

Schreier Coset Graph Rewiring

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September 2025

Abstract

Graph Neural Networks (GNNs) provide a principled framework for learning on graph-structured data, yet their expressiveness is fundamentally limited by over-squashing the exponential compression of information from distant nodes as messages traverse long paths. While graph rewiring methods attempt to alleviate this issue by modifying topology, existing approaches introduce prohibitive computational costs. We propose Schreier-Coset Graph Propagation (SCGP), a group-theoretic rewiring method that augments the input graph with a Schreier coset graph derived from a special linear group $SL(2, Z_n)$. Unlike heuristic rewiring, SCGP provides *provable* theoretical guarantees: the auxiliary graph exhibits a spectral gap and bounded effective resistance, creating low-resistance bypasses for long-range communication. By coupling these two graphs with strength, we ensure that effective resistance between any node pair is bounded, directly mitigating over-squashing. Empirical evaluations demonstrate that SCGP reduces effective resistance by 15-40% across benchmark datasets while maintaining competitive accuracy and less computational overhead, making it practical for both large-scale and resource-constrained applications.

1 Introduction

Graph Neural Networks (GNNs) are designed to process data exhibiting an inherent graph structure [17]. Their versatility has led to widespread adoption and empirical success across diverse domains and numerous graph-related tasks [38, 1].

Several GNN variants have emerged. For instance, the Graph Convolutional Networks (GCN) [22] employs a localized, first-order approximation of spectral graph convolutions. This method aggregates normalized features from neighboring nodes to update node embeddings, achieving a computational complexity that scales linearly with the number of edges denoted as $O(E)$. The Graph Isomorphism Network (GIN) [39] utilizes sum aggregation neighbor features, followed by a multi-layer perceptron (MLP), to maximize its ability to distinguish between different graph structures. When its MLPs process sufficient capacity, GIN’s discriminative power is equivalent to Weisfeiler-Lehman test for graph isomorphism. [20].

Most contemporary GNNs operate under Message Passing Neural Network (MPNN) paradigm [18]. In this framework, nodes iteratively exchange information with their neighbors to refine their representations. While more layer are often necessary to capture long-range interactions within the graph, increasing network depth can lead to challenges. Specifically, the receptive field of nodes grows exponentially with depth. This results in large amounts of information from extensive neighborhoods being compressed into fixed-size embeddings [36]. This phenomenon, known as over-squashing [3], can cause significant information loss [31] and thereby substantially limit the expressive capacity of GNNs [11].

Further the performance and behavior of GNNs are intrinsically linked to the underlying graph topology. For instance, the Jacobian of node features is influenced by topological properties such as graph curvature and effective resistance [11, 33, 6]. Various methods are employed to address over-squashing in graph neural networks. *Graph rewiring* techniques by [10], constructs expander graphs, including Cayley graphs [36] to aid propagation. [36] modifies topology using properties such as curvature [14], spectral expansion [21, 5], and effective resistance [6] to optimize the flow of information.

Feature Augmentation offers an alternative approach. Laplacian Positional Encoding (LapPE) by [12] injects long-range structural context into node features, reducing the need for deep message-passing layers. However, its $O(n^3)$ eigenvector computation limits scalability and makes it sensitive to topological perturbations. Another method, shortest-path distance encoding directly inputs hop counts (all-pair computation is

$O(n(E))$, bypassing intermediate message propagation. This method typically encodes only scalar distances, thus neglecting information about other possible paths and connectivity issues.

This work introduces **SCHREIER-COSET GRAPH PROPAGATION (SCGP)**, a novel graph-rewiring framework that augments input graphs with Schrier-Coset graphs derived from $SL(2, Z_n)$. Unlike prior approaches, that rely solely on Cayley expanders or heavy rewiring, **SCGP** provides a principled alternative: The contribution are summarized as follows:

- **Formalization of Schreier-Coset Rewiring** : Defined the construction of Schreier-Coset graphs and their usage in rewiring augmentations in GNNs. Vertices corresponding to cosets $SL(2, Z_n)$ modulo an upper-triangle subgroup, with constant side generators yielding a d – regular graph.
- **Theoretical Analysis** : Define the Schreier-Graph, its node to coset mapping, spectral properties, effective resistance bounds and augmented graph.
- **Empirical Validation** : Evaluate **SCGP** on node and graph classification benchmarks, additionally we test the accuracy of **SCGP** by varying modularity of a SBM graph. Results demonstrate that **SCGP** consistently matches, attains higher scores against rewiring baselines, while achieving significantly reduced computation overhead.

2 Related Works and Existing Approaches

This section reviews prominent techniques designed to alleviate over-squashing in GNNs. A common underlying strategy involves mitigating structural bottlenecks by de-coupling the input graph from the computational graph that governs message-passing dynamics. [3] proposed rewiring approaches, such as making the GNNs final layer to be fully adjacent. This configuration allows all nodes to interact directly, potentially easing bottlenecks and bypassing the need for extensive full-graph pre-analysis. Graph Transformers [40, 23] further demonstrate this principle by effectively employing full connectivity in every layer. However, such dense approaches $O(|V|^2)$ edge complexity typically limits their application to modest graph sizes. Alternatively, [16] proposed a controller node architecture, introducing a single, central node connected to all other nodes in the graph. While this efficiently reduces the graph’s diameter to 2 with only $O(|V|)$ additional edges, this pivotal controller node can become a new communication bottleneck by over-centralizing information flow.

Feature Augmentation This method enriches node and edge attributes, appending informative signals, mitigating over-squashing while improving propagation. [13] concatenates top- k eigenvectors of the graph Laplacian to every node. Providing each node with global coordination means there is no need for information to travel through many hops. It requires a $O(n^3)$ eigen-decomposition and $O(nk)$ memory with sign ambiguity and dynamic mini-batches leading it to be less efficient.

Graph Rewiring In this approach, the input graph is rewired to optimize the spectral properties of the graph. [21] derived a popular class of approaches based on the spectral quantity of the graph or by reducing the effective resistance [5, 6, 4]. These approaches have provided compelling insights and reduced over-squashing. However, they impose computational complexity when analyzing the entire input graph structure.

Expander Graphs These graph exhibit the desirable properties associated with spectral gap and effective resistance.[5] proposed a construction inspired by expander graphs to rewire the input graph randomly, locally. [32] uses both virtual nodes and expander graphs as a robust foundation to design the graph transformer architecture.[36] introduces a combination of virtual nodes and expander graphs for the design of Cayley propagation, inflating graph nodes to $O(n^3)$, requiring memory intensive padding and truncation.

3 Schreier-Coset Graph Propagation

3.1 Preliminaries

Graphs. Denoted by $G = (V, E)$, where V is the set of nodes and E is the set of edges. G is assumed to be *undirected, connected, and non-bipartite*, and we define an $n \times n$ adjacency matrix A . Here, $A_{i,j}$ denotes the

edge between node i and j , and $|V| = n$ is the number of nodes. Let $D = \text{diag}(d_1, d_2, \dots, d_n)$ be the diagonal degree matrix where $D_{vv} = d_v$ is the degree of node v . The normalized Laplacian $L = \text{lap}(G)$ is defined by

$$L = D^{-1/2}(D - A)D^{-1/2}.$$

The eigenvalues of L are $0 = \lambda_0 \leq \lambda_1 \leq \dots \leq \lambda_{n-2} \leq \lambda_{n-1}$. The eigenvector corresponding to λ_2 is called the *Fiedler vector*. It provides a canonical one-dimensional embedding of the nodes that reflects graph connectivity.

Special Linear Group $SL(2, \mathbb{Z}_n)$. Let $\mathbb{Z}_n = \mathbb{Z}/n\mathbb{Z}$ denote the ring of integers modulo n . The group $\mathcal{G} = SL(2, \mathbb{Z}_n)$ is defined as:

$$\mathcal{G} = SL(2, \mathbb{Z}_n) = \{M \in \mathbb{Z}_n^{2 \times 2} \mid \det(M) \equiv 1 \pmod{n}\}.$$

Here, n depends on the input graph size.

