Chordless Structure: A Pathway to Simple and Expressive GNNs

Hongxu Pan[1], Shuxian Hu[2], Mo Zhou[1], Zhibin Wang[1], Rong Gu[1], Chen Tian[1], Kun Yang[1], and Sheng Zhong[1]

[1]Nanjing University
[2]Alibaba Group

Abstract

Researchers have proposed various methods of incorporating more structured information into the design of Graph Neural Networks (GNNs) to enhance their expressiveness. However, these methods are either computationally expensive or lacking in provable expressiveness. In this paper, we observe that the chords increase the complexity of the graph structure while contributing little useful information in many cases. In contrast, chordless structures are more efficient and effective for representing the graph. Therefore, when leveraging the information of cycles, we choose to omit the chords. Accordingly, we propose a Chordless Structure-based Graph Neural Network (CSGNN) and prove that its expressiveness is strictly more powerful than the k-hop GNN (KPGNN) with polynomial complexity. Experimental results on real-world datasets demonstrate that CSGNN outperforms existing GNNs across various graph tasks while incurring lower computational costs and achieving better performance than the GNNs of 3-WL expressiveness.

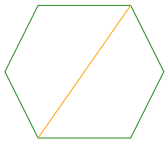
1 Introduction

Graphs have shown their power in representing complex data, from social networks[17] and chemical molecules[51] to recommendation engines[45], by capturing relational dynamics. Graph Neural Networks (GNNs), as a powerful tool for graph representation learning, have been widely used in various fields, such as social network analysis[35], recommendation systems[53], and bioinformatics[15]. Among the various GNNs, Message Passing Neural Networks (MPNNs) [16] is the most popular family of GNNs, including Graph Convolutional Networks (GCNs) [22], GraphSAGE [18], and Graph Attention Networks (GAT) [43]. Specifically, MPNNs recursively update node representations based on the neighborhood structure, which is similar to the Weisfeiler-Lehman (WL) graph isomorphism test[44] that hashes the neighbourhood structure of each node recursively. Therefore, the expressiveness of standard MPNNs is limited by the WL test, which indicates that MPNNs are unable to distinguish some non-isomorphic graphs. The limited expressiveness of MPNNs restricts their performance in analyzing complex graph structures, such as substructure counting, distinguishing graphs with symmetries and automorphisms, reasoning over higher-order interactions, and so on.

In order to enhance the expressiveness of GNNs, researchers have proposed various methods, which can be roughly divided into the following categories.

- **KPGNN** [46, 14]: Different from the standard MPNNs considering 1-hop neighborhood, KPGNN utilizes K-hop neighborhood which further includes the cyclic information among k-hop neighbors. However, as indicate by [46], increasing the depth leads to over-smoothing and incurs high computational costs [42], with complexity $\mathcal{O}(n\overline{d}^k)$ in sparse graphs.

Preprint. Under review.



(a) A chord in a 6-cycle

	IMDB-B	IMDB-M
Number of graphs	1000	1500
Average number of nodes	19.8	13.0
Average number of edges	96.5	65.9
Average number of chordless cycles	393.1	306.2
Average number of cycles	5641.0	5168.6

(b) Statistics of IMDB-B and IMDB-M datasets

Figure 1: Chord and statistics of IMDB datasets.

- **k-GNN** [33]: Observing the MPNNs are bounded by the 1-WL test, researchers imitate the K-WL test to design k-GNNs [33]. However, the computational and memory complexity of k-GNNs is at least $\mathcal{O}(|V|^{k+1})$ and $\mathcal{O}(|V|^k)$ respectively, which is infeasible for large graphs [24].

- **Subgraph GNN** [5]: Recognising that MPNNs are limited to identifying subgraph structures, researchers propose subgraph GNNs to enhance the expressiveness of GNNs by incorporating subgraph information, such as subgraph isomorphism count. However, the subgraph isomorphism count problem is NP-hard and computationally expensive [28]. Moreover, [10] indicates that subgraph GNNs are prone to overfitting by injecting too much structural information.

The existing work highlights the critical role of cycles in enhancing the expressiveness of GNNs. However, vast numbers of cycles in the graph suffer from over-smoothing and high computational costs.
Fortunately, we observe that *if a cycle contains a chord, it can be reconstructed by smaller cycles*. Taking money laundering detection as an example, the fund flow chains of money laundering activities often exhibit a circular structure as funds must ultimately revert to specific entities. Meanwhile, fund flow networks often prefer the shortest path: intuitively, criminals tend to transfer funds through the fewest nodes and edges to avoid tracking [47]. A cycle with a chord can be broken down into smaller cycles or paths. For example, the chord in the 6-cycle shown in Figure 1(a) splits it into two 4-cycles, and such smaller cycles better fit the need for rapid fund diversion in money laundering networks.

Specifically, as shown in Figure 1(a), a chord (highlighted in yellow) in a cycle refers to an edge that is not part of the cycle (green edges) but connects two nodes in the cycle. Therefore, we propose to use chordless cycles and paths [37] to represent the original, where the rest of the substructures can be reconstructed using the chordless cycles and paths. As shown in Figure 1 (b), the number of chordless cycles (CC) is significantly less than the number of cycles(C) while still capturing the necessary structural information, as it enhances the expressiveness of MPNNs by only considering the edge information.

In this paper, we propose a novel framework for enhancing the expressiveness of Graph Neural Networks by incorporating chordless structures into their design[1]. Specifically, we compute chordless paths and cycles in the original graphs whose complexity is $\mathcal{O}(c(G)(|V| + |E|))$ [42]. Subsequently, we conduct message passing on the chordless paths and cycles to aggregate the structural information. Our theoretical analysis in Section section 4.2 shows that even when restricted to a strictly radius-k neighborhood, CSGNN achieves strictly greater expressiveness than KPGNN.

To comprehensively evaluate the effectiveness of CSGNN, we conducted experiments across multiple graph-related tasks, including graph isomorphism testing, graph classification, and molecular regression, under consistent experimental settings. Compared to the CY2C model [10], which relies on extensive cycle-based structural components, CSGNN achieved superior performance despite utilizing fewer structural features (see Table 3a for detailed results). Furthermore, we validated the generalizability of chordless structural information by augmenting existing popular GNNs with this feature, observing consistent performance enhancements across tasks. Remarkably, even when restricted to chordless paths, CSGNN matched the accuracy of PathNN [30], which employs exhaustive path enumeration in its optimal configuration.

[1]The code is available at `https://anonymous.4open.science/r/ul4y4h4/`

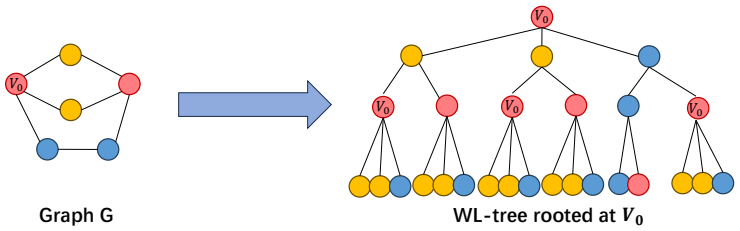


Figure 2: WL-tree of Graph G.

2 Preliminaries

2.1 Notation

Let $G = (V, E)$ be an undirected graph consisting of a set of nodes V and a set of edges $E \subseteq V \times V$. We denote by n the number of nodes in G and by m its number of edges. The set $\mathcal{N}(v)$ represents the neighbors of node v, and the set $\mathcal{N}_k(v)$ represents the k-hop neighborhood of node v. When considering colored graphs $G = (V, E, c)$, we have a color function $c : V \to \mathcal{C}$, where $\mathcal{C}$ is a finite set of colors. When considering attributed graphs, each node $v \in V$ is endowed with an initial node feature vector denoted by x_v that can contain categorical or real-valued properties of v. And $\langle u, v\rangle$ denotes the edge between node u and node v. We denote the natural numbers set $\{1, 2, \cdots, n\} := [n]$.

2.2 MPNNs and WL Test

Definition 2.1. Given a coloring algorithm T, node u and v are called $T - equivalent$, denoted by $u \sim_T v$, if they result in the same color after the termination of the algorithm T.

Currently, most existing GNNs can be designed based on 1-hop message passing framework (MPNNs). Given initial node features $h_v^{(0)} = x_v$, the node representation $h_v^{(t)}$ at layer t is updated by aggregating the features of its neighbors and itself. And finally, the whole graph can be represented by the node features.

$$h_v^{(t+1)} = \text{AGGREGATE}(\{h_u^{(t)} : u \in \mathcal{N}(v)\}), h_G = \text{READOUT}(\{h_v^{(k)} : v \in V\}),$$

where k is the number of iterations in updating processes, and AGGREGATE and READOUT are the aggregation and readout functions. In graph theory, the Weisfeiler-Leman (WL) algorithm[44] is a graph isomorphism test widely used in graph theory and computer science. It is also as knwon as 1-WL. It uses a hash function to encode the neighborhood structure of each node in a graph, and the whole graph can be represented by the value of each node.

$$h_v = \text{hash}(\{x_u : u \in \mathcal{N}(v)\}), h_G = \text{READOUT}(\{h_v : v \in V\})$$

It is acknowledged that the expressiveness of GNNs is limited by the WL test.

