Ego-based Entropy Measures for Structural Representations

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Abstract

In complex networks, nodes that share similar structural characteristics often exhibit similar roles (e.g., type of users in a social network or the hierarchical position of employees in a company). In order to leverage this relationship, a growing literature proposed latent representations that identify structurally equivalent nodes. However, most of the existing methods require high time and space complexity. In this paper, we propose VNEstruct, a simple approach for generating low-dimensional structural node embeddings, that is both time efficient and robust to perturbations of the graph structure. The proposed approach focuses on the local neighborhood of each node and employs the Von Neumann entropy, an information-theoretic tool, to extract features that capture the neighborhood’s topology. Moreover, on graph classification tasks, we suggest the utilization of the generated structural embeddings for the transformation of an attributed graph structure into a set of augmented node attributes. Empirically, we observe that the proposed approach exhibits robustness on structural role identification tasks and state-of-the-art performance on graph classification tasks, while maintaining very high computational speed.

1 Introduction

The amount of data that can be represented as graphs has increased significantly in recent years. Graph representations are ubiquitous in several fields such as in biology, chemistry and social networks [Hamilton et al., 2017]. Many applications require performing machine learning tasks on such type of data. For instance, in chemistry, graph regression can successfully replace expensive quantum mechanical simulation approaches in predicting the quantum properties of organic molecules [Gilmer et al., 2017]. The past few years have witnessed great activity in the field of learning on graphs. This activity has led to the development of several sophisticated approaches. In the supervised setting, graph neural networks have achieved great success in tackling both node and graph-related problems [Scarselli et al., 2009; Kipf and Welling, 2017]. In the unsupervised setting, most of the activity has focused on node embedding algorithms [Hamilton et al., 2017; Ying et al., 2018]. So far, most of these algorithms are designed so that they preserve the proximity between nodes, i.e., nodes that are close to each other in the graph (or belong to the same community) obtain similar representations, while distant nodes are assigned completely different representations [Perozzi et al., 2014; Grover and Leskovec, 2016]. However, some tasks require assigning similar embeddings to nodes that perform similar functions in the network, regardless of their distance. These tasks require structural embeddings, i.e., embeddings that can identify structural properties of a node’s neighborhood. For instance, predicting job positions based on the communication network of a company may be achieved by observing the type of interactions that user have with their colleagues (e.g., broadcasting to a large audience for secretaries or frequent communication to a small group for teammates).

2 Related Work

The major part of the research interest in the field of node embeddings focuses on encouraging nodes close to each other to have similar representations, based on the homophily conditions that satisfy many social and bioinformatics networks. In this work, we focus on the structural equivalence between nodes rather than the homophily, in order to provide structural representations. RolX algorithm [Henderson et al., 2012] is one of the first and still successful approaches to model structural node roles. Specifically, it extracts features for each node and applies non-negative matrix factorization to the emerging matrix in order to automatically discover node roles in the graph. A more recent approach, struc2vec [Ribeiro et al., 2017], constructs a multi-layer graph which encapsulates structural characteristics of the original graph. It then performs random walks to learn structural representations. GraphWave [Donnat et al., 2018] is another approach which capitalizes on the eigenspectrum of the graph to compute diffusion wavelets in the complex space, and uses the real and imaginary parts of these wavelets to generate node embeddings. One main drawback of this method is that it suffers from high space complexity when applied to large graphs. DRNE [Tu et al., 2018] aggregates neighborhood information using an LSTM operator upon the sequence of a node’s neighbors. This method implies an ordering of each node’s neighborhood, hence not satisfying the permutation invariance.
ance criteria and, thus, could affect its performance. Regarding the utilization of structural characteristics in order to decompose the graph structure and the attribute space of the graph nodes, a recent work [Chen et al., 2019b] proposes the augmentation of the node attribute vectors with features that encode the graph structure.

