Exponentially Improving the Complexity of Simulating the Weisfeiler-Lehman Test with Graph Neural Networks

Anders Aamand
MIT
aamand@mit.edu

Justin Y. Chen
MIT
justc@mit.edu

Piotr Indyk
MIT
indyk@mit.edu

Shyam Narayanan
MIT
shyamsn@mit.edu

Nicholas Schiefer
MIT
schiefer@mit.edu

Ronitt Rubinfeld
MIT
ronitt@mit.edu

Sandeep Silwal
MIT
silwal@mit.edu

Tal Wagner[*]
Amazon AWS
tal.wagner@gmail.com

Abstract

Recent work shows that the expressive power of Graph Neural Networks (GNNs) in distinguishing non-isomorphic graphs is exactly the same as that of the Weisfeiler-Lehman (WL) graph test. In particular, they show that the WL test can be simulated by GNNs. However, those simulations involve neural networks for the "combine" function of size polynomial or even exponential in the number of graph nodes n, as well as feature vectors of length linear in n.

We present an improved simulation of the WL test on GNNs with *exponentially* lower complexity. In particular, the neural network implementing the combine function in each node has only $\mathrm{polylog}(n)$ parameters, and the feature vectors exchanged by the nodes of GNN consists of only $O(\log n)$ bits. We also give logarithmic lower bounds for the feature vector length and the size of the neural networks, showing the (near)-optimality of our construction.

1 Introduction

Graph Neural Networks (GNNs) have become a popular tool for machine learning on graph-structured data, with applications in social network prediction [HYL17], traffic prediction [YYZ18], recommender systems [YHC+18], drug discovery [WKK+20], computer vision [LGD+19, FLM+19, MBM+17, QSMG17], and combinatorial optimization [CCK+21]. Standard message passing GNNs use the topology of the input graph to define the network structure: in each step k, a node aggregates messages from each of its neighbors and combines them using a function $\phi^{(k)}$, computed by a neural network, to determine its message for the next round. Crucially, the aggregation function must be *symmetric*, to ensure that the output of GNNs is invariant under node permutation. This restriction raised questions about how expressive such network architectures are, and in particular what classes of graphs are distinguishable using GNNs.

The seminal works of Xu et al. [XHLJ19] and Morris et al. [MRF+19] (see also [Gro21]) showed that GNNs are exactly as powerful in distinguishing graphs as the Weisfeiler-Lehman (WL) test [WL68], also known as *color refinement*. This combinatorial procedure is a necessary but not sufficient test for graph isomorphism. It proceeds in repeated rounds: in each round, a node labels itself with the "hash" of the multiset of labels of its neighbors. The aforementioned papers show that (i) GNNs can simulate the WL test and (ii) GNNs can only distinguish those graphs that the WL test determines to be different. This provides a complete characterization of the expressive power of GNN architectures.

[*] Work done prior to joining Amazon.

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Table 1: Our results compared to prior work on GNNs that simulate the WL test.

Construction	Message size	Parameters in $\phi^{(k)}$	Oblivious*	Deterministic*
Xu et al. [XHLJ19]	$O(n)$	$\Omega(2^n)$	Yes	Yes
Morris et al. [MRF+19]	$O(n)$	$\text{poly}(n)$	No	Yes
This paper	$O(\log n)$	$\text{polylog}(n)$	Yes	No

* Oblivious designs use the same weights for any input graph. Non-deterministic constructions require some weights to be assigned by random samples drawn from some distribution, and may err with small probability.

The connection between GNNs and the WL test has spawned a wave of new results studying GNN variants that either match the distinguishing power of the WL test or adopt new methods beyond message passing on the edges of the input graph to overcome this barrier (see the excellent surveys [MFK21, MLM+21, Gro21] for an overview of this area). However, the results in the original as well the follow up works mostly focus on *qualitative* questions (how expressive GNNs are) as opposed to *quantitative* questions such as the network complexity. In particular, while Xu et al. [XHLJ19] show that there exist GNN architectures that can simulate the WL coloring procedure as long as the aggregation step is injective, they rely on the universal approximation theorem to show that there exists a neural network that can simulate the hash function used in WL. As a result, the size of the network could be exponential in the number of nodes n. In contrast, the construction of Morris et al. [MFK21] uses networks of size polynomial in n. However, the weights of the network implementing $\phi^{(k)}$ in their construction depend on the structure of the underlying graph, which suffices for *node* classification, but is not sufficient for the context of *graph* classification.

Overall, the quantitative understanding of the complexity of simulating WL remains an open problem. Indeed, the survey [Gro21] states *"The size of the GNNs and related parameters like depth and width, which directly affect the complexity of inference and learning, definitely require close attention.*"

Our Results. The main question addressed in this work is: what is the simplest (in terms of the number of neural network units and message length) GNN capable of simulating the WL test? Equivalently, at what point does a GNN become so small that it loses its expressive power?

Our main result is a highly efficient construction of a GNN architecture that is capable of simulating the WL test. For graphs with n nodes, it can simulate $\text{poly}(n)$ steps of the WL test, such that the neural network implementing $\phi^{(k)}$ in each round has $\text{polylog}(n)$ parameters, and the messages exchanged by the nodes of the GNN in each round consist of $O(\log n)$ bits. This offers at least an exponential improvement over the prior bounds obtained in [XHLJ19, MRF+19] (see Table 1), extending the equivalence between the WL test and the expressive power of GNNs to neural networks of reasonable (in fact, quite small) size. Furthermore, our architecture is simple, using vector sum for aggregation and ReLU units for the combine function $\phi^{(k)}$. Finally, our construction can be generalized to yield a depth-size tradeoff: for any integer $t > 0$, we can can construct a neural network of depth $O(t)$ and size $n^{O(1/t)}\,\text{polylog}(n)$.

To achieve this result, our construction is randomized, i.e., some weights of the neural networks are selected at random, and the simulation of the WL test is correct with high probability $1 - 1/\text{poly}(n)$. Thus, our construction can be viewed as creating a *distribution* over neural networks computing the function $\phi^{(k)}$.[2] In particular, this implies that, for each graph, there exists a single neural network implementing $\phi^{(k)}$ that accurately simulates WL on that graph. The size of the network is exponentially smaller than in [MRF+19], although the construction is probabilistic.

We complement this results with two lower bounds for executing a WL iteration. Our first lower bound addresses the *communication complexity* of this problem, and demonstrates that to solve it, each node must communicate labels that are at least $O(\log n)$ bits long, matching the upper bound achieved by our construction. Our second lower bound addresses the *computational complexity*,

[2] Note that selecting $\phi^{(k)}$ at random is quite different from random node initialization, e.g., as investigated in [ACGL21]. In particular, in our model all nodes use *the same* function $\phi^{(k)}$ (with the same parameters), without breaking the permutation invariance property of GNNs, as in the standard GNN model.

namely the parameters of the neural network. It shows that if the messages sent between nodes are vectors with entries in $[F] = \{0, 1, \ldots, F-1\}$, then the network implementing $\phi^{(k)}$ must use $\Omega(\log F)$ ReLU units.

Related work. The equivalence between the discriminative power of GNNs and the WL test has been shown in the aforementioned works [XHLJ19, MRF$^+$19]. A strengthened version of the theorem of [XHLJ19], where the same combine function ϕ is used in all iterations (i.e., $\phi = \phi^{(k)}$ for all k) appeared in the survey [Gro21]. Many works since have studied various representational issues in GNNs; we refer the reader to excellent surveys [Gro21, HV21, MLM$^+$21, Jeg22]. In particular, [Lou19] established connections between GNNs and distributed computing models such as LOCAL and CONGEST, and derived lower bounds for several computational tasks based on this connection. [CVCB19] drew a connection between the expressiveness of GNNs in graph isomorphism testing and in function approximation. [BKM$^+$20] studied the expressiveness of GNNs in computing Boolean node classifiers, and [GMP21] studied the expressiveness of graph convolutional networks (GCNs).

The emergence of WL as a barrier in GNN expressivity has also led to a flurry of work on enhancing their expressivity by means of more general architectures. These include higher-order GNNs inspired by higher-dimensional analogs of WL [MRF$^+$19, MBHSL19], unique node identifiers [Lou19, VLF20], random node initializations [ACGL21, SYK21], relational pooling [MSRR19], incorporating additional information on the graph structure [NM20, BGRR21, BFZB22, CMR21, TRWG21], and more. We refer to [MLM$^+$21] for a comprehensive survey of this line of work.

1.1 Preliminaries

Notation. For the rest of the paper, we use $\mathcal{N}(v)$ to denote the neighborhood of v in a graph $G(V, E)$ *including v itself*, and we use $\{\cdot\}$ to denote *multisets* rather than sets.

GNNs. Let $G = (V, E)$ be a graph with N nodes. GNNs use the graph structure of G to learn node embeddings for all the nodes across multiple iterations. Let $h_v^{(k)}$ denote the embedding vector of node $v \in V$ in the kth iteration. The vectors $h_v^{(0)}$ represent the initial node embeddings. In every iteration $k \geq 1$, each node v sends its current embedding $h_v^{(k-1)}$ to all its neighbors, and then computes its new embedding h_v^k by the equation

$$h_v^{(k)} = \phi^{(k)} \left(f \left(\left\{ h_w^{(k-1)} : w \in \mathcal{N}(v) \right\} \right), h_v^{(k-1)} \right) \tag{1.1}$$

where $\phi^{(k)}$ is implemented by a neural network with ReLU activations (note that $\phi^{(k)}$ may differ across different iterations k). The function f is called the 'aggregate' function, and $\phi^{(k)}$ is called the 'combine' function. The embeddings $h_v^{(K)}$ at the final iteration K can be used for node classification. For graph classification, they can be aggregated into a graph embedding h_G with a 'readout' function,

$$h_G = \text{READOUT}(\{h_v^{(L)} \mid v \in V\}).$$

Weisfeiler-Lehman (WL) Test. The WL test [WL68] is a popular heuristic for the graph isomorphism problem. While the exact complexity of this problem remains unknown [Bab16], the WL test is a powerful heuristic capable of distinguishing a large family of graphs [BK79].

The WL test is as follows. Given a graph $G(V, E)$, initially all nodes are given the same fixed label $\ell_v^{(0)}$, say $\ell_v^{(0)} = 1$ for all $v \in V$. Then, in every iteration $k \geq 1$, each node v is assigned the new label $\ell_v^{(k)} = \text{HASH}(\{\ell_u^{(k-1)} : u \in \mathcal{N}(v)\})$, where HASH is a 1-1 mapping (i.e., different multisets of labels are guaranteed to be hashed into distinct new labels). Performing this procedure on two graphs G, G', the WL test declares them non-isomorphic if the label multiset $\{\ell_v^{(k)} : v \in V\}$ differs between the graphs at some iteration k. Note that the algorithm converges within at most n iterations.

Simulating WL with GNNs. A GNN simulates WL deterministically if the node embeddings $h_v^{(k)}$ at each iteration k constitute valid labels $\ell_v^{(k)}$ for the WL test. We also consider randomized simulation, where the GNN's weights are selected at random and we allow some small failure probability where distinct multisets of labels from iteration $k-1$ are hashed into the same label at iteration k. This is captured by the next definition.