Subgroup. Let H be a subgroup $H \subset SL(2, \mathbb{Z}_n)$ which consists of diagonal matrices with unit determinant within \mathcal{G} :

$$H = \left\{ \begin{pmatrix} a & 0 \\ 0 & d \end{pmatrix} \in \mathcal{G} \mid ad \equiv 1 \pmod{n} \right\}.$$

Generator. Let \mathbb{S} be the generator set:

$$\mathbb{S} = \left\{ \begin{pmatrix} 1 & \pm 1 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ \pm 1 & 1 \end{pmatrix} \right\} \pmod{n}.$$

Expander and Cayley Graphs. An expander graph has a number of edges that scales linearly with the number of nodes. It is both sparse and highly connected. A family of expander graphs has been pre-computed leveraging the theoretical benefits of special linear group $SL(2, \mathbb{Z}_n)$ for which a family of corresponding Cayley Graphs [27] can be derived: $\text{Cay } SL(2, \mathbb{Z}_n); \mathbb{S}$ where, \mathbb{S} denotes a particular generating set for $SL(2, \mathbb{Z}_n)$. For \mathbb{S} , Cayley graphs have expansion properties and are scalable; however, achieving a large specific number of nodes is not always feasible; the node count for $\text{Cay } SL(2, \mathbb{Z}_n); \mathbb{S}$ is given by:

$$|V(\text{Cay}((SL(2, \mathbb{Z}_n); \mathbb{S}))| = n^3 \prod_{\text{prime } p|n} \left(1 - \frac{1}{p^2}\right),$$

rendering them impractical for large n due to excessive memory requirements.

Schreier-Coset Graphs. [28] depicts the standard permutation representation of finitely generated groups on the cosets of subgroups of $SL(2, \mathbb{Z}_n)$ and provides diagrammatic interpretations of combinatorial graph theory. The Schreier-Coset graph plays a central role in our propagation scheme, serving as an auxiliary structure that encodes robust expansion and mixing behavior through group-theoretic symmetries.

4 Methodology

4.1 Schreier-Coset Graph Γ .

For a group \mathcal{G} , a subgroup $H \subseteq \mathcal{G}$, a generating set $\mathbb{S} \subseteq \mathcal{G}$, the Schreier-Coset graph $\Gamma = (V_\Gamma, E_\Gamma)$ is defined as:

- **Vertex Set :** $V_\Gamma = \{gH : g \in \mathcal{G}\}$ (collection of right cosets).
- **Edge Set :** For each coset $gH \in V_\Gamma$ and each generator $s \in \mathbb{S}$, an undirected edge $\{gH, (gs)H \in E_\Gamma\}$.

The graph is d -regular, where $d = |\mathbb{S}|$, since each coset gH has exactly one neighbor $(gs)H$ for each generator $s \in \mathbb{S}$.

In constructing the Schreier Graph, we employ a *canonical construction*. That is, Γ is constructed over the group $\mathcal{G} = SL(2, Z_n)$ with subgroup H consisting of diagonal matrices, and use elementary row operations as generators:

$$\mathbb{S} \approx \left\{ \begin{pmatrix} 1 & \pm 1 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ \pm 1 & 1 \end{pmatrix} \right\} \pmod{n}.$$

The resulting Schreier-Coset graph has $|V_\Gamma| = \frac{|SL(2, Z_n)|}{|H|} = \frac{n(n^2-1)}{\phi(n)}$ vertices, where $\phi(n)$ is Euler's totient function.

4.2 Node to Coset Mapping for Rewiring

For the input graph, $G_{in} = (V_{in}, E_{in})$ and Schreier graph Γ , a locally-preserving map is constructed $\phi : V \rightarrow V_\Gamma$ that enables structure-aware rewiring.

Spectral Mapping Construction . Let $\Phi_{in} : V_{in} \rightarrow \mathbb{R}^r$ be spectral embeddings using the r leading eigenvectors of their respective graph Laplacian's. We defined the locality-preserving mapping $\phi : V_{in} \rightarrow V_\Gamma$ by solving:

Case (i) $|V_{in}| \leq |V_\Gamma|$:

$$\min_{\phi: V_{in} \hookrightarrow V_\Gamma} \sum_{(u,v) \in E_{in}} \text{dist}_\Gamma(\phi(u), \phi(v))$$

subject to $\|\Phi_\Gamma(\phi(v)) - \Phi_{in}(v)\|_2$ being small.

Case (ii) $|V_{in}| > |V_\Gamma|$: Use disjoint copies $\Gamma^{(1)}, \dots, \Gamma^{(q)}$ or a product $\Gamma \times K_q$ and apply case (i) per block.

The optimization ensures that neighborhoods in G_{in} are mapped to neighborhoods in Γ , preserving local structure for effective rewiring.

4.3 Spectral Properties of Γ

We show that the Schreier coset graph Γ is an expander with strong spectral properties that enable efficient information propagation through low effective resistance paths.

Lemma 4.1 (Spectral Gap). *The Schreier coset graph Γ has a spectral gap*

$$\gamma = 1 - \lambda_2(P) > 0,$$

where P is the transition matrix of the random walk on Γ .

Lemma 4.2 (Effective Resistance Bound). *For any vertices $u, v \in V_\Gamma$,*

$$R_{\text{eff}}(u, v) \leq \frac{2}{d\gamma},$$

where $d = |\mathbb{S}|$ is the degree and γ is the spectral gap.

Lemma 4.3 (Expander Mixing). *For the random walk matrix P on Γ and all $t \geq 0$,*

$$\left| (P^t)_{iv} - \frac{1}{n} \right| \leq (1 - \gamma)^t.$$

If $t \geq \frac{\log(2n)}{\gamma}$, then $(P^t)_{iv} \geq \frac{1}{2n}$.

The bounded effective resistance guarantees that any two nodes in the Schreier graph are well-connected, with resistance inversely proportional to the spectral gap γ . This property is crucial for creating efficient rewiring patterns.

4.4 Schreier-Guided Graph Rewiring

Structure-aware rewiring of the input graph G_{in} by adding edges that mirror the connectivity patterns of the Schreier graph Γ .

Rewiring Strategy. Addition of edges to G_{in} between nodes $u, v \in V_{in}$ when their Schreier images $\phi(u), \phi(v) \in V_\Gamma$ are connected by short paths in Γ . This creates an alternative that leverages the expander properties of Γ .

Edge Addition Process :

- **Distance Threshold Selection:** A maximum distance $\ell \geq 1$ in Schreier graph Γ .
- **Schreier Proximity Detection:** For each pair of nodes $u, v \in V_{in}$, compute

$$\text{dist}_\Gamma(\phi(u), \phi(v))$$

- **Conditional Edge Addition:** Add edge u, v to E_{in} if:
 - $u, v \notin E_{in}$ (not already connected).
 - $\text{dist}_\Gamma(\phi(u), \phi(v)) \leq \ell$ (close in Schreier Graph)
 - $\text{dist}_{G_{in}}(u, v) > \ell$ (distant in original graph)
- **Rewired Graph Construction :** The rewired graph $G^{rwd} = (V_{in}, E^{rwd})$ is defined as:

$$E^{rwd} = E_{in} \cup \{(u, v) : u, v \in V_{in}, \text{dist}_\Gamma(\phi(u), \phi(v)) \leq \ell, \text{dist}_{G_{in}}(u, v) > \ell\}$$

- **Weight Assignment.** Added edges receive $w_{uv} = \epsilon \cdot f(\text{dist}_\Gamma(\phi(u), \phi(v)))$, where:
 - $\epsilon > 0$ is the global strength parameter.
 - $f(\cdot)$ is a decreasing function

4.5 Rewired Information Flow

SCGP rests on three key pillars: locality preservation through spectral embeddings, effective resistance reduction via alternative pathways, and quantifiable over-squashing mitigation. We establish formal theoretical guarantees for each component and analyze the computational complexity of the approach:

Bi-Lipschitz Control via Spectral Embeddings. The spectral alignment between G_{in} and Γ preserves distance relationships up to a controlled factor, ensuring that the rewiring preserves meaningful structural relationships.

Theorem 4.1 (Lipschitz Locality). *If Φ_{in} and Φ_Γ are bi-Lipschitz on relevant scales, then there exists $c \geq 1$ such that*

$$\text{dist}_\Gamma(\phi(u), \phi(v)) \leq c \cdot \text{dist}_{in}(u, v)$$

for all $u, v \in V_{in}$.

Effective Resistance Analysis of Rewired Graph. The rewiring process creates alternative pathways between distant nodes, significantly reducing effective resistance and enabling better information flow.

Theorem 4.2 (Effective Resistance in Rewired Graph). *In the rewired graph G^{rwd} , the effective resistance between nodes $u, v \in V_{in}$ satisfies*

$$R_{\text{eff}}^{rwd}(u, v) \leq \min \left\{ R_{\text{eff}}^{in}(u, v), \frac{1}{\epsilon} R_{\text{eff}}^\Gamma(\phi(u), \phi(v)) + \frac{2}{\epsilon} \right\}.$$

The rewired graph can be viewed as an electric network where current can flow either through the original edges in G_{in} or through the alternative Schreier edges. The effective resistance takes the minimum of these pathways.