Contribution. In this paper, we provide a novel and simple structural node embedding algorithm which capitalizes on information-theoretic tools. The algorithm employs the Von Neumann entropy to construct node representations related to the structural identity of the neighborhood of each node. These representations capture the structural symmetries of the neighborhoods of increasing radius of each node. The algorithm is evaluated in node classification and node clustering tasks where it achieves performance comparable to state-of-the-art methods. Moreover, the algorithm is evaluated on standard graph classification datasets where it outperforms recently-proposed graph neural network models. Code will be available at https://github.com/ after the review process.

3 Structural Embeddings based on Von Neumann Entropy

We next present the proposed approach for generating structural node embeddings, employing the Von Neumann entropy, a model-agnostic measure, that quantifies the structural complexity of a graph. Graph entropy methods have been used in recent works [Li and Pan, 2016; Shetty and Adibi, 2005] for graph similarity in network analysis problems. The Von Neumann graph entropy (VNGE) has been proven to have a linear correlation with other graph entropy measures [Anand et al., 2011]. Based on its applications, our method exploits VNGE as a similarity measure between neighborhoods of nodes, in order to extract structural representations.

3.1 Von Neumann Entropy on Graphs

In the field of quantum mechanics, the state of a quantum mechanical system is described by a density matrix $\rho$, i.e., a positive semidefinite, hermitian matrix with unit trace [Gasser, 1970]. Given the above, the Von Neumann entropy of the quantum system is defined as:

$$H(\rho) = -\text{Tr}(\rho \log \rho) = - \sum_{i=1}^{n} \lambda_i \log \lambda_i,$$

where $\text{Tr}(\cdot)$ is the trace of a matrix, and $\lambda_i$’s are the eigenvalues of $\rho$. Correspondingly, given a graph $G = (V, E)$, where $|V| = n$ and its laplacian $L_G = D - A$, where $D$ is the degree matrix and $A$ the adjacency matrix, the ranked eigenvalues of $L_G$ are $\lambda_i$’s. Hence, $H(L_G)$ is symmetric, positive semidefinite and with unit trace, suggesting an analogy with the density matrix. Thus, the Von Neumann graph entropy (VNGE) is defined as:

$$H(\rho(L_G)) = -\text{Tr}(\rho \log \rho(L_G)).$$

Next, for each node $v \in V$, the $r$-hop neighborhood of $v$ is computed using Equation 4. Finally, the $R$ entropies are arranged into a single vector (i.e., node embedding) $h_v \in \mathbb{R}^R$. The method is illustrated in Algorithm 1 below.

$$H(\rho(L_G)) = -\sum_{i=1}^{n} \lambda_i \log \lambda_i,$$

where $\lambda_i$ is the $i$-th eigenvalue of $L_G$, $D$ is the degree matrix of $G$, $A$ is the adjacency matrix of $G$, and $\text{Tr}(\cdot)$ is the trace of a matrix. The Von Neumann entropy of the probability distribution $\{\lambda_i\}_{i=1}^{n}$ is defined as:

$$H(\rho(L_G)) = -\sum_{i=1}^{n} \lambda_i \log \lambda_i,$$

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$$H(\rho(L_G)) = -\sum_{i=1}^{n} \lambda_i \log \lambda_i.$$
As illustrated in Figure 1, VNEstruct is able to identify structural equivalences between nodes, which are distant to each other. Specifically, nodes $u$ and $v$ share structurally identical 1-hop neighborhoods. Therefore, the entropies of their 1-hop neighborhoods are equal to each other. However, this is not the case for the entropies of their 2-hop neighborhoods since the two subgraphs are very dissimilar from each other. Note that in this work, we focus on undirected graphs without edge weights. However, our approach easily extends in the case of weighted and directed graphs.

Algorithm 1: VNEstruct algorithm

```
input : graph $G = (V, E)$, radius $R$
output: An embedding matrix $H \in \mathbb{R}^{n \times R}$

foreach $v \in V$ do
    | foreach $r \in \{1, \ldots, R\}$ do
    |     Extract ego-graph Laplacian $L_{G_r'}$
    |     Derive density matrix $\rho(L_{G_r'}) = \frac{L_{G_r}'}{\text{Tr}(L_{G_r'})}$
    |     $\lambda_{\text{max}} \leftarrow \text{Power-Iteration}(\rho(L_{G_r'}))$
    |     $Q \leftarrow 1 - \frac{1}{\lambda_{\text{max}}} \sum_{i=1}^{n} d_i^2$
    |     $h(v, r) \leftarrow -Q \ln(\lambda_{\text{max}})$
endfor

$H_v \leftarrow \text{CONCAT}(h(v, 1), \ldots, h(v, R))$
```

