Combining Long Short Term Memory and Convolutional Neural Network for Cross-Sentence n-ary Relation Extraction

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Abstract
We propose in this paper a combined model of Long Short Term Memory and Convolutional Neural Networks (LSTM,CNN) that exploits word embeddings and positional embeddings for cross-sentence n-ary relation extraction. The proposed model brings together the properties of both LSTMs and CNNs, to simultaneously exploit long-range sequential information and capture most informative features, essential for cross-sentence n-ary relation extraction. The LSTM,CNN model is evaluated on standard dataset on cross-sentence n-ary relation extraction, where it significantly outperforms baselines such as CNNs, LSTMs and also a combined CNN,LSTM model. The paper also shows that the LSTM,CNN model outperforms the current state-of-the-art methods on cross-sentence n-ary relation extraction.

Introduction
Research in the field of relation extraction has largely focused on identifying binary relations that exist between two entities in a single sentence, known as intra-sentence relation extraction (Bach and Badaskar 2007). However, relations can exist between more than two entities that appear across consecutive sentences. For example, in the text span comprising the two consecutive sentences in Listing 1, there exists a ternary relation response across three entities: EGFR, L858E, gefitinib appearing across sentences. This relation extraction task, focusing on identifying relations between more than two entities – either appearing in a single sentence or across sentences, is known as cross-sentence n-ary relation extraction.

Listing 1: Text span of two consecutive sentences

“The deletion mutation on exon-19 of EGFR gene was present in 16 patients, while the L858E point mutation on exon-21 was noted in 10. All patients were treated with gefitinib and showed a partial response.”

This paper focuses on the cross-sentence n-ary relation extraction task. Formally, let \( \{e_1, \ldots, e_n\} \) be the set of entities in a text span \( S \) containing \( t \) number of consecutive sentences. For example, in the text span comprising 2 sentences \( (t = 2) \) in Listing 1 above, given cancer patients with mutation \( v \) (EGFR) in gene \( g \) (L858E), the patients showed a partial response to drug \( d \) (gefitinib). Thus, a ternary relation response\((EGFR, L858E, gefitinib)\) exists among the three entities spanning across the two sentences in Listing 1.

The entities \( e_1, \ldots, e_n \) in the text span can either appear in a single sentence \( (t = 1) \) or multiple sentences \( (t > 1) \). Thus, given an instance defined as a combined sequence of \( m \) tokens \( x = x_1, x_2, \ldots, x_m \) in \( t \) consecutive sentences and a set of entities \( \{e_1, \ldots, e_n\} \), the cross-sentence n-ary relation extraction task is to predict an n-ary relation (if exists) among the entities in \( x \).

Cross-sentence n-ary relation extraction is particularly challenging compared to intra-sentence relation extraction for several reasons. Lexico-syntactic pattern-based relation extraction methods (Hearst 1992; Brin 1998; Agichtein and Gravano 2000), have shown to be highly effective for intra-sentence relation extraction. Unfortunately, such pattern-based relation extraction methods cannot be readily applied to cross-sentence n-ary relation extraction because it is difficult to match lexico-syntactic patterns across longer text spans such as covering multiple sentences. Features extracted from the dependency parse trees for individual sentences (Culotta and Sorensen 2004; Bunescu and Mooney 2005; Fundel, Küffner, and Zimmer 2006; Xu et al. 2015; Miwa and Bansal 2016) have found to be extremely useful for intra-sentence relation extraction. However, it is non-obvious as how to merge dependency parse trees from different sentences to extract path-based features for cross-sentence relation extraction. Moreover, difficulties in coreference resolution and discourse analysis, further complicate the problem of detecting relations among entities across sentences (Elango 2005).