Information Flow and Over-Squashing Mitigation. The connection between effective resistance and information propagation in neural networks is well established. In message-passing networks, the gradient flow between distant nodes is inversely proportional to their effective resistance.

Theorem 4.3 (Over-Squashing Mitigation). *For nodes $u, v \in V_{in}$ with large distance,*

$$\rho(u, v) = \frac{R_{\text{eff}}^{\text{in}}(u, v)}{R_{\text{eff}}^{\text{rd}}(u, v)} \geq \max \left\{ 1, \frac{R_{\text{eff}}^{\text{in}}(u, v) \cdot \epsilon}{R_{\text{eff}}^{\Gamma}(\phi(u), \phi(v)) + 2} \right\}.$$

When $R_{\text{eff}}^{\text{in}}(u, v)$ grows exponentially with distance, but $R_{\text{eff}}^{\Gamma}(\phi(u), \phi(v)) \leq \frac{2}{d\gamma}$ remains bounded, the improvement factor $\rho(u, v)$ can be exponentially large.

Performance Guarantees. Combining the above results, we can establish comprehensive performance bounds for the SCGP approach.

Theorem 4.4 (Performance Guarantees). *Let G_{in} be an input graph with diameter D and maximum effective resistance $R_{\text{max}}^{\text{in}}$. Using Schreier-guided rewiring with a Schreier graph Γ of spectral gap $\gamma > 0$:*

- For all $u, v \in V_{in}$,

$$R_{\text{eff}}^{\text{rd}}(u, v) \leq \min \left\{ R_{\text{max}}^{\text{in}}, \frac{1}{\epsilon} \left(\frac{2}{d\gamma} + 2 \right) \right\}.$$

- Information can propagate between any nodes with resistance bounded by

$$\frac{1}{\epsilon} \left(\frac{2}{d\gamma} + 2 \right).$$

- The over-squashing factor is reduced by at least

$$\frac{R_{\text{max}}^{\text{in}} \cdot \epsilon d \gamma}{2(d\gamma + 2)}.$$

Complexity and Practical Considerations. The practical implementation of SCGP involves several computational components, each with well-defined complexity bounds.

Graph Construction: The Schreier-Coset graph Γ has $V_{\Gamma} = \theta(n)$ vertices for $(\text{mod } n)$ (and $O(n \cdot \text{polylog}(n))$ in general case), with constant degree $d = |\mathbb{S}| = 4$. Its edge set therefore satisfies $|E_{\Gamma}| = O(|V_{\Gamma}|)$. Constructing Γ via coset representatives and generator multiplications requires $O(|V_{\Gamma}|)$ group operations, which can be cached once and reused across multiple input graphs.

Mapping and Rewiring: The locality-preserving mapping $\phi : V_{in} \rightarrow V_{\Gamma}$ can be computed using spectral embeddings of dimension $r \ll |V|$. This requires $O(r \cdot |E_{in}|)$ operations via power iteration on the Laplacian. For rewiring, distance queries $\text{dist}_{\Gamma}(\phi(u), \phi(v))$ can be approximated using truncated BFS or landmark-based embeddings, avoiding a quadratic scan over all pairs. Thus the edge addition process runs in $\tilde{O}(|E_{in}| + |V_{in}|) \cdot \deg_{\Gamma(\ell)}$ where $\deg_{\Gamma(\ell)}$ is the number of Schreier neighbors within distance ℓ .

Message Passing: Each GNN layer on the rewired graph requires $O(|E^{\text{rd}}|)$ operations. Since $E^{\text{rd}} = O(E_{in} + V_{in}) \cdot \deg_{\Gamma(\ell)}$ and $\deg_{\Gamma(\ell)}$ grows moderately (expander property), the per-layer complexity remains near-linear in the input size.

Space Complexity: The node set is unchanged ($|V^{\text{rd}}| = |V_{in}|$). The added edges are at most $O(|V_{in}| \cdot \deg_{\Gamma(\ell)})$, and $\deg_{\Gamma(\ell)} = O(d^{\ell})$ with $d = 4$. Thus the memory overhead is tunable via ℓ and typically sub-quadratic. All proofs are provided in Appendix.

5 Experiment

The efficacy of SCGP is validated on various node and graph classification datasets and compared with the state-of-the-art methods.

Table 1: Performance comparison of SCGP against baseline models across six standard benchmark datasets.

Model	Am. Comp.	Am. Photo	CiteS.	Co. CS	Cora	PubMed
LogReg	0.6410 \pm 0.0570	0.7300 \pm 0.0650	-	0.8640 \pm 0.0900	-	-
MLP	0.4490 \pm 0.0580	0.6960 \pm 0.0380	0.5880 \pm 0.0220	0.8830 \pm 0.0070	0.5980 \pm 0.0240	0.7010 \pm 0.0070
GAT	0.7800 \pm 0.1900	0.8570 \pm 0.2030	0.6890 \pm 0.0170	0.9050 \pm 0.0060	0.8080 \pm 0.0160	0.7780 \pm 0.0210
GCN	0.8260 \pm 0.0240	0.9120 \pm 0.0120	0.6820 \pm 0.0160	0.9111 \pm 0.0050	0.7910 \pm 0.0180	0.7880 \pm 0.0060
MoNET	0.8350 \pm 0.0220	0.9120 \pm 0.0130	0.7120 \pm 0.0020	0.9080 \pm 0.0600	0.5980 \pm 0.0080	0.7860 \pm 0.0230
LabelProp	0.7080 \pm 0.0810	0.7260 \pm 0.0111	0.6780 \pm 0.0210	0.7360 \pm 0.0390	0.5050 \pm 0.0150	0.7050 \pm 0.0530
LabelProp NL	0.7500 \pm 0.0390	0.8390 \pm 0.0270	0.6670 \pm 0.0220	0.7600 \pm 0.0140	0.5100 \pm 0.0100	0.7230 \pm 0.0290
GS-mean	0.8240 \pm 0.0180	0.9140 \pm 0.0130	0.7160 \pm 0.0190	0.9130 \pm 0.0280	0.5860 \pm 0.0160	0.7740 \pm 0.0220
GS-maxpool	-	0.9040 \pm 0.0130	0.6750 \pm 0.0230	0.8500 \pm 0.0110	0.4700 \pm 0.0150	0.7610 \pm 0.0230
GS-meanpool	0.8960 \pm 0.0090	0.9070 \pm 0.0160	0.6860 \pm 0.0240	0.8960 \pm 0.00090	0.4050 \pm 0.0150	0.7650 \pm 0.0240
+ SCGP	0.9031 \pm 0.0062	0.9400 \pm 0.0026	0.6180 \pm 0.0215	0.9211 \pm 0.0022	0.7957 \pm 0.0058	0.7894 \pm 0.0097

5.1 Node Classification

For Node Classification, we use the following datasets:

Amazon Computers and Amazon Photo [30]: These datasets consist of product co-purchase graphs, where nodes represent items and edges indicate frequent co-purchase relationships. Node features are constructed from bag-of-words representations of product reviews, and class labels correspond to product categories. The Amazon Photo dataset focuses specifically on photographic equipment while preserving identical feature and edge structures.

CoAuthor CS [30]: A co-authorship network where nodes correspond to authors and edges represent collaborations on at least one publication. Node features are extracted from keywords in the authors’ publications, and classes denote major research areas.

CiteSeer [29]: A citation network where nodes represent scientific articles and edges denote citation relationships. The dataset presents moderate feature sparsity and low average node degree, providing a challenging setting for evaluating message-passing effectiveness.

Cora and PubMed [29]: Benchmark citation networks in which nodes correspond to research papers and edges represent citations. Node features are based on word vector embeddings of paper abstracts, and the classification task involves predicting the subject area.

Each model is trained for 200 epochs using four layers and a dropout rate of 0.5, following the hyperparameter settings from [22]. All experiments are repeated 100 times to ensure statistical robustness. In addition to SCGP-enhanced models, comparisons are made against standard baselines including *LogReg* [9], *MLP* [35], *GAT* [34], and *GCN* [22]. Given that the benchmark datasets exhibit balanced class distributions, test accuracy is adopted as the primary evaluation metric, as reported in **Table 1**.

