"Hybrid Topics" -- Facilitating the Interpretation of Topics Through the Addition of MeSH Descriptors to Bags of Words

Zhiguo Yu[a], **Thang Nguyen**[b], **Ferdinand Dhombres**[c], **Todd Johnson**[a], and **Olivier Bodenreider**[c]

[a]The University of Texas of Biomedical Informatics at Houston, Houston, Texas, USA

[b]Department of Computer Science, University of Maryland, College Park, Maryland, USA

[c]U.S. National Library of Medicine, National Institute of Health, Bethesda, Maryland, USA

Abstract

Extracting and understanding information, themes and relationships from large collections of documents is an important task for biomedical researchers. Latent Dirichlet Allocation is an unsupervised topic modeling technique using the bag-of-words assumption that has been applied extensively to unveil hidden thematic information within large sets of documents. In this paper, we added MeSH descriptors to the bag-of-words assumption to generate 'hybrid topics', which are mixed vectors of words and descriptors. We evaluated this approach on the quality and interpretability of topics in both a general corpus and a specialized corpus. Our results demonstrated that the coherence of 'hybrid topics' is higher than that of regular bag-of-words topics in the specialized corpus. We also found that the proportion of topics that are not associated with MeSH descriptors is higher in the specialized corpus than in the general corpus.

Keywords

Medical Subject Headings; Models; Statistical Data; Data Interpretation; Statistical

Introduction

Motivation

Knowledge discovery is a fundamental and important activity in biomedical research. Given that unstructured data is increasing exponentially, extracting and understanding information, themes, and relationships from large collections of documents is increasingly important. PubMed currently comprises more than 26 million articles from the biomedical literature and has been widely used to help researchers keep up with the state of the art in their domains and explore other unfamiliar research areas. To help users better retrieve relevant information and manage this tremendous volume of biomedical literature, the US National

Address for correspondence: Olivier Bodenreider, MD, PhD, 8600 Rockville Pike, 38A/ 09S904, Bethesda, MD 20894, Phone Number: (301) 827-4982, olivier@nlm.nih.gov.

Library of Medicine (NLM) has developed the Medical Subject Headings (MeSH) controlled vocabulary for indexing MEDLINE articles. MeSH has been used to improve PubMed query results [1–2]. However, users are still often overloaded by the tremendous number of relevant articles returned from their PubMed queries [3]. Hence, biomedical researchers need an efficient and convenient way to discover knowledge from large sets of documents.

MeSH Indexing vs. Topics

Latent Dirichlet Allocation (LDA) [4], is a popular topic modeling method that aims to extract the semantic themes (topics) automatically from a corpus of documents. These topics describe the thematic composition of documents and can thus capture the semantic similarity between them. In contrast, MeSH descriptors are manually created and maintained by domain experts to cover all important themes. Topics extracted from a subset of documents are subset-specific [5]. Thus, they may identify corpus-specific themes that may not be covered in MeSH. Such themes may uncover a specific set of concepts for a particular domain or sub-domain.

Related Work

Considerable research has examined the application of topic models to MeSH descriptors. Labeled LDA (labeled LDA) [6] is a supervised topic model developed to uncover latent topics that correlate with user tags in labeled corpora. In other words, each tag will be represented as a topic. Zhu et al. have used labeled LDA in an attempt to automatically assign MeSH descriptors to new publications (not yet indexed with MeSH descriptors) [7]. Elsewhere, Newman et al. presented a resampled author model that combines both general LDA and the author-topic model (in this case MeSH descriptors were treated as the 'authors'). The resampled author model provided an alternative and complementary view of the relationships between MeSH descriptors [8]. All these investigations used topic models to interpret MeSH descriptors. However, they cannot be used to identify themes that are not covered in MeSH. In 2014, a graph-sparse LDA model [9] was developed to generate more interpretable topics by leveraging relationships expressed by controlled vocabulary structure (e.g. MeSH). In this model, a few concept-words from the controlled vocabulary can be identified to represent generated topics. Though MeSH was shown to work well for summarizing biomedical articles, this model cannot identify themes that may not exist in the MeSH vocabulary.

