A NEW PERSPECTIVE ON THE APPROXIMATION CAPABILITY OF GNNs

Giuseppe Alessio D’Inverno
DIISM
University of Siena
Siena
dinverno@diism.unisi.it

Monica Bianchini
DIISM
University of Siena
Siena
monica@diism.unisi.it

Maria Lucia Sampoli
DIISM
University of Siena
Siena
marialucia.sampoli@unisi.it

Franco Scarselli
DIISM
University of Siena
Siena
franco@diism.unisi.it

ABSTRACT

Graph Neural Networks (GNNs) are a broad class of connectionist models for graph processing. Recent studies have shown that GNNs can approximate any function on graphs, modulo the equivalence relation on nodes defined by the Weisfeiler–Lehman test. However, these results suffer from some limitations, both because they were derived using the Stone–Weierstrass theorem — which is existential in nature —, and because they assume that the target function to be approximated must be continuous. In this paper, we propose an alternative way to demonstrate the approximation capability of GNNs that overcomes these limitations. In particular, some new results are proved, which allow to: (1) define GNN architectures capable of obtaining a given approximation; (2) show that the Weisfeiler–Lehman test converges in $r + 1$ steps, where $r$ is the diameter of the graph; (3) derive a formal relationship between the Weisfeiler–Lehman test and the unfolding trees, that is trees that can be built by visiting the graph starting from a given node. These results provide a more comprehensive understanding of the approximation power of GNNs, definitely showing that the 1–WL test and the unfolding tree concepts can be used interchangeably to study the their expressiveness.

1 Introduction

Graph processing is becoming pervasive in many application domains, such as social networks, Web applications, biology and finance. Intuitively, graphs allow to represent patterns along with their relationships. Indeed, graphs can naturally encode high–valued information that is hard to represent with vectors or sequences, the most common data structures used in Machine Learning (ML). Graph Neural Networks (GNNs) are a class of machine learning models that can process information represented in the form of graphs. In recent years, the interest in GNNs has grown rapidly and numerous new models and applications have emerged [34]. The first GNN model was introduced in [30]. Later, several other approaches have been proposed, including Spectral Networks [8], Gated Graph Sequence Neural Networks [17], Graph Convolutional Neural Networks [15], GraphSAGE [12], Graph attention networks [33], and Graph Networks [5].

Despite the differences among the various GNN models, most adopt the same computational scheme, based on a local aggregation mechanism. The information related to a node is stored into a feature vector, which is updated recursively by aggregating the feature vectors of neighboring nodes. After $k$ iterations, the feature vector of a given node $v$ captures both the structural information and the local information attached to it within the $v$’s $k$–hop neighborhood. At the end of the learning process, the node feature vectors can be used to classify or to cluster the objects/concepts represented by a (some) node(s), or by the whole graph.
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Recently, a great effort has been devoted to the study of the expressive power of GNNs [26]. Intuitively, the local computational framework is primarily responsible for the capabilities and limitations of GNNs, since they combine local symbolic and sub-symbolic information available on the graph, i.e. node features and node connectivity, but may not be able to merge information located at distant points in the graph. Therefore, a fundamental question is to define which graphs (nodes) can be distinguished by a GNN, i.e. for which input graphs (nodes) the GNN produces different encodings. In [35], GNNs are proved to be as powerful as the Weisfeiler–Lehman graph isomorphism test (1–WL) [16]. Such an algorithm allows to test whether two graphs are isomorphic or not. The 1–WL algorithm is based on a graph signature which is obtained by assigning a color to each node, where the graph coloring is achieved by iterating a local aggregation function. More generally, there exists a hierarchy of algorithms, called 1–WL, 2–WL, 3–WL, etc., whose elements recognize larger and larger classes of graphs. It has been shown that a GNN can simulate the 1–WL test, provided that a sufficiently general aggregation function is used, but the basic GNN models cannot implement higher order tests [23]. Consequently, the 1–WL test characterizes both the expressiveness and limitations of GNNs, defining the classes of graphs/nodes that GNNs can distinguish.

Another important aspect to define the expressiveness of GNNs is to study their approximation capability. Formally, in node classification/regression tasks, a GNN implements a function \( \varphi(G, v) \rightarrow \mathbb{R}^m \) that takes in input a graph \( G \) and returns an output at each node. Similarly, in graph classification/regression tasks, a GNN implements a function \( \varphi(G) \rightarrow \mathbb{R}^m \). In both cases, the objective is to define which classes of functions can be approximated by a GNN. In [29], the approximation capability of the original GNN model (OGNN), namely the first GNN to be proposed, has been studied using the concept of unfolding trees and unfolding equivalence. The unfolding tree \( T_v \), with root node \( v \), is constructed by unrolling the graph starting from \( v \) (see Fig. 1). Intuitively, \( T_v \) exactly describes the information used by the GNN at node \( v \) and can be employed to study the expressive power of GNNs in node classification/regression tasks. The unfolding equivalence is, in turn, an equivalence relationship defined between nodes having the same unfolding tree. In [29], it was proved that OGNNs can approximate in probability, up to any degree of precision, any measurable function \( \tau(G, v) \rightarrow \mathbb{R}^m \) that respects the unfolding equivalence, namely that produces the same outputs on equivalent nodes. Currently, the idea underlying unfolding trees — also termed computation graphs [9] — is widely used to study the GNN expressiveness. Universal approximation results have been proved for Linear Graph Neural Networks [4, 21], Folklore Graph Neural Networks [20] and, more generally, for the class of the so-called message passing GNNs [35, 4], that includes most of the recent architectures and is considered in this paper.

Figure 1: An example of a graph with some unfolding trees. The symbols outside the nodes represent features. The two nodes on the left part of the graph are equivalent and have equivalent unfolding trees.

Despite the progress of research on approximation theory for GNNs, there are still open problems to be investigated. First of all, the most general results available on modern GNNs are based on the Stone–Weierstrass theorem and state that the functions which can be approximated by GNNs are dense in the invariant continuous function space, modulo

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1It is worth noting that the 1–WL test is inconclusive, since there exist pairs of graphs that the test recognizes as isomorphic even if they are not.
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the 1–WL test \(^2\). However, the Stone–Weierstrass theorem is existential in nature, so that, given a target function to be approximated, it does not allow to construct a GNN architecture that can reach the desired approximation — defining, for example, the number of its layers, and the feature dimension required to build the universal approximator \(^3\). Moreover, the current results apply only to continuous functions on node/edge labels, which are defined on a compact subset of \(\mathbb{R}^L\), a fact that may not hold in practical application domains, since, for instance, the function to be approximated may show step–wise behavior with respect to some inputs.

Finally, while the unfolding trees and the 1–WL test have been used in the approximation theory and provide useful tools to clearly describe the GNN input information and the GNN hidden feature classes, respectively, their relationship is still not formalized from a mathematical point of view. Indeed, it can be observed that the Weisfeiler–Lehman test assigns a color to all the nodes of a graph to make them distinguishable, and it can be assumed that the equivalence classes defined by the colors are related to those defined by the unfolding trees \(^9\). However, which one of the two mechanisms, colors or unfolding trees, is more powerful or whether they are equivalent is still an open question, to which it is advisable to provide a formal and precise answer in order to be able to use them in a targeted or exchangeable way.

In this work, we present an alternative approach to study the approximation capability of recent GNNs that allows to answer to the above questions, also establishing a link between the Weisfeiler–Lehman test and the unfolding tree formalism.

The main contributions of this paper are listed below.

- We show that the 1–WL test induces an equivalence relationship on the graph nodes that exactly equals the unfolding equivalence. Such a result makes it possible to use interchangeably the 1–WL test and the unfolding tree concept, in order to study the expressiveness of GNNs. As a consequence of this result, we deduce that the 1–WL test converges in \(r + 1\) steps, where \(r\) is the diameter of the graph. As far as we know, this result was not known and refines the upper bound on the number of steps to reach convergence, which was known to coincide with the number of nodes in the graph.

