How Powerful are K-hop Message Passing Graph Neural Networks

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Abstract

The most popular design paradigm for Graph Neural Networks (GNNs) is 1-hop message passing—aggregating features from 1-hop neighbors repeatedly. However, the expressive power of 1-hop message passing is bounded by the Weisfeiler-Lehman (1-WL) test. Recently, researchers extended 1-hop message passing to K-hop message passing by aggregating information from K-hop neighbors of nodes simultaneously. However, there is no work on analyzing the expressive power of K-hop message passing. In this work, we theoretically characterize the expressive power of K-hop message passing. Specifically, we first formally differentiate two kinds of kernels of K-hop message passing which are often misused in previous works. We then characterize the expressive power of K-hop message passing by showing that it is more powerful than 1-hop message passing. Despite the higher expressive power, we show that K-hop message passing still cannot distinguish some simple regular graphs. To further enhance its expressive power, we introduce a KP-GNN framework, which improves K-hop message passing by leveraging the peripheral subgraph information in each hop. We prove that KP-GNN can distinguish almost all regular graphs including some distance regular graphs which could not be distinguished by previous distance encoding methods. Experimental results verify the expressive power and effectiveness of KP-GNN. KP-GNN achieves competitive results across all benchmark datasets.

1 Introduction

Currently, most existing graph neural networks (GNNs) follow the *message passing* framework, which iteratively aggregates information from the neighbors and updates the representations of nodes. It has shown superior performance on graph-related tasks [1, 2, 3, 4, 5, 6, 7] comparing to traditional graph embedding techniques [8, 9]. However, as the procedure of message passing is similar to the 1-dimensional Weisfeiler-Lehman(1-WL) test [10], the expressive power of message passing GNNs is also bounded by the 1-WL test [7]. Namely, GNNs cannot distinguish two non-isomorphic graph structures if the 1-WL test would fail.

In normal message passing GNNs, the node representation is updated by the direct neighbors of node, which are called 1-hop neighbors. Recently, some works extend the notion of message passing into K-hop message passing [11, 12, 13, 14, 15]. **K-hop message passing** is a type of message passing where the node representation is updated by aggregating information from not only 1-hop, but all the neighbors within K hops of the node. However, there is no work on theoretically characterizing the expressive power of GNNs with K-hop message passing, e.g., whether it can improve the 1-hop message passing or not, and to what extent it can.

In this work, we theoretically characterize the expressive power of K-hop message passing GNNs. Specifically, 1) we formally distinguish two different kernels of the K-hop neighbors, which are

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often misused in previous works.The first kernel is based on whether node can be reached within k steps of graph diffusion process, which is used in GPR-GNN [14] and MixHop [11]. The second one is based on the shortest path distance of k, which is used in GINE+ [15]. Further, we show that different kernels of K-hop neighbors will result in **different expressive power** of K-hop message passing. 2) We theoretically characterize the expressive power of K-hop message passing GNNs and generalize the proposed theorem to most existing K-hop models. 3) We show that **K-hop message passing is strictly more powerful than 1-hop message passing but bounded by 3-WL** and it failed in distinguishing some simple regular graphs, no matter which kernel is used. This motivates us to further improve K-hop message passing.

Specifically, we introduce **KP-GNN**, a new GNN framework with K-hop message passing, which significantly improves the expressive power of standard K-hop message passing GNNs. In particular, during the aggregation of neighbors in each hop, KP-GNN not only aggregates neighboring nodes in that hop but also aggregates the **peripheral subgraph** (subgraph induced by the neighbors in that hop). This additional information helps the GNN to learn more expressive local structural features around the node. We further prove that KP-GNN is able to distinguish almost all regular graphs and even some distance regular graphs. The proposed KP-GNN has several additional advantages. First, it can be applied to most existing message passing GNNs with little modification. Second, it adds little computational complexity to standard K-hop message passing. We demonstrate the effectiveness of the KP-GNN framework through extensive experiments on both classification and regression tasks.

2 K-hop message passing and its representation power

2.1 Notations

Denote a graph as $G = (V, E)$, where $V = \{1, 2, ..., n\}$ is the node set and $E \subseteq V \times V$ is the edge set. Meanwhile, denote $A \in \{0, 1\}^{n\times n}$ as the adjacency matrix of graph G. Denote x_v as the feature vector of node v and denote e_{uv} as the feature vector of the edge from u to v. Finally, we denote $Q^1_{v,G}$ as the set of 1-hop neighbors of node v in graph G and $\mathcal{N}^1_{v,G}$=$Q^1_{v,G} \cup \{v\}$. Note that when we say K-hop neighbors of node v, we mean **all** the neighbors that have distance from node v less than or equal to K. In contrast, k-th hop neighbors mean the neighbors with **exactly** distance k from node v. The definition of distance will be discussed in section 2.3.

