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 crosssentence 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*, *gefitnib* 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 nary 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 gefitnib and showed a partial response."

This paper focuses on the *cross-sentence n-ary relation* extraction task. Formally, let $\{e_1, ..., e_n\}$ 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 (gefitnib). Thus, a ternary relation response(*EGFR*, *L858E*, *gefitnib*) exists among the three entities spanning across the two sentences in LISTING 1. The entities $e_1, ..., e_n$ 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 $\mathbf{x} = x_1, x_2, ..., x_m$ in t consecutive sentences and a set of entities $\{e_1, ..., e_n\}$, the cross-sentence n-ary relation extraction task is to predict an n-ary relation (if exists) among the entities in \mathbf{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 intrasentence relation extraction. Unfortunately, such patternbased 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 nonobvious as how to merge dependency parse trees from different sentences to extract path-based features for crosssentence 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 crosssentence 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 crosssentence n-ary relation extraction. Although, previous studies have explored LSTMs and CNNs separately for crosssentence *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

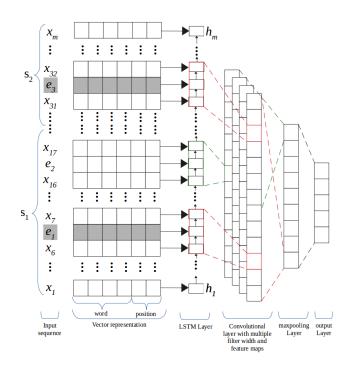


Figure 1: Architecture of the LSTM_CNN+WF+PF model for cross-sentence *n*-ary relation extraction. The input to the network is the sequence of tokens from text span (with two sentences and three entities) shown in LISTING 1. The position features are derived for highlighted entities (e_1 and e_3).

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 $x = x_1, x_2, ..., x_n$ is mapped to a k-dimensional embedding vector using a look-up matrix $\mathbf{W} \in \mathbb{R}^{|V| \times k}$ where |V| is the number of unique words in the vocabulary.

Position Features Following Zeng et al. (2014), positional features (PFs) 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* PFs 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* PFs decreases the performance of the model. Thus, the model defines two sets of PFs PF_1 and PF_n for the entities e_1 and e_n , respectively, as a combination of the relative distances from the current word to the respective entity. The position embedding matrices are randomly initialised and the relative distance of words *w.r.t* entities are transformed into real valued vectors by looking up the position embedding matrices.

Thus, the vector representation for models using position features, transforms an instance into a matrix $\mathbf{S} \in \mathbb{R}^{s \times d}$ by combining the word embeddings and position embeddings, where *s* is the sentence length and $d = d^a + d^b \times 2$ (d^a and d^b are the dimensions of respectively the word and position embeddings).

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. Given the long-range sequential information resulting from combined set of sentences expressing an n-ary relation, LSTM is an excellent choice to learn long-range dependencies. Thus, as shown in Figure 1, the transformed vector representation combining word embeddings and position features is provided as input to the LSTM layer. The LSTM units at each time step t is defined as a collection of vectors in \mathbb{R}^l 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 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.

$$i_t = \sigma(\mathbf{W}_i x_t + \mathbf{U}_i h_{t-1} + b_i) \tag{1}$$

$$f_t = \sigma(\mathbf{W}_f x_t + \mathbf{U}_f h_{t-1} + b_f) \tag{2}$$

$$o_t = \sigma(\mathbf{W}_o x_t + \mathbf{U}_o h_{t-1} + b_o) \tag{3}$$

$$g_t = \tanh(\mathbf{W}_a x_t + \mathbf{U}_a h_{t-1} + b_a) \tag{4}$$

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).

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

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

$$h_t = o_t \odot \tanh(c_t). \tag{6}$$

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

CNN Layer

Let $h_i \in \mathbb{R}^l$ 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:

$$h_{1:m} = h_1 \oplus h_2 \oplus \dots \oplus h_m, \tag{7}$$

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 $\mathbf{w} \in \mathbb{R}^{pl}$, which is 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 $h_{i:i+p-1}$.

