HARP: Hierarchical Representation Learning for Networks

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ABSTRACT

We present HARP, a novel method for learning low dimensional embeddings of a graph's nodes which preserves higher-order structural features. Our proposed method achieves this by compressing the input graph prior to embedding it, effectively avoiding troublesome embedding configurations (i.e. local minima) which can pose problems to non-convex optimization.

HARP works by finding a smaller graph which approximates the global structure of its input. This simplified graph is used to learn a set of initial representations, which serve as good initializations for learning representations in the original, detailed graph. We inductively extend this idea, by decomposing a graph in a series of levels, and then embed the hierarchy of graphs from the coarsest one to the original graph.

HARP is a general meta-strategy to improve *all* of the state-of-the-art neural algorithms for embedding graphs, including *DeepWalk*, *LINE*, and *Node2vec*. Indeed, we demonstrate that applying HARP's hierarchical paradigm yields improved implementations for all three of these methods, as evaluated on classification tasks on real-world graphs such as *DBLP*, *BlogCatalog*, and *CiteSeer*, where we achieve a performance gain over the original implementations by up to 14% Macro F1.

KEYWORDS

social networks, feature learning, latent representations, graph embeddings, multilevel optimization

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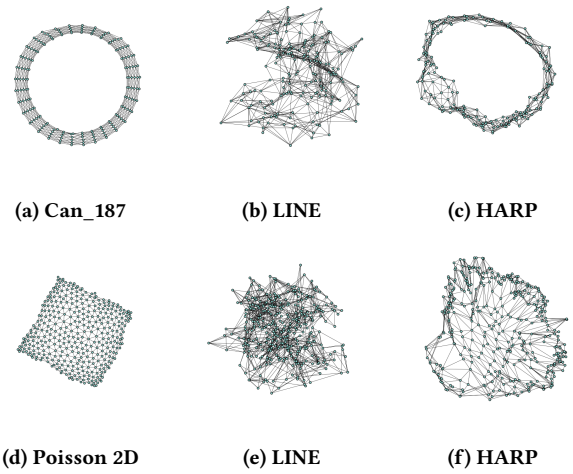
1 INTRODUCTION

From social networks to the World Wide Web, graphs are a ubiquitous way to organize a diverse set of real-world information. Given a network's structure, it is often desirable to predict missing information (frequently called *attributes* or *labels*) associated with each node in the graph. This missing information can represent a variety of aspects of the data – for example, on a social network they could represent the communities a person belongs to, or the categories of a document's content on the web.



(a) Can_187 **(b) LINE** **(c) HARP**

(d) Poisson 2D **(e) LINE** **(f) HARP**

Figure 1: Comparison of two-dimensional embeddings from LINE and our proposed method, for two distinct graphs. Observe how HARP's embedding better preserves the higher order structure of a ring and a plane.

Because many information networks can contain billions of nodes and edges, it can be intractable to perform complex inference procedures on the entire network. One technique which has been proposed to address this problem is *dimensionality reduction*. The central idea is to find a mapping function which converts each node in the graph to a low-dimensional latent representation. These representations can then be used as features for common tasks on graphs such as multi-label classification, clustering, and link prediction.

Traditional methods for graph dimensionality reduction [2, 15, 19] perform well on small graphs. However, the time complexity of these methods are at least quadratic in the number of graph nodes, makes them impossible to run on large-scale networks.

A recent advancement in graph representation learning, DeepWalk [13] proposed online learning methods using neural networks to address this scalability limitation. Much work has since followed [3, 8, 14, 17]. These neural network-based methods have proven both highly scalable and performant, achieving strong results on classification and link prediction tasks in large networks.

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Despite their success, all these methods have several shared weaknesses. Firstly, they are all local approaches – limited to the structure immediately around a node. DeepWalk [13] and Node2vec [8] adopt short random walks to explore the local neighborhoods of nodes, while LINE [17] is concerned with even closer relationships (nodes at most two hops away). This focus on local structure implicitly ignores long-distance global relationships, and the learned representations can fail to uncover important global structural patterns. Secondly, they all rely on a non-convex optimization goal solved using stochastic gradient descent [7, 11] which can become stuck in a local minima (e.g. perhaps as a result of a poor initialization). In other words, all previously proposed techniques for graph representation learning can accidentally learn embedding configurations which disregard important structural features of their input graph.

In this work, we propose *HARP*, a meta strategy for embedding graph datasets which preserves higher-order structural features. *HARP* recursively coalesces the nodes and edges in the original graph to get a series of successively smaller graphs with similar structure. These coalesced graphs, each with a different granularity, provide us a view of the original graph's global structure. Starting from the most simplified form, each graph is used to learn a set of initial representations which serve as good initializations for embedding the next, more detailed graph. This process is repeated until we get an embedding for each node in the original graph.

We illustrate the effectiveness of this multilevel paradigm in Figure 1, by visualizing the two-dimension embeddings from an existing method (*LINE* [17]) and our improvement to it, *HARP(LINE)*. Each of the small graphs we consider has an obvious global structure (that of a ring (1a) and a grid (1d)) which is easily exposed by a force direced layout [9]. The center figures represent the two-dimensional embedding obtained by LINE for the ring (1b) and grid (1e). In these embeddings, the global structure is lost (i.e. that is, the ring and plane are unidentifiable). However, the embeddings produced by using our meta-strategy to improve LINE (right) clearly capture both the local and global structure of the given graphs (1c, 1f).