The principal challenges for cross-sentence n-ary relation extraction arise from (a) difficulties in handling long-range sequences resulting from combining multiple sentences, (b) modeling the contexts of words related to different entities present in different sentences, and (c) the problem of representing a variable-length text span containing an n-ary relation using a fixed-length representation. To address these issues, we propose a combined model consisting a Long Short-Term Memory unit and a Convolutional Neural Network (LSTM,CNN) that exploits both word embedding and positional embedding features for cross-sentence n-ary relation extraction. The LSTM is used as the first layer to encode the combined set of sentences representing an n-ary relation, thereby capturing the long-range sequential information. The hidden state representations obtained from the LSTM is then used with the CNN to further identify the salient
features for relation classification. Our main contributions in this paper can be summarised as follows:

a. Propose an LSTM\_CNN model that exploits word embedding and position embedding features for cross-sentence n-ary relation extraction. We compare the proposed model against multiple baselines such as CNN, LSTM and a combined CNN\_LSTM model. Experimental results show that the proposed model significantly outperforms all baselines.

b. Evaluate the proposed model against state-of-the-art (SOTA) for cross-sentence n-ary relation extraction on two different benchmark datasets. Results show that the proposed model significantly outperforms the current SOTA methods for cross-sentence n-ary relation extraction.

**Related Work**

There is a large body of research on intra-sentence relation extraction (Bach and Badaskar 2007). However, our main focus in this paper is on cross-sentence relation extraction. Therefore, we will limit our discussion below to the cross-sentence relation extraction. Research on cross-sentence relation extraction has extensively used features drawn from dependency trees (Swampillai and Stevenson 2010 [Quirk and Poon 2016] [Peng et al. 2017]), tree kernels (Moschitti, Patwardhan, and Welty 2013 [Nagesh 2016]), and graph LSTMs (Peng et al. 2017). Further, studies on inter-sentence relation extraction have limited their attention on extracting binary relations present across sentences (Swampillai and Stevenson 2010 [Quirk and Poon 2016] Moschitti, Patwardhan, and Welty 2013 [Nagesh 2016]). Recently, Peng et al. (2017) proposed graph-LSTMs not only to consider binary relations, but also for n-ary relations across sentences. Although graph LSTMs are useful to model n-ary relations across sentences, the process of creating directed acyclic graphs covering words in multiple sentences is complex and error-prone. It is non-obvious as where to connect two parse trees and the parse errors compound during the graph creation step. Moreover, co-reference resolution and discourse features used by Peng et al. (2017) do not always improve performance of cross-sentence relation extraction.

We present a neural network-based approach that does not rely on heavy syntactic features such as dependency trees, co-reference resolution or discourse features for cross-sentence n-ary relation extraction. Although, previous studies have explored LSTMs and CNNs separately for cross-sentence n-ary relation extraction, we propose in this paper, a combined model of lstm\_cnn network that simply takes as input the combined sequence of sentences containing n-ary relations. While, LSTMs generate features that preserve long-range relations among words in the combined sequence of sentences, CNNs can generate different weighted combinations of those features and select the most informative ones via pooling. Although recently several studies have explored combining CNNs and RNNs for various NLP tasks such as text classification (Lai et al. 2015 Lee and Dernoncourt 2016 Hsu et al. 2017) and sentiment analysis (Wang, Jiang, and Luo 2016), to the best of our knowledge, we are the first to propose a combined LSTM\_CNN model for cross-sentence n-ary relation extraction.

**Cross-Sentence n-ary Relation Extraction**

The architecture of the proposed LSTM\_CNN+WF+PF model - combined LSTM\_CNN using word features (WF) and positional features (PF) for cross-sentence n-ary relation extraction is shown in Figure 1. Next, we describe the different components of the proposed model.

**Input Representation**

The input to the lstm\_cnn model is the combined sequence of tokens in a text span $S$ comprising $t$ consecutive sentences where an $n$-ary relation exists between two entities. The sequence of tokens is transformed into a combination of word embeddings and position embeddings as follows:

**Word Embeddings** The transformation of words into lower dimensional vectors are observed to be useful in capturing semantic and syntactic information about words (Mikolov et al. 2013 Pennington, Socher, and Manning 2014). Thus, each of the words in the combined sequence $x = x_1, x_2, \ldots, x_n$ is mapped to a $k$-dimensional embedding vector using a look-up matrix $W \in \mathbb{R}^{V \times k}$ where $|V|$ is the number of unique words in the vocabulary.

