Random Features Strengthen Graph Neural Networks

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Abstract

Graph neural networks (GNNs) are powerful machine learning models for various graph learning tasks. Recently, the limitations of the expressive power of various GNN models have been revealed. For example, GNNs cannot distinguish some non-isomorphic graphs (Xu et al., 2019) and they cannot learn efficient graph algorithms (Sato et al., 2019), and several GNN models have been proposed to overcome these limitations. In this paper, we demonstrate that GNNs become powerful just by adding a random feature to each node. We prove that the random features enable GNNs to learn almost optimal polynomial-time approximation algorithms for the minimum dominating set problem and maximum matching problem in terms of the approximation ratio. The main advantage of our method is that it can be combined with off-the-shelf GNN models with slight modifications. Through experiments, we show that the addition of random features enables GNNs to solve various problems that normal GNNs, including GCNs and GINs, cannot solve.

1. Introduction

Graph neural network (GNN) (Gori et al., 2005; Scarselli et al., 2009) is a machine learning method for graph-structured data. GNNs have achieved state-of-the-art performance in various tasks, including chemo-informatics (Gilmer et al., 2017; Zhang et al., 2018), question answering systems (Schlichtkrull et al., 2018), and recommender systems (Ying et al., 2018a; Wang et al., 2019a;b).

Recently, the theoretical power of GNNs have been extensively studied. Morris et al. (2019) and Xu et al. (2019) pointed out that the expressive power of GNNs is at most the same as the first order Weisfeiler-Lehman (WL) test (Weisfeiler & Lehman, 1968), and GNNs cannot solve the graph isomorphism problem. Xu et al. (2019) proposed the most powerful GNN model within the limitation of the first order WL test, and Morris et al. (2019) overcame the limitation by proposing \(k\)-GNN, which has the same representation power as the \(k\)-th order WL test. Maron et al. (2019b) enumerated the invariant (i.e., the output does not change for any node permutation) and equivariant (i.e., the output does not change except the permutation for any node permutation) linear transformations, and Maron et al. (2019c) and Keriven & Peyré (2019) proposed universal equivariant and invariant networks using the invariant and equivariant linear transformations as their building blocks. However, they used the \(n(n-1)/2\)-th order tensors as parameters, where \(n\) is the number of nodes, which is not tractable. Relational Pooling (Murphy et al., 2019b) is another type of universal invariant model. It considers the average of all \((n!)\) ways of permutations of nodes, similar to Janossy Pooling (Murphy et al., 2019a), and they proposed approximation schemes to make the computation tractable in practice. Namely, \(\pi\)-SGD samples a few permutations randomly, similar to randomly sorted Coulomb Matrices (Montavon et al., 2012). The aforementioned works aimed to construct powerful invariant or equivariant models. In contrast, Sato et al. (2019) considered the theoretical power of message-passing GNNs for combinatorial problems, where models are not necessarily equivariant. They demonstrated that the representation power of GNNs is the same as that of distributed local algorithms (Angluin, 1980; Hella et al., 2012; Suomela, 2013), and derived the approximation ratios of the algorithms that can be learned by GNNs considering the theory of distributed local algorithms. However, their approximation ratios are much higher than those of existing algorithms (Chlebík & Chlebíková, 2008; Johnson, 1974). They proposed the use of feature engineering to improve these ratios; however, the improved ratios were far from optimal.

In this paper, we propose a very simple and efficient method to improve the approximation ratios of GNNs, which can achieve near-optimal ratios under the degree-bounded assumption and \(P \neq \text{NP}\) assumption. Namely, we propose the addition of a random feature to each node. An illustrative example is shown in Figure 1. Message-passing GNNs cannot distinguish a node in a ring of three or six nodes if the node features are identical (Figure 1 (a)). This phenomenon is not desirable for graphs comprising categor-
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| Problem | GINs / CPNGNNs | CPNGNNs weak 2-coloring | rGINs | Polynomial Time | Lower Bound |
|---------|----------------|-------------------------|-------|-----------------|-------------|
| MDS     | $\Delta + 1^*$ | $\Delta + 1^*$          | $H(\Delta + 1) + \epsilon$ | $H(\Delta + 1) - \frac{1}{\epsilon}$ | $\ln(\Delta) - C \ln \ln \Delta$ |
| MM      | $\infty^*$     | $\Delta + 1^*$          | $1 + \epsilon^*$            | $1^*$            | $1$          |

Table 1. The summary of approximation ratios of the minimum dominating set problem (MDS) and maximum matching problem (MM). $^*$ indicates that these ratios match the lower bounds. $\Delta$ denotes the maximum degree, $H(k)$ denotes the $k$-th harmonic number, $\epsilon > 0$ is an arbitrary constant, and $C$ is a fixed constant. Since $\ln(k) \leq H(k) \leq \ln(k) + 1$ holds, the approximation ratios of rGINs match the best approximation ratios of polynomial algorithms except constant terms, and they also match the lower bounds except insignificant terms.

In our work, we propose graph isomorphic networks with random features (rGINs). rGINs add a random value to each node each time the procedure is called. We prove that the addition of random features indeed improves the theoretical capability of GNNs in terms of the approximation ratios. Table 1 summarizes our main results. Importantly, our results share a preferable characteristic with Sato et al. (2019)’s result. Our results can be applied to graphs of variable sizes. In other words, we prove that there exist parameters such that for any graph of arbitrary size, the output of rGINs is not far from the optimal solution with high probability. Especially, rGINs assign different random numbers in test time but can guarantee the quality of solution, even in test graphs of arbitrary large sizes. This is the key difference from most of the previous works (Maron et al., 2019c; Keriven & Peyré, 2019; Murphy et al., 2019b), where the upper bound of the graph size was fixed beforehand. Another preferable characteristic of this method is that this can be combined with off-the-shelf GNN models with slight modifications.

In this study, we derive the approximation ratios of the algorithms that rGINs can learn by converting a certain type of constant time algorithms (Nguyen & Onak, 2008; Rubinfeld & Shapira, 2011) to rGINs. Conversely, we also prove that rGINs can be converted to constant time algorithms. This indicates that machine learning researchers also have chances to contribute to the algorithm field by finding effective architectures and features.

2. Related Work

The origin of GNNs dates back to Sperduti & Starita (1997) and Baskin et al. (1997). They aimed to extract features from graph data using neural networks instead of hand-engineered graph fingerprints. Sperduti & Starita (1997) recursively applied a linear aggregation operation and non-linear activation function, and Baskin et al. (1997) used parameter sharing to model the invariant transformations on the node and edge features, which are common with modern GNNs. Gori et al. (2005) and Scarselli et al. (2009) proposed novel graph learning models that used recursive aggregation operations until convergence, and these models were called graph neural networks. Li et al. (2016) extended this idea to Gated Graph Neural Networks. Molecular Graph Network (Merkwirth & Lengauer, 2005) is a concurrent model of the graph neural networks with similar architecture, which uses a constant number of layers. Duvendau et al. (2015) constructed a GNN model inspired by circular fingerprints. Bruna et al. (2014) and Defferrard et al. (2016) utilized the graph spectral analysis and graph signal processing (Shuman et al., 2013) to construct GNN models. Graph Convolutional Networks (GCNs) (Kipf & Welling, 2017) approximate a spectral model using linear filters to reduce it to an efficient spatial model. Gilmer et al. (2017) characterized GNNs using the message passing mechanism to provide a unified view of GNNs. Following these works, many effective GNN models have been proposed, incorporating the attention mechanism (Veličković et al., 2018) and hierarchical pooling (Ying et al., 2018b; Gao & Ji, 2019; Ma et al., 2019), to name a few.

