Knowledge-Rich Self-Supervised Entity Linking

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Abstract

Entity linking faces significant challenges, such as prolific variations and prevalent ambiguities, especially in high-value domains with myriad entities. Standard classification approaches suffer from the annotation bottleneck and cannot effectively handle unseen entities. Zero-shot entity linking has emerged as a promising direction for generalizing to new entities, but it still requires example gold entity mentions during training and canonical descriptions for all entities, both of which are rarely available outside of Wikipedia. In this paper, we explore Knowledge-Rich Self-Supervision (KRISS) for entity linking, by leveraging readily available domain knowledge. In training, it generates self-supervised mention examples on unlabeled text using a domain ontology and trains a contextual encoder using contrastive learning. For inference, it samples self-supervised mentions as prototypes for each entity and conducts linking by mapping the test mention to the most similar prototype. Our approach subsumes zero-shot and few-shot methods, and can easily incorporate entity descriptions and gold mention labels if available. Using biomedicine as a case study, we conducted extensive experiments on seven standard datasets spanning biomedical literature and clinical notes. Without using any labeled information, our method produces KRISSBERT, a universal entity linker for four million UMLS entities, which attains new state of the art across the board, outperforming prior best self-supervised methods by as much as over 20 absolute points in accuracy.

1 Introduction

Entity linking maps mentions to unique entities in a target knowledge base (Roth et al., 2014). It can be viewed as the extreme case of named entity recognition and entity typing, where the category number swells to tens of thousands or even millions. Entity linking is particularly challenging in high-value domains such as biomedicine, where variations and ambiguities abound. For instance, depending on the context, “PDF” may refer to a gene or Portable Document Format. Similarly, “ER” could refer to emergency room, the organelle endoplasmic reticulum, or the estrogen receptor gene. Moreover, the number of entities in domains such as biomedicine can be very large. The Unified Medical Language System (UMLS)1, a representative ontology for biomedicine, contains over four million entities.

Standard classification approaches such as MedLinker (Loureiro and Jorge, 2020) require example gold mentions for each entity and cannot effectively handle new entities for which there are no labeled examples in training. Recently, zero-shot entity linking has emerged as a promising direction for generalizing to unseen entities (Logeswaran et al., 2019; Wu et al., 2020), by learning to encode contextual mentions for similarity comparison against reference entity descriptions. Existing methods, however, require example gold entity mentions during training, as well as canonical descriptions for all entities. While applicable to Wikipedia entities, these methods are hard to generalize to other domains, where such labeled information is rarely available at scale.

In this paper, we explore Knowledge-Rich Self-Supervision (KRISS) for entity linking by leveraging readily available domain knowledge to compensate for the lack of labeled information (Figure 1). For entity linking, the most relevant knowledge source is the domain ontology. The core of an ontology is the entity list, which specifies the unique identifier and canonical name for each entity and is the prerequisite for entity linking. Our method only requires the entity list and unlabeled text that are readily available in any domain.

In training, KRISS uses the entity list to generate self-supervised mention examples from unlabeled

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1https://www.nlm.nih.gov/research/umls/index.html
text, and trains a contextual mention encoder using contrastive learning (Gao et al., 2014; Wu et al., 2020), by mapping mentions of the same entity closer. For inference, KRISS samples prototypes for each entity from the self-supervised mentions. Given a test mention, KRISS finds the most similar prototype and returns the entity it represents.

Prior methods that leverage domain ontology for entity linking often resort to string matching (against entity names and aliases), making them vulnerable to both variations and ambiguities. Recent methods such as SapBERT (Liu et al., 2021) can resolve variations to some extent, but they completely ignore mention contexts and cannot resolve ambiguities. For ambiguous mentions, they simply return all entities with a name or alias matching their predicted surface form, rather than predicting a unique entity for linking (see footnote 2 of Introduction in their paper).

In practice, an ontology may contain additional domain knowledge such as aliases and semantic relations among the entities (e.g., ISA hierarchy). Gold mention examples and canonical descriptions may also be available for some entities. KRISS provides a general framework for incorporating such information and generalizes zero-shot and few-shot entity linking methods. Aliases can be used to generate additional self-supervised mention examples. The ISA hierarchy can be leveraged to aid representation learning for rare entities. Gold mentions and entity descriptions can be used as positive examples in contrastive learning, as well as prototypes at inference.

