AMPNet: Attention as Message Passing for Graph Neural Networks

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Abstract

Feature-level interactions between nodes can carry crucial information for understanding complex interactions in graph-structured data. Current interpretability techniques, however, are limited in their ability to capture feature-level interactions between different nodes. In this work, we propose AMPNet, a general Graph Neural Network (GNN) architecture for uncovering feature-level interactions between different nodes in a graph. Our framework applies a multiheaded attention operation during message-passing to contextualize messages based on the feature interactions between different nodes. We utilize subgraph sampling and node feature downsampling in our experiments to improve the scalability of our architecture to large networks. We evaluate AMPNet on several benchmark and real-world datasets, and develop a synthetic benchmark based on cyclic cellular automata to test the ability of our framework to recover the underlying generation rules of the cellular automata based on feature-interactions.

1 Introduction

Advancements in Deep Learning (DL) have fueled a recent explosion of successful applications on a broad range of tasks where data is represented in Euclidean spaces [Bronstein et al. 2017]. Graph Neural Networks (GNNs) have extended this success to non-Euclidean, graph-structured data, with applications ranging from scene graph generation, text classification, traffic forecasting, and recommender systems [Wu et al. 2020]. GNNs operate on a message passing principle, allowing for nodes to pass information to neighboring nodes which can then be used to update hidden states attributed to either nodes or edges. This allows GNNs to be applied on multiple general tasks, including node classification, edge prediction, and graph classification.
While powerful, Graph Neural Networks suffer from a lack of interpretability in their predictions, which presents challenges for analyzing the importance of different inputs and interactions within the model. Recent works have attempted to address this in various ways: GNNExplainer [Ying et al. 2019] proposed to find subgraph explanations of input graphs by maximizing the mutual information of subgraph explanations to the entire graph, yielding a subgraph explanation of the input graph as well as a node feature mask indicating important node features. Graph Attention Networks [Velickovic et al. 2017] introduced interpretability directly into the model through a self-attention mechanism which generates edge-level attention coefficients used during message-passing. These and other methods, however, are limited in their ability to capture feature-level interactions across different nodes, which may carry important information for node and graph-level tasks.

In this work, we propose a new framework for message-passing in Graph Neural Networks which can uncover inter-node feature interactions during the message passing step. The idea is to use an attention mechanism computed between the feature embeddings of the source and destination node during message passing. This yields attention coefficients for the feature-interactions across different nodes, which are used to contextualize passed messages and update node hidden states. We call this approach attention as message passing, and our implementation of it AMPNet. We evaluate our architecture on the Cora citation network dataset as well as a single-cell gene expression dataset. In addition, we apply AMPNet on a synthetic dataset inspired by cyclic cellular automata, and quantify the ability of AMPNet to recover the transition rules which governs the state of the cellular automata, highlighting the potential of the model to uncover meaningful feature-level relationships in graph-structured data using feature-level attention.

2 Related Work

2.1 Explainable Graph Neural Networks

Previous methods for explaining the predictions of GNNs have focused on explainability at the node, edge, node-feature or sub-graph level. Graph attention networks, described by [Velickovic et al. 2017], compute self-attention between nodes in order to measure attention at the level of edges in the graph. We distinguish ourselves from GATs by applying attention directly between the features of neighboring nodes during message-passing, computing measures of different feature-level interactions for every edge in the graph. Other works have explored post-hoc analysis for explainable predictions in GNNs, notably, GNNExplainer [Ying et al. 2019], PGExplainer [Luo et al. 2020], PGM-Explainer [Vu and Thai 2020], and SubgraphX [Yuan et al. 2021] have all been developed for this purpose. For a more comprehensive overview of explainability methods in GNNs, we refer interested readers to the excellent taxonomic survey by [Yuan et al. 2022].
2.2 Graph Cellular Automata

