Order Embeddings from Merged Ontologies using Sketching

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Abstract

We give a simple, low resource method to produce order embeddings from ontologies. Such embeddings map words to vectors so that order relations on the words, such as hypernymy/hyponymy, are represented in a direct way. Our method uses sketching techniques, in particular countsketch, for dimensionality reduction. We also study methods to merge ontologies, in particular those in medical domains, so that order relations are preserved. We give computational results for medical ontologies and for wordnet, showing that our merging techniques are effective and our embedding yields an accurate representation in both generic and specialised domains.

1 Introduction

While the NLP literature has recently seen one groundbreaking technique after another in feature representation and embedding, there is still work that to be done in imparting knowledge into embeddings, beyond the use of contextual information; moreover, most of the techniques require huge computing time and power, while training from scratch. The medical field is an area where feature representations that are interpretable, and that need limited computing resources to design, can benefit the adoption and acceptance of these systems in practice. Through the OrderSketch algorithm presented in this paper, we aim to provide a step towards a knowledge-rich feature representation technique that is based directly on ontologies and is also computation-resource friendly. The paper is organized as follows: First we present related work on other knowledge representation and order detection techniques. Next we introduce our algorithm OrderSketch, which is simple and yet also effective in capturing knowledge and order information from ontologies. We apply our embedding algorithm to WordNet, and to an augmented medical ontology called SnoMeSHNet that we introduce. After presenting our current constructions and experiments, we discuss future experiments and goals for this work, in progress.

2 Related Work

There has been previous work in representing hierarchical information found in data sources. (Luu et al., 2016) predicts hypernym term given a hyponym and context through concatenation of one hot vector embedding of the hypernym, hyponym, offset vectors of context words and
dynamic weighting of a neural network based on context. There has been work on using a neural network and scoring mechanism to detect hypernymy relations and differentiate from other relations through distributional similarity in (Nguyen et al., 2017). (Chang et al., 2017) presents an approach to a reversed form of order embedding, where an unsupervised embedding method is used to learn embeddings such that the embedding of a hypernym is larger than that of its hyponym in every dimension. There have also been approaches such as, (Vulic and Mrksic, 2017), which is a post-processing mechanism to transform vector space and align vectors to reflect hypernymy presence and directionality, where ontology knowledge representations like ours can be utilized.

When it comes to specialty domains such as medicine, (Perotte et al., 2014) shows that hierarchical representation of ICD codes has more information. (Lu et al., 2019) shows how hierarchical information in ICD codes can be incorporated in hyperbolic embeddings and used to reconstruct input to effectively process EHR data.

2.1 Order embeddings

In the settings of ontologies, especially, it may be that the most effective embedding does not represent synonymy, but other relations between words, such as lexical entailment. (Vendrov et al., 2015) produce maps $g : \text{Tokens} \rightarrow \mathbb{R}^n$ such that for tokens $X$ and $Y$, $Y$ entails $X \iff g(X) < g(Y)$, where the inequality means coordinatewise dominance, that is, every coordinate of $g(X)$ is at most the corresponding coordinate of $g(Y)$. This can be called a conical embedding: if any point in $\mathbb{R}^n$ is a potential concept, the cone

$$c(X) \overset{df}{=} \{ y \in \mathbb{R}^n \mid g(X) < y \}$$

corresponds to the set of concepts that entail $X$. This can also be expressed in terms of subsets:

$$Y \text{ entails } Z \iff c(Y) \subset c(X).$$

Such embeddings extend beyond lexical entailment; for example, Vendrov et al. (2015) map captions and images to $\mathbb{R}^n$, such that a caption is appropriate for an image if its embedding is coordinatewise dominated by the embedding of the image. Such an embedding could also capture entailment among captions: if caption $X$ is appropriate to every image caption $Y$ is, then the embedding of $X$ should be coordinatewise dominated by that of $Y$.

Lexical and caption entailment are partial orders that are transitive: if $X$ is-a $Y$ and $Y$ is-a $Z$, then $X$ is-a $Z$, and such embeddings under coordinatewise dominance capture this transitivity. Other ontological relations are also transitive, such as part-of and causes, so embeddings that represent this structural property are of particular interest.

