ABSTRACT

In recent years, inductive graph embedding models, viz., graph neural networks (GNNs) have become increasingly accurate at link prediction (LP) in online social networks. The performance of such networks depends strongly on the input node features, which vary across networks and applications. Selecting appropriate node features remains application-dependent and generally an open question. Moreover, owing to privacy and ethical issues, use of personalized node features is often restricted. In fact, many publicly available data from online social network do not contain any node features (e.g., demography). In this work, we provide a comprehensive experimental analysis which shows that harnessing a transductive technique (e.g., Node2Vec) for obtaining initial node representations, after which an inductive node embedding technique takes over, leads to substantial improvements in link prediction accuracy. We demonstrate that, for a wide variety of GNN variants, node representation vectors obtained from Node2Vec serve as high quality input features to GNNs, thereby improving LP performance.

1 INTRODUCTION

The link prediction problem (LP) is to predict the set of future edges in a graph which are more likely to appear than the other edges, after observing the graph at a certain time. It has a wide variety of applications, viz., suggesting friends in social networks, connecting people on LinkedIn [15], recommending movies on Netflix [4, 14], etc. LP has been thoroughly studied from the perspectives of both network science and machine learning [8–11, 20, 26, 29] starting from the seminal papers by Adamic and Adar [2] and Liben-Nowell and Kleinberg [15].

1.1 Prior work and limitations

In recent years, there has been a flurry of deep learning models which have shown a great potential in predicting links in online social networks. Such models learn node embedding vectors which compress sparse, high dimensional information about node neighborhoods in the graph into low dimensional dense vectors. These embedding methods predominantly follow two approaches. The first approach consists of transductive neural models which learn the embedding of each node separately by leveraging matrix factorization based models, e.g., Node2Vec [7], DeepWalk [18], etc. Such models suffer from two major limitations, viz., they cannot make predictions using unseen nodes and, the corresponding model complexity grows with the network size [8]. On the other hand, the second approach consists of graph neural networks (GNNs) which train inductive neural models using symmetric aggregator functions [5, 11, 17, 19, 21, 25, 27, 28]. Such models feed the information about the node-neighborhoods into a symmetric aggregator which shares the same parameters globally across the graph. Hence, they can predict links on unseen nodes which were not present during training.

Given a node $u$, a GNN model collects features of the nodes at different distances from $u$ and combine them using a symmetric set aggregator. Therefore, the predictive prowess of GNN is contingent on providing it appropriate node features, which however, are domain dependent and require significant effort to design. Moreover, in the context of link recommendation in online social networks, the use of node features may be restricted due to privacy and ethical issues. As a result, most publicly available datasets on online social networks severely limit access to node features. Therefore, existing works use different proxies, e.g., random features, one-hot encoding of node-IDs, etc.

1.2 Our work

In this work, we provide a detailed experimental study where we first train one set of node embeddings which are agnostic to the graph neural network (GNN), using a transductive embedding model. Such node embeddings contain only structural information about a node. Next, we feed these embedding vectors as input node features into an inductive model. Finally, we train this inductive model using an LP loss function, to obtain the final node
embeddings. We observed that this two step procedure is consistently more effective than introducing other types of ad-hoc proxy node features into the model.

We perform a comparative analysis across seven datasets and four GNN models, which reveal that for online social networks, such a combination of transductive and inductive models consistently improves predictive performance, for all commonly-used LP loss functions\(^1\). However, for citation graphs, such an approach does not provide any improvement, which indicates that the structural properties alone are not enough to capture the generative process of the underlying graph.

2 LINK PREDICTION METHODS

After setting up notation and preliminaries, we will introduce the two major mechanisms through which node representations can be obtained: inductive and transductive embeddings. Then we will describe how to combine their strengths. We will conclude the section with a brief review on standard loss objectives for LP.

2.1 Notation

Given an undirected graph \(G = (V, E)\), we denote \(nbr(u)\) and \(\overline{nbr}(u)\) as the neighbors and non-neighbors of \(u\), respectively. In this context, note that \(nbr(u)\) also contains \(u\), i.e., \(nbr(u) = \{v | (u, v) \in E\} \cup \{u\}\). \(\overline{nbr}(u) = \{v \neq u | (u, v) \notin E\}\). Finally, we denote \(y_{u,v} = 1\) if \(v \in nbr(u)\) and \(y_{u,v} = 0\), otherwise.

