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A thesis submitted in partial fulfilment of the requirement for the degree of Doctor of Philosophy

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Cardiff University
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Dedication

To People you care for their patience and support.

Abstract

We produce interpretable representations, and demonstrate their applicability in interpretable classifiers. Our approach is model-agnostic, given a similarity-based representation, we are able to produce a representation in terms of domain knowledge. We evaluate the interpretability of our representation and provide examples of interpretable classifiers with our representation.

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ML Machine Learning

NLP Natural Language Processing

NDCG Normalized Discounted Cumulative Gain

Chapter 1

Introduction

1.1 Motivation

1.2 Interpretability

Most successful approaches in recent times, like vector-spaces, word-vectors, and others, rely on the distributional model of semantics. This model relies on encoding unstructured text e.g. of a movie review, as a vector, where each dimension corresponds to how frequent each word is, we are able to calculate how similar the entities are, e.g. we know that if two movies have a similar distribution of words in their reviews, like frequent use of the word 'scary', or 'horror', then they would have a higher similarity value. These models, also known as 'semantic spaces' encode this similarity information spatially.

applications/need for good interpretability:

- Safety
- Troubleshooting, bug fixing, model improvement
- Knowledge learning
- EU's "Right to explanation"

2

Discrimination

properties of an interpretable classifier:

- Complexity: 'the magic number is seven plus or minus two' [12] also has many positive effects for its users, like lower response times [11, 8], better question answering and confidence for logical problem questions [8] and higher satisfaction [11].
- Transparancy:
- Explainability:
- Generalizability:

1.3 Thesis Overview / Contributions

In 3, we focus on further experimenting with one relationship that was formalized in [5]: a ranking of entities on properties. In particular, we use this method of building a representation of entities as a way to convert a vector space into an interpretable representation, for use in an interpretable classifier. The reason that we chose this representation to expand on is because by representing each entity e with a vector v that corresponds to a ranking r, the meaning of each dimension is distinct, and we are able to find labels composed of clusters of words for these dimensions. Here, we make the distinction between a property and a word, a property is a natural property of the space that exists in terms of a ranking of entities, and words are the labels we use to describe this property.

Chapter 2

Background

- 2.1 Representation Based Approaches to Interpretability
- 2.1.1 Methods to represent text

Word Vectors

- 2.1.2 Interpretable Methods to represent text
- 2.1.3 Conceptual spaces
- 2.1.4 Word Vectors
- 2.2 Directions and Semantic Relations
- 2.2.1 Obtaining directions/semantic relations and formalizing them from representations

Chapter 3

Converting Vector Spaces into Interpretable Representations

3.1 Introduction

Distributional representations like vector spaces have the ability to represent semantic information spatially. Vector spaces built from a domain-specific corpus of text that represent this kind of information, also known as 'semantic spaces', are used, for instance, to represent items in recommender systems [?, ?, ?], to represent entities in semantic search engines [?, ?], or to represent examples in classification tasks [?]. One way to understand how a semantic space represents information is as a conceptual space [7]. In this space, we can understand domain entities, e.g. movies in a domain of IMDB movie reviews, to be represented as points, and domain properties to be in regions around these points. In figure 3.1, we show an example conceptual space for movies.

The success of these semantic spaces has lead many to investigate how the similarity-based structure can be converted into formal relationships. For example, in word-vectors (see Section ?? for more) [13] found that "equivalent relations tended to correspond to parralel vector differences" [10], while [10] discovered that by decomposing representations into orthogonal semantic and syntactic subspaces they were able to produce substantial improvements on various tasks.

