Improving Attention Mechanism in Graph Neural Networks via Cardinality Preservation

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Abstract

Graph Neural Networks (GNNs) are powerful to learn the representation of graph-structured data. Most of the GNNs use the message-passing scheme, where the embedding of a node is iteratively updated by aggregating the information of its neighbors. To achieve a better expressive capability of node influences, attention mechanism has grown to be popular to assign trainable weights to the nodes in aggregation. Though the attention-based GNNs have achieved state-of-the-art results on several tasks, a clear understanding of their discriminative capacities is missing. In this work, we present a theoretical analysis of the representational properties of the GNN that adopts attention mechanism as an aggregator. Our analysis shows all of the cases when the GNNs always fail to distinguish distinct structures. The finding suggests existing attention-based aggregators fail to preserve the cardinality of the multiset of node feature vectors in the aggregation, thus limits their discriminative power. To improve the performance of attention-based GNNs, we propose cardinality preserved modifications that can be applied to any kind of attention mechanisms. We evaluate their performances in our GNN framework on benchmark datasets for graph classification. The results confirm the theoretical analysis and show the competitive performance of our models.

Introduction

Graphs, as a kind of powerful data structure in non-Euclidean domain, can represent a set of instances (nodes) and the relationships (edges) between them, thus has a broad application in various fields (Zhou et al. 2018a). Different from regular Euclidean data such as texts, images and videos, which have clear grid structures that are relatively easy to generalize fundamental mathematical operations (Shuman et al. 2013), graph structured data are irregular thus it is not straightforward to apply important operations in deep learning (e.g. convolutions). Consequently the analysis of graph-structured data remains a challenging and ubiquitous question.

In recent years, Graph Neural Networks (GNNs) have been proposed to learn the representations of graphs and attract a growing interest (Scarselli et al. 2009; Li et al. 2016; Duvenaud et al. 2015; Niepert, Ahmed, and Kutzkov 2016; Kipf and Welling 2017; Hamilton, Ying, and Leskovec 2017; Zhang et al. 2018; Ying et al. 2018; Morris et al. 2019; Xu et al. 2019). GNNs can iteratively update node embeddings by aggregating/passing node features and structural information in the graph. The generated node embeddings can be fed into extra classification/prediction layer and the whole model is trained end-to-end for the node-level (e.g. node classification, link prediction) or the graph-level (e.g. graph classification) tasks.

Though many GNNs have been proposed with different aggregation schemes, update rules, and pooling methods, it is noted that when updating the embedding of a node \( v_i \) by aggregating the embeddings of its neighbor nodes \( v_j \), most of the GNN variants will assign non-parametric weight between \( v_i \) and \( v_j \). For example, in (Kipf and Welling 2017), the weight is assigned as \( 1/\sqrt{N(v_i)N(v_j)} \), where \( N(v) \) is the number of nearest neighbors of node \( v \). Mean aggregator (Hamilton, Ying, and Leskovec 2017) treats the weight between \( v_i \) and \( v_j \) as \( 1/N(v_i) \), and sum aggregator (Xu et al. 2019) considers all weights as 1. However, such aggregators fail to learn and distinguish the information between a target node and its neighbors during the training. Taking account of different contributions from the nodes in a graph is important in real-world data as not all edges have similar impacts. A natural alternative solution is to make the edge weights trainable to have a better expressive capability.

To assign learnable weights in the aggregation, attention mechanism is incorporated in GNNs. Thus the weights can be directly represented by attention coefficients between nodes (Veličković et al. 2018; Thekumparampil et al. 2018; Xu et al. 2018b; Zhou et al. 2018a). Though GNNs that use the attention-based aggregators achieve promising performance on various tasks, it is not trivial to build a GNN model without knowing the exact power of attention mechanism in graph representation learning (Knyazev, Taylor, and Amer 2019). Recent work (Xu et al. 2019) has theoretically analyzed the expressive power of GNNs that uses non-parametric weights in their aggregators. But for GNNs with attention-based aggregators, a clear understanding of their discriminative power is still missing, thus limits the design of powerful attention-based GNNs.
In this work, we make efforts on theoretically analyzing the discriminative power of GNNs with attention-based aggregators. Our findings reveal that previous proposed attention-based aggregators fail to capture cardinality information and thus exhibit limited representational power. These inspire us to improve the attention mechanism via cardinality preservation. We propose modifications that can be applied to any kind of attention mechanisms to achieve the goal. We further develop Cardinality Preserved Attention Network (CPAN) that adopts our models to solve the graph classification problem. Our experimental results confirm our theoretical analysis. By using the cardinality preservation approach, we can increase the representational power of attention-based aggregator. Moreover, CPAN achieves promising results comparing to other state-of-the-art models. Specifically, our key contributions are summarized as follows:

- We show that previous proposed attention-based aggregators in message-passing GNNs always fail to distinguish certain distinct structures. We strictly give all of those structures and demonstrate that the cardinality information is missing in attention-based aggregation.
- We propose methods to improve the original attention mechanism via cardinality preservation in the aggregator. With those methods, we develop a GNN framework, Cardinality Preserved Attention Network (CPAN), which is universal to adopt any kind of attention mechanisms.
- Experimental results on benchmark graph classification datasets confirm that our approaches can significantly improve the representational power of the original attention mechanism. Moreover, CPAN exhibits comparable or even superior performance to other baselines.

