# Learning Graph Neural Networks using Exact Compression 

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#### Abstract

Graph Neural Networks (GNNs) are a form of deep learning that enable a wide range of machine learning applications on graphstructured data. The learning of GNNs, however, is known to pose challenges for memory-constrained devices such as GPUs. In this paper, we study exact compression as a way to reduce the memory requirements of learning GNNs on large graphs. In particular, we adopt a formal approach to compression and propose a methodology that transforms GNN learning problems into provably equivalent compressed GNN learning problems. In a preliminary experimental evaluation, we give insights into the compression ratios that can be obtained on real-world graphs and apply our methodology to an existing GNN benchmark.


## 1 Introduction

Whereas Machine Learning (ML) has traditionally been most successful in analyzing traditional unstructured data such as text or images, ML over structured data such as graphs has become an active area of research in the past decade. In particular, Graph Neural Networks (GNNs for short) are a form of deep learning architectures that enable a wide range of ML applications on graph-structured data, such as molecule classification, knowledge graph completion, and web-scale recommendations [3, 9, 11, 12, 25]. At their core, GNNs allow to embed graph nodes into vector space. Crucially, the obtained vectors can capture graph structure, which is essential for the ML applications already cited.

While GNNs are hence an attractive mechanism for ML on graphs, learning GNNs is known to be resource-demanding which limits their scalability [23,28]. In particular, for large graphs it becomes difficult to encode all the required information into the limited memory of hardware accelerators like GPUs. For this reason, scalable methods for learning GNNs on large graphs are an active subject of research (e.g., $[5,6,8,12,14,17,18,20-22,26,27])$. Broadly speaking, we can identify three different principles for obtaining scalability in the literature: (1) distributing computation across multiple machines or GPUs [8, 17, 18, 20, 22, 26, 27]; (2) learning on a sample of the input graph instead of the entire graph [5,12,14]; and (3) compression $[6,8,16,21]$. Compression-based approaches limit the memory requirements of learning GNNs on large graphs by reducing the input graph into a smaller graph and then learn on this smaller, reduced graph instead. In this paper, we are concerned with compression.

Compression methods are based on collapsing multiple input nodes into a single reduced node in the compressed graph. Methods vary, however, in how they collapse nodes. For example, Deng et al. [6] use spectral analysis for this purpose; Liang et al. [16] use variants of multi-level graph partitioning; and Generale et al. [8], who specifically consider knowledge graphs, use general heuristics (such as two nodes having equal set of attributes) or bisimulation. While these methods give intuitive reasons to argue that the structure of the obtained compressed graph should be similar to that of the original graph, no formal guarantee is ever given that learning on the compressed graph is in any way equivalent to learning on the original graph. Furthermore, the methods are usually devised and tested for a specific GNN architecture (such as Graph Convolutional Networks, GCN). It is therefore unclear how they fare on other GNN architectures. Inherently, these methods are hence heuristics. At best the compressed graphs that they generate approximate the original graph structure, and it is difficult to predict for which GNN architectures this approximation is good enough, and for which architectures it poses a problem.

Towards a more principled study of learning GNNs on compressed graphs, we propose to take a formal approach and study exact compression instead. We make the following contributions.
(1.) We formally define when two learning problems involving graph neural networks are equivalent. Based on this definition, our goal is to transform a given problem into a smaller, equivalent problem based on compression. (Section 2.)
(2.) We develop a compression methodology that is guaranteed to always yield an equivalent learning problem and that is applicable to a wide class of GNN architectures known as aggregate-combine GNNs [2, 10, 11]. This class includes all Graph Convolutional Networks [11]. Our methodology is based on recent insights into the expressiveness of aggregate-combine GNNs [19, 24]. These results imply that if the local neighborhoods of two nodes $v, w$ in input graph $G$ are equal, then any GNN will treat $v$ and $w$ identically. We may intuitively exploit this property for compression: if $v$ and $w$ are treated identically there is no need for them both to be present during learning; having one of them suffices. We fully develop this intuition in Section 3, where we also consider a more relaxed notion of "local neighborhood" that is applicable only to specific kinds of aggregate-combine GNNs.
(3.) We empirically evaluate the effectiveness of our methodology in Section 4. In particular, we give insights into the compression ratios that can be obtained on real-world graphs. While we find that these ratios are diverse, from compressing extremely well to
compressing only marginally, a preliminary experiment on an existing GNN benchmark shows positive impact on learning efficiency even with marginal compression.

We start with preliminaries in Section 2 and conclude in Section 5. Proofs of formal statements may be found in the Appendix.

## 2 Preliminaries

Background. We denote by $\mathbb{R}$ the set of real numbers, by $\mathbb{N}$ the set of natural numbers, and by $\mathbb{N}_{\infty}$ the set $\mathbb{N} \cup\{\infty\}$ of natural numbers extended with infinity. We will use double curly braces \{\{...\} to denote multisets and multiset comprehension. Formally, we view a multiset over a domain of elements $S$ as a function $M: S \rightarrow \mathbb{N}$ that associates a multiplicity $M(x)$ to each element $x \in S$. As such, in the multiset $M=\{a, a, b\}$, we have that $M(a)=2$ and $M(b)=1$. If $M(x)=0$ then $x$ is not present in $M$. We denote by $\operatorname{supp}(M)$ the set of all elements present in $M, \operatorname{supp}(M):=\{x \in S \mid M(x)>0\}$. Note that if every element has multiplicity at most one, then $M$ is a set. If $M$ is a multiset and $c \in \mathbb{N}_{\infty}$ then we denote by $\left.M\right|_{\leq c}$ the multiset obtained from $M$ by restricting the multiplicity of all elements to be at most $c$, i.e., $\left.M\right|_{\leq c}(x)=\min (M(x), c)$, for all elements $x$. Note in particular that $\left.M\right|_{\leq+\infty}=M$ and that $\left.M\right|_{\leq 1}$ converts $M$ into a set.

Graphs. We work with directed node-colored multigraphs. Formally, our graphs are hence triples $G=(V, E, g)$ where $V$ is a finite set of nodes; $E$ is a multiset of edges over $V \times V$; and $g$ is a function, called the coloring of $G$, that maps every node $v \in V$ to a color $g(v)$. (The term "color" is just an intuitive way to specify that $g$ has some unspecified range.) If $Y$ is the co-domain of $g$, i.e., $g$ is of the form $g: V \rightarrow Y$ then we also call $g$ a $Y$-coloring and say that $G$ is a $Y$-colored graph, or simply a $Y$-graph. When $Y=\mathbb{R}^{n}$ we also call $g$ an $n$-dimensional feature map. To ease notation we write $v \in G$ to indicate that $v \in V$. Furthermore, we write $G(v)$ instead of $g(v)$ to denote the color of $v$ in $G$, and we write $G(v \rightarrow w)$ instead of $E(v \rightarrow w)$ to denote the multiplicity of edge $v \rightarrow w$ in $G$. When $E$ is a set, i.e., when every edge has multiplicity at most one, then we also call $G$ a simple graph. We write $\mathrm{in}_{G}(v)$ for the multiset $\{\{w \in G \mid w \rightarrow v \in E\}$ of all incoming neighbors of $v$. So, if the edge $w \rightarrow v$ has multiplicity 5 in $E$ then $w$ also has multiplicity 5 in $\mathrm{in}_{G}(v)$. We drop subscripts when the graph $G$ is clear from the context. The size of a graph $G$ is the number of nodes $|V|$ plus the number of simple edges $|\operatorname{supp}(E)|$. This is a reasonable definition of the size of a multigraph, since for each edge it suffices to simply store its multiplicity as a number, and storing a number takes unit cost in the RAM model of computation.

Color transformers. If $C$ is a function that maps $X$-colored graphs $G=(V, E, g)$ into $Y$-colored graphs $G^{\prime}=\left(V^{\prime}, E^{\prime}, g^{\prime}\right)$ that leaves nodes and edges untouched and only changes the coloring, i.e., $V=V^{\prime}$ and $E=E^{\prime}$ then we call $C$ a coloring transformer. In particular, if $X=\mathbb{R}^{p}$ and $Y=\mathbb{R}^{q}$ for some dimensions $p$ and $q$ then $C$ is a feature map transformer.

Graph Neural Networks. Graph Neural Networks (GNNs) are a popular form of neural networks that enable deep learning on graphs. Many different forms of GNNs have been proposed in the literature. We refer the reader to the overview by Hamilton [11]. In this paper we focus on a standard form of GNNs that is known
under the name of aggregate-combine GNNs [2], also called messagepassing $G N N s$. These are defined as follows [7, 10].

A GNN layer of input dimension $p$ and output dimension $q$ is a pair (AgG, Comb) of functions where (1) Agg is an aggregation function that maps finite multisets of vectors in $\mathbb{R}^{p}$ to vectors in $\mathbb{R}^{h}$ for some dimension $h$ and (2) Сомв is a combination function Сомв: $\mathbb{R}^{p} \times \mathbb{R}^{h} \rightarrow \mathbb{R}^{q}$. In practice, AGG is usually taken to compute the arithmetic mean, sum, or maximum of the vectors in the multiset, while Сомв is computed by means of a feedforward neural network whose parameters can be learned.

A GNN is a sequence $\bar{L}=\left(L_{1}, \ldots, L_{k}\right)$ of GNN layers, where the output dimension of $L_{i}$ equals the input dimension of $L_{i+1}$, for $1 \leq i<k$. The input and output dimensions of the GNN are the input dimension of $L_{1}$, and the output dimension of $L_{k}$ respectively. In what follows, we write $\bar{L}: p, q$ to denote that $p$ is the input dimension of $\bar{L}$ and $q$ is the output dimension.

Semantically, GNN layers and GNNs are feature map transformers [7] In particular, when GNN layer $L=$ (AgG, Сомв) of input dimension $p$ and output dimension $q$ is executed on $\mathbb{R}^{p}$-colored graph $G=(V, E, g)$ it returns the $\mathbb{R}^{q}$-colored graph $G^{\prime}=\left(V, E, g^{\prime}\right)$ with $g^{\prime}$ the $q$-dimensional feature map defined by

$$
g^{\prime}: v \mapsto \operatorname{Comb}\left(g(v), \operatorname{AGG}\left\{g(w) \mid w \in \operatorname{in}_{G}(v)\right\}\right) .
$$

As such, for each node $v, \bar{L}$ aggregates the (multiplicity-weighted) $\mathbb{R}^{p}$ colors of $v$ 's neighbors, and combines this with $v$ 's own color to compute the $\mathbb{R}^{q}$ output.

A GNN $\bar{L}: p, q$ simply composes the transformations defined by its layers: given $\mathbb{R}^{p}$-colored graph $G$ it returns the $\mathbb{R}^{q}$-colored graph $\left(L_{k} \circ L_{k-1} \circ \cdots \circ L_{1}\right)(G)$.

