Knowledge-Base Enriched Word Embeddings for Biomedical Domain

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1 ABSTRACT
Word embeddings have been shown adept at capturing the semantic and syntactic regularities of the natural language text, as a result of which these representations have found their utility in a wide variety of downstream content analysis tasks. Commonly, these word embedding techniques derive the distributed representation of words based on the local context information. However, such approaches ignore the rich amount of explicit information present in knowledge-bases. This is problematic, as it might lead to poor representation for words with insufficient local context such as domain-specific words. Furthermore, the problem becomes pronounced in domain such as bio-medicine where the presence of these domain specific words are relatively high. Towards this end, in this project, we propose a new word embedding based model for biomedical domain that jointly leverages the information from available corpora and domain knowledge in order to generate knowledge-base powered embeddings. Unlike existing approaches, the proposed methodology is simple but adept at capturing the precise knowledge available in domain resources in an accurate way. Experimental results on biomedical concept similarity and relatedness task validates the effectiveness of the proposed approach.

2 INTRODUCTION
Understanding the semantics behind a text is a fundamental problem in the field of Natural Language Processing (NLP) [3, 4, 8]. Towards this end, recently, modelling the distributed representation of words has attracted considerable attention from the research community. This is primarily due to the development of neural network inspired word embedding models [3, 12–15, 19] that have shown to encode the semantic structure of words at a granular level. Simply put, these embedding models learn continuous low dimensional dense vectors of words, commonly known as word embeddings, in a completely unsupervised manner. While considerable success has been achieved by these embedding models, yet, they are still afflicted with certain drawbacks. The major being their sole reliance on the assumption of distributional hypotheses (words appearing in similar context have similar meaning) [9]. This exclusive reliance on the local-context leads to poor representation of words that have insufficient statistical information such as domain-specific or rare words. Such domain-specific words are present in sizable amount in almost all the domains and particularly in domains such as bio-medicine. As an example, consider a pair of medical concepts “Heart” and “Aorta”. Despite the fact that this pair rarely co-occur together in the corpus (less local-context information), they are still semantically related (aorta is the largest artery in the body that is present in heart) in the knowledge-base. This insight leads us to the crux of the problem that we intend to address in this project.

How to supplement the data-driven embedding model with the curated information from the knowledge-base so that it supplements the insufficient context information and generates knowledge-base enriched vector representations?

To achieve our goal, we leverage both the corpus based information and the KB available in the biomedical domain. As means of corpus information, we choose MEDLINE 1, the popular and perhaps the most comprehensive literature repository in the biomedical domain. Every article in this repository is indexed with a set of medical concepts. Being manually curated by subject-matter-experts, they are highly precise and accurate. In this project, we use these medical concepts as a unit of representation for documents. The same concepts are also present in the biomedical KB (arranged in the form of a hierarchy) thus providing us with another complementary source of information. While MEDLINE provides us with the local-context information for the concepts, the hierarchical KB provides complementary information for those words with insufficient local context-information. We would like to note that, unlike the hierarchies present in general domain such as WordNET [20], the chosen KB in biomedical domain is unique in itself with its own peculiarities. The two main distinctive features are: a) the concepts are strictly arranged in an IS-A relationship, b) the lower the concept pairs in the taxonomy the more specific information they possess. This uniqueness causes the straight-forward portability of existing works [6, 21, 24] to have a limited effect. More specifically, most of the prior works have attempted to augment embeddings with relational/categorical knowledge. The structured representation of these knowledge bases, commonly in the form of triplets (subject-predicate-object), are distinct than the current resource of interest - hierarchical KB. Thus, it is unclear on how the prior works could be applied to the biomedical domain in their plain vanilla form. Motivated with this narrative, in this project, we explore the distinctive features of biomedical KB to generate embeddings that are more suited and optimized for biomedical specific applications. Our main technical challenge lies in jointly modelling the local context information from the natural language text and structural information from human curated KB. To accomplish this objective, we propose a deep-learning based solution that simultaneously exploits the two complementary sources of information. In particular, the proposed model is essentially a recurrent neural networks based concept language model trained on sequential text

[1]https://www.nlm.nih.gov/pubs/factsheets/medline.html
taken from both unstructured corpora (local context) and structured taxonomy (domain knowledge). To validate the effectiveness of proposed model, we performed experiments on biomedical concept similarity/relatedness task.