KPGNN[34] further uses k-hop neighborhood information to enhance the expressiveness of GNNs. The hidden state $h_v^{(t)}$ of KPGNN is shown as follows:

$$a_v^{(t)} = \text{AGGREGATE}(\{h_u^{(t-1)} : u \in \mathcal{N}_k(v)\}), h_v^{(t)} = \text{UPDATE}(h_v^{(t-1)}, a_v^{(t)})$$

where $\mathcal{N}_k(v) = \{u | \exists w \in \mathcal{N}_{k-1}(v), u \in \mathcal{N}(v)\}$for $k > 1$ and $\mathcal{N}_1(v) = \mathcal{N}(v)$ naturally.

2.3 High-order GNNs

In order to understand the expressiveness of GNNs, we can consider showing the expressiveness by comparing it to $KPGNN$, which can be represented by $WL - tree$ of a node, which is given by the computational tree of one node in the graph like [30]. At each iteration of aggregation, level $l + 1$ of the WL-tree is constructed by setting the children of any node at the level l to its direct neighbors. For a node in the l-th layer in $WL - tree$, its children in the $(l + 1)$-th layer are the neighborhood of the node of it.

For high-order graph neural networks, Morris et al. [33] introduced *k-GNNs*, which are based on the *k-dimensional Weisfeiler-Lehman (k-WL) test*. Given a fixed k, the method considers all subsets of nodes of size k from the graph. Each such subset is treated as a *super-node*, and two super-nodes are considered neighbors if they differ in exactly one node.

The k-WL procedure iteratively updates a representation (or "color") for each super-node by incorporating information from its neighboring super-nodes. To better distinguish between structural and topological aspects of the graph, the neighborhood of each super-node is further divided into *local* and *global* parts. Local neighbors are those where the differing nodes are connected by an edge, while global neighbors are those where the differing nodes are not connected.

2.4 Subgraphs GNN

Beyond k-WL-based models, subgraph GNNs like[5] offer another approach to enhance expressive power by leveraging the presence and distribution of local substructures in the graph.

As shown in [56], subgraph GNNs can be formalized as below.

$$h_G^{(l+1)}(u,v) = \mathrm{AGG}^{(l+1)}\left(\left\{f_i(u,v,G,h_G^{(l)})\right\}_{i=1}^{r}\right), f(G) = \mathrm{READ}\left(\left\{h_G^{(L)}(u,v) : u,v \in \mathcal{V}_G\right\}\right),$$

where $h_G^{(l)}(u,v) = h_G^{(0)}(u,v)$ denotes the representation of node v in the subgraph G^u centered at node u, at the l-th layer, $\tilde{h}_G^u(v)$ is the initial input feature of node v in subgraph G^u, determined by the graph generation policy (e.g., node marking, distance encoding) and f_i represents the i-th atomic operation.

2.5 Limitation of existing GNNs

For standard GNNs, the expressiveness is limited by the WL test, which means that GNNs are unable to distinguish some non-isomorphic graphs. For k-hop GNNs, [14] has shown that the expressive power of K-hop message passing is bounded by 3-WL. For k-GNNs based on k-WL, a key limitation of such k-GNNs that achieve WL is their lack of scalability and explainability. [59] shows that these models can only be applied to small graphs with small k in real-world tasks. According to [24], k-WL's memory complexity is at least $\mathcal{O}(n^k)$ and computational complexity is at least $\mathcal{O}(n^{k+1})$, which is infeasible for large graphs.

To solve the problems, we propose a Chordless Structure based Graph Neural Network (CSGNN) that uses chordless paths and cycles to enhance the expressiveness of GNNs. It comes with more expressiveness beyond WL, but with computational efficiency and more explainability.

3 Decomposition of Graph into Chordless Cycles and Paths

3.1 Chord and Chordless Structure

A path is a simple graph whose nodes can be arranged in a linear sequence in such a way that two nodes are adjacent if they are consecutive in the sequence, and are nonadjacent otherwise. Likewise, a cycle is a simple graph whose nodes can be arranged in a cyclic sequence. Given a cycle, if there exists an edge that connects two nodes of the cycle but is not part of the cycle, we call it a *chord*. To put it in another way, a chord decomposes the original cycle into two smaller cycles, conversely, *two smaller cycles can reconstruct the original cycle*.

This observation motivates us to consider the chordless structure, which is enough to encode the whole necessary substructure of the graph.

Formally, for a graph G, a chordless cycle is a cycle that does not contain any chord. Similarly, a chordless path is a path that does not contain any chord. We respectively denote them by CC and CP. In other words, in a chordless cycle CC, we have

$$\forall u, v \in CC, \quad \langle u, v\rangle \notin CC \rightarrow u \notin \mathcal{N}(v).$$

For all chordless cycles/paths of length k, we denote them by CC_k, and We write $u \in CC_k(v)$ if there exists such a chordless cycle containing both u and v, and so does $CP_k(v)$ for chordless paths

and CP_k, and We write $u \in CC_k(v)$ if there exists such a chordless cycle containing both u and v, and so does $CP_k(v)$ for chordless paths.

3.2 Decomposition of Graph

In this subsection, we will discuss why we choose chordless structures to represent the graph structure.

Lemma 3.1. *WL can distinguish all non-isomorphic trees.[21]*

By constructing the $WL - tree$ of the graph, we can get the unique representation of the graph. Since the tree does not contain any cycle, we can get a contrapositive proposition of the lemma.

Corollary 3.2. *If there exists two graphs G_1, G_2, $G_1 \sim_{1-WL} G_2$ but $G_1 \ncong G_2$, then there exists a cycle in the graphs.*

The corollary 3.2 shows the importance of the cycle in the graph structure. Additionally, while the standard GNNs only use the local structure, the cycles can be a better choice to represent the graph global structure. In graph theory, we have a conjecture.

Conjecture (Cycle Double Cover Conjecture)[38] For any undirected graph G, there exists a cycle double cover of G if G is bridgeless.

Since the chordless cycle can be considered as a minimal cycle, we can easily find the lemma below.

Lemma 3.3. *If a node is in a cycle, then the node is in a chordless cycle.*

Lemma 3.4. *With the set of chordless paths, one can find all paths in the graph.*

The detailed proofs and additional visualisations are provided in the Appendix E.1.

Theorem 3.5. *Chordless cycles and chordless paths together provide enough information to describe the structure of a graph.*

The result follows from the preceding lemmas. Thus, the decomposition of the graph is now complete.

4 Chordless Structure based GNN: architecture and expressiveness

In this section, we introduce the architecture of CSGNN, and show the expressiveness of CSGNN by giving provable evidence.

4.1 Model Architecture

The architecture of CSGNN is similar to Message Passing Neural Networks (MPNNs), but with a new aggregation method and spread edges. The overall architecture of CSGNN is as follows:

$$h_{CP}^t(v) = \mathrm{AGG}_1\left(\{h_u^{(t)} : u \in CP_k(v)\}\right) \quad h_{CC}^t(v) = \mathrm{AGG}_2\left(\{h_u^{(t)} : u \in CC_k(v)\}\right)$$
$$h_v^{(t+1)} = h_{CP}^t(v) \oplus h_{CC}^t(v)$$

The implementation above is inherited from the message-passing template. For a more visible representation, we can consider another implementation by encoding the chordless cycles into the representations of the nodes.

$$h_v^{(0)} = x_v \oplus \mathrm{ENCODE}(CC_k(v)) \quad h_v^{(t+1)} = \mathrm{AGG}\left(\{h_u^{(t)} : u \in CP_k(v)\}\right)$$

4.2 Theoretical Background

For further analysis, we will introduce some definitions in the section to quantify the expressiveness of GNNs.

Definition 4.1. A GNN GNN_1 is more expressive (not strictly) than another GNN GNN_2 if GNN_1 can distinguish every pair of the graphs that GNN_2 can distinguish. We denote this relation as $GNN_2 \preccurlyeq GNN_1$.

In order to make analysis easier, we can consider a new definition with intuition from coloring problems. By considering a subset of the graphs with good properties instead of of the graphs, we can head to our result more efficiently.

Definition 4.2. A graph is said to be $1-WL-colorable$ if there is no two vertices sharing the same edge have the same color after the $1-WL$ coloring.

It is clear that not each graph is $1-WL-colorable$, but we can still transform the graphs in $1-WL-colorable$ format, for proving our theory's robustness. We can consider the following lemma, to uniform the form of the graphs' format, to get conclusions easier.