Note that the use of the transitive property of lexical entailment is a simple species of reasoning (indeed, lexical entailment is a special case of NLP entailment), and so exploiting transitivity has the potential to both enable better learning, and improve reasoning.
3 Order embedding algorithm

3.1 Conceptual description

We give a construction for building an approximate embedding for terms with a partial order relation, such as might be given in an ontology. That is, suppose \((U, \leq)\) is a partially ordered set. Our approach, conceptually, is for all \(x \in U\):

1. Construct the upper set Wikipedia contributors (2019) of \(x\), that is, \(\uparrow\{x\} \overset{\text{def}}{=} \{y \mid x \leq y\}\);

2. Construct the characteristic vector \(\text{vec}(x) \in \{0, 1\}^U\) of the upper set of \(x\), that is,
\[
\text{vec}(x)_y \overset{\text{def}}{=} \begin{cases} 1 & y \in \uparrow\{x\}; \\ 0 & \text{otherwise}. \end{cases}
\]

3. Construct the sketch vector \(\text{sk}(\text{vec}(x)) \in \mathbb{R}^d\), for a target dimension \(d\), built so that for \(x, y \in U\),
\[
\text{sk}(\text{vec}(x)) \cdot \text{sk}(\text{vec}(y)) \approx \text{vec}(x) \cdot \text{vec}(y).
\]

Our motivation for considering the upper sets \(\uparrow\{x\}\) is that they represent the partial order via the subset relation, that is,
\[
x \leq y \iff \uparrow\{x\} \supseteq \uparrow\{y\} \iff |\uparrow\{x\} \cap \uparrow\{y\}| = |\uparrow\{y\}|.
\]

Since the characteristic vectors \(\text{vec}(x)\) have the property that \(\text{vec}(x) \cdot \text{vec}(y) = |\uparrow\{x\} \cap \uparrow\{y\}|\), we have that
\[
x \leq y \iff \text{vec}(x) \cdot \text{vec}(y) = \text{vec}(y) \cdot \text{vec}(y),
\]
so the \(\text{vec}(x)\) give a direct representation of \((U, \leq)\) via their dot products. However, they are vectors in \(|U|\) dimensions, which is typically too big to be useful, so in the third step above, we apply a sketching operation, described next, that maps the \(\text{vec}(x)\) to lower-dimensional vectors, while approximately preserving dot products.

3.2 Sketching

There are a variety of sketching methods, but the one we have investigated the most is countsketch Charikar et al. (2002); here we need two hash functions
\[
h_1 : U \to [d] \quad \text{and} \quad h_2 : U \to \{-1, +1\},
\]
where \([d] \overset{\text{def}}{=} \{1, 2, \ldots d\}\). In the ideal setting, \(h_1\) and \(h_2\) are uniformly random, over \([d]\) and \((-1, +1)\) respectively. Given vector \(v \in \{0, 1\}^U\), its sketch in \(\mathbb{R}^d\), via countsketch, has coordinates
\[
\text{sk}_c(v)_i \overset{\text{def}}{=} \sum_{y : h_1(y) = i} v_y h_2(y),
\]
that is, the sum of the bit flips \(h_2(y)\), over the \(y \in U\) such that \(v_y = 1\) and \(y\) hashes (using \(h_1\)) to \(i\).
3.3 More concrete description

Short-cutting the conceptual discussion, our embedding can be described as follows: given \( x \in U \), \( \text{OrderSketch}(x) \) is the vector with

\[
\text{OrderSketch}(x)_i \overset{\text{def}}{=} \sum_{x \leq y \atop h_1(y) = i} h_2(y), \text{ for } i \in [d].
\]  

(1)

If \( h_1 \) and \( h_2 \) are indeed random, then one can show that for \( v, w \in \mathbb{R}^U \), \( sk_c(v) \cdot sk_c(w) \) is an unbiased estimator of \( v \cdot w \), that is,

\[
\mathbb{E}[sk_c(v) \cdot sk_c(w)] = v \cdot w.
\]

In particular, if \( v \) and \( w \) are very sparse, so that there are no collisions in their sketches, that is, \( h_1(y) \neq h_1(y') \) for any \( y, y' \) with \( v_y = v_{y'} = 1 \) or \( w_y = w_{y'} = 1 \), then \( sk_c(v) \cdot sk_c(w) = v \cdot w \). More generally, the sparser \( v \) and \( w \) are, the more accurate the sketch-based estimate of the dot product will be.