Computational Complexity. Algorithm 1 consists of two computational steps: (1) the extraction of the ego-networks and (2) the computation of VNGEs for all subgraphs. The first step is linear in the number of edges of the node’s neighborhood. In the worst case, the complexity is $O(nm)$, but for sparse graphs and for small values of $R$, the complexity is significantly lower (constant in practice). With regards to the second step, as we mentioned above, we do not perform the eigenvalue decomposition of the density matrix (requires $O(n^3)$ time), but we make use of Equation 4. This requires finding the largest eigenvalue $\lambda_{\text{max}}$ and computing simple degree statistics for each $r$-hop neighborhood. We use the power iteration method [Mises and Pollaczek-Geiringer, 1929] to compute $\lambda_{\text{max}}$, which requires $O(nm)$ operations, as the Laplacian matrix has $n+m$ nonzero entries. Hence, the whole approximation exhibits linear complexity $O(n+m)$, while for very sparse graph, it becomes $O(n)$.

Robustness over "small" perturbations. We will next show that utilizing the VNGE, we can acquire robust structural representations over possible perturbations on the graph structure. Clearly, if two graphs are isomorphic to each other, then their entropies will be equal to each other. It is important, though, for structurally similar graphs to have similar entropies, too. So, let $\rho, \rho' \in \mathbb{R}^{n \times n}$ be the density matrices of two graph laplacians $L_{G_1}, L_{G_2}$, as described above. Let also $\rho = \bar{P}\rho'\bar{P}^T + \epsilon$ where $\bar{P}$ is an $n \times n$ permutation matrix equal to $\text{arg min}_P ||\rho - \bar{P}\rho'\bar{P}^T||_F$ and $\epsilon$ is an $n \times n$ symmetric matrix. If $G, G'$ are nearly-isomorphic, then the Frobenius norm of $\epsilon$ is small. By applying the Fannes-Audenaert inequality [Audenaert, 2007], we have that:

$$|H(\rho') - H(\rho)| \leq \frac{1}{2} T \ln(n-1) + S(T),$$

where $T = ||\rho - \rho'||_1$ is the trace distance between $\rho, \rho'$ and $S(T) = -T \log T - (1-T) \log (1-T)$. However, $||\rho - \rho'||_1 = \sum_i |\lambda_i^{\rho} - \lambda_i^{\rho'}| \leq n ||\rho - \rho'||_{\text{op}}$, where $||.||_{\text{op}}$ is the operator norm. Therefore, $|H(\rho') - H(\rho)| \leq \frac{2}{n} \ln(N-1)||\epsilon||_{\text{op}} + S(|T, 1 - T|)$, leading thus to an upper bound of the difference between the entropies of structurally similar graphs.

### 3.3 Graph-level Representations

Next, we propose incorporating the structural embeddings generated by VNEstruct into graph classification algorithms. The majority of the state-of-the-art methods learn node representations using message-passing schemes [Hamilton et al., 2017; Xu et al., 2018], where each node updates its representation $T$ times by aggregating the representations of its neighbors and combining them with its own representation. Clearly, each time the nodes update their representations, the structure of the graph is taken into account. In this work, we do not use any message-passing scheme and we ignore the graph structure. Instead, we employ the VNEstruct and we embed the nodes into a low-dimensional space. These embeddings are then combined with the node attributes (if any). In fact, information about the graph structure is incorporated into the embeddings generated by the proposed algorithm. This approach follows recent studies that propose to augment the node attribute vectors with structural characteristics, in order to avoid performing some message-passing
procedure [Chen et al., 2019b; Errica et al., 2019]. The above pre-processing step transforms the graph into a set of vectors (i.e., one vector for each node). Then, these vectors are passed on to a neural network model which transforms them and then aggregates them using some permutation invariant function [Zaheer et al., 2017]. Specifically, given a matrix of node attributes $X \in \mathbb{R}^{n \times d}$, our approach performs the following steps:

- Computation of $H_v \in \mathbb{R}^{n \times R}$
- Concatenation of node attribute vectors with structural node embeddings: $X' = [X||H] \in \mathbb{R}^{n \times (d+R)}$
- Aggregation of node vectors $X'$ into graph embedding $\hat{H}_G = \psi(\sum_{v \in V_G} \phi(X'_v))$, where $\phi$ and $\psi$ are neural networks.

