IMPRESSING GRAPH PROPERTY PREDICTION WITH GENERALIZED READOUT FUNCTIONS

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ABSTRACT

Graph property prediction is drawing increasing attention in the recent years due to the fact that graphs are one of the most general data structures since they can contain an arbitrary number of nodes and connections between them, and it is the backbone for many different tasks like classification and regression on such kind of data (networks, molecules, knowledge bases, ...). We introduce a novel generalized global pooling layer to mitigate the information loss that typically occurs at the Readout phase in Message-Passing Neural Networks. This novel layer is parametrized by two values ($\beta$ and $p$) which can optionally be learned, and the transformation it performs can revert to several already popular readout functions (mean, max and sum) under certain settings, which can be specified. To showcase the superior expressiveness and performance of this novel technique, we test it in a popular graph property prediction task by taking the current best-performing architecture and using our readout layer as a drop-in replacement and we report new state of the art results. The code to reproduce the experiments can be accessed here: https://github.com/EricAlcaide/generalized-readout-phase

1 Introduction

Geometric Deep Learning

There has been a recent substantial progress during the past decades on Machine Learning and Deep Learning methods for analyzing large amounts of data to identify meaningful patterns that can be latter used for classification, regression, clustering, data generation... Some areas that have experienced such progress include Computer Vision, Speech Recognition and Natural Language Processing.

However, most of the existing machine and deep learning algorithms need structured data defined on Euclidean domains (voxels, grids, etc) to work with. Since there exist several fields which work with data that is not defined on Euclidean domains (physics, biology, complex systems, etc) the need for algorithms that can work with graph and/or manifold structured data is highlighted. In the recent years, the term Geometric Deep Learning has been coined to refer the extension of Deep Learning methods to graphs/manifold data.

Graphs are one of the most general data structures since they can be used to represent Euclidean as well as Non-Euclidean data. Formally $G = (V', E')$, a graph is composed by a set of vertices $V$ (also known as the set of nodes $N$) representing the data points and a set of edges $E$ which model the relations between the vertices. Moreover, graphs are mainly used to capture relational data (social networks, knowledge bases, image entities, maps, etc.) and, thus, are important for reasoning.

Graph Neural Networks

Graph Neural Networks where initially proposed by Scarselli et al. [1] and they are a family of neural networks (universal approximators composed by trainable linear and non-linear transformations[2]) that map graphs to vector representations. This type of neural networks make use of generalized counterparts of traditional neural network functions to work with data with an arbitrary number of nodes and edges.

Recently, Gilmer et al. [3] proposed the Message Passing Neural Network (MPNN) scheme, which is invariant to graph isomorphism and makes use of messages to propagate information across adjacent nodes. The MPNN architecture is comprised of 2 stages: the message passing phase and the readout phase. Formally:
In the massage passing phase (Eqs. 1 and 2), the network learns an embedding vector for each node of the graph via iteratively aggregating and propagating information across adjacent nodes. This part is done in sequential T stages where the network performs 2 functions at each stage: the message function (Eq. 1) and the update function (Eq. 2).

Since graphs can have arbitrary number of nodes and edges, the resulting embedding vectors depend on the original graph, which creates the need for a function that summarizes the arbitrary number of embedding vectors into a fixed vector representation, which is named as readout function (Eq. 3). This fixed output can be later passed to a machine learning algorithm of choice to perform different downstream tasks such as classification, regression, clustering, etc.

Readout functions. A highly desired property for readout functions is permutation invariance since graphs are unordered in nature. Commonly used readout functions are the Mean(·), Max(·) and Sum(·) functions. However, these functions present a problem of information loss at the readout phase. Moreover, the choice of the readout function is sensitive to the nature of the dataset, which makes it difficult to choose the optimal function for a specific task and it often leads to a suboptimal performance in many cases.

Some attempts to mitigate the information loss at the readout phase have been performed, consisting mainly in 3 different types of techniques:

- Fuzzy histograms, which are based on aggregating the arbitrary vector embeddings by calculating the membership probabilities to several fuzzy bins, were implemented by [4].
- Hierarchical clustering, which exploit hierarchical structures present in graphs, was used in [5].
- Multi-Layer Perceptrons, which can also be interpreted as weighted sums of node features and are highly expressive but at the cost of not being order invariant, were reported in [6].

However, the hitherto attempted methods exploit domain-specific graph attributes (i.e., hierarchical structures, order dependency, ...) and have not been compared to modern state of the art architectures which make use of simple Mean(·), Max(·) or Sum(·) functions and exhibit better performance.

