Document Embedding for Scientific Articles: Validation of word embeddings

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Abstract

1 Introduction

2 Background

Introduction and Background

Information retrieval
Information Retrieval(IR)is the activity of gathering relevant information, given another initial piece of information. The most practical example of this is a search engine. Given one or more search words the search engine will attempt to find relevant information. For example, a Google search on "Information Retrieval" (initial piece of information) will give you a list of results (relevant information). To be able to do this, the computer (search engine) must know which texts are related. To achieve this, multiple techniques can be used, such as TF-IDF, Word2Vec, Paragraph Vectors and GloVe. These techiques can be divided into two categories, ones that use a neural network and ones that do not.

Neural Network
Neural Networks are computational structures, based on vector and/or matrix calculations. They can be applied to many different tasks, but need to be trained for each task. This training is the process of iteratively adjusting multiplication matrices or vectors to achieve the optimal result. Which is the result that is as close as possible to the given output for different input and output sets. In some IR techniques, Neural Networks are used to either predict words that may occur around a given word, or predict a word given words that surround it. For example, given the sentence

"The search engine searches for relevant information"

the Neural Network can be trained to either predict the words around "searches" (the, search, engine, for, relevant, information) or to predict the word "searches", given the surrounding (the, search, engine, for, relevant, information). This trained matrix (vector per word) now indicates "word relatedness" which, as mentioned earlier enables association (thus retrieval) with related(relevant) texts.

Embedding
The vector for a word is referred to as a word embedding, which represents the word as a vector. This vector is a distributed representation of the word over the multiple vector dimensions Mikolov et al. [1]. Which can capture both the semantic and syntactic information of the word. The advantage of the machine learning models that create these embeddings is that they do not need human interaction Lai et al. [2]. Once trained, the word embeddings can be used to construct embeddings of larger texts, for example sentence, paragraph, document or corpus embeddings. The usage of word embeddings have improved various Natural Language Processing (NLP) areas such as named entity recognition, part-of-speech tagging, parsing, and semantic role labelling Luong et al. [3].

Text analysis techniques
To enable a computer to process text, for embedding creation or for tasks, the text has to be processed by an algorithm. In this research we used embeddings created by Word2Vec and TF-IDF feature vectors.

> Word2Vec
> Word2vec word embeddings are created using neural network, Word2vec learns word embeddings via maximizing the log conditional probability of the word given the context word(s) occurring within a fixed-sized window. Therefore the learnt embeddings contain useful knowledge about word co-occurrence[4]. There are multiple input/output possibilities for the neural network, best known are Skip-gram and the Continuous Bag-of-Words model (CBOW). The Skip-gram model takes a target word as input and outputs the predicted output words, while CBOW takes the context words as input and outputs the predicted target word[4, 5].
>
> Paragraph vectors
> Variations on the word2vec model have also been proposed, Le and Mikolov [6] introduced the paragraph vector, based on the word2vec model. The paragraph vector model uses additional variables to improve the accuracy of the word-embeddings. An advantage of the paragraph vector model is that it takes the word order into consideration, atleast in a small context [6].

GloVe

Pennington et al. [5] introduced the GloVe (Global Vectors) model. This model captures the global corpus statistics. The model transforms the word co-occurrences of all words in the corpus to chances, it excludes all the zero values and uses that as initial input for the neural network.

TF-IDF

TF-IDF is an abbreviation for Term Frequency times Inverted Document Frequency. This method does not rely on a neural network and therefore does not require training. The TF-IDF score is the product of the term frequency in a text and the inverted document frequency of the same term in a corpus of texts. Both of which can be calculated in a variety of ways. The feature vectors produced by TF-IDF do not capture syntactic or semantic information about words, but capture information about word occurrences.

