
Expander Graph Propagation

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Abstract

1
2 Deploying graph neural networks (GNNs) on whole-graph classification or regres-
3 sion tasks is known to be challenging: it often requires computing node features
4 that are mindful of both local interactions in their neighbourhood and the global
5 context of the graph structure. GNN architectures that navigate this space need
6 to avoid pathological behaviours, such as bottlenecks and oversquashing, while
7 ideally having linear time and space complexity requirements. In this work, we
8 propose an elegant approach based on propagating information over *expander*
9 *graphs*. We leverage an efficient method for constructing expander graphs of a
10 given size, and use this insight to propose the EGP model. We show that EGP is
11 able to address all of the above concerns, while requiring minimal effort to set
12 up, and provide evidence of its empirical utility on relevant graph classification
13 datasets and baselines in the Open Graph Benchmark. Importantly, using expander
14 graphs as a template for message passing necessarily gives rise to negative cur-
15 vature. While this appears to be counterintuitive in light of recent related work
16 on oversquashing, we theoretically demonstrate that negatively curved edges are
17 likely to be **required** to obtain scalable message passing without bottlenecks. To
18 the best of our knowledge, this is a previously unstudied result in the context of
19 graph representation learning, and we believe our analysis paves the way to a novel
20 class of scalable methods to counter oversquashing in GNNs.

21 1 Introduction

22 Graph neural networks (GNNs) are a flexible class of models for learning representations over
23 graph-structured data [1]. Their versatility [2–4] and generality [5, 6] has made them a very attractive
24 approach, leading to considerable application in areas as diverse as virtual drug screening [7], traffic
25 prediction [8], combinatorial chip design [9] and pure mathematics [10, 11].

26 Most GNNs rely on repeatedly propagating information between neighbouring nodes in the graph.
27 This is commonly expressed in the *message passing* [4] paradigm: nodes send vector-based *messages*
28 to each other along the edges of the graph, and nodes update their representations by *aggregating*
29 all the messages sent to them, in a permutation-invariant manner. Under many industrially-relevant
30 tasks, this paradigm is very potent, often allowing for highly scalable model variants [12–14].

31 However, in many areas of scientific interest, purely local interactions are likely insufficient. Among
32 the principal graph tasks, *graph classification* is perhaps most ripe with such situations: to meaning-
33 fully attach a label to a graph, in many cases it is insufficient to treat graphs as “bags of nodes”. For
34 example, when classifying a molecule for its potency as a candidate drug [7], the label is driven by
35 complex substructure interactions in the molecule [15], rather than a naïve sum of atom-level effects.

36 Accordingly, GNNs deployed in this regime need to update node features in a manner that is mindful
37 of the *global* properties of the graph. It quickly became apparent that it is often inadequate to merely
38 stack more message passing layers over the input graph. In fact, for many graph classification tasks,
39 such approaches may be weaker than discarding the graph structure altogether [16, 17]. Now, it is
40 well-understood that stacking many local layers leaves GNNs vulnerable to pathological behaviours
41 such as oversquashing [18]. Intuitively, oversquashing occurs when nodes need to store quantities of
42 information that are *exponentially* increasing with model depth [18, Section 5]. Such nodes often arise
43 in the vicinity of *bottlenecks* in a graph—small collections of edges which are responsible for carrying

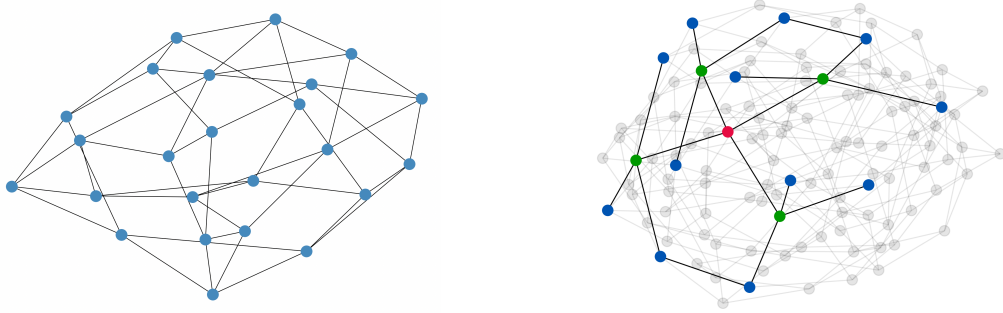
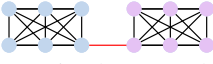


Figure 1: **Left:** The Cayley graph of $SL(2, \mathbb{Z}_3)$, constructed using our method. It has $|V| = 24$ nodes and it is 4-regular (implying $|E| = 2|V|$), hence it is sparse. Despite its sparsity, it is highly interconnected: any node is reachable from any other node by no more than 4 hops. Hence, it can serve as a strong “template” for globally propagating node features with a GNN. **Right:** The Cayley graph of $SL(2, \mathbb{Z}_5)$, constructed in an analogous way (with $|V| = 120$ nodes). A 2-hop neighbourhood of one node (in red) is highlighted, demonstrating its tree-like local structure.

44 representations between large groups of nodes. One typical example of such a bottleneck can be
 45 found in a *barbell graph* , where the red edge is under significant representational
 46 pressure to transport information between the two communities.

47 Within this space, we are interested in proposing a method that satisfies *four* desirable criteria: **(C1)** it
 48 is capable of propagating information *globally* in the graph; **(C2)** it is *resistant* to the oversquashing
 49 effect and does not introduce bottlenecks; **(C3)** its time and space complexity remain *subquadratic*
 50 (tighter than $O(|V|^2)$ for sparse graphs); and **(C4)** it requires *no dedicated preprocessing* of the input.
 51 Satisfying all four of these criteria simultaneously is challenging, and we will survey many of the
 52 popular approaches in the next section—demonstrating ways in which they fail to meet some of them.

53 In this paper, we identify *expander graphs* as very attractive objects in this regard. Specifically, they
 54 offer a family of graph structures that are fundamentally *sparse* ($|E| = O(|V|)$), while having *low*
 55 *diameter*: thus, any two nodes in an expander graph may reach each other in a short number of
 56 hops, eliminating bottlenecks and oversquashing (see Figure 1). Further, we will demonstrate an
 57 efficient way to construct a family of expander graphs (leveraging known theoretical results on the
 58 *special linear group*, $SL(2, \mathbb{Z}_n)$). Once an expander graph of appropriate size is constructed, we
 59 can perform a certain number of GNN *propagation* steps over its structure to globally distribute the
 60 nodes’ features. Accordingly, we name our method *expander graph propagation* (**EGP**).