Contributions The main contribution of this work is a novel and readout layer composed by generalized mean-max-sum function families which substantially improves performance of state of the art GNN architectures and that can be used as a drop-in replacement for existing readout functions with very limited computational overhead. We achieve a state of the art result (improvement by 2 %) in the ogb-molhiv dataset [7].

2 Methods

Generalized Functions. A generalized function \( f_\theta(\cdot) \) is the one parametrized by a set of values \( \theta \) for which exists a set of special cases \( S_\theta \) for which such function reverts to another, more simple function. Generalized functions are useful for defining continuous and intermediate transitions between different existing functions, thus becoming more expressive than their special counterparts. Given the increased expressiveness, we hypothesize that a generalized function can help to mitigate the information loss in the readout phase which Message Passing Neural Networks suffer from.

We define a Generalized Readout layer parametrized by 2 values (\( \beta \) and \( p \)) that is able to represent the majority of the existing and commonly used readout functions (mean, max, sum, min, ...) while maintaining permutation and ordering invariance. Our generalized layer reverts to commonly used functions under certain simple parameter settings, and it is also fully differentiable which allows for the training of the parameters via gradient-based algorithms such as the popular backpropagation.

Proposition 1 (Generalized Mean-Max-Sum Aggregators). A generalized Mean-Max-Sum aggregation function is that for which there exist at least 3 combinations of a set of parameters \( \theta_i \) such that: \( \lim_{\theta \to \theta_1} f_\theta = \text{Mean}(\cdot) \) and \( \lim_{\theta \to \theta_2} f_\theta = \text{Max}(\cdot) \) and \( \lim_{\theta \to \theta_3} f_\theta = \text{Sum}(\cdot) \).
In order to cover the 3 most popular readout phase functions (mean, max and sum), we design 2 mean-max-sum generalized function families (proposition 1). Inspired by [8], we use two different families of generalized mean-max-sum functions: a softmax-based aggregation and a power mean-based aggregation. Both function families are parametrized by two parameters ($\beta$ and $p$) which are optionally learnable and can be set to the initial value of choice.

Both families return graph-level-outputs by transforming node features based on a Generalized Aggr-Mean-Max function, so that for a single graph $G_i$, its output is computed depending on the family of transformations by either Eq.4 for the $\text{Softmax}$ family or by Eq.5 for the $\text{PowerMean}$ family. Let $N_i$ be the number of nodes in the graph $G_i$, $r_i$ the output of the readout function, and $x_n$ the embedding of the $n^{th}$ node from the Message Passing phase:

$$r_i = \frac{N_i}{1 + \beta \cdot (N_i - 1)} \sum_{n=1}^{N_i} \text{softmax} \left( x_n \cdot p \right) \cdot x_n$$

$$r_i = \left( \frac{1}{1 + \beta \cdot (N_i - 1)} \sum_{n=1}^{N_i} x_n^p \right)^{1/p}$$

Here we detail some of the special cases of the 2 function families used:

The softmax-based aggregation family reverts to:

- the Mean function when $\beta = 1$ and $p = 0$
- the Max function when $\beta = 1$ and $p \to +\infty$
- the Min function when $\beta = 1$ and $p \to -\infty$
- the Sum function when $\beta = 0$ and $p = 0$

The power mean based aggregation function family reverts to:

- the Mean function when $\beta = 1$ and $p = 1$
- the Max function when $\beta = 0$ and $p \to +\infty$
- the Min function when $\beta = 0$ and $p \to -\infty$
- the Sum function when $\beta = 0$ and $p = 1$

![Figure 1: Landscape of generalized Mean-Max-Sum functions](image-url)
The power mean based aggregation function family can also revert to different mean functions (quadratic mean, geometric mean, harmonic mean...).

Another advantage of the 2 function families used is that they both keep the permutation-invariance to the ordering of nodes and they support an arbitrary number of messages to be aggregated, two highly desired properties in readout functions.

**Experimental Setup.** The superior expressiveness and performance of the proposed novel readout phase function is tested by comparing the best-performing GCNN on a given graph property prediction dataset (ogb-molhiv [7]) with the Mean(·) readout phase, as indicated by [9], and our new functions under a drop-in replacement scheme.

The ogb-molhiv [7, 10] dataset is a graph property prediction dataset comprised of 41,127 molecules and the goal is a binary classification depending on their experimentally-checked ability to inhibit the HIV virus replication. The evaluation metric for this dataset is the ROC-AUC.