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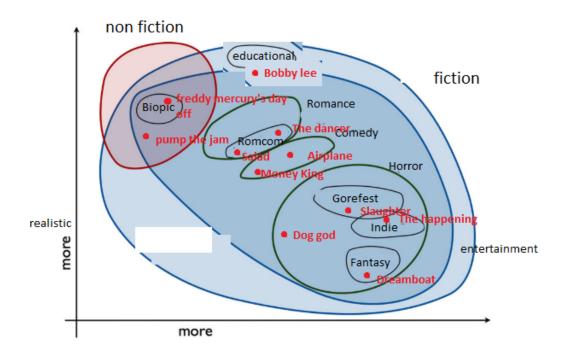


Figure 3.1: A conceptual space of movies, where regions correspond to properties and entities are points..

The semantic relation that we focus in on this paper are directions that correspond to salient features from the considered domain. These kind-of directions have been used in many different ways for different domains, For instance, [?] found that features of countries, such as their GDP, fertility rate or even level of CO₂ emissions, can be predicted from word embeddings using a linear regression model. Similarly, in [?] directions in word embeddings were found that correspond to adjectival scales (e.g. bad < okay < good < excellent) while [?] found directions indicating lexical features such as the frequency of occurrence and polarity of words.

By finding the dot product between entity points in the space and direction vectors, it is possible to induce a ranking of entities on those directions. In this chapter, we more deeply investigate the potential of direction vectors to rank entities on properties to form an interpretable representation.

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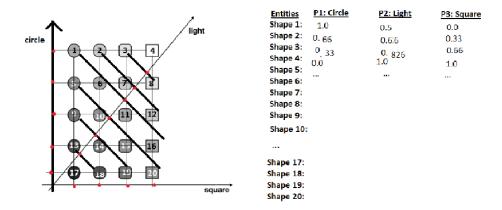


Figure 3.2: This figure shows a 2d toy space where entities are shapes and directions are properties. We demonstrate on the right the method to induce a ranking from the directions, in particular by using the dot-product of the entity point on the directions vector. In the same way for a more complex space, we can understand each entity point to be ranked on thousands of property directions, and the space to be much higher dimensionality..

In this thesis, we refer to these direction vectors as directions to convey the ordinal meaning, and directions as 'properties' if they are sufficiently salient in the space, e.g. In a domain of IMDB movie reviews where movies are entities, a direction on the word "The" would not be a property, but a direction on the word "Horror" would be.

Such properties are useful in a wide variety of applications. The most immediate example is perhaps that they allow for a natural way to implement critique-based recommendation systems, where users can specify how their desired result should relate to a given set of suggestions [?]. For instance, [?] propose a movie recommendation system in which the user can specify that they want to see suggestions for movies that are "similar to this one, but scarier". If the property of being scary is adequately modelled as a direction in a semantic space of movies, such critiques can be addressed in a straightforward way. Similarly, in [?] a system was developed that can find "shoes like these but shinier", based on a semantic space representation that was derived from visual features. Semantic search systems can use such directions to interpret queries

3.1 Introduction 7

involving gradual and possibly ill-defined features, such as "popular holiday destinations in Europe" [?]. While features such as popularity are typically not encoded in traditional knowledge bases, they can often be represented as semantic space directions.

We demonstrate the effect of different filtering methods to find properties, the ability of different clustering methods to label properties, as well as the number and types of directions, for use in a low-depth interpretable linear classifier; a Decision Tree. In Figure 3.3, we demonstrate how depth could affect a Decision Tree that uses salient properties. These trees are not only evaluated quantitatively on key domain tasks, we also evaluate how interpretable the resulting rules are. This gives us a comprehensive idea of how we can use these rankings as an interpretable representation. By using a Decision Tree, we can identify salient properties - if we are able to construct a simple but high-scoring classifier for if a movie is a 'Comedy' using only our ranking of entities on the property p = "Funny", "Hilarious", "Laughing" then we know that this property is salient. Although this is an extreme case, for more complex concepts, if we have salient properties that form the building blocks of this concept, then the model can be less complex and more general, two desirable properties for interpretable classifiers.