- By reusing some ideas originally exploited on OGNNs, we prove that modern GNNs are capable of approximating, in probability and up to any precision, any measurable function on graphs that respects the unfolding equivalence. Intuitively, this means that GNNs are a kind of universal approximators for functions on graphs, modulo the limits enforced by the unfolding equivalence or, analogously, the limits imposed by the 1–WL test. This is the most general result on GNN approximation capability that we are aware of, since holds for generic graphs with real feature vectors and for a broad class of GNNs, which includes most current models. Moreover, it is assumed that the target function is measurable, which allows the approximation of discontinuous and more complex functions w.r.t. existing results, e.g. \(^13\). Finally, the presented proof is constructive and allows us to deduce architectural information that cannot be derived by the Stone–Weierstrass theorem \(^4\). For example, it can be shown that, if the GNN is endowed with sufficiently general aggregation and combination functions, a hidden feature size of 1 is enough to obtain the approximation in \(r + 1\) iterations.

The rest of the paper is organized as follows. In Section \(^2\) some related work is described. Notation and basic concepts are introduced in Section \(^3\) while Section \(^4\) presents the main contribution of this paper. Finally, Section \(^5\) collects some conclusions and presents future perspectives. To make the reading more fluid, the proofs are collected in the Appendix.

2 Related Work

Great attention has recently been paid to the Weisfeiler–Lehman test and its correlation with the expressiveness of GNNs. Xu \textit{et al.} \(^35\) have shown that message passing GNNs are at most as powerful as the 1–WL test; this upper bound could be overcome by injecting the node identity in the message passing procedure, as implemented in \(^36\). Morris \textit{et al.} \(^23\) have gone beyond the 1–WL test, implementing \(k\)–order WL tests as message passing mechanisms into GNNs. In \(^26\), the WL test mechanism applied to GNNs is studied within the paradigm of unfolding trees (also called \textit{computational graphs}), without really establishing an equivalence between the two concepts, so as in \(^37\) (where the unfolding trees are called \textit{rooted subgraphs}). In \(^2\), it is shown that the Weisfeiler–Lehman test tends to oversquash\(^2\).

\(^2\)It is worth noting that an architectural characterization for the number of layers has been obtained in \(^19\), where message passing GNNs, with a number of layers greater or equal than the graph diameter, are proved to be able to realize any Turing computable functions over connected attributed graphs. Anyway, this \textit{representation} result has little practical relevance for the approximation theory, since the target function to be approximated may not be Turing computable, so that we cannot use this result to define the approximation capability of a GNN. Moreover, such architectural characterization is obtained without any restriction on the GNN architecture, except for the number of layers.
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the information coming from the neighbours; moreover, it is claimed that GNNs with at least $K$ layers, where $K$ is the diameter of the graphs in the dataset, do not suffer from under-reaching, which means that the information cannot travel farther than $K$ edges along the graph. Nevertheless, a theoretical proof that GNNs succeed in overcoming the under-reaching behavior is not provided.

Universal approximation properties have been demonstrated for several GNN settings. The OGNN [30] model was proved to be a universal approximator on graphs preserving the unfolding equivalence in [29]. Universal approximation is shown for GNNs with random node initialization in [1] while, in [35], they are shown to be able to encode any graph with countable input features. The universal approximation property has been extended to Folklore Graph Neural Networks in [20], to Linear Graph Neural Networks and general GNNs in [4, 21], both in the invariant and equivariant case, but without any reference to the required number of layers. As already explained in the Introduction, our results differ from these achievements because we allow the approximation of measurable functions and because our proof is constructive and gives some hints on approximator architecture.

A relation between the graph diameter and the computational power of GNNs has been established in [19], where the GNNs are assimilated to the so-called LOCAL models [3, 18, 24] and it is proved that a GNN with a number of layers larger than the diameter of the graph can compute any Turing function of the graph. This result differs from ours, both because we focus on a different question, i.e. which functions can be approximated instead of which functions can be computed, and because was achieved by assuming an infinite amount of memory.

The generalization capability of GNNs has been also studied using different approaches, which include the Vapnik–Chervonenkis dimension for OGNNs [31], and the uniform stability [38] and Rademacher complexity [10] for modern GNNs. Designing GNN architectures that provide good generalization along with good expressive power is a hot research topic (see, e.g., [25]). Moreover, an extensive survey on the theory of Graph Neural Networks can be found in [13].

3 Notation and basic concepts

In this section, we introduce the required notation and the basic definitions used throughout the manuscript.

3.1 Graphs

A graph $G$ is a pair $(V, E)$ where $V$ is a set of vertices or nodes and $E$ is a set of edges between nodes in $V$. Graphs are directed or undirected, according to whether the edge $(v, u)$ is different from the edge $(u, v)$ or not.

In the following, unless otherwise stated, we assume that graphs are undirected.

The set $\text{ne}(v)$ is the neighborhood of $v$, i.e. the set of nodes connected to $v$ by an edge, while $\text{ne}_i(v)$ denote the $i$–th neighbor of $v$. Finally, $|G|$ defines the cardinality of the set of vertices in $G$. From now on, we will always assume finite cardinality graphs, i.e., $|G| = L < \infty$.

Nodes may have attached features, collected into vectors called labels, identified with $\ell_v \in \mathbb{R}^{L}$.

3.2 Graph neural networks

Graph Neural Networks adopt a local computational mechanism to process graphs. The information related to a node $v$ is stored into a feature vector $h_v \in \mathbb{R}^{m}$, which is updated recursively by combining the feature vectors of neighboring nodes. After $k$ iterations, the feature vector $h_v^k$ is supposed to contain a representation of both the structural information and the node information within a $k$–hop neighborhood. After processing is complete, the node feature vectors can be used to classify the nodes or the entire graph.

More rigorously, in this paper, we consider GNNs that use the following general updating scheme:

$$h_v^k = \text{COMBINE}^{(k)}(h_v^{k-1}, \text{AGGREGATE}^{(k)}\{h_u^{k-1}, u \in \text{ne}(v)\}) \quad (1)$$

where the node feature vectors are initialized with the node labels, i.e., $h_v^0 = \ell_v \in \mathbb{R}^{L}$ for each $v$. Here, differently from other approaches, we assume that labels can contain real numbers. Moreover, $\text{AGGREGATE}^{(k)}$ is a function which aggregates the node features obtained in the $(k-1)$–th iteration, and $\text{COMBINE}^{(k)}$ is a function that combines the aggregation of the neighborhood of a node with its feature at the $(k-1)$–th iteration. In graph classification/regression tasks, the GNN is provided with a final READOUT layer that produces the output combining all the feature vectors at the last iteration $K$:

$$o = \text{READOUT}(\{h_v^K, v \in V\}) \quad (2)$$
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whereas, in node classification/regression tasks, the READOUT layer produces an output for each node, based on its features:

\[
o_v = \text{READOUT}(h_v^K)
\]

In this paper, we will focus mainly on node classification/regression tasks. The learning domain of the GNN will be denoted by the graph–node pair \( D = G \times V \), where \( G \) is a set of graphs and \( V \) is a subset of their nodes. Therefore, the function \( \varphi \), implemented by the GNN, takes in input a graph \( G \) and one of its nodes \( v \), and returns an output \( \varphi(G, v) \in \mathbb{R}^o \), where \( o \) is the output dimension.

The framework described by Eqs. (1)–(3) is commonly used to study theoretical properties of modern GNNs (see e.g. [35]). The class of models covered by such a framework is rather wide and includes, for example, GraphSAGE [12], GCN [15], GATs [33], GIN [35], ID-GNN [36], and GSN [7].

It is worth mentioning that the OGNN model is not formally covered, both because in OGNNs the input of AGGREGATE\(^k\) and COMBINE\(^k\) contains the node labels \( \ell_v \) and possibly also the edge features, and because the node features are not initialized to \( \ell_v \). Other models, such as MPNN [11], NN4G [22] and GN [5] are not included as well for similar reasons. Of course, Eq. (2) could easily be extended to include also the OGNNs and the models mentioned above, but here we prefer not to complicate the proposed framework to keep the notation and proofs simple.

3.3 Unfolding trees and unfolding equivalence

**Unfolding trees** and **unfolding equivalence** are two concepts that have been introduced in [29] with the aim of capturing the expressive power of the OGNN model. Intuitively, an **unfolding tree** \( T^d_v \) is the tree obtained by unfolding the graph up to the depth \( d \), using the node \( v \) as its root. Fig. 1 shows some examples of unfolding trees. In the following, a formal recursive definition is provided.

