Integrating Higher-Level Semantics into Robust Biomedical Name Representations

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Abstract

Neural encoders of biomedical names are typically considered robust if representations can be effectively exploited for various downstream NLP tasks. To achieve this, encoders need to model domain-specific biomedical semantics while rivaling the universal applicability of pretrained self-supervised representations. Previous work on robust representations has focused on learning low-level distinctions between names of fine-grained biomedical concepts. These fine-grained concepts can also be clustered together to reflect higher-level, more general semantic distinctions, such as grouping the names *nettle sting* and *tick-borne fever* together under the description *puncture wound of skin*. It has not yet been empirically confirmed that training biomedical name encoders on fine-grained distinctions automatically leads to bottom-up encoding of such higher-level semantics. In this paper, we show that this bottom-up effect exists, but that it is still relatively limited. As a solution, we propose a scalable multi-task training regime for biomedical name encoders which can also learn robust representations using only higher-level semantic classes. These representations can generalise both bottom-up as well as top-down among various semantic hierarchies. Moreover, we show how they can be used out-of-the-box for improved unsupervised detection of hypernyms, while retaining robust performance on various semantic relatedness benchmarks. Our code is open-source and can be found at www.github.com/clips/higherlevelsemantics.

1 Introduction

Recent work on representation learning for biomedical names has mainly involved the training of neural encoder architectures such as LSTMs (Kartsaklis et al., 2018) or Transformers (Sung et al., 2020; Kalyan and Sangeetha, 2020) to finetune name representations for biomedical normalization tasks. Such representations are often tailored towards normalization tasks (e.g. linking names to corresponding concept identifiers), without providing explicit guarantees about their transferability to other use contexts and applications. As a solution for this issue, the Biomedical Name Encoder (BNE) model (Phan et al., 2019) has been proposed as a comprehensive framework for robust and transferable representations.

According to this framework, the robustness of biomedical name representations is characterized along three dimensions. Firstly, semantic similarity between names should be reflected by their closeness in the embedding space. Secondly, the variety of textual contexts in which a name appears should be somehow represented in the encoding. Lastly, a name embedding should be sufficiently close to a pretrained prototypical representation of its conceptual meaning, e.g. a representation of its corresponding concept identifier from a biomedical ontology.

Such a multi-task model can be effectively trained using synonym sets extracted from ontologies such as the UMLS or SNOMED-CT. However, these synonym sets typically reflect only fine-grained distinctions between the lowest-level concepts from ontologies. If robust name representations should truly reflect semantic similarity in general, then the assumption is being made that training on such fine-grained synonym sets learns biomedical semantics in a bottom-up way, expecting names of lower-level concepts to spontaneously form relevant higher-level clusters.
Table 1: Examples of how names from the SNOMED-CT ontology can be grouped into larger classes using parent concepts in the ontological graph. This allows us to investigate higher-level semantic relations, such as grouping poisoning by bombus and nettle sting under the concept of sting of skin, or e.g. grouping them together with tick-borne fever under puncture wound of skin.

However, such assumptions have not yet been empirically validated, for instance by showing that an encoder not only learns the differences between names such as nettle sting and tick-borne fever, but also simultaneously learns that they can be grouped together under the more general description puncture wound of skin. Moreover, research on representation learning and hierarchical classification for e.g. computer vision has indicated that neural models can leverage substantially different discriminative information for higher, more general levels of categorization than for more fine-grained lower levels (Hase et al., 2019). Such hierarchical differences can be exploited to generalize from higher to lower levels (Guo et al., 2017; Taherkhani et al., 2019), but they can also be difficult to integrate consistently into a single neural model (Wu et al., 2019).

In this paper, we investigate to what extent robust biomedical name representations can encode higher-level semantics while retaining relevant lower-level fine-grained information as well. To address this research question, we group synonym sets under increasingly coarse-grained semantic categories, using parent-child relations in the ontological graph. Table 1 gives an example of how names from the SNOMED-CT ontology can be grouped into larger classes. Such a hierarchy can be used to train and test a variety of semantic relations between names. For instance, a model might be able to encode that the names poisoning by bombus and nettle sting can be both described as sting of skin, but fail to represent their similarity to poisoning caused by gila monster venom as a puncture wound of skin. We believe that an evaluation of this nature is a crucial step towards achieving truly robust biomedical name representations, since it clearly requires more semantic inference from the encoder than merely resolving synonyms.