![Figure 1: Architecture of the LSTM\_CNN+WF+PF model for cross-sentence n-ary relation extraction. The input to the network is the sequence of tokens from text span (with two sentences and three entities) shown in LISTING 1. The position features are derived for highlighted entities ($e_1$ and $e_3$).](image-url)
Position Features Following [Zeng et al. 2014], positional features (PFSs) are used to encode the position of entities for n-ary cross-sentence relation extraction. Given entity mentions $e_1, ..., e_n$ in the sequence $x = x_1, x_2, ..., x_n$, although n PFSs can be defined based on n-entities, the proposed model, specifically considers only $e_1$ and $e_n$, to create position embeddings for the input sequence because preliminary experiments show that having n PFSs decreases the performance of the model. Thus, the model defines two sets of PFSs $PF_1$ and $PF_n$ for the entities $e_1$ and $e_n$, respectively, by the input gate and combining word embeddings and position features is an excellent choice to learn long-range dependencies. Thus, as a set of sentences expressing an n-ary relation, the model maintains a separate memory cell that updates and exposes the content only when deemed necessary. Given the content $S$ which exposes the content only when deemed necessary.

LSTM Layer

Although RNNs are useful in learning from sequential data, these networks are observed to suffer from the problem of exploding or vanishing gradient, which makes it difficult for RNNs to learn long distance correlations in a sequence (Hochreiter and Schmidhuber 1997; Hochreiter et al. 2001). To specifically address this issue of learning long-range dependencies, LSTM (Hochreiter et al. 2001) was proposed which maintains a separate memory cell that updates and exposes the content only when deemed necessary. The current memory cell $h_t$ is defined as a collection of vectors in $\mathbb{R}^{d_h}$, an output gate $o_t$, a hidden state $h_t$, a forget gate $f_t$, an input gate $i_t$, a memory cell $c_t$, and a hidden state $h_t$. $l$ is the number of LSTM units in the sequence of length $m$. The LSTM units at each time step $t$ is defined as a collection of vectors in $\mathbb{R}^d$ and comprises the following components: an input gate $i_t$, a forget gate $f_t$, an output gate $o_t$, a memory cell $c_t$, and a hidden state $h_t$. $l$ is the number of LSTM units and the entries of the gating vectors $i_t$, $f_t$, and $o_t$ are in $[0, 1]$. The three adaptive gates $i_t$, $f_t$, and $o_t$ depend on the previous state $h_{t-1}$ and the current input $x_t$ (Equations 1-3). The candidate update vector $g_t$ (Equation 4) is also computed for the memory cell.

$$i_t = \sigma(W_i x_t + U_i h_{t-1} + b_i) \quad (1)$$
$$f_t = \sigma(W_f x_t + U_f h_{t-1} + b_f) \quad (2)$$
$$o_t = \sigma(W_o x_t + U_o h_{t-1} + b_o) \quad (3)$$
$$g_t = \tanh(W_g x_t + U_g h_{t-1} + b_g) \quad (4)$$

The current memory cell $c_t$ is a combination of the previous cell content $c_{t-1}$ and the candidate content $g_t$, weighted respectively by the input gate $i_t$ and forget gate $f_t$ (Equation 5).

$$c_t = i_t \odot g_t + f_t \odot c_{t-1} \quad (5)$$

The hidden state $h_t$, which is the output of the LSTM units is computed using the following equation:

$$h_t = o_t \odot \tanh(c_t) \quad (6)$$

Here $\sigma$ denotes a sigmoid function and $\odot$ denotes element-wise multiplication.

CNN Layer

Let $h_i \in \mathbb{R}^{d_h}$ be the l-dimensional hidden state vector corresponding to the $i$-th token in the combined sequence $x$. The combined hidden state vectors in the sequence of length $m$ is represented as:

$$h_{1:m} = h_1 \oplus h_2 \oplus ... \oplus h_m, \quad (7)$$

where $\oplus$ denotes vector concatenation. In general, let $h_{i:i+j}$ refer to the concatenation of hidden state vectors $h_i, h_{i+1}, ..., h_{i+j}$. The convolution operation involves a filter $w \in \mathbb{R}^{p \times d_h}$, which is applied to a window of $p$ hidden state vectors to generate a new feature. For instance, a feature $c_i$ is generated from a window of hidden state vectors $h_{i:i+p-1}$.

$$c_i = f(w \cdot h_{i:i+p-1} + b). \quad (8)$$

Here $b \in \mathbb{R}$ is the bias term and $f$ is a non-linear function such as the rectified linear unit (ReLU). This filter is applied to each possible window of hidden state vectors in the combined sequence $h_{1:p}, h_{2:p+1}, ..., h_{m-p+1}$ to produce a feature map $c \in \mathbb{R}^{m-p+1}$ given by,

$$c = [c_1, c_2, ..., c_{m-p+1}]. \quad (9)$$

Max-pooling is applied over the feature map to take the maximum value $\hat{c} = \max\{c\}$ as the feature corresponding to this particular filter. The use multiple filters and select the most important feature (one with the highest value) for each feature map. Finally, the use of multiple filters with varying window sizes result in obtaining a fixed length vector $g \in \mathbb{R}^{fw}$, where $f$ is the number of filters and $w$ is the number of different window sizes.