In a case study by [14], giving the business users the option between a model with higher classification score but more input variables and a lower classification score but less input variables resulted in more buy-in for system designers. By accurately representing salient concepts in the domain, we are also able to offer a similar option; less nodes in the decision tree in exchange for more accuracy.

This chapter continues as follows: We begin by describing the work related to this method, giving valuable context for the utility and potential of our approach. This is followed by an explanation of the method, including the variations we have adopted for our experimental work. We follow this with our qualitative experimentation, explaining how these variations affect the results, as well as the interpretability of the method, and

3.2 Related Work

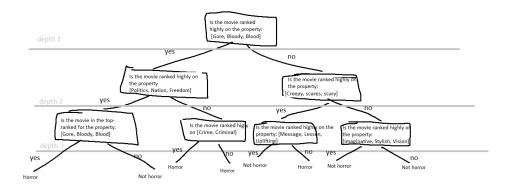


Figure 3.3: This figure shows an example tree from one of our classifiers. Here, we can see that the model increases in complexity as it increases in depth. In this case, we end-up getting better F-score with just a depth-one tree, as the tree begins to overfit at depth three. .

we end with a quantitative analysis on how well we can represent domain knowledge using decision trees constrained to a limited depth.

3.2 Related Work

3.2.1 Interpretable Representations

Vector space models typically use a form of matrix factorization to obtain low-dimensional document representations. By far the most common approach is to use Singular Value Decomposition [?], although other approaches have been advocated as well. Instead of matrix factorization, another possible strategy is to use a neural network or least squares optimization approach. This is commonly used for generating word embeddings [?, ?], but can similarly be used to learn representations of (entities that are described using) text documents [?, ?, ?]. Compared to topic models, such approaches have the advantage that various forms of domain-specific structured knowledge can easily be taken into account. Some authors have also proposed hybrid models, which

3.2 Related Work

combine topic models and vector space models. For example, the Gaussian LDA model represents topics as multivariate Gaussian distributions over a word embedding [?]. Beyond document representation, topic models have also been used to improve word embedding models, by learning a different vector for each topic-word combination [?].

3.2.2 Interpretable Classifiers

The most commonly used representations for text classification are bag-of-words representations, topic models, and vector space models. Bag-of-words representations are interpretable in principle, but because the considered vocabularies typically contain tens (or hundreds) of thousands of words, the resulting learned models are nonetheless difficult to inspect and understand. Topic models and vector space models are two alternative approaches for generating low-dimensional document representations.

Topic models such as Latent Dirichlet Allocation (LDA) represent documents as multinomial distributions over latent topics, where each of these topics corresponds to a multinomial distribution over words [1]. These topics tend to correspond to semantically meaningful concepts, hence topic models tend to be rather interpretable [4]. To characterize the semantic concepts associated with the learned topics, topics are typically labelled with the most probable words according to the corresponding distribution.

There are two ways in which topic models can be used for document classification. First, a supervised topic model can be used, in which the underlying graphical model is explicitly extended with a variable that represents the class label [3]. Second, the parameters of the multinomial distribution corresponding to a given document can be used as a feature vector for a standard classifier, such as a Support Vector Machine (SVM) or Decision Tree. LDA has been extended by many approaches, e.g. aiming to avoid the need to manually specify the number of topics [?], modelling correlations between topics [2], or by incorporating meta-data such as authors [?] or time stamps [?].

Broadly speaking, in the context of document classification, the main advantage of topic models is that their topics tend to be easily interpretable, while vector space models tend to be more flexible in the kind of meta-data that can be exploited. The approach we propose in this paper aims to combine the best of both worlds, by providing a way to derive interpretable representations from vector space models.

3.3 Method

The goal of this method is to obtain a representation composed of salient properties, starting with a domain-specific vector space S_e and its associated bag-of-words (BOW) representation B_w . To obtain these properties, we use a variant of the unsupervised method proposed in [?], which we explain in this section.

