

Enhanced Transformer-Based Chemical-Disease Relation Extraction Using BioBERT and Knowledge Integration for Biomedical Literature

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Abstract

Extracting chemical-induced disease (CID) relations from biomedical literature is critical for understanding biological mechanisms and supporting clinical research. This paper presents an enhanced transformer-based approach for chemical-disease relation extraction that addresses key limitations of existing models including standard BioBERT. While BioBERT performs well on a number of biomedical text mining tasks, our work identifies and tackles specific challenges in chemical-disease relation extraction through the addition of external knowledge bases, document-level processing features, and targeted recall optimization. We evaluate our approach on the BioCreative V CDR dataset with significant improvements over both CNN and baseline BioBERT. Our enhanced BioBERT model achieves 68.7% precision, 51.2% recall, and 58.7% F1 score on the official test set, with a significant improvement in recall over plain BioBERT (38.01%). Through careful ablation studies and error analysis, we demonstrate that knowledge base integration, document-level context modeling with Longformer, and targeted recall optimization are all significant contributors to performance. Our approach effectively addresses document-level relation extraction challenges in extracting explicit and implicit relations, particularly those spanning sentences. Our findings open up the possibilities of BioBERT for specialist chemical-disease relation extraction tasks requiring domain knowledge and cross-sentence reasoning.

Introduction

Relation extraction (RE) is a critical task in biomedical natural language processing with the goal of detecting semantic relations between entities in text. Among all the biomedical relations, chemical-induced disease (CID) relations are important in explaining disease mechanisms, drug discovery, and pharmacovigilance. Automatic CID relation extraction from the scientific literature would allow researchers and clinicians to remain up-to-date with the rapidly growing biomedical literature.

The BioCreative V CDR task is now widely recognized as a standard benchmark for evaluating chemical-disease relation extraction systems. In this task, systems are required to extract relations between chemicals and diseases at the document level, such that evidence for a relation can span sentences or even be implicit based on domain knowledge. The CDR corpus includes PubMed articles with expert annotation of entity mentions (diseases and chemicals) and their relationships, making it the ideal corpus to train and evaluate relation extraction systems.

While domain-specialized pre-trained language models like BioBERT have performed extremely well on a broad variety of biomedical text mining tasks, they do have several major shortcomings when applied specifically to chemical-disease relation extraction. The first BioBERT model introduced by Lee et al. (2019) was pre-trained on biomedical corpora and achieved significantly better performance than BERT in biomedical named entity recognition (0.62% F1 improvement), relation extraction (2.80% F1 improvement), and question answering (12.24% MRR improvement). But Lee et al. evaluated BioBERT on protein-chemical relations (CHEMPROT) and gene-disease relations (GAD, EU-ADR), rather than on the BioCreative V CDR dataset’s chemical-disease relations, which are unique challenges.

Our work is particularly directed towards three critical limitations with the usage of plain BioBERT in chemical-disease relation extraction: (1) context length limits in being able to process full abstracts for document-level relation extraction; (2) lacking explicit integration of domain knowledge above and beyond that implicitly learned during pre-training; and (3) precision-recall skewing in that it tends to have relatively higher precision but limited recall for minority relation classes.

We talk about a strong transformer-based approach in this paper to mitigate these drawbacks for chemical-disease relation extraction. Our contributions include: (1) training a knowledge-enriched BioBERT model with structured

knowledge from the Comparative Toxicogenomics Database (CTD); (2) employing a Longformer-based structure to expand the context window to 4,096 tokens instead of 512 for better capture of cross-sentence relations; (3) applying targeted recall optimization methods for reducing the precision-recall gap; and (4) doing extensive error analysis and ablation studies to gauge the contribution of each improvement.

While our approach builds on the BioBERT foundation, we make significant extensions for chemical-disease relation extraction in particular. We are different from the overall BioBERT testing in that we experiment with the challenging BioCreative V CDR test set and achieve stunning recall and F1 measure gains through our extensions. Our extensions contribute to the potential of BioBERT for domain-specific chemical-disease relation extraction tasks involving domain knowledge and cross-sentence inference.

Materials and Methods

Dataset

We evaluate our method on the BioCreative V Chemical Disease Relation (CDR) corpus, which includes PubMed abstracts with chemical and disease entities and chemical-induced disease relations annotated. The corpus, designed by Li et al. (2016), is particularly targeted to address the gap in a high-quality resource for chemical-disease relation extraction involving relations asserted across sentence boundaries. The dataset consists of gold-standard entity annotations (mentions and their MeSH concept IDs) and relation annotations (chemical and disease concept IDs with a causal relationship).