Predicting n-ary Relations

The task of predicting n-ary relations is modeled both as a binary and multi-classification problem. The output feature vector $g$ obtained from the convolution and max-pooling operation is passed to softmax layer, to obtain the probability distribution over relation labels. Dropout (Srivastava et al. 2014) is used on the output layer to prevent over-fitting. Thus, given a set of instances, with each instance being a text span $S_i$ comprising $t$ consecutive sentences (combined sequence of tokens $x = x_1, x_2, ..., x_m$), entity mentions $e_1, ..., e_n$ and having an n-ary relation $r$, the cross-entropy loss for this prediction is defined as follows:

$$J(\theta) = \sum_{i=1}^{s} \log p(r_i | S_i, \theta) \quad (10)$$

where $s$ indicates the total number of text spans and $\theta$ indicates the parameters of the model.
Implementation details

The proposed model is implemented using Tensorflow (Abadi et al. 2016) and will be made publicly available upon paper acceptance. The hyper-parameters of the models were set based on preliminary experiments on an independent development dataset. Training was performed following minibatch gradient descent (SGD) with batch size of 10. The models were trained for at most 30 epochs, which was sufficient to converge. The dimensions of the hidden vectors for the LSTM was set to 300. The window sizes for CNN was set to 3, 4 and 5, and experiments were conducted with different number of filters set to 10 and 128. Word embeddings were initialised using publicly available 300-dimensional Glove word vectors trained on a 6 billion token corpus from Wikipedia and web text (Pennington, Socher, and Manning 2014). The dimensions for position embeddings was set to 100 and were initialised randomly between [-0.25, 0.25].

Experiments

Datasets

We conduct experiments using the following datasets.

Quirk and Poon (QP) Dataset We use the dataset developed by Quirk and Poon (2016) and Peng et al. (2017) for the task of cross-sentence n-ary relation extraction. Distinct supervision was followed to extract relations involving drug, gene and mutation triples from the biomedical literature available in PubMed Central. The idea of minimal span (Quirk and Poon 2016) was used to avoid co-occurrence of the same entity triples and also to obtain spans with ≤ 3 consecutive sentences to avoid candidates where triples are far apart in the span. A total of 59 drug-gene-mutation triples was used to obtain 3,462 ternary relation instances and 3,192 binary relation instances (involving drug-mutation entities) as positive examples. The dataset has instances with ternary and binary relations, either appearing in a single sentence or across sentences. Each instance is labeled using four labels: ‘resistance’, ‘resistance or non-response’, ‘response’, and ‘sensitivity’. The label ‘none’ is used for negative instances. Negative samples were generated by randomly sampling co-occurring entity triples without known interactions, following the same restrictions used for obtaining positive samples. Negative examples were sampled as the same number of positive samples to develop a balanced dataset.

Chemical Induced Disease (CID) Dataset We also evaluate the proposed model using the CID dataset, which provides binary relation instances between chemicals and related diseases. We followed the methodology of Gu, Qian, and Zhou (2016) to obtain relation instances from the corpus. Accordingly, a total of 1206, 1999 and 1330 positive instances were obtained for binary relations in single sentences and total of 702, 788 and 786 positive instances were binary relations across sentences, respectively. Negative instances were created following the same restrictions, however without any known interactions between entities.

Baselines

We conduct experiments using the following baselines:

(a) CNN: a CNN model using word features alone;
(b) CNN+WF: a CNN model using word features and positional features;
(c) LSTM+WF: an LSTM model using word features alone;
(d) LSTM+WF+PF: an LSTM model using word features and positional features;
(e) CNN+WF+PF: a model that begins with a CNN layer followed by an LSTM layer and uses word features only;
(f) CNN+LSTM+WF+PF: a model that begins with a CNN layer followed by an LSTM layer and employs word features and position features;
(g) LSTM+CNN+WF+PF: a model that begins with an LSTM layer followed by a CNN layer and employs word features only.