61 A key contribution of our work extends the implications of prior art on oversquashing via curvature
 62 analysis [19]. According to [19], negatively curved edges are causing the oversquashing effect—yet,
 63 counterintuitively, the edges of the expander graphs we construct will *always be negatively curved!*
 64 We prove, however, that our expanders can never be sufficiently negatively curved to trigger the
 65 conditions necessary for the results in [19] to be applicable, and show that the existence of negatively
 66 curved edges might in fact be **required** in order to have sparse communication without bottlenecks.

67 2 Related work

68 We begin with a survey of the many prior approaches to handling global context in graph representation
 69 learning, evaluating them carefully against our four desirable criteria **(C1–C4)**; cf. Table 1). This list
 70 is by no means exhaustive, but should be indicative of the most important directions.

71 **Stacking more layers.** As already highlighted, one way to achieve global information propagation is
 72 to have a deeper GNN. In this case, we are capable of satisfying **(C1)** and **(C4)**—no dedicated preprocess-
 73 ing is needed. However, depending on the graph’s diameter, we may need up to $O(|V|)$ layers to
 74 cover the graph, leading to quadratic complexity (violating **(C3)**) and introducing a vulnerability to
 75 bottlenecks **(C2)**, as theoretically and empirically demonstrated in [18].

76 **Master nodes.** An attractive approach to introducing global context is to introduce a *master node*
 77 to the graph, and connect it to all of the graph’s nodes. This can be done either explicitly [4] or

Table 1: A summary of principal approaches to handling global context in graph representation learning (Section 2). “(✓)” indicates that a criterion *may* be satisfied, depending on the method’s tradeoffs. Our proposal, the expander graph propagation (EGP) method, satisfies all four criteria.

Approach	(C1)	(C2)	(C3)	(C4)
	(global prop.)	(no bottlenecks)	(subquadratic)	(no dedicated preproc.)
GNNs	✗	✗	✓	✓
Sufficiently deep GNNs	✓	✗	✗	✓
Master node [4, 20]	✓	✗	✓	✓
Fully connected [18, 21–25]	✓	✓	✗	✓
Feature aug. [26–31]	✓	(✓)	(✓)	✗
Graph rewiring [19, 32, 33]	✓	✓	✓	✗
Hierarchical MP [34–39]	✓	✓	(✓)	✗
EGP (ours)	✓	✓	✓	✓

78 implicitly, by storing a “global” vector [20]. It trivially reduces the graph’s diameter to 2, introduces
 79 $O(1)$ new nodes and $O(|V|)$ new edges, and requires no dedicated preprocessing, hence it satisfies
 80 (C1, C3, C4). However, these benefits come at the expense of introducing a bottleneck in the master
 81 node: it has a very challenging task (especially when graphs get larger) to continually incorporate
 82 information over a very large neighbourhood in a useful way. Hence it fails to satisfy (C2).

83 **Fully connected graphs.** The converse approach is to make *every* node a master node: in this case,
 84 we make all pairs of nodes connected by an edge—this was initially proposed as a powerful method
 85 to alleviate oversquashing by [18]. This strategy proved highly popular in the recent surge of Graph
 86 Transformers [22, 23, 25], and is common for GNNs used in physical simulation [21] or reasoning
 87 [24] tasks. The graph’s diameter is reduced to 1, no bottlenecks remain, and the approach does not
 88 require any dedicated preprocessing. Hence (C1, C2, C4) are trivially satisfied. The main downside
 89 of this approach is the introduction of $O(|V|^2)$ edges, which means (C3) can never be satisfied—and
 90 this approach will hence be prohibitive even for modestly-sized graphs.

91 **Feature augmentation.** An alternative approach is to provide additional features to the GNN which
 92 directly identify the structural role each node plays in the graph [26]. If done properly (i.e., if the
 93 computed features are relevant to the target), this can drastically improve expressive power. Hence, in
 94 theory, it is possible to satisfy (C1) while not violating (C2, C3). However, computing appropriate
 95 features requires either specific domain knowledge, or appropriate pre-training [27–31], in order to
 96 obtain such embeddings. Hence all of these gains come at the expense of failing to satisfy (C4).

97 **Graph rewiring.** Another promising line of research involves modifying the edges of the original
 98 graph to alleviate bottlenecks. Popular examples of this approach involve using diffusion [32]—which
 99 diffuse additional edges through the application of kernels such as the personalised PageRank, and
 100 stochastic discrete Ricci flows [19]—which surgically modify a small quantity of edges to alleviate
 101 the oversquashing effect on the nodes with negative Ricci curvature. Recent concurrent work [33]
 102 also uses constructions inspired by expander graphs to randomly locally rewire a given input graph.
 103 If realised carefully, such approaches will not deviate too far from the original graph, while provably
 104 alleviating oversquashing; hence it is possible to satisfy (C1, C2, C3). However, this comes at a cost
 105 of having to examine the input graph structure, with methods that do not necessarily scale easily with
 106 the number of nodes. As such, dedicated preprocessing is needed, failing to satisfy (C4).

107 **Hierarchical message passing.** Lastly, going beyond modifying the edges, it is also possible to
 108 introduce additional *nodes* in the graph—each of them responsible for a particular *substructure* in
 109 the graph¹. If done carefully, it has the potential to drastically reduce the graph’s diameter while not
 110 introducing bottlenecked nodes (hence, allowing us to satisfy (C1, C2)). However, in prior work,
 111 a cost has to be paid for this, usually in the need for dedicated preprocessing. Prior proposals for
 112 hierarchical GNNs that remain scalable require a dedicated pre-processing step [34–36], sometimes
 113 coupled with domain knowledge [36]—thus failing to satisfy (C4). In addition, such methods may
 114 require adding prohibitively large numbers of substructures [37, 38] or expensive pre-computation,
 115 e.g. computing the graph Laplacian eigenvectors [39]. This might make even (C3) hard to satisfy.

¹Master nodes are a special case: a single node is responsible for a “substructure” spanning the entire graph.

116 We remark that our work is not the first to study expander graph-related topics in the context of
 117 GNNs. Specifically, the ExpanderGNN [40] leverages expander graphs over neural network weights
 118 to sparsify the update step in GNNs. This is a direct application of Deep Expander Networks [41],
 119 which studied such constructs over CNNs. With respect to our contributions, neither of these cases
 120 discuss expanders in the context of the computational graph for a GNN, nor attempt to propagate
 121 messages over such a structure. Further, neither satisfy all four of our desired criteria (C1–C4).

122 3 Theoretical background

123 We now dedicate our attention to the key theoretical results over expander graphs, which will allow
 124 EGP to have favourable properties and be efficiently precomputable.