**Definition 3.3.1.** The unfolding tree \( T^d_v \) of a node \( v \) up to depth \( d \) is

\[
T^d_v = \begin{cases} 
\text{Tree}(\ell_v) & \text{if } d = 0 \\
\text{Tree}(\ell_v, T^{d-1}_{ne[v]}) & \text{if } d > 0 
\end{cases}
\]

where Tree\((\ell_v)\) is a tree constituted of a single node with label \( \ell_v \) and Tree\((\ell_v, T^{d-1}_{ne[v]})\) is the tree with the root node labeled with \( \ell_v \) and having sub–trees \( T^{d-1}_{ne[v]} \). The set \( T^{d-1}_{ne[v]} = \{ T^{d-1}_{a_1}, T^{d-1}_{a_2}, \ldots \} \) collects all unfolding trees having depth \( d - 1 \), with \( u_i \in ne[v], \forall i \).

Moreover, the **unfolding tree of \( v \)**, \( T_v = \lim_{d \to \infty} T^d_v \), is obtained by merging all unfolding trees \( T^d_v \) for any \( d \).

Note that, since a GNN adopts a local computation framework, its knowledge about the graph is updated step by step, every time Eq. (1) is applied. Actually, at the first step, \( k = 0 \), the feature vectors \( h_v^0 \) depends only on the local label. Then, at step \( k \), the GNN updates the feature vector \( h_v^K \) using the neighbour data, with the node feature vector that depends on the \( k \)--distant neighbourhood of \( v \). Thus, intuitively, the unfolding tree \( T^d_v \) describes the information that is theoretically available to the GNN at node \( v \) and step \( k \). Such an observation has been used in [29] to study the expressive power of the OGNN model and will be used also in this paper for the same purpose.

In this context, two questions have been studied.

1. Can GNNs compute and store into the node features a coding of the unfolding trees, namely can GNNs store all the theoretically available information?
2. Since unfolding trees are different from the input graphs, how does this affect GNN’s expressive power?

Regarding the first question, it has been shown that indeed both OGNNs and modern GNNs can compute and store in the node features a coding of the unfolding trees, provided that the appropriate network architectures are used in COMBINE\(^k\) and AGGREGATE\(^k\) [26,29,35]. Regarding question (2), we can easily argue that if two nodes have the same unfolding tree, then GNNs produce the same encoding on those nodes. Such a fact highlights an evident limitation of the expressive power of GNNs. The unfolding equivalence is a formal tool designed to capture such a limit: it is an equivalence relation that brings together nodes with the same unfolding tree, namely it groups nodes that cannot be distinguished by GNNs.

\[\text{Unfolding trees are also referred to as computational graphs [9] or search trees [26,35].}\]
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**Definition 3.3.2.** Two nodes \( u, v \) are said to be **unfolding equivalent** \( u \sim_{ue} v \), if \( T_u = T_v \). Analogously, two graphs \( G_1, G_2 \) are said to be **unfolding equivalent** \( G_1 \sim_{ue} G_2 \), if there exists a bijection between the nodes of the graphs that respects the partition induced by the unfolding equivalence on the nodes. $$\blacksquare$$

Since GNNs have to fulfill the unfolding equivalence, also the functions on graphs that they can realize share this limit. In our results on the approximation capability of GNNs, our focus is on functions that preserve the unfolding equivalence. Those functions are general enough except that they produce the same output on equivalent nodes.

**Definition 3.3.3.** A function \( f : D \to \mathbb{R}^m \) is said to preserve the unfolding equivalence on \( D \) if \( v \sim u \) implies \( f(G, v) = f(G, u) \). $$\blacksquare$$

The class of functions that preserve the unfolding equivalence on \( D \) will be denoted with \( F(D) \). A characterization of \( F(D) \) is given by the following result, demonstrated in [29].

**Proposition 3.3.4 (Functions of unfolding trees).** A function \( f \) belongs to \( F(D) \) if and only if there exists a function \( \kappa \), defined on trees, such that \( f(G, v) = \kappa(T_v) \), for any node \( v \in D \). $$\blacksquare$$

Notice that Proposition 3.3.4 suggests not only that the functions that compute the output on a node using unfolding trees preserve the unfolding equivalence, but also that the converse holds, namely all the functions that preserve the unfolding equivalence can be computed as functions of the unfolding trees. Since GNNs can implement only functions of the unfolding trees, we may expect that there is a tight relationship between what GNNs can do and the class \( F(D) \).

Actually, in [29], it has been shown that the OGNN model can approximate in probability, up to any degree of precision, any function in \( F(D) \) and a similar result will be derived for modern GNNs in this manuscript.

### 3.4 The Weisfeiler–Lehman test

The **first order Weisfeiler–Lehman test** (1–WL test in short) [16] is a method to test whether two graphs are isomorphic, based on a graph coloring algorithm. The coloring algorithm is applied in parallel on the two input graphs. In the end, the number of nodes for each color is counted and the numbers obtained relative to the two graphs are compared: if the numbers match, then the graphs are possibly isomorphic, while if they do not match, then the graphs are certainly non–isomorphic. Note that the test is not conclusive in the case of a positive answer, as the graphs may still be non–isomorphic. Actually, the algorithm just provides an approximate solution to the problem of graph isomorphism.

There exist different versions of the coloring algorithm: in this paper, we adopt a coloring scheme in which also the node labels are considered. Since GNNs process both the structure and the labels of the graphs, it is useful to consider both these sources of information, in order to analyse the GNN expressive power. Such an approach has been used, for example, in [26]. More precisely, the coloring is carried out by an iterative algorithm which, at each iteration, computes a node coloring \( c_v^{(t)} \in \Sigma \), being \( \Sigma \) a subset of values representing the colors. The node colors are initialized on the basis of the node features and then they are updated using the coloring from the previous iteration. The algorithm is sketched in the following.

1. At iteration 0, we set
   \[ c_v^{(0)} = \text{HASH}_0(\ell_v) \]
   where \( \text{HASH}_0 \) is a function that bijectively codes every possible feature with a color in \( \Sigma \).
2. For any iteration \( t > 0 \), we set
   \[ c_v^{(t)} = \text{HASH}(\{c_n^{(t-1)} | n \in n e[v]\}) \]
   where \( \text{HASH} \) bijectively maps the above pair to a unique value in \( \Sigma \), which has not been used in the previous iterations.

The algorithm terminates if the number of colors between two iterations does not change, i.e. when the cardinalities of \( \{c_n^{(t-1)} | n \in V\} \) and \( \{c_n^{(t)} | n \in V\} \) are equal.

Finally, we can introduce the equivalence that is induced on nodes by the WL test.

**Definition 3.4.1 (WL–equivalence).** Two nodes, \( u \) and \( v \), are said to be **WL–equivalent**, \( u \sim_{WL} v \), if they have the same colour at the end of the 1–WL test, i.e. \( c_u = c_v \). Analogously, two graphs, \( G_1 \) and \( G_2 \), are said to be **WL–equivalent**, \( G_1 \sim_{WL} G_2 \), if there exists a bijection between the coloring sets of \( G_1 \) and \( G_2 \) such that the corresponding sets have the same cardinality.

\(^4\)For the sake of simplicity and with notation overloading, we adopt the same symbol \( \sim_{ue} \) both for the equivalence between graphs and the equivalence between nodes.
4 Main results

In this section, the main results of the paper are presented and discussed. For ease of reading the proofs of the theorems are given in the Appendix.

4.1 Unfolding and Weisfeiler–Lehman equivalence

The first proposed result regards the relationship between the unfolding and the Weisfeiler–Lehman equivalence on nodes. Some works in the literature take for granted the interchangeability of these two paradigms, e.g. [21], even if, as far as we know, there is no formal demonstration of their effective equivalence. This equivalence is stated by the following two theorems (demonstrated in the Appendix) in relation respectively to single nodes and entire graphs.

**Theorem 4.1.1.**
Let $G = (V, E)$ be a labeled graph. Then, for each $u, v \in V$, $u \sim_{ue} v$ if and only if $u \sim_{WL} v$ holds.