Our contributions are the following:

- **New Representation Learning Paradigm.** We propose *HARP*, a novel multilevel paradigm for graph representation which seamlessly blends ideas from the graph drawing [6] and graph representation learning [8, 13, 17] communities to build substantially better graph embeddings.
- **Improved Optimization Primitives.** We introduce the Multilevel Hierarchical Softmax, and Multilevel Negative Sampling. Our improvements on these popular methods for learning latent representations illustrate the broad applicability of our hierarchical approach. We demonstrate that our approach leads to improved implementations of **all** state-of-the-art graph representation learning methods, namely *DeepWalk* (DW), *LINE* and *Node2vec* (N2V).
- **Better Embeddings for Downstream Tasks.** We demonstrate that our *HARP(DW)*, *HARP(LINE)* and *HARP(N2V)* embeddings consistently outperform the originals on multi-label classification tasks on several real-world networks, with improvements as large as 14% Macro F_1.

2 PROBLEM FORMULATION

We desire to learn latent representations of nodes in a graph. Formally, let $G = (V, E)$ be a graph, where V is the set of nodes and E is the set of edges. The goal of graph representation learning is to develop a mapping function $\Phi : V \mapsto \mathbb{R}^{|V| \times d}, d \ll |V|$. This mapping Φ defines the latent representation (or *embedding*) of each node $v \in V$. Popular methods for learning the parameters of Φ [8, 13, 17] suffer from two main disadvantages: (1) higher-order graph structural information is not modeled, and (2) their stochastic optimization can fall victim to poor initialization.

In light of these difficulties, we introduce the *hierarchical representation learning* problem for graphs. At its core, we seek to find a graph, $G_s = (V_s, E_s)$ which captures the essential structure of G, but is smaller than our original (i.e. $|V_s| << |V|$, $|E_s| << |E|$). It is likely that G_s will be easier to embed for two reasons. First, there are many less pairwise relationships ($|V_s|^2$ versus $|V|^2$) which can be expressed in the space. As the sample space shrinks, there is less variation in training examples – this can yield a smoother objective function which is easier to optimize. Second, the diameter of G_s may be smaller than G, so algorithms with a local focus can exploit the graph's global structure.

In summary, we define the hierarchical representation learning problem in graphs as follows:

Given a large graph $G(V, E)$ and a function f, which embeds G using initialization θ, $f : G \times \theta \mapsto \Phi_G$,
Simplify G to a series of successively smaller graphs $G_0 \dots G_L$,
Learn a coarse embedding $\Phi_{G_L} = f(G_L, \emptyset)$,
Refine the coarse embedding into Φ_G by iteratively applying $\Phi_{G_i} = f(G_i, \Phi_{G_{i+1}}), 0 \leq i < L$.

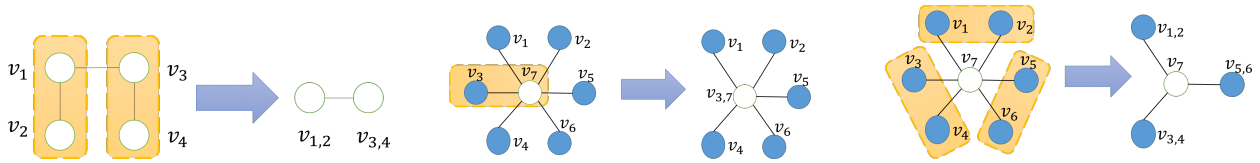
3 METHOD

Here we present our hierarchical paradigm for graph representation learning. After discussing the method in general, we present a structure-preserving algorithm for its most crucial step, graph coarsening.

3.1 Algorithm: HARP

Our method for multi-level graph representation learning, HARP, is presented in Algorithm 1. It consists of three parts - graph coarsening, graph embedding, and representation refinement - which we detail below:

(1) *Graph Coarsening* (line 1): Given a graph G, graph coarsening algorithms create a hierarchy of successively smaller graphs $G_0, G_1, \cdots, G_L$, where $G_0 = G$. The coarser (smaller) graphs preserve the global structure of the original graph, yet have significantly fewer nodes and edges. Algorithms for generating this hierarchy of graphs are discussed in Section 3.2.
(2) *Graph Embedding on the Coarsest Graph* (line 2-3): The graph embedding is obtained on the coarsest graph G_L with the provided graph embedding algorithm. As the size of G_L is usually very small, it is much easier to get a high-quality graph representation.
(3) *Graph Representation Prolongation and Refinement* (line 4-7): We prolong and refine the graph representation from the coarsest to the finest graph. For each graph G_i, we prolong the graph representation of G_{i+1} as its initial embedding Φ'_{G_i}. Then, the



(a) Edge Collapsing. **(b) Edge Collapsing fails to collapse stars.** **(c) Star Collapsing.**

Figure 2: Illustration of graph coarsening algorithms. 2a: Edge collapsing on a graph snippet. 2b: How edge collapsing fails to coalesce star-like structures. 2c: How star collapsing scheme coalesces the same graph snippet efficiently.