Results and Discussion

Performance of the proposed model. The performance of the proposed model LSTM+CNN+WF+PF for cross-sentence n-ary relation extraction on Q&P DATASET is shown in Tables 1 and 2. As seen in Tables 1 and 2 the LSTM+CNN+WF+PF model achieves statistically significant accuracy ($p \leq 0.05$; Friedman Test) against all baseline models such as CNN+WF, CNN+WF+PF, LSTM+WF, LSTM+WF+PF, CNN+LSTM+WF, CNN+LSTM+WF+PF and LSTM+CNN+WF, for both cross-sentence ternary and binary relation extraction. The results showing the performance of the combined LSTM+CNN model higher than CNN and LSTM models in isolation, indicates the usefulness of such combined models for relation extraction. Combining LSTM and

SemEval-2010 Task 8 (SE) Dataset. The SemEval-2010 Task 8 dataset (Hendrickx et al. 2009) is a standard dataset used intra-sentence relation extraction. The SE DATASET defines 9 relation types between nominals. The relation ‘other’ is used to denote negative type. The dataset consists of 8,000 training and 2,717 test sentences.

Evaluation Metrics

We conduct five-fold cross-validation and report average test accuracy on held-out folds experiments using Q&P DATASET, as prior work (Peng et al. 2017) follow similar evaluation measures. To avoid training and test contamination, held-out evaluation is conducted in each fold, based on categorizing instances related to specific entity pairs (binary relations) or entity triples (ternary relations). For example, for binary relations, the instances relating to the first 70% of the entity pairs drawn from a unique list of entity pairs are used as training set. Instances relating to the next 10% and last 20% are used as development set and test set, respectively. For CID DATASET, the Precision, Recall and F-score on test set is reported, since the corpus is already divided in train, development and test set and also for comparison as previous studies (Gu, Qian, and Zhou 2016) have used similar measures for reporting the performance. For SE DATASET, we used 10% of randomly selected instances from the training set as the development set. To evaluate the test set, the official task setting (Hendrickx et al. 2009) was followed and we report the official macro-averaged F1-Score on the 9 relation types.
CNN helps in bringing together the strength of LSTMs to learn from long sequences (input sequence) and the ability of CNNs to identify salient features from the hidden-state output sequence from LSTM for cross-sentence n-ary relation extraction.

Given the above results, it is highly intriguing that a combined model of LSTM and CNN using together word features (WF) and positional features (PF), outperforms the evaluated strong baselines. Interestingly, the use of WF alone already helps the combined model (LSTM_CNN) in achieving higher performance against other baselines, particularly for extracting binary relations in single sentences and across sentences, and also ternary relations in single sentences (Tables 1 and 2 with \( n_f = 128 \)). However, it is the addition of PF that helps in drastically improving the performance for relation extraction. The PF clearly helps the combined LSTM_CNN model by providing useful encoding of the position of words \( w.r.t \) entities in the text span, which helps in achieving higher accuracy.

Further, the higher performance achieved in extracting both ternary and binary relations, particularly from cross-sentence text spans which are longer in sequence, indicates that the LSTM_CNN+WF+PF model is highly suitable for extracting relations from longer sequences. Furthermore, the LSTM_CNN+WF+PF model’s superior performance extracting ternary and binary relations from single sentences also indicates the suitability of the LSTM_CNN+WF+PF model for relation extraction in single sentences. The evaluation results of the LSTM_CNN+WF+PF on Semeval-2010 Task 8 dataset (standard dataset for intra-sentence relation extraction) presented later in this section, further confirms that the combined model (LSTM_CNN) performs better than employing CNN and LSTM in isolation for relation extraction in single sentences.

