RELWIRE: Metric Based Graph Rewiring

Abstract

Oversquashing is a major hurdle to the application of geometric deep learning and graph neural networks to real applications. Recent work has found connections between oversquashing and commute times, effective resistance, and the eigengap (or spectral gap) of the underlying graph. Graph rewiring is the most promising technique to alleviate this issue. Some prior work adds edges locally to highly negatively curved subgraphs. These local changes, however, have a small effect on global statistics such as commute times and the eigengap. Other prior work uses the spectrum of the graph Laplacian to target rewiring to increase the eigengap. These approaches, however, make large structural and topological changes to the underlying graph. We use ideas from geometric group theory to present RELWIRE, a rewiring technique based on the geometry of the graph. We derive topological connections for RELWIRE. We then rewire different real world molecule datasets and show that RELWIRE is Pareto optimal: it has the best balance between improvement in eigengap and commute times and minimizing changes in the topology of the underlying graph.

1 Introduction

Graph neural networks (GNNs) are a promising generalization of (deep) neural networks based upon the premise that many real world data sets exhibit graphical structure. That is, data points are related to one another in complex ways that are best captured by relations on a graph, with vertices being the data points and edges the relations between those points. Hence, GNNs are methods for aggregating information across the relation graph and then propagating those updates. All of these methods, however, seem to suffer from two structural problems: oversquashing and over-smoothing.

Oversquashing has been a challenging problem to define. The problem was initially observed in [2], where the authors setup the neighbors match problem whose task is to match a target subgraph with a template subgraph. They noticed that the feature vectors cannot store enough information, a problem which they called oversquashing. However, since then oversquashing has been defined in a different manner. Influenced by [58], who defined the *influence* of a node on another as the magnitude of the relative derivative, the perspective on oversquashing has shifted. Since then a variety of papers [10, 21, 40, 54] have defined oversquashing to be the problem of having nodes having small influence on each other (i.e., small Jacobian), including theoretical connections between oversquashing and structural properties like commute time [21] and eigengaps.

As a result of these deficiencies, many recent works have introduced the notion of "rewiring" a graph, adding edges or relations amongst the data points so as to improve the performance of GNNs. These methods leverage notions from spectral graph theory (e.g., effective resistance, spectral or eigengap), discrete graph geometry (e.g., graph curvature), and random walks (via commute time). All of these methods make large structural changes to the underlying graph, some more effective than others, which are aimed at affecting one or more of the above quantities.

In this paper, we present a new graph rewiring regime by importing techniques from coarse geometry. We use the geometry of the underlying graph to define two relations between the graph's edges, one which roughly encodes local negative curvature and the other flat curvature. Our rewiring algorithm, called RELWIRE, utilizes this notion of curvature to rewire the underlying graph by targeting certain structural features while minimally affecting the topology of the underlying graph. We develop a framework for analyzing this balancing act of effective rewiring with minimal topological disturbance.

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Contributions. The main contributions of this paper are as follows:

- We define a new topological distance called the rank distance that can be used to measure the structural changes to a graph after rewiring. (Section 3)
- We present a new method for rewiring graphs RELWIRE. Our method uses new ideas and concepts that have not been applied to the field of geometric deep learning before. Specifically, it introduces a global notion of curvature. (Section 4)
- We present topological differences between RELWIRE and prior rewiring techniques. (Section 5)
- We extensively test on real data to show that RELWIRE is Pareto optimal for the graph statistics. That is, it performs the best at improving eigengap and commute times, while simultaneously preserving the graph topology. We also show that it helps for graph regression. (Section 6)

Other Related Work: In this paper we will compare against transductive methods. But there also exist inductive methods for graph rewiring such as [3, 18, 27] and other methods such as [5, 11, 39]. The use of other geometries, especially Hyperbolic geometries, has been widely considered; embeddings [32, 41, 42, 49, 51], and graph neural networks [15, 16, 33, 60]. Finally, other people have also looked at mixed curvature geometries such as [17, 26, 34, 35, 52, 59, 61].

2 Background and Problem Setup

Oversquashing. Prior work has shown that the norm of Jacobian (which controls oversquashing) can be bounded by a variety of graph properties, deriving bounds of the following form:

$$\left\| \frac{\partial x_i^{(\ell)}}{\partial x_j^{(0)}} \right\| \leq c_{act}^{\ell} T_{ij}^{\ell}.$$

Here $x_i^{(\ell)}$ is the feature at the i^{th} node after ℓ layers of message passing. c_{act} is a constant from the architecture of the neural network and T_{ij} is a topological statistic of the graph. Specifically T can be dependent on commute times [21], the curvature [40, 54], or the effective resistance of the graph [10], which is closely related to commute time, see Appendix A.6. Following this in recent work, [20] looked at the Hessian instead of the Jacobian and again showed that it be bounded using the commute times. Importantly, prior work shows that these quantities can be improved via graph rewiring.

In this paper, we are interested in the problem of graph rewiring. That is given a graph G, we want to add k edges to the graph to improve various graph statistics mentioned above while preserving structural information.

Preserving structural information. One of the foundational principles of GNNs was that the structure of the graph had important information, and there are many tasks which illustrate this. One example of this is the NeighborsMatch problem from [2], which was the first paper to identify oversquashing. For this, the task is to identify the labeled node, whose neighbors subgraph is the exactly the same as the given query node. Hence changing the graph structure changes the answer, making structural integrity critical. Another example comes from the (real world) ZINC dataset of molecules, where the task is to predict a value that depends on the number of cycles with at least 6 atoms. Once again, changing the graph structure would change the answer.

