

# Representing and Reconstructing PhySH: Which Embedding Competent?

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## Abstract

In this paper, we conduct a comprehensive comparison of well-known embeddings' capability in capturing the hierarchical Physics knowledge. Several key findings are: (i) Poincaré embeddings do outperform if trained on PhySH, but it fails if trained on co-occurrence pairs which are extracted from raw text. (ii) No algorithm can properly learn hierarchies from the more realistic case of co-occurrence pairs, which contains more noisy relations other than hierarchical relations. (iii) Our statistic analysis of Poincaré embedding's representation of PhySH shows successful hierarchical representation share two characteristics: firstly, upper-level terms have a smaller semantic distance to root; secondly, upper-level hypernym-hyponym pairs should be further apart than lower-level hypernym-hyponym pairs.

## 1 Introduction

Concept hierarchy or taxonomy<sup>1</sup> is highly organized and expertly curated hierarchical hypernym-hyponym sets. How to effectively represent these terms with the hierarchical relation is the main hurdle for automatically taxonomy construction and other downstream applications.

Though embeddings have been taken for granted in most NLP pipelines, none of the previous work has fully explored which embeddings can capture hierarchical scientific knowledge. Even though Poincaré embedding is proved to have a better ability to capture hierarchical relations, it is learned based on existing WordNet hypernym-hyponym pairs. It is never been tested in the scientific domain. In this paper, we conduct a comprehensive comparison of well-known embeddings' performance in reconstructing Physical Subject Headings (PhySH) from raw APS datasets.

<sup>1</sup>In this paper, we use *taxonomy* and *concept hierarchy* as equal term.

Our main contributions are mainly three-fold: Firstly, for the first time, we compare mainstream embeddings' capability to represent and reconstruct Physical Subject Headings (PhySH) both from raw text and PhySH. Secondly, our experiment shows Poincaré embedding is not sufficient for taxonomy induction from raw text. Thirdly, we explore the characteristics of successful representation of PhySH, which might be the inspiration for better taxonomy construction algorithms.

## 2 Related Work

**Representations for Concept Hierarchy.** Representations for concept hierarchy has been receiving quite growing interests in recent years (Kozareva et al., 2008; Carlson et al., 2010; Shen et al., 2018). It is the basis of automatic taxonomy construction. In the survey study of (Wang et al., 2017), there are *Pattern-based* (Hearst, 1992; Wu et al., 2012; Kozareva and Hovy, 2010) methods and *distributional* (Navigli and Velardi, 2004; Luu et al., 2014; Padó and Lapata, 2003; Baroni and Lenci, 2010; Nguyen et al., 2017) methods use hand-crafted rule-based, co-occurrence features, syntactic features or graph features to learn representations of hierarchical pairs. They also apply pretrained neural language models such as Word2Vec (Mikolov et al., 2013), GloVe (Pennington et al., 2014).

Recently, Poincaré embedding (Nickel and Kiela, 2017) is proposed to better represent hierarchical relations. Following works like (Law et al., 2019) use Lorentzian distance to replace the Poincaré metric, (Dhingra et al., 2018) extends Poincaré embedding to apply in raw text with re-parameterization technique, (Leimeister and Wilson, 2019) and (Tifrea et al., 2019) introduce hyperbolic embeddings in word embeddings like Skipgram and GloVe. Effectively in reconstructing WordNet though, the Poincaré embedding is not quite perfect yet (De Sa et al., 2018). It has only been tested on WordNet re-

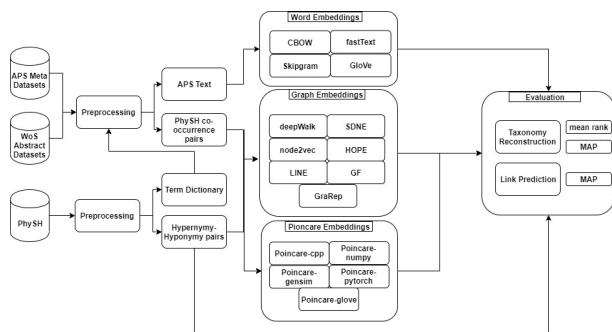


Figure 1: Evaluation Pipeline

construction and Hyperlex entailment (Nickel and Kiela, 2017). Whether it is an effective tool in representing hierarchical relations from raw domain text need to be further explored.

