A Neural Edge-Editing Approach for Document-Level Relation Graph Extraction

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Abstract

In this paper, we propose a novel edge-editing approach to extract relation information from a document. We treat the relations in a document as a relation graph among entities in this approach. The relation graph is iteratively constructed by editing edges of an initial graph, which might be a graph extracted by another system or an empty graph. The way to edit edges is to classify them in a close-first manner using the document and temporally-constructed graph information; each edge is represented with a document context information by a pretrained transformer model and a graph context information by a graph convolutional network model. We evaluate our approach on the task to extract material synthesis procedures from materials science texts. The experimental results show the effectiveness of our approach in editing the graphs initialized by our in-house rule-based system and empty graphs.\(^1\)

1 Introduction

Relation extraction (RE), the task to predict relations between pairs of given entities from literature, is an important task in natural language processing. While most existing work focused on sentence-level RE (Zeng et al., 2014), recent studies extended the extraction to the document level since many relations are expressed across sentences (Christopoulou et al., 2019; Nan et al., 2020). However, such methods do not directly consider interactions among relations in a document, while such relations are often dependent on each other, and other relations can be considered as important contexts for a relation.

We propose a novel, iterative, edge-editing approach to document-level RE. The overview of our approach and an example of the extraction results are illustrated in Figure 1. Our approach treats relations as a relation graph that is composed of entities as nodes and their relations as edges. The relation graph is first initialized using the edges predicted by an existing RE model if provided. Edges are then edited by a neural edge classifier that represents edges using the document information, pre-built graph information, and the current edge information. The document information is represented with pretrained Longformer models (Beltagy et al., 2020), while the graph information is represented with graph convolutional networks (Kipf and Welling, 2017). Edges are edited iteratively in a close-first manner so that the approach can utilize the information of edges between close entity pairs.

\(^1\)The source code is available at https://github.com/tti-coin/edge-editing.
in editing edges of distant entity pairs, which are often difficult to predict. We evaluate our approach on the task to extract synthesis procedures from text (Mysore et al., 2019) and show the effectiveness of our approach.

The contribution of this paper is three-fold. First, we propose a novel edge-editing approach for document-level RE that utilizes contexts in both relation graphs and documents. Second, we build a strong rule-based model and show that our approach can effectively utilize and enhance the output of the rule-based model. Third, we build and evaluate a neural model for extracting synthesis procedures from text for the first time.

2 Approach

Our approach extracts a relation graph on given entities from a document. We formulate the extraction task as an edge-editing task, where the approach iteratively edits edges with a neural edge classifier in a close-first manner (Miwa and Sasaki, 2014).

2.1 Iterative Edge Editing

We build a relation graph by editing the edges iteratively using the edge classifier in Section 2.2. The building finishes when all edges are edited. The edges are edited in a close-first manner (Miwa and Sasaki, 2014; Ma et al., 2019) that edits the close edges first and far edges later. The distance between the entity pair is defined based on the appearing order of entities in a document; if two entities in a pair appear m-th and m + 3-th, the distance becomes 3. Note that each edge is edited only once throughout the entire editing process.

Algorithm 1 shows the method to build the graph by the iterative edge editing. To reduce the computational cost, the pairs with the same distance are edited simultaneously and the pairs with distances more than or equal to the maximum distance \( d_{max} \) are edited simultaneously. This reduces the number of edits from \( |N|^2 \) to \( d_{max} \).

Algorithm 1: Iterative Edge Editing

\[
\text{Distance}(N_i, d_1, d_2) \text{ returns pairs that have distance } d (d_1 \leq d < d_2).
\]

Input: document, \( \mathcal{E} \): initial edges

Output: \( \mathcal{E} \): edited edges

\[
\begin{align*}
\mathcal{N} & \leftarrow \text{EncodeNode}(\text{doc}, \mathcal{N}) \\
\text{while } d \text{ in range}(\max(|\mathcal{N}|, d_{max})) \text{ do} & \\
\mathcal{N}^G & \leftarrow \text{GCN}(\mathcal{N}, \mathcal{E}) \\
\mathcal{E} & \leftarrow \text{EncodeEdge}(\mathcal{N}^G, \mathcal{E}) \\
\text{if } d = d_{max} & \text{ then} \\
\mathcal{P} & \leftarrow \text{Distance}(\mathcal{N}, d_{max}, \infty) \\
\text{else} & \\
\mathcal{P} & \leftarrow \text{Distance}(\mathcal{N}, d, d + 1) \\
\text{end if} & \\
\text{while } (i, j) \text{ in } \mathcal{P} \text{ do} & \\
\mathcal{E}_{ij} & \leftarrow \text{ClassifyEdge}(\mathcal{E}_{ij}) \\
\text{end while} & \\
\text{end while}
\end{align*}
\]