Specific Contribution

This work introduces an alternative LDA approach by migrating its original bag-of-words assumption to a 'bag-of-MeSH&words' approach. By enriching each document with its indexed MeSH descriptors, 'hybrid topics' (mixed vectors of words and MeSH descriptors) can be generated by LDA.

Objectives

We investigated whether the addition of labels (e.g., MeSH descriptors) to bags-of-words can improve the quality and facilitate the interpretation of LDA-generated topics. More

specifically, to assess the quality and interpretability of topics, we tested two hypotheses using one large general biomedical corpus and one smaller specialized biomedical corpus.

1. The coherence (used as a surrogate for quality) of 'hybrid topics' is expected to be higher than that of regular bag-of-words topics.

2. The proportion of topics that are not associated with some MeSH descriptor, which reflects limited interpretability, is expected to be higher in a specialized corpus than in a general corpus.

Background

Medical Subject Headings (MeSH)—The MeSH controlled vocabulary was developed by NLM to help manage, index, and search MEDLINE articles. There were 27,883 descriptors in the 2016 MeSH, with over 87,000 entry terms that assist in finding the most appropriate MeSH descriptor (for example, 'Vitamin C' is an entry term to 'Ascorbic Acid'). In the 2016 MeSH, 82 qualifiers could be attached to MeSH descriptors to describe a particular aspect of a concept, such as 'adverse effects', 'diagnosis', etc. Each year, the MeSH specialists revise and update the MeSH vocabulary to cover emerging research areas and improve indexing consistency and efficiency. MeSH specialists are responsible for areas of the health sciences in which they have knowledge and expertise. MEDLINE indexers make suggestions for new descriptors to MeSH specialists during their indexing processes. Besides, MeSH specialists also collect new terms as they appear in the scientific literature or emerging areas of research. After defining these terms within the context of the existing vocabulary, MeSH specialists recommend their addition(s) to MeSH. During each MEDLINE year-end processing (YEP) activities, changes made to MeSH are applied to MEDLINE (retrospectively) for conformance with the current version of MeSH.

Latent Dirichlet Allocation (LDA)—LDA is a generative model that assumes that each document is generated from a mixture of topics and that each topic corresponds to a distribution over all words in the corpus. Informally, the 'generative story' for LDA is as follows. First, a document is generated by drawing a mixture of topics that the document is about. To generate each word in this document, one draws a topic from this distribution and subsequently selects a word from the distribution over the vocabulary of the whole corpus corresponding to this topic. The LDA algorithm uses this generative model to uncover the latent topics contained within a given a corpus. Specifically, it estimates the parameters that define document topic mixtures and the conditional probabilities of each word given each topic. Parameter estimation is usually done via sampling approaches.

The number of topics produced by LDA must be prespecified. Determining the 'right' number of topics for different datasets remains a challenge. When the number of topics increases, redundant and nonsense topics may be generated. Running LDA with a small number of topics will generate more general themes. In this paper, we used a topic coherence measure to determine the optimal number of topics for our dataset [10]. Details are described in the next section.

Quality of Topics—Recently, O'Callaghan et al. [10] reviewed a number of topic coherence studies using various corpora and proposed a general measure based on distributional semantics, *TC-W2V.* This measures evaluates the relatedness of a set of top terms describing a topic, based on the similarity of their representations in a *word2vec* distributional semantic space. Specifically, the coherence of a topic *n* represented by its top *t* ranked terms is given by the mean pairwise cosine similarity between all relevant term vectors in the *word2vec* space:

$$coh(t_n) = \frac{1}{\binom{t}{2}} \sum_{j=2}^{t} \sum_{i=1}^{j-1} \cos(wv_i, wv_j)$$

An overall score for a topic model *M* consisting of *k* topics is calculated by averaging the individual topic coherence scores:

$$coh(M) = \frac{1}{k} \sum_{n=1}^{k} coh(t_n)$$

In this investigation, we use topic coherence to help determine the optimal number and quality of topics.

