Hierarchies over Vector Space: Orienting Word and Graph Embeddings

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Abstract
Word and graph embeddings are widely used in deep learning applications. We present a data structure that captures inherent hierarchical properties from an unordered flat embedding space, particularly a sense of direction between pairs of entities. Inspired by the notion of distributional generality (Weeds et al., 2004), our algorithm constructs an arborescence (a directed rooted tree) by inserting nodes in descending order of entity power (e.g., word frequency), pointing each entity to the closest more powerful node as its parent.

We evaluate the performance of the resulting tree structures on three tasks: hypernym relation discovery, least-common-ancestor (LCA) discovery among words, and Wikipedia page link recovery. We achieve average 8.98% and 2.70% for hypernym and LCA discovery across five languages and 62.76% accuracy on directed Wiki-page link recovery, with both substantially above baselines. Finally, we investigate the effect of insertion order, the power/similarity trade-off and various power sources to optimize parent selection.

1 Introduction
Word and graph embeddings have important applications outside their primary mission as features for machine learning models, such as word analogy (Gladkova et al., 2016) and graph visualization (Wang et al., 2019). Embeddings generally consist of unordered points in $d$-dimensions where $d$ typically ranges from 50 to 300. But they are flat, with no explicit organization beyond geometrical proximity. In this paper, we aim to expand the power of embeddings for both exploratory analysis and machine learning by building hierarchical structures on top of them.

Directed rooted trees (arborescences) are important structures with many natural applications. When modeling a taxonomy or hierarchy, leaf-to-root paths typically define successively more general concepts or more powerful entities. Sets of nodes in small sub-trees typically share similarities and define natural clusters in the dataset.

Unfortunately, many of the current embeddings have no explicit structure. As Figure 1(a) shows, the distance metric between entities reflects similarity, but the embedding itself does not have an explicit ordered structure, despite that words and graph certainly have underlying hierarchical structures.

Figure 1: Sub-figure(a): 2D PCA projection of words in GLoVe embedding. Sub-figure (b): Discovered solid edges exist in WordNet, while dot edges do not. Associated edge length reflects the $l^2$ distances between words in embedding space. By finding the directed edges among them, a meaningful hierarchy could be discovered.

In this paper, we propose a simple but powerful way to construct meaningful hierarchies, or orientations, from almost any embedding. We incorporate one additional feature, called entity power, which is easily obtained at the time of building the embedding, namely a notion of the frequency, magnitude, or importance of each entity. For words, the word frequency of each token in the training corpus makes for a natural notion of importance, while for graphs the vertex degree of each node or its PageRank (Page et al., 1999) plays a similar role. We further observe the word embedding implicitly
encodes word frequency information, which is consistent with observations found in Schnabel et al. (2015); Gong et al. (2018).

Inspired from distributional generality proposed by Weeds et al. (2004), we assume that general entities have more power than the specific ones, implying a rational entity insertion order when construct arborescences over embeddings. After starting from a single root node at the center of the embedding space, we construct our arborescence in an iterative fashion, inserting nodes in order from most to least powerful, having each new node point to its nearest neighbor already in the tree as its parent, representing similarity in edge length.

We demonstrate that the arborescences we build from word and graph embeddings have several appealing properties as Figure 3 shows. We envision a variety of applications associated with visualization and reasoning via embeddings. Consider the task of discovering hypernym relationships for low resource languages. Hypernyms are “type-of” relations, for example, “color” is the hypernym of “red” and “blue”. WordNet (Miller, 1995) and BabelNet (Navigli and Ponzetto, 2012) are important sources of hypernym relations for popular languages, such resources are rare among the world’s languages. But the oriented embeddings we propose are readily constructed from any text corpus, and provide a first stab at discovering hypernym relationships in the absence of any additional resources.