2.2 Edge Classifier

An edge classifier predicts the class of the target edge \( \mathcal{E}_{ij} \) from inputs that are composed of a document information \( \text{doc} \), a graph of nodes \( \mathcal{N} \) and edges \( \mathcal{E} \), and the node pair \( (N_i, N_j) \) of a target edge. The classifier composed of three modules: EncodeNode that produces document-based node representations \( \mathcal{N} \) using the document \( \text{doc} \) and the entity information of the nodes \( \mathcal{N} \).}

\[
\mathcal{N} = \text{EncodeNode}(\\text{doc}, \mathcal{N}) = \left[ \text{Pool}(\text{Longformer}(\text{doc})); \mathbf{v}^{lab} \right],
\]

where \([; ;]\) denotes concatenation.

To prepare the input to EncodeEdge, the obtained document-based node representation is enriched by GCN to introduce the context of each node in the prebuilt graph: \( \mathcal{N}^G = \text{GCN}(\mathcal{N}, \mathcal{E}) \). We add inverse directions to the graph and assign different weights to different classes in graph convolutional network (GCN) following Schlichtkrull et al. (2018). The produced node representation \( \mathcal{N}^G \) includes both document and prebuilt graph contexts.

EncodeEdge produces the edge representation \( \mathcal{E} \) from \( \mathcal{N}^G \). It individually calculates the repre-
15 directed relation types are defined. The corpus consists of 200 documents for training, 15 for development, and 15 for test. The statistics of the corpus are shown in Appendix A. We chose this corpus since this corpus is publicly available, manually annotated, and it deals with a dense document-level relation graph.

We prepared a rule-based model (RULE) as a baseline and as an existing model to initialize the edges, which was adapted from the rule-based system in Kuniyoshi et al. (2020). The rules are summarized in Appendix B.

We employ the micro F-score for each relation class as the evaluation metric. We maximize the log-likelihood in training the model. We compare the following models on graphs initialized by the rule-based model (with RULE) and empty graphs (without RULE).

**EDIT**: Proposed model

**EDIT-IE**: EDIT without iterative edge editing, i.e., $$d_{\text{max}} = 1$$.

**EDIT-GCN**: EDIT without GCN by replacing $$N^G$$ with $$\bar{N}$$ in Equation (2)

**RANDOM EDIT**: EDIT with random-order editing

**RANDOM INIT**: EDIT with randomly connected edges, the number of which is same as that of the extraction results of RULE, with random classes

Note that although we did not provide the direct comparison with the existing models, our EDIT-GCN without RULE is similar to BRAN (Verga et al., 2018); the only differences are that we use Longformer (Beltagy et al., 2020) instead of transformers, and NER training is not included. Moreover, most of the models for the document-level RE require dataset annotating both entities and their mentions, so the existing models like AT-LOP (Zhou et al., 2021) cannot be directly applied to the current task.

### 3.2 Results without RULE

We show the results with empty initial graphs in Table 1. EDIT shows the highest scores and this indicates the effectiveness of our approach when the initial graphs are empty. When we compare EDIT, EDIT-IE, and RANDOM EDIT, we find that both iterative edge editing and close-first strategy

|                | Dev | Test |
|----------------|-----|------|
| EDIT           | 0.788 | 0.729 |
| EDIT-IE        | 0.732 | 0.685 |
| EDIT-GCN       | 0.744 | 0.703 |
| RANDOM EDIT    | 0.751 | 0.690 |
| RANDOM INIT    | 0.756 | 0.720 |

