Trainability for Universal GNNs Through Surgical Randomness

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December 9, 2021

Abstract

Message passing neural networks (MPNN) have provable limitations, which can be overcome by universal networks. However, universal networks are typically impractical. The only exception is random node initialization (RNI), a data augmentation method that results in provably universal networks. Unfortunately, RNI suffers from severe drawbacks such as slow convergence and high sensitivity to changes in hyperparameters. We transfer powerful techniques from the practical world of graph isomorphism testing to MPNNs, resolving these drawbacks. This culminates in individualization-refinement node initialization (IRNI). We replace the indiscriminate and haphazard randomness used in RNI by a surgical incision of only a few random bits at well-selected nodes. Our novel non-intrusive data-augmentation scheme maintains the networks’ universality while resolving the trainability issues. We formally prove the claimed universality and corroborate experimentally—on synthetic benchmarks sets previously explicitly designed for that purpose—that IRNI overcomes the limitations of MPNNs. We also verify the practical efficacy of our approach on the standard benchmark data sets PROTEINS and NCI1.

1 Introduction

Structured data is omnipresent in the modern world. Graphs are a fundamental data type in machine learning (ML) on structured data and used in a variety of learning algorithms [Shervashidze et al., 2011, Nickel et al. 2016, Hamilton et al. 2017], including graph neural networks (GNNs) [Zhou et al., 2020, Wu et al. 2021]. GNNs, and especially message passing neural networks (MPNNs) [Gilmer et al. 2017], have found wide-spread applications, from drug design to friendship recommendation in social networks [Tang et al. 2020, Song et al. 2019]. However, severe limitations of MPNNs have recently been proven formally. In fact, MPNNs are at most as expressive as color refinement [Xu et al., 2019, Morris et al. 2019]. Color refinement — also known as the 1-dimensional Weisfeiler-Leman algorithm — is a simple algorithm inducing a non-universal similarity measure on graphs. Thus
MPNNs fail to be universal function approximators, a fundamental property known for multilayer perceptrons since the 1980s [Cybenko, 1989].

Addressing this lack, Sato et al. [2021] developed random node initialization (RNI), a data-augmentation scheme provably enabling MPNNs to be universal function approximators [Abboud et al., 2021]. RNI augments the graph’s nodes with random real values, thus artificially breaking its intrinsic symmetries and facilitating the distinction of previously indistinguishable nodes. However, while MPNNs using RNI are universal and thus theoretically appealing, they still have major practical shortcomings. This is in particular true for the limited trainability of the MPNN [Abboud et al., 2021].

To achieve the best of both worlds, universal approximation and high trainability of MPNNs, we propose an algorithm performing surgical insertions of randomness. Rather than introducing randomness haphazardly across all different nodes, it uses just enough randomness to break symmetries and render nodes distinguishable. As we show, limiting the amount of randomness in MPNNs not only improves their trainability while maintaining universal approximation but also facilitates the explainability of MPNNs.

But where should we ideally inject randomness into the graph? Here we draw inspiration from algorithms solving the graph isomorphism problem, the fundamental algorithmic problem of determining whether two graphs are isomorphic (i.e., differing only in the order of nodes). We propose to let individualization refinement (IR) guide us in our choice of a few well-selected nodes where we inject randomness. IR algorithms are procedures that solve the graph isomorphism problem and also compute the symmetries (automorphisms) of graphs. They use node “individualizations” to artificially break symmetries (or similarities) in a graph and then execute a form of backtracking. IR-solvers have been (amongst other things) optimized to choose nodes whose individualization induces distinguishing features into the graph in the most effective way. It is precisely at these nodes where we choose to inject randomness.

Our contributions. Introducing an adaptation of the IR-technique to the machine learning setting, we develop individualization-refinement node initialization (IRNI). This forms a non-intrusive data-augmentation scheme that conservatively introduces binary randomness into the graph. The choice of where to introduce the randomness is outsourced into a highly efficient IR graph isomorphism algorithm. Our empirical analysis demonstrates that our approach yields consistently higher prediction accuracies than other data augmentation schemes while having low execution times and acceptable memory constraints.

- We transfer the IR-framework into the realm of graph neural networks as IRNI. The introduction of IRNI into a GNN does not significantly increase the computation time. In particular, the time for the outsourced IR computation is negligible. (Sec. 4.2)

- We formally prove that IRNI is universal. We even prove that already a very limited version of IRNI is universal on almost all graphs, including all 3-connected planar ones. We also provide a quantification of the amount of randomness required to ensure universality of all but an exponentially small fraction of all graphs (Sec. 4.3)

- We experimentally verify that IRNI is able to distinguish graphs, which are indistinguishable by typical MPNNs, on synthetically generated data sets [Sato et al., 2021, Abboud et al., 2021]. These datasets were specifically designed to challenge non-universal MPNNs. (Sec. 5.2)
• We perform an ablation study to compare IRNI and RNI. Specifically, we also introduce an intermediate approach, one-hot RNI, which helps us to precisely explain the source of the conceptual advantage of IRNI over RNI. (Sec 4.2 and Sec. 5.2)

• We also experimentally verify that in terms of trainability IRNI outperforms RNI, the previously best practical, universal class of GNNs. (Sec. 5.3)

In summary, this gives us the first class of GNN models that are practical, universal, and easily trainable at the same time.

Comparison with RNI  Overall we find that IRNI provides the benefits of RNI, while dramatically reducing RNIs strain on training. Regarding wall-clock time, we want to emphasize that IRNI only marginally increases the per-prediction cost. While one might imagine this leads to a higher wall-clock training time for IRNI, in our experiments the wall-clock training time of IRNI is significantly less than RNI. This is due to the poor trainability of RNI which results from its high sensitivity to its hyperparameters and reduced convergence speed (as discussed in Sec. 5.3). Since IRNI is a form of data augmentation, it can easily be adapted into most if not all message-passing models and beyond. To summarize, IRNI seems to be always preferable over RNI.