Our primary contributions in this paper are:

- **Constructing and Evaluating Oriented Word and Graph Embeddings**: We propose and evaluate a variety of parental selection decision rules for orienting embeddings, differing by insertion order and nearest neighbor criteria. We demonstrate that our favored insertion ordering of most-to-least powerful proves most successful at identifying edges (in graph embeddings) and discovering hypernym relationships (in word embeddings). Figure 2 shows the word frequency relations between hypernym/hyponym word pairs. Rank 0 represents the most frequent word. If multiple hypernyms exist for a word, the minimum rank of hypernym word frequency is shown. The horizontal and vertical axis represent the word frequency rank of hyponym (e.g., banana) and hypernym (e.g., fruit) respectively. Most of the blue dots are placed below the black diagonal line, indicating that the most hypernyms are more frequent than their hyponyms.

- **Identifying Semantic Breaks**: Leaf-to-root paths repeatedly transition in and out of natural neighborhoods to more general concepts. We demonstrate that our accuracy of identifying relationships increases when we exclude natural semantic breaks formed by long edges in the arborescence. This provides natural ways of efficiently constructing fine-grain clusters of entities.

- **Entity Power vs. Similarity in Identifying Relationships**: Nearest neighbor models are widely used in NLP and data science to ascribe possible relationships between pairs of items. But power law distributions imply relatively few entities will account for an outsized fraction of total references or interest. Inspired from Distributional Generality Hypothesis (Weeds et al., 2004). We incorporate notions of power into similarity detection seems valuable in breaking near-ties and prioritizing attention. We perform a series of experiments of the performance of distance measures incorporating various power components, establishing the best trade-off between them.

- **Hidden Power Source from Word Vector**: The frequency rank might be inaccessible from pure word embedding matrix. Fortunately, from our experiment and recent research (Gong et al., 2018; Arora et al., 2016),
we confirm that the first few principal components (PCs) encode the word frequency information. Leveraging this finding, our experiments demonstrate that the power order induced from PCs is significant better than random and helpful in tree construction.

- **Algorithmic Implications of Hierarchical Structures**: For example, the lowest common ancestor (LCA) (Schieber and Vishkin, 1988; Bender et al., 2001) of nodes $x$ and $y$, represents the unique tree node $l$ most distant from the root that is an ancestor of both $x$ and $y$, typically defining the commonalities or superordinate relations between them. After linear-time pre-processing, the lowest common ancestor of $(x, y)$ can be computed in constant time for any node pair, providing a fast way to compare embedded representations.

2 Related Work

Word (Mikolov et al., 2013b; Pennington et al., 2014) and graph embeddings (Perozzi et al., 2014) are widely used to capture the relatedness of symbolic entities in an unsupervised manner.

Rooted on Distributional Hypothesis (Harris, 1954) - the entities in the similar contexts tend to have similar meaning. The co-occurrence based embedding methods capture the correlation of semantic relations. Schnabel et al. (2015) applied intrinsic evaluation on word embeddings and showed that the nearest neighbors of a queried word highly overlap with related words labeled by human (e.g., money is close to cash).

Natural languages inherently have hierarchical structures (Gaume et al., 2006; Polguere, 2009). Distributional Generality was proposed by Weeds et al. (2004), suggesting contexts of a specific word (hyponym) are included in its semantically-related but more general word (hypernym), and hypernysms tend to be more frequent than the hyponyms.

Hearst (1992) leveraged the text surface pattern to discover hypernyms and extended text patterns by bootstrapping. Snow et al. (2005) further built a classifier for hypernym word pair detection in a vector-space model. Herbelot and Ganesalingam (2013) proposed Semantic Content and used KL divergence as the hypernym score, but it does not outperform a simpler frequency measure.

As word embedding and deep learning become popular, many researchers aim at building embedding model dealing with hierarchical information. Alsuhaibani et al. (2018) proposed a hierarchical word embedding model considering not only the contextual information, but also hypernym specific information on a taxonomy for fine-tuning. Fu et al. (2014), Vylomova et al. (2015), Weeds et al. (2014) and Rimell (2014) detect hypernym relations in a supervised word pair classification framework based on the geometric properties of embeddings such as clustering, embedding negation and other vector operations. Recently, Nickel and Kiela (2017); Tifrea et al. (2018) proposed to model tree structure in hyperbolic space, preserving tree-distance in non-Euclidean Poincaré space, and leverage the resulting embedding geometry to reconstruct word hierarchy and predict missing links.

