Unsupervised Approach for Named Entity Recognition in Biomedical Documents Using LDA-BERT Models

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Abstract: Named Entity Recognition (NER) is a crucial task in biomedical text mining, enabling the identification and extraction of entities such as genes, proteins, diseases, and drugs. Existing NER approaches often rely on supervised learning with labeled data, which may be limited and expensive to obtain. This research proposes a novel semantic model featuring weighted distributions focused on unsupervised NER within the biomedical domain. Our methodology leverages an enhanced SciBERT model incorporating LDA topic modeling (SciBERT+LDA) for NER. The model specifically targets identifying three significant entities: *Disease, Chemical, and Protein*. The assessment of the proposed method demonstrates its effectiveness in recognizing named entities within the biomedical domain. Our proposed approach demonstrates promising results, attaining a macro-average F-measure of 86%. Moreover, the proposed approach can readily be expanded to encompass the recognition of more domain-specific entities.

1 INTRODUCTION

Biomedical Named Entity Recognition (BioNER) is a specialized task within Natural Language Processing (NLP) and computational biology that involves identifying and classifying specific entities or terms in biomedical texts. It recognizes the major named entities present in medical records, research articles, and other healthcare documents. Identifying these entities is vital in downstream NLP tasks such as knowledge graph creation, clinical decision support systems, and drug discovery and development. Significant research efforts have been focused on developing open-domain NER systems that utilize cutting-edge machine learning models. Identifying named entities within specific domains poses a notably more challenging task ((Gridach, 2017), (Wei et al., 2019), (Zhang et al., 2021)) due to the semantic complexity of the entities. Current open NER models failed to identify domain-specific entities due to their training on distinct corpora. Furthermore, the challenges of transferability and generalizability persist as significant obstacles. In this work, we formulate BioNER as a classification problem instead of sequence labeling problem, which is used in State-of-the-art NER models. Our methodology uses the extended SciBERT coupled with LDA (SciBERT+LDA) model to generate a Global Vector for each entity. We first use topic modeling to identify the latent topics within the corpus. Specifically, we adopt the widely recognized LDA approach for topic modeling (Blei et al., 2003a). Subsequently, these identified topics undergo vectorization using SciBERT, a contextualized word embedding model tailored for the biomedical and scientific domains. SciBERT captures the context and semantics of scientific language, including the specific vocabulary and structures commonly found in academic papers, research articles, and other scientific documents. By combining LDA and SciBERT, we capitalize on the distinctive capabilities inherent in each model. Furthermore, we extend SciBERT's tokenizer to recognize domain-specific keywords. Additionally, in our process, we use the weighted scores obtained from the LDA modelm to calculate local input word vectors. In the final step of our methodology, we compare these locally generated input vectors and the Global Vectors. This comparison uses the cosine similarity metric to ascertain the ultimate entity tag for the given input phrase.

The primary contributions of our work include:

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- We introduce an unsupervised approach for named entity labeling within the Biomedical domain. The SciBERT+LDA model incorporates elements from both SciBERT and LDA to provide a robust solution for identifying and categorizing named entities in biomedical texts.
- Our approach produces domain-specific word vectors through an enhanced SciBERT, suitable for application in tasks related to relation extraction.

The remainder of the document is organized as follows: Section 2 provides a review of related works. The proposed method is detailed in Section 3. Experimental results and analysis are discussed in Section 4. In conclusion, Section 5 summarizes the paper, providing concluding remarks and suggesting potential directions for future research.

