Abstract

Graph neural networks (GNNs) have emerged recently as a powerful architecture for learning node and graph representations. Standard GNNs have the same expressive power as the Weisfeiler-Leman test of graph isomorphism in terms of distinguishing non-isomorphic graphs. However, it was recently shown that this test cannot identify fundamental graph properties such as connectivity and triangle freeness. We show that GNNs also suffer from the same limitation. To address this limitation, we propose a more expressive architecture, $k$-hop GNNs, which updates a node’s representation by aggregating information not only from its direct neighbors, but from its $k$-hop neighborhood. We show that the proposed architecture can identify fundamental graph properties. We evaluate the proposed architecture on standard node classification and graph classification datasets. Our experimental evaluation confirms our theoretical findings since the proposed model achieves performance better or comparable to standard GNNs and to state-of-the-art algorithms.

1 Introduction

In the past years, the amount of graph-structured data has grown steadily in a wide range of domains, such as in social networks and in chemoinformatics. Learning useful representations from graph data is essential for many real-world applications. For instance, in social network analysis, one might be interested in predicting the interests of users represented by the nodes of a network [35]. In biology, an issue of high interest is the prediction of the functions of proteins modeled as graphs [3]. These applications typically involve either node-focused or graph-focused tasks, the difference lying in the entity of interest, a node or a graph.

Graph Neural Networks (GNNs) have recently emerged as a general framework addressing both node-related and graph-related tasks [4]. Although numerous GNN variants have been proposed in the past years [9, 24, 13, 17, 10, 14, 31, 37], they all share the same basic idea, and can be reformulated into a single common framework. Specifically, GNNs employ a message passing procedure, where each node updates its feature vector by aggregating the feature vectors of its neighbors [7]. After $k$ iterations of the message passing procedure, each node obtains a feature vector which captures the structural information within its $k$-hop neighborhood. These representations can be used as features for node-related tasks. For graph-related tasks, GNNs compute a feature vector for the entire graph using some permutation invariant readout function such as summing the feature vectors of all the nodes of the graph.

Preprint. Work in progress.
The GNN architectures have achieved state-of-the-art performance in many tasks such as in node classification and in link prediction. Furthermore, they have seen considerable success in graph-related tasks even though they have faced intense competition from graph kernels, the approach that dominated the field for more than a decade [21]. With the exception of the work of Scarselli et al. [25], until recently, there has been little attempt to understand the properties and limitations of GNNs. It was clear though that there is a close connection between GNNs and the Weisfeiler-Lehman (WL) test of graph isomorphism [32], a powerful heuristic which can successfully test isomorphism for a broad class of graphs [1]. Similar to GNNs, the WL test iteratively updates a given node’s label by aggregating the labels of its neighbors. Specifically, the algorithm augments the label of each node by the sorted multiset of labels of neighboring nodes, and compresses these augmented labels into new, short labels. To test graph isomorphism, this relabeling procedure is repeated until the label sets of the input graphs are not identical, or the number of iterations reaches a specific value.

Some recent studies have made attempts to formally characterize the expressive power of GNNs [19, 34]. These studies have compared the expressiveness of GNNs with that of the WL test, and have shown that GNNs do not have more power in terms of distinguishing between non-isomorphic graphs than the WL algorithm. To make matters worse, it was recently shown that the WL subtree kernel (which capitalizes on the WL test) has insufficient expressive power for identifying fundamental graph properties [16]. It remains though unclear how GNNs encode subgraph/graph information into their learned representations, and whether they can identify such properties. Since these architectures are directly related to the WL test, they may also lack expressive power, and they may fail to identify these properties. Hence, the need for more powerful representations is more essential than ever.

Present Work. In this paper, we further analyze the representational power of GNNs. Specifically, we study if GNNs can identify specific properties of graphs. We say that a GNN identifies a property if no two graphs are mapped to the same feature vector unless they both have or both do not have the property. We demonstrate that the standard GNN fails to identify fundamental graph properties such as connectivity, bipartiteness and triangle-freeness. We show that this limitation of GNNs stems from the myopic nature of the message-passing procedure which only considers the direct neighbors of each node. To account for that, we propose a novel architecture, called \(k\)-hop-GNNs, which takes into account not only the immediate neighbors of each node, but its whole \(k\)-hop neighborhood. By updating node features using not only the direct neighbors, but taking into account the entire \(k\)-hop neighborhood, we can capture structural information that is not visible when aggregating only the 1-hop neighborhood. The proposed model is strictly more powerful than the standard GNN architecture. Furthermore, in contrast to the GNN framework, the proposed architecture is capable of distinguishing global properties such as connectivity. We demonstrate the proposed architecture in a variety of node and graph classification tasks. The results show that the proposed \(k\)-hop-GNNs are able to consistently outperform traditional GNNs on most datasets. Our main contributions are summarized as follows:

- We show that standard GNNs cannot identify essential graph properties such as connectivity, bipartiteness and triangle-freeness
- We propose \(k\)-hop-GNNs, a novel architecture for performing machine learning on graphs which is more powerful than traditional GNNs.
- We evaluate the proposed architecture on several node classification and graph classification datasets, and achieve performance better or comparable to standard GNNs and to state-of-the-art algorithms.

The rest of this paper is organized as follows. Section 2 introduces some preliminary concepts and summarizes the standard graph neural network model. Section 3 analyzes the expressive power of the graph neural network model highlighting its limitations. Section 4 presents the proposed model for performing machine learning tasks on graph-structured data, and shows that it is theoretically more powerful than the standard graph neural network architecture. Section 5 evaluates the proposed architecture on several standard datasets. Finally, Section 6 concludes.

2 Preliminaries

We start by fixing our notation, and we then present the standard graph neural network framework.
2.1 Notation

Let $G = (V, E)$ be an undirected graph consisting of a set $V$ of nodes and a set $E$ of edges between them. We will denote by $n$ the number of nodes and by $m$ the number of edges. The neighborhood of radius $k$ (or $k$-hop neighborhood) of a node $v \in V$ is the set of nodes at a distance less than or equal to $k$ from $v$ and is denoted by $N_k(v)$. Given a set of nodes $S \subseteq V$, the subgraph induced by $S$ is a graph that has $S$ as its node set and it contains every edge of $G$ whose endpoints are in $S$. The neighborhood subgraph of radius $k$ of a node $v \in V$ is the subgraph induced by the neighborhood of radius $k$ of $v$ and $v$ itself, and is denoted by $G^k_v$. A node-labeled graph is a graph with labels on nodes. That is, given a set of labels $L$, there exists a function $\ell : V \rightarrow L$ that assigns labels to the nodes of the graph. Instead of discrete labels, nodes may also be annotated with multiple categorical or real-valued properties. These graphs are known as attributed graphs.

2.2 Graph Neural Networks

Let $G = (V, E)$ be a graph. Suppose each vertex $v \in V$ is annotated with a feature vector $h_v^{(0)} \in \mathbb{R}^d$. For graphs with discrete node labels, these vectors usually correspond to some representations (e.g., one-hot encoding) such that two nodes $v$ and $u$ have identical feature vectors if and only if $\ell(v) = \ell(u)$. For attributed graphs, these feature vectors may be set equal to the attribute vectors of the nodes. For instance, in biology, proteins are represented as graphs where nodes correspond to secondary structure elements and the feature vector of each secondary structure element contains its physical properties. For graphs without node labels and node attributes, these vectors can be initialized with a collection of local vertex features that are invariant to vertex renumbering (e.g., degree, $k$-core number, number of triangles, etc). A GNN model consists of a series of neighborhood aggregation layers. Each one of these layers uses the graph structure and the node feature vectors from the previous layer to generate new representations for the nodes. The feature vectors are updated by aggregating local neighborhood information.