Relations between MeSH and Topics—Topics are generated based on the bag-of-words assumption, which ignores word order. Each topic is represented as a list of ranked words, which provides the user with a sense of what the topic is about. Each document is displayed as a list of weighted topics, which represents different aspects of the document. Since the tokens within each topic are ranked according to the conditional probabilities *P(w/t)* learned when training the model, where *w* is a word and *t* is a topic, the top few words of each topic provides insight into the subject of the topic. However, the interpretation of the topics (i.e., lists of words) is left as an exercise for the user.

As mentioned earlier, MeSH was developed to cover all important themes and each article in MEDLINE is indexed with a few relevant MeSH descriptors assigned by the MEDLINE indexing staff for retrieval purposes. To capture the potential relationships between MeSH and topics, we simply added the MeSH descriptors assigned to each article to the bag-of-words for a given document, creating a modified 'bag-of-MeSH&word'. Under this 'bag-of-MeSH&word' assumption, 'hybrid topics' are generated and each topic is represented as a list of tokens (i.e., a mixed list of ranked words and MeSH descriptors). The presence of MeSH descriptors among the top tokens for a given topic is expected to facilitate the interpretation of topics. More specifically, if a MeSH descriptor appears among the top *m* (for some *m*) tokens of a topic, we will assume this MeSH descriptor is highly associated with this topic. We consider three types of association patterns:

1.   One topic has no MeSH descriptor in its top *m* tokens (1-0 mapping);

2.   One topic has a single MeSH descriptor in its top m tokens (1-1 mapping);

3.   One topic has multiple MeSH descriptors in the top m tokens (1-many mapping).

Examples of topics for each association pattern are shown in Table 1 along with the top 10 tokens for each topic.

Methods

Data Preparation

One large general corpus and one small specialized corpus were used in this investigation. The general corpus consisted of 200k articles randomly selected from all PubMed articles published in 2013. The specialized corpus consisted of 2,472 articles from the journal *Prenatal Diagnosis*, which focuses on fetal medicine.

General Corpus—There are roughly 1.2 million articles in PubMed for the year 2013. We randomly selected 200k articles (titles and abstracts) from these. This represents an appropriate amount of data given our computing resources.

To reduce the sparsity of the document-to-words distribution, we performed Part of Speech tagging on the dataset and merged several categories, including *NN* and NNS (e.g., patient and patients); *VB*, *VBD*, *VBG*, and VBN (e.g., eat, ate, eaten, and eating); and *JJ*, *JJR*, and *JJS* (e.g., good, better, and best).

We also removed PubMed stop-words and infrequent words (with a frequency lower than 50). A total of 21,922 unique words remained. Similarly, for MeSH descriptors, we treated specific frequently used descriptors known as check tags (e.g., human, male, female, etc.) as stop words, and ignored infrequent descriptors (with a frequency lower than 5). A total of 13,853 MeSH descriptors remained.

Specialized Corpus—We applied similar preprocessing to the specialized corpus, but with different cutoff values due to its smaller size. After setting a cutoff frequency of five for words, we obtained 3,623 unique words. With a cutoff frequency of one for MeSH descriptors, we obtained 919 MeSH descriptors.

Experiment #1

We investigated whether the addition of MeSH descriptors to bags-of-words increased the quality of topics. As a surrogate for the quality of topics, we used topic coherence [11].

In practice, to determine whether our 'hybrid topics' approach (i.e., 'bag-of-MeSH&words') outperformed the original LDA bag-of-words approach (baseline), we generated LDA models under both these assumptions for a various number of topics on the two datasets.

For the general corpus, the number of topics tested 50–600. For the specific corpus, we tested 4–100. For each number of topics, we calculated topic coherence for both the baseline and the 'hybrid topics' approaches.