2.2 1-hop message passing framework

Currently, most existing GNNs are designed based on 1-hop message passing framework [16]. Denote h^l_v as the output representation of node v at layer l and $h^0_v = x_v$. Briefly, given a graph G and a 1-hop massage passing GNN, at layer l of the GNN, h^l_v is computed by h^{l-1}_v and $\{\!\{h^{l-1}_u \mid u \in \mathcal{Q}^1_{v,G}\}\!\}$:

$$m^l_v = \text{MES}^l(\{\!\{(h^{l-1}_u, e_{uv})|u \in Q^1_{v,G}\}\!\}), \quad h^l_v = \text{UPD}^l(m^l_v, h^{l-1}_v), \tag{1}$$

where m^l_v is the message to node v at layer l, MES^l and UPD^l are message and update functions at layer l respectively. After L layers of message passing, h^L_v is used as the final node representation of node v. Such a representation can be used to conduct node-level tasks like node classification and node regression. To get the graph representation, a readout function is used:

$$h_G = \text{READOUT}(\{\!\{h^L_v|v \in V\}\!\}), \tag{2}$$

where READOUT is the readout function for computing final graph representation. Then h_G can be used to conduct graph-level tasks like graph classification and graph regression.

2.3 K-hop message passing framework

The 1-hop message passing framework can be directly generalized to K-hop message passing, as it shares the same message and update mechanism. The difference is that an independent message and update function can be employed for each hop. Meanwhile, a combine function is needed to combine the results from different hops into the final node representation at this layer. First, we differentiate two different kernels of K-hop neighbors, which are interchanged and misused in previous research.

The first kernel of K-hop neighbors is *shortest path distance (spd) kernel*. Namely, the k-th hop neighbors of node v in graph G is the set of nodes that have shortest path distance of k from v.

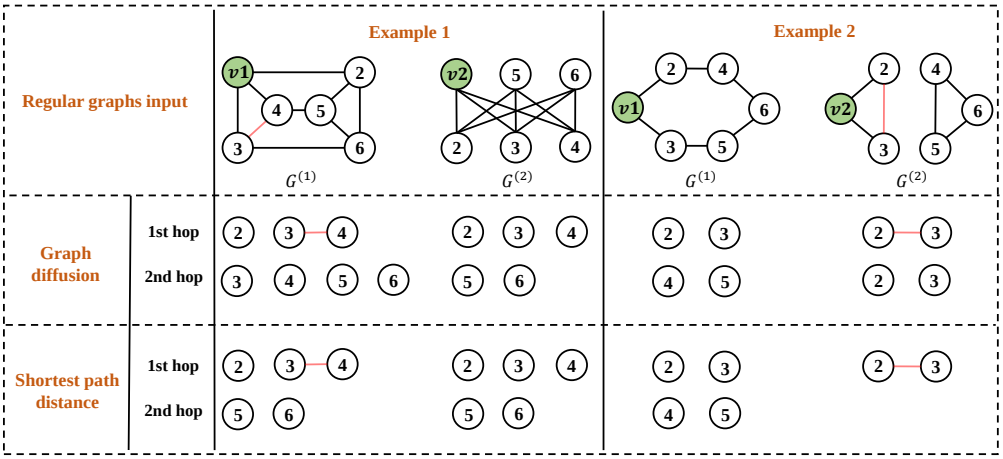

Figure 1: Here are two pairs of non-isomorphic regular graphs. With 2-hop message passing, example 1 can be distinguished by graph diffusion kernel and example 2 can be distinguished by shortest path distance kernel. However, it is indistinguishable if we switch the kernel. Finally, both two examples can be distinguished by adding peripheral edge information.

Definition 1. *For a node v in graph G, the K-hop neighbors $\mathcal{N}_{v,G}^{K,spd}$ of v based on shortest path distance kernel is the set of nodes that have the shortest path distance from node v* ***less than or equal to*** *K. We further denote $Q_{v,G}^{k,spd}$ as the set of nodes in G that are* ***exactly*** *the k-th hop neighbors (with shortest path distance of exactly k) and $\mathcal{N}_{v,G}^{0,spd} = Q_{v,G}^{0,spd} = \{v\}$ is the node itself.*

The second kernel of the K-hop neighbors is based on *graph diffusion (gd)*.