Validation methods

The results produced by the techniques have to be validated to determine their quality (in usage). The quality of the results can be validated through, among others the F1 score and, for classification tasks, the rank of the correct category. The embeddings can furthermore be validated through their performance on tasks such as word analogies, word similarities, categorization and position visualization. These tasks can be designed to produce a score that gives an indication of the performance on a specific task. Schnabel et al. [7] found that a single validation metric cannot produce a representative result for other tasks. Embeddings that perform well on one task do not have to perform well on another task. As a result, the findings about performance of an embedding method are limited to the task on which they are tested, their results cannot be generalized to state that the embedding are overall "performing well". Validation tasks use either labelled or unlabelled data. Labelled data is data that is in some way marked, so that the correct answer can be derived from it, in contrast to unlabelled data.

Word Analogy

Word analogy validation is based on a labelled validation set, containing, commonly, word pairs of four, that can be logically divided into two parts. As Table 1 shows, each last word can be derived from the three words before. The score is the fraction of correctly given fourth words, given the first three words. This validation metric is used in multiple studies[1, 5, 8, 9].

Man	Women	King	Queen
Athens	Greece	Oslo	Norway
great	greater	tough	tougher

Table 1: Word analogies examples

Both this validation technique and the Word Similarity technique use vector distance calculations to validate the embeddings, this can therefore also be written as:

$$X_{\text{Man}} - X_{\text{King}} \approx X_{\text{Women}} - X_{\text{Queen}}$$

This means that the resulting vector of embedding of "Man" minus the embedding of "King" is approximately the embedding of "Woman" minus the embedding of "Queen". This resulting vector may be close to a vector "monarch" for example.

Word Similarity

A method to test the quality of word embeddings is the word similarity test. For these test, the distance between the word embeddings (vectors) is measured and compared to similarity scores defined by humans. Multiple non domain specific validation sets are publicly available including: the Rare-word dataset introduced in the paper "Better Word Representations with Recursive Neural Networks for Morphology" by Luong et al. [3], the MEN test collection by Bruni [10] and the WordSimilarity-353 test collection by Gabrilovich [11]. These sets, among others, have been used in multiple studies of word embeddings[5, 8]. This validation metric also relies on labelled data.

Classification

A classification validation method is a simple task which assigns a label to a text. Lau and

Baldwin [12] used data from StackExchange and tried to determine if a pair was a duplicate. In their setup, the text was a pair of texts, and their categories were duplicate or non-duplicate,

Categorization
Le and Mikolov [6] used for their research a dataset of IMDB with 100,000 movie review. They validated their proposed paragraph vector model by determining whether a review was positive or negative.

Position Visualization
Dai et al. [9] and Hinton and Roweis [13] mapped their word embeddings from a high dimensional vector to a two dimensional vector to be able to display them in a scatter plot and applied colors to various categories. These categories can be created with labelled or unlabelled data. The advantage of this is that a human can directly see the word distributions, and see if it is distributed in a way that seems logical. It gives furthermore insight in the overall spectrum of the words. However, this representation does not give a score, since it is not a evaluation of the data, but an alternative representation.

Motivation

Domain specific
Earlier research, concerning domain specific articles, by Truong [14], found that in-domain training of the word embeddings can improve the process of document clustering. This effect is even stronger than the number of training examples and the model architecture. Lai et al. [2] found that the corpus domain is more important than the corpus size. Using an in-domain corpus significantly improves the performance for a given task, whereas using a corpus in an unsuitable domain may decrease performance. These findings both indicate that an in-domain corpus improves the performance of word embeddings for the specific domains.