Although GNNs have been empirically successful, their limitations have been recently found. Morris et al. (2019) and Xu et al. (2019) pointed out that the expressive power of GNNs is at most the same as the first order Weisfeiler-Lehman (WL) test (Weisfeiler & Lehman, 1968), and they cannot solve the graph isomorphism problem. Maron et al. (2019b) enumerated all the linear equivariant transformations, which are useful for the construction of powerful equivariant GNNs. Maron et al. (2019c) demonstrated that higher-order tensors are sufficient and necessary for universal invariant networks. Keriven & Peyré (2019) extended universality to equivariant networks. Maron et al. (2019a) proposed a second-order tensor GNN model that has the same power as the third order WL test. Relational Pooling (Murphy et al., 2019b) utilized all permutations of the
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nodes, similar to Janossy Pooling (Murphy et al., 2019a),
to construct universal invariant and equivariant networks,
and they proposed approximation schemes to make the
computation tractable. Chen et al. (2019) showed that the
universality of invariant models is essentially equivalent to
the graph isomorphism test. Sato et al. (2019) showed the
representation power of GNNs is the same as that of dis-
tributed local algorithms (Angluin, 1980; Hella et al., 2012;
Suomela, 2013), which have the same representation power
as model logic (Hella et al., 2012). Following this work,
Loukas (2020) and Barceló et al. (2020) demonstrated a
similar connection between GNNs and distributed local al-
gorithms (Loukas, 2020) and modal logic (Barceló et al.,
2020). Our work focuses on randomized algorithms instead
of deterministic algorithms.

The proposed method is similar to π-SGD (Murphy et al.,
2019b), one of approximation schemes for Relational Pool-
ing, but they are different in two aspects: The original π-
SGD uses a random permutation of \( n \) elements, which is
difficult to be applied to graphs of variable sizes, while we
use i.i.d. random variables of a constant support. More-
over, the original π-SGD aims to approximate the equiv-
ariant relational pooling layer, whereas we aim to model
non-equivariant functions using GNNs. Note that our anal-
ysis provides another justification of π-SGD approximation
because the approximation ratios of the algorithms that can
be learned by Relational Pooling GNNs with random sam-
ping approximation can be proved similarly.

3. Background and Notations

For a positive integer \( k \in \mathbb{Z}^+ \), let \([k]\) be the set
\( \{1, 2, \ldots, k\} \). Let \( H(k) = \sum_{i=1}^{k} \frac{1}{i} \) be the \( k \)-th harmonic
number. Let \( G = (V, E) \) be an input graph, where \( V \) is a
set of nodes, and \( E \) is a set of edges. In this work, we only
consider the connected graphs without self loops or multi-
ple edges (i.e., connected simple graphs). \( n = |V| \) denotes
the number of nodes and \( m = |E| \) denotes the number
of edges. We assume \( V = [n] \) without loss of generality.
Let \( V(G) \) be the set of the nodes of \( G \) and \( E(G) \) be the
set of the edges of \( G \). For a node \( v \in V \), \( \deg(v) \) denotes
the degree of node \( v \), \( N_k(v) \) denotes the set of nodes within \( k \)-hop
from node \( v \), and \( N(v) \) denotes the set of neighboring
nodes of node \( v \). Let \( R(G, v, L) = (N_L(v), \{\{x, y\} \in E \mid
x, y \in N_L(v)\}) \) be the induced subgraph of \( G \) by the \( L \)-hop
nodes from node \( v \). In some problem settings, each node
of the input graph has a feature vector \( x_v \in \mathbb{R}^{d_1} \). In
such a case, we include feature vectors into the input graph
\( G = (V, E, X) \), where \( X = [x_1, x_2, \ldots, x_n]^\top \in \mathbb{R}^{n \times d_1} \)
is the matrix for feature vectors. We assume that the sup-
pport \( C \) of the feature vectors is finite (i.e., \( |C| < \infty \)) in this
study. If the input graph involves no features, we use degree
features as the initial embedding, following the works
by Xu et al. (2019) and Sato et al. (2019).

Assumption (Bounded-Degree Graphs). In this paper,
we only consider bounded-degree graphs, following the
work by Sato et al. (2019). There are many degree-
bounded graphs in real world, such as chemical com-
ponents and computer networks. Furthermore, the bounded-
degree assumption is often used in constant time algorithms
(Parnas & Ron, 2007; Nguyen & Onak, 2008). It should
be noted that this assumption is weaker than the bonded-
size assumption because if the maximum degree \( \Delta \) is equal
to the maximum size of nodes, the bounded-degree graphs
contain all bounded-size graphs. For each positive integer
\( \Delta \in \mathbb{Z}^+ \), let \( \mathcal{F}(\Delta) \) be the set of all simple connected graphs
with maximum degrees of \( \Delta \) at most. Let \( \mathcal{F}(\Delta, C) \) be the
set of all simple connected graphs \( G = (V, E, X) \) with
maximum degrees of \( \Delta \) at most with features \( x_v \in C \).

We formally define the graph problems with slight modifi-
cations from Sato et al. (2019).

Definition (Node Problems). A node problem is a function
\( \Pi \) that associates a set \( \Pi(G) \subseteq 2^V \) of feasible solutions
with each graph \( G = (V, E) \).

Definition (Edge Problems). An edge problem is a func-
tion \( \Pi \) that associates a set \( \Pi(G) \subseteq 2^E \) of feasible solutions
with each graph \( G = (V, E) \).

We refer to the node and edge problems as graph problems.
Many combinatorial graph problems aim to obtain a mini-
num or maximum set in feasible solutions. For example,
the minimum dominating set problem can be formulated
by finding a minimum set in \( \Pi(G) = \{U \subseteq V(G) \mid U \)
is a dominating set of \( G \} \). The maximum matching
problem can be formulated by finding a maximum set in
of \( \Pi(G) = \{F \subseteq E(G) \mid F \) is a matching of \( G \} \). Let
\( \text{OPT}_m(\Pi, G) \) and \( \text{OPT}_M(\Pi, G) \) denote the size of the mini-
num and maximum sets in \( \Pi(G) \), respectively.

Definition (Monotonicity). The minimization of a graph
problem \( \Pi \) is monotone if \( \forall G = (V, E), \forall S \subseteq T \subseteq V, \)
\( S \in \Pi(G) \Rightarrow T \in \Pi(G) \). The maximization of a graph
problem \( \Pi \) is monotone if \( \forall G = (V, E), \forall S \subseteq T \subseteq V, \)
\( T \in \Pi(G) \Rightarrow S \in \Pi(G) \).