**Theorem 4.1.2.**
Let $G_1, G_2$ be two graphs. Then, $G_1 \sim_{ue} G_2$ if and only if $G_1 \sim_{WL} G_2$.

Both the unfolding equivalence and the WL–equivalence have been defined using a recursive definition local to nodes. Indeed, the existence of a relationship between those equivalences appears to be a natural consequence of this fact. Figure 2 shows an example in which the unfolding trees and the colors of two nodes are iteratively computed: in the example, the colors of the nodes become different when also the unfolding trees become different.

Theorems 4.1.1 and 4.1.2 are interesting since they formally confirm that the two equivalences are exactly interchangeable and can be used together to study GNNs. While the Weisfeiler–Lehman test has been often adopted to analyse the expressive power of GNNs in terms of their capability of recognizing different graphs, the unfolding equivalence and, more precisely, unfolding trees, can provide a tool to understand the information that a GNN can use at each node to implement its function.

For example, it is known that GNNs cannot distinguish regular graphs where nodes have the same features (see e.g. [26]). Of course, in this case, a GNN is not able to distinguish any node, since all the unfolding trees are equal (see Figure 3d). On the one hand, when a target node has different features with respect to the others, also the unfolding trees incorporate such a difference and the nodes at different distances from this target node belong to different equivalent classes (see Figure 3b). On the contrary, if all the labels are different, then each node belongs to a different class, since all unfolding trees are different (see Figure 3c).

We observe that, in principle, by adding random features to the node labels, we could make all the nodes distinguishable and improve the GNN expressive power. This fact was already mentioned for OGNNs [29] and has been recently
The 1–WL test converges in no more than $8$ steps, where $r = \max(\text{diam}(G_1), \text{diam}(G_2))$.

Corollary 4.1.4.
The 1–WL test converges in no more than $r$ steps, where $r = \max(\text{diam}(G_1), \text{diam}(G_2))$.

In order to address these issues, we consider the class of functions that preserve the unfolding equivalence (see Def. 3.3.3). The following theorem proves that GNNs can approximate in probability, up to any precision, any function of this class. Intuitively, this shows that GNNs are a sort of universal approximators on graphs, modulo the limitations due to the unfolding equivalence. Therefore, we can state that GNNs have no further limits other than those due to the unfolding equivalence and can also approximate any function on graphs within this limit.

**Theorem 4.2.1** (Approximation by GNNs). Let $D$ be a graph domain, with $r = \max_{G \in D} \text{diam}(G)$. For any measurable function $\tau \in \mathcal{F}(D)$ preserving the unfolding equivalence, any norm $\| \cdot \|$ on $\mathbb{R}$, any probability measure $P$ on $D$, there exists a GNN defined by the continuously differentiable functions $\text{COMBINE}^{(k)}$, $\text{AGGREGATE}^{(k)}$, $\forall k \leq r + 1$, and by the function $\text{READOUT}$, with feature dimension $m = 1$, i.e., $h'_{\nu} \in \mathbb{R}$, such that the function $\varphi$ (realized by the GNN) computed after $r + 1$ steps satisfies the condition

$$P(\| \tau(G, v) - \varphi(G, v) \| \leq \varepsilon) \geq 1 - \lambda$$

for any reals $\varepsilon, \lambda$, where $\varepsilon > 0$, $0 < \lambda < 1$.

Theorem 4.2.1 intuitively states that, given a function $\tau$, there exists a GNN that can approximate it. $\text{COMBINE}^{(k)}$ and $\text{AGGREGATE}^{(k)}$ can be any continuously differentiable function, while no assumptions are made on $\text{READOUT}$. This situation does not correspond to practical cases, where the GNN adopts particular architectures and those functions are realized by neural networks or, more generally, parametric models — for example made of layers of sums, max,
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average, etc. Therefore, it is of fundamental interest to clarify whether the theorem still holds when the components COMBINE\(^{(k)}\), AGGREGATE\(^{(k)}\) and READOUT are parametric models.

Let us now study the case when the employed components are sufficiently general to be able to approximate any function. We call this class of networks, \( Q \), GNN models with universal components. In order to simplify our discussion, we introduce the transition function \( f^{(k)} \) to indicate the stacking of the AGGREGATE\(^{(k)}\) and COMBINE\(^{(k)}\), i.e.,

\[
f^{(k)}(h^k, \{ h^k_{v-1}, u \in ne[v] \}) = \text{COMBINE}^{(k)}(h^k_{v-1}, \text{AGGREGATE}^{(k)}(h^k_{v-1}, u \in ne[v])).
\]

Then, we can formally define the class \( Q \).

**Definition 4.2.2.** A class \( Q \) of GNN models is said to have universal components if, for any any \( \epsilon > 0 \) and any continuous target functions \( \text{COMBINE}^{(k)}, \text{AGGREGATE}^{(k)}, \text{READOUT} \), there exists a GNN belonging to \( Q \), with functions \( \text{COMBINE}^{(k)}_w, \text{AGGREGATE}^{(k)}_w, \text{READOUT}_w \) and parameters \( w \) such that

\[
\left\| f^{(k)}(h, \{ h_1, \ldots, h_s \}) - f^{(k)}_w(h, \{ h_1, \ldots, h_s \}) \right\| \leq \epsilon
\]

and

\[
\left\| \text{READOUT}_w(q) - \text{READOUT}_w(q) \right\| \leq \epsilon,
\]

holds, for any input values \( h, h_1, \ldots, h_s, q \). The transition functions \( f^{(k)} \) and \( f^{(k)}_w \) correspond to the target function and the GNN, respectively, and \( \| \cdot \|_\infty \) is the infinity norm.

The following result shows that Theorem 4.2.1 still holds even for GNNs with universal components.

**Theorem 4.2.3.** APPROXIMATION BY NEURAL NETWORKS

Let us assume that the hypotheses of Theorem 4.2.1 are fulfilled and \( Q \) is a class of GNNs with universal components. Then, there exists a parameter set \( w \) and some functions \( \text{COMBINE}^{(k)}_w, \text{AGGREGATE}^{(k)}_w, \text{READOUT}_w \) implemented by neural networks in \( Q \), such that the thesis of Theorem 4.2.1 holds.

The proof of Theorem 4.2.3 is included in the Appendix. However, some related topics are discussed below, to better understand some properties of GNNs.

- In the proof of Theorem 4.2.1 we first define an encoding function \( \nabla \) that maps trees to real numbers. The functions \( \text{COMBINE}^{(k)} \) and \( \text{AGGREGATE}^{(k)} \) are designed so that, at each step, the node feature vector approximates a coding of the unfolding function \( h^k_v = \nabla(T^k_v) \). The function \( \text{READOUT} \) decodes the unfolding and produces the desired outputs.

- In the proof of Theorem 4.2.3 it is shown that Theorem 4.2.1 still holds even when the transition and \( \text{READOUT} \) functions are approximated. Thus, we can use any parametric model to implement those functions. We can expect that also for the GNNs of Theorem 4.2.3 the transition function stores into the feature vector a coding of the unfolding tree while \( \text{READOUT} \) decodes such a coding and gives the desired outputs.

The following remarks may further help to understand our results.

- **GNNs with universal components.** Intuitively, the universality condition means that the architectures used to implement \( f^{(k)}_w \) and \( \text{READOUT}_w \) must be sufficiently general to be able to approximate any possible target function. From the theory of standard neural networks, those architectures must have at least two layers (one hidden and one output layer) \([28]\). Such a conclusion is similar to the one reported in \([35]\), where a related result is described and where it is suggested that, in order to be able to implement the 1–WL test, the GNN must use a two layer transition function. Indeed, in this way, the GNN can implement an injective encoding of the input graph into the node features. The proposed result is slightly different with respect to the one in \([35]\), as, in theory, the encoding may fail to be injective, provided that the approximation remains sufficiently good in probability. However, the conclusion about the architecture is the same.

GNNs with transition functions \( f^{(k)}_w \) exploiting two layer architectures include Graph Isomorphism Networks (GINs) \([35]\), which were claimed to realize an injective encoding. Similarly, also the OGGN model, for which a result similar to Theorem 4.2.1 was proved, adopts a two layer architecture for the transition function: in this case, \( \text{AGGREGATE}^{(k)}_w \) consists of a Multilayer Perceptron (MLP) with a hidden layer and \( \text{COMBINE}^{(k)}_w \) was implemented by a sum. Similar results have been devised also in \([21]\), where a different version of the \( \text{COMBINE}^{(k)}_w \) function has been modeled as a sum of MLPs.
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- **READOUT universality.** The condition on the universality of the READOUT function can be relaxed, provided that a higher dimension for the feature vector is used, namely \( m > 1 \). READOUT\(_w\) can indeed cooperate with the transition function in order to produce the output. In the limit case, the output can be completely prepared by the transition function and stored in some components of \( h^D \), so that READOUT\(_w\) is just a projection function.