Definition 2. *For a node v in graph G, the K-hop neighbors $\mathcal{N}_{v,G}^{K,gd}$ of v based on graph diffusion kernel is the set of nodes that can diffuse information to node v* ***within the number of random walk diffusion steps*** *K with the diffusion kernel A. We further denote $Q_{v,G}^{k,gd}$ as the set of nodes in G that are* ***exactly*** *the k-th hop neighbors (nodes that can diffuse information to node v with k diffusion steps) and $\mathcal{N}_{v,G}^{0,gd} = Q_{v,G}^{0,gd} = \{v\}$ is the node itself.*

Note that a node can be a k-th hop neighbor of v for multiple k based on the graph diffusion kernel. We include more discussions of K-hop kernels in Appendix A. Next, we formally define the K-hop message passing framework as follows:

$$\begin{aligned} m_v^{l,k} &= \mathrm{MES}_k^l(\{\!\{(h_u^{l-1}, e_{uv}) | u \in Q_{v,G}^{k,t}\}\!\}), \quad h_v^{l,k} = \mathrm{UPD}_k^l(m_v^{l,k}, h_v^{l-1}), \\ h_v^l &= \mathrm{COMBINE}^l(\{\!\{h_v^{l,k} | k = 1, 2, ..., K\}\!\}), \end{aligned} \tag{3}$$

where $t = \{spd, gd\}$ indicates the kernel of K-hop neighbors. Here, for each hop, we can apply unique MES and UPD functions. Note that for $k > 1$, there may not exist the edge feature e_{uv} as edges are not directly connected. But we leave it here since we can use another type of feature to replace it, which is described in Appendix H. Compared to the 1-hop message passing framework described in Equation (1), the COMBINE function is introduced to combine the representations of node v at different hops. **It is easy to see that the L layer 1-WL GNNs are actually L layer K-hop message passing GNNs with $K = 1$.** We include more discussion of K-hop message passing GNNs in Appendix A. We also prove that K-hop message passing can injectively encode the neighbor representations at different hops into h_v^l in Appendix K.

2.4 Expressive power of K-hop message passing framework

In this section, we theoretically analyze the expressive power of K-hop message passing. We assume there is no edge feature and all nodes in the graph have the same feature, which means that GNNs can only distinguish two nodes using the local structure of nodes. Note that including node features only increases the expressive power of GNNs as nodes/graphs are more easily discriminated. It has been proved that the expressive power of 1-hop message passing is bounded by the 1-WL test on

discriminating non-isomorphic graphs [7, 17]. In this section, We show that the K-hop message passing is strictly more powerful than 1-WL test when $K > 1$. Across the analysis, we utilize regular graphs as examples to illustrate our theorems since they cannot be distinguished using either 1-hop message passing or the 1-WL test. Note that our analysis is not limited to regular graphs but is capable of describing any graphs.

To begin the analysis, we first define *proper K-hop message passing GNNs*.

Definition 3. *A proper K-hop message passing GNN is a class of GNN models where the message, update and combine functions are all injective given the input from a countable space.*

A proper K-hop message passing GNN is easy to find due to the universal approximation theorem [18] of neural network and the Deep Set for set operation [19]. In the latter sections, by default all mentioned K-hop message passing GNNs are proper. Next, we introduce node configuration:

Definition 4. *The node configuration of node v in graph G within k hops under t kernel is a list $A^{k,t}_{v,G} = (a^{1,t}_{v,G}, a^{2,t}_{v,G}, ..., a^{k,t}_{v,G})$, where $a^{i,t}_{v,G} = |Q^{i,t}_{v,G}|$ is the number of i-th hop neighbors of node v.*

When we say two node configurations $A^{k,t}_{v_1,G^{(1)}}$ and $A^{k,t}_{v_2,G^{(2)}}$ are equal, we mean that these two lists are component-wise equal to each other. Now, we state the first proposition:

Proposition 1. *A proper K-hop message passing GNN is strictly more powerful than 1-hop message passing GNNs when $K > 1$.*

To see why this is true, we first discuss how node configuration is related to the first layer of message passing. In the first layer of K-hop message passing, each node aggregates neighbors from up to K hops. As each node has identical label, an injective message function can only know how many neighbors at each hop (Proof in Appendix K), which is exactly the node configuration. In other words, **The first layer of K-hop message passing is equivalent to inject node configuration for each node label**. Next, we can characterize the expressive power of 1-hop message passing GNNs using node configuration. When $K = 1$, the node configuration of v_1 and v_2 are $d_{v_1,G^{(1)}}$ and $d_{v_2,G^{(2)}}$, where $d_{v,G}$ is the node degree of v. After L layers, GNN can get node configurations of each node within L hops. Given the statement, it is straightforward to see why these GNNs cannot distinguish any n-sized r-regular graph, as each node in the regular graph have same degree. From another prospective, the expressive power of 1-hop message passing GNN is limited because it only has the degree information of each node in the graph within the receptive field of GNN.

