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Abstract

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1 Introduction

The field of ML on graph-structured data has recently become an active topic of research. One reason for this is the wide range of domains and problems that are expressible in terms of graphs.

1.1 Motivation

1.2 Research Questions

1.3 Structure

Chapter 2: Related Work Some text

Chapter 3: Problem Description

Chapter 4: Implementation Some text

Chapter 5: Conclusion Finally, the results of this thesis are summarized and a brief outline of promising directions for future research is given.

2 Related Work

Before describing the problem, and later on the experimental setup, we first

1. Revise three common prediction tasks in graph neural networks (GNNs)

2. Give a general overview of how GNNs organize and process graph structured data

3. We further discuss the relation of messasge passing mechanis to the Weisfeiler-Lehman (WL), an algorithm for inspecting wheather two graphs are isomorph.

4. Give an formal definition and description of two GNN architectures, which will be used in our experiments.

2.1 Prediction Tasks and Typical Problems

Graphs naturally appear in numerous application domains, ranging from social analysis, bioinformatics to computer vision. A Graph $G = (V, E)$, where $V = \{v_1, ..., v_n\}$ is a set of $N = |V|$ nodes and $E \subseteq V \times V$ a set of edges betwen those nodes. The unique capability of graphs enables capturing the structural relations among data, and thus allows to harvest more insights compared to analyzing data in isolation [Zha+19]. Graphs therefore can be seen as a general laguage for describing entities and relationships between those entities. Graph neural networks (GNNs) then organize graph structured data to tackle various prediction and classification tasks. Typically, one is interested in one of the following three tasks:

1. **Link prediction:** Predict whether there are missing links between two nodes e.g., knowledge graph completion

2. **Vertex classification & regression:** Predict a property of a node e.g., categorize online users/items

3. **Graph classification & regression:** Here we are interested in classifying or predicting a continous value for the entire graph e.g., predicting a property of a molecule.

In this work the main focus will be on the latter two, node classification (NC) node regression (NR) and graph classification (GC) graph regression (GR) for small- as well as large-sized graphs.

2.2 Passing Messages in GNNs

Graphs, by nature are unstructured. Vertices in graphs have no natural order and can contatin any type of information. In order for machine learning algorithms to be able to make use of graph structured data, a mechanism is needed to organize them in a suitable way. [Zho+20a] [HYL17] [Zha+19]

Message passing is a mechanism [Xu+19] [Zho+20a], which embedds into every node information about it's neighbourhood. This can be done in several ways and one way of classifying a GNN is by looking at the underlying message passing machanism. In this paper we will look at a network, where message passing is done via convolutions (graph convolutional network (GCN)). We will however ocasionally use the more general term message passing, as the separation is rather blurred and message passing is seen as a generalization of other, more specific mechanisms

Formally, message passing in a GNN can be described as using two functions: AGGREGATE and COMBINE. The expressive and representational power of a GNN can then be determined by looking at the concrete functions and thier properties, used to implement aggregation and combination. AGGREGATE mixes in every iteration the hidden representation of the node with the representation of nodes neighbourhood. COMBINE then combines the mixed representation togheter with the representation of the node. Each node uses the information from its neighbors to update its embeddings, thus a natural extension is to use the information to increase the receptive field by performing AGGREGATE and COMBINE multiple times.

$$a_v^k = \text{AGGREGATE}^{(k)}(\{h_u^{(k-1)} : u \in \mathcal{N}_{(v)}\}), h_v^{(k)} = \text{COMBINE}^{(k)}(h_v^{(k-1)}, a_v^{(k)})$$

One useful type of information, which the message passing framework should be able to capture, is the local graph structure. This can be done by choosing functions with appropriate properties. A more detailed explanation will follow in section 2.2.2. In spatial GNN we make the assumption of the similarity of neighbor nodes. To exploit this spatial similarity, we perform composition by stacking multiple layers togheter and increase the receptive field.