On the other hand, if we are trying to rewire a graph to alleviate oversquashing while not caring about the graph structure, then a natural extreme conclusion might be to use the complete graph. This was explored in [29, 54] among other papers and they saw that this did not have the best performance. At the very least, this indicates that the graph structure is not irrelevant, and moreover that more fine-tuned approaches get better results. However, the process of graph rewiring changes this structure.

Hence we are interested in quantifying this change and keeping it to a minimum. To do this, we introduce two notions of distance which measure the change in relevant topological features of rewired graphs relative to the base graph; see Section 3. The use of topology to measure distances between graphs appears in [44, 47].

2.1 Graph Properties: Eigengap, commute time, and curvature.

In this section, we detail connections between oversquashing and different statistics. See Appendix A.6 for description of prior work that we compare against.

We start by setting up notation for the paper. Throughout the paper $G = (V, E)$ will refer to a graph on vertex set V with edges E. We shall have that G has n nodes and m edges. Let A denote the adjacency matrix of the graph and let D denote the degree matrix of the graph.

Definition 1 (Combinatorial Laplacian)**.** Suppose A is the adjacency matrix for a graph G and D is the degree matrix, the *Combinatorial Laplacian* is $L(G) := D - A$.

Definition 2 (Eigengap)**.** For a connected graph G, the *eigengap* or spectral gap $\lambda_2(G)$ is the second largest eigenvalue of the Combinatorial Laplacian $L(G)$.

Definition 3 (Cheeger Constant)**.** Given a graph $G = (V, E)$ a *cut* $cut(C_1, C_2)$ is a disjoint partition of the nodes V into C_1 and C_2. The *size* of a cut is $|cut(C_1, C_2)| := |\{(u, v) \in E, u \in C_1, v \in C_2\}|$. The *Cheeger constant* h_G is defined as $\min_{(C_1,C_2)} \frac{|cut(C_1,C_2)|}{|C_1||C_2|}$.

Thus, we see that the Cheeger constant tells how connected the graph is, giving it a clear relation to oversquashing. However, the Cheeger constant is difficult to compute, but can be well approximated by the eigengap.

$$\frac{\lambda_2(G)}{2} \leq h_G \leq \sqrt{2\lambda_2(G)} \text{ and } 2h_G \geq \lambda_2(G) \geq \frac{h_G^2}{2}.$$

Thus, having a large $\lambda_2(G)$ results in a large Cheeger constant. Thus, the graph is better connected.

Definition 4 (Commute Times)**.** Let A be the adjacency matrix of a graph G. Consider a random walk on G with transition probabilities given by $P = D^{-1}A$.

1. The *hitting time* $H(i, j)$ is the expected time for a random walk starting at node i to hit node j.
2. The *commute time* is $CT(i, j) = H(i, j) + H(j, i)$.

As discussed in [54], the Ricci curvature is a natural method for measuring information dispersion on a manifold. For instance, two geodesics starting nearby with the same velocity will converge on a sphere (positive curvature), will remain parallel in Euclidean space (zero curvature), or will diverge in Hyperbolic space (negative curvature). This divergence in Hyperbolic space can be used to show that Hyperbolic space is good for representing hierarchical information [51].

Similar to the Ricci curvature on manifolds, Ricci curvature has also been defined for graphs [43] and has been used for rewiring [54]. Recently it has been shown by [56] that the discrete notion of the Ollivier-Ricci curvature defined on metric graphs (i.e. k-nearest neighbor graphs of data on a manifold $\mathcal{M}$) converges pointwise to the Ricci curvature on the manifold $\mathcal{M}$. Thus the information divergence interpretation of the curvature applies to the graphs as well, indicating that graphs with negative curvature are detrimental to oversquashing. This has been formalized by recent work such as [40, Theorem 4.5], where the authors show that negative curvature results in sharply decaying importance of distant nodes. Thus, increasing the curvature of the graphs helps address oversquashing.

3 Capturing topological distortion: Distances from persistent homology

In this paper, we consider two notions of distances between graphs using topological information. The first is based on comparing 1-dimensional information, which is already quite powerful in the context of graphs. The second is based on techniques from topological data analysis, which takes into account higher dimensional features of the graphs. This latter machinery is called *persistence homology*, as it attempts to capture "persistent" homological features as one takes larger samples of the space. The following is a minimal treatment of persistent homology, see [1, 48] for more details.

These topological calculations involve integral *homology groups*. The integral d^{th}*-homology group* of a topological space X, denoted $H_d(X; \mathbb{Z})$, is an abelian group which encodes certain d-dimensional topological features up to a natural topological equivalence. The *rank* of $H_d(X; \mathbb{Z})$—namely the number of its $\mathbb{Z}$-factors—encodes the number of d-dimensional "holes", and is called the d^{th} Betti number β_d. Notably, in dimensions 0 and 1, these numbers have concrete meanings: β_0 encodes the number of connected components of X, and β_1 encodes the number of loops on X (up to homotopy).

In what follows, we will want to consider the homology of simplicial complexes (Definition 14) obtained by iteratively adding higher dimensional simplices, with our starting point being a graph.

Our next goal is to define our two distances. For this, we need a notion of a sequence of simplicial complexes, called a *filtration*, as well as a notion of how topological features can appear and vanish along the filtration, which is called *persistence*; see [6, 30, 31] for more details.

Definition 5 (Filtration)**.** A filtration of simplicial complexes is a collections of nested simplicial complexes $G_0 \subset G_1 \subset \cdots$. The complex G_k is called the k^{th} level of the filtration.

Definition 6 (Persistence)**.** Given a filtration $G_0 \subset G_1 \subset \cdots \subset G_k$, we can compute the homology groups for each G_i. Then for any *feature* (homology class), we can compute the first level k at which the feature appears, called the *birth* of the feature and the level at which the feature disappears, called the *death*. This collection of birth and death tuples is known as the *persistence diagram*.