Suppose we have a GNN model that contains $T$ neighborhood aggregation layers. In the $t$th neighborhood aggregation layer ($t > 0$), the hidden state $h_v^{(t)}$ of a node $v$ is updated as follows:

$$a_v^{(t)} = \text{AGGREGATE}^{(t)} \left( \{ h_u^{(t-1)} | u \in N_1(v) \} \right)$$

$$h_v^{(t)} = \text{MERGE}^{(t)} \left( h_v^{(t-1)}, a_v^{(t)} \right)$$

(1)

By defining different $\text{AGGREGATE}^{(t)}$ and $\text{MERGE}^{(t)}$ functions, we obtain a different GNN variant. For the GNN to be end-to-end trainable, both functions need to be differentiable. Furthermore, since there is no natural ordering of the neighbors of a node, the $\text{AGGREGATE}^{(t)}$ function must be permutation invariant. There are numerous concrete implementations of the above GNN framework. Some of them integrate the $\text{AGGREGATE}^{(t)}$ and $\text{MERGE}^{(t)}$ steps into a single function [14, 37] as follows:

$$h_v^{(t)} = \frac{1}{|N_1(v)| + 1} \sum_{u \in N_1(v) \cup \{v\}} \text{MLP}^{(t)} \left( h_u^{(t-1)} \right)$$

where $\text{MLP}^{(t)}$ is a multi-layer perceptron of the $t$th neighborhood aggregation layer. Note that the majority of the proposed models use 1-layer perceptrons instead of MLPs. Another widely-used GNN model is implemented as follows [17]:

$$a_v^{(t)} = \frac{1}{|N_1(v)|} \sum_{u \in N_1(v)} \text{MLP}_1^{(t)} \left( h_u^{(t-1)} \right)$$

$$h_v^{(t)} = \text{MLP}_2^{(t)} \left( h_v^{(t-1)} + a_v^{(t)} \right)$$

(2)

where again $\text{MLP}_1^{(t)}$ and $\text{MLP}_2^{(t)}$ are multi-layer perceptrons of the $t$th neighborhood aggregation layer.

For node-level tasks, the node feature vectors $h_v^{(T)}$ of the final neighborhood aggregation layer are usually passed on to a fully-connected neural network. For graph-level tasks, GNNs apply a READOUT function to node representations generated by the final neighborhood aggregation layer.
We next study if the standard GNN architecture can identify the above three graph properties. We get

Theorem 1. The standard GNN cannot identify connectivity, bipartiteness or triangle freeness.

To gain theoretical understanding of the properties and weaknesses of GNNs, we capitalize on

Lemma 1. Let \( \mathcal{P} \) be a graph property. If for each \( n \in \mathbb{N} \), a GNN produces different representations for every \( G_1 \in \mathcal{P}_n \) and \( G_2 \notin \mathcal{P}_n \), i.e., it holds that \( h_{G_1} \neq h_{G_2} \), then we say that \( \mathcal{P} \) can be identified by the GNN.

We next study if the standard GNN architecture can identify the above three graph properties. We assume that either all nodes or nodes with the same degree are annotated with the same feature vector. We first show that the standard GNN produces exactly the same representation for the nodes of all regular graphs of a specific degree in \( \mathcal{G}_n \) for some \( n \in \mathbb{N} \).

Lemma 1. The standard GNN maps the nodes of two regular graphs of the same size and degree to the same feature vector.

Proof. Let \( G_1 = (V_1, E_1) \) and \( G_2 = (V_2, E_2) \) be two two non-isomorphic regular graphs of the same degree with the same number of vertices. We show for an arbitrary iteration \( t \geq 1 \) and nodes \( v_1 \in V_1 \), \( v_2 \in V_2 \) that \( h_{v_1}^{(t)} = h_{v_2}^{(t)} \). All nodes have the same initial representation, hence, in iteration 0, it holds that \( h_{v_1}^{(0)} = h_{v_2}^{(0)} \). Assume for induction that \( h_{v_1}^{(t-1)} = h_{v_2}^{(t-1)} \). Let \( \mathcal{M}_{v_1} = \{h_{u_1}^{(t-1)} : u_1 \in \mathcal{N}_1(v_1)\} \) and \( \mathcal{M}_{v_2} = \{h_{u_2}^{(t-1)} : u_2 \in \mathcal{N}_1(v_2)\} \) be the multisets of feature vectors of the neighbors of \( v_1 \) and \( v_2 \), respectively. By the induction hypothesis, we know that \( \mathcal{M}_{v_1} = \mathcal{M}_{v_2} \), and thus \( h_{v_1}^{(t-1)} = h_{v_2}^{(t-1)} \) such that independent of the choice of the AGGREGATE\(^{(t)} \) and MERGE\(^{(t)} \) functions in Equation 1 we get \( h_{v_1}^{(t)} = h_{v_2}^{(t)} \). This holds as the input to both functions AGGREGATE\(^{(t)} \) and MERGE\(^{(t)} \) is identical. This proves that \( h_{v_1}^{(t)} = h_{v_2}^{(t)} \), and thereby the lemma. □

Interestingly, since the standard GNN produces identical feature vectors for the nodes of all regular graphs of a specific degree in \( \mathcal{G}_n \) for some \( n \in \mathbb{N} \), then it also produces identical representations for the graphs themselves. We next show that the GNN architecture cannot identify the three graph properties defined above since for each one of these properties, there exists one regular graph in \( \mathcal{P}_n \) and another regular graph of the same degree in \( \mathcal{G}_n \setminus \mathcal{P}_n \).

Theorem 1. The standard GNN cannot identify connectivity, bipartiteness or triangle freeness.
Proof. Consider a cycle with six vertices (graph $G_2$) and two triangles with three vertices (graph $G_1$) as illustrated in Figure 1. Both $G_1$ and $G_2$ are regular graphs of the same degree with the same number of vertices. Hence, according to Lemma 1, after $T$ neighborhood aggregation steps, the nodes of both graphs have obtained identical representations, i.e., $h^{(T)}_u = h^{(T)}_v$, $\forall u, v \in V_1 \cup V_2$. Therefore, independent of the choice of the READOUT function in Equation 3, the two graphs will have identical representations, $h_{G_1} = h_{G_2}$, since the input to the READOUT function is identical. Clearly, $G_1$ is disconnected, while $G_2$ is connected. Hence, these two graphs correspond to a counterexample to the distinguishability of connectivity. Furthermore, consider the graphs $G_3$ and $G_4$ as illustrated in Figure 2. Note that $G_3$ contains triangles, but is not bipartite, whereas $G_4$ is bipartite, and triangle-free. Both $G_3$ and $G_4$ are regular graphs of the same degree with the same number of vertices. Therefore, they obtain identical representations $h_{G_3} = h_{G_4}$, and correspond thus to a counterexample to the distinguishability of the above two properties.

\[ h_u^{(t)} = \text{AGGREGATE}^{(t)} \left( \{ h_u^{(t-1)} | u \in N_k(v) \} \right) \]

\[ h_v^{(t)} = \text{MERGE}^{(t)} \left( h_v^{(t-1)}, a_v^{(t)} \right) \]

We next present an instance of the proposed architecture which is strictly stronger than standard GNNs in terms of distinguishing non-isomorphic graphs, and is capable of identifying graph properties which are not captured by the standard GNN architecture.