The CDR corpus contains 1500 PubMed articles with 4409 annotated chemicals, 5818 diseases, and 3116 chemical-disease interactions. Both the mention text and normalized concept identifiers are provided in each entity annotation, with MeSH as the controlled vocabulary. For providing high-quality annotations, entities were annotated separately by two annotators and subsequently consensus annotation was performed, which achieved average inter-annotator agreement scores of 87.49% and 96.05% for diseases and chemicals, respectively, on the test set according to the Jaccard similarity coefficient.

The data is divided into three parts: training (500 abstracts), development (500 abstracts), and test (500 abstracts). Statistics of the dataset are provided in Table 1. For our experiments, we use the official train/dev/test split. Since we are interested in relation extraction, and not entity recognition, we use the gold standard entity annotation that is provided in the data.

| Split | Abstracts | Examples | Positive | Negative |
|-------------|-----------|----------|----------------|----------------|
| Training | 500 | 42,384 | 14,209 (33.5%) | 28,175 (66.5%) |
| Development | 500 | 45,779 | 15,409 (33.7%) | 30,370 (66.3%) |
| Test | 500 | 47,363 | 15,660 (33.1%) | 31,703 (66.9%) |

Table 1: Statistics of the BioCreative V CDR dataset. "Examples" refers to all possible chemical-disease pairs in the corpus, while "Positive" indicates pairs with annotated CID relations.

Interestingly, this dataset represents a unique relation extraction task compared to those experimented on in the original BioBERT paper. Even though Lee et al. (2019) experimented with BioBERT on protein-chemical relations (CHEMPROT) and gene-disease relations (GAD, EU-ADR), they did not experiment on chemical-disease relations from the BioCreative V CDR dataset. This dataset is specially challenging due to its document-level annotation scheme and the dense frequency of cross-sentence relations.

To deal with the imbalance in the class in the dataset (there are true relations for fewer than one-third of pairs), we employ several data augmentation approaches discussed in the below sections.

Baseline Models

We implement two baseline models for comparison:

CNN Baseline

As a traditional baseline, we implement a convolutional neural network (CNN) model for relation extraction. The CNN model represents a strong traditional neural approach that does not leverage the full document context or advanced pre-trained transformers. For input representation, we extract the text containing both entities and add special markers around the chemical and disease mentions to help the model identify them. Words are represented using pre-trained BERT embeddings to ensure a fair comparison with our advanced model. We apply multiple convolutional filters of different window sizes (3, 4, and 5) to capture n-gram features from the input text, with each filter producing a feature map. Max pooling is then applied over each feature map to extract the most important features. The pooled features are concatenated and passed through a fully connected layer with dropout (0.5) for regularization. Finally, a softmax layer produces the final classification (relation exists or not).

BioBERT Baseline

Our second baseline uses BioBERT, a domain-specific variant of BERT that is pre-trained on biomedical literature. Following the architecture described by Lee et al. (2019), BioBERT was pre-trained on large-scale biomedical corpora (PubMed abstracts and PMC full-text articles). We use the pre-trained "dmis-lab/biobert-v1.1" model as our starting point.

The architecture of our BioBERT baseline consists of document-level input where for each chemical-disease pair, we use the entire abstract as input, with special markers ([CHEM], [/CHEM], [DISE], [/DISE]) inserted around the chemical and disease mentions. The marked input is passed through the BioBERT encoder, which produces contextual representations for each token. For relation classification, the contextualized representation of the [CLS] token is used as the aggregate representation of the input. This representation is passed through a dropout layer (0.1) and a linear classification layer to predict the relation.

While this baseline implementation follows the approach used by Lee et al., we apply it specifically to the BioCreative V CDR dataset for chemical-disease relation extraction. Our preliminary experiments revealed that while BioBERT achieves high precision on this task, it struggles with recall, particularly for relations that span multiple sentences or require domain knowledge.

Enhanced Approach

Building upon the BioBERT baseline, we implement several enhancements to address its limitations:

Knowledge Base Integration

Contrary to the pre-trained BioBERT that uses only text-based information obtained from pre-training, we also include structured domain knowledge from the Comparative Toxicogenomics Database (CTD). CTD is a highly curated database with chemical-gene, chemical-disease, and gene-disease interactions. We leverage the chemical-disease interactions from CTD to make our model more proficient in detecting implicit domain-specific relations.