In this paper, we will care about two different filtrations where the base complex is a graph. The first is a standard filtration known as the Vietoris-Rips filtration. The second is the filtration defined by the subsequent adding of edges by a graph rewiring procedure, in which every level G_k is a graph. We will use these filtrations to define distances, which the first type of distance being similar to ones used in prior work such as [28, 48].

Definition 7 (Vietoris-Rips filtration)**.** Let $X = \{x_1, \ldots, x_n\}$ be a collection of data points and d a metric on X. Then for any $r \in \mathbb{R}_+$, the *Vietoris-Rips simplicial complex* $VR_r(X)$ is defined by

$$VR_r(X) = \{[x_{i_1}, \ldots x_{i_k}] : \forall j, \ell,\ d(x_{i_j}, x_{i_\ell}) \leq r\}.$$

- We call $\{VR_r(X)\}_{r\in\mathbb{R}_+}$ the *Vietoris-Rips Filtration*.

The idea behind the Vietoris-Rips filtration is that it is a way to transform a metric space to a filtration of simplicial complexes, which in the context of a graph involves introducing higher dimensional topological features which are derived from the geometry of the graph. Using a persistence diagram, we can generalize Betti numbers to a more expressive quantity known as the Betti curve. We can use this to define a distance between persistence diagrams.

Definition 8 (Betti Curve)**.** Let P be a persistence diagram. The *Betti curve* $\beta : \mathbb{R} \to \mathbb{N}$ is a function, where $\beta(r)$ is the number of features that $b \leq r < d$, where b and d are the birth and death.

Definition 9 (Persistence Distance)**.** The *persistence distance* between two persistence diagrams is the L_2 norm of the difference between their respective Betti curves.

Definition 10 (Betti distance)**.** Given two graphs G, G', we will call the persistence distance between their respective Vietoris-Rips filtrations $\{VR_r(G)\}_{r\in\mathbb{R}_+}$ and $\{VR_r(G')\}_{r\in\mathbb{R}_+}$ the *Betti distance* between G, G'.

In practice, we will use the Betti distance to compute the higher dimensional "topological distortion" from a base graph G and some other graph G' built from G by adding edges via a rewiring process.

Our second notion of distance measures 1-dimensional topological distortion. A *graph filtration* $G_0 \subset G_1 \subset \cdots$ has G_i a simplicial graph for each i. Graph filtrations naturally arise in the iterative graph rewiring procedures considered in this paper. Since simplicial graphs have no homology beyond dimension 1 and all edges have length 1, the only relevant features of a graph filtration are loops and each birth and death happens at integer time values. Hence their Betti curves are step functions and we obtain:

Lemma 11 (Rank distance)**.** *If $G_0 \subset G_1 \subset \cdots$ and $G'_0 \subset G'_1 \subset \cdots$ are two graph filtrations, then their persistence distance equals*

$$\text{average}_i |\text{rank } H_1(G_i; \mathbb{Z}) - \text{rank } H_1(G'_i; \mathbb{Z})|.$$

- *Hence we call the persistence distance between a pair of graph filtrations the* rank distance.

Upshot of topological discussion: In this paper, we use the Betti and rank distances to measure of how much a given rewiring procedure changes the topology of the graph. *For GNNs, the structure of the base graph encodes crucial information. Hence we can use these two distances to measure how much a given graph rewiring procedure preserves the underlying graph structure.*

4 RELWIRE: relations on graphs

In this section, we detail our new algorithm, which utilized ideas imported from geometric group theory. We explain the background and motivation first, before describing our algorithm in detail.

4.1 Coarse geometry and relations on graphs

Geometric group theory is interested in the geometry of infinite groups and the metric spaces on which they act. Gromov's work on hyperbolic and CAT(0) spaces [25] introduced various coarse notions

of curvature to the area, which had transformative implications in the study of low-dimensional hyperbolic manifolds via their fundamental groups.

Hierarchical hyperbolicity [8] is an axiomatic framework for studying hybrid spaces which exhibit aspects of coarse negative, flat, and positive curvature. This hierarchical approach builds on work in several areas of low dimensional topology, including mapping class groups ([36], Teichmüller spaces ([13, 22, 46]), and hyperbolic 3-manifolds ([14, 37]). These *hierarchically hyperbolic spaces* (HHSes) are coarsely built out of hyperbolic spaces, which are combined in both negative and flat curvature ways based on various *relations* between the hyperbolic spaces. In this paper, we will apply a simplified version of this hierarchical framework to study curvature properties of graphs. In particular, we will use the geometry of a fixed graph to induce two (mutually exclusive) types of relations among its edges. In the general setting, one starts with an ambient geodesic metric space X with a finite collection of Gromov hyperbolic geodesic metric spaces $\mathcal{V}$. We note that HHSes were developed to study infinite groups where $\mathcal{V}$ is infinite, but we can and will assume $\mathcal{V}$ is finite for simplicity of this discussion. To each space $V \in \mathcal{V}$, there is an associated projection map $\pi_V : X \to V$. The guiding philosophy is that these projections behave like closest-point projections to convex subspaces, and that they collectively coarsely encode most of the geometry of X.

In our setting, the ambient space $X = G$ is a simplicial graph and this philosophy becomes quite simple: the spaces in the hierarchy are the edges, and a projection of a vertex of G to an edge E is a some collection of its endpoints. Specifically, given a vertex $v \in G^{(0)}$ and an edge E of G, the *projection* $\pi_E(v) \subset E^{(0)}$ of v to E is the endpoint of E which is closest in G to v. When both endpoints are equidistant to v, then we set $\pi_E(v) = E^{(0)}$ to be both endpoints. With these projections defined, we define our (simplified) relations.

