Explicitly Capturing Relations between Entity Mentions via Graph Neural Networks for Domain-specific Named Entity Recognition

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Abstract

Named entity recognition (NER) is well studied for the general domain, and recent systems have achieved human-level performance for identifying common entity types. However, the NER performance is still moderate for specialized domains that tend to feature complicated contexts and jargonistic entity types. To address these challenges, we propose explicitly connecting entity mentions based on both global coreference relations and local dependency relations for building better entity mention representations. In our experiments, we incorporate entity mention relations by Graph Neural Networks and show that our system noticeably improves the NER performance on two datasets from different domains. We further show that the proposed lightweight system can effectively elevate the NER performance to a higher level even when only a tiny amount of labeled data is available, which is desirable for domain-specific NER.[1]

1 Introduction

Named entity recognition (NER) has been well studied for the general domain, and recent systems have achieved close to human-level performance for identifying a small number of common NER types, such as *Person* and *Organization*, mainly benefiting from the use of Neural Network models (Ma and Hovy, 2016; Yang and Zhang, 2018) and pretrained Language Models (LMs) (Akbik et al., 2018; Devlin et al., 2019). However, the performance is still moderate for specialized domains that tend to feature diverse and complicated contexts as well as a richer set of semantically related entity types (e.g., *Cell*, *Tissue*, *Organ* etc. for the biomedical domain). With these challenges in view, we hypothesize that being aware of the re-occurrences of the same entity as well as semantically related entities will lead to better NER performance for specific domains.

Therefore, we propose to explicitly connect entity mentions in a document that are coreferential or in a tight semantic relation to better learn entity mention representations. Precisely, as shown in Figure 1, we first connect repeated mentions of the same entity even if they are sentences away. For example, the named entity "tumor vasculature" appears both in the *Title* and sentence *S6* but in quite different contexts. Connecting the repeated mentions in a document enables the integration of contextual cues as well as enables consistent predictions of their entity types.

Second, we also connect entity mentions based on sentence-level dependency relations to effectively identify semantically related entities. For example, the two entities in sentence *S3*, "bone marrow" of the type *Multi-tissue Structure* and "endothelial progenitors" of the type *Cell*, are the subject and object of the predicate "contains" respectively in the dependency tree. If the system can reliably predict the type of one entity, we can infer the type of the other entity more easily, knowing that they are closely related on the dependency tree.

We incorporate both relations by using Graph Neural Networks (GNNs), specifically, we use the Graph Attention Networks (GATs) (Velickovic et al., 2018) that have been shown effective for a range of tasks (Sui et al., 2019; Linmei et al., 2019). Empirical results show that our lightweight method can learn better word representations for sequence tagging models and further improve the NER performance over strong LMs-based baselines on two datasets, the AnatEM (Pyysalo and Ananiadou, 2014) dataset from the biomedical domain and the Mars (Wagstaff et al., 2018) dataset from the planetary science domain. In addition, considering the lack of annotations challenge for

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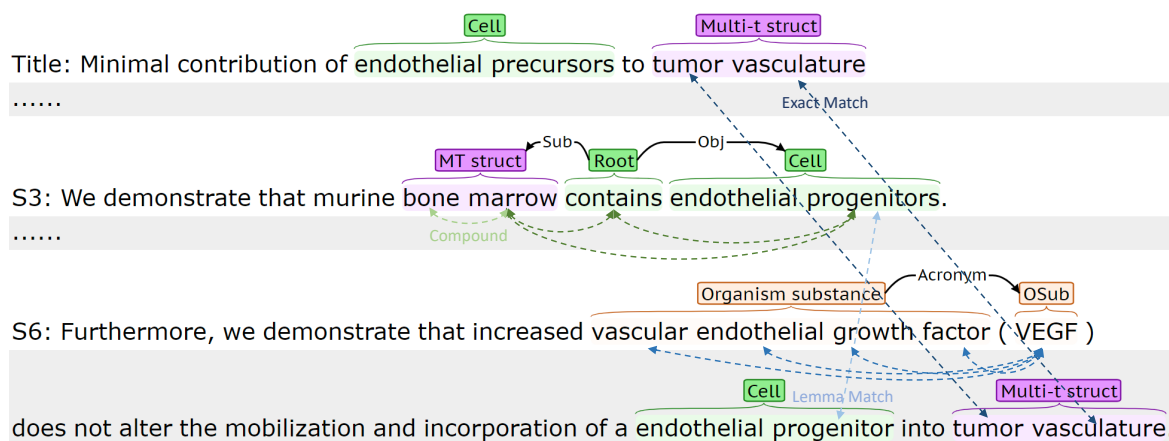[1] The code for the system is available here: https://github.com/brickee/EnRel-G