More specifically, for the large general corpus, we used the indexed PubMed articles (titles and abstracts) published in 2013 as our background corpus when building the *word2vector*

space for the original LDA with the bag-of-words assumption. To build the *word2vector* space containing both MeSH descriptors and words, we simply appended the MeSH descriptors for an article to the end of the document. In this way, we could get a mixed *word2vector* space of MeSH descriptors and words. In our experiment, we tested two different positions of MeSH descriptors in the citation (front and end) and obtained similar topic coherence results. Following [10], we used the same *word2vec* setting and the number of top terms per topic (t=10).

For the small specialized corpus, we used the full-text of these articles as the background corpus when building the *word2vec* space. To build the mixed *word2vector* space of MeSH descriptors and words for this background corpus, we added MeSH descriptors to the end of each full article. In the *word2vec* setting for this dataset, we set vector size to 200, cutoff frequency to three, and window size to 20.

To compare the topic coherence measures obtained within each corpus at different numbers of topics for the baseline and the 'hybrid topics', we used a paired t-test.

Experiment #2

To assess whether the proportion of 'hybrid topics' that were not associated with some MeSH descriptor, which reflects limited interpretability, were higher in a specialized corpus than in a general corpus, we first had to determine the optimal number of topics in each corpus.

Choosing the number of topics k is a key parameter selection decision in topic modeling. Too few topics will produce results that are overly broad, while too many will lead to many small, highly similar topics. One general strategy proposed in the literature is to compare the topic coherence of topic models with different values of k. An appropriate value for k can then be identified by examining a plot of the mean *TC-W2V* coherence scores for a fixed range and selecting a value corresponding to the maximum coherence score. Since we only expected the MeSH descriptors to help interpret topics rather than introduce new topics, we just used LDA's original bag-of-words assumption to determine the optimal number of topics for each test corpus.

Having determined the optimal number of topics for each corpus, we examined the 'hybrid topics' obtained for this number of topics and counted which ones were not associated with MeSH descriptors (i.e., which ones did not contain at least one MeSH descriptor among their top-20 tokens).

We used the chi-square statistic to compare the distribution of topics of two patterns between the 'hybrid topics' and the baseline.

Results

Experiment #1

Figures 1 and 2 display the difference in topic coherence between our 'bag-of-MeSH&words' assumption ('hybrid topics') and LDA's original bag-of-words assumption (baseline) for the general and specialized corpora respectively.

For the general corpus, we computed topic coherence for 10 different numbers of topics for both the baseline and our 'hybrid topics'. As shown in Figure 1, topic coherence scores were very close between the baseline and 'hybrid topics'. The coherence was slightly better with 'hybrid topics' after 100 topics, but slightly lower for 50 and 100 topics.

For the specialized corpus, however, we saw a clear improvement on the coherence of topics in favor of 'hybrid topics' compared to the baseline. As shown in Figure 2, topic coherence scores were systematically higher for 'hybrid topics' across all numbers of topics.

Though 'hybrid topics' are higher the baseline after 100 topics on the general corpus, the paired t-test was not significant (p=0.1624). We could not properly assess the difference between the two approaches on this general corpus. With the specialized corpus, however, the paired t-test was highly significant (p=6.8e-25), demonstrating that the quality of the 'hybrid topics' was better than that of the baseline topics.

Experiment #2

Optimal Number of Topics—For the large general corpus, we generated LDA models containing $k \in [50, 600]$ topics and selected the value of k that maximized the mean *TC-W2V* coherence. As shown in Figure 3, *k=200* is the first maximum and was therefore selected as the optimal number of topics for this dataset.

For the small specialized corpus, we generated LDA models containing $k \in [4, 100]$ topics. As shown in Figure 4, *k=22* was the first maximum and was therefore selected as the optimal number of topics for this dataset.

Proportion of Topics Not Associated with a Mesh Descriptor—Table 2 displays the number of different patterns of association between topics and MeSH descriptors observed in the general and specialized corpus for their respective optimal number of topics.

As shown in Table 2, the proportion of topics not associated with a MeSH descriptor was higher in the specialized corpus (41%) than in the general corpus (3%). The chi-square statistics was 57.36 (p= 3.502e-13), which suggests that the corpora had significantly different distributions.