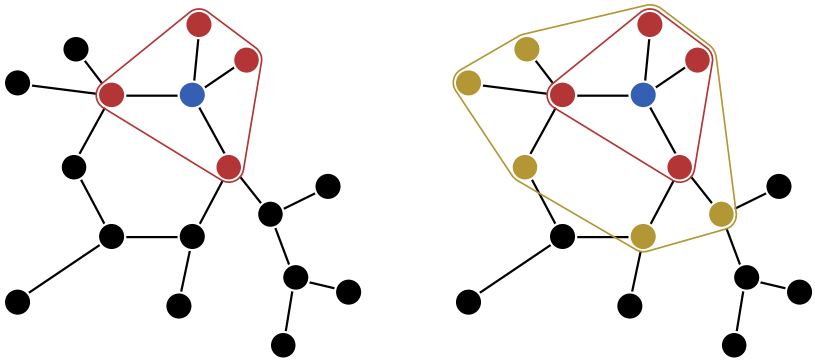

Fig. 2.1.: By performing aggregation k-times we can reach the k-hop neighborhood

2.2.1 Weisfeiler-Lehman Graph Colorings

The Message passing mechanism has a close relation, to the way the Weisfeiler-Lehman (WL) test [WL68] [DMH20] [HV22], an algorithm for deciding wheather two graphs are isomorphic works.

Before describing the WL algorithm, we define preliminaries and introduce some notations.

Definition 2.1. Let $G = (V, E)$ denote a graph where $V = \{v_1, ..., v_n\}$ is a set of $N = |V|$ nodes and $E \subseteq V \times V$ a set of edges between those nodes.

The 1-dimensional WL algorithm (color refinement)

In the 1-dimensional WL algorithm (1-WL), a color is assigned to each vertex of a graph. If the vertices $v \in \mathcal{V}_G$ of the input graph G are labeled, those labels $l_G[v] \in L_\mathcal{V} \subseteq \mathcal{C}$ can be used as the initial graph coloring $\chi^{(0)}_{G,1}(v) \coloneqq l_G[v]$. Since WL colors are inherently discrete, continuous vertex feature vectors $x_G[v]$ are not considered

here. For unlabeled graphs a constant coloring is used, e.g. $\forall v \in \mathcal{V}_G : \chi^{(0)}_{G,1}(v) = \mathbf{A}$ for some initial color $\mathbf{A} \in \mathcal{C}$. In each iteration of the 1-WL color refinement algorithm, the following neighborhood aggregation scheme is used to compute a new color for each vertex:

Definition 2.2. $\chi^{(i+1)}_{G,1}(v) \coloneqq h\left(\chi^{(i)}_{G,1}(v), \{\!\{\chi^{(i)}_{G,1}(u) \mid u \in \Gamma_G(v)\}\!\}\right)$, with $\Gamma_G(v)$ denoting the set of adjacent vertices of $v \in \mathcal{V}_G$ and $h : \mathcal{C}^* \to \mathcal{C}$ denoting an injective hash function that assigns a unique color to each finite combination of colors.

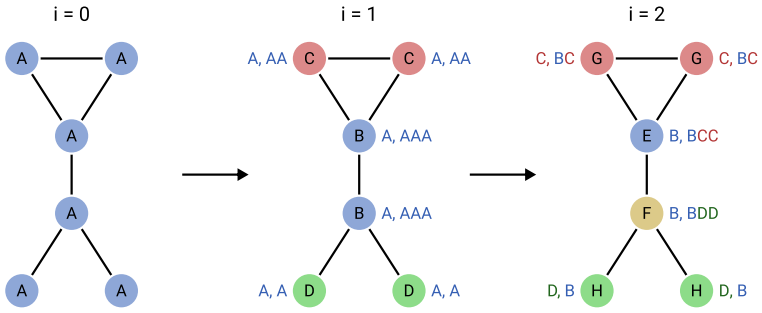

Fig. 2.2.: Example 1-WL color refinement steps. After two iterations the coloring stabilizes. Each vertex v is labeled with its current color and has its previous color and the colors of the hashed neighbors $\Gamma_G(v)$ written next to it (see definition 2.2).

The Weisfeiler-Lehman (WL) algorithm characterizes a graph G by assigning discrete labels $c \in \mathcal{C}$, called *colors*, to vertex k-tuples $(v_1, \ldots, v_k) \in \mathcal{V}^k_G$, where $k \in \mathbb{N}_0$ is the freely choosable *WL-dimension*. A mapping $\chi_{G,k} : \mathcal{V}^k_G \to \mathcal{C}$ is called a *k-coloring* of G.

Definition 2.3. A coloring χ' *refines* χ ($\chi' \preceq \chi$) iff. $\forall a, b \in \mathcal{V}^k_G : \chi(a) \neq \chi(b) \to \chi'(a) \neq \chi'(b)$, i.e. χ' distinguishes at least those tuples that are distinguished by χ.

Definition 2.4. Two colorings χ and χ' are *equivalent* ($\chi \equiv \chi'$) iff. $\chi \preceq \chi' \wedge \chi \succeq \chi'$, i.e. χ is identical to χ' up to color substitutions.

