Improving Scholarly Knowledge Representation: Evaluating BERT-based Models for Scientific Relation Classification

Ming Jiang, Jennifer D’Souza, Sören Auer, and J. Stephen Downie

1 University of Illinois at Urbana Champaign, USA
2 TIB Leibniz Information Centre for Science and Technology and L3S Research Center at Leibniz University of Hannover, Hannover, Germany

{mjiang17|jdownie}@illinois.edu, {jennifer.dsouza|auer}@tib.eu

Abstract. With the rapidly growing number of research publications, there is a vast amount of scholarly information that needs to be organized in digital libraries. To deal with this challenge, digital libraries use semantic techniques to build knowledge-base structures for organizing scientific information. Identifying relations between scientific terms can help with the construction of a representative knowledge-based structure. While advanced automated techniques have been developed for relation extraction, many of these techniques were evaluated under different scenarios, which limits their comparability. To this end, this study presents a thorough empirical evaluation of eight BERT-based classification models by exploring two factors: 1) BERT model variants, and 2) classification strategies. To simulate real-world settings, we conduct our sentence-level assessment using the abstracts of scholarly publications in three corpora, two of which are distinct corpora and the third of which is the union of the first two. Our findings show that SciBERT models perform better than BERTBASE models. The strategy of classifying a single relation each time is preferred in the corpus consisting of abundant scientific relations, while the strategy of identifying multiple relations at one time is beneficial to the corpus with sparse relations. Our results offer recommendations to the stakeholders of digital libraries for selecting the appropriate technique to build a structured knowledge-based system for the ease of scholarly information organization.

Keywords: Digital library · Information extraction · Scholarly text mining · Semantic relation classification · Knowledge graphs · Neural machine learning.

1 Introduction

Today scientific endeavors are increasingly facing a publication deluge [27], which results in the rapid growth of scholarly publications needing to be accessible in digital libraries. While abundant resources have been provided for scholarly communication in digital libraries, it is still challenging for researchers to obtain comprehensive, fine-grained and context-sensitive scholarly knowledge for their research, especially for those who study a research problem that involves multiple disciplines [13]. According to [134], there are three main factors that lead to this issue. First, the set of
keywords used for indexing publication documents may not be able to cover all aspects of knowledge involved in each publication. Second, the traditional keyword search on document-based publications fails to consider the semantic associations among the pieces of scholarly information. Finally, the solely manual processing of unstructured scholarly knowledge does not scale to the number of publications, thus rendering a large part of the scholarly canon unused. To improve this problem, some initiatives advocate for combining human and machine intelligence to build an interlinked and semantically rich graph structure to organize the scholarly information in digital libraries.

A key aspect of building a knowledge graph for the scholarly record is identifying relations between scientific terms. In the natural language processing community, within the context of human-annotated datasets comprising abstracts of scholarly articles, seven relation types between scientific terms are being studied. They are HYPOnym-OF, PART-OF, USAGE, COMPARE, CONJUNCTION, FEATURE-OF, and RESULT. The annotations are in the form of the following generalized relation triples: ⟨experiment⟩COMPARE⟨another experiment⟩; ⟨method⟩USAGE⟨data⟩; ⟨method⟩USAGE⟨research task⟩. Since human language exhibits the phenomenon of paraphrasing where the same concept can be expressed in various ways, the direct identification of a particular relation between scientific terms is impractical—a problem addressed by a classification task. In the framework of an automated pipeline for generating knowledge graphs over massive volumes of scholarly records, scientific relation classification—the task reviewed in this paper—is therefore indispensable. The resulting task is recognizing which particular relation assertion between a pair of scientific terms in scholarly articles holds given a set of possible predefined relations.

In this age of the “deep learning tsunami”, to build automated scientific relation (SR) classification systems, one can combine various neural architectures to achieve high classification accuracy. And with the recent introduction of BERT word embedding models, the opportunity to obtain boosted machine learning systems is further accentuated. While prior studies of SR systems have demonstrated high classifier performances by tapping into these recent deep learning developments, the performances have been reported only on single evaluation scenarios, e.g., based on evaluating on a single dataset. Based on such lean evaluations of prior systems, it is, at present, difficult to obtain conclusive insights about the robustness of the classifiers in real-world diverse application settings: such as within scholarly digital library frameworks hosting diverse collections of articles. Moreover, existing evaluations are not identical between each other, since their evaluated datasets differ greatly; hence results are not comparable. Therefore we have no general insights into the best choice among the SR systems to recommend in practical settings—so far they all seem equally good.