Table 1: Evaluation results in micro F-score without RULE.
We illustrated 6 graphs for an example document (Zhang et al., 2007) in the development data set shown in Figure 2: the result on the right side of Figure 1 shows our best extraction result using EDIT-IE with RULE; Figure 3 shows the correct extraction; Figure 4 shows the extraction result using EDIT without RULE; Figure 5 shows the extraction result using RULE; and Figure 6 shows the extraction result using EDIT with RULE. Figure 3 shows the material synthesis starts from mixed with materials SrCO3, MoO3 and Ni to prefired and so on, and the material SrMo1-xNixO4 is synthesized. When we compare Figure 6 with Figure 5, the extraction results are similar to RULE. Although the overall performance is low, Figure 4, which does not depend on the rule, extracts relations that are not extracted by the other systems and this shows the models with RULE and without RULE capture different relations.

|                | Dev | Test |
|----------------|-----|------|
| RULE           | 0.797 | 0.807 |
| EDIT           | **0.878** | 0.851 |
| EDIT-IE        | 0.863 | **0.863** |
| EDIT-GCN       | 0.857 | 0.834 |
| RANDOM EDIT    | 0.791 | 0.744 |

Table 2: Evaluation results in micro F-score with RULE.

are effective. Since EDIT-GCN extracts from context without graph structure information, the better performance of EDIT over EDIT-GCN shows the effectiveness of the information in the graph structure. The low performance with RANDOM INIT shows that the edge information needs to be reliable.

### 3.3 Results with RULE

We summarize the results with RULE in Table 2. We show the detailed results for EDIT without RULE, RULE, and EDIT-IE with RULE in Appendix D.

When we compare the results with Table 1, the performance with RULE is better than the counterpart without RULE for all the settings. Furthermore, all the scores in Table 2 are better than those in Table 1, which shows the strength of RULE.

Surprisingly, the results with our approach are better than that of RULE even though RULE is better than our approach without RULE. This indicates our EDIT approach can make the prediction accurate. We can conclude that our EDIT approach can utilize the information from the rule-based model and the initialization of the edges by RULE is useful.

As for the performance of the models, most results are consistent with Table 1 except that EDIT-IE shows the highest score on the test set. This may be partly because the initial graph by RULE is already reliable and editing does not help to improve the context. Results with RANDOM EDIT support this since the performance degradation with RANDOM EDIT is large compared to Table 1 and RANDOM EDIT is harmful in this case. Moreover, the different behaviors on the development and test sets indicate an imbalance in the corpus split.

### 4 Case Study

We illustrated 6 graphs for an example document (Zhang et al., 2007) in the development data set shown in Figure 2: the result on the right side

### 5 Related Work

RE has been widely studied to identify the relation between two entities in a sentence. In addition to traditional feature/kernel-based methods (Zelenko et al., 2003; Miwa and Sasaki, 2014), many neural RE methods have been proposed based on convolutional neural networks (CNNs) (Zeng et al., 2014), recurrent neural networks (RNNs) (Xu et al., 2015; Miwa and Bansal, 2016), graph convolutional networks (GCNs) (Zhang et al., 2018; Schlichtkrull et al., 2018), and transformers (Wang et al., 2019). However, sentence-level RE is not enough to cover the relations in a document, and document-level RE has increasingly received research attention in recent years.

Major approaches for document-level RE are graph-based methods and transformer-based methods. For graph-based methods, Quirk and Poon (2017) first proposed a document graph for document-level RE. Christopoulou et al. (2019) constructed a graph that included heterogeneous nodes such as entity mentions, entities, and sentences and represented edges between entities from the graph. Nan et al. (2020) proposed the automatic induction of a latent graph for relational reasoning across sentences. The document graphs in these methods are defined on nodes of linguistic units such as words and sentences, which are different from our relation graphs. Unlike our method, these methods do not directly deal with relation graphs among entities.

For transformer-based methods, Verga et al. (2018) introduced a method to encode a document with transformers to obtain entity embedding and
A series of polycrystalline samples of $\text{SrMo}_{1-x}\text{Ni}_x\text{O}_4$ (0.02 <= x <= 0.08) were prepared through the conventional solid-state reaction method in air. Appropriate proportions of high-purity SrCO$_3$, MoO$_3$, and Ni powders were thoroughly mixed according to the desired stoichiometry, and then pre-fired at 900 [°]C for 24 h. The obtained powders were ground, pelletized, and calcined at 1000, 1100 and 1200 [°]C for 24 h with intermediate grinding twice. White compounds, $\text{SrMo}_{1-x}\text{Ni}_x\text{O}_4$, were obtained. The compounds were ground and pressed into small pellets about 10 mm diameter and 2 mm thickness. These pellets were reduced in a H2/Ar (5%: 95%) flow at 920 [°]C for 12 h, and then the deep red colored products of $\text{SrMo}_{1-x}\text{Ni}_x\text{O}_3$ were obtained.