Apart from introducing this evaluation to the field of biomedical NLP, we also show that we can effectively adapt the BNE framework (Phan et al., 2019) to be trained using such large higher-level semantic classes. Most importantly, we replace the BiLSTM (Graves and Schmidhuber, 2005) encoder architecture of the BNE model with a lightweight Deep Averaging Network (DAN) (Iyyer et al., 2015). This allows us to easily scale to large amounts of training data, caused by the explosive amount of possible pairwise combinations between semantically similar names as classes grow larger.

Training on higher-level classes involves additional challenges such as handling imbalanced data distributions as well as implicit hierarchical and semantic differences among names grouped under the same class. Our aim is not to tailor the proposed approach to such artefacts. Rather, the main contribution of this paper is to show that our simple modification of the BNE model is generally applicable to a range of coarse-grained biomedical
categorizations, without any finetuning apart from the size of the DAN encoder. As of such, it can be used as a low-cost but effective benchmark for future models that are more specialized.

Our experimental results for hierarchical SNOMED-CT data show that our DAN model improves semantic similarity ranking both in a bottom-up as well as top-down manner along various hierarchies. Interestingly, this observation holds even when we train on a few dozens of very broad categories. We also apply extrinsic evaluations to investigate the transferability of our DAN model. Firstly, we validate the robustness of higher-level representations on semantic relatedness benchmarks. Secondly, we perform unsupervised detection of SNOMED-CT hypernym disorder names which were not observed during training. For this task, our DAN model scores substantially better than the publicly released pretrained BNE model, which was trained on a large amount of fine-grained disorder concepts from SNOMED-CT using an elaborate BiLSTM architecture. These results provide tangible evidence that training name representations on large coarse-grained categories can help to encode exploitable higher-level semantics.

3 Encoding model

3.1 Encoder architecture

Our encoder is a Deep Averaging Network (DAN) (Iyyer et al., 2015) which extracts a fixed-size representation for an input name \( n \):

\[
u_n = \frac{1}{|N_t|} \sum_{t \in N_t} u_t
\]

\[f(n) = \text{enc}(u_n)\]  

where \( N_t \) is the bag of tokens from a name, \( u_t \) is a pretrained word embedding of a token, \( u_n \) is a name embedding created by averaging all the pretrained word embeddings of all tokens, and \( \text{enc} \) is a feedforward neural network with Rectified Linear Unit (ReLU) as non-linear activation function. As pretrained word embeddings we use 300-dimensional fastText (Bojanowski et al., 2017) representations which we train on 76M sentences of preprocessed MEDLINE articles released by Hakala et al. (2016). This fastText model also allows for constructing word embeddings for out-of-vocabulary tokens by composing character n-gram embeddings.

3.2 Training objectives

Our proposed approach is a simple modification of the multi-task training regime of the BNE model. We use cosine distance as distance function \( d \) for all three training objectives.

**Semantic similarity** The semantic similarity objective is a generalization from the synonym similarity objective of the BNE model to any level of relevant semantic similarity. To enforce embedding similarity between names that are semantically related, we use a siamese triplet loss (Chechik et al., 2010). This loss forces the encoding of a biomedical name \( f(n) \) to be closer to the encoding of a semantically similar name \( f(n_{pos}) \) than that of an encoded negative sample name \( f(n_{neg}) \), within a
specified (possibly tuned) margin:

\[ \begin{align*}
  pos &= d(f(n), f(n_{pos})) \\
  neg &= d(f(n), f(n_{neg})) \\
  L_{sem} &= \max(pos - neg + \text{margin}, 0)
\end{align*} \] (2)

To select negative names during training we apply distance-weighted negative sampling (Wu et al., 2017) over all training names, since this has been proven more effective than hard or random negative sampling.