Figure 1: An example of NER with both discourse-level and sentence-level entity relations.

domain-specific NER, we plot learning curves and show that leveraging relations between entity mentions can effectively and consistently improve the NER performance when limited annotations are available.

2 Related Work

NER research has a long history and recent approaches (Yang and Zhang, 2018; Jiang et al., 2019; Jie and Lu, 2019; Li et al., 2020) using Neural Network models like BiLSTM-CNN-CRF (Ma and Hovy, 2016) and contextual embeddings such as BERT (Devlin et al., 2019) and FLAIR (Akbik et al., 2018) have improved the NER performance in the general domain to the human-level. However, the NER performance for specific domains is still moderate due to the challenges of limited annotations and dealing with complicated domain-specific contexts.

We aim to further improve NER performance by considering coreference relations and semantic relations between entity mentions. This is in contrast to the usual way of thinking about NER as an up-stream task conducted before coreference resolution or entity relation extraction. The idea aligns with recent works that conduct joint inferences among multiple information extraction tasks (Miwa and Bansal, 2016; Li et al., 2017; Bekoulis et al., 2018; Luan et al., 2019; Sui et al., 2020; Yuan et al., 2020), including NER, coreference resolution and relation extraction, by mining dependencies among the extractions. However, joint inference approaches require annotations for all the target tasks and aim to improve performance for all the tasks as well, while our lightweight approach aims to improve the performance of the basic NER

task requiring no additional annotations (usually unavailable for specific domains).

Our approach is also related to several recent neural approaches for NER that encourage label dependencies among entity mentions. The Pooled FLAIR model (Akbik et al., 2019) proposed a global pooling mechanism to learn word representations. Dai et al. (2019) used a coreference layer with a regularizer to harmonize word representations. Closely related to our work, Qian et al. (2019) used graph neural nets to capture repetitions of the same word as well, but in a denser graph that includes edges between adjacent words and is meant to completely overlay the lower encoding layers. Memory networks (Gui et al., 2020; Luo et al., 2020) were also used to store and refine predictions of a base model by considering repetitions or co-occurrences of words. In addition, dependency relations have been commonly used to connect entities for relation extraction (Zhang et al., 2018; Bunescu and Mooney, 2005), but we aim to better infer the type of an entity by associating it with other closely related entities in a sentence.

3 Model Architecture

Our system with Entity Relation Graphs (EnRel-G) mainly contains 5 layers as in Figure 2: an embedding layer, an encoding layer, a GNNs layer, a fusion layer, and a decoding layer.

