach between multiple sentence models and one word-based model would produce strong results. Yin and Schütze **Yin2015** found this successful when combining different word embedding models.

6.5.3 Limitations

This evaluation has some limitations. As with all such empirical evaluations of machine learning models, a more optimal choice of hyper-parameters and training data will have an impact on the performance. In particular, if the model training was on the evaluation data the models would be expected to be better able to position their embedding. This was however unfeasible due to the small sizes of the datasets used for evaluation, and would not reflect real word application of the models to data not prior seen. Beyond the limitation of the use of the datasets is their contents.

The paraphrase groups were not selected to be independent of the word content overlap – they were simply collected on commonality of meaning from real world sourced corpora. This is a distinct contrast to the work of Ritter et. al. **RitterPosition** discussed in ?? where the classes were chosen to not have meaningful word overlap. However our work is complementary to

theirs, and our findings are well aligned. The key difference in performance is the magnitude of the performance of the sum of word embeddings (comparable to the mean of word embeddings evaluated here). In **RitterPosition** the word embedding model performed similarly to the best of the more complex models. In the results presented above we find that the word embedding based model performs significantly beyond the more complex models. This can be attributed to the word overlap in the paraphrase groups – in real-world speech people trying to say the same thing do in-fact use the same words very often.

6.6 Conclusion

A method was presented, to evaluate the semantic localization of sentence embedding models. Semantically equivalent sentences are those which exhibit bidirectional entailment – they each imply the truth of the other. Paraphrases are semantically equivalent. The evaluation method is a semantic classification task – to classify sentences as belonging to a paraphrase group of semantically equivalent sentences. The datasets used were derived from subsets of existing sources, the MRSP and the Opinosis corpora. The relative performance of various models was consistent across the two tasks, though differed on an absolute scale.

The word embedding and bag of word models performed best, followed by the paragraph vector models, with the URAE trailing in both tests. The strong performance of the sum and mean of word embeddings (SOWE and MOWE) compared to the more advanced models aligned with the results of Ritter et. al.**RitterPosition**. The difference in performance presented here for real-word sentences, were more marked than for the synthetic sentence used by Ritter et. al. This may be attributed to real-world sentences often having meaning overlap correspondent to word overlap – as seen also in the very strong performance of bag of words. Combining the result of this work with those of Ritter et. al., it can be concluded that summing word vector representations is a practical and surprisingly effective method for encoding the meaning of a sentence.

Learning Distributions of Meant Color

This paper is currently under review for Computational Linguistics.

Chapter 8

Learning of Colors from Color Names: Distribution and Point Estimation

Abstract

Color names are often made up of multiple words, as a task in natural language understanding we investigate in depth the capacity of neural networks based on sums of word embeddings (SOWE), recurrence (RNN) and convolution (CNN), to estimate colors from sequences of terms. We consider both point as well as distribution estimates of color. We argue that the latter has a particular value as there is no clear agreement between people as to what a particular color describes – different people have a different idea of what it means to be “very dark orange”. Surprisingly, the sum of word embeddings generally performs the best on almost all evaluations.

8.1 Introduction

Consider that the word `tan` may mean one of many colors for different people in different circumstances: ranging from the bronze of a tanned sunbather, to the brown of tanned leather; `green` may mean anything from `aquamarine` to `forest green`; and even `forest green` may mean the rich shades of a rain-forest, or the near grey of Australian bushland. Thus the *color intended* cannot be uniquely inferred from a color name. Without further context, it does nevertheless remain possible to estimate likelihoods of which colors are intended based on the population’s use of the words.

Color understanding, that is, generating color from text, is an important subtask in natural language understanding, indispensable for *executable semantic parsing*. For example, in a natural language enabled human-machine interface, when asked to select the `dark bluish green` object, it would be much useful if we could rank each object based on how likely its color matches against a learned distribution of the color name `dark bluish green`. This way if the most-likely object is eliminated (via another factor), the second most likely one can be considered. A threshold can be set to terminate the search. This kind of likelihood based approach is not possible when we have only exact semantics based on point estimates.

Color understanding is a challenging domain, due to high levels of ambiguity, the multiple roles taken by the same words, the many modifiers, and the many shades of meaning. In many ways it is a grounded microcosm of natural language understanding. Due to its difficulty, texts containing color descriptions such as `the flower has petals that are bright pinkish purple with white stigma` are used to demonstrate the capability of the-state-of-the-art image generation systems ([reed2016generative](#); [2015arXiv151102793M](#)). The core focus of the work we present here is to address these linguistic phenomena around the short-phrase descriptions of a color, which can be represented in a color-space such as HSV ([smith1978color](#)). Issues of illumination and perceived color based on context are considered out of the scope.

8.1.1 Distribution vs. Point Estimation

As illustrated, proper understanding of color names requires considering *the color intended* as a random variable. In other words, a color name should map to a distribution, not just a single point or region. For a given color name, any number of points in the color-space could be intended, with

some being more or less likely than others. Or equivalently, up to interpretation, it may intend a region but the likelihood of what points are covered is variable and uncertain. This distribution is often multimodal and has a high and asymmetrical variance, which further renders regression to a single point unsuitable. Having said that, we do produce point estimate results for completeness, though we argue the true usefulness of such estimates is limited.

A single point estimate, does not capture the diverse nature of the color names adequately. Moreover, it is impossible to find the single best point estimation method. For example: for a bimodal distribution, using the distribution mean as a point estimate will select a point in the valley between the peaks, which is less likely. Similarly for an asymmetrical distribution, where the mean will be off to one side of the peak. Conversely, using the distribution mode, will select the highest (most likely) peaks, but will on average be more incorrect (as measured by the mean squared error). The correct trade-off, if a point estimate is required, is dependent on the final use of the system. Another problem is that point estimates do not capture the sensitivity. In an asymmetrical distribution, having a point slightly off-centre in one direction may result in a very different probability, this more generally holds for a narrow variance distribution. Conversely for a very wide variance distribution (for example one approaching the uniform distribution) the point estimate value may matter very little with all points providing similar probabilities. Color distributions are almost always multimodal or asymmetrical, and exhibit widely differing variances for different names (this can be seen in the histograms of the training data shown in Section 8.6.1). While by definition the mean color point minimizes the squared error, it may not actually be a meaningful point estimate. Given these issues, producing a point estimate has only limited value and estimating a distribution is more general task. However we do consider the point estimation task, as it allows contrast in assessing the input module (SOWE/CNN/RNN) of our proposed methods across the two different output modules (distribution/point estimation).

The generation of color from text has not received much attention in prior work. To the best of our knowledge, the only similar work is **DBLP:journals/corr/KawakamiDRS16**; which only considers point estimation, and uses a dataset containing far too few observations to allow for learning probability distributions from population usages of the color names. To our knowledge The generation of probability distributions in color-space based on sequences of terms making up the color name, has not been considered at all by any prior work. There has been several works on the reverse problem (**mcmahan2015bayesian**; **meomcmahanstone:color; 2016arXiv160603821M**): the generation of a textual name for a color from a point in a color-space. From the set of work on the reverse problem there is a clear trend on data-driven approaches in recent years where more color names and observations are used.

8.1.2 Contributions

Problem statement: given a set of $\langle \text{color-name}, (h, s, v) \rangle$ pairs, we need to learn a mapping from any color-name, seen or unseen to a color-value or a distribution in HSV space.

We propose a neural network based architecture that can be broken down into an **input module**, which learns a vector representation of color-names, and a connected **output module**, which produces either a probability distribution or a point estimate. The **output module** uses a softmax output layer for probability distribution estimation, or a novel HSV output layer for point estimation. To carry out the representational learning of color-names, three different color-name embedding learning models are investigated for use in the **input module**: Sum Of Word Embeddings (SOWE), Convolutional Neural Network (CNN) and Recurrent Neural Network (RNN). The capacity of these input models is of primary interest to this work.

To evaluate and compare the three learning models, we designed a series of experiments to assess their capability in capturing compositionality of language used in color names. These include: **(1)** evaluation on all color names (full task); **(2)** evaluation on color names when the order of the words matters (order task); **(3)** evaluation on color names which never occur in the training data in that exact form, but for which all terms occur in the training data (unseen combination task); **(4)** qualitative demonstration of outputs for color names with terms which do not occur in the training data at all, but for which we know their word embeddings (embedding only task).