Definition 1.1 (Successful Iteration of the WL Test)**.** *A WL iteration gets existing labels* $\{h_v : v \in V\}$ *for all nodes, and outputs new labels* $\{h'_v : v \in V\}$ *given by*

$$h'_v = \phi\left(f\left(\{h_w : w \in \mathcal{N}(v)\}\right)\right),$$

for an aggregate function f *and neural network* ϕ *with random weights. We say the iteration is* ***successful*** *if for all* $v, u \in V$*, the following holds:*

- *If* $\{h_w : w \in \mathcal{N}(v)\} = \{h_w : w \in \mathcal{N}(u)\}$ *then* $h'_v = h'_u$ *with probability 1, and*
- *If* $\{h_w : w \in \mathcal{N}(v)\} \neq \{h_w : w \in \mathcal{N}(u)\}$ *then* $h'_v \neq h'_u$ *with probability* $1 - p$*,*

where the probability is over the choices of the random weights of ϕ*.*

To ensure the WL simulation is successful across $\text{poly}(n)$ iterations and for all pairs of nodes, we can set failure probability p to $1/\text{poly}(n)$ and apply a union bound (see Prop. A.1 in Appendix A).

1.2 Overview of Our Techniques

In this section we give an overview of our GNN architectures for simulating WL. To explain our ideas in stages, we begin with a simpler construction of a polynomial size GNN. It is far larger than the ultimate polylogarithmic size we are aiming for, but forms a useful intermediate step toward our second and final construction.

Construction 1 (Section 2). Recall that the kth WL iteration, for a node v, aggregates the labels of its neighbors from the previous iteration, $\mathcal{H}_v^{(k-1)} := \{h_w^{(k-1)} : w \in \mathcal{N}(v)\}$, and hashes them into a new label $h_v^{(k)}$ for v. Our GNNs aggregate by summing, i.e., they sum $\mathcal{H}_v^{(k-1)}$ into $\mathcal{S}_v^{(k)} := \sum_{w \in \mathcal{N}(v)} h_w^{(k-1)}$, and then hash the sum into $h_v^{(k)}$ using a ReLU neural network of our choice.

If two nodes u, v satisfy $\mathcal{H}_u^{(k-1)} \neq \mathcal{H}_v^{(k-1)}$, then WL assigns them distinct labels in iteration k, and therefore we want our construction to satisfy $h_u^{(k)} \neq h_v^{(k)}$ with probability at least $1 - p$ (as per Definition 1.1). This can fail in two places: either due to summing (if $\mathcal{S}_u^{(k)} = \mathcal{S}_v^{(k)}$ even though $\mathcal{H}_u^{(k-1)} \neq \mathcal{H}_v^{(k-1)}$) or due to hashing (if $h_u^{(k)} = h_v^{(k)}$ even though $\mathcal{S}_v^{(k)} \neq \mathcal{S}_v^{(k)}$). To avoid the first failure mode (summing), we use one-hot encodings for the node labels, meaning that for every node v and iteration k, $h_v^{(k)}$ is a one-hot vector in $\{0,1\}^F$ (for F to be determined shortly). This ensures that if $\mathcal{H}_u^{(k-1)} \neq \mathcal{H}_v^{(k-1)}$ then $\mathcal{S}_u^{(k)} \neq \mathcal{S}_v^{(k)}$ due to the linear independence of the one-hot vectors. To handle the second failure mode (hashing), we use random hashing into $F = O(1/p)$ buckets, rendering the collision probability no more than p. That is, we let $h_v^{(k)} = \text{One-Hot}(g(\mathcal{S}_v^{(k)}))$ where $g : \mathbb{Z}^F \to \{1, \ldots, F\}$ is chosen at random from an (approximately) universal hash family. We use the simple hash function $g(x) = \langle a, x \rangle \bmod F$ where a is random vector. It can be implemented with a ReLU neural network, since the dot product is just a linear layer, and the mod operation can be implemented with constant width and logarithmic depth, by a reduction to the "triangular wave" construction due to Telgarsky [Tel16] (see Appendix B.1). Finally, we show that turning the index of the hash bucket into a one-hot vector can be done with $O(F)$ ReLU units and constant depth.

Since our desired collision probability is $p = 1/\text{poly}(n)$, we set $F = O(1/p) = \text{poly}(n)$. Since our one-hot vectors are of dimension F, the resulting GNN has width $F = \text{poly}(n)$ (and depth $O(\log n)$ due to implementing the mod operation with ReLUs), and thus total size $\text{poly}(n)$.

Construction 2 (Section 3). We now proceed to describe our polylogarithmic size construction. The weak point in the previous construction was the wasteful use of one-hot encoding vectors, which caused the width to be F. In the current construction, we still wish to hash into F bins — that is, to have F distinct possible labels in each iteration — but we aim to represent them using bitstrings of length $O(\log F)$, thus exponentially improving the width of the network. That is, for every node v and iteration k, the label $h_v^{(k-1)}$ would now be a vector in $\{0,1\}^{O(\log F)}$. The challenge is again to avoid the two failure modes above, ensuring that the failure probability does not exceed p. Since we cannot use one-hot encoding, we need to devise another method to avoid the first failure mode, i.e., ensure that with high probability $\mathcal{S}_u^{(k)} \neq \mathcal{S}_v^{(k)}$ if $\mathcal{H}_u^{(k-1)} \neq \mathcal{H}_v^{(k-1)}$.

To this end, suppose for a moment that we had access to a truly random vector $a \in \{0,1\}^F$. Then each node v, instead of sending the one-hot encoding of its label $h_v^{(k-1)}$, we could instead send

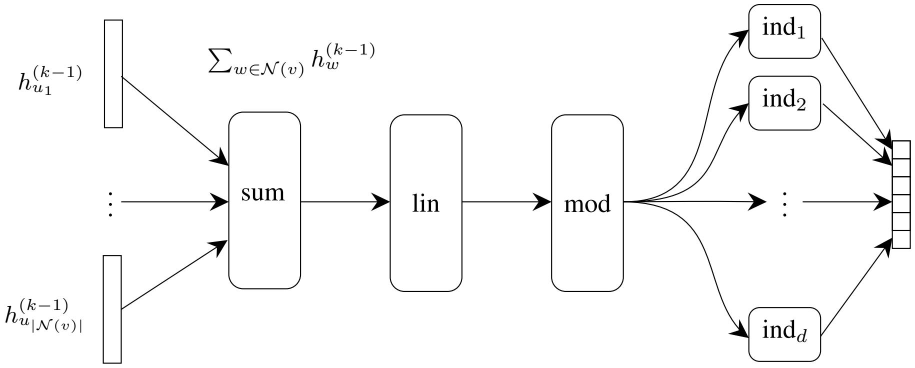

$h_{u_1}^{(k-1)}$
$\sum_{w\in\mathcal{N}(v)} h_w^{(k-1)}$
$h_{u_{|\mathcal{N}(v)|}}^{(k-1)}$
sum
lin
mod
ind_1
ind_2
ind_d

Figure 1: Constructions of our GNNs. Construction 1 (section 2): The layer "sum" sums the input vectors $\{h_w^{(k-1)} : w \in \mathcal{N}(v)\}$. "lin" is a linear layer that computes the dot product with a random vector and outputs a single scalar. "mod" is a neural network that computes the input scalar modulo F, using Theorem 2.2. Each "ind_i" is a neural network that outputs 1 if its input equals i and outputs 0 otherwise, using eq. (2.1). The ith coordinate of the output vector $h_v^{(k)}$ equals the output of ind_i. Construction 2 (section 3): Similar, except that now each ind_i is a neural network that gets an input integer $j \in [F]$ and outputs the jth coordinate of a vector a^i sampled from an ϵ-biased space, using Theorem C.1. This reduces the total number of units of the network from $\text{poly}(n)$ to $\text{polylog}(n)$.

the dot product $\langle a, h_v^{(k-1)}\rangle$, which is the single bit $a_{h_v^{(k-1)}}$. Each node u thus receives the bits $\left\{a_{h_w^{(k-1)}} : w \in \mathcal{N}(w)\right\}$ from its neighbors and aggregates them into the sum $\sum_{w\in\mathcal{N}(u)}\langle a, h_w^{(k-1)}\rangle$, which, by linearity, is equal to $\langle a, \mathcal{S}_u^{(k)}\rangle$ (using the notation from Construction 1). It is easy to observe that if $\mathcal{S}_u^{(k)} \neq \mathcal{S}_v^{(k)}$ then $\langle a, \mathcal{S}_u^{(k)}\rangle \neq \langle a, \mathcal{S}_v^{(k)}\rangle$ with probability at least 0.5. Repeating this process $\log F$ independent times decreases the collision probability to the requisite $1/F$. Thus, we can define a new labeling scheme $\bar{h}_v^{(k)} \in \{0,1\}^{\log F}$ that concatenates $\log F$ dot products with independent random vectors $a^1 \ldots a^{\log F} \in \{0,1\}^F$ as just described, failing at the summing operation with probability at most $1/F$. The second failure mode (hashing) can again be handled as before.

That catch is that, since a has length F, the overall number of parameters in the GNN would again be at least F. To avoid this, we appeal to the computational theory of pseudorandomness. The idea is to replace the random vector a with an efficient pseudorandom analog. Note that the above approach goes through even if the probability that $\langle a, \mathcal{S}_u^{(k)}\rangle \neq \langle a, \mathcal{S}_v^{(k)}\rangle$ is slightly larger than 0.5, say $0.5+\epsilon$ for a small constant ϵ. It is well-known in complexity theory that there exist pseudorandom generators, called *ϵ-biased spaces*, that generate vectors a satisfying this property given only $O(\log F + \log(1/\epsilon))$ truly random bits.[3] Crucially, each bit of a can be computed using a threshold circuit with size polynomial in $O(\log F + \log(1/\epsilon))$ and constant depth (Theorem C.1), which translates to a ReLU neural network with the same parameters (Lemma C.2). Using these generators in our GNN to implement a pseudorandom (ϵ-biased) analog of a yields our final construction.

2 First Construction: Polynomial-size GNN

Our first construction towards Definition 1.1 is exponentially larger compared to our final optimized construction of Section 3. Nevertheless, it is instructive and motivates our optimized construction.

Let $h_u^{(k)}$ denote the label of a vertex u in the kth iteration. For our first construction, we will always maintain the invariant that $h_u^{(k)}$ will be a one-hot encoded vector in $\{0,1\}^F$ for all $u \in V$ and all iterations k. $F > 2n$ will be a prime which also satisfies $F = O(\text{poly}(n))$. As stated previously, the aggregate function f will just be the sum function. Our construction for the neural network used in the kth iteration, $\phi^{(k)}$, will take in the sum of the neighbors labels according to Equation (1.1) and output a one-hot encoded vector in $\{0,1\}^F$.

[3] Technically, they guarantee this property only when $\mathcal{S}_u^{(k)}$ are binary vectors, but Lemma 3.2 shows how to extend this property to general integer vectors as well.

Implementation of Neural Network. Our construction for $\phi^{(k)}$ is the following: First recall the notation from (simplified) Equation 1.1:

$$h_v^{(k)} = \phi^{(k)}\left(f\left(\left\{h_w^{(k-1)} : w \in \mathcal{N}(v)\right\}\right)\right).$$

1. For every node v, the input to $\phi^{(k)}$ is the sum of feature vectors of neighbors from the prior iteration, $\sum_{w \in \mathcal{N}(v)} h_w^{(k-1)}$, which is returned by the summing function f. Given any such input $x \in \mathbb{Z}^F$, $\phi^{(k)}$ computes the inner product of x with a vector $a \in \mathbb{Z}^F$ where each entry of a is a uniformly random integer in $[F] := \{0, \ldots, F-1\}$.
2. $\phi^{(k)}$ then computes $\langle x, a\rangle \bmod F$.
3. Finally, we represent the value of $z = \langle x, a\rangle$ as a one-hot encoded vector in $\mathbb{Z}^F$ where the z-th entry is equal to 1 and all other entries are 0's.