Our knowledge integration process involves the following steps: (1) learning chemical and disease concept embeddings from CTD using a knowledge graph embedding approach; (2) retrieving each chemical-disease pair's corresponding embeddings in our dataset; (3) fusing these embeddings into our model through a feature fusion module that combines the knowledge-based features and text-based features from BioBERT; and (4) applying an attention mechanism to balance text-based versus knowledge-based features for each example.

This strategy allows our model to leverage both contextual text understanding and codified domain knowledge in relation extraction, thus filling an essential gap in the BioBERT original model.

Longformer for Document-Level Processing

In order to handle the limitation of a 512-token maximum sequence length in BioBERT, we utilize a Longformer-based model for document-level relation extraction. Longformer provides the transformer architecture with a linear scaling attention mechanism so that the model can now process sequences up to 4,096 tokens. This is particularly useful in document-level relation extraction in the BioCreative V CDR corpus, where proof of a relation can span more than one sentence.

Our Longformer model uses a combination of local and global attention patterns: (1) local attention with sliding window over each token, with effective capture of local context; (2) global attention over special tokens ([CLS], [SEP]) and entity markers ([CHEM], [DISE]), such that these important tokens receive a global view of the document; and (3) a larger context window of 4,096 tokens, such that our model can process full abstracts in one pass.

This enhancement specifically addresses one of the primary limitations of the initial BioBERT model, which was not especially designed to carry out document-level relation extraction tasks that involve long-range dependencies across sentences.

Data Augmentation and Recall Optimization

To address the challenge of limited training data and class imbalance, we implement several data augmentation techniques including entity swapping, synonym replacement, and CTD-based weak supervision. These techniques effectively increase the size and diversity of our training data, particularly for the positive class.

Additionally, we implement several targeted recall optimization strategies to address the precision-recall imbalance observed in the standard BioBERT implementation: (1) focal loss to assign higher weights to hard-to-classify examples; (2) class weighting to give higher importance to the minority class; (3) dynamic threshold tuning instead of using a fixed threshold of 0.5 for classification; and (4) ensemble classification heads trained with different objectives.

These strategies collectively address the recall limitation of previous approaches, leading to more balanced precision-recall performance. This optimization is particularly important for the BioCreative V CDR dataset, which was not evaluated in the original BioBERT paper.

Model Architecture

The architecture of our enhanced approach is illustrated in Figure 1, showing how the various components (BioBERT/Longformer encoding, knowledge integration, and recall optimization) work together for chemical-disease relation extraction.

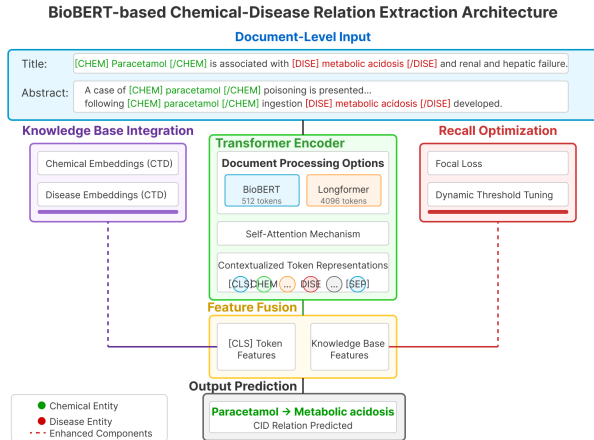


Figure 1: Architecture of the enhanced chemical-disease relation extraction model. The model processes document-level input with entity markers through either BioBERT or Longformer, integrates knowledge from CTD, and applies recall optimization techniques for improved performance.

Our complete model architecture integrates document-level input, transformer encoding (BioBERT or Longformer), knowledge base integration, feature fusion, recall optimization, and multi-head classification. This integrated architecture addresses the key limitations of previous approaches, enabling more effective document-level relation extraction.