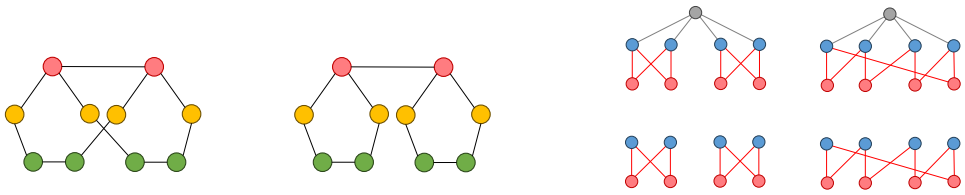
Lemma 4.3. *For a finite set of graphs, each of them can be map in the form of* $1-WL-colorable$ *graph.*

The detailed proof and visual interpretation are provided in Appendix E.2.

Definition 4.4. For two graphs G_1 and G_2, if they have the same colored form(under isomorphism) after 1-WL coloring, we say they are 1-WL-equivalent, and denote $G_1 \sim_{1-WL} G_2$.

Lemma 4.5. *For two graphs* G_1 *and* G_2*, if they are* $1-WL-equivalent$ *but not isomorphic, there exist minimal subgraphs* G_1' *and* G_2' *of* G_1 *and* G_2 *such that* G_1' *and* G_2' *are not isomorphic but* $G_1' \sim_{1-WL} G_2'$.

The proof of the lemma is obvious since the minimal subgraphs can be itself whatever. Hence, in order to generate the structure of the graph after 1-WL coloring, we can start with the nodes in the same color and then add colors adjacent to the previous layer, layer by layer based on the color. But the structure of the graph is complex, we turn to consider the minimal subgraph that is defined in the Lemma 4.5, and consider a more common form in which each layer has only one color, estimate whether each graph is $1-WL-colorable$ in the follow-up analysis.



(a) Two WL-equivalent graphs can be distinguished through chordless cycles.

(b) Two pairs of WL-equivalent graphs that are distinguishable by CSGNN.

Figure 3: Examples of WL-indistinguishable graphs where CSGNN succeeds: (a) distinction by chordless cycles; (b) distinction via component structures.

In order to describe CSGNN's expressiveness, we need to introduce the concept below, which is similar to the definition of graph isomorphism naturally.

Definition 4.6. A colored graph $G=(V,E,c)$ is $color-equivalent$ if for any pair of nodes u_1,u_2 of the same color, there exists a map $\phi: V \to V$ that satisfies the following conditions:

- ϕ is a bijection which satisfies $\phi(u_1)=u_2$, and $\phi(u_2)=u_1$.
- For any $v_1, v_2 \in V$, v_1 and v_2 are adjacent if and only if $\phi(v_1)$ and $\phi(v_2)$ are adjacent.
- For any $v \in V$, the color of v is the same as the color of $\phi(v)$.

4.3 Expressiveness of CSGNN

First, by showing the expressiveness based on aggregating the chordless paths, we can get a lower bound of the expressiveness of CSGNN.

Theorem 4.7. *CSGNN is more expressive than the k-hop GNN (KPGNN) with* $CP_{[k]}$.

Proof. Since every chordless path of length $\leq k$ is within the computational scope of $KPGNN$, we have $CP_{[k]} \preccurlyeq KPGNN$, we only need to prove the other direction. By considering theorem 3.2, we can get the proof of the theorem. □

Furthermore, to observe the benefit of the chordless cycle, we can consider the following lemma.

Lemma 4.8. *If G_1, G_2 are two non-isomorphic bipartite graphs that have different amounts of connected components, then CSGNN can distinguish G_1 and G_2.*

In some special cases, we can consider the following example 3b, showing the hybrid capability of considering minimal graphs in Lemma 4.5 and using the Lemma 4.8.

For a more general case, we limit the condition of the graphs. Because we have realized that the upper bound of standard GNNs is caused by cycles. We try to construct the graph first by formatting from a node to a tree by layers, and finally, we form the cycle in the last layer. The process aims to constrain regular representations of graphs. In other words, the reasonableness can be shown, since two non-isomorphic graphs must have different nodes, and we form the graph from the different nodes, which also matches the minimal subgraph in Lemma 3.6.

Theorem 4.9. *Let G_1, G_2 be two non-isomorphic graphs satisfies the following conditions:*

- *G_1 and G_2 are $color - equivalent$*
- *G_1 and G_2 have different amounts of connected components.*

Then CSGNN can distinguish G_1 and G_2.

The proof is left at appendix E.3.

Notice that the cut-edge is a symbol of components, we have the following corollary.

Corollary 4.10. *CSGNN is cut-edge sensitive.*

From the content above, we get the expressiveness of CSGNN. GNN has limited expressiveness since graphs don't have a uniform structure. But after processing by CSGNN, we can get a more regular form of the graph, which improves the expressiveness of GNNs, see Figure **??** for an example.

4.4 Feature Encoding

To realize the topological structure of the graph better, we can introduce the concept of **regular cell complex** from [19], and get inspiration from design

Definition 4.11. A **regular cell complex** is a topological space X with a partition into subspaces $\{X_\alpha\}_{\alpha \in P_X}$ satisfying the following conditions:

- $\forall x \in X$, every sufficiently small the neighborhood of x intersects only finitely many X_α.
- $\forall \alpha, \beta \quad \bar{X_\alpha} \cap X_\beta \neq \emptyset$ only if $X_\beta \subseteq \bar{X_\alpha}$
- Every X_α is homeomorphic to $\mathbf{R}^{n_\alpha}$ for some n_α.
- For every α, there is a homeomorphism of a closed ball in $\mathbf{R}^{n_\alpha}$ to $\bar{X_\alpha}$ that maps the interior of the ball homomorphically onto X_α

Here we can consider P_X denotes the set of the minimal cycles in the graph, since the intersections of the minimal cycles are always empty set.

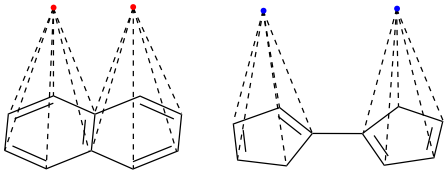
We can encode the structure with an intuition from chemistry. In some ways, the nodes on the cycle compose an equivalent class (example: carbon on the benzene ring have similar properties), so we want the encoding to be a mapping from the original topological space to a quotient space, which corresponds to the concept of **Topological cone**

Definition 4.12. For a topological space X, the **topological cone** of X is the quotient space $CX := (X \times I)/(X \times \{1\})$, where I denotes the interval $[0, 1]$.

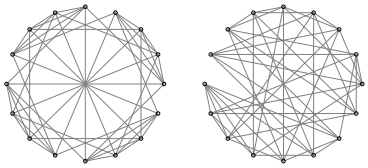
So the encoding can be realized as a mapping from the subspaces of the regular cell to the topological cone of the graph such as in Figure 4a. Hence the feature can be encoded as the following:

$$Feature_i(u) = \mathbf{1}\Big[\exists CC_i \in X, \quad s.t. \quad u \in CC_i\Big]$$

where u is the node in the graph, and CC_i is the chordless cycle(always minimal cycle) in the graph, and $\mathbf{1}$ is the indicator function. So with the encoding, we can get an equivalent class on the cycle since all the node on the cycle is encoded in 1. The model can be realized as a mapping $M \to CM$ with more information from the topological structure of the graph, where M is the original structure. While the structural features in [5] rely on symmetry group counts, our approach emphasizes preserving the structural similarity of nodes within cyclic (ring) substructures.



(a) Topological cones on Decalin and Bicyclopenty, two 1-WL indistinguishable molecules.



(b) Two 3-WL indistinguishable graphs from SR(16,6,2,2).

Figure 4: Examples of non-isomorphic graphs indistinguishable by WL tests. (a) 1-WL failure on molecular graphs; (b) 3-WL failure on strongly regular graphs.

In another way, we can consider the encoding as a binary molecular Fingerprint[29] embedding into the node features. And our model performs well in the chemical graph data sets in the experiments, which are shown in the following section.

5 Experiments

Dataset	Task	Size/Type	Special Property
GRAPH8C	Isomorphism	11117 graphs (8 nodes)	All non-isomorphic graphs
EXP	Isomorphism	600 pairs	1-WL indist. / 2-WL dist.
SR	Isomorphism	105 pairs (25 nodes)	3-WL indist.
ZINC	Regression	250K molecules	Predict chemical properties
TUDataset	Classification	120+ datasets	Chem. / social graphs
ogbg-MOLHIV	Classification	40K+ molecules	MoleculeNet; HIV activity

Table 1: Overview of datasets.

To qualify the expressiveness of CSGNN in distinguishing graphs, we apply CSGNN on the synthetic dataset in Section 5.1 and real-world datasets in Section 5.2, which include graph isomorphism tasks, regression tasks, and classification tasks. The detailed experimental setup is provided in Appendix B, and the detailed dataset introduction is in Appendix D.

5.1 Synthetic Datasets

Results The performance is given by the table and the figure, we find that CSGNN performs well on graph isomorphism tasks. According to the results of SR datasets, CSGNN has stronger expressiveness than 3-WL. Additionally, by running the code in [3] and checking their results, we can find that the expressiveness of fundamental GNNs is limited by 1-WL test, then less than 3-WL test. Above all, our experiments show that CSGNN has excellent expressiveness.