Altogether, $\phi^{(k)}$ can be summarized as: $h_v^{(k)} = \text{One-Hot}\left(\left\langle \sum_{w \in \mathcal{N}(v)} h_w^{(k-1)}, a\right\rangle \bmod F\right)$.

Note that we set the initial labels $h_u^{(0)}$ to be the same starting vector for all vertices (any one-hot vector). This matches the WL test which also initializes all nodes with the same initial label. Furthermore, the weights of $\phi^{(k)}$ are independent: the random vector a is sampled independently for each iteration.

Correctness of Construction. The following lemma proves that the above construction satisfies the requirement of Definition 1.1. Its proof is given in Appendix B.

Lemma 2.1. *Let $\{h_w^{(k-1)} : w \in \mathcal{N}(v)\}$ and $\{h_w^{(k-1)} : w \in \mathcal{N}(u)\}$ denote the multiset of neighborhood labels for vertices v and u respectively. If the multisets are distinct then the labels computed for v and u in the kth iteration are the same with probability at most $O(1/F)$. If the multisets are the same then the labels are the same, i.e., the kth iteration is successful according to Definition 1.1.*

Complexity of the GNN. We now evaluate the size complexity of implementing our construction via a neural network ϕ. Note that Step 1 of the construction can be done with 1 layer as it simply involves taking an inner product. The main challenge is to implement the modulo function. We give the following construction in Section B.1 of the appendix.

Theorem 2.2. *Suppose $F = \text{poly}(n)$. There exists an explicit construction of a network which computes modulo F in the domain $\{0, \ldots, nF\}$ using a ReLU network with $O(\log n)$ hidden units and $O(\log n)$ depth. More generally, given an integer parameter $t > 0$, the function can be computed with $O((Fn)^{O(1/t)} \log n)$ hidden units and $O(t)$ depth.*

Directly appealing to the theorem above, we can implement modulo F required in Step 2 of the construction using a neural network with $O(\log n)$ units, depth $O(\log n)$. In addition, we need only $O(\log n)$ bits to represent the weights.

Finally, Step 3 of our construction requires outputting a one hot encoding. We can do this by inputting z (the output of Step 2 of the construction) into F indicator functions, each of which detect if z is equal to a particular integer in $[F]$. Each indicator function can be implemented via $O(1)$ ReLU nodes as follows. Let

$$g(x) = \text{ReLU}(\min(-\text{ReLU}(2x - 1/2) + 1, \text{ReLU}(2x + 1))) \tag{2.1}$$

which can be easily implemented as a ReLU network. (Note $\min(a, b) = a + b - \max(a, b)$ and $\max(a, b) = \max(a - b, 0) + b = \text{ReLU}(a - b) + b$.) It can be checked that $g(0) = 1$ and $g(x) = 0$ for all other integers $x \neq 0$ and that g can be implemented with $O(1)$ ReLU function compositions. Thus, Step 3 of the construction requires $O(1)$ hidden layers and $O(F)$ total hidden units. Altogether we have proven the following result.

Theorem 2.3. *There exists a construction of a neural network ϕ which performs a successful iteration according to Definition 1.1 with failure probability $p = O(1/|F|)$. ϕ has depth $O(\log n)$, $O(F)$ hidden units, and requires $O(\log(nF))$ bits of precision. Furthermore, all labels in all iterations are vectors in $\{0, 1\}^F$. More generally, given an integer parameter $t > 0$, the function can be computed with $n^{O(1/t)}\,\text{polylog}(n)$ hidden units and $O(t)$ depth.*

Remark 2.4. *In the standard WL test, the number of iterations is chosen to be $O(n)$. Thus the right setting of F in Theorem 2.3 is $F = O(\mathrm{poly}(n))$ which gives us depth $O(\log n)$, $O(\mathrm{poly}(n))$ hidden units, and requires $O(\log n)$ bits of precision in addition to labels in dimension $O(\mathrm{poly}(n))$.*

3 Second Construction: Polylogarithmic-size GNN via Pseudo-randomness

We now present a more efficient construction of a GNN which simulates the WL test with an exponential improvement in the number of hidden units and label size. To motivate the improvement, we consider Step 3 of the prior construction which outputs a one-hot encoding. The one-hot encoding was useful as it allowed us to index into a uniformly random vector a (which we then sum over mod F in order to hash the neighborhood's labels). However, this limited us to use feature vectors of a large dimension and required many hidden units to create one-hot vectors. Instead of working with one-hot encodings as an intermediary, we will directly compute the entries of the random vector a as needed. This has two advantages: we can significantly reduce the dimension of the feature vectors as well as reduce the total size of the neural networks used. We accomplish this via using *pseudo-random* vectors whose entries can be generated as needed with a small ReLU neural network (see Corollary 3.3). This allows us to use node labels in dimension $O(\log n)$ as opposed to $O(n)$.

The random vectors we employ have their entries generated from an ε-biased sample space. These are random vectors which are approximately uniform and they have been well-studied in the complexity-theory literature. We recall some definitions below.

Definition 3.1 (Bias)**.** *Let X be a probability distribution over $\{0,1\}^m$. The bias of X with respect to a set of indices $I \subseteq \{1,\dots,m\}$ is defined as* $\mathrm{bias}_I(X) = \left|\mathbb{P}_{x\sim X}\left[\sum_{i\in I} x_i = 0\right] - \mathbb{P}_{x\sim X}\left[\sum_{i\in I} x_i = 1\right]\right|$ *where each sum is taken modulo 2 and the empty sum is defined to be 0.*

Definition 3.2 (ε-biased Sample Space)**.** *A probability distribution over $\{0,1\}^m$ is called an ε-biased sample space if* $\mathrm{bias}_I(X) \le \varepsilon$ *holds for all non-empty subsets $I \subseteq \{1,\dots,m\}$.*

Note that the uniform distribution has bias 0. We now state our construction for the neural network used in the kth iteration, $\phi^{(k)}$. We recall that $h_u^{(k)}$ denotes the label of a vertex u in the kth iteration.

Implementation of Neural Network. Our construction for $\phi^{(k)}$ is the following:

1. The input vectors of $\phi^{(k)}$, which are of the form $h_v^{(k-1)}$ for the kth iteration, are each assumed to be a feature vector in $\mathbb{Z}^{C\log n}$ for a sufficiently large constant C. The output of $\phi^{(k)}$ will also be a feature vector in $\mathbb{Z}^{C\log n}$. Our aggregation function f will again be the summation function.
2. Let F be a prime of size $\mathrm{poly}(n)$ which is at least $2n$.
3. For each node v, $\phi^{(k)}$ computes $z_v = \langle b, \sum_{w\in\mathcal{N}(v)} h_w^{(k-1)}\rangle \bmod F$ where every entry of b is uniformly random in $\{0,\dots,F-1\}$. Note $\sum_{w\in\mathcal{N}(v)} h_w^{(k-1)}$ is the output of the aggregation f.
4. Let $a^t \in \{0,1\}^F$ for $t = 1,\dots,C\log n$ be vectors which are independently drawn from an ε-biased sample space for a sufficiently small constant ε.
5. The output $h_v^{(k)}$ will be a $C\log n$ dimensional binary vector where the t-th coordinate is equal to the z_v-th coordinate of the vector a^t. In other words, $h_v^{(k)} = (a^t(z_v))_{t=1}^{C\log n}$ where $a^t(z_v)$ denotes the z_v-th coordinate of a^t.

Correctness of Construction. We now prove the correctness of our construction. We will refer to z_v computed in Step 3 of the construction as the *index* of v for the kth iteration. To prove the correctness of the above construction, it suffices to prove the lemma below which shows our construction satisfies Definition 1.1.

Lemma 3.1. *Let $\{h_w^{(k-1)} : w \in \mathcal{N}(v)\}$ and $\{h_w^{(k-1)} : w \in \mathcal{N}(u)\}$ denote the multiset of neighborhood labels for vertices v and u respectively. If the multisets are distinct then the labels computed for v and u in the kth iteration are distinct with probability $1 - 1/\mathrm{poly}(n)$. If the multisets are the same then the labels are the same, i.e., the kth iteration is successful according to Definition 1.1.*

We first need the following auxiliary lemma about ε-biased sample spaces, proven in Section C.

Lemma 3.2. *Let $\mathcal{D}$ be a probability distribution over $\{0,1\}^m$ that is an ε-biased sample space. Then, for any $x, y \in \mathbb{Z}^m$ such that $x \neq y$, $\mathbb{P}_{a \sim \mathcal{D}}[\langle a, x\rangle = \langle a, y\rangle] \leq \frac{1}{2} + \frac{\varepsilon}{2}$.*

Note that this lemma is necessary, as we will be computing dot products of a with integer vectors (over integers), not with binary vectors modulo 2.

We are now ready to prove Lemma 3.1.

Proof of Lemma 3.1. Let $x' = \sum_{w \in \mathcal{N}(v)} h_w^{(k-1)}$ denote the input for v and analogously, define $y' = \sum_{w \in \mathcal{N}(u)} h_w^{(k-1)}$ to be the input for u. We first show that if $\{h_w^{(k-1)} : w \in \mathcal{N}(v)\}$ is not equal to (as multisets) $\{h_w^{(k-1)} : w \in \mathcal{N}(u)\}$ then $x' \neq y'$ with sufficiently large probability. We further consider the case that $k \geq 2$ since for $k = 1$ (the first iteration), the statement follows since all node labels are initialized to be the same. Let z'_v be the indices computed in Step 3 of iteration $k-1$ (which are used to construct the node labels $h_v^{(k-1)}$ in iteration $k-1$). Note that there is a one to one mapping between z'_v and $h_v^{(k-1)}$. Thus we can assume $\{z'_w : w \in \mathcal{N}(v)\} \neq \{z'_w : w \in \mathcal{N}(u)\}$ without loss of generality.

Let $\tilde{a}^1$ be the first ε-biased vector used in the previous neural network $\phi^{(k-1)}$. Note that the first entry of x' is equal to $\sum_{w \in \mathcal{N}(v)} \tilde{a}^1(z_w)$, i.e., it is the dot product of $\tilde{a}^1$ with a suitable vector x which is the sum of one-hot encoding of the neighborhood of v. The same statement is true for y': the first entry of y' is equal to the dot product of $\tilde{a}^1$ with a vector y which represents the one-hot encoding of the neighborhood of u. This is because we computed the index z'_v of every node in the previous iteration, as defined in Step 3 of the construction, and passed along the coordinate of $\tilde{a}^1$ which corresponds to this computed index. By assumption, we know that $x \neq y$. Therefore by Lemma 3.2, we have that $\mathbb{P}_{\tilde{a}^1}[(x')_1 = (y')_1] = \mathbb{P}_{\tilde{a}^1}(\langle \tilde{a}^1, x\rangle = \langle \tilde{a}^1, y\rangle) \leq 2/3$ for a suitable ε. By independence of vectors $\tilde{a}^t$, it follows that $\mathbb{P}[x' = y'] \leq (2/3)^{C \log n} \leq 1/\operatorname{poly}(n)$ for a suitable constant $C > 0$.

We now condition on $x' \neq y'$. Without loss of generality, suppose that their first coordinates, x'_1 and y'_1, differ. We know $x'_1 \neq y'_1 \bmod F$ since $x'_1 \neq y'_1$, they are both non-negative and bounded by n, and $|x'_1 - y'_1| \leq O(n)$ whereas F is a prime at least $2n$. It follows that the probability of the event $\langle (x' - y'), b\rangle = 0 \bmod F$ is at most $1/F$. To see this, condition on all the entries of b except b_1. Then $(x' - y')_1 \cdot b_1$ must be equal to a specific value modulo F for $\langle (x' - y'), b\rangle = 0 \bmod F$ to hold, as desired. We now condition on this event which equivalently means we condition on $z_v \neq z_u$ (see Step 3 of the construction).