**Preliminaries**

**Notations**

Let $G = (V, E)$ be a graph where $V$ is the set of $n$ nodes and $E$ is the set of $m$ edges between nodes. Let $X$ to denote the input feature of node $i \in V$ or edge $(i,j) \in E$. The structure of $G$ can be represented by the adjacency matrix, $A \in \mathbb{R}^{n \times n}$, where $A_{ij} = 1$ if $(i,j) \in E$ and $A_{ij} = 0$ if $(i,j) \notin E$. The degree of a node $i$ is defined as $\text{degree}(i) = \sum A_{ii}$. The nearest neighbors of node $i$ are defined as $\mathcal{N}(i) = \{j | d(i, j) = 1\}$, where $d(i, j)$ is the shortest distance between node $i$ and $j$. Moreover, we denote the set of node $i$ and its nearest neighbors as $\tilde{\mathcal{N}}(i) = \mathcal{N}(i) \cup \{i\}$.

For the nodes in $\tilde{\mathcal{N}}(i)$, their feature vectors form a multiset $M(i)$. A multiset is defined as a pair $M = (S, \mu)$, where $S = \{s_1, \ldots, s_N\}$ is the ground set of $M$, and $\mu : S \rightarrow \mathbb{N}^*$ is the multiplicity function that gives the multiplicity of each $s_i \in S$. The cardinality of a multiset is the number of elements (with multiplicity) in the multiset. We denote it as $|M| = \sum_{s \in S} \mu(s)$. Thus for $M(i)$, $|M(i)| = |\tilde{\mathcal{N}}(i)|$, which is also the number of nodes in $\tilde{\mathcal{N}}(i)$.

**Graph Neural Networks**

In general, GNNs adopt element (node or edge) features $X$ and the graph structure $A$ as input to learn the representation of each element, $h_i$, or graph, $h_G$, for different tasks. In this work, the term “GNNs” especially means those GNNs under neighborhood aggregation framework, which update the node embeddings by aggregating neighbor node embeddings iteratively. In previous surveys, this type of GNNs is referred as Graph Convolutional Networks in (Wu et al. 2019) or the GNNs with convolutional aggregator in (Zhou et al. 2018b). Under the framework, a learned representation of the node after $l$ aggregation layers can contain the features and structural information within $l$-step neighborhoods of the node. The $l$-th layer of a GNN can be formally represented as:

$$h_i^l = f^l(h_i^{l-1}, \{h_j^{l-1}, \forall j \in \mathcal{N}(i)\}) \quad (1)$$

where the superscript $l$ denotes the $l$-th layer and $h_i^0$ is initialized as $X_i$. Equation (1) propagates information between nodes and updates the hidden state of nodes. Different aggregation function $f$ will result in different GNNs. Common used functions include sum (Xu et al. 2019), mean (Kipf and Welling 2017), and max-pooling (Hamilton, Ying, and Leskovec 2017).

In the final layer, the node representation $h_i^L$ can be directly used after a total of $L$ iterations for node-level tasks. While for graph-level tasks, the whole graph representation $h_G$ is needed. Thus an extra readout function $g$ is used to compute $h_G$ from all $h_i^L$:

$$h_G = g(\{h_i^L, \forall i \in G\}) \quad (2)$$

**Attention-Based Aggregator**

When an aggregator in a GNN adopts attention mechanism to assign learnable weights between nodes, we name it “attention-based aggregator”. We also denote the GNN as “attention-based GNN”. In a previous survey (Section 6 of (Lee et al. 2018)), this is referred to as the first two types of attentions which have been applied to graph data.