**Where exactly does LSTM_CNN model score?** To assess the contribution of LSTM_CNN+WF+PF against the baseline models, we divided each dataset into three groups based on the distance between entity \( e_1 \) and \( e_n \) in the text span. Specifically, we calculated the average number of tokens (\( \mu \)) between \( e_1 \) and \( e_n \) and the standard deviation (\( \sigma \)) over different lengths of tokens between \( e_1 \) and \( e_n \) in the dataset.

|    | single sentence |    | cross sentences |    |
|----|----------------|----|----------------|----|
|    | \( n_f = 10 \) | \( n_f = 28 \) | \( n_f = 10 \) | \( n_f = 128 \) |
| CNN+WF | 72.5 | 75.5 | 75.2 | 76.3 |
| CNN+WF+PF | 73.3 | 73.9 | 78.5 | 78.7 |
| LSTM+WF \( \dagger \) | - | 75.0 | - | 78.2 |
| LSTM+WF+PF \( \dagger \) | - | 74.5 | - | 78.9 |
| LSTM_CNN+WF \( \dagger \) | 77.6 | 75.4 | 76.9 | 75.3 |
| LSTM_CNN+WF+PF \( \dagger \) | 72.0 | 53.0 | 68.6 | 62.6 |
| LSTM_CNN+WF | 78.3 | 78.4 | 77.5 | 78.8 |
| LSTM_CNN+WF+PF | 73.1 | 79.6 \( \ast \) | 80.5 | 82.9 \( \ast \) |

Table 1: Average test accuracy in five-fold cross-validation for drug-gene-mutation ternary interactions in QP DATASET. \( n_f \) - number of filters. \( \dagger \) LSTM+WF and LSTM+WF+PF models does not use filters

Thus, if \( k \) is the total number of tokens between \( e_1 \) and \( e_n \), the dataset was divided into the following three groups: (a) short-distance spans (\( \mu \leq \mu - \sigma \)); (b) medium-distance spans (\( \mu - \sigma < k < \mu + \sigma \)); (c) long-distance spans (\( k \geq \mu + \sigma \)).

Analysing the performance of models on different groups of spans divided in the above manner will provide insights into the model’s performance on different sequence lengths and the contribution of different features for relation extraction.

The performance of various models on three groups of sentences, divided based on the number of tokens between entities \( e_1 \) and \( e_n \) in the text span is provided in Table 3.

As seen in Table 3, the proposed LSTM_CNN+WF+PF model score higher particularly for medium-distance spans (\( \mu - \sigma < k < \mu + \sigma \)) and long-distance spans (\( k \geq \mu + \sigma \)). For example, for short-distance and long-distance spans involving ternary relations across sentences, the LSTM_CNN+WF+PF model predicts ternary relations correctly for a higher percent of 81.3 and 82.9 spans, respectively. Similarly, the percentage of correct predictions for binary relation extraction in single sentences and across sentences is significantly higher than the performance of other models. These results clearly indicate that the combined LSTM_CNN model is more useful compared to using CNN and LSTM models in isolation for cross-sentence n-ary relation extraction, particularly where the distance between the first (\( e_1 \)) and the last entity (\( e_2 \)) is large. In other words the combined LSTM_CNN models are more useful in extracting relations from larger spans of consecutive sentences.

