Towards Scale-Invariant Graph-related Problem Solving by Iterative Homogeneous Graph Neural Networks

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Abstract

Current graph neural networks (GNNs) lack generalizability with respect to scales (graph sizes, graph diameters, edge weights, etc..) when solving many graph analysis problems. Taking the perspective of synthesizing graph theory programs, we propose several extensions to address the issue. First, inspired by the dependency of iteration number of common graph theory algorithms on graph size, we learn to terminate the message passing process in GNNs adaptively according to the computation progress. Second, inspired by the fact that many graph theory algorithms are homogeneous with respect to graph weights, we introduce homogeneous transformation layers that are universal homogeneous function approximators, to convert ordinary GNNs to be homogeneous. Experimentally, we show that our GNN can be trained from small-scale graphs but generalize well to large-scale graphs for a number of basic graph theory problems. It also shows generalizability for applications of multi-body physical simulation and image-based navigation problems.

1. Introduction

Graph, as a powerful data representation, arises in many real-world applications (Schlichtkrull et al., 2018; Shang et al., 2019; Fan et al., 2019; Battaglia et al., 2016; Sanchez-Gonzalez et al., 2018; Liu et al., 2018). On the other hand, the flexibility of graphs, including the different representations of isomorphic graphs, the unlimited degree distributions (Muchnik et al., 2013; Seshadri et al., 2008), and the *boundless graph scales* (Ying et al., 2018; Zang et al., 2018), also presents many challenges to their analysis. Recently, Graph Neural Networks (GNNs) have attracted broad attention in solving graph analysis problems. They are permutation-invariant/equivariant by design and have shown superior performance on various graph-based applications (Wu et al., 2020; Zhang et al., 2020; Zhou et al., 2018; Gilmer et al., 2017; Battaglia et al., 2018).

However, investigation into *the generalizability of GNNs with respect to the graph scale* is still limited. Specifically, we are interested in GNNs that can learn from small graphs and perform well on new graphs of arbitrary scales. Existing GNNs (Wu et al., 2020; Zhang et al., 2020; Zhou et al., 2018; Battaglia et al., 2018) are either ineffective or inefficient under this setting. In fact, even ignoring the optimization process of network training, the representation power of existing GNNs is yet too limited to achieve graph scale generalizability. There are at least two issues: 1) By using a pre-defined layer number (Li & Zemel, 2014; Zheng et al., 2015; Tamar et al., 2016), these GNNs are not able to approximate graph algorithms whose complexity depends on graph size (most graph algorithms in textbook are of this kind). The reason is easy to see: For most GNNs, each node only uses information of the 1-hop neighborhoods to update features by message passing, and it is impossible for k-layer GNNs to send messages between nodes whose distance is larger than k. More formally, Loukas (Loukas, 2020) proves that GNNs, which fall within the message passing framework, lose a significant portion of their power for solving many graph problems when their width and depth are restricted; and 2) a not-so-obvious observation is that, the range of numbers to be encoded by the internal representation may deviate greatly for graphs of different scales. For example, if we train a GNN to solve the shortest path problem on small graphs of diameter k with weight in the range of $[0, 1]$, the internal representation could only need to build the encoding for the path length within $[0, k]$; but if we test this GNN on a large graph of diameter $K \gg k$ with the same weight range, then it has to use and transform the encoding for $[0, K]$. The performance of classical neural network modules (e.g. the multilayer perceptron in GNNs) are usually highly degraded on those out-of-range inputs.

To address the pre-defined layer number issue, we take a program synthesis perspective, to design GNNs that have stronger representation power by mimicking the control flow of classical graph algorithms. Typical graph algorithm, such

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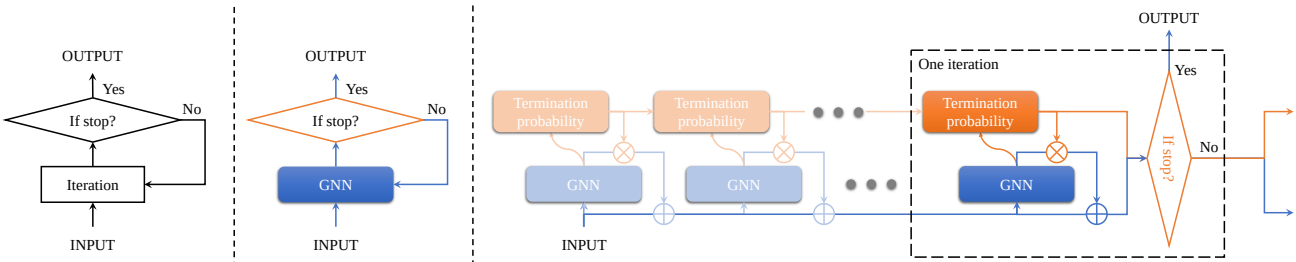


(a) iterative algorithms (b) general illustration of Iterative GNN (c) concrete unfolded illustration of Iterative GNN at one iteration

Figure 1. (a) The illustration of general iterative algorithms. The iteration body is repeated until the stopping criterion is satisfied. (b) Illustration of IterGNN as a combination of GNNs and iterative module. (c) A detailed illustration of Iterative GNN. It unfolds the computational flow of IterGNN. Other than the normal data flow (marked as blue), there is another control flow (marked as orange) that serves both as an adaptive stopping criterion and as a data flow controller.

as the Dijkstra's algorithm for shortest path computation, are iterative. They often consist of two sub-modules: an iteration body to solve the sub-problem (e.g., update the distance for the neighborhood of a node as in Dijkstra), and a termination condition to control the loop out of the iteration body. By adjusting the iteration numbers, an iterative algorithm can handle arbitrary large-scale problems. We, therefore, introduce our novel Iterative GNN (IterGNN) that equips ordinary GNN with an adaptive and differentiable stopping criterion to let GNN iterate by itself, as shown in Figure 1. Our stopping condition is adaptive to the inputs, supports arbitrarily large iteration numbers, and interestingly, is able to be trained in an end-to-end fashion *without any direct supervision*.

We also give a partial solution to address the issue of out-of-range number encoding, if the underlying graph algorithm is in a specific hypothesis class. More concretely, the solutions to many graph problems, such as shortest path and TSP, are homogeneous with respect to the input graph weights, i.e., the solution scales linearly with the magnitudes of the input weights. To build GNNs with representation power to approximate the solution to such graph problems, we further introduce the homogeneous inductive-bias. By assuming the message processing functions are homogeneous, the knowledge that neural networks learn at one scale can be generalized to different scales. We build HomoMLP and HomoGNN as powerful approximates of homogeneous functions over vectors and graphs, respectively.

2. Related Works.

We briefly describe the most related ones here due to space limitation and include a more complete review in Appendix C. Recently, (Veličković et al., 2020) and (Xu et al., 2020) achieved positive performance on solving the shortest path problem using GNNs. However, (Veličković et al., 2020) requires per-layer supervisions to train and models in (Xu et al., 2020) theoretically lack the generalizability w.r.t. graph scales due to their bounded number of message passing steps. The final formulation of our iterative module is generally similar to the previous adaptive computation time algorithm (ACT) (Graves, 2016) for RNNs or spatially ACT (Figurnov et al., 2017; Eyzaguirre & Soto, 2020) for CNNs, however, with distinct motivations and formulation details. The numbers of iterations for ACT are usually small by design (e.g.the formulation of regularizations and halting distributions). The recent flow-based methods (Poli et al., 2019) , although potential for providing adaptive layer numbers, are not a straightforward solution to approximate iterative algorithms with no explicit iteration controller.

3. Backgrounds

Graphs and graph scales. Each graph $G := (V, E)$ consists of a set of nodes V and a set of edges (pairs of nodes) E. To notate graphs with attributes, we use $\vec{x}_v$ for node attributes of node $v \in V$ and use $\vec{x}_e$ for edge attributes of edge $e \in E$. We consider three graph properties to quantify the graph scales, which are the number of nodes $N := |V|$, which is also called the graph size, and the graph diameter $\delta_G := \max_{u,v \in V} d(u, v)$. Here, $d(u, v)$ denotes the length of the shortest path from node u to node v, which is also called the distance between node u and node v for undirected graphs.

4. Method

We propose Iterative GNN (IterGNN) and Homogeneous GNN (HomoGNN) to improve the generalizability of GNNs with respect to graph scales. IterGNN is first introduced, in Section 4.1, to enable adaptive and unbounded iterations of GNN layers so that the model can generalize to graphs of arbitrary scale. We further introduce HomoGNN, in Section 4.2, to partially solve the problem of out-of-range

number encoding, for graph-related problems. We describe PathGNN layers that improves the generalizability of GNNs for distance-related problems by improving the algorithm alignments (Xu et al., 2020) to the Bellman-Ford algorithm in Appendix D.2.