Next, when $K > 1$, the K-hop message passing is at least equally powerful as 1-hop message passing since node configuration up to k hops includes all the information the 1 hop has. To see why it is more powerful, we use two examples to illustrate it. The first example is shown in the left part of Figure 1. Suppose here we use graph diffusion kernel and we want to learn the representation of node v_1 and node v_2 in the two graphs, we know that the 1-hop message passing framework produces the same representation for two nodes as they are both nodes in 6-sized 3-regular graphs. However, it is easy to see that v_1 and v_2 have different local structures and should have different representations. Instead, if we use the 2-hop message passing with the graph diffusion kernel, we can easily distinguish the two nodes by checking the 2nd hop neighbors of the node, as node v_1 has four 2nd hop neighbors but node v_2 only has two 2nd hop neighbors. The second example is shown in the right part of Figure 1. Two graphs in the example are still regular graphs and the 1-hop message passing continue to fail in distinguishing node v_1 and node v_2. In contrast, suppose here we use shortest path distance kernel, node v_1 and v_2 have different numbers of 2nd hop neighbors thus will have different representations by performing 2-hop message passing. These two examples convincingly demonstrate that the K-hop message passing with $K > 1$ can have better expressive power than $K = 1$.

The above discussion can be applied to any existing K-hop GNNs using shortest path distance kernel like GINE [15], Graphormer [20]. However, for K-hop GNNs using graph diffusion kernel like MixHop [11], GPR-GNN [14], MAGNA [13], we find they actually use a weak version of K-hop than the definition of us. We leave the detailed discussion in Appendix B. Further, Distance Encoding [21] also uses shortest path distance information to augment the 1-hop message passing, which is similar to K-hop GNNs with shortest path distance kernel. However, we find the expressive power of the two frameworks are actually different from each other. We leave the detailed discussion in Appendix C.

2.5 Limitation of K-hop message passing framework

Although we show that K-hop message passing with $K > 1$ is better at distinguishing non-isomorphic structures than 1-hop message passing, there are still limitations. In this section, we discuss the limitation of K-hop message passing. Specifically, we show that **the choice of the kernel can affect the power of K-hop message passing**. Furthermore, even with K-hop message passing, we **cannot distinguish some simple non-isomorphic structures and the expressive power of K-hop message passing is bounded by 3-WL.**

Continue looking at the provided examples. In example 1, we know that node v_1 and v_2 have different numbers of 2nd hop neighbors with the graph diffusion kernel. However, if we use the shortest path distance kernel, the two nodes have the same number of neighbors in the 2nd hop, which means that we cannot distinguish two nodes using 2-hop message passing with the shortest path distance kernel. Similarly, in example 2, two nodes have the same number of neighbors in both 1st hop and 2nd hops with graph diffusion kernel. These results highlight that the choice of kernel can affect the expressive power of K-hop message passing. Furthermore, **none of them can distinguish both two examples** with 2-hop message passing.

Recently, Frasca et al. [22] show that any subgraph-based GNNs can be implemented by 3-IGN [23, 24] and thus their power is bounded by 3-WL. Here, we show that the K-hop message passing can also be implemented by 3-IGN and thus:

Theorem 1. *The expressive power of a proper K-hop message passing GNN of any kernel is bounded by 3-WL.*

We include the proof in Appendix D. Given all these observations, we may wonder if there is a way to further improve the expressive power of K-hop message passing?

3 KP-GNN: improving the power of K-hop message passing by peripheral subgraph

In this section, we describe how to improve the expressive power of K-hop message passing by adding additional features to message passing. Specifically, by adding the *peripheral subgraph* information, we can improve the representation power of K-hop message passing by a large margin.

3.1 Peripheral edge and peripheral subgraph

First, we define *peripheral edge* and *peripheral subgraph*.

Definition 5. *The peripheral edges $E(Q^{k,t}_{v,G})$ are defined as the set of edges that connect nodes within set $Q^{k,t}_{v,G}$. We further denote $|E(Q^{k,t}_{v,G})|$ as the number of peripheral edges. The peripheral subgraph $G^{k,t}_{v,G} = (Q^{k,t}_{v,G}, E(Q^{k,t}_{v,G}))$ is defined as the subgraph induced by $Q^{k,t}_{v,G}$ from the whole graph G.*

Briefly speaking, the peripheral edges $E(Q^{k,t}_{v,G})$ record all the edges whose two ends are both from $Q^{k,t}_{v,G}$ and the peripheral subgraph is a graph constituted by peripheral edges. It is easy to see that the peripheral subgraph $G^{k,t}_{v,G}$ automatically contains all the information of peripheral edges $E(Q^{k,t}_{v,G})$. Next, we show that the power of K-hop message passing can be improved by leveraging the information of peripheral edges and peripheral subgraph. We again refer to the examples in Figure 1. Here we only consider the peripheral edge information. In example 1, we notice that at the 1st hop, there is an edge between node 3 and node 4 in the left graph. More specifically, $E(Q^{1,t}_{v_1,G^{(1)}}) = \{(3,4)\}$. In contrast, we have $E(Q^{1,t}_{v_2,G^{(2)}}) = \{\}$ in the right graph, which means there is no edge between the 1st hop neighbors of v_2. Therefore, by adding this information to the message passing, we can successfully distinguish these two nodes. Similarly, in example 2, there is one edge between the 1st hop neighbors of node v_2 but no such edge exists for node v_1. By leveraging peripheral edge information, we can distinguish the two nodes as well. The above examples demonstrate the effectiveness of the peripheral edge and peripheral subgraph information.

