Distance Encoding – Design Provably More Powerful Graph Neural Networks for Structural Representation Learning

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Abstract

Learning structural representations of node sets from graph-structured data is crucial for applications ranging from node-role discovery to link prediction and molecule classification. Graph Neural Networks (GNNs) have achieved great success in structural representation learning. However, most GNNs are limited by the 1-Weisfeiler-Lehman (WL) test and thus possible to generate identical representation for structures and graphs that are actually different. More powerful GNNs, proposed recently by mimicking higher-order-WL tests, only focus on entire-graph representations and cannot utilize sparsity of the graph structure to be computationally efficient. Here we propose a general class of structure-related features, termed Distance Encoding (DE), to assist GNNs in representing node sets with arbitrary sizes with strictly more expressive power than the 1-WL test. DE essentially captures the distance between the node set whose representation is to be learnt and each node in the graph, which includes important graph-related measures such as shortest-path-distance and generalized PageRank scores. We propose two general frameworks for GNNs to use DEs (1) as extra node attributes and (2) further as controllers of message aggregation in GNNs. Both frameworks may still utilize the sparse structure to keep scalability to process large graphs. In theory, we prove that these two frameworks can distinguish node sets embedded in almost all regular graphs where traditional GNNs always fail. We also rigorously analyze their limitations. Empirically, we evaluate these two frameworks on node structural roles prediction, link prediction and triangle prediction over six real networks. The results show that DE-assisted GNNs outperform GNNs without DEs by up-to 15% improvement in average accuracy and AUC. DE-assisted GNNs also significantly outperform other state-of-the-art baselines particularly designed for those tasks.

1 Introduction

Structural representation learning aims to learn representation vectors of graph-structured data [1]. Representations of node sets embedded in a graph can be leveraged in a wide range of applications, such as discovery of functions/roles of nodes based on individual node representations [2][6], link or
Graph neural networks (GNNs), inheriting the power of neural networks [13], have recently become almost the default choice to learn structural representations in graphs [19]. In general, GNNs use message passing procedure over graphs, which can be summarized in three steps: (1) Initialize node representations as their initial attributes (if given) or structural features such as node degrees; (2) Iteratively update the representation of each node by aggregating the representations of its neighboring nodes; (3) Readout the final representation of a single node, a set of nodes or the entire node set as requested by the task. Under the above framework, researchers have proposed many well-known GNNs [14–16, 20–23]. Interested readers may refer to tutorials on GNNs for more details [24].

Despite the success of GNNs in a variety of graph-related domains, their representation power in structural representation learning was found limited [16, 25]. Recent works proved that the structural representation power of GNNs that follow the above framework is bounded by the 1-WL test [16, 25] (we shall refer to these GNNs as WLGNNs). Concretely, WLGNNs yield same vector representations for any structure that the 1-WL test cannot distinguish, as they are not structurally equivalent (or say “isomorphic”) as defined in Section 2. Furthermore, WLGNN cannot distinguish all the node-pairs highlighted by the dashed circles no matter whether these node-pairs correspond to edges or not. However, we may use shortest-path-distances (SPDs) between nodes as features to distinguish blue nodes from green or red nodes because there is another blue node with SPD= 3 to the blue node of interest (e.g., the pair of blue nodes highlighted by red boxes), while all SPDs between other nodes to red/green nodes are less than 3. To distinguish red nodes and green nodes, one needs in-depth analysis of the computation graphs (trees) of GNNs (see Figure 3 in Appendix C). Note that the structural equivalence between any two horizontally-aligned nodes can be obtained from the vertical reflexivity of the graph while the equivalence between two vertically-aligned blue nodes can be further obtained from the node permutation shown in the right. (b) WLGNN to represent a p-sized node set — f_i(·)’s are arbitrary neural networks; AGG(·)’s are set-pooling; L is the number of layers.

In this work, we address the limitations of WLGNNs and propose a class of structural features, termed Distance Encoding (DE). DE comes with both theoretical guarantees and empirical efficiency. Given a node set whose structural representation is to be learnt, DE for a node over the graph is defined as a mapping of a set of landing probabilities of random walks from each node of the node set of interest to this node. DE generally includes measures such as shortest path distance (SPD) and generalized PageRank scores [34], which essentially captures the graph structural information. DE can be merged into the design of GNNs in simple but effective ways: First, we propose DEGNN that utilizes DE as extra node features. We further enhance DEGNN by allowing DE to control the aggregation procedure of WLGNNs, which yields another model DEAGNN. Since DE purely depends on the graph structure and is independent from node identifiers, it has inductive and generalization ability. We have contributions as follows.

1. Theoretically, we analyze the additional expressive power of DEGNN and DEAGNN as opposed to WLGNN for structural representation learning. Regarding the expressive power, these two models
are able to distinguish two non-isomorphic equal-sized node sets (including nodes, node-pairs, ..., entire-graphs) that are embedded in almost all sparse regular graphs where WLGNN always fails if no discriminatory node/edge attributes are available.

(2) We also prove that these two models are not more powerful than WLGNN without discriminatory node/edge attributes to learn the structural representations of nodes over distance regular graphs [35], which implies the limitation of DEs. However, we show that they have extra power to learn the structural representations of node-pairs over distance regular graphs [35].

(3) Empirically, we evaluate these two models on three levels of tasks including node-structural-role classification (node-level), link prediction (node-pair-level), triangle prediction (node-triad-level). Our methods significantly outperform WLGNN on all three tasks by up-to 15% improvement in prediction average accuracy. Our methods also outperform other baselines specifically designed for these tasks.

Roadmap. Section 2 introduces the definition of structural representation learning and reviews WLGNNS and WL tests. Section 3 defines Distance Encoding and introduces how DE is used to improve the design of GNNs. Section 4 reviews related works. Section 5 compares DE-assisted GNNs with other models. We postpone the proof of all the theoretical results to the appendix.

2 Preliminaries

In this section, we formally define the notion of structural representation and review how WLGNN learns structural representation and its relation to the 1-WL test.

2.1 Structural Representation

Definition 2.1. We consider an undirected graph which can be represented as $G = (V, E, \mathbf{A})$, where $V = [n]$ is the node set, $E \subseteq V \times V$ is the edge set, and $\mathbf{A}$ contains all features in the space $\mathcal{A} \subset \mathbb{R}^{n \times n \times k}$. Its diagonal component, $\mathbf{A}_{vv}$, denotes the node attributes of node $v$ ($v \in V$), while its off-diagonal component in $\mathbf{A}_{uv}$ denotes the node-pair attributes of $(v, u)$. We set $\mathbf{A}_{uv}$ as all zeros if $(v, u) \notin E$. In practice, graphs are usually sparse, i.e., $|E| \ll n^2$. We introduce $\mathbf{A} \in \{0, 1\}^{n \times n}$ to denote the adjacency matrix of $G$ such that $A_{uv} = 1$ iff $(u, v) \in E$. Note that $\mathbf{A}$ can be also viewed as one slice of the feature tensor $\mathbf{A}$. If no node/edge attributes are available, we let $\mathbf{A} = A$.

Definition 2.2. The node permutation denoted by $\pi$ is a bijective mapping from $V$ to $V$. All possible $\pi$’s are collected in the permutation group $\Pi_n$. We denote $\pi$ acting on a subset of $V$, say $S$ as $\pi(S) = \{\pi(i) | i \in S\}$. We further define $\pi(A)_{uv} = A_{\pi(u)\pi(v)}$ for any $(u, v) \in V \times V$.

Definition 2.3. Denote all $p$-sized subsets of $V$ as $\mathcal{P}_p(V)$ and define the space $\Omega_p = \mathcal{P}_p(V) \times \mathcal{A}$. For two tuples $\mathcal{T}_1 = (S^{(1)}, \mathbf{A}^{(1)})$ and $\mathcal{T}_2 = (S^{(2)}, \mathbf{A}^{(2)})$ in $\Omega_p$, we call that they are isomorphic (otherwise non-isomorphic), if $\exists \pi \in \Pi_n$ such that $S^{(1)} = \pi(S^{(2)})$ and $\mathbf{A}^{(1)} = \pi(\mathbf{A}^{(2)})$.

Definition 2.4. A function $f$ defined on $\Omega_p$ is invariant if $\forall \pi \in \Pi_n$, $f(S, \mathbf{A}) = f(\pi(S), \pi(\mathbf{A}))$.

Definition 2.5. The structural representation of a tuple $(S, \mathbf{A})$ is an invariant function $\Gamma(\cdot) : \Omega_p \rightarrow \mathbb{R}^d$ where $d$ is the dimension of representation. Therefore, if two tuples are isomorphic, they should have the same structural representation.

The invariant property is critical for the inductive and generalization capability as it frees structural representations from node identifiers and effectively reduces the problem dimension by incorporating the symmetry of the parameter space [28] (e.g., the convolutional layers in GCN [20]). The invariant property also implies that structural representations do not allow encoding the absolute positions of $S$ in the graph.

Suppose we set two node sets $S^{(1)}$, $S^{(2)}$ of interest as two single nodes respectively and set two graph structures $\mathbf{A}^{(1)}$ and $\mathbf{A}^{(2)}$ as the ego-networks around these two nodes respectively. Then, the definition of structural representation essentially provides a mathematical characterization the concept “structural roles” of nodes [3, 5, 9], where two far-away nodes could have the same structural roles (representations) as long as their ego-networks have the same structures.

By adjusting the size of the node set $S$ of interest, the definition of structural representation becomes a general concept. Specifically, when $S = V$, structural representations reduce to entire graph representations. However, to restrict the scope of this work that is already too broad, we will primarily...
focus on the case that the node set $S$ has a fixed and small size $p$, where $p$ does not depend on $n$. Although Corollary 5.4 later shows the potential of our techniques on learning the entire graph representations, this is not the main focus of this work. We expect the techniques proposed in this work can be further used for entire graph representations while we leave the detailed discussion for future.

Although structural representation defines a more general concept, it shares some properties with graph representation. For example, the universal approximation theorem regarding graph representation [29] can be directly generalized to the case of structural representations:

**Theorem 2.6.** If structural representations $\Gamma$ are different over any two non-isomorphic tuples $T_1$ and $T_2$ in $\Omega_p$, then for any invariant function $f : \Omega_p \to \mathbb{R}$, $f$ can be universally approximated by feeding $\Gamma$ into a 3-layer feed-forward neural network with ReLu as the activation function, as long as (1) the feature space $\mathcal{A}$ is compact and (2) $f(S, \cdot)$ is continuous over $\mathcal{A}$ for any $S \in \mathcal{P}_p(V)$.

Theorem 2.6 formally establishes the importance of learning structural representations that may distinguish non-isomorphic structures, i.e., $\Gamma(T_1) \neq \Gamma(T_2)$ iff $T_1$ and $T_2$ are non-isomorphic. However, no polynomial algorithms have been found even to learn such representations of the entire graphs without node/edge attributes (known as the graph isomorphism problem) [36]. In this work, we will use the range of non-isomorphic structures that GNNs cannot distinguish to characterize their expressive power of structural representation learning.

### 2.2 Weisfeiler-Lehman Tests and WLGNN for Structural Representation Learning

Weisfeiler-Lehman tests (WL-test) are a family of algorithms used in graph isomorphism problems [26]. 1-WL test, the simplest one among this family, starts with coloring nodes with their degrees, iteratively aggregates the colors of nodes and their neighborhoods, and hashes the aggregated colors into unique new colors. The coloring procedure finally converges to some static node-color configuration. Here a node-color configuration is a multiset that records the types and the number of each type of colors. Different node-color configurations indicate two graphs are non-isomorphic. However, the reverse statement is not always true.

More than the graph isomorphism problem, the node colors obtained by the 1-WL test also indicate that different node-color configurations of nodes in $S^{(1)}$ and in $S^{(2)}$ obtained by the 1-WL test also indicate $T_1$ and $T_2$ are not isomorphic.

WLGNNS refer to those GNNs that mimic the 1-WL test to learn structural representation, which is summarized in Fig. 1(b). It covers many well-known GNNs of which difference may appear in the implementation of neural networks $f_i$ and set-poolings $AGG(\cdot)$ (Fig. 1(b)), including GCN [20], GraphSAGE [21], GAT [22], MPNN [14], GIN [16] and many more [28]. Note that we use WLGNN-$p$ to denote the WLGNN that is to learn structural representations of node sets $S$ with size $|S| = p$. One may directly choose $S = V$ to obtain the entire-graph representation. Theoretically, the graph representation power of WLGNN-$p$ is provably bounded by the 1-WL test [16]. The result can be also generalized to the case of structural representations as follows.