The k-dimensional WL algorithm (k-WL) works by iteratively refining k-colorings $\chi^{(0)}_{G,k} \succeq \chi^{(1)}_{G,k} \succeq \ldots$ of a given graph G until the convergence criterion $\chi^{(i)}_{G,k} \equiv \chi^{(i+1)}_{G,k}$ is satisfied. We denote the final, maximally refined k-WL coloring with $\chi^*_{G,k}$.

Definition 2.5. The color distribution $dist_{\chi_{G,k}} : \mathcal{C} \to \mathbb{N}_0$ of a k-coloring $\chi_{G,k}$ counts each color $c \in \mathcal{C}$ in the coloring, i.e. $dist_{\chi_{G,k}}(c) \coloneqq \left|\left\{v \in \mathcal{V}^k_G \mid \chi_{G,k}(v) = c\right\}\right|$.

Definition 2.6. Two graphs G and H are k-WL *distinguishable* ($G \not\simeq_k H$) iff. there exists a color $c \in \mathcal{C}$ s.t. $dist_{\chi^*_{G,k}}(c) \neq dist_{\chi^*_{H,k}}(c)$.

As we will see, the way in which WL colorings are refined is vertex order invariant; thus any difference in the final coloring of two graphs always implies the non-isomorphism of the colored graphs, i.e. $G \not\simeq_k H \implies G \not\simeq H$. The opposite does however not necessarily hold; two k-WL indistinguishable graphs are not always isomorphic, i.e. $\exists\, G, H : G \simeq_k H \wedge G \not\simeq H$.

In addition to the binary aspect of WL distinguishability and its relation to the graph isomorphism (GI) problem, WL colorings are also useful for more fuzzy graph similarity comparisons as we will see in section 2.2.4 when we look at graph kernels. Before that however, the details of the WL color refinement strategy have to be described. We begin with the color refinement algorithm for the most simple case of $k = 1$. Then the definitions and intuitions from the 1-dimensional case are extended to its higher-dimensional generalization. Lastly we will discuss the discriminative power of the WL algorithm and its relation to the WL-dimension k.

2.2.2 GNN Architectures in this Paper

Experiments will be conducted on two types of GNNs: GCN and graph isomorphism network (GIN)

Graph Convolutional Network (GCN)

Graph Convolutional Network GCN as proposed by the authors [KW17] has the following layer-wise propaation rule

$$H^{(l+1)} = \sigma(\tilde{D}^{-\frac{1}{2}}\tilde{A}\tilde{D}^{-\frac{1}{2}}H^{(l)}W^{(l)})$$

and is very broadly used for a variety of different tasks, such as for instance node Classification tasks. Despite not being as powerful as the GIN architecture, this

architecture is sufficient for a lot of tasks, especially when there is no need for distinguishing different structures/ substructures of a graph and the prediction can be done with.

The authors claim, the model scales linearly in the number of graph edges and learns hidden layer representations that encode both local graph structure and features of nodes.

Graph Isomorphism Network (GIN)

To overcome the lack of expressivity of popular GNN architectures, Xu et al. designed a new type of GNN, the graph isomorphism network GIN. They proved that GINs are strictly more expressive than a variety of previous GNNs and that they are in fact as powerful as the commonly used Weisfeiler-Lehman graph isomorphism test.

The key idea is to use injective functions, so that the function would never map two different neighbourhoods to the same representations. [Xu+19]

The following layer- wise propagation rule shows a forward pass in a GIN

$$h_v^{(k)} = \mathrm{MLP}^{(k)}((1+\epsilon^{(k)}) * h_v^{(k-1)} + \sum_{u \in \mathcal{N}(v)} h_u^{(k-1)}$$

$$x = \mathcal{A} : \mathcal{G} \to \mathbb{R}^d$$

Assuming, that the following conditions hold, with a sufficient number of GNN - layer A is as powerful as the WL Test

2.2.3 Weaknesses and Obstacles in GNN Architectures

Because of the way GNNs operate, they tend to suffer from two main obstacles: overfitting and oversmoothing.

Overfitting hinders the generalization ability of a neural network (NN), making it perform poorly on previously unseen data. This problematic occurs expecially when using small datasets, since the model thends to 'memorize' instead of learn the pattern.