The initial study on cellular automata (CA) was done by von Neumann [1966]. CA was inspired by biological organisms and proposed as models that might imitate some fascinating characteristics of biological creatures, such as multicellular development, reproduction, and resilience. Previous extensive studies of DL for CA were primarily concerned with identifying the underlying transition rule, extrapolating the training history, and learning asymptotic dynamical behavior. An early-stage experiment by Wulff and Hertz [1992] successfully trained a small Neural Network (NN) to imitate 1-D and 2-D binary CA with chaotic behavior and complex dynamics. Other studies have implemented the NN approach to understand the hidden rules for CA. Compositional Pattern Producing Networks (CPPNs) proposed by Stanley [2007] is capable to produce structural motifs of 2-D CA with discrete states. A further extended work by Nichole et al. [2018] proposed a new principle of CPPNs-based morphogenesis to investigate 2-D CA pattern replication. Elmenreich and Fehevar [2011] introduce an algorithm that uncovers the NN transition rule, which can generate a complex self-organizing multicellular system based on CA.

Recent seminal work by Gilpin [2019] showed how CNN represents CA rules. Gilpin using just one convolutional layer with small kernel size and enough adjustments, can achieve a promising prediction result for predicting any binary CA with a Moore neighborhood of size $3 \times 3$. Mordvintsev et al. [2020] developed Neural Cellular Automata (NCA), which constructs a CNN to learn the transition rules of 2-D CA-based images with a continuous and multi-dimensional state space. Additionally, Aach et al. [2021] designed a deep convolutional encoder-decoder network to learn 2-D CA transition rules. Furthermore, Grattarola et al. [2021] proposed the Graph Neural Cellular Automata (GNCA) that uses GNN to learn the transition rules of conventional CA as a general extension of the previous CNN approaches.

It has long been known that cellular automata are closely related to partial differential equations (PDEs) and can be seen as discretized versions of the latter Arnold [2012]. Interestingly, the connection between automata and PDEs is bidirectional, in the sense while cellular automata are successful methods for studying properties of PDEs in a discretized and computationally inexpensive manner, it is possible to construct PDE systems that reproduce any cellular automaton on a given grid Omohundro [1984]. By virtue of such connection, the CNN approaches mentioned above can be thought of a natural implementation of spectral methods for solving PDEs in a discrete grid.

Interestingly, however, graph neural network based approaches such as AMPNet, as we will argue below, further generalize this correspondence since the geometric support of a graph can naturally encode non-euclidean (and non-flat) geometries. This perspective has been for instance championed in the loop quantum gravity literature Rovelli [2004], where manifolds are discretized through a CW decomposition (e.g. a simplicial decomposition) and a spin-network entails such procedure.

3 Formulation

In this section, we provide a formulation for the attention as message-passing operator which can be used in arbitrary graph neural network architectures.

3.1 Notation

We denote $G = (V, E)$ as a graph with edge set $E$ and vertex set $V$. Let each node $v_i \in V$ have a feature vector $h_i \in \mathbb{R}^F$ where $F$ is the number of features in each node. We define a mapping $\tau : \mathbb{R}^F \rightarrow \mathbb{R}^{F \times D}$ where $D$ denotes the size of vectors which will be used for attention computation. We may apply this mapping to the feature vectors to obtain an $F \times D$ feature matrix $H_i = \tau(h_i)$.

3.2 Message Passing

We first define an attention-as-message-passing layer, which performs attention on each node pair $(v_j, v_i) \in E$ denoting an edge from $v_j$ to $v_i$. For each node $v_i$, an update step may be defined by a
scaled dot-product attention with \(L\) attention heads between the feature matrices as in Vaswani et al. [2017], followed by a mean aggregator over the messages from all neighbors:

\[
H'_{i} = \text{AGGREGATE} \left( \text{Attention} \left( Q = H_{i}W_{Q}, K = H_{j}W_{K}, V = H_{j}W_{V} \right) \right)
= \text{AGGREGATE} \left( \text{softmax} \left( \frac{H_{i}W_{Q} (H_{j}W_{K})^{T}}{\sqrt{D}} \right) H_{j}W_{V} \right)
\]

Where \(\mathcal{N}(i) = \{j \mid (i, j) \in E\}\) is the neighborhood of node \(i\), \(\cdot^{T}\) is the transposition operator, and AGGREGATE is an aggregation operator, such as mean pooling. We note that this is not a self attention operation but rather a directed attention operation, where the "values" in the query-key-value attention framework are provided by the node passing the message \((v_{j} \text{ for the edge } v_{i} \rightarrow v_{j} \in E)\). If desired for a particular application, a node may be included in its own neighborhood through the use of self (loop) edges.