Why individualization refinement.  We explain why the IR-framework is a natural choice for the development of efficient universal GNNs. (For general strengths and weaknesses beyond ML see [Mckay and Piperno, 2014, Neuen and Schweitzer, 2017].) First of all, the introduction of graph isomorphism techniques in the context of machine learning on graphs already lead to two success stories, namely the highly efficient Weisfeiler-Leman (WL) Kernels [Shervashidze et al., 2011] based on color refinement (1-WL) and the more theoretical higher-order graph neural networks [Morris et al., 2019] based on higher-dimensional WL.

However, when it comes to practical graph isomorphism the use of the 2-dimensional WL is already prohibitive. This is not only due to excessive running time but also due to excessive memory consumption. In the world of isomorphism testing, higher-dimensional Weisfeiler-Leman algorithms remain on the theoretical side. In truth, without fail, modern solvers are IR algorithms [Mckay and Piperno, 2014, Anders and Schweitzer, 2021a, Juntila and Kaski, 2011, McKay, 1981]. They only use color refinement and instead of higher-dimensional WL rather use individualizations to achieve universality. In contrast to higher-dimensional WL, the IR-approach is generic, universal, and practical. Uncontested for more than 50 years, IR algorithms have the fastest computation times and acceptable memory consumption for graph isomorphism [Mckay and Piperno, 2014]. In that sense, the IRNI approach we introduce in this paper is the first time in which universal graph isomorphism techniques that are truly used in practice are transferred into a machine learning context. An important consequence of this is that ML practitioners can now readily transfer existing IR-related results to ML on graphs (Sec. 4.3).

2 Related Work  
Graphs are a powerful means of representing semantic information. Since graphs are a very general data type, of which most other data types are special cases, graphs have a plethora of applications. They can be used to extend or combine other data types like text, images, or time series [Vazirgianiss et al., 2018, Noble and Cook, 2003] and there are also data sets specific to graphs. Most commonly these data sets are related to biology or chemistry, however, computer vision, social networks, and synthetic graphs without a related field are also present [Morris et al.,]
We interpret the node representations as colors using the Weisfeiler-Leman algorithm and expanded on it by proposing the \( \delta \)-\( k \)-GNN, a local variant of the \( k \)-GNN. Cybenko \[1989\] proved the first universality result for one of the earliest deep learning models, the smallest possible multilayer perceptron (MLP), with exactly one hidden layer and the sigmoid activation. This result has since then been expanded to different activation functions \[Leshno et al., 1993, Barron, 1994\], to width-bounded MLPs \[Lu et al., 2017, Liang and Srikant, 2017\], and more recently to different layered artificial neural networks like the convolutional neural network \[Zhou, 2020\]. Analogous results had been lacking for MPNNs, which are now well-established to be non-universal \[Ku et al., 2019, Morris et al., 2019, Abboud et al., 2021\]. Following this finding, multiple attempts were made to establish universal ML models on graph data. Sato et al. \[2021\] proposed random node initialization, which Abboud et al. \[2021\] proved to provide universality to MPNNs. Dasoulas et al. \[2020\] proposed the CLIP model, a method closely related to RNI (more specifically ORNI in Sec. 4.2). Morris et al. \[2019, 2020\] proposed \( k \)-GNNs based on the \( k \)-dimensional Weisfeiler-Leman algorithm and expanded on it by proposing the \( \delta \)-\( k \)-GNN a local variant of the \( k \)-GNN. Maron et al. \[2019a, b\] propose provably powerful graph networks, which are \( 2 \)-WL powerful, and invariant graph networks, which are proven to be universal.

### 3 Background

#### 3.1 Graphs and Colorings

We consider undirected, finite graphs \( G = (V, E)\) which consist of a set of vertices \( V \subseteq \mathbb{N} \) and a set of edges \( E \subseteq V^2 \), where \( E \) is symmetric. From this point onward, let \( n := |V| \) and \( V = \{v_1, \ldots, v_n\} \). Additionally, we let \( \mathcal{G} \) denote the set of all graphs, while \( \mathcal{G}_n \) denotes the set of all graphs on \( n \) vertices.

In ML contexts, graphs typically carry a node representation in \( \mathbb{R}^d \), which we denote by \( \{x_{v_1}, \ldots, x_{v_n}\} \). IR-tools require these node representations to be discrete, i.e., in \( \mathbb{N} \). For other approaches, discretization can be difficult and techniques are being actively researched \[Morris et al., 2016\]. However, for our purpose, the discretization is not critical, since we only require this encoding to compute a tuple of nodes \( (w_1, w_2, \ldots) \) from an IR algorithm. After that, our approach continues on the original node representation. Let \( \text{enc} : \mathbb{R}^d \times \mathcal{G} \rightarrow \mathbb{N} \) be an arbitrary isomorphism-invariant encoding of the node representations. In practice, it is best to choose an encoding for which \( \text{enc}(x_v, G) = \text{enc}(x_w, G) \) if and only if \( x_v = x_w \), however, this is not a requirement for any of the results we present.