Model	EXP ↓	Graph8c ↓
GCN [22]	600	$7.727 * 10^{-5}$
GAT [43]	600	$2.958 * 10^{-5}$
GIN[48]	600	$6.247 * 10^{-6}$
GNNML1[3]	600	$5.389 * 10^{-6}$
PathNN[30]	0	N/A
ChebNet[11]	0	$7.120 * 10^{-7}$
PAIN[12]	0	N/A
CSGNN	0	0

(a) Undistinguished pairs in EXP and failure rate on Graph8c.

No.	Model	Test MAE↓	T/A
1	ESA[7]	$0.0122^{(0.0004)}$	✓
2	TIGT[9]	0.014	✓
3	CSGIN (Ours)	0.0216	
4	GRIT[27]	0.023	✓
5	GraphGPS[36]	$0.024^{(0.007)}$	✓
6	SignNet[25]	$0.024^{(0.003)}$	✓
7	Graphormer[52]	$0.036^{(0.002)}$	✓
8	δ-2-GNN[32]	$0.042^{(0.003)}$	

(b) Test MAE on ZINC dataset. T/A = Transformer/Attention-Based.

Table 2: Comparative evaluation of GNN expressiveness and real-world performance. (a) Number of indistinguishable pairs on the EXP dataset and failure rate on Graph8c (lower is better). (b) Test MAE on the ZINC dataset, sorted by performance. Models marked with ✓are Transformer/Attention-based.

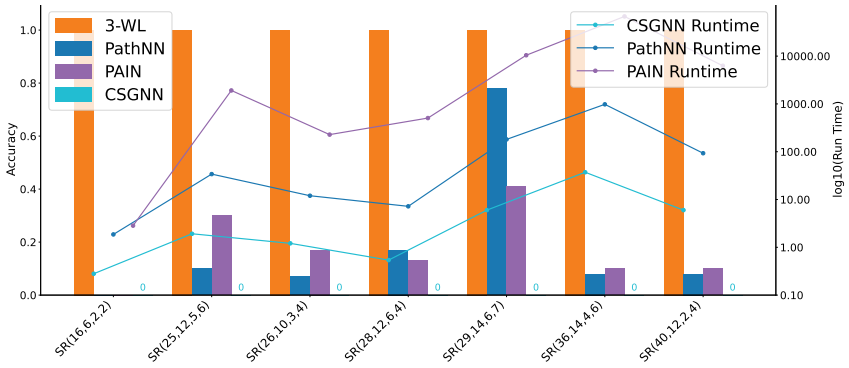


Figure 5: Accuracy and Run time(s) comparison on SR datasets

5.2 Real-World Datasets

Result According to the benchmark table from `https://paperswithcode.com/sota/`, our CSGNNs achieve strong performance[2] on the full ZINC dataset 2b. Compared to CY2C-GCN [10], our models are more robust and resource-efficient, notably avoiding out-of-memory errors on the DD dataset when tested on an A100 GPU (see Table 3a). Moreover, compared to PathNN, our model significantly reduces memory usage, as shown in Table 4. Our method outperforms many classical models on the ogbg-MolHIV dataset, as shown in Table 3b.

	DD	PROTEINS	IMDB-B	IMDB-M
DGCNN[57]	76.6 ± 4.5	72.9 ± 3.5	69.2 ± 3.0	45.6 ± 3.4
DiffPool[54]	75.0 ± 4.3	73.7 ± 3.5	68.4 ± 3.3	45.6 ± 3.4
ECC [39]	72.6 ± 4.1	72.3 ± 3.4	67.7 ± 2.8	43.5 ± 3.1
GIN [48]	75.3 ± 2.9	73.3 ± 4.0	71.2 ± 3.9	48.5 ± 3.3
GraphSAGE [18]	72.9 ± 2.0	73.0 ± 4.5	68.8 ± 4.5	47.6 ± 3.5
GAT [43]	73.9 ± 3.4	70.9 ± 2.7	69.2 ± 4.8	48.2 ± 4.9
SPN [2]	77.4 ± 3.8	74.2 ± 2.7	N/A	N/A
PathNet [40]	OOM	70.5 ± 3.9	70.4 ± 3.8	49.1 ± 3.6
Nested GNN [58]	77.8 ± 3.9	74.2 ± 3.7	N/A	N/A
PathNN [30]	77.0 ± 3.1	75.2 ± 3.9	72.6 ± 3.3	$\mathbf{50.8 \pm 4.5}$
CY2C-GCN [10]	OOM	61.0 ± 5.3	58.0 ± 4.1	35.3 ± 2.1
KAGNN [6]	73.3 ± 4.5	$\mathbf{75.6 \pm 3.6}$	72.6 ± 4.5	50.0 ± 4.1
CSGNN	$\mathbf{78.1 \pm 2.6}$	75.4 ± 3.4	$\mathbf{72.8 \pm 3.6}$	50.6 ± 4.1

(a) Performance comparison across DD, PROTEINS, IMDB-B, and IMDB-M datasets. OOM = out-of-memory; N/A = not available.

Model	**ROC-AUC**
GIN	75.58 ± 1.40
GCN	76.06 ± 0.97
ESAN	78.00 ± 1.22
CIN	80.94 ± 0.57
GSN	77.99 ± 1.00
Graphormer	80.51 ± 1.06
GPS	78.80
pathNN	79.17 ± 1.09
PAIN	78.50 ± 1.40
CSGIN	82.22

(b) ROC-AUC results on the ogbg-MolHIV dataset.

Table 3: (a) Performance comparison on four benchmark datasets; (b) ROC-AUC results for ogbg-MolHIV.

6 Conclusion

In this paper, we observe that chord is a key factor in achieving simple and expressive GNNs. Accordingly, we propose a new GNN framework, CSGNN, which is based on chordless structures. Theoretical analysis shows that CSGNN achieves expressiveness beyond KPGNN but only with $\mathcal{O}(c(G)(|V|+|E|))$ complexity. Extensive experiments demonstrate that CSGNN outperforms existing GNN models by embedding cycles' feature into graph but only introduces $\mathcal{O}(|CC|(|V|+|E|))$ additional computational cost.

[2]We merged the results of ESA and retained the best one

References

[1] Ralph Abboud, Ismail Ilkan Ceylan, Martin Grohe, and Thomas Lukasiewicz. The surprising power of graph neural networks with random node initialization. *arXiv preprint arXiv:2010.01179*, 2020.

[2] Ralph Abboud, Radoslav Dimitrov, and Ismail Ilkan Ceylan. Shortest path networks for graph property prediction. In *Learning on Graphs Conference*, pages 5–1. PMLR, 2022.

[3] Muhammet Balcilar, Pierre Héroux, Benoit Gauzere, Pascal Vasseur, Sébastien Adam, and Paul Honeine. Breaking the limits of message passing graph neural networks. In *International Conference on Machine Learning*, pages 599–608. PMLR, 2021.

[4] Cristian Bodnar, Fabrizio Frasca, Nina Otter, Yuguang Wang, Pietro Lio, Guido F Montufar, and Michael Bronstein. Weisfeiler and lehman go cellular: Cw networks. *Advances in neural information processing systems*, 34:2625–2640, 2021.

[5] Giorgos Bouritsas, Fabrizio Frasca, Stefanos Zafeiriou, and Michael M. Bronstein. Improving graph neural network expressivity via subgraph isomorphism counting. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 45(1):657–668, 2023.

[6] Roman Bresson, Giannis Nikolentzos, George Panagopoulos, Michail Chatzianastasis, Jun Pang, and Michalis Vazirgiannis. Kagnns: Kolmogorov-arnold networks meet graph learning, 2024.

[7] David Buterez, Jon Paul Janet, Dino Oglic, and Pietro Lio. An end-to-end attention-based approach for learning on graphs, 2024.

[8] Zhengdao Chen, Lei Chen, Soledad Villar, and Joan Bruna. Can graph neural networks count substructures? *Advances in neural information processing systems*, 33:10383–10395, 2020.

[9] Yun Young Choi, Sun Woo Park, Minho Lee, and Youngho Woo. Topology-informed graph transformer. *arXiv preprint arXiv:2402.02005*, 2024.

[10] Yun Young Choi, Sun Woo Park, Youngho Woo, and U Jin Choi. Cycle to clique (cy2c) graph neural network: A sight to see beyond neighborhood aggregation. In *The Eleventh International Conference on Learning Representations*, 2022.

[11] Michaël Defferrard, Xavier Bresson, and Pierre Vandergheynst. Convolutional neural networks on graphs with fast localized spectral filtering. *Advances in neural information processing systems*, 29, 2016.

[12] Tamara Drucks, Caterina Graziani, Fabian Jogl, Monica Bianchini, Franco Scarselli, and Thomas Gärtner. The expressive power of path based graph neural networks. In *ICML*, 2024.

[13] Federico Errica, Marco Podda, Davide Bacciu, and Alessio Micheli. A fair comparison of graph neural networks for graph classification. *arXiv preprint arXiv:1912.09893*, 2019.