In this work, we comprehensively surveyed eight deep learning techniques for scientific relation classification based on two different classification strategies and four BERT model variants. Further, we evaluated these systems on all available evaluation resources for the SR task including: a dataset of scholarly articles from the ACL anthology; a more diverse dataset of scholarly articles from various Artificial Intelligence conference proceedings; and a third resource that leveraged the two datasets combined, thereby offering a more realistic setting of unbalanced distribution of data domains and, further, offering robust training for classification models on annotations.
made by two different groups of annotators. Our ultimate goal is to help the stakeholders of digital libraries select the optimal tool to implement knowledge-based scientific information flows. In summary, we address the following research questions in this paper:

1. What is the impact of the eight classifiers on scientific relation classification?
2. Which of the seven relation types studied are easy or challenging for classification?
3. What is the practical relevance of the seven relation types in a scholarly knowledge graph?

2 Related Work

Relations Mined from Scientific Publications. Overall, knowledge is organized in digital libraries based on the following three aspects of the digital collections: 1) metadata, 2) free-form content, and 3) ontologized content [23,12]. In this context, the main categories of relations that have been explored for scholarly publications belong to two groups. One group includes metadata relations such as authorship, co-authorship, and citations [24,22]. Research in this group mainly focuses on examining the social dimension of scholarly communication such as co-author prediction [22] and scholarly community analysis [24]. The second group includes semantic relations, either as free-form semantic content classes [15,14] or as ontologized classes [21,19]. In the framework of automatic systems, content relations have been examined for: 1) scientific relation identification that involves determining which scientific term pairs are related [10,14], and 2) scientific relation classification that involves determining which relation type exists between related term pairs, where the relation types are typically pre-defined [26,6,16]. With respect to ontologized relation classes, prior work primarily considers the conceptual hierarchy based on formal concept analysis [21,19].

We attempt the task of classifying semantic relations that were created from free-form text. Given that the digital libraries are interested in the creation of linked data [11], our attempted task directly facilitates the creation of scholarly knowledge graphs [3], offering structured data for use by librarians to generate linked data.

Techniques Developed for Relation Classification. Both rule-based [1] and learning-based [7,28] methods have been developed for relation classification. Traditionally, learning-based systems relied on hand-crafted semantic and/or syntactic features [17]. In recent years, the success of deep learning techniques have nearly obviated the need to manually design features since they can more effectively learn latent feature representations for discriminating between relations. An attention-based bidirectional long short-term memory network (BiLSTM) [28] was one of the first top-performing systems that leveraged neural attention mechanisms to capture important information per sentence for relation classification. Another advanced system [17] leveraged a dynamic span graph framework based on BiLSTMs to simultaneously extract terms and infer their pairwise relations. Aside from these neural methods considering the word sequence order, transformer-based models [25] that use self-attention mechanisms to quantify the semantic association of each word to its context have become the current state-of-the-art in relation classification. E.g. BERT word embeddings [8]. It can be trained
to model data from any domain—the original BERT models were trained on books and Wikipedia. Now with the newly introduced SciBERT [6], there are BERT models trained on scholarly publications as well.

With respect to the classification strategy, the single-relation-at-a-time classification (SRC) that identifies the relation type for an entity pair each time are regularly adopted by prior work [28,17,6]. To improve the classification efficiency, [26] designed a BERT-based classifier that can recognize multiple pairwise relationships at one time, which can be regarded as a multiple-relations-at-a-time classification (MRC). Differing from prior work that emphasizes classification improvement, we focus on providing a fine-grained analysis of existing resources for selecting the proper tool to extract and organize scientific information in digital libraries.

3 Corpus

For our comprehensive evaluations, we select both the publicly available NLP datasets [10,16] annotated for the scientific relation classification task. These datasets contain a set of manually annotated scholarly abstracts for their scientific terms and the scientific relations between pairs of terms. Additionally, we combine the two datasets into a third new dataset, which offers a more realistic evaluation setting since it provides a larger, more diverse task representation. In the sequel, we describe our evaluation corpora.

