Clustering-based Inference for Zero-Shot Biomedical Entity Linking

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Abstract

Due to large number of entities in biomedical knowledge bases, only a small fraction of entities have corresponding labelled training data. This necessitates a zero-shot entity linking model which is able to link mentions of unseen entities using learned representations of entities. Existing zero-shot entity linking models however link each mention independently, ignoring the inter/intra-document relationships between the entity mentions. These relations can be very useful for linking mentions in biomedical text where linking decisions are often difficult due mentions having a generic or a highly specialized form. In this paper, we introduce a model in which linking decisions can be made not merely by linking to a KB entity but also by grouping multiple mentions together via clustering and jointly making linking predictions. In experiments on the largest publicly available biomedical dataset, we improve the best independent prediction for zero-shot entity linking by 2.5 points of accuracy, and our joint inference model further improves entity linking by 1.8 points.

1 Introduction

Ambiguity is inherent in the way entities are mentioned throughout natural language text. Grounding such ambiguous mentions to their corresponding entities, the task of entity linking, is critical to many applications: automated knowledge base construction and completion (Riedel et al., 2013; Surdeanu et al., 2012), information retrieval (Meij et al., 2014), smart assistants (Balog and Kenter, 2019), question answering (Dhingra et al., 2020), text mining (Leaman and Lu, 2016; Murty et al., 2018).

Consider the excerpt of text from a biomedical research paper in Figure 1, the three highlighted mentions (expression, facial expressions, and facially expressive) all link to the same entity, namely \texttt{C0517243} – Facial Expression in the leading biomedical KB, Unified Medical Language System (UMLS).

The mention expression is highly ambiguous and easily confused with the more prevalent entity, Gene expression. With sufficient training examples (or sufficiently rich structured information in the knowledge-base) this linking decision may become easier. However, in biomedical (Mohan and Li, 2019) and other specialized domains (Logeswaran et al., 2019), it is often the case that the knowledge-base information is largely incomplete and furthermore the scarcity of training data leads to a setting in which most entities have not been observed at training (i.e., zero-shot setting).

State-of-the-art methods for zero-shot entity linking make predictions for each mention independently (Logeswaran et al., 2019; Wu et al., 2019). In this way, the methods may have difficulty linking mentions which, as in the example above, have little lexical similarity with the entities in the knowledge-base, as well as mentions for which...
the context is highly ambiguous. These mentions cannot directly use information from one mention (or its linking decision) to inform the prediction of another mention. On the other hand, entity linking methods that do jointly consider entity linking decisions (Ganea and Hofmann, 2017; Le and Titov, 2018) are not well suited for the zero-shot domain as they were designed for all of the entities in the knowledge-base to have example mentions or metadata, e.g., pre-trained embeddings, at training time.

In this paper, we propose a zero-shot entity linking model in which entity mentions are either (1) linked directly to an entity in the knowledge-base or (2) join a cluster of other mentions and link as a cluster to an entity in the knowledge-base. Some mentions may be difficult to link directly to their referent ground truth entity, but may have very clear coreference relationships to other mentions. So long as one mention among the group of mentions clustered together links to the correct entity the entire cluster can be correctly classified. We describe both an inference procedure as well as training objective for optimizing the model’s inference procedure, based on recent work on supervised clustering (Yadav et al., 2019).

It is important to note that our approach does not aim to do joint coreference and linking, but rather makes joint linking predictions by clustering together mentions that are difficult to link directly to the knowledge-base. For instance, in Figure 1, the mention expression may be difficult to link to the ground truth Facial expression entity in the knowledge-base because the mention can refer to a large number of entities. However, the local syntactic and semantic information of the paragraph give strong signals that expression is coreferent with facial expression, which is easily linked to the correct entity.

We perform experiments on MedMentions (Mohan and Li, 2019), the largest publicly available biomedical research paper entity linking dataset. Over 42% of the entities in the test set of this data are not seen at training, making it appropriate for the zero-shot task. We find that our approach improves 1.8% over the baseline method and perform an comprehensive analysis of where the improvements take place for our method.

2 Background

Each document $D \in \mathcal{D}$, has a set of mentions $\mathcal{M}(D) = \{m_1^{(D)}, m_2^{(D)}, \ldots, m_N^{(D)}\}$. The task of entity linking is to classify each mention $m_i$ as referent to a single entity $e_i$ from a KB of entities. We use $\mathcal{E}(m_i)$ to refer to the ground truth entity of mention $m_i$ and $\hat{e}_i$ to refer to the predicted entity.