Discussion

Findings and Significance

This investigation demonstrates that the addition of MeSH descriptors to the traditional bag-of-words approach to creating topic models ('hybrid topics') can improve the quality of the

topics and facilitate their interpretation, but the impact is different on a general corpus and on a specialized corpus. The quality of the 'hybrid topics', assessed by their coherence, was better than that of the baseline topics in the specialized corpus, but it did not seem to be the case in the general corpus.

MeSH terms are created and maintained by MeSH specialists to cover all general themes in biomedicine. However, topics extracted from a subset of documents are often specific to these documents. For the general corpus, most of the topics captured by LDA were general themes. Hence, this addition of MeSH descriptors to the bag-of-words approach did not contribute too much to the topic quality. This could be the reason that we did not see a significant improvement of the topic coherence score between regular and 'hybrid topics' in the general corpus. In contrast, for the specialized corpus, adding MeSH descriptors can provide additional information for LDA to better differentiate between general and specific themes and to improve topics quality.

In terms of interpretability, however, the general corpus benefited from 'hybrid topics' more than the specialized corpus did, because over 40% (9/22) of the 'hybrid topics' remained unlabeled (i.e., not associated with any MeSH descriptors) in the specialized corpus, compared to 3% (6/200) in the general corpus.

Applications to Corpus Exploration

From the general corpus, we saw that only 6/200 topics (3%) contained no MeSH descriptors in their top 20 terms. For the specialized corpus, 9/22 topics (40%) were generated with no MeSH descriptors in their top 20 terms. General themes from the MeSH vocabulary may not be able to cover in detail all aspects of a specialized corpus. In contrast, the topics generated by LDA from a corpus are corpus-specific. It is therefore logical that more topics with no MeSH descriptors are generated from a specialized corpus than a general corpus. Hence LDA will be more useful for a specialized corpus on the task of exploring concepts that may not be covered by MeSH.

From the general corpus, we also saw that 178/194 topics were associated with MeSH descriptors (92%) generated with multiple MeSH descriptors. MeSH descriptors were characterized in 16 top-level categories, such as category A for anatomic terms, category B for organisms, C for diseases, etc. Of these 178 topics, 140 (79%) contained MeSH descriptors from different top-level MeSH categories. These topics were most likely interdisciplinary topics. For the specialized corpus, 7/13 topics associated with MeSH descriptors (54%) were generated with multiple MeSH descriptors. Topics associated with multiple MeSH descriptors from different top-level MeSH categories could be used to explore the intersection of multiple domains. LDA clearly offers an advantage for discovering interdisciplinary topics.

Limitations and Future Work

One limitation of this work is that we ignored the MeSH qualifiers and only considered the MeSH descriptors when constructing our 'hybrid topics'. In the future, we will include the qualifiers to our 'hybrid topics' to test whether it improves the interpretation of topic models. We are also planning to run LDA with a larger number of topics.

Conclusion

In this paper, we introduced an alternative LDA model by adding labels (here, MeSH descriptors) to the bag-of-words assumption. With this setting, 'hybrid topics' can be generated to reveal relationships between topics and labels. In our evaluation, these 'hybrid topics' resulted in higher topic coherence scores compared the original LDA, but only on the specialized biomedical corpus. For the general corpus, we did not see a significant difference on topic quality between our 'hybrid topics' and baseline topics. From our results, we can also conclude that LDA is more useful in the specialized corpus to explore concepts that may not be covered by the MeSH vocabulary and where topic models can capture aggregate concepts from different domains.

Topic models have a strong potential for analyzing the content of large text corpora. However, the deployment of topic models in the real world has been limited. Our goals in the future are to find more practical ways to apply topic models to help people better understand the massive amount of unstructured data available to us.