An interesting challenge when considering this discretization is the smoothness of the estimate. The true space is continuous, even if we are discretizing it at a resolution as high as the original color displays which were used to collect the data. Being continuous means that a small change in the point location in the color-space should correspond to a small change in how likely that point is according to the probability distribution. Informally, this means the histograms should look smooth, and not spiky. We investigated using a Kernel Density Estimation (KDE) based method for smoothing the training data, and further we conclude that the neural networks learn

this smoothness. To qualify our estimate of the distribution, we discretize the HSV color-space to produce a histogram. This allows us to take advantage of the well-known softmax based methods for the estimation of a probability mass distribution using a neural network.

We conclude that the SOWE model is generally the best model for all tasks both for distribution and point estimation. It is followed closely by the CNN; with the RNN performing significantly worse (see Section 8.6). We believe that due to the nature of color understanding as a microcosm of natural language understanding, the results of our investigations have some implications for the capacity of the models for their general use in short phrase understanding.

To the best of knowledge, this is the first of such investigation in term-wise mapping color names to values that can generate a visual representation, which bring the future of natural language controlled computer graphics generation and executable semantic parsing one step closer to reality.

8.2 Related Work

The understanding of color names has long been a concern of psycholinguistics and anthropologists (**berlin1969basic**; **heider1972universals**; **HEIDER1972337**; **mylonas2015use**). It is thus no surprise that there should be a corresponding field of research in natural language processing.

The earliest works revolve around explicit color dictionaries. This includes the ISCC-NBS color system (**kelly1955iscc**) of 26 words, that are composed according to a context free grammar, such that phrases are mapped to single points in the color-space; and the simpler, non-compositional, 11 basic colors of **berlin1969basic**. Works including **Berk:1982:HFS:358589.358606**; **conway1992experimental**; **ele1994computational**; **mojsilovic2005computational**; **menegaz2007discrete**; **van2009learning** which propose methods for the automatic mapping of colors to and from these small manually defined sets of colors. We note that **menegaz2007discrete**; **van2009learning** both propose systems that discretize the color-space, though to a much coarser level than we consider in this work.

More recent works, including the work presented in this article, function with a much larger number of colors, larger vocabularies, and larger pools of respondents. In particular making uses of the large Munroe dataset **Munroe2010XKCDdataset**, as we do here. This allows a data driven approach towards the modelling.

mcmahan2015bayesian and **meomcmahanstone:color** present color naming methods. Their work primarily focuses on mapping from colors to their exact names, the reverse of our task. These works are based on defining fuzzy rectangular distributions in the color-space to cover the distribution estimated from the data, which are used in a Bayesian system to non-compositionally determine the color name.

2016arXiv160603821M map a point in the color-space, to a sequence of probability estimates over color words. They extend beyond, all prior color naming systems to produce a compositional color namer based on the Munroe dataset. Their method uses a recurrent neural network (RNN), which takes as input a color-space point, and the previous output word, and gives a probability of the next word to output – this is a conditional language model. We tackle the inverse problem to the creation of a conditional language model. Our distribution estimation models map from a sequence of terms, to a distribution in color-space. Similarly, our point estimation models map from a sequence of terms to a single point in color-space.

DBLP:journals/corr/KawakamiDRS16 proposes another compositional color naming model. They use a per-character RNN and a variational autoencoder approach. It is in principle very similar to **2016arXiv160603821M**, but functioning on a character, rather than a word level. The work by Kawakami et al. also includes a method for generating colors. However they only consider the generation of point estimated, rather than distributions. The primary focus of our work is on generating distributions. The datasets used by Kawakami et al. contain only very small numbers of observations for each color name (often just one). These datasets are thus not suitable for modelling the distribution in color-space as interpreted by a population. Further, given the very small number of examples they are not well suited for use with word-based modelling: the character based modelling employed by Kawakami et al. is much more suitable. As such, we do not attempt to compare with their work.

DBLP:journals/corr/MonroeHGP17 present a neural network solution to a communication game, where a speaker is presented with three colors and asked to describe one of them, and the listener is to work out which color is being described. Speaker and listener models are trained, using LSTM-based decoders and encoders, respectively. The final time-step of their model produces a 100 dimensional representation of the description provided. From this, a Gaussian distributed score function is calculated, over a high dimensional color-space from **2016arXiv160603821M**,

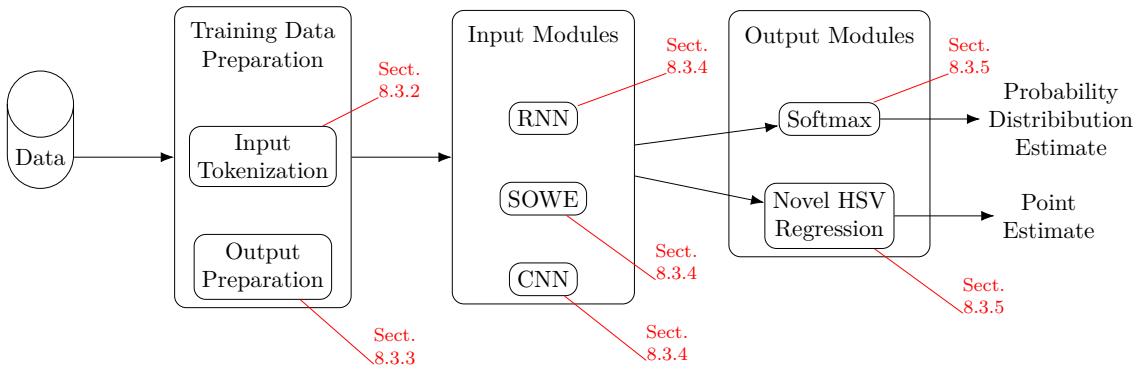


Figure 8.1: The overall architecture of our systems

which is then used to score each of the three options. While this method does work with a probability distribution, as a step in its goal, this distribution is always both symmetric and unimodal – albeit in a high-dimensional color-space.

acl2018WinnLighter demonstrates a neural network for producing point estimates of how colors change based on the use of comparative terms such as `lighter`. The network’s input is word embedding for a comparative adjective, and a point in RGB color-space; the model outputs a point in predicted RGB space that is the modified version of the input color point according to the given adjective. For example mapping from green to a darker green is: $((164, 227, 77), \text{darker}) \mapsto (141, 190, 61)$. The color adjectives may have up to two words, to allow for expressions such as `more neon`. This is allowed by taking as the fixed sized input two embeddings – when only one input is required, the other is replaced by zero vector. Their training and evaluation is based on data sourced from the Munroe dataset.

The work presented here closes the gap, that while we have language models conditional upon color, we do not have color models conditional upon language.

8.3 Method

8.3.1 System Architecture

Our overall system architecture for all models is shown in Figure 8.1. This shows how color names are transformed into distribution or point estimates over the HSV color-space.

8.3.2 Input Data Preparation

We desire a color prediction model which takes as input a sequence of words that make up the color’s name; rather than simply mapping from the whole phrase (whole phrase mapping does not scale to new user input, given the combinatorial nature of language). Towards this end, color names are first tokenized into individual words. For the input into our neural network based models, these words are represented with pretrained word embeddings.

Tokenization

During tokenization a color name is split into terms with consistent spelling. For example, `bluish kahki` would become the sequence of 3 tokens: `[blue, ish, khaki]`. Other than spelling, the tokenization results in the splitting of affixes and combining tokens (such as hyphens). Combining tokens and related affixes affect how multiple colors can be combined. The full list of tokenization rules can be found in the accompanying source code. Some further examples showing how combining tokens and affixes are used and tokenized:

- `blue purple` \mapsto `[blue, purple]`.
- `blue-purple` \mapsto `[blue, -, purple]`.
- `bluish purple` \mapsto `[blue, ish, purple]`
- `bluy purple` \mapsto `[blue, y, purple]`
- `blurple` \mapsto `[blue-purple]`

The final example of `blurple` is a special-case. It is the only portmanteau in the dataset, and we do not have a clear way to tokenize it into a series of terms which occur in our pretrained embedding’s vocabulary (see Section 8.3.2). The portmanteau `blurple` is not in common use in any training set used for creating word embeddings, so no pretrained embedding is available.¹ As such we handle it by treating it as the single token `blue-purple` for purposes of finding an embedding. There are many similar hyphenated tokens in the pretrained embeddings vocabulary, however (with that exception) we do not use them as it reduces the sequential modelling task to the point of being uninteresting.