**End-to-end linking.** End-to-end entity linking refers to the task of beginning with the tokens in the document $D$, predicting mention spans and then predicting entity linking assignments for the mention spans.

**Knowledge-bases.** We assume that we are given a knowledge-base corresponding to a closed world of entities. These KBs are typically massive: English Wikipedia contains just over 6M entities\(^1\) and the 2020 release of the UMLS contains 4.28M entities\(^2\). We describe in Section 5.1 the details of the KB used in this work.

**Candidate Generation.** Given the massive number of entities that a mention may refer to, previous work (Ganea and Hofmann, 2017; Le and Titov, 2018; Logeswaran et al., 2019; Wu et al., 2019) typically uses a candidate generation step to reduce the restrict the number of entities considered for a given mention, $m$, to a candidate set $\Gamma(m)$. The recall of this step is critical to the final performance of entity linking models.

**Zero-Shot Setting.** We refer to the zero-shot setting as one in which we have entities appearing at test time for which there are no training examples.

3 Model

In this section, we describe our clustering-based approach for jointly making entity linking predictions for a set of mentions. Our proposed inference method builds a graph where the nodes are the union of all of the mentions and entities and the edges have weights denoting the affinities between the endpoints. To make linking decisions, we cluster the nodes of the graph such that each cluster contains exactly one entity, following which each mention is assigned to the entity in its cluster.

3.1 Clustering-based Entity Linking

Let $\varphi : \mathcal{M} \times \mathcal{M} \to \mathbb{R}$ and $\psi : \mathcal{M} \times \mathcal{E} \to \mathbb{R}$ be parameterized functions which compute mention-mention and mention-entity affinities, respectively. The exact parameterizations of these functions are detailed in Section 3.2.

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\(^1\)number of content pages as of May 20, 2020, https://en.wikipedia.org/wiki/Special:Statistics

\(^2\)https://www.nlm.nih.gov/research/umls/knowledge_sources/metathesaurus/release/notes.html
Define the graph $G = (V, E)$ where $V = \mathcal{M} \cup \mathcal{E}$ and $E = \mathcal{M} \times \mathcal{M} \cup \{(m, e) : e \in \Gamma(m)\}$. The weight of each edge, $w(v_i, v_j)$ for $v_i, v_j \in V$, is determined by $\varphi$ or $\psi$ depending on the vertices of the edge: $w(m_i, m_j) = \varphi(m_i, m_j)$ and $w(m_i, e_l) = \psi(m_i, e_l)$. Linking decisions for each mention are determined by clustering the vertices of $G$ under the constraint that every entity must appear in exactly one cluster.

Given the graph $G$, we start with every node in their own individual cluster. We define affinity between a pair of clusters as the strongest cross-cluster edge between nodes in the two clusters. iteratively, we greedily merge clusters by choosing a pair of clusters with largest affinity between them under the constraint that we cannot merge two clusters which both contain an entity. When every cluster contains exactly one entity, this process can no longer merge any clusters, and thus terminates. Each mention is linked to the entity present in its cluster at the end of inference. Algorithm 1 describes this process of constructing the graph and clustering nodes to make linking decisions more formally.

Figure 2 shows the proposed inference in action on five entities and six mentions. Initially, every mention and entity start in a singleton cluster. In the first round, clusters $\{m_1\}$ and $\{m_2\}$ are merged, followed by merger of $\{e_3\}$ and $\{m_6\}$ in the second round, and so on. Note that in fifth round, clusters $c_1 = \{m_4, e_2\}$ has higher affinity with $c_2 = \{m_1, m_2, m_3, e_1\}$ than with $c_3 = \{m_5\}$, yet $c_1$ and $c_3$ are merged instead of $c_1$ and $c_2$ due to the constraint that we cannot merge two clusters which both contain an entity. At the end, every mention is clustered together with exactly one entity, and there could be entities present as singleton clusters such as $\{e_4\}$ and $\{e_5\}$. Note that $m_3$ correctly links to its gold entity $e_1$ as a result of being clustered with mentions $m_1$, $m_2$ even though it has higher affinity with entity $e_3$: $w(m_3, e_3) > w(m_3, e_1)$.

### 3.2 Affinity Models

We parameterize $\psi(\cdot, \cdot)$ and $\phi(\cdot, \cdot)$ using two separate deep transformer encoders (Vaswani et al., 2017) for our mention-mention affinity model and mention-entity affinity model — specifically we use the BERT architecture (Devlin et al., 2019) initialized using the weights from BioBERT (Lee et al., 2019).