Now our task is to show that $h_v^{(k)} \neq h_u^{(k)}$ with sufficiently high probability. The first coordinate of $h_v^{(k)}$ is equal to $\langle a^1, e_{z_v}\rangle$ where a^1 is the first ε-biased vector considered in Step 4 of the construction and e_{z_v} is the basis vector in dimension $C \log n$ which has a 1 entry only in the z_v coordinate and 0 otherwise. Therefore by Lemma 3.2, we have that , $\mathbb{P}_{a^1}[(h_v^{(k)})_1 = (h_u^{(k)})_1] = \mathbb{P}_{a^1}[\langle a^1, e_{z_v}\rangle = \langle a^1, e_{z_u}\rangle] \leq 2/3$ for a suitable choice of ε since e_{z_u} and e_{z_v} are distinct. By independence of vectors a^t, it follows that $\mathbb{P}[h_v^{(k)} = h_u^{(k)}] \leq (2/3)^{C \log n} \leq 1/\operatorname{poly}(n)$ for a suitable constant $C > 0$. This exactly means that the node labels of u and v in the next iteration are different with probability at least $1 - 1/\operatorname{poly}(n)$, as desired. Lastly, it is clear that if the multiset of neighborhood labels of u and v are the same, then $x' = y'$ and it's always the case that $h_v^{(k)} = h_u^{(k)}$. □

Complexity of the GNN. We now analyze the overall complexity of representing $\phi^{(k)}$ as a ReLU neural network. First we state guarantees on generating ε-based vectors using a ReLU network. The following corollary is proven in Appendix C.

Corollary 3.3. *Let $s = O(\log F + \log(1/\varepsilon))$. For every ε and F, there exists an explicit ReLU network $C : \{0,1\}^s \cup [F] \to \{0,1\}^F$ which takes as input s uniform random bits and an index $i \in F$ and outputs the ith coordinate of an ε-biased vector in $\{0,1\}^F$. C uses $O(\log F)$ bits of precision and has $\operatorname{poly}(s)$ hidden units. More generally, given an integer parameter $t > 0$, the function can be computed with $n^{O(1/t)} \operatorname{polylog}(n)$ hidden units and $O(t)$ depth.*

We can now analyze the complexity of our construction. The complexity can be computed by analyzing each step of the construction separately as follows:

1. For every node v, the sum of feature vectors of neighbors from the prior iteration, $\sum_{w \in \mathcal{N}(v)} h_w^{(k-1)}$, is returned by the aggregate function f.
2. The inner product with the random vector b in Step 3 of the construction can be computed using one layer of the network. Then computing modulo F can be constructed via Theorem 2.2.
3. Given the inner product value z_v which is the output of Step 3 of the construction, we compute all of the $O(\log n)$ coordinates of $h_v^{(k)}$ in parallel. We recall that each coordinate of $h_v^{(k)}$ is indexing onto $O(\log n)$ ε-biased random vectors and we use the *same* index for all vectors, namely the z_v-th index. This can be done as follows. We first have $O(\log n)$ edges fanning-out from the node which computes z_v. For all $t = 1, \ldots, O(\log n)$, the other endpoint of the t-th fan-out edge computes the value $a^t(z_v)$ where a^t is the t-th ε-biased vector as stated in Steps 4 and 5 of the construction. This can be done by appealing to the construction guaranteed by Corollary 3.3. The result of this computation is exactly $h_v^{(k)}$.

Altogether, we have proven the following theorem.

Theorem 3.4. *There exists a construction of ϕ which performs a successful WL iteration according to Definition 1.1 with $p \leq 1/\operatorname{poly}(n)$. ϕ has depth $O(\log n)$, $O(\operatorname{poly}(\log n))$ hidden units, and requires $O(\log n)$ bits of precision. All labels in all iterations are binary vectors in $\{0,1\}^{O(\log n)}$. More generally, given an integer parameter $t > 0$, the function can be computed with $n^{O(1/t)} \operatorname{polylog}(n)$ hidden units and $O(t)$ depth.*

4 Lower Bounds

We complement our construction with lower bounds on the label size and number of ReLU units required to simulate the WL test. We outline these two lower bounds below and defer the full details to Appendix D.

Message Size. Recall that in our construction, the message (label) size was $O(\log n)$ bits. Via communication complexity, we give a corresponding lower bound. In particular, we construct a graph on which any (randomized) communication protocol which simulates WL as in Definition 1.1 must send at least $\Omega(\log n)$ bits along one edge of the graph. As message-passing GNNs are a specific class of communication protocols, this immediately implies that the message sizes must have $\Omega(\log n)$ bits, so our construction is optimal in that respect.

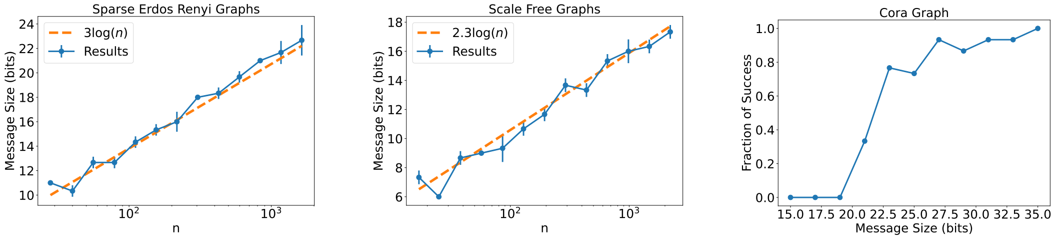
The hard instance is formed by a graph which is a collection of disjoint star subgraphs of sizes ranging from 2 to $\Theta(\sqrt{n})$. In order to perform a valid WL coloring, each node must essentially learn the size of its subgraph, requiring $\Omega(\log(\sqrt{n})) = \Omega(\log n)$ bits of communication. In addition, this must be done in only 2 iterations as the depth of each subgraph is 2, so some node must send $\Omega(\log n)$ bits to its neighbors in a single round. See Appendix D.1 for the full details and proof.

Number of ReLU Units. In order to show a lower bound on the number of units needed to implement a successful WL iteration, we rely on prior work lower bounding the number of linear regions induced by a ReLU network (for instance [MPCB14]). In particular, these works show that ReLU networks induce a partition of the input space into N convex regions (where N is a function of the size of the network) such that the network acts as a linear function restricted to any given region. Using these results, we describe a fixed graph and a distribution over inputs to the neural network $S_u^{(k-1)}$ for all $u \in V$ (sums of the labels from the previous round) which includes $O(F)$ potential special pairs of nodes (where F is defined such that inputs $S_u^{(k-1)} \in [F]^t$ for some t). For each such pair u, v, their neighborhoods $N(u), N(v)$ have different multisets of inputs, but both multisets of inputs sum to the same value. We show that if the number of linear regions is small, $N = o(F)$, then it is relatively likely that u, v will be in the same linear region and thus their sums will collide: $S_u^{(k)} = S_v^{(k)}$ even while their neighborhoods had distinct inputs in the $(k-1)$st round.

This immediately gives a $\Omega(\log F)$ lower bound on the number of ReLU units (and thus number of parameters) with more refined depth/width tradeoffs given in Appendix D.2.1. Note that F is the size of each coordinate in the *sum* of labels. Even if the labels are binary, F can be as large as n, depending on the max degree in the graph, which implies a $\Omega(\log n)$ lower bound on the number of ReLU units. See Appendix D.2 for full details and proof.

5 Experiments

To demonstrate the expressivity of our construction, i.e., that our small-sized GNN reliably simulates the WL test, we perform experiments on both synthetic and real world data sets. Common to all of our experiments is that we start with some graph $G = (V, E)$ (either real world or generated with respect to some probability distribution). We then simulate a perfect run of the WL test on G where any two nodes which receive different multisets of labels in iteration $k - 1$ get distinct labels in iteration k with probability 1 as well as a run of our construction from[4] Section 3. At any point in time, the node labels induce partitions of V where two nodes are in the same class if they have the same labels. Denote the partitions after k-iterations using the perfect simulation and our construction respectively by $\mathcal{P}_k$ and $\mathcal{P}'_k$. Letting k_0 be minimal such that $\mathcal{P}_{k_0-1} = \mathcal{P}_{k_0}$ (at which point the WL labels have converged), we consider the implementation using our GNN successful if $\mathcal{P}_k = \mathcal{P}'_k$ for all $k \leq k_0$, i.e., if the the simulation using our implementation induced the same partitions as a perfect runs. For all of our experiments it turned out that $k_0 \leq 5$ (see [BK22] for a discussion of this fast convergence).



(a) (b) (c)

Figure 2: Plots of our experimental results on Erdős-Rényi graphs, scale free graphs, and the real world Cora graph. The vertical blue lines in (a) and (b) are the empirical standard deviations over the 5 independent samples of random graphs. Note that the x-axes in (a) and (b) are logarithmic.

Sparse Erdős-Rényi Graphs We generated Erdős-Rényi random graphs $G(n, p)$ with $p = 20/n$ for a varying number of vertices n. For each value of n, we generated five such graphs and for each of these five graphs, we ran 10 independent trials of our GNN implementation with message sizes $t = 1, 2, \ldots$. Averaging over the five graphs, we report the minimal t such that at least 70% of the 10 iterations successfully simulated the WL test. See Figure 2a. The average message size needed to achieve this is approximately $3 \log n$ where the logarithmic dependence on n is as predicted theoretically and significantly improves on the linear message size required for prior constructions.

Scale Free Graphs We generated samples of the scale free graphs from [BBCR03] with a varying number of vertices n using the implementation from [HSS08]. Our experiment design was the same as for Erdős-Rényi random graphs. See Figure 2b.

Cora Graph We finally ran experiments on the real world graph Cora[5] which is the citation network of $n = 2708$ scientific publications. We simulated our GNN with varying message lengths, for each message length reporting the fraction of successful runs of 30 independent trials. See Figure 2c for a plot of the results. We see that with message length 35, all of the 30 trials successfully simulated the WL test.

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[4] Since our goal is to test whether our protocol correctly simulates WL test with small messages, we are not implementing the actual GNNs but instead we are simulating their computation. Further, for simplicity, we replaced the ε-biased sample space with a random string, which guarantees $\varepsilon = 0$.