2.2 Inductive node embeddings

Suppose, through some means, we obtain an initial node representation \(z_u\) for each node \(u\). These can be used by an inductive model to obtain graph-context sensitive node representations. Various graph neural networks (GNNs) are standard examples of inductive models. At a very high level, given a node \(u\) and an integer \(K\), a GNN takes the underlying graph \(G = (V, E)\) and the initial node embeddings \(\{z_u | u \in V\}\) as input, and then computes inductive node embeddings \(\{emb_u | u \in V\}\) by iteratively aggregating structural information from the nodes \(k = 1, 2, ..., K\) hops away from \(u\).

\[
x_u(0) = z_u
\]

\[
x_u(k) = F_\theta(x_u(k-1) | v \in nbr(u))
\]

In Eqs. (2) \& (3), \(x_u(\bullet)\) are intermediate node embeddings. Moreover, \(F_\theta\) and \(G_\theta\) are neural networks parameterized with \(\theta\). The exact form of \(F_\theta\) and \(G_\theta\) vary across different GNN models. In this paper, we consider four competitive GNNs, viz., GCN [11], GraphSAGE [8], GIN [26] and DGCNN [29]. For a downstream task such as LP, we compute the score for the node-pair \((u, v)\) as

\[
s_\theta(u, v) = H_\theta(\overline{emb}_u, \overline{emb}_v)
\]

Here \(H_\theta\) is another network that compares embeddings \(\overline{emb}_u, \overline{emb}_v\) to arrive at a link score. We call this scheme ‘inductive’ because, once \(F_\theta, G_\theta, H_\theta\) are trained for a task, the induced model can be applied to a completely new graph in the same problem domain, to get meaningful node representations.

\(^1\)Our code is available at https://www.cse.iith.ac.in/~abhir/codes/linkPredCIKM2021.zip

2.3 Transductive node embeddings

For each application, a key question is how to set initial node representations \(\{z_u\}\). If rich local signals (such as text or demographics) are available at each node, these can be suitably featureized using classical feature engineering or deep techniques. In the absence of node features, GNN practitioners have tried fixed random vectors, one-hot codes for (arbitrary) node IDs, and a row or column of the adjacency matrix corresponding to each node. One may argue that the GNNs are in charge of network signal aggregation, so local features should suffice for setting up \(\{z_u\}\). Our key noteworthy observation is that when graph features are used to also determine the initial \(\{z_u\}\), the GNNs may behave better and lead to better end-task accuracy. We will now describe two ways in which how graph-based transductive methods can be used to obtain these initial node representations.

**Node2Vec (N2V) [7]** Given a node \(u\), Node2Vec first samples nodes \(N_\theta(u)\) using different random walk based heuristics. Then it models the likelihood of the sampled nodes using a multinomial distribution informed by the proximity of the nodes, measured in terms of \(\exp(z_u^\top z_w)\). More specifically, we have:

\[
Pr(N_\theta(u) | z_u) = \prod_{v \in N_\theta(u)} \frac{\exp(z_u^\top z_v)}{\sum_{w \in V} \exp(z_u^\top z_w)}
\]

Finally, the node embeddings \(z_u\) are estimated by solving the following training problem.

\[
\max_{\{z_u\}} \sum_{u \in V} -\sum_{v \in V} \log \sum_{w \in N_\theta(u)} \exp(z_u^\top z_w) + \sum_{v \in N_\theta(u)} z_u^\top z_v
\]

**Matrix factorization (MF) [16]** Apart from Node2Vec, we also consider Matrix factorization as a candidate transductive model, i.e., we train the node embeddings \(\{z_u\}\) as:

\[
\min_{\{z_u\}} \sum_{u \in V} \sum_{v \in V} (y_{u,v} - z_u^\top z_v)^2 + \lambda \sum_u ||z_u||_2^2
\]

where \(\lambda\) is a regularizing constant.