Unfortunately, these aforementioned approaches need labeled structured data (e.g., hypernyms from WordNet (Miller, 1995)), word pairs with known relations or hand-crafted patterns, and they may not be easily expandable to resource-poor languages. Different from the previous works, our goal is **not** to design a supervised model for word pairs classification, but to discover a meaningful hierarchy over embeddings of symbolic data in an unsupervised manner, then evaluate the hierarchy’s rationality with external ground truth.
3 Methods

We propose an unsupervised method to build an arborescence over symbolic data, enhancing embeddings with a measure of the power or importance of each data point, like word frequency or vertex degree. After initializing the tree with a maximally powerful root node artificially, simulating the ultimate parent of all entities, at the center of the embedding space, we insert entities into the tree in descending order of entity power.

Each new node is connected to the closest current tree node as the parent by some measure of similarity. Here we evaluate a family of similarity measures based on geometric distance (Euclidean or cosine distance) in embedding space and node power of the parent candidates. With the selected parent $P_i$ for the $i^{th}$ inserted node, we define the similarity measures below:

$$P_i = \text{argmax}_{\text{Node}_j \in T_{i-1}} p \cdot \frac{\text{dist}^{-2}(\vec{v}_i, \vec{v}_j)}{\text{Max}(\text{dist}^{-2}(\vec{v}_i, \vec{v}_k \in \{0, \ldots, j\}))} + (1 - p) \cdot \frac{\log(d_j)}{\text{Max}(\log(d_k \in \{0, \ldots, j\}))}$$

where $T_{i-1}$ is the total tree nodes prior to the new node being inserted, $p \in [0, 1]$ is the weight on distance, $d_j$ is the entity power of the candidate parent $\text{Node}_j$, $\vec{v}_i$ is the embedding vector of $\text{Node}_i$, and $\text{dist}(\cdot, \cdot)$ is either $l^2$ or cosine distance function.

The range of edge scores is scaled to be $[0, 1]$ by separately normalizing the contributions from node distance and node power, and then linearly combining them according to the weight $p$. In this manner, the edge score is proportional to the square root of node distance and logarithm of node power.

Meanwhile, to avoid the power dominance of the artificial root, we dynamically change root’s power to be the average power of the inserted entities. Therefore, the first inserted nodes are more prone to connect to the root, preserving the natural high-level categorization or semantic base. As insertion continues, the root becomes less influential.

Inserting each of the $n$ nodes requires searching for the nearest neighbor among all current tree nodes, so the complete tree can be constructed in $O(n^2)$ time. The bottleneck here is in finding the nearest neighbor. Instead of using brute force, a geometric search data structure such as a ball-tree (Omahundro, 1989) can be pre-computed over all the points. Although we are only interested in the nearest more-powerful point instead of the closest point over all, we can heuristically reduce the search space using ball-trees, so the expected time complexity can be reduced to $O(n^{3/2})$.

Besides the explicit word frequency counted from the corpus, Arora et al. (2016) theoretically explains the relation between word frequency and $l^2$-norm of the word vector, showing that high-frequency words tend to have large $l^2$-norm, as we observed in Figure 4.

![Figure 4: We select the vocabularies overlapped with the WordNet, roughly 10K for each language. Word frequency decreases from left to right along horizontal-axis. Concurrently, the $l^2$-norm of the word vector tends to decrease, indicating a strong correlation between word frequency and vector length. The value is smoothed using a window of size 50.](image_url)

Based on this justification, (Mu et al., 2017) proposed a simple but effective post-processing method for word embedding, arguing that the undesirable word frequency is encoded in the first few principal components (PCs) of word embedding. Their post-processed embedding, by projecting PCs away from word vectors, presumably removes the frequency bias, and gain better performance consistently on various word similarity tasks.