Many combinatorial graph problems are monotone, such
as the minimum dominating set problem, minimum vert-
ex cover problem, and maximum matching problem. This
property is used to ensure that the learned algorithm always
outputs a feasible solution by including or excluding the un-
certain nodes or edges.

Definition (Consistent Algorithm). An algorithm \( \mathcal{A} \) that
takes a graph \( G = (V, E) \) as input and outputs a set of
nodes or a set of edges is a consistent algorithm of a graph
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Figure 1. Illustrative example: GNNs with identical features (such as degree features) cannot distinguish a node in a cycle of three nodes with a node in a cycle of six nodes, whereas GNNs with random features can.

Problem II if for all $G = (V, E), A(G) \in \Pi(G)$.

Note that An algorithm $A$ may involve randomized processes but it must always output a feasible solution to be consistent.

**Definition (Approximation Ratio).** The objective value $y$ of a minimization problem $\Pi$ is said to be an $(\alpha, \beta)$-approximation if $\OPT_{\alpha}(\Pi, G) \leq y \leq \alpha \OPT_{\beta}(\Pi, G) + \beta$, and an objective value $y$ of a maximization problem $\Pi$ is an $(\alpha, \beta)$-approximation if $\frac{1}{\beta} \OPT_{\alpha}(\Pi, G) - \beta \leq y \leq \OPT_{\alpha}(\Pi, G)$. The solution $S$ of a graph problem is also said to be an $(\alpha, \beta)$-approximation if $|S|$ is an $(\alpha, \beta)$-approximation. A consistent algorithm $A$ is an $(\alpha, \beta)$-approximation algorithm for a graph problem $\Pi$ w.h.p. if for all graphs $G = (V, E), A(G)$ is an $(\alpha, \beta)$-approximation of $\Pi$ w.h.p. Especially, we refer to an $(\alpha, 0)$-approximation algorithm as an $\alpha$-approximation algorithm, and we call $\alpha$ the approximation ratio of the algorithm.

**GINs.** Graph Isomorphism Network (GIN) (Xu et al., 2019) is a powerful machine learning model that takes a graph $G = (V, E, X)$ as input and outputs an embedding $z_v \in \mathbb{R}^{d_0}$ of each node $v \in V$. A GIN with parameters $\theta$ calculates the embeddings $z_v = z_v^{(L)}$ by the following equations:

$$z_v^{(0)} \leftarrow \text{MLP}_{\theta_0}(x_v),$$

$$z_v^{(l)} \leftarrow \text{MLP}_{\theta_l} \left( (1 + \varepsilon^{(k)})z_v^{(l-1)} + \sum_{w \in \mathcal{N}(v)} z_w^{(l-1)} \right),$$

where $\text{MLP}_{\theta_l}$ is a multi layer perceptron with parameters $\theta_l$. Here, $\theta$ includes $\theta_0, \theta_1, \ldots, \theta_L$ and $\varepsilon^{(1)}, \varepsilon^{(2)}, \ldots, \varepsilon^{(L)}$. The existence of the parameters $\theta$ implies that there exists an architecture (such as the number of layers and dimensions of hidden vectors) along with its parameters. We build a GNN model with random features based on GINs because GINs have the strongest power among message-passing GNNs (Xu et al., 2019). Especially, GINs can distinguish the neighboring node sets if the multisets of features of neighboring nodes are different.

4. Main Results

4.1. Intuitive Explanation

We first provide an intuition using Figure 1 (b). Here, we use a toy model CAT that concatenates all features of all nodes for simplicity, whereas we use GINs in the main section. We further assume that the maximum degree is two in this example. The first dimension $v_1$ of the embedding $v$ is the random feature of the center node. The second and third dimensions are the random features of the one-hop nodes (e.g., in the sorted order) with appropriate zero paddings. The fourth to seventh dimensions are the random features of the two-hop nodes. The eighth to fifteenth dimensions are the random features of the three-hop nodes. Then, as Figure 1 (b) shows, irrespective of the random features, the center node is involved in a cycle of length three if and only if there exists a leaf node of the same color as the center node unless the random features accidentally coincide. This condition can be formulated as $v_1 = v_8$ or $v_1 = v_9$ or $\ldots$ or $v_1 = v_{15}$. Therefore, we can check whether the center node is involved in a cycle of length three by checking the embedding on the union of certain hyperplanes. This property is valid even if the random features are re-assigned; a center node involved in a cycle of length three always falls on the union of these hyperplanes irrespective of the random features. A similar property is valid for substructures other than a cycle of length three. Therefore, if the positive examples of a classification problem have characteristic substructures, the model can classify the nodes by checking the embedding on certain hyperplanes. It is noteworthy that the values of random features are not important; however, the relationship between the values is important because the values are random.

In the main results, we use GINs, which do not concatenate the features but apply nonlinear transformation and summation per layer. However, according to the theory
of GINs, this model does not lose information, and similar discussion as that mentioned above can be applied by replacing the hyperplanes with curved surfaces. The aggregation functions of GINs are parameterized, and appropriate features or substructures are selected according to the downstream task. For example, if the downstream task relies only on the existence of a cycle of length three, GINs can learn to discard the second to seventh dimensions in the example above. These intuitions are formally stated in Theorem 1.

In this paper, we further show that the GINs with random features can solve the combinatorial problems with lower approximation ratios than the existing GNNs, where distinguishing the local structures is not sufficient. For example, if the input graph is a clique, all nodes are isomorphic. However, the empty set does not form a dominating set and the entire nodes contain too many nodes because the minimum dominating set contains only one node. We show that random features can help select the nodes appropriately. This type of mechanism is not required for ordinary node classification tasks, but important for combinatorial problems and cannibalization-aware recommendation (Gong et al., 2019).

4.2. GINs with Random Features (rGINs)

In this section, we introduce GINs with random features (rGINs). rGINs assign a random value \(r_v \in D \subseteq \mathbb{R}^{d_r}\) to each node \(v\) every time the procedure is called and calculate the embeddings of a node using GINs, and let \(R = [r_1, r_2, \ldots, r_n]^\top \in \mathbb{R}^{n \times d_r}\). Here, \(D\) is the support of random features. We show the pseudo code of rGINs in Algorithm 1, where \(\text{CONCAT}([X, R]) \in \mathbb{R}^{n \times (d_t + d_r)}\) denotes concatenation along the feature dimension. We show that this slight modification theoretically strengthens the representation power of GINs.

In the following analysis, we use discrete random features to ensure consistency in the learned algorithm. Continuous random features cannot ensure consistency because the theoretical analysis of GINs assumes that the input feature is countable (Xu et al., 2019). However, continuous random features can be used in practice. For consistency algorithms, the continuous features can be discretized. We then introduce the property that random features should satisfy. We prove in the following sections that the quality of solutions generated by rGINs can be guaranteed if the random distribution of random features are i.i.d. with the following property.