The first relation, called *orthogonal*, encodes flat curvature. In the setting of an HHS X, when two hyperbolic spaces U, V in the hierarchy are orthogonal, the product map $\pi_U \times \pi_V : X \to U \times V$ is surjective, and there is a coarsely isometrically embedded flat subspace of X (see e.g. Subsection 5B of [7]). For instance, $\mathbb{R}^2$ is an HHS where the hyperbolic spaces are the coordinate axes (i.e., copies of $\mathbb{R}$), and the flat subspace corresponding to their product is the whole ambient space $\mathbb{R} \times \mathbb{R} = \mathbb{R}^2$.

In our graphical setting, we will say two edges E_1, E_2 are *independent* when $\pi_{E_1} \times \pi_{E_2} : G \to E_1^{(0)} \times E_2^{(0)}$ is surjective. Otherwise, we will say that E_1, E_2 are *transverse*. Roughly, this notion of transversality encodes negative curvature (see e.g. [9]).

While the connection between independence/transversality and flat/negative curvature is not exact, the connection is more than moral:

(a) 4 cycle **(b)** Cross

Figure 1: Here are two simple graphs in which: (a) all adjacent edges are independent and (b) all edges are transverse.

Lemma 12. *Let E_1, E_2 be edges of a simplicial graph G. If for E_1, E_2 we have that they*

1. *are contained in a clique subgraph of G, then E_1, E_2 are independent;*
2. *are separated by vertex v with $\pi_{E_1}(v)$ and $\pi_{E_2}(v)$ both singletons, then E_1, E_2 are transverse.*

Much more is true in practice. For instance, most edges in a given loop will be pairwise independent, while the condition in item (2) of Lemma 12 is fairly generic. More refined relations are capable of exactly encoding, e.g. that independence and being in a loop are equivalent, but these conditions are difficult to state and even slower to implement algorithmically.

Remark 13 (Global vs. local curvature)**.** As every pair of edges in a graph satisfies one of our two relations, they are both capable of capturing local and global properties of the graph. While item (2) of Lemma 12 says that independence is frequently more locally focused, transversality captures negative curvature in a fundamentally different way than existing notions of graph curvature.

4.2 RELWIRE

We present our new rewiring technique RELWIRE. The pseudocode for the method can be seen in Algorithm 1. The basic idea is to eliminate negative curvature by adding edges, so the main task is to

identify pairs of vertices which belong to the most transverse edge pairs, weighted by their distance in the graph.

We begin by determining for each pair of edges if they are independent or transverse. Then for each pair of nodes u, a, we consider all neighboring edges of the form (u, v) and (a, b) for all $v \in \mathcal{N}(u)$ and $b \in \mathcal{N}(a)$. Then we define

$$r(u,a) = d(u,a) \sum_{\substack{v\in\mathcal{N}(u)\\ b\in\mathcal{N}(a)}} \mathbb{1}\{(u,v) \not\perp (a,b)\}.$$

We then connect the k node pairs that are not adjacent in the graph that have the highest r values, where k is our rewiring parameter. That is, for a pair of nodes, we count the number of transverse edge pairs that the two nodes are in. We then weight this count by the distance between the two nodes, and connect the pairs of nodes with the highest weighted r value.

Algorithm 1 RELWIRE

function RELWIRE(G - Graph, k - number of edges added)
  Compute shortest distance $d(u, v)$ between all pairs of nodes u, v.
  Compute $T : E \times E \to \{0, 1\}$ such that $T(e_1, e_2) = 1$ if and only if $e_1 \not\perp e_2$.
  Compute $r(u,a) = d(u,a) \sum_{v\in\mathcal{N}(u)} \sum_{b\in\mathcal{N}(a)} T\big((u,v),(a,b)\big)$.
  Connect the k non-adjacent node pairs with largest r value.
  return Rewired Graph
end function

As discussed above, tranversality captures some notion of negative curvature, at both the local and global scale of the graph. Hence connecting a highly transverse distant pair morally helps remove negative curvature at a global level.

Time complexity. Let n be the number of nodes in the graph, m be the number of edges we start with, and k the number of edges we want to add. For RelWire, there are 4 steps. The first step is All Pair Shortest Path which takes $O(n^2 \log(n) + nm)$. Next is to determine independence, this can be done naively in $O(m^2 n)$ time. Specifically for each pair of edges E_1, E_2, we look at all the projections and see if the map $\pi_{E_1} \times \pi_{E_2} : G \to E_1^{(0)} \times E_2^{(0)}$ is surjective. Finally, determining which edges to add can be done in $O(k \log(m))$ time. Thus the total time complexity is $O(n^2 \log(n) + m^2 n + k \log(m))$.

Connecting RelWire to topology. By Lemma 12, one should expect that RelWire, applied to a very large graph, will identify a "maximally transverse" pair of vertices p, q which are very far apart in the graph. Many of the vertices v occurring along any geodesic between p, q will likely be separators, in the sense of item 2 of that lemma. Adding an edge between p, q then creates a number of loops containing these separators. On the other hand, one should expect any such separator v to participate in a comparable number of transverse pairs with both p, q, making it likely that RelWire will fill in the loops it creates. This philosophy is most clearly illustrated in Figure 2.