**Embeddings Analysis.** With the fast pacing of text representation technology, it is also important to revisit existing embedding methods for different downstream tasks. Several previous works have explicitly done this work based on their unique perspectives. Gladkova et al. (2016) explores GloVe’s ability to encode different morphological and semantic relations. (Zuccon et al., 2015) analyze word embeddings for information retrieval. Nooralahzadeh et al. (2019) compared COW and Skipgram by using Gensim implementation (Řehůřek and Sojka, 2010) with several different hyper-parameters settings and different domain corpus. Sanchez and Riedel (2017) explored different datasets in evaluation hypernyms identification by using GloVe. (Lastra-DÁmaz et al., 2019) surveys main word embeddings for word similarity.

Despite the above-mentioned work, there is still a missing part describing which embedding is the optimal choice for taxonomy induction. In this paper, we design our evaluation pipeline to choose the optimal embedding scheme for taxonomy learning and construction. In our paper, we consider two perspectives to represent and construct concept hierarchy: (i) Learn and construct from raw texts by word embeddings; (ii) Learn and construct from extracted co-occurrence pairs from raw texts by graph embeddings and Poincaré embeddings.

### 3 Method

In our pipeline (Figure 1), we follow three steps: raw text and PhySH preprocessing; learn various embeddings with different hyperparameters; evaluate embeddings by reconstructing PhySH.

We evaluate the following embeddings:

Model Name	Metric	Dimensions						
		5	10	20	50	100	200	
Word Embeddings	GloVe	mean rank	2168-30	2568-93	2237-33	2142-94	2188-83	2271-32
		MAP	0-18	0-05	0-06	0-07	0-06	0-06
	COW	mean rank	2883-64	3196-44	2937-09	3162-85	1894-02	3096-82
		MAP	0-69	0-63	0-70	0-63	<b>0-72</b>	0-64
	Skipgram	mean rank	2595-87	3939-61	3091-23	2732-08	3683-61	2893-45
		MAP	0-68	0-60	0-67	0-68	0-63	0-70
fastText	mean rank	2461-97	3004-28	2903-78	3391-16	3456-85	2493-87	
	MAP	0-67	0-67	0-69	0-66	0-59	0-65	
Graph Embeddings	deepWalk	mean rank	<b>244-03</b>	469-47	624-21	726-95	780-47	811-30
		MAP	0-18	0-05	0-06	0-05	0-05	0-05
	GF	mean rank	1189-78	1003-12	916-56	825-82	682-73	629-40
		MAP	0-01	0-01	0-01	0-01	0-02	0-03
	GraRep	mean rank	676-07	944-67	849-28	813-40	828-20	840-75
		MAP	0-05	0-01	0-02	0-03	0-03	0-03
	HOPE	mean rank	-	749-61	776-90	803-42	838-26	874-51
		MAP	-	0-12	0-11	0-10	0-08	0-06
	LINE	mean rank	387-65	360-36	459-23	432-79	423-59	425-38
		MAP	0-07	0-06	0-06	0-05	0-06	0-08
	node2vec	mean rank	490-53	458-11	462-65	459-00	453-37	450-80
		MAP	0-02	0-03	0-04	0-04	0-04	0-04
SDNE	mean rank	917-78	836-11	823-17	960-99	931-31	991-00	
	MAP	0-04	0-10	0-10	0-02	0-04	0-02	
Poincaré Embeddings	Poincaré Gensim	mean rank	765-08	734-58	747-20	750-99	739-38	745-25
		MAP	0-03	0-03	0-03	0-03	0-03	0-03
	Poincaré Cpp	mean rank	438-84	428-82	441-85	449-64	452-56	457-11
		MAP	0-06	0-09	0-09	0-09	0-09	0-09
	Poincaré Numpy	mean rank	935-95	880-16	861-51	874-15	892-52	879-84
		MAP	0-01	0-02	0-02	0-02	0-02	0-02
	Poincaré Pytorch	mean rank	1169-85	1151-57	1167-01	1164-53	1169-49	1165-13
		MAP	0-08	0-08	0-08	0-08	0-08	0-08
	Poincaré GloVe	mean rank	1268-48	1263-33	1250-31	1169-00	1165-30	1003-67
		MAP	0-01	0-01	0-01	0-03	0-04	0-06