[14] Jiarui Feng, Yixin Chen, Fuhai Li, Anindya Sarkar, and Muhan Zhang. How powerful are k-hop message passing graph neural networks. *Advances in Neural Information Processing Systems*, 35:4776–4790, 2022.

[15] Pablo Gainza, Freyr Sverrisson, Frederico Monti, Emanuele Rodola, Davide Boscaini, Michael M Bronstein, and Bruno E Correia. Deciphering interaction fingerprints from protein molecular surfaces using geometric deep learning. *Nature Methods*, 17(2):184–192, 2020.

[16] Justin Gilmer, Samuel S Schoenholz, Patrick F Riley, Oriol Vinyals, and George E Dahl. Neural message passing for quantum chemistry. In *International conference on machine learning*, pages 1263–1272. PMLR, 2017.

[17] Will Hamilton, Zhitao Ying, and Jure Leskovec. Inductive representation learning on large graphs. *Advances in neural information processing systems*, 30, 2017.

[18] William L. Hamilton, Rex Ying, and Jure Leskovec. Inductive representation learning on large graphs, 2018.

[19] Jakob Hansen and Robert Ghrist. Toward a spectral theory of cellular sheaves. *Journal of Applied and Computational Topology*, 3(4):315–358, 2019.

[20] John J Irwin, Teague Sterling, Michael M Mysinger, Erin S Bolstad, and Ryan G Coleman. Zinc: a free tool to discover chemistry for biology. *Journal of chemical information and modeling*, 52(7):1757–1768, 2012.

[21] Sandra Kiefer. *Power and limits of the Weisfeiler-Leman algorithm*. PhD thesis, Dissertation, RWTH Aachen University, 2020, 2020.

[22] Thomas N. Kipf and Max Welling. Semi-supervised classification with graph convolutional networks, 2017.

[23] Lecheng Kong, Yixin Chen, and Muhan Zhang. Geodesic graph neural network for efficient graph representation learning. *Advances in neural information processing systems*, 35:5896–5909, 2022.

[24] Pan Li and Jure Leskovec. The expressive power of graph neural networks. *Graph Neural Networks: Foundations, Frontiers, and Applications*, pages 63–98, 2022.

[25] Derek Lim, Joshua Robinson, Lingxiao Zhao, Tess Smidt, Suvrit Sra, Haggai Maron, and Stefanie Jegelka. Sign and basis invariant networks for spectral graph representation learning. *arXiv preprint arXiv:2202.13013*, 2022.

[26] Ziqi Liu, Chaochao Chen, Longfei Li, Jun Zhou, Xiaolong Li, Le Song, and Yuan Qi. Geniepath: Graph neural networks with adaptive receptive paths. In *Proceedings of the AAAI conference on artificial intelligence*, volume 33, pages 4424–4431, 2019.

[27] Liheng Ma, Chen Lin, Derek Lim, Adriana Romero-Soriano, Puneet K Dokania, Mark Coates, Philip Torr, and Ser-Nam Lim. Graph inductive biases in transformers without message passing. In *International Conference on Machine Learning*, pages 23321–23337. PMLR, 2023.

[28] Ciaran McCreesh, Patrick Prosser, Christine Solnon, and James Trimble. When subgraph isomorphism is really hard, and why this matters for graph databases. *Journal of Artificial Intelligence Research*, 61:723–759, 2018.

[29] Malcolm J McGregor and Peter V Pallai. Clustering of large databases of compounds: using the mdl "keys" as structural descriptors. *Journal of chemical information and computer sciences*, 37(3):443–448, 1997.

[30] Gaspard Michel, Giannis Nikolentzos, Johannes F Lutzeyer, and Michalis Vazirgiannis. Path neural networks: Expressive and accurate graph neural networks. In *International Conference on Machine Learning*, pages 24737–24755. PMLR, 2023.

[31] Christopher Morris, Nils M Kriege, Franka Bause, Kristian Kersting, Petra Mutzel, and Marion Neumann. Tudataset: A collection of benchmark datasets for learning with graphs. *arXiv preprint arXiv:2007.08663*, 2020.

[32] Christopher Morris, Gaurav Rattan, and Petra Mutzel. Weisfeiler and leman go sparse: Towards scalable higher-order graph embeddings. *Advances in Neural Information Processing Systems*, 33:21824–21840, 2020.

[33] Christopher Morris, Martin Ritzert, Matthias Fey, William L Hamilton, Jan Eric Lenssen, Gaurav Rattan, and Martin Grohe. Weisfeiler and leman go neural: Higher-order graph neural networks. In *Proceedings of the AAAI conference on artificial intelligence*, volume 33, pages 4602–4609, 2019.

[34] Giannis Nikolentzos, George Dasoulas, and Michalis Vazirgiannis. K-hop graph neural networks. *Neural Networks*, 130:195–205, 2020.

[35] Jiezhong Qiu, Jian Tang, Hao Ma, Yuxiao Dong, Kuansan Wang, and Jie Tang. Deepinf: Social influence prediction with deep learning. In *Proceedings of the 24th ACM SIGKDD international conference on knowledge discovery & data mining*, pages 2110–2119, 2018.

[36] Ladislav Rampášek, Michael Galkin, Vijay Prakash Dwivedi, Anh Tuan Luu, Guy Wolf, and Dominique Beaini. Recipe for a general, powerful, scalable graph transformer. *Advances in Neural Information Processing Systems*, 35:14501–14515, 2022.

[37] Hiroko Satoh, Hiroyuki Koshino, Takeaki Uno, Shungo Koichi, Satoru Iwata, and Tadashi Nakata. Effective consideration of ring structures in cast/cnmr for highly accurate 13c nmr chemical shift prediction. *Tetrahedron*, 61(31):7431–7437, 2005.

[38] P. D. Seymour. Sums of circuits. In J. A. Bondy and U. S. R. Murty, editors, *Graph Theory and Related Topics*, pages 341–355. Academic Press, New York, 1979.

[39] Martin Simonovsky and Nikos Komodakis. Dynamic edge-conditioned filters in convolutional neural networks on graphs. In *Proceedings of the IEEE conference on computer vision and pattern recognition*, pages 3693–3702, 2017.

[40] Yifei Sun, Haoran Deng, Yang Yang, Chunping Wang, Jiarong Xu, Renhong Huang, Linfeng Cao, Yang Wang, and Lei Chen. Beyond homophily: Structure-aware path aggregation graph neural network. In *IJCAI*, pages 2233–2240, 2022.

[41] Quang Truong and Peter Chin. Weisfeiler and lehman go paths: Learning topological features via path complexes. In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 38, pages 15382–15391, 2024.

[42] Takeaki Uno and Hiroko Satoh. An efficient algorithm for enumerating chordless cycles and chordless paths. In *International Conference on Discovery Science*, pages 313–324. Springer, 2014.

[43] Petar Veličković, Guillem Cucurull, Arantxa Casanova, Adriana Romero, Pietro Lio, and Yoshua Bengio. Graph attention networks. *arXiv preprint arXiv:1710.10903*, 2017.

[44] Boris Weisfeiler and Andrei Leman. The reduction of a graph to canonical form and the algebra which appears therein. *nti, Series*, 2(9):12–16, 1968.

[45] Jiancan Wu, Xiang Wang, Fuli Feng, Xiangnan He, Liang Chen, Jianxun Lian, and Xing Xie. Self-supervised graph learning for recommendation. In *Proceedings of the 44th international ACM SIGIR conference on research and development in information retrieval*, pages 726–735, 2021.

[46] Xinyi Wu, Zhengdao Chen, William Wang, and Ali Jadbabaie. A non-asymptotic analysis of oversmoothing in graph neural networks. *arXiv preprint arXiv:2212.10701*, 2022.

[47] Jennifer J Xu and Hsinchun Chen. Fighting organized crimes: using shortest-path algorithms to identify associations in criminal networks. *Decision Support Systems*, 38(3):473–487, 2004.

[48] Keyulu Xu, Weihua Hu, Jure Leskovec, and Stefanie Jegelka. How powerful are graph neural networks? *CoRR*, abs/1810.00826, 2018.

[49] Zuoyu Yan, Tengfei Ma, Liangcai Gao, Zhi Tang, and Chao Chen. Cycle representation learning for inductive relation prediction. In Kamalika Chaudhuri, Stefanie Jegelka, Le Song, Csaba Szepesvari, Gang Niu, and Sivan Sabato, editors, *Proceedings of the 39th International Conference on Machine Learning*, volume 162 of *Proceedings of Machine Learning Research*, pages 24895–24910. PMLR, 17–23 Jul 2022.

[50] Zuoyu Yan, Tengfei Ma, Liangcai Gao, Zhi Tang, Chao Chen, and Yusu Wang. Cycle invariant positional encoding for graph representation learning. In *Learning on Graphs Conference*, pages 4–1. PMLR, 2024.