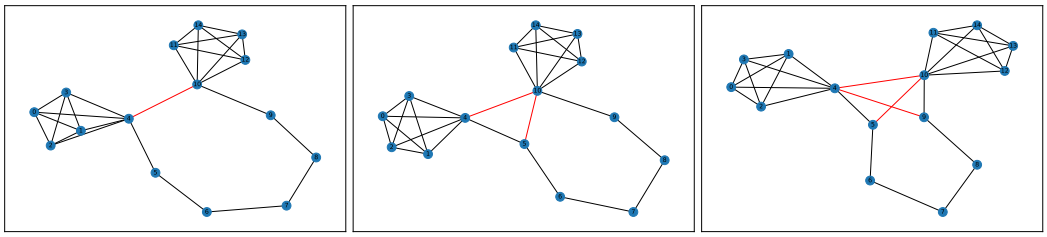
5 Preserving the topology: barbell example

In this section we explore the topological differences between RELWIRE, FOSR, GTR, and SDRF. We will do this using the standard example of a barbell graph G (Figure 3a) that has been used in prior work such as [20, 21, 29, 54]. We shall use all four methods to add between one and nine edges, and we shall see that the results are quite different. To understand the topological distortion caused by rewiring, we compute both the rank and Betti distances relative to the underlying graph.

Figure 2 shows the rewired graphs for $k = 1, 2, 3$ and Figure 3b shows the ranks for adding up to 9 edges. Here we see that RELWIRE initially introduces a loop and the rank increases to 1, while successive edges fill in that loop. On the other hand, both FOSR and GTR create a loop with each successive edge addition. Finally, it is not clear what SDRF does to the topology and the topological rank is not very stable.

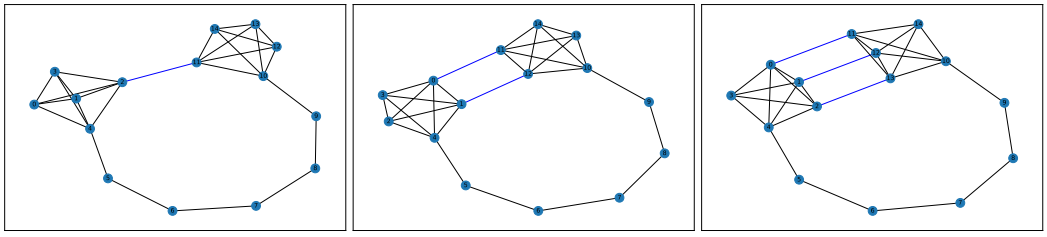
We also analyze how rewiring affects the statistics related to oversquashing, i.e. average commute times and eigengaps of the graph. These quantities, along with Betti distance to the original graph, are plotted in Figure 4. As we can see, RELWIRE, GTR, and FOSR have the best average commute times and eigengaps, whereas SDRF is ineffective. On the other hand, we see that FOSR and GTR result in large topological changes, whereas RELWIRE has relatively little effect on the topology.

6 Experiments



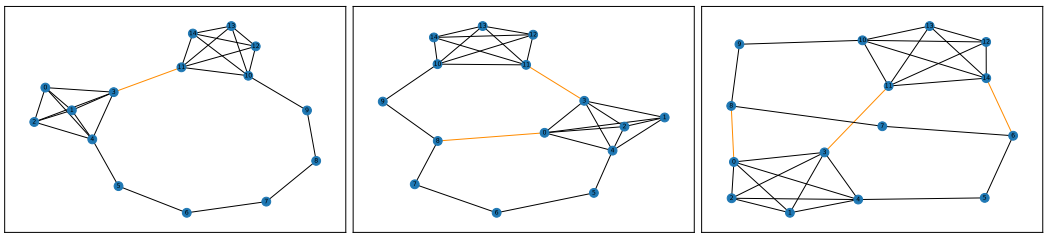
(a) $k = 1$ **(b)** $k = 2$ **(c)** $k = 3$

(d) RELWIRE rewiring of the barbell graph



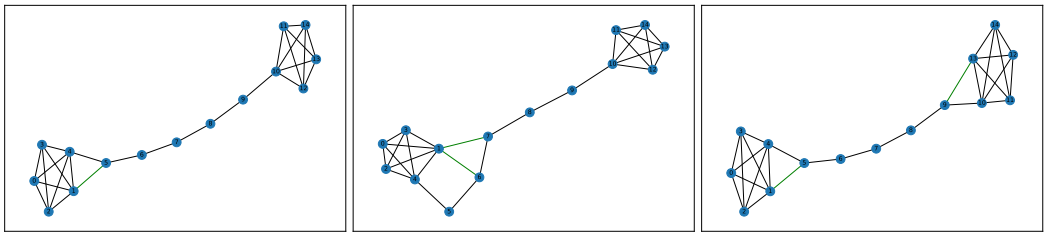
(e) $k = 1$ **(f)** $k = 2$ **(g)** $k = 3$

(h) FOSR rewiring of the barbell graph



(i) $k = 1$ **(j)** $k = 2$ **(k)** $k = 3$

(l) GTR rewiring of the barbell graph



(m) $k = 1$ **(n)** $k = 2$ **(o)** $k = 3$

(p) SDRF rewiring of the barbell graph

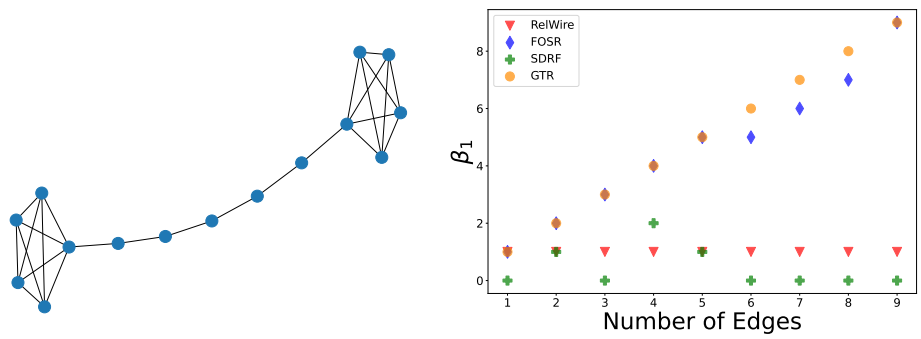
Figure 2: Rewired barbell graph.