C1: The SemEval18 Corpus. This corpus was created for the SemEval-2018 Task 7 [10] as a community-wide research initiative. It provided 500 manually annotated abstracts from scholarly articles in computational linguistics from the ACL Anthology. In the abstracts, originally, six discrete semantic relations were defined that were studied to capture the predominant information content. For our evaluation, we omit one of the six, viz. Topic, since it is not well-represented in the corpus, and simply consider the following five relations: Usage, Result, Model, Part Whole, and Comparison. In all, the dataset comprised 500 annotated abstracts partitioned into a training dataset

| Id | Relation | SemEval18 Total | SciER Total | Combined Total |
|----|----------|-----------------|-------------|---------------|
| 1  | USAGE: a scientific entity that is used for/by/on another scientific entity. E.g. MT system is applied to Japanese | 658 | 2.437 | 52.33% | 3,095 | 49.84% |
| 2  | FEATURE-OF: An entity is a characteristic or abstract model of another entity. E.g. computational complexity of unification | 392 | 25.10% | 526 | 9.77% |
| 3  | CONJUNCTION: Entities that are related in a lexical conjunction i.e., with ‘and’ or ‘or’. E.g. videos from Google Video and a NatGeo documentary | 582 | 12.52% | 582 | 9.37% |
| 4  | PART-OF: scientific entities that are in a part-whole relationship. E.g. describing the processing of utterances in a discourse | 304 | 19.46% | 573 | 9.23% |
| 5  | RESULT: An entity affects or yields a result. E.g. With only 12 training speakers for SI recognition we achieved a 7.5% word error rate | 92 | 5.89% | 546 | 8.99% |
| 6  | HYPERnym-OF: An entity whose semantic field is included within that of another entity. E.g. Image matching is a problem in Computer Vision | 409 | 8.80% | 409 | 6.59% |
| 7  | COMPARE: An entity is compared to another entity. E.g. conversation transcripts have features that differ significantly from neat texts | 116 | 7.43% | 349 | 5.62% |
| Overall | 1,562 | 100% | 4,648 | 100% | 6,210 | 100% |

Table 1: Overview of corpus statistics. ‘Total’ and ‘%’ columns show the number and percentage of instances annotated with the corresponding relation over all abstracts, respectively. Generated in the Open Research Knowledge Graph [3] https://www.orkg.org/orkg/c/SldTAX.
for machine learning containing 350 abstracts and a test dataset of 150 abstracts for evaluating the trained machine learning model.

**C2: The SciERC Corpus.** Our second evaluation corpus \[16\], also contains a set of 500 manually annotated abstracts of scholarly articles with their scientific terms and their pairwise relations. Unlike the SemEval18 corpus, the SciERC corpus represents diverse underlying data domains where the abstracts were taken from 12 AI conference/workshop proceedings in five research areas: artificial intelligence, natural language processing, speech, machine learning, and computer vision. These abstracts were annotated for the following seven relations: \texttt{COMPARE}, \texttt{PART-OF}, \texttt{CONJUNCTION}, \texttt{EVALUATE-FOR}, \texttt{FEATURE-OF}, \texttt{USED-FOR}, and \texttt{HYPONYM-OF}. And, for machine learning, the corpus was prepartitioned into a 350/50/100 train/dev/test split. Between the two corpora, except the \texttt{CONJUNCTION} and \texttt{HYPONYM-OF} relations, five of the defined relations are semantically identical.

**C3: The Combined Corpus.** To create this corpus, we merged \textit{C1} and \textit{C2}. This involved renaming relations. Specifically, \texttt{USED-FOR} in \textit{C2} which is semantically similar to \texttt{USAGE} in \textit{C1}, was renamed as \texttt{USAGE}. Further, based on our observations of the two corpora, for \texttt{RESULT} in \textit{C1} and \texttt{EVALUATE-FOR} in \textit{C2}, we found that the arguments of these relations were in reverse order. E.g. [accuracy] for [semantic classification] is labeled as “accuracy” \rightarrow \texttt{EVALUATE-FOR} \rightarrow “semantic classification” in \textit{C2}, which can be regarded as “semantic classification” \rightarrow \texttt{RESULT} \rightarrow “accuracy”. In this way, we renamed all instances annotated with relation \texttt{EVALUATE-FOR} in corpus \textit{C2} into \texttt{RESULT} by flipping their argument order. The two additional relations in \textit{C2}, i.e., \texttt{HYPONYM-OF} and \texttt{CONJUNCTION}, that were not in \textit{C1} were preserved as is. Thus, we created a third evaluation corpus of 1000 abstracts presenting a more realistic evaluation scenario of large and heterogeneous data.