2.4 Combining inductive and transductive approaches

Once we train the transductive embeddings \(\{z_u\}\) using Eq. (6) or (7), we feed them into the GNN model (1)–(3) to learn \(\overline{emb}_u\).

**Training losses** We learn the parameters \(\theta\) used to parameterize Eqs. (2), (3) by minimizing a LP loss function — the two most popular of which binary cross entropy (BCE) loss and ranking loss are considered in this work.

**BCE loss** We compute the binary cross entropy loss as follows:

\[
\ell_{\text{BCE}}(\theta; G) = - \sum_{(u,v) \in E} \log[\sigma(s_\theta(u, v))] - \sum_{(u,v) \notin E} \log[1 - \sigma(s_\theta(u, v))]
\]

**Pairwise ranking loss** We compute the pairwise ranking loss as follows:

\[
\ell_{\text{rank}}(\theta; G) = \sum_{u \in V} \sum_{v \in nbr(u)} \text{ReLU}(s_\theta(w, u) - s_\theta(v, u) + \delta)
\]

where \(\sigma\) is the sigmoid function and \(\delta\) is a tunable margin.

3 EXPERIMENTS

In this section, we provide a comprehensive evaluation of our proposed approach, and comparisons with standard alternatives.
In the document, there is a table labeled as Table 1: Dataset statistics. The table contains the following columns: Dataset, |V|, |E|, $d_{avg}$, Diameter, |Q|. The dataset statistics are as follows:

| Dataset   | |V|  | |E|  | $d_{avg}$ | Diameter | |Q| |
|-----------|----|----|----------|-----------|----------|----------|
| Twitter-1 | 213 | 12173 | 115.38   | 3         | 209      |
| Twitter-2 | 235 | 10862 | 92.44    | 3         | 235      |
| Twitter-3 | 193 | 7790  | 79.73    | 4         | 190      |
| Google+   | 769 | 22515 | 57.56    | 7         | 718      |
| PB        | 1222| 17936 | 28.36    | 8         | 999      |
| Citeseer  | 3312| 7848  | 3.74     | 28        | 1010     |
| Cora      | 2708| 7986  | 4.90     | 19        | 1470     |

The table represents the statistics of various datasets, including the number of nodes (|V|), edges (|E|), average degree ($d_{avg}$), diameter, and the number of queries (|Q|) for each dataset.

3.1 Datasets

We use seven datasets from diverse domains. Among them, the first three datasets, viz., Twitter-1, Twitter-2, Twitter-3 are three separate connected components from Twitter [13]. The other datasets are Google+ [12], PB [1], Cora [6, 22], and Citeseer [6, 22]. Among them, the first five datasets are online social networks, whereas, the last two datasets are citation networks. Refer Table 1 for details.

3.2 Setup

Candidates for inductive and transductive models We consider four candidates for the inductive GNNs — GCN [11], GIN [26], DGCNN [29] and GraphSAGE [8]. On the other hand, we consider two candidates for transductive models—N2V [7] and MF [16].

LP methods As described in Section 2, we first train the transductive node embeddings ($z_q$) and then feed them into the inductive models as input. While doing so, we also augment these transductive embeddings with the one-hot encodings of node labels obtained using Double-Radius Node Labeling (DRNL) algorithm [29, 30]. In addition, we also compare our approach with the corresponding transductive model which only uses the DRNL node features.

Implementation details We used Adam optimizer with learning rate $10^{-3}$. We use early stopping during training with patience parameter $P = 6$, i.e., we stop training when validation fold performance does not improve within the last $P$ epochs. For the ranking losses, we cross validate our method across three values of the tunable margin $\delta \in \{0.1, 1, 10\}$.

3.3 Evaluation

Protocol As suggested in previous works [3, 20], we consider predicting only on those node pairs whose one of the nodes participate in at least one triangle. We call such nodes query nodes $Q$. Then for each query node $q$, we randomly split both nbr($q$) and nbr($q$) into 70% training, 10% validation and 20% test sets. We use the training set to supervise training of the GNN model. Next, we rank the node pairs in the test set based on the scores computed by the trained LP model.