To validate our method on real data[1], we took ten different datasets with roughly $\sim 27,000$ graphs for rewiring (see the Appendix A for more details). We rewired these datasets by adding three edges using RELWIRE, FOSR, GTR, and SDRF. We then computed the spectral gap for each of the graphs in the dataset and

Dataset	RELWIRE	FOSR	GTR	SDRF
Zinc	9.96	10.9	9.22	12.7
ESOL	6.1	6.3	5.7	7.0
BACE	13.9	15.4	12.7	17.7
Mutag	7.7	8	7.2	8.8
AIDS700nef	4.5	4.4	4.1	4.8
Alkane	4.8	4.6	4.2	5.2
Linux	3.9	3.8	3.6	4.3

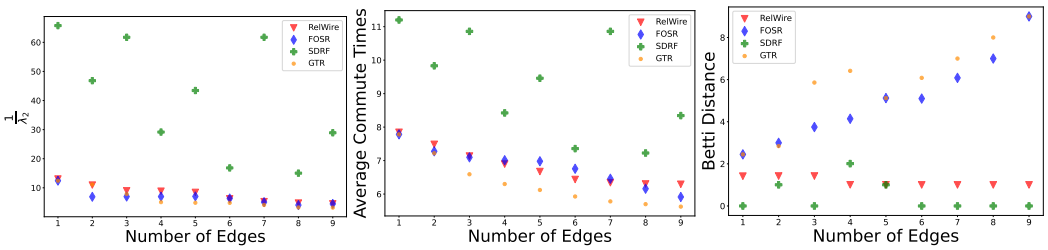
Table 1: Average commute times after rewiring.

[1]All code can be found anonymized at Github



(a) Barbell Graph **(b)** Ranks

Figure 3: (a) Barbell Graph. (b) The ranks of the first homology group of the rewired graphs.



(a) $\frac{1}{\lambda_2}$ **(b)** Average Commute Times **(c)** Betti Distance

Figure 4: Figure showing $\frac{1}{\lambda_2}$, the average commute times, as well as the Betti distance between the rewired graph and the original graph for RELWIRE, SDRF, GTR, and FOSR.

took the average spectral gap for each dataset.
Similarly, we computed the average commute times for each of the graphs and then averaged that as well. Note that for three of the datasets (Lipo, Tox21, and Enzymes) we had disconnected graphs post rewiring, hence we did not compute the commute times for these datasets. Finally, we computed the Betti and rank distances. Table 2 shows the spectral gap and the Betti distance, while Table 1 displays the commute times. The values in green are the best observed values, while those in blue are the second best.

Here we can see there is a give-and-take between the eigengap and commute times with the Betti distance. In particular, GTR greatly decreases the eigengap and commute times at the expense of transforming the topology, as measured by large Betti distance. On the other hand, SDRF relatively preserves the topology as well as the eigengap and commute times. Hence if we are to reduce oversquashing while preserving the graph, we must find a balance.

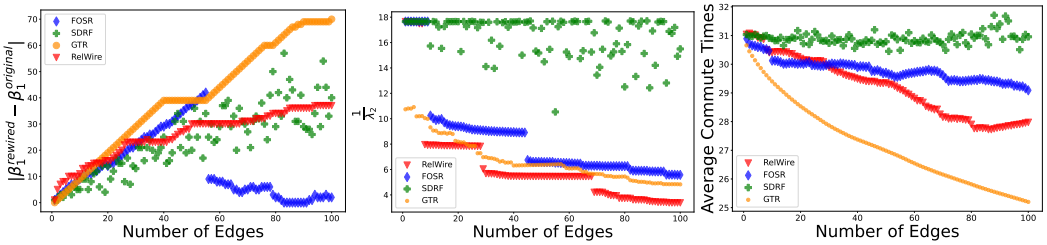
In this regard, we see that RELWIRE is Pareto optimal, in that we have the second best eigengap, commute times, and Betti distance. This can be visually seen in Figure 5, which plots λ_2^{-1} versus Betti distance for the 10 datasets from Table 2. If we consider each data point as a vector and then compute the average norm squared of the 10 vectors for each method, we see that the average for RELWIRE is 114.7, for GTR is 454.0, for FOSR is 275.8, and SDRF is 627.7. In this sense, RELWIRE has the best performance. We test the performance of our method on the downstream task of Graph Regression. The results can be seen in Appendix A.2.

Betti Curve for Rank Persistence. In the previous experiments we only added a fixed number of edges to the graphs. As with the barbell graph example, it is interesting to see how the statistics change as we vary the number of edges added. Hence, we took Texas and Cornell from the WebKb dataset [45] and added up to 100 edges. Figure 6 shows the results for Texas. The one for Cornell can be seen in the Appendix. Here we see that RELWIRE has the best eigengap, FOSR has the best rank distance, and GTR has the best commute times. There are many other interesting aspects to the curves. The first is the jump discontinuity in the rank of the first homology group from FOSR. This