[5] https://graphsandnetworks.com/the-cora-dataset/

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Checklist

1. For all authors...
   (a) Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope? [Yes]
   (b) Did you describe the limitations of your work? [Yes]
   (c) Did you discuss any potential negative societal impacts of your work? [N/A] This paper is focused on fundamental research on graph neural networks with no direct social impacts.
   (d) Have you read the ethics review guidelines and ensured that your paper conforms to them? [Yes]
2. If you are including theoretical results...
   (a) Did you state the full set of assumptions of all theoretical results? [Yes]
   (b) Did you include complete proofs of all theoretical results? [Yes]
3. If you ran experiments...
   (a) Did you include the code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL)? [N/A]
   (b) Did you specify all the training details (e.g., data splits, hyperparameters, how they were chosen)? [N/A]
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    (a) Did you include the full text of instructions given to participants and screenshots, if applicable? [N/A]
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A Omitted Proofs of Section 1

Proposition A.1. *Let $\ell_v^{(T)}$ be the labels of nodes after running the WL test for T iterations on an input graph G with initial labels $\ell_v^{(0)}$ all equal and suppose $p \leq \delta/(n^2T)$. Suppose T independent GNN iterations are successful according to Definition 1.1 and the output labels of iteration i are the input labels of iteration $i+1$ for all i with the initial labels being equal to $\ell_v^{(0)}$. Let $h_v^{(T)}$ denote the node labels which are the output of the final iteration of the GNN. Then for all $v_1, v_2 \in V$, the following statements hold with probability $1-\delta$:*

- *If $\ell_v^{(T)} = \ell_u^{(T)}$ then $h_v^{(T)} = h_u^{(T)}$ and*
- *If $\ell_v^{(T)} \neq \ell_u^{(T)}$ then $h_v^{(T)} \neq h_u^{(T)}$.*

Proof. Consider some iteration $i \leq T$. Suppose we have the following guarantee on the node label inputs for the ith iteration (note the inputs are the output labels of the previous iteration):

- If $\ell_v^{(i-1)} = \ell_u^{(i-1)}$ then $h_v^{(i-1)} = h_u^{(i-1)}$ and
- If $\ell_v^{(i-1)} \neq \ell_u^{(i-1)}$ then $h_v^{(i-1)} \neq h_u^{(i-1)}$.

Given the guarantee for iteration $i-1$, we show that the same guarantee is true for the labels outputted in the ith iteration with probability $1-p$. Consider what the WL test does given input labels $\ell_{v_1}^{(i-1)}$: it assigns the same node labels to all pairs of vertices with the same multiset of neighborhood (input) labels and different labels for all pairs of vertices with different multiset of neighborhood (input) labels. This is exactly the same guarantee as Definition 1.1, except we also have to union bound over all $\leq n^2$ pairs of nodes in Definition 1.1. Thus, the invariant stated in the beginning of the proof also holds for the ith iteration with probability $1-n^2p$. Now applying a union bound across all T iterations, the total failure probability is $n^2Tp \leq \delta$, as desired. □

B Omitted Proofs of Section 2

Proof of Lemma 2.1. Since all vectors $h_u^{(k)}$ are always one-hot encoded vectors, if two nodes have differing neighborhood multisets of labels, then the sum of the one-hot encoding vectors of each neighborhoods will also be different. Suppose we are in this case and let y and y' denote the sum of the neighborhood labels of v and u respectively. Without loss of generality, suppose y and y' differ in the first coordinate, y_1 and y_1'. Then $\langle a, y-y' \rangle \equiv 0 \bmod F$ if and only if $a_1(y_1 - y_1') \equiv c \bmod F$ where $c = \sum_{i=2}^{F} a_i(y_i' - y_i)$. Condition on the event that $a_1 \not\equiv 0 \bmod F$ which happens with probability $1 - 1/F$. We now claim that $y_1' - y_1 \not\equiv 0 \bmod F$. Indeed, $0 \leq y_1 \neq y_1' \leq n$ so $0 \neq |y_1 - y_1'| \leq n$. Since $F > 2n$, it cannot be the case that $y_1 - y_1' \equiv 0 \bmod F$ which means that the multiplicative inverse of $(y_1 - y_1') \bmod F$, denoted as $(y_1 - y_1')^{-1}$, is well-defined and unique. Thus for $a_1(y_1 - y_1') \equiv c \bmod F$, we must have $a_1 \equiv c(y_1 - y_1')^{-1} \bmod F$ which happens with probability $O(1/F)$. Altogether, we have that $\mathbb{P}_a[\langle a, y \rangle \equiv \langle a, y' \rangle \bmod F] \leq O(1/F)$, as desired. Conditioning on $\langle a, y \rangle \not\equiv \langle a, y' \rangle \bmod F$, we have that $h_v^{(k)} \neq h_u^{(k)}$ as their single non-zero coordinates are distinct. Finally, we can easily check that if the multiset of neighborhoods of u and v are the same, then $h_v^{(k)} = h_u^{(k)}$ always holds. □

B.1 Implementation of Modulo F via ReLU Network

We now give an efficient ReLU network construction of the function computing modulo F, thereby proving Theorem 2.2. First we define the function $\mathrm{TW}_F : \{0, \ldots, NF\} \to \{0, \ldots, F-1\}$, also known as the “triangular wave" function:

$$\mathrm{TW}_F(x) = \mathrm{T}_F(x \bmod 2F)$$

where

$$\mathrm{T}_F(x) = \begin{cases} x, \text{ if } x \leq F \\ 2F - x, \text{ if } x > F. \end{cases}$$

A result of [Tel16] implements the function TW_F using low-depth ReLU networks.

Theorem B.1 (Lemma 3.8 and Corollary 3.9 in [Tel16])**.** *Suppose $F = \mathrm{poly}(n)$. The function $\mathrm{TW}_F : \{0, \dots, nF\} \to \{0, \dots, F-1\}$ can be implemented using a neural network with $O(\log n)$ hidden units and $O(\log n)$ depth.*

We now reduce the modulo F case to the construction of the triangular wave function.

Theorem 2.2. *Suppose $F = \mathrm{poly}(n)$. There exists an explicit construction of a network which computes modulo F in the domain $\{0, \dots, nF\}$ using a ReLU network with $O(\log n)$ hidden units and $O(\log n)$ depth. More generally, given an integer parameter $t > 0$, the function can be computed with $O((Fn)^{O(1/t)} \log n)$ hidden units and $O(t)$ depth.*

Proof. Assume without loss of generality that F is odd. Given an integer $z \in \mathbb{Z}$, we first compute $\mathrm{TW}_F(z)$ and $\mathrm{TW}_{F/2}(z)$. Note that even though $F/2$ is non-integral, we can still compute it. Looking for a general real number $z \in [0, 2F]$, we have that $\mathrm{TW}_F(z) = \mathrm{TW}_{F/2}(z)$ if and only if $z \in [0, F/2]$ or $z \in [3F/2, 2F]$. In addition, if z is an integer in $[0, 2F]$ but not in $[0, F/2] \cup [3F/2, 2F]$, then $\mathrm{TW}_F(z) - \mathrm{TW}_{F/2}(z) \ge 1$. Noting that $\mathrm{ReLU}(1 - \mathrm{ReLU}(1 - x)) = 0$ for $x = 0$ and $\mathrm{ReLU}(1 - \mathrm{ReLU}(1 - x)) = 1$ for any $x \ge 1$, we therefore have that

$$\mathrm{ReLU}(1 - \mathrm{ReLU}(1 - \mathrm{TW}_F(z) + \mathrm{TW}_{F/2}(z)))$$

equals 0 if $z \in \mathbb{Z}$ and $0 \le (z \bmod 2F) \le (F-1)/2$ or $(3F+1)/2 \le (z \bmod 2F) \le 2F - 1$, and equals 1 if $z \in \mathbb{Z}$ and $(F+1)/2 \le (z \bmod 2F) \le (3F-1)/2$. So, if we consider shifting z by $(F-1)/2$, we can make this equal 1 if and only if z is between F and $2F - 1$ mod F. Therefore, for integers z,

$$\mathrm{ReLU}\left(1 - \mathrm{ReLU}\left(1 - \mathrm{TW}_F\left(z - \frac{F-1}{2}\right) + \mathrm{TW}_{F/2}\left(z - \frac{F-1}{2}\right)\right)\right)$$
$$= \begin{cases} 0 & 0 \le (z \bmod 2F) \le F - 1 \\ 1 & F \le (z \bmod 2F) \le 2F - 1 \end{cases}.$$

Now, for simplicity, let us define the function above as $g(z)$. Note that when $g(z) = 0$, then $\mathrm{TW}_F(z) = z \bmod F$, and when $g(z) = 1$, then $\mathrm{TW}_F(z) = F - (z \bmod F)$, so $z \bmod F = F - \mathrm{TW}_F(z)$. Therefore, we have that for any integer z, $z \bmod F = |F \cdot g(z) - \mathrm{TW}_F(z)|$. But note that we can write

$$|x| = \max(x, -x) = \max(2x, 0) - x = \mathrm{ReLU}(2x) - x.$$

Therefore, we have that

$$z \bmod F = \mathrm{ReLU}(2F \cdot g(z) - 2 \cdot \mathrm{TW}_F(z)) - F \cdot g(z) + \mathrm{TW}_F(z). \qquad \square$$

C Omitted Proofs for Section 3

Proof of Lemma 3.2. Since $\langle a, x\rangle - \langle a, y\rangle = \langle a, x - y\rangle$, by writing $z = x - y \in \mathbb{Z}^m$, it suffices to show that if z is nonzero, then $\mathbb{P}_{a\sim\mathcal{D}}[\langle a, z\rangle = 0] \le \frac{1}{2} + \frac{\varepsilon}{2}$.

Let k represent the largest nonnegative integer such that $2^k | z_i$ for all $i \in [m] := \{1, 2, \dots, m\}$, and let $z' = z/2^k$. Then, by replacing z with z', we have that $\mathbb{P}_{a\sim\mathcal{D}}[\langle a, z\rangle = 0]$ if and only if $\mathbb{P}_{a\sim\mathcal{D}}[\langle a, z'\rangle = 0]$ (since we are just dividing by 2^k) and z'_i is odd for at least one value of $i \in [m]$. So, it suffices to show that $\mathbb{P}_{a\sim\mathcal{D}}[\langle a, z'\rangle = 0] \le \frac{1}{2} + \frac{\varepsilon}{2}$. Note that by reducing modulo 2, it suffices to show that over $\mathbb{GF}_2$, $\mathbb{P}_{a\sim\mathcal{D}}[\langle a, z'\rangle \equiv 0 \bmod 2] \le \frac{1}{2} + \frac{\varepsilon}{2}$, because then the probability over the integers is either the same or lower.

Let I be the subset of $i \in [m]$ for which z'_i is odd. Note that I is nonempty since we know z'_i is odd for at least one value of $i \in [m]$. So, by the definition of ε-biased sample spaces, we know that over $\mathbb{GF}_2$, $\left|2 \cdot \mathbb{P}_{a\in\mathcal{D}}\left[\sum_{i\in I} a_i = 0\right] - 1\right| \le \varepsilon$, which means that $\mathbb{P}_{a\in\mathcal{D}}\left[\sum_{i\in I} a_i = 0\right] \le \frac{1}{2} + \frac{\varepsilon}{2}$. But indeed $\sum_{i\in I} a_i \equiv \langle a, z'\rangle$ since $i \in I$ precisely when z'_i is odd, so this completes the proof. $\square$

C.1 Proof of Corollary 3.3

We first need to define the circuit class TC^0.

Definition C.1 (Threshold Gate). *For inputs $x_1, \ldots, x_m \in \{0,1\}$ the output of a threshold gate,* TH, *is*

$$\mathrm{TH}(x_1, \ldots, x_m) = \begin{cases} 1 & \sum_{i=1}^m a_i x_i \geq \theta \\ 0 & \textit{otherwise} \end{cases}$$

where $\theta, a_1, \ldots, a_m \in \mathbb{Z}$. $\theta, a_1, \ldots, a_m$ may depend on n but they do not depend on the input $x_1, \ldots, x_m$.

Definition C.2 (TC^0 Circuit Class). TC^0 *is the class of boolean functions computed by constant-depth* $\mathrm{poly}(m)$*-size circuits with threshold gates.*

It is known that ε-biased vectors can be generated using an efficient circuit in TC^0.