#### 3.2.1 Mention-Mention Model

The mention-mention model is also a cross-encoder, taking as input a pair of mention in context and producing a single scalar affinity for every pair. The input tokens take the form:

$$[CLS] < m_i > [SEP] < m_j > [SEP]$$

where $< m_i > := c_l [START] m_i [END] c_r$

where $m_i$ is the mention tokens and $c_l$ and $c_r$ are the left and right context of the mention in the text, respectively. The [START] and [END] tokens are special tokens fine-tuned to signify the start and end of the mention in context, respectively. We restrict the length of each input sequence to have

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3This process is equivalent to single-linkage hierarchical agglomerative clustering with the constraint that two entities cannot be in the same cluster.
Algorithm 1 Clustering Inference for Linking

1: Input: \((\mathcal{M}, \mathcal{E}, \Gamma, \varphi, \psi)\)  
2: Output: \(\{(m_i, e_i)\}_{i=1}^{\mathcal{M}}\)  
3: \(\triangleright\) Construct the graph \(G\)  
4: \(E = \emptyset\)  
5: for \(m_i \in \mathcal{M}\) do  
6: \(\quad\) for \(m_j \in \mathcal{M}_{(D_i)} \setminus \{m_i\}\) do  
7: \(\quad\) \(E = E \cup \{(m_i, m_j, \varphi(m_i, m_j))\}\)  
8: \(\quad\) for \(e_l \in \Gamma(m_i)\) do  
9: \(\quad\) \(E = E \cup \{(m_i, e_l, \psi(m_i, e_l))\}\)  
10: Construct \(G = (V, E)\) from edge set \(E\)  
11: Let \(S\) be the edges sorted in descending order  
12: \(\triangleright\) Cluster nodes of \(G\) under linking constraint  
13: \(\quad\hat{C} = \{\{v\} | v \in V\}\)  
14: for \((s, t) \in S\) do  
15: \(\quad\) if \(\hat{C}(s) \cap \mathcal{E} = \emptyset\) or \(\hat{C}(t) \cap \mathcal{E} = \emptyset\) then  
16: \(\quad\) \(\hat{C} = \hat{C} \setminus \{\hat{C}(s), \hat{C}(t)\}\)  
17: \(\quad\) \(\hat{C} = \hat{C} \cup \{\hat{C}(s) \cup \hat{C}(t)\}\)  
18: \(\triangleright\) Make linking decisions based on clustering  
19: \(\quad L = \{\}\)  
20: for \(C \in \hat{C}\) do  
21: \(\quad\) \(M = C \cap \mathcal{M}\)  
22: \(\quad\) \(\{\hat{e}\} = C \cap \mathcal{E}\)  
23: for \(m \in M\) do  
24: \(\quad\) \(L = L \cup \{(m, \hat{e})\}\)  
25: return \(L\)

For training purposes, we use triplet max-margin based training objectives to train both models. The most important aspect of our procedure is how we pick negatives during training. For the mention-entity model, we restrict our negatives to be from the candidate set. For the mention-mention model, we restrict our negatives to come from mentions within the same document. From these sets of possible negatives we choose the top-\(k\) most offending ones according to the instantaneous state of the model – i.e. the negatives with highest predicted affinities according to the model at that point during training. The following sections detail the training procedures for both models.

4.1 Mention-Mention Affinity Training

To train the mention-mention affinity model we use a variant of the maximum spanning tree (MST) supervised single linkage clustering algorithm presented in Yadav et al. (2019). Let \(\mathcal{M}_{e_l}^{(D)} = \{m \in \mathcal{M}(D) | E(m) = e_l\}\) be the set of mentions referring to entity \(e_l\) in any one document and the set of ground truth clusters be represented by \(C^* = \mathcal{M}_{e_l}^{(D)} | e_l \in \mathcal{E}\). Let \(P\) be the set of positive training edges: the edges of the MST of the complete graph on the cluster \(C \in C^*\). Let \(N_{\varphi}(m_s)\) be the \(k\)-nearest within document negatives to the anchor point \(m_s \in C\) according to the current state of the model during training. The objective of this training procedure is to minimize the following triplet max-margin loss\(^4\) with margin \(\mu\) for each cluster \(C \in C^*\):

\[
\mathcal{L}_{\varphi}(\theta; C) = \sum_{m_s, m_+, m_- \in P} \sum_{m_- \in N_{\varphi}(m_s)} \ell_{\varphi,\mu}(m_s, m_+, m_-),
\]

where \(\ell_{\varphi,\mu}(a, p, n) = [\varphi(a, n) - \varphi(a, p) + \mu]_+\).