In general, the attention-based aggregator is a special version of Equation (1) and the aggregation in $l$-th layer can be formulated as follows:

$$e_{ij}^{l-1} = \text{Att}(h_i^{l-1}, h_j^{l-1}) \quad (3)$$

$$\alpha_{ij}^{l-1} = \text{softmax}(e_{ij}^{l-1}) = \frac{\exp(e_{ij}^{l-1})}{\sum_{k \in \mathcal{N}(i)} \exp(e_{ik}^{l-1})} \quad (4)$$

$$h_i^l = f^l\left(\sum_{j \in \mathcal{N}(i)} \alpha_{ij}^{l-1} h_j^{l-1}\right) \quad (5)$$

where the superscript $l$ denotes the $l$-th layer and $e_{ij}$ is the attention coefficient computed by an attention function $\text{Att}$ to measure the relation between node $i, j$. And $\alpha_{ij}$ is the attention weight calculated by the softmax function. Equation (5) is a weighted summation that uses all $\alpha$ as weights followed with a nonlinear function $f$. Note that the weighted summation is done on $\tilde{\mathcal{N}}(i)$, which includes $\mathcal{N}(i)$ and $i$.

**Limitation of Attention-Based Aggregator**

In this section, we theoretically analyze the discriminative properties of attention-based aggregator and show its limitation. We start with the upper bound for the discriminative capacity of any attention-based GNN when solving the graph
isomorphism problem. We find that the conditions cannot be always satisfied for attention-based GNN to reach the upper bound. Furthermore, we theoretically find all cases when such conditions are always failed to be satisfied for all attention-based aggregators. For the proof sketches in this section, we contain the full proofs in the Supplemental Material.

Upper Bound for Representational Capacity
With the assumption of a countable node input feature space, the Theorem 3 of (Xu et al. 2019) has proved that for any aggregation-based GNN, the upper bound for its discriminative capacity is the Weisfeiler-Lehman (WL) test (Weisfeiler and Lehman 1968) when deciding the graph isomorphism. Our analysis also assumes the node input feature space is countable. For any attention-based GNN, the WL test is still the upper bound for its representational power and the conditions to reach the upper bound is given in Lemma 1.

Lemma 1. Let \( A : G \rightarrow \mathbb{R}^n \) be a GNN following the neighborhood aggregation scheme with the attention-based aggregator. For any graphs \( G_1 \) and \( G_2 \) that the Weisfeiler-Lehman test of isomorphism decides as non-isomorphic, \( A \) maps them to different embeddings after sufficient iterations with the following conditions:

- \( A \) computes node features \( h_i \) with Equation 5. Function \( f \) and the weighted summation in Equation 5 are injective.
- \( A \)'s readout function (Equation 2) is injective.

Proof. (sketch) The proof bases on that of Theorem 3 in (Xu et al. 2019) by modifying the aggregator to our attention-based version.

With Lemma 1, we are interested in whether its conditions can always be satisfied, thus to guarantee the highest discriminative capacity of an attention-based GNN. For all functions in attention-based GNN, since the function \( f \) and the graph-level readout function can be predetermined to be injective, we only focus on whether the weighted summation function is injective. In the next section, we will show the answer is no from our theoretical analysis.

The Non-Injectivity of Attention-Based Aggregator
Given a countable feature space \( \mathcal{H} \), a weighted summation function is a mapping \( W : \mathcal{H} \rightarrow \mathbb{R}^n \). However, the exact \( W \) is determined by the attention weights \( \alpha \), which are computed from \( Att \) in Equation 6. Function \( Att \) are learned during the training using a stochastic optimization algorithm like stochastic gradient descent (SGD), which will introduce stochasticity. Thus we have to decide the injectivity of the weighted summation function when having any possible choices of \( Att \). In Theorem 1, we theoretically find and show all of the cases where the weighted summation functions in attention mechanism will always map distinct multisets to the same embedding no matter how function \( Att \) is learned. This shows attention-based aggregators are not injective. So that the attention-based GNNs can never met the upper bound to be as powerful as the WL test, which is stated in Corollary 1.

Theorem 1. Assume the input feature space \( \mathcal{X} \) is countable. Given a multiset \( X \subset \mathcal{X} \) and the feature node \( c \) of the central node, the weighted summation function \( h(c, X) \) in aggregation is defined as

\[
h(c, X) = \sum_{x \in X} \alpha_{cx} f(x),
\]

where \( f : \mathcal{X} \rightarrow \mathbb{R}^n \) is a mapping of input feature vector and \( \alpha_{cx} \) is the attention weight between \( f(c) \) and \( f(x) \) calculated by the attention function \( Att \) in Equation 3 and the softmax function in Equation 4. For all \( f \) and \( Att \), \( h(c_1, X_1) = h(c_2, X_2) \) if and only if \( c_1 = c_2, X_1 = (S, \mu) \) and \( X_2 = (S, k \cdot \mu) \) for \( k \in \mathbb{N}^+ \).

