Improving BERT Model Using Contrastive Learning for Biomedical
Relation Extraction

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Abstract

Contrastive learning has been used to learn a high-quality representation of the image in
computer vision. However, contrastive learning is not widely utilized in natural language
processing due to the lack of a general method of data augmentation for text data. In this
work, we explore the method of employing contrastive learning to improve the text repre-
sentation from the BERT model for relation extraction. The key knob of our framework
is a unique contrastive pre-training step tailored for the relation extraction tasks by seam-
lessly integrating linguistic knowledge into the data augmentation. Furthermore, we inves-
tigate how large-scale data constructed from the external knowledge bases can enhance the
generality of contrastive pre-training of BERT. The experimental results on three relation ex-
traction benchmark datasets demonstrate that our method can improve the BERT model rep-
resentation and achieve state-of-the-art performance. In addition, we explore the inter-
pretability of models by showing that BERT with contrastive pre-training relies more on ra-
tionales for prediction. Our code and data are publicly available at: https://github.
com/udel-biotm-lab/BERT-CLRE.

1 Introduction

Contrastive learning is a family of methods to learn a discriminative model by comparing input pairs
(Le-Khac et al., 2020). The comparison is performed between positive pairs of “similar” inputs
and negative pairs of “dissimilar” inputs. The positive pairs can be generated in an automatic way
by transforming the original data to variants without changing the key information (e.g., rotate an
image). Contrastive learning can encode general properties (e.g. invariance) in the learned represen-
tation while it is relatively hard for other representation learning methods to achieve (Bengio et al.,
2013; Le-Khac et al., 2020). Therefore, contrastive learning provides a powerful approach to learn rep-
resentations in a self-supervised manner and has shown great promise and achieved the state of the
art results in recent years (He et al., 2020; Chen et al., 2020).

Despite its advancement, contrastive learning has not been well studied in biomedical natural
language processing (BioNLP), especially for relation extraction (RE) tasks. One obstacle lies in the
discrete characteristics of text data. Compared to computer vision, it is more challenging to design a
general and efficient data augmentation method to construct positive pairs. Instead, there have been
significant advances in the development of pre-trained language models to facilitate downstream
BioNLP tasks (Devlin et al., 2019; Radford et al., 2019; Peng et al., 2019). Therefore, leveraging con-
trastive learning in the large pre-trained language models to learn more general representation for RE
tasks remains unexplored.

To bridge this gap, this paper presents an innovative method of contrastive pre-training to improve
the language model representation for biomedical relation extraction. As the main difference from
the existing contrastive learning framework, we augment the datasets for RE tasks by randomly
changing the words that do not affect the relation expression. Here, we hypothesize that the short-
est dependency path (SDP) between two entities (Bunescu and Mooney, 2005) captures the required
knowledge for the relation expression. We hence keep words on SDP fixed during the data augmenta-
tion. In addition, we utilize external knowledge bases to construct more data to make the learned
representation generalize better, which is a method that is frequently used in distant supervision (Mintz
et al., 2009; Peng et al., 2016).

To verify the effectiveness of the proposed method, we use the transformer-based BERT model
as a backbone (Devlin et al., 2019) and evaluate
our method on three widely studied RE tasks in
the biomedical domain: the chemical-protein inter-
actions (ChemProt) (Krallinger et al., 2017), the
drug-drug interactions (DDI) (Herrero-Zazo et al.,
2013), and the protein-protein interactions (PPI)
(Krallinger et al., 2008). The experimental results
show that our method boosts the BERT model per-
formance and achieves state-of-the-art results on
all three tasks.

Interest has also grown in designing interpretable
BioNLP models that are both plausible (accurate)
and rely on a specific part of the input (faithful
rationales) (DeYoung et al., 2020; Lei et al., 2016).
Here rationale is defined as the supporting evidence
in the inputs for the model to make correct predic-
tions. In this direction, we propose a new metric,
"prediction shift", to measure the sensitivity degree
to which the small changes (out of the SDP) of
the inputs will make model change its predictions.
We show that the contrastively pre-trained model
is more robust than the original model, suggesting
that our model is more likely to make predictions
based on the rationales of the inputs.

In sum, the contribution of this work is four-
fold. (1) We propose a new method that utilizes
contrastive learning to improve the BERT model
on biomedical relation extraction tasks. (2) We
utilize external knowledge to generate more data
for learning more generalized text representation.
(3) We achieve state-of-the-art performance on
three benchmark datasets of relation extraction
tasks. (4) We propose a new metric that aims to
reveal the rationales that the model uses for pre-
dicting relations. The code and the new rationale
test datasets are available at https://github.
com/udel-biotm-lab/BERT-CLRE.