To summarize, in this study, we made the following particular contributions:

1. We proposed a new word embedding model for biomedical domain that jointly exploits both the corpus based information and hierarchical knowledge-base to produce knowledge-base augmented word embeddings.

2. Compared to the existing approaches, the proposed model is relatively simple but adept at capturing the explicit semantic knowledge in an accurate fashion.

3 RELATED WORK
Improving the distributed representation of words is an important problem in the research area of natural language processing [3, 4, 7]. For a recent survey, please refer [1, 16]. In our chosen domain of interest (i.e., biomedical domain), recent years have witnessed some early attempts towards applying word embedding models for several bioNLP tasks. Chiu et al. [6] studied and reported the effects of input corpora, dimension size, parameters on the quality of embeddings. Similarly, [21] conducted intrinsic evaluations on multitude of linguistic tasks such as Part-of-Speech tagging, chunking, named entity recognition, mention detection.

While these studies were important in demonstrating the salient aspects of biomedical embedding models, they did not focus on making model level innovation. Furthermore, the quality of embeddings generated by these models for domain-specific words are relatively poor [25]. To overcome this, in this study, we leverage the rich domain knowledge present in biomedical domain and explore effective ways to integrate them. We would like to note that there have been studies conducted in NLP domain that integrate certain forms of prior knowledge [5, 23]. In [24], the authors proposed a simple but effective method to encode relational knowledge. In particular, they extended the objective function of skip-gram by incorporating the prior knowledge in the form of a regularizer. Likewise, in another related study [17], the authors proposed an alternate method to encode the semantic knowledge via ordinal constraints. Although these models made important advances, their application is limited to the biomedical domain. This is mainly due to the unique challenges posed by the hierarchical KB present in biomedical domain.

4 MODEL ARCHITECTURE
In this section we discuss our proposed model to generate word embedding for biomedical domain. A complete pipeline of the proposed framework is illustrated in Figure 1.

4.1 Continuous Bag-of-Words Model
In general, the word embeddings are generated using neural networks with majority of them modelling the objective function as a one trying to predict either the word under consideration based on a context described through a window or the vice-versa. The two most popular word embedding models are Continuous Bag-of-Words Model (CBOW) and Skip-gram models [18, 19]. Both CBOW and Skip-gram models are three-layer neural networks, containing input, projection, and output layers. In this project, we base our proposed model on CBOW. The CBOW model learns word embedding by using context words to predict the center word \(w_c\), where the context words refer to the neighboring words within a window size \(c\) near the center word in a sentence. Given a sequence of training words \(w_1, w_2, ..., w_T\), the CBOW model has the following objective function:

\[
J\hat{c} = \frac{1}{T} \sum_{t=1}^{T} \log p(w_t|w_{t-c}, ..., w_{t-1}, w_{t+1}, ..., w_{t+c}).
\]

The CBOW model first computes the hidden layer \(h_t\) for word \(w_t\) by averaging the input embeddings for its context words.

\[
h_t = \frac{1}{2c} \sum_{-c < j < c, j \neq 0} v_{t+j},
\]

where \(v_t\) is the input representation for word \(w_t\). Then \(p(w_0|w_{t-c}, ..., w_{t-1}, w_{t+1}, ..., w_{t+c})\) is calculated based on hidden state \(h_t\) using a softmax function:

\[
P(w_0|h_t) = \frac{\exp(v_0^T h_t)}{\sum_{i=1}^{N} \exp(v_i^T h_t)},
\]

where \(v_i\) is the output representation for word \(w_i\). Note that, the representation vector for \(v_0\) is between input layer and projection layer. \(v_0\) is the output vector between projection layer and output layer.

In this project, we use CBOW to incorporate the corpus based information into the model. Having incorporated the local context, the next step is to integrate the domain knowledge from external KB. As mentioned before, the chosen KB is hierarchical in nature. Consequently, every medical concept is associated with a sequence of ancestors. To model this sequential nature of ancestors, we use recurrent neural network (RNN). The hidden layer of RNN contains the history of ancestors linked as an input to the word-level recurrent neural network to predict the next word together with the word-level history vector. This allows the language model to predict the next word probability distribution beyond the words in the current sentence. In Figure 1, RNN could be any RNN variants, such as Long Short Term Memory (LSTM)[11] and Gated Recurrent Unit (GRU). In our implementation, we use LSTM to deal with the vanishing gradient problem.