In Table 1, we present corpus statistics for each of the evaluation corpora. Across all three, \texttt{USAGE} is the most predominant. Particularly pertinent in the context of the digital libraries are the columns ‘SemEval18’ and ‘SciERC’ in Table 1 that were generated from the Open Research Knowledge Graph \[3\]. The contributions in each scholarly article about the respective SemEval18 and SciERC datasets \[10,16\] are encoded via subject-predicate-object triples and were customized for comparability and merged in a single view. This customized comparison view of the scholarly knowledge graph of the two articles is persistently accessible \[3\] for all researchers to access or edit. While this customized graph with machine-actionable data from the scholarly article is not based upon the triples that are addressed in this work, the relations we study can be harnessed similarly.

### 4 BERT-based Scientific Relation Classifiers

BERT \[8\], Bidirectional Encoder Representations from Transformers, as a pretrained language representation built on cutting-edge neural technology, provides NLP practitioners with high-quality language features from text data simply out-of-the-box that
improves performance on many NLP tasks. These models return contextualized embeddings for tokens which can be directly employed as features for various NLP tasks. Further, with minimal task-specific extensions over the core BERT architecture, the embeddings can be relatively inexpensively fine-tuned to the task at hand, in turn facilitating even greater boosts in task performance.

In this work, for scientific relation classification, we employ BERT embeddings and we also fine-tune them within two different neural extensions: 1) for single-relation-at-a-time classification (SRC); and 2) for multiple-relation-at-a-time classification (MRC). In the remainder of the section, we first describe the BERT models we employ followed by the SRC and MRC classifiers that implement different classification objectives.

4.1 Pre-trained BERT Variants

BERT models as pretrained language representations are available in several variants depending on the model configuration parameters and on the underlying training data. While there are over 16 types, in this work we select the following four core variants.

**BERT\textsubscript{BASE}** The first two models we use are in the category of the pretrained BERT\textsubscript{BASE}. They were pretrained on billions of words from text data comprising the BooksCorpus (800M words) \footnote{https://github.com/google-research/bert} and English Wikipedia (2,500M words). The two models we select are: a cased model (where the case of the underlying words were preserved when training BERT\textsubscript{BASE}) and an uncased model (where the underlying words were all lowercased when training BERT\textsubscript{BASE}).

**SciBERT** The next two models employed in this study are in the category of the pretrained scientific BERT called SciBERT. They are language models based on BERT but trained on a large corpus of scientific text. Specifically, they are trained on a random sample of 1.14M papers from Semantic Scholar \footnote{https://github.com/allenai/scibert} consisting of full text of 18% papers from the computer science domain and 82% from the broad biomedical domain. Like BERT\textsubscript{BASE}, for SciBERT, we use its cased and uncased variants.

4.2 Fine-tuned BERT-based Classifiers

We implement the aforementioned BERT models within two neural system extensions that respectively adopt different classification strategies.

**Single-relation-at-a-time Classification (SRC)** Classification models built for SRC generally extend the core BERT architecture with one additional linear classification layer that has $K \times H$ dimensions, where $K$ is the number of labels and $H$ denotes the size of hidden states. The label probabilities are further normalized by using a softmax function and the classifier assigns the label with the maximum probability to the target.
Multiple-relations-at-a-time Classification (MRC)  This strategy is a more recent innovation on the classification problem in which the classifier can be trained with all the relation instances in a sentence at a time or predicts all the instances in one pass, as opposed to separately for each instance. In this case, however, the core BERT architecture’s self-attention mechanism is modified to efficiently consider representations of the relative positions of tokens that represent scientific terms [20,26]. While this modification enables encoding the novel multiple-relations-at-a-time problem, for obtaining the classification probabilities, the MRC is also extended with a linear classification layer, though not identical to the SRC since it has to model the modified architecture.