The role of the bit-flip hash function \( h_2 \) is to reduce the effect of collisions, by averaging out their effects, but with enough sparsity, \( h_2 \) is not needed.

Other possible sketching methods involve simhash Charikar (2002) and minhash Broder (1997), for which the application to dot-product estimation is less direct, and processing is more complex and expensive, but which may well be more effective in sketching vectors that are not sparse. Our preliminary experiments suggested that simhash is not competitive with countsketch for the cases we considered.

4 OrderSketch applied to WordNet

We apply our order embedding technique to WordNet Miller (1998), mainly to the hypernym relation. Here the relation is between specific word meanings, where a word meaning is represented in WordNet as a synset. Our hashes \( h_1 \) and \( h_2 \) are implemented as Python's native hash applied to the synsets and to synset names, respectively. The upper sets \( \uparrow \{ x \} \) are, for each synset, the set of all synsets that hypernyms of it (including transitively), and each lemma name, considered as a union of synsets, is represented as the union of their upper sets.

We obtain representations \( \text{OrderSketch}(x) \) of synsets and lemma names, using countsketch. When synset \( y \) is a hypernym of lemma name \( x \), \( |\uparrow \{ x \} \cap \uparrow \{ y \}| = |\uparrow \{ y \}| \), by construction, and so we expect

\[
R_{x,y} \overset{\text{def}}{=} \frac{\text{OrderSketch}(x) \cdot \text{OrderSketch}(y)}{\text{OrderSketch}(y) \cdot \text{OrderSketch}(y)}
\]

to be close to one. If \( x \) and \( y \) are not related, we expect \( R_{x,y} \approx 0 \).

To test our representation, we consider \( R_{x,y} \) in these two situations, where we consider for the positive case all synsets \( y \), and all lemma names \( x \) in WordNet that have one sense (synset) that is a hyponym of \( y \). Our proxy for the negative, unrelated case, is choosing for each synset \( y \) a number of lemma names \( x \) at random, and computing \( R_{x,y} \).
We used this scheme with embedding dimension $d = 100$, and 20 random $x$ per synset in the negative case. The average deviation from $R_{x,y} = 1$ in the positive case was 6%, and from zero in the negative case was 9%. By considering a decision rule $R_{x,y} \geq T$ for different $T$, we obtain a range of true and false classifications, with ROC curve shown in Figure 1. We also explored AUROC, the area under the ROC, as a function of $d$; see Figure 1 in the Appendix, and further results in Section A.3 there. A similar experiment for part-of, that is, the part-meronym relation, yielded a classifier with 0.985 AUROC, and AUROC 0.986 for the substance-meronym relation.

![Figure 1: ROC of hypernymy classification based on OrderSketch; the area under the curve is 0.9733.](image)

5 **OrderSketch applied to SnoMeSHNet**

Before beginning with applying the embedding algorithm to medical ontologies just as with Wordnet, we needed to perform an intermediate step of organizing the ontology elements as synsets and lemmas, during which we formed SnoMeSH, in which we composed related elements across SNOMEDCT and MeSH (Rogers, 1963) The ordering information in SnoMeSH is based on the is-a relationship in SNOMEDCT, as it aligns more with how hypernymy is represented in Wordnet, although there are more ordering relations such as part-of to exploit as well.

It can also be noted that the provision of synonymous concepts from one ontology as the lemmas of a synset, corresponding to matching a concept of another ontology, enables contextual information to be captured along with ordering information. While this is explicit during construction of the SnoMeSH dataset, such synonymy amidst hypernymy can also be present in synsets of Wordnet for our embedding algorithm to capture. One more point to notice is that unlike Wordnet, where a single lemma can have multiple senses, here in SnoMeSH we assume there is only one medical sense, although there is potential in future to explore the granularity of sense even within medical usage.