Discussion. It is important to stress that in the literature GNNs are defined to operate on simple graphs, whereas we have generalized their semantics above to also work on multigraphs. We did so because, as we will see in Section 3, the result of compressing a simple graph for the purpose of learning naturally yields a multigraph.
Learning problems. GNNs are used for a wide range of supervised learning tasks on graphs. For example, for a node $v$, the $\mathbb{R}^{q_{-}}$ vector $\bar{L}(G)(v)$ computed for $v$ by GNN $\bar{L}$ can be interpreted, after normalisation, as a probability distribution over $q$ new labels (for node classification), or as predicted values (for node regression). Similarly, an edge prediction for nodes $v$ and $w$ can be made based on the pair $(\bar{L}(G)(v), \bar{L}(G)(w))$. Finally, by aggregating $\bar{L}(G)(v)$ over all nodes $v \in G$, one obtains graph embeddings that can be used for graph classification, regression and clustering [11].

In this work, we focus on the tasks of node classification and regression. Our methodology is equally applicable to the other tasks, however.

In order to make precise what we mean by learning GNNs on compressed graphs for node classification, we propose the following formal definition.

Definition 2.1. A learning problem of input dimension $p$ and output dimension $q$ is a tuple $\mathcal{P}=(G, T$, Loss, $\mathcal{S})$ where

- $G$ is the $\mathbb{R}^{p^{p}}$-colored graph on which we wish to learn;
- $T$ is a subset of $G$ 's nodes, representing the training set;
- Loss: $T \times \mathbb{R}^{q} \rightarrow \mathbb{R}$ is a loss function that allows to quantify, for each node $v \in T$ the dissimilarity $\operatorname{Loss}(v, c)$ of the $\mathbb{R}^{q_{-}}$ color $c$ that is predicted for $v$ by a GNN and the desired $\mathbb{R}^{q}$-color for $v$ as specified in the training set;
- $\mathcal{S}$ is the hypothesis space, a (possibly infinite) collection of GNNs of input dimension $p$ and output dimension $q$.
Given a learning problem $\mathcal{P}$, a learning algorithm produces a "learned" GNN in $\mathcal{S}$ by traversing the search space $\mathcal{S}$. For each currently considered GNN $\bar{L} \in \mathcal{S}$, the observed loss of $\bar{L}$ on $G$ w.r.t. $T$ is computed as

$$
\operatorname{Loss}(\bar{L}(G), T):=\sum_{v \in T} \operatorname{Loss}(v, \bar{L}(G)(v))
$$

The learning algorithm aims to minimize this loss, but possibly returns an $\bar{L}$ for which this is only a local minimum.

In practice, $\mathcal{S}$ is usually a collection of GNNs with the same topology: they all have the same number of layers (with each layer $d$ having the same input and output dimensions accross GNNs in $\mathcal{S}$ ) and are parametrized by the same number of learnable parameters. Each concrete parametrization constitutes a concrete GNN in $\mathcal{S}$ in our framework. Commonly, the learned GNN $\bar{L}$ is then found by means of gradient descent, which updates the learnable parameters of the GNNs in $\mathcal{S}$ to minimize the observed error.

No matter which concrete learning algorithm is used to solve a learning problem, the intent is that the returned $\bar{L}$ generalizes well: it makes predictions on $G$ for the nodes not in $T$, and can also be applied to other, new $\mathbb{R}^{p}$-colored graphs to predict $\mathbb{R}^{q}$-vectors for each node.

## Our research question in this paper is the following.

Given a GNN learning problem $\mathcal{P}=(G, T$, Loss, $\mathcal{S})$, is it possible to transform this into a new problem $\mathcal{P}^{\prime}=$ $\left(G^{\prime}, T^{\prime}\right.$, Loss $\left.^{\prime}, \mathcal{S}\right)$ that is obtained by compressing $G$, $T$, and Loss into a smaller graph $G^{\prime}$, training set $T^{\prime}$, and loss function Loss' such that instead of learning a $G N N$ on $\mathcal{P}$ we could equivalently learn a GNN on $\mathcal{P}^{\prime}$ instead?
Here "equivalently" means that ideally, no matter which learning algorithm is used, we would like the learned GNN to be identical in both cases. Of course, this is not possible in practice because the learning process is itself non-deterministic, e.g., because the learning algorithm makes random starts; because of stochasticity in stochastic gradient descent; or because of non-deterministic dropout that is applied between layers. Nevertheless, we expect the GNN obtained by learning on the compressed problem would perform "as good" as the GNN obtained by the learning on the uncompressed problem, in the sense that it generalizes to unseen nodes and unseen colored graphs equally well.

To ensure that we may hope any learning algorithm to perform equally well on $\mathcal{P}^{\prime}$ as on $\mathcal{P}$, we formally define:

Definition 2.2. Two learning problems $\mathcal{P}$ and $\mathcal{P}^{\prime}$ are equivalent, written $\mathcal{P} \equiv \mathcal{P}^{\prime}$, if they share the same hypothesis space of GNNs $\mathcal{S}$ and, for every $\bar{L} \in \mathcal{S}$ we have $\operatorname{Loss}(\bar{L}(G), T)=\operatorname{Loss}^{\prime}\left(\bar{L}\left(G^{\prime}\right), T^{\prime}\right)$.

In other words, when traversing the hypothesis space for a GNN to return, no learning algorithm can distinguish between $\mathcal{P}$ and $\mathcal{P}^{\prime}$. All other things being equal, if the learning algorithm then
returns a GNN $\bar{L}$ when run on $\mathcal{P}$, it will return $\bar{L}$ on $\mathcal{P}^{\prime}$ with the same probability.

Note that, while the hypothesis space $\mathcal{S}$ remains unchanged in this definition, it is possible (and, as we will see, actually required) to adapt the loss function Loss into a modified loss function Loss' during compression.

The benefit of a positive answer to our research question, if compression is efficient, is computational efficiency: learning on smaller graphs is faster than learning on larger graphs and requires less memory.

## 3 Methodology

To compress one learning problem into an equivalent, hopefully smaller, problem we will exploit recent insights into the expressiveness of GNNs [2, 19, 24]. In particular, it is known that if the local neighborhoods of two nodes $v, w$ in input graph $G$ are equal, then any GNN will treat $v$ and $w$ identically. In particular, it will assign the same output colors to $v$ and $w$. We may intuitively exploit this property for compression: since $v$ and $w$ are treated identically there is no need for them both to be present during learning; having one of them suffices. So, we could compress by removing nodes that are redundant in this sense. We must take care, however, that by removing one, we do not change the structure (and hence, possibly, the predicted color) of the remaining node. Also, of course, we need to make sure that by removing nodes we do not lose training information. I.e., if $T$ specifies a training color for $v$ but not $w$ then if we decide to remove $v$, we somehow need to "fix" $T$, as well as the loss function.

This section is devoted to developing this intuitive idea. In Section 3.1 we first study under which conditions GNNs treat nodes identically. Next, in Section 3.2 we develop compression of colored graphs based on collapsing identically-treated nodes, allowing to remove redundant nodes while retaining the structure of the remaining nodes. Finally, in Section 3.3, we discuss compression of the training set and loss function. Together, these three ingredients allow us to compress a learning problem into an equivalent problem, cf. Definition 2.2.

We close this section by proposing an alternative definition of compression that works only for a limited class of learning problems. It is nevertheless interesting as it may allow better compression, as we will show in Section 4.

### 3.1 Indistinguishability

The following definition formalizes when two nodes, not necessarily in the same graph, are treated identically by a class of GNNs.

Definition 3.1. Let $\mathcal{S}$ be a class of GNNs, let $G$ and $H$ be two $\mathbb{R}^{p}$-colored graphs for some $p$, and let $v \in G, w \in H$ be two nodes in these graphs. We say that $(G, v)$ is $\mathcal{S}$-indistinguishable from ( $H, w$ ), denoted $(G, v) \sim \mathcal{S}(H, w)$, if for every GNN $\bar{L} \in \mathcal{S}$ of input dimension $p$ it holds that $\bar{L}(G)(v)=\bar{L}(H)(w)$.

In other words, two nodes are indistinguishable by a class of GNNs $\mathcal{S}$ if no GNN in $\mathcal{S}$ can ever assign a different output color to these nodes, when started on $G$ respectively $H$. We call $(G, v)$ and (H,w) $\mathcal{S}$-distinguishable otherwise.


|  | $\mathrm{cr}^{0}$ | $\mathrm{cr}^{1}$ | $\mathrm{cr}^{2}$ |
| :---: | :---: | :---: | :---: |
| $a_{1}$ | $a$ | (1) $=(a,\{\{a\})$ | (1), \{(2)\}) |
| $a_{2}$ | $a$ | (2) $=(a,\{a, a\})$ | ( (2), \{(1), (2) \}) |
| $a_{3}$ | $a$ | (2) $=(a,\{a, a\})$ | (2), \{(1), (2)\}) |
| $b_{1}$ | $b$ | (3) $=(b,\{a, a\})$ | (3), \{(1), (2) \}) |
| $b_{2}$ | $b$ | (3) $=(b,\{a, a\})$ | (3), \{[1, (2)\}) |
| $b_{3}$ | $b$ | (3) $=(b,\{a, a\})$ | (3), \{[2, (2)\}) |

Figure 1: Example of color refinement. Nodes $a_{1}, a_{2}, a_{3}$ have the same color $a$; nodes $b_{1}, b_{2}, b_{3}$ have the same color $b$. All edges have multiplicity 1 .

For the purpose of compression, we are in search of sets of nodes in the input graph $G$ that are pairwise $\mathcal{S}$-indistinguishable, with $\mathcal{S}$ the hypothesis space of the input learning problem. It is these nodes that we can potentially collapse in the input learning problem. Formally, let $[G, v]_{\mathcal{S}}$ denote the set of all nodes in $G$ that are $S$-indistinguishable from $v$,

$$
[G, v]_{\mathcal{S}}:=\left\{w \in G \mid(G, v) \sim_{\mathcal{S}}(G, w)\right\}
$$

We aim to calculate $[G, v]_{\mathcal{S}}$ and subsequently compress $G$ by removing all but one node in $[G, v]_{\mathcal{S}}$ from $G$.
Color refinement. To calculate $[G, v]_{\mathcal{S}}$, we build on the work of Morris et al. [19] and Xu et al. [24]. They proved independently that a GNN can distinguish two nodes if an only if the so-called color refinement algorithm assigns different colors to these nodes. Color refinement is equivalent to the one-dimensional Weisfeiler-Leman (WL) algorithm [10], and works as follows.

Definition 3.2. The (one-step) color-refinement of colored graph $G=(V, E, g)$, denoted $\operatorname{cr}(G)$, is the colored graph $G^{\prime}=\left(V, E, g^{\prime}\right)$ where $g^{\prime}$ maps every node $v \in G$ to a pair, consisting of $v$ 's original color and the multiset of colors of its incoming neighbors:

$$
g^{\prime}: v \mapsto\left(G(v),\left\{G(w) \mid w \in \operatorname{in}_{G}(v)\right\}\right)
$$

As such, we can think of $\operatorname{cr}(G)(v)$ as representing the immediate neighborhood of $v$ (including $v$ ), for any node $v$.

We denote by $\mathrm{cr}^{d}(G)$ the result of applying $d$ color refinement steps on $G$, so $\mathrm{cr}^{0}(G)=G$ and $\mathrm{cr}^{d+1}(G)=\operatorname{cr}\left(\operatorname{cr}^{d}(G)\right)$. Using this notation, we can think of $\mathrm{cr}^{d}(G)(v)$ as representing the local neighborhood of $v$ "up to radius $d$ ".