The computational resources used for the experiments have been:

- **Hardware:** All the experiments in this work were carried on an Intel i7-6700-K 4.0Ghz and 16gb RAM computer with an Nvidia GTX 1060 6gb graphics card.

- **Software:** In order to design and train the Deep Learning models, we employed the PyTorch [11] and PyTorch Geometric [12] python libraries.

Our new technique has been implemented as a PyTorch Geometric [12] layer for ease of use. The code to reproduce the experiments can be accessed here: [https://github.com/EricAlcaide/generalized-readout-phase](https://github.com/EricAlcaide/generalized-readout-phase)

### 3 Results

**Experiment 1.** In order to prove the superior performance of our novel technique, we performed a drop-in replacement with our readout phase and the Hierarchical Inter-Message Passing GNN (HIMP) [12] original architecture for the ogb-molhiv dataset [7] (which was the best-performing (which had its code in open source) in the OGB leaderboard [13] at the time of writing this paper). We trained the new model architecture for 10 independent runs consisting of 100 epochs each. We used the Adam optimizer [14] with the following hyperparameters (lr=1e-4, β₁=0.9, β₂=0.999, ε=1e-8). The hyperparameter combinations that were tried were:

- Softmax₁ (β=1, p=1) and Softmax₂ (β=1e-5, p=1e-5)
- PowerMean₁ (β=1, p=1) and PowerMean₂ (β=1e-5, p=10)

The results from the experiment are showcased in table 1 and the comparison with current SoTA is done in table 2. The final metric for every configuration for each of the 10 independent runs can be found, alongside with the mean ± std. For comparison with previous models, we use the best-performing model from table 1.

| Our results          | Softmax₁ | Softmax₂ | PowerMean₁ | PowerMean₂ |
|----------------------|----------|----------|------------|------------|
|                      | 83.50    | 80.79    | 82.56      | 82.55      |
|                      | 83.90    | 81.54    | 82.54      | 80.38      |
|                      | 83.46    | 81.30    | 82.80      | 81.50      |
|                      | 84.95    | 80.09    | 82.96      | 80.98      |
|                      | 84.32    | 81.50    | 83.25      | 81.57      |
|                      | 83.06    | 80.08    | 80.69      | 81.76      |
|                      | 84.81    | 80.81    | 81.23      | 80.67      |
|                      | 84.91    | 79.21    | 82.49      | 79.37      |
|                      | 84.54    | 80.19    | 82.29      | 79.12      |
|                      | 84.86    | 81.50    | 82.45      | 78.21      |
| **84.23 ± 0.70**     | 80.70 ± 0.79 | 82.33 ± 0.78 | 80.61 ± 1.35 |
Table 2: Comparison between our model and previous SoTA (ROC-AUC mean ± std)

| HIMP+GenReadout (Ours) | GraphNorm [15] | HIMP [9] | DeeperGCN [8] | GIN+VirtualNodes [13] |
|------------------------|----------------|----------|---------------|-----------------------|
| 84.23 ± 0.70           | 78.83 ± 1.0    | 78.80 ± 0.82 | 78.58 ± 1.17  | 77.07 ± 1.49          |

4 Discussion

Our results from Experiment 1 represent a new state of the art result in the ogb-molhiv dataset [7] with an increase of 5.4% over the next top-performing model. Remarkably, all the different hyperparameter combinations tried exhibited better performance when compared to previous state of the art architectures. We attribute this to the superior expressiveness of our new function, which might help to mitigate the information that usually takes place at the readout phase.

We encourage the adoption of this new framework of generalized readout functions for graph property prediction, especially in different GNN architectures and bigger datasets than ogb-molhiv [7], since its superior performance has been proven in a small dataset probably due the fact that this novel mitigates the information loss typically occurring at the Readout phase in MPNN.

Due to computational limitations, it has not been possible to test this novel technique on bigger and perhaps more challenging datasets and other architectures which recently exhibited good performance. Thus, its superior performance on bigger datasets can not be guaranteed, but only expected by logical extrapolation. This is likely to be addressed in future work.

5 Conclusion

In this work, we have introduced a generalized readout function, which can revert to many already popular functions under certain parameter settings, to address the information loss problem that typically occur in Graph Neural Networks during the readout phase. We have successfully proven its superior expressiveness & performance by achieving new SoTA results in a standardized graph property prediction task from the Open Graph Benchmark [7]. The scalability of the proposed technique to bigger datasets and different model architectures is to be addressed in future work.

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