4.1. Iterative module

Algorithm 1 Iterative module. g is the stopping criterion and f is the iteration body

input: initial feature x; stopping threshold ϵ
$k \leftarrow 1$
$h^0 \leftarrow x$
while $\prod_{i=1}^{k-1}(1-c^i) > \epsilon$ **do**
  $h^k \leftarrow f(h^{k-1})$
  $c^k \leftarrow g(h^k)$
  $k \leftarrow k+1$
end while
return $h = \sum_{k=1}^{\infty} c^k \prod_{i=1}^{k-1}(1-c^i)h^k$

The core of IterGNN is a differentiable iterative module. It executes the same GNN layer repeatedly until a learned stopping criterion is met. We present the pseudo-codes in Algorithm 1. This module includes a stopping criterion function g and an iteration body f. At step k, the iteration body f firstly calculates the new hidden state h^k from previous hidden state h^{k-1}; the stopping criterion function g then calculates a confidence score, which we denote as $c^k \in [0,1]$. The score c^k describes the probability of the iteration to terminate at the current time step. We can then determine the iteration numbers using a random process. In detail, at time step i, we sample from a binomial distribution with probability c^i to decide if the iteration terminates and returns the current hidden states as the output. The probability for the iteration to terminate at time step k is then $p^k = \prod_{i=1}^{k-1}(1-c^i)c^k$, which is also the probability of the network to output h^k in the random process. We take the expectation $E[h] = \sum_{i=1}^{\infty} p^k h^k$ as the output of the iterative module. The gradient to the output h can thus optimize the hidden state h^k and confidence score c^k directly. The iteration stops when the probability $\prod_{i=1}^{k-1}(1-c^i)$, which we also call the left confidence, is smaller than a pre-defined threshold ϵ.

By setting f and g as GNNs, we obtain our novel IterGNN, as shown in Figure 1. The features are associated with nodes in graph as $\{\vec{h}_v^{(k)} : v \in V\}$. GNN layers are adopted as the body function f to update the node features iteratively $\{\vec{h}_v^{(k+1)} : v \in V\} = \text{GNN}(G, \{\vec{h}_v^{(k)} : v \in V\}, \{\vec{h}_e : e \in E\})$. We build the termination probability module as g by integrating a readout function and a MLP. The readout function (e.g. max/mean pooling) summarizes all node features $\{\vec{h}_v^{(k+1)} : v \in V\}$ into a fixed-dimensional vector $\vec{h}^{(k+1)}$. The MLP predicts the confidence score as $c^k = \text{sigmoid}(\text{MLP}(\vec{h}^{(k+1)}))$. The sigmoid function is utilized to ensure the output of g is between 0 and 1. With the help of our iterative module, IterGNN can adaptively adjust the number of iterations. Moreover, it can be trained without any supervision of the stopping condition.

4.2. Homogeneous prior

The homogeneous prior is introduced to improve the generalizability of GNNs for out-of-range number encoding. We first define the positive homogeneous property of a function:

Definition 1. *A function f over vectors is positive homogeneous iff $f(\lambda\vec{x}) = \lambda f(\vec{x})$ for all $\lambda > 0$.*

A function f over graphs is positive homogeneous iff for any graph $G = (V, E)$ with node attributes $\vec{x}_v$ and edge attributes $\vec{x}_e$, $f(G, \{\lambda\vec{x}_v : v \in V\}, \{\lambda\vec{x}_e : e \in E\}) = \lambda f(G, \{\vec{x}_v : v \in V\}, \{\vec{x}_e : e \in E\})$

The solutions to most graph-related problems are positive homogeneous, such as the length of shortest path, the maximum flow, graph radius, and the optimal distance in the travelling salesman problem.

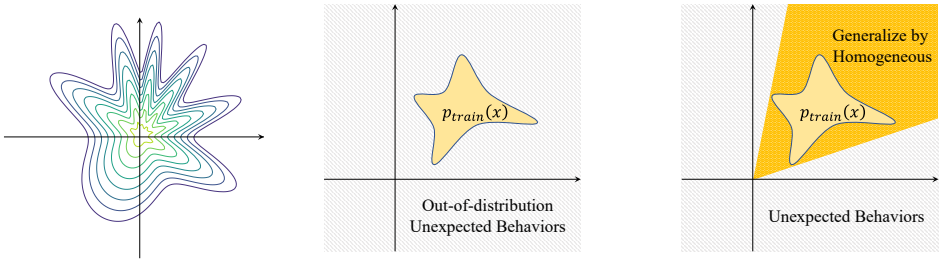
The homogeneous prior tackles the problem of different magnitudes of features for generalization. As illustrated in Figure 2, by assuming functions as positive homogeneous, models can generalize knowledge to the scaled features/attributes of different magnitudes. For example, let's assume two datasets D and D_λ that are only different on magnitudes, which means $D_\lambda := \{\lambda x : x \in D\}$ and $\lambda > 0$. If the target function f and the function $F_{\mathcal{A}}$ represented by neural networks $\mathcal{A}$ are both homogeneous, the prediction error on dataset D_λ then scales linearly w.r.t. the scaling factor λ:

$$\sum_{x \in D_\lambda} ||f(x) - F_{\mathcal{A}}(x)|| = \lambda \sum_{x' \in D} ||f(x') - F_{\mathcal{A}}(x')||. \quad (1)$$

We design the family of GNNs that are homogeneous, named HomoGNN, as follows: simply remove all the bias terms in the multi-layer perceptron (MLP) used by ordinary GNNs, so that all affine transformations degenerate to linear transformations. Additionally, only activation functions that are homogeneous are allowed to be used. Note that ReLU is a homogeneous activation function. The original MLP used in ordinary GNNs become HomoMLP in HomoGNNs afterwards.

5. Experiments

We evaluate the generalizability of models with respect to graph scales on three graph theory problems, i.e. shortest path, component counting, and Traveling Salesman Problem (TSP). We build a benchmark by combining multiple



(a) $f(\lambda x) = \lambda f(x),\ \forall \lambda > 0, x \in R^2$ (b) Behaviors of MLP (c) Behaviors of Homogeneous MLP

Figure 2. (a) An example of homogeneous functions. (b-c) Illustration of the improved generalizability by applying the homogeneous prior. Knowledge learned from the training samples not only can be generalized to samples of the same data distribution as ordinary neural networks, as shown in (b), but also can be generalized to samples of the scaled data distributions, as shown in (c).

Table 1. Generalization performance on graph algorithm learning . Models are trained on graphs of sizes within $[4, 34)$ and are tested on graph of larger sizes such as 100 and 500. The metric for shortest path and TSP is the relative loss. The metric for component counting is the accuracy. The metric for the unweighted shortest path problem is the success rate of identifying shortest paths.

Models	Shortest Path - weighted				Component Cnt.		TSP	Shortest Path - unweighted				
	ER	PL	KNN	Lob	ER	Lob	2D	20	100	500	1000	5000
GCN (Kipf & Welling, 2017)	0.1937	0.202	0.44	0.44	0.0%	0.0%	0.52	66.6	25.7	5.5	2.4	0.4
GAT (Veličković et al., 2018)	0.1731	0.127	0.26	0.28	0.0%	0.0%	0.18	**100.0**	42.7	10.5	5.3	0.9
Path	0.0014	0.084	0.16	0.29	82.3%	36.9%	0.16	**100.0**	62.9	20.1	10.3	1.6
Homo-Path	**0.0008**	0.015	0.07	0.27	**91.9%**	83.9%	0.14	**100.0**	72.7	58.3	53.7	50.2
Iter-Homo-Path	**0.0007**	**0.003**	**0.03**	**0.02**	86.6%	**95.4%**	**0.11**	**100.0**	**100.0**	**100.0**	**100.0**	**100.0**

graph generators, including Erdos-Renyi (ER), K-Nearest-Neighborhoods graphs (KNN), planar graphs (PL), and lobster graphs (Lob), so that the generated graphs can have more diverse properties. The generation processes and the properties of datasets are listed in the Appendix E.

Models and baselines. We stack 30 GCN (Kipf & Welling, 2017)/GAT (Veličković et al., 2018) layers to build the baseline models. GIN (Xu et al., 2019) is not enlisted since 30-layer GINs do not converge in most of our preliminary experiments. Our "Path" model stacks 30 PathGNN layers. Our "Homo-Path" model replaces GNNs and MLPs in the "Path" model with HomoGNNs and HomoMLPs. The "Iter-Homo-Path" model adopts the iterative module to control the iteration number of the GNN layer in the "Homo-Path" model.

Training Details. We utilize the default hyper-parameters to train models. We generate 10000 samples for training, 1000 samples for validation, and 1000 samples for testing. The only two tunable hyper-parameter in our experiment is the epoch number (10 choices) and the formulation of PathGNN layers (3 choices). Validation datasets are used to tune them. More details are presented in Appendix E.3.

Results and analysis. We present the generalization performance for all three graph theory problems in Table 1. Models are trained on graphs of sizes within $[4, 34)$ and are evaluated on graphs of larger sizes such as 100 (for shortest path and TSP) and 500 (for component counting so that the diameters of components are large enough). The relative loss metric is defined as $|y - \hat{y}|/|y|$, given a label y and a prediction $\hat{y}$. The results demonstrate that each of our proposals improves the generalizability on almost all problems. Exceptions happen on graphs generated by ER. It is because the diameters of those graphs are 2 with high probability even though the graph sizes are large. Our final model, Iter-Homo-Path, which integrates all proposals, performs much better than the baselines such as GCN and GAT.

We then explore models' generalizability on much larger graphs on the shortest path problem using Lob to generate graphs with larger diameters. As shown in Table 1, our model achieves 100% success rate of identifying the shortest paths on graphs with as large as 5000 nodes even though they are trained on graphs of sizes within $[4, 34)$. As claimed, the iterative module is necessary for generalizing to graphs of much larger sizes and diameters due to the message passing nature of GNNs.

6. Conclusion

We propose IterGNN and HomoGNN to improve the generalizability of GNNs w.r.t. graph scales. Experiments show that our proposals do improve the generalizability for solving multiple graph-related problems and tasks.