SCGP in **Table 1** consistently enhances model performance across the node classification tasks. It achieves the highest accuracies on four of the six benchmark datasets, particularly notable improvements on Amazon Computers, Amazon Photo, Coauthor-CS and PubMed. It remains **SCGP** competitive in Cora. The consistent performance gains across most datasets, combined with notably reduced variance (as evidenced by smaller standard deviations), suggest that **SCGP** provides a robust enhancement to existing GNN architectures. The method’s effectiveness is particularly pronounced on the Amazon datasets and Computer Science, where the spectral properties and community structure align well with the Schreier-Coset graph’s expander properties, enabling more effective long-range information propagation during message passing.

5.2 Graph Classification

TU Dataset (see Morris et al. [25]) comprises over 120 graph classification and regression datasets. Representative datasets include chemical graphs (MUTAG), protein structures (PROTEINS), social networks (IMDB-BINARY, REDDIT-BINARY), and research collaboration graphs (COLLAB). The topology of the graphs about the task is identified as requiring long-range interactions. While certain node classification tasks have also been considered in previous works, these are tractable with nearest neighbor information Brockschmidt [7]. *SCGP* is compared against *CGP* Wilson et al. [36], *EGP* Deac et al. [10], **FA** Alon and Milman [2] as well as the following state-of-the-art graph rewiring techniques that require dedicated

Table 2: Results of SCGP compared against CGP, EGP, FA and the approaches that require dedicated preprocessing for GCN and GIN on the TUDataset. The colors highlight **First**, **Second** and **Third** positions respectively.

Model	REDDIT-BINARY	IMDB-BINARY	MUTAG	ENZYMES	PROTEINS	COLLAB
GCN	77.735 \pm 1.586	60.500 \pm 2.729	74.750 \pm 4.030	29.083 \pm 2.363	66.652 \pm 1.933	70.490 \pm 1.628
+ FA	OOM	48.950 \pm 1.652	70.250 \pm 4.608	28.667 \pm 3.693	71.071 \pm 1.506	72.039 \pm 0.771
+ DIGL	77.350 \pm 1.206	49.600 \pm 2.435	70.500 \pm 5.045	30.833 \pm 1.537	72.723 \pm 1.420	56.470 \pm 0.865
+ SDRF	77.975 \pm 1.479	59.000 \pm 2.254	74.000 \pm 3.462	26.667 \pm 2.000	67.277 \pm 2.170	71.330 \pm 0.807
+ FoSR	77.750 \pm 1.385	59.750 \pm 2.357	75.250 \pm 5.722	24.167 \pm 3.005	70.848 \pm 1.618	67.220 \pm 1.367
+ BORF	OOT	48.900 \pm 0.900	76.750 \pm 0.037	27.833 \pm 0.029	67.411 \pm 0.016	OOT
+ GTR	79.025 \pm 1.248	60.700 \pm 2.079	76.500 \pm 4.189	25.333 \pm 2.931	72.991 \pm 1.956	72.600 \pm 1.025
+ PANDA	87.275 \pm 1.033	68.350 \pm 2.346	76.750 \pm 5.531	30.667 \pm 2.019	70.134 \pm 1.518	73.850 \pm 0.695
+ EGP	67.550 \pm 1.200	59.700 \pm 2.371	70.500 \pm 4.738	27.583 \pm 3.262	73.304 \pm 2.516	69.470 \pm 0.970
+ CGP	67.050 \pm 1.483	56.200 \pm 1.825	83.750 \pm 3.597	31.000 \pm 2.397	73.036 \pm 1.291	69.630 \pm 0.730
+ SCGP	88.430 \pm 2.0600	61.600 \pm 4.870	76.670 \pm 1.320	52.750 \pm 7.800	72.590 \pm 4.330	73.620 \pm 1.620
GIN	84.600 \pm 1.454	71.250 \pm 1.509	80.500 \pm 5.143	35.667 \pm 2.803	70.312 \pm 1.749	71.490 \pm 0.746
+ FA	OOM	69.900 \pm 2.332	80.250 \pm 5.314	47.833 \pm 2.529	72.902 \pm 1.419	72.740 \pm 0.786
+ DIGL	84.575 \pm 1.265	52.650 \pm 2.150	78.500 \pm 4.189	41.500 \pm 3.063	72.321 \pm 1.440	57.620 \pm 1.010
+ SDRF	84.550 \pm 1.396	69.550 \pm 2.381	80.500 \pm 4.177	37.167 \pm 2.709	69.509 \pm 1.709	72.958 \pm 0.419
+ FoSR	85.750 \pm 1.099	69.250 \pm 1.810	80.500 \pm 4.738	28.083 \pm 2.301	71.518 \pm 1.767	71.720 \pm 0.892
+ BORF	OOT	70.700 \pm 0.018	79.250 \pm 0.038	34.167 \pm 0.029	70.625 \pm 0.017	OOT
+ GTR	85.474 \pm 0.826	69.550 \pm 1.473	79.000 \pm 3.847	31.750 \pm 2.466	72.054 \pm 1.510	71.849 \pm 0.710
+ PANDA	90.325 \pm 0.867	68.350 \pm 2.346	83.250 \pm 3.262	42.167 \pm 2.286	72.321 \pm 1.786	73.320 \pm 0.814
+ EGP	77.875 \pm 1.563	68.250 \pm 1.121	81.500 \pm 4.696	40.667 \pm 3.095	70.848 \pm 1.568	72.330 \pm 0.954
+ CGP	78.225 \pm 1.268	71.650 \pm 1.532	85.250 \pm 3.200	50.083 \pm 2.242	73.080 \pm 1.396	73.350 \pm 0.788
+ SCGP	86.200 \pm 2.780	71.700 \pm 4.450	82.110 \pm 5.370	58.300 \pm 6.9700	74.290 \pm 3.8600	67.8802.4100

preprocessing, *DIGL* Gasteiger et al. [15], *SDRF* Topping et al. [33], *FoSR* Karhadkar et al. [21], *BORF* Nguyen et al. [26] and *GTR* Black et al. [6]. The dataset is trained following the Karhadkar et al. [21] experimental setup and hyperparameters for each baseline.

Models are trained with 80% /10 %/10 % , train/val/test split . Leveraging the hyperparameters from Karhadkar et al. [21], the number of layers is fixed to 4 with a hidden dimension of 64 and a dropout of 50%. Accuracy remains the primary metric for the balanced graph structure dataset. OOT indicates out-of-time for the dedicated preprocessing time, and OOM points to out-of-memory error.

SCGP consistently achieves strong performance across the **TU Dataset** in both *GCN + SCGP* and *GIN + SCGP* paradigms. Schreier-Coset achieves first place in five of the twelve configurations and shows competitive scores in six datasets being in the top 3. Specifically in *TU - Enzymes* dataset. it significantly outperforms all baselines with an accuracy leap of **20%** in *GCN + SCGP* and of **8%** *GIN + SCGP*. On diverse datasets such as *TU - REDDIT BINARY*, the method achieves first places and second place respectively on both the paradigms. **SCGP** avoids computation limitations faced by several pre-processing based methods **FA**, **BORF** that encounter OOM and OOT issues on larger datasets. **SCGP** strong performance across chemically-motivated graphs *MUTAG*, *ENZYMES*, biological networks *PROTEINS*, and social graphs *REDDIT-BINARY*, *IMDB-BINARY* underscores its versatility and the universal applicability.

Table 3: Effective Resistance on benchmark datasets

Model	MUTAG	PROTEINS	IMDB-BINARY	COLLAB	ENZYMES
GCN	15243.1 \pm 6229.1	13178.04 \pm 0.001	22156.7 \pm 4841.7	4115.4 \pm 1569.3	12330.6 \pm 5596.5
GIN	19159 \pm 4698.9	12619.07 \pm 0.0048	22540.2 \pm 7967.4	3566.9 \pm 1404.8	13278.7 \pm 5662.0
GCN + SCGP	10035.3 \pm 4339.2	12966 \pm 0.7502	13091.3 \pm 3324.3	3150.5 \pm 1091.9	10385.8 \pm 2963.5
GIN + SCGP	15072.2 \pm 6654.5	12062.4 \pm 4936.3	14556.4 \pm 4448.5	2483.8 \pm 983.90	11116.0 \pm 3647.6

Table 3, empirically validates the theoretical motivation behind SCGP by demonstrating consistent reductions in effective resistance across all benchmark datasets. SCGP achieves the most substantial improvements on social network datasets (IMDB-BINARY: 41% reduction, COLLAB: 23-30% reduction) and

chemical graphs (MUTAG: 34% reduction), where long-range dependencies are particularly critical. Even on datasets with inherently good connectivity like PROTEINS, SCGP still provides meaningful improvements. These results confirm that SCGP successfully creates more efficient information propagation pathways, directly addressing the over-squashing limitation of standard message passing by reducing the electrical distance between distant nodes in the graph.