2 RELATED WORKS

In the present era, state-of-the-art performance in NER systems is accomplished by utilising deep learning models, which demand minimal feature engineering (Brundha et al., 2023), (Srivastava et al., 2022). We conducted an exhaustive literature review to develop a NER system tailored to the biomedical domain, concentrating on unsupervised approaches for identifying named entities. These models autonomously uncover latent features within raw text and have found applications across diverse domains (Shahina et al., 2019). Their versatility has enabled effective application in various fields, ranging from biomedical research and healthcare to finance and legal domains. A deep neural network based NER model in the Biomedical Domain (BioNER) is presented in (Yao et al., 2015). Bio-NER reported a 71.01% F-measure on the GENIA corpus. Wei et al.(Wei et al., 2016) present a Conditional Random Field (CRF)-based neural system designed for identifying disease entities in PubMed abstracts. Gopalakrishnan et al. (Gopalakrishnan et al., 2019) proposed an RNN, LSTM, and GRU approach on GENIA version 3.02 corpus and achieved an F score of 90%. Chiu and Eric Nichols (Chiu and Nichols, 2016) proposed an approach utilizing bidirectional LSTM-CNN for named entity identification, achieving a 91.62% F-measure on the CoNLL-2003 dataset. Li et al. (Li et al., 2020) propose a detailed survey of deep learning based NER systems.

Several recent research works have explored Pretrained language models for downstream NLP applications, yielding substantial success (Veena et al., 2023b), (G et al., 2023), (Veena et al., 2023a). Bidirectional Encoder Representations from Transformers for Biomedical Text Mining (BioBERT) is a domain-specific language representation model pretrained on large-scale biomedical corpora (Lee et al., 2020). BioBERT is fine-tuned on specific biomedical NLP tasks, NER, relation extraction, and classification (Zhu et al., 2020), (KafiKang and Hendawi, 2023), etc. ABioNER, a BERT-based model to identify biomedical named entities in the Arabic text, is proposed in (Boudjellal et al., 2021). A detailed survey of transformer based pretrained models for biomedical NER systems can be found in (Kalyan et al., 2022).

Conventional supervised approaches necessitate the availability of manually annotated datasets for training, a process that can be both resource-intensive and time-consuming. In contrast, unsupervised models offer a more flexible and adaptable alternative by alleviating the dependency on annotated data, enabling them to be applied across diverse domains and languages. Unsupervised methodologies are specifically crafted to unveil latent patterns or structures inherent within datasets lacking explicit labeling. A notable illustration of such an approach is exemplified by Zhang and Elhadad (Zhang and Elhadad, 2013), who introduce an unsupervised technique for biomedical named-entity recognition. The efficacy of their method is assessed on the i2b2 and GENIA corpora, yielding reported accuracies of 69.5% and 53.8%, respectively. Another unsupervised strategy, CycleNER (Iovine et al., 2022), is centered around learning the mapping between sentences and entities. This approach undergoes evaluation on the CoNLL and BC2GM datasets, with resulting average F measures of 68.6% and 38%, respectively. After the literature survey, we identified the following research gaps:

- Traditional supervised approaches require manually annotated datasets for training, which can be resource-intensive and time-consuming to create.
- Models trained on specifically labeled datasets may have difficulty generalizing to new, unseen data that differs significantly from the training set.
- Supervised models can be influenced by biases present in annotated data.

Considering these gaps, we propose an unsupervised approach for SciBert with LDA. After applying LDA, each document can be represented as a distribution over topics, and each topic is represented as a distribution over words. These distributions can serve as features for the documents. Detailed explanations of the proposed architecture and the analysis of results are provided in the following sections.

3 METHODOLOGY

The subsequent steps involve the labeling of entities within the sentence by the proposed model, categorizing them into three distinct classes, viz., *Disease, Chemical, and Protein*.