We conduct our study on biomedicine, which serves as a representative high-value domain where prior methods are hard to apply. Among the four million biomedical entities in UMLS, less than 6% have some description available. Likewise, gold mention labels are available for only a tiny fraction of the entities. E.g., MedMentions (Mohan and Li, 2019), the largest biomedical entity linking dataset, only covers 35 thousand entities.

We applied our method to train KRISSBERT, a universal entity linker for all four million biomedical entities in UMLS, using only the entity list in UMLS and unlabeled text in PubMed². KRISSBERT can also incorporate additional domain knowledge in UMLS such as entity aliases and ISA hierarchy. We conducted extensive evaluation on seven standard biomedical entity linking datasets spanning biomedical literature and clinical notes.

²https://pubmed.ncbi.nlm.nih.gov/
KRISSBERT demonstrated clear superiority, outperforming prior state of the art by 10 points in average accuracy and by over 20 points in MedMentions.

KRISSBERT can be directly applied to few-shot or supervised entity linking with no additional training, by just adding gold mention examples as prototypes during inference. This simple universal model already attains comparable results as dataset-specific state-of-the-art supervised entity linking systems, each tailored to an individual dataset by limiting entity candidates and using additional supervision sources and more complex methods (e.g., coreference rules and joint inference).

To facilitate research and applications, we will release KRISSBERT upon publication.

2 Related Work

Entity linking Many end applications require mapping mentions to unique entities. E.g., knowing that some drug can treat some disease is not very useful, unless we know which drug and disease. Entity linking is inherently challenging given the large number of unique entities. Prior work often adopts a pipeline approach that first narrows entity candidates to a small set (candidate generation) and then learns to classify contexts of the mention and a candidate entity (candidate ranking) (Bunescu and Pașca, 2006; Cucerzan, 2007; Ratinov et al., 2011). Candidate generation often resorts to string matching or TF-IDF variants (e.g., BM25), which are vulnerable to variations. Ranking features are manually engineered or learned via various neural architectures (He et al., 2013; Ganea and Hofmann, 2017; Kolitsas et al., 2018). Additionally, entity relations (e.g., concept hierarchy) and joint inference have been explored for improving accuracy (Gupta et al., 2017; Murty et al., 2018; Cheng and Roth, 2013; Le and Titov, 2018). These methods are predominantly supervised, and suffer from the scarcity of annotated examples, especially given the large number of entities to cover. By contrast, KRISSBERT leverages self-supervision using readily available domain knowledge and unlabeled text, and can effectively resolve variations and ambiguities for millions of entities.

Zero-shot entity linking Recent work (Logeswaran et al., 2019) enables generalization to unseen entities by learning a cross-attention BERT model over the mention and entity contexts for candidate ranking. Gillick et al. (2019); Wu et al. (2020) introduce a bi-encoder that encodes the mention context and entity context separately, thus scaling to candidate generation and reducing recall loss due to mention variations. These methods, however, still require labeled information such as gold mention examples, which are not readily available in many high-value domains. This restricts their applicability to the Wikipedia domain, where labeled mentions can be gleaned from hyperlinks and entity pages. KRISSBERT, however, does not require labeled information and can learn from entity list and unlabeled text alone.

Knowledge-rich self supervision Domain ontology such as UMLS has been applied to self-supervise biomedical named entity recognition (Zhang and Elhadad, 2013; Almgren et al., 2016). Recently, Sung et al. (2020); Liu et al. (2021) propose SapBERT for mention normalization by conducting contrastive learning over synonyms from UMLS. However, SapBERT completely ignores mention contexts. It can resolve some variations but not ambiguity. As Angell et al. (2021) points out, given an ambiguous mention, SapBERT would return all possible entities with matching surface form and stop short of linking. Their evaluation is overly optimistic, considering an instance correct if any of the proposed entities matches the gold one. By contrast, we apply contrastive learning on mention contexts, and leverage unlabeled text to generate self-supervised examples. SapBERT relies on synonyms to learn spelling variations. Our approach can learn with just the canonical name for each entity, as self-supervised mention examples naturally capture contexts where synonymous mentions may appear in.