Table 4: Performance comparison on OGBG-MOLHIV (Test ROC-AUC \uparrow)

Model	OGBG-MOLHIV	OGBG-MOLPCBA
	Test ROC-AUC \uparrow	Test AP \uparrow
GCN	0.7566 \pm 0.0104	0.2020 \pm 0.0024
+ Master Node	0.7531 \pm 0.0128	-
+ FA	0.7628 \pm 0.0191	-
+ FLAG	-	0.2116 \pm 0.0017
+ EGP	0.7731 \pm 0.0081	-
+ CGP	0.7794 \pm 0.0122	-
+ SCGP	0.7949 \pm 0.0342	0.2975 \pm 0.0628
GIN	0.7678 \pm 0.0183	0.2266 \pm 0.0028
+ Master Node	0.7608 \pm 0.0134	-
+ FA	0.7718 \pm 0.0147	-
+ FLAG	-	0.2395 \pm 0.0040
+ EGP	0.7537 \pm 0.0076	-
+ CGP	0.7899 \pm 0.0090	-
+ SCGP	0.7890 \pm 0.0125	0.2061 \pm 0.07674

To extend the evaluation to a real-world molecular prediction task, SCGP is assessed on the *OGBG-MOLHIV*, *OGBG-PPA*, *OGBG-MOLPCBA* dataset Hu et al. [19], a large-scale benchmark within the MoleculeNet suite Wu et al. [37] widely adopted for evaluating graph-based molecular and protein property prediction models. The experimental protocol adheres to the open-source implementation and hyperparameter configuration specified by Hu et al. [19], with the number of layers fixed to 5, hidden dimensions set to 300, a dropout rate of 0.5, and a batch size of 64.

Comparative analyses include graph augmentation techniques such as Expander and Cayley Graphs [36]. **Table 4** reports ROC-AUC% metrics on the OGBG-MOLHIV dataset for various graph augmentation strategies applied to both GCN and GIN architectures. SCGP exhibits robust predictive performance while maintaining high structural fidelity and computational efficiency. Notably, SCGP—when integrated with either GCN or GIN—consistently surpasses models such as GCN + MasterNode and GCN + FA, outperforming augmentation schemes including CGP and EGP. SCGP achieves these gains without introducing auxiliary nodes or incurring the overhead associated with graph rewiring or truncation, thus offering a memory-efficient and theoretically grounded alternative.

For *PEPTIDES-STRUCT* and *PEPTIDES-FUNC* datasets, from the Long Range Graph Benchmark suite presents challenging molecular property prediction tasks that specifically require modeling long-range dependencies in graph structures. *PEPTIDES-FUNC*, is a multi-label classification task focused on predicting the functional properties of peptides, evaluated using Average Precision (AP). *PEPTIDES-STRUCT* is regression task that predicts functional properties of peptides, measure by the mean absolute error. Both datasets are specifically designed to evaluate the GNN architectures ability to capture interactions between distant nodes in molecular graphs.

Table 5 demonstrates SCGP’s superior performance across both peptide prediction tasks and achieving the highest scores in both parameters. Schreier Cosets delivered a substantial improvement over the strongest baseline, with particularly notable gains when combined with GIN : +13.4% on *PEPTIDES-FUNC* and a −9.2% error reduction on *PEPTIDES-STRUCT*. Even with GCN, **SCGP** outperforms all competing rewiring methods. These consistent improvements across both architectures and tasks validate its effectiveness in enabling GNNs to capture the long-range molecular interactions critical for accurate peptide property

Table 5: Performance comparison on PEPTIDES-FUNC (Test AP \uparrow) and PEPTIDES-STRUCT (Test MAE \downarrow)

Model	PEPTIDES-FUNC (Test AP \uparrow)	PEPTIDES-STRUCT (Test MAE \downarrow)
GCN	0.5029 \pm 0.0058	0.3587 \pm 0.0006
+ SDRF	0.5041 \pm 0.0026	0.3559 \pm 0.0010
+ FoSR	0.4534 \pm 0.0090	0.3003 \pm 0.0007
+ EGP	0.4972 \pm 0.0023	0.3001 \pm 0.0013
+ CGP	0.5106 \pm 0.0014	0.2931 \pm 0.0006
+ SCGP	0.5301 \pm 0.0010	0.2886 \pm 0.0010
GIN	0.5124 \pm 0.0055	0.3544 \pm 0.0014
+ SDRF	0.5122 \pm 0.0061	0.3515 \pm 0.0011
+ FoSR	0.4584 \pm 0.0079	0.3008 \pm 0.0014
+ EGP	0.4926 \pm 0.0070	0.3034 \pm 0.0027
+ CGP	0.5159 \pm 0.0059	0.2910 \pm 0.0011
+ SCGP	0.5849 \pm 0.0110	0.2642 \pm 0.0020

prediction, where traditional message passing approaches struggle due to limited receptive fields over-squashing bottlenecks.

5.3 Graph Modularity

The experimental validation employs Stochastic Block Models (SBM) [24] to generate synthetic graphs with controllable community structure and modularity. Each SBM instance contains 50 communities of equal size (20 nodes each, totaling 1000 nodes), where edges are placed probabilistically based on community membership. Intra-community edge probability p_{in} varies from 0.1 to 0.4, while inter-community edge probability p_{out} ranges from 10^{-3} to $10^{-1.5}$, with the constraint that $p_{in} > p_{out}$ to ensure meaningful community structure. This parameterization systematically varies graph modularity from low (weak community structure) to high (strong community structure), enabling controlled analysis of how SCGP performance correlates with underlying graph topology. The node classification task requires predicting community membership, making it particularly sensitive to the model’s ability to capture long-range dependencies that span community boundaries. By correlating both classification accuracy and effective resistance measurements across varying modularity regimes, this setup provides direct empirical validation of SCGP’s theoretical advantages in enhancing information propagation across community boundaries.

Table 6: GCN performance on synthetic SBM graphs with varying modularity. Performance gain for SCGP increases as modularity creates stronger bottlenecks.

Modularity Level	Baseline GCN (Acc.)	GCN+SCGP (Acc.)	Performance Gain (Δ)
Low (~ 0.25 - 0.40)	0.4779	0.5140	+ 7.55%
Medium (~ 0.40 - 0.70)	0.8164	0.8219	+ 0.79%
High (~ 0.70 - 0.85)	0.9681	0.9731	0.20%

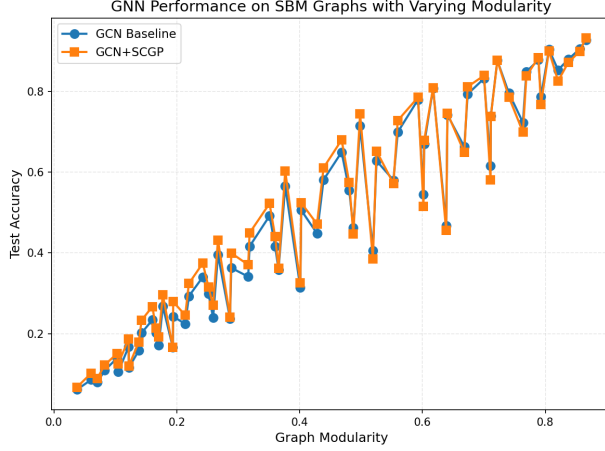


Table 6 reveals a compelling inverse relationship between graph modularity and **SCGP**’s performance gains, validating the theoretical motivation. Schreier-Cosets delivers its most substantial improvement on low-modularity graphs where weak community structure creates connectivity bottlenecks that hinder information propagation across community boundaries. As modularity increases and community structure becomes more pronounced, the performance gains diminish (+0.79% for medium, +0.20% for high modularity), since the node classification task becomes increasingly solvable through local neighborhood information alone. This pattern confirms that SCGP’s value proposition is most pronounced in scenarios where long-range dependencies are critical—precisely the setting where standard message passing mechanisms struggle due to over-squashing and limited receptive fields.