Dataset	Eigengap				Betti Distance			
	RELWIRE	FOSR	GTR	SDRF	RELWIRE	FOSR	GTR	SDRF
Zinc	0.094	0.065	0.13	0.029	2.7	3.5	5.2	0.9
ESOL	0.4	0.37	0.4	0.21	1.7	3	3.5	0.7
BACE	0.048	0.033	0.08	0.017	3.5	3.8	5.9	1
Lipophilicity	0.083	0.056	0.12	0.03	3.1	3.7	5.3	1
Tox21	0.24	0.22	0.26	0.12	2.2	3.2	4.3	0.7
Mutag	0.18	0.15	0.23	0.1	2.2	3.2	4.2	1.3
Enzymes	1.1	1.1	1.3	0.06	2.5	3.5	4.6	1.2
AIDS700nef	0.46	0.44	0.49	0.31	1.0	2.9	3	0.65
Alkane	0.46	0.47	0.43	0.24	0.43	2.9	3.0	0.41
Linux	0.6	0.62	0.57	0.3	0.68	2.9	2.7	0.4

Table 2: Table showing the eigengap λ_2 and the Betti distance for the rewired graphs.

implies that FOSR reaches a critical number of edges after which adding loops is no longer beneficial and starts eliminating loops. On the other, GTR and SDRF seem to always add loops. RELWIRE on the other hand, seems to always want to eliminate topological loops. The jump discontinuity in the rank of the first homology group for FOSR seems to correlate with the jump discontinuity in the eigengap curve. However, interestingly we see no discontinuity in the commute times curve.



(a) Rank distance **(b)** $1/\lambda_2$ **(c)** Commute Time

Figure 6: Comparing the four rewiring methods after many edge additions: in (a), rank distance; (b) eigengap (λ_2^{-1}), and (c) the average commute times, each as a function of the number of edges added.

7 Conclusion

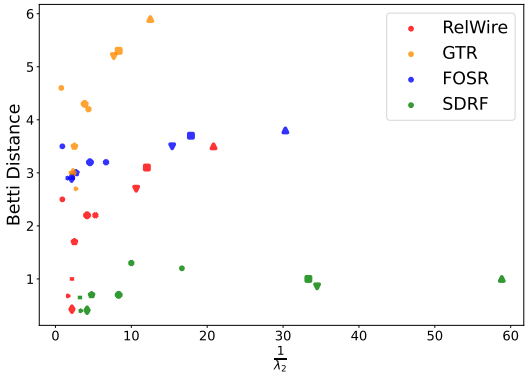


Figure 5: Betti distance versus $1/\lambda_2$. The closer the points are to the origin the better.

In conclusion, we use ideas from geometric group theory to develop a new rewiring technique known as RELWIRE using a new curvature-like relation on edges. We also introduce a new topological distance which measures how rewiring changes the structure of a graph. We show that compared to other method RELWIRE is Pareto optimal in that it makes small topological changes to the graph and makes big changes to statistics connected to oversquashing such as eigengap and commute times. We test RELWIRE on the downstream task of graph regression and report positive results.

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	Zinc	ESOL	BACE	Lipo	Tox21	Mutag	Enzymes	AIDS	Alkane	Linux
Nodes	23.2	13.3	34.1	27	18.6	17.9	32.6	8.9	8.9	7.6
Edges	49.8	27.4	73.7	59	38.6	39.6	124.3	17.6	15.8	13.9

Table 3: Table showing the average sizes of the graphs in each dataset.

A Appendix

A.1 Datasets

Specifically, we look at The ZINC dataset [24, 53] which consists of 10,000 molecular graphs. From [57], we look at ESOL which is the water solubility of 1,128 compounds, BACE which 1,522 compounds representing the inhibitors or human β-secretase 1, Lipophilicity which is 4,200 drug compounds, and Tox21 measure the toxicity of 7831 compounds. From the TUDataset [38], we use MUTAG [19] with consists of 188 nitroaromatic compounds and ENZYMES [12] which is a dataset of 600 protein tertiary structures obtained from the BRENDA enzyme database. Finally, we use three datasets from [4] consisting of 1520 graphs in total. The statistics for the datasets can be seen in Table 3.

A.2 Graph Regression

We also do preliminary experiments to show that RELWIRE helps improve the performance for graph regression. Four out of the ten data are for graph regression. For each dataset we split into train, test, and validation sets. We train 5 two layer Transformer Convolution networks [50]. We then pick the network with the best validation accuracy and report the test accuracies. These can be see in Table 4. As we see from the Table, we don't have any consistent trends. However, we do see that RELWIRE does perform well on average. This lack of trends is further supported by [55], where they do node classification tests on different data sets. This suggests that more work needs to be done to understand when graph rewiring is helpful.

Data Split. For Zinc we used a random split of 8000 training datapoints, 1000 validation data points and 1000 test datapoints. For BACE we use 1100 training, 200 validation and 222 test datapoints. For Lipo we used 3600 training data points and 300 for validation and test east. Finally, for ESOL we used 700 graphs as the training data and 100 each for validation and test.

	Original	RELWIRE	SDRF	FOSR	GTR
Zinc	185.092	185.089	185.091	185.091	185.090
Lipo	0.7067	0.6662	0.6325	0.7543	1.1388
BACE	0.5142	0.5556	0.5724	0.6284	0.6174
ESOL	0.8605	0.7631	1.4253	0.6936	0.6012

Table 4: Test mean squared error for the model with the best validation mean squared error over five trials.

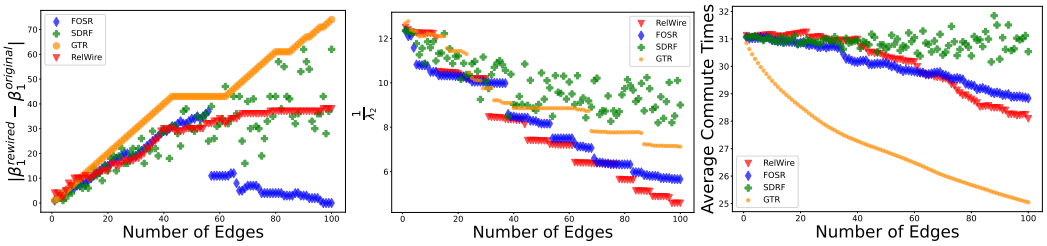
Optimization. For all methods we used Adam optimizer with the default parameters. We also used cosine annealing as the learning rate decay.