**Theorem 2.7.** Consider two tuples $T_1 = (S^{(1)}, \mathbf{A}^{(1)})$ and $T_2 = (S^{(2)}, \mathbf{A}^{(2)})$ in $\Omega_p$. If $T_1, T_2$ cannot be distinguished by the 1-WL test, then the corresponding outputs of WLGNN-$p$ satisfy $\Gamma(T_1) = \Gamma(T_2)$. On the other side, if $\Gamma(T_1) \neq \Gamma(T_2)$, then for any invariant function $f : \Omega_p \to \mathbb{R}$, $f$ can be universally approximated by feeding $\Gamma$ into a 3-layer feed-forward neural network with ReLu as the activation function, as long as (1) the feature space $\mathcal{A}$ is compact and (2) $f(S, \cdot)$ is continuous over $\mathcal{A}$ for any $S \in \mathcal{P}_p(V)$.

Because of Theorem 2.7, WLGN5 inherits the limitation of the 1-WL test. For example, WLGN5 cannot distinguish two equal-sized node sets embedded in all $r$-regular graphs unless node/edge features are discriminatory. Here, a $r$-regular graph means all its nodes have degree $r$. Therefore, researchers have recently focused on designing GNNs with expressive power greater than the 1-WL test. Here, we will improve the power of GNNs by incorporating a general class of structural features.
3 Distance Encoding and Its Power

3.1 Distance Encoding

Suppose we are to learn the structural representation of the target node set $S$. Intuitively, we propose DE to encode certain distance from $S$ to a node $u$. Rigorously, we define DE as follows.

**Definition 3.1.** Given a target set of nodes $S \in 2^V \setminus \emptyset$ of $G$ with the adjacency matrix $A$, denote **distance encoding** as a function $\zeta(\cdot | S, A) : V \to \mathbb{R}^k$. $\zeta$ should also be permutation invariant, i.e., $\zeta(u|S,A) = \zeta(\pi(u)|\pi(S),\pi(A))$ for all $u \in V$ and $\pi \in \Pi_n$. We denote DEs w.r.t. the size of $S$ and call them as $DE-p$ if $|S| = p$.

Later we use $\zeta(u|S)$ for brevity where $A$ could be inferred from the context. For simplicity, we choose DE as a set aggregation (e.g., the sum-pooling) of DEs between nodes $u$, $v$ where $v \in S$:

$$\zeta(u|S) = \text{AGG}({\zeta(u|v)|v \in S})$$

(1)

More complicated DE may be used while this simple design can be efficiently implemented and achieves good empirical performance. Then, the problem reduces to choosing a proper $\zeta(u|v)$. Again for simplicity, we consider the following class of functions that is based on the mapping of a list of landing probabilities of random walks from $v$ to $u$ over the graph, i.e.,

$$\zeta(u|v) = f_3(\ell_{uv}), \ell_{uv} = ((W)^2)_{uv}, \ldots, (W^k)_{uv}, \ldots$$

(2)

where $W = AD^{-1}$ is the random walk matrix, $f_3$ may be simply designed by some heuristics or be parameterized and learnt as a feed-forward neural network. In practice, a finite length of $\ell_{uv}$, say 3,4, is enough. Note that (2) covers many important measures. First, setting $f_3(\ell_{uv})$ as the first non-zero position in $\ell_{uv}$ gives the shortest-path-distance (SPD) from $v$ to $u$. We denote this specific choice as $\zeta_{spd}(u|v)$. Second, one may choose generalized PageRank scores [34].

$$\zeta_{gpr}(u|v) = \sum_{k \geq 1} \gamma_k(W^k)_{uv} = \left(\sum_{k \geq 1} \gamma_k W^k\right)_{uv}, \gamma_k \in \mathbb{R}, \text{ for all } k \in \mathbb{N}.$$  

(3)

Note that permutation invariance of DE is beneficial for inductive learning, which fundamentally differs from positional node embeddings such as node2vec [37] or one-hot node identifiers. In the rest of this work, we will show that DE improves the expressive power of GNNs in both theory and practice. In Section 3.2, we use DE as extra node features. We term this model as DEGNN, and theoretically demonstrate its expressive power. In the next subsection, we further use DE-1 to control the aggregation procedure of WLGNN. We term this model as DEAGNN and extend our theory there.

3.2 DEGNN — Distance Encodings as Node Features

DE can be used as extra node features. Specifically, we improve WLGNNS by setting $h^{(0)}_u = A_{uv} \oplus \zeta(v|S)$ where $\oplus$ is the concatenation. We call the obtained model DEGNN. We similarly use DEGNN-$p$ to specify the case when $|S| = p$. For simplicity, we give the following definition.

**Definition 3.2.** DEGNN is called proper if $f_1$, $f_2$, AGGs in the WLGN (Fig. 1(b)), and AGG in Eq. (1), $f_3$ in Eq. (2) are injective mappings as long as the input features are all countable.

We know that a proper DEGNN exists because of the universal approximation theorem of feed-forward networks (to construct $f_i$, $i \in \{1,2,3\}$) and Deep Sets [38] (to construct AGGs).

3.2.1 The Expressive Power of DEGNN

Next, we demonstrate the power of DEGNN to distinguish structural representations. Recall that the fundamental limit of WLGNN is the 1-WL test for structural representation (Theorem 2.7). One important class of graphs that cannot be distinguished by the 1-WL test are regular graphs, although, in practice, node/edge attributes may help diminish such difficulty by breaking the symmetry. In theory, we may consider the most difficult case by assuming that no node/edge attributes are available. In the following, our main theorem shows that even in the most difficult case, DEGNN is able to distinguish two equal-sized node sets that are embedded in almost all $r$-regular graphs. One example where DEGNN using $\zeta_{spd}(\cdot)$ (SPD) is shown in Fig. 1(a): The blue nodes can be easily distinguished from the green or red nodes as SPD=3 may appear between two nodes when a blue node is the node
What’s more, for any $i,j$, the capability of DE indicated by Theorem 3.3 may still help with breaking such regularity. In practice, we do not need to work on each subgraph individually. Mostly, the capability of DE indicated by Theorem 3.3 may still help with breaking such regularity. Actually, the power of structural representations of small node sets can be used to further characterize the power of graph representation. Consider that we directly aggregate all the representations of nodes of a graph output by DEGNN-1 via set-pooling as the entire-graph representation, which is a common
strategy adopted to learn graph representation via WLGNN-1 \cite{14,15,23}. So how about the power of DEGNN-1 to represent graphs? To answer this question, suppose two \( n \)-sized \( r \)-regular graphs \( A^{(1)} \) and \( A^{(2)} \) satisfy the condition in Theorem 3.3. Then, by using a union bound, Theorem 3.3 indicates that for a node \( v \in V \), its representation \( \Gamma((v, A^{(1)})) \) \( \not\in \{(u, A^{(2)})|u \in V\} \) with probability \( 1 - no(n^{-1}) = 1 - o(1) \). Therefore, these two graphs \( A^{(1)} \) and \( A^{(2)} \) can be distinguished via DEGNN-1 with high probability. We formally state this result in the following corollary.

**Corollary 3.4.** Suppose two graphs are uniformly independently sampled from all \( n \)-sized \( r \)-regular graphs over \( V \) where \( 3 \leq r < (2 \log n)^{1/2} \). Then, within \( L \leq \left(\frac{1}{2} + \epsilon\right) \frac{\log n}{\log^2(\epsilon^{-1})} \) layers, DEGNN-1 can distinguish these two graphs with probability \( 1 - o(1) \) by being concatenated with injective set-pooling over all the representations of nodes.

### 3.2.2 The Limitation of DEGNN

Next, we show the limitation of DEGNN. We prove that over a subclass of regular graphs, distance regular graphs (DRG), on which DE-1 is useless for structural representation. We provide the definition of DRG as follows while we refer interested readers to check more properties of DRGs in \cite{35}.

**Definition 3.5.** A *distance regular graph* is a regular graph such that for any two nodes \( v, u \in V \), the number of vertices \( w \) s.t. \( SPD(w, v) = i \) and \( SPD(w, u) = j \), only depends on \( i, j \) and \( SPD(v, u) \).

Shrikhande graph and \( 4 \times 4 \) Rook’s graph are two non-isomorphic DRGs shown in Fig. 2(b) (We temporarily ignore the nodes colors which will be discussed later). For simplicity, we only consider connected DRGs that can be characterized by arrays of integers termed intersection arrays.

**Definition 3.6.** The *intersection array* of a connected DRG with diameter \( \Delta \) is an array of integers \( \{b_0, b_1, \ldots, b_{\Delta - 1}; c_1, c_2, \ldots, c_{\Delta}\} \) such that for any node pair \( (u, v) \in V \times V \) that satisfies \( SPD(v, u) = j \), \( b_j \) is the number of nodes \( w \) that are neighbors of \( v \) and satisfy \( SPD(w, u) = j + 1 \), and \( c_j \) is the number of nodes \( w \) that are neighbors of \( v \) and satisfy \( SPD(w, u) = j - 1 \).

It is not hard to show that the two DRGs in Fig. 2(b) share the same intersection array \( \{6, 3; 1, 2\} \). The following theorem shows that over distance regular graphs, DEGNN-1 must distinguish structures with discriminatory node/edge attributes, which indicates the limitation of DE-1.

**Theorem 3.7.** Given any two nodes \( v, u \in V \), consider two tuples \( T_1 = (v, A^{(1)}) \) and \( T_2 = (u, A^{(2)}) \) with graph structures \( A^{(1)} \) and \( A^{(2)} \) that correspond to two connected DRGs with a same intersection array. Then, DEGNN-1 must use discriminatory node/edge attributes to distinguish \( T_1 \) and \( T_2 \).

Note Theorem 3.7 only works for node representations using DE-1. Therefore, DEGNN-1 may not associate distinguishable node representations in the two DRGs in Fig. 2(b).

However, if we are to learn higher-order structural representations \( (|S| \geq 2) \) with DE-\( p \) \( (p \geq 2) \), DEGNN-\( p \) may have even stronger representation power. We illustrate this point by considering structural representations of two node-pairs that form edges of the two DRGs respectively. Consider two node-pairs that correspond to two edges of these two graphs in Fig. 2(b) respectively. Then, there exists a proper DEGNN-2 via using SPD as DE-2, whose outputs associate these two node-pairs with different representations. Moreover, by simply aggregating the obtained representations of all node-pairs into graph representations via a set-pooling, we may also distinguish these two graphs. Note that distinguishing the node-pairs of the two DRGs is really hard, because even the 2-WL test \footnote{1} will fail to distinguish any edges in the DRGs with a same intersection array and diameters exactly equal to 2. This means that the recently proposed more powerful GNNs, such as RingGNN \footnote{2} and PPGN \footnote{3}, will also fail in this case. However, it is possible to use DEGNN-2 to distinguish those two DRGs.

It is interesting to generalize Theorem 3.3 to DRGs to demonstrate the power of DEGNN-\( p \) \( (p \geq 2) \). However, missing analytic-friendly random models for DRGs makes such generalization challenging.
3.3 DEAGNN — Distance Encoding-1’s as Controllers of the Message Aggregation

DEGNN only uses DEs as initial node features. In this subsection, we further consider leveraging DE-1 between any two nodes to control the aggregation procedure of DEGNN. Specifically, we propose DE-Aggregation-GNN (DEAGNN) to do the following change

\[ \text{AGG}(\{f_2(h_u^{(l)}, A_{vu})\}_{u \in V_u}) \rightarrow \text{AGG}(\{f_2(h_u^{(l)}, A_{vu}), \zeta(u|v)\}_{u \in V}) \]  \hspace{1cm} (4)

Note that the representation power of DEAGNN is at least no worse than DEGNN because the latter one is specialized by aggregating the nodes with \( \zeta_{spd}(u|v) = 1 \), so Theorem 3.3, Corollary 3.4 are still true. Interestingly, its power is also limited by Theorem 3.7. We conclude as the follows.

**Corollary 3.8.** Theorem 3.3, Corollary 3.4 and Theorem 3.7 are still true for DEAGNN.

The general form Eq. (4) that aggregates all nodes in each iteration holds more theoretical significance than practical usage due to scalability concern. In practice, the aggregation procedure of DEAGNN may be trimmed by balancing the tradeoff between complexity and performance. For example, we may choose \( \zeta(u|v) = \zeta_{spd}(u|v) \), and only aggregate the nodes \( u \) such that \( \zeta(u|v) \leq K \), i.e., \( K \)-hop neighbors. Multi-hop aggregation avoids training issues of deep architecture, e.g., gradient degeneration. Particularly, we may prove that \( K \)-hop aggregation decreases the number of layers \( L \) requested to \( \lceil \frac{1}{2} \log \frac{n}{K} \rceil \) in Theorem 3.3, and Corollary 3.4 with proof in Appendix E.