Embeddings

All our neural network based solutions incorporate an embedding layer. This embedding layer maps from tokenized words to vectors. We make use of 300 dimensional pretrained FastText embeddings ([bojanowski2016enriching](#))².

The embeddings are not trained during the task, but are kept fixed. As per the universal approximation theorem ([leshno1993uat](#); [SONODA2017uat](#)) the layers above the embedding layer allow for arbitrary continuous transformations. By fixing the embeddings, and learning this transformation, we can produce estimates of colors from embeddings alone, without any training data at all, as shown in Section 8.6.3.

8.3.3 Output Data Preparation for Training Distribution Estimation Models

To train the distribution estimation models we need to preprocess the training data into a distribution. The raw training data itself, is just a collection of $\langle \text{color-name}, (h, s, v) \rangle$ pairs – samples from the distributions for each named-color. This is suitable for training the point estimation models, but not for the distribution estimation models . We thus convert it into a tractable form, of one histogram per output channel – by assuming the output channels are conditionality independent of each other.

Conditional Independence Assumption

We make the assumption that given the name of the color, the distribution of the hue, saturation and value channels are independent. That is to say, it is assumed if the color name is known, then knowing the value of one channel would not provide any additional information as to the value of the other two channels. The same assumption is made, though not remarked upon, in [meomcmahanstone:color](#) and [mcmahan2015bayesian](#). This assumption of conditional independence allows considerable saving in computational resources. Approximating the 3D joint distribution as the product of three 1D distributions decreases the space complexity from $O(n^3)$ to $O(n)$ in the discretized step that follows.

Superficial checks were carried out on the accuracy of this assumption. Spearman’s correlation on the training data suggests that for over three quarters of all color names, there is only weak correlation between the channels for most colors ($Q3 = 0.187$). However, this measure underestimates correlation for values which have a circular relative value, such as hue. Of the 16 color-spaces evaluated, HSV had the lowest correlation by a large margin. Full details, including the table of correlations, are available in supplementary materials (Appendix .1.1). These results are suggestive, rather than solidly indicative, on the degree of correctness of the conditional independence assumption. We consider the assumption sufficient for this investigation; as it does not impact on the correctness of results. A method that does not make this assumption may perform better when evaluated using the same metrics we use here.

Discretization

For distribution estimation, our models are trained to output histograms. This is a discretized representation of the continuous distribution. Following standard practice, interpolation-based methods can be used to handle it as a continuous distribution. By making use of the conditional independence assumption (see Section 8.3.3), we output one 256-bin histogram per channel. We note that 24-bit color (as was used in the survey that collected the dataset) can have all the

¹Methods do exist to generate embeddings for out of vocabulary words (like `blurple`), particularly with FastText embeddings ([bojanowski2016enriching](#)). But we do not investigate those here.

²Available from <https://fasttext.cc/docs/en/english-vectors.html>

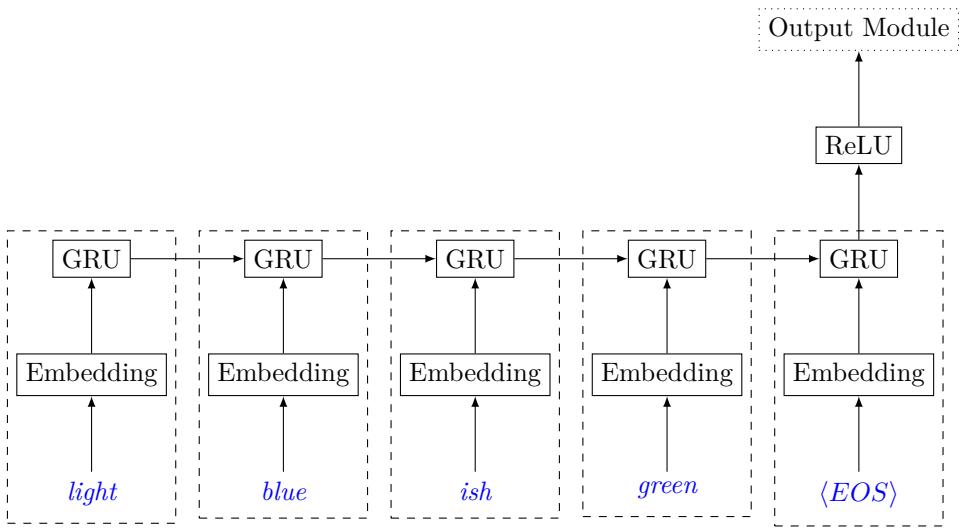


Figure 8.2: The RNN Input module for the example input `light greenish blue`. Each dashed box represents 1 time-step.

information captured by a 256 bin discretization per channel. 24 bit color allows for a total of 2^{24} colors to be represented, and even one-hot encoding for each of the 256 bin discretization channels allows for the same. As such there is no meaningful loss of information when using histograms over a truly continuous estimation method, such as a Gaussian mixture model. Although such models may have other advantages (such as the a priori information added by specifying the distribution), we do not investigate them here, instead considering the simplest non-parametric estimation model (the histogram), which has the simple implementation in a neural network using a softmax output layer.

Discretizing the data in this way is a useful solution used in several other machine learning systems. **oord2016pixel**; **DBLP:journals/corr/OordDZSVGKSK16** apply a similar discretization step and found that their method to outperform the more complex truly continuous distribution outputting systems.

For training purposes we thus convert all the observations into histograms. One set of training histograms is produced per color description present in the dataset – that is to say a training histogram is created for `brownish green`, `greenish brown`, `green` etc. We perform uniform weight attribution of points to bins as described by **jones1984remark**. In short, this method of tabulation is to define the bins by their midpoints, and to allocate probability mass to each bin based on how close an observed point is to the adjacent midpoints. A point precisely on a midpoint would have all its probability mass allocated to that bin; whereas a point halfway between midpoints would have 50% of its mass allocated to each. This is the form of tabulation commonly used during the first step of performing kernel density estimation, prior to the application of the kernel.

8.3.4 Color Name Representation Learning (Input Modules)

For each of the models we investigate we define an input module. This module handles the input of the color name, which is provided as a sequence of tokens. It produces a fixed sized dense representation of the color name, which is the input to the output module (Section 8.3.5). In all models the input and output modules are trained concurrently as a single system.

Recurrent Neural Network(RNN)

A Recurrent Neural Network is a common choice for this kind of task, due to the variable length of the input. The general structure of this network, shown in Figure 8.2 is similar to **2016arXiv160603821M**, or indeed to most other word sequence learning models. Each word is first transformed to an embedding representation. This representation is trained with the rest of the network allowing per word information to be efficiently learned. The embedding is used as the input for a Gated Recurrent Unit (GRU). The stream was terminated with an End of Stream (`<EOS>`) pseudo-token, represented using a zero-vector. The output of the last time-step is fed to a Rectified Linear Unit (ReLU).

We make use of a GRU (**cho2014properties**), which we found to marginally out-perform the

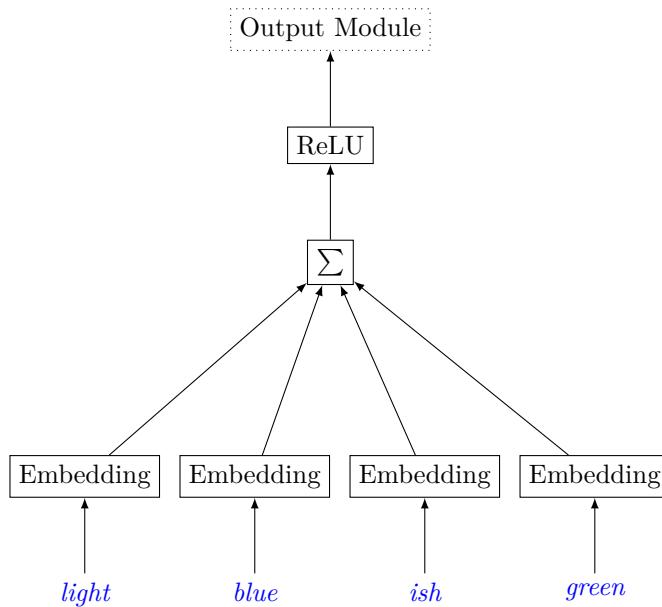


Figure 8.3: The SOWE input module for the example input `light bluish green`

basic RNN in preliminary testing. The small improvement is unsurprising, as the color names have at most 5 terms, so longer short term memory is not required.