**Contextual meaningfulness** The contextual meaningfulness objective forces the encoding of a biomedical name to be similar to its local contexts. The summary of these local contexts is approximated by taking the pretrained embedding representation of the name:

\[ L_{cont} = d(f(n), u_n) \] (3)

This constraint implies that the dimensionality of the encoder output should be the same as that of the input. However, if the input dimensionality is smaller than the desired output dimensionality, this could be solved using e.g. random projections, which work well for increasing the dimensionality of neural encoder inputs (Wieting and Kiela, 2019).

**Conceptual grounding** The conceptual grounding objective is a modification of the conceptual meaningfulness objective of the BNE model. The conceptual meaningfulness objective forces the encoding of a biomedical name to be similar to a prototypical representation of its concept. This concept representation is approximated by averaging the pretrained embedding representations of all the names belonging to the concept:

\[ u_p = \frac{1}{|C_n|} \sum_{n \in C_n} u_n \] (4)

While converging to this pretrained target is feasible for small synonym sets, such convergence is unnecessary and overfitting for larger classes of names with graded differences in semantic similarity among the class members. To retain the robustness of the encodings, we only want to pull the names in the direction of their pretrained concepts, rather than minimizing their distance entirely. To this end, we simply take the average of the pretrained name representation and the pretrained concept representation:

\[ v_{ground} = \frac{u_p + u_n}{2} \]

\[ L_{ground} = d(f(n), v_{ground}) \] (5)

**Multi-task setup** Our multi-task setup sums the losses of the 3 training objectives:

\[ L = \alpha L_{sem} + \beta L_{cont} + \gamma L_{ground} \] (6)

where \( \alpha \), \( \beta \), and \( \gamma \) are possible weights for the individual losses. Since the 3 losses all directly reflect cosine distances, they are similarly scaled and don’t require weighting to work properly. In our experiments, \( \alpha = \beta = \gamma = 1 \) showed the most robust performance along all settings.

**4 Data and task setup**

**4.1 Extracting hierarchical data**

Following previous research (Kotitsas et al., 2019; Camacho-Collados et al., 2018), we use IS-A relations between concepts from the SNOMED-CT\(^1\) ontology as biomedical hypo-hyponymy relations. For direct comparison with the publicly released BNE embeddings, which were trained on all disorder concepts of SNOMED-CT, we use the 2018AB release of the UMLS\(^2\) to extract only those SNOMED-CT concepts which are included in the semantic group of disorders\(^3\), and extract their reference terms as disorder names. While the resulting directed graph should be acyclic, there are many inconsistencies, which we resolve by removing all cyclic edges, similar to the naive approach used by Mougou and Bodenreider (2005).

For our experiments, we select 3 different (yet slightly overlapping) subgraphs of IS-A relations by sampling 3 high-level concepts which have around 10K child concepts in our cleaned graph. We extract consistent taxonomies from these subgraphs by removing relations which form shortcuts between otherwise non-consecutive levels of the taxonomy, and by leaving out dead-end concepts which don’t have a path to the required level of specification down the taxonomy. Child concepts can have mutually inclusive relations to multiple higher-level concepts on the same level of categorization.

\(^1\)https://www.snomed.org
\(^2\)https://uts.nlm.nih.gov/home.html
\(^3\)https://metamap.nlm.nih.gov/SemanticTypesAndGroups.shtml
|        | min | max | mean | stdev |
|--------|-----|-----|------|-------|
| Level 1 | 1   | 10203 | 1015 | 2053  |
| Level 2 | 1   | 10203 | 291  | 1101  |
| Level 3 | 1   | 3840  | 118  | 411   |
| Level 4 | 1   | 2607  | 48   | 195   |

Table 2: Descriptive statistics about the number of names per class for the different levels sampled from the subgraph with parent concept C1290864 (disorder of abdomen). These statistics show that lower levels have less extreme imbalances between classes.

4.2 Data setup

For each subgraph, we select 4 consecutive levels of parent concepts (level 1 is highest, level 4 is lowest). The concepts on these 4 levels are used as class labels for the names from all concepts below level 4. In other words, names belonging to the parent concepts themselves are not used during training: the parent concepts are only used as reference to cluster the names from the lower levels. Table 1 visualizes an example of this process.