Theorem C.1 (Theorem 14 in [HV06], Restated). *Let $s = O(\log F + \log(1/\varepsilon))$. For every ε and F, there exists an explicit* TC^0 *circuit $C : \{0,1\}^s \cup \{0,1\}^{\lceil log_2 F \rceil} \rightarrow \{0,1\}$ which takes as input s uniform random bits and an index $i \in [F]$ and outputs the ith coordinate of an ε-biased vector in $\{0,1\}^F$. C uses* $\mathrm{poly}(s)$ *threshold gates.*

Note that the guarantees of Theorem C.1 are not directly applicable since we need to use a ReLU network instead of threshold gates. Nevertheless, since the circuit C guaranteed by Theorem C.1 has integer inputs in all gates, we can easily approximate each threshold gates using an appropriately scaled ReLU. This is a straightforward and known reduction but we briefly outline a procedure in Lemma C.2.

Lemma C.2. *Consider the threshold gate* TH*: $\{0,1\}^m \rightarrow \{0,1\}$ which computes the threshold $\sum_{i=1}^m a_i x_i \geq \theta$. Assume that a_i, θ are all integers bounded by* $\mathrm{poly}(m)$*.* TH *can be computed by a ReLU network using $O(\log m)$ bits of precision and a constant number of parameters.*

Proof. Consider the function

$$g(x) = \mathrm{ReLU}(-\mathrm{ReLU}(-x+2)).$$

It is 0 for all integers $x \leq 0$ and 1 for all integers ≥ 1, i.e., it computes the threshold "$x \geq 0$". By shifting and scaling g, we can now compute the threshold "$x \geq \theta$" for any integer θ. Finally, the sum $\sum_{i=1}^m a_i x_i$ can be computed using one additional layer. Since all parameters are integers, we only require $O(\log m)$ bits of precision to store the shifting and scaling factors. □

Lastly, we remark that as per the definition of a threshold gate in Definition C.1, Theorem C.1 requires the index $i \in [F]$ to be inputted as a binary string with its bits given on individual nodes. However, this presents a slight inconsistency with the statement of Theorem C.1 and its corollary, Corollary 3.3 which is used in the construction of Section 3. Specifically, Step 3 of the construction of Section 3 outputs the actual integer $i \in [F]$ which we use as the index for our ε-biased vector, which does not match the format required by Theorem C.1. This inconsistency is straightforward to fix without having any impact whatsoever in the asymptotic size complexity of the neural network. We simply take the integer i outputted by Step 3 of the construction and compute the jth bit of i for all $1 \leq j \leq O(\log F)$ in parallel. The jth bit is exactly equal to 0 if and only if $(i \bmod 2^{j+1}) < 2^j$ and 1 otherwise. Note that $2^{j+1} = O(F)$ for all j and we can easily compute each $\mathrm{mod} 2^{j+1}$ by appealing to Theorem 2.2. This only requires $O(1)$ extra depth and an additional $O(\mathrm{poly}(\log n))$ hidden units and $O(\log n)$ bits of precision. The more general trade-off of Theorem 3.4 also readily holds.

D Lower bounds

In this appendix we provide lower bounds on the complexity of graph neural networks that are able to simulate the WL test. We present both a communication complexity lower bound and a lower bound on the number of ReLU units of the GNN. More concretely, in Section D.1, we prove that in order to maintain the invariant that with at least some constant probability, nodes with isomorphic neighborhoods get the same label while nodes with non-isomorphic neighborhoods get different

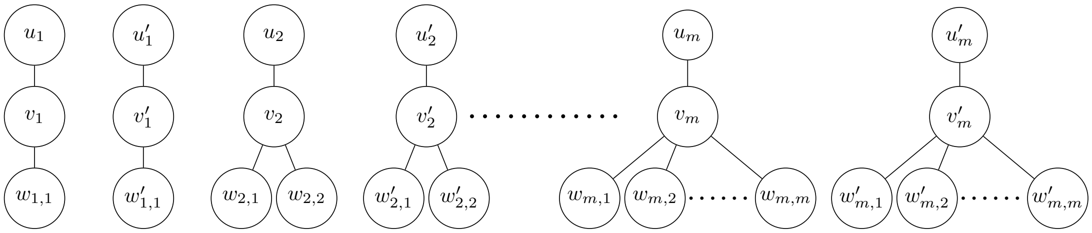

Figure 3: The graph G used for Theorem D.1, showing the disconnected pieces $G_1, G'_1, G_2, G'_2, \ldots, G_m, G'_m$. Note that for all k, G_k and G'_k are isomorphic.

labels, some message sent between nodes must be of length at least $\Omega(\log n)$. This bound matches the upper bound of Theorem 3.4. Second, in Section D.2, we consider a more specific although still fairly general lower bound model which captures the implementation of the WL test using neural networks. We suppose that the messages sent between nodes are t-dimensional vectors with integral entries. We moreover suppose that each node combines its received messages by summing them to get a vector in $[F]^t$ (here, $[F] = \{0, 1, \ldots, F-1\}$) and applying a collectively agreed upon neural network ϕ with at most H ReLU units to this sum. We show that if the combination of summing neighborhoods and applying the neural network maps distinct multisets to distinct elements with at least some constant probability, then $H = \Omega(\log F)$. Moreover, parametrizing in terms of the depth and width of the neural network, we obtain a more fine-grained lower bound, demonstrating that for shallow neural networks, we need even more ReLU units. In Remark D.5, we point out that our lower bound holds even if the aggregation function f is itself a neural network with a bounded number of ReLU units. As a node in an n-node graph could have up to $n-1$ neighbours, we need at least $F = \Omega(n)$ in order to store the sum of the messages from the neighbors of the nodes. With this assumption, the lower bound thus becomes $\Omega(\log n)$ which matches our upper bound up to $\text{polylog}(n)$ factors. It remains an interesting open problem to bridge the gap between the upper and lower bound.

For both our lower bounds we assume that the nodes have access to an infinite public string of random bits. In Section D.2, this is the string which the nodes use to collectively agree on some neural network network f with respect to some distribution on such networks with at most H ReLU units.

D.1 Lower Bound: Communication Complexity

We consider a forest graph G composed of pieces $G_1, G'_1, G_2, G'_2 \ldots, G_m, G'_m$, for $m = \Theta(\sqrt{n})$. Each piece G_k consists of a "top" node u_k, which is only connected to a "middle" node v_k, which in turn is connected to k "bottom" nodes $w_{k,1}, \ldots, w_{k,k}$, and G'_k is simply a duplicate of G_k (with vertices u'_k, v'_k, and $w'_{k,j}$ for $1 \le j \le k$). See Figure 3 for a depiction of G. We note that after two rounds, each u_k (and u'_k) should know the respective value of k, because the local graph of depth 2 around u_k is distinct for each $k \in [m]$.

Theorem D.1. *Suppose there exists a public random string r that every node of G has access to, and each node additionally has some independent private randomness. Suppose there is a communication protocol where by the end, with probability at least $3/4$, the following hold.*

- *For every $k \in [m]$, the top nodes u_k and u'_k output the same value.*
- *For every $k \neq \ell \in [m]$, the top nodes u_k, u_ℓ output distinct values.*

Then, there must be some k such that the edge (u_k, v_k) or the edge (u'_k, v'_k) has at least $\Omega(\log n)$ total bits of communication. Hence, if there are only $O(1)$ rounds of communication, one of those rounds must have sent $\Omega(\log n)$ bits of communication across the edge.

Remark D.2. *In comparison to Definition 1.1, we note that our lower bound works for $p = \frac{1}{4m^2} = \Theta\left(\frac{1}{n}\right)$ in Definition 1.1. This is because we require all nodes u_k, u_ℓ to simultaneously have different outputs with probability at least $\frac{3}{4}$, which is implied by a union bound if every u_k, u_ℓ for $k \neq \ell$ have different outputs with probability at least $1 - \frac{1}{4m^2}$. In addition, we actually prove a stronger lower* *bound against Definition 1.1, because our lower bound holds even if we allow each node to have its own independent private randomness, and only requires nodes with the same local neighborhood to output the same answer simultaneously with probability* $3/4$ *instead of probability* 1.

Proof. First, we note that we may assume the communication is one-way from v_k to u_k. This is because the node v_k can simulate all communication from u_k, as u_k has no information about neighbors apart from v_k. So, we just need to show the one-way communication complexity is $\Omega(\log n)$. Next, we will assume there is no public randomness - we will remove this assumption at the end. So, each u_k (resp., u'_k) receives at most b bits of information from v_k (resp., v'_k). If v_k sends a randomized message of length b to u_k and u_k uses this message to produce some output o_k, with probability at least $\frac{3}{4}$ the outputs o_k must all be distinct. In addition, for each k, the outputs of the duplicate copies of u_k must be the same with probability at least $\frac{3}{4}$. Our goal is to show that $b = \Omega(\log n)$.

Let f be a randomized function from $[m]$ to $\{0,1\}^b$, representing the randomized message v_k sends to u_k assuming it has full knowledge of its number of neighbors. Let g be a randomized function from $\{0,1\}^b$ to some arbitrary output space $\mathcal{O}$, which represents the final output of u_k after it has seen the message from v_k. Then, for all $k \neq \ell \in [m]$, $\mathbb{P}[g_1(f_1(k)) \neq g_2(f_2(\ell))] \geq \frac{3}{4}$, but for all $k \in [m]$, $\mathbb{P}[g_1(f_1(k)) = g_2(f_2(k))] \geq \frac{3}{4}$. Here, g_1, g_2 represent the function g with different instantiations of the randomness, and f_1, f_2 represent the function f with different instantiations of the randomness.

Fix some $k \in [m]$ and for each output $o \in \mathcal{O}$, let $p_k(o)$ represent the probability of outputting $g(f(k)) = o$. Note that $p_k(o)^2$ is the probability that u_k outputs o *and* u'_k outputs o, so the probability that u_k and u'_k have the same output equals $\sum_{o \in \mathcal{O}} p_k(o)^2$, which we are assuming is at least $\frac{3}{4}$. This means that $\max_{o \in \mathcal{O}} p_k(o) = \sum_{o \in \mathcal{O}} p_k(o) \cdot \max_{o \in \mathcal{O}} p_k(o) \geq \sum_{o \in \mathcal{O}} p_k(o)^2 \geq \frac{3}{4}$. Therefore, for all $k \in [m]$, there exists an output $\tilde{o}_k$ such that $\mathbb{P}[g(f(k)) = \tilde{o}_k] \geq \frac{3}{4}$. Therefore, there must exist a value $s_k \in \{0,1\}^b$ such that $\mathbb{P}[g(s_k) = \tilde{o}_k] \geq \frac{3}{4}$. Indeed, if not, then for any distribution over $s_k \in \{0,1\}^b$, we have that $\mathbb{P}[g(s_k) = \tilde{o}_k] < \frac{3}{4}$, which means that $\mathbb{P}[g(f(k)) = \tilde{o}_k] < \frac{3}{4}$. In addition, $\tilde{o}_k$ is different across all k, as if $\tilde{o}_k = \tilde{o}_\ell$ for some $k \neq \ell$, then $\mathbb{P}[g(f(k)) = g(f(\ell)) = \tilde{o}_k] \geq \left(\frac{3}{4}\right)^2 \geq \frac{1}{2}$, which means that $\mathbb{P}[g(f(k)) \neq g(f(\ell))] \leq \frac{1}{2}$.

But now, note that the s_k's must be distinct, because if $s_k = s_\ell$, then because $\mathbb{P}[g(s_k) = \tilde{o}_k] \geq \frac{3}{4}$ and $\mathbb{P}[g(s_\ell) = \tilde{o}_\ell] \geq \frac{3}{4}$, this means that $\tilde{o}_k = \tilde{o}_\ell$. Therefore, $s_1, \dots, s_m$ are all distinct. But since each s_i lies in $\{0,1\}^b$, this means that $b = \Omega(\log m) = \Omega(\log n)$, as desired.