4.2 Mention-Entity Affinity Training

For the mention-entity model, we use a triplet max-margin based objective with margin \(\mu\) where

\[^4\text{Define } [x]_+ = \max(x, 0)\]
|        | Train | Dev   | Test  |
|--------|-------|-------|-------|
| # Mentions | 119.8K | 39.8K | 39.9K |
| # Entities  | 18.5K  | 8.6K  | 8.4K  |
| % Entities seen | 100%  | 57.7% | 57.5% |

Table 1: Statistics train/dev/test split of MedMentions dataset, including the percent of ground truth entities seen during training.

anchor is a mention \( m \) in the training set, the positive is the ground truth entity \( e_+ = E(m) \), and the negatives are chosen from the candidate set \( \Gamma(m) \). Denote the \( k \) most offending negatives according to the current state of the model during training as \( N_\psi(m) \subseteq \Gamma(m) \setminus \{E(m)\} \). Formally, the loss is

\[
L_\psi(\theta; M) = \sum_{m, e_+} \sum_{e_- \in N_\psi(m)} \ell_\psi,\mu(m, e_+, e_-),
\]

where \( \ell_\psi,\mu(a, p, n) = [\psi(a, n) - \psi(a, p) + \mu]_+ \).

4.3 Training Details

We optimize both the models with mini-batch stochastic gradient descent using the Adam optimizer (Kingma and Ba, 2014) with recommended learning rate of 5e-5 (Devlin et al., 2019) for one epoch. We compute the top-\( k \) most offending negatives on-the-fly for each batch by running the model in inference mode proceeding each training step.

5 Experiments

We evaluate on biomedical entity linking using the MedMentions dataset (Mohan and Li, 2019). We compare to state-of-the-art methods. We then analyze the performance of our method in more detail and provide qualitative examples demonstrating our approaches’ ability to use mention-mention relationships to improve candidate generation and linking.

5.1 MedMentions

MedMentions is a publicly available\(^5\) dataset consisting of the titles and abstracts of 4,392 PubMed articles. The dataset is hand-labeled by annotators and contains labeled mention spans and entities linked to the 2017AA full version of UMLS. Following the suggestion of Mohan and Li (2019), we use the ST21PV subset, which restricts the entities linked in documents to a set of 21 entity types that were deemed most important for building scientific knowledge-bases. We refer the readers to Mohan and Li (2019) for a complete analysis of the dataset and provide a few important summary statistics here. The train/dev/test split partitions the PubMed articles into three non-overlapping groups. This means that some entities seen at training time will appear in dev/test and other entities will appear in dev/test but not at training time. In fact, a large number of entities that appear in dev/test time are unseen at training, about 42% of entities.

Previous work has evaluated on MedMentions using unfairly optimistic candidate generation settings such as using only 10 candidates including the ground truth (Zhu et al., 2019) or restricting candidates to entities appearing somewhere in the MedMentions corpus (Murty et al., 2018). We instead work in a much more general setting where all entities in UMLS are considered at candidate generation time and the generated candidates might not include the ground truth entity.

5.1.1 Preprocessing

The MedMentions ST21PV corpus is processed as follows: (i) Abbreviations defined in the text of each paper are identified using AB3P (Sohn et al., 2008). Each definition and abbreviation instance is then replaced with the expanded form. (ii) The text of each paper in the corpus is tokenized and split into sentences using CoreNLP (Manning et al., 2014). (iii) Overlapping mentions are resolved by preferring longer mentions that begin earlier in each sentence, and mentions are truncated at sentence boundaries. This results in 379 mentions to be dropped from the total of 203,282. (iv) Finally, the corpus is saved into the IOB2 tag format. Full dataset statistics are available in Table 1.