5 Evaluation

5.1 Experimental Setup

Experimental datasets, BERT word embeddings, and Classification strategies. Our comprehensive evaluation setup involved three different corpora, four BERT embedding variants, and two classification strategies. Given this, we trained a total of eight different classifiers, which for each of the three corpora resulted in 24 trained models. Each corpus was already prepartitioned three ways as training/dev/test by the original creators, which we adopt. To train optimal classifiers on the respective corpus, we tuned the learning rate parameter $\eta$ for values $\{2e^{-5}, 3e^{-5}, 5e^{-5}\}$.

Evaluation Metrics. We employ the standard machine learning classification evaluation indicators, i.e., Precision ($P$), Recall ($R$), F1-score ($F_1$), and Accuracy ($Acc$).

5.2 Results and Analysis

In this section, we present results from our comprehensive evaluations with respect to the three main research questions that undergird this study.

| SRC                  | MRC                  | Avg±Std             |
|----------------------|----------------------|---------------------|
|                      | SemEval18 | SciERC | Combined | SemEval18 | SciERC | Combined | SemEval18 | SciERC | Combined | SciEval18 | SciERC | Combined |
| Acc.     | F1       | Acc.     | F1       | Acc.     | F1       | Acc.     | F1       | Acc.     | F1       | Acc.     | F1       | Acc.     | F1       |
|----------------------|-----------|----------|----------|-----------|----------|-----------|----------|-----------|----------|-----------|----------|-----------|----------|
| Bert-base uncased    | 76.42     | 71.74    | 84.6     | 77.25     | 81.75    | 77.38     | 80.4     | 79.98     | 83.42    | 74.84     | 80.84    | 76.29     | 81.24    | 76.25±0.78|
| Bert-base cased      | 73.58     | 71.14    | 85.32    | 77.92     | 78.73    | 74.38     | 79.55    | 78.44     | 83.72    | 75.07     | 79.42    | 74.8      | 80.05±0.41| 75.29±0.65|
| SciBERT cased        | 73.58     | 69.72    | 86.86    | 79.65     | 84.46    | 81.60     | 80.11    | 78.32     | 83.42    | 74.35     | 81.80    | 77.68     | 81.71±0.40| 76.89±0.25|
| SciBERT uncased      | 80.97     | 79.42    | 86.14    | 79.49     | 83.11    | 80.27     | 81.82    | 80.54     | 84.33    | 77.44     | 81.06    | 76.76     | 82.91±0.04| 78.99±1.54|
| Avg. Scores          | Acc. 84.10| F1 80.22 | Acc. 82.55| F1 77.52  | Acc. 82.55| F1 77.52  | Acc. 82.55| F1 77.52  | Acc. 82.55| F1 77.52  | Acc. 82.55| F1 77.52  | Acc. 82.55| F1 77.52  |

Table 2: Scientific relation classification results over three datasets (SemEval18, SciERC, & Combined), four BERT model variants (BERT cased & uncased; SciBERT cased & uncased), and two classification strategies (SRC & MRC). Acc. is accuracy and $F_1$ is the macro $F_1$-score; Top scores are in bold; Scores in red from our surveyed systems are those that are on par with the state-of-the-art reported results [6,20] on SemEval18 and SciERC.
RQ1: What is the impact of the eight classifiers on scientific relation classification?

The eight classifiers are obtained from two classification strategies built over four BERT model variants. We examine their classification results (depicted in Table 2) in terms of the following three key characteristics of the classifiers.

The classification strategy, i.e., SRC vs. MRC. From the Acc and F1 shown in Table 2, we see that SRC outperforms MRC on two corpora except the SemEval18 corpus. One characteristic of the SemEval18 corpus is that it has significantly lower number of annotations than the other two corpora. Thus we infer that the novel MRC strategy is more robust than SRC because its performance level is unaffected by a drop in the number of the annotations.

Word embedding features, i.e., BERT vs. SciBERT. Regarding the BERT word embedding models, SciBERT outperformed BERT on all three corpora with higher accuracy and F1 scores. Since our experimental corpora are all scholarly data, as an expected result, word embeddings trained on the similar data domains are better suited.

Vocabulary case in BERT models, i.e., cased vs. uncased. We observe that the uncased BERT models (SciBERT: 82.91, BERT: 81.24) show higher classification accuracy than their cased counterpart (SciBERT: 81.71, BERT: 80.05) on average. Further, the uncased models have a lower standard deviation in accuracy overall (SciBERT: 2.04, BERT: 2.84) than the cased models (SciBERT: 4.60, BERT: 4.14); comparisons on F1 are along similar lines. Hence, our results suggest that uncased BERT models can achieve more stable performances than cased variants.