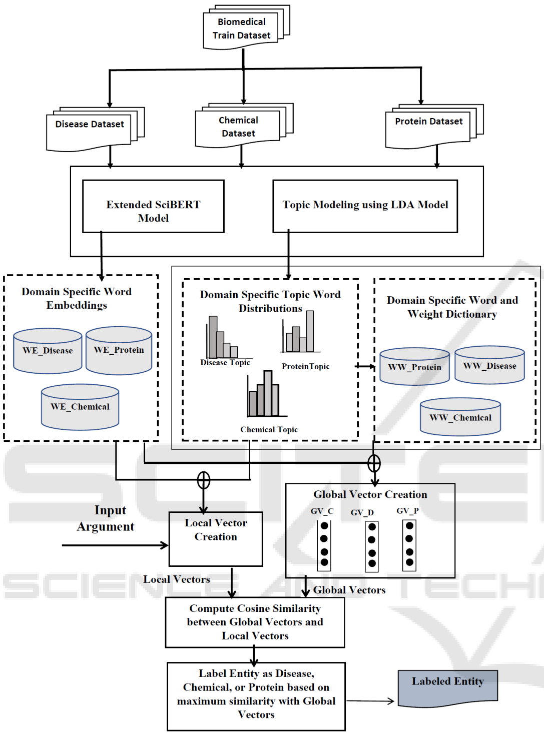


Figure 1: The Pipeline model of the Proposed Unsupervised Named Entity Recognition in Biomedical text.

3.1 Dataset Creation Module

We created distinct datasets for each Biomedical subdomain: Disease, Chemical, and Protein. To extract data, we used key phrases associated with Disease, Chemical, and Protein subdomains, focusing on BC4CHEMD ((Krallinger et al., 2015)), NCBI-Disease((Doğan et al., 2014)), and BC2GM ((Smith et al., 2008)) datasets. The list of keyphrases contains 550 disease names, 250 names of genes, and 100 chemical names. Examples of key phrases include {*'arthralgia', 'atherogenesis', 'Duchenne muscular dystrophy', 'pancreatic cysts and tumors', 'breast and prostate cancer', 'Erythropoietin receptor', 'leptin receptor', 'phalloidin', 'cyclin-dependent kinase 1'*,..}. Examples of retrieved sentences related to each subdomain are displayed in Table 3.

Table 1: Sample Sentences extracted using Keywords

Domain	Phrases
Disease	Duchenne muscular dystrophy (DMD) is a severe type of muscular dystrophy affecting boys. Retinoblastoma (Rb) is a rare cancer developing in retinal cells. Soft-tissue sarcoma (STS) is a malignant tumor in soft tissue, often growing painlessly over months or years.
Protein	The long-chain fatty acyl-CoA ligase enzyme activates fatty acid oxidation. ACSL5 gene encodes the long-chain-fatty-acid—CoA ligase 5 enzyme.
Chemical	The glycine transporter-1 inhibitor SSR103800 exhibits an antipsychotic-like profile in mice. Schizophrenia is linked to dopamine dysfunction. High doses of catecholamines, sedatives, and relaxants via a central venous catheter were ineffective.

In the process of constructing the training set, 80% of the key phrases are used. Detailed information regarding the data statistics for the combined training and test datasets within each subdomain is available in Table 3.

Table 2: Statistics of the Dataset

Sub-domain	Sentences	Avg. Length	Unique Words
Disease	2906	12.40	7836
Chemical	2837	11.88	16060
Protein	3503	11.90	18113

Following data acquisition, we undertake fundamental pre-processing procedures. In the subsequent subsection, a detailed explanation of the Entity Identification process is provided.

3.2 Entity Identification Module

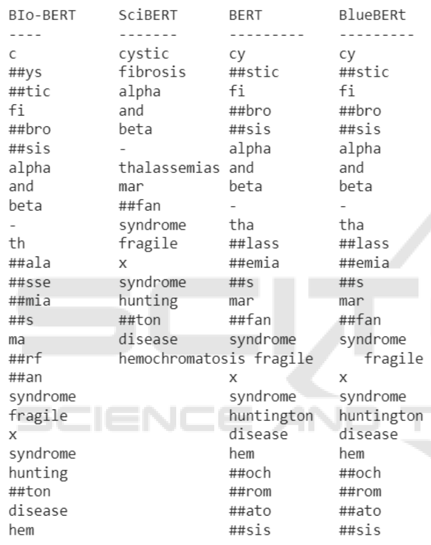
The test sentences undergo an Entity Identification module, which recognizes meaningful noun phrases representing entities within the input sentence. For entity extraction, we employed Open Information Extraction systems (Del Corro and Gemulla, 2013). After obtaining the entities, the subsequent step involves labeling each entity into one of the three categories or assigning it to the 'OTHER' category. This process is further detailed in the subsequent subsection.