Contrastive learning conducts representation learning by mapping semantically similar instances to nearby points and dissimilar ones away from each other (Hadsell et al., 2006). Contrastive loss is often a variant of noise-contrastive estimation (NCE) that normalizes against negative (dissimilar) examples (Gutmann and Hyvärinen, 2010). A popular choice is InfoNCE (Oord et al., 2018), where each mini-batch samples a query instance $(q)$, one positive (similar) example $k+$, a few negative (dissimilar) examples $k_1$’s, and optimizes the softmax of the query’s dot product with the positive example $L(q) = -\log(\exp(q \cdot k+)/\sum_i \exp(q \cdot k_i))$.

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3 The SapBERT paper states: “In this work, biomedical entity refers to the surface forms of biomedical concepts”. As aforementioned, many surface forms of biomedical entities are highly ambiguous (e.g., “PDF”, “ER”).
In computer vision, contrastive learning is often synonymous with self-supervised learning, where “similar” images are generated using data augmentation techniques assumed to preserve semantics (e.g., crop, resize, recolor) (Wu et al., 2018; Oord et al., 2018; He et al., 2019; Chen et al., 2020). In NLP, contrastive estimation has been applied to probabilistic unsupervised learning (by approximating the partition function with a tractable neighborhood) (Smith and Eisner, 2005; Poon et al., 2009). With the rise of neural representation, contrastive learning has also been applied to information retrieval (Huang et al., 2013; Shen et al., 2014), knowledge graph embedding (Bordes et al., 2013; Yang et al., 2015), entity linking (Loureiro and Jorge, 2020; Logeswaran et al., 2019; Wu et al., 2020), question answering (Karpukhin et al., 2020), typically with supervised labeled examples. In this paper, we apply contrastive learning to self-supervised entity linking where “similar” mentions are derived from unlabeled text using entity names and other relevant domain knowledge, without required any labeled information.

3 Knowledge-Rich Self-Supervision for Entity Linking

Entity linking grounds textual mentions to unique entity entries in a given database/dictionary. Formally, the goal of entity linking is to learn a function \( \text{Link} : m^t \rightarrow e \) that maps a mention \( m \) in text span \( t \) to the unique entity \( e \) that \( m \) represents in the context of \( t \). For brevity, we will drop the superscript \( t \) when the context is clear.

Supervised entity linking has access to labeled mention examples \((m, e)\). Zero-shot (few-shot) entity linking has access to zero (a few) labeled mention examples for test entities; it may also have access to labeled mentions for non-test entities. For example, Logeswaran et al. (2019); Wu et al. (2020) uses gold mentions derived from Wiki hyperlinks.

By contrast, self-supervised entity linking assumes no access to any gold mention examples. In the knowledge-rich self-supervision setting (KRISS), we assume that only a domain ontology \( O \) and an unlabeled text corpus \( T \) are available. In particular, we require the availability of an entity list, which specifies for each entity the unique identifier and canonical name. Entity list is the prerequisite for entity linking, as it provides the targets for linking. Our framework can also incorporate other knowledge that might be available in an ontology, as shown in subsection 3.5.

3.1 Generating Self-Supervision

For each entity, KRISS searches its canonical name (with case preserved) in \( T \) and returns a fixed-size window as context. This instantly yields a large collection of noisy mention examples \((m, e)\).

3.2 Contrastive Learning

Given contextual mention examples, we train a mention encoder using contrastive learning by mapping mentions of the same entity closer and mentions of different entities farther apart. Specifically, we adopt the InfoNCE loss (Oord et al., 2018) that uses in-batch negative for normalization.

A mini-batch comprises \( B \) samples from \( B/2 \) unique entities, with two sampled contextual mentions for each: \( \{m_{b,i} : b \in \ldots B/2, i \in \{-1, 1\}\} \). Each contextual mention is used as the query in turn to compute the InfoNCE loss against others in the batch, with the average loss being:

\[
\frac{1}{B} \sum_{b,i} - \log \frac{\exp(C(m_{b,i}) \cdot C(m_{b,-i}))}{\sum_{(b',i') \neq (b,i)} \exp(C(m_{b,i}) \cdot C(m_{b',i'}))}
\]

Here, \( C(\cdot) \) refers to the contextual mention encoder. We use a transformer-based model with entity markers added around each mention, and return the [CLS] representation as the encoding. See Appendix Figure 3.