Rankings entities on words

We can understand that only some words will be properties, as only some correspond to domain knowledge, e.g. in a domain of IMDB movies, the word "the" does not correspond to a property of the domain, but the word "horror" does. Initially, we obtain rankings of entities for each word in the space.

As an initial filtering step, we remove words that do not meet a frequency threshold, with the understanding that words that do not occur in a minimum amount of documents are unlikely to correspond to properties as they are too specific to a subset of movies, which would make them difficult to learn. This leaves us with w_n words. We show the kind of words that would be poorly represented in ??.

Then, for each considered word w, a logistic regression classifier is trained to find a hyperplane H_w in the space that separates entities e which contain w in their BOW B_e representation from those that do not. The vector v_w perpendicular to this hyperplane is then taken as a direction that models the word w. In $\ref{eq:word_w}$, we show an example of

this in a toy domain. To rank the objects on the entity, if e is the representation of an entity in the given vector space S_e then we can think of the dot product $v_w \cdot e$ as the value $r_e w$ of object e for vector v_w , and in particular, we take $r_e 1 < r_e 2$ to mean that e_2 has the property labelled with the word w to a greater extent than e_1 . The result of this is shown in e?? Example entities, with their associated highest and lowest ranking properties, are shown in e??

Filtering directions to obtain salient properties

With the rankings R_r , we could create a representation of each entity Se, composed of w_n dimensions, where each dimension is a ranking of the entity e on that word w_re . However, many of the words do not properties. In-order to filter these words out, we evaluate them using a scoring metric, and remove the words that are not sufficiently well scored. We use three different metrics:

Classification accuracy. Evaluating the quality in terms of the accuracy of the logistic regression classifier: if this classifier is sufficiently accurate, it must mean that whether word w relates to object o (i.e. whether it is used in the description of o) is important enough to affect the semantic space representation of o. In such a case, it seems reasonable to assume that w describes a salient property for the given domain.

Cohen's Kappa. One problem with accuracy as a scoring function is that these classification problems are often very imbalanced. In particular, for very rare words, a high accuracy might not necessarily imply that the corresponding direction is accurate. For this reason, X proposed to use Cohen's Kappa score instead. In our experiments, however, we found that accuracy sometimes yields better results, so we keep this as an alternative metric.

Normalized Discounted Cumulative Gain This is a standard metric in information retrieval which evaluates the quality of a ranking w.r.t. some given relevance scores [?]. In our case, the rankings r_e of the entity e are those induced by the dot products $v_w \cdot e$

and the relevance scores are determined by the Pointwise Positive Mutual Information (PPMI) score ppmi(w,e), of the word w in the BoW representation of entity e where $ppmi(w,e) = \max\left(0,\log\left(\frac{p_{we}}{p_{w*}\cdot p_{*o}}\right)\right)$, and

$$p_{wo} = \frac{n(w, o)}{\sum_{w'} \sum_{o'} n(w', o')}$$

where n(w,e) is the number of occurrences of w in the BoW representation of object e, $p_{w*} = \sum_{e'} p_{we'}$ and $p_{*e} = \sum_{w'} p_{w'e}$.

In principle, we may expect that accuracy and Kappa are best suited for binary features, as they rely on a hard separation in the space between objects that have the word in their BoW representation and those that do not, while NDCG should be better suited for gradual features. In practice, however, we could not find such a clear pattern in the differences between the words chosen by these metrics despite often finding different words. In Table ??, we show examples of properties scored highly for each domain.

Clustering salient properties

Although we are able to find the words that are most salient, the properties in the domain may not correspond directly to words. Further, the properties may not be well described by their associated word. In-order to find better representations of properties, we cluster together similar vectors v_w , following the assumption that those vectors which are similar are representing some property more general than their individual words, and we can find it between them. As the final step, we cluster the best-scoring candidate feature directions v_w . Each of these clusters will then define one of the feature directions to be used in applications. The purpose of this clustering step is three-fold: it will ensure that the feature directions are sufficiently different (e.g. in a space of movies there is little point in having *funny* and *hilarious* as separate features), it will make the features easier to interpret (as a cluster of terms is more descriptive than an individual term), and it will alleviate sparsity issues when we want to relate

features with the BoW representation, which will play an important role for the finetuning method described in the next section.