A (node) coloring is a surjective map \( \pi : V \rightarrow \{1, \ldots, k\} \). In our context \( \pi(v_i) := \text{enc}(x_{v_i}, G) \). We interpret the node representations as colors using \( \text{enc} \). We call \( \pi^{-1}(i) \subseteq V \) the \( i \)-th cell for \( i \in \{1, \ldots, k\} \). If \( |\pi(V)| = n \) then \( \pi \) is discrete. This means every node has a unique color in \( \pi \). Note that in the following, we always use “discrete” in this sense. Furthermore, we say a coloring \( \pi \) is finer than \( \pi' \) if \( \pi(v) = \pi(v') \implies \pi'(v) = \pi'(v') \) holds for every \( v, v' \in V \). We may also say \( \pi' \) is coarser than \( \pi \).

We should remark that the IR machinery described in this work effortlessly generalizes to directed
Figure 1: Two graphs which are indistinguishable by MPNNs as well as color refinement.

and edge-colored graphs [Piperno, 2018]. We denote by $N_G(v)$ the neighborhood of node $v$ in graph $G$.

### 3.2 Message Passing Neural Networks

Formally, given a graph $G$ and the vector representation $x_{v,t}$ of node $v$ at time $t$, a message passing update can be formulated as:

$$x_{v,t+1} := \text{combine}(x_{v,t}, \text{aggregate}(\{x_{w,t} | w \in N_G(v)\}))$$ (1)

In this context, the aggregate function is typically required to be invariant under isomorphisms, to prevent learning spurious features from the arbitrary node ordering of the input. Common instances of the MPNN are graph convolutional networks (GCNs) [Duvenaud et al., 2015], graph attention networks [Velickovic et al., 2018], and graph isomorphism networks (GIN) [Xu et al., 2019]. We will be using the GIN throughout this paper.

A GIN is characterized by being simple and yet as powerful as the color refinement algorithm. It updates its node representations $h_v^{(k)}$ in layer $k$ as follows

$$h_v^{(k)} := \text{MLP}^{(k)}\left(\left(1 + \epsilon^{(k)}\right)h_v^{(k-1)} + \sum_{u \in N_G(v)} h_u^{(k-1)}\right),$$ (2)

where $\text{MLP}^{(k)}$ is an arbitrary multi-layer perceptron (MLP) in layer $k$, $\epsilon^{(k)}$ is a learnable parameter of layer $k$, and $h_v^{(0)}$ is the input representation of node $v$. A GIN layer has far fewer parameters than other MPNN layers, since it depends on only one MLP in each of its layers instead of for instance three in the case of a GCN layer.

### 3.3 Universality of MPNNs and Random Node Initialization

MPNNs with no data-augmentation are not universal [Xu et al., 2019, Sato et al., 2021, Abboud et al., 2021]. Consider, e.g., the graphs in Fig. 1. Since each node has the same color and the same number of neighbors, the MPNN update is equal for each node. This continues through each layer of the MPNN and results in a uniformly colored output graph. Thus, no nodes can be distinguished and since we use only the node colors for prediction and each graph has six equally colored nodes, both graphs have an equal prediction. Thus the graphs are not distinguished. MPNNs are exactly as powerful in distinguishing graphs as color refinement [Xu et al., 2019], which for instance cannot distinguish regular graphs of the same degree (e.g., the graphs in Fig. 1).

As a remedy for the non-universality of MPNNs, Sato et al. [2021] proposed RNI. Precisely, let $G$ be a graph with node representations $\{x_{v_1}, \ldots, x_{v_n}\}$ and $d \in \mathbb{N}$ a constant (see Section 3.1). Random node initialisation (RNI) concatenates $d$ features sampled from a random distribution $\mathcal{X}$ to each node $\forall i \in \{1, \ldots, n\}$: $x_{v_i} \leftarrow x_{v_i} \odot (r_1, \ldots, r_d), r_1 \ldots, r_d \sim \mathcal{X}$. Abboud et al. [2021] then proved that an MPNN with RNI is universal.
4 Data Augmentation by Individualization Refinement

We introduce individualization-refinement node initialization (IRNI), a data-augmentation that,—as we prove—when used together with MPNNs results in universal function approximators on graphs.

4.1 Individualization Refinement Trees

Individualization refinement (IR) trees are the backtracking trees of practical graph isomorphism algorithms. We use randomly sampled leaves of these trees for data augmentation purposes, which have very specific properties that we describe below. These leaves correspond to sequences of nodes \((w_1, \ldots, w_k)\) of the graph, which we translate into features of the MPNN. One major property of the sequence is that distinguishing (individualizing) its nodes from other nodes in the graph and applying color refinement yields a discrete coloring.

In the following, we describe all the necessary ingredients for the purposes of this paper. Knowledge of all the particular details is not required to understand how our data augmentation scheme itself is built, however, the theoretical results in Section 4.3 do depend on the details. We remark that the IR paradigm is a complex machinery refined over many decades into sophisticated software libraries. We refer to McKay and Piperno [2014] and Anders and Schweitzer [2021a] for a more exhaustive description. We briefly describe the components of IR trees.

**Refinement.** A coloring \(\pi\) is equitable if for every pair of (not necessarily distinct) colors \(i, j\) the number of \(j\)-colored neighbors is the same for all \(i\)-colored vertices. Equitable colorings are precisely the colorings for which color refinement cannot be employed to further distinguish nodes. For a colored graph \((G, \pi)\) there is (up to renaming of colors) a unique coarsest equitable coloring finer than \(\pi\) [McKay, 1981]. This is precisely the coloring computed by color refinement. We denote this coloring by Ref\((G, \pi, \epsilon)\), where \(\epsilon\) denotes the empty sequence. A more algorithmic way to describe the refinement is to define for a colored graph \((G, \pi)\) the naively refined graph \((G, \pi^r)\) where \(\pi^r(v) := (\pi(v), \{\pi(v') \mid v' \in N_G(v)\})\). The naive refinement \(r\) is applied exhaustively, i.e., until vertices cannot be partitioned further. The result is precisely the coarsest equitable coloring. We want to point out the similarity between the refinement \(r\) and the message passing update (Equation 1). We refer to Xu et al. [2019] and Morris et al. [2019] for a formal comparison.