Sum of Word Embeddings (SOWE)

Using a simple sum of word embeddings as a layer in a neural network is less typical than an RNN structure. Though it is well established as a useful representation, and has been used as an input to other classifiers such as support vector machines (e.g. as in **White2015SentVecMeaning; novelperspective**). Any number of word embeddings can be added to the sum, thus allowing it to handle sequences of any length. However, it has no representation of the order. The structure we used is shown in Figure 8.3.

Convolutional Neural Network(CNN)

A convolutional neural network (shown in Figure 8.4) can be applied to the task by applying 2D convolution over the stacked word embeddings. We use 64 filters of size between one and five. Five is number of tokens in the longest color-name, so this allows it to learn full length relations.

8.3.5 Distribution and Point Estimation (Output Modules)

On top of the input module, we define an output module to suit the neural network for the task of either distribution estimation or point estimation. The input module defines how the terms are composed into the network. The output module defines how the network takes its hidden representation and produces an output.

Distribution Estimation

The distributions are trained to produce the discretized representation as discussed in Section 8.3.3. Making use of the conditional independence assumption (see Section 8.3.3), we output the three discretized distributions. As shown in Figure 8.5, this is done using three softmax output layers – one per channel. They share a common input, but have separate weights and biases. The loss function is given by the sum of the cross-entropy for each of the three softmax outputs.

Point Estimation

Our point estimation output module is shown in Figure 8.6. The hidden-layer from the top of the input module is fed to four single output neurons.³ Two of these use the sigmoid activation

³Equivalently these four single neurons can be expressed as a layer with four outputs and two different activation functions.

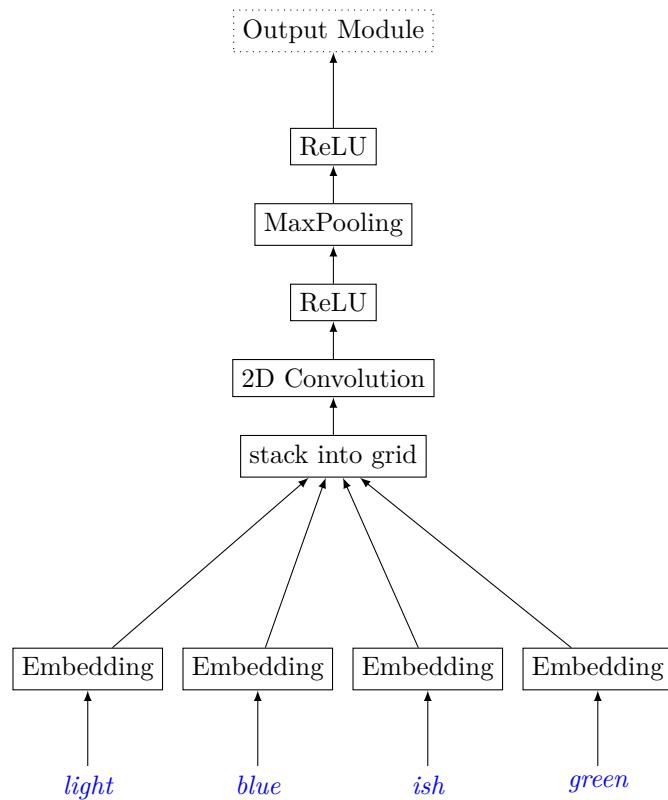


Figure 8.4: The CNN input module for the example input `light greenish blue`

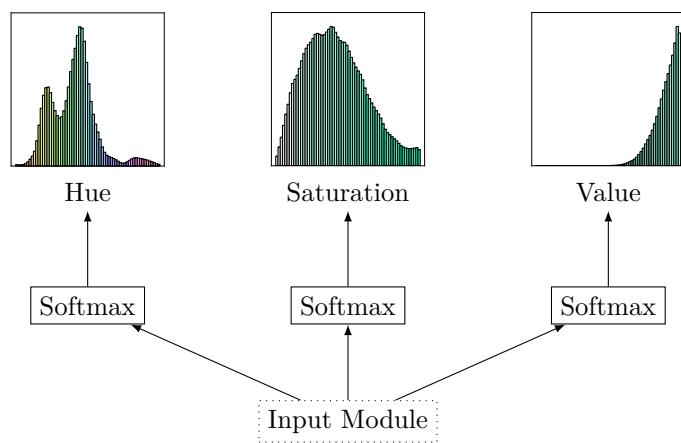


Figure 8.5: The Distribution Output Module

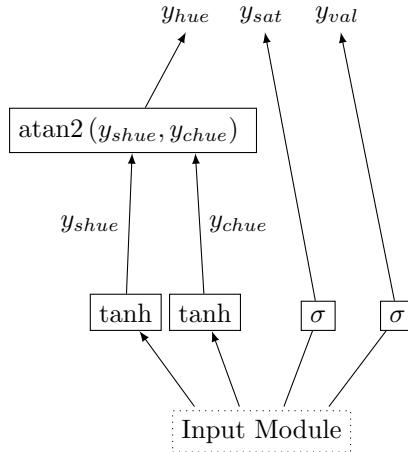


Figure 8.6: The Point Estimate Output Module. Here atan2 is the quadrant preserving arctangent, outputting the angle in turns.

function (range 0:1) to produce the outputs for the saturation and value channels. The other two use the tanh activation function (range -1:1), and produce the intermediate output that we call y_{shue} and y_{chue} for the sine and cosine of the hue channel respectively. The hue can be found as $y_{hue} = \text{atan2}(y_{shue}, y_{chue})$. We use the intermediate values when calculating the loss function. During training we use the following loss function for each observation y^* , and each corresponding prediction y .

$$\begin{aligned}
loss = & \frac{1}{2} (\sin(y_{hue}^*) - y_{shue})^2 \\
& + \frac{1}{2} (\cos(y_{hue}^*) - y_{chue})^2 \\
& + (y_{sat}^* - y_{sat})^2 \\
& + (y_{val}^* - y_{val})^2
\end{aligned} \tag{8.1}$$

This mean of this loss is taken over all observations in each mini-batch during training. This loss function is continuous and correctly handles the wrap-around nature of the hue channel (**WhiteRepresentingAnglesSE**).

8.4 Evaluation

8.4.1 Perplexity in Color-Space

Perplexity is a measure of how well the distribution, estimated by the model, matches the reality according to the observations in the test set. Perplexity is commonly used for evaluating language models. Here however, it is being used to evaluate the discretized distribution estimate. It can be loosely thought of as to how well the model's distribution does in terms of the size of an equivalent uniform distribution. Note that this metric does not assume conditional independence of the color channels.

Here τ is the test-set made up of pairs consisting of a color name t , and a color-space point \tilde{x} ; and $p(\tilde{x} | t)$ is the output of the evaluated model. Perplexity is defined as:

$$PP(\tau) = \exp_2 \left(\left(\frac{-1}{|\tau|} \sum_{\forall(t, (\tilde{x})) \in \tau} \log_2 p(\tilde{x} | t) \right) \right) \tag{8.2}$$

As the perplexity for a high-resolution discretized model will inherently be very large and difficult to read, we define the standardized perplexity: $\frac{PP(\tau)}{n_{res}}$, where n_{res} is the total number of bins in the discretization scheme. For all the results we present here $n_{res} = 256^3$. This standardized perplexity gives the easily interpretable values *usually* between zero and one. It is equivalent to comparing the relative performance of the model to that of a uniform distribution of the same total resolution. $\frac{PP(\tau)}{n_{res}} = 1$ means that the result is equal to what we would see if we had distributed the probability mass uniformly into all bins in a 3D histogram. $\frac{PP(\tau)}{n_{res}} = 0.5$ means the result is

twice as good as if we were to simply use a uniform distribution: it is equivalent to saying that the correct bin is selected as often as it would be had a uniform distribution with half as many bins been used (i.e. larger bins with twice the area). The standardised perplexity is also invariant under different output resolutions. Though for brevity we only present results with 256 bins per channel, our preliminary results for using other resolutions are similar under standardized perplexity.

8.4.2 Angularly Correct Calculations on HSV

We use the HSV color-space ([smith1978color](#)) through-out this work. In this format: hue, saturation and value all range between zero and one. Note that we measure hue in *turns*, rather than the more traditional degrees, or radians. Having hue measured between zero and one, like the other channels, makes the modelling task more consistent. Were the hue to range between 0 and 2π (radians) or between 0 and 360 (degrees) it would be over-weighted in the loss function and evaluation metrics compared to the other channels. This regular space means that errors on all channels can be considered equally. Unlike many other colors spaces (CIELab, Luv etc.) the gamut is square and all combinations of values from the different channels correspond to realizable colors.