3.2 K-hop peripheral-subgraph-enhanced graph neural network

In this section, we propose the **K**-hop **P**eripheral-subgraph-enhanced **G**raph **N**eural **N**etwork (KP-GNN), which equipes the K-hop message passing with peripheral subgraph information for more powerful GNN design. Recall the K-hop message passing defined in Equation (3). The only difference of KP-GNN is that we revise the message function as follows:

$$\hat{h}_v^{l,k} = \text{MES}_k^l(\{\!\{(h_u^{l-1},\ e_{uv}) | u \in Q_{v,G}^{k,t}\}\!\},\ G_{v,G}^{k,t}). \tag{4}$$

Briefly speaking, in the message step at the k-th hop, we not only aggregate information of the neighbors but also the peripheral subgraph at the k-th hop. The implementation of KP-GNN can be very flexible as any graph encoding function can be used. To maximize the information the model can encode while keeping it simple, we implement the message function as:

$$\text{MES}_k^l = \text{MES}_k^{l,normal}(\{\!\{(h_u^{l-1}, e_{uv}) | u \in Q_{v,G}^{k,t}\}\!\}) + \sum_{c \in C} \frac{1}{|C|} \sum_{(i,j) \in E(Q_{v,G}^{k,t})_c} e_{ij}\ , \tag{5}$$

where $\text{MES}_k^{l,normal}$ denotes the message function in the original GNN model, C is the set of connected components in $G_{v,G}^{k,t}$, $E(Q_{v,G}^{k,t})_c$ is the edge set of the c-th connected component in $G_{v,G}^{k,t}$. Such implementation helps the KP-GNN to not only encode the $E(Q_{v,G}^{k,t})$ but also partial information of $G_{v,G}^{k,t}$ (number of components). With this implementation, any GNN model can be incorporated into and be enhanced by the KP-GNN framework by replacing $\text{MES}_k^{l,normal}$ and UPD_k^l with the corresponding functions for each hop k. We leave the detailed implementation in Appendix H.

3.3 The expressive power of KP-GNN

In this section, we theoretically characterize the expressive power of KP-GNN and compare it with the original K-hop message passing framework. The key insight is that, according to Equation (4), the message function at the k-th hop additionally encodes $G_{v,G}^{k,t}$ compared to normal K-hop message passing. Next, we show that even with very simple information, the KP-GNN can become powerful enough for distinguishing regular graphs.

Theorem 2. *Consider all pair of n-sized r-regular graphs, where $3 \leq r < \sqrt{2logn}$. For any small constant $\epsilon > 0$, there exists a KP-GNN using shortest path distance as kernel and only peripheral edge information with at most $K = \lceil (\frac{1}{2} + \epsilon \frac{logn}{log(r-1-\epsilon)}) \rceil$, which distinguishes almost all $(1 - o(1))$ such pair of graphs with only 1-layer message passing.*

We include the proof in Appendix E. The above theorem proves that a simple implementation of KP-GNN leveraging only peripheral edge information can distinguish almost all regular graphs with some K and 1 layer.

Moreover, K-hop message passing with shortest path distance kernel cannot distinguish any distance regular graphs with the same intersection array according to the Theorem 3.7 in Distance Encoding [21]. Here we show that KP-GNN is more powerful than Distance Encoding on **distinguishing distance regular graphs**.

Theorem 3. *For two non-isomorphic distance regular graphs $G^{(1)} = (V^{(1)}, E^{(1)})$ and $G^{(2)} = (V^{(2)}, E^{(2)})$ with the same intersection array $(b_0, b_1, ..., b_{d-1}; c_1, c_2, ..., c_d)$, we pick two nodes v_1 and v_2 from two graphs respectively. Given a proper 1-layer K-hop KP-GNN with message functions defined in Equation (5), it can distinguish v_1 and v_2 if $b_0 - b_j - c_j = 2$ for some $j \leq K$ and $G_{v_1,G^{(1)}}^{j,t}$ and $G_{v_2,G^{(2)}}^{j,t}$ are non-isomorphic.*

We include the proof in Appendix F. Theorem 3 shows that the KP-GNN with a simple implementation can distinguish some distance regular graphs, which further distinguishes KP-GNN from Distance Encoding [21] and subgraph-based GNNs [25, 26, 27, 28] as they cannot distinguish distance regular graphs. We include further discussion in Appendix F. However, with the current implementation, KP-GNN cannot distinguish all distance regular graphs.