4 k-hop Graph Neural Networks

In this section, we propose a generalization of GNNs, so-called $k$-hop Graph Neural Networks ($k$-hop GNNs). This new model consists of neighborhood aggregation layers that do not take into account only the direct neighbors of the nodes, but their entire $k$-hop neighborhood. Hence, instead of the neighborhood aggregation layer shown in Equation 1, the proposed model updates the hidden state $h_v^{(t)}$ of a node $v$ as follows:

\[ a_v^{(t)} = \text{AGGREGATE}^{(t)} \left( \{ h_u^{(t-1)} | u \in N_k(v) \} \right) \]

\[ h_v^{(t)} = \text{MERGE}^{(t)} \left( h_v^{(t-1)}, a_v^{(t)} \right) \]

We next present an instance of the proposed architecture which is strictly stronger than standard GNNs in terms of distinguishing non-isomorphic graphs, and is capable of identifying graph properties which are not captured by the standard GNN architecture.

4.1 Proposed Architecture

Let $G = (V, E)$ be a graph. In what follows, we will focus on a single node $v \in V$, and we will present how the representation of this node is updated during the neighborhood aggregation phase. Node $v$ will also be referred as the root of the $k$-hop neighborhood subgraph $G_v^k$. For a given iteration/layer $t$, and a root node $v$, we define an inner representation $x_u$ of each node $u \in N_k(v)$ and we initialize it as $x_u = h_u^{(t-1)}$. We will next describe how the hidden state $h_v^{(t)}$ of the root $v$ is
After we refer to as the nodes at level $d$ where MLP
The proposed approach starts from the most distant nodes and follows a sequential procedure updating
$u$ the two updates aggregate information from the neighbors of $v$, which are located at the immediately higher and at the same level of the neighborhood subgraph, respectively. Hence, the proposed model performs the following two types of updates of inner representations: (1) updates across rings of nodes, and (2) updates within a ring of nodes. We next present these two updates in detail:

- Updates across rings of nodes: Let $u \in R_d(v)$ be a node that belongs to the k-hop neighborhood of $v$ and whose shortest path distance from $v$ is equal to $d$. Let also $B = N_1(u) \cap R_{d+1}(v)$ denote the neighbors of $u$ that belong to level $d + 1$ of $G^k_v$. Note that $B$ is empty if $k = d$ or if all the neighbors of $u$ belong to levels $d - 1$ and $d$ of $G^k_v$. If $B$ is not empty, the representation $x_u$ of $u$ is updated as follows:
  $$ x_u = \text{UPDATE}^{(t)}_{d,across}(u, B) $$
  Otherwise, if $u$ has no neighbors at the next higher level (i.e., $N_1(u) \cup R_{d+1}(v)$ is empty), then its representation is not updated.

- Updates within a ring of nodes: If $u$ has one or more neighbors at the same level of $G^k_v$, and hence $D = N_1(u) \cap R_d(v)$ is not empty, the representation $x_u$ of $u$ is re-updated as follows:
  $$ x_u = \text{UPDATE}^{(t)}_{d,within}(u, D) $$

The proposed approach starts from the most distant nodes and follows a sequential procedure updating
the feature vectors of nodes that are gradually closer to the root. The first type of update (across rings) precedes the second (within a ring). After all its direct neighbors $u \in N_1(v)$ have been processed, the hidden state of the root node $v$ is computed as follows:

$$ h_v^{(t)} = \text{UPDATE}^{(t)}_{0,across}(v, N_1(v)) $$

As mentioned above, although the model learns a new inner representation $x_u$ for some of the nodes in $N_k(v)$, these representations are only learned for the purpose of updating the root node’s hidden state. Furthermore, it is clear that for a single neighborhood aggregation layer, the proposed model needs at most $2k$ UPDATE modules. As we will show next, the proposed model can capture the structural information within the root node’s k-hop neighborhood even if it comprises of a single neighborhood aggregation layer. Hence, instead of using multiple neighborhood aggregation layers/iterations, it is more suitable to increase the value of $k$. The various steps of the proposed model are illustrated in Algorithm 1.

After $T$ iterations (i.e., $T$ neighborhood aggregation layers), the emerging node feature vectors $h^{(T)}_v$ can be used in any node-related task. For graph-level tasks, the proposed model can compute a vector representation over the whole graph by applying a READOUT function similar to the one shown in Equation 4.
Algorithm 1: k-hop GNN

**Input:** Graph $G = (V, E)$, node features \( \{h_v : v \in V\} \), number of neighborhood aggregation layers $T$, number of hops $k$

**Output:** node features \( \{h_v^{(T)} : v \in V\} \)

for $t \in \{1, \ldots, T\}$ do

  for $v \in V$ do

    for $u \in R_k(v)$ do

      $x_u \leftarrow \text{UPDATE}_{k, \text{within}}^{(t)}$

    end

    for $i \in \{k - 1, \ldots, 1\}$ do

      for $u \in R_i(v)$ do

        $x_u \leftarrow \text{UPDATE}_{i, \text{across}}^{(t)}(u, B)$
        $x_u \leftarrow \text{UPDATE}_{i, \text{within}}^{(t)}(u, D)$

      end

    end

  end

  $h_v^{(t)} = \text{UPDATE}_{0, \text{across}}^{(t)}(v, \mathcal{N}_1(v))$

end

4.2 Example

We next provide a simple example that illustrates the update procedure that was presented above. Specifically, Figure 3 shows the 2-hop neighborhood graph $G_{v_1}^2$ of a node $v_1 \in V$. As mentioned above, we first consider the most distant nodes (i.e., nodes $v_4$ and $v_5$ since $v_4, v_5 \in R_2(v_1)$). The representations of nodes $v_4$ and $v_5$ are not updated since these two nodes are at the frontier of $G_{v_1}^2$. Furthermore, there is no edge between the two nodes. However, these two nodes contribute to the update of the representation of node $v_2$. Specifically, the inner representation of node $v_2$ is updated as follows:

$$x_{v_2} = \text{UPDATE}_{1, \text{across}}^{(t)}(v_2, \{v_4, v_5\})$$

Then, we update the inner representations of nodes whose shortest path distance from the root is 1 and which are connected with other nodes with the same distance from the root. There is one such pair of nodes (i.e., nodes $v_2$ and $v_3$) which are updated as:

$$x_{v_2} = \text{UPDATE}_{1, \text{within}}^{(t)}(v_2, \{v_3\})$$

$$x_{v_3} = \text{UPDATE}_{1, \text{within}}^{(t)}(v_3, \{v_2\})$$

Finally, we update the root by aggregating information from its direct neighbors:

$$h_{v_1}^{(t)} = \text{UPDATE}_{0, \text{across}}^{(t)}(v_1, \{v_2, v_3\})$$

4.3 Expressive Power

We next study the identifiability of the proposed $k$-hop GNN. The following Theorem comprises the main results about graph properties that can be identified by the proposed model.