We obtain representations $\text{OrderSketch}(x)$ of synsets and lemma names of SnoMeSHNet, using countsketch. We use 500,000 synsets, out of which 100,000 have more than one lemma, and produced an embedding of dimension $d = 500$. The area under the ROC curve for this is 0.9723. Further results are given in Section A.4 in the Appendix.

5.1 **Additional findings from SnoMeSH**

While building an order embedding using the SnoMeSH dataset, we discovered loops in the is-a relationship in SNOMEDCT, which we currently handle by detecting strongly connected components and merging them into single synsets, also altering the concerned synset’s hypernyms and hyponyms. This also presents an opportunity to involve a human-in-the-loop domain...
expert, to verify these bad links and directly fix shortcomings in ontologies. In addition to the ordering information provided through SNOMEDCT, ordering information can also be derived from MeSH through applied heuristics: when a MeSH concept has synonyms, and the synonyms are not given as synonyms of each other, then the initial MeSH concept can be regarded as the hypernym of each of these synonyms, with all the hypernymy chains being of depth 1. Due to the low depth, we preferred not to use it for our experiments, but is still worth noting.

6 Execution times

The experiments were run on a personal Macbook pro with 16GB memory and processor 2.7 GHz Quad-Core Intel Core i7 with no graphics processor engaged. The following observations were made: There was an average 103.2% increase in end-to-end execution time for a doubling up of dataset size (number of synsets with hypernymy relations) to be processed, while embedding dimension was kept the same. There was an average of 47.3% increase in end-to-end execution time for a doubling up of embedding dimension, with size of synsets maintained. A dataset of 500,000 synsets with 100,000 of them having more than one lemma, and an embedding dimension of 300, takes an end-to-end execution time of 901.898 seconds, that is, about 15 minutes. See also Section A.5.

7 Future experiments

We have shown that embeddings that embody ordering knowledge from ontologies are readily built; we plan to use these embeddings standalone or in combination with contextual embeddings on real-world applications and benchmarks such as BLESS dataset. In addition to widely used benchmarks for this category of embedding technique, we also plan to test the usefulness of our embedding on specialty real-world applications with sufficient vocabulary overlap, such as on medical applications, including disease code detection on MIMIC NOTEEVENTS, and other textual data with sufficient vocabulary overlap with SNOMEDCT and MeSH concepts. In addition to using our technique for feature representation, we also plan to use our embedding algorithm to detect cycles in ontologies when the ontology is intended to be hierarchical but is not (as with SNOMEDCT for example), infer relationships within it (as in MeSH) and across (as in SnoMeSH) ontologies. We plan to do this more automatically, rather than involving applying heuristics as we do currently, and use these verified and established relationships to suggest completion to properties of entities within and across ontologies.

Given the quick execution time and ability to run on any configuration of even personal systems, we hope to have our embedding algorithm deployed where domain experts, such as doctors in the case of medical ontology embedding, can add or edit their local version of the ontology, and then retrain and obtain new embeddings for text processing nearly instantaneously. We would also like to develop prototype systems to drive this line of usage.
8 Conclusion

In this work, we presented a low-carbon-footprint method to capture ordering knowledge from ontologies of any given domain from partial orders, specifically is-a relationships, and amending this knowledge using synonymy for synsets or lemmas. Along with this, we provided some insights into what the graphical representation of the embeddings tell us regarding our current experiments, and the scope for future work.

References

Andrei Z Broder. 1997. On the resemblance and containment of documents. In Proceedings. Compression and Complexity of SEQUENCES 1997 (Cat. No. 97TB100171), pages 21–29. IEEE.

Haw-Shiuan Chang, ZiYun Wang, Luke Vilnis, and Andrew McCallum. 2017. Unsupervised hypernym detection by distributional inclusion vector embedding. CoRR, abs/1710.00880.

Moses Charikar, Kevin Chen, and Martin Farach-Colton. 2002. Finding frequent items in data streams. In International Colloquium on Automata, Languages, and Programming, pages 693–703. Springer.