To finish, we revisit the fact that we assumed there was no public randomness. Let us reintroduce the random string r that every node of G is given. We assume that with probability at least $3/4$, the top nodes u_k, u'_k have the same output for all $k \in [m]$ and that the nodes $u_1, \dots, u_m$ output pairwise distinct values. But as this event happens with probability at least $3/4$ over a random string r, there must exist a choice of r for which it happens with probability at least $3/4$ conditioned on r. But then we are back to the case where there is no public randomness, as desired. □

D.2 Lower Bound: ReLU Units

We next prove a lower bound on the number of ReLU units that we need to implement the WL test as a graph neural network. To do so, we will use that any neural network $\phi : \mathbb{R}^t \to \mathbb{R}^\ell$ which uses ReLU's as activation functions induces a partition of $\mathbb{R}^t$ into convex polytopes $R_1, \dots, R_N$ such that ϕ restricted to each R_i is just a linear function. Moreover, the number of such regions can be bounded using the following theorem.

Theorem D.3 (Proposition 4 in [MPCB14]). *The number of linear regions of any ReLU network* $\phi : \mathbb{R}^t \to \mathbb{R}^d$ *with a total of* H *ReLU units is at most* 2^H.

Let $t, \ell, F \in \mathbb{N}$ be given and denote by $[F] = \{0, 1, \dots, F-1\}$. Let Φ_H denote the family of neural networks $\phi : \mathbb{R}^t \to \mathbb{R}^\ell$ with at most H ReLU units mapping. We will consider the following model (see Figure 4): The algorithm designer picks a distribution D over Φ_H. Let G be an arbitrary n-node graph and recall that $\mathcal{N}(i)$ denotes the neighborhood of node i (including i itself). For arbitrary inputs $x_1, \dots, x_n \in [F]^t$ to the n nodes (which we think of as the sums of the messages that the

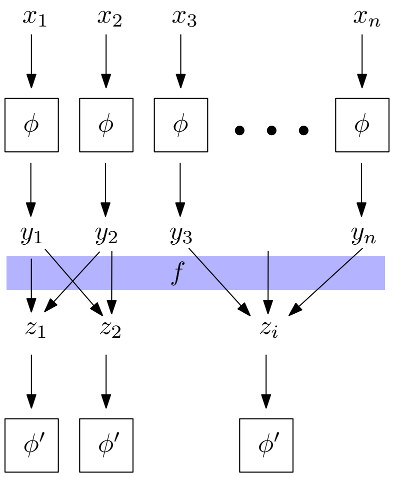

Figure 4: The structure of the GNN in our lower bound model. For every node i, node i receives the message x_i which is the sum of the labels of the neighbors of i. The algorithm then picks a random $\phi \in \Phi_H$ with respect to D and for each $i = 1, \ldots, n$, calculates $y_i = \phi(x_i)$ which is the new label of node i. Next, each node i, sends y_i to each of its neighbors and every node i then calculates $z_i = f(\{y_j \mid j \in \mathcal{N}(i)\}) = \sum_{j \in \mathcal{N}(i)} y_i$. The z_i's then form the node inputs at the next iteration to a new randomly chosen $\phi' \in \Phi_H$.

nodes receive), the GNN operates as follows: Using the publicly available random string, the nodes collectively pick a random neural network $\phi \in \Phi_H$ with respect to D. For $i = 1, \ldots, n$, node i then calculates $y_i = \phi(x_i)$ (which we think of as the new label of node i). Then each node i sends y_i to each node in its neighborhood $\mathcal{N}(i)$ and calculates $z_i = \sum_{j \in \mathcal{N}(i)} y_j$. We remark that this notation is different from what we introduced in Section 1.1 and 1.2. Referring back to those sections, i corresponds to node u, x_i corresponds to $\mathcal{S}_u^{(k-1)}$, i.e., the sum of the received messaged of node u in iteration $k-1$, ϕ corresponds to $\phi^{(k)}$, y_i corresponds to $h_u^{(k)}$, i.e., the new label of node u, and z_i corresponds to $\mathcal{S}_u^{(k)}$, i.e., the sum of the received messaged of node u in iteration k. We have made this switch in notation to make the argument that follows less unwieldy.

We would like our GNN to satisfy that for any n-node graph G, and arbitrary inputs $x_1, \ldots, x_n$ to the nodes, it holds with probability at least $9/10$ over the randomness of D that $z_i \neq z_j$ for all i, j such that the multisets $\{x_k \mid k \in \mathcal{N}(i)\}$ and $\{x_k \mid k \in \mathcal{N}(j)\}$ are different. The following theorem provides a lower bound on the number of ReLU units H needed for this property to hold.

Theorem D.4. *Suppose that the neural networks in Φ_H have at most $H \leq \lg F - 4$ ReLU units. Then there exists a graph G on n nodes and inputs $x_1, \ldots, x_n \in [F]^t$ such that if $\mathcal{N}(1), \ldots, \mathcal{N}(n)$ are the neighborhoods of the nodes of G, then with probability at least $1 - \left(\frac{3}{4}\right)^{n/6}$, there exists $i, j \in [n]$ such that $z_i = z_j$ even though the multisets $\{x_k \mid k \in \mathcal{N}(i)\}$ and $\{x_k \mid k \in \mathcal{N}(j)\}$ are different. Thus, to simulate the WL test with neural networks from Φ_H, we need $H > \log F - 3$ ReLU units.*

Before proving the theorem, we first explain how to interpret it as a lower bound for the computational complexity of implementing a WL iteration as in Definition 1.1 as a neural network. As an initial observation, note that in any iteration k, if for two nodes u and v, the sums $S_u^{(k-1)}$ and $S_v^{(k-1)}$ are distinct (recall that $\mathcal{S}_u^{(k-1)} = \sum_{u' \in \mathcal{N}(u)} h_u^{(k-1)}$), then for the WL iteration to be successful, we must also have that $h_u^{(k)} \neq h_v^{(k)}$. This is because, $S_u^{(k-1)} \neq S_v^{(k-1)}$ implies that the multisets $\{h_{u'}^{(k-1)} \mid u' \in \mathcal{N}(u)\}$ and $\{h_{v'}^{(k-1)} \mid v' \in \mathcal{N}(v)\}$ are also distinct. But then Definition 1.1 yields that we need $h_u^{(k)} \neq h_v^{(k)}$ (at least with some probability $1-p$). Now, consider two nodes $i = u$ and $j = v$ such that in some iteration of the WL test, the multisets of sums $\{\mathcal{S}_{u'}^{(k-1)} \mid u' \in \mathcal{N}(u)\}$ and $\{\mathcal{S}_{v'}^{(k-1)} \mid v' \in \mathcal{N}(v)\}$ are different. This corresponds to the multisets $\{x_k \mid k \in \mathcal{N}(i)\}$ and $\{x_k \mid k \in \mathcal{N}(j)\}$ being different. We would like to argue that for the WL iteration to be successful

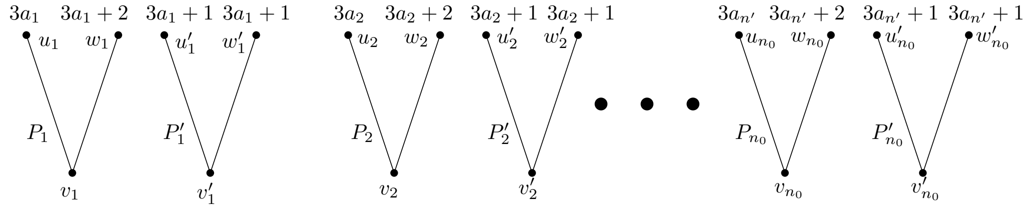

Figure 5: The graph of our lower bound construction of Theorem D.4. It consists of $n/3$ copies of a path of length 3 grouped into pairs of two. For each such pair of paths (P, P'), the two end nodes of P are assigned (random) inputs (which we think of as the sum of their received messages) that are guaranteed to have the same sum as the sum of the inputs to the end nodes of P'. The idea of the proof is that if the neural network ϕ has too few ReLU unit, then this linear dependence is preserved with probability $\Omega(1)$ even after applying ϕ.

according to Definition 1.1, for each such pair of nodes u, v, we must have that also $\mathcal{S}_u^{(k)} \neq \mathcal{S}_v^{(k)}$ with some good probability (the sums of labels in the next iteration differ). Theorem D.4 tells us that the probability of this happening is very low if we use too few ReLU units. Now why do we require that $\mathcal{S}_u^{(k)} \neq \mathcal{S}_v^{(k)}$ for such a pair of nodes u, v?

Since the multisets $\{\mathcal{S}_{u'}^{(k-1)} \mid u' \in \mathcal{N}(u)\}$ and $\{\mathcal{S}_{v'}^{(k-1)} \mid v' \in \mathcal{N}(v)\}$ are different, by the initial observation, the multisets $\{h_{u'}^{(k)} \mid u' \in \mathcal{N}(u)\}$ and $\{h_{v'}^{(k)} \mid v' \in \mathcal{N}(v)\}$ must also be distinct for the WL test to be successful. But since the multisets of labels $\{h_{u'}^{(k)} \mid u' \in \mathcal{N}(u)\}$ and $\{h_{u'}^{(k)} \mid v' \in \mathcal{N}(v)\}$ are distinct it follows by another application of Definition 1.1, that we must also have that $h_u^{(k+1)} \neq h_v^{(k+1)}$. However, the only way this can happen is if $\mathcal{S}_u^{(k)} \neq \mathcal{S}_v^{(k)}$ as otherwise these two sums will be mapped to the same label by $\phi^{(k+1)}$.

We remark that this lower bound applies to an isolated WL iteration rather than a full sequence of iterations. In particular, the inputs $x_1, \ldots, x_n \in [F]^t$ (corresponding to the sums $\{\mathcal{S}_u^{(k-1)} \mid u \in G\}$) are adversarially chosen while in reality these inputs are not arbitrary but are the result of a prior WL iteration. Our construction in Section 3 indeed works against such adversarially chosen sums in the sense that different multisets of sums are mapped (via applying $\phi^{(k)}$ and summing the outputs for each multisets) to different sums with high probability, and as such our lower bound is exactly a lower bound for this harder problem. However, in general the sums $S_v^{(k-1)}$ are not adversarially chosen, and it would very be interesting to find a lower bound that does not require this assumption but works all the way from a graph and its initial labels.

Proof of Theorem D.4. We exhibit a graph G and a distribution D_0 over the possible inputs, such that for any neural network $\phi : [F]^t \to \mathbb{R}^\ell$ with at most H ReLU units, if $(x_1, \ldots, x_n) \in ([F]^t)^n$ is chosen with respect to D_0, then with probability at least $1 - \left(\frac{3}{4}\right)^{n/6}$, there exists i, j such that $z_i = z_j$ even though the multisets $\{x_k \mid k \in \mathcal{N}(i)\}$ and $\{x_k \mid k \in \mathcal{N}(j)\}$ are different. It then follows from Yao's minimax principle that for any distribution D over Φ_H, there exists an input $x = (x_1, \ldots, x_n)$ such that the same bad event occurs with the same high probability. As desired.