Proof. (sketch) We prove Theorem 1 in both two directions:

1. If given \( c_1 = c_2 = c, X_1 = (S, \mu) \) and \( X_2 = (S, k \cdot \mu) \) for all \( f \) and \( Att \), we know that \( X_2 \) has \( k \) copies of the elements in \( X_1 \). For each element \( x \in X_1 \) or \( X_2 \), we can define a pair \((c, x)\) correspondingly. So the number of pair \((c, x)\) that according to \( X_2 \) is also \( k \) times larger than that to \( X_1 \). Then by considering the definition of the attention weight \( \alpha \) in Equation 5, we have that each \( \alpha_{cx} \) belongs to \( X_1 \) is \( k \) times as large as the corresponding one belongs to \( X_2 \). Finally, as the number of pair \((c, x)\) equals to the number of terms that contain \( \alpha_{cx} \) in the weighted summation, by computing the weighted summation we can always get \( h(c_1, X_1) = h(c_2, X_2) \).

2. If given \( h(c_1, X_1) = h(c_2, X_2) \) for all \( f \) and \( Att \), we have

\[
\sum_{x \in X_1} \alpha_{cx_1} f(x) = \sum_{x \in X_2} \alpha_{cx_2} f(x), \quad \forall f, Att,
\]

where \( \alpha_{cx_1} \) is the attention weight belongs to \( X_1 \), and between \( f(c_1) \) and \( f(x) \), \( x \in X_1, i \in \{1, 2\} \).

We denote \( X_1 = (S_1, \mu_1) \) and \( X_2 = (S_2, \mu_2) \), so that:

\[
\sum_{s \in S_1} \mu_1(s) \alpha_{cs_1} f(s) = \sum_{s \in S_2} \mu_2(s) \alpha_{cs_2} f(s), \quad \forall f, Att,
\]

where \( \mu_i(s) \) is the multiplicity function of \( X_i, i \in \{1, 2\} \). Moreover, \( \alpha_{cs_1} \) is the attention weight belongs to \( X_1 \), and between \( f(c_i) \) and \( f(s) \), \( s \in S_i, i \in \{1, 2\} \).

When considering the relations between \( S_1 \) and \( S_2 \), we have:

\[
\sum_{s \in S_1 \setminus S_2} (\mu_1(s) \alpha_{cs_1} - \mu_2(s) \alpha_{cs_2}) f(s) + \sum_{s \in S_1 \setminus S_2} \mu_1(s) \alpha_{cs_1} f(s) - \sum_{s \in S_2 \setminus S_1} \mu_2(s) \alpha_{cs_2} f(s) = 0. \quad (6)
\]

If we assume the equality of Equation 6 is true for all \( f \) and \( S_1 \neq S_2 \), we can define such two functions \( f_1 \) and \( f_2 \):

\[
f_1(s) = f_2(s), \forall s \in S_1 \setminus S_2; \quad f_1(s) = f_2(s) - 1, \forall s \in S_1 \setminus S_2, \quad f_2(s) = f_2(s) + 1, \forall s \in S_2 \setminus S_1.
\]

As \( \mu_i(s) \geq 1 \) due to the definition of multiplicity, \( \alpha_{cs_1} > 0 \) due to the softmax function, we have \( \mu_1(s) \alpha_{cs_1} > 0, \forall s \in S_i, i \in \{1, 2\} \). Thus if given the previous equality is true for \( f_1 \), it is obvious that the equality is not true for \( f_2 \) (the LHS of Equation 6 > 0). So the assumption of \( S_1 \neq S_2 \) is false. We denote \( S = S_1 = S_2 \). To let the remaining summation term always equal to 0, we have

\[
\mu_1(s) \alpha_{cs_1} - \mu_2(s) \alpha_{cs_2} = 0, \quad \forall Att.
\]
Considering Equation \[4\] we rewrite the equation above:
\[
\frac{\mu_1(s)}{\mu_2(s)} = \frac{\exp(e_{cx_2}) \sum_{x \in X_1} \exp(e_{cx_1})}{\exp(e_{cx_1}) \sum_{x \in X_2} \exp(e_{cx_2})}, \quad \forall \text{Att}, \tag{7}
\]
where \(e_{cx_1}\) is the attention coefficient belongs to \(X_1\), and between \(f(c_i)\) and \(f(s)\), \(s \in S\). And \(e_{cx_2}\) is the attention coefficient belongs to \(X_2\), and between \(f(c_i)\) and \(f(x)\), \(x \in X, i \in \{1, 2\}\).