**Definition** \((\mathcal{U}(p))\). For a real number \(p \in \mathbb{R}^+\), a discrete probability measure \(\mu\) with support \(D \subseteq \mathbb{R}^{d_r}\) has the property \(\mathcal{U}(p)\) or \(\mu \in \mathcal{U}(p)\) if \(\mu(x) \leq p\) for all \(x \in D\).

**Example.** For all \(p \in \mathbb{R}^+\), the uniform distribution \(\text{Unif}(D)\) on \(D = [\text{ceil}(\frac{1}{p})]\) has the property \(\mathcal{U}(p)\).

**How to solve node problems using rGINs.** We solve the node problems using node classification models. We first calculate the embeddings \(z_1, \ldots, z_n \in \mathbb{R}\) using rGINs with output dimension \(d_O = 1\) and the sigmoid activation in the last layer. For each node \(v\) that is assigned the same random number as an \(L\)-hop node from \(v\), we fix the embedding \(z_v = 1\) and \(z_v = 0\) for the monotone minimization and maximization problem, respectively. This step ensures that the learned algorithm is consistent, but this step is optional and can be skipped for some applications. Finally, we decide the solution \(U = \{v \in V \mid z_v > 0.5\}\) by setting a threshold for the output probabilities. Let \(\text{rGIN}_v(G, \mu, \theta)\) denote the function that takes a graph \(G = (V, E, X)\) as input and returns \(U\) by the procedure above.

**How to solve edge problems using rGINs.** We solve the edge problems using link prediction models. We first calculate the embeddings of each node using rGINs. For each node \(v\) that is assigned the same random number as an \(L\)-hop node from \(v\), we fix the embedding \(z_v = 1\) and \(z_v = 0\) for the monotone minimization and maximization problem, respectively, where \(1 \in \mathbb{R}^{d_O}\) and \(0 \in \mathbb{R}^{d_O}\) are vectors of ones and zeros, respectively. Finally, we decide the solution \(F = \{\{u, v\} \in E \mid z_u \cdot z_v > 0.5\}\) by setting a threshold for the inner product of embeddings, following a standard method for the link prediction task (Liben-Nowell & Kleinberg, 2003). Let \(\text{rGIN}_e(G, \mu, \theta)\) denote the function that takes a graph \(G = (V, E, X)\) as input and returns \(F\) by the procedure above.

4.3. Expressive Power of rGINs

In this section, we demonstrate the expressive power of rGINs. Especially, we prove that rGINs can distinguish any isomorphism between the pairs of a graph and a node.

**Definition** Let \(G = (V, E, X)\) and \(G' = (V', E', X')\) be graphs and \(v \in V\) and \(v' \in V'\) be nodes. \((G, v)\) and \((G', v')\) are isomorphic if there exists a bijection \(f : V \rightarrow V'\) such that \((x, y) \in E \iff (f(x), f(y)) \in E', x_x = x'_{f(x)} (\forall x \in V)\), and \(f(v) = (v')\). \((G, v) \simeq (G', v')\) denotes \((G, v)\) and \((G', v')\) are isomorphic.

**Theorem 1.** \(\forall L \in \mathbb{Z}^+, \text{ for all finite feature spaces } C (|C| < \infty), \forall \mathcal{G} \in 2^{\mathcal{F}(\Delta, C)}\times|\Delta|, \text{ there exists } p \in \mathbb{R}^+ \text{ such that } \forall \mu \in \mathcal{U}(p), \text{ there exist parameters } \theta \text{ such that } \forall G = (V, E, X) \in \mathcal{F}(\Delta, C), \forall v \in V\).
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• if $\exists (G', v') \in \mathcal{G}$ such that $(G', v') \simeq (R(G, v, L), v)$ holds, $r\text{GIN}(G, \mu, \theta)_v > 0.5$ holds w.h.p.

• if $\forall (G', v') \in \mathcal{G}$, $(G', v') \not\simeq (R(G, v, L), v)$ holds, $r\text{GIN}(G, \mu, \theta)_v < 0.5$ holds w.h.p.

All proofs have been provided in the supplementary material. For example, let $L = 2$ and $\mathcal{G}$ be a set of all pairs of a graph and a node $v$ with at least one triangle incident to $v$. Then Theorem 1 shows that rGINs can classify the nodes by presence of the triangle structure, while GINs cannot determine the existence of a triangle in general. We confirm this fact by numerical experiments in Section 5. Moreover, let $\mathcal{G}$ be a set of all graphs with certain chemical functional groups, then rGINs can classify nodes based on the functional groups that the node belongs to.

4.4. Approximation Ratios with rGINs

4.4.1. Minimum Dominating Set Problems

In this section, we modify a constant time algorithm for the minimum dominating set problem $\Pi_{\text{MDS}}$ and prove that rGINs can simulate this algorithm. Nguyen & Onak (2008) converted a sequential greedy algorithm for the minimum dominating set problem (Johnson, 1974; Lovász, 1975) into a constant time algorithm. We use a slightly different version of the sequential greedy algorithm.

1. Assign a random value $r_v \sim \mu$ to each node $v \in V$.
2. Add nodes $v$ into the solution if there exists a node $u \in N_2(v)$ with the same random value as $v$.
3. Add a node that covers the most number of uncovered nodes into the solution until all nodes are covered. Ties are broken by the lexicographical order of $r_v$.

This is a consistent algorithm for the minimum dominating set problem by its stop criterion. Moreover, this satisfies the following property.

Lemma 2. For all $\varepsilon > 0$, there exists $p \in \mathbb{R}^+$ such that for any distribution $\mu \in \mathcal{U}(p)$, the algorithm above is an $(H(\Delta + 1) + \varepsilon)$ approximation algorithm for the minimum dominating set problem.

We construct a constant time algorithm using this sequential algorithm by constructing oracles $O_0, O_1, \ldots, O_{\Delta + 1}$ as Nguyen & Onak (2008). Intuitively, $O_0(v)$ is the indicator function that decides whether node $v$ is included in the solution after the second step of the greedy algorithm, and $O_k$ is the indicator function that decides whether node $v$ is included in the solution when no node covers more than $\Delta + 1 - k$ uncovered nodes in the third step of the algorithm.

$O_0(v)$ returns 1 if there exists a node $u \in N_2(v)$ with the same random value as $v$ and returns 0 otherwise.

$O_k(v)$ returns 1 if $O_{k-1}(v) = 1$. Otherwise, it queries $\{O_{k-1}(u) \mid u \in N_2(v) \text{ and } r_u > r_v\}$ and $\{O_k(u) \mid u \in N_2(v) \text{ and } r_u < r_v\}$ to determine that the number of uncovered nodes covered by $v$. If $v$ covers $\Delta + 2 - k$ uncovered nodes, $O_k(v)$ returns 1 and returns 0 otherwise, where $r_u < r_v$ is a lexicographical comparison.

$O_{\Delta + 1}(v)$ decides whether $v$ is in the solution of the greedy algorithm. Irrespective of the size of the input graph, this oracle stops within a constant number of steps w.h.p. by the locality lemma (Nguyen & Onak, 2008). Therefore, the following lemma holds true.