3.1 Embedding Layer

We choose the BERT-base LM as our embedding layer. For domain-specific datasets, we use BioBERT (Lee et al., 2020) for the biomedical domain and SciBERT (Beltagy et al., 2019) for the planetary science domain. Specifically, for an input
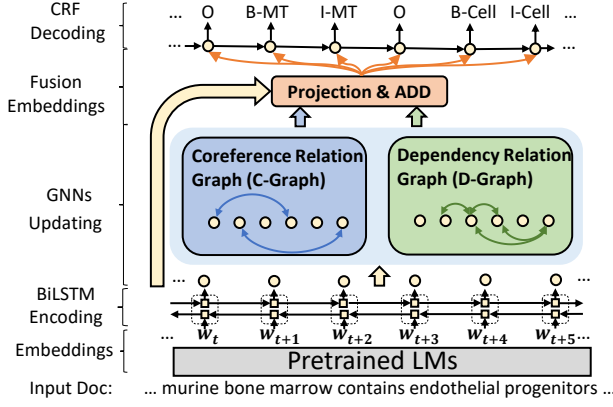
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Figure 2: Overall Architecture of the EnRel-G system

document $D = [w_1, w_2, ..., w_n]$ with n words, the BERT model will output a contextual word embeddings matrix $\boldsymbol{E} = [\boldsymbol{w}_1, \boldsymbol{w}_2, ..., \boldsymbol{w}_n] \in \mathbb{R}^{n \times d_1}$ with a d_1 dimension vector for each word.

3.2 Encoding Layer

To capture the sequential context information, we use a BiLSTM layer to encode the word embeddings from the BERT model. We concatenate the forward and backward LSTM hidden states as the encoded representations and then obtain embedding matrix $\boldsymbol{E}^{lstm} = BiLSTM(\boldsymbol{E}) \in \mathbb{R}^{n \times d_2}$ with a d_2 dimension vector for each word.

3.3 Graph Neural Networks Layer

For the GNNs layer, we first introduce how to build Entity Relation Graphs using global coreference relations (coreference graph, C-graph) and local dependency relations (dependency graph, D-graph) between entities, and then describe how the GNNs model incorporates them into the word representations.

Coreference Relation Graph For each document, we build a graph $G^C = (\mathcal{V}, \mathcal{A}^C)$ based on coreference relations, in which $\mathcal{V}$ is a set of nodes denoting all the words in a document and $\mathcal{A}^C$ is the adjacency matrix. Specifically, we approximate the entity coreference relations using 3 syntactic coreference clues as in Figure 1: (1) *Exact Match*, two nouns are connected if they are the same, e.g., "tumor vasculature" in both the *Title* and *S6*; (2) *Lemma Match*, two nouns are linked together if they have the same lemma, e.g., "progenitors" and "progenitor" in the *S3* and *S6*; (3) *Acronym Match*, the acronym word is connected to all full expression words, e.g., "VEGF" and "vascular endothelial growth factor" in the *S6*. For each connected node

pair (i, j), we set $\mathcal{A}^C_{i,j} = 1$. We also add a self-connection to each node ($\mathcal{A}^C_{i,i} = 1$) to maintain the words' original semantic information.

Dependency Relation Graph We build a Dependency Relation Graphs $G^D = (\mathcal{V}, \mathcal{A}^D)$ for each document based on sentence-level dependency relations. We first parse each sentence using the scispaCy[2] tool and then connect the following word pairs in the dependency tree: (1) *subject head word & object head word & their predicate*, we connect them to enhance the interactions between the entities from the subject and object. e.g., "marrow" and "progenitors" with the predicate "contains" in the *S3*; (2) *compound & head word*, we connect the compounds with their head words because they often both exist in an entity. e.g., the "bone" and "marrow" in the *S3*. Same as before, We set $\mathcal{A}^D_{i,j} = 1$ for each connect pair (i, j), and also add self-connection ($\mathcal{A}^D_{i,i} = 1$) for each node.