Learning from their investigations, we leverage the $l^2$-norm of the projected PCs as a new source of word power, called PCA-induced Power. Formally:

$$u_0, u_1, \ldots, u_d = \text{PCA}(V - \mu)$$

$$d_w = \| \sum_{i=0}^{k} (v_w u_i^\top u_i) \|_2$$

(1)

$$\vec{v}_w = v_w - \mu - \sum_{i=0}^{k} (v_w u_i^\top u_i)$$

where $V$ is the word embedding matrix, $\mu$ is the center of the embedding vectors, $u_i$ is the $i^{th}$ principal component of the embedding centered at $\vec{0}$, $d_w$ is the PCA-induced power for the word.
\( w, \ v_w \) is the row-vector embedding of the word \( w \), \( \tilde{v}_w \) is the de-biased word vector, \( k \) is the parameter controlling how many PCs should be projected. We fix \( k \) to be 3 for all experiments.

4 Experiments

We construct our proposed trees for two types of embedding datasets: the Wikipedia-people graph embedding and word embeddings of multiple languages. We investigate effects of three node insertion orders (descending, random and ascending), the power/distance trade-off parameter \( p \), and the word power induced from word vector. In the following section, we will describe the datasets, report our results on Wiki-people and WordNet (English) in detail, then extend our experiments to WordNet of other languages (French, Italian, Japanesees and Chinese), finally discuss the effect of word power information encoded in the word vector.

4.1 Dataset Description

The Wiki-people dataset is a directed graph of links between biographical Wikipedia pages (Leskovec and Krevl, 2014; Skiena and Ward, 2014). We sampled a sub-graph of 100K nodes from the largest weakly-connected component of the Wiki-people graph. Then we run Deepwalk (Perozzi et al., 2014) on the undirected version of the sub-graph to obtain the node embeddings. We expect our algorithm can recover the directed relations from the embeddings trained from an undirected hierarchy.

WordNet (Miller, 1995; Bond and Foster, 2013) contains a directed graph of words in major languages, where certain edges represent hypernym relationships, specifically, the hypernyms within a five-closure of a word.\(^1\) For example, President is Man, Man is Vertebrate, so President is a Vertebrate. We leverage pre-trained English GLoVe embedding (Pennington et al., 2014) with 100-dimension, and Word2Vec (Mikolov et al., 2013a) embeddings of five languages with 300-dimension. All the embeddings are pre-trained on Wikipedia data, without any explicit hypernym information.

We restrict attention here to the intersection between embedding vocabulary and the words involved in WordNet hypernym relations. The embeddings are ordered by frequency rank, so we estimate the word power as underlying word frequencies using Zipf’s law (Li, 1992), called Zipf-induced frequency. Furthermore, we investigate the effect of word power directly induced from Principal Components of word embeddings, mentioned earlier as PCA-induced power.

The gross statistics of both data sets are presented in Table 1. Figure 3 shows several examples of generated sub-trees. Our algorithm recovers edges (solid lines) in the datasets and discovers new edges (dotted lines), while the edge length represents the inter-node distance.

4.2 Detailed Analysis on Wiki-people and WordNet (En)

In this section, we evaluate our constructed trees by edge accuracy: what percentage of the reported tree edges are ground-truth relationships in the associated dataset. We investigate the effect of insertion orders and varying \( p \), as well as the edge accuracy from the perspective of edge length and node power. In all evaluations, we exclude the edges linking to the artificial root.

4.2.1 Edge Accuracy vs. Power/Distance

Figure 5 presents edge accuracy as a function of \( p \), the trade-off parameter between power and distance. We measure this accuracy in three ways: undirected edge accuracy accepts edges regardless of direction, directed edge accuracy requires getting the edge orientation to match that of the ground-truth relation, and reverse directed edge accuracy counts the edges having reversed direction to the ground truth.

Figure 5: Accuracy as \( 0 \leq p \leq 1 \). Increased weight on distance over power results in trees with more qualified edges. “Syn. Acc.” reflects the edges capturing synonym word pairs.