Problems in validation
To assess the performance of the embeddings, validation methods are used. This are tasks designed to produce a metric that gives an indication of the usability of the provided embeddings. Schnabel et al. [7] found that the validation method indicates only the quality of an embedding for a specific task. There is (yet) no methtod that can asses the usability of an embedding on all possible tasks, since each task may require other information to be embedded into the embedding. Validation methods use either labelled or unlabelled data. Labelled data is data that is in some way marked, so that the correct answer can be derived from it. Unlabelled is the opposite, this data is not marked.
The usage of labelled data is common practice for validation methods, since the results produced by this data can be easily checked checked. Unpublished results of the study by Truong encounter this problem, they show high error rates on the validation scores, presented in Table 2. However, the word embeddings created correct document clusterings[14], this seems to indicate that the word-vectors are able to represent the words correctly but that the available validation sets cannot confirm this.
Furthermore, a study by Schnabel et al. [7] found that the quality of embeddings are tasks specific, *different tasks favour different embeddings.* They also found that the embeddings encode information about word frequency, even in models that are created to prevent this. *This casts doubt on the common practice of using vanilla cosine similarity as a similarity measure.*
Therefore, we propose the validation of domain specific word-embeddings through a classification tasks, using multiple vector-distance calculations. This eliminates the need for labelled data in the validation of these domain specific word embeddings, will validate the quality of word embeddings for domain specific texts, and will validate the impact of different vector-distance measures on a categorization task.

	WordSim	Men	RareWords
Best results from the research by Truong:	0.49	0.61	0.32
Average results from the research by Truong	0.45	0.59	0.32

Table 2: Results for the different validation sets of word simularity validations on domain specific texts from the study by Truong [14]

Research Questions

- Have word-embeddings a higher accuracy for academic texts than TF-IDF for article classification?
- Which metric(s) can be used to measure the accuracy of word embeddings for scientific articles?

Related work

3 Work context

Data

Experiment setup

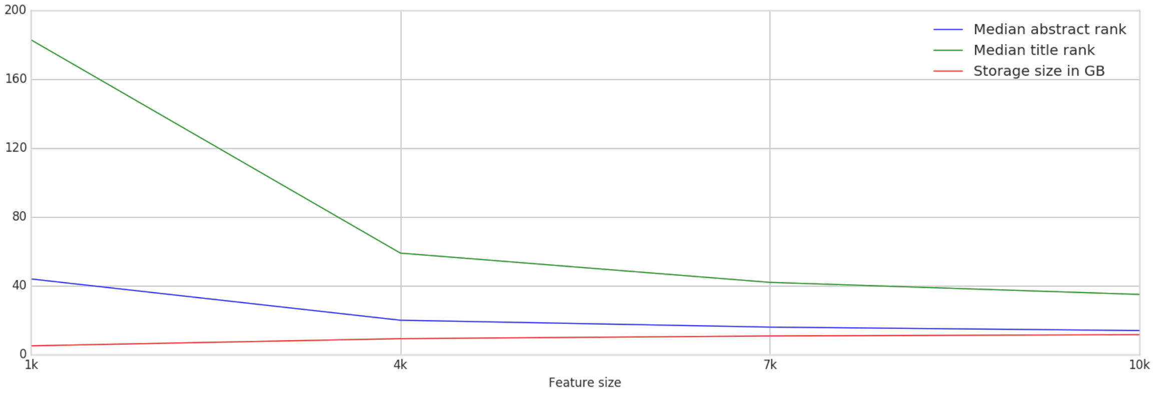
We used the following pipeline to collect the performance metrics for the categorization task:

1. Create embeddings
2. Filter articles
3. Create training and validation set
4. Create journal embeddings
5. Categorize validation articles
6. Calculate performance metrics

Create embeddings
For this research, we used word-embeddings (created using the word2vec model) and TF-IDF embeddings. The word-embeddings were created with the word2vec model from PySparks MlLib library[15]. The embeddings were pre-trained and have a vector size of 300, which is an industry default. The TF-IDF embeddings were created with the TF-IDF model from pyspark's MlLib library[15], in combination with a token hasher (HashingTF) from the same library. We used multiple hashing dimensions and multiple vocabulary sizes. Since the TF-IDF uses the output of the term hasher, the TF-IDF model produces the same dimensions. We will denote the tfidf sets as vocabulary size/hashing size. All of our sets, both embedding and TF-IDF, use tokenized texts.