- **GNN architectures that are not universal approximators.** Most of GNN models, e.g. Graph Convolutional Neural Networks, GraphSAGE and so on, use a single layer architecture to implement the transition function. Thus, even if they do employ universal components, such as those specified by Def. 4.2.2, they have a limited computational power with respect to two layer architectures and this is supported by theoretical results. In [35], Lemma 7, it is shown that, if the transition function is made up by a single layer with ReLU activation functions, the encoding function cannot be injective. A similar result was obtained for linear recursive neural networks in [6]. However, in general, it is not correct to assert that GNNs with single layer transition functions cannot be universal approximators for functions on graphs, as this property depends on the used GNN model and on other architectural/training details. For example, a GNN model with a single layer transition component can use several iterations of Eq. (1) to emulate a GNN with a deeper transition component. In the former model, the node features emulate the transition network hidden layers and COMBINE must have a self–loop, namely must have access to the previous features of each node.

- **Feature dimension.** Surprisingly, Theorems 4.2.1 and 4.2.3 suggest that a feature vector of dimension \( m = 1 \) is sufficient to establish the universal approximation capability of GNNs. It is obvious, however, that the dimension of the feature vector plays an important role in determining the complexity of the coding function for a given domain. We expect that the larger the dimension, the smaller the complexity of the coding. This complexity, in turn, affects the complexity of the transition function, the difficulty in learning such a function, the number of patterns required for training the GNN and so on.

Notice that, throughout the manuscript, we used the idea that the unfolding tree represents the information available to a GNN to compute the output, and we mentioned that a similar approach has been applied also by other authors. From a formal point of view, Theorem 4.2.1 defines a method by which a GNN can actually encode an unfolding tree into the node features, so that it has been proved that all the information collected into the unfolding trees can be used by GNNs. However, also the reverse implication holds true, that is a GNN cannot encode more information into features than that contained into the unfolding trees. Indeed, this is a consequence of the fact that GNNs have no greater discriminatory capability than the 1–WL test (see [23], Theorem 1). Therefore, the unfolding trees totally represent the information used by a GNN.

Finally, the following corollaries provide an alternative way to describe the approximation capability of GNNs in function of their unfolding trees.

**Corollary 4.2.4.** Let \( D \) be a domain of graphs.

1. A function \( f \) preserves the unfolding equivalence if and only if it can be written as a function \( \kappa \) of the unfolding tree \( f(G, v) = \kappa(T^r_{v+1}) \), where the depth \( r + 1 \) of the tree is such that \( r = \text{diam}(G) \).

2. A function \( \varphi(G, v) \), implemented by a GNN, preserves the unfolding equivalence and can be written as a function of the unfolding tree of depth \( r + 1 \), i.e., \( \varphi(G, v) = \kappa(T^r_{v+1}) \) for some \( \kappa \).

3. The class of functions implemented by a GNN with universal components is dense in probability in the class \( \mathcal{F}(D) \) of functions preserving the unfolding equivalence.

Point (1) is an extension of Proposition 3.3.4 and can be easily proved considering Theorem 4.1.3. Point (2) can be demonstrated by observing that GNNs cannot have a greater discriminatory capability than the 1–WL test [23], based on the established relationship between 1–WL and unfolding trees. Finally, Point (3) is simply a rephrasing of Theorem 4.2.3.

**Conclusion**

In this paper, we have shown that GNNs can approximate, in probability, any function that preserves the unfolding equivalence (i.e., that passes the 1–WL test). Our proof improves existing results both because it is constructive and because it is more general, since it holds for measurable functions. Moreover, by using the developed theory, we have provided details on the GNN architectures that can reach a given approximation, we have shown that the unfolding

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5 Recursive neural networks [32] are the ancestors of GNNs and assume that the input graph is acyclic.
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trees and the 1–WL test result in the same equivalence between nodes, and that the 1–WL test converges in $r + 1$ steps, where $r$ is the diameter of the graph.

Future developments in this theoretical framework may include further extensions of our results beyond the 1–WL domain and covering GNN models not considered by the framework used in this paper. Moreover, the proposed results are mainly focused on the expressive power of GNNs, but GNNs with the same expressive power may differ for other fundamental properties, e.g., the computational and memory requirements and the generalization capability. Understanding how the architecture of AGGREGATE$(k)$, COMBINE$(k)$ and READOUT impact on those properties is of fundamental importance for practical applications of GNNs.

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A Appendix

Proof of Theorems 4.1.1, 4.1.2, 4.1.3 and 4.1.4

Since both the unfolding equivalence and the WL-equivalence have been defined using a recursive definition localized on the nodes, it is natural to investigate the possible connections between these two equivalence relations. Indeed, in the following, we show that they are equivalent, namely they define the same relationship between nodes. To this aim, we start by proving Theorem 4.1.3.

Proof of Theorem 4.1.3

• (v ⇝ \_ue u \rightarrow T^r_v = T^r_u) – By definition, u ⇝ \_ue v iff T_v = T_u, which implies T^k_u = T^k_v for all k and, in particular, also for k = r + 1.

• (T^{r+1}_v = T^{r+1}_u \rightarrow v ⇝ \_ue u) – We prove by reductio ad absurdum that

\[
T^k_v = T^k_u \rightarrow T^{k+1}_v = T^{k+1}_u \quad \forall k \geq r + 1
\]

In fact, let us assume that \( \exists k \geq r + 1 \) such that \( T^k_v = T^k_u \) but \( T^{k+1}_v \neq T^{k+1}_u \). This means that there would be a node \( \mu \) in \( T^{k+1}_v \) and a node \( \nu \) in \( T^{k+1}_u \) such that \( \mu = \nu \) and \( T^k_\mu = T^k_\nu \), which is impossible, because in \( T^k_v \) and \( T^k_u \) all nodes have already been explored (since \( k \geq r + 1 \)). Moreover, some \( i \), with \( i \leq r \), exists such that, at depth \( i \), an equality holds between subtrees of depth 1 so as \( T^k_\mu = T^k_\nu \). Therefore, \( \exists k \geq r + 1 \) such that \( T^k_v = T^k_u \) but \( T^{k+1}_v \neq T^{k+1}_u \), which proves the theorem.

To prove the remaining theorems, the following lemma is required.

Lemma A.0.1.

Let \( G = (V, E) \) be a graph and let \( u, v \in V \), with features \( \ell_u, \ell_v \). Then, \( \forall t \in \mathbb{N} \)

\[
T^t_u = T^t_v \quad \text{iff} \quad c^t_u = c^t_v
\]

where \( c^t_u \) and \( c^t_v \) represent the node coloring of \( u \) and \( v \) at time \( t \), respectively.

Proof. The proof is carried out by induction on \( t \), which represents both the depth of the unfolding trees and the iteration step in the WL colouring.

For \( t = 0 \), \( T^0_u = \text{Tree}(\ell_u) = \text{Tree}(\ell_v) = T^0_v \) if and only if \( \ell_u = \ell_v \) and \( c^0_u = \text{HASH}_0(\ell_u) = \text{HASH}_0(\ell_v) = c^0_v \). Let us suppose that Eq. 4 holds for \( t - 1 \), and prove that it holds also for \( t \).