5.1.2 Candidate Generation

We use a character \( n \)-gram TF-IDF model to produce candidates for all of the mentions in all splits. The candidate generator utilizes the 200k most frequent character \( n \)-grams, \( n \in \{2 \ldots 5\} \) and the 200k most frequent words in the names in \( E \) to produce sparse vectors for all of the mentions and entity descriptions (which in our case is the canonical name, the type, and a list of known aliases and synonyms). We restrict our candidate set to be of size at most 50. The recall for this candidate generator is 85.5%, 85.5%, and 85.4% on the train, dev, and test splits respectively.
Table 2: Linking accuracy on MedMentions dataset.

|               | Overall Acc. | Acc. on Seen | Acc. on Unseen |
|---------------|--------------|--------------|---------------|
| INDEPENDENT   | 72.0         | 75.2         | 60.7          |
| JOINT (ours)  | 72.7         | 76.0         | 61.1          |

Table 3: Linking accuracy on MedMentions dataset conditioned on the gold mention type.

|               | Overall Acc. | Acc. on Seen | Acc. on Unseen |
|---------------|--------------|--------------|---------------|
| TaggerOne     | 73.8         | -            | -             |
| Independent   | 76.3         | 78.8         | 67.4          |
| Joint (ours)  | 78.1         | 80.7         | 69.2          |

5.2 Results

This section presents the results of our clustering-based inference procedure, JOINT, in comparison to the previous state-of-the-art model TaggerOne and independent inference, INDEPENDENT, using our mention-entity affinity model. In this section, we use seen and unseen to refer to the sets of entities seen and unseen at training, respectively.

Table 2 shows performance of INDEPENDENT and JOINT inference procedure on MedMentions dataset using gold mention segmentations. Overall, JOINT improves accuracy by 0.7, making 0.8 and 0.4 improvement for seen and unseen entities respectively. Table 3 shows performance of INDEPENDENT, JOINT, and TaggerOne when the candidates are limited to ground-truth type of the mention. Performance of both INDEPENDENT and JOINT improve when using gold type information as it rules out some candidate entities based on a type mismatch, and JOINT inference offers 1.8 points improvement over INDEPENDENT and 4.3 points over TaggerOne.

Finally, Table 4 shows end-to-end entity linking results for different inference methods using TaggerOne’s predicted mention segmentation. Overall performance of all these models is penalized due errors in mention detection step. Many of the errors made in the mention detection step are more obscure mentions where our inference approach is designed to succeed. Nevertheless, JOINT inference outperforms both TaggerOne and INDEPENDENT.

6 Related Work

Entity linking is widely studied and often focused on linking mentions to Wikipedia entities (also known as Wikification) (Mihalcea and Csomai, 2007; Cucerzan, 2007; Milne and Witten, 2008; Hoffart et al., 2011; Ratinov et al., 2011; Cheng and Roth, 2013). Entity linking is often done independently for each mention in the document (Ratinov et al., 2011; Raiman and Raiman, 2018) or by modeling dependencies between predictions of entities in a document (Cheng and Roth, 2013; Ganea and Hofmann, 2017; Le and Titov, 2018).

In the biomedical domain, Unified Medical Language System (UMLS) is often used as a knowledge-base for entities (Mohan and Li, 2019; Leaman and Lu, 2016). While UMLS is a rich ontology of concepts and relationships between them, this domain is low resource compared to Wikipedia with respect to number of labeled training data for each entity mention. This leads to a zero-shot setting in datasets such as MedMentions (Mohan and Li, 2019) where new entities are seen at test time. Previous work has addressed this zero-shot setting using models of the type hierarchy (Murty et al., 2018; Zhu et al., 2019). This previous work (Murty et al., 2018; Zhu et al., 2019) uses an unrealistic candidate generation setting where the true positive candidate is within the candidate set and/or entities are limited to those in the dataset rather than those in the knowledge-base. The only candidate generation results on this data is using UMLS aliases.

Mention-mention relationships are also explored in (Le and Titov, 2018) which extends the pairwise CRF model (Ganea and Hofmann, 2017) to use mention-level relationships in addition to entity relationships. These works use attention in a way to build the context representation of the mentions. However, as mentioned by (Logeswaran et al., 2019) is not well suited for zero-shot linking.

Coreference (both within and across documents)
has also been explored by past work (Dutta and Weikum, 2015). This work uses an iterative procedure that performs hard clustering for the sake of aggregating the contexts of entity mentions. Durrett and Klein (2014) presents a CRF-based model for joint NER, within-document coreference, and linking. They show that jointly modeling these three tasks improves performance over the independent baselines. This differs from our work since we do not require coreference decisions to be correct in order to make correct linking decisions. Other work performs joint entity and event coreference (Barhom et al., 2019) but does not consider linking.

7 Conclusion

In this work, we presented a novel clustering-based inference procedure which enables joint entity linking predictions. We evaluate the effectiveness of our approach on the largest biomedical entity linking dataset and obtain new state-of-the-art results.

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