To illustrate, Figure 1 shows a colored graph $G$ and two steps of color refinement.

The following property was observed by Morris et al. [19] and Xu et al [24] for GNNs operating on simple graphs. We here extend it to multigraphs.
Proposition 3.3. Let $\bar{L}$ be a $G N N$ composed ofd $\in \mathbb{N}$ layers, $d \geq 1$. If $\operatorname{cr}^{d}(G)(v)=\operatorname{cr}^{d}(H)(w)$ then $\bar{L}(G)(v)=\bar{L}(H)(w)$. As a consequence, if $\mathcal{S}$ is a hypothesis space consisting of GNNs of at most $d$ layers and $\operatorname{cr}^{d}(G)(v)=\operatorname{cr}^{d}(H)(w)$ then $(G, v) \sim \mathcal{S}(H, w)$.

In other words, $d$-layer GNNs cannot distinguish nodes that are assigned the same color by $d$ steps of color refinement.

Let $[G, v]_{d}$ denote the set of all nodes in $G$ that receive the same color as $v$ after $d$ steps of color refinement,

$$
[G, v]_{d}:=\left\{w \in G \mid \operatorname{cr}^{d}(G)(v)=\operatorname{cr}^{d}(G)(w)\right\}
$$

Then it follows from Proposition 3.3 that $[G, v]_{d}$ is a refinement of $[G, v]_{\mathcal{S}}$ in the sense that $[G, v]_{d} \subseteq[G, v]_{\mathcal{S}}$, for all $v \in G$. Morris et al. [19] and Xu et al. [24] have also shown that for every graph $G$ and every depth $d$ there exists a GNN $\bar{L}$ of $d$ layers such that $[G, v]_{d}=[G, v]_{\{\bar{L}\}}$, for every node $v \in G$. Consequently, if, in addition to containing only GNNs with at most $d$ layers, $\mathcal{S}$ includes all possible $d$-layer GNNs, then $[G, v]_{d}=[G, v]_{\mathcal{S}}$ coincide, for all $v \in G$. Hence, for such $\mathcal{S}$ we may calculate $[G, v]_{\mathcal{S}}$ by calculating $[G, v]_{d}$ instead. When $\mathcal{S}$ does not include all $d$-layer GNNs we simply use $[G, v]_{d}$ as a proxy for $[G, v]_{\mathcal{S}}$. This is certainly safe: since $[G, v]_{d} \subseteq[G, v]_{\mathcal{S}}$ no GNN in $\mathcal{S}$ will be able to distinguish the nodes in $[G, v]_{d}$ and we may hence collapse nodes in $[G, v]_{d}$ for the purpose of compression. In this case, however, we risk that $[G, v]_{d}$ contains too few nodes compared to $[G, v]_{\mathcal{S}}$, and therefore may not provide enough opportunity for compression. We will return to this issue in Section 3.4.

What happens if there is no bound on the number of layers of GNNs in $\mathcal{S}$ ? In that case we can still use color refinement to compute $[G, v]_{\mathcal{S}}$ as follows. It is known that after a finite number of color refinements steps we reach a value $d$ such that for all nodes $v \in G$ we have $[G, v]_{d}=[G, v]_{d+1}$. The smallest value $d$ for which this holds is called the stable coloring number of $G$, and we denote the colored graph obtained by this value of $d$ by $\mathrm{cr}^{\infty}(G)$ in what follows. Similarly we denote the equivalence classes at this value of $d$ by $[G, v]_{\infty}$. From Proposition 3.3 it readily follows:

Corollary 3.4. For any class $\mathcal{S}$ of $G N N s$, ifcr ${ }^{\infty}(G)(v)=\operatorname{cr}^{\infty}(H)(w)$ then $(G, v) \sim_{\mathcal{S}}(H, w)$.

We note that it is very efficient to compute the set $\left\{[G, v]_{d} \mid\right.$ $v \in G\}$ of all color refinement classes: this can be done in time $O((n+m) \log n)$ with $n$ the number of vertices and $m$ the number of edges of the input graph [4].

Example 3.5. To illustrate, consider the colored graph from Figure 1, as well as the color refinement steps illustrated there. (Recall that nodes $a_{1}, a_{2}, a_{3}$ share the same color, as do $b_{1}, b_{2}, b_{3}$.) Then after one step of color refinement we have

$$
\begin{aligned}
& {\left[G, a_{1}\right]_{1}=\left\{a_{1}\right\}} \\
& {\left[G, a_{2}\right]_{1}=\left[G, a_{3}\right]_{1}=\left\{a_{2}, a_{3}\right\}} \\
& {\left[G, b_{1}\right]_{1}=\left[G, b_{2}\right]_{1}=\left[G, b_{3}\right]_{1}=\left\{b_{1}, b_{2}, b_{3}\right\}}
\end{aligned}
$$

while after two steps of color refinement we obtain the following color refinement classes:

$$
\begin{array}{ll}
{\left[G, a_{1}\right]_{2}=\left\{a_{1}\right\}} & {\left[G, b_{1}\right]_{2}=\left[G, b_{2}\right]_{2}=\left\{b_{1}, b_{2}\right\}} \\
{\left[G, a_{2}\right]_{2}=\left[G, a_{3}\right]_{2}=\left\{a_{2}, a_{3}\right\}} & {\left[G, b_{3}\right]_{2}=\left\{b_{3}\right\} .}
\end{array}
$$

We invite the reader to check that for every node $v$ in this graph, $[G, v]_{3}=[G, v]_{2}$. As such, the stable coloring is obtained when $d=2$ and $[G, v]_{2}=[G, v]_{\infty}$.

### 3.2 Graph reduction

Having established a way to compute redundant nodes, we now turn our attention to compression. Assume that we have already computed the color refinement classes $\left\{[G, v]_{d} \mid v \in G\right\}$ for $d \in \mathbb{N}_{\infty}$. For each $v \in G$, we wish to "collapse" all nodes in $[G, v]_{d}$ into a single node. To that end, define a $d$-substitution on a graph $G$ to be a function that maps each color refinement class in $\left\{[G, v]_{d} \mid v \in G\right\}$


Figure 2: Reduction of the graph of Figure 1 by the 1substitutions $\rho_{1}$ and $\rho_{2}$ from Example 3.7.
to a node $\rho\left([G, v]_{d}\right) \in[G, v]_{d}$. Intuitively, $\rho\left([G, v]_{d}\right)$ is the node that we wish to keep; all other nodes in $[G, v]_{d}$ will be removed. In what follows we extend $\rho$ to also operate on nodes in $G$ by setting $\rho(v)=\rho\left([G, v]_{d}\right)$.

Definition 3.6. The reduction of graph $G$ byd-substitution $\rho$ on $G$ is the graph $H=(V, E, h)$ where

- $V=\{\rho(v) \mid v \in G\}$
- For all $v, w \in V$ we have

$$
E(v \rightarrow w)=\sum_{v^{\prime} \in[G, v]_{d}} G\left(v^{\prime} \rightarrow w\right)
$$

In particular, if there is no edge into $w$ in $G$, there will be no edge into $w$ in $H$, as this sum is then zero.

- nodes retain colors: for each node $v \in H$ we have $h(v)=$ $G(v)$.
In what follows, we denote by $G / \rho$ the reduction of $G$ by $\rho$. A graph obtained by reducing $G$ according to some $d$-substitution $\rho$ is called a $d$-reduct of $G$.

Example 3.7. Reconsider the colored graph $G$ of Figure 1. Let $\rho_{1}$ and $\rho_{2}$ be the following $d=1$-substitutions:

$$
\begin{array}{lll}
\rho_{1}:\left\{a_{1}\right\} \mapsto a_{1} & \left\{a_{2}, a_{3}\right\} \mapsto a_{2} & \left\{b_{1}, b_{2}, b_{3}\right\} \mapsto b_{1} \\
\rho_{2}:\left\{a_{1}\right\} \mapsto a_{1} & \left\{a_{2}, a_{3}\right\} \mapsto a_{2} & \left\{b_{1}, b_{2}, b_{3}\right\} \mapsto b_{3}
\end{array}
$$

Then $G / \rho_{1}$ and $G / \rho_{2}$ are illustrated in Figure 2.
The following proposition is an essential property of our compression methodology.

Proposition 3.8. For every graph $G$, everyd-substitution $\rho$ of $G$ with $d \in \mathbb{N}_{\infty}$, and every nodev $\in G$ we have $\mathrm{cr}^{d}(G)(v)=\operatorname{cr}^{d}(G / \rho)(\rho(v))$.

It hence follows from Proposition 3.3 and Corollary 3.4 that if $\mathcal{S}$ consists of GNNs of at most $d \in \mathbb{N}_{\infty}$ layers, then $(G, v) \sim \mathcal{S}$ ( $G / \rho, \rho(v)$ ).
Discussion Example 3.7 shows that the choice of $d$-substitution determines the reduct $G / \rho$ that we obtain. In particular, the example shows that distinct substitutions can yield distinct, non-isomorphic reducts. This behavior is unavoidable, unless $d$ is the stable coloring number of $G$. Indeed, we are able to show:

Proposition 3.9. There is a single d-reduct of a graph $G$ up to isomorphism if and only if d is greater than or equal to the stable coloring number of $G$.

A direct consequence of having different non-isomorphic reducts when $d$ is less than the coloring number is that some of these reducts may be smaller than others. In Example 3.7, $G / \rho_{1}$ has 3 nodes and 4 edges while $G / \rho_{2}$ has 3 nodes and only 3 edges. We may always obtain a $d$-reduct of minimal size as follows. For $d \in \mathbb{N}_{\infty}$, define


Figure 3: Reduction of a tree-shaped simple graph (left) into a small multigraph (right).
the $d$-incidence of a node $w \in G$, denoted incidence ${ }_{G}^{d}(w)$, to be the number of color refinement classes in $\left\{[G, v]_{d} \mid v \in G\right\}$ that contain an incoming neighbor of $w$. That is, the $d$-incidence of $w$ is the number of distinct classes in $\left\{[G, u]_{d} \mid u \in \operatorname{in}_{G}(w)\right\}$. The following proposition shows that we obtain a $d$-reduct of minimal size by by choosing a $d$-substitution that maps color refinement classes to nodes of minimal $d$-incidence.
Proposition 3.10. Let $G$ be a graph, let $d \in \mathbb{N}_{\infty}$ and let $\rho$ be a $d$-substitution such that

$$
\text { incidence }_{G}^{d}(\rho(v))=\min _{v^{\prime} \in[G, v]_{d}} \text { incidence }_{G}^{d}\left(v^{\prime}\right)
$$

for every node $v \in G$. Then the size of $G / \rho$ is minimal among all $d$-reducts of $G$.