\((\rightarrow)\) Assuming that \( T^t_u = T^t_v \), we have

\[
T^{t-1}_u = T^{t-1}_v
\]

and

\[
\text{Tree}(\ell_u, T^{t-1}_{ne[u]}) = \text{Tree}(\ell_v, T^{t-1}_{ne[v]})
\]

By induction, Eq. 5 is true if and only if

\[
c^{(t-1)}_u = c^{(t-1)}_v
\]

Eq. 6 implies that \( \ell_u = \ell_v \) and \( T^{t-1}_{ne[u]} = T^{t-1}_{ne[v]} \), which means that an ordering on \( ne[u] \) and \( ne[v] \) exists s.t.

\[
T^{t-1}_{ne[u]} = T^{t-1}_{ne[v]} \quad \forall \ i = 1, \ldots, |ne[u]|
\]

Hence, Eq. 8 holds iff an ordering on \( ne[u] \) and \( ne[v] \) exists s.t.

\[
c^{t-1}_{ne(u)} = c^{t-1}_{ne(v)}, \forall i = 1, \ldots, |ne[u]|
\]

that is

\[
\{c^{t-1}_m | m \in ne[u]\} = \{c^{t-1}_n | n \in ne[v]\}
\]

Putting together Eqs. 6 and 9, we obtain:

\[
\text{HASH}(c^{t-1}_u, \{c^{t-1}_m | m \in ne[u]\}) = \text{HASH}(c^{t-1}_v, \{c^{t-1}_n | n \in ne[v]\})
\]

which implies that \( c^t_u = c^t_v \).
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The proof of the converse implication follows a similar reasoning, but some different steps are required in order to reconstruct the unfolding equivalence from the equivalence based on the 1–WL test.

Let us assume that
\[ c_t(u) = c_t(v) \]
by definition,
\[
\text{HASH}(\{c_{t-1}(m) | m \in \text{ne}[u]\}) = \\
\text{HASH}(\{c_{t-1}(n) | n \in \text{ne}[v]\})
\]

Being the HASH function bijective, Eq. (10) implies that:
\[ c_{t-1}(u) = c_{t-1}(v) \] (11)
and
\[ \{c_{t-1}(m) | m \in \text{ne}[u]\} = \{c_{t-1}(n) | n \in \text{ne}[v]\} \] (12)

Eq. (11) is true if and only if, by induction,
\[ T_{t-1}^u = T_{t-1}^v \] (13)
which implies
\[ \ell_u = \ell_v \] (14)

Moreover, Eq. (12) means that an ordering on \( \text{ne}[u] \) and \( \text{ne}[v] \) exists such that
\[ c_{t-1}^{\text{ne}(u)} = c_{t-1}^{\text{ne}(v)}, \forall i = 1, \ldots, |\text{ne}[u]| \] (15)

Instead, by induction, Eq. (15) holds if an ordering on \( \text{ne}[u] \) and \( \text{ne}[v] \) exists so as \( T_{t-1}^{\text{ne}(u)} = T_{t-1}^{\text{ne}(v)} \) \forall i = 1, \ldots, |\text{ne}[u]|, \) i.e.
\[ T_{t-1}^{\text{ne}[u]} = T_{t-1}^{\text{ne}[v]} \] (16)

Finally, putting together Eqs. (14) and (16), we obtain
\[ \text{Tree}(\ell_u, T_{t-1}^{\text{ne}[u]}) = \text{Tree}(\ell_v, T_{t-1}^{\text{ne}[v]}) \]
that means \( T_u^t = T_v^t \)

Theorem 4.1.1 is therefore proven, as its statement just rephrases the statement of Lemma A.0.1 in terms of the equivalence notation. Theorem 4.1.2 is the natural extension of Theorem 4.1.1 to graphs, while Corollary 4.1.4 can be obtained by putting together Theorem 4.1.3 and Theorem 4.1.2.

Proof of Theorem 4.2.1 (Approximation by GNNs)

First, we need a preliminary lemma, for the proof of which we refer to [29]. Intuitively, this lemma suggests that a graph domain with continuous features can be partitioned into small subsets so that the features of the graphs are almost constant in each partition. Moreover, a finite number of partitions is sufficient, in probability, to cover a large part of the domain.

Lemma A.0.2. (Lemma 1 in [29]) For any probability measure \( P \) on \( D \), and any reals \( \lambda, \delta \), where \( 0 < \lambda \leq 1, \delta \geq 0 \), there exist a real \( b > 0 \), which is independent of \( \delta \), a set \( \mathcal{D} \subseteq \mathcal{D} \), and a finite number of partitions \( D_1, \ldots, \delta \) of \( \mathcal{D} \), where \( \mathcal{D} = G \times \{v_i\} \), with \( G_i \subseteq G \) and \( v_i \in G_i \), such that:

1. \( P(\mathcal{D}) \geq 1 - \lambda \) holds;
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2. for each i, all the graphs in \(G_i\) have the same structure, i.e., they differ only for the values of their labels;

3. for each set \(D_i\), there exists a hypercube \(H_i \in \mathbb{R}^a\) such that \(\ell_G \in H_i\) holds for any graph \(G \in G_i\), where \(\ell_G\) denotes the vector obtained by stacking all the feature vectors of \(G\);

4. for any two different sets \(G_i, G_j, i \neq j\), their graphs have different structures or their hypercubes \(H_i, H_j\) have a null intersection, i.e. \(H_i \cap H_j = \emptyset\);

5. for each i and each pair of graphs \(G_1, G_2 \in G_i\), the inequality \(\|\ell_{G_1} - \ell_{G_2}\|_\infty \leq \delta\) holds;

6. for each graph \(G \in D\), the inequality \(\|\ell_G\|_\infty \leq \bar{b}\) holds.

By adopting an argument similar to that in [29], it is proved that Theorem 4.2.1 is equivalent to the following, where the domain contains a finite number of graphs and the features are integers.

**Theorem A.0.3.** For any finite set of patterns \(\{(G_i, v_i) | G_i \in G, v_i \in \mathcal{N}, 1 \leq i \leq n\}\), with \(r = \max \text{diam}(G_i)\) and with graphs having integer features, for any function \(\tau : D \rightarrow \mathbb{R}^m\), which preserves the unfolding equivalence, and for any real \(\varepsilon > 0\), there exist continuously differentiable functions \(\text{AGGREGATE}^{(k)}, \text{COMBINE}^{(k)}, \forall k \leq r + 1\), s.t.

\[
\ell^k_h = \text{COMBINE}^{(k)}(\ell^{k-1}_h, \text{AGGREGATE}^{(k)}\{\ell^{k-1}_u, u \in ne[v]\})
\]

and a function \(\text{READOUT}\), with feature dimension \(m = 1\), i.e. \(\ell^k_h \in \mathbb{R}\), so that the function \(\varphi\) (realized by the GNN), computed after \(r + 1\) steps, satisfies the condition

\[
|\tau(G_i, v_i) - \varphi(G_i, v_i)| \leq \varepsilon
\]

for any \(i, 1 \leq i \leq n\).

The equivalence is formally proved by the following lemma.

**Lemma A.0.4.** Theorem 4.2.1 holds if and only if Theorem A.0.3 holds.

**Proof.** Although the proof is quite identical to the one contained in [29], we report it here with the new notation.

Theorem 4.2.1 is more general than Theorem A.0.3 which makes this implication straightforward. Suppose instead that Theorem A.0.3 holds and show that this implies Theorem 4.2.1. Let us apply Lemma A.0.2 with values for \(P\) and \(\lambda\) equal to the corresponding values of Theorem 4.2.1 being \(\delta\) any positive real number. It follows that there is a real \(\bar{b}\) and a subset \(D\) of \(D\) s.t. \(P(D) > 1 - \lambda\). Let \(M\) be the subset of \(D\) that contains only the graphs \(G\) satisfying \(\|\ell_G\|_\infty \leq \bar{b}\).

Note that, since \(\bar{b}\) is independent of \(\delta\), then \(D \subset M\) for any \(\delta\). Since \(\tau\) is integrable, there exists a continuous function which approximates \(\tau\), in probability, up to any degree of precision. Thus, without loss of generality, we can assume that \(\tau\) is equi–continuous on \(M\). By definition of equi–continuity, a real \(\delta > 0\) exists such that

\[
|\tau(G_1, v) - \tau(G_2, v)| \leq \frac{\varepsilon}{2}
\]

holds for any node \(v\) and for any pair of graphs \(G_1, G_2\) having the same structure and satisfying \(\|\ell_{G_1} - \ell_{G_2}\|_\infty \leq \delta\).