Definition 1. For a finite connected graph $G = (V(G), E(G))$, we consider functions $f: V(G) \rightarrow \mathbb{R}$.
 The *Laplacian* $Lf: V(G) \rightarrow \mathbb{R}$ of such a function is defined to be

$$Lf(v) = \deg(v)f(v) - \sum_{vw \in E(G)} f(w),$$

125 where $\deg(v)$ is the degree of the vertex v .

The mapping $L: \mathbb{R}^{V(G)} \rightarrow \mathbb{R}^{V(G)}$ sending a function f to its Laplacian Lf is a linear transformation.
 It is not hard to show [42] that L is symmetric with respect to the standard basis for $\mathbb{R}^{V(G)}$ and
 positive semi-definite and hence has non-negative real eigenvalues

$$0 = \lambda_0(G) < \lambda_1(G) \leq \lambda_2(G) \leq \dots$$

126 The smallest eigenvalue is 0 and its associated eigenspace consists of the constant functions (assuming
 127 G is connected). The smallest positive eigenvalue, $\lambda_1(G)$, is central to the definition of expander
 128 graphs, as the next definition shows.

129 **Definition 2.** An infinite collection $\{G_i\}$ of finite connected graphs is an *expander family* if there is
 130 a constant $c > 0$ such that for all G_i in the collection, $\lambda_1(G_i) \geq c$.

131 Expander families [43–45] have many remarkable and useful properties, particularly when there is a
 132 uniform upper bound on the degree of the vertices of G_i .

Definition 3. Let G be a finite graph. For $A \subset V(G)$, its *boundary* ∂A is the collection of edges
 with one endpoint in A and one endpoint not in A . The *Cheeger constant* $h(G)$ is defined to be

$$h(G) = \min \left\{ \frac{|\partial A|}{|A|} : A \subset V(G), 0 < |A| \leq |V(G)|/2 \right\}.$$

133 Thus, having a small Cheeger constant is equivalent to the graph having a ‘bottleneck’, in the sense
 134 that there is a collection of edges ∂A that, when removed, disconnects the vertices into two sets
 135 (A and its complement, $V(G) \setminus A$), with the property that the sizes of A and its complement are
 136 significantly larger than the size of ∂A .

137 Expander families can be reinterpreted using Cheeger constants, as follows (see, e.g., [46–49]):

138 **Theorem 4.** Let $\{G_i\}$ be an infinite collection of finite connected graphs with a uniform upper bound
 139 on their vertex degrees. Then the following are equivalent:

- 140 1. $\{G_i\}$ is an expander family;
- 141 2. there is a constant $\epsilon > 0$ such that for all graphs in the collection, $h(G_i) \geq \epsilon$.

142 Hence, expander graphs have higher Cheeger constants and will hence experience less severe problems
 143 arising due to bottleneck edges. The following result is one of the many useful properties of expander
 144 families, and it concerns their *diameter*. It was proved by Mohar [50, Theorem 2.3]. See also [47].

Theorem 5. The diameter $\text{diam}(G)$ of a graph G satisfies

$$\text{diam}(G) \leq 2 \left\lceil \frac{\Delta(G) + \lambda_1(G)}{4\lambda_1(G)} \log(|V(G)| - 1) \right\rceil,$$

where $\Delta(G)$ is the maximal degree of any vertex of G . Hence, if $\{G_i\}$ is an expander family of finite
 graphs with a uniform upper bound on their vertex degrees, then there is a constant $k > 0$ such that
 for all graphs in the family,

$$\text{diam}(G_i) \leq k \log V(G_i).$$

145 Therefore, if we want to globally propagate information over an expander graph which has $|V|$ nodes,
 146 we only need $O(\log |V|)$ propagation steps to do so—yielding subquadratic complexity.

147 We showed that expanders will experience less severe problems arising due to bottleneck edges, with
 148 favourable propagation qualities. What is missing is an efficient method of constructing an expander
 149 of (roughly) $|V|$ nodes. To demonstrate such a method, we leverage known results from group theory.

150 **Definition 6.** A group (Γ, \circ) is a set Γ equipped with a *composition* operation $\circ : \Gamma \times \Gamma \rightarrow \Gamma$ (written
 151 concisely by omitting \circ , i.e. $g \circ h = gh$, for $g, h \in \Gamma$), satisfying the following axioms:

- 152 • (*Associativity*) $(gh)l = g(hl)$, for $g, h, l \in \Gamma$.
- 153 • (*Identity*) There exists a unique $e \in \Gamma$ satisfying $eg = ge = g$ for all $g \in \Gamma$.
- 154 • (*Inverse*) For every $g \in \Gamma$ there exists a unique $g^{-1} \in \Gamma$ such that $gg^{-1} = g^{-1}g = e$.

155 A group is hence a natural construct for reasoning about transformations that leave an object invariant
 156 (unchanged). Further, we define a relevant notion of a group’s generating set:

157 **Definition 7.** Let Γ be a group. A subset $S \subseteq \Gamma$ is a *generating set* for Γ if it can be used to “generate”
 158 all of Γ via composition. Concretely, any element $g \in \Gamma$ can be expressed by composing elements in
 159 the generating set, or their inverses; that is, we can express $g = s_1^{\pm 1} s_2^{\pm 1} s_3^{\pm 1} \cdots s_{n-1}^{\pm 1} s_n^{\pm 1}$ for $s_i \in S$.

160 Now we are ready to define a Cayley graph of a group w.r.t. its generating set.

161 **Definition 8.** Let Γ be a group with a finite generating set S . Then the associated *Cayley graph*
 162 $\text{Cay}(\Gamma; S)$ has vertex set Γ and it has an edge $g \rightarrow gs$ for each $g \in \Gamma$ and each $s \in S$. We say that
 163 s is the *label* on this edge. This is a potentially non-simple graph, as it may have edges with both
 164 endpoints on the same vertex and it may have multiple edges between a pair of vertices. In particular,
 165 when s has order 2, then we view the edge $g \rightarrow gs$ and the edge $gs \rightarrow gs^2 = g$ as distinct edges.

166 Note that the degree of each vertex of a Cayley graph $\text{Cay}(\Gamma; S)$ is $2|S|$. This is because each vertex
 167 g is joined by edges to gs and gs^{-1} for each $s \in S$. Thus, we shall be particularly interested in the
 168 case where there is a uniform upper bound on $|S|$. The specific group we use for EGP is as follows.

For each positive integer n , the *special linear group* $\text{SL}(2, \mathbb{Z}_n)$ denotes the group of 2×2 matrices
 with entries that are integers modulo n and with determinant 1. One of its generating sets is:

$$S_n = \left\{ \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix} \right\}.$$

169 Central to our constructions is the following important result.

170 **Theorem 9.** *The family of Cayley graph $\text{Cay}(\text{SL}(2, \mathbb{Z}_n); S_n)$ forms an expander family.*

171 The proof uses a result of Selberg [51] who showed that the smallest positive eigenvalue of the
 172 Laplacian of certain hyperbolic surfaces is at least $3/16$. One can use this to produce a lower bound
 173 on the first eigenvalue of the Laplacian on $\text{Cay}(\text{SL}(2, \mathbb{Z}_n); S_n)$. Full proofs are given in [44, 45].