Lemma 3. For all $\varepsilon > 0$, there exist $L \in \mathbb{Z}^+$, $p \in \mathbb{R}^+$, and a function $f$ that takes a graph and a node as input and outputs a binary value s.t. $\forall \mu \in \mathcal{U}(p)$, $G = (V, E) \in \mathcal{F}(\Delta)$, let $r_v \sim \mu (\forall v \in V)$. Then $(G, v) \simeq (G', v') \Rightarrow f(G, v) = f(G', v')$, $F = \{v \in V \mid f(R(V, E, R), v, L), v) = 1\}$ always forms a dominating set, $\{v \in V \mid \exists s, t \in N_k(v) s.t. r_s = r_t \subseteq F\}$ always holds, and $|F| \leq (H(\Delta + 1) + \varepsilon) \cdot \text{OPT}_m(\Pi_{\text{MDS}}, G)$ holds w.h.p.

It can be proved that rGINs can simulate the function $f$ above and can learn an approximation algorithm for the minimum dominating set problem with a small approximation ratio (Table 1).

Theorem 4. For all $\varepsilon > 0$, there exist parameters $\theta, p \in \mathbb{R}^+$ such that for all distributions $\mu \in \mathcal{U}(p)$ and graphs $G \in \mathcal{F}(\Delta)$, $r\text{GIN}_V(G, \mu, \theta) \in \Pi_{\text{MDS}}(G)$ always holds and $|r\text{GIN}_V(G, \mu, \theta)| \leq (H(\Delta + 1) + \varepsilon) \cdot \text{OPT}_m(\Pi_{\text{MDS}}, G)$ holds w.h.p.

4.4.2. Maximum Matching Problems

In this section, we study the maximum matching problem. We assume the existence of at least one edge because; otherwise, the problem becomes trivial. We modify a constant time algorithm for the maximum matching problem $\Pi_{\text{MM}}$ and prove that rGINs can simulate this algorithm. Nguyen & Onak (2008) converted a sequential greedy algorithm into a constant time algorithm. We use a slightly different version of the sequential algorithm. This algorithm constructs the solution $M$ from the empty set by the following procedure.

1. Assign a random value $r_v \sim \mu$ to each node $v \in V$.
2. Let $F \subseteq E$ be a set of edges $e = \{u, v\}$ such that there exist nodes $s, t \in N_k(u) \cup N_k(v)$ such that $r_s = r_t$.
3. for $k = 1, 2, \ldots, t$.
This sequential algorithm satisfies the following property.

**Lemma 5.** For all \( \varepsilon > 0 \), there exist \( t \in \mathbb{Z}^+ \) and \( p \in \mathbb{R}^+ \) such that for any distribution \( \mu \in \mathcal{U}(p) \), the algorithm is a consistent \((1 + \varepsilon)\)-approximation algorithm for the maximum matching problem.

Similar to the minimum dominating set problem (Section 4.4.1), this sequential algorithm can be converted to a constant time algorithm and simulated by rGINs.

**Theorem 6.** For all \( \varepsilon > 0 \), there exist parameters \( \theta, p \in \mathbb{R}^+ \) such that for all distributions \( \mu \in \mathcal{U}(p) \) and graphs \( G \in \mathcal{F}(\Delta) \), \( r\text{GIN}_E(G, \mu, \theta) \in \Pi_{\text{MM}}(G) \) always holds and \[ |r\text{GIN}_E(G, \mu, \theta)| \geq \frac{1}{1 + \varepsilon} \text{OPT}_M(\Pi_{\text{MM}}, G) \] holds w.h.p.

### 4.5. Opposite Direction

So far, we have demonstrated that a certain type of constant algorithm can be converted to randomized GNNs. Next, we prove the opposite direction. The next theorem indicates that the advancement of GNN theory promotes the theory of constant time algorithms.

**Theorem 7.** If there exist parameters of rGINs that represent a consistent minimization (resp. maximization) algorithm of \( \Pi \) with approximation ratio \( \alpha \), there exists a constant time algorithm that estimates an \((\alpha, \varepsilon)\)-approximation of \( \text{OPT}_m(\Pi, G) \) (resp. \( \text{OPT}_M(\Pi, G) \)) w.h.p.

Owing to this theorem, machine learning researchers have chances to contribute to the algorithm field by demonstrating a new problem that rGINs or GINs can solve or finding effective architectures or features of GNNs.

### 5. Experiments

We confirm the theoretical results via numerical experiments. We slightly modify the original implementation of GINs\(^1\) to introduce random features. We also use Graph Convolutional Networks (GCNs) and GCNs with random features (rGCNs) to confirm that the addition of the random features can improve the expressive power of GNN architectures other than GINs. In the experiments, we use the uniform distribution over \( D = \{0, 0.01, 0.02, \ldots, 0.99\} \) as the random distribution \( \mu \). The experimental setup and implementation details have been described in the supplementary material.

#### 5.1. Learning Substructures

We confirm that rGINs can distinguish local substructures, proven in Theorem 1. We use four synthetic datasets in this experiment.

- **TRIANGLE**: This dataset contains random 3-regular graphs for a binary node classification problem. Both training and test data contain 1000 graphs. The training graphs have 20 nodes, and test graphs have 20 nodes for the normal dataset (denoted by (N)) and 100 nodes for the extrapolation dataset (denoted by (X)). A node \( v \) is positive if \( v \) has two neighboring nodes that are adjacent to each other.

- **LCC**: This dataset contains random 3-regular graphs for a multi-label node classification problem. Both training and test data contain 1000 graphs. The training graphs have 20 nodes, and test graphs have 20 nodes for the normal dataset and 100 nodes for the extrapolation dataset. The class of node \( v \) is the local clustering coefficient (Watts & Strogatz, 1998) of \( v \).

Learning the local clustering coefficient is important because this is a useful feature for spam detection and estimating content quality (Becchetti et al., 2008; Welser et al., 2007). The training data and test data of TRIANGLE(N) and LCC(N) contain the same number of nodes, but the test graphs of TRIANGLE(X) and LCC(X) have more nodes than the training graphs. As stated in Sections 1 and 4, the advantage of rGINs is that they can generalize to graphs with variable size, whereas relational pooling (Murphy et al., 2019) cannot. We confirm this using extrapolation datasets.

We measure the ROC-AUC scores for TRIANGLE(N) and TRIANGLE(X), and measure the average of the AUC score for each category of the LCC(N) and LLC(X) datasets because they are multi-label problems. The first four columns of Table 2 report the AUC scores for the test data of these datasets. This indicates that rGINs and rGCNs can learn substructures from data whereas GINs and GCNs cannot distinguish substructures in these datasets. Indeed, the existence of a triangle or the local clustering coefficient can be added as a node feature by hand. However, it is important to note that rGINs and rGCNs can learn these structures from the data without including these structures as node features explicitly. This indicates that rGINs and rGCNs can implicitly utilize the characteristic substructures for positive or negative examples (e.g., chemical functional groups) for classification. This is desirable because there are too many...