As input to the clustering algorithm, we consider the N best-scoring candidate feature directions v_w , where N is a hyperparameter. To cluster these N vectors, we have followed the approach proposed in [?], which we found to perform slightly better than K-means. The main idea underlying their approach is to select the cluster centers such that (i) they are among the top-scoring candidate feature directions, and (ii) are as close to being orthogonal to each other as possible. We refer to [?] for more details. The output of this step is a set of clusters $C_1, ..., C_K$, where we will identify each cluster C_j with a set of words. We will furthermore write v_{C_j} to denote the centroid of the directions corresponding to the words in the cluster C_j , which can be computed as $v_{C_j} = \frac{1}{|C_j|} \sum_{w_l \in C_j} v_l$ provided that the vectors v_w are all normalized. These centroids $v_{C_1}, ..., v_{C_k}$ are the feature directions that are identified by our method.

Table ?? displays some examples of clusters that have been obtained for three of the datasets that will be used in the experiments, modelling respectively movies, placetypes and newsgroup postings. For each dataset, we used the scoring function that led to the best performance on development data(see Section ??). Only the first four words whose direction is closest to the centroid v_C are shown. K-Means Derrac's K-Means Variation Mean-shift Hdbscan

3.3.1 Quantitative Results

We use the data provided by [5], but differ from them in a few ways. First, rankings are done differently (we combine them differently or something?), as well as duplicates being removed from the data. This makes it difficult to directly compare our results to theirs, although they are sometimes similar.

"Second, as the classification problems are heavily imbalanced, most methods are able to achieve a similar accuracy score. Differences between the F1 score, on the other

hand, are more pronounced. Overall," [5]

We demonstrate the effectiveness of our approach on five datasets, each with their associated tasks.

- The IMDB Movie Dataset: 15,000 movies represented by aggregated reviews.
 On the tasks of Movie Genres, 100 IMDB Keywords, and UK + US Age Certificates.
- Flickr Place-types: 1,383 place-types. On the tasks of three different place-types, Foursquare, Geonames and OpenCYC.
- The 20-Newsgroups dataset: 18,846 newsgroup posting in 20 different categories. On the task of identifying which of the 20 categories the posting is from.
- The IMDB Sentiment Dataset: 50,000 movie reviews, with binary tags for either positive or negative. On the task of identifying if the review is positive or negative.
- The Reuters Dataset: 10655 News articles. On the task of identifying the category of the article.

To test the ability of the identified directions to accurately represent domain concepts in a ranking, we use low-depth decision-trees. Although these classifiers are not intended to be competitive with more complex classifiers like unbounded decision trees or SVM's, we find that our rankings are sometimes able to outperform these approaches using only a single decision node (equivalent to finding the best cutoff in a single ranking for classification). We use the F1 metric for our experiments, as almost all classes in each dataset are unbalanced.

We obtain the unsupervised representations as follows:

• To obtain the PPMI representation, we first remove terms from the corpus that do not appear at least (length of the corpus * 0.001) documents. We additionally

remove any terms that are in (length of corpus * 0.95) documents. Unlike when finding directions, we are not interested in finding salient properties, rather we simply want to remove noise from the dataset. For some corpuses, this means that we end-up with some empty entities that contained only infrequent terms. In particular, reuters goes from X documents to Y documents. In terms of vocabulary changes, reuters goes from X to 6432 terms, for the newsgroups, we go from 51064 terms to 9001. and then trim all entities that were exclusively composed of these terms. We then we apply standard PPMI based on the implementation from sydmi ¹.