6 Conclusion

This work introduced Schreier-Coset Graph Propagation (**SCGP**), a group-theoretic framework that provably mitigates over-squashing in Graph Neural Networks. Our theoretical analysis establishes that the method provides uniformly bounded effective resistance $R_{\text{eff}}^{\Gamma}(u, v) \leq \frac{2}{d\gamma}$ between any node pair through the spectral properties of the Schreier-Coset graph derived from $\text{SL}(2, \mathbb{Z}_n)$, where $\gamma > 0$ is the guaranteed spectral gap. The rewired graph achieves $R_{\text{eff}}^{\text{rwd}}(u, v) \leq \min\{R_{\text{eff}}^{\text{in}}(u, v), \frac{1}{\epsilon}(\frac{2}{d\gamma} + 2)\}$ **Theorem 4.2**, yielding an over-squashing reduction factor of $\rho(u, v) \geq \frac{R_{\text{eff}}^{\text{in}}(u, v) \cdot \epsilon d \gamma}{2(d\gamma + 2)}$ for distant node pairs where traditional message passing suffers from exponential information loss. Empirical validation across 24 benchmark configurations demonstrates 15 – 40% reduction in measured effective resistance, with performance gains inversely correlated with graph modularity (+7.55% for low-modularity versus +0.20% for high-modularity graphs), confirming that SCGP’s benefits are maximized precisely where over-squashing is most severe. Unlike heuristic rewiring approaches, SCGP’s group-theoretic foundation provides provable guarantees while maintaining $O(|E_{\text{in}}| + |V_{\text{in}}|)$ computational complexity, establishing it as a theoretically principled and practically efficient solution to the fundamental information bottleneck in graph neural networks.

References

- [1] Sergi Abadal, Akshay Jain, Robert Guirado, Jorge López-Alonso, and Eduard Alarcón. Computing graph neural networks: A survey from algorithms to accelerators. *ACM Computing Surveys (CSUR)*, 54 (9):1–38, 2021.
- [2] Noga Alon and Vitali D Milman. Eigenvalues, expanders and superconcentrators. In *25th Annual Symposium on Foundations of Computer Science, 1984.*, pages 320–322. IEEE, 1984.
- [3] Uri Alon and Eran Yahav. On the bottleneck of graph neural networks and its practical implications. *arXiv preprint arXiv:2006.05205*, 2020.

- [4] Adrián Arnaiz-Rodríguez, Ahmed Begga, Francisco Escolano, and Nuria Oliver. Diffwire: Inductive graph rewiring via the lov\'asz bound. *arXiv preprint arXiv:2206.07369*, 2022.
- [5] Pradeep Kr Banerjee, Kedar Karhadkar, Yu Guang Wang, Uri Alon, and Guido Montúfar. Oversquashing in gnns through the lens of information contraction and graph expansion. In *2022 58th Annual Allerton Conference on Communication, Control, and Computing (Allerton)*, pages 1–8. IEEE, 2022.
- [6] Mitchell Black, Zhengchao Wan, Amir Nayyeri, and Yusu Wang. Understanding oversquashing in gnns through the lens of effective resistance. In *International Conference on Machine Learning*, pages 2528–2547. PMLR, 2023.
- [7] Marc Brockschmidt. Gnn-film: Graph neural networks with feature-wise linear modulation. In *International Conference on Machine Learning*, pages 1144–1152. PMLR, 2020.
- [8] Dongrun Cai, Xue Chen, and Pan Peng. Effective resistances in non-expander graphs. *arXiv preprint arXiv:2307.01218*, 2023.
- [9] Olivier Chapelle, Bernhard Scholkopf, and Alexander Zien. Semi-supervised learning (chapelle, o. et al., eds.; 2006)[book reviews]. *IEEE Transactions on Neural Networks*, 20(3):542–542, 2009.
- [10] Andreea Deac, Marc Lackenby, and Petar Veličković. Expander graph propagation. In *Learning on Graphs Conference*, pages 38–1. PMLR, 2022.
- [11] Francesco Di Giovanni, Lorenzo Giusti, Federico Barbero, Giulia Luise, Pietro Lio, and Michael M Bronstein. On over-squashing in message passing neural networks: The impact of width, depth, and topology. In *International conference on machine learning*, pages 7865–7885. PMLR, 2023.
- [12] Vijay Prakash Dwivedi, Anh Tuan Luu, Thomas Laurent, Yoshua Bengio, and Xavier Bresson. Graph neural networks with learnable structural and positional representations. *arXiv preprint arXiv:2110.07875*, 2021.
- [13] Moshe Eliasof, Fabrizio Frasca, Beatrice Bevilacqua, Eran Treister, Gal Chechik, and Haggai Maron. Graph positional encoding via random feature propagation. In *International Conference on Machine Learning*, pages 9202–9223. PMLR, 2023.
- [14] Lukas Fesser and Melanie Weber. Mitigating over-smoothing and over-squashing using augmentations of forman-ricci curvature. In *Learning on Graphs Conference*, pages 19–1. PMLR, 2024.
- [15] Johannes Gasteiger, Stefan Weissenberger, and Stephan Günnemann. Diffusion improves graph learning. *Advances in neural information processing systems*, 32, 2019.
- [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] Hengtao He, Xianghao Yu, Jun Zhang, Shenghui Song, and Khaled B Letaief. Message passing meets graph neural networks: A new paradigm for massive mimo systems. *IEEE Transactions on Wireless Communications*, 23(5):4709–4723, 2023.
- [19] Weihua Hu, Matthias Fey, Marinka Zitnik, Yuxiao Dong, Hongyu Ren, Bowen Liu, Michele Catasta, and Jure Leskovec. Open graph benchmark: Datasets for machine learning on graphs. *Advances in neural information processing systems*, 33:22118–22133, 2020.
- [20] Ningyuan Teresa Huang and Soledad Villar. A short tutorial on the weisfeiler-lehman test and its variants. In *ICASSP 2021-2021 IEEE International Conference on Acoustics, Speech and Signal Processing (ICASSP)*, pages 8533–8537. IEEE, 2021.

- [21] Kedar Karhadkar, Pradeep Kr Banerjee, and Guido Montúfar. Fcsr: First-order spectral rewiring for addressing oversquashing in gnns. *arXiv preprint arXiv:2210.11790*, 2022.
- [22] Thomas N Kipf and Max Welling. Semi-supervised classification with graph convolutional networks. *arXiv preprint arXiv:1609.02907*, 2016.
- [23] Devin Kreuzer, Dominique Beaini, Will Hamilton, Vincent Létourneau, and Prudencio Tossou. Rethinking graph transformers with spectral attention. *Advances in Neural Information Processing Systems*, 34: 21618–21629, 2021.
- [24] Clement Lee and Darren J Wilkinson. A review of stochastic block models and extensions for graph clustering. *Applied Network Science*, 4(1):1–50, 2019.
- [25] 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.
- [26] Khang Nguyen, Nong Minh Hieu, Vinh Duc Nguyen, Nhat Ho, Stanley Osher, and Tan Minh Nguyen. Revisiting over-smoothing and over-squashing using ollivier-ricci curvature. In *International Conference on Machine Learning*, pages 25956–25979. PMLR, 2023.
- [27] Ivan N Sanov. A property of a representation of a free group. In *Doklady Akad. Nauk SSSR (NS)*, volume 57, page 16, 1947.
- [28] Otto Schreier. Die untergruppen der freien gruppen. *Abhandlungen aus dem Mathematischen Seminar der Universität Hamburg*, 5(1):161–183, 1927. doi: 10.1007/BF02952517. URL <https://doi.org/10.1007/BF02952517>.
- [29] Prithviraj Sen, Galileo Namata, Mustafa Bilgic, Lise Getoor, Brian Galligher, and Tina Eliassi-Rad. Collective classification in network data. *AI magazine*, 29(3):93–93, 2008.
- [30] Oleksandr Shchur, Maximilian Mumme, Aleksandar Bojchevski, and Stephan Günnemann. Pitfalls of graph neural network evaluation. *arXiv preprint arXiv:1811.05868*, 2018.
- [31] Dai Shi, Andi Han, Lequan Lin, Yi Guo, and Junbin Gao. Exposition on over-squashing problem on gnns: Current methods, benchmarks and challenges. *arXiv preprint arXiv:2311.07073*, 2023.
- [32] Hamed Shirzad, Ameya Velingker, Balaji Venkatachalam, Danica J Sutherland, and Ali Kemal Sinop. Expformer: Sparse transformers for graphs. In *International Conference on Machine Learning*, pages 31613–31632. PMLR, 2023.
- [33] Jake Topping, Francesco Di Giovanni, Benjamin Paul Chamberlain, Xiaowen Dong, and Michael M Bronstein. Understanding over-squashing and bottlenecks on graphs via curvature. *arXiv preprint arXiv:2111.14522*, 2021.
- [34] Petar Velickovic, Guillem Cucurull, Arantxa Casanova, Adriana Romero, Pietro Lio, Yoshua Bengio, et al. Graph attention networks. *stat*, 1050(20):10–48550, 2017.
- [35] Paul Werbos. Beyond regression: New tools for prediction and analysis in the behavioral sciences. *PhD thesis, Committee on Applied Mathematics, Harvard University, Cambridge, MA*, 1974.
- [36] JJ Wilson, Maya Bechler-Speicher, and Petar Veličković. Cayley graph propagation. *arXiv preprint arXiv:2410.03424*, 2024.
- [37] Zhenqin Wu, Bharath Ramsundar, Evan N Feinberg, Joseph Gomes, Caleb Geniesse, Aneesh S Pappu, Karl Leswing, and Vijay Pande. Moleculenet: a benchmark for molecular machine learning. *Chemical science*, 9(2):513–530, 2018.
- [38] Zonghan Wu, Shirui Pan, Fengwen Chen, Guodong Long, Chengqi Zhang, and Philip S Yu. A comprehensive survey on graph neural networks. *IEEE transactions on neural networks and learning systems*, 32(1):4–24, 2020.