Tokenization
== TODO ==

TF-IDF selection
To limit computational expenses, we used only the top performing which can reasonably be kept in RAM. The plot displays the ranking & size for the 1000/1000, 4000/4000, 7000/7000 and 10.000/10.000 sets respectively.



The plot show the median abstract & title rank and the storage size in Gigabytes (1024 based) plotted over feature size, which is equal to the hashing size for these sets. The plot shows that both title and abstract are stagnating, while the memory usage is, slowly, going up. At a feature size of 10.000, we have a storage size of 11.6GB. Given this size and the stagnation of the rankings, we chose to use the 10.000/10.000 feature size tfidf vectors, we furthermore used the 10.000/5000 set and the 5000/5000 set for comparison.

Embeddings
We have made use of multiple embedding sets for this research. All sets share the same (default) embedding and have been (uniquely) modified. For this research we have used the following embedding sets:

1. Default embedding

   The embedding as generated by word2vec, without further enhancements.

2. TF-IDF embedding

   The embedding as generated by the word2vec, multiplied by their tfidf weights to embed word priorities. We use this enhancement to give the embeddings more information about the corpus.

3. 10K TF-IDF Embedding

   The embedding as generated by the word2vec, filtered on the top 10.000 most common words, multiplied by their tfidf weights.
   We use this enhancement to try to filter out possible noise created by lots of words with few occurrences.

4. 5K TF-IDF Embedding

   The embedding as generated by the word2vec, filtered on the top 5.000 most common words, multiplied by their tfidf weights.
   We use this enhancement to cancel out the noise caused be rare words more aggressively

5. 1K 6K TF-IDF Embedding

   The embeddings as generated by the word2vec, filtered on the top top 1.000 till top 5.000 most common words, multiplied by their tfidf weights.
   We use this enhancement to ignore the top 1.000 most common words, which are most likely generic words, since they occur often. And to cancel out the rare-words, by cutting off all words after 6K. This gives us a set of 5K words.

Filter articles
We create our initial set of articles by collecting all articles from the journals that were published in the year 2017, and have at least 200 publications in 2017. This reduces the journal set to $3,759$ thousand journals, resulting in a set of $1,391,543$ million articles ().

Create training and validation set
We split our initial set 80% - 20%,. We use the 80% set as the training set for the journal representations, and the 20% set as the validation set for the journal representations.

Create journal embeddings
From our training set we create the journal embeddings by averaging all title embeddings as the journal title embedding, and by averaging all abstract embeddings as the journal abstract embedding. We also normalized both embeddings.

Categorize validation articles
To categorize the articles, we calculate the distance between the title- and abstract embedding of each article, from the validation set, to the title- and abstract embedding of each journal. To calculate the distance, we use cosine similarity (as provided by the SciPy library[16]). During this process we keep track of:

- Title-based-rank of the actual journal
- Abstract-based-rank of the actual journal
- Best scored journal on the abstract similarity
- Best scored journal on the title similarity
- Abstract similarity between the actual journal and the article
- Title similarity between the actual journal and the article

Performance measurement
We use multiple metrics to indicate the performance of the embeddings on a categorization task. These metrics are:

1. F1-score
2. Median & average rank

3. Rank distribution

F1-score

We define the positive & negative metrics as follows:

$$\begin{aligned}
TruePositive &= \text{Articles that are correctly matched to the current journal}\\
FalsePositive &= \text{Articles that are incorrectly matched to other journals}\\
FalseNegative &= \text{Articles that are incorrectly matched to the current journal}
\end{aligned}$$

We used these metrics to calculate the Recall, Precision & F1 as follows:

$$Recall = \frac{TruePositive}{TruePositive + FalseNegative}$$

$$Precision = \frac{TruePositive}{TruePositive + FalsePositive}$$

$$F1 = \frac{2 * Precision * Recall}{Precision + Recall}$$

Median & average rank

We use the median rank to indicate around which rank the 'standard' article would be ranked, based on its title or abstract. We do this by taking the median of the respective rank from each article. This gives us an indication of the behaviour of most articles in our validation set. This median rank (mostly) ignores the outliers, we therefore also use the average rank, which gives a more global indication, although this rank may be over-influenced by some outliers.