**Individualization.** IR algorithms make use of individualization, a process that artificially forces a node into its own color class, distinguishing it. To record which vertices have been individualized we use a sequence \(\nu = (v_1, \ldots, v_k) \in V^*\) (note that \(^*\) denotes the Kleene star). We extend the refinement function so that Ref\((G, \pi, \nu)\) is the unique coarsest equitable coloring finer than \(\pi\) in which every node in \(\nu\) is a singleton with its own artificial color. I.e., the artificial distinctions caused by individualizations are taken into account.

**Cell selector.** In a backtracking fashion, the goal of an IR algorithm is to reach a discrete coloring using color refinement and individualization. For this, color refinement is first applied. If this does not yield a discrete coloring, individualization is applied, branching over all vertices in one non-singleton cell. The task of the cell selector is to (isomorphism-invariantly) pick the non-singleton cell. Figure 2 illustrates this process. While many choices within certain restrictions are possible, for the purposes of this paper we define Sel\((G, \pi)\) to simply choose the first, largest non-singleton cell of \(\pi\).
Figure 2: The figure shows how in IR, refinement and individualization are alternately applied. The process continues until the coloring of the graph becomes discrete. Two nodes connected by a squiggly line are considered one node of the IR tree: they illustrate the coloring of the graph before and after the refinement is applied.

**IR trees.** We first give a formal definition of the IR tree $\Gamma(G, \pi)$, followed by a more intuitive explanation.

Nodes of $\Gamma(G, \pi)$ are sequences of vertices of $G$. The root of $\Gamma(G, \pi)$ is the empty sequence $\epsilon = ()$. If $\nu = (v_1, \ldots, v_k)$ is a node in $\Gamma(G, \pi)$ and $C = \text{Sel}(G, \text{Ref}(G, \pi, \nu))$, then the set of children of $\nu$ is $\{(v_1, \ldots, v_k, v) \mid v \in C\}$, i.e., all extensions of $\nu$ by one node $v$ of the selected cell $C$.

The root represents the graph (with no individualizations) after refinement (see Figure 2). A node $\nu$ represents the graph after all nodes in $\nu$ have been individualized followed by refinement (see Figure 2). A root-to-$\nu$ walk of the tree is naturally identified with a sequence of individualizations in the graph: in each step $i$ of the walk, one more node $v_i$ belonging to a non-trivial color class $C$ is individualized (followed by refinement). The sequence of individualizations $(v_1, \ldots, v_k)$ uniquely determines the node of the IR tree in which this walk ends up. This is why we identify the name of the node with the sequence of individualizations necessary to reach the node: the sequence of individualizations necessary to reach $\nu$ is $(v_1, \ldots, v_k) = \nu$.

By $\Gamma(G, \pi, \nu)$ we denote the subtree of $\Gamma(G, \pi)$ rooted in $\nu$. Isomorphism invariance of the IR tree follows from the isomorphism invariance of Sel and Ref:

**Lemma 1** (Mckay and Piperno [2014]). Let $\varphi: V \rightarrow V$ denote an automorphism of $(G, \pi)$, i.e., $(G, \pi)^\varphi = (\varphi(V), \varphi(E), \varphi(\pi)) = (V, E, \pi) = G$, and $\text{Aut}(G, \pi)$ denotes all automorphisms of $(G, \pi)$. Then, if $\nu$ is a node of $\Gamma(G, \pi)$ and $\varphi \in \text{Aut}(G, \pi)$, then $\nu^\varphi$ is a node of $\Gamma(G, \pi)$ and $\Gamma(G, \pi, \nu)^\varphi = \Gamma(G, \pi, \nu^\varphi)$.

**Random IR walks.** There are various ways to traverse and use IR trees. Traditionally, solvers (e.g., nauty) solely used deterministic strategies, such as depth-first traversal [Mckay and Piperno, 2014]. Only recently, with the introduction of dejavu [Anders and Schweitzer, 2021a], competitive strategies based solely on random traversal have been developed (see Section 4.3). We make use of this recent development.

Specifically, we make use of random root-to-leaf walks of the IR tree $\Gamma(G, \pi)$. We begin such a
walk in the root node of $\Gamma(G, \pi)$. We repeatedly choose uniformly at random a child of the current node, until we reach a leaf $\nu$ of the tree. Then, we return the leaf $\nu = (w_1, \ldots, w_k)$ (recall that a node $\nu$ of the IR tree is named after the sequence of individualizations necessary to reach $\nu$).

A crucial property is that since $\Gamma(G, \pi)$ is isomorphism-invariant (Lemma 1), random walks of $\Gamma(G, \pi)$ are isomorphism-invariant as well:

**Lemma 2** (Anders and Schweitzer [2021a]). As a random variable, the graph colored with the coloring of the leaf resulting from a random IR walk is isomorphism-invariant.

Lemma 2 is also true when restricting random walks to prefixes of a certain length $d$. We stress that random IR walks are conceptually unrelated to random walks in the graph itself considered elsewhere [Nikolentzos and Vazirgiannis, 2020].

Our next step is to insert the sequence of nodes defined by random IR walks into MPNNs.