Then we update the encoded word embeddings with the entity relations graphs based on GNNs, particularly the GATs. Since nodes represent the words in a document, we initialize the node representations in the graphs from the encoding layer as $\boldsymbol{E}^{lstm} = [\boldsymbol{w}_1^{lstm}, \boldsymbol{w}_2^{lstm}, ..., \boldsymbol{w}_n^{lstm}]$. The graph attention mechanism updates the initial representation of node $\boldsymbol{w}_i^{lstm}$ to $\boldsymbol{w}_i^{gnn}$ by aggregating its neighbors' representations with their corresponding normalized attention scores.

$$\boldsymbol{w}_i^{gnn} = \mathop{\|}_{k=1}^{K} \sigma \left(\sum_{j \in \mathcal{N}_i} \alpha_{ij}^k W^k \boldsymbol{w}_j^{lstm} \right) \quad (1)$$

As in equation (1), and we have K attention heads and concatenate ($\|$) them as the final representation. For head k, we weighted all the adjacent nodes ($\mathcal{N}_i$, obtained from the adjacent matrix $\mathcal{A}$) by W^k and and then aggregate them with the attention score α_{ij}^k. σ is the activation function LeakyReLU. The attention score α_{ij}^k is obtained as followed ($\boldsymbol{a}^T$ is a weight vector):

$$\alpha_{ij}^k = \frac{\exp \left(\sigma \left(\boldsymbol{a}^T \left(W^k \boldsymbol{w}_i^{lstm} \| W^k \boldsymbol{w}_j^{lstm} \right) \right) \right)}{\sum_{z \in \mathcal{N}_i} \exp \left(\sigma \left(\boldsymbol{a}^T \left(W^k \boldsymbol{w}_i^{lstm} \| W^k \boldsymbol{w}_z^{lstm} \right) \right) \right)}$$

(2)

For each of the two relation graphs, we use an independent graph attention layer. The output word representations from the two GATs are denoted as: $\boldsymbol{G}^C = [\boldsymbol{w}_1^{gnn(C)}, \boldsymbol{w}_2^{gnn(C)}, ..., \boldsymbol{w}_n^{gnn(C)}] \in \mathbb{R}^{n \times d_3}$ and $\boldsymbol{G}^D = [\boldsymbol{w}_1^{gnn(D)}, \boldsymbol{w}_2^{gnn(D)}, ..., \boldsymbol{w}_n^{gnn(D)}] \in \mathbb{R}^{n \times d_3}$, with d_3 dimension for each word.

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[2]https://allenai.github.io/scispacy/

Methods	Datasets	
	AnatEM	Mars
Wagstaff et al. (2018)	–	94.5 / 77.7 / 85.3
NCRF++	83.40±0.34 / 76.96±0.46 / 80.05±0.12	91.28±1.08 / 80.57±0.55 / 85.59±0.23
FLAIR	81.07±0.29 / 75.28±0.57 / 78.06±0.39	90.67±1.02 / 81.45±1.41 / 85.81±0.62
Pooled FLAIR	82.11±0.50 / 77.55±0.40 / 79.76±0.34	87.79±1.31 / 86.57±1.10 / 87.17±0.17
Tuning Bio/SciBERT	83.94±0.40 / 83.12±0.30 / 83.53±0.32	90.93±0.66 / 88.99±1.61 / 89.95±0.64
EnRel-G (C)	84.65±0.67 / 83.69±0.31 / 84.17±0.41	91.21±1.05 / **89.35**±1.76 / 90.27±0.45
EnRel-G (D)	**84.98**±0.83 / 83.50±0.45 / 84.23±0.54	**92.66**±1.16 / 88.03±1.46 / 90.29±0.53
EnRel-G (CD)	84.86±0.50 / **83.96**±0.32 / **84.41**±0.24	92.57±1.00 / 88.65±1.50 / **90.57**±0.47

Table 1: Test results of baselines and our system (Average Precision/Recall/F1 Scores±standard deviation,%)[3]

3.4 Fusion Layer

Similar to Sui et al. (2019), we also use a fusion layer to blend the encoded word embeddings and the GNNs updated word embeddings. We first project these embeddings into the same hidden space using liner transformation and then add them, as in $\boldsymbol{F} = W_N \boldsymbol{E}^{lstm} + W_C \boldsymbol{G}^C + W_D \boldsymbol{G}^D$, where W_N, W_C, W_D are trainable weights. Then we will have a feature matrix $\boldsymbol{F} \in \mathbb{R}^{n \times d_4}$ for the n words blended with both the sequential context information and global entity relations.