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Appendix

In the appendix, we seek to answer the following questions: **(1)** How powerful is our iterative module on approximating the iterative algorithms? **(2)** Are low generalization errors achievable when using homogeneous neural networks to approximate the homogeneous functions? What is the generation error bound? **(3)** Are low training errors achievable when using HomoMLP to approximate the homogeneous functions? **(4)** How does each of our proposals improve the generalizability w.r.t. graph scales? How much improvements do our proposals achieve compared with the baselines? **(5)** What kind of stopping criterion does our iterative module learn in practice? **(6)** Is the iterative module harmful to the standard generalizability in practice? **(7)** What are the experimental setups?

To answer the question **(1)**, we present the theoretical analysis of the representation power of our iterative module in Section A.1. To answer the question **(2)**, we present and prove the generalization error bounds of homogeneous neural networks on approximating homogeneous functions with independent scaling assumptions in Section A.2.1. To answer the question **(3)**, we present and prove the universal approximation theorem of HomoMLP on approximating the homogeneous functions in Section A.2.3. To answer question **(4)**, we perform the ablation studies in Section B.1. To answer question **(5)**, we show that our iterative module actually learns an optimal and interpretable stopping criterion in Section B.2. To answer question **(6)**, we show that our IterGIN model, which wraps each layer of the state-of-art GIN (Xu et al., 2019) model with our iterative module, achieves competitive performance to GIN, in Section B.3. To answer question **(7)**, we describe all omitted details of the experimental setups in Section E.

A. Theoretical analysis

We present the theoretical analysis of our proposals in this section. In detail, we analyze the representation power of our iterative module in Section A.1. We prove the generalization error bounds of homogeneous neural networks in Section A.2.1. We show that HomoMLP and HomoGNN can only represent homogeneous functions in Section A.2.2. We also prove the universal approximation theorem of HomoMLP on approximating homogeneous functions in Section A.2.3.

A.1. Representation powers of iterative module

We first state the intuition that our iterative module as described in the main body can approximate any iterative algorithms as defined in Algorithm 2, as long as the $body$ and $condition$ functions are available or can be perfectly reproduced by neural networks.

Algorithm 2 Iterative algorithm

input initial feature x
$k \leftarrow 1$
$h^0 \leftarrow x$
while not $condition(h^k)$ **do**
  $h^k \leftarrow body(h^{k-1})$
  $k \leftarrow k + 1$
end while
return $h = h^k$

More formally, we build an ideal class of models, named as Iter-Oracle, by combining our iterative module with the oracles $\mathcal{F}_\theta$ that can perfectly reproduce the $body$ function and the $condition$ function, which means there exist θ' and θ'' such that for all x, $\mathcal{F}_{\theta'}(x) = body(x)$ and $\mathcal{F}_{\theta''}(x) = condition(x)$. We can then show the representation power of our iterative module using the following theorem:

Theorem A.1.1. *For any iterative algorithm, iter-alg, defined as in Algorithm 2, for any initial feature x, and for any $\epsilon > 0$, there exist an Iter-Oracle model $\mathcal{A}$, which represents the function $\mathcal{F}_\mathcal{A}$, satisfying*

$$||\textit{iter-alg}(x) - \mathcal{F}_\mathcal{A}(x)|| < \epsilon. \tag{2}$$

We prove it by construction. We build the function f in our iterative module using $\mathcal{F}_{\theta'}$ such that $\mathcal{F}_{\theta'}(x) = body(x)$ for all x. The function g in our iterative module is built as $\text{sigmoid}(\alpha(\mathcal{F}_{\theta''}(x) - 0.5))$, where $\mathcal{F}_{\theta''}(x) = condition(x)$ for all x and

we utilize similar rules to the python language for type conversion, which means $condition(x)$ outputs 1 if the condition is satisfied and outputs 0 otherwise. By setting $\alpha \to +\infty$, we have

$$c^k \to \begin{cases} 1 & \text{if } condition(h^k) \\ 0 & \text{if not } condition(h^k). \end{cases}$$

Therefore, $\sum_{j=1}^{\infty} c^j h^j \prod_{i=1}^{j-1}(1-c^i) \to h^k$, where k is the time step that $condition(h^k)$ is firstly satisfied. More formally, assume Λ bounds the norm of features h^j for the specific iterative algorithm $iter\text{-}alg$, for the specific initial feature x, and for any j, we can set α as

$$\alpha > 2\ln\left(\frac{(k+1)\Lambda}{\epsilon} - 1\right) \text{ and } \alpha > -2\ln\left(\left(1 + \frac{\epsilon}{(k+1)\Lambda}\right)^{-\frac{1}{k}} - 1\right), \tag{3}$$

so that Eq. 2 is satisfied, since for $j < k$,

$$\left\| c^j h^j \prod_{i=1}^{j-1}(1-c^i) - 0 \right\| < \left\| c^j h^j \right\| < \frac{1}{1+e^{\frac{\alpha}{2}}}\Lambda = \frac{\epsilon}{k+1}, \tag{4}$$

for $j = k$,

$$\left\| c^k h^k \prod_{i=1}^{k-1}(1-c^i) - h^k \right\| < \left(\left(\frac{1}{1+e^{-\frac{\alpha}{2}}}\right)^k - 1\right)\Lambda = \frac{\epsilon}{k+1}, \tag{5}$$

for $j > k$,

$$\left\| \sum_{j=k+1}^{\infty} c^j h^j \prod_{i=1}^{j-1}(1-c^i) - 0 \right\| < (1-c^k)\Lambda < \frac{1}{1+e^{\frac{\alpha}{2}}}\Lambda = \frac{\epsilon}{k+1}. \tag{6}$$

Together, we have

$$\begin{aligned} \left\| \sum_{j=1}^{\infty} c^j h^j \prod_{i=1}^{j-1}(1-c^i) - h^k \right\| \quad \leq \quad & \sum_{j=1}^{k-1} \left\| c^j h^j \prod_{i=1}^{j-1}(1-c^i) - 0 \right\| + & (7) \\ & \left\| c^k h^k \prod_{i=1}^{k-1}(1-c^i) - h^k \right\| + & (8) \\ & \left\| \sum_{j=k+1}^{\infty} c^j h^j \prod_{i=1}^{j-1}(1-c^i) - 0 \right\| & (9) \\ < \quad & (k+1)\frac{\epsilon}{k+1} = \epsilon \quad \square \end{aligned}$$

We then derive a more practical proposition of IterGNN, based on Theorem A.1.1, stating the intuition that IterGNN can achieve adaptive and unbounded iteration numbers:

Proposition A.1.1. *Under the assumptions that IterGNN can calculate graph sizes N with no error and the multilayer perceptron used by IterGNN is a universal approximator of continuous functions on compact subsets of $\mathbb{R}^n$ ($n \geq 1$) (i.e. the universal approximation theorem), there exist IterGNNs whose iteration numbers are constant, linear, polynomial or exponential functions of the graph sizes.*

The proofs are simple. Let g' be the function that maps the graph sizes N to iteration numbers k. we can then build GNNs as f to calculate the graph sizes N and the number of current time step j, and build g as sigmoid$(\alpha(0.5 - |g'(N) - j|))$.

The α can be set similarly to the previous proof except for one scalar that compensates the approximation errors of neural networks. More formally, assume ϵ' bounds the error of predicting $g'(N)$ and j using neural networks $\mathcal{A}$, which means for any input, there exists neural networks that represent functions $\mathcal{F}_g$ and $\mathcal{F}_j$ satisfying $|g'(N) - \mathcal{F}_g| < \epsilon'$ and $|j - \mathcal{F}_j| < \epsilon'$. We can then set α as

$$\alpha > \frac{2}{1-4\epsilon'} \ln\left(\frac{(k+1)\Lambda}{\epsilon} - 1\right) \text{ and } \alpha > -\frac{2}{1-4\epsilon'} \ln\left(\left(1 + \frac{\epsilon}{(k+1)\Lambda}\right)^{-\frac{1}{k}} - 1\right), \tag{10}$$

so that Proposition A.1.1 is satisfied. Note that it is easy to build GNNs to exactly calculate the graph sizes N and the number of current time step j. Given the universal approximation theorem of MLP, the stopping condition function g can also be easily approximated by MLPs. Our iterative module is thus able to achieve adaptive and unbounded iteration numbers using neural networks.

A.2. Homogeneous prior

We formalize the generalization error bounds of homogeneous neural networks on approximating homogeneous functions under proper conditions, by extending the example in the main body to more general cases, in Section A.2.1. To make sure functions represented by neural networks are homogeneous, we also prove that HomoGNN and HomoMLP can only represent homogeneous functions, in Section A.2.2. To show that low training errors are achievable, we further analyze the representation powers of HomoMLP and demonstrate that it is a universal approximator of homogeneous functions under some assumptions, based on the universal approximation theorem of MLPs (Cybenko, 1989), in Section A.2.3.