Let us apply Lemma A.0.2 again, where, now, the \(\delta\) of the hypothesis is set to \(\delta\), i.e. \(\delta = \delta\). From then on, \(D = G_i \times \{v_i\}\), \(1 \leq i \leq n\), represents the set obtained by the new application of Lemma A.0.2 and \(I_i^{b, \hat{b}}\), \(1 \leq i \leq 2d\), denotes the corresponding intervals defined in the proof of the same lemma. Let \(\theta : \mathbb{R} \rightarrow \mathbb{Z}\) be a function that encodes reals into integers as follows: for any \(i\) and any \(z \in I_i^{b, \hat{b}}\), \(\theta(z) = i\). Thus, \(\theta\) assigns to all the values of an interval \(I_i^{b, \hat{b}}\) the index \(i\) of the interval itself. Since the intervals do not overlap and are not contiguous, \(\theta\) can be continuously extended to the entire \(\mathbb{R}\). Moreover, \(\theta\) can be extended also to vectors, being \(\theta(Z)\) the vector of integers obtained by encoding all the components of \(Z\). Finally, let \(\Theta : \mathcal{G} \rightarrow \mathcal{G}\) represent the function that transforms each graph by replacing all the feature labels with their coding, i.e. \(\text{L}_{\Theta(G)} = \theta(\text{L}_{G})\). Let \(G_1, \ldots, G_n\) be graphs, each one extracted from a different set \(G_i\).

Consider, now, the problem of approximating \(\tau \circ \Gamma\) on the set \((\Theta(G_1), v_1), \ldots, (\Theta(G_n), v_n)\). Theorem A.0.3 can be applied to such a set, because it contains a finite number of graphs with integer labels. Therefore, there exists a GNN that implements a function \(\tilde{\varphi}\) s.t., for each \(i\),

\[
|\tau(\Gamma(\Theta(G_i), v_i)) - \tilde{\varphi}(\Theta(G_i), v_i)| \leq \frac{\varepsilon}{2}
\]
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However, this means that there is also another GNN that produces the same result operating on the original graphs \( G_i \), namely a GNN for which
\[
\psi(G_i, v_i) = \hat{\varphi}(\Theta_i(G_i), v_i)
\]
holds. Actually, the graphs \( G_i \) and \( G_i \) are equal except that the former have the coding of the feature labels attached to the nodes, while the latter contain the whole feature labels. Thus, the GNN that operates on \( G_i \) is that suggested by Theorem A.0.3 except that AGGREGATE\(^{(0)}\) creates a coding of \( \theta(\epsilon_v) \) before the rest of the tasks.

Putting together the above equality with Eqs. (18) and (19), it immediately follows that, for any \((G, v) \in \mathcal{D}_i,\)
\[
|\tau(G, v) - \psi(G, v)| = \\
= |\tau(G, v) - \tau(G_i, v) + \tau(G_i, v) - \psi(G, v)| \\
\leq |\tau(G_i, v) - \psi(G, v)| + \frac{\varepsilon}{2} \\
= |\tau(\Gamma(\Theta_i(G_i), v)) - \hat{\varphi}(\Theta_i(G_i), v)| + \frac{\varepsilon}{2} \leq \varepsilon
\]
Thus, the GNN described by Eq. (20) satisfies \(|\tau(G, v) - \psi(G, v)| \leq \varepsilon\) in the restricted domain \( \mathcal{D} \). Since \( P(\mathcal{D}) \geq 1 - \lambda \), we have:
\[
P(\|\tau(G, v) - \psi(G, v)\| \leq \varepsilon) \geq 1 - \lambda
\]
which proves the lemma.

Now, we can proceed to prove Theorem A.0.3

Proof of Theorem A.0.3. For the sake of simplicity, the theorem will be proved assuming \( n = 1 \), i.e. \( \tau(G, v) \in \mathbb{R} \). However, the result can be easily extended to the general case when \( \tau(G, v) \in \mathbb{R}^n \). Indeed, in this case, the GNN that satisfies the theorem can be defined by stacking \( n \) GNNs, each one approximating a component of \( \tau(G, v) \).

According to Theorem 3.3.4 there exists a function \( \kappa \) s.t. \( \tau(G, v) = \kappa(T_v) \). Theorem 4.1.3 suggests that an unfolding tree of depth \( r + 1 \), where \( r \) is the diameter of the graph, is enough to store the graph information, so that \( \kappa \) can be designed to satisfy \( \tau(G, v) = \kappa(T_v) = \kappa(T_v^{r+1}) \). Thus, the main idea of the proof consists of designing a GNN that is able to encode the unfolding trees into the node features, i.e., for each node \( v \), we want to have \( h_v = \nabla(T_v^{r+1}) \), where \( \nabla \) is an encoding function that maps trees into real numbers. More precisely, the encodings are constructed recursively by the AGGREGATE\(^{(k)}\) and the COMBINE\(^{(k)}\) functions using the neighbourhood information. After \( t \) steps, the node features contain the encoding of the unfolding tree \( \nabla(T_v^t) \), of depth \( t \). Then, after a number of steps \( t \) larger than the diameter of the graph, the GNN, by the READOUT function, can produce the desired output \( \kappa(T_v^{r+1}) \).

Therefore, the theorem can be proved provided that we can implement the above mentioned procedure, which means that there exist appropriate functions \( \nabla \), AGGREGATE\(^{(k)}\), COMBINE\(^{(k)}\) and READOUT. The existence of the READOUT function is obvious, since, given that unfolding trees can be encoded in node features, READOUT has just to decode the representation and compute the target output. Then, let use focus on the other functions. They will be defined in two steps. Initially, AGGREGATE\(^{(k)}\), COMBINE\(^{(k)}\), and READOUT will be defined without taking into account that they have to be continuously differentiable. Later, this farther constraint will be considered.

The coding function \( \nabla \)

Let \( \nabla \) be a composition of any two injective functions \( \alpha \) and \( \beta, \alpha \circ \beta, \) with the properties described in the following.

\begin{itemize}
  \item \( \alpha \) is an injective function from the domain of the unfolding trees \( T_v^{r+1} \), calculated on the nodes in the graph \( G_i \), to the Cartesian product \( \mathbb{N} \times \mathbb{N}^P \times \mathbb{Z}^{\ell} = \mathbb{N}^{P+1} \times \mathbb{Z}^{\ell} \), where \( r = \max \text{diam}(G_i) \) and \( P \) is the maximum number of nodes a tree could have.

Intuitively, in the Cartesian product, \( \mathbb{N} \) represents the tree structure, \( \mathbb{N}^P \) denotes the node numbering, while, for each node, an integer vector \( \in \mathbb{Z}^{\ell} \) is used to encode the node features. Notice that \( \alpha \) exists and is injective, since the maximal information contained in an unfolding tree is given by the union of all its node features and all its structural information, which just equals the dimension of the codomain of \( \alpha \).
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- $\beta$ is an injective function from $\mathbb{N}^{P+1} \times \mathbb{Z}^V$ to $\mathbb{R}$, whose existence is guaranteed by the cardinality theory, since the two sets have the same cardinality.

Since $\alpha$ and $\beta$ are injective, also the existence and the injectiveness of $\nabla$ are ensured.

**The functions AGGREGATE$^{(k)}$ and COMBINE$^{(k)}$**

The functions AGGREGATE$^{(k)}$ and COMBINE$^{(k)}$ must satisfy

$$\nabla(T^t_u) = h^t_u = \text{COMBINE}^{(k)}(h^{t-1}_u, \text{AGGREGATE}^{(k)}\{h^{t-1}_u, \; u \in ne[v]\})$$

$$= \text{COMBINE}^{(k)}(\nabla(T^{t-1}_u), \text{AGGREGATE}^{(k)}\{\nabla(T^{t-1}_u), \; u \in ne[v]\})$$

\forall k \leq r. In a simple solution, AGGREGATE$^{(k)}$ decodes the trees of the neighbour $T^{t-1}_u$ of $v$ and stores them into a data structure to be accessed by COMBINE$^{(k)}$. For example, the trees can be collected into the coding of a new tree, i.e., $\text{AGGREGATE}^{(k)}(\nabla(T^{t-1}_u), \; u \in ne[v]) = \nabla(\bigcup_{u \in ne[v]} \nabla^{-1}(\nabla(T^{t-1}_u)))$, where $\bigcup_{u \in ne[v]}$ denotes an operator that constructs a tree with a root having void features from a set of sub–trees (see Figure 4). Then, COMBINE$^{(k)}$ assigns the correct features to the root by extracting them from $T^{t-1}_v$, i.e.,

$$\text{COMBINE}^{(k)}(\nabla(T^{t-1}_v), b) = \nabla(\text{ATTACH}(\nabla^{-1}(\nabla(T^{t-1}_v)), \nabla^{-1}(b)))$$

where ATTACH is an operator that returns a tree constructed by replacing the features of the root in the latter tree with those of the former tree and $b$ is the result of the AGGREGATE$^{(k)}$ function.