### 4.2 Individualization Refinement Node Initialization

Let $G$ be a graph with node representations $\{x_{v_1}, \ldots, x_{v_n}\}$ and $d \in \mathbb{N}$ a constant. Individualization-refinement node initialization (IRNI) computes a random IR walk $w = (w_1, \ldots, w_k)$ in $\Gamma(G, \pi)$, where $\pi(v_i) := enc(x_{v_i}, G)$ as defined in Sec. 3.1. Assuming for the moment that $k \geq d$, we take a prefix of length $d$, i.e., $(w_1, \ldots, w_d)$, providing $d$ nodes to be individualized. IRNI then concatenates $d$ features that are either 0 or 1 depending on this prefix: We set $\forall i \in \{1, \ldots, n\}$:

$$x_{v_i} \leftarrow x_{v_i} \circ (\mathbb{I}_{w_1=v_i}, \ldots, \mathbb{I}_{w_d=v_i}),$$

which means that the $j$-th feature of node $v_i$ is set to 1 if $v_i$ is the $j$-th node that was individualized (i.e., $w_j = v_i$) and 0 otherwise. This implies that in each added feature dimension there is exactly one node to which a 1 is assigned and all other values in the dimension are 0. Overall this guarantees that node $v_i$ is individualized if and only if it appears in the prefix. If $k < d$, that is the random IR walk returns a walk of length shorter than $d$, then we simply “fill up” the walk with nodes in an isomorphism-invariant manner using the discrete coloring $\text{Ref}(G, \pi, (w_1, \ldots, w_k))$: we add nodes in order of their color, i.e., first the node with the smallest color, then with the second smallest color, and so forth. We abbreviate IRNI with constant $d$ as $d$-IRNI.

IRNI depends on the random walk in the IR tree and is thus a randomized data augmentation. This justifies ensembling over this randomization, which we include as an integral part of IRNI. Specifically, we apply an MPNN with IRNI $e$ times for $e$ ensembles and average the prediction scores.

To study the specific advantage IRNI grants over RNI we define one-hot RNI (ORNI), which eases the comparison between IRNI and RNI. Consider the case where RNI adds a feature to each node, which is randomly drawn from a finite set $R \subset \mathbb{Q}$. This set $R$ represents a discretization of the randomness introduced by RNI. We can then define one-hot RNI (ORNI) as concatenating the one-hot encoding of the randomly chosen element from $R$ onto each node. RNI and ORNI are then exactly equivalent.

This one-hot encoding, however, can also be interpreted as the order in which nodes should be individualized under IRNI. In this sense, IRNI specifies an order for the random values in $R$ and guarantees each random value is used only once. IRNI is a partial counterpart to RNI, where the order of individualization is chosen according to the IR tree. As an ablation study of IRNI we will include ORNI in our experiments, where exactly $d$ nodes are individualized to mimic IRNI.

### 4.3 IR algorithms and IRNI

We now discuss the relationship of IR algorithms and MPNNs using IRNI. First, we remark that in terms of solving graph isomorphism, the use of repeated random IR walks has recently been
proven to be a near-optimal traversal strategy of IR trees. This is in contrast to deterministic traversal strategies such as depth-first search or breadth-first search which have a quadratic overhead \textcolor{green}{[Anders and Schweitzer, 2021b]}. The data augmentation scheme is thus closely related to optimal strategies of traversing the IR tree itself.

Interestingly, when taking a closer look, the ensembling defined in the previous section even seems to mimic the way the aforementioned near-optimal IR algorithm operates \textcolor{green}{[Anders and Schweitzer, 2021b]}. In fact, the currently fastest practical graph isomorphism algorithm \textcolor{green}{deja vu \cite{Anders and Schweitzer, 2021a}} uses essentially the same strategy. Moreover, the use of random IR walks has additional inherent benefits, such as “implicit automorphism pruning”, i.e., the automatic exploitation of symmetry in the input \textcolor{green}{[Anders and Schweitzer, 2021a]}. This translates to MPNNs with IRNI, in that if individualizations across multiple random walks are made on nodes that are symmetrical to each other, this does not truly introduce any additional randomness: due to their isomorphism-invariance (or equivariance) symmetrical nodes are naturally indistinguishable by MPNNs.

Previously, we discussed that a crucial property of MPNNs is that their result is isomorphism-invariant, i.e., it only depends on the isomorphism type. While this is not true in the deterministic sense for IRNI, because of Lemma 2, the result only depends on the isomorphism type and the randomness.

**Lemma 3.** Let $f$ be the function computed by $d$-IRNI, mapping a graph $G$ and a random seed $s \in \Omega$ from the sample space of random IR walks $\Omega$ to a value $f(G, s) \in \mathbb{R}$. Then for every permutation $\pi$, we have that the random variables $s \mapsto f(G, s)$ and $s \mapsto f(\pi(G), s)$ have the same distribution.

We now provide a universality theorem for IRNI, in a similar fashion as \textcolor{green}{Abboud et al. \cite{2021}} does for RNI. The theorem proven by \textcolor{green}{Abboud et al. \cite{2021}} is based on the fact that RNI fully individualizes a graph with high probability, and all fully individualized representations of a graph together constitute a complete isomorphism invariant. The crucial insight we exploit is that IR trees constitute a complete isomorphism invariant as well. To be more precise, even the set of all leaves of an IR tree suffice to provide such an invariant.

**Theorem 4.** Let $n \geq 1$ and let $f: G_n \rightarrow \mathbb{R}$ be invariant. Then, for all $\epsilon, \delta > 0$, there is an MPNN with $(n-1)$-IRNI that $(\delta, \epsilon)$-approximates $f$.