3.4 Time, space complexity, and limitation

In this section, we discuss the time and space complexity of K-hop message passing GNN and KP-GNN. Suppose a graph has n nodes and m edges. Then, the K-hop message passing and KP-GNN have both the space complexity of $O(n)$ and time complexity of $O(n^2)$ for shortest path distance kernel. Note that the complexity of graph diffusion is no less than the shortest path distance kernel. We can see that KP-GNN only requires the same space complexity as vanilla GNNs and much less time complexity than the $O(nm)$ of subgraph-based GNNs. We leave the detailed discussion on complexity and limitation of KP-GNN in Appendix G

4 Related Work

Expressive power of GNN. Analyzing the expressive power of GNN is a crucial problem as it can serve as a guidance on how to improve GNNs. Xu et al. [7] and Morris et al. [17] first proved that the power of 1-hop message passing is bounded by the 1-WL test. In other words, 1-hop message passing cannot distinguish any non-isomorphic graphs that the 1-WL test fails to. In recent years, many efforts have been put into increasing the expressive power of 1-hop messaging passing. The first line of research tries to mimic the higher-order WL tests, like 1-2-3 GNN [17], PPGN [23], ring-GNN [29]. However, they require exponentially increasing space and time complexity w.r.t. node number and cannot be generalized to large-scale graphs. The second line of research tries to enhance the rooted subtree of 1-WL with additional features. Some works [30, 31, 32] add one-hot or random features into nodes. Although they achieve good results in some setting, they deteriorate the generalization ability as such features produce different representations for nodes even with the same local graph structure. Instead, ID-GNN [33] enhances the rooted subtree by labeling the root node with a different color. However, the additional expressive power of ID-GNN only comes from the rooted node's labeling, which may not be powerful enough to distinguish more complex structures. Some works like Distance Encoding [21], SEAL [34], labeling trick [35] and GLASS [36] introduce node labeling based on either distance or distinguishing target node set. Specifically, Distance Encoding can be regarded as K-hop message passing with the shortest path distance kernel. On the other hand, GraphSNN [37] introduces a hierarchy of local isomorphism and proposes structural coefficients as additional features to identify such local isomorphism. However, the function designed to approximate the structural coefficient cannot fully achieve its theoretical power. The third line of research attends to revising the rooted subtree. Specifically, NGNN [25] encodes a rooted subgraph instead of a rooted subtree thus achieving superior expressive power on distinguishing regular graphs. However, it needs to run an inner GNN on every node of the graph thus introducing much more computation overhead. GNN-AK [26] applies a similar idea as NGNN. The only difference lies in how to compute the node representation from the local subgraph.

K-hop message passing GNN. There are some existing works that instantiate the K-hop message passing framework. For example, MixHop [11] performs messing passing on each hop with graph diffusion kernel and concatenates the representation on each hop as the final representation. K-hop [12] sequentially performs the message passing from hop K to hop 1 to compute the representation of the center node. However, it is not parallelizable due to its computational procedure. MAGNA [13] introduces an attention mechanism to K-hop message passing. GPR-GNN [14] use graph diffusion kernel to perform graph convolution on K-hop and aggregate them with learnable parameters. However, none of them give a formal definition of K-hop message passing and theoretically analyze its representation power and limitations.

5 Experiments

In this section, we conduct extensive experiments to evaluate the performance of KP-GNN. Specifically, we 1) empirically verify the expressive power of KP-GNN on 3 simulation datasets and demonstrate the benefits of KP-GNN compared to normal K-hop message passing GNNs and existing models; 2) show that the KP-GNN can achieve state-of-the-art performance on 5 TU datasets; 3) demonstrate that the KP-GNN achieves comparable performance on 3 molecular prediction datasets; 4) analyze the running time of KP-GNN. The detail of each variant of KP-GNN is described in Appendix H and the detailed experimental setting is described in Appendix I.

Table 1: Simulation dataset result. The top two are highlighted by **First**, **Second** . (*: with encoding)

Method	EXP(ACC)	Node Properties ($\log_{10}$(MAE))			Graph Properties ($\log_{10}$(MAE))			Counting Substructures (MAE)			
		SSSP	Ecc.	Lap.	Connect.	Diameter	Radius	Tri.	Tailed Tri.	Star	4-Cycle
GIN	50	-2.0000	-1.9000	-1.6000	-1.9239	-3.3079	-4.7584	0.3569	0.2373	0.0224	0.2185
PNA	50	**-2.8900**	**-2.8900**	-3.7700	-1.9395	3.4382	-4.9470	0.3532	0.2648	0.1278	0.2430
PPGN	100	-	-	-	-1.9804	-3.6147	-5.0878	**0.0089**	**0.0096**	0.0148	**0.0090**
GIN-AK+	100	-	-	-	-2.2268	-3.7585	-5.1044	0.0885	0.0696	0.0162	0.0668
K-GIN+	100	**-2.7651**	-2.6159	**-4.4309**	-2.0725	-3.9732	**-5.3113**	0.1180	0.0747	**0.0009**	0.0840
KP-GIN+	100	**-2.7651**	**-2.6193**	**-4.6107**	**-4.1803**	**-3.9952**	-5.2206	0.0377	0.0314	**0.0024**	0.0258
GIN-AK+*	100	-	-	-	-2.7513	-3.9687	5.1846	0.0123	0.0112	0.0150	0.0126
KP-GIN+*	100	-2.7628	-2.6164	-4.3540	**-3.7229**	**-4.0160**	**-5.2357**	**0.0029**	**0.0027**	0.0029	**0.0082**