A.2.1. Generalization error bounds of homogeneous neural networks

Extending the example in the main body to more general cases, we present the out-of-distribution generalization error bounds of homogeneous neural networks on approximating homogeneous functions under the assumption of independent scaling of magnitudes during inference:

Let training samples $D_m = \{x_1, x_2, \cdots x_m\}$ be independently sampled from the distribution $\mathcal{D}_x$, then if we scale the training samples with the scaling factor $\lambda \in \mathbb{R}^+$ which is independently sampled from the distribution $\mathcal{D}_\lambda$, we get a "scaled" distribution $\mathcal{D}_x^\lambda$, which has a density function $P_{\mathcal{D}_x^\lambda}(z) := \int_\lambda \int_x \delta(\lambda x = z) P_{\mathcal{D}_\lambda}(\lambda) P_{\mathcal{D}_x}(x) \,\mathrm{d}x \,\mathrm{d}\lambda$. The following theorem bounds the generalization error bounds on $\mathcal{D}_x^\lambda$:

Theorem 1. (Generalization error bounds of homogeneous neural networks with independent scaling assumption). *For any positive homogeneous functions function f and neural network $F_\mathcal{A}$, let β bounds the generalization errors on the training distribution D_x , i.e., $\mathbb{E}_{x\sim\mathcal{D}_x}|f(x) - \mathcal{F}_\mathcal{A}(x)| \le \frac{1}{m}\sum_{i=1}^m |f(x_i) - F_\mathcal{A}(x_i)| + \beta$, then the generalization errors on the scaled distributions $\mathcal{D}_x^\lambda$ scale linearly with the expectation of scales $\mathbb{E}_{\mathcal{D}_\lambda}[\lambda]$:*

$$\mathbb{E}_{x\sim\mathcal{D}_x^\lambda}|f(x) - F_\mathcal{A}(x)| = \mathbb{E}_{\mathcal{D}_\lambda}[\lambda]\mathbb{E}_{x\sim\mathcal{D}_x}|f(x) - F_\mathcal{A}(x)| \le \mathbb{E}_{\mathcal{D}_\lambda}[\lambda](\frac{1}{m}\sum_{i=1}^m |f(x_i) - F_\mathcal{A}(x_i)| + \beta) \tag{11}$$

The proof is as simple as re-expressing the formulas:

$$\begin{aligned}
\mathbb{E}_{z\sim\mathcal{D}_x^\lambda}|f(z) - F_\mathcal{A}(z)| &= \int_\lambda \int_x P_{\mathcal{D}_\lambda}(\lambda) P_{\mathcal{D}_x}(x) |f(\lambda x) - F_\mathcal{A}(\lambda x)| \,\mathrm{d}x \,\mathrm{d}\lambda & (12)\\
&= \int_\lambda P_{\mathcal{D}_\lambda}(\lambda)\lambda \,\mathrm{d}\lambda \int_x P_{\mathcal{D}_x}(x)|f(x) - F_\mathcal{A}(x)| \,\mathrm{d}x & (13)\\
&= \mathbb{E}_{\mathcal{D}_\lambda}[\lambda]\mathbb{E}_{x\sim\mathcal{D}_x}|f(x) - F_\mathcal{A}(x)| & (14)\\
&\le \mathbb{E}_{\mathcal{D}_\lambda}[\lambda](\frac{1}{m}\sum_{i=1}^m |f(x_i) - F_\mathcal{A}(x_i)| + \beta) \quad \square
\end{aligned}$$

Theorem 1 can be considered as a meta-bound and can thus be integrated with any specific generalization error bounds with classical i.i.d. assumptions to create a concrete generation error bounds of homogeneous neural networks on approximating homogeneous functions with independent scaling assumptions. For example, when integrated a generation error bounds in

the PAC-Bayesian framework (Eq.7 in (Neyshabur et al., 2017)), we obtain the following lemma: Let $f_{\boldsymbol{w}}$ be any predictor learned from training data. We consider a distribution $\mathcal{Q}$ over predictors with weights of the form $\boldsymbol{w}+\boldsymbol{v}$, where $\boldsymbol{w}$ is a single predictor learned from the training set, and $\boldsymbol{v}$ is a random variable.

Lemma A.2.1. *Assume all hypothesis h and $f_{\boldsymbol{w}+\boldsymbol{v}}$ for any $\boldsymbol{v}$ are positive homogeneous functions, as defined in Definition 1. Then, given a "prior" distribution P over the hypothesis that is independent of the training data, with probability at least $1-\delta$ over the draw of the training data, the expected error of $f_{\boldsymbol{w}+\boldsymbol{v}}$ on the scaled distribution $\mathcal{D}_x^{\lambda}$ can be bounded as follows*

$$\begin{aligned}\mathbb{E}_{\boldsymbol{v}}\left[\mathbb{E}_{x\sim\mathcal{D}_x^{\lambda}}\left[\left|f(x)-f_{\boldsymbol{w}+\boldsymbol{v}}(x)\right|\right]\right] \leq \mathbb{E}_{\mathcal{D}_\lambda}[\lambda]\Bigg(&\frac{1}{m}\sum_{i=1}^{m}\left|f(x_i)-f_{\boldsymbol{w}}(x_i)\right|+\mathbb{E}_{\boldsymbol{v}}\left[\frac{1}{m}\sum_{i=1}^{m}\left|f(x_i)-f_{\boldsymbol{w}+\boldsymbol{v}}(x_i)\right|\right]\\ &-\frac{1}{m}\sum_{i=1}^{m}\left|f(x_i)-f_{\boldsymbol{w}}(x_i)\right|+4\sqrt{\frac{1}{m}\left(KL(\boldsymbol{w}+\boldsymbol{v}||P)+\ln\frac{2m}{\delta}\right)}\Bigg). \qquad (15)\end{aligned}$$

A.2.2. HomoMLP and HomoGNN are homogeneous functions

We present that HomoGNN and HomoMLP can only represent homogeneous functions:

Proposition A.2.1. *For any input x, we have HomoMLP$(\lambda x)=\lambda$HomoMLP(x) for all $\lambda>0$.*

Proposition A.2.2. *For any graph $G=(V,E)$ with node attributes $\vec{x}_v$ and edge attributes $\vec{x}_e$, we have for all $\lambda>0$,*

$$\textit{HomoGNN}(G,\{\lambda\vec{x}_v:v\in V\},\{\lambda\vec{x}_e:e\in E\})=\lambda\textit{HomoGNN}(G,\{\vec{x}_v:v\in V\},\{\vec{x}_e:e\in E\}). \qquad (16)$$

Both propositions are derived from the following lemma:

Lemma A.2.2. *Compositions of homogeneous functions are homogeneous functions.*

We compose functions by taking the outputs of functions as the input of other functions. TThe inputs of functions are either the outputs of other functions or the initial features x. For example, we can compose functions f,g,h as $h(f(x),g(x),x)$. If f,g,h are all homogeneous functions, we have for all x and all $\lambda>0$,

$$h(f(\lambda x),g(\lambda x),\lambda x)=\lambda h(f(x),g(x),x). \qquad (17)$$

More formally, we can prove the lemma by induction. We denote the composition of a set of functions $\{f_1,f_2,\cdots,f_n\}$ as $O(\{f_1,f_2,\cdots,f_n\})$. Note that there are multiple ways to compose n functions. Here, $O(\{f_1,f_2,\cdots,f_n\})$ just denotes one specific way of composition, and we can use $O'(\{f_1,f_2,\cdots,f_n\})$ to denote another. We want to prove that the composition of homogeneous functions is still a homogeneous function, which means for all $n>0$, for all $\lambda>0$, and for all possible ways of compositions O, $O(\{f_1,f_2,\cdots,f_n\})(\lambda x)=\lambda O(\{f_1,f_2,\cdots,f_n\})(x)$.

The base case: $n=1$. The composition of a single function $O(\{f_1\})$ is itself f_1. Therefore, $O(\{f_1\})$ is homogeneous by definition as $O(\{f_1\})(\lambda x)=f_1(\lambda x)=\lambda O(\{f_1\})(x)$.

Assume the composition of the k functions is homogeneous, for any composition of $k+1$ functions $O(\{f_1,f_2,\cdots,f_{k+1}\})$, let f_{k+1} be the last function of the compositions, which means $O(\{f_1,f_2,\cdots,f_{k+1}\})(x):=f_{k+1}(O'(\{f_1,f_2,\cdots,f_k\})(x),O''(\{f_1,f_2,\cdots,f_k\})(x),O'''(\{f_1,f_2,\cdots,f_k\})(x),\cdots)$, it's easy to see that, according to the definition of homogeneous functions,

$$O(\{f_1,f_2,\cdots,f_{k+1}\})(\lambda x)=\lambda O(\{f_1,f_2,\cdots,f_{k+1}\})(x). \quad \square$$

Therefore, we prove the Lemma A.2.2. Proposition A.2.1 and Proposition A.2.1 can all be considered as specializations of this lemma.

A.2.3. Universal approximation theorem for HomoMLP

We first introduce a class of neural networks that can be proved as a universal approximator of homogeneous functions (Theorem A.2.1) and then show that our HomoMLP is as powerful as this class of neural networks to prove that our HomoMLP is a universal approximator of homogeneous functions (Theorem A.2.2).

We construct a class of neural networks as the universal approximator of positive homogeneous functions, as defined in the main body, as follows:

$$G_{\text{MLP}}(x) = |x|\mathcal{F}_{\text{MLP}}(\frac{x}{|x|}), \tag{18}$$

where $|\cdot|$ denotes the L1 norm, the MLP denotes the classical multilayer perceptrons with positive homogeneous activation functions and $\mathcal{F}_{\text{MLP}}$ is the function represented by the specific MLP.

Proposition A.2.3. *For any input x, we have $G_{MLP}(\lambda x) = \lambda G_{MLP}(x)$.*

This proposition can be easily proved by re-expressing the formulas:

$$G_{\text{MLP}}(\lambda x) = |\lambda x|\mathcal{F}_{\text{MLP}}(\frac{\lambda x}{|\lambda x|}) = \lambda|x|\mathcal{F}_{\text{MLP}}(\frac{x}{|x|}) = \lambda G_{\text{MLP}}(x) \quad \square$$

We show that it is a universal approximator of homogeneous functions: Let $\mathbb{X}$ be a compact subset of $\mathbb{R}^m$ and $C(\mathbb{X})$ denotes the space of real-valued continuous functions on $\mathbb{X}$.