**Theorem 2.** For the $k$-hop GNN, there exists a sequence of modules \( \text{UPDATE}_{0, \text{across}}^{(0)}, \text{UPDATE}_{1, \text{within}}^{(0)}, \text{UPDATE}_{1, \text{across}}^{(0)}, \ldots, \text{UPDATE}_{k-1, \text{across}}^{(0)}, \text{UPDATE}_{k, \text{within}}^{(0)} \) such that

1. it can identify triangle-freeness for $k \geq 1$
2. connectivity for $k > \delta_{\min}$ where $\delta_{\min}$ is the minimum of the diameters of the connected components
3. bipartiteness for $k \geq \frac{l-1}{2}$ where $l$ is the length of the smallest odd cycle in the graph (if any)

**Proof.** The proof is left to the Appendix.
4.4 Computational Complexity.

Of course, the increase of expressiveness does not come without a price. Clearly the time complexity of the \(k\)-hop GNN is higher than that of the standard GNN. The model needs to extract the \(k\)-hop neighborhoods of all nodes. This can be done in linear time in the number of edges in the neighborhood of each node. Hence, its complexity is \(O(nm)\) in the worst case. Furthermore, to update the representations of the nodes, the model requires the use of three MLPs for each edge of the \(k\)-hop neighborhood subgraphs. However, for sparse graphs and small values of \(k\), the number of edges in each \(k\)-hop neighborhood is small and therefore, the complexity is low (constant in practice).

5 Experimental Evaluation

In this Section, we evaluate the performance of the proposed \(k\)-hop GNN in two tasks: (1) node classification, (2) graph classification. We compare the performance of the proposed model against the standard GNN architecture and against strong baselines.

5.1 Node Classification

The main objective of node classification is to assign class labels to unlabeled nodes. Each node \(v_i \in V\) has an associated class label \(y_i\) and the goal is to learn a representation vector \(h_i^{(T)}\) of \(v_i\) such that \(v_i\)'s label can be predicted as \(y_i = f(h_i^{(T)})\).

Datasets. We evaluate the proposed model on synthetic graphs with planted structural equivalences. To generate the graphs, we follow the same procedure as in [5]. Structurally equivalent nodes are assigned the same class labels. All the generated graphs consist of a cycle of length 40 and some basic shapes (“house”, “fan”, “star”) which are regularly placed along the cycle. In the “basic” setup, 10 instances of only one of the three types (randomly chosen with uniform probability) are placed along the cycle. In the “varied” setup, 10 instances of each one of the three shapes are randomly placed along the cycle. The use of multiple shapes increases the number and complexity of the structural role patterns, posing a challenge to the learning algorithms. To assess how the algorithms perform in noisy scenarios, we introduce two additional configurations (“basic perturbed” and “varied perturbed”) where we add edges uniformly at random on the generated graphs. The number of edges that are added is equal to 10% of the edges of the graph.

Baselines. We compare the proposed model against three recent state-of-the-art techniques for learning structural node representations: (1) RolX, a method based on non-negative matrix factorization of a node-feature matrix that describes each node based on this given set of latent features [11], (2) struc2vec, a method which learns structural node embeddings through a sequence of walks on a multilayered graph [24], and (3) GraphWave, an algorithm that builds upon techniques from signal processing and generates a structural embedding for each node based on the diffusion of a spectral graph wavelet centered at the node [5]. Note that these three algorithms are unsupervised, in the sense that they only take a graph as input and not any class labels of the nodes. We also compare the \(k\)-hop GNN model against DeepWalk, a method for learning node representations such that nodes that reside in close network proximity are assigned similar latent representations [22]. Besides the above four methods, we also compare the proposed model against the standard GNN architecture as described in Equation [1].

Experimental setup. For each configuration, we generate 20 graphs using the procedure described above. For each graph, we perform 10-fold cross validation. We repeat the whole process 25 times. We measure the performance of the different algorithms using the following two evaluation metrics: (1) average accuracy and (2) average F1-score.

For the unsupervised algorithms, we learn an embedding for each node, and we predict the class label of each node in the test set using a 4-nearest neighbors classifier. For all baselines, we use the default parameter values. Specifically, for struc2vec, we set the probability that the random walks stays in current layer to 0.5, the dimensionality of the embeddings to 128, the number of epochs to 5, the number of walks per node to 10, the walk length to 80 and the context window size to 10. Furthermore, we make use of all approximations OPT1, OPT2, and OPT3. For GraphWave, we use the multiscale version, set \(d = 50\) and use evenly spaced sampling points \(t_i\) in range \([0, 100]\).
For DeepWalk, we set the dimensionality of the embeddings to 128, the number of epochs to 5, the number of walks per node to 80, the walk length to 40 and the context window size to 10. Finally, for RolX, we did not use any approach for automatically detecting the number of different roles, but we directly provided the algorithm with the correct number of roles. For the proposed \(k\)-hop GNN model and the standard GNN model, we train the models on the training set of each fold and use the models to classify the nodes of the test set. We use 2 and 3 neighborhood aggregation layers for the standard GNN, and 1 layer for the proposed 2-hop and 3-hop GNNs. The neighborhood aggregation layers of all architectures consist of MLPs with 2 layers. Batch normalization is applied to the output of every neighborhood aggregation layer. The hidden-dimension size of the MLPs was set equal to 8. Moreover, we used the Adam optimizer with a learning rate of \(10^{-3}\), and we trained the neural networks for 200 epochs.

**Results.** Table 1 shows that the instances of the proposed \(k\)-hop GNN architecture outperform all the baselines in the node classification task. DeepWalk is the worst-performing method. This is not surprising since this method cannot capture structural similarity. Regarding the remaining methods, in the least challenging configuration (“basic”), the \(k\)-hop GNN models, and RolX perform the best. All these methods yield perfect performance, while the standard GNN models and GraphWave exhibit slightly worse performance. In the presence of noise (“basic perturbed” configuration), the performance of all methods degrades a lot. Specifically, the 2-hop GNN model is the best-performing method followed by the 3-hop GNN model, RolX, GraphWave, and the two standard GNN models, in that order. DeepWalk and struc2vec perform much worse than the other methods in that configuration. In the “varied” configuration, the \(k\)-hop GNN models are once again the best-performing methods along with RolX. In the “varied perturbed” configuration, the 2-hop GNN model yields the best performance. The 3-hop GNN model achieves slightly worse performance, while the performance of the remaining methods is much lower. From the two noisy configurations, it is clear that the baseline methods are more prone to noise compared to the \(k\)-hop GNN model. Furthermore, regarding the

### Table 1: Performance of the baselines and the proposed \(k\)-hop GNN models for learning structural embeddings averaged over 20 synthetically generated graphs for each configuration. Dashed lines denote perturbed graphs (obtained by randomly adding edges).