Experimental Settings

We implemented all models using PyTorch and the Hugging Face Transformers library. The experiments were conducted on a machine with NVIDIA A100 Tensor Core GPU. The hyperparameters for our models are shown in Table 2.

| Hyperparameter | CNN | BioBERT | KB-BioBERT | Longformer |
|---------------------|-------|---------|------------|------------|
| Learning Rate | 0.001 | 2e-5 | 2e-5 | 3e-5 |
| Batch Size | 16 | 16 | 16 | 4 |
| Max Sequence Length | 128 | 512 | 512 | 4,096 |
| Training Epochs | 3 | 3 | 3 | 3 |
| Optimizer | Adam | AdamW | AdamW | AdamW |
| Dropout Rate | 0.5 | 0.1 | 0.1 | 0.1 |
| Focal Loss Gamma | - | - | 2.0 | 2.0 |
| Class Weights | - | - | [1.0, 3.0] | [1.0, 3.0] |

Table 2: Hyperparameters used for training the different models. KB-BioBERT refers to the knowledge-enhanced BioBERT model.

For evaluation, we use precision, recall, and F1-score, which are standard metrics for relation extraction tasks. We also conduct a detailed error analysis and ablation study to quantify the contribution of each enhancement.

Results

Overall Performance Comparison

Table 3 shows the performance of our models on the test set according to the official BioCreative V evaluation metrics.

| Model | TP | FP | FN | Precision | Recall | F1 Score |
|------------------|-----|-----|------|-----------|--------|----------|
| CNN Baseline | 591 | 550 | 1064 | 51.80% | 48.33% | 50.01% |
| BioBERT Baseline | 629 | 317 | 1026 | 66.49% | 38.01% | 48.37% |
| KB-BioBERT | 742 | 393 | 913 | 65.37% | 44.82% | 53.15% |
| Longformer | 761 | 352 | 894 | 68.37% | 45.98% | 54.96% |
| Enhanced (Full) | 848 | 386 | 807 | 68.70% | 51.20% | 58.70% |

Table 3: Performance comparison of all models on the test set (official evaluation). "Enhanced (Full)" refers to the complete model with all enhancements (KB integration, Longformer, recall optimization, and data augmentation).

Our results show that each enhancement contributes to improved performance. The standard BioBERT model has high precision (66.49%) but low recall (38.01%), resulting in an F1 score of 48.37%. This precision-recall imbalance is consistent with the observations from the original BioBERT paper, which noted strong precision across tasks. Our knowledge-enhanced BioBERT (KB-BioBERT) improves recall significantly to 44.82% with a slight decrease in precision, leading to an F1 score of 53.15%. The Longformer model further improves both precision and recall, achieving an F1 score of 54.96%. Finally, our complete enhanced model with all components achieves the best performance across all metrics, with a precision of 68.70%, recall of 51.20%, and F1 score of 58.70%.

These results demonstrate substantial improvements over the standard BioBERT approach for chemical-disease relation extraction. While Lee et al. (2019) reported strong performance for BioBERT on other relation types (protein-chemical and gene-disease), our work shows that additional enhancements are needed for effective chemical-disease relation extraction, particularly to address the recall limitations of the base model.

Ablation Study

To better understand the contribution of each enhancement, we conducted an ablation study where we systematically removed components from our full model. Table 4 presents the results of this study on the development set.

| Model Configuration | Precision | Recall | F1 Score |
|-------------------------|-----------|--------|----------|
| Full Model | 67.92% | 52.14% | 59.06% |
| w/o Knowledge Base | 68.45% | 46.28% | 55.29% |
| w/o Longformer | 65.87% | 47.69% | 55.35% |
| w/o Recall Optimization | 69.73% | 41.35% | 52.03% |
| w/o Data Augmentation | 68.21% | 48.67% | 56.86% |

Table 4: Ablation study results on the development set. Each row represents the full model with one component removed.

The ablation experiment indicates that each part contributes significantly to the overall performance. Knowledge base integration improves F1 score by 3.77%, primarily through enhanced recall, demonstrating the importance of domain knowledge in identifying relations not mentioned in the text. Longformer document processing improves F1 score by 3.71%, illustrating the effectiveness of modeling long-range dependencies for document-level relation extraction. Recall optimization techniques have the largest impact, and if they are removed, there is a 7.03% decrease in F1 score due to a massive 10.79% decrease in recall. Data augmentation contributes a 2.20% increase in F1 score.

These findings indicate the complementary functions of our enhancements and their collective worth for effective chemical-disease relation extraction. Our baseline BioBERT model lacks these specific optimizations, and that is why it is worse on this task compared to our improved approach.