Metrics We evaluate the predicted ranked list (of node pairs belonging to a query node $q \in Q$) via average precision (AP) and reciprocal rank (RR). Finally, we report Mean Average Precision (MAP) and Mean Reciprocal Rank (MRR) as follows:

$$\text{MAP} = \frac{1}{|Q|} \sum_{q \in Q} AP_q,$$

$$\text{MRR} = \frac{1}{|Q|} \sum_{q \in Q} RR_q,$$

where $AP_q$ and $RR_q$ are the average precision and reciprocal rank corresponding to the ranked list given by $q \in Q$.

3.4 Results

Comparative analysis First, we compare our approach against the corresponding inductive embedding model trained only with the DRNL features. Here, we consider N2V as the transductive embedding model. Table 2 summarizes the results for both BCE loss and Ranking loss, which shows that: (i) for all datasets, except for citation graphs, our method outperforms the other method; (ii) the trained N2V embeddings provide significant performance boost in GraphSAGE; and, (iii) the performance of GCN and GraphSAGE are comparable in the absence of N2V embeddings, as they share similar neural architectures. N2V computes the node embeddings by performing long range random walk, whereas, the GNN models limit their aggregation operation within $K \leq 3$ hop distance. As a result, our approach is able to capture the structural information better than a GNN model trained alone with the DRNL features.

Query-wise analysis Next, we look into the performance at the individual query level. Specifically, we probe the gain/loss achieved by our model in terms of Gain = $AP$(Our method) − $AP$(GNN-Only) for each query $q \in Q$. Figure 1 summarizes the results which show that, for GCN model (GIN model), our method provides superior performance for 71% and 53% (81% and 61%) queries for Twitter-3 and Google+ datasets, respectively.

Effect of Matrix Factorization (MF) as the inductive model Then, we investigate if the superior performance of our approach is consistent across transductive models. We show this to be the case, when MF is the candidate transductive model in Table 3.

Effected of raw node attributes instead of N2V features Recall that, the alternative GNN models use the node features computed via DRNL algorithm [29, 30]. Here, we augment them with the available node attributes and compare its performance with our proposed approach. We find out that the performance of the two methods is comparable, as shown in Table 4.

| Dataset   | r = 0.02|V| | r = 0.05|V| |
|-----------|---------|--------|---------|--------|
| Twitter-3 | 0.769   | 0.775  |
| Google+   | 0.615   | 0.618  |

Table 5: Effect of length of random walk $r$ in N2V on MAP for Twitter-3 and Google+ datasets with GCN model (our approach) and BCE loss.
Table 2: Performance comparison in terms of MAP (left half) and the MRR (right half) of our proposed method — which integrates the transductive and inductive models — against the inductive model which does not receive any input from the transductive model, across all datasets and all inductive models, i.e., GCN [11], GIN [26], DGCNN [29] and GraphSAGE [8]. We choose N2V as the transductive embedding model. The top and bottom halves of the table report the results for BCE loss and Ranking loss objective, respectively. We observe that for all datasets except citation networks, our proposed approach outperforms the inductive model trained without transductive embeddings.

Table 3: Performance comparison in terms of MAP of our proposal when we use MF [16] as the transductive model against the inductive model trained without any transductive embedding for the first five datasets with BCE loss.

Effect of random walk length in Node2Vec Finally, we change the length $r$ of the random walk in N2V and observe the MAP values obtained by our approach. Table 5 summarizes the results, which shows that the MAP values improves with increasing the value of $r$. This is because a larger value of $r$ can encode the structural information of the graph neighborhood of node $u$ better into the node embedding $\{z_u\}$ compared to smaller values of $r$.

4 CONCLUSION

There are two dominant paradigms to represent graph nodes using continuous embedding vectors. The transductive approach, typified by Node2Vec and Matrix Factorization, scales up the number of parameters with the number of nodes, but can effectively exploit long-range influence in the graphs. The inductive approach has a globally-tied, smaller-capacity local neighborhood feature aggregator that is rarely applied beyond two hops. In this paper we establish that combining their strengths can give notable accuracy improvements for social networks where access to intrinsic node features may be restricted or prohibited.

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