Theorem A.2.1. (Univeral approximation theorem for G_{MLP}.) *Given any $\epsilon > 0$ and any function $f \in C(\mathbb{X})$, there exist a finite-layer feed-forward neural networks $\mathcal{A}$ with positive homogeneous activation functions such that for all $x \in \mathbb{X}$, we have $|G_{\mathcal{A}}(x) - f(x)| = \left||x|\,\mathcal{F}_{\mathcal{A}}\left(\frac{x}{|x|}\right) - f\left(x\right)\right| < \epsilon$.*

The prove is as simple as applying the universal approximation theorem of MLPs (Cybenko, 1989) and applying the definition of the homogeneous functions. In detail, as $\mathbb{X}$ is a compact subset, the magnitudes of inputs x is bounded. We use M denote the bound, which means $|x| \leq M$ for all $x \in \mathbb{X}$. According to the universal approximation theorem of MLPs (Cybenko, 1989), there exists a finite-layer feed-forward layer $\mathcal{A}$ with ReLU as activation functions such that $\left|\mathcal{F}_{\mathcal{A}}\left(\frac{x}{|x|}\right) - f\left(\frac{x}{|x|}\right)\right| < \frac{\epsilon}{M}$ for all $x \in \mathbb{X}$. Then, according to definition of homogeneous functions, we have

$$|G_{\mathcal{A}}(x) - f(x)| = \left||x|\,\mathcal{F}_{\mathcal{A}}\left(\frac{x}{|x|}\right) - |x|\,f\left(\frac{x}{|x|}\right)\right| < |x|\,\frac{\epsilon}{M} < \epsilon \tag{19}$$

Note that ReLU is positive homogeneous. Therefore, we finish the proof of Theorem A.2.1. $\square$

We then prove that HomoMLP is a universal approximator of homogeneous functions: Let $\mathbb{X}$ be a compact subset of $\mathbb{R}^m$ and $C(\mathbb{X})$ denotes the space of real-valued continuous functions on $\mathbb{X}$.

Theorem A.2.2. (Universal approximation theorem for HomoMLP.) *Given any $\epsilon > 0$ and any function $f \in C(\mathbb{X})$, there exist a finite-layer HomoMLP $\mathcal{A}'$, which represents the function $F_{\mathcal{A}'}$, such that for all $x \in \mathbb{X}$, we have $|F_{\mathcal{A}'}(x) - f(x)| < \epsilon$.*

We prove it based on Theorem A.2.1 by construction. In detail, according to Theorem A.2.1, there exists a finite-layer MLP $\mathcal{A}$ such that for all $x \in \mathbb{X}$, $|G_{\mathcal{A}}(x) - f(x)| = \left||x|\,\mathcal{F}_{\mathcal{A}}\left(\frac{x}{|x|}\right) - f\left(x\right)\right| < \epsilon$. Without loss of generality, we assume $\mathcal{A}$ as a two-layer ReLU feed-forward neural networks, which means $\mathcal{F}_{\mathcal{A}}(x) = W^2\text{ReLU}(W^1x + b^1) + b^2$, where $W^1 \in \mathbb{R}^{n\times m}, W^2 \in \mathbb{R}^{1\times n}$ are weight matrices and $b^1 \in \mathbb{R}^n, b^2 \in \mathbb{R}$ are biases. The function $G_{\mathcal{A}}$ can then be expressed as

$$G_{\mathcal{A}}(x) = |x|\left(W^2\text{ReLU}\left(W^1\frac{x}{|x|} + b^1\right) + b^2\right) = W^2\text{ReLU}\left(W^1x + b^1|x|\right) + b^2|x|. \tag{20}$$

Therefore, we just need to prove that the L1 norm $|\cdot|$ can be exactly calculated by HomoMLP to show that HomoMLP is a universal approximator homogeneous functions. Typically, we construct a two-layer HomoMLP as follows

$$\mathbf{1}^T\text{ReLU}\left(\begin{bmatrix}\mathbf{I}\\-\mathbf{I}\end{bmatrix}x\right) \equiv |x|, \text{for all } x \in \mathbb{R}^m, \tag{21}$$

Iter-Homo-Path	
100.0	
Homo-Path	Iter-Path
53.7	48.9
ACT-Homo-Path	Iter-Homo-GAT
52.7	2.9
Shared-Homo-Path	Iter-Homo-GCN
91.7	1.4

Table 2. Ablation studeis of generalization performance for the shortest path problem on lobster graphs with 1000 nodes. Metric is the success rate.

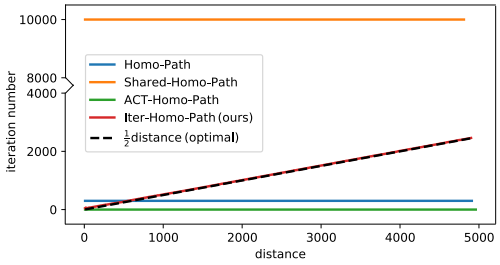


Figure 3. The iteration numbers of GNN layers w.r.t. the distances from the source node to the target node for the shortest path problem.

where $\mathbf{1}$ is a vertical vector containing $2m$ elements whose values are all one, and $\mathbf{I}$ denotes the identity matrix of size $m \times m$. Together with Eq. 20, we show that $G_{\mathcal{A}}(x)$ is a specification of HomoMLP, denoted as $\mathcal{A}'$, as follows:

$$G_{\mathcal{A}}(x) = W^2\text{ReLU}\left(W^1x + b^1|x|\right) + b^2|x| \tag{22}$$

$$= W^2\text{ReLU}\left(W^1x + b^1\mathbf{1}^T\text{ReLU}\left(\begin{bmatrix}\mathbf{I}\\-\mathbf{I}\end{bmatrix}x\right)\right) + b^2\mathbf{1}^T\text{ReLU}\left(\begin{bmatrix}\mathbf{I}\\-\mathbf{I}\end{bmatrix}x\right) \tag{23}$$

$$= \begin{bmatrix}W^2 & b^2\end{bmatrix}\text{ReLU}\left(\begin{bmatrix}W^1 + b^1 & -W^1 + b^1\\ \mathbf{1}^T & \mathbf{1}^T\end{bmatrix}\text{ReLU}\left(\begin{bmatrix}\mathbf{I}\\-\mathbf{I}\end{bmatrix}x\right)\right) \tag{24}$$

$$= F_{\mathcal{A}'}(x) \tag{25}$$

Here, we use $\mathbf{1}$ to denote a vertical vector containing m elements whose values are all one, and $\mathbf{I}$ still denotes the identity matrix of size $m \times m$. The summation of the weight matrix $W \in \mathbb{R}^{n\times m}$ and the bias $b \in \mathbb{R}^n$ outputs a new weight matrix W_b such that $W_b[i,j] = W[i,j] + b[i]$ for all $i = 1, 2, \cdots, n$ and $j = 1, 2, \cdots, m$, where $W[i,j]$ is the element in the ith row and the jth column of matrix W and $b[i]$ is the ith element of vertex b. Consequently, we build a three-layer HomoMLP $\mathcal{A}'$ with ReLU as activation functions such that for all $x \in \mathbb{X}$,

$$|F_{\mathcal{A}'}(x) - f(x)| = |G_{\mathcal{A}}(x) - f(x)| < \epsilon. \quad \square$$

B. Experiment Results

B.1. Ablation studies and comparison

We conduct ablation studies to exhibit benefits of our proposals using the unweighted shortest path problem on lobster graphs with 1000 nodes in Table 2. The models are built by replacing each proposal in our best Iter-Homo-Path model with other possible substitutes in the literature. For the iterative module, other than the simplest paradigm utilized in Homo-Path that stacks GNN layers sequentially, we also compare it with the ACT algorithm (Graves, 2016) and the fixed-depth weight-sharing paradigm (Tamar et al., 2016; Li & Zemel, 2014), resulting in the "ACT-Homo-Path" and "Shared-Homo-Path" models. The ACT algorithm provides adaptive but usually short iterations of layers (analyzed later). The weight-sharing paradigm iterates modules for predefined times and assumes that the predefined iteration number is large enough. We set its iteration number to the largest graph size in the dataset. Homo-Path and ACT-Homo-Path perform much worse than Iter/Shared-Homo-Path because of the limited representation powers of shallow GNNs. Shared-Homo-Path performs worse than our Iter-Homo-Path, possibly because of the accumulated errors after unnecessary iterations. For the homogeneous prior, we build "Iter-Path" by simply removing the homogeneous prior. It performs much worse than Iter-Homo-Path because of the poor performance of MLPs on out-of-distribution features. For PathGNN, we build "Iter-Homo-GCN" and "Iter-Homo-GAT" by replacing PathGNN with GCN and GAT. Their bad performance verifies the benefits of better algorithm alignments (Xu et al., 2020).

The iteration numbers learned by ACT are usually small. As shown in Figure 3, the ACT-Homo-Path model learns much smaller iteration numbers than other models. It is because of the formulations of the ACT algorithm. In detail, the

Dataset	GIN	Iter-GIN
IMDB-B	75.1±5.1	**75.7±4.2**
IMDB-M	**52.3±2.8**	51.8±4.0
MUTAG	89.4±5.6	**89.6±8.6**
PROTEINS	76.2±2.8	**76.3±3.4**
PTC	**64.6±7.0**	64.5±3.8

Table 3. The performance of our iterative module on graph classification on five popular benchmarks. Iter-GIN is built by wrapping each GIN module in the previous state-of-art method (Xu et al., 2019) using our iterative module. Metric is the averaged accuracy and STD in 10-fold cross-validation.