Acknowledgments

References

1. Lu Z, Kim W, Wilbur WJ. Evaluation of query expansion using MeSH in PubMed. Information retrieval. 2009; 12:69–80. [PubMed: 19774223]

2. Richter RR, Austin TM. Using MeSH (medical subject headings) to enhance PubMed search strategies for evidence-based practice in physical therapy. Physical therapy. 2012; 92:124–132. [PubMed: 21979271]

3. Dogan RI, Murray GC, Névéol A, Lu Z. Understanding Pub-Med® user search behavior through log analysis. Database. 2009; 2009:bap018. [PubMed: 20157491]

4. Blei DM, Ng AY, Jordan MI. Latent dirichlet allocation. Journal of machine Learning research. 2003; 3:993–1022.

5. Yu, Z., Johnson, TR., Kavuluru, R. Phrase based topic modeling for semantic information processing in biomedicine. Machine Learning and Applications (ICMLA), 2013 12th International Conference on; IEEE; 2013. p. 440-445.

6. Ramage, D., Hall, D., Nallapati, R., Manning, CD. Labeled LDA: A supervised topic model for credit attribution in multi-labeled corpora. Proceedings of the 2009 Conference on Empirical Methods in Natural Language Processing: Volume 1-Volume 1; Association for Computational Linguistics; 2009. p. 248-256.

7. Zhu, D., Li, D., Carterette, B., Liu, H. BioASQ@ CLEF. Citeseer; 2013. An Incremental Approach for MEDLINE MeSH Indexing.

8. Newman, D., Karimi, S., Cavedon, L. Using topic models to interpret MEDLINE's medical subject headings. Australasian Joint Conference on Artificial Intelligence; Springer; 2009. p. 270-279.

9. Doshi-Velez F, Wallace B, Adams R. Graph-sparse LDA: a topic model with structured sparsity. 2014 arXiv preprint arXiv:1410.4510.

10. O'Callaghan D, Greene D, Carthy J, Cunningham P. An analysis of the coherence of descriptors in topic modeling. Expert Systems with Applications. 2015; 42:5645–5657.