**Figure 2:** Example document

**Figure 3:** Gold graph for the document in Figure 2

**Figure 4:** Example extraction results from the document in Figure 2 by EDIT without RULE

**Figure 5:** Example extraction results from the document in Figure 2 by RULE

**Figure 6:** Example extraction results from the document in Figure 2 by our EDIT with RULE

classify the relations between entities using the embedding. Tang et al. (2020) proposed a Hierarchical Inference Network (HIN) for document-level RE, which aggregates information from entity level to document level. Zhou et al. (2021) tackled document-level RE with an Adaptive Thresholding and Localized cOntext Pooling (ATLOP) model that introduces a learnable entity-dependent threshold for classification and aggregated local mention-level contexts that are relevant to both entities.

Several studies focus on procedural texts such as cooking recipes (Bosselut et al., 2018), scientific processes (Dalvi et al., 2018) and open domain procedures (Tandon et al., 2020). They, however, do not directly treat relation graphs. Several efforts have been made to annotate procedural or action graphs in procedural text (Mori et al., 2014; Mysore et al., 2019; Kuniyoshi et al., 2020). Kuniyoshi et al. (2020) and Mehr et al. (2020) individually proposed rule-based systems to extract procedures from a document, but no neural methods have been proposed for the extraction.

**6 Conclusions**

We proposed a novel edge editing approach for document-level relation extraction. This approach treats the task as the edge editing of relation graphs, given nodes. It edits edges considering contexts in the document and the relation graph. We evaluated the approach on the material synthesis procedure corpus, and the results showed the usefulness of initializing edges by the rule-based model, utilizing prebuilt graph information for editing and editing in a close-first manner. As a result, our model performed an F-score of 86.3% for edge prediction. In future work, we plan to improve the approach to obtain more consistent and accurate relation graphs. We also would like to apply the approach to other data sets such as cooking recipes (Mori et al., 2014) and temporal graphs (Pustejovsky et al., 2003; Cassidy et al., 2014).
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### A Statistics of the Materials Science Procedural Text Corpus

We present the statistics of the materials science procedural text corpus\(^2\) proposed by Mysore et al. (2019). Table 3 and Table 4 summarize the numbers of entities and relations, respectively.

\(^2\)https://github.com/olivettigroup/annotated-materials-syntheses
B Rule-based Relation Extraction Model

We built a rule-based model by defining the rules to extract relations between entity pairs for the materials science procedural text corpus (Mysore et al., 2019). The rules were adapted from the rule-based model in (Kuniyoshi et al., 2020) for the target corpus. The rules depend on labels of the entities of an entity pair, distance, and the order of occurrence of the entities. According to the combination of labels of the entities, our rules are divided into three types: OPERATION–OPERATION, OPERATION–MATERIAL, and other relations. In the following, the starting point of a relation is called head and the ending point is called tail, and an edge is denoted as HEAD–TAIL.

B.1 OPERATION–OPERATION

The relation OPERATION–OPERATION takes only a NEXT_OPERATION label, which means the progress of operation.

NEXT_OPERATION: Close OPERATION entities are linked with the relation from the beginning to the end in the document order, in which the entities of OPERATION appear.

B.2 OPERATION–MATERIAL

For the edges of OPERATION–MATERIAL, there are five relation labels: RECIPE_PRECURSOR indicates the input of a material; RECIPE_TARGET indicates the generation of a product; PARTICIPANT_MATERIAL indicates the generation of an intermediate product; SOLVENT_MATERIAL indicates the solvent material of an operation; and ATMOSPHERIC_MATERIAL indicates the atmosphere of an operation.

For SOLVENT_MATERIAL, ATMOSPHERIC_MATERIAL and PARTICIPANT_MATERIAL labels, a dictionary is prepared manually for each label. The relations are linked from the nearest OPERATION to a MATERIAL in the sentence if the MATERIAL match in the dictionary since these relations take specific MATERIAL entities. The dictionary is included in the source code.

RECIPE_PRECURSOR is linked from all MATERIAL that do not match the dictionary of SOLVENT_MATERIAL, ATMOSPHERIC_MATERIAL, and PARTICIPANT_MATERIAL to the nearest OPERATION. This rule-based model does not produce the relation RECIPE_TARGET. The reason for these decisions is that it is difficult to classify these relations with simple rules.