2 Related Work

The history of contrastive representation learning
can be traced back to (Hadsell et al., 2006), in
which the authors explore the method of represen-
tation learning that similar inputs are mapped
to nearby points in the representation space. Re-
cently, with the development of data augmentation
techniques, deep neural network architectures, con-
trastive learning regains attention and achieves su-
perior performance on visual representation learn-
ing (He et al., 2020; Chen et al., 2020). In (He et al.,
2020), the Momentum Contrast (MoCo) framework
is designed to learn representation using the me-
chanism of dictionary look-up: an encoded example
(the query) should be similar to its matching key
(augmented sample from the same data example)
and dissimilar to others. In (Chen et al., 2020),
the authors propose the SimCLR frame to learn
the representations by maximizing the agreement
between augmented views of the same data point.

The contrastive representation has all the prop-
erties that a good representation should have: 1) Distrbuted property; 2) Abstraction and invariant
property; 3) Disentangled representation (Bengio
et al., 2013; Le-Khac et al., 2020). The distributed
property emphasizes the expressive aspect of the
representation (different data points should have
distinguishable representations). The capture of
abstract concepts and the invariance to small and
local changes are concerned in the abstraction and
invariant property. From the disentangled repre-
sentation’s perspective, it should encode as much
information as possible. In this work, we will show
contrastive learning can improve the invariant as-
pect of the representation.

In the natural language processing (NLP) field,
several works have utilized the contrastive learning
 technique. Fang et al. (2020) propose a pre-trained
language representation model (CERT) using con-
trastive learning at the sentence level to benefit
the language understanding tasks. Klein and Nabi
(2020) employ contrastive self-supervised learn-
ing to solve the commonsense reasoning problem.
Peng et al. (2020) propose a self-supervised pre-
training framework for relation extraction to ex-
plore the encoded information for the textual con-
text and entity type. Compared with the previous
works, we employ different data augmentation tech-
niques and utilize data from external knowledge
bases in contrastive learning to improve the model
for relation extraction tasks.

Relation extraction is usually seen as a classifi-
cation problem when the entity mentions are given
in the text. Many different methods have been
proposed to solve the relation extraction problem
(Culotta and Sorensen, 2004; Sierra et al., 2008;
Sahu and Anand, 2018; Zhang et al., 2019; Su et al.,
2019). However, the language model methods re-
define this field with their superior performance
(Dai and Le, 2015; Peters et al., 2018; Devlin
et al., 2019; Radford et al., 2019; Su and Vijay-
Shanker, 2020). Among all the language models,
BERT (Devlin et al., 2019) --a language represen-
tation model based on bidirectional Transformer
(Vaswani et al., 2017), attracts lots of attention in
Our goal is to learn a text representation by maximizing agreement between inputs from positive pairs. At the end of training, we only keep the encoder $f$ as in (Chen et al., 2020). For any text input $x$, $h = f(x)$ will be the representation of $x$ from contrastive learning.

### 3.1 Data augmentation for relation extraction

The data augmentation module is a key component of contrastive learning, which needs to randomly generate two correlated views for the original data point. At the same time, the generated data should be different from each other to make them distinguishable (from the model’s perspective), but should not be significantly different to change the structure and semantics of the original data. It is especially difficult to augment the text data of relation extraction. In this work, we only focus on binary relations. Given $< s, e_1, e_2, r >$, where $e_1$ and $e_2$ are two entity mentions in the sentence $s$ with the relation type $r$, we keep $e_1$ and $e_2$ in the sentence and retain the relation expression between $e_1$ and $e_2$ in the augmented views.

Specifically, we propose a data augmentation method utilizing the shortest dependency path (SDP) between the two entities in the text. We hypothesize that the shortest dependency path captures the required information to assert the relationship of the two entities (Bunescu and Mooney, 2005). Therefore we fix the shortest dependency path, and randomly change the other tokens in the text to generate the augmented data. This idea is inspired by (Wei and Zou, 2019), which
employed easy data augmentation techniques to improve model performance on text classification tasks.

As the preliminary study, we experiment with three techniques to randomly replace the tokens to generate the augmented data and choose the best one for our contrastive learning method: 1) Synonym replacement (SR), 2) Random swap (RS), and 3) Random deletion (RD).

Table 1 gives some samples after applying the three operations on a sentence from the PPI task. For the synonym replacement, we randomly replace \( n \) words with their synonyms. To acquire the synonym of a word, we utilize the WordNet database (Miller, 1995) to extract a list of synonyms and randomly choose one from the list. For the random swap, we swap the positions of two words and repeat this operation \( n \) times. For the random deletion, we delete some words with the probability \( p \). The probability \( p \) is set to 0.1 in our experiments and the parameter \( n \) for SR and RS is calculated by \( p \times l \), where \( l \) is the length of the sentence.

To examine which operation performs better for relation extraction tasks, we train three BERT models using the three types of augmented data (combined with the original training data). Table 4 shows that the synonym replacement (SR) operation achieves the best performance on all three tasks and we will employ this operation in our data augmentation module in our contrastive learning experiments (We will further discuss it in Section 5.2).