When performing calculations with the HSV color-space, it is important to take into account that hue is an angle. As we are working with the color-space regularized to range between zero and one for all channels, this means that a hue of one and a hue of zero are equivalent (as we measure in turns, in radians this would be 0 and 2π).

The square error of two hue values is thus calculated as:

$$SE(h_1, h_2) = \min((h_1 - h_2)^2, (h_1 - h_2 - 1)^2) \quad (8.3)$$

This takes into account that the error can be calculated clockwise or counter-clockwise; and should be the smaller. Note that the -1 term is related to using units of turns, were we using radians it would be -2π

The mean of a set of hues ($\{h_1, \dots, h_N\}$) is calculated as:

$$\bar{h} = \text{atan2}\left(\frac{1}{N} \sum_{i=1}^{i=N} \sin(h_i), \frac{1}{N} \sum_{i=1}^{i=N} \cos(h_i)\right) \quad (8.4)$$

This gives the mean angle.

8.4.3 Operational Upper-bounds

To establish a rough upper-limit on the modelling results we evaluate a direct method which bypasses the language understanding component of the task. These direct methods do not process each term in the name:, they do not work with the language at all. They simply map from the exact input text (no tokenization) to the pre-calculated distribution or mean of the training data for the exact color name. This operational upper bound bypass the compositional language understanding part of the process. It is as if the input module (as discussed in Section 8.3.4) would perfectly resolve the sequence of terms into a single item.

They represent an approximate upper bound, as they fully exploit all information in the training data for each input. There is no attempt to determine how each term affects the result. We say approximate upper-bound, as it is not strictly impossible that the term-based methods may happen to model the test data better than can be directly determined by training data as processed per exact color name. This would require learning how the terms in the color name combine in a way that exceeds the information directly present in the training data per class. It is this capacity of learning how the terms combine that allow for the models to predict the outputs for combinations of terms that never occur in the training data (Section 8.4.4). Doing this in a way that generalizes to get better results than the direct exploitation of the training data, would require very well calibrated control of (over/under)f fitting.

Operational Upper-bound for Distribution Estimation: KDE

To determine an operational upper-bound for the distribution estimation tasks, we use kernel-density estimation (KDE) in a formulation for non-parametric estimation ([silverman1986density](#)). The KDE effectively produces a smoothed histogram from the training data as processed in Section 8.3.3. It causes adjacent bins to have most similar probabilities, thus matching to the mathematical notion of a continuous random variable. This is applied on-top of the histogram

used for the training data. We use the Fast Fourier Transform (FFT) based KDE method of the **silverman1982algorithm**. We use a Gaussian kernel, and select the bandwidth per color description based on leave-one-out cross validation on the training data. A known issue with the FFT-based KDE method is that it has a wrap-around effect near the boundaries, where the mass that would be assigned outside the boundaries is instead assigned to the bin on the other side. For the value and saturation channels we follow the standard solution of initially defining additional bins outside the true boundaries, then discarding those bins and rescaling the probability to one. For the hue channel this wrap-around effect is exactly as desired.

In our evaluations using KDE rather than just the training histograms directly proved much more successful on all distribution estimation tasks. This is because it avoids empty bins, and effectually interpolates probabilities between observations. We found in preliminary investigations that using KDE-based method to be much better than add-one smoothing.

We also investigated the application of KDE to the training data, before training our term-based neural network based distribution models. Results for this can be found in Appendix .1.2. In brief, we found that smoothing the training data does not significantly affect the result of the neural network based models. As discussed in Section 8.6.2, this is because the neural networks are able to learn the smoothness relationship of adjacent bins.

Our KDE-based operational upper bound for distribution estimation bypasses the natural language understanding part of the task, and directly uses the standard non-parametric probability estimation method to focus solely on modelling the distributions. Matching its performance indicates that a model is effectively succeeding well at both the natural language understanding component and the distribution estimation component.

Operational Upper-bound for Point Estimation: Mean-point

In a similar approach, we also propose a method that directly produces a point estimate from a color name. We define this by taking the mean of all the training observations for a given exact color name. The mean is taken in the angularly correct way (as discussed in Section 8.4.2). Taking the mean of all the observations gives the theoretically optimal solution to minimize the squared error on the training data set. As with our direct distribution estimation method, this bypasses the term based language understanding, and directly exploits the training data. It thus represents an approximate upper bound on the point estimation performance of the term based models. Though, as discussed in Section 8.1, the notion of mean and of minimizing the square error is not necessarily the correct way to characterize selecting the optimal point estimate for colors. It is however a consistent way to do so, and so we use it for our evaluations.

8.4.4 Evaluation Strategies

Full Task

We make use of the Munroe dataset as prepared by **mcmahan2015bayesian** from the results of the XKCD color survey. The XKCD color survey (**Munroe2010XKCDdataset**), collected over 3.4 million observations from over 222,500 respondents. McMahan and Stone take a subset from Munroe’s full survey, by restricting it to the responses from native English speakers, and removing very rare color names with less than 100 uses. This gives a total of 2,176,417 observations and 829 color names. They also define a standard test, development and train split.

Unseen combination Task

A primary interest in using the term based models is to be able to make predictions for never before seen descriptions of colors. For example, based on the learned understanding of **salmon** and of **bright**, from examples like **bright green** and **bright red**, we wish for the system to make predictions about **bright salmon**, even though that description never occurs in the training data. The ability to make predictions, such as these, illustrates term-based natural language understanding. This cannot be done with the operational upper bound models, which by-passes the term processing step. To evaluate this generalisation capacity, we define new sub-datasets for both testing and training. We select the rarest 100 color descriptions from the full dataset, with the restriction that every token in a selected description must still have at least 8 uses in other descriptions in the training set. The selected examples include multi-token descriptions such as: **bright yellow green** and also single tokens that occur more commonly as modifiers than as stand-alone descriptions such as **pale**.

The unseen combination testing set has only observations from the full test set that do use those rare descriptions. We define a corresponding restricted training set made up of the data from the full training set, excluding those corresponding to the rare descriptions. Similar restriction is done to create a restricted development set, so that no direct knowledge of the combined terms can leak during early-stopping.

By training on the restricted training set and testing on the unseen combination, we can assess the capacity of the models to make predictions for color descriptions not seen during training. A similar approach was used in **acl2018WinnLighter** and in **DBLP:journals/corr/AtzmonBKG16**. We contrast this to the same models when trained on the full training set to see how much accuracy was lost.

Order Task

It is believed that the order of words in a color description matters, at least to some extent, for its meaning. For example, `greenish brown` and `brownish green` are distinct, if similar, colors. To assess the models on their ability to make predictions when order matters we construct the order test set. This is a subset of the full test set containing only descriptions with terms that occur in multiple different orders. There are 76 such descriptions in the full dataset. Each of which has exactly one alternate ordering. This is unsurprising as while color descriptions may have more than 2 terms, normally one or more of the terms is a joining token such as `ish` or `-`. We only construct an order testing set, and not a corresponding training set, as this is an evaluation using the model trained on the full training data.

8.5 Experimental Setup

8.5.1 Implementation

The implementation of all the models was in the julia programming language (**Julia**). The full implementation can be downloaded from the GitHub repository.⁴ The machine learning components make heavy use of the `MLDataUtils.jl`⁵ and `TensorFlow.jl`,⁶ packages. The latter of which we enhanced significantly to allow for this work to be carried out. The discretization and the KDE for the Operational Upper Bound is done using `KernalDensityEstimation.jl`.⁷

8.5.2 Common Network Features

Drop-out(**srivastava2014dropout**) is used on all ReLU layers and on the GRU in the RNN, with threshold of 0.5 during training. The network is optimized using Adam (**kingma2014adam**), and a learning rate of 0.001. Early stopping is checked every 10 epochs using the development dataset. Distribution estimation methods are trained using the full batch (where each observation is a distribution) for every epoch. Point Estimation methods are trained using randomized mini-batches of 2^{16} observations (which are each color-space triples). All hidden-layers, except as otherwise precluded (inside the convolution, and in the penultimate layer of the point estimation networks) have the same width 300, as does the embedding layer.