Further, the highest margin between LSTM_CNN+WF+PF and the baselines is recorded for binary interactions in single sentences and across sentences with an accuracy of 85.8 and 88.6, respectively (Table 3). This is followed by ternary interactions in single sentences and across sentences with an accuracy of 79.6 and 82.9, respectively (Table 1). It is interesting to note that the average length of tokens (\( \mu \)) between entities in text spans in the datasets relating to binary and ternary interactions in single sentences and across sentences is of the order 19, 29, 34 and 44, respectively. Based on these results, it can be broadly concluded that the contribution of PF decreases with the increase in the distance between entities in the text span.
| Model                                      | $k < \mu - \sigma$ (%) | $\mu - \sigma < k < \mu + \sigma$ (%) | $k \geq \mu + \sigma$ (%) |
|-------------------------------------------|-------------------------|----------------------------------------|---------------------------|
| **drug-gene-mutation - ternary relations - cross sentence ($\mu=44$)** |                         |                                        |                           |
| CNN+WF                                    | 82.9                    | 74.9                                   | 79.8                      |
| CNN+WF+PF                                 | 84.7                    | 76.5                                   | 80.3                      |
| LSTM+WF                                   | 46.2                    | 77.0                                   | 79.5                      |
| LSTM+WF+PF                                | 54.2                    | 77.6                                   | 80.4                      |
| CNN_LSTM+WF                               | 51.4                    | 74.9                                   | 79.0                      |
| CNN_LSTM+WF+PF                           | 86.2                    | 74.8                                   | 78.8                      |
| LSTM_CNN+WF                               | 52.0                    | 76.0                                   | 79.1                      |
| LSTM_CNN+WF+PF                           | 81.3                    | 81.3                                   | 82.9                      |
| **drug-gene-mutation - ternary relations - single sentence ($\mu=34$)** |                         |                                        |                           |
| CNN+WF                                    | 20.0                    | 73.1                                   | 86.6                      |
| CNN+WF+PF                                 | 10.0                    | 72.0                                   | 83.4                      |
| LSTM+WF                                   | 20.0                    | 73.5                                   | 85.8                      |
| LSTM+WF+PF                                | 20.0                    | 73.0                                   | 85.6                      |
| CNN_LSTM+WF                               | 20.0                    | 76.2                                   | 87.3                      |
| CNN_LSTM+WF+PF                           | 20.0                    | 69.7                                   | 88.8                      |
| LSTM_CNN+WF                               | 20.0                    | 76.8                                   | 88.0                      |
| LSTM_CNN+WF+PF                           | 20.0                    | 79.5                                   | 86.6                      |
| **drug-mutation - binary relations - cross sentence ($\mu=29$)** |                         |                                        |                           |
| CNN+WF                                    | 0.0                     | 79.6                                   | 78.1                      |
| CNN+WF+PF                                 | 20.0                    | 83.9                                   | 82.7                      |
| LSTM+WF                                   | 20.0                    | 80.7                                   | 79.9                      |
| LSTM+WF+PF                                | 20.0                    | 81.2                                   | 80.5                      |
| CNN_LSTM+WF                               | 20.0                    | 78.0                                   | 81.3                      |
| CNN_LSTM+WF+PF                           | 20.0                    | 84.8                                   | 87.3                      |
| LSTM_CNN+WF                               | 20.0                    | 81.6                                   | 83.2                      |
| LSTM_CNN+WF+PF                           | 20.0                    | 90.9                                   | 90.2                      |
| **drug-mutation - binary relations - single sentence ($\mu=19$)** |                         |                                        |                           |
| CNN+WF                                    | 16.1                    | 73.5                                   | 66.6                      |
| CNN+WF+PF                                 | 18.4                    | 74.8                                   | 67.3                      |
| LSTM+WF                                   | 17.6                    | 77.7                                   | 66.5                      |
| LSTM+WF+PF                                | 16.9                    | 75.7                                   | 64.9                      |
| CNN_LSTM+WF                               | 15.3                    | 72.7                                   | 62.5                      |
| CNN_LSTM+WF+PF                           | 19.2                    | 76.8                                   | 65.8                      |
| LSTM_CNN+WF                               | 16.1                    | 76.4                                   | 67.6                      |
| LSTM_CNN+WF+PF                           | 17.6                    | 84.9                                   | 68.5                      |

Table 3: Performance of models on different groups of sentences. $k$ - length of tokens between entities $e_1$ and $e_n$, $\mu$ average number of tokens between $e_1$ and $e_n$, $\sigma$ standard deviation over the length of tokens.

**LSTM_CNN vs. CNN_LSTM.** The results shown above clearly indicate that it is more useful to start with an LSTM layer followed by CNN layer (LSTM_CNN model) than having a CNN_LSTM model for cross-sentence $n$-ary relation extraction. As seen from Tables 1 and 2, the LSTM_CNN models perform significantly higher than CNN_LSTM models both for ternary and binary relations in single sentences and across sentences. A LSTM_CNN model is more useful in that, it initially learns from the sequential information available in the input, which is further exploited by CNN max-pooling layer to identify salient features. However, in the CNN_LSTM model, the use of CNN layer with max-pooling as the fist component though helps in identifying salient features from the input, the output from the CNN layer does not retain the sequential information. The CNN output feature vector without sequential information when fed to LSTM layer, results in poor performance. This indicates that an LSTM_CNN model is more useful than CNN_LSTM model for cross-sentence $n$-ary relation extraction. Further, as the results show, the addition of position embeddings in the CNN_LSTM model (CNN_LSTM+WF+PF) results in poor performance in comparison to the use of word embeddings alone (CNN_LSTM+WF). This is particularly true for ternary relation extraction (Table 1). Further as seen in Table 1 the use of higher number of filters combining word embeddings and position embeddings, dramatically lowers the performance. This indicates that position embeddings along with higher number of filters are not useful for CNN_LSTM models. However, it is also worthwhile to note that as seen from Table 3 the CNN_LSTM+WF+PF model extracts ternary relations in single sentences for the higher number of long-distance spans (88.8%), indicating that CNN_LSTM models are useful in certain cases.