[51] Kevin Yang, Kyle Swanson, Wengong Jin, Connor Coley, Philipp Eiden, Hua Gao, Angel Guzman-Perez, Timothy Hopper, Brian Kelley, Miriam Mathea, et al. Analyzing learned molecular representations for property prediction. *Journal of chemical information and modeling*, 59(8):3370–3388, 2019.

[52] Chengxuan Ying, Tianle Cai, Shengjie Luo, Shuxin Zheng, Guolin Ke, Di He, Yanming Shen, and Tie-Yan Liu. Do transformers really perform badly for graph representation? *Advances in neural information processing systems*, 34:28877–28888, 2021.

[53] Rex Ying, Ruining He, Kaifeng Chen, Pong Eksombatchai, William L Hamilton, and Jure Leskovec. Graph convolutional neural networks for web-scale recommender systems. In *Proceedings of the 24th ACM SIGKDD international conference on knowledge discovery & data mining*, pages 974–983, 2018.

[54] Zhitao Ying, Jiaxuan You, Christopher Morris, Xiang Ren, Will Hamilton, and Jure Leskovec. Hierarchical graph representation learning with differentiable pooling. *Advances in neural information processing systems*, 31, 2018.

[55] Bingxu Zhang, Changjun Fan, Shixuan Liu, Kuihua Huang, Xiang Zhao, Jincai Huang, and Zhong Liu. The expressive power of graph neural networks: A survey. *arXiv preprint arXiv:2308.08235*, 2023.

[56] Bohang Zhang, Guhao Feng, Yiheng Du, Di He, and Liwei Wang. A complete expressiveness hierarchy for subgraph gnns via subgraph weisfeiler-lehman tests. In *International Conference on Machine Learning*, pages 41019–41077. PMLR, 2023.

[57] Muhan Zhang, Zhicheng Cui, Marion Neumann, and Yixin Chen. An end-to-end deep learning architecture for graph classification. In *Proceedings of the AAAI conference on artificial intelligence*, volume 32, 2018.

[58] Muhan Zhang and Pan Li. Nested graph neural networks. *Advances in Neural Information Processing Systems*, 34:15734–15747, 2021.

[59] Qi Zhao, Ze Ye, Chao Chen, and Yusu Wang. Persistence enhanced graph neural network. In *International Conference on Artificial Intelligence and Statistics*, pages 2896–2906. PMLR, 2020.

NeurIPS Paper Checklist

1. **Claims**

   Question: Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope?

   Answer: [Yes]

   Justification: The claims in the abstract and introduction accurately reflect the scope and contributions of the paper, as detailed in Sections 1.

   Guidelines:

   - The answer NA means that the abstract and introduction do not include the claims made in the paper.
   - The abstract and/or introduction should clearly state the claims made, including the contributions made in the paper and important assumptions and limitations. A No or NA answer to this question will not be perceived well by the reviewers.
   - The claims made should match theoretical and experimental results, and reflect how much the results can be expected to generalize to other settings.
   - It is fine to include aspirational goals as motivation as long as it is clear that these goals are not attained by the paper.

2. **Limitations**

   Question: Does the paper discuss the limitations of the work performed by the authors?

   Answer: [No]

   Justification: The limitations of our work are discussed at the points in the paper where they naturally arise.

   Guidelines:

   - The answer NA means that the paper has no limitation while the answer No means that the paper has limitations, but those are not discussed in the paper.
   - The authors are encouraged to create a separate "Limitations" section in their paper.
   - The paper should point out any strong assumptions and how robust the results are to violations of these assumptions (e.g., independence assumptions, noiseless settings, model well-specification, asymptotic approximations only holding locally). The authors should reflect on how these assumptions might be violated in practice and what the implications would be.
   - The authors should reflect on the scope of the claims made, e.g., if the approach was only tested on a few datasets or with a few runs. In general, empirical results often depend on implicit assumptions, which should be articulated.
   - The authors should reflect on the factors that influence the performance of the approach. For example, a facial recognition algorithm may perform poorly when image resolution is low or images are taken in low lighting. Or a speech-to-text system might not be used reliably to provide closed captions for online lectures because it fails to handle technical jargon.
   - The authors should discuss the computational efficiency of the proposed algorithms and how they scale with dataset size.
   - If applicable, the authors should discuss possible limitations of their approach to address problems of privacy and fairness.
   - While the authors might fear that complete honesty about limitations might be used by reviewers as grounds for rejection, a worse outcome might be that reviewers discover limitations that aren't acknowledged in the paper. The authors should use their best judgment and recognize that individual actions in favor of transparency play an important role in developing norms that preserve the integrity of the community. Reviewers will be specifically instructed to not penalize honesty concerning limitations.

3. **Theory assumptions and proofs**

   Question: For each theoretical result, does the paper provide the full set of assumptions and a complete (and correct) proof?

Answer: [Yes]

Justification: All theoretical results are stated with their full assumptions and accompanied by complete proofs in section 4 and the appendix.

Guidelines:

- The answer NA means that the paper does not include theoretical results.
- All the theorems, formulas, and proofs in the paper should be numbered and cross-referenced.
- All assumptions should be clearly stated or referenced in the statement of any theorems.
- The proofs can either appear in the main paper or the supplemental material, but if they appear in the supplemental material, the authors are encouraged to provide a short proof sketch to provide intuition.
- Inversely, any informal proof provided in the core of the paper should be complemented by formal proofs provided in appendix or supplemental material.
- Theorems and Lemmas that the proof relies upon should be properly referenced.

4. **Experimental result reproducibility**

   Question: Does the paper fully disclose all the information needed to reproduce the main experimental results of the paper to the extent that it affects the main claims and/or conclusions of the paper (regardless of whether the code and data are provided or not)?

   Answer: [Yes]

   Justification: We provide full implementation details in Appendix to enable reproduction of all key experiments.

   Guidelines:

   - The answer NA means that the paper does not include experiments.
   - If the paper includes experiments, a No answer to this question will not be perceived well by the reviewers: Making the paper reproducible is important, regardless of whether the code and data are provided or not.
   - If the contribution is a dataset and/or model, the authors should describe the steps taken to make their results reproducible or verifiable.
   - Depending on the contribution, reproducibility can be accomplished in various ways. For example, if the contribution is a novel architecture, describing the architecture fully might suffice, or if the contribution is a specific model and empirical evaluation, it may be necessary to either make it possible for others to replicate the model with the same dataset, or provide access to the model. In general. releasing code and data is often one good way to accomplish this, but reproducibility can also be provided via detailed instructions for how to replicate the results, access to a hosted model (e.g., in the case of a large language model), releasing of a model checkpoint, or other means that are appropriate to the research performed.
   - While NeurIPS does not require releasing code, the conference does require all submissions to provide some reasonable avenue for reproducibility, which may depend on the nature of the contribution. For example
     (a) If the contribution is primarily a new algorithm, the paper should make it clear how to reproduce that algorithm.
     (b) If the contribution is primarily a new model architecture, the paper should describe the architecture clearly and fully.
     (c) If the contribution is a new model (e.g., a large language model), then there should either be a way to access this model for reproducing the results or a way to reproduce the model (e.g., with an open-source dataset or instructions for how to construct the dataset).
     (d) We recognize that reproducibility may be tricky in some cases, in which case authors are welcome to describe the particular way they provide for reproducibility. In the case of closed-source models, it may be that access to the model is limited in some way (e.g., to registered users), but it should be possible for other researchers to have some path to reproducing or verifying the results.

5. **Open access to data and code**

Question: Does the paper provide open access to the data and code, with sufficient instructions to faithfully reproduce the main experimental results, as described in supplemental material?

Answer: [Yes]

Justification: We include anonymized link to our code and data in the footnote, along with detailed instructions to reproduce results.

Guidelines:

- The answer NA means that paper does not include experiments requiring code.
- Please see the NeurIPS code and data submission guidelines (`https://nips.cc/public/guides/CodeSubmissionPolicy`) for more details.
- While we encourage the release of code and data, we understand that this might not be possible, so "No" is an acceptable answer. Papers cannot be rejected simply for not including code, unless this is central to the contribution (e.g., for a new open-source benchmark).
- The instructions should contain the exact command and environment needed to run to reproduce the results. See the NeurIPS code and data submission guidelines (`https://nips.cc/public/guides/CodeSubmissionPolicy`) for more details.
- The authors should provide instructions on data access and preparation, including how to access the raw data, preprocessed data, intermediate data, and generated data, etc.
- The authors should provide scripts to reproduce all experimental results for the new proposed method and baselines. If only a subset of experiments are reproducible, they should state which ones are omitted from the script and why.
- At submission time, to preserve anonymity, the authors should release anonymized versions (if applicable).
- Providing as much information as possible in supplemental material (appended to the paper) is recommended, but including URLs to data and code is permitted.

6. **Experimental setting/details**

Question: Does the paper specify all the training and test details (e.g., data splits, hyperparameters, how they were chosen, type of optimizer, etc.) necessary to understand the results?

Answer: [Yes]

Justification: All relevant training and evaluation details, including hyperparameters and data splits, are described in Section 5 and Appendix.