### 3.3 AMPNet as a non-local DD operator

Delay differential equations (DDEs) are a class of differential equations where the derivative of the unknown function \(y\) depends on the previous temporal values of \(y\). More generally, non-local equations are functional equations where the value of the unknown function depends only on a small local neighborhood of each spatio-temporal point.

AMPNet can be naturally interpreted as a non-local delay differential operator in that it incorporates temporal intervals for the evaluation of time points, implementing delays. Moreover, iterating over the procedure of computing attention between edges, local information relative to adjacent nodes diffuses to other nodes, i.e. neighbors of neighbors, therefore capturing long-distance spatial relations between the features of far nodes. During the iterations, each temporal feature is determined by an increasingly large, and therefore non-local, neighborhood.

Therefore, the functioning of AMPNet can be schematically described as follows. A feature (e.g. time) interval is initialized and evaluation of attention between adjacent nodes according to the geometric support of the graph \(G\) produces a feature output (e.g. future time points) at a single-iteration degree of approximation. A second iteration now propagates the information previously exchanged between nodes regarding the predicted features to farther nodes, and so on.

In this perspective, AMPNet models cellular automata as a result of an operator learning task where the corresponding PDE is learned in the form of a DDE. See Subsection 2.2. Moreover, as previously observed, employing the notion of graph neural networks the geometric support can correspond to non-euclidean manifolds seen in a discretized manner (e.g. spin-network formalism) and AMPNet can be interpreted as applying an operator learning task over a topological manifold.

### 3.4 Feature Embedding

Given input node features \(h_{i} \in \mathbb{R}^{F}\) where a node is represented by an \(F\)-dimensional feature vector representing the \(F\) features of node \(i\), we realize mapping \(\tau\) through a concatenation of two learned linear projections: one of the feature identity and one of the feature value. The feature identity is embedded through a lookup embedding table which is learned alongside the model, while the value embedding is done through a learned linear projection of the feature value.

\[
H_{i} = \tau(h_{i}) = [W_{E} \parallel \omega(h_{i})]
\]

Where \(W_{E} \in \mathbb{R}^{F \times C_{f}}\) represents the embedding table of \(C_{f}\)-dimensional feature embeddings, \(\omega: \mathbb{R}^{F} \rightarrow \mathbb{R}^{F \times C_{v}}\) is a learned linear projection of the feature value, and \(D = C_{f} + C_{v}\).

### 3.5 Sparse Sampling of Feature Matrix

In cases where there are many node features and high-dimensionality, the computational complexity of performing attention on across all node features will grow quadratically with respect to the number of features. An example of this would be gene expression data, where cells may contain thousands of
genes that need to be embedded. To limit the complexity of the AMPNet operator, in practice we randomly sample $M$ non-zero node features with replacement to represent the given node on each forward pass. This limits the amount of vectors participating in attention, and provides a regularizing effect on the representation of each node.

### 3.6 Subgraph Sampling

Attention mechanisms performed between all pair of nodes within a network introduces a large computational burden during the message-passing step in relation to the number of edges in the graph. To address this, we mitigate the time and computational complexity during training by sampling subgraphs from the network and train the model on these subgraphs. We follow the findings of Leskovec and Faloutsos [2006], and use random-walk based methods for subgraph sampling in order to obtain subgraphs with properties similar to that of the entire graph. Specifically, we utilize the GraphSAINT random walk subgraph sampler described in Zeng et al. [2019], which constructs subgraphs through multiple random walks and uses a loss normalization term in order to reduce bias in node minibatch estimation. In contrast to layer-wise subgraph samplers Hamilton et al. [2017], Ying et al. [2018] which sample neighboring nodes at each GNN layer, GraphSAINT samples the training graph itself to construct subgraphs.