| Configuration | Shapes Placed along a Cycle Graph | Method | Accuracy | F1-score |
|---------------|----------------------------------|--------|----------|----------|
| **BASIC**     | ![OR](image)                     | DeepWalk | 0.442    | 0.295    |
|               |                                  | RolX    | 1.000    | 1.000    |
|               |                                  | struc2vec | 0.784    | 0.708    |
|               |                                  | GraphWave | 0.995    | 0.993    |
|               |                                  | 2-GNN   | 0.996    | 0.993    |
|               |                                  | 3-GNN   | 0.998    | 0.997    |
|               |                                  | 2-hop GNN | 1.000   | 1.000    |
|               |                                  | 3-hop GNN | 1.000   | 1.000    |
| **BASIC PERTURBED** | ![OR](image) | DeepWalk | 0.488    | 0.327    |
|               |                                  | RolX    | 0.928    | 0.886    |
|               |                                  | struc2vec | 0.703    | 0.632    |
|               |                                  | GraphWave | 0.906    | 0.861    |
|               |                                  | 2-GNN   | 0.903    | 0.863    |
|               |                                  | 3-GNN   | 0.905    | 0.849    |
|               |                                  | 2-hop GNN | 0.959   | 0.933    |
|               |                                  | 3-hop GNN | 0.955   | 0.929    |
| **VARIED**    | ![AND](image)                   | DeepWalk | 0.329    | 0.139    |
|               |                                  | RolX    | 0.998    | 0.996    |
|               |                                  | struc2vec | 0.738    | 0.592    |
|               |                                  | GraphWave | 0.982    | 0.965    |
|               |                                  | 2-GNN   | 0.987    | 0.974    |
|               |                                  | 3-GNN   | 0.998    | 0.989    |
|               |                                  | 2-hop GNN | 0.999   | 0.998    |
|               |                                  | 3-hop GNN | 0.998   | 0.997    |
| **VARIED PERTURBED** | ![AND](image) | DeepWalk | 0.313    | 0.128    |
|               |                                  | RolX    | 0.856    | 0.768    |
|               |                                  | struc2vec | 0.573    | 0.412    |
|               |                                  | GraphWave | 0.793    | 0.682    |
|               |                                  | 2-GNN   | 0.831    | 0.725    |
|               |                                  | 3-GNN   | 0.845    | 0.743    |
|               |                                  | 2-hop GNN | 0.944   | 0.901    |
|               |                                  | 3-hop GNN | 0.942   | 0.897    |
two instances of the $k$-hop GNN model, the 2-GNN model outperforms the 3-hop GNN model in all but one ("basic" where they achieve the same performance) configurations. This is probably related to the structure of the employed shapes. It should be mentioned that the diameter of all three shapes is equal to 2. Finally, the proposed $k$-hop GNN models outperform the two standard GNN models in all experiments, thereby validating our theoretical results. Overall, the proposed $k$-hop GNN model is robust and achieves good performance, demonstrating that it can learn high-quality node representations.

5.2 Graph Classification

We next apply the proposed architecture to the problem of graph classification, i.e., the supervised learning task of assigning a graph to a set of predefined categories. Specifically, given a set of graphs $\{G_1, \ldots, G_N\} \subseteq \mathcal{G}$ and their class labels $\{y_1, \ldots, y_N\}$, the goal is to learn a representation vector $h_{G_i}$ such that the class label of every graph of the test set can be predicted as $y_i = f(h_{G_i})$. For this task, we are going to evaluate the performance of the proposed model in two different types of datasets: (1) synthetic datasets containing graphs that satisfy or do not satisfy the considered graph properties, and (2) standard widely-used datasets from real-world scenarios.

5.2.1 Synthetic Datasets

In this set of experiments, we seek to identify potential benefits of our proposed $k$-hop GNN architecture over the standard GNN model.

Datasets. In order to investigate if the proposed model can distinguish triangle-freeness, bipartiteness and connectivity, we created three synthetic datasets. Each one of these datasets consists of 800 4-regular graphs. All the graphs have the same size (60 nodes), and each graphs is assigned a class label which denotes whether it satisfies the corresponding property or not (i.e., binary classification task). All the nodes are assigned identical labels. Furthermore, all three datasets are balanced, i.e., half of the graphs (400 graphs) satisfy the examined graph property, while the rest of the graphs (400 graphs) do not satisfy it.

Baselines. We compare our model against the standard GNN architecture of Equations 1 and 3. Based on our theoretical results, we expect the standard GNN model to perform much worse than the proposed model on these 3 datasets.

Experimental Setup. To measure the performance of the 4 models, 10-fold cross-validation was employed.

For the proposed $k$-hop GNN models (2-hop GNN and 3-hop GNN), we used a single neighborhood aggregation layer, while for the standard GNN, we used 2 and 3 layers. The hidden-dimension size of these layers was chosen from $\{16, 32, 64\}$. To generate graph representations, we employed a readout function that sums the vector representations of the nodes. The generated graph representations are then fed into a two layer MLP, with a softmax output. We used the ReLU activation function, and we chose the batch size from $\{32, 64, 128\}$. We used the Adam optimizer with a learning rate of $10^{-2}$, while we set the number of epochs to 100.

Results. We report in Table 2 average prediction accuracies across the 10 folds. It is clear that the standard GNN architectures are unable to distinguish the 3 graph properties. Specifically, they all achieve an average accuracy equal to 50% on all three datasets which can be attributed to the balanced splits of the training/test sets. On the other hand, the proposed $k$-hop GNN architectures achieved much higher average accuracies, indicating that the proposed architecture can distinguish the 3 properties in regular graphs. In the case of bipartiteness, the 3-hop GNN model yielded

| Method | Connectivity | Bipartiteness | Triangle-freeness |
|-------|--------------|---------------|-------------------|
| 2-GNN | 50.0         | 50.0          | 50.0              |
| 3-GNN | 50.0         | 50.0          | 50.0              |
| 2-hop GNN | 81.2       | 98.7          | 84.0              |
| 3-hop GNN | 94.7       | 100.0         | 82.5              |

Table 2: Average classification accuracy of GNNs and the proposed $k$-hop GNN models on the 3 synthetic datasets.
We chose parameters for the graph kernels as follows. For the Weisfeiler-Lehman subtree kernel (WL) [27], (2) PROTEINS, (3) NCI1. We also use the following 2 social interaction datasets: (1) IMDB-BINARY, (2) IMDB-MULTI. We next give more details about the employed datasets. MUTAG consists of 188 mutagenic aromatic and heteroaromatic nitro compounds. The task is to predict whether or not each chemical compound has mutagenic effect on the Gram-negative bacterium Salmonella typhimurium. PROTEINS comprises of 1, 113 proteins represented as graphs where vertices are secondary structure elements and there is an edge between two vertices if they are neighbors in the amino-acid sequence or in 3D space. The task is to classify proteins into enzymes and non-enzymes. NCI1 contains 4, 110 chemical compounds screened for activity against non-small cell lung cancer and ovarian cancer cell lines. Each enzyme is a member of one of the Enzyme Commission top level enzyme classes (EC classes) and the task is to correctly assign the enzymes to their classes. IMDB-BINARY and IMDB-MULTI contain 1, 000 and 1, 500 movie collaboration graphs, respectively.

Note that the social network graphs are unlabeled, while all other graph datasets come with discrete node labels. Hence, for the social network graphs, we assign an one-dimensional feature to each node which is equal to its degree, while for the remaining datasets, we use one-hot encodings of the node labels.

Baselines. We compare our methods against four graph kernels: (1) the graphlet kernel (GK) [28], (2) the shortest-path kernel (SP) [2], (3) the Weisfeiler-Lehman subtree kernel (WL) [27], and (4) the Weisfeiler-Lehman Optimal Assignment kernel (WL-OA) [15]. The first three kernels are available in the GraKeL library [29], while for WL-OA we used the code provided by the authors. Besides graph kernels, we also compare the proposed model against the basic GNN architecture of Equations 1 and 3 against GS-SVM [6] which makes use of geometric scattering features, and against the following state-of-the-art deep learning architectures: (1) PatchySan [20], (2) Deep Graph CNN (DGCNN) [37], (3) CapsGNN [33], (4) VRGC [23], (5) 1-2-3-GNN [19]. For the deep learning methods and GS-SVM, we compare against the accuracies reported in the original papers.

Experimental Setup. We performed 10-fold cross-validation where 10% of the graphs of each training fold was used as a validation set. The whole process was repeated 10 times for each dataset and each approach.