Guidelines:

- The answer NA means that the paper does not include experiments.
- The experimental setting should be presented in the core of the paper to a level of detail that is necessary to appreciate the results and make sense of them.
- The full details can be provided either with the code, in appendix, or as supplemental material.

7. **Experiment statistical significance**

Question: Does the paper report error bars suitably and correctly defined or other appropriate information about the statistical significance of the experiments?

Answer: [Yes]

Justification: We report standard deviation over runs for each metric and explain the computation method in Section 5.

Guidelines:

- The answer NA means that the paper does not include experiments.
- The authors should answer "Yes" if the results are accompanied by error bars, confidence intervals, or statistical significance tests, at least for the experiments that support the main claims of the paper.

- The factors of variability that the error bars are capturing should be clearly stated (for example, train/test split, initialization, random drawing of some parameter, or overall run with given experimental conditions).
- The method for calculating the error bars should be explained (closed form formula, call to a library function, bootstrap, etc.)
- The assumptions made should be given (e.g., Normally distributed errors).
- It should be clear whether the error bar is the standard deviation or the standard error of the mean.
- It is OK to report 1-sigma error bars, but one should state it. The authors should preferably report a 2-sigma error bar than state that they have a 96% CI, if the hypothesis of Normality of errors is not verified.
- For asymmetric distributions, the authors should be careful not to show in tables or figures symmetric error bars that would yield results that are out of range (e.g. negative error rates).
- If error bars are reported in tables or plots, The authors should explain in the text how they were calculated and reference the corresponding figures or tables in the text.

8. **Experiments compute resources**

   Question: For each experiment, does the paper provide sufficient information on the computer resources (type of compute workers, memory, time of execution) needed to reproduce the experiments?

   Answer: [Yes]

   Justification: We specify the hardware and compute time used for each experiment in Section 5 and Appendix.

   Guidelines:

   - The answer NA means that the paper does not include experiments.
   - The paper should indicate the type of compute workers CPU or GPU, internal cluster, or cloud provider, including relevant memory and storage.
   - The paper should provide the amount of compute required for each of the individual experimental runs as well as estimate the total compute.
   - The paper should disclose whether the full research project required more compute than the experiments reported in the paper (e.g., preliminary or failed experiments that didn't make it into the paper).

9. **Code of ethics**

   Question: Does the research conducted in the paper conform, in every respect, with the NeurIPS Code of Ethics `https://neurips.cc/public/EthicsGuidelines`?

   Answer: [Yes]

   Justification: Our work adheres fully to the NeurIPS Code of Ethics, and no ethical concerns are raised by our methodology or data usage.

   Guidelines:

   - The answer NA means that the authors have not reviewed the NeurIPS Code of Ethics.
   - If the authors answer No, they should explain the special circumstances that require a deviation from the Code of Ethics.
   - The authors should make sure to preserve anonymity (e.g., if there is a special consideration due to laws or regulations in their jurisdiction).

10. **Broader impacts**

    Question: Does the paper discuss both potential positive societal impacts and negative societal impacts of the work performed?

    Answer: [NA]

    Justification: There is no societal impact of the work performed.

    Guidelines:

    - The answer NA means that there is no societal impact of the work performed.

- If the authors answer NA or No, they should explain why their work has no societal impact or why the paper does not address societal impact.
- Examples of negative societal impacts include potential malicious or unintended uses (e.g., disinformation, generating fake profiles, surveillance), fairness considerations (e.g., deployment of technologies that could make decisions that unfairly impact specific groups), privacy considerations, and security considerations.
- The conference expects that many papers will be foundational research and not tied to particular applications, let alone deployments. However, if there is a direct path to any negative applications, the authors should point it out. For example, it is legitimate to point out that an improvement in the quality of generative models could be used to generate deepfakes for disinformation. On the other hand, it is not needed to point out that a generic algorithm for optimizing neural networks could enable people to train models that generate Deepfakes faster.
- The authors should consider possible harms that could arise when the technology is being used as intended and functioning correctly, harms that could arise when the technology is being used as intended but gives incorrect results, and harms following from (intentional or unintentional) misuse of the technology.
- If there are negative societal impacts, the authors could also discuss possible mitigation strategies (e.g., gated release of models, providing defenses in addition to attacks, mechanisms for monitoring misuse, mechanisms to monitor how a system learns from feedback over time, improving the efficiency and accessibility of ML).

11. **Safeguards**

    Question: Does the paper describe safeguards that have been put in place for responsible release of data or models that have a high risk for misuse (e.g., pretrained language models, image generators, or scraped datasets)?

    Answer: [NA]

    Justification: The paper poses no such risks.

    Guidelines:

    - The answer NA means that the paper poses no such risks.
    - Released models that have a high risk for misuse or dual-use should be released with necessary safeguards to allow for controlled use of the model, for example by requiring that users adhere to usage guidelines or restrictions to access the model or implementing safety filters.
    - Datasets that have been scraped from the Internet could pose safety risks. The authors should describe how they avoided releasing unsafe images.
    - We recognize that providing effective safeguards is challenging, and many papers do not require this, but we encourage authors to take this into account and make a best faith effort.

12. **Licenses for existing assets**

    Question: Are the creators or original owners of assets (e.g., code, data, models), used in the paper, properly credited and are the license and terms of use explicitly mentioned and properly respected?

    Answer: [Yes]

    Justification: All datasets and code used are properly cited with licensing terms.

    Guidelines:

    - The answer NA means that the paper does not use existing assets.
    - The authors should cite the original paper that produced the code package or dataset.
    - The authors should state which version of the asset is used and, if possible, include a URL.
    - The name of the license (e.g., CC-BY 4.0) should be included for each asset.
    - For scraped data from a particular source (e.g., website), the copyright and terms of service of that source should be provided.

- If assets are released, the license, copyright information, and terms of use in the package should be provided. For popular datasets, `paperswithcode.com/datasets` has curated licenses for some datasets. Their licensing guide can help determine the license of a dataset.
- For existing datasets that are re-packaged, both the original license and the license of the derived asset (if it has changed) should be provided.
- If this information is not available online, the authors are encouraged to reach out to the asset's creators.

13. **New assets**

    Question: Are new assets introduced in the paper well documented and is the documentation provided alongside the assets?

    Answer: [Yes]

    Justification: We release a new code along with complete documentation, licensing, and usage instructions in the repository provided in the footnote.

    Guidelines:

    - The answer NA means that the paper does not release new assets.
    - Researchers should communicate the details of the dataset/code/model as part of their submissions via structured templates. This includes details about training, license, limitations, etc.
    - The paper should discuss whether and how consent was obtained from people whose asset is used.
    - At submission time, remember to anonymize your assets (if applicable). You can either create an anonymized URL or include an anonymized zip file.

14. **Crowdsourcing and research with human subjects**

    Question: For crowdsourcing experiments and research with human subjects, does the paper include the full text of instructions given to participants and screenshots, if applicable, as well as details about compensation (if any)?

    Answer: [NA]

    Justification: The paper does not involve crowdsourcing nor research with human subjects.

    Guidelines:

    - The answer NA means that the paper does not involve crowdsourcing nor research with human subjects.
    - Including this information in the supplemental material is fine, but if the main contribution of the paper involves human subjects, then as much detail as possible should be included in the main paper.
    - According to the NeurIPS Code of Ethics, workers involved in data collection, curation, or other labor should be paid at least the minimum wage in the country of the data collector.

15. **Institutional review board (IRB) approvals or equivalent for research with human subjects**

    Question: Does the paper describe potential risks incurred by study participants, whether such risks were disclosed to the subjects, and whether Institutional Review Board (IRB) approvals (or an equivalent approval/review based on the requirements of your country or institution) were obtained?

    Answer: [NA]

    Justification: The paper does not involve crowdsourcing nor research with human subjects.

    Guidelines:

    - The answer NA means that the paper does not involve crowdsourcing nor research with human subjects.
    - Depending on the country in which research is conducted, IRB approval (or equivalent) may be required for any human subjects research. If you obtained IRB approval, you should clearly state this in the paper.

- We recognize that the procedures for this may vary significantly between institutions and locations, and we expect authors to adhere to the NeurIPS Code of Ethics and the guidelines for their institution.
- For initial submissions, do not include any information that would break anonymity (if applicable), such as the institution conducting the review.

16. **Declaration of LLM usage**

    Question: Does the paper describe the usage of LLMs if it is an important, original, or non-standard component of the core methods in this research? Note that if the LLM is used only for writing, editing, or formatting purposes and does not impact the core methodology, scientific rigorousness, or originality of the research, declaration is not required.

    Answer: [NA]

    Justification: The core method development in this research does not involve LLMs as any important, original, or non-standard components.

    Guidelines:

    - The answer NA means that the core method development in this research does not involve LLMs as any important, original, or non-standard components.
    - Please refer to our LLM policy (`https://neurips.cc/Conferences/2025/LLM`) for what should or should not be described.