As expected, the edge accuracy generally increases as \( p \) increases, but peaks at \( p = 0.6 \). This shows the importance of distance over power. Further, under our preferred descent insertion order the accuracy of the directed edges (“Dir. Acc.”) is consistently higher than the reversed directed edges.

\(^1\)We also did experiments with the hypernym closures from 1 to 4, with similar results.
Table 1: We use CBOW version of Word2Vec in all experiments. Since WordNet (Fr, Zh, It, Ja) only share a small portion of vocabulary (~10K) with the pre-trained embedding, we limit the size of all WordNet datasets to the similar scale. Multilingual WordNet data is organized by Bond and Foster (2013); Bond and Paik (2012). The versions of each language are created by Fellbaum (1998); Wang and Bond (2013); Isahara et al. (2008); Toral et al. (2010); Sagot and Fišer (2008)

(“Rev. Dir. Acc.”), which supports our hypothesis that nodes of less power should point to more powerful ones.

Table 2 presents model performance using the best $p$ for three different insertion orders, as well as a random selection baseline model that links to completely arbitrary parent nodes. The model using the descending insertion order significantly outperform the others in both undirected and directed edge accuracy. The WordNet-Random wins for reverse directed accuracy is a Pyrrhic victory because it puts edges in backwards, but still smaller than the accuracy (0.0507 to 0.0828) of our preferred insertion heuristic. The extremely low performance of the random selection baseline demonstrates the complexity of the edge linking task.

### 4.2.2 Edge Accuracy vs. Edge Length

Figure 6 reports the accuracy of tree edges as a function of the embedding distance between points (Edge length). It shows that closer pairs generally have higher edge accuracy, matching our expectation that close embedding pairs are more suggestive of genuine relationships than distant pairs. The initial low accuracy in WordNet reflects that many of the closest words are synonyms, not hypernyms. Generally short edges have higher accuracy, preserving more semantic and hierarchy information. Long edges create semantic breaks, forming weak links between entities. More fine-grain sub-trees can be extracted by excluding those long edges.

### 4.2.3 Edge Accuracy vs. Node Power

Figure 7 reports the edge accuracy as a function of node power. With the preferred insertion order, high power (of high percentile) entities are first inserted. The Wiki-people result shows the overall accuracy keeps steady, while the low accu-
racy of the least powerful nodes represents the lack of community linkages in the least significant persons. From right to left, the WordNet result shows that directed edge accuracy initially increases as we keep inserting words, demonstrating the ability to capture hypernym relations after constructing a semantic base above the artificial root.

Figure 7: Accuracy by node power. Under the preferred descending insertion order (from high percentile to low percentile), the directed edge accuracy increases and keeps steady.

4.3 Multilingual WordNets and PCA-induced Word Power

Table 3 aggregates the result of the best directed edge accuracy for three insertion orders of multiple languages (English, French, Italian, Japanese and Chinese). The results of the top-half (using Zipf-induced frequency) are consistent with the previous experiments: our preferred descent order always achieves the best accuracy across languages with a significant improvement, demonstrating that the core assumption (Distribution Generality Hypothesis (Weeds et al., 2004)) exists in multiple languages and can be leveraged to discover hypernym hierarchy from various word embeddings.

As we expected, after alternating Zipf-induce frequency to PCA-induced power, the performance is also consistent in Table 3, proving that the word vector encodes not only semantic meaning, but also a notion of frequency or generality, leading to the success of hypernym discovery.

4.4 Least Common Ancestors Discovery

One of the appealing properties in our proposed tree is least-common-ancestor (LCA) of a word pair \((w_1, w_2)\). We expect LCA can capture the common high level semantic meaning, providing a hierarchical understanding of word pairs. In WordNet, the function Lowest-Common-Hypernyms (LCH) plays the similar role. For example, \(LCH(\text{policeman}, \text{chef}) = \text{person}\).