We chose parameters for the graph kernels as follows. For the Weisfeiler-Lehman subtree kernel and for the Weisfeiler-Lehman optimal assignment kernel, we chose the number of iterations from \( h = \{4, 5, 6, 7\} \), while the graphlet kernel that we implemented samples 500 graphlets of size up to 6 from each graph. For the proposed \( k \)-hop GNN models (2-hop GNN and 3-hop GNN), we used a single neighborhood aggregation layer, while for the standard GNN, we used 2 and 3 layers. The parameters of the neighborhood aggregation layers correspond to MLPs with 2 layers. Batch normalization is applied to the output of every neighborhood aggregation layer. The hidden-dimension size of the MLPs was chosen from \( \{16, 32, 64\} \). To generate graph representations, we employed a readout function that sums the vector representations of the nodes. The generated graph representations are then fed into a two layer MLP, with a softmax output. We used the ReLU activation function, and we chose the batch size from \( \{32, 64, 128\} \). We used the Adam optimizer with an initial learning rate of \( 10^{-3} \) and decay the learning rate by 0.5 every 50 epochs. We set the number of epochs to 500, and we select the epoch with the best validation accuracy.

Results. We report in Table 3 average prediction accuracies and standard deviations. Note that the graphs contained in the IMDB-BINARY and IMDB-MULTI datasets correspond to the ego-networks

\[1\] The datasets, further references and statistics are available at https://ls11-www.cs.tu-dortmund.de/staff/morris/graphkerneldatasets
of actors and actresses. The diameter of these graphs is at most equal to 2, and therefore, the 3-hop neighborhoods of the nodes are identical to their 2-hop neighborhoods. This is why we do not report the performance of the 3-hop GNN on these two datasets.

In general, we observe that the variants of the proposed model achieve high levels of performance. Specifically, they achieve the second best performance on MUTAG, the third best performance on IMDB-BINARY, and the fourth best performance on the NCI1 and IMDB-MULTI datasets. On most datasets, the proposed model yields only slightly worse accuracies compared to the best performing method, the WL-OA kernel. Interestingly, the two $k$-hop GNN models perform equally well in general. More specifically, the 3-hop GNN achieves slightly better accuracy than the 2-hop GNN on most datasets. However, the difference in performance is not very large. Furthermore, it should be mentioned that the proposed $k$-hop GNN models outperform the two standard GNN models on all datasets, demonstrating their superiority. Overall, the proposed architecture yields good performance, demonstrating that it can learn not only high-quality node representations, but also graph representations.

6 Conclusion

In this paper, we analyzed the expressive power of GNNs, showing that a wide class of GNN architectures cannot identify fundamental properties of graphs such as triangle-freeness and bipartiteness. To account for that, we proposed a generalization of GNNs, so-called $k$-hop GNNs, which update a node’s representation by aggregating information not only from its direct neighbors, but from its $k$-hop neighborhood. This new model is strictly stronger than GNNs in terms of distinguishing non-isomorphic graphs and is capable of identifying graph properties that are not captured by standard GNNs. We evaluated the proposed model on standard node classification and graph classification datasets. The empirical results validated our theoretical findings since the proposed model achieved performance better or comparable to standard GNNs and to state-of-the-art algorithms.

Acknowledgment

Giannis Nikolentzos is supported by the project “ESIGMA” (ANR-17-CE40-0028). We gratefully acknowledge the support of the NVIDIA Corporation, who donated the Titan Xp GPU that was used for this research in the context of the NVIDIA GPU Grant program.

| METHOD | MUTAG | PROTEINS | NCI1 | IMDB BINARY | IMDB MULTI | AVERAGE |
|--------|-------|----------|------|-------------|------------|---------|
| GR     | 69.97 (± 2.22) | 71.23 (± 0.38) | 65.47 (± 0.14) | 60.33 (± 0.25) | 36.53 (± 0.93) | 13.4 |
| SP     | 84.03 (± 1.49) | 75.36 (± 0.61) | 72.85 (± 0.24) | 60.21 (± 0.58) | 39.62 (± 0.57) | 10.6 |
| WL     | 83.63 (± 1.57) | 73.12 (± 0.52) | 84.42 (± 0.25) | 73.36 (± 0.38) | 51.06 (± 0.47) | 6.2 |
| WL-OA  | 86.63 (± 1.49) | 75.35 (± 0.45) | 85.74 (± 0.37) | 73.61 (± 0.60) | 50.48 (± 0.33) | 3.0 |
| 2-GNN  | 85.92 (± 2.19) | 75.24 (± 0.45) | 76.32 (± 0.41) | 71.40 (± 0.74) | 47.73 (± 0.86) | 8.4 |
| 3-GNN  | 85.74 (± 1.48) | 74.59 (± 0.71) | 79.62 (± 0.45) | 71.60 (± 0.84) | 47.33 (± 1.01) | 8.6 |
| PATCHY| 88.95 (± 4.37) | 75.00 (± 2.51) | 76.34 (± 1.68) | 71.00 (± 2.29) | 45.23 (± 2.84) | 8.0 |
| GCN    | 85.83 (± 1.66) | 75.54 (± 0.94) | 74.44 (± 0.47) | 70.03 (± 0.56) | 47.83 (± 0.85) | 8.4 |
| CAPS    | 86.67 (± 6.88) | 76.28 (± 3.63) | 78.35 (± 1.55) | 73.10 (± 4.83) | 50.27 (± 2.65) | 4.4 |
| VRGC   | 86.3 | 74.8 | 80.7 | - | - | 6.3 |
| 1-2-3-GNN | 86.1 | 75.2 | 76.2 | 74.2 | 49.5 | 5.6 |
| 2-HOP GNN | 87.93 (± 1.22) | 75.03 (± 0.42) | 79.31 (± 0.57) | 73.33 (± 0.30) | 49.79 (± 0.25) | 5.0 |
| 3-HOP GNN | 87.56 (± 0.72) | 75.28 (± 0.36) | 80.61 (± 0.34) | - | - | 4.4 |

Table 3: Average classification accuracy (± standard deviation) of the baselines and the proposed $k$-hop GNN models on the 5 graph classification benchmark datasets. The “Average Rank” column illustrates the average rank of each method. The lower the average rank, the better the overall performance of the method.
Appendix

Proof of Theorem\textsuperscript{2}

We assume that the feature vectors of the nodes come from a countable set. This set may correspond to a subset of an uncountable set such as $\mathbb{R}^d$. Furthermore, the feature vectors of a set of nodes form a multiset (i. e., since some nodes may have identical feature vectors).

We will show that if a graph has one of the three considered properties (i. e., triangle-freeness, bipartiteness, and connectivity), some of its nodes can be mapped to different feature vectors compared to the nodes of a graph that does not have the property. Then, by applying an injective readout function, the two graphs can also be mapped to different feature vectors.

For simplicity of presentation, we will assume that the proposed model consists of a single neighborhood aggregation layer. The same results also hold for multiple neighborhood aggregation layers. We first show that the aggregation scheme that our model employs can represent universal functions over the pairs of a node and the multiset of its neighbors. The following Lemma generalizes the setting in Xu et al.\textsuperscript{34}.

**Lemma 2.** Assume $X$ is countable, and let $r \in \mathbb{N}$. There exist functions $f : X \to \mathbb{R}^d$ and $f' : X \to \mathbb{R}^d$ such that $h_i(c, X) = f(c) + \sum_{x \in X} f'(x)$ is unique for each $i \in \{0, \ldots, r\}$ and each pair $(c, X)$, where $c \in X$ and $X \subseteq X'$ is a finite multiset. Moreover, any function $g_i$ over such pairs can be decomposed as $g_i(c, X) = \phi(f(c) + \sum_{x \in X} f'(x))$ for some function $\phi$.