We may also choose \( \zeta(u|v) = \zeta_{gpr}(u|v) \) with non-negative \( \gamma_k \) in Eq. (3) and aggregate the nodes whose \( \zeta(u|v) \) are top-\( K \) ranked among all \( u \in V \). This manner is able to control fix-sized aggregation sets. As DEAGNN does not show provably better representation power than DEGNN, all the above approaches share the same theoretical power and limitations. However, in practice their specific performance may vary across datasets and applications.

4 Related Works

Recently, extensive effort has been taken to improve the structural representation power of WLGNN. From the theoretical perspective, most previous works only considered representations of entire graphs \([25, 27, 30, 43, 44]\) while Srinivasan & Ribeiro initialized the investigation of structural representations of node sets \([45]\) from the view of joint probabilistic distributions. Some works view GNNS as general approximators of invariant functions but the proposed models hold more theoretical implication than practical usage because of their dependence on polynomial \( (n) \)-order tensors \([28, 46, 47]\). Ring-GNN \([29]\) (or equivalently PPGN \([30]\), a relatively scalable model among them, was based on 3-order tensors and was proposed to achieve the expressive power of the 2-WL test (a brief introduction in Appendix G). However, Ring-GNN (PPGN) was proposed for entire-graph representations and cannot leverage the sparsity of the graph structure to be scalable enough to process large graphs \([29, 30]\). DEGNN still benefits from such sparsity and are also used to represent node sets of arbitrary sizes. Moreover, our models theoretically behave orthogonal to Ring-GNN, as DE-2 can distinguish some non-isomorphic node-pairs that Ring-GNN fails to distinguish because the power of Ring-GNN is limited by the 2-WL test (Fig. 2 (b)).

Some works with empirical success inspire the proposal of DE, though we are the first one to derive theoretical characterization and leverage our theory to better those models as a return. SEAL \([9]\) predicts links by reading out the representations of ego-networks of node-pairs. Although SEAL leverages a specific DE-2, the representations of those ego-networks are extracted via complex SortPooling \([23]\). However, we argue against such complex operations as DE-2 yields all the benefit of representations of node-pairs, as demonstrated by our experiments. PGN\(N \) \([10]\) uses SPDs between each node and some anchor nodes to encode distance between nodes. As those encodings are not permutation invariant, PGN\(N \) holds worse inductive/generalization capability than our models.

Quite a few works targeted at revising neighbor aggregation procedure of WLGNN and thus are related to the DEAGNN. However, none of them demystified their connection to DE or provided theoretical characterization. MixHop \([48]\), PAGTN \([51]\), MAT \([17]\) essentially used \( \zeta_{spd}(u|v) \) to change the way of aggregation (Eq. (3)) while GDC \([32]\) and PowerGNN \([49]\) used variants of \( \zeta_{gpr}(u|v) \). MixHop, GDC and PowerGNN are evaluated for node classification while PAGTN and MAT are evaluated for graph classification. GDC claims that the aggregation based on \( \zeta_{gpr}(u|v) \) does not help link prediction. However, we are able to show its empirical success for link prediction, as the key point missed by GDC is using DEs as extra node attributes (Appendix F.2).
5 Experiments

Extensive experiments are conducted to evaluate our DEGNN and DEAGNN over three levels of tasks involving target node sets with sizes 1, 2 and 3 respectively: roles of nodes classification (Task 1), link prediction (Task 2), and triangle prediction (Task 3). Triangle prediction is to predict for any node-pair triad (u, v, w), whether links uv, uw, and vw all exist. This task belongs to the more general class of higher-order network motif prediction tasks and has recently attracted much significance to [52] [56]. We briefly introduce the experimental settings and save the details of the datasets and the model parameters to Appendix F.

Dataset & Training. We use the following six real graphs for the three tasks introduced above: Brazil-Airports (Task 1), Europe-Airports (1), USA-Airports (1), NS (2 & 3), PB (2), C.ele (2 & 3). For Task 1, the goal is to predict the passenger flow level of a given airport based solely on the flight traffic network. These airports datasets are chosen because the labels indicate the structural roles of nodes (4 levels in total from hubs to switches) rather than community identifiers of nodes as traditionally used [20] [21]. For Tasks 2 & 3, the datasets were used by the strongest baseline [9], which consist of existing links/triangles plus the the same number of randomly sampled negative instances from those graphs. The positive test links/triangles are removed from the graphs during the training phase. For all tasks, we use 80%, 10%, 10% dataset splitting for training, validation, testing respectively. All the models are trained until loss converges and the testing performance of the best model on validation set is reported. We also report the experiments without validation sets that follow the original settings of the baselines [5] [9] in Appendix F.5

Baselines. We choose six baselines. GCN [20], GraphSAGE(SAGE) [21], GIN [16] are representative methods of WLGGN. These models use node degrees as initial features when attributes are not available to keep inductive ability. Struc2vec [5] is a kernel-based method, particularly designed for structural representations of single nodes. PGNN [10] and SEAL [9] are also GNN-based methods: PGNN learns node positional embeddings and is not inductive for node classification; SEAL is particularly designed for link prediction by using entire-graph representations of ego-networks of node-pairs. SEAL outperforms other link prediction approaches such as VAE [58]. The node initial features for these two models are set as the inductive setting suggested in their papers. We tune parameters of all baselines (Appendix F.5) and list their optimal performance here.

Instantiation of DEGNN and DEAGNN. We choose GCN as the basic WLGGN and implement three variants of DEGNNs over it. Note that GIN could be a more powerful basis while we tend to keep our models simple. The first two variants of Eq. (2) give us DEGNN-SPD and DEGNN-LP. The former uses SPD-based one-hot vectors ζ_{u|v} as extra nodes attributes, and the latter uses the sequence of landing probabilities Eq. (2). Next, we consider an instantiation of Eq. (4), DEAGNN-SPD that uses SPDs, ζ_{u|v} = ζ_{sdp}(u|v) ≤ K, to control the aggregation, which enables K-hop aggregation (K = 2, 3) and the better performance will be used. DEAGNN-SPD uses SPD-based one-hots vectors as extra nodes attributes. Appendix F.5 provides thorough discussion on implementation of the three variants and another implementation that uses Personalized PageRank scores to control the aggregation. Experiments are repeated 20 times using different seeds and we report the average.

Results are shown in Table 1. Regarding the node-level task, GIN outperforms other WLGGNs, which matches the theory in [16] [25] [28]. Struc2vec is also powerful though it is kernel-based. DEGNNs significantly outperform the baselines (except Eur.-Airport) which imply the power of DE-1’s. Among them, landing probabilities (LP) work slightly better than SPDs as DE-1’s.
Regarding node-pairs-level tasks, SEAL is the strongest baseline, as it is particularly designed for link prediction by using a special DE-2 plus a graph-level readout [23]. However, our DEGNN-SPD performs even significantly better than SEAL: The numbers are close, but the difference is still significant; The decreases of error rates are always greater than 10% and achieve almost 30% over NS. This indicates that DE-2 is the key signal that makes SEAL work while the complex graph-level readout adopted by SEAL is not necessary. Moreover, our set-pooling form of DE-2 (Eq. (1)) decreases the dimension of DE-2 adopted in SEAL, which also better the generalization of our models (See the detailed discussion in Appendix F.3). Moreover, for link prediction, SPD seems to be much better to be chosen as DE-2 than LP.

Regarding node-triads-level tasks, no baselines were particularly designed for this setting. We have not expected that GIN outperforms PGNN as PGNN captures node positional information that seems useful to predict triangles. We guess that the distortion of absolute positional embeddings learnt by PGNN may be the reason that limits its ability to distinguish structures with nodes in close positions: For example, the three nodes in a path of length two are close in position and the three nodes in a triangle are also close in position. However, this is not a problem for DE-3. We also conjecture that the gain based on DEs grows w.r.t. their orders (i.e., \( |S| \) in Eq. (1)). Again, for triangle prediction, SPD seems to be much better to be chosen as DE-3 than LP.

Note that DEAGNN-SPD further improves DEGNN-SPD (by almost 1% across most of the tasks). This demonstrates the power of multi-hop aggregation (Eq. (4)). However, note that DEAGNN-SPD needs to aggregate multi-hop neighbors simultaneously and thus pays an additional cost of scalability.

6 Conclusion and Discussion

This work proposes a novel angle to systematically improve the structural representation power of GNNs. We break from the convention that previous works characterize and further improve the power of GNNs by intimating different-order WL tests [25, 29, 30, 59]. As far as we know, we are the first one to provide non-asymptotic analysis of the expressive power of the proposed GNN models. Therefore, the proof techniques of Theorems 3.3,3.7 may be expected to inspire new theoretical studies of GNNs and further better the practical usage of GNNs. Moreover, our models have good scalability by avoiding using the framework of WL tests, as higher-order WL tests are not able to leverage the sparsity within graph structures. To be evaluated over extremely large graphs [60], our models can be simply trimmed and work on the ego-networks sampled with a limited size around the target node sets, just as the strategy adopted by GraphSAGE [21] and GraphSAINT [61].

Distance encoding unifies the techniques of many GNN models [9, 17, 31, 32, 48] and provides a extremely general framework with clear theoretical characterization. In this paper, we only evaluate four specific instantiations over three levels of tasks. However, there are some other interesting instantiations and applications. For example, we expect a better usage of PageRank scores as edge attributes (Eq. (4)). Currently, our instantiation DEAGNN-PR simply uses those scores as weights in a weighted sum to aggregate node representations. We also have not considered any attention-based mechanism over DEs in aggregation while it seems to be practically useful [17, 22]. Researchers may try these directions in a more principled manner based on this work. Our approaches may also help other tasks based on structural representation learning, such as graph-level classification/regression [14, 16, 23, 25, 30] and subgraph counting [59], which we leave for future study.

There are also two important implications coming from the observations of this work. First, Theorem 5.7 and Corollary 5.8 show the limitation of DE-1 over distance regular graphs, including the cases when DE-1’s are used as node attributes or controllers of message aggregation. As distance regular graphs with the same intersection array have the important co-spectral property [35], we guess that DE-1 is a bridge to connect GNN frameworks to spectral approaches, two fundamental approaches in graph-structured data processing. This point sheds some light on the question left in [29] while more rigorous characterization is still needed. Second, as observed in the experiments, higher-order DE’s induce larger gains as opposed to WLGNN, while Theorem 5.3 is not able to characterize this observation as the probability \( 1 - \alpha(\frac{1}{n}) \) does not depend on the size \( p \). We are sure that the probabilistic quantization in Theorem 5.3 is not tight, so it is interesting to see how such probability depends on \( p \) by deriving tighter bounds.
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Appendix

A Proof of Universal Approximate Theorem for Structural Representation

We restate Theorem 2.6. If the structural representation $\Gamma$ can distinguish any two non-isomorphic tuples $T^{(1)}$ and $T^{(2)}$ in $\Omega_p$, then for any invariant function $f : \Omega_p \rightarrow \mathbb{R}$, $f$ can be universally approximated by $\Gamma$ via 3-layer feed-forward neural network with ReLU as rectifiers, as long as

- The feature space $A$ is compact.
- $f(S, \cdot)$ is continuous over $A$ for any $S \in \mathcal{P}_p(V)$.

**Proof.** This is a direct generalization of Theorem 4 [29]. Specifically, we extend the statement of representing graphs featured by $A$ to that of representing structures featured by $(S, A)$.

Recall the original space $A \subset \mathbb{R}^{n \times n \times k}$. We define a space $A' \subset \mathbb{R}^{n \times n \times (k+1)}$: For any $A' \in A'$, its slice in the first $k$ dimensions of 3-rd mode, i.e., $A'_{:, :, 1:k}$, is in $A$ and the slice corresponds to the last dimension of 3-rd mode, i.e., $A'_{:, :, k+1}$ is a diagonal matrix where the diagonal components could be only 0 or 1. Then, we may build a bijective mapping between $A' \in A'$ and $(S, A) \in \Omega_p$ by

$$A'_{:, :, 1:k} = A, \quad A'_{u, u, k+1} = 1 \text{ if } u \in S \text{ or } 0 \text{ if } u \notin S$$

As $A$ is compact in $\mathbb{R}^{n \times n \times k}$ and we have only finite possible choices of $A'_{:, :, k+1}$, $(\binom{n}{|S|})$, the space $A'$ is compact in $\mathbb{R}^{n \times n \times (k+1)}$.