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

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 $h_{1:p}, h_{2:p+1}, \ldots, h_{m-p+1:n}$ to produce a feature map $c \in \mathbb{R}^{m-p+1}$ given by,

$$c = [c_1, c_2, \dots, c_{m-p+1}].$$
(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 $\mathbf{g} \in \mathbb{R}^{fw}$, 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-class classification problem. The output feature vector **g** obtained from the convolution and maxpooling 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 $\mathbf{x} = x_1, x_2, ..., x_m$), entity mentions $e_1, ..., e_n$ and having an *n*-ary relation *r*, the cross-entropy loss for this prediction is defined as follows:

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

where s indicates the total number of text spans and θ 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.

Ouirk and Poon (OP) Dataset We use the dataset¹ developed by Quirk and Poon (2016) and Peng et al. (2017) for the task of cross-sentence *n*-ary relation extraction. Distant supervision was followed to extract relations involving drug, gene and mutation triples from the biomedical literature available in PubMed Central². 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 instances 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 dataset³, 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.

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; Gu et al. 2017; Zhou et al. 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.

Baseline models

The proposed LSTM_CNN+WF+PF model is evaluated against the following baseline models: (a) CNN+WF: a CNN model using word features alone; (b) CNN+WF+PF: 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_LSTM+WF: a model that begins with a CNN layer followed by an LSTM layer and uses word features only; (f) CNN_LSTM+WF+PF: model that begins with a CNN layer followed by LSTM layer and employs word features and position features; (g) LSTM_CNN+WF: 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 crosssentence *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 ($p \le 0.05$; 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

¹http://hanover.azurewebsites.net

²http://www.ncbi.nlm.nih.gov/pmc

³https://github.com/JHnlp/BC5CIDTask

	single sentence		cross sentences	
	nf=10	nf=128	nf=10	nf=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
CNN_LSTM+WF	77.6	75.4	76.9	75.3
CNN_LSTM+WF+PF	72.0	53.0	76.8	62.6
LSTM_CNN+WF	78.3	78.4	77.5	78.8
LSTM_CNN+WF+PF	73.1	79.6*	80.5	82.9*

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

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 nf = 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.tentities in the text span, which helps in achieving higher accuracy.

Further, the higher performance achieved in extracting both ternary and binary relations, particularly from crosssentence 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 (μ) between e_1 and e_n and the standard deviation (σ) over different lengths of tokens between e_1 and e_n in the dataset.

	single sentence		cross sentences	
	nf=10	nf=128	nf=10	nf=128
CNN+WF	68.9	72.4	73.2	76.6
CNN+WF+PF	74.0	74.2	81.3	81.3
$LSTM+WF^{\dagger}$	-	75.4	-	80.3
LSTM+WF+PF [†]	-	74.4	-	80.8
CNN_LSTM+WF	71.2	72.3	76.5	76.5
CNN_LSTM+WF+PF	74.7	56.2	81.2	74.4
LSTM_CNN+WF	74.9	76.7	79.7	82.0
LSTM_CNN+WF+PF	85.3	85.8*	85.1	88.6*

Table 2: Average test accuracy in five-fold cross-validation for *drug-gene binary interactions* in QP DATASET. nf - 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 $(k \le \mu - \sigma)$; (b) medium-distance spans $(\mu - \sigma < k < \mu + \sigma)$; (c) long-distance spans $(k \ge \mu + \sigma)$. 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 ($k \ge \mu + \sigma$). 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 2). 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 (μ) 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	$k \leq \mu - \sigma$	$\mu - \sigma < k < \mu + \sigma$	$k \ge \mu + \sigma$		
	(%)	(%)	(%)		
drug-gene-mutation -	drug-gene-mutation - ternary relations - cross sentence (μ =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 rela	tions - single sente	nce (μ =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 - b	inary relatio	ns - cross sentence	(µ=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 - bi	nary relatio	ns - single sentence	e (µ=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	86.5		

Table 3: Performance of models on different groups of sentences. k - length of tokens between entities e_1 and e_n , μ average number of tokens between e_1 and e_n , σ 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 maxpooling 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 longdistance 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 drugmutation (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 drugmutation (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_CNNW-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