Algorithm 1 HARP(G, *Embed*(), *Prolongate*())

Input:
graph $G(V, E)$
arbitrary graph embedding algorithm EMBED()
embedding prolongation algorithm PROLONGATE()
Output: matrix of vertex representations $\Phi \in \mathbb{R}^{|V| \times d}$

1: $G_0, G_1, \cdots, G_L \leftarrow$ GRAPHCOARSENING(G)
2: Initialize Φ'_{G_L} by assigning zeros
3: $\Phi_{G_L} \leftarrow$ EMBED(G_L, Φ'_{G_L})
4: **for** $i = L - 1$ to 0 **do**
5: $\quad \Phi'_{G_i} \leftarrow$ PROLONGATE($\Phi_{G_{i+1}}, G_{i+1}, G_i$)
6: $\quad \Phi_{G_i} \leftarrow$ EMBED(G_i, Φ'_{G_i})
7: **end for**
8: **return** Φ_{G_0}

Algorithm 2 GraphCoarsening(G)

Input: graph $G(V, E)$
Output: Series of Coarsened Graphs $G_0, G_1, \cdots, G_L$

$L \leftarrow 0$
$G_0 \leftarrow G$
while $|V_L| \geq$ *threshold* **do**
$\quad L \leftarrow L + 1$
$\quad G_L \leftarrow$ EDGECOLLAPSING(STARCOLLAPSING(G))
end while
return $G_0, G_1, \cdots, G_L$

embedding algorithm *Embed*() is applied to (G_i, Φ'_{G_i}) to further refine Φ'_{G_i}, resulting in the refined embedding Φ_{G_i}. We discuss this step in detail in Section 4.

(4) *Graph Embedding of the Original Graph* (line 8): We return Φ_{G_0}, which is the graph embedding of the original graph.

We can easily see that this paradigm is algorithm independent, relying only on the provided functions *Embed*() and *Prolongate*(). Thus, with minimum effort, this paradigm can be incorporated into any existing graph representation learning methods, yielding a multilevel version of that method.

3.2 Graph Coarsening

In Algorithm 2, we develop a hybrid graph coarsening scheme which preserves global graph structural information at different scales. Its two key parts, namely edge collapsing and star collapsing, preserve *first-order proximity* and *second-order proximity* [17] respectively. First-order proximity is concerned with preserving the observed edges in the input graph, while second-order proximity is based on the shared neighborhood structure of the nodes.

Edge Collapsing. Edge collapsing [9] is an efficient algorithm for preserving first-order proximity. It selects $E' \subseteq E$, such that no two edges in E' are incident to the same vertex. Then, for each $(u_i, v_i) \in E'$, it merges (u_i, v_i) into a single node w_i, and merge the edges incident to u_i and v_i. The number of nodes in the coarser graph is therefore at least half of that in the original graph. As illustrated in Figure 2a, the edge collapsing algorithm merges node pairs (v_1, v_2) and (v_3, v_4) into supernodes $v_{1,2}$ and $v_{3,4}$ respectively, resulting in a coarser graph with 2 nodes and 1 edge. The order of merging is arbitrary; we find different merging orders result in very similar node embeddings in practice.

Star Collapsing. Real world graphs are often scale-free, which means they contain a large number of star-like structures. A star consists of a popular central node (sometimes referred to as *hubs*) connected to many peripheral nodes. Although the edge collapsing algorithm is simple and efficient, it cannot sufficiently compress the star-like structures in a graph. Consider the graph snippet in Figure 2b, where the only central node v_7 connects to all the other nodes. Assume the degree of the central node is k, it is clear that the edge collapsing scheme can only compress this graph into a coarsened graph with $k - 1$ nodes. Therefore when k is large, the coarsening process could be arbitrarily slow, takes $O(k)$ steps instead of $O(\log k)$ steps.

One observation on the star structure is that there are strong second-order similarities between the peripheral nodes since they share the same neighborhood. This leads to our star collapsing scheme, which merges nodes with the same neighbors into supernodes since they are similar to each other. As shown in Figure 2c, (v_1, v_2), (v_3, v_4) and (v_5, v_6) are merged into supernodes as they share the same neighbors (v_7), generating a coarsened graph with only $k/2$ nodes.

Hybrid Coarsening Scheme. By combining edge collapsing and star collapsing, we present a hybrid scheme for graph coarsening in Algorithm 2, which is adopted on all test graphs. In each coarsening step, the hybrid coarsening scheme first decomposes the input graph with star collapsing, then adopts the edge collapsing scheme to generate the coalesced graph. We repeat this process until a small enough graph (with less than 100 vertices) is obtained.