- We obtain the MDS spaces for the movies, place-types and wines datasets from the data made available by [5], to obtain the MDS spaces for the other datasets, we use the same method as [5] and using default parameters for the MDSJ library. For each domain, we obtain 20, 50, 100 and 200 dimensional spaces.
- So that we can use the sparse PPMI matrices when obtaining the space, we the TruncatedSVD method from scikit-learn method² with default parameters. For each domain, we obtain 20, 50, 100 and 200 dimensional spaces.
- For the averaged word-vectors (AWV) and the weighted averaged word vectors (AWVw), we average the glove 6B word-vectors³ obtained from the Wikipedia 2014 + Gigaword 5 corpuses. As these are only available in size 50, 100 and 200, and there are not many other commonly used pre-trained word-vectors that offer multiple dimension sizes, differing from other methods we only obtain AWV and AWVw representations of size 50, 100 and 200. As these dimension sizes are hyper-parameters, we can consider average word vectors to be disadvantaged on some tasks, but as it is unlikely that there is too much benefit in training our own word-vectors from the relatively small domains, we opted to simplify the process and simply remove this as a hyper-parameter for this method, as well as

¹https://github.com/Bollegala/svdmi/blob/master/src/svdmi.py

²https://scikit-learn.org/stable/modules/generated/sklearn.decomposition.TruncatedSVD.htm

³https://nlp.stanford.edu/projects/glove/

the averaged method. The averaged word vectors are obtained by multiplying the vectors by the PPMI values, and finding the weighted average of all vectors multiplied in this way.

• For the Doc2Vec vectors, we use hyperparameter optimization to select the appropriate parameters, as the quality of the end space is typically reliant on welltuned hyperparameters for the dataset. We use [9] as a guideline for which parameters to optimize, re-using the parameters that stayed constant for both their datasets in their tests, specificially the dbow method, glove6B pre-trained 300-dimensional word-vectors, training those word vectors while training the representation, a sub-sampling of 10(-5), and a negative sample of 5. We tune and select between the values of the window size 5, 15, 50, the minimum frequency count 1, 5, 20, and epoch size 20, 40, 100, and as in the other methods, we obtain vectors of size 20, 50, 100, 200, but the hyperparameters for each of these is found individually, as the different space sizes are later evaluated on how well they can produce good directions. We evaluate the quality of the space using a Gaussian SVM on a selected task for each dataset, in the case of Reuters, Newsgroups and Sentiment, we use their associated tasks, for Movies we use the Genres task and Place-types the Foursquare task, as these tasks represent essential concepts in the domain.

Table 1 shows how well unsupervised representations perform. Topic models are included to demonstrate the difference between other simple and interpretable approaches, and Random Forest's are included to demonstrate the difference between our simple but interpretable approach and a model that typically performs well at the task [6], but is difficult to interpret.

Table 2 demonstrates the difference between unsupervised representations and salient properties, and Table 3 demonstrates the difference between salient properties and clustered salient properties.

3.3.2 Interpretability Results

Chapter 4

Fine-tuning Vector Spaces to Improve Their Directions

"Commonly, these representations are made in a single vector space with similarity being the main structure of interest. However, recent work by Mikolov et al. (2013b) on a word-analogy task suggests that such spaces may have further use- ful internal regularities. They found that seman- tic differences, such as between big and small, and also syntactic differences, as between big and bigger, were encoded consistently across their space. In particular, they solved the word-analogy problems by exploiting the fact that equivalent re- lations tended to correspond to parallel vector- differences.

[10] "Explicitly designing such structure into a neural network model results in representations that decompose into orthog- onal semantic and syntactic subspaces. We demonstrate that using word-order and morphological structure within En- glish Wikipedia text to enable this de- composition can produce substantial im- provements on semantic-similarity, pos- induction and word-analogy tasks."

4.1 Experiments

We find that non-linearity is useful.

Chapter 5

Investigating Neural Networks In Terms Of Directions

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