3.3 Linking with Self-Supervised Prototypes

For linking at test time, we sample a small set of self-supervised mentions for each entity \( e \) as reference prototypes, denoted as \( \text{Proto}(e) \). Given a test mention \( m \), we return the entity with the most similar reference prototype:

\[
\text{Link}(m) = \arg \max_e \max_{m' \in \text{Proto}(e)} C(m) \cdot C(m')
\]

3.4 Cross-Attention Candidate Ranking

In contrastive learning (subsection 3.2), we follow Wu et al. (2020) to adopt the bi-encoder formulation (Humeau et al., 2020), where each contextual mention is encoded independently. This helps scale linking with millions of entities without separating candidate generation from ranking, as reference prototype encoding can be pre-computed offline. As will be shown in experiments, this bi-encoder version of KRISSBERT already attains substantial gain over prior state of the art in self-supervised entity linking. Similar to Wu et al. (2020), we can further improve linking accuracy by replacing the bi-encoder with a cross-attention transformer-based method.
model over the contextual mention pairs. Similar to the bi-encoder setting, entity markers are appended to mentions and the [CLS] representation is used to classify whether the mention pair refer to the same entity. See Appendix Figure 4.

3.5 Incorporate Additional Knowledge

Our self-supervised entity linking formulation can easily incorporate other knowledge available in an ontology, either by generating additional mention examples from unlabeled text, or by creating special entity-centric examples.

**Aliases** Ontology often includes aliases for some entities. The alias lists are generally incomplete and aliases such as acronyms are highly ambiguous. So they can’t be used as a definitive source for candidate generation. However, aliases can be used in KRISS to generate additional self-supervised mentions from unlabeled text, just like the canonical name. To avoid introducing too much noise, aliases shared by multiple entities are skipped.

**Semantic hierarchy** Ontology often organizes entities in a hierarchy via ISA relations among entities. E.g., in UMLS, the ER gene is assigned a Semantic Tree Number (A1.2.3.5), which specifies the ISA path from root to its entity type (Gene or Genome): Entity → Physical Object → Anatomical Structure → Fully Formed Anatomical Structure → Gene or Genome. KRISS uses this information to generate an entity-centric reference, by concatenating the entity type and semantic hierarchy components, separated by [SEP]. It is used just like mention examples. (We have experimented with learning a separate encoder for them but there is negligible difference in performance.)

**Entity description** For a small fraction of common entities, manually written descriptions may be available. In UMLS, less than 6% of entities have description, so they can’t be used as the main source for contrastive learning and linking. Still, the information may be useful and can be incorporated in KRISS by concatenating with semantic hierarchy in generating the entity-centric reference.

3.6 Supervised Entity Linking

KRISS has no access to any labeled mention examples in training, let alone labeled mentions for test entities. So by definition, it always conducts zero-shot entity linking. Given a new entity at test time, KRISS generates self-supervised mention prototypes by searching its canonical name in unlabeled text. Unlike prior work on zero-shot entity linking (Logeswaran et al., 2019; Wu et al., 2020), KRISS doesn’t require manually written entity descriptions that are scarcely available, thus is more generally applicable.

If labeled mention examples are available, KRISS can also be used for few-shot or supervised entity linking, with zero additional training, as in lazy learning (Wettschereck et al., 2004). In this case, gold mention examples from target training data are used as mention prototypes for linking, replacing the noisy self-supervised ones. KRISS can also use labeled examples to fine-tune the self-supervised model, which should yield additional accuracy gains; we leave it to future work.

4 Experiments

We use biomedicine as a representative high-value domain and conduct a thorough study on knowledge-rich self-supervised entity linking.