When we report the size of $d$-reducts in our experiments (Section 4), we always report the minimal size among all $d$-reducts.
Discussion Example 3.7 illustrates that, depending on the substitution used, the result of reducing a simple graph may be a multigraph. In the literature, however, GNNs and color refinement are normally defined to operate on simple graphs. One may therefore wonder whether it is possible to define a different notion of reduction that always yields a simple graph when executed on simple, instead of a multigraph as we propose here. To answer this question, consider the tree-shaped graph $G$ in Figure 3(left), whose root $v$ has $m$ $b$-colored children, each having $n c$-labeled children. It is straightforward to see that when $d \geq 2$, any simple graph $H$ that has a node $w$ such that $\operatorname{cr}^{d}(G)(v)=\operatorname{cr}^{d}(H)(w)$ must be such that $w$ has $m$ $b$-colored children in $H$, each having $n c$-labeled children. As such, because $H$ is simple, it must be of size at least as large as $G$. Instead, by moving to multigraphs we are able to compress this "regular" structure in $G$ by only three nodes, as show in Figure 3(right). This illustrates that for the purpose of compression we naturally need to move to multigraphs.

### 3.3 Problem compression

We next combine the insights from Sections 3.1 and 3.2 into a method for compressing learning problems.

Let $\mathcal{P}=(G, T$, Loss, $\mathcal{S})$ be a learning problem. Let $\rho$ be a $d$ substitution. We then define the reductions $T / \rho$ and Loss $/ \rho$ of $T$ and Loss by $\rho$ as follows:

$$
\begin{aligned}
T / \rho & =\{\rho(v) \mid v \in T\} \\
\operatorname{Loss} / \rho(v, c) & =\sum_{w \in T \cap[G, v]_{d}} \operatorname{Loss}(w, c)
\end{aligned}
$$

We denote by $\mathcal{P} / \rho$ the learning problem $(G / \rho, T / \rho$, Loss $/ \rho, \mathcal{S})$.

Theorem 3.11. Let $\mathcal{P}$ be a learning problem with hypothesis space $\mathcal{S}$ and assume that $d \in \mathbb{N}_{\infty}$ is such that every $G N N$ in $\mathcal{S}$ has at most $d$ layers. (In particular, $d=\infty$ if there is no bound on the number of layers in $\mathcal{S}$.) Then $\mathcal{P} \equiv \mathcal{P} / \rho$ for every $d$-substitution $\rho$.

### 3.4 Graded Color Refinement

So far, we have focused on compression based on the depth of the GNNs present in the hypothesis space, where the depth of a GNN equals its number of layers and the depth of a hypothesis space $\mathcal{S}$ is the maximum depth of any of its GNNs, or $\infty$ if this maximum is unbounded. In particular, the notion of $d$-reduct hinges on this parameter $d$ through the calculated color refinement classes $[G, v]_{d}$.

As we have already observed in Section 3.1, however, when $\mathcal{S}$ does not contain all $d$-layer GNNs the color refinement classes $[G, v]_{d}$ that we base compression on may contain too few nodes compared to $[G, v]_{\mathcal{S}}$ and may therefore not provide enough opportunity for compression.

In such cases, it may be beneficial to move to more fine-grained notions of color refinement that better capture $[G, v]_{\mathcal{S}}$. In this section we propose one such fine-grained notion, which takes into account the "width" of $\mathcal{S}$. We say that $G N N \bar{L}$ has width $c \in \mathbb{N}_{\infty}$ if for every layer in $\bar{L}$ the aggregation function AgG is such that $\operatorname{AgG}(M)=\operatorname{AgG}\left(\left.M\right|_{\leq c}\right)$ for every multiset $M$. In other words: AGG can only "count" up to $c$ copies of a neighbor's color. When $c=\infty$ there is no limit on the count. The width of $\mathcal{S}$ is then the maximum width of any of its GNNs, or $\infty$ if this maximum is unbounded. Hypothesis spaces of bounded width clearly do not contain all $d$-layer GNNs, for any depth $d$.

While we know of no practical GNN architectures that explicitly limit the width, there are influential learning algorithms that implicitly limit the width. For example, to speed up learning, GraphSAGE [12] can be parametrized by a hyperparameter $c$. When $c<\infty$ GraphSAGE does not consider all of a node's neighbors in each layer, but only a random sample of at most $c$ neighbors of that node. Such sampling effectively limits the width of $\mathcal{S}$.

We next define a variant of color refinement, called graded color refinement, that takes width into account. It may lead to larger color refinement classes, and therefore potentially also to better compression.

Definition 3.12. Let $c \in \mathbb{N}_{\infty}$. The (one-step) c-graded color refinement of colored graph $G=(V, E, g)$, denoted $\operatorname{cr}_{c}(G)$, is the colored graph $G^{\prime}=\left(V, E, g^{\prime}\right)$ with

$$
g^{\prime}: v \mapsto\left(G(v),\left\{\left\{G(w) \mid w \in \operatorname{in}_{G}(v)\right\} \mid \leq c\right)\right.
$$

Note that $\mathrm{cr}_{\infty}$ equals normal, non-graded, color refinement. We also remark that $\mathrm{cr}_{c}$ with $c=1$ corresponds to standard bisimulation on graphs [1]. We denote by $\operatorname{cr}_{c}^{d}(G)$ the result of applying $d$ refinement steps of $c$-graded color refinement, $\operatorname{so~}_{\operatorname{cr}}^{c}(G)=G$ and $\operatorname{cr}_{c}^{d+1}=\operatorname{cr}\left(\operatorname{cr}_{c}^{d}(G)\right)$. We denote by $[G, v]_{c, d}$ the set of all nodes in $G$ that receive the same color after $d$ steps of $c$-graded color refinement. The concept of $(c, d)$-substitution is then defined analogously to $d$-substitution, as mappings from the $[G, v]_{c, d}$ color refinement classes to nodes in these classes. The reduction of a graph $G$ by a ( $c, d$ ) substitution is similar to reductions by $d$-substitution except that the edge multiplicity $E(v \rightarrow w)$ for $v, w$ in the reduction is

| Graph | Type | \#Nodes | \#Edges |
| :--- | :--- | ---: | ---: |
| ogbn-arxiv | directed | 169.343 | 1.166 .243 |
| ogbn-arxiv-inv | directed | 169.343 | 1.166 .243 |
| ogbn-arxiv-undirected | undirected | 169.343 | 2.315 .598 |
| ogbn-products | undirected | 2.449 .029 | 61.859 .140 |
| snap-roadnet-ca | undirected | 1.965 .206 | 5.533 .214 |
| snap-roadnet-pa | undirected | 1.088 .092 | 3.083 .796 |
| snap-roadnet-tx | undirected | 1.379 .917 | 3.843 .320 |
| snap-soc-pokec | directed | 1.632 .803 | 30.622 .564 |

Table 1: Datasets
now limited to $c$, i.e.,

$$
E(v \rightarrow w)=\left.\sum_{v^{\prime} \in[G, v]_{c, d}} G\left(v^{\prime} \rightarrow w\right)\right|_{\leq c} .
$$

With these definitions, we can show that for any $\mathcal{P}$ with hypothesis space $\mathcal{S}$ of width $c$ and depth $d$ we have $\mathcal{P} \equiv \mathcal{P} / \rho$ for any $(c, d)$ reduction $\rho$. The full development is omitted due to lack of space.

We note that $[G, v]_{d} \subseteq[G, v]_{c, d}$, always. Graded color refinement hence potentially leads to better compression, but only applies to problems with hypothesis spaces of width $c$. We will empirically contrast the compression ratio obtained by $(c, d)$-reducts to those obtained by $d$-reducts (i.e., where $c=\infty$ ) in Section 4. There, we also study the effect of $c$ on learning accuracy for problems whose width is not bounded.

## 4 Evaluation

In this section, we empirically evaluate the compression methodology described in Section 3. We first give insights into the compression ratios that can be obtained on real-world graphs in Section 4.1. Subsequently, we evaluate the learning on compressed graphs versus learning on the original graphs.

### 4.1 Compression

We consider the real-world graphs listed in Table 1. The ogbn-* graphs are from the Open Graph Benchmark (OGB), a collection of realistic, large-scale, and diverse benchmark datasets for machine learning on graphs [13], where they belong to the OGB node property prediction benchmark (OGBN). Specifically, ogbn-arxiv is a network of academic papers, where edge $x \rightarrow y$ indicates that $x$ cites $y$. Graph ogbn-arxiv-inv is the inverted version of ogbn-arxiv; it is obtained by reversing edges, so that edge $x \leftarrow y$ indicates that $y$ was cited by $x$. Graph ogbn-arxiv-undirected is the undirected version of ogbn-arxiv; it is obtained by adding inverse edges to ogbn-arxiv. Next, there is ogbn-products, an undirected graph representing an Amazon product co-purchasing network. The other datasets are from the Stanford Large Network Dataset Collection (SNAP) [15]. Here, snap-roadnet-ca, snap-roadnet-pa, and snap-roadnet-tx are undirected graphs representing road networks, and snap-soc-pokec is a directed graph containing an online social network.

The input colors used for learning on these graphs typically depend on the application. To get an understanding of the maximum amount of compression that we can obtain independent of the target application, we assign a shared single color $c$ to each node, in all graphs. As such, the color refinement classes $[G, v]_{d}$ that we obtain
are maximal, in the sense that for any other colorored graph $G^{\prime}$ whose topology equals $G$ we will have $\left[G^{\prime}, v\right]_{d} \subseteq[G, v]_{d}$. In this setting, we hence reach maximal compression.

We consider three versions of ogbn-arxiv to get an indication of how edge directionality impacts compression. Recall that GNN layers propagate color information following the direction of edges. Hence, because in ogbn-arxiv an edge $x \rightarrow y$ indicates that $x$ cites $y$, color information flows from citing papers to cited papers. In ogbn-arxiv-inv, by contrast, it flows from cited papers to citing papers while in ogbn-arxiv-undirected it flows in both directions. The direction in which the information can flow impacts the number of color refinement classes that we obtain, and hence the compression, as we will see.

Ungraded compression Figures 4(a) and 4(b) shows the fraction of nodes and edges remaining in $d$-reducts of these graphs, plotted as a function of the number of color refinement rounds $d$. (Consistent with our definition of the size of a multigraph, the number of edges plotted is the number of unique edges, i.e., ignoring edge multiplicities.) We see that in terms of the number of nodes, compression is effective for $d \leq 2$, obtaining compression ratios of $0.03 \%-0.05 \%$ on the road network datasets, to $77 \%$ on ogbnproducts. For $d=3$, compression becomes ineffective for ogbn-arxiv-undirected, ogbn-products and snap-soc-pokec as these retain $88 \%$ of their nodes or more. Compression on the other datasets is satsifactory for $d=3$, as shown in Table 2. From $d>3$ onwards, node compression becomes ineffective for most datasets, with all datasets except ogbn-arxiv retaining at least $86 \%$ of their nodes when $d \geq 5$. By contrast, ogbn-arxiv stabilizes at $d=4$, retaining only $36 \%$ of its nodes.

In terms of the number of edges, we see that ogbn-arxiv-inv, ogbn-arxiv-undirected, ogbn-products, and snap-soc-pokec retain almost $100 \%$ of their edges from $d \geq 2$ onwards, while ogbn-arxiv retains only $56 \%$ of its edges when $d=3$ and the road networks compress to $5 \%-8 \%$ of the edges when $d=3$.