B.3 Remaining Relations

The remaining 9 relation labels are defined between the other pairs of entity labels: PROPERTY_OF, which indicates a condition of a material; CONDITION_OF, which indicates a condition of an operation; NUMBER_OF, which indicates the relationship between a number and a unit; AMOUNT_OF, which indicates a condition of a quantity; TYPE_OF, which indicates a condition of a numerical condition; BRAND_OF, which indicates the brand of a material or equipment; APPARATUS_OF, which indicates equipment used in an

| Entity class                  | Train | Dev | Test |
|-------------------------------|-------|-----|------|
| MATERIAL                      | 4,271 | 277 | 316  |
| OPERATION                     | 3,249 | 212 | 242  |
| NUMBER                        | 2,872 | 224 | 219  |
| CONDITION-UNIT               | 1,363 | 101 | 87   |
| MATERIAL-DESCRIPTOR           | 1,214 | 67  | 89   |
| AMOUNT-UNIT                   | 1,193 | 96  | 98   |
| PROPERTY-MISC                | 481   | 25  | 16   |
| CONDITION-MISC               | 468   | 32  | 20   |
| SYNTHESIS-APPARATUS          | 433   | 20  | 34   |
| NONRECIPE-MATERIAL           | 329   | 33  | 25   |
| BRAND                         | 291   | 30  | 27   |
| APPARATUS-DESCRIPTOR         | 165   | 10  | 9    |
| AMOUNT-MISC                  | 149   | 14  | 7    |
| META                          | 128   | 12  | 13   |
| PROPERTY-TYPE                | 124   | 10  | 4    |
| CONDITION-TYPE               | 119   | 2   | 1    |
| REFERENCE                     | 106   | 10  | 11   |
| PROPERTY-UNIT                | 92    | 7   | 8    |
| APPARATUS-UNIT               | 89    | 6   | 16   |
| CHARACTER-APPARATUS          | 54    | 2   | 11   |
| APPARATUS-PROPERTY-TYPE      | 26    | 0   | 6    |

Table 3: Entities in the materials science procedural text corpus

| Relation class             | train | dev | test |
|----------------------------|-------|-----|------|
| NEXT_OPERATION             | 2,898 | 184 | 202  |
| RECIPE_PRECURSOR           | 876   | 67  | 89   |
| RECIPE_TARGET              | 363   | 31  | 22   |
| PARTICIPANT_MATERIAL       | 1,723 | 113 | 124  |
| SOLVENT_MATERIAL           | 463   | 28  | 33   |
| ATMOSPHERIC_MATERIAL       | 183   | 11  | 14   |
| PROPERTY_OF                | 586   | 35  | 21   |
| CONDITION_OF               | 1,810 | 132 | 107  |
| NUMBER_OF                  | 2,805 | 219 | 209  |
| AMOUNT_OF                  | 1,512 | 130 | 121  |
| DESCRIPTOR_OF              | 1,495 | 91  | 102  |
| BRAND_OF                   | 423   | 42  | 41   |
| TYPE_OF                    | 164   | 7   | 13   |
| APPARATUS_OF               | 455   | 20  | 36   |
| APPARATUS_ATTR_OF          | 90    | 6   | 11   |
| COREF_OF                   | 267   | 12  | 14   |

Table 4: Relations in the materials science procedural text corpus
operation; **Apparatus_Attr**. **of**, which indicates a numerical condition of on equipment; and **Descriptor**. **of**, which indicates other conditions. For these labels, the rules are defined based only on the labels of head and tail entities and the distance between them. We explain the detailed rules in the remainder of this section.

**Property_Of:** The relation can take **Property-Unit** or **Property-Misc** as the head and **Material** or **NonRecipe-Material** as the tail. When **Property-Unit** is a head, it is linked to the nearest **Material** in the sentence. When **Property-Misc** is a head, it is linked to the nearest **Material** or **NonRecipe-Material** in the sentence.

**Condition_Of:** **Condition-Unit** and **Condition-Misc** are linked to the nearest **Operation** with the relation in the sentence.

**Number_Of:** **Number** is linked to the nearest **Property-Unit**, **Condition-Unit**, or **Apparatus-Unit** that appear after the **Number** in the sentence.