Quantitatively, we evaluate the tree LCA quality by hit-rate, comparing the set \(LCA_{tree}(w_1, w_2)\) to the set \(LCH_{WordNet}(w_1, w_2)\). If \(LCA_{tree}\) contains any element in \(LCH_{WordNet}\), we consider it as a successful hit. We also add measure relaxation by including words within two-closure of LCA and
LCH. The hit-rate $s$ is defined as:

$$s = \frac{\sum_{W_i \in W} 1[LCAtree(W_i) \cap LCH_{WordNet}(W_i) \neq \emptyset]}{\sum_{W_i \in W} 1[LCH_{WordNet}(W_i) \neq \emptyset]}$$

(2)

where $W$ is the set of word pairs. The $i^{th}$ word pair $W_i$ consists of a randomly sampled word $w_i^1$ and another word $w_i^2$ which is sampled from 20-nearest neighbors of $w_i^1$ in the embedding space, making sampled word pair shares semantic meaning with subtle difference. Since the coverage of human annotation in WordNet is limited, we only count for the pairs having non-zero LCH.

We report the best hit-rate for different insertion orders in Table 4. As expected, our favored insertion order consistently achieves the highest hit-rate across different languages.

| Lang. | Descent | Random | Ascent |
|-------|---------|--------|--------|
|       | Zipf-induced Frequency |        |        |
| $En_{GloVe}$ | 0.0269 | 0.0136 | 0.0101 |
| $En$ | 0.0385 | 0.0143 | 0.0109 |
| $Fr$ | 0.0202 | 0.0010 | 0.0027 |
| $It$ | 0.0199 | 0.0051 | 0.0028 |
| $Ja$ | 0.0238 | 0.0038 | 0.0065 |
| $Zh$ | 0.0327 | 0.0081 | 0.0071 |
|       | PCA-induced Power |        |        |
| $En_{GloVe}$ | 0.0299 | 0.0132 | 0.0097 |
| $En$ | 0.0151 | 0.0055 | 0.0078 |
| $Fr$ | 0.0195 | 0.0075 | 0.0027 |
| $It$ | 0.0222 | 0.0115 | 0.0020 |
| $Ja$ | 0.0127 | 0.0020 | 0.0033 |
| $Zh$ | 0.0382 | 0.0055 | 0.0054 |

Table 4: The best tree LCA hit-rate of different insertion order of each language. Our favored descending order consistently outperforms others. We use GloVe embedding in $En_{GloVe}$ and Word2Vec (CBOW) for others. 10K word pairs are sampled as mentioned above.

LCA Result Analysis: We dive deep into the LCA results of English (GloVe) and categorize the results into four cases with examples:

- **Success** case represents the tree LCA overlaps the LCH from WordNet.

  Word Pair : (soup, potato)
  LCA : \{food\}
  LCH : \{food, substance, nutrient ... \}

- **FailureTrue** case represents the tree LCA fails to overlap LCH. It usually happens when Distributional Generality does not hold and should be improved in the future work.

  Word Pair : (september, april)
  LCA : \{june\}
  LCH : \{month, period, measure, ...\}

- **FailureFalse** case represents the tree LCA fails to overlap LCH, but with rationality.

  Word Pair : (thoroughfare, waterway)
  LCA : \{road\}
  LCH : \{physical entity, way\}

- **Complement** case represents LCH can not be found in WordNet, but our discovered LCA can be complementary.

  Word Pair : (ford, chevy)
  LCA : \{car\}
  LCH : \{\}

  Word Pair : (convalescence, recuperate)
  LCA : \{recover\}
  LCH : \{\}

5 Conclusions

We have proposed an algorithm to construct arborescences from embeddings. Our experiment shows this arborescence can achieve 62.76% of directed edge accuracy for Wiki-people graph, and a corresponding 8.98% and 2.70% average accuracy in hypernym & LCA discovery across different languages. We have restricted attention to directed trees, where each node has only one parent. Allowing each node to have multiple parents among higher-ranked nodes turns our arborescence into a directed acyclic graph (DAG). Such expressibility would allow us to capture alternate word senses, and is left for future work.
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