8.6 Results

8.6.1 Qualitative Results

To get an understanding of the problem and how the models are performing, we consider some of the outputs of the model for particular cases. To illustrate the models trained on the full dataset, Figure 8.7 shows examples of distribution estimates, and Figure 8.8 shows similar examples for point estimates. It can be seen that the models' outputs using term based estimation are generally similar to the non-term-based operational upper-bound, as is intended. This shows that the models are correctly fitting to estimate the colors. This aligns with the strong results found in the quantitative evaluations discussed in Section 8.6.2.

⁴Implementation source is at <https://github.com/oxinabox/ColoringNames.jl>

⁵MLDataUtils.jl is available from <https://github.com/JuliaML/MLDataUtils.jl>

⁶TensorFlow.jl is available from <https://github.com/malmaud/TensorFlow.jl>

⁷KernalDensityEstimation.jl is available from <https://github.com/JuliaStats/KernelDensity.jl>

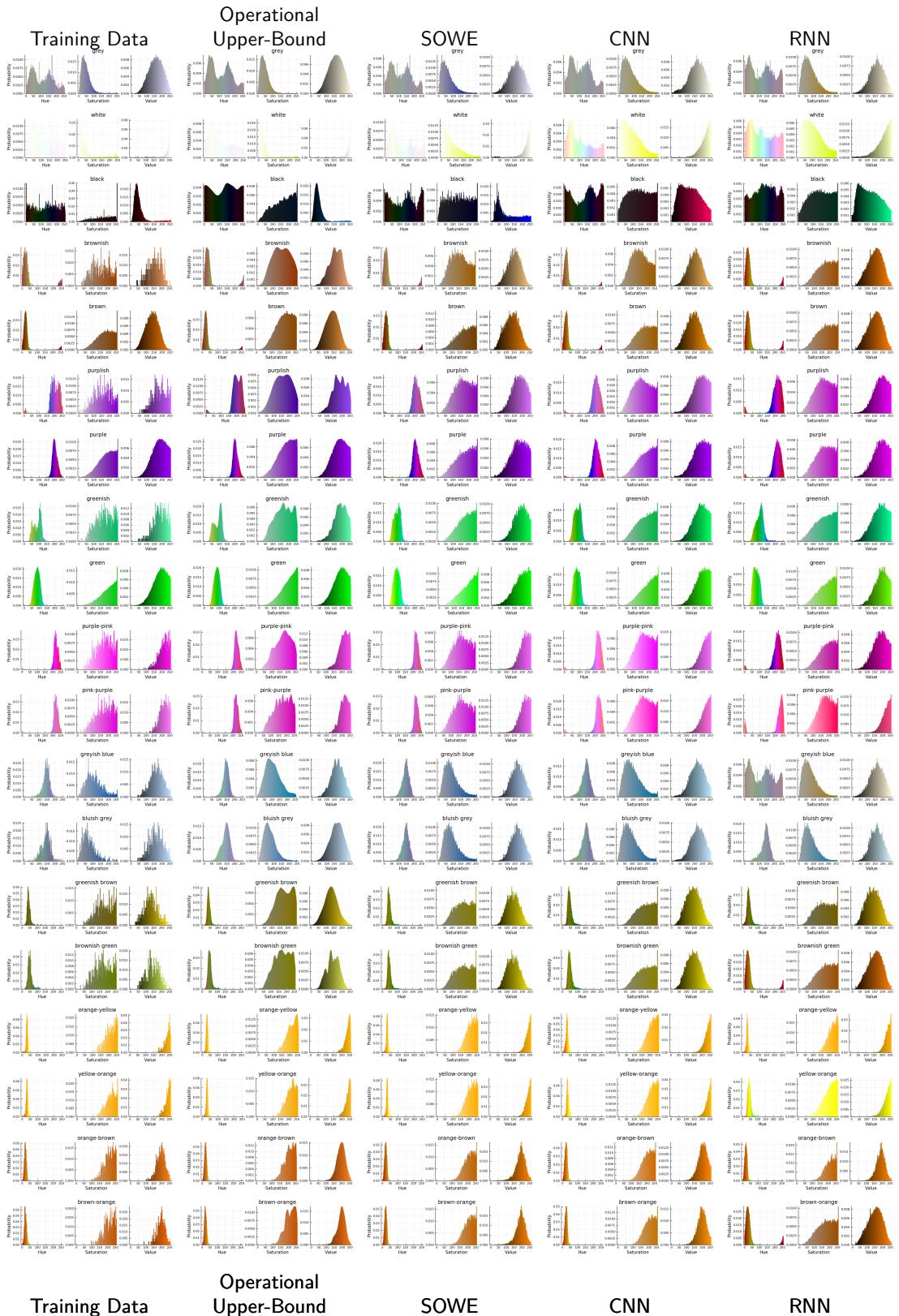


Figure 8.7: Some examples of the output distribution estimates from the models trained on the full dataset



Figure 8.8: Some examples of the output point estimates from the models trained on the full dataset

On the effects of word-order

The different input modules have a different capacity to leverage word-order. This is reflected in Figures 8.7 and 8.8, when considering the pairs of outputs that differ only in word order, such as **purple-pink** and **pink-purple**. The plots presented for the training data and for the Operational Upper-Bound show that such color name pairs are subtly different but similar. The SOWE model is unable to take into account word order at all, and so produces identical outputs for all orders. The CNN models produce very similar outputs but not strictly identical – spotting the difference requires a very close observation. This is in-line with the different filter sizes allowing the CNN to effectively use n-gram features, and finding that the unigram features are the most useful. The RNN produces the most strikingly different results. It seems that the first term dominates the final output: **purple-pink** is more purple, and **pink-purple** is more pink. We can see that the first term is not solely responsible for the final output however, as **purple-pink**, **purple** and **purplish** (tokenized as **purple**, **ish**) are all different. It is surprising that the RNN is dominated by the first term and not the latter terms⁸. This shows that the GRU is functioning to remember the earlier inputs. This is happening too strongly however, as it is causing incorrect outputs.

On the smoothness of the distribution estimates

In Figure 8.7 it can be seen that the term-based distribution estimation models are much smoother than the corresponding histograms taken from the training data. They are not as smooth as the Operational Upper-Bound which explicitly uses KDE. However, they are much smoother than would be expected, had the output bins been treated independently. Thus it is clear that the models are learning that adjacent bins should have similar output values. This is a common feature of all the training data, no matter which color is being described. This learned effect is in line with the fact that color is continuous, and is only being represented here as discrete. We note in relation to this learned smoothness: that while the models capture the highly asymmetrical shapes of most distributions well, they do not do well at capturing small dips. Larger multi-modes as seen in the achromatic colors such as **white**, **grey**, **black**, **white**, are captured; but smaller dips such as the hue of **greenish** being more likely to be on either side of the green spectrum are largely filled in. In general, it seems clear that additional smoothing of the training data is not required for the neural network based models. This aligns with the results presented in Appendix .1.2.

8.6.2 Quantitative Results

Overall, we see that our models are able to learn to estimate colors based on sequences of terms. From the consideration of all the results shown in Tables 8.1 to 8.6. The CNN and SOWE models perform almost as well as the operational upper-bound. With the SOWE having a marginal lead for distribution estimation, and the CNN and SOWE being nearly exactly equal for most point estimation tasks. We believe the reason for this is that the SOWE is an easier to learn model from a gradient descent perspective: it is a shallow model with only one true hidden layer. The RNN did not perform as well at these tasks. While it is only marginally behind the SOWE and CNN on the full point estimation task (Table 8.2), on all other tasks for both point estimation and distribution estimation it is significantly worse. This may indicate that it is hard to capture the significant relationships between terms in the sequence. However, as shown Section 8.6.2 it did learn generally acceptable colors, but it is not as close a match to the population’s expectation.

Ordered Task

The performance of SOWE on the order tasks (Tables 8.3 and 8.4) is surprising. For the distribution estimation it outperforms the CNN, and for point estimation it ties with the CNN. The CNN and RNN, can take into account word order, but the SOWE model cannot. The good results for SOWE suggest that the word-order is not very significant for color names. While word order matters, different colors with the same terms in different order are similar enough that it still performs very well. In theory the models that are capable of using word order have the capacity to ignore it, and thus could achieve a similar result. An RNN can learn to perform a sum of its inputs (the word embeddings), and the CNN can learn to weight all non-unigram filters to zero. In practice we see that for the RNN in particular this clearly did not occur. This can be attributed to the more complex networks being more challenging to train via gradient descent. It seems that color-naming is not a task where word order substantially matters, and thus the simpler SOWE model excels.