While we may hence conclude that in general compression becomes ineffective for deeper layer numbers, $d>4$, we note that in practice most GNN topologies use only $d=3$ layers. For such GNNs, compression on ogbn-arxiv and the road networks is promising.

One may wonder why the inverted and undirected variants of ogbn-arxiv differ so much in terms of compression. The short answer is that that, their graph topology is completely different. As such, the local neighborhood information that $\mathrm{cr}^{d}$ calculates is also completely different, yielding different reductions. For example, a manual inspection of ogbn-arxiv reveals a number of highly cited papers that have no outgoing edges. While these papers are the "sink nodes" in ogbn-arxiv, they are "source nodes" in ogbn-arxivinv. Quite quickly we may then distinguish nodes in ogbn-arxiv-inv based solely on the number of highly cited papers that they cite. This behavior does not occur in ogbn-arxiv, because the highly cited papers are outgoing neighbors, which $\mathrm{cr}^{d}$ ignores.
Graded compression We next evaluate the effect of moving to compression based on c-graded color refinement. Figure 4(c) and (d) shows the fraction of nodes and edges remaining in (c,3)-reducts of our graphs, relative to the number of nodes and edges in the corresponding $d=3$-reduct, plotted as a function of $c$. In terms of the number of nodes we see that, as expected, moving to graded

| Graph | Nodes (\%) | Edges (\%) |
| :--- | ---: | ---: |
| ogbn-arxiv | 32.9 | 56.3 |
| ogbn-arxiv-inv | 65.9 | 92.7 |
| ogbn-arxiv-undirected | 93.3 | 98.9 |
| ogbn-products | 88.5 | 98.6 |
| snap-roadnet-ca | 4.4 | 5.9 |
| snap-roadnet-pa | 6.1 | 7.9 |
| snap-roadnet-tx | 3.9 | 5.2 |
| snap-soc-pokec | 87.9 | 99.1 |

Table 2: Compression at $d=3$.

| Problem | Nodes <br> $(\%)$ | Edges <br> $(\%)$ | Accurracy <br> $(\%)$ | Training |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| time $(s)$ | mem (GiB) |  |  |  |  |
| $\boldsymbol{P}_{1}$ | 100.0 | 100.0 | 66.7 | 61.66 | 2.14 |
| $\boldsymbol{P}_{2}$ | 100.0 | 100.0 | 65.9 | 58.99 | 2.02 |
| $\mathcal{P}_{3}^{1}$ | 76.9 | 95.9 | 60.9 | 48.10 | 1.59 |
| $\boldsymbol{P}_{3}^{3}$ | 79.2 | 97.1 | 64.5 | 49.71 | 1.65 |
| $\boldsymbol{\mathcal { P }}_{3}^{5}$ | 79.3 | 97.2 | 64.9 | 49.55 | 1.65 |
| $\boldsymbol{P}_{3}^{\infty}$ | 79.4 | 97.2 | 63.8 | 49.16 | 1.65 |

Table 3: Comparison of learning on the original uncompressed problem $\mathcal{P}_{1}$, the uncompressed problem with discretized labels $\mathcal{P}_{2}$, and ( $c, d=3$ )-compressed variants $\mathcal{P}_{3}^{c}$.
compression yields better compression than non-graded compression. In particular, for $c=1$ all datasets retain $<1 \%$ of their nodes while for $c=3$, compression is $27 \%$ or less for ogbn-arxiv, ogbn-arxiv-undirected, and the road networks. In the latter setting, ogbnproducts is at $75 \%$ of nodes and snap-soc-pokec at $55 \%$. Compression hence becomes less effective as $c$ increases.

In terms of the number of edges, compression is most effective when $c=1$ or $c=2$ in which case it significantly improves over ungraded compression. From $c \geq 3$ onwards, graded compression becomes only marginally better than ungraded compression.

We conclude that graded compression has the potential to yield significantly smaller graphs than ungraded compression, but only for small gradedness values, $c=1$ (i.e., bisimulation) or $c=2$.
Conclusion Overall, we see that real-world graphs have diverse non-graded compression ratios: road networks compress extremely well (to $4 \%$ of nodes and $5 \%$ of edges when $d=3$ ); while other graphs such as ogbn-arxiv-inv compress reasonably in terms of number of nodes ( $65 \%$ ) but only marginally in terms of edges ( $93 \%$ or more); and graphs such as ogbn-products compress only marginally in both (retaining $90 \%$ or more of nodes and edges). This diversity is to be expected: our exact compression methodology is based on exploiting redundancy in local neighborhoods of nodes. For graphs where few nodes have equal local neighborhoods, we cannot expect reduction in size. Moving to graded compression for those graphs improves reduction in size, but will yield approximate compression unless the learning problem hypothesis space has small width.

### 4.2 Learning

We next turn to validating empirically the effect of learning on compressed problems according to our methodology. Specifically, we apply our methodology to learning on ogbn-arxiv-inv with $d=3$. We know from Section 4.1 that compression on this graph is reasonable in terms of nodes, but only marginal in terms of edges.


Figure 4: Normalized reduction in nodes and edges using $d$-reduction ( $\mathbf{a}$ and $\mathbf{b}$ ) and ( $c, 3$ )-reduction ( $\mathbf{c}$ and d).

Despite the modest compression, the effect on learning efficiency in terms of learning time and memory consumption is still positive, as we will see.

We hence focus in this section on ogbn-arxiv-inv and the associated learning problem from the OGBN benchmark: predict, for every paper in ogbn-arxiv-inv, its subject area (e.g., cs.AI, cs.LG, and cs.OS, $\ldots$ ). There are 40 possible subject areas. In addition to the citation network, we have available for each paper a 128-dimensional feature vector obtained by averaging the embeddings of words in its title and abstract. Our learning problem $\mathcal{P}_{1}$ hence consists of the ogbn-arxiv-inv graph in which each node is colored with this feature vector. The training set $T$ consists of 90941 nodes, obtained conform the OGBN benchmark. The hypothesis space $\mathcal{S}$ consists of GNNs that all share the same topology and vary only in their concrete parameters. The topology consists of 3 GNN layers whose Agg function computes the mean of all colors of incoming neighbors. The Сомв function applies a linear transformation to $G(v)$, applies a linear transformation to the result of the aggregation, and finally sums these two intermediates together. Each layer, except the final one, is followed by a batch normalisation as well ReLU to introduce non-linearity. The layers have dimensions $(128,256)$, $(256,256)$ and $(256,40)$, respectively. We apply a $50 \%$ dropout between layers during training. Softmax is applied after the last layer to turn feature vectors into subject areas, and we use cross-entropy as loss function.

Unfortunately, the initial coloring in $\mathcal{P}_{1}$ is such that every node has a distinct color. Therefore, every node is in its own unique color refinement class, and compression is not possible. We therefore transform $\mathcal{P}_{1}$ into a problem $\mathcal{P}_{2}$ that can be compressed by first converting the 128 -dimensional word embedding vectors into estimates of paper areas by means of a multilayer perceptron (MLP) that is trained on the nodes in $T$ but without having the graph structure available. This hence yields an initial estimate of the paper area for each node. By learning a GNN on the graph that is colored by one-hot encodings of these initial estimates, the estimates can be refined based on the graph topology. We denote the new problem hence obtained by $\mathcal{P}_{2}$. Note that $\mathcal{P}_{2}$ has the same training set, hypothesis space, and loss function as $\mathscr{P}_{1}$. The MLP has input
dimension 128 , one hidden layer of dimension 256 , and output layer of dimension 40 .
We next compress $\mathcal{P}_{2}$ using $(c, d)$-reduction with $d=3$. The resulting compressed problems are denoted $\mathcal{P}_{3}^{c}$. The corresponding compressed graph sizes are shown in Table 3. We note that, because we consider labeled graphs here, the compression ratio is worse than the maximum-compression scenario of Section 4.1.

We gauge the generalisation power of the learned GNNs by computing the accurracy on the test set, determined by the OGBN benchmark, comprising 48603 nodes. We learn for 256 epochs with learning rate 0.01 on all problems. All experiments are run on an HP ZBook Fury G8 with Intel Core i9 11950H CPU, 32 GB of RAM and NVIDIA RTX A3000 GPU with 6 GB RAM.

The results are summarized in Table 3. Comparing $\mathcal{P}_{1}$ with $\mathcal{P}_{2}$ we see that estimating the paper area through an MLP has marginal effect on the test accurracy, training time and memory consumption. Further comparing $\mathcal{P}_{2}$ with $\mathcal{P}_{3}^{c}$, which are equivalent by Theorem 3.11, we see that training accurracy is indeed comparable between $\mathcal{P}_{2}$ and $\mathcal{P}_{3}^{\infty}$; we attribute the difference in accurracy to the stochastic nature of learning. There is a larger difference in accurracy between $\mathcal{P}_{2}$ and $\mathcal{P}_{3}^{c}$ when $c=1$, i.e., when we compress based on bisimulation, than when $c>1$. This is because $c$-graded compression is an approximation, as explained in Section 3.4, and because, as we can see, $c$-graded compression for $c>1$ is nearly identical in size to ungraded compression. For $c>1$ we may hence expect there to be only marginal differences w.r.t. ungraded compression. Learning the compressed problems $\mathcal{P}_{3}^{c}$ is more efficient than learning on the uncompressed $\mathcal{P}_{2}$, taking only 81.5-84.3\% of the learning time and $78.7-81.6 \%$ of the memory respectively which is comparable to the reduction in number of nodes when compressing.
Our evaluation in this section is on a single learning problem; it should hence be interpreted as a preliminary insight that requires further evaluation. Based on these preliminary findings, however, we conclude that compressed learning can yield observable improvements in training time and memory consumption.

## 5 Conclusion and Future Work

We have proposed a formal methodology for exact compression of GNN-based learning problems. While the attainable exact compression ratio depends on the input graph, our experiment in Section 4.2 nevertheless indicates that observable improvements in learning efficiency are possible, even when the compression in terms of the number of edges is negligible.

In terms of future work, first and foremost our preliminary empirical evaluation should be extended to more learning tasks. Second, as we have seen $c$-graded color refinement offers a principled way of approximating exact compression, which becomes exact for hypothesis spaces of width $c$. It is an interesting question whether other existing approximate compression proposals $[6,16]$ can similarly be tied to structural properties of the hypothesis space.

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## A Proofs for Section 3 (Methodology)

Proposition 3.3. Let $\bar{L}$ be a $G N N$ composed of $d \in \mathbb{N}$ layers, $d \geq 1$. If $\operatorname{cr}^{d}(G)(v)=\operatorname{cr}^{d}(H)(w)$ then $\bar{L}(G)(v)=\bar{L}(H)(w)$. As a consequence, if $\mathcal{S}$ is a hypothesis space consisting of GNNs of at most d layers and $\operatorname{cr}^{d}(G)(v)=\operatorname{cr}^{d}(H)(w)$ then $(G, v) \sim \mathcal{S}(H, w)$.