A Related Work

GNNs that use paths As [30] wrote in their paper, Graphormer[52], PEGN[59], SP-MPNN[2], Geodesic GNN[23] use the shortest paths to embed the graph structure, which aims to use fewer paths to represent the graph structure. There are some other GNNs that use specific paths to represent the graph structure. [30] introduce PathNN that uses the sp-path, [12] develop PathNN focus on single shortest paths, all shortest paths and all simple paths, and [26] uses GeniePath adaptively as receptive paths for breadth/depth exploration and filter useful/noisy signals. [41] introduces topological message-passing scheme PCN(Path Complex Networks) operating on path complexes and a novel graph isomorphism test PWL, with the the theoretical connection between PWL and the latter higher-order WL tests.

GNNs that use cycles At the same time, starting from the subgraph count GNN, cycle as an important subgraph, has been widely used in graph representation. [49] uses the SPT cycle bases family to learn cycle representations to enhance the expressiveness of GNN for inductive relation prediction tasks in knowledge graphs.[4] proposes a new message-passing aggregation method based on cell complexes(including cycles) to enhance the expressiveness of GNNs. [10] introduces a way of using cycle structures in aggregation and shows its expressiveness by universal covers. They connect the nodes in the same cycle and then aggregate them as cliques in some additional GNN layers. [50] proposes a novel edge structure encoding CycleNet based on the position of the edge in the cycle spaces.

The limitation(expressiveness) of MPNNs It has shown that [48] MPNNs are at most as powerful as the WL test in distinguishing isomorphic graphs. On the other hand, the limitation leads to a lack in counting simple substructures[8] like cycles. At the same time, there is a lot of work that tries to enhance the expressiveness of GNNs by using graph features, graph topology, and enhancing the architecture of GNNs, see the survey[55] for more details.

B Experimental Setup

B.1 Experimental Setup on synthetic datasets

Experimental setup Following [30], for all experiments in synthetic datasets, the aggregation function is set to the identity function. We set initial node features to be vectors of ones and process them with MLPs.

For the SR, EXP, and graph8c datasets, we investigate whether the proposed models have the right inductive bias to distinguish the graphs. Like [13] , we consider two graphs to be non-isomorphic if the Euclidean distance between their representations is not below a threshold ϵ, where the presentation

is generated by an untrained model. And we set the radius to 3 for detecting cycles in use. Then we use some cycle-convolution layers to aggregate and apply a GCN layer and a linear layer at last.

B.2 Experimental Setup on real-world datasets

Experimental Setup For regression tasks on ZINC, we add the feature introduced in Section 4.4 to the node features, followed by a linear layer for encoding. We apply simple MLP models with various convolution layers, using batch normalization between them and an LSTM before the final linear layer.

For classification tasks on TUDatasets, we incorporate cycle convolutions similar to [10], aggregating nodes along chordless cycles step by step based on their distance in the original graph. This helps the model differentiate structures like ortho, meta, and para. We also use GAT layers based on MPNNs, where edge indices are given by chordless paths.

For classification on ogbg-MOLHIV, we add the feature from Section 4.4 into a GIN model. We follow the evaluation protocol of [13] on TUDatasets, using 10-fold cross-validation and predefined data splits. Hidden dimensions are chosen from $\{32, 64\}$, and dropout rates from $\{0, 0.5\}$ are applied to the final MLP. For all datasets, we use a consistent batch size of 1. We also test various convolution strategies, including path-first and cycle-first approaches, to systematically assess their impact.

C Statistics of Chordless Cycles in various datasets

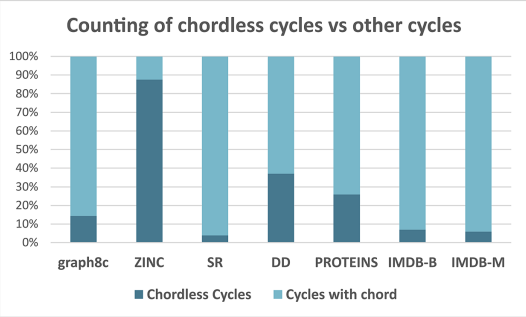


Figure 6: By comparing the counts between chordless cycles and other cycles, we can see that the chordless cycles demonstrate superior performance, achieving significantly lower costs

Dataset	CSGNN	PathNN
Protein	248	408
DD	704	2664
IMDB-B	386	390
IMDB-M	584	444

Table 4: Model Memory Usage (MB)

D Dataset introduction

D.1 Synthetic Datasets

Dataset Overview We evaluate the performance of our CSGNN in three publicly available datasets. **Graph8c** consists of all the 11117 possible connected non-isomorphic simple graphs with 8 nodes. **EXP dataset** [1]includes 600 pairs of 1-WL equivalent graphs which is distinguishable under the 2-WL algorithm. **SR dataset** [3]consists of strongly regular graphs which is undistinguishable under

[3]EXP and SR dataset can be found in `https://users.cecs.anu.edu.au/~bdm/data/graphs.html`

the 3-WL algorithm. Where each graph in SR25 has 25 nodes, and contains 15 graphs generating 105 pairs for isomorphism comparison.

D.2 Real-World Datasets

Dataset Overview We evaluate CSGNN in real-world tasks, including regression tasks and classification tasks in three datasets.

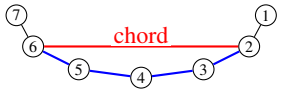
ZINC[20] It is a molecular graph regression dataset with 250,000 molecules, used for predicting molecular properties, and ZINC(subset) takes a 12k subset of it.

TUDatasets[31] It is a collection of over 120 datasets for graph classification, covering various applications such as chemistry and bioinformatics.

ogbg-MOLHIV It is a molecular property prediction dataset adopted from the MoleculeNet, and among the largest of the MoleculeNet datasets, used for predicting the target molecular properties.

E the proofs of the theorems

E.1 proof of Lemma 3.4



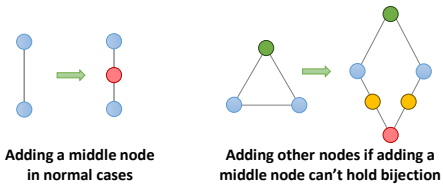
chordless paths

Proof. Given a path containing a chord, we focus on the decomposition of the subpath that includes the chord, as the remaining subpaths are already chordless. In such cases, it suffices to select a single chord—preferably one whose endpoints are near the middle of the path—to partition it into chordless segments. This approach avoids exhaustive decomposition over all edges or chords, and is sufficient for our purposes. □

E.2 proof of Lemma 4.3

Proof. After considering the $1-WL$ coloring, if there is an edge that has the same color as its neighbor, we can add a node in the middle of the edge, and then we can get a $1-WL-colorable$ graph. If the graph after adding the middle node has existed in the set, we can again add another two nodes in the middle of the edge, and so on (refer to Figure **??**). By considering the finity of the set, we can get the $1-WL-colorable$ graphs in the set.

□



Lemma 4.3: Construct $1-WL-colorable$ graphs by adding nodes.

E.3 proof of Theorem 4.9

Proof. After removing the nodes in the last layer, we can get two trees that are 1-WL-equivalent, so they are isomorphic. So we pay attention to the nodes in the last layer to see their connection to the second-last layer. Note that if there exists cycles that including each node in the last layer in each connected components, then we can distinguish the graphs with different number of nodes in the last layer in each connected components (As shown in the figure 7, double 1 vs a single 2).

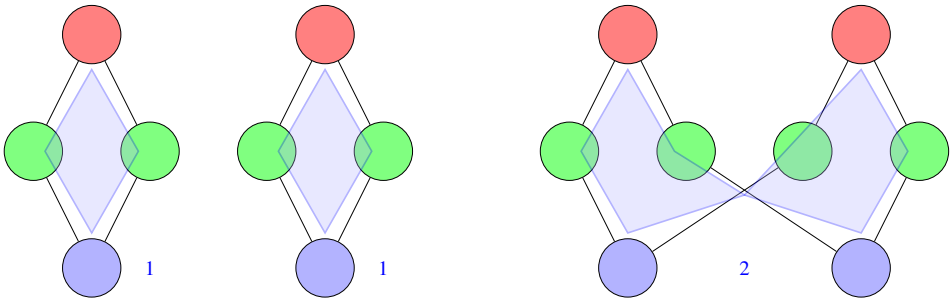


Figure 7: Two WL-equivalent graphs that have different number of connected components

Otherwise, that is the case that there exists a unique way between two nodes in the last layer since two paths help build a cycle. And then we can simplify the form of the graph to a three-layer form, since the equivalence of WL-tree above. We consider the color-equivalent mapping ϕ of a pair of nodes u_1, u_2 in the last layer of the same WL-tree. And we denote the neighborhood of u^* in another WL-tree by u_3.

(1) if $\phi(u^*) = u^*$ then the nodes in the last layer of the same WL-tree are connected by u^* by color-equivalence.

(2) if $\phi(u^*) = u^{'} \neq u^*$ then u_1 and $\phi(u_3)$ are neighbors of $u^{'}$ then we can find two paths. $\square$