Datasets:To evaluate the expressive power of KP-GNN, we choose: 1) EXP dataset [38], which contains 600 pairs of 1-WL-indistinguishable but non-isomorphic graphs. 2) Graph property regression (connectedness, diameter, radius) and node property regression (single source shortest path, eccentricity, Laplacian feature) task on graph random dataset [39]. 3) Graph substructure counting (triangle, tailed triangle, star and 4-cycle) tasks on random graph dataset [40]. For TU datasets evaluation, we choose MUTAG [41],D&D [42],PROTEINS [42],PTC-MR [43], and IMDB-B [44] from TU database. For molecule prediction datasets, we pick QM9 [45, 46], ZINC [47], and MolHIV [48]. The detailed statistics of the datasets are described in Appendix J.Without further highlight, all error bars in the result tables are standard deviation of multiple runs (more details are in Appendix I).

Table 2: Ablation study on EXP

kernel	K	K-GIN+	KP-GIN+
GD	K=1	50	50
	K=2	50	100
	K=3	66.17	100
	K=4	100	100
SPD	K=1	50	50
	K=2	50	100
	K=3	100	100
	K=4	100	100

Empirical verification of the expressive power: To evaluate the power of KP-GNN, we compare it with several existing models. For the baseline model, we use GIN [7], which has the same expressive power as 1-WL test. For more powerful baselines, we use GIN-AK+ [26], PNA [39] and PPGN [23]. For KP-GNN, we implement the KP-GIN+. To evaluate the effectiveness of peripheral subgraph, we also implement the normal K-hop version of GINE+, denote as K-GIN+. The results are shown in Table 1. Baseline results are taken from [26] and [39]. We also compare results of GIN-AK+ for both with and without D2C encoding and KP-GIN+ both with and without path encoding. We can see both K-GIN+ and KP-GIN+ achieve perfect performance on EXP dataset. Further, we conduct an ablation study on KP-GIN+ and K-GIN+ using EXP dataset. Table 2 presents the results. We can see that KP-GNN achieves perfect results with only $K \geq 2$ for both two kernels. However, K-GIN requires $K \geq 3$ and $K \geq 4$ to get perfect results for shortest path distance kernel and graph diffusion kernel respectively. Results on various property regression tasks further demonstrate the advantage of KP-GNN over existing models and normal K-hop message passing GNNs.

Table 3: TU dataset evaluation result.

Method	MUTAG	D&D	PTC-MR	PROTEINS	IMDB-B
WL	90.4±5.7	79.4±0.3	59.9±4.3	75.0±3.1	73.8±3.9
GIN	89.4±5.6	-	64.6±7.0	75.9±2.8	75.1±5.1
DGCNN	85.8±1.7	79.3 ±0.9	58.6 ±2.5	75.5±0.9	70.0±0.9
GraphSNN	91.24±2.5	82.46 ±2.7	66.96±3.5	76.51 ±2.5	76.93±3.3
GIN-AK+	91.30±7.0	-	68.20±5.6	77.10±5.7	75.60±3.7
KP-GCN	91.1±6.0	78.9±3.9	64.1±7.9	76.4±4.8	75.1±3.6
KP-GraphSAGE	91.1±3.9	78.2±3.7	65.9±7.6	76.1±4.4	74.7±3.7
KP-GIN	91.1±5.4	78.6±4.3	64.7±6.8	76.1±5.4	74.4±3.4
GIN-AK+*	95.0±6.1	00M	74.1±5.9	78.9±5.4	77.3±3.1
GraphSNN*	94.70±1.9	83.93±2.3	70.58±3.1	78.42±2.7	78.51±2.8
KP-GCN*	**96.1±4.6**	83.1±2.8	72.4±5.8	**80.0±3.8**	**79.0±2.7**
KP-GraphSAGE*	**96.1±4.6**	**84.0±3.4**	**74.4±6.5**	79.9±4.2	78.7±4.0
KP-GIN*	95.6±5.1	82.9±2.3	71.8±6.8	79.8±3.8	78.0±3.7

Evaluation on TU datasets: For baseline models, we select: 1) graph kernel based method WL subtree kernel [49]; 2) 1-hop message passing based GNN methods: GIN [7] and DGCNN [6]; 3) advanced GNN methods: GraphSNN [37] and GIN-AK+ [26]. For the proposed KP-GNN, we implement GCN [1], GraphSAGE [3], and GIN [7] using the KP-GNN framework, denoted as KP-