Then, we may transfer all definitions from $\Omega_p$ to $A'$. Specifically, the structural representation $\Gamma$ that distinguishes any two non-isomorphic tuples $T^{(1)}$ and $T^{(2)}$ in $\Omega_p$ defines $\Gamma' : A' \rightarrow \mathbb{R}^d$ that distinguishes any two non-isomorphic tensors $A^{(1)}$ and $A^{(2)}$ in $A'$, as $T^{(i)}$ and $A^{(i)}$ form a bijective mapping for $i = 1, 2$. Moreover, one invariant function $f : \Omega_p \rightarrow \mathbb{R}$ also defines another invariant function $f' : A' \rightarrow \mathbb{R}$, as $T^{(i)}$ and $A^{(i)}$ form a bijective mapping for $i = 1, 2$.

Suppose the original metric over $A$ is denoted by $\mathcal{M} : A \times A \rightarrow \mathbb{R}_{\geq 0}$. Define a metric defined over $A'$ as

$$\mathcal{M}'(A^{(1)}, A^{(2)}) = \mathcal{M}(A^{(1)}_{:, :, 1:k}, A^{(2)}_{:, :, 1:k}) + \sum_{u \in V} 1_{A^{(1)}_{u, u, k+1} \neq A^{(2)}_{u, u, k+1}}$$

Then, it is easy to show that we have the following lemma based on the definition of continuity.

**Lemma A.1.** If $f(S, \cdot)$ is continuous over $A$ for any $S \in \mathcal{P}_p(V)$ with respect to $\mathcal{M}$, then $f'$ is continuous over $A'$ with respect to $\mathcal{M}'$.

Now, we only need to use Theorem 4 [29] to prove the statement. Actually, the dimensions of $\Gamma'$ overall forms a set of one-dimensional functions $\Xi = \{\Gamma'[i]\}_{i \in [d]}$, where $\Gamma'[i]$ is the $i$th component of $\Gamma' \in \mathbb{R}^d$. According to the definition of $\Gamma'$, we know $\Xi$ distinguishes all the non-isomorphic $A^{(1)}$ and $A^{(2)}$ in $A'$. Moreover, because $A$ is compact and $f'$ is continuous over $A'$, Theorem 4 [29] shows that the arbitrary invariant function $f'$ defined on $A'$ can be universally approximated by $\Xi$ via 3-layer feed-forward neural networks with ReLU as rectifiers. Recall $f$ and $f'$ are bijective, and $\Gamma, \Gamma'$, and $\Xi$ are mutually bijective. Therefore, we claim that $f$ can be universally approximated $\Gamma$ via 3-layer feed-forward neural networks with ReLu as rectifiers.

B Proof for The Power of WLGGN for Structural Representation

We restate Theorem 2.7. Consider two tuples $T_1 = (S^{(1)}, A^{(1)})$ and $T_2 = (S^{(2)}, A^{(2)})$ in $\Omega_p$. If $T_1, T_2$ cannot be distinguished by the 1-WL test, then the corresponding outputs of WLGGN satisfy $\Gamma(T_1) = \Gamma(T_2)$. On the other side, if they can be distinguished by the 1-WL test and suppose aggregation operations (AGG) and feed-forward neural networks $f_1, f_2$ are all injective mappings, then a large enough number of layers $L$, the outputs of WLGGN satisfy $\Gamma(T_1) \neq \Gamma(T_2)$. 

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We restate Theorem 3.3: Given two fixed-sized sets $S^{(1)}, S^{(2)} \subset V$, $|S^{(1)}| = |S^{(2)}| = p$. Consider two tuples $T^{(1)} = (S^{(1)}, A^{(1)})$ and $T^{(2)} = (S^{(2)}, A^{(2)})$ in the most difficult setting when features $A^{(1)}$ and $A^{(2)}$ are uniformly independently sampled from all $r$-regular graphs over $V$ where $3 \leq r < (2\log n)^{1/2}$. Then, for some constant $\epsilon > 0$, there exists a proper DEGNN with layers $L < (\frac{1}{2} + \epsilon) \frac{\log n}{\log(r-1)}$, using DE-$p$ $\zeta(u|S^{(1)})$, $\zeta(u|S^{(2)})$ for all $u \in V$ such that with probability $1 - o(n^{-1})$, its outputs $\Gamma(T^{(1)}) \neq \Gamma(T^{(2)})$. Specifically, $f_3$ can be simply chosen as SPD, i.e., $\zeta(u|v) = \zeta_{spd}(u|v)$. The big-O notation is with respect to $n$.

Proof. To prove the statement, we only need to prove the case that $|S^{(1)}| = |S^{(2)}| = 1$, $\zeta(u|v) = \zeta_{spd}(u|v)$ because of the following lemma.

Lemma C.1. Suppose the statement is true when $|S^{(1)}| = |S^{(2)}| = 1$, $\zeta(u|v) = \zeta_{spd}(u|v)$. Then, the statement is also true for the case when $|S^{(1)}| = |S^{(2)}| = p > 1$ for some fixed $p$, and $\zeta(u|v)$ is a neural network fed with the list of landing probabilities.

Proof. We first focus on the case when DE is chosen as SPD, i.e., $\zeta(u|v) = \zeta_{spd}(u|v)$. Suppose $|S^{(1)}| = |S^{(2)}| > 1$. We choose an arbitrary node from $S^{(1)}$, say $w_1$. As we assume the statement is true for the single node case, for any node in $S^{(2)}$, say $w_2$, DEGNN with DEs $\zeta_{spd}(u|w_1)$, $\zeta_{spd}(u|w_2)$ is able to distinguish two tuples $(w_1, A^{(1)})$ and $(w_2, A^{(2)})$, with probability at least $1 - o(n^{-1})$. Given that the space of SPD is countable and AGG in Eq. 1 is injective, $\zeta_{spd}(u|S^{(1)})$ and $\zeta_{spd}(u|S^{(2)})$ are different if $\zeta_{spd}(u|w_1)$ and $\zeta_{spd}(u|w_2)$ are different. Therefore, DEGNN with DEs $\zeta_{spd}(u|S^{(1)})$, $\zeta_{spd}(u|S^{(2)})$ is also able to distinguish two tuples $(w_1, A^{(1)})$ and $(w_2, A^{(2)})$, with probability at least $1 - o(n^{-1})$. Based on the union bound, we know that DEGNN with DEs $\zeta_{spd}(u|S^{(1)})$, $\zeta_{spd}(u|S^{(2)})$ is able to distinguish two tuples $(w_1, A^{(1)})$ and $(v, A^{(2)})$ for any $v \in S^{(2)}$, with probability at least $1 - |S^{(2)}|o(n^{-1}) = 1 - o(n^{-1})$. Therefore, we prove the capability to generalize the result from the single node case to the multiple node cases.

Now, let us generalize the result from $\zeta_{spd}(u|v)$ to arbitrary $\zeta(u|v)$ represented by neural networks fed with the list of landing probabilities. As $\zeta_{spd}(u|v)$ is indeed a function of the list of landing probabilities (Eq. 2), the general $\zeta(u|v)$ should have stronger discriminative power unless neural networks cannot provide a good mapping from the list of landing probabilities to SPD. However, we do not have to worry this because the list of landing probabilities fortunately lies a countable space for unweighted graphs: 1) The dimension of this list is countable (finite in practice); 2) Each component of this list is always a rational number if the graph is unweighted. According to our assumption, $f_3$ is allowed to have an injective mapping over the list of landing probabilities. Therefore, neural networks on the list of landing probabilities will not decrease the representation power based on $\zeta_{spd}(u|v)$.

Outline: From now on, we focus on the single node case, i.e., $|S^{(1)}| = |S^{(2)}| = 1$, with SPD as $f_3$, i.e., $\zeta(u|v) = \zeta_{spd}(u|v)$. Without loss of generality, we suppose $S^{(1)} = S^{(2)} = \{u\}$. As SPD is countable, there exists a proper DEGNN that guarantees that all the operations are injective, which follows the basic condition used in [16]. Because of the iterative procedure of DEGNN and all mappings are injection, the label of node $u$ only depends on the subtree with depth $L$ rooted at $u$ (See the illustration of the subtree rooted at a given node in Fig. 3). Therefore, we only need to show that $A^{(1)}$ and $A^{(2)}$, which are uniformly sampled $r$-regular graphs, with probability at most $o(n^{-1})$, have the same subtrees rooted at $u$ given SPDs as initial node labels. To show this, our proof contains four steps. Note that all through the following proof, we assume that $n$ is very large and $\epsilon$ is a small positive constant that depends on $n$.
we first explain that we are able work on the configuration model of r-regular graphs proposed in [62] which associates uniform measure over all r-regular graphs. Given the condition r < (2 \log n)^{1/2}, there are a large portion (\Omega(n^{-1/2})) of all the graphs generated by this model are simple (without self-loops and multi-edges) r-regular graphs. Since the configuration model alleviates the difficulty to analyze dependence of edges in r-regular graphs, we consider the graphs generated by the configuration model for the next two steps.

Suppose the set of nodes that are associated with SPD= k from u is denoted by Q_k, and the number of edges that connect the nodes in Q_k and those in Q_{k+1} is denoted by p_k. We prove that with probability 1 - o(n^{-2}), for all k \in (\frac{\log n}{\log(r-1)} + 1, (\frac{2}{3} - \epsilon) \frac{\log n}{\log(r-1)}), |Q_k| \geq (r - 1 - \epsilon)^{k-1} and p_k \geq (r - 1 - \epsilon)|Q_k| based on the configuration model.

Next, we define the edge configuration between Q_k and Q_{k+1} as a list C_k = (a_{1,k}, a_{2,k}, \ldots) where a_{i,k} means the number of nodes in Q_{k+1} of which each has exactly i edges from Q_k. We prove that for each k \in (\frac{\log n}{\log(r-1-\epsilon)}, \frac{1}{2} \frac{\log n}{\log(r-1-\epsilon)}), as the edges between Q_k and Q_{k+1} are so many, there are too much randomness that makes each type of edge configuration C_k appear with only limited probability \mathbb{P}(C_k) = O(\frac{n^{1/2}}{p^k}). Then, given any \epsilon \frac{\log n}{\log(r-1-\epsilon)} many k’s, the probability that A^{(1)} and A^{(2)} have all the same edge configurations for these k’s is bounded by \Pi_k \mathbb{P}(C_k) \sim o(n^{-2}). Therefore, we only need to consider edge configurations for k \in (\frac{1}{2} \frac{\log n}{\log(r-1-\epsilon)}, (\frac{2}{3} + \epsilon) \frac{\log n}{\log(r-1-\epsilon)}) to distinguish A^{(1)} and A^{(2)}.

Since there are at least \Omega(n^{-1/2}) of all the graphs generated by the configuration model that are simple r-regular graphs, and there are at most o(n^{-2}) probability that A^{(1)} and A^{(2)}
We start from the set \( W \), an edge who two end-nodes are in \( Q_k \). Now, we go back to prove the bound for \( |Q_k| \).

Step 1: We first introduce the configuration model proposed in [62] for \( r \)-regular graphs of \( n \) nodes. Suppose we have \( n \) sets of items, \( W_u, u \in [n] \), where each set corresponds to one node in \([n]\). Each set \( W_u \) has \( r \) items. Now, we randomly partition all these \( nr \) items into \( \frac{nr}{2} \) pairs. Then, each partitioning result corresponds to a \( r \)-regular graph: if a pair contains items from \( W_u \) and \( W_v \), then there is an edge between nodes \( u \) and \( v \) in the graph. Note that such partitioning results may render self-loops and multi-edges. Of course, we would like to consider only simple graphs which do not have self-loops and multi-edges. For this, the theory in [62] shows that for all these \( r \)-regular graphs, if \( r < (2 \log n)^{1/2} \), there are about \( \exp(-n^{3/4}) \) portion among them, i.e., \( \Omega(n^{-1/2}) \), which are simple graphs.

Step 2: Now, we consider a graph that is uniformly sampled from the configuration model. Suppose the set of nodes that are associated with SPD = \( k \) from \( u \) is denoted by \( Q_k \), and the number of edges that connect the nodes in \( Q_k \) and those in \( Q_{k+1} \) is denoted by \( p_k \). Now, we prove that there exists a small \( \epsilon > 0 \), such that with probability \( 1 - o(n^{-2\epsilon}) \), for all \( k \in (\frac{\log n}{\log(r-1)} - 1, (\frac{\log n}{\log(r-1)}) \), \( |Q_k| \geq (r-1-\epsilon)^k - 1 \) and \( p_k \geq (r-1-\epsilon)|Q_k| \). We prove an even stronger lemma that gives the previous argument via a union bound and doing induction over all \( k \in (\frac{\log n}{\log(r-1)} - 1, (\frac{\log n}{\log(r-1)}) \).