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\(^1\)https://github.com/weihua916/powerful-gnnns
Table 2. Each value stands for an ROC-AUC score. * means a statistically significant improvement for the paired t-test with α = 0.05.

|      | TRI(N) | TRI(X) | LCC(N) | LCC(X) | MDS(N) | MDS(X) | MUTAG | NCI1 | PROTEINS |
|------|--------|--------|--------|--------|--------|--------|-------|------|----------|
| GINs | 0.500  | 0.500  | 0.500  | 0.500  | 0.500  | 0.500  | 0.946 | 0.870 | 0.806    |
| rGINs| 0.908  | 0.926  | 0.811  | 0.852  | 0.659  | 0.652  | 0.949 | 0.876 | 0.810    |
| GCNs | 0.500  | 0.500  | 0.500  | 0.500  | 0.500  | 0.500  | 0.890 | 0.819 | 0.804    |
| rGCNs| 0.855  | 0.877  | 0.784  | 0.785  | 0.651  | 0.644  | 0.904 | 0.816 | 0.812    |

Figure 2. Scatter plot of node embeddings generated by rGINs with different random feature seeds.

5.2. Learning Algorithms

We confirm that rGINs can learn algorithms for combinatorial problems. In particular, we confirm that rGINs can learn the sequential greedy algorithm (Johnson, 1974; Lovász, 1975) for the minimum dominating set problem, as shown in Theorem 4. In this experiment, the training graphs and test graphs are random 3-regular graphs. Both the training and test data contain 1000 graphs. The training graphs have 20 nodes and the test graphs of MDS(N) and MDS(X) have 20 and 100 nodes, respectively. The labels of nodes depend on the assigned random features. We simulate the greedy algorithm using the order of assigned random features. We set the label of a node as positive if that node is included into the solution of the algorithm and negative otherwise. The fifth and sixth columns of Table 2 report the AUC scores for the test data of these datasets. This result shows that rGINs and rGCNs can learn some concept of the sequential algorithm whereas GINs and GCNs cannot. Note that the AUC score of rGINs is not significantly high because we used a predetermined architecture, which may be insufficient to completely imitate the algorithm, and the learned parameters are suboptimal due to the learning process. However, it is clearly higher than the AUC score of the ordinary GINs.

5.3. Real World Datasets

In this section, we confirm the effect of random features on real world datasets. We assess the performance of rGINs using three biological datasets: MUTAG, NCI1, and PROTEINS. We measure the cross validation scores following the works of Xu et al. (2019) and Niepert et al. (2016) because the evaluation is unstable due to the small dataset sizes. It should be noted that the hyperparameters to be tuned are the same for GINs and rGINs because the distribution of random features was fixed beforehand. The sixth to eighth columns of Table 2 summarize the AUC scores, which show that rGINs are comparable or slightly outperform the ordinary GINs. The performance gain is less drastic compared to TRIANGLE and LCC datasets because the degrees of nodes differ in the real world datasets, and the original GINs can distinguish most nodes using the degree signals. However, this experiment shows that adding random features does not harm the performance for real world datasets. As shown in the above experiments, and known as a folklore, GINs cannot distinguish regular graphs of the same size, whereas rGINs can. For example, GINs cannot distinguish between the decaprismane C_{20}H_{20} (Schultz, 1965) and the dodecahedrane C_{20}H_{20} (Paquette et al., 1983), which means that GINs always fail to classify these molecules if they belong to different categories. In contrast, rGINs can distinguish them by the existence of cycles of length four. This result suggests that the addition of the random features is a handy practice to ensure the capability of GNNs without harming the performance even with slight improvements.
6. Conclusion

In this paper, we show that the addition of the random features theoretically strengthens the capability of GINs. Especially, GINs with random features (rGINs) can distinguish any local substructures w.h.p. and solve the minimum dominating set problem and maximum matching problem with almost optimal approximation ratios. The main advantage of rGINs is that they can guarantee the capability even in the test time with arbitrarily large test graphs. In the experiments, we show that rGINs can solve three problems that the normal GINs cannot solve, i.e., determining the existence of a triangle, computing local cluster coefficients, and learning the greedy algorithm for the minimum dominating set problem. We also show that rGINs slightly outperform the normal GINs for biological real world datasets.

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A. Experimental Setups

A.1. General Setups

In the experiments, we use five-layered GNNs (including the input layer). In our experiments, the Graph Convolutional Networks (GCNs) aggregate the features by average pooling, following the work of Xu et al. (2019) whereas the original model (Kipf & Welling, 2017) uses symmetrized normalization. We train models with the Adam optimizer (Kingma & Ba, 2015) with an initial learning rate of 0.01 and batch size of 32. We decay the learning rate by 0.5 every 50 epochs. We use dropout in the final layer with a dropout rate of 0.5 for graph classification datasets (i.e., MUTAG, NCI1, and PROTEINS). We do not train the parameters ε because Xu et al. (2019) showed that it does not affect the performance. We train models for 350 epochs for the TRIANGLE, LCC, and MDS datasets, and select the number of epochs from \{1, 2, \ldots, 350\} by cross-validation for MUTAG, NCI1, and PROTEINS datasets. It is noteworthy that these hyperparameter settings are the default values of the open implementation of GINs https://github.com/weihua916/powerful-gnns, which have been shown to be effective in practice.

A.2. Graph Synthesis Process

We generate graphs for TRIANGLE, LCC, and MDS datasets by the random_degree_sequence_graph function of networkx package (Bayati et al., 2010; Hagberg et al., 2008). All graphs are generated by the same process with different seeds. Figures below show examples of test graphs of the TRIANGLE(S) dataset.

B. Proofs

Lemma 8. \(\forall L \in \mathbb{Z}^+, \epsilon > 0, \exists p > 0\) s.t. \(\forall \mu \in U(p), \forall G = (V, E) \in \mathcal{F}(\Delta), \) let \(r_v \sim \mu, \) then \(\forall v \in V, Pr[\exists x, y \in \mathcal{N}_L(v), r_x = r_y] < \epsilon.\)

Proof of Lemma 8. Let \(L \in \mathbb{Z}^+\) be an arbitrary positive integer and \(\epsilon > 0\) be an arbitrary positive number. Let \(p = \Delta^{-2(L+2)} \epsilon. \) \(\forall \mu \in U(p), \forall G = (V, E) \in \mathcal{F}(\Delta) \forall s, t \in V, Pr[r_s = r_t] \leq p.\) Because \(|\mathcal{N}_L(v)| < \Delta^{L+2},\)

\[\forall v \in V, Pr[\exists x, y \in \mathcal{N}_L(v), r_x = r_y] < \Delta^{2(L+2)}p = \epsilon.\]

Definition (T): For \(G \in \mathcal{F}(\Delta, C), R \in \mathbb{D}^n, v \in G,\) and \(l \in \mathbb{Z}^+\), let \(T(G, v, l)\) be

\[T(G, v, 0) = (x_v, r_v)\]

\[T(G, v, l) = (T(G, v, l - 1), \text{MULTISET}(T(G, u, l - 1) \mid u \in \mathcal{N}(v)))\]

We call \(T(G, v, l)\) a level-l tree.