4 USE CASE: THE SKIP-GRAM MODEL

In this section, we discuss the application of HARP to a specific class of representation learning models (without loss of generality). First, we describe the Skip-gram model's details in Section 4.1, since it is the basis of many previous graph representation learning algorithms, such as DeepWalk, LINE and Node2vec. Next, we present

Algorithm 3 Prolongate$_{MHS}(G_{i+1}, \Phi_{G_{i+1}}, B_{i+1}, G_i)$

Input:
the coarser graph G_{i+1}
node representations $\Phi_{G_{i+1}}$ of G_{i+1}
hierarchical softmax tree B_{i+1} of G_{i+1}
the finer graph G_i
Output: node representations Φ_{G_i} prolonged from $\Phi_{G_{i+1}}$

1: $M \leftarrow$ GetNodeMappings(G_{i+1}, G_i)
2: $B_i \leftarrow B_{i+1}$
3: **for** $v \in G_{i+1}$ **do**
4: ExtendSubTree$(B_{i+1}, v, B_i, M(v))$
5: **for** $u \in M(v)$ **do**
6: $\Phi_{G_i}(u) \leftarrow \Phi_{G_{i+1}}(v)$
7: **end for**
8: **end for**
9: **return** Φ_{G_i}

our improvements to its two popular optimization strategies: the Multilevel Hierarchical Softmax (Section 4.2) and Multilevel Negative Sampling (Section 4.3).

4.1 Model Details

Skip-gram is a probabilistic model which has been extended to learn node representations in a graph [13]. Given a node $v \in G$, the Skip-gram model maximizes the probability of generating its context nodes $C(v)$. The definition of context nodes varies with different graph representation learning algorithms. For random walk-based algorithms like DeepWalk and Node2vec, $C(v)$ is defined as the nodes within window size w of v in a truncated random walk. For LINE first order, $C(v)$ is simply the nodes adjacent to v. Specifically, the Skip-gram model minimizes the following objective:

$$J = -\sum_{u \in C(v)} log\, Pr(u|v) \tag{1}$$

Where $Pr(u|v)$ is defined by the softmax function:

$$Pr(u|v) = \frac{exp(\Phi(u) \cdot \Phi'(v))}{\sum_{u \in V} exp(\Phi(u) \cdot \Phi'(v))} \tag{2}$$

Here $\Phi'(v)$ is the representation of v when served as the context node. However, calculating the denominator requires the probability summation over all vertices, which is computationally expensive. To solve this problem, two strategies for faster model optimization have been proposed: the hierarchical softmax and negative sampling [7]. The hierarchical softmax creates a Huffman tree, where each leaf node corresponds to a node in the original graph. Then, it learns a binary classifier on each inner node of the binary tree to maximize the probability of reaching the desired leaf node. This reduces the time complexity of calculating the denominator from $O(|V|)$ to $O(log|V|)$. This approach is used by *DeepWalk* [13]. The negative sampling method first constructs negative edges which do not exist in the graph. Then, it jointly minimizes the probability of generating negative samples and maximizes the probability of generating samples in the training data. This is the approach adopted by *LINE* [17] and *Node2vec* [8].

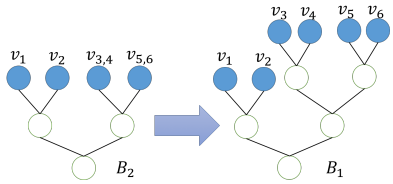


Figure 3: Visualization of $ExtendSubTree()$**.**

4.2 Multilevel Hierarchical Softmax

In our paradigm, a graph embedding method requires a $Prolongate()$ function - an approach for extending representations from a coarse graph to a finer one. Here we detail one such function for the hierarchical softmax.

Our prolongation scheme, the Multilevel Hierarchical Softmax, is presented in Algorithm 3. In line 1, the node mappings M from each node in G_{i+1} to a list of nodes in G_i is obtained. Then, the binary hierarchical softmax tree B_{i+1} is copied to B_i (line 2), and further extended (lines 3-8). Specifically, each node $v \in G_{i+1}$ is merged from a list of nodes $M(v)$ in G_i. Thus, we call the subroutine $ExtendSubTree()$ to extend node $B_{i+1}(v)$ to a subtree consisting of nodes in $M(v)$. Finally, node representation of v is copied to each $u \in M(v)$ (line 6). Figure 3 shows an example of this process. In the graph coarsening phase, (v_3, v_4) and (v_5, v_6) are merged into $v_{3,4}$ and $v_{5,6}$ respectively. Thus, $ExtendSubTree()$ splits $B_2(v_{3,4})$ to a subtree consisting of $B_1(v_3)$, $B_1(v_4)$ and an inner node. The representation of v_3 and v_4 are both initialized with the representation of $v_{3,4}$. For $B_2(v_{5,6})$ it is the same.

4.3 Multilevel Negative Sampling

Negative sampling is an alternate method to hierarchical softmax for speeding up Skip-gram. The representation prolongation for Skip-gram with negative sampling is simpler than that for the hierarchical softmax, but we sketch it here for completeness.

After the graph representation for G_{i+1} is learned, we prolong it into the initial representation for G_i. We observe that each node $v \in G_{i+1}$ is either a member of the finer representation ($v \in G_i$), or the result of a merger, $(v_1, v_2, \cdots, v_k) \in G_i$. In both cases, we can simply reuse the representation of the parent node $v \in G_i$ - the children are quickly separated by gradient updates.

4.4 Complexity Analysis

In this section, we discuss the time complexity of *HARP(DW)* and *HARP(LINE)* and compare with the time complexity of *DeepWalk* and *LINE* respectively. *HARP(N2V)* has the same time complexity as *HARP(DW)*, thus it is not included in the discussion below.