4.1 Entity Linking Benchmark

We conduct our experiments on seven standard entity linking datasets, spanning biomedical literature and clinical notes. See Table 1 for a summary. In particular, MedMentions (MM) (Mohan and Li, 2019) is the largest and most comprehensive dataset for biomedical entity linking, covering diverse UMLS entities (including all entity types in other datasets). See subsection A.2 for details. Training and development sets are not used in any way during self-supervised learning. Only test sets are used to evaluate self-supervised entity linking. Following standard practice in prior work on entity linking (Logeswaran et al., 2019; Wu et al., 2020; Angell et al., 2021), we assume that gold mention boundaries are given and focus on evaluating link-

| Datasets       | Mentions | Entities | Domain Entities |
|---------------|----------|----------|-----------------|
| NCBI          | 6,892    | 790      | 16,317          |
| BC5CDR-d      | 5,818    | 1,076    | 16,317          |
| BC5CDR-c      | 4,409    | 1,164    | 233,632         |
| ShARe         | 17,809   | 1,866    | 82,763          |
| N2C2          | 13,609   | 3,791    | 423,670         |
| MM (full)     | 352,496  | 34,724   | 3,416,210       |
| MM (st21pv)   | 203,282  | 25,419   | 2,325,023       |

Table 1: Summary of entity linking datasets used in our evaluation. MM refers to MedMentions; st21pv refers to the subset with 21 most common semantic types. Domain entities refer to candidates in the UMLS sub-domains (e.g., disease) considered in the dataset.
Table 2: Comparison of test accuracy of self-supervised entity linking on standard entity linking datasets. MM refers to MedMentions, st21pv refers to the subset with 21 most common semantic types. Top four systems only use UMLS and unlabeled text. KRISSBERT (self-supervised) uses self-supervised mention examples for learning and linking, whereas KRISSBERT (supervised only) only uses training-set mentions instead. KRISSBERT (lazy supervised) augments KRISSBERT (self-supervised) with training-set mentions for linking (as in lazy learning). \(^\dagger\) SapBERT returns all entities with the predicted surface form; we randomly select one as its prediction for linking.

| Entity Type | MM (full) | MM (st21pv) | Mean |
|-------------|-----------|-------------|------|
| NCBI        | 39.7      | 49.0        | 63.0 |
| BC5CDR-d    | 47.5      | 83.6        | 64.0 |
| BC5CDR-c    | 34.9      | 96.2        | 66.8 |
| ShARe       | 42.1      | 80.6        | 62.0 |
| N2C2        | 29.6      | 80.4        | 63.3 |
| ShARe       | 29.8      | 59.7        | 59.7 |
| N2C2        | 13.9      | 37.6        | 37.6 |
| MM (full)   | 12.1      | 32.6        | 32.6 |
| MM (st21pv) | 20.0      | 44.2        | 44.2 |

Table 3: Comparison of test accuracy of KRISSBERT with lazy learning and supervised state of the art. MM refers to MedMentions; st21pv refers to the subset with 21 most common semantic types. \(^\dagger\) Prior work generally avoids evaluating on the full MM dataset; we can only find one published result which combines mention boundary detection and linking.

| Entity Type | KRISSBERT (lazy supervised) | Supervised State of the Art |
|-------------|-----------------------------|------------------------------|
| NCBI        | 89.9                        | 89.1 (Li et al., 2020)      |
| BC5CDR      | 93.7                        | 91.3 (Angell et al., 2021) |
| ShARe       | 90.4                        | 91.1 (Li et al., 2020)     |
| N2C2        | 80.2                        | 81.6 (Xu et al., 2020)     |
| MM (full)   | 70.7                        | 45.3 \(^\dagger\) (Mohan and Li, 2019) |
| MM (st21pv) | 70.6                        | 74.1 \(^\dagger\) (Angell et al., 2021) |

To generate self-supervised mention examples, we use a window of 64 tokens for context. We sample three self-supervised mention examples per entity for training, and sample sixteen as prototypes for inference at test time.

We use PubMedBERT (Gu et al., 2021) to initialize the contextual mention encoder. For contrastive learning, we use $B = 512$ for mini-batch size, and train the encoder for two epochs with a learning rate of $10^{-5}$ using Adam, linear scheduling with warm-up, and dropout rate 0.1. We conduct fine-tuning all the way and denote the end model as KRISSBERT. For the cross-attention model, the top 100 most similar prototypes returned by the bi-encoder model are used as candidates for ranking.