The LHS of Equation \[7\] is a rational number. However, if \(c_1 \neq c_2\), the RHS of Equation \[7\] can be irrational: We assume \(S\) contains at least two elements \(s_0\) and \(s \neq s_0\). If not, we can directly get \(c_1 = c_2\). We consider any attention mechanism that results in: \(e_{cx_1} = 1, \forall s \in S\); \(e_{cx_2} = 1\) for \(s = s_0, e_{cx_2} = 2, \forall s \neq s_0 \in S\). Thus when \(s = s_0\), the RHS of the equation becomes:
\[
e \frac{|X_1|}{e (|X_2| - n)e^2 + ne} = \frac{|X_1|}{(|X_2| - n)e + n},
\]
where \(n\) is the multiplicity of \(s_0\) in \(X_2\). It is obvious that the value of RHS is irrational. So we have \(c_1 = c_2\) to always hold the equality.

With \(c_1 = c_2\), we know \(e_{cx_1} = e_{cx_2}, \forall s \in S\) and \(e_{cx_1} = e_{cx_2}, \forall x \in X_1, X_2\). We denote \(e_{cx} = e_{cx_1} = e_{cx_2}\). Equation \[7\] becomes
\[
\frac{\mu_1(s)}{\mu_2(s)} = \frac{\sum_{x \in X_1} \exp(e_{cx})}{\exp(e_{cx}) \sum_{x \in X_2} \exp(e_{cx})} = \text{const.}, \quad \forall \text{Att}.
\]

We further denote \(k = \frac{\mu_1(s)}{\mu_2(s)}\), \(\forall s \in S\). So that \(\mu_2 = k \cdot \mu_1\). Finally by denoting \(\mu = \mu_1\), we have \(X_1 = (S, \mu), X_2 = (S, k \cdot \mu)\) and \(c_1 = c_2\).

**Corollary 1.** Let \(A : G \rightarrow \mathbb{R}^n\) be a GNN following the neighborhood aggregation scheme with the attention-based aggregator. There exits \(G_1\) and \(G_2\) that the Weisfeiler-Lehman test decides as non-isomorphic while \(A\) always maps to the same embeddings after sufficient iterations.

**Proof.** (sketch) Let \(G_1\) be a fully connect graph with \(n\) nodes and \(G_2\) be a ring-like graph with \(n\) nodes. All nodes in \(G_1\) and \(G_2\) have the same feature. It’s obvious that the Weisfeiler-Lehman test of isomorphism decides \(G_1\) and \(G_2\) as non-isomorphic. Considering Theorem \[1\] and Equation \[5\], we know that an attention-based GNN will always map \(G_1\) and \(G_2\) to the same set of multisets of node features in each iteration \(l\) and finally get the same embedding for each graph.

When the node features seldom repeat in a graph, the cases shown in Theorem \[1\] will rarely happen. That’s why the attention-based GNN, for example GAT (Veličković et al. 2018; Qu et al. 2018), works well for node classification tasks on citation networks and social influence predictions on social networks, where the node features are diverse.

**Attention Mechanism Fails to Preserve Cardinality**

For all of the cases listed in Theorem \[1\] we find that those distinct multisets have the same distribution. The attention-based aggregator will assign similar weights to identical elements in the multiset. While for distinct elements in the multiset, attention-based aggregator can assign different weights to them, which means a learnable distribution of the elements in the multiset is assigned via the attention mechanism. To summarize, the multiplicity of each element is missing and the cardinality of the multiset is not preserved.

In the next section, we propose improved attention-based models to preserve the cardinality in aggregation.

**Improving Attention Mechanism via Cardinality Preservation**

As the cardinality of the multiset is not preserved for an attention-based aggregator to distinguish different multisets, our goal is to propose modifications to any attention mechanisms so that they can capture the cardinality information. With preserved cardinality, the distinct multisets with the same distribution can be distinguished. Thus all of the cases listed in Theorem \[1\] can be avoided.

**Cardinality Preserved Attention Model**

To achieve our goal, we modify the weighted summation function in Equation \[5\] to incorporate the cardinality information and don’t change the attention function in Equation \[3\] so as to keep its original expressive power. Two different models named as *Additive* and *Scaled* are proposed:

**Model 1.** *(Additive)* Equation \[5\] is modified as
\[
h'_i = f\left( \sum_{j \in \tilde{N}(i)} \alpha_{ij} l^{-1} h_j l^{-1} + w \odot \sum_{j \in \tilde{N}(i)} h_j l^{-1} \right), \tag{8}
\]
where \(w\) is a trainable or fixed vector \(\in \mathbb{R}^n\), \(\odot\) denotes the element-wise multiplication.

**Model 2.** *(Scaled)* Equation \[5\] is modified as
\[
h'_i = f\left( \psi\left(\left|\tilde{N}(i)\right|\right) \odot \sum_{j \in \tilde{N}(i)} \alpha_{ij} l^{-1} h_j l^{-1} \right), \tag{9}
\]
where \(\left|\tilde{N}(i)\right|\) equals to the cardinality of the multiset \(\tilde{N}(i)\), \(\psi : \mathbb{Z}^+ \rightarrow \mathbb{R}^n\) is an injective function for the cardinality value, \(\odot\) denotes the element-wise multiplication.