Moses S Charikar. 2002. Similarity estimation techniques from rounding algorithms. In Proceedings of the thirty-fourth annual ACM symposium on Theory of computing, pages 380–388.

Qiuhao Lu, Nisansa de Silva, Sabin Kafle, Jiazhen Cao, Dejing Dou, Thien Huu Nguyen, Prithviraj Sen, Brent Hailpern, Berthold Reinwald, and Yunyao Li. 2019. Learning electronic health records through hyperbolic embedding of medical ontologies. In Proceedings of the 10th ACM International Conference on Bioinformatics, Computational Biology and Health Informatics, BCB ’19, page 338–346, New York, NY, USA. Association for Computing Machinery.

Anh Tuan Luu, Yi Tay, Siu Cheung Hui, and See Kiong Ng. 2016. Learning term embeddings for taxonomic relation identification using dynamic weighting neural network. In Proceedings of the 2016 Conference on Empirical Methods in Natural Language Processing, pages 403–413, Austin, Texas. Association for Computational Linguistics.

George A Miller. 1998. WordNet: An electronic lexical database. MIT press.

Kim Anh Nguyen, Maximilian Köper, Sabine Schulte im Walde, and Ngoc Thang Vu. 2017. Hierarchical embeddings for hypernymy detection and directionality. CoRR, abs/1707.07273.

A. Perotte, R. Pivovarov, K. Natarajan, N. Weiskopf, F. Wood, and N. Elhadad. 2014. Diagnosis code assignment: models and evaluation metrics. Journal of the American Medical Informatics Association : JAMIA. 2014 Mar-Apr;21(2):231-7. Epub 2013 Dec 2. PMID: 24296907; PMCID: PMC3932472.

Frank B Rogers. 1963. Medical subject headings. Bulletin of the Medical Library Association, 51(1):114–116.
A Appendices

A.1 Creating the SnoMeSH dataset

For each SNOMEDCT concept, a compound BioOntology (Whetzel et al., 2011) query containing tokens of the concept is launched on MeSH ontology. Out of the accepted MeSH return results that contain both `prefLabel` and `synonym` attributes, the results are further validated such that there is an overlap of at least one token between the snomed concept and MeSH `prefLabel` and between the snomed concept and at least one `synonym`. This ensures sufficient contextual match of snomed entry and MeSH entry and also between the MeSH `prefLabel` and its `synonyms` with respect to the snomed concept.

An example of some SnoMeSH entries for the SNOMEDCT concept of `Entire occipitomastoid suture of skull (body structure)` are presented in Table 1 to show how the SnoMeSH entries can provide contextual knowledge on related anatomical parts, medical procedures and related medical findings for this instance. Since MeSH terms are more descriptive labels than the phrase like nature of SNOMEDCT concepts, the MeSH entries that pass the validation are most likely to contain essential information and exclude returning non-informative parts like prepositions and determinants.

![Table 1](image)

| MeSH synonyms                     | MeSH prefLabel         |
|-----------------------------------|-------------------------|
| ‘Cranium’, ‘Skulls’,              | Skull                   |
| ‘Calvaria’, ‘Calvarium’           |                         |
| ‘Suture Technique’,               | Suture Techniques       |
| ‘Technique, Suture’,...           |                         |
| ‘Technics, Suture’                |                         |
| ‘Fractures, ... ’Non-Depressed    | Skull Fractures         |
| Skull Fractures’                  |                         |
| Skull Fractures’                  |                         |

Table 1: Example for how a single SNOMEDCT concept `Entire occipitomastoid suture of skull (body structure)` gets augmented in SnoMeSH

Also SNOMEDCT is noisier compared to MeSH wherein it has related entries such as `Sandals (physical object)` is-a `Footwear (physical object)` which is not much relevant to medical domain. The MeSH match and curation step will not include this entry in SnoMeSHNet and hence also excluded from `synset` and lemmas used by our embedding algorithm. In a way, the amending of SNOMEDCT using MeSH to create a SnoMeSH entry, is a realization for curating
more domain relevant entries, since now we have two domain specific ontologies, to verify the relevance of a particular concept against.