HARP(DW): The time complexity of *DeepWalk* is linear to the number of nodes in the graph and the number of walks γ, which is $O(\gamma|V|)$. For *HARP(DW)*, coarsening a graph with $|V|$ nodes produces a coarser graph with about $|V|/2$ nodes. The total number of nodes in all levels is approximately $|V| \sum_{i=0}^{log_2|V|} (\frac{1}{2})^i = 2|V|$. Therefore, the time complexity is $O(|V|)$ for copying binary tree and $O(\gamma|V|)$ for random walking. Thus, the overall time complexity of *HARP(DW)* is also $O(\gamma|V|)$.

Name	DBLP	Blogcatalog	CiteSeer
# Vertices	29,199	10,312	3,312
# Edges	133,664	333,983	4,732
# Classes	4	39	6
Task	Classification	Classification	Classification

Table 1: Statistics of the graphs used in our experiments.

HARP(LINE): The time complexity of *LINE* is linear to the number of edges in the graph and the number of iterations r over edges, which is $O(r|E|)$. For *HARP(LINE)*, coarsening a graph with $|E|$ nodes produces a coarsened graph with about $|E|/2$ edges. The total number edges in all levels is approximately $|E| \sum_{i=0}^{log_2|E|} (\frac{1}{2})^i = 2|E|$. Thus, the time complexity of *HARP(LINE)* is also $O(r|E|)$.

5 EXPERIMENT

In this section, we provide an overview of the datasets and methods used for experiments and evaluate the effectiveness of our method on challenging multi-label classification tasks in several real-life networks. We further illustrate the scalability of our method and discuss its performance with regard to several important parameters.

5.1 Datasets

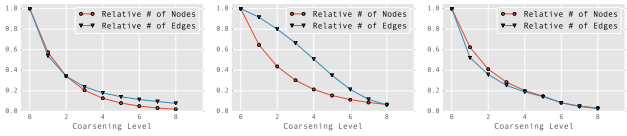
Table 1 gives an overview of the datasets used in our experiments.

- *DBLP* [14] – DBLP is a co-author graph of researchers in computer science. The labels indicate the research areas a researcher publishes his work in. The 4 research areas included in this dataset are DB, DM, IR, and ML.
- *BlogCatalog* [18] – BlogCatalog is a network of social relationships between users on the BlogCatalog website. The labels represent the categories a blogger publishes in.
- *CiteSeer* [16] – CiteSeer is a citation network between publications in computer science. The labels indicate the research areas a paper belongs to. The papers are classified into 6 categories: Agents, AI, DB, IR, ML, and HCI.

5.2 Baseline Methods

We compare our model with the following graph embedding methods:

- *DeepWalk* — *DeepWalk* is a two-phase method for embedding graphs. Firstly, *DeepWalk* generates random walks of fixed length from all the vertices of a graph. Then, the walks are treated as sentences in a language model and the Skip-Gram model for learning word embeddings is utilized to obtain graph embeddings. *DeepWalk* uses hierarchical softmax for Skip-gram model optimization.
- *LINE* — *LINE* is a method for embedding large-scale networks. The objective function of *LINE* is designed for preserving both first-order and second-order proximities, and we use first-order *LINE* for comparison. Skip-gram with negative sampling is used to solve the objective function.
- *Node2vec* — *Node2vec* proposes an improvement to the random walk phase of *DeepWalk*. By introducing the return parameter p and the in-out parameter q, *Node2vec* combines DFS-like and BFS-like neighborhood exploration. *Node2vec* also uses negative sampling for optimizing the Skip-gram model.



(a) DBLP **(b) BlogCatalog** **(c) CiteSeer**

Figure 4: The ratio of nodes/edges of the coarsened graphs to that of the original test graphs. For disconnected graphs, the graph coarsening result on the largest connected component is shown.

For each baseline method, we combine it with *HARP* and compare their performance.

5.3 Parameter Settings

Here we discuss the parameter settings for our models and baseline models. Since *DeepWalk*, *LINE* and *Node2vec* are all sampling based algorithms, we always ensure that the total number of samples seen by the baseline algorithm is the **same** as that of the corresponding *HARP* enhanced algorithm.

DeepWalk. For *DeepWalk* and *HARP(DW)*, we need to set the following parameters: the number of random walks γ, walk length t, window size w for the Skip-gram model and representation size d. In *HARP(DW)*, the parameter setting is $\gamma = 40, t = 10, w = 10, d = 128$. For *DeepWalk*, all the parameters except γ are the same as in *HARP(DW)*. Specifically, to ensure a fair comparison, we increase the value of γ for *DeepWalk*. This gives *DeepWalk* a larger training dataset (as large as all of the levels of *HARP(DW)* combined). We note that failure to increase γ in this way resulted in substantially worse *DeepWalk* (and *Node2vec*) models.

LINE. For *HARP(LINE)*, we run 50 iterations on all graph edges on all coarsening levels. For *LINE*, we increase the number of iterations over graph edges accordingly, so that the amount of training data for both models remain the same. The representation size d is set to 64 for both *LINE* and *HARP(LINE)*.