**Amount_Of:** The relation is linked from **Amount-Unit** and **Amount-Unit** to the nearest **Material** or **NonRecipe-Material** in the sentence.

**Descriptor_Of:** When **Material-Descriptor** is a head, it is linked to the nearest **Material** or **NonRecipe-Material** in the sentence. When **Apparatus-Descriptor** is a head, it is linked to the nearest **Synthesis-Apparatus** in the sentence.

**Apparatus_Of:** The relation is linked from **Synthesis-Apparatus** and **Characterization-Apparatus** to the nearest **Operation** with the priority given to the **Operation** that appear before the **Apparatus** in the sentence.

**Type_Of:** **Property-Type** and **Apparatus-Property-Type** are linked to the nearest **Property-Unit** and **Apparatus-Unit** in the sentence with the relation, respectively. When **Condition-Type** is a head, it is linked to the nearest **Condition-Unit** that appears before the **Condition-Type** in the sentence.

**Brand**. **of:** The relation is linked from **Brand** to the nearest entities that may have brands (i.e., **Material**, **NonRecipe-Material**, **Synthesis-Apparatus**, and **Characterization-Apparatus**) in the sentence.

| Parameter             | Range            | Value      |
|-----------------------|------------------|------------|
| Learning rate         | [1e-5, 1e-2]     | 0.001      |
| No. of GCN layers     | [0, 4]           | 3          |
| $d_{max}$             | [1, 10]          | 4          |
| Dimension of hidden layers | [32, 128]    | 85         |
| No. of FC$^u$ layers  | [1, 5]           | 4          |
| No. of FC$^t$ layers  | [1, 5]           | 1          |
| Dropout rate          | [0.0, 1.0)       | 0.46       |
| Dimension of $e^{old}_{ij}$ | [1, 32]    | 3          |
| Maximum distance for $b_{ij}$ | [1, 32]   | 3          |
| Dimension of $b_{100}$ | [1, 100]      | 1          |
| Use bidirectional GCN | True or False    | True       |

Table 5: Search space for optimization of hyper-parameters and the selected values after optimization

| Relation | Prec. | Recall | F-score |
|----------|-------|--------|---------|
| NEXT_OPERATION | 0.622 | 0.693 | 0.656   |
| RECIPE_PRECURSOR   | 0.632 | 0.539 | 0.582   |
| RECIPE_TARGET    | 0.640 | 0.727 | 0.681   |
| PARTICIPANT_MATERIAL | 0.641 | 0.476 | 0.546   |
| SOLVENT_MATERIAL  | 0.491 | 0.818 | 0.614   |
| ATMOSPHERIC_MATERIAL   | 0.733 | 0.786 | 0.759   |
| PROPERTY_Of   | 0.773 | 0.810 | 0.791   |
| CONDITION_Of   | 0.798 | 0.850 | 0.824   |
| NUMBER_Of      | 0.874 | 0.962 | 0.916   |
| AMOUNT_Of      | 0.722 | 0.645 | 0.681   |
| DESCRIPTOR_Of  | 0.761 | 0.814 | 0.787   |
| BRAND_Of       | 0.567 | 0.415 | 0.479   |
| TYPE_Of       | 0.900 | 0.692 | 0.783   |
| APPARATUS_Of   | 0.657 | 0.639 | 0.648   |
| APPARATUS_Attr_of | 0.769 | 0.909 | 0.833   |
| COREF_Of       | 0.875 | 0.500 | 0.636   |
| Overall       | 0.717 | 0.722 | 0.720   |

Table 6: Detailed results using **EDIT** without **RULE** on the test set

**Apparatus_Attr**. **of:** **Apparatus-Unit** is linked to the nearest **Synthesis-Apparatus** or **Characterization-Apparatus**.