### 4 Experiments

#### 4.1 Datasets

Citation graphs have been extensively used to benchmark GNNs. We benchmark AMPNet on the Cora citation network Sen et al. [2008], which consists of 2708 nodes which represent published scientific documents, categorized into one of 7 topics. Edges are created based on citation relations between documents, and each node is represented by a 1433-dimensional binary feature vector representing the presence or absence (0/1) of a word in the Cora dataset vocabulary. Feature embedding in Cora experiments is done using a learned, randomly-initialized feature embedding table.

We also construct a synthetic dataset inspired by multicolor cyclic cellular automata Hillemann [2008]. We start with a 2D 30x30 cellular automata, where each cell may take on one of 6 different color states. To run the automata for 1 step, we apply a cyclical rule where if a cell has a neighbor with the next indexed color, the cell takes on that color in the next iteration. This can be formalized as $\{0, 1 \in C_N\} \rightarrow 1$, where a cell with state 0 and at least one neighbor with state 1 will transition to...
Figure 3: Attention heatmaps depicting feature-level interactions in the (a) Slide-seqV2 dataset and the (b) Cora citation network. Rows represent features of the source node, and columns represent features of the destination node. For brevity, both subplots show the top 30 features (or genes) present in the chosen node classes along the axes. (a) shows the average attention coefficients across all edges connecting a Polydendrocyte to an Oligodendrocyte cell in the Slide2Seq dataset. (b) shows average attention coefficients across all edges linking two nodes of class 0 in the Cora dataset.

color state 1 at the next timestep. We do not add any noise to this rule (probability of transition is 100% if condition is met), and with this simple state transition logic we obtain a cellular automaton which enters a cyclical stable state from a random initialization of the board. To transform this into a graph, we create a node for each cell in the 30x30 grid, with node features comprising of a one-hot encoding of the cell’s color index, as shown in Figure 2. We then perform feature embedding to obtain a matrix representation for a node given its cell state at the current time step. We use this dataset to evaluate the ability of AMPNet to recover the transition rule used to generate the cellular automata.

Finally, we evaluate AMPNet on the publicly available mouse hippocampal Slide-seqV2 dataset [Stickels et al. 2021]. This is a gene expression dataset with high RNA capture efficiency and near-cellular spatial resolution. The data consists of 41786 cells, expressed in 4000 genes. The cells are categorized into one of 14 different cell types. The location of each cell is provided using two spatial coordinates. We generate a graph from the dataset by using cells as nodes, genes as features, and applying k-nearest neighbors to the spatial coordinates to create edges based on spatial proximity. We use the first 50 principle components of each gene as the feature embedding in Slide-seqV2 experiments.

4.2 Experimental Setup

All models were implemented in Pytorch [Paszke et al. 2019], an open-source deep learning library for Deep Learning. For all tasks we apply a two-layer AMPNet model with ReLU activations [Nair and Hinton 2010]. Average pooling is performed before the final classification layer for node classification tasks in all three datasets. Hyperparameters were optimized using the validation set of Cora, and subsequently evaluated on the test set and reused across the gene expression and cellular automata dataset. We use $L = 4$ attention heads per Multihead attention layer [Vaswani et al. 2017] within AMPNet message passing layers, and train all models with the Adam optimizer [Kingma and Ba 2014] using a learning rate of 0.01. On the Cora dataset, we apply $L_2$ regularization with $\lambda = 0.0005$ in order to reduce model capacity and prevent overfitting on the datasets.

For all attention visualizations, we take the attention coefficients from the Multihead attention mechanism of the first AMPNet message-passing layer, and visualize the coefficients generated on a forward pass of unseen test data post-training.
### Cyclic Cellular Automata Transition Table

| Transition | Ground Truth Probability | AMPNet Attention |
|------------|--------------------------|------------------|
| \(\{0, 1 \in C_N\} \rightarrow 1\) | 1.0 | 1.0 |
| \(\{1, 2 \in C_N\} \rightarrow 2\) | 1.0 | 0.98 |
| \(\{2, 3 \in C_N\} \rightarrow 3\) | 1.0 | 0.97 |
| \(\{3, 4 \in C_N\} \rightarrow 4\) | 1.0 | 0.99 |
| \(\{4, 5 \in C_N\} \rightarrow 5\) | 1.0 | 0.99 |
| \(\{5, 0 \in C_N\} \rightarrow 0\) | 1.0 | 1.0 |

Table 1: Transition table for 6-color cyclic cellular automata. AMPNet attention coefficients reliably attend to the correct color feature in the neighboring containing the next color state.