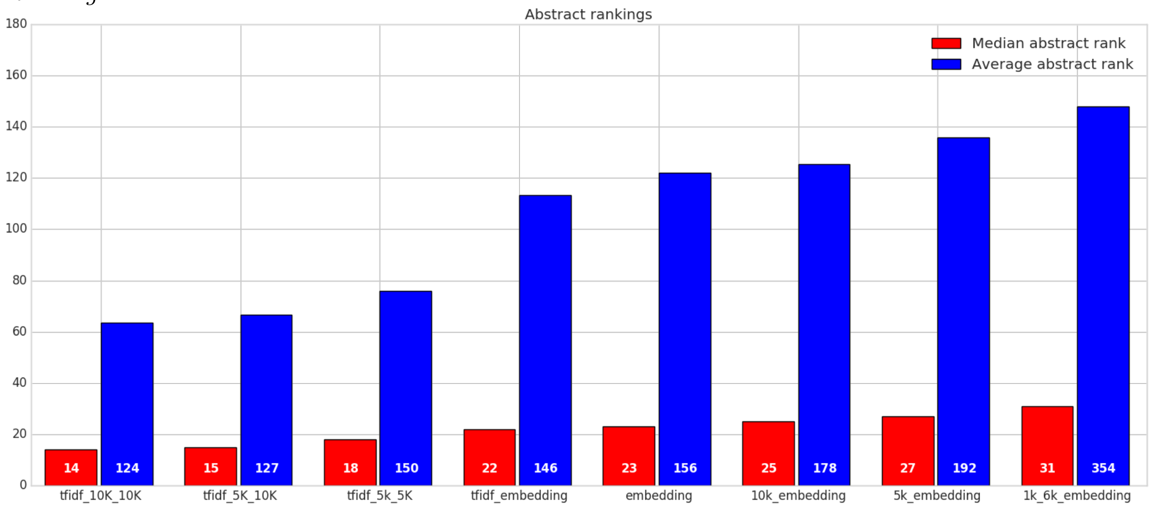
Rank distribution

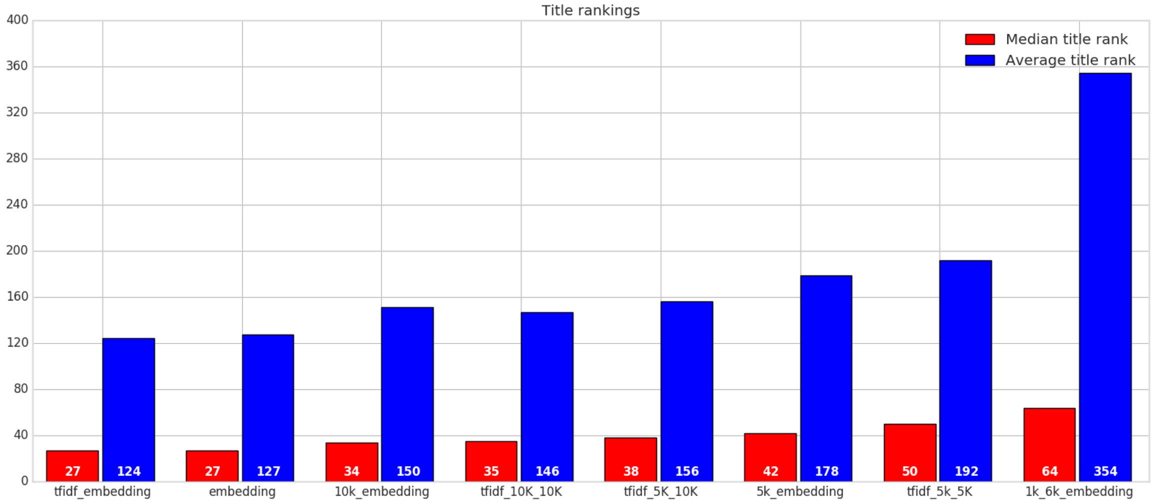
To further analyse the ranking results, we plot the rank distribution to get an indication of the ranking-landscape. We limit ourselves to the following categories: 1 (absolute hits), top-10, top-20, top-30, top-40, top-50, top-100 and 100+.