ACT algorithm considers a different random process from our iterative module while designing the stopping criterion. The expected output has the form as $\sum_{i=1}^{k-1} c^i h^i + (1 - \sum_{i=1}^{k-1} c^i) h^k$. The notations are the same as our iterative module described in the main body. And the stopping criterion is $\sum_{i=1}^{k} c^i > 1$. Compared with the expected output $\sum_{j=1}^{k} c^j h^j \prod_{i=1}^{j-1}(1 - c^i)$ and the stopping criterion $\prod_{i=1}^{k}(1 - c^i) < \epsilon$ of our iterative module, it is generally easier for the stopping criterion of ACT to be satisfied since $1 - \sum_{i=1}^{k} c^i < \prod_{i=1}^{k}(1 - c^i)$ if $k > 1$ and $0 < c^i < 1$ for all $i <= k$. In the paper that proposes ACT (Graves, 2016), the author also states similar intuitions that the formulation in our iterative module will not stop in a few steps. In fact, as far as we know, all works (Graves, 2016; Figurnov et al., 2017; Eyzaguirre & Soto, 2020) that utilize the ACT algorithm adopt a noisy regularization term to encourage fewer iteration numbers. They have distinct motivations and objectives from our work. For example, most of them are designed for more efficiencies by fewer iterations (Figurnov et al., 2017; Eyzaguirre & Soto, 2020). On the other hand, our iterative module is designed to improve the generalizability of GNNs with respect to scales by generalizing to much larger iterations.

B.2. Interpreting stopping criterion learned by the iterative module.

We show that our Iter-Homo-Path model learned the optimal stopping criterion for the unweighted shortest path problem in Figure 3. Typically, to accurately predict the shortest path of lengths d on undirected graphs, the iteration number of GNN layers is at least $d/2$ due to the message passing nature of GNNs. In detail, both the source node and the target node need to send and to collect information along the shortest path towards each other, so that each iteration of GNNs could collect information of two more edges on the shortest path. No less iteration numbers can be achieved using 1-hop message passing GNNs as the path length is already the shortest. Our iterative module actually learns such optimal stopping criterion. The Iter-Homo-Path model adaptively increases the iteration numbers w.r.t. the distances and moreover stops timely when the information is enough.

B.3. Graph Classification

We evaluate models on standard graph classification benchmarks to show that our proposals don't hurt GNNs' powers as well as the standard generalizability while improving their generalizability w.r.t. scales. More descriptions of the task are available in (Xu et al., 2019). The experimental setups are presented in Section E.2.

As stated in Table 3, our model performs competitively with the previous state-of-art backbone, GIN, on all five benchmarks. It suggests that our iterative module is a safe choice for improving generalizability w.r.t. scales while still maintaining the performance for normal tasks. Note that, due to the shortage of time, little hyper-parameter search was conducted in our experiments. Default hyper-parameters such as learning rate equal to 0.001 and hidden size equal to 64 were adopted. Therefore, the performance of Iter-GIN is potentially better than those stated in Table 3.

C. Related Work

Graph Neural Networks. Graph neural networks (GNNs) have become popular in many fields (Zhou et al., 2018; Goyal & Ferrara, 2018; Wu et al., 2020) , because of their abilities to handle irregular graph structures, to approximate permutation invariant/equivalent functions, and to exploit relational inductive biases such as locality (Battaglia et al., 2018). Most of those popular GNN variants come within a generalized framework called message passing (Gilmer et al., 2017; Battaglia et al., 2018). We will describe it in Section 3.

Graph Algorithm Learning. Despite the success of GNNs (mostly come within the message passing framework (Gilmer

et al., 2017; Battaglia et al., 2018)) in many fields (Zhou et al., 2018; Goyal & Ferrara, 2018; Wu et al., 2020), few works have reported remarkable results on solving traditional graph-related problems, such as the shortest path problem, by neural networks, especially when the generalizability with regard to scales is taken into account. Previously, in the period with limited computation power, people explored the possibility of approximating graph algorithms by neural networks for more efficiencies by distributed computation (Araujo et al., 2001). After the resurgence of deep neural networks, Neural Turing Machine (Graves et al., 2014; 2016) first reported performance on solving shortest path on small graphs using deep neural networks to demonstrate its representation powers. Recently, (Veličković et al., 2020) and (Xu et al., 2020) achieved positive performance on solving the shortest path problem on relatively large graphs using the GNNs. However, methods in (Veličković et al., 2020) require per-layer supervisions to train and models in (Xu et al., 2020) theoretically lack the generalizability w.r.t. graph scales due to their bounded number of message passing steps. As far as we know, no previous work has solved the shortest path problem by neural networks on graphs of diameters larger than 100. There is either no work reporting notable generalization performance with respect to graph scales.

Iterative Algorithm Approximation. Traditional iterative algorithms have been successfully applied in solving the classical graph problems (Dijkstra, 1959) as well as in many application fields such as controlling, network analysis (Page et al., 1999), and Bayesian statistics (Blei et al., 2017). Inspired by their success, several works were proposed to incorporate the iterative architecture into neural networks for better generalizability (Tamar et al., 2016), more efficiency (Dai et al., 2018), or to support end-to-end training (Li & Zemel, 2014; Zheng et al., 2015). However, none of them supports adaptive and unbounded iteration numbers and is therefore not applicable for approximating general iterative algorithms over graphs of any sizes. Dai (Dai et al., 2018) adopted GNNs to improve the efficiency and scalability of a special class of iterative algorithms whose solutions are characterized by a set of steady-state conditions. However, it is not applicable to approximate general iterative algorithms and the iteration numbers are usually pre-defined as done in their experiments.

Differentiable Controlling Flows. In recent years, multiple works have been proposed in the graph representation learning field that integrate controlling into neural networks to achieve flexible data-driven control. For example, DGCNN (Zhang et al., 2018) implemented a differentiable sort operator (sort pooling) to build more powerful readout functions. Graph U-Net (Gao & Ji, 2019; Cangea et al., 2018) designed an adaptive pooling operator (TopK pooling) to support flexible data-driven pooling operations. All these methods achieved the differentiability by relaxing and multiplying the controlling signals with the neural networks' hidden representations. Inspired by their works, our method also differentiates the iterative algorithm by relaxing and multiplying the stopping criterion's output into neural networks' hidden representations.

Adaptive Depth of Neural Networks. The final formulation of our method is generally similar to the previous adaptive computation time algorithm (ACT) (Graves, 2016) for RNNs or spatially ACT (Figurnov et al., 2017; Eyzaguirre & Soto, 2020) for CNNs, however, with distinct motivations and formulation details. The numbers of iterations for ACT are usually small by design (e.g.the formulation of regularizations and halting distributions). Other than to achieve more representation powers through repeating operations for multiple times, or to achieve more efficiency by selectively iterating for fewer times, our method is designed to fundamentally improve the generalizability of GNNs w.r.t. scales by generalizing to much larger iteration numbers. Several improvements are proposed accordingly. Recently, there are also flow-based methods that (e.g. the Graph Neural ODE (Poli et al., 2019)) are also potentially able to provide adaptive layer numbers. However, with no explicit iteration controller, they are not a straightforward solution to approximate iterative algorithms and to encode related inductive biases. For example, it's not easy to transform the solution of the shortest path into an ODE.

D. Method

We present the decaying confidence mechanism to achieve much larger iteration numbers during inference in practice in Section D.1. We show the formulation of PathGNN layers in detail in Section D.2. There are three variants of PathGNN, each of which corresponds to different degrees of flexibilities of approximating functions.

D.1. Decaying confidence mechanism of our iterative module

Although the vanilla IterGNN, as described in the main body, theoretically supports infinite iteration numbers, models can hardly generalize to much larger iteration numbers during inference in practice. In detail, we utilize the sigmoid function to ensure that confidence scores are between 0 and 1. However, the sigmoid function can't predict zero confidence scores to continue iterations forever. Alternatively, the models will predict small confidence scores when they are not confident enough to terminate at the current time step. As a result, the models will still work well given the IID assumption, but can't generalize well when much larger iteration numbers are needed than those met during training. For example, while solving

the shortest path problem, 0.05 is a sufficiently small confidence score during training, because no iteration number larger than 30 is necessary and 0.95^{30} is still quite larger than 0. However, such models can not generalize to graphs with node numbers larger than 300, since $0.95^{300} \to 0$ and the models will terminate before time step 300 in any case. During our preliminary experiments, the vanilla IterGNN can not iterate for more than 100 times.

The key challenge is the difference between iteration numbers during training and inference. We then introduce a simple decaying mechanism to achieve larger iteration numbers during inference. The improved algorithm is shown in Algorithm 3. The termination probabilities will manually decay/decrease by λ at each time step. The final formulation of IterGNN can then generalize to iterate for 2500 times during inference in our experiments.

We compare the choices of decaying ratios as $0.99, 0.999, 0.9999$ in our preliminary experiments and fix it to 0.9999 afterwards in all experiments.

Algorithm 3 IterGNN with decay. g is the stopping criterion and f is the iteration body

Input: initial feature x; stop threshold ϵ; decay constant λ;
$k \leftarrow 1$
$h^0 \leftarrow x$
while $\lambda^k \prod_{i=1}^{k-1}(1-c^i) > \epsilon$ **do**
  $h^k \leftarrow f(h^{k-1})$
  $c^k \leftarrow g(h^k)$
  $k \leftarrow k+1$
end while
return $h = \lambda^k \sum_{j=1}^{k} c^j h^j \prod_{i=1}^{j-1}(1-c^i)$

D.2. Path Graph Neural Networks

As stated in (Battaglia et al., 2018), the performance of GNNs, especially their generalizability and zero-shot transferability, is largely influenced by the relational inductive biases. Xu (Xu et al., 2020) further formalized the relational inductive biases as sample efficiencies from algorithm alignments. For solving path-related graph problems such shortest path, a classical algorithm is the Bellman-Fold algorithm. Therefore, to achieve more effective and generalizable solvers for path-related graph problems, we design several specializations of GN blocks, as described in (Battaglia et al., 2018), by exploiting the inductive biases of the Bellman-Fold algorithms.