Table 1: PhySH reconstruction from APS datasets, with word embeddings trained on raw text, graph embeddings and Poincaré embeddings trained on co-occurrence of PhySH terms in raw text. We only include each embedding’s optimal result in the table.

- Word embeddings: CBOw and Skipgram (Mikolov et al., 2013), fastText (Joulin et al., 2017), GloVe (Pennington et al., 2014)<sup>2</sup>.
- Graph embeddings: deepWalk (Perozzi et al., 2014), node2vec (Grover and Leskovec, 2016), LINE (Tang et al., 2015), LLE (Roweis and Saul, 2000), HOPE (Ou et al., 2016), GF (Ahmed et al., 2013), SDNE (Wang et al., 2016)<sup>3</sup>.
- Poincaré embeddings: Poincaré-gensim<sup>4</sup>, Poincaré-cpp<sup>5</sup>, Poincaré-pytorch<sup>6</sup>, Poincaré-numpy<sup>7</sup>, Poincaré-glove<sup>8</sup> (Tifrea et al., 2019).

Word embeddings are trained on *title* and *abstract* of APS publications. The PhySH terms’ embedding vectors will be extracted for taxonomy

<sup>2</sup>CBOw, Skipgram and fastText are trained by [https://github.com/NIHOPA/word2vec\\_pipeline](https://github.com/NIHOPA/word2vec_pipeline). GloVe is trained by <https://github.com/stanfordnlp/GloVe>

<sup>3</sup>Graph embeddings are implemented by OpenNE repository <https://github.com/thunlp/OpenNE>

<sup>4</sup><https://radimrehurek.com/gensim/models/poincare.html>

<sup>5</sup><https://github.com/TatsuyaShirakawa/poincare-embedding.git>

<sup>6</sup><https://github.com/facebookresearch/poincare-embeddings>

<sup>7</sup>[https://github.com/nishnik/poincare\\_embeddings.git](https://github.com/nishnik/poincare_embeddings.git)

<sup>8</sup>[https://github.com/alex-tifrea/poincare\\_glove](https://github.com/alex-tifrea/poincare_glove)

Model Name	Metric	Dimensions						
		5	10	20	50	100	200	
Graph Embeddings	deepWalk	<i>mean rank</i>	357-26	496-36	546-02	537-64	525-74	519-82
		<i>MAP</i>	0-22	0-19	0-21	0-22	0-22	0-23
	GF	<i>mean rank</i>	277-24	125-89	50-67	8-90	2-93	9-79
		<i>MAP</i>	0-10	0-35	0-58	0-65	0-66	0-66
	GraRep	<i>mean rank</i>	-	78-87	34-45	22-19	13-45	82-18
		<i>MAP</i>	-	0-49	0-53	0-56	0-58	0-57
	HOPE	<i>mean rank</i>	-	561-03	758-32	691-95	615-45	515-47
		<i>MAP</i>	-	0-64	0-47	0-43	0-43	0-45
	LINE	<i>mean rank</i>	489-49	344-14	141-35	34-32	15-84	10-00
		<i>MAP</i>	0-04	0-07	0-23	0-52	0-60	0-62
	node2vec	<i>mean rank</i>	265-65	264-94	265-69	264-81	269-52	265-20
		<i>MAP</i>	0-33	0-34	0-35	0-35	0-34	0-35
SDNE	<i>mean rank</i>	72-58	33-18	478-27	517-55	512-10	492-46	
	<i>MAP</i>	0-37	0-54	0-12	0-04	0-02	0-02	
Poincaré Embeddings	Poincare	<i>mean rank</i>	8-08	6-58	7-04	7-43	6-63	6-20
		<i>MAP</i>	0-61	0-61	0-62	0-61	0-62	0-61
	Gensim	<i>mean rank</i>	12-04	11-74	8-12	6-75	8-17	6-95
		<i>MAP</i>	0-61	0-61	0-62	0-62	0-62	0-62
	Poincare	<i>mean rank</i>	382-52	291-56	272-80	232-12	249-01	247-75
		<i>MAP</i>	0-46	0-53	0-56	0-58	0-58	0-59
	Numpy	<i>mean rank</i>	3-83	3-22	2-88	2-61	2-80	2-82
		<i>MAP</i>	0-93	0-94	0-94	0-94	0-94	0-94