**Proof.** We first show that there exists a mapping $f'$ such that $\sum_{x \in X} f'(x)$ is unique for each finite multiset $X$. Because $X$ is countable, there exists a mapping $Z : X \to \mathbb{N}$ from $x \in X$ to natural numbers. Because the multisets $X$ are finite, there exists a number $N \in \mathbb{N}$ such that $|X| < N$ for all $X$. Then, an example of such $f'$ is $f'(x) = N - Z(x)$. The sum of the above function for all finite multisets $X$ takes values less than 1, i. e., $\sum_{x \in X} f'(x) < 1$. Hence, if we also set $f(x) = Z(x) + (r - i)|X|$, then it holds that $h_i(c, X) = f(c) + \sum_{x \in X} f'(x)$ is an injective function over pairs of elements and multisets, and is also unique for each $i \in \{0, \ldots, r\}$.

For any function $g_i$ over the pairs $(c, X)$, we can construct such $\phi$ for the desired decomposition by letting $g_i(c, X) = \phi(f(c) + \sum_{x \in X} f'(x))$. Note that such $\phi$ is well-defined because $h_i(c, X) = f(c) + \sum_{x \in X} f'(x)$ is injective. $\square$

In our setting, the UPDATE modules correspond to $g_i(c, X)$ functions. These modules use multi-layer perceptrons (MLPs) to model and learn $f, f'$ and $\phi$ in the above Lemma, thanks to the universal approximation theorem [12]. Note that given two nodes $v, v'$, if a node $u \in N_r(v)$ obtains a representation that is never obtained by any node $u' \in N_r(v')$, then based on the above Lemma, there exist UPDATE modules such that the root nodes $v, v'$ are assigned different representations. Hence, for all three properties, it is sufficient to show that at some point of the algorithm, a node of the graph that satisfies the property can obtain a representation that is never obtained by any node of a graph that does not satisfy the property.

**Triangle-freeness** If a graph is not triangle-free, then there exist at least three nodes whose 1-hop neighborhoods contain a triangle. Let $v$ be such a node. Then, clearly there are at least two nodes $u \in R_1(v)$ which are connected to each other by an edge. The representations of these nodes are updated as follows: $x_u = \text{UPDATE}^{(0)}_{1, \text{within}}(u, D)$. On the other hand, no such update takes place in the case of triangle-free graphs since $D = \emptyset$. Hence, based on Lemma\textsuperscript{2}, the above UPDATE module can generate different representations for the nodes that participate in a triangle from the representations of the nodes of the neighborhood subgraph of each node of a triangle-free graph.

**Connectivity** Let $G$ be a disconnected graph and $C$ its component which has the minimum diameter $\delta_{\min}$. Then, for an arbitrary node $v$ of component $C$, it holds that $R_i(v) = \emptyset$ for all $i > \delta_{\min}$. On the other hand, if the graph is connected, for some node $v$, it holds that $|R_i(v)| > 0$ for all $i \leq \delta$ where $\delta > \delta_{\min}$ is the diameter of the connected graph. Hence, the representations of the nodes $u \in R_i(v)$ and $u' \in R_{i-1}(v)$ are updated as $x_u = \text{UPDATE}^{(0)}_{i, \text{within}}(u, D)$ and $x_{u'} = \text{UPDATE}^{(0)}_{i-1, \text{across}}(u', D')$, respectively. Based on Lemma\textsuperscript{2}, the above two UPDATE
modules can generate different representations for the nodes of a neighborhood subgraph of a disconnected graph compared to those of the nodes of the neighborhood subgraph of a connected graph.

**Bipartiteness** It is well-known that a graph is bipartite if and only if it does not contain an odd cycle. If \( G \) is bipartite and \( l \) is the length of the smallest odd cycle in \( G \), then the \( k \)-hop neighborhood subgraphs \( (k \geq \frac{l+1}{2}) \) of more than one nodes contain a cycle of odd length. According to Lemma 3 (below), the \( k \)-hop neighborhood subgraph of a node \( v \) contains a cycle of odd length if and only if the shortest path lengths from two adjacent nodes \( u, w \in N_k(v) \) to \( v \) are identical. In other words, there exist two nodes both at the same level \( i \) of the \( k \)-hop neighborhood subgraph of node \( v \) that are connected to each other with an edge. During the process of updating the representation of the root \( v \), the feature vectors of these nodes are also updated as follows: \( x_u = \text{UPDATE}_{i, \text{within}}^{(0)}(u, D) \).

This update does not take place in the case of a non-bipartite graph since \( D = \emptyset \) for all nodes of all neighborhood subgraphs. Based on Lemma 2, these nodes can obtain different representations from all the representations of the nodes of a neighborhood subgraph extracted from a bipartite graph.

**Lemma 3.** Let \( G^k_v \) be the \( k \)-hop neighborhood subgraph of a node \( v \). Then, \( G^k_v \) contains a cycle of odd length if and only if the shortest path lengths from two adjacent nodes \( u, w \in N_k(v) \) to \( v \) are identical.

**Proof.** Let \( u, w \) be two vertices such that \( u, w \in N_k(v) \). Assume that the shortest path lengths between each of these two vertices and the root \( v \) are identical and equal to \( d \in \mathbb{N} \) such that \( d \leq k \). If \( u \) and \( w \) are connected by an edge, then \( G^k_v \) contains a cycle of length \( 2d + 1 \) which is clearly an odd number. This proves the first statement. For the second statement, assume that \( G^k_v \) contains a cycle of odd length and there is no edge between two vertices whose shortest path lengths from the root \( v \) are identical. Then, from all the nodes of the cycle, there is a single node \( u \) such that the shortest path distance \( d \in \mathbb{N} \) from the root \( v \) to \( u \) is maximum. Since this is a cycle, there are two paths from \( v \) to \( u \) of length \( d \). Hence, the length of the cycle is \( 2d \) which is an even number, contradicting the assumption.

**References**

[1] László Babai and Ludik Kucera. Canonical labelling of graphs in linear average time. In *Foundations of Computer Science, 1979., 20th Annual Symposium on*, pages 39–46. IEEE, 1979.

[2] Karsten M Borgwardt and Hans-Peter Kriegel. Shortest-path kernels on graphs. In *Proceedings of the 5th International Conference on Data Mining*, pages 74–81, 2005.

[3] Karsten M Borgwardt, Cheng Soon Ong, Stefan Schönauer, SVN Vishwanathan, Alex J Smola, and Hans-Peter Kriegel. Protein function prediction via graph kernels. *Bioinformatics*, 21(suppl_1):i47–i56, 2005.

[4] Michael M Bronstein, Joan Bruna, Yann LeCun, Arthur Szlam, and Pierre Vandergheynst. Geometric Deep Learning: Going beyond Euclidean data. *IEEE Signal Processing Magazine*, 34(4):18–42, 2017.

[5] Claire Donnat, Marinka Zitnik, David Hallac, and Jure Leskovec. Learning Structural Node Embeddings via Diffusion Wavelets. In *Proceedings of the 24rd International Conference on Knowledge Discovery and Data Mining*, pages 1320–1329, 2018.

[6] Feng Gao, Guy Wolf, and Matthew Hirn. Geometric Scattering for Graph Data Analysis. In *Proceedings of the 36th International Conference on Machine Learning*, pages 2122–2131, 2019.