3.3 Biomedical Entity Recognition using the extended SciBERT with LDA model

The three major entities in the biomedical documents, namely, Disease, Chemical, and Protein entities, are identified and labeled using the SciBERT+LDA model. The overall architecture of the SciBERT+LDA model is depicted in Figure 1. The entire process is divided into four submodules and explained in the following subsections.

3.3.1 Subdomain Word Vectorization

The training datasets from the three biomedical subdomains are fed into the extended SciBERT and LDA models. The extended SciBERT model produces domain-specific word vectors that capture semantic information. At the same time, the LDA model creates domain-specific topic distributions and word distributions, offering insights into the thematic content of the respective subdomains.



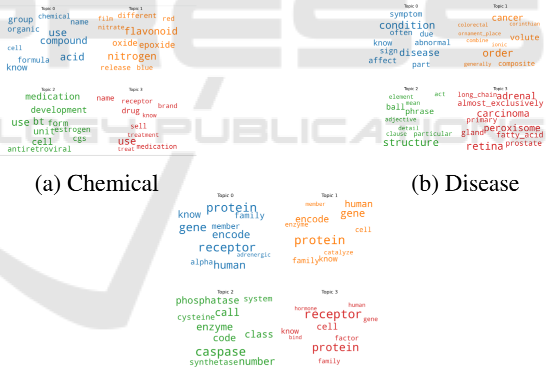
```
BIo-BERT    SciBERT      BERT         BlueBERt
----        -------      ---------    ---------
c           cystic       cy           cy
##ys        fibrosis     ##stic       ##stic
##tic       alpha        fi           fi
fi          and          ##bro        ##bro
##bro       beta         ##sis        ##sis
##sis       -            alpha        alpha
alpha       thalassemias and          and
and         mar          beta         beta
beta        ##fan        -            -
-           syndrome     tha          tha
th          fragile      ##lass       ##lass
##ala       x            ##emia       ##emia
##sse       syndrome     ##s          ##s
##mia       hunting      mar          mar
##s         ##ton        ##fan        ##fan
ma          disease      syndrome     syndrome
##rf        hemochromatosis fragile    fragile
##an                     x            x
syndrome                 syndrome     syndrome
fragile                  huntington   huntington
x                        disease      disease
syndrome                 hem          hem
hunting                  ##och        ##och
##ton                    ##rom        ##rom
disease                  ##ato        ##ato
hem                      ##sis        ##sis
```

Figure 2: Comparison of different versions of BERT Models

SciBERT (Beltagy et al., 2019)is an extension of the BERT model tailored for scientific and biomedical text. Its architecture retains the transformer-based design of BERT but incorporates domain-specific pretraining and an expanded vocabulary to better handle scientific language characteristics. As depicted in Figure 2, the number of tokens generated by various BERT models for the following list of words *cystic fibrosis alpha and beta-thalassemias Marfan syndrome fragile X syndrome Huntington disease hemochromatosis* are higher compared to SciBERT. This is because of generating more subwords by the BERT models. Consequently, for our experiments, we opted for the SciBERT model. However, the SciBERT model presents challenges, particularly concerning the inclusion of domain-specific terms. To address this issue, in our approach we augment the SciBERT tokenizer's vocabulary with domain-specific terms ((Tai et al., 2020)). Once the training dataset is vectorized, the resulting subdomain word vectors are stored in separate dictionaries named WE_Disease, WE_Protein, and WE_Chemical. These dictionaries are then used to generate both Global Vectors and Local Vectors, as detailed in the following sections.