In the *Additive* model, each element in the multiset will contribute to the term that we added to preserve the cardinality information. In the *Scaled* model, the original weighted summation is directly multiplied by a representation vector of the cardinality value. So with these models, distinct multisets with the same distribution will result in different embedding \(h\). Note that both of our models don’t change the *Att* function, thus can keep the learning power of the original attention mechanism.

With these modifications, attention-based aggregators can now distinguish the multisets mentioned in Theorem \[1\].

**Corollary 2.** Assume \(X\) is countable. Given two finite multisets \(X_1 = (S, \mu)\) and \(X_2 = (S, k \cdot \mu) \subset X\) for some \(k \in \mathbb{N}^+\) and \(c \in S\), there exists \(w \in \mathbb{R}^n\), function \(f : X \rightarrow \mathbb{R}^n\) and \(\psi : \mathbb{Z}^+ \rightarrow \mathbb{R}^n\) so that the aggregation function \(h_1(c, X) = \sum_{x \in X} \alpha_{cx} f(x) + w \odot \sum_{x \in X} f(x)\) and \(h_2(c, X) = \psi (|X|) \odot \sum_{x \in X} \alpha_{cx} f(x)\) can always distinguish them by \(h_1(c, X_1) \neq h_1(c, X_2), i \in \{1, 2\}\).
Proof. By Theorem 1, given \(X_1 = (S, \mu)\) and \(X_2 = (S, k \cdot \mu) \subset X\) for some \(k \in \mathbb{N}^+\) and \(c \in S\), we have \(\sum_{x \in X_1} \alpha_{cex} f(x) = \sum_{x \in X_2} \alpha_{cex} f(x)\), where \(\alpha_{cex}\) is the attention weight belongs to \(X_i\), and between \(f(c)\) and \(f(x)\), \(x \in X_i, i \in \{1, 2\}\). We denote \(H = \sum_{x \in X_i} \alpha_{cex} f(x) = \sum_{x \in X_2} \alpha_{cex} f(x)\), so the aggregation functions can be rewritten as:

\[
\begin{align*}
\sum_{x \in X_i} f(x), & \quad i \in \{1, 2\}, \\
\psi(|X_i|) & \circ H, & \quad i \in \{1, 2\}.
\end{align*}
\]

We consider the following example: All elements in \(w\) equal to 1. Function \(\psi\) maps \(|X|\) to a n-dimensional vector which all elements in it equal to \(|X|\). And \(f(x) = N^{-z(x)}\), where \(Z : X \to \mathbb{N}\) and \(N > |X|\). So that the aggregation functions become:

\[
\begin{align*}
\sum_{x \in X_i} f(x), & \quad i \in \{1, 2\}, \\
|X_i| & \circ H, & \quad i \in \{1, 2\}.
\end{align*}
\]

For \(h_1\), we have \(h_1(c, X_1) - h_1(c, X_2) = \sum_{x \in X_1} f(x) - \sum_{x \in X_2} f(x)\). According to Lemma 5 of \(Xu et al. 2019\), when \(X_1 \neq X_2\), \(\sum_{x \in X_1} f(x) \neq \sum_{x \in X_2} f(x)\). So \(h_1(c, X_1) \neq h_1(c, X_2)\).

For \(h_2\), we have \(h_2(c, X_1) - h_2(c, X_2) = (|X_1| - |X_2|) \cdot H\). As \(\alpha_{cex} > 0\) due to the softmax function, and \(f(x) > 0\) in our example, we know \(H > 0\). Moreover as \(|X_1| - |X_2| \neq 0\), we can get \(h_2(c, X_1) \neq h_2(c, X_2)\).

While the original attention-based aggregator is never injective as we mentioned in previous sections, our cardinality preserved attention-based aggregator can be injective with certain learned attention weights, thus could be as powerful as the WL test. As a future direction, it would be interesting to find the conditions when our cardinality preserved attention-based aggregator is injective and analyze the effects of different attention mechanisms.