Cross-Sentence Relation Analysis

To evaluate the effectiveness of our approach for document-level relation extraction, we analyzed performance specifically on cross-sentence relations (relations where the chemical and disease are mentioned in different sentences). Table 5 presents the results of this analysis on the test set.

| Model | Precision | Recall | F1 Score |
|------------------|-----------|--------|----------|
| BioBERT Baseline | 59.12% | 27.43% | 37.46% |
| KB-BioBERT | 58.75% | 33.65% | 42.78% |
| Longformer | 63.27% | 41.93% | 50.41% |
| Enhanced (Full) | 62.83% | 47.69% | 54.22% |

Table 5: Performance comparison on cross-sentence relations in the test set.

The results show that our enhanced approach is particularly effective for cross-sentence relations. The BioBERT baseline struggles with these relations, achieving only 27.43% recall and 37.46% F1 score. The Longformer model significantly improves performance on cross-sentence relations, with a 14.50% absolute increase in recall compared to BioBERT. The full enhanced model further improves recall to 47.69%, achieving an F1 score of 54.22% on cross-sentence relations, a remarkable 16.76% improvement over the baseline.

This analysis highlights a key limitation of the original BioBERT model that is not addressed in the work by Lee et al. (2019): the inability to effectively capture relations that span multiple sentences. Our approach specifically addresses this limitation through Longformer’s extended context window and knowledge base integration.

Error Analysis

To better understand the strengths and limitations of our approach, we conducted a detailed error analysis, categorizing errors into different types. Table 6 presents the distribution of errors for the BioBERT baseline and our enhanced model.

| Error Type | BioBERT | Enhanced | Reduction |
|--------------------------|-------------|------------|---------------|
| Distant relation errors | 387 | 193 | 50.13% |
| Implicit relation errors | 294 | 127 | 56.80% |
| Entity ambiguity errors | 155 | 139 | 10.32% |
| Negation errors | 104 | 91 | 12.50% |
| Knowledge gap errors | 86 | 71 | 17.44% |
| Total Errors | 1026 | 621 | 39.47% |

Table 6: Distribution of error types for BioBERT baseline and enhanced model on the test set, with percentage reduction in each error type.

Our error analysis reveals significant improvements across all error categories. Distant relation errors (where the chemical and disease are mentioned far apart in the text) are reduced by 50.13%, primarily due to Longformer’s ability to capture long-range dependencies. Implicit relation errors (where the relation is not explicitly stated but must be inferred) are reduced by 56.80% through knowledge base integration. Entity ambiguity errors, negation errors, and knowledge gap errors are also reduced, though to a lesser extent.

Overall, our enhanced model reduces the total number of errors by 39.47% compared to the BioBERT baseline. This comprehensive error analysis provides insights that were not available in the original BioBERT paper, which did not perform such detailed categorization of error types.

Discussion

Impact of Knowledge Integration

Our results indicate that the inclusion of structured domain knowledge from the CTD significantly improves relation extraction performance, particularly for implicit relations requiring biomedical expertise. The knowledge base provides informative information about known chemical-disease associations that are not necessarily textually explicit, allowing our model to capture relations lost with text-only approaches like the original BioBERT.

The ablation study shows that knowledge base integration contributes a 3.77% improvement in F1 score, primarily through increased recall. This finding extends the capabilities of BioBERT beyond what was demonstrated in the original paper by Lee et al. (2019), which relied solely on textual information learned during pre-training without explicit domain knowledge integration.

Advantages of Document-Level Processing

Longformer document processing exhibits notable benefit in document-level relation extraction, particularly in cross-sentence relations. With the window of context set from 512 tokens to 4,096 tokens, our model is capable of processing abstracts in one pass since it captures relations extending beyond sentence boundaries.

Cross-sentence relation analysis demonstrates that Longformer improves F1 score from 37.46% to 50.41% on these challenging cases, with a 12.95% absolute improvement. This is also lifted to 54.22% with our complete model. This capacity is crucial for the BioCreative V CDR dataset, in which roughly 30% of the relations have crossings of sentence boundaries. The base BioBERT model as introduced by Lee et al. (2019) was not rigorously evaluated on document-level relation extraction tasks with long-range dependencies, making our contribution unique.

Effectiveness of Recall Optimization

Our recall-enhancing techniques combined address the precision-recall trade-off in the default BioBERT model. Ablation analysis shows that our techniques provide an additional 7.03% increase in F1 score, the largest among all the gains. Specifically, focal loss leads the model to focus on difficult-to-classify positive samples, and dynamic thresholding optimizes the precision-recall trade-off.