Oversmoothing is a condition, where the performance and predictive power of a NN does not imporve of even gets worse when more layers are added. This happens because by stacking multiple layers togheter togheter aggregation is being performed over and over again. This way, the representation of a node is being smoothed - mixed with features of very distant, possibly unrelated nodes. Oversmoothing is a problem mainly for node classification tasks. There is a trade-off between the expressivness of the model (capturing) graph structure by applying multiple layers and oversmoothing, which leads to a model where nodes have the same representation, because they all converge to indistinguishable vectors.[Zho+20b][Has+20] (In spatial GNNs we make the assumption of relatedness by proximity)

A closer examination of underlying causes of oversmoothing was conducted by [Che+20], who suggested, that not message passing itself, but the type of interacting nodes cause this issue. For node classification (NC) tasks, intra-class communication (interaction between two nodes sharing the same class) is useful (signal), whereas inter-class communication (the communication between two nodes sharing different lables) is considered harmful, because it brings interference noise into the feature-representations by mixing unrelated features and therefore making unrelated nodes more similar to each other. Because of that, the the quality of shared information is essencial and should therefore be considered as a benchmark for improvement.

2.2.4 Regularization Techniques

[KGC17] define Regularization as any supplementary technique that aims at making the model generalize better, i.e. produce better results on the test set, which can include various properties of the loss function, the loss optimization algorithm, or other techniques.

One subgroup of regularization is via data, where the training set $\mathcal{D}$ is transformed into a new set $\mathcal{D}_R$ using some stochastic parameter θ, which can be used in various ways, including to manipulate the feature space, create a new, augmented dataset or to change (e.g, thin out the hidden layers of the NN)

In the scope of this work we will look at various regularization techniques and thier efficacy in terms of dealing with the issues of overfitting and oversmoothing The four regularization approaches, as described by [Has+20] are:

DropOut (DO)
DO randomly removes elements of its previous hidden layer $H^{(l)}$ based on independent Bernoulli random draws with a constant success rate at each training iteraration: [Has+20]

$$H^{(l+1)} = \sigma(\mathfrak{R}(A)(Z^{(l)} \odot H^{(l)})W^{(l)})$$

Originally this method was proposed by [Sri+14], who proposed to randomly drop units (along with their connections) from the neural network during training and thus prevent units from co-adapting too much. During training dropout samples from an exponential number of different "thinned" networks.At test time, it is easy to approximate the effect of averaging the predictions of all these thinned networks by simply using a single unthinned network that has smaller weights. This signifcantly reduces overftting and gives major improvements over other regularization methods.

Exspecially when working with small datasets we have much noize, which then leads the model to overfit. DropEdge (DE)

$$H^{(l+1)} = \sigma(\mathfrak{R}(A \odot Z^{(l)})H^{(l)}W^{(l)})$$

NodeSampling (NS)

$$H^{(l+1)} = \sigma(\mathfrak{R}(A)diag(z^{(l)})H^{(l)}W^{(l)})$$

GraphDropConnect (GDC)

$$H^{(l+1)}[:, j] = \sigma(\sum_{i=1}^{f_t} \mathfrak{R}(A \odot Z_{i,j}^{(l)})H^{(l)}[:, i]W^{(l)}[i, j])$$

2.3 Conclusion

GNNs are widely used. They make use of a mechanism called message passing, which is done specifically by using two functions AGGREGATE and COMBINE. The concrete choice of these functions determines the type of GNN and it's expressive power. If we want the network to have the same expressive and representational as the WL, the functions need to be injective in order to map different neighbourhoods to different representations.

Also, since graphs have no natural order, the functions need to be permutation invariant.

There are three typeical prediction tasks in GNNs, two of which we will concider in this work. (We focus on node classification regression as well as graph classification regression)

3 Problem Description

[Has+20]

4 Implementation

This section provides a brief overview of experimental setup as well as used libraries and frameworks and gives an explanation for the choices. Despite GNNs being such a big deal and widely used in various domains, there is a lack of standartisation in machine learning on graphs. Tensorflow has no build-in structure for graph representation and expects the input to be tensors or dictionaries. A few attempts were made towards dealing with graph-structured data in a standardized way Spektral is Despite graph neural networks (GNNs) being a hot topic, there still is no standardized way of dealing with graphs in terms of representation, ...

A few efforts have been made to create standardized frameworks and libraries. Such examples are Spektral, and NetworX

4.1 Scope and Limitations

4.2 Experimental Setup

4.3 Evaluation

5 Conclusion

5.1 Future Work

Another proposed regularization technique https://arxiv.org/pdf/2106.07971.pdf

Appendix A

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Colophon

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Munich, February 4, 2022

Olga Yakobson