⁸So much so that we double checked our implementation to be sure that it wasn’t processing the inputs backwards.

Method	$\frac{PP}{256^3}$
Operational Upper Bound	0.071
SOWE	0.075
CNN	0.078
RNN	0.089

Table 8.1: The results for the **full distribution estimation task**. Lower perplexity (PP) is better.

Unseen Combinations of Terms

The SOWE and CNN models are able to generalize well to making estimates for combinations of color terms that are not seen in training. Tables 8.5 and 8.6 show the results of the model on the test set made up of rare combinations of color names (as described in Section 8.4.4) for the restricted training set (which does not contain those terms). These results on this test set are compared with the same models when trained on the full training set. The Operation Upper Bound models are unable to produce estimates from the unseen combinations testing set as they do not process the color names term-wise. The RNN models continue to perform badly on the unseen combination of terms task for both point and distribution estimation.

On distribution estimation (Table 8.5) the SOWE results are only marginally worse for the restricted training set as they are for the full training set. The CNN results are worse again, but they are still better than the results on the full test-set. The distribution estimates are good on absolute terms, having low evaluated perplexity.

In the point estimation task (Table 8.6) the order is flipped with the CNN outperforming the SOWE model. In-fact the CNN actually performs better with the restricted training set. This may be due to the CNN not fitting to the training data as well as the SOWE, as on the full training set (for this test set) we see the SOWE outperforms the CNN. This suggests that the CNN point estimation model may be better at capturing the shared information about term usages, at the expense of fitting to the final point. Unlike for distribution estimates, the unseen color point estimates are worse than the overall results from the full task (Table 8.2), though the errors are still small on an absolute scale.

Extracting the mean from the distribution estimates

In the point estimation results discussed so far, have been from models trained specifically for point estimation (as described by Section 8.3.5). However, it is also possible to derive the mean from the distribution estimation models. Those results are also presented in Tables 8.2, 8.4 and 8.6. In general these results perform marginally worse (using the MSE metric) than their corresponding modules using the point estimation output module. We note that for the operational upper-bound, the distributions mean is almost identical to the true mean of points, as expected.

Beyond the output module there are a few key differences between the point estimation modules and the distribution estimate modules. When training distribution estimation models, all examples of a particular color name is grouped into a single high information training observation using the histogram as the output. Whereas when training for point estimation, each example is processed individually (using minibatches). This means that the distribution estimating models fit to all color names with equal priority. Whereas for point estimates, more frequently used color names have more examples, and so more frequent color names are fit with priority over rarer ones. Another consequence of using training per example using random minibatches, rather than aggregating and training with full batch, is increased resilience to local minima. One of the upsides of the aggregated training used in distribution estimation is that it trains much faster as only a small number of high-information training examples are processed, rather than a much larger number of individual observations. It may be interesting in future work to consider training the distribution estimates per example using one-hot output representations; thus making the process similar to that used in the point estimate training. We suspect that such a method may have trouble learning the smoothness of the output space (as discussed in Section 8.6.1).

8.6.3 Completely Unseen Color Estimation From Embeddings

As an interesting demonstration of how the models function by learning the transformation from the embedding space to the output ,we briefly consider the outputs for color-names that do not occur in the training or testing data at all. This is even more extreme than the unseen combination

Method	<i>MSE</i>
Operational Upper Bound	0.066
SOWE	0.067
CNN	0.067
RNN	0.071
Distribution Mean Operational Upper Bound	0.066
Distribution Mean SOWE	0.068
Distribution Mean CNN	0.069
Distribution Mean RNN	0.077

Table 8.2: The results for the **full point estimation task**. Lower mean squared error (MSE) is better.

Method	$\frac{PP}{256^3}$
Operational Upper Bound	0.053
SOWE	0.055
CNN	0.057
RNN	0.124

Table 8.3: The results for the **order distribution estimation task**. Lower perplexity (PP) is better. This is a subset of the full test set containing only tests where the order of the words matters.

Method	<i>MSE</i>
Operational Upper Bound	0.065
SOWE	0.066
CNN	0.066
RNN	0.096
Distribution Mean Operational Upper Bound	0.065
Distribution Mean SOWE	0.066
Distribution Mean CNN	0.066
Distribution Mean RNN	0.095

Table 8.4: The results for the **order point estimation task**. Lower mean squared error (MSE) is better. This is a subset of the full test set containing only tests where the order of the words matters.

Method	Full Training Set	Restricted Training Set
	$\frac{PP}{256^3}$	$\frac{PP}{256^3}$
Operational Upper Bound	0.050	—
SOWE	0.050	0.055
CNN	0.052	0.065
RNN	0.117	0.182

Table 8.5: The results for the **unseen combinations distribution estimation task**. Lower perplexity (PP) is better. This uses the extrapolation subset of the full test set. In the extrapolating results certain rare word combinations were removed from the training and development sets. In the non-extrapolating results the full training and development set was used.

Method	Full Training Set	Restricted Training Set
	<i>MSE</i>	<i>MSE</i>
Operational Upper Bound	0.062	—
SOWE	0.065	0.079
CNN	0.072	0.070
RNN	0.138	0.142
Distribution Mean Operational Upper Bound	0.062	—
Distribution Mean SOWE	0.073	0.076
Distribution Mean CNN	0.073	0.084
Distribution Mean RNN	0.105	0.152

Table 8.6: The results for the **unseen combinations point estimation task**. Lower mean squared error (MSE) is better. This uses the extrapolation subset of the full test set. In the extrapolating results certain rare word combinations were removed from the training and development sets. In the non-extrapolating results the full training and development stet was used.

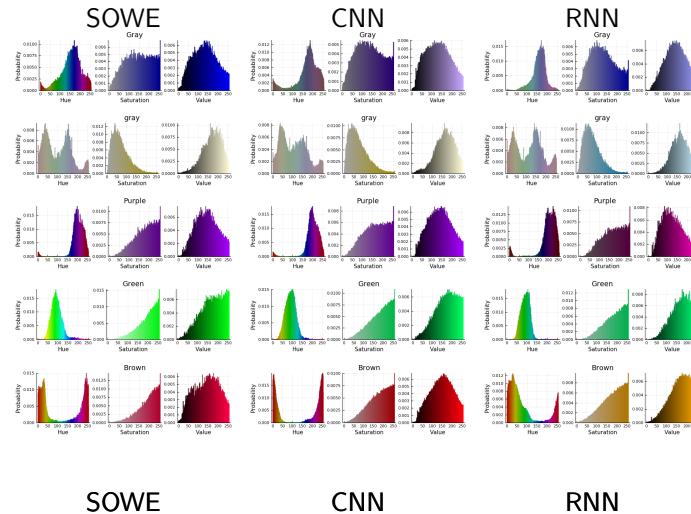


Figure 8.9: Some example distribution estimations for colors names which are completely outside the training data. The terms: **Brown**, **gray**, **Gray**, **Green**, and **Purple**, do not occur in any of the color data; however **brown**, **grey**, **green**, and **purple** do occur.

task considered in Tables 8.5 and 8.6 where the terms appeared in training, but not the combination of terms. In the examples shown in Figures 8.9 and 8.10, where the terms never occurred in the training data at all, our models exploit the fact that they work by transforming the word-embedding space to predict the colors. There is no equivalent for this in the direct models. While **Grey** and **gray** never occur in the training data; **grey** does, and it is near-by in the word-embedding space. Similar is true for the other colors that vary by capitalization. We only present a few examples of single term colors here, and no quantitative investigation, as this is merely a matter of interest.

It is particularly interesting to note that the all the models make similar estimations for each color. This occurs both for point estimation and for distribution estimation. They do well on the same colors and make similar mistakes on the colors they do poorly at. The saturation of **Gray** is estimated too high, making it appear too blue/purple, this is also true of **grey** though to a much lesser extent. **Purple** and **Green** produce generally reasonable estimates. The hue for **Brown** is estimated as having too much variance, allowing the color to swing into the red or yellowish-green parts of the spectrum. This suggests that in general all models are learning a more generally similar transformation of the space. In general the overall quality of each model seems to be in line with that found in the results for the full tests.