### 4.3 Baseline Systems

We conduct head-to-head comparison against five baseline systems, including popular tools and prior state-of-the-art methods: QuickUMLS (Solaimani and Goharian, 2016), entity linking by reading descriptions (Logeswaran et al., 2019; Wu et al., 2020), SapBERT (Liu et al., 2021), MedLinker (Loureiro and Jorge, 2020), ScispaCy (Neumann et al., 2019). See subsection A.3.

### 4.4 Main Results

Table 2 shows the main results on self-supervised entity linking. KRISSBERT results are averaged among three runs with identical hyperparameters but different random seeds. As expected, QuickUMLS provides a reasonable dictionary-based baseline but can’t effectively handle variations and ambiguities. Prior approach on zero-shot entity linking (Reading Entity Descriptions) attained promising results in the Wikipedia domain, but per-
formed poorly in biomedical entity linking, due to the scarcity of available entity descriptions. Sap-BERT performed well on largely unambiguous entity types such as chemicals but faltered in more challenging datasets such as MedMentions (MM). By contrast, KRISSBERT performed substantially better across the board, establishing new state of the art in self-supervised biomedical entity linking, outperforming prior best systems by 10 points in average and by over 20 points in MedMentions.

By leveraging knowledge-rich self-supervision, KRISSBERT even substantially outperformed supervised entity linkers such as MedLinker and SciSpaCy, which used MM labeled data for supervision, gaining over 10-20 absolute points in average.

Amazingly, self-supervised KRISSBERT even substantially outperforms KRISSBERT (supervised only). It is particularly remarkable as KRISSBERT (self-supervised) learns a single, unified model for all four million UMLS entities, whereas KRISSBERT (supervised only) learns separate supervised models that tailor to individual datasets. This seemingly counter-intuitive result can be explained by the unreasonable effectiveness of data (Halevy et al., 2009). Knowledge-rich self-supervision produces a large dataset comprising diverse entity and mention examples. Despite the inherent noise, it confers significant advantage over supervised learning with small training data. This manifests most prominently in small clinical datasets like ShARe and N2C2.

### 4.5 Supervised Entity Linking

KRISSBERT can also make much better use of labeled data when available. Even lazy learning yields results comparable to supervised state of the art. See Table 3. KRISSBERT (lazy supervised) is based on a single, unified model (KRISSBERT (self-supervised)), and simply uses training examples as prototypes for linking. By contrast, prior supervised state-of-the-art results were attained using separate models that tailored to individual datasets. They may use additional supervision such as coreference and joint inference (Angell et al., 2021), which can also be incorporated into KRISSBERT.

### 4.6 Ablation Studies

We conducted a series of ablation studies to understand the impact of domain knowledge and model choices. Table 4 shows the results. By modeling non-linear interdependencies among mention context pairs, cross-attention encoder produces consistent gains compared to bi-encoder. Domain-specific pretraining (PubMedBERT; Gu et al., 2021) offers a substantial advantage for biomedical entity linking, gaining 6.5 points in average accuracy over BERT initialization. Self-supervised mention examples and additional domain knowledge such as semantic hierarchy both provide important signals for contrastive learning. The bi-encoder setting also admits several ways to use prototypes at test time: entity-only (using entity-centric prototype generated from semantic type), mention-only (using self-supervised mentions), hybrid (mixing both), default (add scores for both entity-centric prototype and mention prototype). Adding both entity and mention scores is more robust to outlier and generally yields better performance.

### 4.7 Discussion

Aside from BC5CDR-C where KRISSBERT already performs very well, there is a large gap (10-15 points) between top-1 and top-5 accuracy, in both self-supervised and lazy supervised settings. See Figure 2. This suggests that there is much room for KRISSBERT to gain by further improving ranking. KRISSBERT also facilitates efficient few-shot learning, with a single example per entity yielding over 10 point gain in N2C2.