Proof. It suffices to show that, for all graphs $G, H$ and nodes $v \in G, w \in H$ it holds that, if $\operatorname{cr}(G)(v)=\operatorname{cr}(H)(w)$ then $L(G)(v)=$ $L(H)(w)$ for any GNN layer $L$. Using this observation, the proposition then follows for GNNs by straightforward induction on the number of layers $d$ and the fact that if $\mathrm{cr}^{d}(G)(v)=\operatorname{cr}^{d}(H)(w)$, then also $\mathrm{cr}^{d^{\prime}}(G)(v)=\mathrm{cr}^{d^{\prime}}(H)(w)$ for all $d^{\prime} \leq d .{ }^{1}$

So, assume that $\operatorname{cr}(G)(v)=\operatorname{cr}(H)(w)$. Since, by definition,

$$
\begin{aligned}
\operatorname{cr}(G)(v) & =\left(G(v),\left\{\left\{G\left(v^{\prime}\right) \mid v^{\prime} \in \operatorname{in}_{G}(v)\right\}\right)\right. \\
\operatorname{cr}(H)(w) & =\left(H(w),\left\{H\left(w^{\prime}\right) \mid w^{\prime} \in \operatorname{in}_{H}(w)\right\}\right)
\end{aligned}
$$

we may conclude that, $G(v)=H(w)$ and $\left\{G\left(v^{\prime}\right) \mid v^{\prime} \in \operatorname{in}_{G}(v)\right\}=$ $\left\{H\left(w^{\prime}\right) \mid w^{\prime} \in \operatorname{in}_{H}(w)\right\}$. Let $L=$ (AgG, Сомв) be an arbitrary GNN layer. Then,

$$
\begin{aligned}
\bar{L}(G)(v) & =\operatorname{ComB}\left(G(v), \operatorname{AgG}\left\{G\left(v^{\prime}\right) \mid v^{\prime} \in \operatorname{in}_{G}(v)\right\}\right) \\
& =\operatorname{ComB}\left(H(w), \operatorname{AgG}\left\{H\left(w^{\prime}\right) \mid w^{\prime} \in \operatorname{in}_{H}(w)\right\}\right) \\
& =\bar{L}(H)(w)
\end{aligned}
$$

Proposition 3.8. For every graph $G$, everyd-substitution $\rho$ of $G$ with $d \in \mathbb{N}_{\infty}$, and every nodev $\in G$ we havecr ${ }^{d}(G)(v)=\operatorname{cr}^{d}(G / \rho)(\rho(v))$.

Proof. Fix $d \in \mathbb{N}_{\infty}$ arbitrarily. When $d \neq \infty$, the statement follows from Proposition A. 1 below. It hence remains to prove the case where $d=\infty$. To that end, let $c_{1} \in \mathbb{N}$ be the stable coloring number of $G$, and let $c_{2} \in \mathbb{N}$ be the stable coloring number of $G / \rho$. We prove that $c_{1}=c_{2}$. From this, the claimed equality directly follows:

$$
\begin{aligned}
\operatorname{cr}^{\infty}(G)(v) & =\operatorname{cr}^{c_{1}}(G)(v) \\
& =\operatorname{cr}^{c_{2}}(G)(v) \\
& =\operatorname{cr}^{c_{2}}(G / \rho)(\rho(v)) \\
& =\operatorname{cr}^{\infty}(G / \rho)(\rho(v))
\end{aligned}
$$

Here, the first and last equality are by definition of $\mathrm{cr}^{\infty}$; the second equality is because $c_{1}=c_{2}$; and the third equality is by Proposition A.1.

To prove that $c_{1}=c_{2}$ it suffices to show that $c_{1} \geq c_{2}$ and $c_{1} \leq c_{2}$. We only explain how to obtain the inequality $c_{1} \geq c_{2}$; the other direction is similar.

To show that $c_{1} \geq c_{2}$, we must show that $[G / \rho, \rho(v)]_{c_{1}}=$ $[G / \rho, \rho(v)]_{c_{1}+1}$ for all nodes $\rho(v) \in G / \rho$. Since $[G / \rho, \rho(v)]_{c_{1}} \supseteq$ $[G / \rho, \rho(v)]_{c_{1}+1}$ trivially holds by definition of cr, it remains to show that if $\rho(w) \in[G / \rho, \rho(v)]_{c_{1}}$ then also $\rho(w) \in[G / \rho, \rho(v)]_{c_{1}+1}$, for all nodes $\rho(w) \in G / \rho$. Hence, fix $\rho(w) \in G / \rho$ and assume $\operatorname{cr}^{c_{1}}(G / \rho)(\rho(v))=\operatorname{cr}^{c_{1}}(G / \rho)(\rho(w))$. Then, by Proposition A. 1 we derive

$$
\operatorname{cr}^{c_{1}}(G)(v)=\operatorname{cr}^{c_{1}}(G / \rho)(\rho(v))=\operatorname{cr}^{c_{1}}(G / \rho)(\rho(w))=\operatorname{cr}^{c_{1}}(G)(w)
$$

[^0]Since $c_{1}$ is the stable coloring number of $G$ and $\mathrm{cr}^{c_{1}}(G)(v)=$ $\operatorname{cr}^{c_{1}}(G)(w)$, also $\mathrm{cr}^{c_{1}+1}(G)(v)=\mathrm{cr}^{c_{1}+1}(G)(w)$. Therefore, again by Proposition Proposition A.1,

$$
\begin{aligned}
\operatorname{cr}^{c_{1}+1}(G / \rho)(\rho(v)) & =\operatorname{cr}^{c_{1}+1}(G)(v) \\
& =\operatorname{cr}^{c_{1}+1}(G)(w) \\
& =\operatorname{cr}^{c_{1}+1}(G / \rho)(\rho(w)) .
\end{aligned}
$$

As such, $\rho(w) \in[G / \rho, \rho(v)]_{c_{1}+1}$, as desired.
Proposition A.1. For every graph $G$, every d-substitution $\rho$ of $G$ with $d \in \mathbb{N}(i . e ., d \neq \infty)$, and every node $v \in G$ we have $\mathrm{cr}^{d}(G)(v)=$ $\operatorname{cr}^{d}(G / \rho)(\rho(v))$.

Proof. Let $d$ be an arbitrary but fixed natural number, and let $\rho$ be a $d$-substitution of $G$. For ease of readability, let us abbreviate $G / \rho$ by $H$.

Throughout the proof, we will use the following observations.
(O1.) By definition of $d$-substitutions, $\rho\left([G, v]_{d}\right) \in[G, v]_{d}$ for every node $v \in G$. Because we have extended $d$-substitutions to nodes by setting $\rho(v)=\rho\left([G, v]_{d}\right)$, it follows in particular that $\rho(v) \in[G, v]_{d}$ for every node $v$. Therefore, by definition of $[G, v]_{d}$ we have $\mathrm{cr}^{d}(G)(v)=\operatorname{cr}^{d}(G)(\rho(v))$ for every $v \in G$. Because $d$ step color refinement includes $d$-1-step color refinement in the first component of the pair that it outputs, this also implies that $\operatorname{cr}^{l}(G)(v)=\operatorname{cr}^{l}(G)(\rho(v))$ for every $l \leq d$.
(O2.) In addition, we note that for every node $w \in H=G / \rho$ we have $\rho(w)=w$. Indeed: only nodes that appear in the image of $\rho$ are in $G / \rho$. As such, if $w \in G / \rho$ there exists some $w^{\prime}$ such that $w=\rho\left(\left[G, w^{\prime}\right]_{d}\right)$. Because $\rho\left(\left[G, w^{\prime}\right]_{d}\right) \in\left[G, w^{\prime}\right]_{d}$, it follows that $w \in\left[G, w^{\prime}\right]_{d}$ and as such, $[G, w]_{d}=\left[G, w^{\prime}\right]_{d}$. Hence, $w=$ $\rho\left([G, w]_{d}\right)=\rho(w)$.
(O3.) In addition, we note that for every node $w \in H$ and every node $w^{\prime} \in[G, w]_{d}$ we have $\rho\left(w^{\prime}\right)=w$. Indeed, because $w^{\prime} \in[G, w]_{d}$ we have $\left[G, w^{\prime}\right]_{d}=[G, w]_{d}$. As such $\rho\left(w^{\prime}\right)=$ $\rho\left(\left[G, w^{\prime}\right]_{d}\right)=\rho\left([G, w]_{d}\right)=\rho(w)=w$, where the last equality is due to observation (O2).
(O4.) For every node $v \in H$ we have $\operatorname{in}_{H}(v)=\{\rho(w) \mid w \in$ $\left.\operatorname{in}_{G}(v)\right\}$. Indeed, let $E_{H}$ denote the multiset of edges of $H$ and $E_{G}$ the multiset of edges of $G$. Then

$$
\begin{aligned}
\operatorname{in}_{H}(v) & =\left\{w \mid(w \rightarrow v) \in E_{H}\right\} \\
& =\left\{w \mid w^{\prime} \in[G, w]_{d},\left(w^{\prime} \rightarrow v\right) \in E_{G}\right\} \\
& =\left\{\left\{w \mid \rho\left(w^{\prime}\right)=w,\left(w^{\prime} \rightarrow v\right) \in E_{G}\right\}\right. \\
& =\left\{\rho\left(w^{\prime}\right) \mid\left(w^{\prime} \rightarrow v\right) \in E_{G}\right\} \\
& =\left\{\rho\left(w^{\prime}\right) \mid w^{\prime} \in \operatorname{in}_{G}(v)\right\} \\
& =\left\{\rho(w) \mid w \in \operatorname{in}_{G}(v)\right\}
\end{aligned}
$$

The first equality is by definition of $\mathrm{in}_{H}$; the second because by definition the multiplicity of $w \rightarrow v$ in $E_{H}$ equals $\sum_{w^{\prime} \in[G, w]_{d}} E_{G}\left(w^{\prime} \rightarrow\right.$ $v)$; and the third by (O3).

To prove the proposition, we now prove the stronger statement that for every $l \leq d$ and every node $v \in G$ we have $\operatorname{cr}^{l}(G)(v)=$ $\operatorname{cr}^{l}(G / \rho)(\rho(v))$. Clearly $\mathrm{cr}^{d}(G)(v)=\operatorname{cr}^{d}(G / \rho)(\rho(v))$ then follows when $l=d$.

The proof of this stronger statement is by induction on $l$. For the base case when $l=0$ we have, for every $v \in G$,

$$
\operatorname{cr}^{0}(H)(\rho(v))=H(\rho(v))=G(\rho(v))=\operatorname{cr}^{0}(G)(\rho(v))=\operatorname{cr}^{0}(G)(v)
$$

as desired. Here, the first equality is by definition of $\mathrm{Cr}^{0}$; the second is by definition of $H=G / \rho$; the third is again by definition of $\mathrm{cr}^{0}$; and the final equality is by observation (O1).