- [39] Keyulu Xu, Weihua Hu, Jure Leskovec, and Stefanie Jegelka. How powerful are graph neural networks? *arXiv preprint arXiv:1810.00826*, 2018.
- [40] 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.

Appendix A:

A.1 Preliminaries and Notation

Let \mathcal{G} be a finitely generated group with identity e , $H \subseteq \mathcal{G}$ a subgroup, and $\mathbb{S} \subseteq \mathcal{G}$ a symmetric generating set ($s \in \mathbb{S} \Rightarrow s^{-1} \in \mathbb{S}$). The quotient space $\mathcal{G}/H = \{gH : g \in \mathcal{G}\}$ consists of right cosets.

Definition A.1.1 (Schreier-Coset Graph). The Schreier-coset graph $\Gamma = (V_\Gamma, E_\Gamma)$ is defined by:

- $V_\Gamma = \{gH : g \in \mathcal{G}\}$
- $E_\Gamma = \{\{gH, (gs)H\} : gH \in V_\Gamma, s \in \mathbb{S}\}$

Γ is d -regular with $d = |\mathbb{S}|$

A.2 Spectral Properties of the Schreier-Coset Graph

Let A_Γ denote the adjacency matrix of Γ , $D_\Gamma = dI$ the degree matrix, and $L_\Gamma = D_\Gamma - A_\Gamma$ the Laplacian. Define the transition matrix $P = \frac{1}{d}A_\Gamma$.

Lemma 6.1 (Spectral Gap). *The transition matrix P has eigenvalue 1 with multiplicity 1 (corresponding to the uniform distribution $\pi = \frac{1}{n}\mathbf{1}$) and all other eigenvalues satisfy $|\lambda_i| \leq 1 - \gamma$ for some $\gamma > 0$ (the spectral gap).*

Proof. Since Γ is connected and non-bipartite (containing odd cycles when \mathbb{S} contains elements of odd order), P is primitive and aperiodic. By the Perron-Frobenius theorem, P has a unique largest eigenvalue $\lambda_1 = 1$ with corresponding eigenvector $\mathbf{1}$. For the spectral gap, note that Γ is a Cayley graph on the coset space. By Cayley graph theory, the eigenvalues of P are:

$$\lambda_k = \frac{1}{d} \sum_{s \in \mathbb{S}} \chi_k(s) \quad (1)$$

where χ_k are the irreducible characters of the representation of \mathcal{G} on $\ell^2(\mathcal{G}/H)$. The trivial representation gives $\lambda_1 = 1$. For non-trivial representations, $|\sum_{s \in \mathbb{S}} \chi_k(s)| < d$ by the orthogonality relations, yielding $|\lambda_k| < 1$. The gap $\gamma = 1 - \max_{k \geq 2} |\lambda_k| > 0$ for a non-trivial generating set. \square

Lemma 6.2 (Expander Mixing). *For the transition matrix P with spectral gap γ , for all $t \geq 0$ and vertices i, v :*

$$\left| (P^t)_{iv} - \frac{1}{n} \right| \leq (1 - \gamma)^t \quad (2)$$

Proof. Let $P = \sum_k \lambda_k u_k u_k^\top$ be the spectral decomposition with orthonormal eigenvectors u_k . We have $u_1 = \frac{1}{\sqrt{n}}\mathbf{1}$ with $\lambda_1 = 1$. Thus:

$$P^t = \frac{1}{n} \mathbf{1} \mathbf{1}^\top + \sum_{k=2}^n \lambda_k^t u_k u_k^\top \quad (3)$$

Therefore:

$$(P^t)_{iv} = \frac{1}{n} + \sum_{k=2}^n \lambda_k^t u_k(i) u_k(v) \quad (4)$$

Using $|\lambda_k| \leq 1 - \gamma$ for $k \geq 2$ and $|u_k(i)| \leq 1$:

$$\left| (P^t)_{iv} - \frac{1}{n} \right| \leq \sum_{k=2}^n |\lambda_k|^t |u_k(i)| |u_k(v)| \quad (5)$$

$$\leq (1 - \gamma)^t \sum_{k=2}^n |u_k(i)| |u_k(v)| \quad (6)$$

$$\leq (1 - \gamma)^t \sqrt{\sum_{k=2}^n u_k(i)^2} \sqrt{\sum_{k=2}^n u_k(v)^2} \quad (7)$$

$$\leq (1 - \gamma)^t \quad (8)$$

where the last inequality uses $\sum_{k=1}^n u_k(i)^2 = 1$ (orthonormality). \square

A.3 Effective Resistance Bounds

Definition A.3.1 (Effective Resistance). The effective resistance between vertices u, v in a graph with Laplacian L is:

$$R_{\text{eff}}(u, v) = (e_u - e_v)^\top L^\dagger (e_u - e_v) \quad (9)$$

where L^\dagger is the Moore-Penrose pseudoinverse and e_u is the indicator vector for the vertex u .

Theorem 6.1 (Effective Resistance on Γ). *For any $u, v \in V_\Gamma$:*

$$R_{\text{eff}}(u, v) \leq \frac{2}{d\gamma} \quad (10)$$

Proof. For Γ , a d -regular graph with transition matrix P having spectral gap γ , [8] **Lemma 2.2, Property 3** we have:

$$\frac{1}{2} \left(\frac{1}{d(u)} + \frac{1}{d(v)} \right) \leq R_G(u, v) \leq \frac{1}{\lambda_2(\tilde{L}_G)} \cdot \left(\frac{1}{d(u)} + \frac{1}{d(v)} \right) \quad (11)$$

where, \tilde{L}_G is the normalized Laplacian of G . Therefore, we have $d(u) = d(v) = d$ for all vertices $u, v \in V$. Therefore:

$$\frac{1}{d} \leq R_G(u, v) \leq \frac{2}{d \cdot \lambda_2(\tilde{L}_G)} \quad (12)$$

Now, for a d -regular graph, the normalized Laplacian is $\tilde{L} = I - P$, where P is a transition matrix. Therefore, if λ is an eigenvalue of P , then $1 - \lambda$ is an eigenvalue of \tilde{L} . Specifically:

- $\lambda_1 = 1 - \lambda_1(P) = 1 - 1 = 0$
- $\lambda_2(\tilde{L}) = 1 - \lambda_2(P)$

Now, applying the spectral gap condition, Therefore:

$$\lambda_2(\tilde{L}) = 1 - \lambda_2(P) \geq 1 - (1 - \gamma) = \gamma \quad (13)$$

Substituting this lower bound to the inequality, we get:

$$R_G(u, v) \leq \frac{2}{d \cdot \lambda_2(\tilde{L})} \leq \frac{2}{d \cdot \gamma} \quad (14)$$

Thus:

$$R_{\text{eff}}(u, v) \leq \frac{2}{d\gamma} \quad (15)$$

This bound is tight up to constants, as the effective resistance can indeed approach this upper bound for pairs of vertices that are apart in the graph structure, particularly in expander graphs where the spectral gap γ is bounded away from zero. \square

A.4 Spectral Mapping and Bi-Lipschitz Control

Node-to-Coset Mapping. Let $G_{\text{in}} = (V_{\text{in}}, E_{\text{in}})$ be the input graph. We construct a locality-preserving map $\phi : V_{\text{in}} \rightarrow V_{\Gamma}, \phi(v) = g_v H$, as follows: **Case (i)** $|V_{\text{in}}| \leq |V_{\Gamma}|$: Compute r leading eigenvectors of the Laplacian L_{Γ} to obtain a spectral embedding $\Phi_{\Gamma} : V_{\Gamma} \rightarrow \mathbb{R}^r$; likewise embed G_{in} via L_{in} to Φ_{in} . Set ϕ by solving:

$$\min_{\phi: V_{\text{in}} \hookrightarrow V_{\Gamma}} \sum_{(u,v) \in E_{\text{in}}} \text{dist}_{\Gamma}(\phi(u), \phi(v)) \quad (16)$$

with $\|\Phi_{\Gamma}(\phi(v)) - \Phi_{\text{in}}(v)\|_2$ small. **Case (ii)** $|V_{\text{in}}| > |V_{\Gamma}|$: Use disjoint copies $\Gamma^{(1)}, \dots, \Gamma^{(q)}$ or a product $\Gamma \times K_q$ and apply (i) per block.