Let us start out by describing the graph G. Assume with no loss of generality that 6 divides n, i.e. $n = 6n_0$ for some natural number n_0. The graph G simply consists of $2n_0$ copies of a path of length 2 grouped into pairs $(P_1, P_1'), \ldots, (P_{n_0}, P_{n_0}')$ (see Figure 5). Denote the vertices of path P_i by (u_i, v_i, w_i) and similarly the vertices of path P_i' by (u_i', v_i', w_i'). We next proceed to describe the distribution D_0 over inputs $(x_1, \ldots, x_n) \in ([F]^t)^n$. Here, for each $i < n_0$, we let $x_{3i}, x_{3i+1}, x_{3i+2}$ be the inputs to nodes u_i, v_i and w_i respectively and $x_{3i+3}, x_{3i+4}, x_{3i+5}$ be the inputs to nodes u_i', v_i' and w_i'. To do so, let $\ell = \lfloor F/3 \rfloor$ and define for each $0 \leq a < \ell$ and $b \in [F]^{t-1}$ the set $F_{a,b} = \{(3a, b), (3a+1, b), (3a+2, b)\}$. Thus, $F_{a,b} \subseteq [F]^t$ consists of the three vectors which have their first coordinate equal to respectively $3a$,$3a+1$ and $3a+2$, and b as their last $t-1$ coordinates. For each $i < n_0$, we independently pick uniformly random $0 < a \leq \ell$ and $b \in [F]^{t-1}$. We then define $x_{6j} = (3a, b)$, $x_{6j+2} = (3a+2, b)$, and $x_{6j+3} = x_{6j+5} = (3a+1, b)$ (see Figure 5). We further define $x_{6j+1} = x_{6j+4} = 0$ (the exact value is unimportant, as long as they are equal). Note that $x_{6j} + x_{6j+1} + x_{6j+2} = x_{6j+3} + x_{6j+4} + x_{6j+5}$. In particular, if the random $\phi \in \mathcal{F}$ was a linear map, we would have that

$$z_{6j+1} = \phi(x_{6j}) + \phi(x_{6j+1}) + \phi(x_{6j+2}) = \phi(x_{6j+3}) + \phi(x_{6j+4}) + \phi(x_{6j+5}) = z_{6j+4}, \quad \text{(D.1)}$$

in spite of the multisets, $\{x_{6j}, x_{6j+1}, x_{6j+2}\}$ and $\{x_{6j+3}, x_{6j+4}, x_{6j+5}\}$ being different. Now, ϕ is a neural network, so this identity does not need to hold. The idea is however, that if ϕ has only few ReLU units, then we obtain a good upper bound on the number of *linear regions* by Theorem D.3 and since a and b are random, the set $F_{a,b}$ is likely to be fully contained in one of these regions. And since ϕ restricted to this region in linear, (D.1) holds in this case.

To formalize this, assume that $\phi : [F]^t \to \mathbb{R}^\ell$ is a neural network in Φ_H with at most H ReLU units. Using Theorem D.3, it follows that $[0, F-1]^t$ can then be partitioned into at most 2^H convex regions $R_1, \ldots, R_N$, such that for each region R_i, it holds that ϕ restricted to R_i is simply a linear function. For $0 \le a < \ell$ and $b \in [F]^{t-1}$, we let $L_{a,b}$ be the straight line segment connecting the two points $(3a, b)$ and $(3a+2, b)$. By convexity, for a fixed R_i and a fixed $b \in [F]^{t-1}$, at most 2 of the line segments in $\{L_{a,b} \mid 0 \le a < \ell\}$ can intersect the boundary of R_i. Since there are F^{t-1} distinct choices for b and $N \le 2^H$ choices for i, this implies that the number of line segments $L_{a,b}$ that can cross *any* of the boundaries of the convex regions is at most $2^{H+1}F^{t-1}$. Each of the remaining segments $L_{a,b}$ must be fully contained in some region R_i. There are $\lfloor F/3 \rfloor F^{t-1}$ choices of a and b in total, and thus, at least $\lfloor F/3 \rfloor F^{t-1} - 2^{H+1}F^{t-1}$ of the segments $L_{a,b}$ are fully contained in one of the regions R_i, which means that ϕ restricted to $L_{a,b}$ acts as a linear map. For such a segment $L_{a,b}$, we get by linearity that

$$\phi(3a, b) + \phi(3a+2, b) = 2\phi(3a+1, b).$$

In other words, if for a fixed $i \le n_0$, (a, b) is chosen such that $L_{a,b}$ is fully contained in one of the convex regions, then (D.1) is satisfied. It follows that for any given $i < n_0$,

$$\Pr[z_{6i+1} = z_{6i+4}] \ge 1 - \frac{2^{H+1}F^{t-1}}{\lfloor F/3 \rfloor F^{t-1}} \ge 1 - \frac{12 \cdot 2^H}{F}. \quad \text{(D.2)}$$

Since the event $(z_{6i+1} = z_{6i+4})_{i \le n_0}$ are independent (as we choose independent (a, b) for each pair of paths (P_i, P_i')), it follows that

$$\Pr[\exists 0 \le i \le n_0 : z_{6i+1} = z_{6i+4}] \ge 1 - \left(\frac{12 \cdot 2^H}{F}\right)^{n_0}.$$

If in particular, $H \le \lg F - 4$, we obtain that

$$\Pr[\exists 0 \le i \le n_0 : z_{6i+1} = z_{6i+4}] \ge 1 - \left(\frac{3}{4}\right)^{n/6},$$

As the multisets $\{x_k \mid k \in \mathcal{N}(6i+1)\}$ and $\{x_k \mid k \in \mathcal{N}(6i+4)\}$ are different, this completes the proof. □

Remark D.5. *In analogue with our construction in Section 2 and Section 3, we assumed in the above proof that the aggregate function f is the summation function. As such, f is just another neural network but without a single ReLU unit. We can therefore think of the combined computation performed by f and ϕ (illustrated in Figure 5) as the result of applying a single neural network. It follows from this observation (and the proof of Theorem D.4) that in the more general setting where f is a function in Φ_{H_1} and where the neural network $\phi \in \Phi_{H_2}$, then we must have that $H_1 + H_2 > \log F - 4$ in order to successfully simulate the WL test.*

D.2.1 Better bounds on the number of linear regions.

The proof of Theorem D.4 used that the number of convex linear regions of any neural network with at most H ReLU's is at most 2^H. However, in many cases one can obtain better upper bounds on the number of such regions, and this directly translates to a better lower bound than the one given in Theorem D.4. Indeed, if the family of neural networks Φ satisfies that the domain of any $\phi \in \Phi$ can be partitioned into at most K convex regions such that ϕ restricted to each of these regions is linear, then the lower bound in (D.2) instead becomes

$$\Pr[z_{6i+1} = z_{6i+4}] \ge 1 - \frac{12 \cdot K}{F}.$$

In particular, when using independence of the events $(z_{6i+1} = z_{6i+4})_{i<n_0}$, we just need $K \leq \frac{F}{24}$, say, to get that an error occur with probability at least $1 - 2^{-\Omega(n)}$. Plugging in the bound $K \leq 2^H$ of Theorem D.3 gave the desired bound of Theorem D.4 which led to the $\Omega(\log F)$ lower bound. If we instead use the more fine grained theorem below, we obtain better bounds for shallow neural networks with low input dimension as stated in Corollary D.7.

Theorem D.6 (Theorem 1 in [RPK$^+$17])**.** *Any ReLU neural network with input dimension t, width w, and depth d has at most $O(w^{d\cdot t})$ linear regions.*

Corollary D.7. *Let $\Phi_{t,d,w}$ consist of all ReLU neural networks with input dimension t, depth d, and width w. Suppose that we are in the setting of Theorem D.4, except that the neural network is picked from $\Phi_{t,d,w}$. Then the conclusion of the theorem holds as long as $w^{d\cdot t} \leq cF$ for a small enough constant c. In particular, to simulate the WL test with neural networks from $\Phi_{t,d,w}$, we need $dw = \Omega(dF^{\frac{1}{dt}})$ ReLU units.*

As an example, for shallow neural networks with low input dimension, say with $d, t = O(1)$, this lower bound becomes $dw = F^{\Omega(1)}$, i.e. polynomial rather than logarithmic in the size of the underlying field.

For certain architectures of the neural networks one can obtain even stronger bounds on the number of linear regions (see e.g., Proposition 3 in [Mon17] and Theorem 1 in [STR18]). These bounds are parametrized in the number of ReLU units in each of the d layers of the neural networks. One can therefore obtain even more fine grained lower bounds on the number of ReLU units if one makes more assumptions on the family of neural networks but the bounds are more opaque and we refrain from stating them here.

D.2.2 Description complexity

In this subsection, we consider more general function classes Φ that do not necessarily have to consist of neural networks. We prove that for any aggregation function f, if for any two distinct multisets of labels each of size at most n, there exists a function $\phi \in \Phi$ such that the multisets are mapped to different labels by $\phi \circ f$, then $|\Phi| = \Omega\left(\frac{n}{\log n}\right)$. It follows that the description complexity of Φ must be $\Omega(\log n)$. Our bound is combinatorial, and does not employ the linear structure of F^t. Hence we may just put $t = 1$ and think of F as a set rather than a vector space.

Theorem D.8. *Let F and n be natural numbers and let $N = \sum_{i=0}^{n} \binom{i+F-1}{i}$ be the number of multisets of $[F]$ of size at most n. Suppose that f is any aggregation function mapping multisets of $[F]$ to some range $\mathcal{R}$. Let Φ be any set of functions from $\mathcal{R}$ to F and assume that $|\Phi| < \frac{\log N}{\log F}$. Then there exists distinct multisets A and B each with at most n elements from $[F]$ such that $\phi(f(A)) = \phi(f(B))$ for all $\phi \in \Phi$.*

Proof. Note that each function $\phi \in \Phi$ induces a partition $\mathcal{P}_\phi$ on the set of these multisets induced by the equivalence relation defined by $X \sim_\phi Y \iff \phi(f(X)) = \phi(f(Y))$. By repeated application of the pidgeonhole principle, there must exists a collection $\mathcal{C}$ of multisets each containing at most n elements from $[F]$ such that (1) for all $\phi \in \Phi$ and all $X, Y \in \mathcal{C}$, $X \sim_\phi Y$ and (2) $|\mathcal{C}| \geq N/F^{|\Phi|}$. If in particular $|\Phi| < \frac{\log N}{\log F}$, we must have that $|\mathcal{C}| \geq 2$. Letting A and B be distinct elements of $\mathcal{C}$, we have that $\phi(f(A)) = \phi(f(B))$ for all $\phi \in \Phi$. □

Note that number of distinct degrees of the vertices of a simple n-node graph could be as large as $\Omega(n)$, so it is a natural assumption that also $F = \Omega(n)$. Indeed, if F is smaller, then for such a graph, the simulation of the WL test will fail with probability 1 since it must inevitably assign two nodes of distinct degrees the same label in F. With this assumption, it follows that

$$\begin{aligned}\log N = \log \sum_{i=0}^{n} \binom{i+F-1}{i} &\geq \log \binom{n+F-1}{n} \geq \log \left(1 + \frac{F-1}{n}\right)^n \\ &= \Omega\left(n \cdot \max\left\{1, \log \frac{F}{n}\right\}\right),\end{aligned}$$

using the inequality $\binom{n}{k} \geq \left(\frac{n}{k}\right)^k$. Thus,

$$\frac{\log N}{\log F} = \Omega\left(n \cdot \frac{\max\left\{1, \log \frac{F}{n}\right\}}{\log F}\right) = \Omega\left(\frac{n}{\log n}\right).$$

In particular, the description complexity of Φ has to be $\Omega(\log n)$ in order to separate any two distinct multisets $X, Y \subset F$ each consisting of at most n elements. We note that the description complexity of the construction in Section 3 is $\operatorname{poly}\log n$.