Lemma C.2. There exists a small constant \( \epsilon > 0 \), with probability \( 1 - O(n^{-2\epsilon}) \), such that: 1) For any \( k < (\frac{2}{3} - \epsilon) \frac{\log n}{\log(r-1)} \), if \( |Q_k| \geq n^{\epsilon/5} \), \( |Q_{k+1}| \geq p_k \geq |Q_k|^{1/2} \) and \( p_k \geq (r-1)|Q_k| - |Q_k|^{1/2} \); 2) When \( k = \lceil \frac{\log n}{\log(r-1)} \rceil + 1 \), \( |Q_k| \geq (r-1)^{k-1} = n^{\epsilon/5} \).

Proof. We consider the following procedure to generate the graph based on the configuration model. We start from the set \( W_u \) and generate the \( r \) pairs with at least one item in \( W_u \). Then, we have all the nodes in \( Q_1 \). Based on the set \( \cup v \in Q_1 W_v \), we generate all the \((r-1)|Q_1|\) pairs with at least one item in \( \cup v \in Q_1 W_v \), and we have all the nodes in \( Q_2 \). The procedure goes on so on and so forth.

Now, we prove 1). First, we prepare some inequalities. We have \( |Q_k| \leq (r-1)^{k-1} < n^{2/3-\epsilon} \). For \( i \geq \lceil |Q_k|^{1/2} \rceil \), we have

\[
\frac{|Q_k| \cdot (r-1)|Q_k|}{n \cdot i} \leq n^{-\epsilon}
\]

Moreover, Recall \( |Q_k| < n^{2/3-\epsilon} \). As \( |Q_k| \geq n^{\epsilon/5} \), then

\[
\frac{(\epsilon(r-1)|Q_k|^{3/2})^{\lceil |Q_k|^{1/2} \rceil}}{n} = O(n^{-2+\epsilon}).
\]

This inequality is very crude.

Now, we go back to prove the bound for \( p_k \). Recall the definition of \( p_k \) that is the number of edges between \( Q_k \) and \( Q_{k+1} \). Then, the number of edges that are generated with both end-nodes are in \( Q_k \) is \((r-1)|Q_k| - p_k \). As we suppose the edges are generated sequentially, the probability to generate an edge who two end-nodes are in \( Q_k \) is upper bounded by \( \frac{(r-1)|Q_k|}{n - \sum_{j=0}^{\lceil |Q_k|^{1/2} \rceil} (r-1)|Q_k|} < \frac{|Q_k|}{n} \) where we use \( \sum_{j=0}^{\lceil |Q_k|^{1/2} \rceil} (r-1)|Q_k| = O(n^{2/3}) \). Then, the probability that \((r-1)|Q_k| - p_k > |Q_k|^{1/2} \) is upper bounded by

\[
\sum_{i=\lceil |Q_k|^{1/2} \rceil}^{(r-1)|Q_k|} \left[ \frac{|Q_k|}{n} \right]^i \left( \frac{(r-1)|Q_k|}{n} \right) \left[ \frac{|Q_k|^{1/2}}{|Q_k|^{1/2}} \right] \sum_{i=0}^{\lceil |Q_k|^{1/2} \rceil} n^{-i} - \frac{c_1 |Q_k|^{1/2}}{|Q_k|^{1/2}} \left( \frac{(r-1)|Q_k|}{|Q_k|^{1/2}} \right) \left( \frac{|Q_k|^{1/2}}{|Q_k|^{1/2}} \right) O(n^{-2+\epsilon})
\]

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where \( c_1, c_2 \) are constants, the numbers above the equality/inequality signs refer to which equations are used.

Next, we prove the bound for \( |Q_{k+1}| \geq p_k - |Q_k|^{1/2} \). Again, if the edges are generated sequentially, \( p_k - Q_{k+1} \) indicates the number of edges whose end-nodes in \( Q_{k+1} \) also belong to other edges that has been generated between \( Q_k \) and \( Q_{k+1} \). The probability of this edge is upper bounded by

\[
\frac{(r-1)|Q_k|}{n} \left( \frac{(r-1)|Q_k|}{n} \right)^i = O(n^{-2+c})
\]

Till now, we have proved the statement 1).

Now, we prove the statement 2). Actually, at the time when \( Q_k \) is generated, the number of edges having been generated is at most \( r(r - 1)^k - 2 \). These edges cover at most \( r(r - 1)^k - 1 \) nodes. When \( k = \left[ \frac{\log n}{\log(r-1)} \right] + 1 \), we claim that with probability \( 1 - O(n^{-2+c}) \), at most 1 edge among these edges when generated is not connected to a new node. This is because if there are more than 1 edges, the probability is at most

\[
\sum_{i=2}^{r(r-1)^k} \left[ \frac{r(r-1)^k}{n} \right]^i \left( \frac{r(r-1)^k}{n} \right)^i \leq c_3 \left( \frac{r^2 n^c/5}{n} \right)^2 = O(n^{-2+c})
\]

We use this result to give a lower bound of \( |Q_k| \) for \( k = \left[ \frac{\log n}{\log(r-1)} \right] + 1 \). Because there is at most 1 edge when generated do not connect to a new node. The worst case appears when two items in \( W_k \) are mutually connected, which leads to \( |Q_1| \geq r - 2 \geq 1 \). All edges after \( Q_1 \) are generated are connected to new nodes and furthermore \( |Q_k| \geq (r - 1)^k - 1 \geq n^{\epsilon/5} \).

**Step 3**: We start to consider the edge configuration between \( Q_k \) and \( Q_{k+1} \) for \( k \in (\frac{1}{2} \frac{\log n}{\log(r-1)}, \frac{4}{7} \frac{\log n}{\log(r-1)-c}) \). We focus our attention on the graphs that satisfy the properties developed in Step 2, which, as demonstrated in Step 2, are with high probability \( 1 - o(n^{-3/2}) \). For those graphs, we know that for \( k \in (\frac{1}{2} \frac{\log n}{\log(r-1)-c}, \frac{4}{7} \frac{\log n}{\log(r-1)-c}) \), \( p_k \geq (r - 1 - \epsilon)|Q_k| \geq (r - 1 - \epsilon)^k \geq n^{\epsilon/2} \) and \( p_k \leq r(r - 1)^k < n^{2\epsilon/3 - \epsilon} \). Moreover, \( \sum_{i=1}^{k} |Q_i| \leq (r - 1)|Q_k| = o(n) \) and therefore at the time when \( Q_k \) is generated, there are still \( q_k = n - o(n) = \Theta(n) \) nodes that have not been connected.

Recall that we define the edge configuration between \( Q_k \) and \( Q_{k+1} \) is a list \( C_k = (a_{i,k}, a_{2,k}, \ldots) \) where \( a_{i,k} \) means the number of nodes in \( Q_{k+1} \) of which each has exactly \( i \) edges from \( Q_k \). According to the definition of \( C_k \), it satisfies

\[
\sum_{i=1}^{r} i \times a_{i,k} = p_k \tag{7}
\]

Note that if DEGNN cannot distinguish \( u, A^{(1)} \) and \( u, A^{(2)} \), then \( A^{(1)} \) and \( A^{(2)} \) must share the same edge configuration between \( Q_k \) and \( Q_{k+1} \). Otherwise, after one iteration, the intermediate representation of nodes in \( Q_{k+1} \) are different between \( A^{(1)} \) and \( A^{(2)} \). Such difference will be propagated to \( u \) later. To bound the probability that \( A^{(1)} \) and \( A^{(2)} \) must share the same edge configuration between \( Q_k \) and \( Q_{k+1} \), for simplicity, we consider the probability of \( C_k \) given the number of edges between \( Q_k \) and \( Q_{k+1} \), i.e., \( p_k \) and the number remaining nodes, i.e., \( q_k = |n|/\cup_{i=1}^{k} q_i = \Theta(n) \). We are to derive a upper bound of \( P(C_k) \) based on the configuration model in the following lemma.

**Lemma C.3**: Suppose \( p_k \in [n^{1/2}, n^{2/3-\epsilon}] \) and \( q_k = \Theta(n) \). Consider the configuration model to generate edges: there are \( p_k \) edges that correspond to two items that are one in \( \cup_{i \in Q_k} W_i \) and one among the rest \( q_k r \) items. Then, for any possible edge configuration \( C_k \) obtained based on this generating procedure, \( P(C_k) \leq c_5 q_k^{1/2}/p_k \) for some constant \( c_5 \).
Proof. First, for the configuration $C_k = (a_1,k, a_2,k, ...)$, we claim that the most probable $C_k$ is achieved when $a_{i,k} = 0$ for $i \geq 3$. We prove this statement via the adjustment method: We fix the value of $a_{1,k} + i a_{i,k}$ and all the other $a_{i',k}$’s. We compare the probability of $(a_{1,k} = x, a_{i,k} = y)$ and that of $(a_{1,k} = x + i, a_{i,k} = y - 1)$. Because $x, y \leq p_k = O(n^{2/3-r})$, for some constant $c_6$, we have

$$
\frac{\mathbb{P}(a_{1,k} = x, a_{i,k} = y)}{\mathbb{P}(a_{1,k} = x + i, a_{i,k} = y - 1)} = \frac{(q_k x)^r (q_k x + y)^y}{(q_k x + i)^{x+i} (q_k x - y + 1)^{y-1}} \leq c_6 \frac{x^i}{q_k} \leq c_6 \frac{x^3}{q_k} < 1.
$$

Therefore, we only need to consider the case when $a_{1,k}, a_{2,k} > 0$ so $a_{1,k} + 2a_{2,k} = p_k$. Define a function $g(x)$ to denote the probability of the edge configuration $(a_{1,k} = p_k - 2y, a_{2,k} = y)$. We compare $g(y)$ and $g(y + 1)$

$$
g(y + 1) = \frac{(p_k - 2y)^y}{y^{y+1}} = 2r \frac{(y + 1)(q_k - p_k + y + 1)}{(p_k - 2y)(p_k - 2y - 1)}.
$$

Consider the choice $y = y^*$ to make $g(y^*)/g(y^* + 1) \geq 1$ while $g(y^* - 1)/g(y^*) \leq 1$ that corresponds to $g(y^*) = \max_y g(y)$. Then, we must have $y^* = o(p_k)$ and otherwise $g(y^* - 1)/g(y^*) > 1$. As $y^* = o(p_k)$ and $p_k = O(n)$, $y^*$ according to Eq. 8 is about $\frac{(r-1)p_k}{2r}$. We define $y_0 = \frac{(r-1)p_k}{2r}$. Consider $y_0 + \delta$ where $\delta = o(y_0)$. Then, using $p_k = O(n^{2/3-r})$ and hence $\frac{\log p_k}{q_k} = o(1) = o(\delta)$, we have

$$
\frac{g(y_0 + \delta)}{g(y_0 + \delta + 1)} = 1 + \frac{\delta}{y_0} + o\left(\frac{\delta}{y_0}\right).
$$

Moreover, for $\delta > 0$

$$
g(y_0) = \prod_{j=0}^{c_0} \left(1 + \frac{j}{y_0} + o\left(\frac{j}{y_0}\right)\right) \leq 1 + \frac{\delta}{y_0} + o\left(\frac{\delta}{y_0}\right).
$$

Choose $\delta = y_0^{1/2}$, then

$$
g(y_0 + y_0^{1/2}), g(y_0 - y_0^{1/2}) \geq \left(\frac{2}{3} + o(1)\right)g(y_0).
$$

As $\sum_{j=-y_0^{1/2}}^{y_0^{1/2}} g(j) \leq 1$ and $y^*$ should be in $[y_0 - y_0^{1/2}, y_0 + y_0^{1/2}]$, we obtain

$$
g(y^*) \leq \frac{3}{4y_0^{1/2}} = c_5 \frac{q_k^{1/2}}{p_k},
$$

which concludes the proof.