For the inductive case $l>0$, consider an arbitrary node $v \in G$. Then, by definition,

$$
\begin{aligned}
\operatorname{cr}^{l}(G)(v) & =\left(\operatorname{cr}^{l-1}(G)(v),\left\{\left\{\operatorname{cr}^{l-1}(G)(w) \mid w \in \operatorname{in}_{G}(v)\right\}\right)\right. \\
\operatorname{cr}^{l}(H)(\rho(v)) & =\left(\operatorname{cr}^{l-1}(H)(\rho(v)),\left\{\operatorname{cr}^{l-1}(H)\left(w^{\prime}\right) \mid w^{\prime} \in \operatorname{in}_{H}(\rho(v))\right\}\right)
\end{aligned}
$$

To show that $\mathrm{cr}^{l}(G)(v)=\mathrm{cr}^{l}(H)(\rho(v))$ we hence need to show:
(i) $\mathrm{cr}^{l-1}(G)(v)=\mathrm{cr}^{l-1}(H)(\rho(v))$; and
(ii) $\left\{\left\{\mathrm{cr}^{l-1}(G)(w) \mid w \in \operatorname{in}_{G}(v)\right\}\right)=\left\{\left\{\mathrm{cr}^{l-1}(H)\left(w^{\prime}\right) \mid w^{\prime} \in\right.\right.$ $\left.\operatorname{in}_{H}(\rho(v))\right\}$.
Equality (i) follows directly from the induction hypothesis. To show (ii), we reason as follows:

$$
\begin{aligned}
& \left.\left\{\mathrm{cr}^{l-1}(H)\left(w^{\prime}\right) \mid w^{\prime} \in \operatorname{in}_{H}(\rho(v))\right\}\right) \\
& \left.\quad=\left\{\left\{\operatorname{cr}^{l-1}(H)\left(w^{\prime}\right) \mid w^{\prime} \in\left\{\rho(w) \mid w \in \operatorname{in}_{G}(\rho(v))\right\}\right\}\right\}\right) \\
& =\left\{\left\{\operatorname{cr}^{l-1}(H)(\rho(w)) \mid w \in \operatorname{in}_{G}(\rho(v))\right\}\right. \\
& =\left\{\left\{\operatorname{cr}^{l-1}(G)(w) \mid w \in \operatorname{in}_{G}(\rho(v))\right\}\right. \\
& =\left\{\operatorname{cr}^{l-1}(G)(w) \mid w \in \operatorname{in}_{G}(v)\right\}
\end{aligned}
$$

The first equality is due to observation (O3); the second is an elementary equality of multiset comprehensions; the third is by induction hypothesis; and the fourth is because $\mathrm{cr}^{l}(G)(v)=\operatorname{cr}^{l}(G)(\rho(v)$ by Observation (O1). In particular, the next-to-last line is exactly the second component of the color $\mathrm{cr}^{l}(G)(\rho(v)$ and the last line is the second component of $\operatorname{cr}^{l}(G)(v)$, which must hence be equal.

Lemma A.2. Let $H_{1}=G / \rho_{1}$ and $H_{2}=G / \rho_{2}$ be two d-reducts of $G$ and let $f$ be an isomorphism from $H_{1}$ to $H_{2}$. Then $f$ agrees with $\rho_{2}$ : $f(u)=\rho_{2}(v)$ for all $u \in H_{1}$.

Proof. It is straightforward to verify by induction on $d$ that $\mathrm{cr}^{d}$ is invariant under isomorphism, in the sense that $\mathrm{cr}^{d}\left(H_{1}\right)(u)=$ $\operatorname{cr}^{d}\left(H_{2}\right)(f(u))$ for all $u \in H_{1}$. Therefore, for all $u \in H_{1}$

$$
\begin{aligned}
\operatorname{cr}^{d}(G)(u) & =\operatorname{cr}^{d}\left(H_{1}\right)\left(\rho_{1}(u)\right) \\
& =\operatorname{cr}^{d}\left(H_{1}\right)(u) \\
& =\operatorname{cr}^{d}\left(H_{2}\right)(f(u)) \\
& =\operatorname{cr}^{d}\left(H_{2}\right)\left(\rho_{2}(f(u))\right) \\
& =\operatorname{cr}^{d}(G)(f(u))
\end{aligned}
$$

The first equality is by Proposition 3.8; the second by the fact that $\rho_{1}(u)=u$ for all $u \in H_{1}$; the third by invariance under isomorphisms; the fourth by the fact that $f(u) \in H_{2}$ and $\rho_{2}\left(u^{\prime}\right)=u^{\prime}$ for every $u^{\prime} \in H_{2}$; and the last again by Proposition 3.8.

In other words, $f(u) \in[G, u]_{d}$, for every $u \in H_{1}$. Then, because $f(u) \in H_{2}$ and $H_{2}$ contains only one node for each color refinement class in $\left\{[G, u]_{d} \mid u \in G\right\}$, it follows that $\rho_{2}(u)=f(u)$, for every $u \in H_{1}$ (including $v$ ).

Proposition 3.9. There is a single d-reduct of a graph Gup to isomorphism if and only if d is greater than or equal to the stable coloring number of $G$.

Proof. (If.) For the if-implication, assume that $c$ is the stable coloring number of $G$ and let $d \geq c, d \in \mathbb{N}$. Then, for all nodes
$v \in G$ we have $[G, v]_{d}=[G, v]_{d+1}$. Let $H_{1}=G / \rho_{1}$ and $H_{2}=G / \rho_{2}$ be two $d$-reducts of $G$. Let $V_{1}=\left\{\rho_{1}(v) \mid v \in G\right\}$ be the set of nodes in $H_{1}$ and $V_{2}=\left\{\rho_{2}(v) \mid v \in G\right\}$ be the set of nodes in $H_{2}$. It is clear that $V_{1}$ and $V_{2}$ are of the same cardinality, as they have one node for each color refinement class in $\left\{[G, v]_{d} \mid v \in G\right\}$. It is furthermore straightforward to obtain that $\rho_{1}(v)=v$ for all $v \in V_{1}$, and similarly $\rho_{2}(v)=v$ for all $v \in V_{2}$.

We claim that the function $f=\left.\rho_{2}\right|_{V_{1}}$ is an isomorphism from $H_{1}$ to $H_{2}$.
(1) This function is injective: assume that $v, w \in V_{1}$ and $\rho_{2}(v)=$ $\rho_{2}(w)$. Since, by defintion of $d$-substitutions, we have $\rho_{2}(v) \in$ $[G, v]_{d}$ and $\rho_{2}(w) \in[G, w]_{d}$ it follows that $[G, v]_{d}=[G, w]_{d}$. Because $v, w \in V_{1}$ we have $\rho_{1}(v)=v$ and $\rho_{1}(w)=w$. As such $v=\rho_{1}(v)=\rho_{1}\left([G, v]_{d}\right)=\rho_{1}\left([G, w]_{d}\right)=w$ as desired.
(2) Since $f$ is an injective function from $V_{1}$ to $V_{2}$ and $V_{1}$ and $V_{2}$ are finite sets of the same cardinality, it is also surjective. Hence $f$ is a bijection between $V_{1}$ and $V_{2}$.
(3) It remains to show that for all $v, w \in V_{1}$ we have

$$
H_{1}(v \rightarrow w)=H_{2}\left(\rho_{2}(v) \rightarrow \rho_{2}(w)\right)
$$

Fix $v, w \in V_{1}$ arbitrarily. By definition of $\rho_{2}$ we have $\rho_{2}(w) \in$ $[G, w]_{d}$ and because $[G, w]_{d}=[G, w]_{d+1}(d$ is larger than the stable coloring number of $G$ ) it follows that $\rho_{2}(w) \in[G, w]_{d+1}$. Therefore, $\operatorname{cr}^{d+1}(G)(w)=\mathrm{cr}^{d+1}(G)\left(\rho_{2}(w)\right)$. In particular,

$$
\left.\left\{\operatorname{cr}^{d}(G)\left(v^{\prime}\right) \mid v^{\prime} \in \operatorname{in}_{G}(w)\right\}\right\}=\left\{\operatorname{cr}^{d}(G)\left(v^{\prime}\right) \mid v^{\prime} \in \operatorname{in}_{G}\left(\rho_{2}(w)\right)\right\}
$$

Hence, for any $v \in G$ we also have

$$
\begin{align*}
& \left\{\left\{\operatorname{cr}^{d}(G)\left(v^{\prime}\right) \mid v^{\prime} \in \operatorname{in}_{G}(w), v^{\prime} \in[G, v]_{d}\right\}\right. \\
& =\left\{\operatorname{cr}^{d}(G)\left(v^{\prime}\right) \mid v^{\prime} \in \operatorname{in}_{G}\left(\rho_{2}(w)\right), v^{\prime} \in[G, v]_{d}\right\}
\end{align*}
$$

Let us denote the total multplicity of a finite multiset $M$ by $\# M$, i.e., $\# M=\sum_{x} M(x)$. Then we reason as follows.

$$
\begin{aligned}
H_{1}(v \rightarrow w) & =\sum_{v^{\prime} \in[G, v]_{d}} G\left(v^{\prime} \rightarrow w\right) \\
& =\#\left\{\left\{v^{\prime} \mid v^{\prime} \in \operatorname{in}_{G}(w), v^{\prime} \in[G, v]_{d}\right\}\right. \\
& =\#\left\{\left\{\mathrm{cr}^{d}\left(G, v^{\prime}\right) \mid v^{\prime} \in \operatorname{in}_{G}(w), v^{\prime} \in[G, v]_{d}\right\}\right. \\
& =\#\left\{\left\{\mathrm{cr}^{d}\left(G, v^{\prime}\right) \mid v^{\prime} \in \operatorname{in}_{G}\left(\rho_{2}(w)\right), v^{\prime} \in[G, v]_{d}\right\}\right. \\
& \left.=\#\left\{\operatorname{cr}^{d}\left(G, v^{\prime}\right) \mid v^{\prime} \in \operatorname{in}_{G}\left(\rho_{2}(w)\right), v^{\prime} \in\left[G, \rho_{2}(v)\right]_{d}\right\}\right\} \mid \\
& =\#\left\{\left\{v^{\prime} \mid v^{\prime} \in \operatorname{in}_{G}\left(\rho_{2}(w)\right), v^{\prime} \in\left[G, \rho_{2}(v)\right]_{d}\right\}\right\} \\
& =\sum \sum^{\prime} \in\left[G, \rho_{2}(v)\right]_{d} \\
= & H_{2}\left(\rho_{2}(v) \rightarrow \rho_{2}(w)\right)
\end{aligned}
$$

The first equality is by definition of $H_{1}$; the second is by rewriting the sum in multiset notation; the third because we are only interested in the total multiplicity of the multiset and not its elements; the fourth by $(\star)$; the fifth because $[G, v]_{d}=[G, \rho(v)]_{d}$ by definition of $d$-substitutions; the sixth again because we care only about multiplicity and not the actual elements; the seventh by rewriting the multiset notation into a sum; and the last by definition of $H_{2}$.
(Only if). Assume that all $d$-reducts of $G$ are isomorphic. We need to show that for all $v \in G$ we have $[G, v]_{d}=[G, v]_{d+1}$. The containment $[G, v]_{d} \supseteq[G, v]_{d+1}$ trivially holds by definition of cr. For
the other containment, assume that $w \in[G, v]_{d}$, i.e., $\mathrm{cr}^{d}(G)(v)=$ $\operatorname{cr}^{d}(G)(w)$. We will show that also $\mathrm{cr}^{d+1}(G)(v)=\operatorname{cr}^{d+1}(G)(w)$, which is equivalent to saying that $w \in[G, v]_{d+1}$.