**Coref**. **of:** The relation is not detected by the rules because it is difficult to describe rules.

**C Tuning Details**

We tuned our model using a hyper-parameter optimization framework Optuna (Akiba et al., 2019). We searched for the hyper-parameters that maximize micro-F scores within 600 trials on the development set. We employed the tree-structured Parzen estimator algorithm (Bergstra et al., 2011) for the sampler and the successive halving algorithm (Li et al., 2020) for the pruner with default options in Optuna. In each trial of the search, we trained our model for 100 epochs, which was confirmed by preliminary experiments to be sufficient for convergence. We searched hyper-parameters on 20 NVIDIA GPUs, which include Tesla V100, TITAN V, RTX 3090, and GTX TITAN Xp GPUs.
We defined the search space as shown in Table 5; the hyper-parameters for the search are composed of the learning rate for Adam, the number of GCN layers, the maximum edit distance $d_{\text{max}}$, the dimensions of all hidden layers, the number of $\text{FC}^{\text{out}}$ layers, the number of $\text{FC}^h$ and $\text{FC}^t$ layers, the dropout rate, the dimension of $e_{ij}^{\text{old}}$, the maximum distance and the dimension for $b_{ij}$ and whether to use bidirectional GCNs or uni-directional GCNs. In the table, the range column shows the range of values to search and the final value column shows the rounded selected values after the optimization.

## D Detailed Evaluation Results

Our editing models for evaluation are trained with a TITAN V GPU for EDIT with RULE and a Tesla V100 GPU for the others. The training takes about 6 hours 30 minutes with EDIT-IE using RULE and 21 hours with EDIT not using RULE.

We show the detailed evaluation results with precision (Prec.), recall, and F-score on the test set in Table 6 for EDIT without RULE, Table 7 for RULE, and Table 8 for EDIT-IE without RULE. The results show the relations that are not covered by RULE, i.e., Recipe_Precursor and Coref.Of, are extracted by our approach, and for these classes, EDIT without RULE show the better performance than the models with RULE. Some relations with high performance by RULE, including Next_Operation, Condition_Of, and Descriptor_Of, are extracted by EDIT-IE with RULE in high performance. This shows our approach can effectively utilize the outputs of RULE.

### Table 7: Detailed results with RULE on the test set

| Relation         | Prec. | Recall | F-score |
|------------------|-------|--------|---------|
| Next_Operation   | 0.905 | 0.990  | 0.946   |
| Recipe_Precursor | 0.810 | 0.573  | 0.671   |
| Recipe_Target    | 0.560 | 0.636  | 0.596   |
| Solvent_Material | 0.733 | 0.667  | 0.698   |
| Participant_Material | 0.624 | 0.790  | 0.698   |
| Atmospheric_Material | 0.778 | 1.000  | 0.875   |
| Property_Of      | 0.905 | 0.905  | 0.905   |
| Condition_Of     | 0.953 | 0.944  | 0.948   |
| Number_Of        | 0.958 | 0.990  | 0.974   |
| Amount_Of        | 0.854 | 0.868  | 0.861   |
| Descriptor_Of    | 0.941 | 0.931  | 0.936   |
| Brand_Of         | 0.880 | 0.537  | 0.667   |
| Type_Of          | 1.000 | 0.692  | 0.818   |
| Apparatus_Of     | 0.833 | 0.972  | 0.897   |
| Apparatus_Attr_Of| 0.769 | 0.909  | 0.833   |
| Coref_Of         | 0.750 | 0.429  | 0.545   |
| Overall          | 0.807 | 0.808  | 0.807   |

### Table 8: Detailed results using EDIT-IE with RULE on the test set

| Relation         | Prec. | Recall | F-score |
|------------------|-------|--------|---------|
| Next_Operation   | 0.905 | 0.990  | 0.946   |
| Recipe_Precursor | 0.730 | 0.414  | 0.528   |
| Recipe_Target    | 0.000 | 0.000  | 0.000   |
| Participant_Material | 0.419 | 0.800  | 0.550   |
| Solvent_Material | 0.697 | 0.418  | 0.522   |
| Atmospheric_Material | 1.000 | 0.378  | 0.549   |
| Property_Of      | 0.905 | 1.000  | 0.950   |
| Condition_Of     | 0.963 | 0.981  | 0.972   |
| Number_Of        | 0.943 | 0.961  | 0.952   |
| Amount_Of        | 0.744 | 0.865  | 0.800   |
| Descriptor_Of    | 0.931 | 0.979  | 0.955   |
| Brand_Of         | 0.561 | 0.920  | 0.697   |
| Type_Of          | 0.769 | 1.000  | 0.870   |
| Apparatus_Of     | 0.972 | 0.854  | 0.833   |
| Apparatus_Attr_Of| 0.909 | 0.769  | 0.833   |
| Coref_Of         | 0.000 | 0.000  | 0.000   |
| Overall          | 0.807 | 0.808  | 0.807   |