The above procedure does not apply any message-passing scheme. This reduces the computational complexity of the training procedure since each graph is represented as a set of node representations.

4 Experiments

Next, we evaluate the performance of the proposed approach in two scenarios: (1) the structural role identification task, where we extract the role of a node in the graph and (2) the graph classification task, where given a graph (attributed or not), we predict the class that it belongs, based on the graph-level representation. For the structural role identification task we use both synthetic and real-world graphs, while for the graph classification task we use 5 well-studied real-world datasets.

4.1 Structural Role Identification

We first experiment with some synthetic datasets and then we compare the performance of VNENstruct and baselines on a real-world dataset.

Toy network: Barbell Graph

This toy graph consists of two cliques of size 10 that are connected through a path of length 7. The graph is shown in Figure 2 (right). The different colors indicate the roles of the nodes in the graph. Figure 2 (left) illustrates the 2-dimensional representations of the 27 nodes of the graph. These representations were generated by the VNENstruct algorithm (we set $R = 3$ and then applied PCA to project them to the 2-dimensional space). We should mention that the proposed algorithm can identify the structural role of the nodes in the barbell graph and produce similar/identical embeddings for structurally similar/identical nodes.

Highly-symmetrical synthetic networks

In order to evaluate the expressiveness of the structural embeddings generated by our method, we measure its performance on synthetic datasets, which were introduced in [Donnat et al., 2018; Ribeiro et al., 2017]. We perform both classification and clustering with the same experimentation setup as [Donnat et al., 2018].

Evaluation.

For the classification task, we measure the accuracy and the F1-score. For the clustering task, we report the 3 evaluation metrics, that were also calculated in [Donnat et al., 2018]: Homogeneity, Completeness and Silhouette. Specifically, the homogeneity evaluates the conditional entropy of the structural roles in the generated clustering, based on each method: $H(C) = -\sum_{c=1}^{\lvert C \rvert} \frac{\sum_{k=1}^{\lvert K \rvert} a_{ck}}{\lvert n \rvert} \log \frac{\sum_{k=1}^{\lvert K \rvert} a_{ck}}{\lvert n \rvert}$ where $C = \{c_1, c_2, ..., c_{\lvert C \rvert}\}$, $K$ is the set of the assigned clusters $K = \{k_1, k_2, ..., k_{\lvert K \rvert}\}$ and $a_{ij}$ is the number of nodes with structural role $c$ and assigned in the cluster $j$. The completeness evaluates how many nodes with equivalent structural roles are assigned to the same cluster: $H(C) = -\sum_{k=1}^{\lvert K \rvert} \frac{\sum_{c=1}^{\lvert C \rvert} a_{ck}}{\lvert n \rvert} \log \frac{\sum_{c=1}^{\lvert C \rvert} a_{ck}}{\lvert n \rvert}$. The silhouette measures the mean intra-cluster distance vs the mean inter-cluster distance. Regarding our method, the only hyperparameter that we optimized was the radius of the considered ego-networks. We chose $R$ from $\{1, ..., 3\}$.

Dataset setup.

The generated synthetic datasets are identical to those used in [Donnat et al., 2018]. They consist of basic symmetrical shapes, as shown in Table 1, that are regularly placed along a cycle of length 30. The basic setups use 10 instances of only one of the shapes of Table 1, while the varied setups use 10 instances of every shape, randomly placed along the cycle. The perturbed instances are formed by randomly rewiring edges. The colors in the shapes indicate the different classes.