Corollary 9 (from (Xu et al., 2019)). For all \(l \in \mathbb{Z}^+,\) there exist parameters \(\theta\) of GINs such that for all \(G = (V, E, X), G' = (V', E', X') \in \mathcal{F}(\Delta, C), R \in \mathbb{D}^{|V|}, R' \in \mathbb{D}^{|V'|}, v \in V, v' \in V'\) if \(T(G, v, L) \neq T(G', v', L)\) holds, \(\text{GIN}_\theta((V, E, [X, R]), v) \neq \text{GIN}_\theta((V', E', [X', R']), v')\) holds.

Lemma 10. For all \(L \in \mathbb{Z}^+,\) there exists a function \(f\) such that for all \(G = (V, E, X) \in \mathcal{F}(\Delta, C), R \in \mathbb{D}^n, v \in G,\) if for all \(s, t \in \mathcal{N}_{L+1}(v), r_s \neq r_t\) holds,

\[f(T(R(G, v, L), v, L + 1)) \simeq (R(G, v, L), v).\]
Proof of Lemma 10. We construct $f(T) \in \mathcal{F}(\Delta)$. Let the node set $V'$ be all $r_p$ of level-0 sets $[x_p, r_p]$ that $T[0]$ (i.e., the left element of $T$) contains, and the feature vector $x'_{r_p}$ be equal to one of $x_p$ (e.g., the smallest one). If for all $s, t \in \mathcal{N}_L(v), r_s \neq r_t$, holds, the choice of $x'_{r_p}$ is unique, and the number of nodes is the same as $G$. Let the center node be $v' = T[0][0] \ldots [0][1]$ (i.e., the right element of the leftmost level-0 set), $v'$ is equal to $r_v$ by construction. For $p, q \in V'$, $(p, q)$ is included in $E'$ if and only if there exists a level-1 set $T'$ such that the right element of the rightmost level-0 set to $T'$ is equal to $p$, and a level-0 set whose right element is equal to $q$ is included in the right element of $T'$. There exists an edge between $s, t \in E$ if and only if there exists an edge between $r_s, r_t \in E'$ by construction. Therefore, $f(T) = ((V', E', X', v')) \approx (R(G, v, L), v)$ holds.

Proof of Theorem 1. From Corollary 9 and Lemma 10, for all $L \in \mathbb{Z}_+$, there exist parameters $\theta$ of GINs such that for all $G = (V, E, X), G' = (V', E', X') \in \mathcal{F}(\Delta, C), R \in D^{V_s}, R' \in D^{V'_s}, v \in V, v' \in V'$ if (1) for all $s, t \in \mathcal{N}_{L+1}(v), r_s \neq r_t$, (2) for all $s', t' \in \mathcal{N}_{L+1}(v'), r_{s'} \neq r_{t'},$ and (3) $(R(G, v, L), L) \neq (R(G', v', L), L')$ hold, $\text{GL}(G, v, L, v, X) \neq \text{GL}(G', v', L, v', X')$ holds. The cardinality of $\{R((V, E, [X, R]), v, L) | G = (V, E, X) \in \mathcal{F}(\Delta, C), v \in V, R \in D^{V_s}\}$ is finite. Therefore, there exists a multi layer perceptron MLP such that if the first and second conditions are valid, $\text{MLP}(\text{GL}(G, v, L, v, X)) > 0.5$ if $G', v' \in G$ such that $(G', v') \approx (R(G, v, L), L)$ holds and $\text{MLP}(\text{GL}(G', v', L, v, X')) < 0.5$ otherwise. This MLP can be considered as the last layer of the GIN. From Lemma 8, there exists $p$ such that for all $\mu \in \mathcal{U}(p), the probability of the first and second conditions being true is arbitrarily small.

Proof of Lemma 2. Let $U = \{v \in V | \exists u \in \mathcal{N}_2(v) \text{ s.t. } r_v = r_u \}$ and $U^+ = \{v \in V | \exists u \in \mathcal{N}(v) \text{ s.t. } u \in U\}$. The solution $S$ our sequential algorithm outputs for $G$ is the same as the union of $U^+$ and the solution $T$ the sequential algorithm (Nguyen & Onak, 2008; Lovász, 1975; Johnson, 1974) outputs for the induced graph $G' \setminus (U^+)$ by construction. From Lemma 8, there exists $p$ such that for all $\mu \in \mathcal{U}(p), |U| \leq \frac{\varepsilon}{\Delta + 1} \cdot n$ with high probability. It means that $|U| \leq \varepsilon \text{OPT}_m(\Pi_{\text{MDS}}, G')$ because for any $G = (V, E) \in \mathcal{F}(\Delta), \text{OPT}_m(\Pi_{\text{MDS}}, G) \geq \frac{\Delta}{\Delta + 1} \cdot n$ holds. Therefore, with high probability,$S \leq |U| + |T| 
\leq (H(\Delta + 1) + \varepsilon) \text{OPT}_m(\Pi_{\text{MDS}}, G') 
\leq (H(\Delta + 1) + \varepsilon) \text{OPT}_m(\Pi_{\text{MDS}}, G)$

Proof of Lemma 3. Let $S_L = \{v \in V | \text{ the computation of } C_{\Delta+1}(v) \text{ stops within } R(G, v, L)\}, U_L = \{v \in V | \exists s, t \in \mathcal{N}_L(v) \text{ s.t. } r_s = r_t\}, A = \{v \in V | \mathcal{O}_{\Delta+1}(v) = 1\}$. For fixed $R$, let $f$ be a function that outputs 1 if $v \in f = S_L \cup U_L \cup A$, and 0 otherwise. This value can be computed online from $(R(G, v, L), v)$. From the locality lemma (Nguyen & Onak, 2008), there exists $L \in \mathbb{Z}_+$ such that $|S_L| \leq \frac{\varepsilon}{3(\Delta + 1)} \cdot n \leq \frac{\varepsilon}{5} \text{OPT}_m(\Pi_{\text{MDS}}, G)$ holds w.h.p. From Lemma 8, $|U_L| \leq \frac{\varepsilon}{3(\Delta + 1)} \cdot n \leq \frac{\varepsilon}{5} \text{OPT}_m(\Pi_{\text{MDS}}, G)$ holds w.h.p. if $p$ is sufficiently large. From Lemma 2, there exists $p$ such that for all $\mu \in \mathcal{U}(p), |A| \leq (H(\Delta + 1) + \frac{\varepsilon}{5}) \text{OPT}_m(\Pi_{\text{MDS}}, G)$ holds w.h.p. $F$ always forms a dominating set because $A \subseteq F$. From the above equations, $|f| \leq |S_L| + |U_L| + |A| \leq (H(\Delta + 1) + \varepsilon) \text{OPT}_m(\Pi_{\text{MDS}}, G)$ holds w.h.p.