In conclusion, with respect to the classification strategy, we find SRC outperforms MRC (see averaged scores in the last row in Table 2). Nevertheless, the advanced MRC strategy demonstrates consistently robust performance that remains relatively unaffected by smaller dataset sizes compared to the SRC (e.g. SRC vs. MRC results on the SemEval18 corpus). On the other hand, with respect to BERT word embedding variants, from the averaged scores in the last column in Table 2 the SciBERT uncased model posits as the optimal word embedding features model on scholarly articles.

RQ2: Which of the seven relation types studied are easy/challenging to classify?

Examining the fine-grained per-relation classification results in Tables 3 to 5 across all our evaluation corpora for both SRC and MRC, we note the classification ranked

| Relationship Type  | SRC       | MRC       |
|--------------------|-----------|-----------|
|                    | P        | R | F1 | P | R | F1 |
| USAGE              | 87.22    | 89.71 | 88.45 | 90.53 | 87.43 | 88.95 |
| RESULT             | 78.26    | 90.00 | 83.72 | **100.00** | 75.00 | 85.71 |
| COMPARE            | 85.71    | 85.71 | 85.71 | 75.00 | 85.71 | 80.00 |
| MODEL-FEATURE      | 66.67    | 75.76 | 70.92 | 70.83 | 77.27 | 73.91 |
| PART-WHOLE         | 79.25    | 60.00 | 68.29 | 70.83 | 72.86 | 71.83 |

Table 3: Per-relation classification scores of SRC and MRC best systems on SemEval18.
Table 4: Per-relation classification results of SRC and MRC best systems on SciERC.

| Relationship Type | SciERC       |          |           |          |          |          |          |          |          |
|-------------------|--------------|----------|----------|----------|----------|----------|----------|----------|----------|
|                   | SRC          | MRC      | SRC      |          | MRC      |          | SRC      |          | MRC      |
|                   | P  | R  | F1 | P  | R  | F1 | P  | R  | F1 | P  | R  | F1 |
| Used-For          | 93.30 | 91.37 | 92.32 | 88.75 | 90.24 | 89.49 | 88.75 | 90.24 | 89.49 |        |        |    |
| Conjunction       | 87.97 | 95.12 | 91.41 | 80.69 | 95.12 | 87.31 | 80.69 | 95.12 | 87.31 |        |        |    |
| Hyponym-Of        | 92.31 | 89.55 | 90.91 | 80.00 | 82.93 | 81.44 | 80.00 | 82.93 | 81.44 |        |        |    |
| Evaluate-For      | 82.29 | 86.81 | 84.49 | 84.44 | 83.52 | 83.98 | 84.44 | 83.52 | 83.98 |        |        |    |
| Compare           | 72.73 | 84.21 | 78.05 | 83.87 | 68.42 | 75.36 | 83.87 | 68.42 | 75.36 |        |        |    |
| Part-Of           | 66.04 | 55.56 | 60.34 | 65.52 | 60.32 | 62.81 | 65.52 | 60.32 | 62.81 |        |        |    |
| Feature-Of        | 59.02 | 61.02 | 60.00 | 73.68 | 47.46 | 57.73 | 73.68 | 47.46 | 57.73 |        |        |    |

Table 5: Per-relation classification results of the best SRC and MRC systems on the Combined corpus.