Model	Single	Cross	
	Sent.	Sents.	
drug-gene-mutation - ternary relations			
FEATURE-BASED	74.7	77.7	
BILSTM	75.3	80.1	
GRAPH LSTM-EMBED	76.5	80.6	
GRAPH LSTM-FULL	77.9	80.7	
BILSTM+MULTI-TASK	-	82.4	
GRAPH LSTM+MULTI-TASK	-	82.0	
LSTM_CNN+WF+PF (proposed model)	79.6	82.9	
drug-mutation - binary relations			
FEATURE-BASED	73.9	75.2	
BILSTM	73.9	76.0	
BILSTM-SHORTEST-PATH	70.2	71.7	
TREE-LSTM	75.9	75.9	
GRAPH LSTM-EMBED	74.3	76.5	
GRAPH LSTM-FULL	75.6	76.7	
BILSTM+MULTI-TASK	-	78.1	
GRAPH LSTM+MULTI-TASK	-	78.5	
LSTM_CNN+WF+PF (proposed model)	85.8	88.5	

Table 4: Average test accuracy in five-fold cross validation of the proposed model and SOTA methods on n-ary cross-sentence relation extraction (Q&P DATASET)

tress, co-reference and discourse features, which are timeconsuming 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 make 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. As seen in Table 5, the LSTM_CNN+WF+PF model achieves statistically significant performance for extracting binary relations from text spans with two sentences (t = 2) against methods based on supervised learning using linguistic features and maximum entropy models. The LSTM_CNN+WF+PF model also performs well in extracting binary relations in single sentences (t = 2). The combined LSTM_CNN+WF+PF model achieves higher F-score (0.63) against various SOTA methods⁴ on CID DATASET as shown in Table 5. The combination of LSTM_CNN provides a slight increase than using CNN and LSTM separately on CID DATASET. The CNN-based models proposed by Nguyen and Verspoor (2018) although achieve a higher recall, they tend to achieve a lower precision. The same is the case with CNN+ME+PP (Gu et al. 2017) and CNN (Zhou et al. 2016). On the other hand, LSTMs achieve higher precision, but suffer from poor recall (LSTM, LSTM+SVMP (Zhou et al. 2016)). In comparison to CNN models and LSTM models, the combined LSTM_CNN achieve a higher precision and at the same time do not lose on recall, resulting in achieving a higher F-score on CID DATASET.

Model	P	R	F
Single sentences (text span whe	ere $t = 1$	L)	
LINGUISTIC FEATURES	0.67	0.68	0.68
(Gu, Qian, and Zhou 2016)			
CNN (Gu et al. 2017)	0.59	0.55	0.57
LSTM_CNN+WF+PF (proposed model)	0.69	0.70	0.69
Across sentences (text span who	ere $t = 2$	2)	
LINGUISTIC FEATURES	0.51	0.29	0.37
(Gu, Qian, and Zhou 2016)			
MAXIMUM ENTROPY (Gu et al. 2017)	0.51	0.07	0.11
LSTM_CNN+WF+PF (proposed model)	0.57	0.57	0.57*
Across sentences (text span who	ere $t \leq t$	2)	
LINGUISTIC FEATURES + ME	0.62	0.55	0.58
(Gu, Qian, and Zhou 2016)			
CNN+ME (Gu et al. 2017)	0.60	0.59	0.60
CNN+ME+PP (Gu et al. 2017)	0.55	0.68	0.61
CNN (Zhou et al. 2016)	0.41	0.55	0.47
LSTM (Zhou et al. 2016)	0.54	0.51	0.53
LSTM+SVMP (Zhou et al. 2016)	0.64	0.49	0.56
LSTM+SVM+PP (Zhou et al. 2016)	0.55	0.68	0.61
SVM (Xu et al. 2016)	0.55	0.68	0.61
CNN	0.54	0.69	0.61
CNN+CNNCHAR	0.57	0.68	0.62
CNN+LSTMCHAR	0.56	0.68	0.62
(Nguyen and Verspoor 2018)			
LSTM_CNN+WF+PF (proposed model)	0.63	0.63	0.63

Table 5: Comparison of performance of LSTM_CNN+WF+PF with state-of-the-art models on CID DATASET. t = number of sentences, P - precision, R - recall, F - F-score.