[7] Justin Gilmer, Samuel Schoenholz, Patrick F Riley, Oriol Vinyals, and George E Dahl. Neural Message Passing for Quantum Chemistry. In *Proceedings of the 34th International Conference on Machine Learning*, pages 1263–1272, 2017.

[8] Oded Goldreich. *Introduction to property testing*. Cambridge University Press, 2017.

[9] Marco Gori, Gabriele Monfardini, and Franco Scarselli. A New Model for Learning in Graph Domains. In *Proceedings of the 2005 IEEE International Joint Conference on Neural Networks*, volume 2, pages 729–734, 2005.

[10] Will Hamilton, Zhitao Ying, and Jure Leskovec. Inductive Representation Learning on Large Graphs. In *Advances in Neural Information Processing Systems*, pages 1024–1034, 2017.

[11] Keith Henderson, Brian Gallagher, Tina Eliassi-Rad, Hanghang Tong, Sugato Basu, Leman Akoglu, Danai Koutra, Christos Faloutsos, and Lei Li. RolX: Structural Role Extraction & Mining in Large Graphs.
[12] Kurt Hornik, Maxwell Stinchcombe, and Halbert White. Multilayer Feedforward Networks are Universal Approximators. *Neural networks*, 2(5):359–366, 1989.

[13] Steven Kearnes, Kevin Mccloskey, Marc Berndl, Vijay Pande, and Patrick Riley. Molecular graph convolutions: moving beyond fingerprints. *Journal of computer-aided molecular design*, 30(8):595–608, 2016.

[14] Thomas N Kipf and Max Welling. Semi-Supervised Classification with Graph Convolutional Networks. In *Proceedings of the 5th International Conference on Learning Representations*, 2017.

[15] Nils M Kriege, Pierre-Louis Giscard, and Richard Wilson. On valid optimal assignment kernels and applications to graph classification. In *Advances in Neural Information Processing Systems*, pages 1623–1631, 2016.

[16] Nils M Kriege, Christopher Morris, Anja Rey, and Christian Sohler. A Property Testing Framework for the Theoretical Expressivity of Graph Kernels. In *Proceedings of the 27th International Joint Conference on Artificial Intelligence*, pages 2349–2354, 2018.

[17] Tao Lei, Wengong Jin, Regina Barzilay, and Tommi Jaakkola. Deriving Neural Architectures from Sequence and Graph Kernels. In *Proceedings of the 34th International Conference on Machine Learning*, pages 2024–2033, 2017.

[18] Yujia Li, Daniel Tarlow, Marc Brockschmidt, and Richard Zemel. Gated Graph Sequence Neural Networks. arXiv preprint arXiv:1511.05493, 2015.

[19] Christopher Morris, Martin Ritzert, Matthias Fey, William L Hamilton, Jan Eric Lenssen, Gaurav Rattan, and Martin Grohe. Weisfeiler and Leman Go Neural: Higher-order Graph Neural Networks. In *Proceedings of the 33rd AAAI Conference on Artificial Intelligence*, 2019.

[20] Mathias Niepert, Mohamed Ahmed, and Konstantin Kutzkov. Learning Convolutional Neural Networks for Graphs. In *Proceedings of the 33rd International Conference on Machine Learning*, 2016.

[21] Giannis Nikolentzos, Giannis Siglidis, and Michalis Vazirgiannis. Graph Kernels: A Survey. arXiv preprint arXiv:1904.12218, 2019.

[22] Bryan Perozzi, Rami Al-Rfou, and Steven Skiena. DeepWalk: Online Learning of Social Representations. In *Proceedings of the 20th International Conference on Knowledge Discovery and Data Mining*, pages 701–710, 2014.

[23] Edouard Pinoeau and Nathan de Lara. Variational Recurrent Neural Networks for Graph Classification. In *Representation Learning on Graphs and Manifolds Workshop*, 2019.

[24] Leonardo FR Ribeiro, Pedro HP Saverese, and Daniel R Figueiredo. struc2vec: Learning Node Representations from Structural Identity. In *Proceedings of the 23rd International Conference on Knowledge Discovery and Data Mining*, pages 385–394, 2017.

[25] Franco Scarselli, Marco Gori, Ah Chung Tsoi, Markus Hagenbuchner, and Gabriele Monfardini. Computational Capabilities of Graph Neural Networks. *IEEE Transactions on Neural Networks*, 20(1):81–102, 2008.

[26] Franco Scarselli, Marco Gori, Ah Chung Tsoi, Markus Hagenbuchner, and Gabriele Monfardini. The Graph Neural Network Model. *IEEE Transactions on Neural Networks*, 20(1):61–80, 2009.

[27] Nino Shervashidze, Pascal Schweitzer, Erik Jan van Leeuwen, Kurt Mehlhorn, and Karsten M Borgwardt. Weisfeiler-Lehman Graph Kernels. *The Journal of Machine Learning Research*, 12:2539–2561, 2011.

[28] Nino Shervashidze, SVN Vishwanathan, Tobias Petri, Kurt Mehlhorn, and Karsten Borgwardt. Efficient Graphlet Kernels for Large Graph Comparison. In *Proceedings of the International Conference on Artificial Intelligence and Statistics*, pages 488–495, 2009.

[29] Giannis Siglidis, Giannis Nikolentzos, Stratis Limnios, Christos Giatsidis, Konstantinos Skianis, and Michalis Vazirgiannis. GraKeL: A Graph Kernel Library in Python. arXiv preprint arXiv:1806.02193, 2018.

[30] Felipe Petroski Such, Shagan Sah, Miguel Alexander Dominguez, Suhas Pillai, Chao Zhang, Andrew Michael, Nathan D Cahill, and Raymond Ptucha. Robust Spatial Filtering With Graph Convolutional Neural Networks. *IEEE Journal of Selected Topics in Signal Processing*, 11(6):884–896, 2017.

[31] Petar Veličković, Guillem Cucurull, Arantxa Casanova, Adriana Romero, Pietro Lio, and Yoshua Bengio. Graph Attention Networks. In *Proceedings of the 6th International Conference on Learning Representations*, 2018.

[32] Boris Weisfeiler and AA Lehman. A reduction of a graph to a canonical form and an algebra arising during this reduction. *Nauchno-Technicheskaya Informatsia*, 2(9):12–16, 1968.
[33] Zhang Xinyi and Lihui Chen. Capsule Graph Neural Network. In Proceedings of the 7th International Conference on Learning Representations, 2019.

[34] Keyulu Xu, Weihua Hu, Jure Leskovec, and Stefanie Jegelka. How Powerful are Graph Neural Networks? arXiv preprint arXiv:1810.00826, 2018.

[35] Shuang-Hong Yang, Bo Long, Alex Smola, Narayanan Sadagopan, Zhaohui Zheng, and Hongyuan Zha. Like like alike - Joint Friendship and Interest Propagation in Social Networks. In Proceedings of the 20th International Conference on World Wide Web, pages 537–546. ACM, 2011.

[36] Zhitao Ying, Jiaxuan You, Christopher Morris, Xiang Ren, Will Hamilton, and Jure Leskovec. Hierarchical Graph Representation Learning with Differentiable Pooling. In Advances in Neural Information Processing Systems, pages 4801–4811, 2018.

[37] Muhan Zhang, Zhicheng Cui, Marion Neumann, and Yixin Chen. An End-to-End Deep Learning Architecture for Graph Classification. In Proceedings of the 32nd AAAI Conference on Artificial Intelligence, pages 4438–4445, 2018.