Table 2: PhySH reconstruction from PhySH hypernym-hyponym pairs. Since there is no context information, word embeddings are not applicable here.

reconstruction. Graph embeddings and Poincaré embeddings are trained on the co-occurrence of PhySH terms in each of APS publications. As with (Nickel and Kiela, 2017), we also train graph embeddings and Poincaré embeddings on PhySH hypernym-hyponym pairs.

**Taxonomy Reconstruction:** We follow (Nickel and Kiela, 2017) to reconstruct taxonomy based on embedding vectors. For each embedding vector in Poincaré disk space, which is denoted as  $\mathcal{B}^d = \{x \in \mathbb{R}^d, \|x\|_2 \leq 1\}$ . The norm of each vector can measure the radius of each vector, while the hyperbolic distance can measure the closeness of two vectors. The closest two are assigned as hypernym-hyponym pairs. The hyperbolic distance of two vector points  $u, v \in \mathcal{B}^d$  is calculated follow as (Nickel and Kiela, 2017).

$$d_H(u, v) = \operatorname{arcosh} \left( 1 + 2 * \frac{\|u - v\|^2}{(1 - \|u\|^2)(1 - \|v\|^2)} \right) \quad (1)$$

The distance could only tell how semantically close are the node pairs  $(u, v)$ . But which one is the parent node is not answered. One property that makes hyperbolic space outstanding for the hierarchical structure is that the hyperbolic disc area and circle length grow exponentially with its radius. Node with the smaller norm is the higher-level term.

## 4 Evaluation and Results

### 4.1 Evaluation Datasets

APS (American Physical Society) has made available their publications data for researchers with the total number of 661, 209 articles and citations and dates back to 1893<sup>9</sup>. We utilize the article metadata datasets. PhySH (Physics Subject Headings) is the Physics concept hierarchy. It is used to organize publications of APS. It is open-source on Github<sup>10</sup>. APS metadata datasets only contain *title* field, we retrieve *abstract* from Web of Sciences database<sup>11</sup>.

### 4.2 Evaluation Metrics

*mean rank* and *MAP* metrics are used to measure taxonomy reconstruction performance. *mean rank* is calculated for each node’s distance of ground truth children against all other nodes. *MAP* is the mean average precision at the threshold of each correctly retrieved child.

$$\operatorname{mean\_rank}(u) = \frac{sp(u)}{sp(u) + lp(u)} \in [0, 1] \quad (2)$$

$lp(u)$  is the furthest length from node  $u$  to its descendants.  $sp(u)$  is the shortest length from node  $u$  to root node. The optimal embedding should score a low *mean rank* and a high *MAP*.

### 4.3 PhySH Reconstruction Evaluation

**PhySH Reconstruction From Raw Text.** In this experiment, we extract co-occurrence of PhySH terms in each APS publication. The graph embeddings are trained on the co-occurrence graph. Poincaré embeddings are trained on the noisy co-occurrence pairs. Word embeddings are trained on APS publication raw texts. PhySH terms’ representation vectors are extracted from word vectors in the postprocessing step.

Table 1 is the performance of PhySH reconstruction by learning representation from raw APS datasets<sup>12</sup>. None of the embeddings get the best result in both metrics. Word embeddings like CBOW achieve better *MAP*, while graph embeddings like deepWalk outperform in *mean rank*. Poincaré embeddings did not show any superior. Learn PhySH

<sup>9</sup><https://journals.aps.org/datasets>

<sup>10</sup><https://github.com/physh-org/PhySH>

<sup>11</sup>Web of Science is a commercial database of Clarivate Analytics, it can be accessed by most universities and institutions

<sup>12</sup>We experiment each embedding with different hyperparameters by grid search, we present the optimal performance of each embedding in the tables.