This method of aggregating names can lead to very imbalanced classes. Table 2 shows how large this imbalance can get as we go up the hierarchy. While the training regime of our proposed model should be robust against such data artefacts, we want to take a representative test sample across all classes to empirically validate our approach. Therefore, for multiple iterations, we sample one held-out test name for each class on level 4. This test name is then also used for levels 1-3. Afterwards, we carry out the same procedure to sample validation data for calculating the stopping criterion during training. Table 3 shows the distributions of concepts and names used during training, validation, and testing.

4.3 Task setup

We perform 2 tasks on the held-out SNOMED-CT test data to validate our approach. Evidently, we always evaluate on individual levels of categorization. As intrinsic evaluation, we evaluate trained encoders on semantic similarity ranking. We also include the task of unsupervised hypernym detection as extrinsic evaluation. As we don’t use the names of higher-level concepts during training, we can exploit them as previously unobserved hypernymic data to show how much higher-level semantics are being modeled by encoders. If the encoder has learned to represent biomedical semantics more effectively, then the name embedding space can reflect that by being more suited for unsupervised detection of hypernyms.

Table 1 gives examples of hypernym names on all 4 levels. Successful hypernym detection for this data implies e.g. that we rank the previously unobserved hypernym bite wound over another previously unobserved hypernym sting of skin for the name tick-borne fever. This task clearly requires more semantic inference than merely resolving synonyms. In this case, the encoder has to represent that ticks are insects that bite instead of sting.

Semantic similarity ranking We evaluate encoders on the ability to reflect semantic similarity between names by their cosine similarity. Given a mention $m$ of a biomedical name which belongs to the higher-level class $c$, we have to rank the set of all training names $S$ which includes $C_n \subset S$, a set of training names which belong to the same class $c$ as the test mention. To rank the biomedical names according to their similarity to the mention, we first encode both the mention $m$ as well as every name $n \in S$, and then rank every name $n$ using the cosine similarity between the encoded mention $f(m)$ and the encoded name $f(n)$. We then calculate the Mean Average Precision (mAP) over all test mentions for retrieving training names from the same higher-level class.

Unsupervised hypernym detection Given a test mention $m$ of a biomedical name which belongs to the higher-level class $c$, we have to rank the set of all hypernym names $H$ belonging to a specific level of categorization. This set includes $C_h \subset H$, the set of hypernym names which belong to the same class $c$ as the test mention. To rank the biomedical names according to their similarity to the mention, we first encode both the mention $m$ as well as every hypernym name $h \in H$, and then rank every hypernym name $h$ using the cosine similarity between the encoded mention $f(m)$ and the encoded hypernym $f(h)$. We then calculate the Mean Reciprocal Rank (MRR) over all test mentions for retrieving hypernym names from the same higher-level class.

5 Experiments and results

5.1 Reference model and baselines

We compare our DAN model against the publicly released pretrained BNE model with skip-gram word embeddings, BNE + SG\textsubscript{w},\textsuperscript{4} which was

\textsuperscript{4}https://github.com/minhcp/BNE
Table 3: An overview of the distribution of higher-level classes for the 3 subgraphs used in our experiments. The lower-level names are divided into train / test / validation.

|                | C1290864 (disorder of abdomen) | C0560169 (osteoarthropathy) | C0263661 (dermatological finding) |
|----------------|--------------------------------|------------------------------|-----------------------------------|
| Level 1        | 27                             | 30                           | 35                                |
| Level 2        | 98                             | 86                           | 80                                |
| Level 3        | 248                            | 236                          | 231                               |
| Level 4        | 610                            | 536                          | 602                               |
| Lower-level names | 24737 / 1557 / 763           | 20574 / 1335 / 649           | 25659 / 1567 / 814                |

5.2 Training and implementation details

The DAN model is implemented in PyTorch (Paszke et al., 2019). Both the input and output dimensionality are 300 (which is the dimensionality of the input fastText embeddings described in Section 3.1). All encoders for which we report results are finetuned to one hidden layer, which has 76,800 dimensions. Adam optimization (Kingma and Ba, 2015) is performed on a batch size of 64, using a learning rate of 0.001 and a dropout rate of 0.5. Input strings are first tokenized using the Pattern tokenizer (Smedt and Daelemans, 2012) and then lowercased. We use a triplet margin of 0.1 for the siamese triplet loss $L_{sem}$ defined in Equation 2.