3.1.2 The neural network encoder

In this work, we employ the BERT model (Devlin et al., 2019) as our encoder for the text data and the classification token ([CLS]) output in the last layer will be the representation of the input.

3.1.3 Projection head

As demonstrated in (Chen et al., 2020), adding a nonlinear projection head on the model output will improve the representation quality during training. Following the same idea, a multi-layer perceptron (MLP) will be applied to the model output \( h \). Formally,

\[
z = g(h) = W^2 \phi(W^1 h)
\]

and \( \phi \) is the ReLU activation function, \( W^1 \) and \( W^2 \) are the weights of the perceptron in the hidden layers.

3.1.4 Contrastive loss

Contrastive learning is designed to make similar representations be learned for the augmented samples (positive pairs) from the same data point. We follow the work of (Chen et al., 2020) to design the loss function (Algorithm 1). During contrastive learning, the contrastive loss is calculated based on the augmented batch derived from the original batch. Given \( N \) sentences in a batch, we first employ the data augmentation technique to acquire two views for each sentence in the batch. Therefore, we have \( 2N \) views from the batch. Given one positive pair (two views from the same sentence), we treat the other \( 2(N - 1) \) within the batch as negative examples. Similar to (Chen et al., 2020), the loss for a positive pair is defined as:

\[
l(z', z'') = -\log \frac{\exp(sim(z', z'')/\tau)}{\sum_{k=1}^{2N} \mathbb{1}_{[z_k \neq z']} \exp(sim(z', z_k)/\tau)}
\]

where \( sim(\cdot, \cdot) \) is the cosine similarity function, \( \mathbb{1}_{[z_k \neq z']} \) is the indicator function and \( \tau \) is the temperature parameter. The final loss \( L \) is computed across all positive pairs, both \((z', z'')\) and \((z'', z')\), in a batch.

For computation convenience, we arrange the \((2k - 1)\)-th example and the \(2k\)-th example in the batch are generated from the same sentence, a.k.a., \((2k - 1, 2k)\) is a positive pair. Please see Algorithm 1 for calculating the contrastive loss in one batch. Then we can update the parameters of the BERT model and projection head \( g \) to minimize the loss \( L \).
Algorithm 1: Contrastive loss in a batch

Input: encoder \( f \) (BERT), project head \( g \)

data augmentation module, data batch
\[\{s_k\}_{k=1}^N;\]

for \( k=1,\ldots,N \) do

\[v',v'' = \text{data} \_\text{augment}(s_k);\]
\[z_{2k-1} = g(f(v'));\]
\[z_{2k} = g(f(v''));\]

end

\[L = \frac{1}{2N} \sum_{k=1}^N [l(z_{2k-1}, z_{2k}) + l(z_{2k}, z_{2k-1})].\]

3.2 Training procedure

Figure 2 shows the training procedure of our framework. It consists of three stages. First, we pretrain the BERT model on a large amount of unlabeled data from a specific domain (e.g., biomedical domain). Second, we conduct contrastive pre-training on task-specific data as a continual pre-training step after the domain pre-training of BERT model. In this way, we retain the learned knowledge from general pre-training, and add the new features from contrastive learning. Finally, we fine-tune the model on the RE tasks to further gain task-specific knowledge through supervised training on the labeled datasets.

The domain pre-training stage follows that of the BERT using the masked language model and next sentence prediction technique (Devlin et al., 2019). In our experiments, we use two pre-trained versions for the biomedical domain: BioBERT (Lee et al., 2020) and PubMedBERT (Gu et al., 2021).

3.3 A knowledge-based method to enrich training dataset for contrastive learning

Contrastive pre-training requires a large-scale dataset to generalize the representation. Also, our data augmentation for contrastive learning needs SDP between two given entities, so we need to construct the augmented dataset with the entities mentioned in the text. For these purposes, we utilize external databases for the relations to acquire extra instances for contrastive learning.

Formally, assuming a curated database for relation \( r \) contains all the relevant entities and text, we consider every combination of the entity pairs in one sentence and use them as examples for this relation. For instance, there are three proteins in the sentence: "Thus NIPP1 works as a molecular sensor for PP1 to recognize phosphorylated Sap155." We will generate three examples for PPI task from this sentence: \(<s,\text{NIPP1},\text{PP1},\text{PPI}>,<s,\text{NIPP1},\text{Sap155},\text{PPI}>,<s,\text{PP1},\text{Sap155},\text{PPI}>.\"

We use the IntAct database (Orchard et al., 2014) as the interacting protein pairs database for the PPI task. Similarly, DrugBank (Wishart et al., 2008) and BioGRID (Stark et al., 2006) are utilized for DDI and ChemProt, respectively. In the column "EK" of Table 2, we show the statistics of datasets for each task generated by external knowledge bases. We can see that the datasets from the external database are much larger than that of the human-labeled datasets.