Now, we go back to consider any $c \frac{\log n}{\log(r-1-\epsilon)}$ many $k$’s in $(\frac{1}{2} \log\frac{n}{\log(r-1-\epsilon)}, \frac{2}{3} \log\frac{n}{\log(r-1-\epsilon)})$. Based on Lemma C.3, the probability that $A^{(1)}$ and $A^{(2)}$ share the same edge configurations between $Q_k$ and $Q_{k+1}$ for all these $k$’s is bounded by

$$
\prod_{k = c_7}^{c_7+\epsilon \frac{\log n}{\log(r-1-\epsilon)}} \mathbb{P}(C_k) \leq \prod_{k = c_7}^{c_7+\epsilon \frac{\log n}{\log(r-1-\epsilon)}} c_5 \frac{q_k^{1/2}}{p_k} < n^{r \log c_6} \frac{n^{c_{7} \frac{\log n}{\log(r-1-\epsilon)}}}{n^{(c_{7} \frac{\log n}{\log(r-1-\epsilon)})}} = o(n^{-3/2}).
$$

**Step 4:** From step 2, we know that the graphs that do not satisfy $|Q_k| \geq (r - 1 - \epsilon)k^{k-1}$ and $p_k \geq (r - 1 - \epsilon)|Q_k|$ for $k \in (\frac{2}{3} \log\frac{n}{\log(r-1-\epsilon)}, 1, \frac{2}{3} - \epsilon)\log\frac{n}{\log(r-1-\epsilon)}$ are only $o(n^{-3/2})$ portion of all
graphs generated from the configuration model. From step 3, we know that $A^{(1)}$ and $A^{(2)}$ that satisfy the properties of step 2, with probability at most $o(n^{-3/2})$, their subtrees rooted at node $u$ are the same even with DE-1’s. Even if all these graphs belong to simple regular graphs, as step 1 tells the portion of simple regular graphs among the graphs generated from the configuration model is $\Omega(n^{-1/2})$, we arrive at the final conclusion that if $A^{(1)}$ and $A^{(2)}$ are sampled from all simple $r$-regular graphs, with probability at least $1 - o(n^{-3/2})/\Omega(n^{-1/2}) = 1 - o(n^{-1})$, a proper DEGNN can distinguish $(u, A^{(1)})$ and $(u, A^{(2)})$. □

Theorem [3.3] focuses on node sets embedded in regular graphs. A natural question therefore arises: how about the power of DEs to distinguish non-isomorphic node sets embedded in irregular graphs that the 1-WL test (also WLGNN) may not distinguish. A full investigation of this question is out of the scope of this work. However, there is some important connection between irregular graphs and regular graphs under the umbrella of the 1-WL test. Actually, the partition of nodes over irregular graphs according to their representations (colors) stably associated by the 1-WL test has equitable property [39].

Basiclly, suppose that the whole node set $V$ can be partitioned into several parts based on the representations (colors) of nodes, $V = \bigcup_{i=1}^{n} V_i$, where for an arbitrary $i$, nodes in $V_i$ share the same representations based on the 1-WL test. Then, the induced subgraph of the nodes in $V_i$ is a regular graph for all $i$’s. What’s more, for any $i,j$, the number of nodes in $V_i$ that are neighbors of a certain node in $V_i$ is shared by all the nodes in $V_i$, which again shows certain regularity. In some sense, the capability of DE indicated by Theorem 3.3 may still help with breaking such regularity.

D Proof for The Limitation of DE-1 — Theorem 3.7

We restate Theorem 3.7: Consider any two nodes $v, u$ with DE-1 corresponding to SPD $(\Delta_0, c_0, \ldots, c_\Delta)$; $\Delta_0$ is the number of nodes $w$ that are neighbors of $v$ and satisfy $\text{SPD}(w, u) = j + 1$, and $c_j$ is the number of nodes $w$ that are neighbors of $v$ and satisfy $\text{SPD}(w, u) = j - 1$.

We recall the definition of the intersection array of a connected DRG as the following.

**Definition D.1.** The intersection array of a connected DRG with diameter $\Delta$ is an array of integers $\{b_0, b_1, \ldots, b_{\Delta-1}; c_1, c_2, \ldots, c_{\Delta}\}$ such that for any node pair $(u, v) \in V \times V$ that satisfies $\text{SPD}(v, u) = j$, $b_j$ is the number of nodes $w$ that are neighbors of $v$ and satisfy $\text{SPD}(w, u) = j + 1$, and $c_j$ is the number of nodes $w$ that are neighbors of $v$ and satisfy $\text{SPD}(w, u) = j - 1$.

The definition of DRG implies the following lemma.

**Lemma D.2.** Suppose each node is associated with SPD as DE-1. Consider a graph with the intersection array $\{b_0, b_1, \ldots, b_{\Delta-1}; c_1, c_2, \ldots, c_{\Delta}\}$. For an arbitrary node $u$, any node $v$ in the subtree rooted at $u$, with $\text{SPD}(v, u) = j$, has children including $b_j$ nodes $w$ with DE-1 corresponding to $\text{SPD}(w, u) = j + 1$, $c_j$ nodes with DE-1 corresponding to $\text{SPD}(w, u) = j - 1$, and $b_0 - b_j - c_j$ nodes $w$ with DE-1 corresponding to $\text{SPD}(w, u) = j + 1$.

**Proof.** A DRG with the intersection array $\{b_0, b_1, \ldots, b_{\Delta-1}; c_1, c_2, \ldots, c_{\Delta}\}$ is a $b_0$-regular graph and thus $v$ has $b_0$ neighbors. All the neighbors of $v$ become children of $v$ in the subtree. As $\text{SPD}(v, u) = j$, we know that SPDs from the neighbors of $v$ to $u$ are in $\{j - 1, j, j + 1\}$. According to the definition of intersection array, we know the numbers of neighbors of $v$ with different SPDs, $j - 1, j, j + 1$, exactly are $c_j, b_0 - b_j - c_j, b_j$ respectively. □

We start from any node $u$ and construct the subtree rooted at $u$. By using the Lemma [D.2], it is obvious that subtrees for any nodes from DRGs with a same intersection array are all the same even if all the nodes use SPD as DE-1. An illustrative example of this result is shown in Fig. A.
An interesting case in practice is to set the DE-1 in Eq. (4) as SPD. Actually, Lemma D.3 is closely related the argument in [63], which claims the same result for walks over one DRG. However, Lemma D.3 extends the argument to any DRGs with the same intersection array, the configuration of colors (DE-1) of children only depends on the color (DE-1) of their father node.

The next step is to generalize SPD as DE-1 to the list of landing probability as DE-1. Actually, the following lemma indicates that in DRGs, SPD and the list of landing probability are bijective.

**Lemma D.3.** In any connected DRG with the same intersection array, the number of walks of given length between nodes depends only on the SPD between these vertices.

**Proof.** Given any node \( u \in V \) over the DRG with the intersection array \( \mathcal{L} = \{b_0, b_1, \ldots, b_\Delta, c_1, c_2, \ldots, c_\Delta\} \), denote the number of walks of length \( l \) from \( u \) to another node \( v \) is \( f(v, l) \). We need to prove that \( f(v, l) \) can be written as a function \( g(\text{SPD}(u, v), l, \mathcal{L}) \). We prove this result via induction over the length of walks denoted by \( l \). The statement is trivial for \( l = 1 \). Suppose the statement is true for \( l = l_0 - 1 \), we consider the case \( l = l_0 \).

Because of the definition of walks, there is recurrence relation

\[
f(u, v, l_0) = \sum_{w \in \mathcal{N}_v} f(u, w, l_0 - 1)
\]

\[
= \sum_{w : \text{SPD}(w, u) = \text{SPD}(v, u) - 1} f(u, w, l_0 - 1) + \sum_{w : \text{SPD}(w, u) = \text{SPD}(v, u) + 1} f(u, w, l_0 - 1)
\]

Because the assumption of induction, we have

\[
f(u, v, l_0) = c_{\text{SPD}(v, u)} g(\text{SPD}(v, u) - 1, l_0 - 1, \mathcal{L}) + b_{\text{SPD}(v, u)} g(\text{SPD}(v, u) + 1, l_0 - 1, \mathcal{L})
\]

which only depends on \( \text{SPD}(v, u), l_0 \) and \( \mathcal{L} \) and thus can be written as \( g(\text{SPD}(u, v), l_0, \mathcal{L}) \). \( \square \)

Actually, Lemma D.3 is closely related the argument in [63], which claims the same result for walks over one DRG. However, Lemma D.3 extends the argument to any DRGs with the same intersection array. As DRGs are \( b_0 \)-regular graphs, there is a bijective mapping between the list of landing probabilities and the list of walks of different length. Therefore, this is a bijective mapping between SPD and the list of landing probabilities, which concludes the proof. \( \square \)

### E Proof for DEAGNN — Corollary 3.8 and Further Discussion

DEAGNN contains a general aggregation procedure assisted by DE-1 (Eq. (4)). As we discussed in Section 3.3 as DEAGNN allows to use DEs as extra node features as DEGNN in the same time, it has at least the same representation power as DEGNN. Therefore, Theorem 3.3 and Corollary 3.4 are still true for DEAGNN. So our first question is whether DEAGNN shares the same limitation with DEGNN with DE-1 for node representation learning over DRGs.

An interesting case in practice is to set the DE-1 in Eq. (4) as SPD \( \zeta(u|v) = \zeta_{\text{spd}}(u|v) \). For some \( K \geq 1 \), we specify the aggregation as

\[
\text{AGG}(\{f_2(h_u^{(l)}, \mathbf{A}_{uv})\}_{u \in \mathcal{N}_v}) \rightarrow \text{AGG}(\{(f_2(h_u^{(l)}, \mathbf{A}_{uv}), \zeta_{\text{spd}}(u|v))\}_{\zeta_{\text{spd}}(u|v) \leq K}), \tag{9}
\]
We choose SPD as DE-1. Both models require at least two layers to distinguish two black nodes. DEAGNN-1 cannot decrease the number of layers by a factor of 2.

which means that the aggregation happens among K-hop neighbors. If the model is to learn the representation of a node subset with size p, We term this model as DEAGNN-p-K-hop. The second question is to investigate whether DEAGNN-p-K-hop may decrease the number of layers of DEGNN required in Theorem 3.3 and Corollary 3.4 by a factor of K. This result is not trivial. For example, Fig. 5 shows two trees whose root nodes are the target nodes to learn structural representation. Obviously, DEGNN-1 needs two layers to distinguish these two root nodes. However, DEAGNN-1-K-hop may not decrease the number of layers by a factor of 2 and thus still needs two layers. This is because the set aggregation in Eq. (9) may decrease the discriminatory power of those features interacted with graph structures. Next, we will prove the confirmation to these two questions.

**Confirmation to the first question.** We formally restate the conclusion to prove: Consider any two nodes \( w_1, w_2 \in V \). Consider two tuples \( T_1 = (w_1, A^{(1)}) \) and \( T_2 = (w_2, A^{(2)}) \) with graph topologies \( A^{(1)} \) and \( A^{(2)} \) that correspond to two connected DRGs with a same intersection array. Then, DEAGNN-1 must depend on discriminatory node/edge attributes to distinguish \( T_1 \) and \( T_2 \).

**Proof.** Because Lemma D.3 implies that in all DRGs with the same intersection array, there is a bijective mapping between SPD and the list of landing probabilities. Therefore, we only need to focus on the case that uses SPDs as DE-1, which both appears as extra node attributes and features in aggregation (see Eq. 4). As the statement is about the limitation, we consider the most expressive case, i.e., the aggregation appearing among every pair of nodes.

Recall the tree structure to compute DAGNN is termed as the subtree rooted at some node. Now, we call the tree structure to compute DEAGNN for the structural representation of a node \( w \) as the extended subtree rooted at \( w \), which has the same utility as the tree structure for DEGNN (Fig. 3). Suppose we are to learn the structural representation of \( w \). We are going to prove by induction that with arbitrary number of layers, if no discriminatory node/edge attributes are available, any node \( v \) will be associated with an representation vector that only depends on SPD(\( v \)) and the intersection array of the graph. If this is true, then we know that any nodes in DRGs with a same intersection array will have the same representation output by DEAGNN with an arbitrary number of layers.