A.2 Evaluating our representations

As discussed in the main text, to test our representations, we consider $R_{x,y}$ in two situations, where we consider for the positive case all synsets $y$, and all lemma names $x$ in WordNet that have at least one sense (synset) that is a hyponym of $y$. Our proxy for the negative, unrelated case, is choosing for each synset $y$ a number of lemma names $x$ at random, and computing $R_{x,y}$.

One aspect we will address in future work is to ensure that when $x \preceq y$, the approximations we use do not result in our reporting that $y \preceq x$. A scheme to do this is as follows: rather than $R_{x,y}$, we store for each $x$ also $N_x \overset{def}{=} |\uparrow\{x\}|$, and test

$$\hat{R}_{x,y} \overset{def}{=} \text{OrderSketch}(x) \cdot \text{OrderSketch}(y)/N_y,$$

instead of using

$$\text{OrderSketch}(y) \cdot \text{OrderSketch}(y) \approx N_y.$$  

Moreover, we test also if $N_y < N_x$, and only report $x \preceq y$ if that is true, in addition to $\hat{R}_{x,y} \approx 1$. Such a scheme would be more accurate, at the cost of a representation with one more coordinate, and a more complicated representation.

A.3 Evaluating WordNet representations

For wordnet, we used our evaluation scheme with embedding dimension $d = 100$, and 20 random $y$ per synset in the negative case. The average deviation from $R_{x,y} = 1$ in the positive case was 6% (shown in Figure 2a), and from zero in the negative case was 9% (shown in Figure 2b).

For convenience, in all our tests, we ignore the verbs in WordNet, as they have a loop.

As discussed in the main text, we also computed the AUROC (area under the ROC), for part and substance holonyms as well as hypernyms. For hypernyms, we computed the AUROC for different values of $d$, from 10 to 500; please see Figure 2c.
A.4 Evaluating SnoMeSHNet representations

For SnoMeSHNet, we used our evaluation scheme with embedding dimension $d = 500$. The average deviation from $R_{x,y} = 1$ in the positive case was 15% (shown in Figure 3a), and from zero in the negative case was 7% (shown in Figure 3b). By considering a decision rule $R_{x,y} \geq T$ for different $T$, we obtain a range of true and false classifications, with ROC curve shown in Figure 3c.

A.5 Execution times

The experiments were run on a personal Macbook pro with 16GB memory and processor 2.7 GHz Quad-Core Intel Core i7 with no graphics processor engaged. The following observations were made:

- There was an average of 103.2% increase in end-to-end execution time for a doubling up of dataset size (number of synsets with hypernymy relations) to be processed while embedding dimension was kept the same.

- There was an average of 6.4% increase in end-to-end execution time for a 10-fold increase in the number of synsets that had more than one lemma, while size of synsets and embedding dimension were maintained.

- There was an average of 47.3% increase in end-to-end execution time for a doubling up of embedding dimension, with size of synsets maintained.

- A dataset of 500,000 synsets with 100,000 of them having more than one lemma, and an embedding dimension of 300, takes an end-to-end execution time of 901.898 seconds, that is, about 15 minutes.

A few profiling entries from an array of experiments we ran with SnoMeSHNet can be found in Table 2.
| No. of synsets | Component          | Secs  |
|---------------|--------------------|-------|
| 10,000        | Hypernym chains    | 0.038 |
| 100,000       | Hypernym chains    | 0.687 |
| 500,000       | Hypernym chains    | 4.714 |
| 10,000        | No loops seen      | 0.000 |
| 100,000       | Fix 27 loops       | 0.006 |
| 500,000       | Fix 835 loops      | 0.049 |
| 10,000        | Two hash functions | 0.062 |
| 100,000       | Two hash functions | 0.674 |
| 500,000       | Two hash functions | 13.298|
| 10,000        | Create vectors     | 0.455 |
| 100,000       | Create vectors     | 4.534 |
| 500,000       | Create vectors     | 55.988|
| 10,000        | End-to-end $d = 100$ | 16.539|
| 100,000       | End-to-end $d = 200$ | 207.712|
| 500,000       | End-to-end $d = 300$ | 901.898|

Table 2: Profiling across different size runs, components and embedding dimensions