3.5 Decoding Layer

Finally, a Conditional Random Field (CRF) (Lafferty et al., 2001) layer is used to decode the enriched embeddings $\boldsymbol{F} = [\boldsymbol{f}_1, \boldsymbol{f}_2, ..., \boldsymbol{f}_n]$ into a sequence of labels $y = \{y_1, y_2, ..., y_n\}$. In the training phrase, we optimize the whole model by minimizing the negative log-likelihood loss with respect to gold labels.

4 Experiments[4]

We test our model on two domain-specific datasets: the AnatEM (Pyysalo and Ananiadou, 2014) from the biomedical domain and the Mars (Wagstaff et al., 2018) from the planetary science domain. The AnatEM has annotated 12 types of entities in 1,212 documents with 13,701 entity mentions; the Mars has 117 longer documents with 4,458 entity mentions containing 3 types.

4.1 Baselines

NCRF++ (Yang and Zhang, 2018) is an open-source Neural Sequence Labelling Toolkit. We use the BiLSTM-CNN-CRF structrue as a baseline.

FLAIR (Akbik et al., 2018) is a character-level pretrained LM based on BiLSTM, which has been used in many NER systems (Jiang et al., 2019; Wang et al., 2019). We use the embeddings from it with a BiLSTM-CRF architecture as a baseline.

Pooled FLAIR (Akbik et al., 2019) is an extended version of the FLAIR model with global memory and pooling mechanism for the same word, which helps consistent predictions of coreferential entity mentions. We also use the embeddings from it with a BiLSTM-CRF architecture as a baseline.

Tuning Bio/SciBERT We also use Bio/SciBERT with a BiLSTM-CRF architecture as baselines for the AnatEM/Mars datasets, which do not have the GNNs layer or Fusion layer as compared with our system.

4.2 Results

To alleviate random turbulence, we train all the systems five times using different random seeds and evaluate their average performance on the test sets using the same script[5], as in the Table 1.

We can see that our system with both the global entity coreference and local dependency relations performs the best among all the systems. It improves the average F1 score by 0.88 points (84.41% vs. 83.53%) compared to BioBERT on the AnatEM, and 0.62 points (90.57% vs. 89.95%) compared to SciBERT on the Mars. Further, both the coreference and dependency relations help to improve the NER performance. Specifically, our model with either the coreference or dependency relation graph improves the F1 scores by 0.64 point or 0.7 point on the AnatEM dataset, and by 0.32 point or 0.34 point on the Mars dataset.

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[3]Previous systems on the AnatEM dataset either evaluate the NER performance by head match or only evaluate the performance on span identification; therefore, so we do not include their results here.

[4]More details about the datasets, data preprocessing, and model settings can be found in the appendices.

[5]https://github.com/sighsmile/conlleval

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Methods	Datasets	
	AnatEM	Mars
Tuning Bio/SciBERT	83.94±0.40 / 83.12±0.30 / 83.53±0.32	90.93±0.66 / 88.99±1.61 / 89.95±0.64
EnRel-G (D) (Key Edges Only)	83.79±0.70 / 83.39±0.39 / 83.59±0.40	91.71±0.63 / 88.30±0.86 / 89.97±0.33
EnRel-G (D) (Compound + Key Edges)	**84.98**±0.83 / 83.50±0.45 / **84.23**±0.54	**92.66**±1.16 / 88.03±1.46 / **90.29**±0.53
EnRel-G (D) (All Modifiers + Key Edges)	84.38±0.72 / **83.83**±0.31 / 84.10±0.40	91.06±1.94 / **89.19**±1.07 / 90.11±0.55
EnRel-G (D) (All Dependency Edges)	84.32±0.36 / 83.52±0.44 / 83.92±0.30	90.71±2.85 / 89.62±1.87 / 90.16±1.23