174 Lastly, it is useful to state a known result: the number of nodes of $\text{Cay}(\text{SL}(2, \mathbb{Z}_n); S_n)$ is:

$$|V(\text{Cay}(\text{SL}(2, \mathbb{Z}_n); S_n))| = n^3 \prod_{\text{prime } p|n} \left(1 - \frac{1}{p^2}\right), \quad (10)$$

175 hence, it is of the order of $O(n^3)$. We now study the local properties of Cayley graphs in detail.

176 4 Local structure of the Cayley graphs, and the utility of negative curvature

177 Recent work [19] has suggested that the local structure of the graph G underlying a GNN may play
 178 an important role in the way that information propagates around G . In particular, various notions of
 179 ‘Ricci curvature’ such as Forman curvature [52], Ollivier curvature [53, 54] and balanced Forman
 180 curvature [19] have been examined. These are all local quantities, in the sense that they depend on the
 181 structure of the graph within a small neighbourhood of each edge. In this section, we will therefore
 182 examine the local structure of the Cayley graphs $G_n = \text{Cay}(\text{SL}(2, \mathbb{Z}_n); S_n)$.

183 The various notions of curvature given above are defined for each e of the graph G . Since, as defined
 184 by [19], the balanced Forman curvature of an edge depends only on local structures (i.e. triangles

185 and squares) around that edge, they can be determined by only observing the immediate 2-hop
 186 surrounding of that edge. Formally, for an edge e of a graph G , let $N_2(e)$ be the induced subgraph
 187 with vertices that are at most two hops away from at least one endpoint of e . Then the curvature of e
 188 only depends on the isomorphism type of $N_2(e)$. More specifically, if e and e' are edges in possibly
 189 distinct graphs, and there is a graph isomorphism between $N_2(e)$ and $N_2(e')$ that sends e to e' , then
 190 this guarantees that the curvatures of e and e' are equal.

191 This situation arises prominently in the Cayley graphs that we are considering, as follows.

Proposition 11. *Let s be one of*

$$\begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}, \quad \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}.$$

192 *Let $n, n' > 18$ and let e and e' be s -labelled edges in G_n and $G_{n'}$. Then there is a graph isomorphism
 193 between $N_2(e)$ and $N_2(e')$ taking e to e' .*

194 We prove Proposition 11 in Appendix A. This immediately allows us to characterise the balanced
 195 Forman curvature and Ollivier curvature for all of the Cayley graphs we generate:

Proposition 12. *The balanced Forman curvatures $\text{Ric}(n)$, and the Ollivier curvatures $\kappa(n)$ of all
 edges of Cayley graphs G_n are given by:*

$$\text{Ric}(n) = \begin{cases} 0 & \text{if } n = 2 \\ -1/4 & \text{if } n = 3 \\ -1/2 & \text{if } n = 4 \\ -1 & \text{if } n \geq 5, \end{cases} \quad \kappa(n) = \begin{cases} 0 & \text{if } n = 2 \\ -1/8 & \text{if } n = 3 \\ -1/4 & \text{if } n = 4 \\ -3/8 & \text{if } n = 5 \\ -1/2 & \text{if } n \geq 6. \end{cases}$$

196 *Proof.* Proposition 11 implies that the balanced Forman and Ollivier curvatures are all equal for
 197 $n > 18$. Their values for $2 \leq n \leq 19$ can all be empirically computed, and are given as above. \square

198 Prior work [19] suggests it is preferable for GNNs to operate on graphs with positive Ricci curvature,
 199 whereas our graphs G_n ($n > 2$) all have negative Ricci curvature. However, we contend that negative
 200 Ricci curvature is not in itself an impediment to efficient propagation around a GNN. Indeed, it was
 201 shown in [19, Theorem 4] that poor propagation arises when the balanced Forman curvature is close
 202 to -2 , specifically if it is at most $-2 + \delta$ for some $\delta > 0$. Here, δ is required to satisfy certain
 203 inequalities. But, with certainty, $\delta = 1$ can *never* be satisfied in the hypotheses of [19, Theorem 4].

204 Furthermore, positive Ricci curvature may have *downsides* when used for GNNs. One significant
 205 downside can be derived using the main result of [55], which says that the three properties of
 206 expansion, sparsity and non-negative Ollivier curvature are incompatible, in the following sense.

207 **Theorem 13.** *For any $\delta > 0$ and $\Delta > 0$, there are only finitely many graphs with maximum vertex
 208 degree Δ , Cheeger constant at least δ and non-negative Ollivier curvature.*

209 We prove Theorem 13 in Appendix B. Furthermore, quoting directly from [55]:

210 *“The high-level message is that on large sparse graphs, non-negative curvature (in an even weak sense)
 211 induces extremely poor spectral expansion. This stands in stark contrast with the traditional idea
 212 – quantified by a broad variety of functional inequalities over the past decade – that non-negative
 213 curvature is associated with good mixing behavior.”*

214 In our view, it is highly desirable that the graphs used for GNNs have high Cheeger constants, in
 215 the sense of globally lacking bottlenecks. Having bounded vertex degree is certainly useful too,
 216 since it implies that the graphs will be sparse, and the nodes will not have to handle ever-increasing
 217 neighbourhoods for message passing as graphs grow larger in size.

218 However, by proving Theorem 13, we showed non-negative Ollivier curvature is *incompatible* with
 219 these properties for sufficiently large graphs. Specifically, given the *finite* supply of non-negatively
 220 curved sparse graphs, we can define N' as the largest number of nodes of such graphs. Then, for
 221 all graphs G where $|V(G)| > N'$, we will be *unable* to produce a computational graph for a GNN
 222 which is non-negatively curved everywhere.

223 The negative curvature of each edge in G_n implies that they are locally ‘tree-like’. In Appendix C,
 224 we make this statement precise by showing that G_n is ‘tree-like’ up to scale $c \log(n)$ about each node,
 225 for $c \simeq (1/2)(\log((1 + \sqrt{5})/2))^{-1}$ (see Figure 1 (Right) for a schematic view).