Table 4: QM9 results. The top two are highlighted by **First**, **Second**

Target	DTNN	MPNN	Deep LRP	PPGN	Nested 1-2-3-GNN	KP-GIN+
μ	**0.244**	0.358	0.364	**0.231**	0.433	0.365
α	0.95	0.89	0.298	0.382	**0.265**	**0.249**
$\varepsilon_{\text{HOMO}}$	0.00388	0.00541	**0.00254**	0.00276	0.00279	**0.00243**
$\varepsilon_{\text{LUMO}}$	0.00512	0.00623	0.00277	0.00287	**0.00276**	**0.00252**
$\Delta\varepsilon$	0.0112	0.0066	**0.00353**	0.00406	0.00390	**0.00346**
$\langle R^2 \rangle$	17.0	28.5	19.3	**16.7**	20.1	**16.64**
ZPVE	0.00172	0.00216	0.00055	0.00064	**0.00015**	**0.00017**
U_0	2.43	2.05	0.413	0.234	**0.205**	**0.06632**
U	2.43	2.00	0.413	0.234	**0.200**	**0.09447**
H	2.43	2.02	0.413	**0.229**	0.249	**0.06037**
G	2.43	2.02	0.413	0.238	**0.253**	**0.04752**
C_v	0.27	0.42	0.129	0.184	**0.0811**	**0.0977**

GCN, KP-GraphSAGE, and KP-GIN respectively. The results are shown in Table 3. For a detailed comparison, we report the results of two different settings. The first setting follows Xu et al. [7] and the second setting follows Wijesinghe and Wang [37]. We denote the second setting with * in the table. We can see that under the setting of Wijesinghe and Wang [37], KP-GNN achieves state-of-the-art performance across all datasets, which demonstrates the performance of KP-GNN on real-world datasets. Under the setting of Xu et al. [7], KP-GNN still achieves comparable performance.

Evaluation on molecular prediction tasks: For QM9 dataset, we report results of DTNN, MPNN from [46]. We further select Deep LRP [40], PPGN [23], and Nested 1-2-3-GNN [25]. For ZINC dataset, we report results of MPNN [16] and PNA [39] from [47]. We further pick Graphormer [20], GSN [50], GIN-AK+ [26], and CIN [51] . For MolHIV dataset, we report results of PNA [39], DeepLRP [40], GINE [15], NGNN [25], GIN-AK+[26] and GraphSNN [37]. The results of QM9 dataset are shown in Table 4. We can see KP-GNN achieves state-of-the-art performance on most of targets. The results of MolHIV and ZINC dataset are shown in Table 5 and Table 6. Although KP-GNN does not achieve the best result, it is still comparable to other methods.

Table 5: OGB-MolHIV result.

Method	Test AUC
PNA	79.05 ±1.32
DeepLRP	77.19±1.40
GINE-VN	76.60±1.40
NGNN	78.34±1.86
GIN-AK+	79.61±1.19
GraphSNN-VN	**79.72±1.83**
KP-GIN+-VN	78.48±0.87

Table 6: ZINC result.

Method	# param.	test MAE
MPNN	480805	0.145±0.007
PNA	387155	0.142±0.010
Graphormer	489321	0.122±0.006
GSN	~500000	0.101±0.010
GIN-AK+	-	0.080±0.001
CIN	-	**0.079±0.006**
KP-GIN+	500790	0.119±0.002

Table 7: Running time (ms/epoch)

Method	D&D	ZINC	Graph property
GIN	1.15	5.00	1.80
K-GIN	6.55	11.00	3.77
KP-GIN	7.84	13.00	6.82
KP-GIN+	7.96	9.00	8.74

Running time comparison: In this section, we compare the running time of KP-GNN to 1-hop message passing GNN and K-hop message passing GNN. We use GIN [7] as the base model. We also include the KP-GIN+. All models use the same number of layers and hidden dimensions for a fair comparison. The results are shown in Table 7. For D&D, ZINC, Graph property dataset, we set $K = 5$, $K = 4$, $K = 6$ respectively. We can see the computational overhead does not seem to grow quadratically as in our theoretical analysis. This is reasonable as practical graphs are sparse and the number of K-hop neighbors are far less than n when using a small K.

6 Conclusion

In this paper, we theoretically characterize the power of K-hop message passing GNNs and propose the KP-GNN to improve the expressive power by leveraging the peripheral subgraph information at each hop. Theoretically, we prove that KP-GNN can distinguish almost all regular graphs including some distance regular graphs. Empirically, KP-GNN achieves competitive results across all simulation and real-world datasets.

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1. For all authors...
   (a) Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope? [Yes]
   (b) Did you describe the limitations of your work? [Yes]
   (c) Did you discuss any potential negative societal impacts of your work? [N/A]
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2. If you are including theoretical results...
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3. If you ran experiments...
   (a) Did you include the code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL)? [Yes] The implementation of KP-GNN can be found at https://github.com/anoncodesub/KP-GNN.
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