Recall that the number of layers is \( L \). Obviously, when \( L = 0 \), the node representations only depend on SPD(\( v \)) and thus satisfy the statement. Suppose the statement is true when \( L = L_0 - 1 \), consider the case when \( L = L_0 \). Denote the representation of a node \( v \) after \( L_0 - 1 \) layers as \( h^{(L_0-1)}_v \). Then, its representation after \( L_0 \) layers is

\[
h^{(L_0)}_v = f_1(h^{(L_0-1)}_v, \text{AGG} \{ (f_2(h^{(L_0-1)}_u, \zeta_{spd}(u | v)) \}_{u \in V}) \).
\]

Note that we omit the edge attributes \( A_{uv} \) due to the requirement of the statement. Consider another node \( v' \) who satisfies SPD\( (v' | w) = \text{SPD}(v | w) \). For this, we only need to prove that the following two components are the same and thus \( h^{(L_0)}_v = h^{(L_0)}_{v'} \):

\[
h^{(L_0-1)}_v = h^{(L_0-1)}_{v'},
\]

\[
\{ (h^{(L_0-1)}_u, \zeta_{spd}(u | v)) \}_{u \in V} = \{ (h^{(L_0-1)}_u, \zeta_{spd}(u | v')) \}_{u \in V}.
\]

The Eq. (11) is directly due to the assumption of induction. To prove Eq. (10), we first partition all nodes in \( V \) according to \( \zeta_{spd}(u | v), \zeta_{spd}(u | v') \) by defining \( S_v(\alpha) = \{ u \in V | \zeta_{spd}(u | v) = \alpha \} \)
and $S_w(a) = \{ u \in V : \zeta_{spd}(u|v') = a \}$. We further partition these two sets according to $\zeta_{spd}(u|w), \zeta_{spd}(u|w')$ by defining $S_u(a, b) = \{ u \in S_u(a) \mid \zeta_{spd}(u|w) = b \}$ and $S_{w'}(a, b) = \{ u \in S_{w'}(a) \mid \zeta_{spd}(u|w') = b \}$. By using the definition of DRG, we know that $|S_u(a, b)| = |S_{w'}(a, b)|$ and such cardinality only depends on the intersection array $\mathcal{L}$. Moreover, using the assumption of induction, all nodes $u$ in $S_u(a, b), S_{w'}(a, b)$ share the same representation $h_u^{(2)}$. Combining the fact that $|S_u(a, b)| = |S_{w'}(a, b)|$ and the fact that the nodes in these two sets hold the same representation, we may claim the second Eq. (11) is true, which completes the proof.

\[ \square \]

**Confirmation to the second question.** We formally restate the conclusion to prove: Given two fixed-sized sets $S^{(1)}, S^{(2)} \subseteq V, |S^{(1)}| = |S^{(2)}| = p$. Consider two tuples $T^{(1)} = (S^{(1)}, A^{(1)})$ and $T^{(2)} = (S^{(2)}, A^{(2)})$ in the most difficult setting when features $A^{(1)}$ and $A^{(2)}$ are only different in graph topologies specified by $A^{(1)}$ and $A^{(2)}$ respectively. Suppose $A^{(1)}$ and $A^{(2)}$ are uniformly independently sampled from all $r$-regular graphs over $V$ where $3 \leq r < (2 \log n)^{1/2}$. Then, for some constant $\epsilon > 0$ and constant positive integer $K$, there exist a proper DEAGNN-$p$-$K$-hop with layers $L < \lceil (\frac{1}{2} + \epsilon) \frac{\log n}{K \log (r-1)} \rceil$, using DE-$p$ $\zeta(u|S^{(1)}), \zeta(u|S^{(2)})$ for all $u \in V$ such that with probability $1 - o(n^{-1})$, its outputs $\Gamma(T^{(1)}) \neq \Gamma(T^{(2)})$.

**Proof.** Similar to the proof of Theorem 3.3, we use Lemma C.1 and focus on the case $S^{(1)} = S^{(2)} = \{ w \}$ and the initial node attribute for each node $u$ are $\zeta_{spd}(u|w)$. Most of the logic of the proof is the same as that of Theorem 3.3. We only need to take care of the step 3 of the proof of Theorem 3.3, as in DEAGNN-1-$K$-hop, a node $v$ with $\text{SDP}(v|w) = k$ will aggregation representations of nodes $u$ even with SDP$(u|w) \in [k - K, k + K]$. Therefore, we need to redefine the edge configuration in the step 3 of the proof of Theorem 3.3.

Recall $Q_k = \{ v \in V : \text{SDP}(v|w) = k \}$. We define the edge configuration between $Q_k$ and $\bigcup_{t \in [k+1, k+K]} Q_t$, as a list $C_k = \{(a_{1,1}, a_{2,1}, a_{3,1}, \ldots), (a_{1,2}, a_{2,2}, a_{3,2}, \ldots), \ldots (a_{1,k}, a_{2,k}, a_{3,k}, \ldots)\}$, where $a_{m,k,j}$ is the number of nodes in $Q_{k+j}$ of which each connects to exactly $m$ nodes in $Q_{k+j-1}$.

Note that two different $C_k$’s will lead to two different representations of $(uA^{(1)})$ and $(uA^{(2)})$ after layers $\lceil \frac{k}{r} \rceil + 1$ as DEAGNN-1-$K$-hop uses at most 2 layers yield $\{h_u^{(2)} | \zeta_{spd}(u|w, A^{(1)}) = k \} \neq \{h_u^{(2)} | \zeta_{spd}(u|w, A^{(2)}) = k \}$ and uses at most $\lceil \frac{k}{r} \rceil$ layers to propagate such difference to the target node $w$.

Actually, this definition of edge configuration is nothing but a concatenation of the edge configurations $(C_t)_{t \in [k+1, k+K]}$, where $C_t$ is the edge configuration between $Q_t$ and $Q_{t+1}$ as defined in the proof of Theorem 3.3. Then, we use the statement of step 3 on $C_t$ to characterize the probabilistic property of $C_k$.

For each $k \in \left( \frac{1}{2} \frac{\log n}{\log (r-1) - \epsilon}, \frac{1}{2} \frac{\log n}{\log (r-1) - \epsilon} \right)$, each type of edge configuration $C_k$ appears with probability $\Pi_{t=k}^{k+K-1} C_k = \Pi_{t=k}^{K-1} O(\frac{n^{1/2}}{p_t})$. Then, we consider $\epsilon \frac{\log n}{K \log (r-1)}$ many $k$’s in the following interval $\left( \frac{1}{2} \frac{\log n}{\log (r-1) - \epsilon}, \frac{1}{2} \frac{\log n}{\log (r-1) - \epsilon} \right)$ such that these $k$’s hold the same integral interval $K$ and can be denoted as $k_0, k_0 + K, \ldots$. The probability that $A^{(1)}$ and $A^{(2)}$ have all the same edge configurations for these $k$’s is bounded by

$\Pi_{k \in \{k_0, k_0+K, \ldots\}} P(C_k) = \Pi_{t=k_0}^{k_0+K-1} P(C_t) \sim o(n^{-\frac{3}{2}})$.

Therefore, we only need to consider edge configurations for $k \in \left( \frac{1}{2} \frac{\log n}{\log (r-1) - \epsilon}, (\frac{1}{2} + \epsilon) \frac{\log n}{\log (r-1) - \epsilon} \right)$ to distinguish $A^{(1)}$ and $A^{(2)}$. And within $\left( \frac{1}{2} + \epsilon \right) \frac{\log n}{\log (r-1) - \epsilon}$, DEAGNN-1-$K$-hop yields different representations for $(u, A^{(1)})$ and $(u, A^{(2)})$. Note that the constant 2 may be merged in $\epsilon$ for simplicity, which concludes the proof. $\square$

**F Details of the Experiments**

**F.1 Datasets**

The three air traffic networks for Task 1, Brazil-Airports, Europe-Airports, and USA-Airports were collected by [64] from government websites throughout the year 2016 and were used to evaluate
algorithms to learn structural representations of nodes [5,6]. Networks are built such that nodes represent airports and there exists an edge between two nodes if there are commercial flights between them. Brazil-Airports is a network with 131 nodes, 1,038 edges and diameter 5; Europe-Airports is a network with 399 nodes, 5,995 edges and also diameter 5; USA-Airports is a network with 1,190 nodes, 13,599 edges and diameter 8. In each dataset, the airports are divided into 4 different levels according to the annual passengers flow distribution by 3 quantiles: 25%, 50%, 75%. The goal is to infer the level of an airport using solely the connectivity pattern of them.

Tasks 2 & 3 were carried out on three other datasets used by SEAL [9] to facilitate comparison study: C.ele, NS and PB. C.ele [65] is a neural network of C. elegans with 297 nodes, 2,148 edges and 3,241 triangles (closed node triads), and diameter of 5, in which nodes are neurons and edges are neural linkage between them. NS [66] is a network of collaboration relationship between scientists specialized in network science, comprising of 1461 nodes 2742 edges and 3,764 triangles. PB [64] is a network of reference relationships between political post web-pages, consisting of 1,222 nodes, 16,714 edges, and of diameter 8. Following [9][10], for Task 2 & 3, we remove all links or triangles in testing sets from graph structure during the training phase to avoid label leakage.

F.2 Baseline Details

We have five baselines based on GNNs and one baseline, struc2vec [5], based on kernels using handcrafted structural features. We first introduce the implementation of struc2vec and then discuss other baselines.

**Struc2vec** is implemented in a 2-phase manner. In the first phase, embeddings for all the nodes are learned by running the n-gram framework over a constructed graph based on structural similarity kernels. We directly use the code provided by the original paper [5]. In the second phase, the embeddings of nodes that in the target node set are concatenated and further fed into an one-layer fully connected neural network to make further inference.

Regarding other GNN-based baselines, **GCN** is implemented according to Equation (9) of [20] with self-loops added. **SAGE** is implemented according to Algorithm 1 of Section 3.1 in [21]. **GIN** is implemented by adapting the code provided by the original paper [16] where we use the sum-pooling aggregation and multi-linear perception to aggregate neighbors. In all three baselines described above, ReLU nonlinearities are applied to the output of each hidden layer, followed by a Dropout layer. **PGNN** layer is implemented by adapting the code provided by the original paper [10]. **SEAL** is implemented by adapting the code provided by the original paper [7]. As we focus on learning structural representation with inductive capability, all the five GNN-based methods use node degrees as input features if node attributes are not available.

Final readout layers are tailored to suit different tasks. For Task 1 since the task is node classification, the final layer for all baselines is a one-layer neural network followed by a cross entropy loss. Tasks 2 & 3 have slightly more complex readout layers since the target entity for prediction is a node set of size 2 or 3. Note that SEAL is specifically designed for Task 2 and has its own readout that uses SortPooling over all node representations over the ego-networks of node-pairs [23]. We refer the readers to the original paper for details [9]. For all the other baselines, to make a fair comparison, we use the following difference-pooling: Suppose the target node set is $S$ and the representation of node $v$ for $v \in S$ is denoted by $h_v$, then we readout the representation of $S$ as

$$z = \sum_{u,v \in S} |h_v - h_u|$$

where $| \cdot |$ denotes component-wise absolute value. Note that Tasks 2 & 3 are to predict the existence of a link / triangle. So we use the inner product $\langle w, z \rangle$ where $w \in \mathbb{R}^d$ is a trainable final projection vector, and feed this product into the binary cross entropy loss to train the models.

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4https://github.com/leoribeiro/struc2vec
5https://github.com/weihua916/powerful-gnns
6https://github.com/JiaxuanYou/P-GNN
7https://github.com/muhanzhang/SEAL
F.3 DEGNN Variants Details.

**Minibatch training based on ego-network extraction.** To understand our detailed framework it is helpful to first discuss the minibatch training of GCN, although the original GCN is trained in a full-batch manner [20]. To train GCN in minibatches, we first extract, for each target node \( v \) in a given minibatch, an ego-network centering at \( v \) within \( L \)-hop neighbors by doing a depth-\( L \)-BFS from \( v \), denoted by \( G_v \). Here, \( L \) is the number of GCN layers intended to be used in the model. Note that the representation of node \( v \) via using \( L \)-layer GCN over \( G_v \) is the same as that via using \( L \)-layer GCN over the whole graph. If node attributes are not available for GCN or other WLGGNNs, we may use the degree of each node as its node attributes.

Our models are implemented by following the above mini-batch training framework. For a target node set \( S \), we first extract the union of ego-networks centering at any nodes in \( S \) within \( L \)-hop neighbors. We call the union of ego-networks as the ego-network around \( S \), denoted by \( G_S = \bigcup_{v \in S} G_v \). Note that even if \( S \) has multiple nodes, \( G_S \) can be extracted as a whole by running BFS. All the edges of \( G_S \) between nodes that are both in \( S \) will be further removed, which is denoted by \( G'_{S} \). For \( G'_{S} \), we associate each node \( u \) in these ego-networks with the DE \( \zeta(u|S) \) as extra node attributes. Specifically, we use a simple aggregation for Eq. (1):

\[
\zeta(u|S) = \frac{1}{|S|} \sum_{v \in S} \zeta(u|v)
\]

(13)

Next, we detail the different versions of \( \zeta(u|v) \) used by different variants of DEGNN.

**DEGNN-SPD.** This variant sets \( \zeta(u|v), v \in S \) and \( u \in G_S \) as a one-hot vector of the truncated shortest-path-distance between \( u \) and \( v \). That is,

\[
\zeta_{spd}(u|v) = \text{one hot}(\min(\text{SPD}(u, v), \max_{u,v} d)),
\]

(14)

where \( d_{\max} \) is the maximum distance to be encoded. As a result, the \( \zeta_{spd}(u|v) \) is a vector of length \( d_{\max} + 1 \). The pairwise SPDs can either be pre-computed in preprocessing stage, or be computed by traversing the extracted ego-networks on the fly. The \( d_{\max} \leq L \) helps prevent overfitting the noise in an overly large neighborhood.