226 This tree-like structure might seem, at first, to be counter-productive for good propagation across
 227 the graphs G_n . Indeed, GNNs based on trees have been shown to have provably poor performance
 228 [18]. The reason for this seems to be two-fold. On the one hand, trees have small Cheeger constant.
 229 Indeed, any tree G on n vertices has a Cheeger constant $1/\lfloor n/2 \rfloor$, since we may find an edge that,
 230 when removed, decomposes the graph into subgraphs with $\lfloor n/2 \rfloor$ and $\lceil n/2 \rceil$ vertices. As discussed
 231 in Section 3 and in [19], when a graph has small Cheeger constant, its performance when used as
 232 a template for a GNN is likely to become poor. Secondly, GNNs based on trees are susceptible
 233 to oversquashing. For a k -regular infinite tree, there are $k(k-1)^{r-1}$ vertices at distance r from a
 234 given vertex. Hence, if information is to be propagated at least distance r from a given vertex, then
 235 seemingly an exponential amount of information is required to be stored.

236 However, neither of these issues are problematic for a GNN based on the Cayley graph G_n . By
 237 Theorem 9, their Cheeger constants are bounded away from 0. Secondly, although they are tree-like
 238 locally, this is only true up to scale $O(\log n)$. In fact, the r -neighbourhood of any vertex is the whole
 239 graph G_n as soon as $r > C \log n$, for some constant C , by Theorem 5. Being tree-like up to distance
 240 $O(\log n)$ does not lead to a requirement to store too much information as the message propagates.
 241 This is because $k(k-1)^{r-1}$ is polynomial in n when $r \leq O(\log n)$.

242 Beyond this scale, there exist many additional connections, which lead to many possible paths joining
 243 any pair of vertices. Each of these paths can be a potential route of transfer of information from one
 244 vertex to another. The perspective of information transfer also gives rise to another perspective in
 245 which expanders fare very favourably: the *mixing time* of their corresponding Markov chain. We
 246 state several known facts about the favourable mixing times of expanders in Appendix D, to further
 247 supplement our claims on their efficient communication properties.

248 5 Expander graph propagation

249 Let an input to a graph neural network be a node feature matrix $\mathbf{X} \in \mathbb{R}^{|V| \times d}$, and an adjacency matrix
 250 $\mathbf{A} \in \mathbb{R}^{|V| \times |V|}$. This setup is such that the feature vector of node u , $\mathbf{x}_u \in \mathbb{R}^d$, can be recovered by
 251 taking an appropriate row from \mathbf{X} . Note that the adjacency information can also be fed in an edge-list
 252 manner, which is desirable from a scalability perspective. Further, each edge in the graph may be
 253 endowed with additional features rather than a single real scalar. None of the above modifications
 254 would change the essence of our findings; we use a matrix formalism here purely for simplicity.

255 There exist many ways in which the computed Cayley graph $\text{Cay}(\text{SL}(2, \mathbb{Z}_n); S_n)$ can be leveraged
 256 for message propagation, and exploring these variations could be very useful for future work. Here,
 257 we opt for a simple construction: interleave running a standard GNN over the given input structure,
 258 followed by running another GNN layer over the relevant Cayley graph. If we let $\mathbf{A}^{\text{Cay}(n)}$ be an
 259 adjacency matrix derived from $\text{Cay}(\text{SL}(2, \mathbb{Z}_n); S_n)$, this implies:

$$\mathbf{H} = \text{GNN}(\text{GNN}(\mathbf{X}, \mathbf{A}), \mathbf{A}^{\text{Cay}(n)}) \quad (14)$$

260 Here, GNN refers to any preferred GNN layer, such as the graph isomorphism network [56, GIN]:

$$\mathbf{h}_u = \phi \left((1 + \epsilon) \mathbf{x}_u + \sum_{v \in \mathcal{N}_u} \mathbf{x}_v \right) \quad (15)$$

261 where \mathcal{N}_u is the neighbourhood of node u , i.e. in our setup, the set of all nodes v such that $a_{vu} \neq 0$.
 262 $\epsilon \in \mathbb{R}$ is a learnable scalar, and $\phi: \mathbb{R}^d \rightarrow \mathbb{R}^d$ is a two-layer MLP.

263 This procedure is iterated for a certain number of steps, after which the computed node embeddings
 264 in \mathbf{H} can be used for any downstream task of interest—such as node classification, link prediction
 265 or graph classification. Note that, unlike [18], who apply their custom layer only at the *tail* of the
 266 architecture, we apply the expander graph immediately after each layer over the input graph. We find
 267 that if the input graph given by \mathbf{A} contains bottlenecks, applying the GNN over $\mathbf{A}^{\text{Cay}(n)}$ only at the
 268 end may result in oversquashing occurring before any expander graph propagation can take place.

269 The setup so far assumed the number of nodes in our input graph to line up with the Cayley graph,
 270 that is, $\mathbf{A}^{\text{Cay}(n)} \in \mathbb{R}^{|V| \times |V|}$. However, there is no guarantee that we can find an appropriate n such
 271 that $\text{Cay}(\text{SL}(2, \mathbb{Z}_n); S_n)$ would have $|V|$ nodes. What we can do in practice, as an approximation, is
 272 choose the smallest n such that the number of nodes of $\text{Cay}(\text{SL}(2, \mathbb{Z}_n); S_n)$ is $\geq |V|$, then consider
 273 $\mathbf{A}_{1:|V|, 1:|V|}^{\text{Cay}(n)}$ —i.e. only the subgraph containing the first $|V|$ nodes in the Cayley graph.

274 There is a slight misalignment to our theory in this slicing choice—if the $|V|$ vertices in this subgraph
 275 are chosen completely arbitrarily, we risk disconnecting the graph. However, in all our experiments
 276 we construct the Cayley graph in a breadth-first manner, starting from the identity element as “node
 277 zero”. Hence, the node at index i is always guaranteed to be reachable from the nodes at lower indices
 278 ($j < i$), and the graph cannot be disconnected under this construction. More interesting strategies for
 279 this step can also be considered in the future. Note that, much like the fully connected graph used by
 280 [18], we interpret the Cayley graph mainly as a *template* for global information propagation, in order
 281 to relieve bottlenecks in a scalable way. Our interpretation, hence, assumes that the efficient diffusion
 282 of information over the whole graph is of benefit to the learning task we perform. When this is not
 283 the case, it might be worthwhile to construct expanders that somehow align with the input graph, but
 284 no such expander constructions are currently known, to the best of our knowledge. There is also a
 285 possible effect of *stochasticity* due to arbitrarily having to align the Cayley graph’s nodes to the input
 286 graph—which would not appear when using master nodes or fully-connected graphs—though our
 287 preliminary experiments did not observe any such negative effects.

288 Algorithm 1 summarises the steps of our proposed EGP model. As direct corollaries of results we
 289 proved or demonstrated, we note that EGP satisfies all four of our desirable criteria: **(C1)** by Theorem
 290 5 (so long as logarithmically many layers are applied), **(C2)** by Theorem 4 (high Cheeger constant
 291 implies no bottlenecks), **(C3)** by the fact our Cayley graphs are 4-regular and hence sparse, and
 292 **(C4)** by the fact we can generate a Cayley graph of appropriate size without detailed analysis of the
 293 input—we may precompute a “bank” of Cayley graphs of various sizes to use in an ad-hoc manner.