3.3.2 Topic Modeling using LDA Model

As shown in Figure 1, to identify the topics and associated word distributions, we employ topic modeling on the training datasets within each subdomain. The main objective of topic modeling is to identify the thematic structures within an extensive corpus of text data. Common techniques for topic modeling include Latent Dirichlet Allocation (LDA) and Nonnegative Matrix Factorization (NMF), Latent Semantic Analysis (LSA) and Probabilistic Latent Semantic Analysis (pLSA). We have used the most popular approach, LDA (Blei et al., 2003b), for topic modeling. Subsequently, these topics undergo vectorization using SciBERT, a semantic model leveraging the distributional properties of words. We used the two crucial hyperparameters in our experimental setup: α and η. The parameter α governs document-topic density, while η controls the topic-word density. For these hyperparameters, we opted for the default values provided by the Gensim library ([1]). Additionally, We also focused on the determination of two critical parameters: the number of topics required (T) and the number of words required in a topic (K). In the context of LDA, the optimal number of topics (T) is selected based on coherence scores. The topics identified for each subdomain are presented in Figures 3.



(a) Chemical (b) Disease

(c) Protein

Figure 3: Topic Distribution of Three LDA Models

[1] https://pypi.org/project/gensim/

3.3.3 Weighted Local Vector Generation

The Entity Identification module identifies the input arguments to be labeled. Subsequently, these input arguments undergo vectorization through the weighted Local Vector creation module. We employ a weighted scoring mechanism to adjust the significance of words relative to each subdomain. Specifically, if *Arg* represents an input argument with m words $(w_1, w_2, w_3, \dots w_m)$, we calculate the Local Vector (LV) as the weighted average of all the m words in *Arg* using the equation 1.

$$LV(Arg) = \frac{\sum_{i=1}^{m}, W_{wi} * Vec(w_i)}{m} \tag{1}$$

$$= \begin{cases} LV\_C; & if\ W_{wi} \in WW\_C\ \&\ Vec(w_i) \in WE\_C \\ LV\_D; & if\ W_{wi} \in WW\_D\ \&\ Vec(w_i) \in WE\_D \\ LV\_P; & if\ W_{wi} \in WW\_G\ \&\ Vec(w_i) \in WE\_P \end{cases}$$

$$GV(subdomain) = \frac{\sum_{j=1}^{T} (\sum_{i=1}^{K} W_{w\mathrm{ij}} * Vec(w_{\mathrm{ij}}))}{T} \tag{2}$$

$$= \begin{cases} GV\_C; & if\ W_{w\mathrm{ij}} \in TV\_C\ \&\ Vec(w_{ij}) \in WE\_C \\ GV\_D; & if\ W_{w\mathrm{ij}} \in TV\_D\ \&\ Vec(w_{ij}) \in WE\_D \\ GV\_P; & if\ W_{w\mathrm{ij}} \in TV\_P\ \&\ Vec(w_{ij}) \in WE\_P \end{cases}$$

In Equation (1), w_i represents the ith word, and $W_{w\mathrm{i}}$ denotes the weight associated with the word w_{i}. The vector corresponding to each of the m words is derived from the domain-specific word vectors which is stored in the dictioneries *WE_C, WE_D, and WE_G*. These weights are obtained from the word-weight dictionaries *WW_C (Chemical), WW_D (Disease), and WW_P (Protein).*