#### 4.3 Results

For the node classification task on the Cora citation network, we report mean test set accuracy compared to standard baseline architectures in Table 1, and reuse reported performance on the benchmark from Veličković et al. [2017] and Kipf and Welling [2016]. We demonstrate comparable performance to standard architectures Kipf and Welling [2016], Veličković et al. [2017] on the Cora benchmark, in addition to our model's ability to uncover feature-level interactions across nodes. In Fig. 3b, we visualize the average attention coefficients between the top 30 occurring word features across edges connecting class 0 nodes in the Cora dataset. The structure in the attention matrix suggests that a subset of the source node word features is important for the cross-node interaction.

The Cora dataset, however, has the limitation of not having human-interpretable features, since the identities of words within scientific documents (nodes) is unknown.

To address this, we evaluate AMPNet on our synthetic multicolor cellular automata dataset. We define a node classification objective on the cellular automata, predicting the next state given the current cellular automata encoded state. We obtain a square attention matrix between the one-hot encoded color features of a source and destination node. What we wish to demonstrate however, is that these attention patterns can capture the transition rules used to generate the cellular automata, which are written out in Table 1. We do this by calculating for each color transition (e.g. color 0 changes to 1) the percentage of times the correct color feature was highly attended to when that color transition occurred. Given a predicted next cell state \(C_i\) for cell \(i\), we are interested in the number of times AMPNet predicted the correct next color state based on neighbor information, as well as what color features were attended to in important neighbors. Focusing on neighbors with color state \(C_i\), we sum attention coefficients associated with each of their six color features. The color feature with the highest total attention becomes the "predicted" color based on attention scores. We then calculate the number of times AMPNet predicts the correct next color state and attends to the correct color feature in the neighbor with that color feature. In the case that multiple neighbors of a cell have state \(C_i\), we see if either of those cells had attention on the correct color feature.

On the gene expression dataset, we evaluate the ability of AMPNet to uncover gene-gene interactions between different cells in the dataset. In Figure 3a, which depicts the average attention coefficients across edges connecting Polydendrocyte cells with Oligodendrocytes, we note an example of high gene interaction between the MOBP gene in polydendrocytes and the Cryab gene in Oligodendrocytes. Crystallin beta (cryab) and myelin oligodendrocyte basic protein (MOBP) are both associated with aging Alerie et al. [2020], and are also relevant targets for autoreactive T cells in multiple sclerosis Vojdani et al. [2003]. The identification of attention between these genes should be further explored in the context of oligodendrocyte development, and the maintenance of myelination in the mammalian central nervous system.

#### 5 Conclusions

In this work, we propose a new operator for message passing in Graph Neural Networks, which we term attention as message-passing. The AMPNet operator uncovers cross-node feature-level interactions, and we demonstrate the utility of the attention mechanism during the message passing step for analysing feature-level interactions and recovering the patterns in cellular automata systems.
| Architecture   | Cora  |
|---------------|------|
| MLP           | 55.1%|
| GCN [Kipf and Welling, 2016] | 81.5%|
| GAT [Veličković et al., 2017] | 83.0 ± 0.7%|
| AMPNet (ours) | 82.3%|

Table 2: Comparison of test set classification accuracies on the Cora dataset. Performance measures for GAT and GCN are taken from [Veličković et al., 2017].

We benchmark AMPNet on multiple datasets against standard Graph Neural Architectures, and provide multiple methods for managing the computational complexity of the operator.

There are several avenues for improvement upon the AMPNet operator, which could be addressed in further research. A better selection strategy for node features might outperform random sampling, yielding better representations for nodes during forward passes through the architecture. Alternatively, different formulations of sparse attention across the entire node feature set might be an interesting research direction. Finally, edge features, or possibly features assigned to the relationship between specific features, may also be an interesting direction for further contextualizing feature-level interactions in graph-structured data.

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