**Compare DEGNN-SPD with SEAL.** DEGNN-SPD, when used for link prediction, is similar to SEAL [9] in a sense that we both encode the distance between any node and the two nodes in the target node-pairs. However, we are fundamentally different from SEAL as SEAL uses graph-level readout of all nodes in the ego-networks. SEAL also has no discussion on the expressive power of distance encoding. Their intention of node labeling as they reported is just to let the model know which node-pair in the extracted ego-networks is the target node-pair. Moreover, the specific DE \( \zeta(u|S) \) for a node-pair \( S = \{v_1, v_2\} \) used in SEAL is a one-hot encoding of the value \( 1 + \min(\text{SPD}(u, v_1), \text{SPD}(u, v_2)) + (d/2)\lfloor (d/2) + (d/2) - 1 \rfloor \), where \( d = \text{SPD}(u, v_1) + \text{SPD}(u, v_2) \). The dimension of this DE is \( O(d^2_{\max}) \) which is higher than our DE (Eq. (14)) used in DEGNN-SPD, which may result in model overfitting for large \( d_{\max} \).

**DEGNN-LP.** This variant sets \( \zeta(u|v), v \in S \) and \( u \in G_S \) as landing probabilities of random walks (of different lengths) from node \( v \) to node \( u \):

\[
\zeta_{lp}(u|v) = ((W^{(0)})_{vu}, (W^{(1)})_{vu}, (W^{(2)})_{vu}, \ldots, (W^{(d_{\max})})_{vu})
\]

(15)

where \( W^{(k)} = (AD^{-1})^k \) is the \( k \)-step random walk matrix, \( d_{\max} \) is the max step number of random walks. Notice that in principle, \( \zeta_{lp}(u|v) \) encodes the distance information at a finer granularity than \( \zeta_{spd}(u|S) \). This is because SPD(\( u, v \)) can be inferred from \( \zeta_{lp}(u|v) \) as the index of the first non-zero random walk feature. However, in practice we observe that such encoding does not always bring a significant performance gain.

For both DEGNN-SPD and DEGNN-LP, we use the same 1-hop neighborhood aggregation as GCN. DE can also be used to control the message passing as shown in Eq. (4). We further discuss two variants by incorporating DEGNN-SPD and Eq. (4).

**DEAGNN-SPD.** DEAGNN-SPD is built on top of DEGNN-SPD, using the same extra node features \( \zeta_{spd}(u|S) \), but allows for multi-hop aggregation by specifying Eq. (4) as

\[
\text{AGG}(\{f_2(h_u^{(l)}, A_{vu})\}_{u \in N_v}) \rightarrow \text{AGG}(\{f_2(h_u^{(l)}, A_{vu}), \zeta_{spd}(u|v)\}_{\zeta_{spd}(u|v) \leq K}).
\]
In experiments, we choose $K = 2, 3$, which means that each node aggregates representations of other nodes that are not only its direct neighbors but also its (exclusive) 2-hop and even 3-hop neighbors. As we do not have edge attributes in our data, we omit $A_{vu}$. Our implementation of the aggregation for the layer $l$ follows

$$h_v^{(l+1)} = \sum_{k=1}^{K} \text{Relu} \left( \frac{1}{|S_v,k|+1} \left( h_v^{(l)} + \sum_{u \in S_v,k} h_u^{(l)} \Theta^{(lk)} \right) \right), \quad S_v,k = \{ u | \zeta_{spd}(u|v) = k \}.$$

where $\Theta^{(lk)}$ is a trainable weight matrix and for each $k$, we aggregate $k$-hop neighbors via a GCN layer with a self-loop. Note that when implementing DEAGNN-SPD, we need to extract the ego-network of nodes within $L$-hops, if DEAGNN-SPD has $L$ layers.

**DEAGNN-PR.** DEAGNN-SPD is also built on top of DEGNN-SPD, but the propagation is by specifying Eq. (4) as

$$AGG(\{ f_2(h_u^{(l)}, A_{vu}) \}_{u \in \mathcal{N}_v}) \to AGG(\{ f_2(h_u^{(l)}, A_{vu}), \zeta_{prr}(u|v) \}_{v \in V}).$$

As the aggregation is over the whole node set, this model does not extract the ego-networks but uses the entire graphs. For the layer $l$, we further specify the above aggregation by using

$$h_v^{(l+1)} = \text{Relu} \left( \sum_{u \in V} \zeta_{prr}(u|v) h_u^{(l)} \Theta^{(l)} \right),$$

where $\Theta^{(l)}$ is a trainable weight matrix and $\zeta_{prr}(u|v)$ is a specific form of $\zeta_{prr}(u|v)$ based on Personalized Pagerank scores [67], i.e.,

$$\zeta_{prr}(u|v) = \sum_{k=0}^{\infty} (0.9W)^k u v = [(I - 0.9W)^{-1}]_{uv}.$$

Note that the above 0.9 is a hyper-parameter. As we are just willing to show the use case, 0.9 is set as a heuristic and is not obtained via parameter tuning. Other values may yield better performance. Other types of PageRank scores may be used, e.g., heat-kernel PageRank scores [68], time-dependent PageRank scores [69].

We compare DEAGNN-PR with all other methods, which yields the following Table 2. DEAGNN-PR performs worse than DEAGNN-SPD while it still works much better than WLGNNs in link and triangle predictions. Comparing these observations with the statements on GDC [32], we argue that missing DEs as node attributes is the key that limits the performance of link prediction via GDC.

| Method          | Data          | Nodes (Task 1): Average Accuracy | Node-pairs (Task 2): AUC | Node-triads (Task 3): AUC |
|-----------------|---------------|---------------------------------|--------------------------|---------------------------|
|                 | Bra.-Airports | Eur.-Airports | USA-Airports | Bra.-Airports | Eur.-Airports | USA-Airports | C.elegans | NS | PR | C.elegans | NS | PR |
| DEAGNN-SPD      | 64.55±±.18    | 54.83±±.29    | 56.58±±.11    | 74.03±±.09    | 74.21±±.12    | 98.79±±.09    | 80.94±±.51    | 81.72±±.56    | 97.82±±.32    | 98.30±±.40    | 98.64±±.14    | 98.40±±.14    | 98.40±±.14    | 98.30±±.40    |
| DEAGNN-LP       | 70.65±±.33    | 56.29±±.21    | 50.85±±.83    | 73.91±±.32    | 73.96±±.14    | 90.23±±.74    | 84.72±±.40    | 84.06±±.14    | 90.83±±.34    | 93.74±±.50    | 93.74±±.50    | 93.74±±.50    | 93.74±±.50    |
| DEAGNN-PR       | 71.89±±.60    | 57.05±±.08    | 58.87±±.12    | 75.58±±.59    | 87.75±±.56    | 91.11±±.52    | 86.42±±.12    | 94.59±±.66    | 94.59±±.66    | 94.59±±.66    | 94.59±±.66    | 94.59±±.66    | 94.59±±.66    | 94.59±±.66    |
| Struc2vec [5]   | 70.88±±.26    | 57.94±±.01    | 61.92±±.61    | 72.11±±.03    | 82.76±±.59    | 90.47±±.60    | 77.72±±.58    | 81.93±±.61    | 81.93±±.61    | 81.93±±.61    | 81.93±±.61    | 81.93±±.61    | 81.93±±.61    | 81.93±±.61    |
| PGNN [10]       | N/A           | N/A           | N/A           | 78.20±±.33    | 94.88±±.77    | 89.72±±.32    | 86.36±±.74    | 79.36±±.14    | 98.68±±.55    | 98.68±±.55    | 98.68±±.55    | 98.68±±.55    | 98.68±±.55    | 98.68±±.55    |
| SEAL [9]        | N/A           | N/A           | N/A           | 118.26±±.86   | 98.55±±.32    | 94.18±±.57    | N/A           | N/A           | 98.68±±.55    | 98.68±±.55    | 98.68±±.55    | 98.68±±.55    | 98.68±±.55    | 98.68±±.55    |

Table 2: Model performance (including DEAGNN-PR) in Average Accuracy and Area Under the ROC Curve (AUC) (mean in percentage ± 95% confidence level). $\ast$ highlights the best baselines. "bold font, bold font" respectively highlights the case where our proposed model’s performance: exceeds the best baseline on average, exceeds by 70% confidence, exceeds by 95% confidence.

**F.4 Model performance without validation datasets**

We have confirmed with the original authors of Struc2vec [5] and SEAL [9] that the performance of these two baselines reported in their papers do not use validation set. The performance therein is the best testing results ever achieved when models are being trained till convergence. We think that it is necessary to include validation datasets to achieve fair comparison and therefore reported the results with validation datasets in the main text. We put the results without validation datasets here. Under both experimental settings, we draw similar conclusions for our models in comparison with the baselines.
We report additional results of our model on Task 2 and 3 versus other baselines, measured by average accuracy without validation set in Table 4. Similar observations as reported in the main text can be drawn from both Table 3 and 4: the strongest baselines are given by SEAL \cite{9} and GIN \cite{16}, while our DEAGNN variants further significantly outperform those baselines on all tasks.

F.5 Hyperparameters Tuning.

Table 5 lists the most important hyperparameters’ at a glance, which applies to both the baselines and our proposed models. Grid search is used to find the best hyperparameters combination. The models are sufficiently trained till the cross entropy loss converges and we report the best model by running each for 20 times over different random seed. For more details please refer to the code attached.

| Hyperparameters | Value / Range | Notes |
|-----------------|---------------|-------|
| batch size      | 64, 128       |       |
| learning rate   | 1e-4          |       |
| optimizer       | SGD           | stochastic gradient descent |
| conv. layers    | 1, 2, 3       | struc2vec does not follow this setting |
| conv. hidden dim.| 20, 50, 80, 100 | struc2vec does not follow this setting |
| dropout         | 0, 0.2        |       |
| $d_{rw}$        | 3, 4          | #steps of random walk, valid only for DEGNN-RW |
| $d_{spd}$       | 3, 4          | maximum shortest path distance for DEGNN-SPD variants |
| prop. depth     | 1, 2, 3       | the number of hops of message in one layer, only valid for DEAGNN-SPD, 1 for all the others |

| Table 5: List of hyperparameters and their value / range. |
the $k$-WL test here also corresponds to the $k$-WL’ test in [41] and the $k$-FWL test in [30], and are equivalent to the $k + 1$-WL tests in [25][30].

The $k$-WL test ($k \geq 2$) follows the following coloring procedure:

1. For each $k$-tuple of node set $V_i = (v_{i1}, v_{i2}, ..., v_{ik}) \in V^k$, $i \in [n^k]$, we initialize $V_i$ with a color denoted by $C_i^{(0)}$. These colors satisfies that for two $k$-tuples, $V_i$ and $V_j$, $C_i^{(0)}$ and $C_j^{(0)}$ are the same if and only if for $a, b \in [k]$ (1) $v_{ia} = v_{ib} \iff v_{ja} = v_{jb}$ and (2) $(v_{ia}, v_{ib}) \in E \iff (v_{ja}, v_{jb}) \in E$.

2. For each $k$-tuple $V_i$ and $u \in V$, define $N(V_i; u)$ as a sequence of $k$-tuples such that $N(V_i; u) = ((u, v_{i2}, ..., v_{ik}), (v_{i1}, u, ..., v_{ik}), (v_{i1}, v_{i2}, ..., u))$. Then, the color of $V_i$ can be updated via the following mapping:

$$C_i^{(l+1)} \leftarrow g(C_i^{(l)}, \{C_j^{(l)} | V_j \in N(V_i; u)\}_{u \in V}),$$

where $g(\cdot)$ is injective coloring.

3. For each step $l$, $\{C_i^{(l)}\}_{i \in [n^k]}$ is a coloring configuration of the graph $G$, which is essentially a multi-set. If two graphs have different coloring configurations, these two graphs are determined to be non-isomorphic, while the inverse is not true.

Note that the step 2 essentially requires to aggregate colors of $nk$-tuples and thus even when $k = 2$, the 2-WL test may not leverage the sparsity of graph structure to keep good scalability. Ring-GNN [29] and PPGN [30] essentially try to achieve the expressive power of the 2-WL test. They are not scalable to process large graphs and they were only evaluated for entire-graph-level tasks such as graph classification and graph regression [29][30].