3.3.4 Global Vector(GV) Generation

The Global Vector creation commences with the application of Topic modeling to the subdomain dataset, where major topics are identified based on coherence scores. The topics undergo vectorization, and the Global Vector is created utilizing Equation (2). To break down the steps further, the Global Vector is derived by first calculating the average of all subdomain Topic Vectors, denoted as *TV_C, TV_D, and TV_P*. This involves computing the vector representation for each word (w_{ij}) within a topic, where T signifies the total number of topics, K represents the number of words in a topic, and W_{wij} denotes the weight assigned to that word as defined by the LDA in a subdomain. The function *Vec(w_{ij})* extracts the embedding vector associated with the word w_{ij} from the subdomain dictionaries. This ensures that the contextual embeddings of the words, as captured in the subdomain-specific dictionaries, contribute to the overall composition of the Global Vector. This entire process is repeated for each subdomain, leading to the generation of three distinct Global Vectors, viz., *GV_C, GV_D, and GV_P.*

3.3.5 Bio Named Entity Labeling- Chemical, Disease, and Protein Entities

In this section, the labeling of the input argument is determined based on its resemblance to subdomains. As depicted in Figure 1, the input argument undergoes a vectorization procedure, generating Local Vectors tailored to each subdomain. Subsequently, these Local Vectors are compared with the corresponding set of four Global Vectors, namely *GV_C, GV_D, and GV_P*. The rationale behind this comparison is to evaluate the relevance of the input argument within the distinct contexts represented by the global characteristics of each subdomain. In Equation (3), $Cos(LV, GV)$ calculates the cosine similarity between the Local and Global Vectors. Following the computation of the cosine similarity scores, the next step involves identifying the Global Vector that exhibits the maximum similarity with the Local Vector. The maximum similarity score is computed using Equation (4), which shows the resemblance between the input argument and the identified subdomain's Global Vector. The final named entity label is determined by assigning the tag (label) associated with the Global Vector, as specified in Equation (5).

$$Label = \arg\max_i \{Cos(LV\_i, GV\_i) : i \in \{C, D, G\}\} \tag{3}$$

$$Score = \max_i \{Cos(LV\_i, GV\_i) : i \in \{C, D, G\}\} \tag{4}$$

$$\text{ArgLabel=} \begin{cases} C; & if\ Label = C\ and\ Score \geq \theta_{\text{chemical}} \\ D; & if\ Label = D\ and\ Score \geq \theta_{\text{disease}} \\ P; & if\ Label = P\ and\ Score \geq \theta_{\text{protein}} \\ OTHER\ or\ Place; & Otherwise \end{cases} \tag{5}$$

Individual threshold values are assigned to establish precise criteria for each subdomain. The threshold parameter, θ, is the average similarity score between the training seed phrases and their corresponding Global Vectors. To illustrate, consider the disease domain, where the threshold value $\theta_{\text{disease}} = 0.65$ is derived. This value is computed by determining the average cosine similarity score across one thousand training phrases compared to the Global Vector *GV_D* representative of the disease domain. Similar procedures are employed to find threshold values for other domains. In the chemical domain, the threshold is set at $\theta_{\text{chemical}} = 0.61$, representing the average similarity score between training phrases and the corresponding Global Vector *GV_C* for chemicals. Likewise, in the protein domain, the threshold is determined as

$\theta_{\text{protein}} = 0.60$, reflecting the average cosine similarity score obtained from the training phrases in relation to the Global Vector GV_P specific to proteins.

4 RESULTS ANALYSIS

This section provides a detailed examination of the outcomes and assessment of the introduced unsupervised BioNER model. A test corpus comprising 600 sentences from each subdomain is utilized to conduct the evaluation. The entities are identified using the OpenIE system. In Table 3 the similarity score is presented.

Table 3: Similarity Score of Global and Local Vectors

No.	Phrase	Cos Sim. GV_D	Cos Sim. GV_C	Cos Sim. GV_P	Pred.	Actual
1	Abnormal color vision	0.74	0.54	0.10	**DISEASE**	**DISEASE**
2	Colorectal cancers	0.67	0.53	0.00	**DISEASE**	**DISEASE**
3	Glycine	0.00	0.62	0.30	**Chemical**	**Chemical**
4	Palinurin	0.00	0.00	0.00	**Chemical**	**Other**
5	5-hydroxytryptamin	0.53	0.63	0.43	**Protein**	**Protein**
6	5-kinase	0.53	0.63	0.43	**Chemical**	**Protein**

The model's performance is rigorously assessed using key metrics, including Precision, Recall, Accuracy, and F Score. The comprehensive performance metrics of the proposed model are depicted in Figure 4. For a more in-depth understanding, we delve into an entity-level analysis, the findings of which are presented in Figure 5. This analysis allows us to explore the model's performance at a granular level, offering insights into how well it performs for each specific entity.