To train the model, we iterate over all names in the training data and apply the 3 training objectives for each name in a batch. To avoid overfitting on the largest classes, we always sample one siamese triplet per name, using random sampling for the positive name and distance-weighted sampling for the negative name. As stopping criterion we use the mAP of semantic similarity ranking (as defined in Section 4.3) for held-out validation names: we stop training once this score hasn’t improved anymore over 10 epochs. This relaxed stopping criterion allows the model to optimize the subsampled siamese triplet loss in a balanced stochastic way over many epochs without quitting too early.

5.3 Results and discussion

Semantic similarity ranking  Table 4 shows the test performance for semantic similarity ranking. First and foremost, the robustness of the Level 1 DAN models is consistently great for all 3 subgraphs. For instance, in the case of the subgraph C1290864 (disorder of abdomen), the DAN is trained on only 27 large classes but outperforms the fastText baseline for the 610 classes on Level 4. Secondly, all DAN models generalize both bottom-up and top-down along the hierarchical levels to the extent that they consistently outperform the fastText baseline by a substantial margin.

Thirdly, the slight superiority of BioBERT over fastText for this task is most pronounced for the lowest levels. As we go up in the hierarchy, the difference grows smaller, which leads us to believe that the improvements are not so much of a semantic nature. Interestingly, the pretrained BNE model is competitive with our DAN models for the lower levels, which are still more coarse-grained than the fine-grained distinctions on which the BNE was trained. However, such a bottom-up effect is lacking for the highest levels of categorization. These observations reinforce the notion that both the size (the BNE was trained on 156K disorder names, our models on 20-25K) and the granularity of the data matter for deep representation learning.

Unsupervised hypernym detection  Table 5 shows the test performance for unsupervised hypernym detection. These results clearly show trends which are similar to the semantic similarity ranking. Most remarkably, the bottom-up and bottom-down effects are almost as consistent here: the highest-level DAN still outperforms the baselines for the lowest levels and vice versa. One major difference with the results for semantic similarity ranking is the relatively worse performance from BioBERT.
Table 4: Test performance of semantic similarity ranking per level, as measured by mAP. The highest score per level of each subgraph is denoted in bold; the second highest score is underlined.

|            | C1290864 |            | C0560169 |            | C0263661 |
|------------|----------|------------|----------|------------|----------|
| DAN level 1| 0.57     | 0.50       | 0.39     | 0.43       | 0.70     | 0.44 | 0.36 | 0.37 | 0.64 | 0.55 | 0.36 | 0.36 |
| DAN level 2| 0.49     | 0.58       | 0.46     | 0.48       | 0.55     | 0.58  | 0.44 | 0.44 | 0.58 | 0.59 | 0.40 | 0.39 |
| DAN level 3| 0.43     | 0.51       | 0.56     | 0.54       | 0.51     | 0.51  | 0.52 | 0.54 | 0.52 | 0.52 | 0.51 | 0.48 |
| DAN level 4| 0.38     | 0.43       | 0.47     | 0.60       | 0.45     | 0.45  | 0.48 | 0.58 | 0.45 | 0.44 | 0.41 | 0.54 |

fastText: 0.26
BioBERT: 0.27
BNE: 0.35

Table 5: Test performance for unsupervised hypernym detection per level, as measured by MRR. The highest score per level of each subgraph is denoted in bold; the second highest score is underlined.

|            | C1290864 |            | C0560169 |            | C0263661 |
|------------|----------|------------|----------|------------|----------|
| DAN level 1| 0.60     | 0.58       | 0.59     | 0.68       | 0.48     | 0.54  | 0.52 | 0.63 | 0.52 | 0.57 | 0.55 | 0.62 |
| DAN level 2| 0.52     | 0.59       | 0.62     | 0.70       | 0.45     | 0.58  | 0.56 | 0.67 | 0.50 | 0.60 | 0.57 | 0.63 |
| DAN level 3| 0.55     | 0.57       | 0.66     | 0.73       | 0.41     | 0.54  | 0.58 | 0.70 | 0.48 | 0.57 | 0.62 | 0.67 |
| DAN level 4| 0.53     | 0.52       | 0.63     | 0.74       | 0.39     | 0.53  | 0.58 | 0.74 | 0.46 | 0.54 | 0.59 | 0.71 |

fastText: 0.46
BioBERT: 0.41
BNE: 0.43

here compared to fastText. This is in line with the findings by Yu et al. (2020), who report that BERT does not yield considerable improvement for hypernym detection in their experiments. It also puts into perspective to what extent we can expect higher-level semantics to be encoded solely through self-supervised methods.