Algorithm 1: Expander graph propagation (EGP) forward pass

Inputs : Node features $\mathbf{X} \in \mathbb{R}^{|V| \times d}$, Adjacency matrix $\mathbf{A} \in \mathbb{R}^{|V| \times |V|}$

Output : Node embeddings \mathbf{H}

// Choose the smallest Cayley graph from our family that has number of nodes equal to, or greater than, $|V|$
 $n \leftarrow \operatorname{argmin}_{m \in \mathbb{N}} |V(\operatorname{Cay}(\operatorname{SL}(2, \mathbb{Z}_m); S_m))| \geq |V|$; // We can use Equation 10 to determine n

$G^{\operatorname{Cay}(n)} \leftarrow \operatorname{Cay}(\operatorname{SL}(2, \mathbb{Z}_n); S_n)$

$\mathbf{A}_{uv}^{\operatorname{Cay}(n)} \leftarrow \begin{cases} 1 & (u, v) \in E(G^{\operatorname{Cay}(n)}) \\ 0 & \text{otherwise} \end{cases}$; // Populate adjacency matrix of the Cayley graph

$\mathbf{H}^{(0)} \leftarrow \mathbf{X}$; // Initialise GNN inputs

for $t \in \{1, \dots, T\}$ **do**

if $t \bmod 2 = 0$ **then**

$\mathbf{H}^{(t)} \leftarrow \operatorname{GNN}^{(t)}(\mathbf{H}^{(t-1)}, \mathbf{A})$; // GNN layer over input graph; e.g. Equation 15

end

else

$\mathbf{H}^{(t)} \leftarrow \operatorname{GNN}^{\operatorname{Cay}(t)}(\mathbf{H}^{(t-1)}, \mathbf{A}_{1:|V|, 1:|V|}^{\operatorname{Cay}(n)})$; // GNN layer over Cayley graph; e.g. Eq. 15

end

end

return $\mathbf{H}^{(T)}$; // Return final embeddings for downstream use

294 6 Empirical evaluation

295 Our work provides mainly a theoretical contribution: demonstrating a simple, theoretically-grounded
 296 approach to relieving bottlenecks and oversquashing in GNNs without requiring quadratic complexity
 297 or dedicated preprocessing. Further, we prove several additional results which deepen our understand-
 298 ing of curvature-based analysis of GNNs, showing how our expanders can be favourable in spite of
 299 their negatively-curved edges.

300 We now provide several direct comparative experiments in order to ascertain that our EGP addition
 301 can directly help existing graph classification baselines, even without further hyperparameter tuning.

302 **Datasets** To show this, we leverage the established Open Graph Benchmark collection of tasks
 303 [57, OGB]. Specifically, we provide results on all of its graph classification datasets: ogbg-molhiv,

Table 2: Statistics of the three graph classification datasets studied in our evaluation.

Name	Number of graphs	Avg. nodes/graph	Avg. edges/graph	Metric
ogbg-molhiv	41, 127	25.5	27.5	ROC-AUC
ogbg-molpcba	437, 929	26.0	28.1	Avg. precision
ogbg-ppa	158, 100	243.4	2, 266.1	Accuracy
ogbg-code2	452, 741	125.2	124.2	F ₁ score

Table 3: Comparative evaluation performance on the four datasets studied. Our baseline model is a GIN [56], using exactly the same implementation as in [57].

Model	ogbg-molhiv	ogbg-molpcba	ogbg-ppa	ogbg-code2
GIN	0.7558 ± 0.0140	0.2266 ± 0.0028	0.6892 ± 0.0100	0.1495 ± 0.0023
GIN + EGP	0.7934 ± 0.0035	0.2329 ± 0.0019	0.7027 ± 0.0159	0.1497 ± 0.0015

ogbg-molpcba, ogbg-ppa and ogbg-code2. The first two are among the largest molecule property prediction datasets in the MoleculeNet benchmark [58]. The third dataset is concerned with classifying species into their taxa, from their protein-protein association networks [59, 60] given as input. The fourth dataset is a *code summarisation* task: it requires predicting the tokens in the name of a Python method, given the abstract syntax tree (AST) of its implementation.

We provide a summary of important dataset statistics in Table 2; please see [57] for detailed information on the data. These datasets are designed to span a wide variety of domains (virtual drug screening, molecular activity prediction, protein-protein interactions, code summarisation) and sizes (from small molecules to very large syntax trees—the largest graph in ogbg-code2 has 36, 123 nodes).

Models In all four datasets, we want to *directly* evaluate the empirical gain of introducing an EGP layer and completely rule out any effects from parameter count, or similar architectural decisions.

To enable this, we take inspiration from the experimental setup of [18]. Our baseline model is the GIN [56], with hyperparameters as given by [57]. We use the *official* publicly available model implementation from the OGB authors [57], and modify all *even* layers of the architecture to operate over the appropriately-sampled Cayley graph.

Note that our construction leaves both the parameter count and latent dimension of the model *unchanged*, hence any benefits coming from optimising those have been diminished.

Results The results of our evaluation are presented in Table 3. It can be observed that, in all four cases, propagating information over the Cayley graph yields improvements in mean performance—these improvements are most apparent on ogbg-molhiv, where our approach significantly outperforms even the “virtual node” version of GIN, which uses $\sim 1.8\times$ more parameters and achieves 0.7707 ± 0.0149 AUC [57]. We believe that these results provide encouraging empirical evidence that propagating information over Cayley graphs is an elegant idea for alleviating bottlenecks.

7 Conclusion

In this paper, we have presented expander graph propagation (EGP), a novel and elegant approach to alleviating bottlenecks in graph representation learning, which provably supports global communication while not requiring quadratic complexity or dedicated preprocessing of the input.

To this end, we offered a detailed theoretical overview of Cayley graphs of special linear groups, $\text{Cay}(\text{SL}(2, \mathbb{Z}_n); S_n)$. We cite proofs that these graphs have highly favourable properties for information propagation in graph neural networks: they are sparse and 4-regular, they have logarithmic diameter, and they can be efficiently precomputed by a simple procedure that does not rely on the input structure. We show that, in spite of having negatively curved edges, our findings do not violate any prior results on understanding oversquashing via curvature. Even under a simple intervention—interleaving EGP layers inbetween standard GNN layers—we have been able to recover significant performance returns without changing the parameter count or latent space dimensionality.