Performance of LSTM_CNN model 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.

References

[Abadi et al. 2016] Abadi, M.; Agarwal, A.; Barham, P.; Brevdo, E.; Chen, Z.; Citro, C.; Corrado, G. S.; Davis,

⁴Note that the SOTA methods listed in Table 5 does not use any knowledge base or the development set for learning the model.

A.; Dean, J.; Devin, M.; et al. 2016. Tensorflow: Largescale machine learning on heterogeneous distributed systems. *arXiv preprint arXiv:1603.04467*.

- [Agichtein and Gravano 2000] Agichtein, E., and Gravano, L. 2000. Snowball: Extracting relations from large plaintext collections. In *Proceedings of the fifth ACM conference on Digital libraries*, 85–94. ACM.
- [Bach and Badaskar 2007] Bach, N., and Badaskar, S. 2007. A survey on relation extraction. *Language Technologies Institute, Carnegie Mellon University.*
- [Brin 1998] Brin, S. 1998. Extracting patterns and relations from the world wide web. In *International Workshop on The World Wide Web and Databases*, 172–183. Springer.
- [Bunescu and Mooney 2005] Bunescu, R. C., and Mooney, R. J. 2005. A shortest path dependency kernel for relation extraction. In *Proceedings of the conference on human language technology and empirical methods in natural language processing*, 724–731. Association for Computational Linguistics.
- [Culotta and Sorensen 2004] Culotta, A., and Sorensen, J. 2004. Dependency tree kernels for relation extraction. In *Proceedings of the 42nd annual meeting on association for computational linguistics*, 423. Association for Computational Linguistics.
- [Elango 2005] Elango, P. 2005. Coreference resolution: A survey. University of Wisconsin, Madison, WI.
- [Fundel, Küffner, and Zimmer 2006] Fundel, K.; Küffner, R.; and Zimmer, R. 2006. Relexrelation extraction using dependency parse trees. *Bioinformatics* 23(3):365–371.
- [Gu et al. 2017] Gu, J.; Sun, F.; Qian, L.; and Zhou, G. 2017. Chemical-induced disease relation extraction via convolutional neural network. *Database* 2017.
- [Gu, Qian, and Zhou 2016] Gu, J.; Qian, L.; and Zhou, G. 2016. Chemical-induced disease relation extraction with various linguistic features. *Database* 2016.
- [Hearst 1992] Hearst, M. A. 1992. Automatic acquisition of hyponyms from large text corpora. In *Proceedings of the 14th conference on Computational linguistics-Volume 2*, 539–545. Association for Computational Linguistics.
- [Hendrickx et al. 2009] Hendrickx, I.; Kim, S. N.; Kozareva, Z.; Nakov, P.; Ó Séaghdha, D.; Padó, S.; Pennacchiotti, M.; Romano, L.; and Szpakowicz, S. 2009. Semeval-2010 task 8: Multi-way classification of semantic relations between pairs of nominals. In *Proceedings of the Workshop on Semantic Evaluations: Recent Achievements and Future Directions*, 94–99. Association for Computational Linguistics.
- [Hochreiter and Schmidhuber 1997] Hochreiter, S., and Schmidhuber, J. 1997. Long short-term memory. *Neural computation* 9(8):1735–1780.
- [Hochreiter et al. 2001] Hochreiter, S.; Bengio, Y.; Frasconi, P.; Schmidhuber, J.; et al. 2001. Gradient flow in recurrent nets: the difficulty of learning long-term dependencies.
- [Hsu et al. 2017] Hsu, S. T.; Moon, C.; Jones, P.; and Samatova, N. 2017. A hybrid cnn-rnn alignment model for phrase-aware sentence classification. In *Proceedings of the*

15th Conference of the European Chapter of the Association for Computational Linguistics: Volume 2, Short Papers, volume 2, 443–449.