**CNN and LSTM models.** The results provided above clearly shows that, when used in isolation, LSTM-based models are more useful for cross-sentence $n$-ary relation extraction, compared to CNN-based models. Interestingly, the use of PF helps only longer sequences (accuracy of 78.9 (LSTM+WF+PF) vs. 78.2 (LSTM+WF) and 80.8 (LSTM+WF+PF) vs. 80.3 (LSTM+WF+PF) scored for ternary relations in drug-mutation-gene (Table 1) and drug-mutation (Table 2), respectively). However, for shorter sequences, the use of PF results in decrease in accuracy (accuracy of 74.5 (LSTM+WF+PF) vs. 75.0 (LSTM+WF) and 74.4 LSTM+WF+PF) vs. 75.4 (LSTM+WF+PF) scored for binary relations in drug-mutation-gene (Table 1) and drug-mutation (Table 2), respectively). The contribution of WF in CNN model significantly improves with the use of higher number of filters, so much so that the model performs better than combining WF and PF. This is particularly true for extracting ternary relations in single sentences (Table 1).

**$n$-positional embeddings.** Given entities $e_1,..e_n$ in the text span, the proposed LSTM_CNN+WF+PF model employed only $e_1$ and $e_n$ to create positional embeddings. However, we could also create $n$-positional embeddings for each of the n entities in the text span. To this end, we evaluated the LSTM_CNN+WF+PF model using $n$-positional embeddings. The use of $n$-positional embeddings resulted in a lower accuracy of 80.5 and 77.9 (compared to 82.5 and 79.6 using position embeddings for $e_1$ and $e_n$) for ternary relation extraction across sentence and single sentences, respectively. This indicates that using positional embeddings for $e_1$ and $e_n$ is more useful for cross-sentence relation extraction.

**Comparison against the state-of-the-art.** As seen from Table 4 the proposed LSTM_CNN+WF+PF model outperforms various state-of-the-art methods for cross-sentence $n$-ary relation extraction on Q&P DATASET. These models include GRAPH LSTM (Peng et al. 2017), feature-based models (Quirk and Poon 2016), RNN-based networks such as BiLSTM (Miwa and Bansal 2016) and TREE-LSTM, and also combining multi-task learning with BiLSTM and GRAPH LSTM (Peng et al. 2017). The strength of the proposed model comes from the fact that the previous state-of-the-art methods heavily rely on syntactic features such as dependency
tress, co-reference and discourse features, which are time-consuming and less accurate particularly in the biomedical domain. However, in comparison to these models, the proposed LSTM,CNN+WF+PF model does not use any such sophisticated features, but uses much simpler features such as WF and PF. The ability to provide significantly higher performance with much simpler features makes the proposed LSTM,CNN+WF+PF an attractive choice for cross-sentence n-ary relation extraction.

The performance of LSTM,CNN+WF+PF model on CID DATASET is provided in Table 5.

### Performance of LSTM,CNN on SE DATASET.

To examine the performance of the proposed model on standard relation extraction dataset, the LSTM,CNN model was evaluated on SE DATASET (Hendrickx et al. 2009). The LSTM,CNN+WF and LSTM,CNN+WF+PF models achieved F1-scores of 71.6 and 81.5, respectively. These scores are slightly better than employing CNN with WF to obtain an F1-score of 69.7 and combining WF and PF with CNN to achieve an F1-score of 78.9, further suggesting that combining LSTM and CNN is useful for relation extraction.

### Conclusion

To conclude, we presented in this paper a combined LSTM,CNN model that exploits both word embeddings and position embeddings for the task of cross-sentence n-ary relation extraction. The experimental results provided in this paper clearly establish that combining LSTMs and CNNs offer the ability to harness together the strength of LSTMs to learn from longer sequences and the usefulness of CNNs to learn salient features, vital for cross-sentence n-ary relation extraction. The comparison with state-of-the-art results further proves the usefulness of combined LSTM and CNN model for cross-sentence n-ary relation extraction.

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