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507 A Proof of Proposition 11

Let s be one of

$$\begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}, \quad \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}.$$

508 Let $n, n' > 18$ and let e and e' be s -labelled edges in G_n and $G_{n'}$. Then there is a graph isomorphism
 509 between $N_2(e)$ and $N_2(e')$ taking e to e' .

510 *Proof.* Note first that, by the homogeneity of the Cayley graphs G_n and $G_{n'}$, we may assume that e
 511 and e' emanate from the identity vertex of each graph.

Let G_∞ be the Cayley graph of $\text{SL}(2, \mathbb{Z})$ with respect to the generators

$$S_\infty = \left\{ \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix} \right\}.$$

Let e_∞ be the s -labelled edge emanating from the identity vertex of G_∞ . The quotient homomorphism

$$\text{SL}(2, \mathbb{Z}) \rightarrow \text{SL}(2, \mathbb{Z}_n)$$

induces a graph homomorphism $G_\infty \rightarrow G_n$ sending e_∞ to e . We will show that it restricts to a graph
 isomorphism

$$N_2(e_\infty) \rightarrow N_2(e).$$

512 As there is a similar graph isomorphism $N_2(e_\infty) \rightarrow N_2(e')$, the proposition will follow.

Note that two elements of $\text{SL}(2, \mathbb{Z})$ map to the same element of $\text{SL}(2, \mathbb{Z}_n)$ if and only if they differ
 by multiplication by an element of the kernel K_n . This is

$$K_n = \left\{ \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \text{SL}(2, \mathbb{Z}) : a \equiv d \equiv 1 \pmod{n} \text{ and } b \equiv c \equiv 0 \pmod{n} \right\}.$$

513 The graph homomorphism sends edges to edges, and so it is distance non-increasing. Hence it
 514 certainly sends $N_2(e_\infty)$ to $N_2(e)$. It is also clearly surjective, because any element of $N_2(e)$ is
 515 reached from an endpoint of e by a path of length at most 2, and there is a corresponding path in
 516 $N_2(e_\infty)$.

517 We just need to show that this is an injection. If not, then two distinct vertices g_1 and g_2 in $N_2(e_\infty)$
 518 map to the same vertex in $N_2(e)$. Note then that as elements of $\text{SL}(2, \mathbb{Z})$, $g_2 = g_1 k$ for some $k \in K_n$.
 519 There are paths with length at most 3 joining the identity 1 to g_1 and g_2 respectively. Hence, the
 520 distance in G_∞ between g_1 and g_2 is at most 6. Therefore, the distance between 1 and $g_1^{-1}g_2$ is at
 521 most 6. This element $g_1^{-1}g_2$ lies in K_n . We will show that when $n > 18$, the only element of K_n
 522 that has distance at most 6 from the identity is the identity itself. This will imply that $g_1^{-1}g_2 = 1$ and
 523 hence $g_1 = g_2$. But this contradicts the assumption that g_1 and g_2 are distinct vertices. Our argument
 524 follows that of [61].

The operator norm $\|A\|$ of a matrix $A \in \text{SL}(2, \mathbb{Z})$ is

$$\|A\| = \sup\{|A(v)| : v \in \mathbb{R}^2, |v| = 1\}.$$

This is submultiplicative: $\|AB\| \leq \|A\| \|B\|$ for matrices A and B . It can be calculated as the square root of the largest eigenvalue of $A^t A$. In our case, the operator norms satisfy

$$\left\| \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} \right\| = \left\| \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix} \right\| = \frac{1 + \sqrt{5}}{2}.$$

Consider an element

$$K = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

of K_n that is not the identity. Since $a \equiv d \equiv 1$ modulo n and $b \equiv c \equiv 0$ modulo n , we deduce that at least one $|a|$, $|b|$, $|c|$ and $|d|$ is at least $n - 1$. Therefore, this matrix acts on one of the vectors $(1, 0)^t$ or $(0, 1)^t$ by scaling its length by at least $n - 1$. Therefore, $\|K\| \geq n - 1$. Suppose now that K has distance at most 6 from the identity. Then K can be written as a word in the generators of $\text{SL}(2, \mathbb{Z})$ with length at most 6. Therefore, we obtain the inequality

$$\|K\| \leq \left(\frac{1 + \sqrt{5}}{2} \right)^6 < 17.95.$$

525 Hence, $n < 18.95$ and therefore, as n is integral, $n \leq 18$. □

526 B Proof of Theorem 13

527 For any $\delta > 0$ and $\Delta > 0$, there are only finitely many graphs with maximum vertex degree Δ ,
528 Cheeger constant at least δ and non-negative Ollivier curvature.

529 *Proof.* This is a consequence of the main result of Salez [55, Theorem 3]. This states if $G_n =$
530 (V_n, E_n) is a sequence of graphs with the following properties:

$$\sup_{n \geq 1} \left\{ \frac{1}{|V_n|} \sum_{v \in V_n} \deg(v) \log \deg(v) \right\} < \infty \quad (16)$$

531

$$\forall \epsilon > 0, \quad \frac{1}{|E_n|} |\{e \in E_n : \kappa(e) < -\epsilon\}| \rightarrow 0 \text{ as } n \rightarrow \infty, \quad (17)$$

then

$$\forall \rho < 1, \quad \liminf_{n \rightarrow \infty} \left\{ \frac{1}{|V_n|} |\{i : \mu_i(G_n) \geq \rho\}| \right\} > 0.$$

Here, $\kappa(e)$ is the Ollivier curvature of an edge e and

$$1 = \mu_0(G) \geq \mu_1(G) \geq \dots \geq 0$$

are the eigenvalues of the lazy random walk operator. To prove the theorem, we suppose that on the contrary, there are infinitely many distinct graphs $G_n = (V_n, E_n)$ with maximum vertex degree Δ , Cheeger constant at least δ and non-negative Ollivier curvature. Then

$$\sum_{v \in V_n} \deg(v) \log \deg(v) \leq |V_n| \Delta \log \Delta$$

and so condition 16 is satisfied. Condition 17 is trivially satisfied because the Ollivier curvature of each graph is non-negative. Thus, we deduce that the conclusion of Salez' theorem holds. Setting $\rho = 1 - (\delta^2/4\Delta^2)$, we deduce that a definite proportion of the eigenvalues of the lazy random walk operator are at least $1 - (\delta^2/4\Delta^2)$. In particular, $\mu_1(G_n) \geq 1 - (\delta^2/4\Delta^2)$. Denote the eigenvalues of the normalised Laplacian by

$$0 = \lambda'_0(G_n) \leq \lambda'_1(G_n) \leq \dots$$

These are related to the eigenvalues of the lazy random walk operator by $\lambda'_i(G_n) = 2 - 2\mu_i(G_n)$. Hence, $\lambda'_1(G_n) \leq \delta^2/(2\Delta^2)$. There is a variation of Cheeger's inequality that relates λ'_1 to the *conductance* of the graph. To define this, one considers subsets A of the vertex set, and defines their *volume* to be $\text{vol}(A) = \sum_{v \in A} \deg(v)$. The conductance $\phi(G)$ of a graph G is

$$\phi(G) = \min \left\{ \frac{|\partial A|}{\text{vol}(A)} : A \subset V(G), 0 < \text{vol}(A) \leq \text{vol}(V(G))/2 \right\}.$$