Table 2: Edge Selection in the Dependency Graph (Average Precision/Recall/F1 Scores±standard deviation,%)
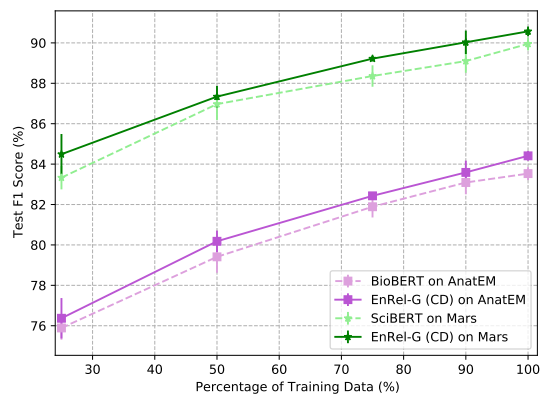
4.3 Learning Curves

Figure 3: Learning Curves, each point shows the average performance of 5 system runs.

One main limitation of domain-specific NER systems is the lack of annotations, therefore, it is vital to make the best use of labeled data. The learning curves (Figure 3) shows that leveraging the relations between entity mentions can effectively elevate the NER performance to a higher level even when only a tiny amount of labeled data (a quarter of training data) is available, and this is true on both the AnatEM dataset and the Mars dataset.

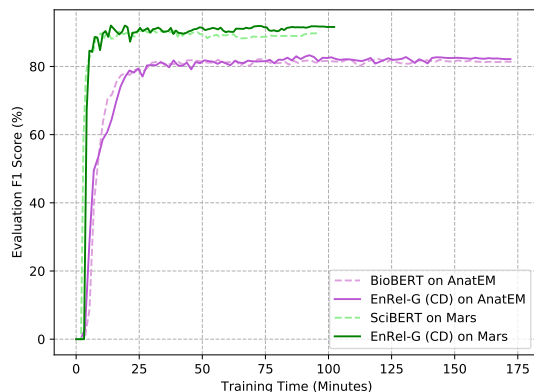## 4.4 Analysis of Computation Cost

Figure 4: Comparison of Training Time

Although fine-tuning pretrained LMs has im-

proved the performance of many NLP tasks, one limitation is the increase of training time. Therefore, it is important to build computing efficient models based on pretrained LMs. As shown in Figure 4, our model with the GNNs layer does not increase the time cost for fine-tuning the BERT models. The training time of methods with or without the GNNs layer is similar.

4.5 Edge selection in the Dependency Graph

To build the sentence-level dependency graph, we selected only two types of dependency relations: between the subject, object and their predicate (*Key Edges*) and between a compound modifier and its head word. As shown in the Table 2, we also tried to connect all the modifiers with their head word and found that this yields slightly worse performance, and the reason may be that many modifiers other than compounds are not entities themselves. In addition, including all the dependency edges also yields worse performance than using the two selected types of dependency relations, probably for the same reason that many of the nodes in a dependency tree are not parts of entity mentions and many dependency relations do not directly contribute to capturing relations between entities.

5 Conclusion

In this work, we explicitly capture the global coreference and local dependency relations between entity mentions, and use graph neural nets to incorporate the relations to improve domain-specific NER tasks. Experimental results on two datasets show the effectiveness of this lightweight approach. We also find that the selection of entity relations is important to the system performance. Future work may consider about using GNNs to incorporate external knowledge for performance improvement.

Acknowledgments

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Appendices

Appendix A: Dataset Details

The AnatEM (Pyysalo and Ananiadou, 2014) dataset is an extended Anatomical Entity Mention corpus combining both the Anatomical Entity Mention (AnEM) (Ohta et al., 2012) dataset and Multilevel Event Extraction (MLEE) (Pyysalo et al., 2012) corpus. All the documents are selected from PubMed[6] abstracts or full-text papers. AnatEM is manually annotated by biological experts and it has 12 types of entities annotated, namely *Anatomical System, Cancer, Cell, Cellular Component, Developing Anatomical Structure, Immaterial Anatomical Entity, Multi-tissue Structure, Organ, Organism Subdivision, Organism Substance, Pathological Formation, Tissue*. In total, this dataset consists of 1,212 documents and 13,701 entities annotated.