4.2 Long Short-Term Memory
LSTMs address the vanishing gradient problem commonly found in RNNs by incorporating gating functions into their state dynamics. At each time step, an LSTM maintains a hidden vector \(h\) and a memory vector \(m\) responsible for controlling state updates and outputs. More concretely, we define the computation at time step \(t\) as follows:
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5 EXPERIMENTS

5.1 Dataset Preparation

To examine the applicability of the model, we sampled a subset of entire dataset (MEDLINE). For this project, the total number of article used from MEDLINE are 100,000. The proposed model was trained on this subset. Before we delve into the details of our evaluation, we briefly describe our unit of representation (MeSH terms) and chosen external knowledge base.

5.2 Medical Subject headings (MeSH)

Medical Subject Heads (MeSH) are National Library of Medicine (NLM) controlled vocabulary that human experts use to index journal articles in the life sciences domains. Mesh terms are classified into three categories a) Descriptors, b) Qualifiers and c) Supplementary concept records. Descriptors represent the conceptual meaning of the article. In this work, we use Descriptors as the unit of representation for documents.

5.3 External knowledge base

Our chosen KB is MeSH hierarchy. MeSH terms are organized in the form of a tree hierarchy based on their level of specificity. Every MeSH term has a corresponding tree code which represents its level of specificity in the tree. As an example, the tree code for concept Migraine Disorders is: C10.228.140.546.399.750.

5.4 Evaluation Datasets

To evaluate the output embeddings on biomedical concept similarity/relatedness task, we borrow evaluation set from [2]. The description of both datasets are provided below:

- **MeSH-1**: The first dataset (MeSH-1) [22] was created by experts from Mayo Clinic and consists of a set of word pairs that are related to general medical disorders. The similarity of each concept pair was assessed by 3 physicians and 9 medical coders. Each pair was annotated on a 4 point scale: practically synonymous, related, marginally, and unrelated. The average correlation between physicians is 0.68 and between experts is 0.78. In this project, we use 19 concepts that were present in our vocabulary as our evaluation set.

- **MeSH-2**: The second biomedical benchmark (MeSH-2) was introduced in [10]. It consists of a set of 36 word pairs extracted from the MeSH repository. The similarity between word pairs was assessed by 8 medical experts and assigned a score between 0 (non-similar) to 1 (synonym). In this project, we use 20 concepts that were present in our vocabulary as our evaluation set.

5.5 Results

Table 1 and Table 2 reports the Spearman ($\rho$) coefficient values obtained by applying the proposed model on the datasets MeSH-1 and MeSH-2 respectively. In order to have a baseline for comparison, we generated word embeddings using only the domain knowledge and corpus information respectively. As it can be observed from the table 1 and table 2, the proposed model outperforms the baseline and achieves a higher correlation with human experts.

Discussion: Although the proposed model outperforms the baseline the overall Spearman coefficient is relatively low. We believe...
Table 1: Correlation values relative to human judgments for MeSH-1

| Methods                  | Spearman coefficient |
|--------------------------|----------------------|
| Domain knowledge only    | 0.228                |
| CBOW                     | 0.304                |
| Proposed Model           | 0.312                |

Table 2: Correlation values relative to human judgments for MeSH-2

| Methods                  | Spearman coefficient |
|--------------------------|----------------------|
| Domain knowledge only    | 0.280                |
| CBOW                     | 0.363                |
| Proposed Model           | 0.371                |

the reason for this lies in the insufficient training. As mentioned before, due to limited time constraint and computational challenges, the training was performed on a small subset of entire dataset. In future, we intend to train of model on the entire massive dataset. One insight to note from the experiments is the higher correlation of proposed model. This result validates the importance of incorporating both local context and explicit semantic knowledge to generate semantically meaningful embeddings. Furthermore, the higher correlation also points the effectiveness of model in capturing the human intuition of similarity/relatedness.

6 CONCLUSION

In this project, we proposed a new recurrent neural network based language model for biomedical domain that leverages both corpus based contextual information and explicit semantic knowledge (present in the form of hierarchy) to produce high-quality word embeddings. The fusion of taxonomical knowledge that are hand-engineered by subject matter experts into corpus based embedding model provides additional semantic evidence to words with poor local context, thereby, enriching the quality of overall embeddings. Experiments on biomedical concept similarity/relatedness task have illustrated that the proposed knowledge-based powered approach significantly improves the quality of word representation. In future work, we intend to explore more effective ways of integrating this knowledge base and to develop strategies in order to make the system computationally efficient.

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