Then, by Chung [42, Theorem 2.2],

$$\phi(G) \leq \sqrt{2\lambda_1(G)}$$

Hence, in our case,

$$\phi(G_n) \leq \delta/\Delta.$$

Consider any subset A_n of the vertex set that realises $\phi(G_n)$. Thus $0 < \text{vol}(A_n) \leq \text{vol}(V_n)/2$ and $|\partial A_n|/\text{vol}(A_n) = \phi(G_n) \leq \delta/\Delta$. If A_n is at most half the vertices of G_n , then this implies that the Cheeger constant $h(G_n) \leq \delta$. On the other hand, if A_n is more than half the vertices of G_n , we consider its complement A_n^c . Its cardinality $|A_n^c|$ satisfies

$$|A_n^c| \geq \text{vol}(A_n^c)/\Delta.$$

Hence,

$$h(G_n) \leq \frac{|\partial A_n^c|}{|A_n^c|} \leq \frac{|\partial A_n|\Delta}{\text{vol}(A_n^c)} \leq \frac{|\partial A_n|\Delta}{\text{vol}(A_n)} = \phi(G_n)\Delta \leq \delta.$$

532 In either case, we deduce that the Cheeger constant of G_n is at most δ , contradicting one of our
 533 hypotheses. Hence, there must have been only finitely many graphs satisfying the conditions of the
 534 theorem. \square

535 C Cayley graph at infinity is quasi-isometric to a tree

536 As all vertices of G_n look the same, we focus attention on $N_r(1)$, the r -neighbourhood of the identity
 537 vertex. The proof of Proposition 11 immediately gives the following.

Proposition 18. *Let r be a positive integer satisfying*

$$r < \frac{1}{2} \left(\log \left(\frac{1 + \sqrt{5}}{2} \right) \right)^{-1} \log(n - 1).$$

538 *Then there is a graph isomorphism between the r -neighbourhood of the identity vertex in G_n and*
 539 *the r -neighbourhood of the identity vertex in G_∞ . This isomorphism takes the identity vertex to the*
 540 *identity vertex.*

Proof. As shown in the proof of Proposition 11, there is a graph homomorphism from $N_r(1)$ in G_∞ to $N_r(1)$ in G_n that is a surjection. If it fails to be an injection, then there is a non-trivial element K in the kernel K_n of $\text{SL}(2, \mathbb{Z}) \rightarrow \text{SL}(2, \mathbb{Z}_n)$ satisfying

$$\|K\| \leq \left(\frac{1 + \sqrt{5}}{2} \right)^{2r}.$$

But any non-trivial element K in K_n satisfies

$$\|K\| \geq n - 1.$$

541 Rearranging gives the required inequality. \square

542 This raises the question of the local structure of G_∞ . The answer is well-known: it is ‘tree-like’.
 543 Specifically, it is quasi-isometric to a tree. The formal definition of quasi-isometry is as follows.

544 **Definition 19.** A *quasi-isometry* between two metric spaces (X_1, d_1) and (X_2, d_2) is a function
 545 $f: X_1 \rightarrow X_2$ that satisfies the following two conditions:

1. there are constants $c, C > 0$ such that, for every $x, x' \in X_1$

$$c d_1(x, x') - c \leq d_2(f(x), f(x')) \leq C d_1(x, x') + C,$$

- 546 2. there is a constant $K \geq 0$ such that for every $y \in X_2$, there is an $x \in X_1$ with $d_2(f(x), y) \leq K$.

547 If there is such a quasi-isometry, we say that (X_1, d_1) and (X_2, d_2) are *quasi-isometric*.

548 This forms an equivalence relation on metric spaces. When two metric spaces are quasi-isometric,
 549 they are viewed as being ‘essentially the same’ at large scales.

550 When S and S' are finite generating sets for a group Γ , the graphs $\text{Cay}(\Gamma; S)$ and $\text{Cay}(\Gamma; S')$ are
 551 quasi-isometric. Hence, the quasi-isometry type of a finitely generated group is well-defined, and this
 552 is the central object of study in geometric group theory.

553 The group $\text{SL}(2, \mathbb{Z})$ has a finite-index subgroup that is a free group F [62]. If S' denotes a free
 554 generating set for F , then $\text{Cay}(F; S')$ is a tree. As passing to a finite-index subgroup preserves
 555 its quasi-isometry class, we deduce that the Cayley graph $G_\infty = \text{Cay}(\text{SL}(2, \mathbb{Z}); S_\infty)$ is indeed
 556 quasi-isometric to a tree, as claimed above.

557 D Mixing time properties of expander graphs

558 Expanders are well known to have small mixing time, in the following sense.

559 Let G be a graph. We will consider probability distributions π on $V(G)$. The lazy random walk
 560 operator M acts on probability distributions as follows. We think of $\pi(v)$ as being the probability of
 561 the random walk being at vertex v . If the current location of the walk is at v , then at the next step
 562 of the walk, either we stay put with probability $1/2$ or we move to one of its neighbours with equal
 563 probability. Then $M\pi$ is the new probability distribution.

564 In the case when G is k -regular, this takes a particular simple form. The operator M is represented by
 565 the matrix $(1/2)I + (1/2k)A$, where A is the adjacency matrix. In that case, any initial distribution
 566 π converges under powers of M to the uniform distribution.

This is true for any reasonable notion of convergence, but we will use the $\|\cdot\|_1$ norm, where for two probability distributions π and π' ,

$$\|\pi - \pi'\|_1 = \sum_{v \in V(G)} |\pi(v) - \pi'(v)|.$$

Definition 20. The *mixing time* for a regular graph G is the minimum value of ℓ such that for any starting probability distribution π on the vertex set of G ,

$$\|M^\ell \pi - u\|_1 \leq \frac{1}{4}.$$

567 Here, u is the uniform probability distribution on the vertex set, and M is the lazy random walk
 568 operator.

569 Expanders have small mixing times in the following very strong sense.

570 **Theorem 21.** For any $k > 0$ and $\delta > 0$, there is a constant $c > 0$ with the following property. If G is
 571 a connected k -regular graph on n vertices with Cheeger constant at least $\delta > 0$, then the mixing time
 572 for G is at most $c \log(n)$.