Node2vec. For *HARP(N2V)*, the parameter setting is $\gamma = 40, t = 10, w = 10, d = 128$. Similar to *DeepWalk*, we increase the value of γ in *Node2vec* to ensure a fair comparison. We use *Node2vec* in an unsupervised way by setting both in-out and return hyperparameters to 1.0.

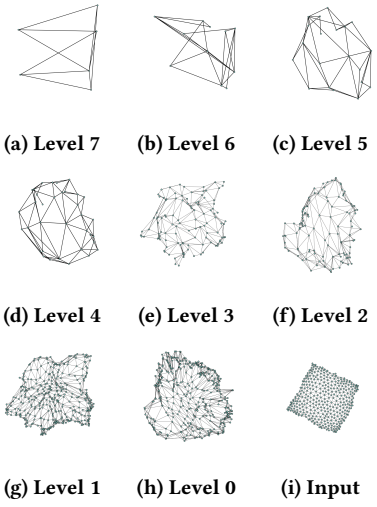
For all models, the initial learning rate and final learning rate are set to 0.025 and 0.001 respectively.

5.4 Graph Coarsening

Figure 4 demonstrates the effect of our hybrid coarsening method on all test graphs. The first step of graph coarsening for each graph eliminates about half the nodes, but the number of edges only reduce by about 10% for *BlogCatalog*. This illustrates the difficulty of coarsening real-world graphs. However, as the graph coarsening process continues, the scale of all graphs drastically decrease. At level 8, all graphs have less than 10% nodes and edges left.

5.5 Visualization

To show the intuition of the *HARP* paradigm, we set $d = 2$, and visualize the graph representation generated by *HARP(LINE)* at each level. Figure 5 shows the level-wise 2D graph embeddings



(a) Level 7 (b) Level 6 (c) Level 5

(d) Level 4 (e) Level 3 (f) Level 2

(g) Level 1 (h) Level 0 (i) Input

Figure 5: Two-dimensional embeddings generated with *HARP(LINE)* on different coarsening levels on *Poisson 2D*. Level 7 denotes the smallest graph, while level 0 denotes the original graph. The last subfigure is the graph layout generated by a force-direct graph drawing algorithm.

obtained with *HARP(LINE)* on *Poisson 2D*. The graph layout of level 5 (which has only 21 nodes) already highly resembles the layout of the original graph. The graph layout on each subsequent level is initialized with the prolongation of the previous graph layout, thus the global structure is kept.

5.6 Multi-label Classification

We evaluate our method using the same experimental procedure in [13]. Firstly, we obtain the graph embeddings of the input graph. Then, a portion (T_R) of nodes along with their labels are randomly sampled from the graph as training data, and the task is to predict the labels for the remaining nodes. We train a one-vs-rest logistic regression model with L2 regularization on the graph embeddings for prediction. The logistic regression model is implemented by LibLinear [5]. To ensure the reliability of our experiment, the above process is repeated for 10 times, and the average Macro F_1 score is reported. The other evaluation metrics such as Micro F_1 score and accuracy follow the same trend as Macro F_1 score, thus are not shown.

Table 2 reports the Macro F_1 scores achieved on *DBLP*, *BlogCatalog*, and *CiteSeer* with 5%, 50%, and 5% labeled nodes respectively. The number of class labels of *BlogCatalog* is about 10 times that of the other two graphs, thus we use a larger portion of labeled nodes. We can see that our method improves all existing neural embedding techniques on all test graphs. In *DBLP*, the improvements introduced by *HARP(DW)*, *HARP(LINE)* and *HARP(N2V)* are 7.8%, 3.0% and 0.3% respectively. Given the scale-free nature of *BlogCatalog*, graph coarsening is much harder due to a large amount of star-like structures in it. Still, *HARP(DW)*, *HARP(LINE)* and *HARP(N2V)* achieve gains of 4.0%, 4.6% and 4.7% over the corresponding baseline methods respectively. For *CiteSeer*, the performance improvement is also striking: *HARP(DW)*, *HARP(LINE)* and *HARP(N2V)* outperforms the baseline methods by 4.8%, 13.6%, and 2.8%.

Algorithm	Dataset		
	DBLP	BlogCatalog	CiteSeer
DeepWalk	57.29	24.88	42.72
HARP(DW)	**61.76***	**25.90***	**44.78***
Gain of HARP[%]	**7.8**	**4.0**	**4.8**
LINE	57.76	22.43	37.11
HARP(LINE)	**59.51***	**23.47***	**42.95***
Gain of HARP[%]	**3.0**	**4.6**	**13.6**
Node2vec	62.64	23.55	44.84
HARP(N2V)	**62.80**	**24.66***	**46.08***
Gain of HARP[%]	**0.3**	**4.7**	**2.8**

Table 2: Macro F_1 scores and performance gain of *HARP* on *DBLP*, *BlogCatalog*, and *CiteSeer* in percentage. * indicates statistically superior performance to the corresponding baseline method at level of 0.001 using a standard paired t-test. Our method improves all existing neural embedding techniques.