As Table 1 shows, VNENstruct outperforms the competitors on the perturbed instances of the synthetic graphs. Specifically, while on the basic and the varied configurations RolX and GraphWave achieve higher F1-scores, on the perturbed configurations GraphWave and VNENstruct show better performance, with our approach outperforming all the others in the varied perturbed configuration. The results in Table 1 suggest a comparison of VNENstruct, RolX and GraphWave on noisy setting. This comparison is provided in Figure 3. Here, we use the same dataset, but we report the classification and clustering performance with respect to the number of rewired edges (from 0 to 20). As we can see, the presence of noise has a less impact on VNENstruct than on GraphWave and RolX, especially in the clustering task.

Role identification on Email-dataset

We next evaluate the performance of VNENstruct algorithm and of its competitors on a real-world dataset, the Enron Email dataset [Klimt and Yang, 2004]. This is an email
| Configuration | Shapes | Algorithm  | Homogeneity | Completeness | Silhouette | Accuracy | F1-score |
|--------------|--------|------------|-------------|--------------|------------|---------|----------|
| Basic        |        | DeepWalk   | 0.178       | 0.115        | 0.163      | 0.442   | 0.295    |
|              |        | RolX       | **0.983**   | **0.976**    | 0.846      | **1.000**| **1.000**|
|              |        | struc2vec  | 0.803       | 0.595        | 0.402      | 0.784   | 0.708    |
|              |        | GraphWave  | 0.868       | 0.797        | 0.730      | 0.995   | 0.993    |
|              |        | VNEstruct  | 0.966       | 0.963        | **0.891**  | 0.920   | 0.901    |
| Perturbed    |        | DeepWalk   | 0.172       | 0.124        | 0.171      | 0.488   | 0.327    |
|              |        | RolX       | 0.764       | 0.458        | 0.429      | 0.928   | **0.886**|
|              |        | struc2vec  | 0.625       | 0.543        | 0.424      | 0.703   | 0.632    |
|              |        | GraphWave  | 0.714       | 0.326        | 0.287      | 0.906   | 0.861    |
|              |        | VNEstruct  | **0.882**   | **0.701**    | **0.478**  | **0.940**| **0.881**|
| Varied       |        | DeepWalk   | 0.327       | 0.220        | 0.216      | 0.329   | 0.139    |
|              |        | RolX       | **0.984**   | **0.939**    | 0.748      | **0.998**| **0.996**|
|              |        | struc2vec  | 0.805       | 0.626        | 0.422      | 0.738   | 0.592    |
|              |        | GraphWave  | 0.941       | 0.843        | **0.756**  | 0.982   | **0.965**|
|              |        | VNEstruct  | 0.950       | 0.892        | 0.730      | 0.988   | 0.95     |
| Perturbed    |        | DeepWalk   | 0.300       | 0.231        | 0.221      | 0.313   | 0.128    |
|              |        | RolX       | 0.682       | 0.239        | 0.062      | 0.856   | 0.768    |
|              |        | struc2vec  | 0.643       | 0.524        | **0.433**  | 0.573   | 0.412    |
|              |        | GraphWave  | 0.670       | 0.198        | 0.005      | 0.793   | 0.682    |
|              |        | VNEstruct  | **0.722**   | **0.678**    | 0.399      | **0.899**| **0.878**|

Table 1: Performance of the baselines and the VNEstruct method for learning structural embeddings averaged over 20 synthetically generated graphs. Dashed lines denote perturbed graphs.

4.2 Graph Classification

Graph classification on molecular and social networks

We next evaluate VNEstruct algorithm and the baselines in the task of graph classification. We compare our proposed algorithm against well-established message-passing algorithms for learning graph representations. Note that in contrast to the majority of the baselines, we pre-compute the entropy-based structural representations, and then we represent each graph as a set of vectors (i.e., its node representations) which encode structural characteristics of the neighborhood of each node.