**Proof.** We prove the theorem using a combination of Theorem 2 from \textcolor{green}{Morris et al. \cite{2019}}, the universality result of RNIs given in \textcolor{green}{Abboud et al. \cite{2021}}, and the basic definition of IR trees, as follows. First of all, since graphs have $n$ nodes—by definition—all possible random IR walks considered by $(n-1)$-IRNI are random IR walks ending in a leaf node of the IR tree $\Gamma(G, \pi)$ (see Section 3). If we were to individualize the sequence of nodes $(w_1, \ldots, w_k)$ corresponding to a leaf and apply color refinement, the coloring of the entire graph would become discrete, i.e., fully individualized.

By the definition of $(n-1)$-IRNI, the nodes contained in $\{w_1, \ldots, w_k\}$ all have distinct features not shared by any of the other nodes in the graph. This means that the vertices in $\{w_1, \ldots, w_k\}$ are indeed initially individualized in the MPNN. Now, Theorem 2 of \textcolor{green}{Morris et al. \cite{2019}} (see also \textcolor{green}{Xu et al. \cite{2019}}) proves that there is an MPNN that produces the same partitioning of colors that color refinement would, i.e., in our case yields a discrete partitioning of vertices. In other words, we may assume that the graph is fully individualized. This suffices to apply the universality result of \textcolor{green}{Abboud et al. \cite{2021}} (see Lemma A2 and Lemma A4 in \textcolor{green}{Abboud et al. \cite{2021}}, which build upon \textcolor{green}{Barceló et al. \cite{2020}}), which solely depends on fully individualizing the given graph.

The IR paradigm opens up more opportunities to transfer results into the realm of MPNNs. In particular, IR itself includes many hyperparameters that can be used to show more specific results.
Below, we give one such example. We argue that with a specific cell selector, 3-connected planar graphs can be detected with random IR walks of length at most 4.

Let $\mathcal{P}_n$ denote the class of 3-connected planar graphs. We now show that 4-IRNI is universal for $\mathcal{P}_n$.

**Theorem 5.** Let $n \geq 1$ and let $f : \mathcal{P}_n \to \mathbb{R}$ be invariant. Then, for all $\epsilon, \delta > 0$, there is a cell selector (which does not depend on $n$) and an MPNN with 4-IRNI that $(\delta, \epsilon)$-approximates $f$.

**Proof.** First of all, we argue that individualizing a node of degree 5 and 3 of its neighbors surely suffices to make the graph discrete: this follows from Lemma 22 of Kiefer et al. [2017], which proves that individualizing 3 vertices on a common face followed by color refinement suffices to make the coloring discrete. Note that individualizing a node of degree 5 and 3 of its neighbors surely individualizes 3 vertices on a common face. Using the arguments from the proof of Theorem 4 again, we can see that this would indeed suffice to show the claim.

It remains to be shown that there is a cell selection strategy achieving the above. In the first step, the cell selector chooses an (isomorphism-invariant) color class consisting of degree 5 vertices. We remark that, due to Euler’s formula, the average degree of a planar graph is less than 6, so such a node always exists. In the next step, we choose a non-trivial class containing only neighbors of the individualized degree 5 node $v$. We argue that unless all neighbors of $v$ have been individualized, there is a non-trivial color class consisting of neighbors of $v$. Indeed, if there is a non-trivial class containing neighbors of $v$, the class may only contain such neighbors, since color refinement distinguishes neighbors of $v$ from non-neighbors of $v$. Here we use that $v$ is individualized. We repeat the step of choosing a non-singleton class of neighbors of $v$ and individualizing a node within it. If at any point no non-trivial class of neighbors exists, we are done: this means that the neighbors are fully discrete. This in turn suffices to show the claim.

More results of this kind can be shown. For example, it is known that strongly regular graphs require at most $O(\sqrt{n} \log n)$ individualizations [Babai, 1980]. In fact for all but an exponentially small fraction of graphs, $d$-IRNI with small $d$ suffices.

**Theorem 6.** There is an absolute constant $c > 1$ such that the following holds. Let $n \geq 1$ and $d \in \mathbb{N}$, then there is a graph class $\mathcal{G}'_n$ containing all but at most a $1/c^{dn}$ fraction of all graphs for which the following holds. Let $f : \mathcal{G}'_n \to \mathbb{R}$ be invariant, then, for all $\epsilon, \delta > 0$, there is an MPNN with $d$-IRNI that $(\delta, \epsilon)$-approximates $f$.

**Proof.** To prove the theorem we use the same technique as before. We only need to observe that for most graphs, after color refinement is applied, $d$ arbitrary individualizations in non-singleton cells cause discretization of the graph. This, however, is a classic theorem by Babai and Kucera [1979, Theorem 4.1] showing the fraction of graphs for which this fails is at most $1/c^{dn}$.

## 5 Experiments

In this section we first experimentally confirm that IRNI increases the discriminatory power of MPNNs. We do so by applying it on synthetically generated—specifically designed to be hard—data sets. It seems that most methods of increasing expressibility result in substantial increases in running time and/or memory consumption while not always guaranteeing universality. For this reason we only consider RNI for our comparisons, which is the closest related method. We compare IRNI to ORNI and RNI on practical data sets. In addition, we compare the trainability of IRNI to RNI.
5.1 Experimental Setup

Network architectures and optimization. For all experiments we use the same GIN architecture. It closely resembles the network design by Sato et al. [2021]. We use 5 layers as described in Equation 2, where the MLP has 3 layers (input, hidden, output) that widen to a fixed number of features $f$ as soon as possible. In this fashion the MLP’s hidden layer and output layer have $f$ features. If we do not state otherwise we use $f = 64$. The hidden layer of each MLP is followed by a batch-norm operation. The final layer of the GIN is followed by a dropout layer with a dropout rate of 0.5. For the activations we use ReLU. If the task is a graph classification task, we use graph mean pooling and a final fully connected layer with sigmoid activations, otherwise, the task is node classification, where we use a fully connected layer with sigmoid activations directly on the nodes. We train for 256 epochs with a learning rate of 0.001 that decays by 0.5 every 32 epochs and a batch size of 32. The optimizer used is ADAM. Unless we state otherwise we are using 1-IRNI with 1 ensemble. To compute the node sequence for IRNI we use DEJAVU [Anders and Schweitzer, 2021a].