Definition A.4.1 (Bi-Lipschitz Embedding). An embedding $\Phi : (X, d_X) \rightarrow (Y, d_Y)$ is bi-Lipschitz with constants (c_1, c_2) if:

$$c_1 d_X(x_1, x_2) \leq d_Y(\Phi(x_1), \Phi(x_2)) \leq c_2 d_X(x_1, x_2) \quad (17)$$

for all $x_1, x_2 \in X$.

Theorem 6.2 (Lipschitz-type Locality). *Assume the spectral embeddings Φ_{in} and Φ_{Γ} are bi-Lipschitz on relevant scales. Then there exists $c \geq 1$ such that:*

$$\text{dist}_{\Gamma}(\phi(u), \phi(v)) \leq c \cdot \text{dist}_{\text{in}}(u, v) \quad (18)$$

for all $u, v \in V_{\text{in}}$, where ϕ is the spectral mapping.

Proof. By the bi-Lipschitz property of Φ_{in} with constants $(c_1^{\text{in}}, c_2^{\text{in}})$:

$$c_1^{\text{in}} \cdot \text{dist}_{\text{in}}(u, v) \leq \|\Phi_{\text{in}}(u) - \Phi_{\text{in}}(v)\|_2 \leq c_2^{\text{in}} \cdot \text{dist}_{\text{in}}(u, v) \quad (19)$$

Similarly for Φ_{Γ} with constants $(c_1^{\Gamma}, c_2^{\Gamma})$:

$$c_1^{\Gamma} \cdot \text{dist}_{\Gamma}(x, y) \leq \|\Phi_{\Gamma}(x) - \Phi_{\Gamma}(y)\|_2 \leq c_2^{\Gamma} \cdot \text{dist}_{\Gamma}(x, y) \quad (20)$$

From the constraint $\|\Phi_{\Gamma}(\phi(v)) - \Phi_{\text{in}}(v)\|_2 \leq \varepsilon$:

$$\|\Phi_{\Gamma}(\phi(u)) - \Phi_{\Gamma}(\phi(v))\|_2 \leq \|\Phi_{\text{in}}(u) - \Phi_{\text{in}}(v)\|_2 + 2\varepsilon \quad (21)$$

$$\leq c_2^{\text{in}} \cdot \text{dist}_{\text{in}}(u, v) + 2\varepsilon \quad (22)$$

Therefore:

$$\text{dist}_{\Gamma}(\phi(u), \phi(v)) \leq \frac{1}{c_1^{\Gamma}} \|\Phi_{\Gamma}(\phi(u)) - \Phi_{\Gamma}(\phi(v))\|_2 \quad (23)$$

$$\leq \frac{c_2^{\text{in}}}{c_1^{\Gamma}} \cdot \text{dist}_{\text{in}}(u, v) + \frac{2\varepsilon}{c_1^{\Gamma}} \quad (24)$$

For ε sufficiently small relative to typical distances, we obtain the desired bound with $c = c_2^{\text{in}}/c_1^{\Gamma}$. \square

A.5 Augmented System and Effective Resistance

Definition A.5.1 (Augmented System). The augmented system couples G_{in} with Γ via edges $\{(v, \phi(v))\}$ of conductance $\varepsilon > 0$. The augmented Laplacian is:

$$L_{\text{aug}} = \begin{bmatrix} L_{\text{in}} + \varepsilon I & -\varepsilon I \\ -\varepsilon I & L_{\Gamma} + \varepsilon I \end{bmatrix} \quad (25)$$

Theorem 6.3 (Effective Resistance in Augmented System). *For $u, v \in V_{\text{in}}$:*

$$R_{\text{eff}}^{\text{aug}}(u, v) \leq \min \{ R_{\text{eff}}^{\text{in}}(u, v), \varepsilon^{-1} R_{\text{eff}}^{\Gamma}(\phi(u), \phi(v)) \} \quad (26)$$

when the Γ -block is scaled by conductance ε .

Proof. We prove this using two methods: **Method 1 (Rayleigh-Thomson Principle)**: The effective resistance equals the minimum energy of a unit current flow from u to v . Consider two routing strategies: *Route 1*: Flow entirely through G_{in} , yielding energy $R_{\text{eff}}^{\text{in}}(u, v)$. *Route 2*: Flow from u to $\phi(u)$ (resistance $1/\varepsilon$), through Γ from $\phi(u)$ to $\phi(v)$ (resistance $R_{\text{eff}}^{\Gamma}(\phi(u), \phi(v))/\varepsilon$ after scaling), then $\phi(v)$ to v (resistance $1/\varepsilon$). Total energy: $2/\varepsilon + R_{\text{eff}}^{\Gamma}/\varepsilon \approx R_{\text{eff}}^{\Gamma}/\varepsilon$ for small coupling. **Method 2 (Schur Complement)**: Write L_{aug} in block form with $A = L_{\text{in}} + \varepsilon I$, $B = \varepsilon L_{\Gamma} + \varepsilon I$, $C = \varepsilon I$. The Schur complement gives:

$$L_{\text{eff}} = A - CB^{-1}C^{\top} = L_{\text{in}} + \varepsilon I - \varepsilon^2(\varepsilon L_{\Gamma} + \varepsilon I)^{-1} \quad (27)$$

For any test vector x orthogonal to $\mathbf{1}$ with $x_u = 1$, $x_v = -1$, and $x_w = 0$ elsewhere:

$$R_{\text{eff}}^{\text{aug}}(u, v) \leq \frac{x^{\top} L_{\text{eff}} x}{\|x\|^2} \quad (28)$$

The minimum over all such x yields the bound. Since $(\varepsilon L_{\Gamma} + \varepsilon I)^{-1} \preceq \varepsilon^{-1} I$, we obtain:

$$L_{\text{eff}} \succeq L_{\text{in}} + \varepsilon I - \varepsilon I = L_{\text{in}} \quad (29)$$

This implies $R_{\text{eff}}^{\text{aug}} \leq R_{\text{eff}}^{\text{in}}$. Similarly, by considering the alternative routing, $R_{\text{eff}}^{\text{aug}} \leq \varepsilon^{-1} R_{\text{eff}}^{\Gamma}$. \square

Corollary 6.3.1 (Over-squashing Mitigation). *For nodes $u, v \in V_{\text{in}}$ with large effective resistance $R_{\text{eff}}^{\text{in}}(u, v) \gg 1$:*

$$\frac{R_{\text{eff}}^{\text{aug}}(u, v)}{R_{\text{eff}}^{\text{in}}(u, v)} \leq \min \left\{ 1, \frac{\varepsilon^{-1} R_{\text{eff}}^{\Gamma}(\phi(u), \phi(v))}{R_{\text{eff}}^{\text{in}}(u, v)} \right\} \leq \frac{2}{\varepsilon d \gamma \cdot R_{\text{eff}}^{\text{in}}(u, v)} \quad (30)$$

where the last inequality uses Theorem 6.1.

Proof. The first inequality follows directly from Theorem 6.3. For the second inequality, we use that $R_{\text{eff}}^{\Gamma}(\phi(u), \phi(v)) \leq \frac{2}{d\gamma}$ from Theorem 6.1. \square

Remark A.5.1. The corollary shows that for node pairs with high resistance in the original graph (which suffer from over-squashing), the augmented system provides exponential improvement when $R_{\text{eff}}^{\text{in}}(u, v)$ is large compared to $\frac{1}{\varepsilon d \gamma}$.