Datasets. We use 4 graph classification datasets (3 are from bioinformatics: MUTAG, PROTEINS, PTC-MR and 1 dataset comes from social-networks: IMDB-BINARY). The datasets have been examined in a variety of graph kernels and graph neural networks methods [Xu et al., 2018; Shervashidze et al., 2011; Kipf and Welling, 2017]. As they have been previously described, the bioinformatics datasets contain node attributes, while the social network does not and following previous works, we create the attributes by employing one-hot encodings of the node degrees. In the case of VNEstruct, we append to the attributes the generated structural embeddings.
Baselines. The goal of the comparison is to show that decomposing the graph structure and the attribute space, we can achieve comparable results to the state-of-the-art algorithms. Thus, we use as baselines graph neural network variants and specifically: DGCNN [Zhang et al., 2018], Capsule GNN [Xinyi and Chen, 2019], Graph Isomorphism Network [Xu et al., 2018], Graph Convolutional Network [Kipf and Welling, 2017]. Moreover, in a more recent work [Chen et al., 2019b], the authors propose Graph Feature Network, which, also, augments the attributes with structural features and then ignores the graph structure during the learning procedure.

Model setup. For the baselines, we followed the same experimentation setup, as described on [Chen et al., 2019b] and, thus, we report the achieved accuracies. Regarding the VNEstruct, we performed 10-fold cross-validation with Adam optimizer and learning rate decay every 50 epochs by a factor of 0.3. In all experiments, we set the number of epochs to 300. As hyper-parameters, we set the radius of the ego-networks $r \in \{1, 2, 3, 4\}$ and the number of hidden layers $d \in \{8, 16, 32\}$ on the MLPs of the node representation aggregator.

With regards to the running time of the different methods, Figure 4 illustrates the average training time per epoch of VNEstruct and some baselines that apply message-passing schemes. The proposed approach is generally more efficient than the baselines. Specifically, it is 0.31 times faster than GIN and 0.60 times faster than GCN on average. This improvement in efficiency is mainly due to the fact that the graph structural features are computed in a preprocessing step, are then concatenated with the node attributes, and are passed on the neural network model. Furthermore, we should mention that due to the low dimensionality of the generated embeddings ($d \leq 4$), our method does not have any significant requirements in terms of memory.

5 Conclusion

In this paper, we proposed an algorithm for generating structural node representations, based on the entropies of egonetworks. We evaluated the proposed algorithm in node classification and clustering tasks where it either outperformed or performed comparably to strong baselines. We also proposed an approach for performing graph-related tasks which combines these representations with the nodes’ attributes, and then passes the new representations into a neural network model, avoiding the computational cost of message passing schemes. The proposed approach yielded high classification accuracies on standard datasets.

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| Method      | MUTAG      | IMDB-BINARY | PTC-MR     | PROTEINS   |
|-------------|------------|-------------|------------|------------|
| DGCNN       | 85.83 ± 1.66 | 70.03 ± 0.86 | 58.62 ± 2.34 | 75.54 ± 0.94 |
| CapsGNN     | 86.67 ± 6.88 | 73.10 ± 4.83 | -          | 76.28 ± 3.63 |
| GIN         | 89.40 ± 5.60 | 75.10 ± 5.10 | 64.6 ± 7.03 | 76.20 ± 2.60 |
| GCN         | 87.20 ± 5.11 | 73.30 ± 5.29 | 64.20 ± 4.30 | 75.65 ± 3.24 |
| GFN         | 90.84 ± 7.22 | 73.00 ± 4.29 | -          | 77.44 ± 3.77 |
| VNEstruct   | 91.08 ± 5.65 | 75.40 ± 3.33 | 65.39 ± 8.57 | 77.41 ± 3.47 |

Table 3: Average classification accuracy (± standard deviation) of the baselines and the proposed VNEstruct algorithm on the 5 graph classification datasets.

![Figure 4](https://via.placeholder.com/150)

Figure 4: Training time per epoch (in sec) of VNEstruct and competitors for the graph classification tasks.

Performance and efficiency results. Table 3 illustrates the average classification accuracies of the proposed approach and the baselines on the 5 graph classification datasets. Interestingly, the proposed approach achieves accuracies comparable to some of the state-of-the-art message-passing models. VNEstruct outperformed all the baselines on 3 out of 4 datasets, while achieved the second best accuracy on the remaining dataset PROTEINS.
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