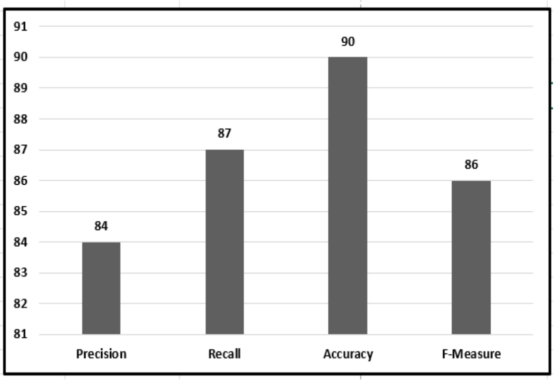


Figure 4: Average performance metrics including Accuracy, Precision, Recall, and F-Measure of the Proposed Unsupervised BioNER Model.

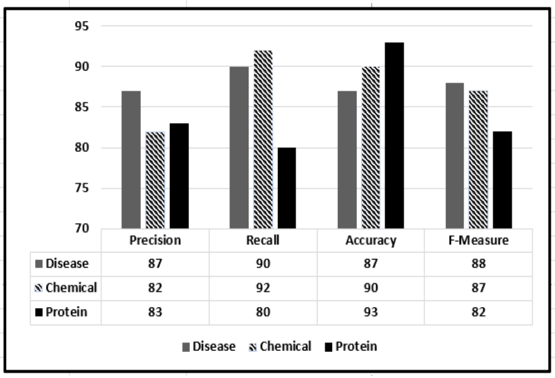


Figure 5: Performance Metrics of the Proposed Unsupervised BioNER Model for Identifying Disease, Chemical, and Protein Entities

5 CONCLUSION

The presented methodology introduces an innovative unsupervised approach for NER within the Biomedical domain, known as the unsupervised BioNER Model. This model specifically targets and labels biomedical entities, including *Disease, Chemical, and Protein*. The core of the proposed approach lies in the SciBERT+LDA model, which plays a pivotal role in the NER process. This model is designed to create Global Vectors, essentially representative vectors, for each distinct biomedical entity. These Global Vectors encapsulate the overall characteristics and significance of the respective entities within the biomedical context. To enhance the model's adaptability to various domain-specific entities, a crucial suggestion is made to extend the SciBERT tokenizer. For the recognition of new inputs, the model generates Local Vectors using a sophisticated mechanism involving a weighted score derived from the LDA model and uses the cosine similarity of Local vectors with Global vectors. Moreover, the proposed BioNER Model offers seamless integration with any Open Information Extraction (OIE) System. This means that the model can be effortlessly incorporated into existing OIE frameworks to carry out the labeling of arguments. The presented approach represents a comprehensive and effective strategy for unsupervised biomedical entity recognition. The suggested methodology yielded an average F Measure of 86%, a noteworthy achievement, particularly within the context of an unsupervised setting. The attainment of an 86% F Measure implies a commendable level of accuracy and effectiveness in the proposed approach for the given task.

In our future endeavours, we aim to identify entities, properties and relations that extend beyond the confines of two sentences. The outcomes hold significant promise for downstream applications, particularly in creating knowledge bases. By incorporating the extracted information into existing healthcare systems, professionals can access a wealth of structured and interrelated data. This, in turn, can contribute decision making regarding patient care and treatment plans.

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