Our first observation of the Bellman-Fold algorithm is that it directly utilizes the input attributes such as the edge weights and the source/target node identifications at each iteration. We further observe that the input graph attributes of classical graph-related problems are all informative, well defined and also well represented as discrete one-hot encodings or simple real numbers (e.g. edge weights). Therefore, we directly concatenate the input node attributes with the hidden node attributes as the new node attributes before fed into our Graph Networks (GN) blocks. The models then don't need to extract and later embed the input graph attributes into the hidden representations in each GN block.

Our second observation is that Bellman-Fold algorithm can be perfectly represented by Graph Networks as stated in Algorithm 4. Typically, for each iteration of the Bellman-Fold algorithm, the message module sums up the sender node's attributes (i.e. distance) with the edge weights, the node-level aggregation module then selects the minimum of all edge messages, and finally the attributes of the central node are updated if the new message (/distance) is smaller. The other modules of GN blocks are either identity functions or irrelevant. Therefore, to imitate the Bellman-Fold algorithm by GN blocks, we utilize max pooling for both aggregation and update modules to imitate the min poolings in the Bellman-Fold algorithm. The edge message module is MLP, similarly to most GNN variants. The resulting module is then equal to replacing the MPNN (Gilmer et al., 2017)'s aggregation and update module with max poolings. Therefore, we call it MPNN-Max as in (Veličković et al., 2020). The concrete formulas are as follows

$$\begin{aligned} \mathbf{e}'_k &= MLP(\mathbf{v}_{s_k}, \mathbf{v}_{r_k}, \mathbf{e}_k) \\ \bar{\mathbf{e}}_j &= \max(\{\mathbf{e}'_k : r_k = j\}) \\ \mathbf{v}'_j &= \max(\mathbf{v}_j, \bar{\mathbf{e}}_j) \end{aligned}$$

Moreover, we notice that the Bellman-Ford algorithm is only designed for solving the shortest path problem. Many

Algorithm 4 The Bellman-Fold algorithm

Input: node attributes $V = \{\mathbf{v}_i, i = 1, 2, \cdots, N_v\}$, edge attributes $E = \{(w_k, s_k, r_k), k = 1, 2, \cdots, N_e\}$, and the source node $source$.
Output: The shortest path length from the source node to others, $distance = \{dist_i, i = 1, 2, \cdots, N_v\}$.

Initialize the intermediate node attributes $V' = \{dist_i, i = 1, 2, \cdots, N_v\}$ as $dist_i = \begin{cases} 0 & if.\ i = source \\ \infty & o.w. \end{cases}$.
for i=1 **to** $N_v - 1$ **do**
  for (w_k, s_k, r_k) **in** E **do**
    $\mathbf{e}'_k = dist_{s_k} + w_k$ ◁ edge message module
  end for
  for j=1 **to** N_v **do**
    $\bar{\mathbf{e}}_j = \min(\{\mathbf{e}'_k : r_k = j\})$ ◁ aggregation module
    $dist_j = \min(dist_j, \bar{\mathbf{e}}_j)$ ◁ update module
  end for
end for

Algorithm 5 One step of PathGNN

Input: graph $G = (V, E)$
Output: updated graph $G' = (V', E)$

for (w_k, s_k, r_k) **in** E **do**
  $\tilde{\mathbf{e}}_k = MLP(\mathbf{v}_{s_k}, \mathbf{v}_{r_k}, \mathbf{e}_k)$
  $score_k = MLP'(\mathbf{v}_{s_k}, \mathbf{v}_{r_k}, \mathbf{e}_k)$
  $\mathbf{e}'_k = (score_k, \tilde{\mathbf{e}}_k)$ ◁ edge message module
end for
for j=1 **to** N_v **do**
  $\bar{\mathbf{e}}_j = \text{attention}(\{\mathbf{e}'_k : r_k = j\})$ ◁ aggregation module
  $\mathbf{v}'_j = \max(\mathbf{v}_j, \bar{\mathbf{e}}_j)$ ◁ update module
end for

path-related graph problems can not be solved by it. Therefore, we further relax the max pooling to attentional poolings to increase the models' flexibility while still maintaining the ability to approximate min pooling in a sample efficient way. Typically, we propose the PathGNN by replacing the aggregation module with attentional pooling. The detailed algorithm is stated in Algorithm 5, where the global attributes are omitted due to their irrelevance.

Another variant of PathGNN is also designed by exploiting a less significant inductive bias of the Bellman-Fold algorithm. Specifically, we observe that only the sender node's attributes and the edge attributes are useful in the message module while approximating the Bellman-Fold algorithm. Therefore, we only feed those attributes into the message module of our new PathGNN variant, PathGNN-sim. The detailed algorithm is stated in Algorithm 7.

In summary, we introduce Path Graph Neural Networks (PathGNN) to improve the generalizability of GNNs for distance related problems by improving the algorithm alignment (Xu et al., 2020). It is a specially designed GNN layer that imitates one iteration of the classical Bellman-Ford algorithm. There are three variants of PathGNN, i.e. MPNN-Max, PathGNN,

Algorithm 6 Attention Pooling in GNNs

Input: set of messages $\{\mathbf{e}'_k = (score_k, \tilde{\mathbf{e}}_k)\}$
Output: aggregated messages $\bar{\mathbf{e}}_j$

$\alpha = softmax(score)$
$\bar{\mathbf{e}}_j = \sum_k \alpha_k \tilde{\mathbf{e}}_k$

Algorithm 7 One step of PathGNN-sim

Input: graph $G = (V, E)$
Output: updated graph $G' = (V', E)$

for (w_k, s_k, r_k) **in** E **do**
  $\tilde{\mathbf{e}}_k = MLP(\mathbf{v}_{s_k}, \mathbf{e}_k)$
  $score_k = MLP'(\mathbf{v}_{s_k}, \mathbf{v}_{r_k}, \mathbf{e}_k)$
  $\mathbf{e}'_k = (score_k, \tilde{\mathbf{e}}_k)$ ◁ edge message module
end for
for j=1 **to** N_v **do**
  $\bar{\mathbf{e}}_j = \text{attention}(\{\mathbf{e}'_k : r_k = j\})$ ◁ aggregation module
  $\mathbf{v}'_j = \max(\mathbf{v}_j, \bar{\mathbf{e}}_j)$ ◁ update module
end for

and PathGNN-sim, each of which corresponds to different degrees of flexibilities. In our experiments, they perform much better than GCN and GAT for all path-related tasks regarding the generalizability, as stated in Section 5 in the main body.

E. Experiment Setups

We present the experimental setups in this subsection. Typically, we first present details of three graph theory problems, i.e. the shortest path problem in Section E.1.2, the component counting problem in Section E.1.3, and the traveler salesman problem in Section E.1.4. We also describe the experimental setups of graph classification in Section E.2. The training details are presented in Section E.3.

E.1. Graph theory problems

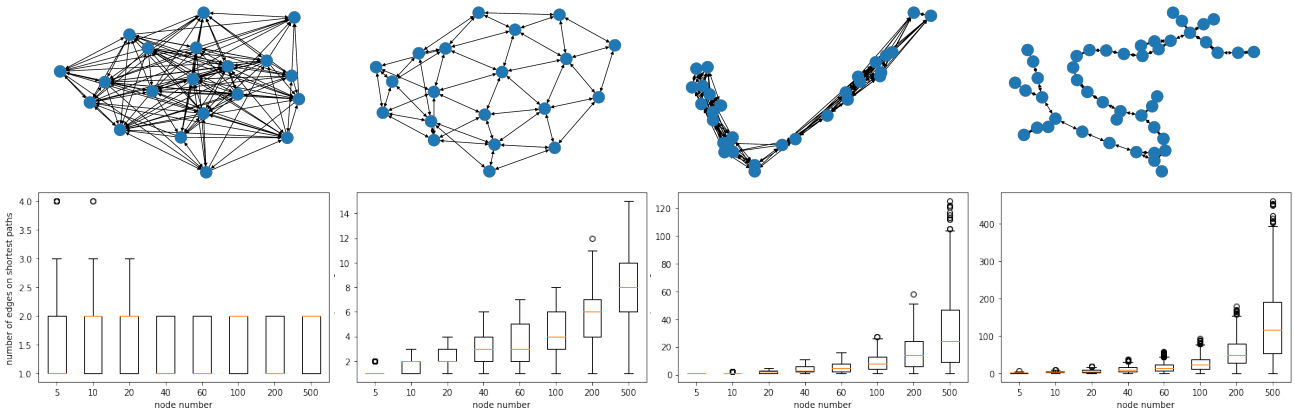
We evaluate our proposals on three classical graph theory problems, i.e. shortest path, component counting, and the Traveling Salesman Problem (TSP). We present the properties of graph generators in Section E.1.1, the setups for the shortest path problem in Section E.1.2, the setups for the component counting in Section E.1.3, and the setups for the TSP problem in Section E.1.4.