4 Results

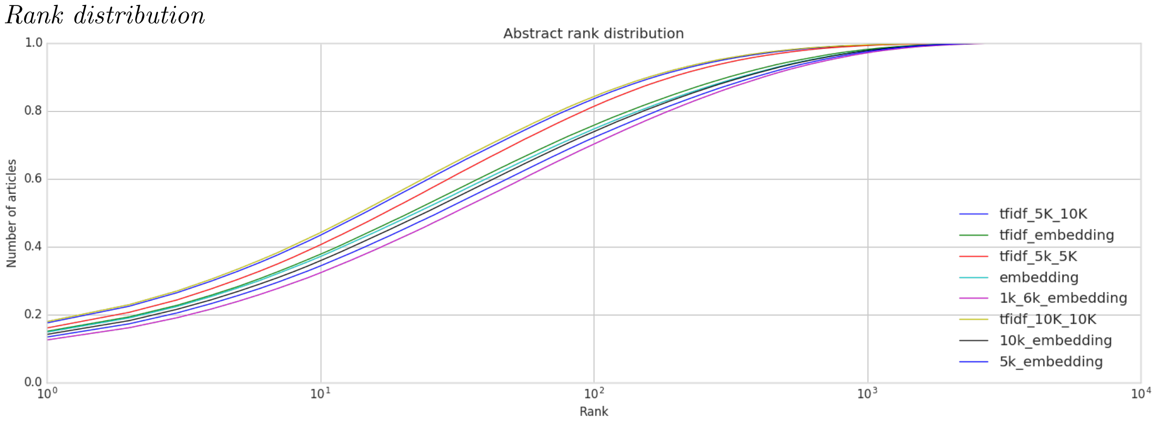
Research results

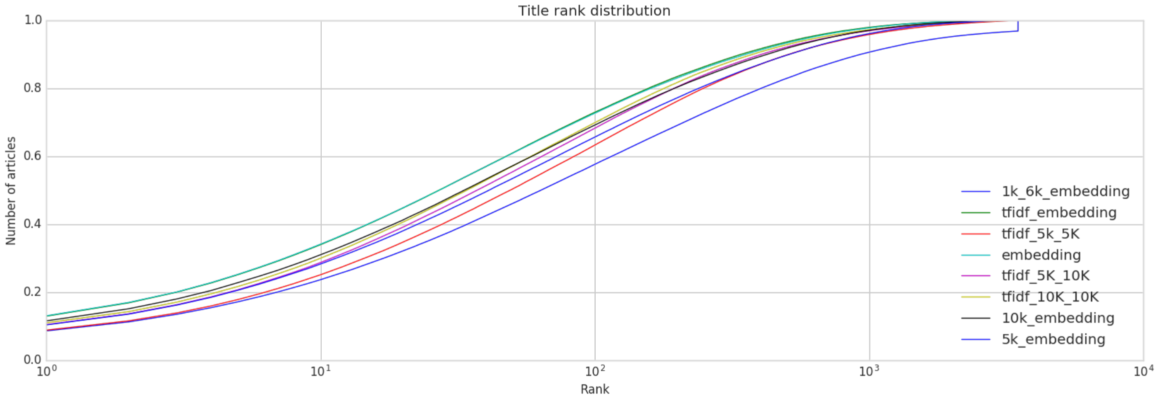
Ranking



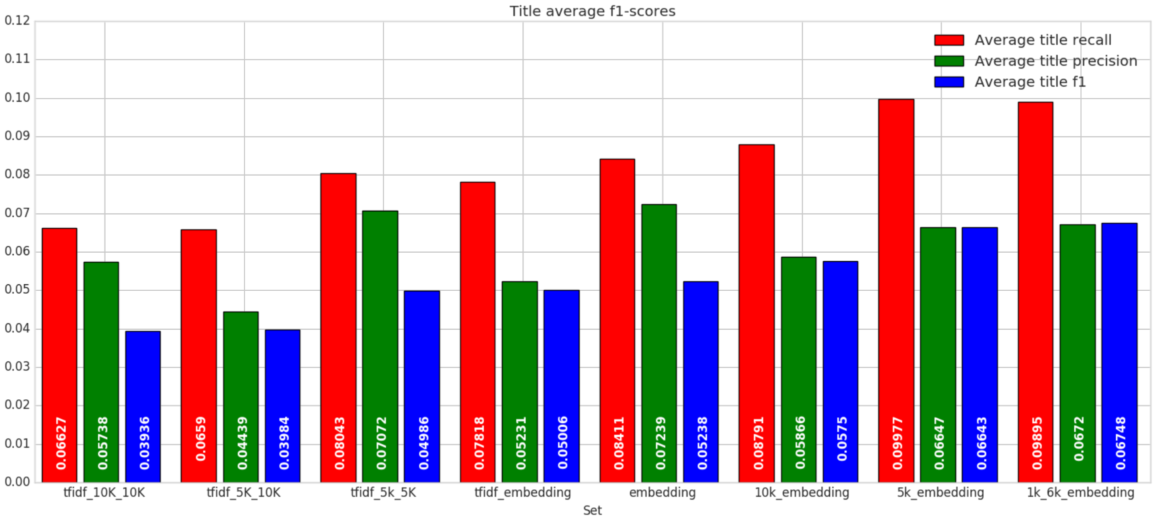


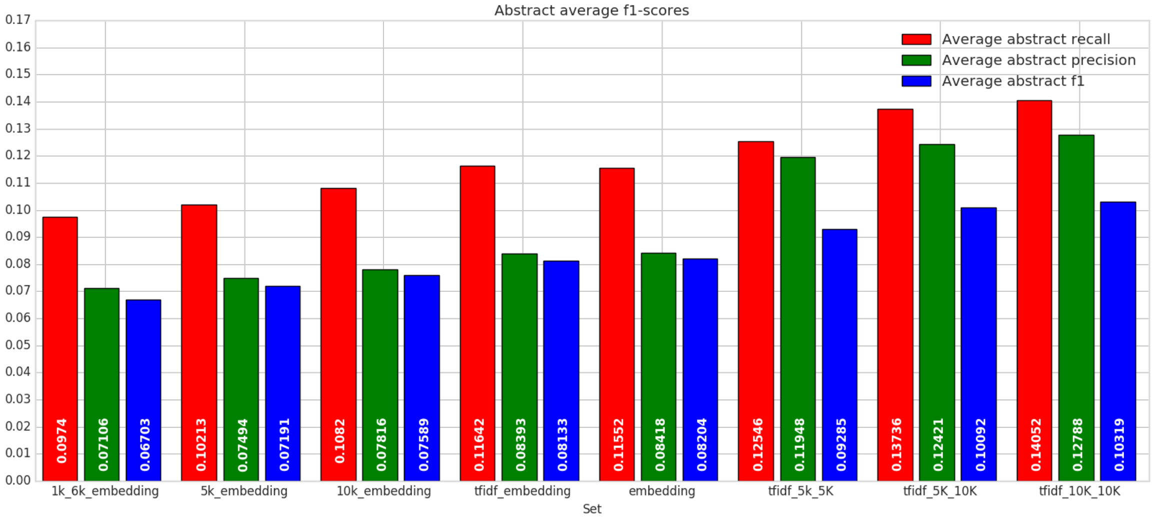
Rank distribution





F1-Score





Memory usage

Set	Size in GB
tfidf 5k 5K	9.82
tfidf 5K 10K	11.47
tfidf 10K 10K	**11.61**
embedding	3.13
5k embedding	3.13
10k embedding	3.13
tfidf embedding	**3.13**
1k 6k embedding	3.06

Discussion

1k 6k behaviour

1k 6k embedding has lower storage than the other embeddings, this is most likely due to it's word filtering. Cutting off most-used words results probably in empty titles/abstracts which reduce the space that is needed for this embedding variant. All other embeddings have the same size, which indicates that this does not occur in the other situations, even in the 5k set, where the same amount of words are cut off.