8.7 Conclusion

We have presented three input modules (SOWE, CNN, RNN), and two output modules (distribution estimate, and point estimate) that are suitable for using machine learning to make estimates

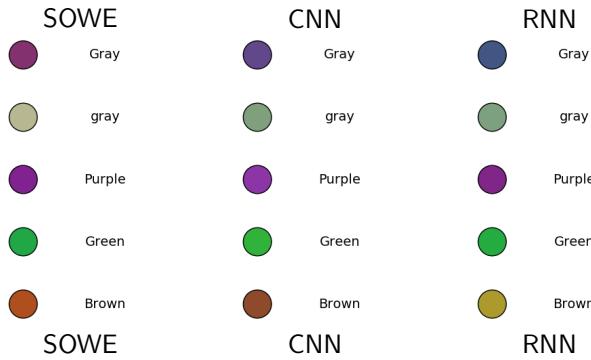


Figure 8.10: Some example point estimates for colors names which are completely outside the training data. The terms: **Brown**, **gray**, **Gray**, **Green**, and **Purple**, do not occur in any of the color data; however **brown**, **grey**, **green**, and **purple** do occur.

about color based on the terms making up its name. We contrasted these to an operational upper bound model for each task which bypassed the term-wise natural language understanding component of the problem. We found the results for SOWE, and CNN were very strong, approaching this upper bound.

A key take away from our results is that using a SOWE should be preferred over an RNN for short phrase natural language understanding tasks when order is not a very significant factor. The RNN is the standard type of model for problems with sequential input, such as color names made up of multiple words as we considered here. However, we find its performance to be significantly exceeded by the SOWE and CNN. The SOWE is an unordered model roughly corresponding to a bag of words. The CNN similarly roughly corresponds to a bag of ngrams, in our case a bag of all 1,2,3,4 and 5-grams. This means the CNN can readily take advantage of both fully ordered information, using the filters of length 5, down to unordered information using filters of length 1. The RNN however must fully process the ordered nature of its inputs, as its output comes only from the final node. It would be interesting to further contrast a bidirectional RNN.

In a broader context, we envisage the distribution learned for a color name can be used as a prior probability and when combining with additional context information, this can be used for better prediction in areas such as document classification and sentiment detection.

A further interesting avenue for investigation would condition the model not only on the words used but also on the speaker. The original source of the data **Munroe2010XKCDdataset**, includes some demographic information which is not exploited by any known methods. It is expected that color-term usage may vary with subcultures.

.1 Appendix

.1.1 On the Conditional Independence of Color Channels given a Color Name

As discussed in the main text, we conducted a superficial investigation into the truth of our assumption that given a color name, the distributions of the hue, value and saturation are statistically independent.

We note that this investigation is, by no means, conclusive though it is suggestive. The investigation focusses around the use of the Spearman's rank correlation. This correlation measures the monotonicity of the relationship between the random variables. A key limitation is that the relationship may exist but be non-monotonic. This is almost certainly true for any relationship involving channels, such as hue, which wrap around. In the case of such relationships Spearman's correlation will underestimate the true strength of the relationship. Thus, this test is of limited use in proving conditional independence. However, it is a quick test to perform and does suggest that the conditional independence assumption may not be so incorrect as one might assume.

In Monroe Color Dataset the training data given by $V \subset \mathbb{R}^3 \times T$, where \mathbb{R}^3 is the value in the color-space under consideration, and T is the natural language space. The subset of the training data for the description $t \in T$ is given by $V_{|t} = \{(\tilde{v}_i, t_i) \in V \mid t_i = t\}$. Further let $T_V = \{t_i \mid (\tilde{v}, t_i) \in V\}$ be the set of color names used in the training set. Let $V_{\alpha|t}$ be the α channel component of $V_{|t}$, i.e. $V_{\alpha|t} = \{v_\alpha \mid ((v_1, v_2, v_3), t) \in V_{|t}\}$.

The set of absolute Spearman's rank correlations between channels a and b for each color name is given by $S_{ab} = \{|\rho(V_{a|t}, V_{b|t})| \mid t \in T_V\}$.

Color-Space	$Q3(S_{12})$	$Q3(S_{13})$	$Q3(S_{23})$	max
HSV	0.1861	0.1867	0.1628	0.1867
HSL	0.1655	0.2147	0.3113	0.3113
YCbCr	0.4005	0.4393	0.3377	0.4393
YIQ	0.4088	0.4975	0.4064	0.4975
LCHab	0.5258	0.411	0.3688	0.5258
DIN99d	0.5442	0.4426	0.4803	0.5442
DIN99	0.5449	0.4931	0.5235	0.5449
DIN99o	0.5608	0.4082	0.5211	0.5608
RGB	0.603	0.4472	0.5656	0.603
Luv	0.5598	0.6112	0.4379	0.6112
LCHuv	0.6124	0.4072	0.3416	0.6124
HSI	0.2446	0.2391	0.6302	0.6302
CIELab	0.573	0.4597	0.639	0.639
xyY	0.723	0.5024	0.4165	0.723
LMS	0.968	0.7458	0.779	0.968
XYZ	0.9726	0.8167	0.7844	0.9726

Table 7: The third quartile for the pairwise Spearman’s correlation of the color channels given the color name.

We consider the third quartile of that correlation as the indicative statistic in Table 7. That is to say for 75% of all color names, for the given color-space, the correlation is less than this value.

Of the 16 color-spaces considered, it can be seen that the HSV exhibits the strongest signs of conditional independence – under this (mildly flawed) metric. More properly put, it exhibits the weakest signs of non-independence. This includes being significantly less correlated than other spaces featuring circular channels such as HSL and HSI.

Our overall work makes the conditional independence assumption, much like n-gram language models make the Markov assumption. The success of the main work indicates that the assumption does not cause substantial issues.

1.2 KDE based smoothing of Training Data

It can be seen that smoothing has very little effect on the performance of any of the neural network based distribution estimation models. All three term based models (SOWE, CNN, RNN) all perform very similarly whether or not the training data is smoothed. This is seen consistently in all the distribution estimation tasks. Contrast Tables 8 to 10 to the tables for the unsmoothed results Tables 8.1, 8.3 and 8.5.

If however, smoothing is not applied to the operational upper bound, it works far worse. In Tables 8 to 10 the Direct result refers to using the training histograms almost directly, without any smoothing or term-based input processing. This is the same as the operational upper bound, minus the KDE. It works very poorly (by comparison). This is because the bins values are largely independent: a very high probability in one bin does not affect the probability of the adjacent bin – which by chance of sampling may be lower than would be given by the true distribution.

This is particularly notable in the case of the direct, full training set result on the unseen combinations task reported in Table 10. As these were some of the rarest terms in the training set, several did not coincide with any bins for observations in testing set. This is because without smoothing it results in estimating the probability based on bins unfilled by any observation. We do cap that empty bin probability at $\epsilon_{64} \approx 2 \times 10^{-16}$ to prevent undefined perplexity. We found capping the lower probability for bins like this to be far more effective than add-on smoothing.

Conversely, on this dataset the neural network models do quite well, with or without smoothing. As the network can effectively learn the smoothness, not just from the observations of one color but from all of the observations. It learns that increasing the value of one bin should increase the adjacent ones. As such smoothing does not need to be applied to the training data.

Method	$\frac{PP}{256^3}$
Direct	0.164
Operational Upper Bound	0.071
SOWE-smoothed	0.075
CNN-smoothed	0.079
RNN-smoothed	0.088

Table 8: The results for the **full distribution estimation task** using smoothed training data. Lower perplexity (PP) is better. This corresponds to the main results in Table 8.1.

Method	$\frac{PP}{256^3}$
Direct	0.244
Operational Upper Bound	0.053
SOWE-smoothed	0.055
CNN-smoothed	0.058
RNN-smoothed	0.122

Table 9: The results for the **order distribution estimation task** using smoothed training data. Lower perplexity (PP) is better. This is a subset of the full test set containing only tests where the order of the words matters. This corresponds to the main results in Table 8.3.

Method	Full	Restricted
	Training Set	Training Set
	$\frac{PP}{256^3}$	$\frac{PP}{256^3}$
Direct	175.883	—
Operational Upper Bound	0.050	—
SOWE-smoothed	0.050	0.056
CNN-smoothed	0.053	0.063
RNN-smoothed	0.112	0.183

Table 10: The results for the **unseen combinations distribution estimation task** using smoothed training data. Lower perplexity (PP) is better. This uses the extrapolation subset of the full test set. In the extrapolating results certain rare word combinations were removed from the training and development sets. In the non-extrapolating results the full training and development set was used. This corresponds to the main results in Table 8.5.