The official test results confirm this progress, with a progress in recall from 38.01% for the BioBERT baseline to 51.20% on our enhanced model, with only a slight increase in precision from 66.49% to 68.70%. This more balanced performance is especially desirable for real-world usage where both recall and precision are important. The BioBERT paper never really emphasized optimizing recall for imbalanced relation extraction tasks as an objective goal, so this is yet another significant contribution of our work.

Comparison with Previous Work

Table 7 compares our results with previous work on the BioCreative V CDR dataset, including the original BioBERT results reported by Lee et al. (2019) for relation extraction on other datasets.

| System | Dataset | Precision | Recall | F1 Score |
|---------------------------|----------|-----------|--------|----------|
| Co-occurrence Baseline | BC V CDR | 16.43% | 76.45% | 27.05% |
| Best BioCreative V System | BC V CDR | 55.67% | 58.44% | 57.03% |
| BioBERT (Lee et al.) | CHEMPROT | 76.05% | 74.33% | 75.18% |
| BioBERT (Lee et al.) | GAD | 76.43% | 87.65% | 81.61% |
| BioBERT (Lee et al.) | EU-ADR | 78.04% | 93.86% | 84.44% |
| CNN Baseline (Ours) | BC V CDR | 51.80% | 48.33% | 50.01% |
| BioBERT Baseline (Ours) | BC V CDR | 66.49% | 38.01% | 48.37% |
| Enhanced Model (Ours) | BC V CDR | 68.70% | 51.20% | 58.70% |

Table 7: Comparison with previous work on the BioCreative V CDR dataset and BioBERT results on other relation extraction datasets.

Our enhanced model achieves competitive performance compared to the best BioCreative V system and outperforms our BioBERT baseline by a significant margin. Interestingly, our results show that while the original BioBERT achieves strong performance on protein-chemical relations (CHEMPROT) and gene-disease relations (GAD, EU-ADR) as reported by Lee et al., its performance on chemical-disease relations from the BioCreative V CDR dataset is considerably lower without our enhancements.

This comparison highlights the differences between relation types and the need for task-specific optimizations beyond the general-purpose BioBERT model. Chemical-disease relations in the CDR dataset appear to be more challenging than the relation types evaluated in the original BioBERT paper, requiring the additional enhancements we’ve developed.

Limitations and Future Work

Despite the significant improvements, our approach has several limitations that can be addressed in future work. Entity disambiguation remains difficult, with only a 10.32% reduction in entity ambiguity errors. More sophisticated entity disambiguation techniques, perhaps drawing on entity linking to knowledge bases, can further enhance performance. Negation handling is also an area where progress can still be made, with only a 12.50% reduction in negation errors.

Computation cost is yet another issue in that the Longformer-based one is more computation-costly compared to the standard BioBERT. Subsequent research might pursue better document-level computation processes, for instance, sparse attention or hierarchical models.

Both of our integration techniques utilize a static knowledge database. Subsequent work could test dynamic knowledge recollection based on the context and entities in view, or consume more than a single knowledge base apart from CTD.

While this effort has focused on chemical-disease relations, follow-up work could apply our enhanced model to other biomedical relation extraction tasks, such as those that were experimented on in the initial BioBERT paper, to determine if similar improvements arise from enhancement across relation types.

Conclusion

In this paper, we presented an enhanced transformer-based approach to chemical-disease relation extraction that addresses key limitations of the baseline BioBERT model on the BioCreative V CDR dataset. Our approach integrates structured domain knowledge from the CTD, employs Longformer for document-level processing, and exploits targeted recall optimization techniques.

Our experimental results show a significant advance of the BioBERT baseline with a 10.33% absolute F1 score improvement (from 48.37% to 58.70%) and a 13.19% recall improvement (from 38.01% to 51.20%). The detailed error analysis and ablation study provide sharp observations about the impact of each improvement and the limitations that still exist in biomedical relation extraction.

While the original BioBERT model of Lee et al. (2019) achieved great performance across a variety of biomedical text mining tasks, our work identifies and addresses specific challenges in chemical-disease relation extraction that were beyond the scope of their evaluation. By extending BioBERT with knowledge incorporation, document-level processing, and recall optimization, we push its capabilities to specialized relation extraction tasks requiring domain knowledge and cross-sentence inference.

The intersection of domain expertise and advanced transformer models is a promising direction for biomedical NLP, enabling the mining of more complex relationships from the scientific literature. It can be used to enhance numerous applications in biomedical research, drug development, and pharmacovigilance, as well as ultimately contribute to an enhanced understanding of disease mechanisms and potential treatments.

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