- [Lai et al. 2015] Lai, S.; Xu, L.; Liu, K.; and Zhao, J. 2015. Recurrent convolutional neural networks for text classification. In *AAAI*, volume 333, 2267–2273.
- [Lee and Dernoncourt 2016] Lee, J. Y., and Dernoncourt, F. 2016. Sequential short-text classification with recurrent and convolutional neural networks. *arXiv preprint arXiv:1603.03827*.
- [Mikolov et al. 2013] Mikolov, T.; Chen, K.; Corrado, G.; and Dean, J. 2013. Efficient estimation of word representations in vector space. *arXiv preprint arXiv:1301.3781*.
- [Miwa and Bansal 2016] Miwa, M., and Bansal, M. 2016. End-to-end relation extraction using lstms on sequences and tree structures. *arXiv preprint arXiv:1601.00770*.
- [Moschitti, Patwardhan, and Welty 2013] Moschitti, A.; Patwardhan, S.; and Welty, C. 2013. Long-distance time-event relation extraction. In *IJCNLP*, 1330–1338.
- [Nagesh 2016] Nagesh, P. 2016. Exploiting tree kernels for high performance chemical induced disease relation extraction. In *4TH ANNUAL DOCTORAL COLLOQUIUM*, 15.
- [Nguyen and Verspoor 2018] Nguyen, D. Q., and Verspoor, K. 2018. Convolutional neural networks for chemicaldisease relation extraction are improved with characterbased word embeddings. arXiv preprint arXiv:1805.10586.
- [Peng et al. 2017] Peng, N.; Poon, H.; Quirk, C.; Toutanova, K.; and Yih, W.-t. 2017. Cross-sentence n-ary relation extraction with graph lstms. *Transactions of the Association for Computational Linguistics* 5:101–115.
- [Pennington, Socher, and Manning 2014] Pennington, J.; Socher, R.; and Manning, C. 2014. Glove: Global vectors for word representation. In *Proceedings of the 2014 conference on empirical methods in natural language processing (EMNLP)*, 1532–1543.
- [Quirk and Poon 2016] Quirk, C., and Poon, H. 2016. Distant supervision for relation extraction beyond the sentence boundary. *arXiv preprint arXiv:1609.04873*.
- [Srivastava et al. 2014] Srivastava, N.; Hinton, G. E.; Krizhevsky, A.; Sutskever, I.; and Salakhutdinov, R. 2014. Dropout: a simple way to prevent neural networks from overfitting. *Journal of machine learning research* 15(1):1929–1958.
- [Swampillai and Stevenson 2010] Swampillai, K., and Stevenson, M. 2010. Inter-sentential relations in information extraction corpora. In *LREC*.
- [Wang, Jiang, and Luo 2016] Wang, X.; Jiang, W.; and Luo, Z. 2016. Combination of convolutional and recurrent neural network for sentiment analysis of short texts. In *Proceedings of COLING 2016, the 26th International Conference on Computational Linguistics: Technical Papers*, 2428–2437.
- [Xu et al. 2015] Xu, Y.; Mou, L.; Li, G.; Chen, Y.; Peng, H.; and Jin, Z. 2015. Classifying relations via long short term memory networks along shortest dependency paths. In *EMNLP*, 1785–1794.

- [Xu et al. 2016] Xu, J.; Wu, Y.; Zhang, Y.; Wang, J.; Lee, H.-J.; and Xu, H. 2016. Cd-rest: a system for extracting chemical-induced disease relation in literature. *Database* 2016.
- [Zeng et al. 2014] Zeng, D.; Liu, K.; Lai, S.; Zhou, G.; Zhao, J.; et al. 2014. Relation classification via convolutional deep neural network. In *COLING*, 2335–2344.
- [Zhou et al. 2016] Zhou, H.; Deng, H.; Chen, L.; Yang, Y.; Jia, C.; and Huang, D. 2016. Exploiting syntactic and semantics information for chemical–disease relation extraction. *Database* 2016.