Recall that $\mathrm{cr}^{d+1}(G)(v)$ and $\mathrm{cr}^{d+1}(G)(w)$ are pairs by definition. Since $\mathrm{cr}^{d}(G)(v)=\operatorname{cr}^{d}(G)(w)$ by assumption, the first components of of these pairs are certainly equal. To prove $\mathrm{cr}^{d+1}(G)(v)=$ $\mathrm{cr}^{d+1}(G)(w)$, we hence only need to show that also their second components are equal, i.e., that

$$
\underbrace{\left\{\left\{\operatorname{cr}^{d}(G)(u) \mid u \in \operatorname{in}_{G}(v)\right\}\right\}}_{=: M_{1}}=\underbrace{\left\{\left\{\operatorname{cr}^{d}(G)(u) \mid u \in \operatorname{in}_{G}(w)\right\}\right.}_{=: M_{2}}
$$

To obtain this equality, consider two $d$-substitutions $\rho_{1}$ and $\rho_{2}$ s.t.

$$
\rho_{1}:[G, v]_{d} \mapsto v \quad \quad \rho_{2}:[G, v]_{d} \mapsto w
$$

In other words, $\rho_{1}(v)=\rho_{1}(w)=v$ and $\rho_{2}(v)=\rho_{2}(w)=w$. By assumption, $H_{1}=G / \rho_{1}$ and $H_{2}=G / \rho_{2}$ are isomorphic. Let $f$ be an isomorphism from $H_{1}$ to $H_{2}$. By Lemma A. $2 f$ agrees with $\rho_{2}: f(u)=\rho_{2}(u)$ for all $u \in H_{1}$ (including $v$ ). Furthermore, by definition of isomorphism, for all $u \in H_{1}$ we have $H_{1}(u \rightarrow v)=$ $H_{2}(f(u) \rightarrow f(v))=H_{2}\left(\rho_{2}(u) \rightarrow \rho_{2}(v)\right)=H_{2}\left(\rho_{2}(u) \rightarrow w\right)$.

To show that $M_{1}=M_{2}$ we show that for every $x, M_{1}(x) \leq M_{2}(x)$ and $M_{2}(x) \leq M_{1}(x)$. We only illustrate the reasoning for $M_{1}(x) \leq$ $M_{2}(x)$, the converse direction is similar. Consider an element $x$ in $M_{1}$, and let $m=M(x)$ be its multiplicity. Then there exists some $u \in \operatorname{in}_{G}(v)$ such that $x=\operatorname{cr}^{d}(G)(u)$, and $x$ occurs as many times in $M_{1}$ as there are elements in $M_{1}^{\prime}:=\left\{u^{\prime} \mid u^{\prime} \in \operatorname{in}_{G}(v), u^{\prime} \in[G, u]_{d}\right\}$, i.e., $m_{1}=\# M_{1}^{\prime}$. Because $[G, u]_{d}=\left[G, \rho_{1}(u)\right]_{d}$ for all $u \in G$, it follows that

$$
\begin{aligned}
m_{1} & =\#\left\{u^{\prime} \mid u^{\prime} \in \operatorname{in}_{G}(v), u^{\prime} \in[G, u]_{d}\right\} \\
& =\#\left\{u^{\prime} \mid u^{\prime} \in \operatorname{in}_{G}(v), u^{\prime} \in\left[G, \rho_{1}(u)\right]_{d}\right\} \\
& =H_{1}\left(\rho_{1}(u) \rightarrow v\right) \\
& =H_{2}\left(\rho_{2}\left(\rho_{1}(u)\right) \rightarrow w\right) \\
& =\#\left\{u^{\prime} \mid u^{\prime} \in \operatorname{in}_{G}(w), u^{\prime} \in\left[G, \rho_{2}\left(\rho_{1}(u)\right)\right]_{d}\right\} \\
& =\#\left\{u^{\prime} \mid u^{\prime} \in \operatorname{in}_{G}(w), u^{\prime} \in[G, u]_{d}\right\}
\end{aligned}
$$

The last equality is because $\left[G, \rho_{2}\left(\rho_{1}(u)\right)\right]_{d}=[G, u]_{d}$ by definition of $d$-reducts. Notice that all elements $u^{\prime}$ in the multiset on the last line will create one copy of $\mathrm{cr}^{d}(G)\left(u^{\prime}\right)=\operatorname{cr}^{d}(G)(u)$ in $M_{2}$. As such, $x=\operatorname{cr}^{d}(G)(u)$ occurs at least $m$ times in $M_{2}$, as desired.

Proposition 3.10. Let $G$ be a graph, let $d \in \mathbb{N}_{\infty}$ and let $\rho$ be a $d$-substitution such that

$$
\text { incidence }{ }_{G}^{d}(\rho(v))=\min _{v^{\prime} \in[G, v]_{d}} \text { incidence }_{G}^{d}\left(v^{\prime}\right)
$$

for every node $v \in G$. Then the size of $G / \rho$ is minimal among all $d$-reducts of $G$.

Proof. Since $\infty$-substitutions are simply $d$-substitutions with $d \in \mathbb{N}$ the stable coloring number of $G$, it suffices to show the statement for all $d \in \mathbb{N}$.

Fix $d \in \mathbb{N}$, let $C=\left\{[G, v]_{d} \mid v \in G\right\}$ be the color refinement classes of $G$ of depth $d$, and let $\rho$ be a $d$-substitution such that

$$
\text { incidence }_{G}^{d}(\rho(c))=\min _{v^{\prime} \in c} \operatorname{incidence}_{G}^{d}(v),
$$

for every refinement class $c \in C$. Let $H=G / \rho$. Furthermore, let $\mu$ be another $d$-substitution and let $U=G / \mu$. We will show that $H$, viewed as a simple graph by ignoring edge multiplicities, has no more edges than $U$.

Note that for each class $c \in C$ there is exactly one corresponding node in $H$ (namely, $\rho(c)$ ) and one corresponding node in $U$ (namely $\mu(c))$. We claim that, for every $c \in C$, the indegree ${ }^{2}$ of $\rho(c)$ in $H$ is at most the indegree of $\mu(c)$ in $U$. Since the total number of simple edges in $H$ equals $\sum_{c \in C}$ indegree $_{H}(\rho(c))$ and the total number of simple edges in $U$ similarly equals $\sum_{c \in C}$ indegree $_{U}(\mu(c))$, it follows that $H$, viewed as a simple graph, has no more edges than $U$.

To prove the claim, let $c \in C$. There is an edge from $\rho\left(c^{\prime}\right) \rightarrow$ $\rho(c)$ in $H$ if and only if $\left[G, \rho\left(c^{\prime}\right)\right]_{d} \cap \mathrm{in}_{G}(\rho(c))$ is non-empty. Hence, since $\left[G, \rho\left(c^{\prime}\right)\right]_{d}=c^{\prime}$, the indegree of $\rho(c)$ in $H$ is exactly incidence ${ }_{G}^{d}(\rho(c))$. Similar reasoning shows that the indegree of $\mu(c)$ in $U$ equals incidence ${ }_{G}^{d}(\mu(c))$. As such,

$$
\begin{aligned}
\operatorname{indegree}_{H}(\rho(c)) & =\operatorname{incidence}_{G}^{d}(\rho(c)) \\
& =\min _{v^{\prime} \in c} \operatorname{incidence}_{G}^{d}\left(v^{\prime}\right) \\
& \leq \operatorname{incidence}_{G}^{d}(\mu(c)) \\
& =\operatorname{indegree}_{U}(\mu(c))
\end{aligned}
$$

The inequality in the third line is because $\mu(c) \in c$ by definition of $d$-substitution.
Theorem 3.11. Let $\mathcal{P}$ be a learning problem with hypothesis space $\mathcal{S}$ and assume that $d \in \mathbb{N}_{\infty}$ is such that every $G N N$ in $\mathcal{S}$ has at most $d$ layers. (In particular, $d=\infty$ if there is no bound on the number of layers in $\mathcal{S}$.) Then $\mathcal{P} \equiv \mathcal{P} / \rho$ for every $d$-substitution $\rho$.

Proof. Let $\mathcal{P} / \rho=\left(G^{\prime}, T^{\prime}\right.$, Loss $\left.{ }^{\prime}\right)$, so $G^{\prime}=G / \rho ; T^{\prime}=T / \rho$, and Loss $^{\prime}=$ Loss $/ \rho$. Consider an arbitrary but fixed GNN $\bar{L} \in \mathcal{S}$. We need to show that $\operatorname{Loss}(\bar{L}(G), T)=\operatorname{Loss}^{\prime}\left(\bar{L}\left(G^{\prime}\right), T^{\prime}\right)$. To that end, first observe that for every node $v \in G^{\prime}$ and every node $w \in[G, v]_{d}$ we have $\rho(w)=v$. Consequently,

$$
\operatorname{cr}^{d}\left(G^{\prime}, v\right)=\operatorname{cr}^{d}\left(G^{\prime}, \rho(w)\right)=\operatorname{cr}^{d}(G / \rho, \rho(w))=\operatorname{cr}^{d}(G, w)
$$

Here, the last equality follows from Proposition 3.8. Hence, by Proposition 3.3 (or Corollary 3.4 when $d=\infty),\left(G^{\prime}, v\right) \sim_{\mathcal{S}}(G, w)$ and such $\bar{L}\left(G^{\prime}\right)(v)=\bar{L}(G)(w)$ for every $v \in G^{\prime}$ and $w \in[G, v]_{d}$.

Using this observation we now reason as follows.

$$
\begin{aligned}
\operatorname{Loss}^{\prime}\left(\bar{L}\left(G^{\prime}\right), T^{\prime}\right) & =\sum_{v \in T^{\prime}} \operatorname{Loss}^{\prime}\left(v, \bar{L}\left(G^{\prime}\right)(v)\right) \\
& =\sum_{v \in T^{\prime}} \sum_{w \in T \cap[G, v]_{D}} \operatorname{Loss}\left(w, \bar{L}\left(G^{\prime}\right)(v)\right) \\
& =\sum_{v \in T^{\prime}} \sum_{w \in T \cap[G, v]_{D}} \operatorname{Loss}(w, \bar{L}(G)(w)) \\
& =\sum_{w \in T} \operatorname{Loss}(w, \bar{L}(G)(w)) \\
& =\operatorname{Loss}(\bar{L}(G), T)
\end{aligned}
$$

The second equality is by definition of Loss' ${ }^{\prime}$. The third equality follows from our observation. The fourth equality is because $T=$ $\cup_{v \in T^{\prime}}[G, v]_{d} \cap T$.

[^1]
[^0]:    ${ }^{1}$ This latter fact is because $\mathrm{cr}^{d}(G)(v)$ is a pair, whose first component is $\mathrm{cr}^{d-1}(G)(v)$ (which is a pair, whose first component is $\mathrm{cr}^{d-2}(G)(v)$, and so on), and similarly for $\mathrm{cr}^{d}(H)(w)$.

[^1]:    ${ }^{2}$ That is, the number of nodes $w$ in $H$ having an outgoing edge to $\rho(c)$.