| Relationship Type | Combined     |          |           |          |          |          |          |          |          |
|-------------------|--------------|----------|----------|----------|----------|----------|----------|----------|----------|
|                   | SRC          | MRC      | SRC      |          | MRC      |          | SRC      |          | MRC      |
|                   | P  | R  | F1 | P  | R  | F1 | P  | R  | F1 | P  | R  | F1 | P  | R  | F1 |
| Conjunction       | 92.56 | 91.06 | 91.80 | 85.07 | 92.68 | 88.72 | 85.07 | 92.68 | 88.72 |        |        |    |
| Usage             | 91.30 | 88.98 | 90.13 | 87.96 | 87.71 | 87.84 | 87.96 | 87.71 | 87.84 |        |        |    |
| Hyponym-Of        | 89.39 | 88.06 | 88.72 | 83.12 | 78.05 | 80.50 | 83.12 | 78.05 | 80.50 |        |        |    |
| Compare           | 86.89 | 89.83 | 88.33 | 73.85 | 81.36 | 77.41 | 73.85 | 81.36 | 77.41 |        |        |    |
| Result            | 76.36 | 75.68 | 76.02 | 84.69 | 74.77 | 79.43 | 84.69 | 74.77 | 79.43 |        |        |    |
| Part-Of           | 75.86 | 66.17 | 70.68 | 68.33 | 61.65 | 64.82 | 68.33 | 61.65 | 64.82 |        |        |    |
| Feature-Of        | 58.02 | 75.20 | 65.51 | 60.28 | 68.00 | 63.91 | 60.28 | 68.00 | 63.91 |        |        |    |

order. Of all relations, Usage (Used-For) is the easiest classification target, since in all three tables, it is in the two topmost. Usage is the most predominant type in all corpora. This accounts, in part, for its high-scored classification, since the classifiers are trained on a significant number of training instances for Usage compared to the rest.

For the challenging relations, we examine the results per corpus. Starting with the Table 4 results for the SemEval18 corpus, we observe that both SRC and MRC find Part-Whole most challenging to classify. We surmise that this relation displays high diversity in the underlying natural language text from which it is induced; hence the classifier is unable to generalize a consistent set of patterns for it. Observing classification performance ranks, for three of the five relations (i.e., Usage, Model-Feature and Part-Whole), SRC and MRC obtain the same classification rank order. For Result and Compare, they are opposites, where SRC classifies Result better than MRC.

In Table 5 results for SciERC, both classifiers perform significantly low on two relations, viz. Feature-Of and Part-Of. Since these two relations are not the most underrepresented in the corpus, we theorize that their low classification performance is owed to the natural language text diversity from which they are deduced. In this case, obtaining more annotated instances is one way to boost classifier performance. In terms
of the ranked order of performances on the relations, SRC and MRC perform identically on SciERC data.

And lastly in Table 5 results on the Combined corpus, for the challenging relations, both SRC and MRC have the same result as they did on SciERC—i.e., FEATURE-OF followed by PART-OF are the most challenging. And we theorize the same reason for the low scores on these relations, since Combined contains SciERC data. Given the two corpora in the Combined dataset, SciERC additionally introduced CONJUNCTION which SemEval18 did not have. CONJUNCTION is among the top two easiest relations to classify, with USAGE as the other, for the classifiers trained on SciERC and on the Combined corpus. Further, its classification is better in the Combined corpus than in SciERC. This lends an understanding to the realistic evaluation settings that the Combined corpus presents. To elaborate, for USAGE, instances from SemEval18 and SciERC (i.e. USED-FOR) are combined, resulting in an insignificant dip in performance (on the Combined corpus, USAGE ranks second easiest compared with SemEval18 and SciERC) since they are now non-uniform annotation signals. As opposed to the case of CONJUNCTION, the Combined corpus obtains a uniform annotation signal from just the SciERC corpus and ranks a minor degree higher at classifying it.

Finally, a list summarizing the top-scoring per-relation performances for scientific relation classification across all three tables, includes the following: USAGE (SRC in SciERC), CONJUNCTION (SRC in Combined), HYPONYM-OF (SRC in SciERC), RESULT (MRC in SemEval18), PART-OF (MRC in SemEval18 for PART-WHOLE), and FEATURE-OF (MRC in SemEval18 for MODEL-FEATURE). Since the SemEval18 corpus appears the most times in the top-ranked results, we conclude that its annotations obtain a relatively better trained classifier. However, the SemEval18 corpus only includes scholarly abstracts from one AI domain i.e. NLP (in the ACL Anthology), whereas SciERC is more comprehensively inclusive across various AI domains. Thus, an additional factor that classifiers trained on SciERC handle is domain diversity.