Table 6 gives an example of hypernym rankings for the test mention poisoning caused by mexican beaded lizard bite. By clustering similar names together with other bite wounds during training, the DAN model has learned to recognize the test mention as a bite wound. The BNE has failed to do so.

The effectiveness of our unsupervised method using only cosine similarity contrasts with earlier approaches which explicitly require more than cosine similarity to properly work. For example, Vulić and Mrkšić (2018) use vector norms to encode hierarchical hypernymic relations, while other research into hypernymy even requires other geometric spaces than Euclidean space, such as hyperbolic space (Dhingra et al., 2018). Our results can indicate that cosine similarity in Euclidean space still shows potential for encoding these hierarchical relations given the right training objectives.

5.4 Semantic relatedness benchmarks

We also evaluate our name encoders on two biomedical benchmarks of semantic similarity, which allow to compare cosine similarity between name embeddings with human judgments of relatedness. MayoSRS (Pakhomov et al., 2011) contains multi-word name pairs of related but different fine-grained concepts. UMNSRS (Pakhomov et al., 2016) contains only single-word pairs, which also stem from different fine-grained concepts. This benchmark makes a distinction between similarity and relatedness.

The correlations in Table 7 show that the majority of our trained encoders remain robust out-of-the box, with a large portion of them outperforming the fastText baseline which they use as input. The highest-level model trained on the C0560169 subgraph (dermatological finding) is even competitive with the pretrained BNE, having been trained on only 30 classes. All in all, these results confirm that our proposed model is relatively robust against variable granularity of clustering, and is not overly tailored to the data artefacts of one specific sub-
Table 6: A comparison between our DAN encoder and the BNE reference model for unsupervised hypernym ranking of the Level 3 test mention *poisoning caused by mexican beaded lizard bite*. The DAN model generalizes from the training data to associate the test mention correctly with bite wounds. In the training process, it seems to have clustered bite wounds together with open dislocations. The BNE model apparently associates lizards with infestations by fly larvae, but fails to recognize that there is a bite wound mentioned in the test mention.

### 5.5 Discussion

While our empirical results are certainly encouraging, the true robustness of our proposed framework remains an open question. Whereas our proposed DAN model remains robust over entire hierarchies for semantic similarity ranking and unsupervised hypernym detection, its relative performance for the semantic relatedness benchmarks is not entirely predictable from those tasks. One the one hand, this likely has to do with the modest sizes of the benchmarks, for which small to very small margins in performance are not very reliable or indicative.

On the other hand, we also have to consider that our finetuned DAN only contains a single, yet very wide, hidden layer. This implies that the encoder network relies more on what can considered to be an elaborate weighted average than a deep multi-layer transformation of the input. While this is not very surprising in the context of transferable representations (and emphasizes the effectiveness of exploiting word embeddings according to their full potential in simple ways, as suggested by WieEtting and Kiela (2019)), it still raises the question whether there are straightforward regularization alternatives to the contextual meaningfulness objective which can allow for deep transformations with the DAN.

### 6 Conclusion and future work

In this paper, we have introduced the challenge of integrating higher-level semantics into robust biomedical name representations. We provide a framework to both train and evaluate encoders for
this task. Moreover, we have proposed a modification of the Biomedical Name Encoder model which is directly applicable to a variety of coarse-grained categorizations. This modification replaces more complex neural architectures with a lightweight Deep Averaging Network encoder, which is easily scalable to the large amounts of required training data, while remaining sufficiently robust. The only important hyperparameter to tune for this encoder is the size of the Feedforward Neural Network.

Experiments indicate that our proposed framework can even be effective using only around 30 coarse-grained classes. This opens up possibilities for applying our framework to data beyond carefully curated ontologies, for instance in self-supervised or semi-supervised settings. Future work will try to understand and define the limits of applying our framework to such settings.

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