4 Experiments

As discussed before, we will utilize the BERT model as the encoder for the inputs. In particular, we will employ two BERT models pre-trained for the biomedical domain in our experiments: BioBERT (Lee et al., 2020) and PubMedBERT (Gu et al., 2021).

4.1 Datasets and evaluation metrics

We will evaluate our method on three benchmark datasets. The statistics of these datasets is shown in Table 2. For ChemProt and DDI tasks, we employ the corpora in (Krallinger et al., 2017) and (Herrero-Zazo et al., 2013) respectively, and we use the same split of training, development and test sets with the
Table 3: BERT model performance on ChemProt, DDI and PPI tasks. BioBERT/PubMedBERT: original BERT model; BioBERT/PubMedBERT+CL: BioBERT/PubMedBERT with contrastive pre-training on the training set of human-labeled dataset; BioBERT/PubMedBERT+CLEK: BioBERT/PubMedBERT with contrastive pre-training on the data from the external knowledge base.
Table 4: BioBERT model performance (F1 score) using different types of augmented data. RS: random swap; RD: random deletion; SR: synonym replacement.

| Training data | ChemProt | DDI | PPI |
|---------------|----------|-----|-----|
| Original      | 75.3     | 79.0| 81.0|
| +RS           | 75.6     | 78.4| 75.4|
| +RD           | 75.4     | 79.8| 81.2|
| +SR           | 76.0     | 80.1| 81.9|

Table 5: Examples of prediction shift. (1): Original sentence; (2): Augmented sentence.

| Task   | Model               | Prediction Shift |
|--------|---------------------|------------------|
| ChemProt | BioBERT             | 246              |
|         | BioBERT+CLEK        | 191 (22%↓)       |
|         | PubMedBERT          | 248              |
|         | PubMedBERT+CLEK     | 189 (24%↓)       |
| DDI     | BioBERT             | 111              |
|         | BioBERT+CLEK        | 89 (20%↓)        |
|         | PubMedBERT          | 90               |
|         | PubMedBERT+CLEK     | 75 (17%↓)        |
| PPI*    | BioBERT             | 51               |
|         | BioBERT+CLEK        | 33 (35%↓)        |
|         | PubMedBERT          | 49               |
|         | PubMedBERT+CLEK     | 34 (31%↓)        |

Table 6: Count of prediction shift on the "augmented" test set. *: The sum of counts on the 10 folds.

5.3 Measurement of rationale faithfulness

As discussed previously, we hypothesize the words on the shortest dependency path (SDP) as the rationales in the input. Therefore, the model should make its predictions based on them. If the model predictions are all made based on a specific part of the input, we can define this specific part of the input to be the completely faithful rationales. In practice, the rationales are more faithful means they are more influential on the model predictions.

In this work, we define a new metric to measure the faithfulness of the rationales: "prediction shift". If the model predicts one test example (non-negative) with label $L_t$, but changes its prediction on its neighbor (the augmented data point) with another label $L'_t$, we will say a "prediction shift" happens (In Table 5, we give two examples of pre-
diction shift on PubMedBERT model). Fewer "prediction shift" indicates the information outside of SDP influences the prediction less, which means the rationales are more faithful.

To generate a similar set (with test set) for the measurement of "prediction shift", we apply the same synonym replacement (SR) technique on the original test data. Since we retain the words that are on the shortest dependency path between the two entities, the generated data should express the same relation with the original ones. The trained model should predict them with the same labels if the rationales of input are utilized during inference, and in that case, we say the rationales are faithful.

We compare the number of "prediction shift" on two types of BERT model: the original BERT and the BERT model with contrastive pre-training. Table 6 illustrates that the BERT models with contrastive pre-training dramatically reduce the number of "prediction shift". Those results indicate that the BERT models with contrastive pre-training rely more on the information of shortest dependency path for prediction, a.k.a., the rationales are more faithful. From another perspective, the results in Table 6 also demonstrate that the BERT models with contrastive pre-training are resilient to small changes of the inputs, which means the models are more robust.

6 Conclusion and Future Directions

In this work, we propose a contrastive pre-training method to improve the text representation of the BERT model. Our approach differs from previous studies in the choice of text data augmentation with linguistic knowledge and the use of the external knowledge bases to construct large-scale data to facilitate contrastive learning. The experimental results demonstrate that our method outperforms the original BERT model on three relation extraction benchmarks. Additionally, our method shows robustness to slightly changed inputs over the BERT models. In the future, we will investigate different settings of data augmentation and contrastive pre-training to exploit their capability on language models. We also hope that our work can inspire researchers to design better metrics and create high-quality datasets for the exploration of model interpretability.

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