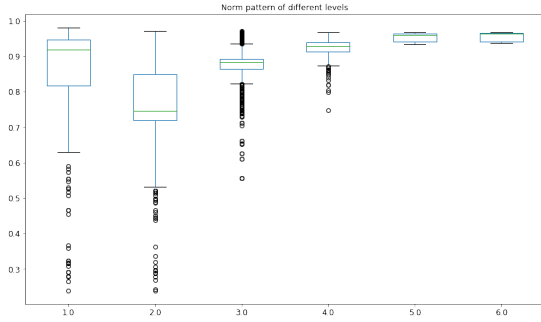


Figure 2: Norm of Poincaré embedding vector at different taxonomy levels

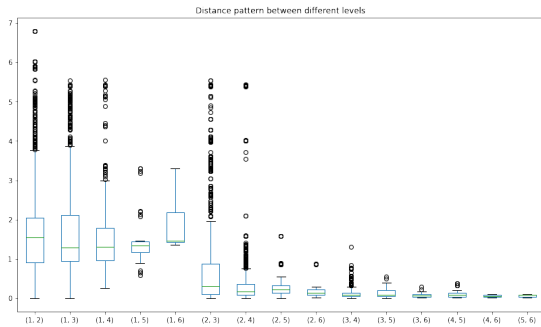


Figure 3: Distance of Poincaré embedding vector across different taxonomy levels

from noisy co-occurrence pairs are much more complicated than the mammal tree of the WordNet described in the origin paper (Nickel and Kiela, 2017). We can conclude Poincaré embeddings are not sufficient for learning and representing from the co-occurrence pairs.

**PhySH Reconstruction From PhySH.** Table 2 is the performance of PhySH reconstruction by learning representation from PhySH hypernym-hyponym pairs. The graph embeddings are trained on the PhySH hypernym-hyponym graph. Poincaré embeddings are trained on the PhySH hypernym-hyponym pairs.

In this experiment, Poincaré’s official implementation *Poincaré-Pytorch* wins with far better results than other algorithms. This is because Poincaré is trained with the loss function designed to learn hierarchies, while graph embeddings are trained to learn from neighbors and global graph structure. However, *GF* at dimension 100 and *LINE* at dimension 200 also get very good performance.

#### 4.4 The Hierarchical Characteristics of PhySH Poincaré embedding

If we understand the successful representation characteristics of taxonomy hierarchical relations, it

will be the help of taxonomy construction. We will analyze what are the hierarchical characteristics of PhySH preserved by Poincaré embeddings in this section.

In Figure 2, we visualize how the norm value varies in different PhySH level. There is a clear pattern from taxonomy level 2 to level 6: lower-level terms have bigger norm values. It means lower terms are further from the root term. The pace of the decrease of the norm in lower levels seems to decelerate, which needs to be further validated. However, the norm of level 1 terms is rather distributed, which we think is the points where Poincaré embedding fails.

In Figure 3, we compare the distance of terms over different PhySH levels. The ancestor nodes are further than parent nodes. For each node, its distance to the child is smaller than the distance to parent, and the distance to the child is nearly half as the distance to parent. These patterns are important for a successful representation of taxonomy.

## 5 Conclusion and Future Work

we compare word embeddings, graph embeddings, and Poincaré embeddings by reconstructing PhySH. We consider two scenario case: reconstructing from raw texts and reconstructing from existing PhySH. The experiment shows even though Poincaré embeddings far outweigh other embeddings in reconstructing PhySH from PhySH, it is also not competent as other embeddings in reconstructing PhySH from raw APS texts.

We further demystify what is the success of Poincaré embeddings in reconstructing PhySH from PhySH. The future work would be how to design a powerful taxonomy induction algorithm which could benefit from the characteristics of our paper.

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