To have a detailed comparison between HARP and the baseline methods, we vary the portion of labeled nodes for classification, and present the macro F_1 scores in Figure 6. We can observe that *HARP(DW)*, *HARP(LINE)* and *HARP(N2V)* consistently perform better than the corresponding baseline methods.

DBLP. In *DBLP*, the relative gain of *HARP(DW)* is over 9% with 4% labeled data. With only 2% labeled data, *HARP(DW)* achieves higher macro F_1 score than *DeepWalk* with 8% label data. *HARP(LINE)* also consistently outperforms *LINE* given any amount of training data, with macro F_1 score gain between 1% and 3%. *HARP(N2V)* and *Node2vec* have comparable performance with less than 5% labeled data, but as the ratio of labeled data increases, *HARP(N2V)* eventually distances itself to a 0.7% improvement over *Node2vec*. We can also see that *Node2vec* generally has better performance when compared to *DeepWalk*, and the same holds for *HARP(N2V)* and *HARP(DW)*. The difference in optimization method for Skip-gram (negative sampling for *Node2vec* and hierarchical softmax for *DeepWalk*) may account for this difference.

BlogCatalog. As a scale-free network with complex structure, *BlogCatalog* is challenging for graph coarsening. Still, by considering both first-order proximity and second-order proximity, our hybrid coarsening algorithm generates an appropriate hierarchy of coarsened graphs. With the same amount of training data, *HARP(DW)* always leads *HARP(DW)* by at least 3.0%. For *HARP(LINE)*, it achieves a relative gain of 4.8% with 80% labeled data. For *HARP(N2V)*, its gain over *Node2vec* reaches 4.7% given 50% labeled nodes.

Citeseer. For *CiteSeer*, the lead of *HARP(DW)* on Macro F_1 score varies between 5.7% and 7.8%. For *HARP(LINE)*, its improvement over *LINE* with 4% labeled data is an impressive 24.4%. *HARP(N2V)* also performs better than *Node2vec* on any ratio of labeled nodes.

5.7 Scalability

In Section 4.4, we show that introducing *HARP* does not affect the time complexity of the underlying graph embedding algorithms.

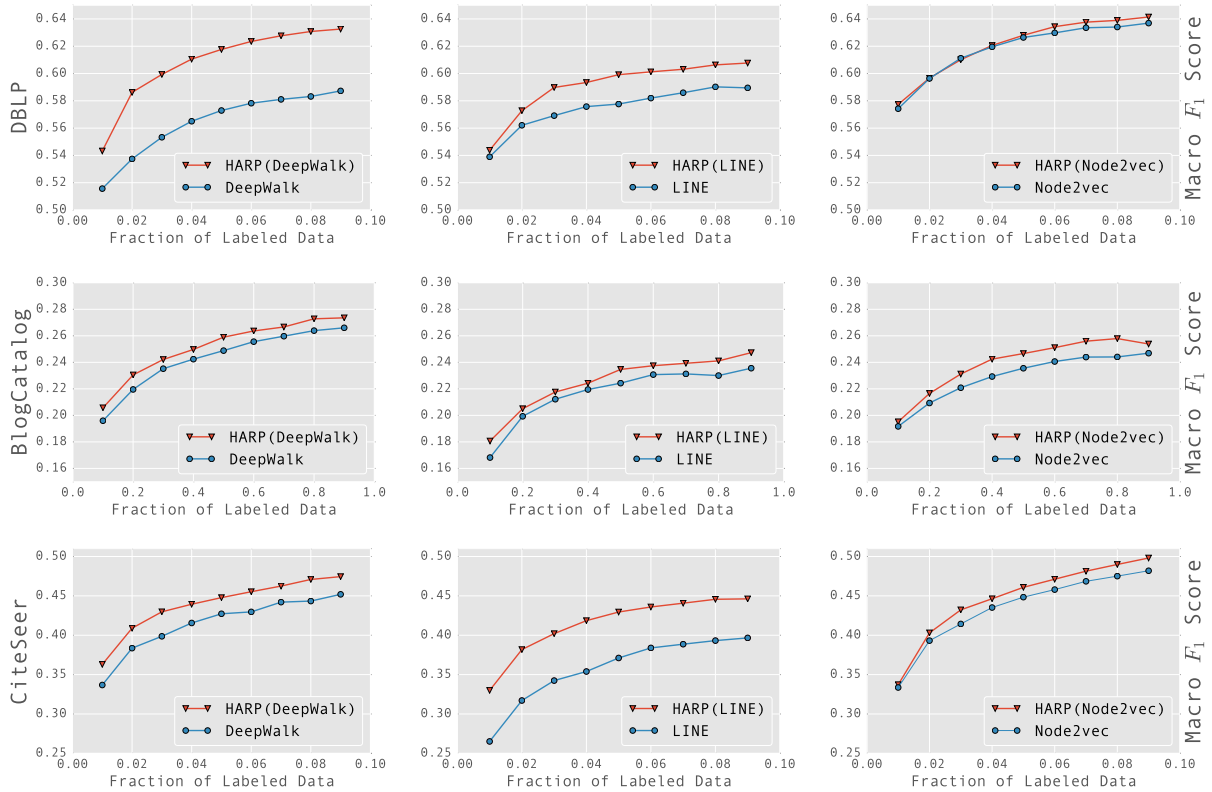
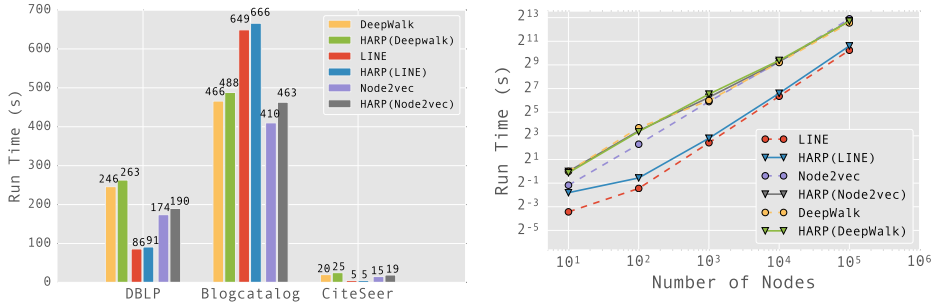