The, relatively, much higher average rank compared to the median rank of the 1k 6k embedding can be explained with the data of table (RANKING DISTRIBUTION TABLE). This shows that the embedding goes up at the start, indicating that there are articles in the low ranks, flats out in the center more than the others do, indicating a relatively low amount of articles in the middle ranks, and a strong increase at the end. Indicating that there are many titles on the high end of the distribution. This explains the relatively low median, which is dawn towards the lower end of the distribution, and the high average, which is drawn to the higher end of the distribution.

Best performers

The data shows that the 10.000/10.000 set preforms better than all other TF-IDF sets, although the difference with the 5.000/10.000 is low, 1 (7.14%) on abstract and 3 (8.57%) on title. For the embeddings the TF-IDF weighted embedding works better than the others, although it is near equal to the default embeddings, which 1 rank higher on abstract, and equal on title.

TF-IDF weighting on embeddings

The difference between the TFIDF weighted embedding and the default embedding can be explained as follows: The embeddings seem to outperform the TF-IDF in situation when there is little information available, the titles in our case. This indicates that the embeddings store some kind of word meaning that enables them to perform relatively well on the titles. The abstracts on the other hand contain much more information. Our data seems to indicate that the amount of information available in the abstracts enable the TF-IDF to cope with the lack of embedded information. If this is the case, we could expect that there would little performance increase on the title, since the TF-IDF lacks the information to perform well. This can be seen in our data, only the average rank increased by 3, indicating that there is a difference between the two embeddings, but not a major one. We could expect on the abstract an increase in performance, since the TF-IDF has more information in this context. We would expect that the weighting applied by the TF-IDF improves the performance of the embedding by indicating word importance. Our data shows a minor improvement in performance of 1(4.35%) median rank and 10(6.41%) average ranks.

Raw, readable results

The TF-IDF outperform the embeddings on the abstract with a difference of 8 ranks for the best of each. On the title however, the best embedding outperforms the best TF-IDF by 8 ranks.

Memory usage

Although the TF-IDF outperforms the embeddings on the abstracts, the memory usage of the TF-IDF is higher than the memory usage of the embeddings. The top-performing embedding, TF-IDF weighted embedding, uses 3.13 GB, the top performing TF-IDF, 10.000/10.000 uses 11.61 GB, which is 270.93% more. The closest TF-IDF configuration we used was 1.000/1.000, which uses 5.13 GB (SEE GRAPH XXX). This TF-IDF set has a median title rank of 183 and a median abstract rank of 44. Which is worse than the embedding, which also uses less memory.

Conclusion

This research shows that the article embeddings, created with word embeddings, perform better than the reasonable TF-IDF alternatives for our categorization task, based on article titles. The TF-IDF alternatives give better results than the embeddings based on abstracts. The performance of the embeddings have been improved by weighting them with the TF-IDF values on word level. This improved embedding results in a median rank decrease of 8 on title and an median rank increase of 8 on title, compared to the best performing TF-IDF alternative. The embedding also results in a memory decrease of 73.04% making it more viable to keep it in memory. We have furthermore shown that limiting vocabulary size to exclude rare words or common words decreases the performance of the embeddings. We thus come to the following conclusions:

1. Article based embeddings perform better than TF-IDF on small texts
2. TF-IDF performs better than article based embeddings on larger texts
3. Embeddings give a significant decrease in memory usage compared to TF-IDF

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