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[6] https://pubmed.ncbi.nlm.nih.gov/

Datasets		#Doc	#Words	#Entities	#Words/Doc
AnatEM	Train	606	153,823	6,946	254
	Dev	202	58,785	2,139	291
	Test	404	99,976	4,616	247
	Total	1,212	312,584	13,701	258
Mars	Train	62	99,952	2,431	1,612
	Dev	20	33,743	906	1,687
	Test	35	58,392	1,121	1,668
	Total	117	192,087	4,458	1,642

Table 3: Statistics of the AnatEM and Mars datasets.[7]

Methods	Optimizer	Learning Rate	Batch Size
NCRF++	SGD	1e-2	10
(pooled) FLAIR	Adam	2e-3	8
Tuning Bio/SciBERT	Adam	5e-5	32
EnRel-G	Adam	5e-5	32

Table 4: Model Settings

Mars is from the scientific literature domain, and it is about planetary science. All documents come from the Lunar and Planetary Science Conference (LPSC)[8], and the entity mentions are annotated manually. It has 3 types of entities: *Element*, *Mineral*, *Target*. The corpus consists of 117 documents. 62 of them are from LPSC 2015 and they are for training and 55 of them are from LPSC 2016 for evaluation. Same as previous work, we divide the 2016 documents into a validation set with 20 documents and a testing set with 35 documents.

Appendix B: Data Preprocessing

We want our model to take advantage of the document-level information, but some of the documents are extremely too long. Moreover, the BERT model also has a limitation of 512 subtokens for input texts. So we need to split the long documents. Besides, the BERT language model needs a big enough batch size (e.g., 16 or 32) to be well fine-tuned, which is also a burden for the GPU memory consumption. In consideration of these restrictions, we limit the max subtoken count of a split document to 128 in the data preprocessing. Future work with more computing resources may try longer input documents.

Moreover, we also add the POS and Dependency Tree information into the data using scispaCy for constructing the Coreference Graph and the Dependency Graph in our model.

Appendix C: Model Settings

For the **NCRF++** baseline, we use one layer of BiLSTM for word sequence representation with 300-dim Glove (Pennington et al., 2014) embeddings, four layers of CNN for character sequence representation with 50-dim random initialized character embeddings, and a CRF layer for inference.

For the **FLAIR** and **Pooled FLAIR** baselines, we use the PubMed version (pretrained on the biomedical corpus) for the AnatEM dataset and the general English version (pretrained on the English news articles) for the Mars dataset. Particularly, for the Pooled FLAIR model, we set the *mean* pooling mechanism to calculate the average of embeddings for multiple occurrences of a word, and then use it as the representation for the word.

For the **Tuning BERT** baselines, we use *BioBERT-Base v1.1* for the AnatEM dataset and *SciBERT-scivocab-uncased* for the Mars dataset.

For our **EnRel-G** system, we keep the embeddings layer the same as the Tuning BERT baselines. As for the GNNs layer, we use one layer of the graph attention mechanism with 4 heads, and each head has a hidden dimension of 128.

For the optimization related parameters, as in the Table 4, we mainly use the recommended settings for the baseline models. For our EnRel-G system, we keep the same parameters as in the Tuning BERT baseline for fair comparison.

We train all the systems on a single Nvidia GEFORCE GTX 2080Ti GPU. We set the maximum epoch as 100 and use the best-performed model on the development set to evaluate the test data.

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[7]We remove the redundantly annotated entities in the Mars.
[8]https://www.hou.usra.edu/meetings/