Proof of Theorem 4. From Corollary 9, Lemma 10, and Lemma 3, there exist parameters $\theta$ of GINs such that $\forall G = (V, E) \in \mathcal{F}(\Delta), \forall R \in D^{V_s}$,

$\{v \in V | \text{GIN}_\theta((V, E, R)) > 0.5\} \cup \{v \in V | \exists s, t \in \mathcal{N}_L(v) \text{ s.t. } r_s = r_t\} = \{v \in V | f(R((V, E, R), v, L), v) = 1\}$,

where $f$ is the function in the proof of Lemma 3. Therefore, $r\text{GINs}$ can simulate $f$, which is $(H(\Delta + 1) + \varepsilon)$-approximation w.h.p.

Proof of Lemma 5. Let $F = \{u \in u, v \in E | \exists s, t \in \mathcal{N}_L(u) \cup \mathcal{N}_L(v) \text{ s.t. } r_s = r_t\}$. The solution $S$ our sequential algorithm outputs for $G$ is the same as the solution $T$ the sequential algorithm (Nguyen & Onak, 2008) outputs for $G' = (V, E, F)$. Let $\varepsilon' = \frac{\varepsilon}{5}$. From (Nguyen & Onak, 2008), the sequential algorithm (Nguyen & Onak, 2008) is $(1 + \varepsilon')$-approximation by setting $t = \text{ceil}(\frac{1}{\Delta})$. From Lemma 8, there exists $p \in \mathbb{R}^+$ such that for all $\mu \in \mathcal{U}(p), |F| \leq \frac{\varepsilon'}{\Delta + 1} \cdot n$
because $|E| \leq \frac{2}{\Delta} n$ by the degree-bounded assumption. When an edge is added to the solution, at most $2\Delta$ candidate edges are excluded. Therefore,

$$\text{OPT}_M(\Pi_{\mathcal{MM}}, G) \geq \frac{m}{2\Delta} \geq \frac{n-1}{2\Delta} \geq \frac{n}{4\Delta}$$

holds. Furthermore,

$$\frac{1}{1 + \varepsilon'} - \frac{1}{1 + \varepsilon} = \frac{\varepsilon - \varepsilon'}{(1 + \varepsilon')(1 + \varepsilon)} \geq \frac{\varepsilon - \varepsilon'}{2(1 + \varepsilon)^2}$$

holds. Therefore,

$$|S| = |T| \geq \frac{1}{1 + \varepsilon'} \text{OPT}_M(\Pi_{\mathcal{MM}}, G') \geq \frac{1}{1 + \varepsilon'} (\text{OPT}_M(\Pi_{\mathcal{MM}}, G) - |F|) \geq \frac{1}{1 + \varepsilon'} \text{OPT}_M(\Pi_{\mathcal{MM}}, G) - \frac{\varepsilon}{8(1 + \varepsilon)^2} n \geq \frac{1}{1 + \varepsilon} \text{OPT}_M(\Pi_{\mathcal{MM}}, G) - \frac{\varepsilon}{2(1 + \varepsilon)^2} \text{OPT}_M(\Pi_{\mathcal{MM}}, G) \geq \frac{1}{1 + \varepsilon} \text{OPT}_M(\Pi_{\mathcal{MM}}, G).$$

This concludes that our sequential algorithm is $(1 + \varepsilon)$-approximation.

**Proof of Theorem 6.** We assume $D = [k]$ for some $k \in \mathbb{Z}^+$ without loss of generality. Let $S$ be the solution that our algorithm outputs for $G = (V, E)$. By the locality lemma and Lemma 7 of \cite{Nguyen&Onak:2008}, there exists $L \in \mathbb{Z}^+$ such that there exists an algorithm $A$ that takes $G' = (V, E, R)$ and $e = \{v, u\} \in E$ and decides $e \in S$ or not with the following property: Let $T = \{e \in E \mid A$ accesses $G \setminus (R(G', u, L) \cap R(G', v, L))$ to decide $e \in S$ or not $\}$, then $|T| \leq \frac{\varepsilon}{16\Delta} n$ w.h.p. with respect to the randomness of $R$. Take $L$ such that $|S| \geq \frac{1}{1 + \varepsilon/4} \text{OPT}_M(\Pi_{\mathcal{MM}}, G)$ holds w.h.p. Let $F = \{e = \{u, v\} \in E \mid \exists s, t \in N_L(u) \cap N_L(v) \text{ s.t. } r_s = r_t\}$ and $U = \{v \in V \mid \exists s, t \in N_L(v) \text{ s.t. } r_s = r_t\}$. Let $g(R(G', v, L), v) \in \mathbb{R}^{k^2}$ be $0 \in \mathbb{R}^{k^2}$ if $v \in U$. Otherwise, $g(R(G', v, L), v)i = 1$ if there is an edge $\{u, v\} \in E$ such that $e \in S \setminus (F \cup T)$ and $i = \min\{r_u, r_v\} + \max\{r_u, r_v\} - k$ hold, and 0 otherwise. $g$ can be computed only from $R(G', v, L)$ and $v$ by construction. For any pair of nodes $u, v \in (V \setminus U)$, $e = \{u, v\} \in S \setminus (F \cup T)$ holds if and only if $g(R(G', u, L), u)^\top g(R(G', v, L), v) = 1$ by construction. Therefore, $A = \{g(R(G', u, L), u)^\top g(R(G', v, L), v) > 0.5 \} \subseteq \Pi_{\mathcal{MM}}(G)$ holds because $A \subseteq S$. By Lemma 8 and Lemma 5, there exists $p$ such that for all $\mu \in \mathcal{U}(p)$, $|A| \geq \frac{1}{1 + \varepsilon} \text{OPT}_M(\Pi_{\mathcal{MM}}, G)$ w.h.p. By the same argument as Theorem 4, $g$ can be simulated by rGINs because $g$ only depends on $R(G', v, L)$, and $g(R(G', v, L), v) = 0$ if $v \in U$.

**Proof of Theorem 7.** Let $\theta$ and $\mu$ be the parameters and distributions of rGINs that represent an $\alpha$ approximation algorithm of $\Pi$. Let $L$ be the number of layers in the rGIN. Draw the random feature $r_u$ when the rGINs first accesses the node $u \in V$. Then, for each $v \in V$, rGINs$(G, \mu, \theta)_v$ can be computed in a constant time because the size of $R(G, v, L)$ is bounded by a function of $L$ and $\Delta$, which are constant. For a node problem, sample $O(\frac{1}{\Delta})$ nodes $U \subseteq V$ uniformly randomly, and decide each node $v \in U$ is included in the solution by computing rGINs$(G, \mu, \theta)_v$. For an edge problem, sample $O(\frac{1}{\Delta})$ edges $F$ uniformly randomly, and decide each edge $e = \{u, v\} \in F$ is included in the solution by computing the rGINs$(G, \mu, \theta)_u$ and rGINs$(G, \mu, \theta)_v$. From the Hoeffding bound, the size of the solution can be estimated with additive error $\varepsilon n$ w.h.p.