11. Lau JH, Newman D, Baldwin T. Machine Reading Tea Leaves: Automatically Evaluating Topic Coherence and Topic Model Quality, in. EACL. 2014:530–539.
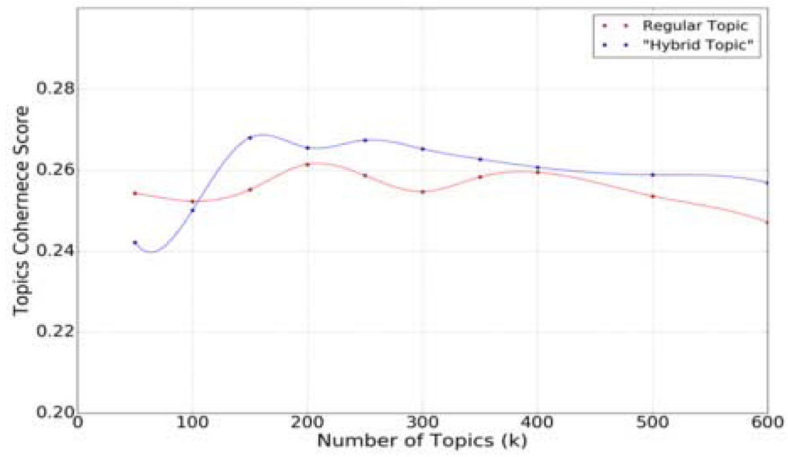
Figure 1.
Comparison of mean TC-W2V topic coherence scores for different numbers of topics k, generated from the general corpus
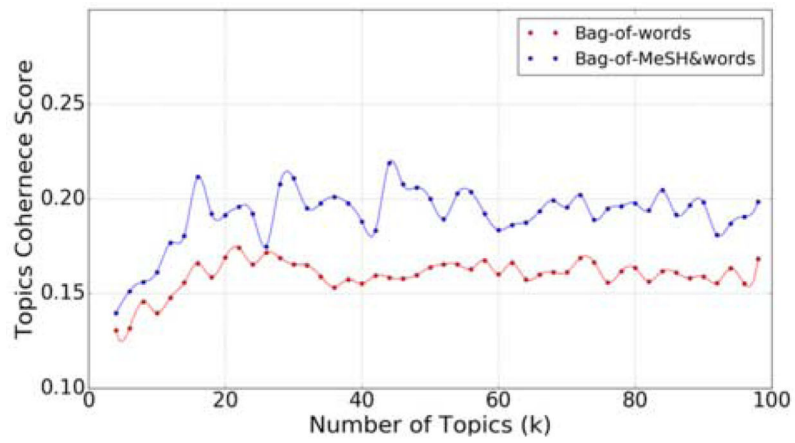
Figure 2.
Comparison of mean TC-W2V topic coherence scores for different numbers of topics k, generated from the specialized corpus
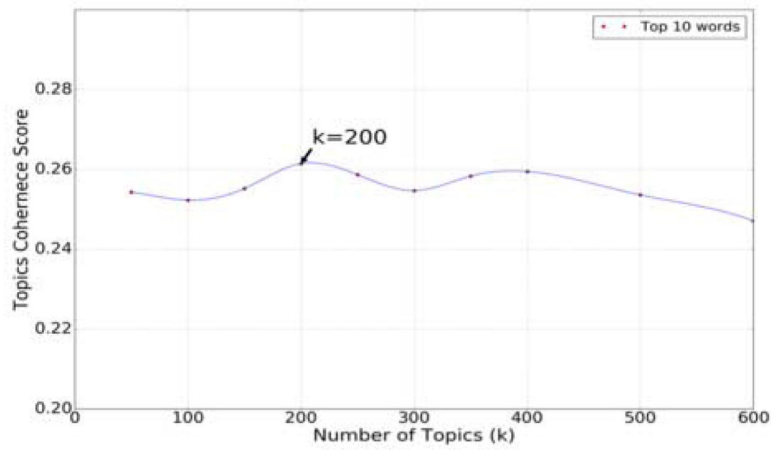
Figure 3.
Plot of mean TC-W2V topic coherence scores for different numbers of topics k, generated from the general corpus
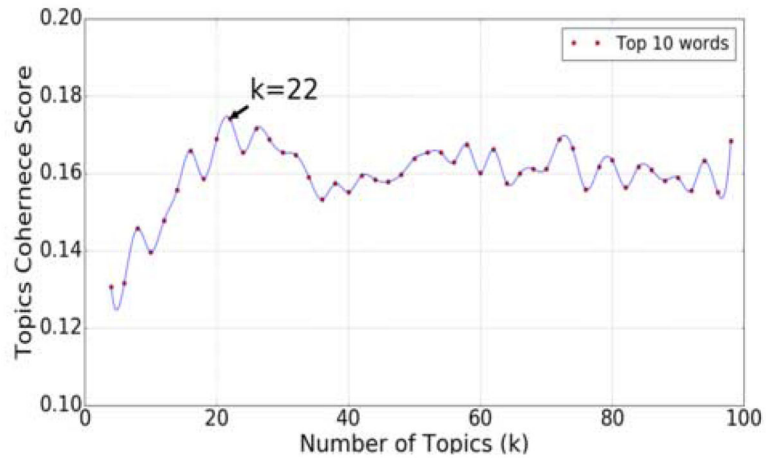
Figure 4.
Plot of mean TC-W2V topic coherence scores for different numbers of topics k, generated from the specialized corpus

Table 1

Generated 'bag-of-MeSH&word' topics (*MeSH descriptors)

Topic 1	Topic 2	Topic 3
model	*brain	motor
predict	cortex	visual
value	region	*movement
prediction	functional	*face
analysis	cortical	right
predictive	activity	response
regression	neural	*hand
datum	network	processing
estimate	change	object
predictor	area	stimuli
1-0 mapping	1-1 mapping	1-many mapping

Table 2

# of topics with 0,1,n MeSH descriptors (n>1)

Data Set	Optimal *K*	# of Topic with 0 MD	# of Topic with 1 MD	# of Topic with n MD
General Corpus	200	6(3%)	16(8%)	178(89%)
Spec. Corpus	22	9(41%)	6(27%)	7(32%)