In the following, we refer to a GIN without any node initialization just as a GIN, while we refer to a GIN with some initialization as X-GIN, where X is RNI, IRNI, or ORNI.

Data sets. We evaluate the different models on EXP, CEXP, TRI, TRIX, PROTEINS, and NCI1 [Sato et al., 2021, Abboud et al., 2021, Borgwardt et al., 2005, Wale and Karypis, 2006]. EXP, CEXP, TRI, and TRIX are synthetic data sets made up of graphs not distinguishable by the color refinement algorithm. TRI and TRIX contain 3-regular graphs and have the same training set while differing in their respective test set. EXP and CEXP consist of graphs encoding SAT-formulas. These graphs are carefully constructed so that each graph is in a pair that is indistinguishable by color refinement while encoding a satisfiable and unsatisfiable formula respectively. CEXP is a corrupted counterpart to EXP, where 50% of all satisfiable graphs are modified to be distinguishable by color refinement from their unsatisfiable counterparts.

5.2 Comparing IRNI to RNI

We investigate and compare the performance of IRNI, RNI, ORNI, and simple GIN without data augmentation. For the RNI-GIN we use the code or results from [Sato et al., 2021]. For EXP and CEXP we include the RNI-GCN defined in [Abboud et al., 2021]. For GIN on EXP, CEXP, TRI, and TRIX we report the theoretically optimal AUROC (AUROC is used in the related literature). For GIN on PROTEINS and NCI1 we use the result from [Sato et al., 2021]. For EXP and CEXP the performance is averaged over 100 trained models derived from 10-times 10-fold cross-validation. For TRI and TRIX, 10 models are trained. For PROTEINS we follow the experimental setup from [Sato et al., 2021]. On TRI and TRIX, we ensemble 64 IRNI (and ORNI) initializations. The results can be found in Table 1.

Results. On all data sets IRNI outperforms—or equals—all other approaches. Without the biased evaluation from [Sato et al., 2021] the performance on PROTEINS and NCI1 is 0.814 ± 0.038 on PROTEINS and 0.885 ± 0.017 on NCI1. This verifies that IRNI is just as applicable as RNI, while typically outperforming it.

5.3 Trainability of IRNI

Abboud et al. [2021] note that MPNNs using RNI converge slower and are sensitive to changes in learning rate, activation function, and/or randomization distribution. Our experiments corroborate these findings. In stark contrast to this, we empirically find that our IRNI-GIN converges as fast
Table 1: The AUROC of a GIN network with RNI, IRNI, ORNI, and without any of these, as well as an RNI-GCN on selected data sets. The symbol * indicates results were taken from related literature or obtained by executing the code of other authors. O indicates the theoretically optimal value. Bold entries indicate statistical significance.

| Method   | EXP     | CEXP    | TRI     | TRIX    | PROTEINS | NCI1    |
|----------|---------|---------|---------|---------|----------|---------|
| GIN      | 0.500 ± 0.000  | 0.750 ± 0.000  | 0.500 ± 0.000  | 0.500 ± 0.000  | 0.806 ± 0.029* | 0.870 ± 0.009* |
| RNI-GIN  | NA      | NA      | 0.908 ± NA* | 0.926 ± NA* | 0.810 ± 0.030* | 0.876 ± 0.010* |
| RNI-GCN  | 0.998 ± 0.003* | 0.998 ± 0.002* | 0.855 ± NA*  | 0.877 ± NA*  | 0.812 ± 0.029* | 0.816 ± 0.016* |
| ORNI-GIN | 0.852 ± 0.052  | 0.959 ± 0.018  | 0.995 ± 0.000  | 0.998 ± 0.000  | 0.816 ± 0.037  | 0.881 ± 0.010  |
| IRNI-GIN | 1.000 ± 0.002  | 0.999 ± 0.003  | 0.995 ± 0.000  | 0.998 ± 0.000  | 0.817 ± 0.033  | 0.886 ± 0.017  |

as typical MPNNs, is not sensitive to changes in learning rate or activation function, and is not dependent on a randomization distribution. Results demonstrating small sensitivity to variation of the activation can be found in the supplementary material.

We evaluate the convergence in Fig. 3a. One epoch in Fig. 3a takes approximately the same time for RNI and IRNI, so it can also be understood as a plot of wall-clock time (see supplement for a comparison of per prediction cost). We include 1.6%-partial RNI introduced in [Abboud et al., 2021], which reduces the random dimensions added to only 1. Each curve in Fig. 3a is the average of 100 trained models derived from 10-times 10-fold cross-validation. We can see that the IRNI-GIN converges significantly faster than the RNI-GIN and this convergence can even be sped up by increasing the number of individualized nodes. We were unable to apply any speed-up to the convergence of the RNI-GIN, using for instance a dropping learning rate, due to its sensitivity to changes in learning rate.