E.1.1. Properties of Graph Generators

How to sample graphs turns to be intricate in our exploration to deeply investigate the generalizability power. Four generators are adopted in our experiments:

- The Erdos-Renyi model (Erdos & Renyi, 1959), $G(n, p)$, generates graphs with n nodes and each pair of nodes is connected with probability p.
- The KNN model, KNN(n, d, k), first generates n nodes whose positions are uniformly sampled from a d-dimensional unit cube. The nodes are then connected to their k nearest neighbors. The edge directions are from the center node to its neighborhoods.
- The planar model, PL(n, d), first generates n nodes whose positions are uniformly sampled from a d-dimensional unit cube. Delaunary triangulations are then computed (Barber et al., 1996) and nodes in the same triangulation are connected to each other.
- The lobster model, Lob(n, p_1, p_2), first generates a line with n nodes. $n_1 \sim \mathcal{B}(n, p_1)$ nodes are then generated as first-level leaf nodes, where $\mathcal{B}$ denotes the binomial distribution. Each leaf node uniformly selects one node in the line as the parent. Afterwards, $n_2 \sim \mathcal{B}(n_1, p_2)$ are generated as second-level leaf nodes. Each second-level leaf node also uniformly selects one first-level leaf node as the parent. The parents and children are connected to each other and the graph is therefore undirected.

For the Erdos-Renyi model, we assign p equal to 0.5 so that all graphs of n nodes can be generated with equal probabilities. However, the expectation of graph diameters decreases dramatically as graph sizes increase for such model. As illustrated in



(a) Erdős–Rényi model (b) Planar graph (dim=2) (c) KNN graph (dim=1, k=8) (d) Lobster graph (p1=p2=0.2)

Figure 4. Properties of different random graph generators. The upper row illustrates graph samples generated by the corresponding generator. The lower row demonstrates the relationships between the graph sizes (i.e. node numbers) and the distributions of random node pairs' distances. Typically, for each generator and each graph size, 1000 sample graphs are generated by the corresponding generator for estimating the distributions. Box plots are utilized for visualizing the distributions.

Figure 4, the graph diameters are just 2 with high probability when the node number is larger than 50.

The other three graph generators are therefore designed to generate graphs with larger diameters for better evaluation of models' generalizabilities w.r.t. scales. We manually select their hyper-parameters to efficiently generate graphs of diameters as large as possible. Specifically, we set $d = 1$ and $k = 8$ for the KNN model, $d = 2$ for the planar model, $p_1 = 0.2$ and $p_2 = 0.2$ for the lobster model. Their properties are illustrated in Figure 4. Note that the distances are positively related to the graph sizes for all three graph generators. Moreover, for the lobster model, the distances increase almost linearly with respect to the graph sizes.

E.1.2. Shortest Path

In this task, given a source node and a target node, the model needs to predict the length of the shortest path between them. The edge weights are positive and uniformly sampled. We consider both unweighted graphs and weighted graphs (edge weights uniformly sampled between 0.5 and 1.5). Groundtruth is calculated by Dijkstra's algorithm.

We utilize a three-dimensional one-hot representation to encode the location of the source and target nodes (100 for source, 010 for destination, and 001 for other nodes). Edge weights are encoded as the edge attributes. Two metrics are used to measure the performance of GNNs. The relative loss is first applied to measure the performance of predicting shortest path lengths. To further examine the models' ability in tracing the shortest path, we implemented one simple post-processing method leveraging the noisy approximation of path lengths (presented later). In detail, we define the relative loss as $|l - l_{pred}|/l$ and the success rate of identifying the shortest path by post-processing as $\mathbb{1}(l = l_{post\text{-}pred})$, where l is the true shortest path length, l_{pred} is the predicted length by GNNs, and $l_{post\text{-}pred}$ is the length of the predicted path after post-processing.

Post-Processing After training, our model can predict the shortest path length from source to target nodes. The post-processing method is then applied to find the shortest path based on the learned models. Specifically, the post-processing method predicts the shortest path

$$p = [p_1, p_2, \cdots, p_n] = \text{post-processing}(G; GNN)$$

given the input graph $G = (V_{i,j}, E)$, as defined in Section 5.1.1., and the noisy shortest path length predicting model GNN, where i, j are the indexes of source and target nodes, $V_{i,j}$ is the node attributes with one-hot encodings, and p_k denotes the index of the kth node on the shortest path.

The post-processing algorithm is stated in Algorithm.8. Concretely, we first denote the shortest path length between any two nodes i' and j' predicted by the trained model GNN as $dist_{i',j'} = GNN(G_{i',j'}) = GNN((V_{i',j'}, E))$, where $V_{i',j'}$

Algorithm 8 Post-processing to predict the shortest path

Input: graph $G = (V_{i,j}, E)$; source node index i; target node index j; trained models GNN that predict the shortest path length from nodes i' to node j' as $dist_{i',j'} = GNN((V_{i',j'}, E))$
Output: shortest path $p = [p_1, p_2, \cdots, p_n]$

Initialize $p_1 = i, k = 1$.
while $p_k \neq j$ **do**
  if $|\{l : dist_{l,j} + w_{p_k,l} \leq dist_{p_k,j}\}| > 0$ **then**
    $p_{k+1} = \arg\min_{l:dist_{l,j}+w_{p_k,l} \leq dist_{p_k,j}} |dist_{l,j} + w_{p_k,l} - dist_{p_k,j}|$.
  else
    return $p = []$
  end if
  $k = k + 1$.
end while
return p

represents the one-hot node attributes when nodes i' and j' are the source and target nodes. For further convenience, we also defined $w_{i',j'}$ as the weight of edge connecting node i' and node j' ($w_{i',j'} = \infty$ if node i' and node j' are not connected by an edge.). Then, the post-processing algorithm sequentially predicts the next node p_{k+1} of node p_k by minimizing the difference between the predicted shortest path length approximated by GNNs $dist_{p_k,j}$ and the length of shortest path predicted by the post-processing method $dist_{p_{k+1},j} + w_{p_k,p_{k+1}}$. To further reduce the effect of models' noises, another constrain is added as $dist_{p_{k+1},j} + w_{p_k,p_{k+1}} \leq dist_{p_k,j}$ so that the method will always convergence.

E.1.3. Component Counting

In component counting task, the model counts the number of connected components of an undirected graph. To generate a graph with multiple components, we first sample a random integer m between 1 to 6 as the number of components, and then divide the nodes into m parts. In detail, for n nodes and m components, we first uniformly sample $m - 1$ positions from 1 to $n - 1$ and then divide the n nodes into m parts by the $m - 1$ positions. We then connect nodes in each component using the random graph generator defined above, e.g., Erdos-Renyi graph and lobster graph. The metric is the accuracy of correct counting. We initialize the node attributes by random values$\in [0, 1)$ to distinguish different nodes.

E.1.4. Traveler Salesman Problem (TSP)

In the Euclidean travelling salesman problem (TSP), there are several 2D points located in the Euclidean plane, and the model generates a shortest route to visit each point. The graph is complete. The weight of an edge is the Euclidean distance between the two ends. Points $\{(x_i, y_i)\}$ are uniformly sampled from $\{x, y \in \mathbb{Z} : 1 \leq x, y \leq 1000\}$. We use the standard solver for TSP, Concorde (Applegate et al.) to calculate the ground truth. The node attributes are the 2D coordinates of each node. We use relative loss defined the same as the shortest path problem to evaluate the networks.

E.2. Graph Classification

Note that models' abilities to utilize the information of long-term relationships are necessary for accurately solving most of the previous tasks and problems. Therefore, the benefits of adaptive and unbounded depths introduced by the iterative module are distinguished. In this sub-section, we show that our IterGNN can also achieve competitive performance on graph-classification benchmarks, demonstrating that our iterative module doesn't hurt the standard generalizability of GNNs while improving the generalizability w.r.t. graph scales. The results are presented in Section B.3.

In detaile, we evaluate models on five small datasets, which are two social network datasets (IMDB-B and IMDB-M) and three bioinformatics datasets (MUTAG, PROTEINS and PTC). Readers are referred to (Xu et al., 2019) for more descriptions of the properties of datasets. We adopt the same evaluation method and metrics as previous state-of-art (Xu et al., 2019), such as 10-fold cross validation and classification accuracies as the metric. The dataset splitting strategy and pre-processing methods are all identical to (Xu et al., 2019) by directly integrating their public codes[1].

[1] https://github.com/weihua916/powerful-gnns

Regarding the models, we adopt the previous state-of-art, GIN (Xu et al., 2019) as GN-blocks and the JK connections (Xu et al., 2018) plus average/max pooling as the readout module. To integrate the iterative architecture, we wrap each GN-block in original backbones with the iterative module with maximum iteration number equal to 10. The tunable hyper-parameters include the number of IterGNNs, the epoch numbers, and whether or not utilizing the random initialization of node attributes.

E.3. Training Details

All models are trained with the same set of hyper-parameters: the learning rate is 0.001, and the batch size is 32. We use Adam as the optimizer. The hidden neuron number is 64. For models using the iterative module or the ACT algorithm, we train the networks with 30 maximal iterations and test them with no additional constraints. For the fixed-depth shared-weights paradigm, we train the networks with 30 iterations and test them with 1000 iterations (maximum node numbers in the datasets). The only two tunable hyper-parameter within our proposals are the epoch number=20, 40, $\cdots$, 200 and the degree of flexibilities of PathGNN, each corresponding to one variation of the PathGNN layer as described in Section D.2. Another hyper-parameter within the ACT algorithm (Graves, 2016) is $\tau = 0, 0.1, 0.01, 0.001$. We utilize the validation dataset to select the best hyper-parameter and report its performance on the test datasets.