|               | NCBI | BC5CDR-d | BC5CDR-c | ShARe | N2C2 | MM (full) | MM (st21pv) | Mean |
|---------------|------|----------|----------|-------|------|-----------|-------------|------|
| KRISSBERT (cross-attention) | 83.2 | 85.5     | 96.5     | 84.0  | 67.8 | 61.4      | 63.5        | 77.4 |
| — semantic hierarchy         | 79.5 | 82.7     | 95.6     | 78.3  | 60.2 | 54.4      | 56.8        | 72.5 |
| — mention pair contrast       | 77.9 | 82.2     | 93.3     | 75.0  | 56.3 | 47.8      | 49.9        | 68.9 |
| Initialize w. BERT            | 79.3 | 80.6     | 94.4     | 74.5  | 58.4 | 53.9      | 55.3        | 70.9 |
| KRISSBERT (bi-encoder)       | 82.8 | 85.0     | 95.1     | 83.4  | 65.0 | 59.4      | 61.3        | 76.0 |
| Entity-only prototype         | 78.0 | 83.5     | 94.1     | 79.3  | 61.3 | 52.7      | 54.5        | 71.9 |
| Mention-only prototype        | 81.9 | 84.4     | 95.6     | 78.4  | 62.8 | 57.6      | 59.5        | 74.3 |
| Hybrid prototype              | 81.4 | 84.6     | 95.7     | 80.6  | 63.7 | 58.1      | 60.1        | 74.9 |

Table 4: Ablation study of KRISSBERT. Top: impact of knowledge components and domain-specific pretraining. Bottom: KRISSBERT with bi-encoder and various prototype settings.
Figure 2: Test accuracy (oracle) with top $K$ predictions shows that improving ranking has the potential to yield large gains. Few-shot learning results are averaged over three runs.

**Mention:** "... Hence, we aimed to find drug targets using the 2DE / MS proteomics study of a dexamethasone - resistant cell line ..."

**SapBERT prediction:** Master of Science (C1513009), Montserrat Island (C0026514), Mass Spectrometry (C0037813), ...

**KRISSBERT prediction:** Mass Spectrometry (C0037813)

**KRISSBERT predicted prototype:** "... mass spectrometry is a widely used technique for enrichment and sequencing of phosphopeptides ..."

**Example:** "... every patient followed up accordingly within ten days of discharge ...

**SapBERT prediction:** Discharge, Body Substance, Sample (C0600083), Body Fluid Discharge (C0012621), Patient Discharge (C0030685)

**KRISSBERT prediction:** Patient Discharge (C0030685)

**KRISSBERT predicted prototype:** "Performance of the Hendrich Fall Risk Model II in Patients Discharged from Rehabilitation Wards ..."

**Example:** "... we added separately, live cells and heat-killed cells of E. coli C600 ...

**SapBERT prediction:** Clone Cells (C0009013), Cell Count (C0007584), Cell Line, Tumor (C0085983), Cells (C0007634), ...

**KRISSBERT prediction:** Cells (C0007634)

**KRISSBERT predicted prototype:** "... gram-positive rods such as C. liquefaciens activate T and A cells ...

Table 5: Examples of ambiguous mentions: SapBERT struggles whereas KRISSBERT predicts correctly.

| Ambiguous (%) | KRISSBERT | SapBERT |
|---------------|-----------|---------|
| NCBI          | 43.2      | 64.5    | 57.1   |
| ShArC        | 48.5      | 72.4    | 67.5   |
| N2C2         | 67.5      | 58.2    | 50.7   |
| MM (full)    | 67.8      | 48.9    | 24.8   |
| MM (st21pv)  | 69.4      | 52.5    | 29.6   |

Table 6: Accuracy comparison on ambiguous cases.

Table 5 shows ambiguous test examples where SapBERT struggles while KRISSBERT predicts accurate linking results. Ambiguous mentions are prevalent in biomedical text; see Table 6. KRISSBERT performs much better than Sap-BERT (Liu et al., 2021), but still has much room for growth.

**Mention:** "... NTeff cells appeared to have lower expression of Foxp1 ...

**Gold entity:** Protein Expression (C1171362)

**KRISSBERT prediction:** Expression Procedure (C0185117)

**KRISSBERT predicted prototype:** "... expression of a myeloid differentiation antigen, M01 ...

**Mention:** "... On admission included BUN / creatinine of 33/2.1 : Sodium 141 : ...

**Gold entity:** Creatinine Measurement (C0201975)

**KRISSBERT prediction:** Creatinine (C0010294)

**KRISSBERT predicted prototype:** "... Sorbent binding of urea and creatinine in a Roux-Y intestinal segment. ...

Table 7: Examples of common errors by KRISSBERT.