Error Analysis A closer look at the misclassifications is portrayed in the confusion matrices in Figure 1 for the SRC and MRC strategies on the Combined corpus. Four of the seven relations, i.e. HYPONOMY-OF, RESULT, PART-OF, and FEATURE-OF, are highly likely to be misclassified as USAGE. This shows that our classifiers are biased by
The predominant USAGE relation. In general, unbalanced distribution of training samples (see the details in the corpus section) is, more often than not, one of the main factors for confusion learned in machine learning systems. For the most challenging relations FEATURE-OF and PART-OF, after USAGE, are highly likely to be confused with each other (FEATURE-OF as PART-OF (~10% confusion), and vice-versa (~9.4% confusion)). For the relations HYPONYM-OF and FEATURE-OF that loosely demonstrate a relation hierarchy such that HYPONYM-OF subsumes FEATURE-OF, but not the other way around, we find the classification confusion demonstrates a consistent pattern to this data. From the matrices, we see that HYPONYM-OF has ~6% likelihood to be predicted as FEATURE-OF, but none of the FEATURE-OF (0%) instances were confused with HYPONYM-OF.

To offer another pertinent angle on the classifier error analysis, we compute the word distance distributions between related scientific term pairs in the Combined corpus. This data is depicted in Figure 2. In general, most box plots shown in the figure are skewed with a long upper whisker and a short lower whisker, which indicates that the majority of paired scientific terms are close in the text. Specifically, the scientific term pairs in the CONJUNCTION relation, which in linguistic terms should necessarily be close. This consistent pattern could be another reason why CONJUNCTION is among the easiest relations to classify. Further, the average word distance of FEATURE-OF, PART-OF, HYPONYM-OF, and COMPARE is closer to the lower quartile than the other relations. Such varied distribution may bring challenges for a classifier to identify these relations. Notably, the similar median value and spread range between FEATURE-OF and PART-OF could account for why they are challenging to classify.

Finally, we examine the third research question that undergirded this study.

**RQ3: What is the practical relevance of the seven relations studied in this paper in a scholarly knowledge graph?** As a practical illustration of the relation triples studied in this work, we build a knowledge graph from their annotations in the 1000 scholarly abstracts in the Combined dataset. This is depicted in Figure 3. Looking at the corpus-level graph (the right graph), we observe that generic scientific terms such as “method,” “approach,” and “system” are the most densely connected nodes, as expected since generic terms are found across research areas. In the zoomed-in ego-network of the term “machine_translation” (the left graph), HYPONYM-OF is meaningfully highlighted by its role linking “machine_translation” and its sibling nodes as the
research tasks “speech_recognition,” and “natural_language_generation” to the parent node “NLP_problems.” The term “lexicon” is related by USAGE to “machine_translation” and “operational_foreign_language.” The CONJUNCTION link joins “machine_translation” and “speech_recognition” both aim at translating information from one source to the other one. This knowledge graph now enables various property comparisons across 1000 scholarly abstracts (consider the corpus statistics Table 1 generated from the Open Research Knowledge Graph presented in the corpus section).

6 Conclusions and Recommendations

We have investigated the scientific relation classification task for improving scholarly knowledge representations in digital libraries. Our surveyed systems offer a comprehensive view of results that are attainable given advanced neural technology when put together in varying combinations, including the ones that produce the state-of-the-art results. We have categorized neural technology in terms of four BERT-based embedding models and two classification strategies. Our results indicate that, of the various word embedding models, SCIBERT is the optimal choice for a corpus of scholarly data. In terms of classification strategies, the single-relation-at-a-time system outperforms the multiple-relations-at-a-time classification system. Nevertheless, the latter is robust over all datasets, even in settings with lean annotated data, in which case it outperforms the former. Our findings are obtained over a broad scenario of model performances for scientific relation classification now available to the stakeholders of the digital libraries.

7 Future Work

To further facilitate the choice of the proper technique for classifying scientific relations toward the creation of structured, semantic representations over scholarly articles,
there are two main avenues that are worthwhile for future exploration. As we have seen in the course of examining our RQ2, there exist label biases in the annotated corpora such that some relations are better represented than others (e.g. USAGE). Toward this end, such data needs to be further curated by experts to enable a well-represented domain. Further, digital libraries deal with various domains in Science in general. While our evaluations have been performed on corpus that covers the Artificial Intelligence research area, there still remains a plenty of potentials to explore other research domains that are unrelated to Computer Science specifically. Finally, we have examined scientific relation classification in terms of seven relations, ontologized models of the scientific world [9,19] posit a larger set of relations or properties. For this, techniques such as open information extraction or ontology-based extraction are viable alternatives for future developments.

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