![Figure 4: The ATTACH operator on trees.](image)

Now, notice that, with this definition, AGGREGATE$^{(k)}$, COMBINE$^{(k)}$, and READOUT may not be differentiable. Nevertheless, Eq. (17) has to be satisfied only for a finite number of graphs, namely $G_i$. Thus, we can specify other functions $\overline{\text{AGGREGATE}}^{(k)}$, $\overline{\text{COMBINE}}^{(k)}$, and $\overline{\text{READOUT}}$, which produce exactly the same computations when they are applied on the graphs $G_i$, but that can be extended to the rest of their domain, so that they are continuously
differentiable. Obviously, such an extension exists since those functions are only constrained to interpolate a finite number of points.

Proof sketch of Theorem 4.2.3

Proof. As in the proof of Theorem 4.2.1, without loss of generality, we will assume that the feature dimension is \( n = 1 \). First of all, note that Theorem 4.2.1 ensures that we can find \( \text{COMBINE}^{(k)}, \text{AGGREGATE}^{(k)}, \forall k \leq r \), and \( \text{READOUT} \) so that, for the corresponding function \( \bar{\varphi} \) implemented by the GNN,

\[
P(\|\tau(G, v) - \bar{\varphi}(G, v)\| \leq \varepsilon/2) \geq 1 - \lambda
\]

holds. Let us consider the corresponding transition function \( \bar{f} \), defined by

\[
\bar{f}^k(h_{v}^{k-1}, \{h_{u}^{k-1}, u \in ne[v]\}) = \\
\text{COMBINE}^{(k)}(h_{v}^{k-1}, \text{AGGREGATE}^{(k)}\{h_{u}^{k-1}, u \in ne[v]\})
\]

Since \( \text{COMBINE}^{(k)} \) and \( \text{AGGREGATE}^{(k)} \) are continuously differentiable, \( \bar{f}^k \) is continuously differentiable. Considering that the theorem has to hold only in probability, we can also assume that the domain is bounded, so that \( \bar{f}^k \) is bounded and has a bounded Jacobian. Let \( B \) be a bound on the Jacobian/derivative of \( \bar{f}^k \) for any \( k \) and any input. The same argument can also be applied to the function \( \text{READOUT} \), which is continuously differentiable w.r.t. its input and can be assumed to have a bounded Jacobian/derivative. Let us assume that \( B \) is also a bound for the Jacobian/derivative of \( \text{READOUT} \). Moreover, let \( \text{COMBINE}^{(k)}_{\text{ne}}, \text{AGGREGATE}^{(k)}_{\text{ne}} \) be functions implemented by universal neural network that approximate \( \text{COMBINE}^{(k)}, \text{AGGREGATE}^{(k)}, \forall k \leq r \), respectively, and such that

\[
f^k_w(h_v^{k-1}, \{h_u^{k-1}, u \in ne[v]\}) = \\
\text{COMBINE}^{(k)}_{\text{ne}}(h_{v}^{k-1}, \text{AGGREGATE}^{(k)}_{\text{ne}}\{h_{u}^{k-1}, u \in ne[v]\})
\]

and let us assume that

\[
\|\bar{f}^k - f^k_w\|_{\infty} \leq \eta
\]

holds for every \( k \) and a \( \eta > 0 \). Let \( \text{READOUT}_w \) be the function implemented by a universal neural network that approximates \( \text{READOUT} \), so that

\[
\|\text{READOUT} - \text{READOUT}_w\|_{\infty} \leq \eta
\]

In the following, it will be shown that, when \( \eta \) is sufficiently small, the GNN implemented by the approximating neural networks is sufficiently close to the GNN of Theorem 4.2.1 so that the thesis is proved.

Let \( \bar{F}^k, F^k_w \) be the global transition functions of the GNNs that are obtained by stacking all the \( \bar{f}^k \) and \( f^k_w \) for all the nodes of the input graph. The node features are computed at each step by \( \bar{H}^k = \bar{F}^k(\bar{H}^{k-1}), \quad H^k = F^k_w(H^{k-1}) \), where \( \bar{H}^k, H^k \) denote the stacking of all the node features of the graph obtained by the two transition functions, respectively. Then,

\[
\|\bar{H}^1 - H^1\|_{\infty} = \|\bar{F}^1(H^0) - F^1_w(H^0)\|_{\infty} \leq \eta N
\]

where \( N = |G| \) is number of nodes in the input graph. Moreover,

\[
\|\bar{H}^2 - H^2\|_{\infty} = \\
= \|\bar{F}^2(\bar{H}^1) - F^2_w(H^1)\|_{\infty} \\
= \|\bar{F}^2(\bar{H}^1) - \bar{F}^2(\bar{H}^1) + \bar{F}^2(\bar{H}^1) - F^2_w(H^1)\|_{\infty} \\
\leq \|\bar{F}^2(\bar{H}^1) - \bar{F}^2(\bar{H}^1)\|_{\infty} + \|\bar{F}^2(\bar{H}^1) - F^2_w(H^1)\|_{\infty} \\
\leq \eta NB + \eta N = \eta N(B + 1).
\]

Here, \( \|\bar{F}^2(\bar{H}^1) - \bar{F}^2(\bar{H}^1)\|_{\infty} \leq \eta NB \) holds because of Eq. (23), which bounds the difference between \( \bar{H}^1 \) and \( H^1 \), and due to the fact that the Jacobian/derivative of \( \bar{F}^2 \) is bounded by \( B \). Moreover, \( \|\bar{F}^2(\bar{H}^1) - F^2_w(H^1)\|_{\infty} \leq \eta N \) holds by Eq. (22).

\footnote{Notice that a similar extension can also be applied to the coding function \( \varphi \) and to the decoding function \( \varphi^{-1} \). In this case, the coding function is not injective on the whole domain, but only on the graphs mentioned in the theorem.}
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The above reasoning can then be applied recursively to prove that
\[
\|\bar{H}^k - H^k_w\|_\infty \leq \eta N \sum_{i=0}^{k-1} B^i
\]

Finally, since the output of the GNN is computed using the encoding at the step \(r + 1\), we have
\[
\|\varphi(G, v) - \varphi_w(G, v)\|_\infty = \\
\|\text{READOUT}(H^{r+1}) - \text{READOUT}_w(H^{r+1})\|_\infty \\
\leq \eta N + B(\eta N \sum_{i=0}^{r} B^i)
\]

Finally, since we can consider the maximum number of nodes \(N\) as bounded\(^7\), then we can find a GNN based on neural networks so that \(\eta\) is small enough to achieve
\[
\|\varphi(G, v) - \varphi_w(G, v)\|_\infty \leq \epsilon/2
\]
which, together with Eq. (21), produces the bound of Theorem 4.2.1.

**Proof of Corollary 4.2.4**

**Proof.** Point 1) is a consequence of Theorem 3.3.4 and Theorem 4.1.3. Concerning Point 2), a function \(\varphi(G, v)\) implemented by a GNN is, by construction, a function \(f\) which preserves the unfolding equivalence: in fact, a GNN induces (as shown in the proof of Theorem 4.2.1) an equivalence on nodes at least as refined as the unfolding equivalence, because the GNN is capable of coding the unfolding tree; on the other hand, as shown in [35], the GNN could be at most as powerful as the 1–WL test, which we have proven to be equivalent to the unfolding equivalence. Therefore, \(\varphi(G, v)\) preserves exactly the unfolding equivalence, and so we can apply Point 1) to it. Finally, as already stated, Point 3) is a rephrasing of Theorem 4.2.3.

---

\(^7\)For the sake of simplicity, we skip over a very formal proof of this claim. Intuitively, note that the theorem has to be proved and Lemma A.0.2 clarifies that any graph domain can be covered in high probability by a finite number of structures, which obviously have a bounded number of nodes.