Cardinality Preserved Attention Network (CPAN)

Now with our novel proposed cardinality preserved attention models, we build a simple GNN framework named Cardinality Preserved Attention Network (CPAN) that adopts them. In detail, we take advantage of the approximation capability of multi-layer perceptron (MLP) \(\text{Hornik, Stinchcombe, and White 1989, Hornik 1991}\) to model \(f^l\) and \(\psi^l\) in Equation 3 and Equation 9. Weight \(w^l\) in Equation 8 is set as trainable. Thus the aggregating step in the \(l\)-th layer of CPAN can be chosen as one of bellow:

\[
\begin{align*}
\sum_{j \in \mathcal{N}(i)} \alpha^{-1}_{ij} h^{-1}_j + w^l \odot \sum_{j \in \mathcal{N}(i)} h^{-1}_j, & \quad (10) \\
\psi_{MLP}(|\mathcal{N}(i)|) & \circ \sum_{j \in \mathcal{N}(i)} \alpha^{-1}_{ij} h^{-1}_j. & \quad (11)
\end{align*}
\]

Besides, we further simplify Equation 10 and Equation 11 by fixing the additional weights embedded in \(w^l\) and \(\psi_{MLP}\) and get two more variants:

\[
\begin{align*}
\sum_{j \in \mathcal{N}(i)} \alpha^{-1}_{ij} h^{-1}_j + \sum_{j \in \mathcal{N}(i)} h^{-1}_j, & \quad (12) \\
\psi_{MLP}(|\mathcal{N}(i)|) & \circ \sum_{j \in \mathcal{N}(i)} \alpha^{-1}_{ij} h^{-1}_j. & \quad (13)
\end{align*}
\]

Note that we can still use the original version of attention mechanism in the aggregator for comparison:

\[
\begin{align*}
\sum_{j \in \mathcal{N}(i)} \alpha^{-1}_{ij} h^{-1}_j, & \quad (14)
\end{align*}
\]

For the graph pooling function, a naive way is to only consider the node embeddings from the last iteration. Although a sufficient number of iterations can help to avoid the cases in Theorem 1 and exhibit good discriminative power by aggregating more diverse node features, the features from the latter iterations may generalize worse and the GNNs are constrained to have shallow structures \(Xu et al. 2019, Zhou et al. 2018b\). So CPAN adopts the same function as used in \(Xu et al. 2018a, Xu et al. 2019, Lee, Lee, and Kang 2019, Li et al. 2019\), which concatenates graph embeddings from all iterations to fuse multi-scale features together:

\[
\begin{align*}
\bigg| \bigg| & \bigg( \text{Readout}(|\{h_i^l| i \in G\}|) \bigg) \bigg| \\
& \quad k=0 \quad \bigg| \bigg| \quad \bigg| \bigg|
\end{align*}
\]

where \(\big| \big|\) represents concatenation. \(\text{Readout}\) function can be sum or mean. With our proposed aggregators, the cases in Theorem 1 can be avoided in each iteration to guarantee a good discriminative power.

Experiments

In this section, we evaluate the performance of CPAN on graph classification tasks. Note that the discriminative power of the CPAN variants can be directly shown by the accuracies on training sets. Higher training accuracy indicates better fitting ability on a given dataset to distinguish graphs. To empirically investigate the generalization power of CPAN, the accuracies on testing sets are provided. With the testing accuracies, we can further compare our models with other baselines.

Experimental Setup

Datasets In our experiments on graph classification tasks, we use 6 benchmark datasets: 4 bioinformatics datasets (MUTAG, PROTEINS, ENZYMES, NCI1) and 2 social network datasets (REDDIT-BINARY (RE-B), REDDIT-MULTISIK (RE-MSK)). Details of the datasets are listed in Supplemental Material. For the bioinformatics datasets, we use the one-hot encodings of the original node features. While for the social network datasets, we assign all the node features to be the same because there are no original node features.

\footnote{All of the datasets are available at https://ls11-www.cs.tudortmund.de/staff/morris/raphernaldatasets}
Baselines We compare CPAN with several state-of-the-art baselines: WL kernel (WL) (Shervashidze et al. 2011), PATCHY-SAN (PSCN) (Niepert, Ahmed, and Kutzkov 2016), Deep Graph CNN (DGCNN) (Zhang et al. 2018), Graph Isomorphism Network (GIN) (Xu et al. 2019) and Capsule Graph Neural Network (CapsGNN) (Verma and Zhang 2019). For all models, we report the original accuracies in papers. Especially for WL kernel, we report the results shown in (Xu et al. 2019).

Choices of Attention Mechanism As our CPAN framework is universal enough to adopt any kind of attention mechanisms in Equation 3, we choose 2 typical ones to evaluate the performance of our models: GAT and Bilinear.

GAT is proposed in (Veličković et al. 2018):

\[ e_{ij} = \text{LeakyReLU} (a^\top [W_h_i][W_h_j]) \tag{16} \]

where \( a \) and \( W \) are trainable, and \( \parallel \) is the concatenation.

Bilinear is given in (Luong, Pham, and Manning 2015):

\[ e_{ij} = h_i^\top W h_j \tag{17} \]

where \( W \) is trainable.