In Fig. 3b we evaluate the sensitivity of IRNI and RNI to changes in learning rate. For better comparability, IRNI does not drop its learning rate and RNI’s number of epochs are matched with IRNI to 256. Each curve is the average of 10 trained models derived from 10-fold cross-validation. The RNI used here is the 1.6%-partial RNI, which we find to outperform regular RNI. IRNI seems to be stable for a learning rate in (2^{-6}, 2^2)·0.001, while RNI is stable between (2^{-2}, 2^0)·0.001. For RNI this interval is very small, which explains the difficulty in tuning its learning rate. For IRNI, on the other hand, the size of this interval is wide and far more typical, and even outside of this IRNI’s drop in performance is slower than RNI.

6 Discussion and Conclusion

We successfully transferred the IR-technique to the world of MPNNs, demonstrating universality, practicality, and trainability. We also performed a wide-ranging comparison to RNI. Overall we conclude that IRNI enables MPNNs to be universal while being substantially more trainable than RNI and variants.

Future work. The construction of the IR tree used for IRNI comes with many hyperparameters that we did not investigate for this work. In fact, the compatibility of IRNI with MPNNs opens up various new research avenues. First, we used an IR algorithm as is, but one could optimize aspects. A cell selector specifically tailored for machine learning tasks might perform better. Using other refinements, color refinement with limited rounds, might align better with MPNNs. Second, experimenting with other network architectures also remains as future work.
Figure 3: A plot of the AUROC on EXP for (a) different models throughout training (b) different learning rates. (a) compares the RNI-GIN to the IRNI-GIN with varying amounts of individualized nodes. (b) compares the sensitivity of RNI and IRNI to the learning rate.

Limitations and broader impact. A limitation of this work is that we did not investigate IRNIs effects on graphs that are considered large. This, however, is mainly due to these large graphs not being included in typical benchmark data sets. The proposed method does not introduce any new avenues to impact society but potentially amplifies existing effects.

Acknowledgments and Disclosure of Funding

The research leading to these results has received funding from the European Research Council (ERC) under the European Union’s Horizon 2020 research and innovation programme (EngageS; grant agreement No. 820148).

The authors also acknowledge support by the Carl-Zeiss Foundation, the DFG awards KL 2698/2-1 and KL 2698/5-1, the BMWi award 01MK20014U, and the BMBF awards 01|S18051A, 03|B0770E, and 01|S21010C.

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Table 2: Performance of RNI, ORNI, and IRNI, for different activation functions on the EXP dataset.

| Method    | RELU       | ELU        | tanh       |
|-----------|------------|------------|------------|
| RNI-GIN   | 0.889 ± 0.170 | 0.998 ± 0.003 | 0.993 ± 0.007 |
| ORNI-GIN  | 0.849 ± 0.049 | 0.772 ± 0.038 | 0.786 ± 0.044 |
| IRNI-GIN  | 1.000 ± 0.000 | 1.000 ± 0.000 | 0.999 ± 0.003 |

Appendix

A Implementation Details

The implementation was done in PyTorch Geometric. We used DejaVu to compute the leaves in the IR tree. All experiments were run on one personal machine with the following specs:

- Processor: Intel Core i7-8700 with 3.20 GHz.
- RAM: 16 GB.
- GPU: NVIDIA GeForce GTX 960 with 4 GB memory.

Running multiple experiments in parallel, maximizing GPU utilization, all experiments took \( \approx 7 \) days.

B Sensitivity to Activations

Table 2 shows the sensitivity of RNI, ORNI, and IRNI to changes in activation function on the EXP dataset. Each of the models was trained as described in Section 5 of the paper. It is clearly observable that IRNI is quite stable while RNI and ORNI vary in their performance. RNI varies by at most 0.109, while ORNI varies by at most 0.077. This indicates that ORNI is less sensitive than RNI.

C Runtime of IRNI

Table 3 shows the average time per prediction on multiple datasets, comparing RNI, ORNI, and IRNI. These values are the average of 10 trials predicting all data points in each data set using a randomly initialized model. On TRI and TRIX ensembling over 64 initializations is considered, which increases their prediction times by at least an order of magnitude. Clearly RNI has the lowest prediction times overall, while ORNI comes in a close second, excluding TRI and TRIX. However, IRNI does not significantly increase prediction time. IRNI at most doubles and typically only increases prediction time by around 35% making it a viable practical method.

D Ensembling

As stated in the body of this work 64 IRNI walks were ensembled on the TRI and TRIX datasets. This is because performance increases with the amount of ensembles used. Figure 4 shows the
Table 3: Average time per prediction in milliseconds for RNI, ORNI, and IRNI, on different data sets.

| Method      | EXP | CEXP | TRI  | TRIX | PROTEINS | NCI1 |
|-------------|-----|------|------|------|----------|------|
| RNI-GIN     | 1.140 | 1.440 | 0.440 | 0.493 | 1.123    | 0.910 |
| ORNI-GIN    | 1.141 | 1.460 | 21.97 | 21.53 | 1.219    | 0.998 |
| IRNI-GIN    | 1.451 | 1.893 | 20.14 | 20.36 | 1.580    | 1.957 |

Figure 4: A plot of the performance of the IRNI-GIN on TRI and TRIX with varying amounts of ensembling. This plot includes standard deviation, which is very small and only barely visible.

average performance, over 10 trials, of one trained model for varying amounts of ensembling. This behavior is natural: to detect a triangle using an MPNN, at least one node of the triangle has to be differentiated from the other nodes. The task for TRI and TRIX is to detect triangles. Thus it follows that a node within at most \( k - 1 \) hops of each triangle has to be individualized for the triangle to be detectable, where \( k \) is the number of layers of the MPNN. Thus the performance of 1-IRNI on TRI and TRIX is dependent on the probability that a node within \( k - 1 \) hops of each triangle is individualized as well as the number of triangles in each graph. Ensembling then simply increases the chance that in at least one of the ensembles the triangle can be detected.