For Lipo, we used a batch size of 40 and trained for 100 epochs. For Zinc we used a batchsize of 80 and also trained for a 100 epochs. For ESOL and BACE, we used a bigger batchsize of 100 but trained for 1000 epochs.

Computing Test Error. We trained each model five times. We then picked the trial with the smallest validation accuracy and then reported the corresponding test accuracy.

Computer Resource. All datasets were accessed using Pytorch Geometric [23]. The models were all trained on Google Colab using a V100 GPU and pytorch geometric.

For rewiring, for used the official implementations of FOSR and GTR. For SDRF, we used the implementation from the LOG conference tutorial on graph rewiring [3].



(a) Rank Betti Curve **(b)** $1/\lambda_2$ **(c)** Commute Time

Figure 7: Graph properties for Cornell for the different rewiring methods.

A.3 WebKd Experiments

In Figure 7, we show the graphs for Cornell.

A.4 Proof

Lemma 12. *Let E_1, E_2 be edges of a simplicial graph G. If for E_1, E_2 we have that they*

1. *are contained in a clique subgraph of G, then E_1, E_2 are independent;*
2. *are separated by vertex v with $\pi_{E_1}(v)$ and $\pi_{E_2}(v)$ both singletons, then E_1, E_2 are transverse.*

Proof. We start by proving (1). For this let $E_i = (u, v)$ and $E_2 = (a, b)$. Then since this is a clique with all edge weights equal to 1. We have that

$$\pi_{E_1}(a) = \{u, v\} \text{ and } \pi_{E_2}(u) = \{a, b\}.$$

Thus, we have independence.

For (2), we note that since v separates tthe graph into at least two components G_1, G_2 such that $E_1 \in G_1$ and $E_2 \in G_2$. Then we see that for all $x \in G_1$, we have that

$$\pi_{E_2}(x) = \pi_{E_2}(v).$$

Similarly for all $x \in G_2$, we have that

$$\pi_{E_1}(x) = \pi_{E_1}(v).$$

Then since $\pi_{E_1}(v), \pi_{E_2}(v)$ are singletons, we see that we cannot get all four projection pairs. Thus, the edges are transverse. □

A.5 Topology Definitions

Definition 14 (Simplicial Complexes)**.** A *k-simplex* C is the convex hull of $k+1$ affinely independent vectors. A *simplicial complex* $\mathcal{K}$ is a collection of simplices such that for every $C \in \mathcal{C}$ every face of C is in $\mathcal{K}$ and for every $C_1, C_2 \in \mathcal{K}$, if $C_1 \cap C_2$ is not empty then $C_1 \cap C_2$ is a face of both. The *d-skeleton* of $\mathcal{K}$, denoted $\mathcal{K}^{(d)}$, is the simplicial subcomplex of $\mathcal{K}$ consisting of simplices of dimension at most d.

A.6 Prior Rewiring Works: SDRF, FOSR, and GTR

We review the existing rewiring methods against which we compare our own method RELWIRE.

SDRF. As we have seen, the curvature of a graph is related to oversquashing. Thus, [54] design a method to increase the curvature of negatively curved areas. However, the Ollivier Ricci curvature is computationally expensive to calculate, hence they approximate it using a notion called Balanced Forman Curvature $Ric(i, j)$. In [54] show that if $Ric(i, j) > k$ for all edges then we have that $\frac{k}{2} \leq h_G \leq \frac{\lambda_2}{2}$. Thus, showing the connection between the curvature and other quantities such as the eigengap and the Cheeger constant. They then create a method that finds the most negatively curved edge and then add the edge that increases the curvature of this edge the most.

FOSR. In [29], they showed that if f is the second eigenvector for the normalized Laplacian $(I - D^{-1/2}AD^{-1/2})$) then adding an edge i, increases the second eigenvalue by

$$\frac{2f_i f_j}{\sqrt{1+d_i}\sqrt{1+d_j}} + 2\lambda_2 \left[f_i^2 \left(\frac{\sqrt{d_i}}{\sqrt{1+d_i}} - 1 \right) + f_j^2 \left(\frac{\sqrt{d_j}}{\sqrt{1+d_j}} - 1 \right) \right].$$

They use this method to design an algorithm FOSR, that maximizes the first order term.

GTR. Another notion of relevance is the total resistance of a graph, G. Let L be the Combinatorial Laplacian of a graph. Then the resistance $R(i,j)$ between nodes i and j is given by $R(i,j) = (1_i - 1_j)^T L^\dagger (1_i - 1_j)$. Here 1_i is the indicator vector for the ith node and $L^\dagger$ is the pseudoinverse of the Combinatorial Laplacian. The total resistance R_{tot} is $R_{tot} = \sum_{i,j} R(i,j)$. Then the biharmonic distance $B(i,j)$ between nodes i and j is given by $B(i,j) = \sqrt{(1_i - 1_j)^T (L^\dagger)^2 (1_i - 1_j)}$.

[10] show that the increase in the total resistance of adding an edge (i,j) is given by $\frac{B(i,j)^2}{1+R(i,j)}$. Hence they design a method GTR that maximizes this quantity. This quantity is related to the eigengap as well [10], where the maximum resistance between any two pairs of nodes R_{max} is bounded by

$$\frac{1}{n\lambda_2} \leq R_{max} \leq \frac{1}{\lambda_2}.$$