Model Settings To evaluate the performance of our cardinality preserved models, we use 5 variants of our CPAN framework: (1) Additive: CPAN with Additive model in Equation 10; (2) Scaled: CPAN with Scaled model in Equation 11; (3) \( f \)-Additive: CPAN with Additive model and fixed weights in Equation 12; (4) \( f \)-Scaled: CPAN with Scaled model and fixed weights in Equation 13; (5) Original: CPAN with the original attention mechanism in Equation 14. Each CPAN variant can adopt GAT and Bilinear as its attention mechanism.

We evaluate the performance by using 10-fold cross-validation, and repeating the experiments 10 times for each dataset and each model. The average accuracies and their standard deviations are reported based on the results across the folds in all runs. In all CPAN variants, we use 4 GNN layers besides the input layer. MLP classifier is used to perform the graph classification. We apply Batch normalization (Ioffe and Szegedy 2015) on every hidden layer in MLP except the MLP classifier. All MLPs in the models have 2 layers with ReLU activation. For the Readout function in all variants, we use sum for bioinformatics datasets and mean for social network datasets. The hidden dimensionality is set as 32 for bioinformatics datasets and 64 for social network datasets. The negative input slope of LeakyReLU in the GAT attention mechanism is 0.2. The models are trained using the Adam optimizer (Kingma and Ba 2018). We use an initial learning rate of 0.01 for the bioinformatics datasets and 0.0025 for the social network datasets. The learning rate is dropped by a factor of 0.5 every 50 epochs. For each dataset, the following hyper-parameters are tuned: (1) Batch size in \{32, 128\}; (2) Dropout ratio in \{0, 0.5\} after dense layer; (3) \( L_2 \) regularization from 0 to 0.001; (4) Number of epochs. On each dataset, we use the same hyper-parameter configurations for all CPAN variants.

Results and Discussion

Performance on training set. We first compare the training accuracies of CPAN variants to validate that our cardinality preserved attention models can increase the representational power of the original attention-based aggregator to reach the upper bound.

For bioinformatics datasets, we show the training curves of CPAN variants that use the GAT attention mechanism in Figure 1. From these curves, we can see our proposed models (Additive, Scaled, \( f \)-Additive and \( f \)-Scaled) all fit the training data better than Original and bring gains in different percentages on different datasets. For CPAN variants that use the Bilinear attention mechanism, we also find those patterns in the curves (see in Supplemental Material).

Compared to the WL kernel, our proposed models can get training accuracies close to 100% on several datasets, which reach those obtained from the WL kernel (equal to 100% as shown in (Xu et al. 2019)). However, the accuracies of Original always exist gaps comparing with those of the WL kernel. This validates that our proposed models can approach the upper bound to be as powerful as the WL test with certain learned weights, while the original attention-based GNNs are constrained. On social network datasets, we find that our proposed models can get training accuracies close to 100% on RE-B and > 60% on RE-M5K, which are all significantly higher than the accuracies of Original (50% on RE-B and 20% on RE-M5K).

To further understand why our proposed models fit better than Original on the datasets we tested, we calculate the proportion \( P \) of multisets that hold the properties in Theorem 1 among all multisets for each dataset: MUTAG: 56.9%; PROTEINS: 29.3%; ENZYMES: 29.4%; NCI1: 43.3%; RE-B: 100.0%; RE-M5K: 100.0%. Note that on social network datasets, we assign all the same node features for the unlabeled graphs, thus all multisets will hold the properties in Theorem 1 and \( P = 100.0\% \). The results directly show the existence of the multisets that hold the properties in The-
models clearly show the good generalization power of our proposed models. Moreover, the good performance of attention mechanism. Compared to other state-of-the-art baselines, our proposed models achieve results comparable with or better than that of the baselines. It should be noted that our CPAN framework is universal enough to adopt any kind of attention mechanism, it is expected that even better performance can be achieved with certain choice of attention mechanism.

**Conclusion**

In this paper, we theoretically analyze the representational power of GNNs with attention-based aggregators. We find all cases when those GNNs always fail to distinguish distinct structures. The finding shows that attention mechanism fails to preserve cardinality and thus limits its discriminative ability. To improve, we develop models that can preserve cardinality information to solve this issue. With our models, a GNN framework is designed and evaluated on several benchmark datasets for graph classification. Results on the datasets validate our theoretical analysis and confirm our models can improve the discriminative power of attention mechanism. Compared to other state-of-the-art baselines, our framework can achieve better or comparable performance. In future work, a challenging problem is how to better learn the attention weights in order to let our proposed models easily reach the upper bound for the discriminative capacity. Besides, it would be interesting to investigate how our models affect the generalization power of the original GNNs.
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