Figure 6: Detailed multi-label classification result on *DBLP*, *BlogCatalog*, and *CiteSeer*.



(a) Test graphs. **(b) Erdos-Renyi graphs.**

Figure 7: Runtime analysis.

Here, we compare the actual run time of *HARP* enhanced embedding algorithms with the corresponding baseline methods on all test graphs. All models run on a single machine with 128GB memory, 24 CPU cores at 2.0GHZ with 20 threads. As shown in Figure 7a, applying *HARP* typically only introduces an overhead of less than 10% total running time. The time spent on sampling and training the Skip-gram model dominates the overall running time.

Additionally, we learn graph embeddings on Erdos-Renyi graphs with node count ranging from 100 to 100,000 and constant average degree of 10. In Figure 7b, we can observe that the running time of *HARP* increases linearly with the number of nodes in the graph. Also, when compared to the corresponding baseline method, the overhead introduces by the graph coarsening and prolongation process in HARP is negligible, especially on large-scale graphs.

6 RELATED WORK

The related work is in the areas of graph representation learning and graph drawing, which we briefly describe here.

Graph Representation Learning. Most early methods treated representation learning as performing dimension reduction on the Laplacian and adjacency matrices [2, 4, 19]. These methods work

well on small graphs, but the time complexity of these algorithms is too high for the large-scale graphs commonly encountered today.

Recently, neural network-based methods have been proposed for constructing node representation in large-scale graphs. Deepwalk [13] presents a two-phase algorithm for graph representation learning. In the first phase, Deepwalk samples sequences of neighboring nodes of each node by random walking on the graph. Then, the node representation is learned by training a Skip-gram model [11] on the random walks. A number of methods have been proposed which extend this idea. First, several methods use different strategies for sampling neighboring nodes. LINE [17] learns graph embeddings which preserve both the first-order and second-order proximities in a graph. Walklets [14] captures multiscale node representation on graphs by sampling edges from higher powers of the graph adjacency matrix. Node2vec [8] combines DFS-like and BFS-like exploration within the random walk framework. Second, matrix factorization methods and deep neural networks have also been proposed [1, 3, 12, 23] as alternatives to the Skip-gram model for learning the latent representations.

Although these methods are highly scalable, they all rely on optimizing a non-convex objective function. With no prior knowledge of the graph, the latent representations are usually initialized with random numbers or zero. With such an initialization scheme, these methods are at risk of converging to a poor local minima. *HARP* overcomes this problem by introducing a multilevel paradigm for graph representation learning.

Graph Drawing. Multilevel layout algorithms are popular methods in the graph drawing community, where a hierarchy of approximations is used to solve the original layout problem [6, 9, 21]. Using an approximation of the original graph has two advantages - not only is the approximation usually simpler to solve, it can also be extended as a good initialization for solving the original problem. In addition to force-directed graph drawing, the multilevel framework [22] has been proved successful in various graph theory problems, including the traveling salesman problem [20], and graph partitioning [10].

HARP extends the idea of the multilevel layout to neural representation learning methods. We illustrate the utility of this paradigm by combining *HARP* with three state-of-the-art representation learning methods.

7 CONCLUSION

Recent literature on graph representation learning aims at optimizing a non-convex function. With no prior knowledge of the graph, these methods could easily get stuck at a bad local minima as the result of poor initialization. Moreover, these methods mostly aim to preserve local proximities in a graph but neglect its global structure. In this paper, we propose a multilevel graph representation learning paradigm to address these issues. By recursively coalescing the input graph into smaller but structurally similar graphs, *HARP* captures the global structure of the input graph. By learning graph representation on these smaller graphs, a good initialization scheme for the input graph is derived. This multilevel paradigm is further combined with the state-of-the-art graph embedding methods, namely *DeepWalk*, *LINE*, and *Node2vec*. Experimental results on various real-world graphs show that introducing *HARP* yields graph embeddings of higher quality for all these three methods.

In the future, we would like to combine *HARP* with other graph representation learning methods. Specifically, as Skip-gram is a shallow method for representation learning, it would be interesting to see if *HARP* also works well with deep representation learning methods. For the On the other hand, our method could also be applied to language networks, possibly yielding better word embeddings.

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