Table 7 shows examples of common errors by KRISSBERT. They are inherently subtle and challenging. E.g., the top example is labeled with the concept of expression, while KRISSBERT predicts the procedure of expression. By contrast, the bottom example is labeled with the measurement of creatinine, whereas KRISSBERT predicts the concept of creatinine. Learning to differentiate such intricate distinctions would be a key future direction to explore.

5 Conclusion

We propose knowledge-rich self-supervised entity linking by conducting contrastive learning on mention examples generated from unlabeled text using readily available domain knowledge. Experiments on seven standard biomedical entity linking datasets demonstrate the promise in this approach, with our proposed KRISSBERT outperforming prior state of the art by as much as over 20 points in accuracy. Future directions include: further improving self-supervision quality; incorporating additional knowledge; applications to other domains.
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A Appendix

A.1 Contextual Mention Encoders

![Contextual Mention Encoder](image)

Figure 3: Contextual mention encoder for self-supervised entity linking (bi-encoder).

![Contextual Mention Encoder](image)

Figure 4: Contextual mention encoder for self-supervised entity linking (cross-attention). Computation of similarity scores between query mention and prototype mention by the cross-attention encoder.
A.2 Entity Linking Datasets

NCBI (Doğan et al., 2014) contains 793 PubMed abstracts annotated with 6892 disease mentions, which are mapped to 790 unique concepts in MeSH⁵ or OMIM⁶, both part of UMLS. BC5CDR (Li et al., 2016) contains 1,500 PubMed abstracts with 5,818 annotated disease mentions (BC5CDR-d) and 4,409 chemical mentions (BC5CDR-c), which are mapped to MeSH.

ShARe (Pradhan et al., 2014) contains 431 de-identified clinical reports with 17,809 disease mentions mapped to the SNOMED-CT (Spackman et al., 1997) subset of UMLS.

N2C2 (2019 n2c2/UMass Lowell shared task 3) (Luo et al., 2020) adds entity linking annotations to a subset of the 2010 i2b2/VA shared task dataset (Uzuner et al., 2011). The resulting dataset contains 100 de-identified discharge summaries with 13,609 mentions (including medical problems, treatments, and tests) linked to RxNorm (Liu et al., 2005) and SNOMED-CT (Spackman et al., 1997) within UMLS.

MedMentions (Mohan and Li, 2019) (MM) is the largest publicly available dataset for biomedical entity linking, which contains 4,392 PubMed abstracts and 350,000 mentions annotated with UMLS linking. MM (st21pv) is a sub-corpus limited to 21 most common entity types.

A.3 Baseline Systems

QuickUMLS (Soldaini and Goharian, 2016) conducts entity linking by approximate matching of mentions against UMLS entity lexicon (canonical name and aliases). It serves as a representative baseline for ontology-based entity linking.

Zero-shot entity linking by reading entity descriptions (Logeswaran et al., 2019; Wu et al., 2020) learns to encode contextual mentions against entity descriptions and attains state-of-the-art zero-shot entity linking results in the Wikipedia domain. Prior work uses gold mention examples in supervised learning. We adapt it to self-supervised learning using the self-supervised mention examples and available entity descriptions in UMLS. Prior work initializes the encoder with general-domain BERT models. To ensure head-to-head comparison, we followed KRISSBERT to use PubMedBERT (Gu et al., 2021) instead, which yielded better results.

SapBERT (Liu et al., 2021) learns to resolve variations in entity surface forms using synonyms in UMLS, using PubMedBERT (Gu et al., 2021). It ignores the mention context and returns all entities with a matching surface form. To use SapBERT for linking, we randomly select an entity when SapBERT returns multiple ones.

MedLinker (Loureiro and Jorge, 2020) is a strong supervised entity linking baseline that trains a BERT model on MedMentions. At test time, it augments the BERT-based prediction with approximate dictionary match for entities unseen in training.

ScispaCy (Neumann et al., 2019) provides another strong entity linking baseline that leverages labeled data in MedMentions to tune an elaborate biomedical linking system that uses TF-IDF based approximate matching and sophisticated abbreviation expansion.

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⁵https://www.nlm.nih.gov/mesh/meshhome.html
⁶https://omim.org/