

GRAPH ATTENTION NETWORKS 图注意力网络

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ABSTRACT

GAT针对：图结构数据
目标：用自注意力层-->解决图卷积及其近似方法的缺点

We present graph attention networks (GATs), novel neural network architectures that operate on graph-structured data, leveraging masked self-attentional layers to address the shortcomings of prior methods based on graph convolutions or their approximations. By stacking layers in which nodes are able to attend over their neighborhoods' features, we enable (implicitly) specifying different weights to different nodes in a neighborhood, without requiring any kind of costly matrix operation (such as inversion) or depending on knowing the graph structure upfront. In this way, we address several key challenges of spectral-based graph neural networks simultaneously, and make our model readily applicable to inductive as well as transductive problems. Our GAT models have achieved or matched state-of-the-art results across four established transductive and inductive graph benchmarks: the *Cora*, *Citeseer* and *Pubmed* citation network datasets, as well as a *protein-protein interaction* dataset (wherein test graphs remain unseen during training).

通过叠加节点可以参与其邻域特征的层，
可以为不同节点指定不同的权重
1.不需要代价高昂的矩阵操作
2.不需要预先知道图形结构

优点：1.解决基于频谱的图神经网络的关键挑战
2.使模型易于适用于归纳问题和转换问题

1 INTRODUCTION

卷积神经网络CNN的应用：

- 1.图像分类
- 2.语义分割
- 3.机器翻译

卷积神经网络CNN的底层数据：网格状结构（矩阵）

Convolutional Neural Networks (CNNs) have been successfully applied to tackle problems such as image classification (He et al., 2016), semantic segmentation (Jégou et al., 2017) or machine translation (Gehring et al., 2016), where the underlying data representation has a grid-like structure. These architectures efficiently reuse their local filters, with learnable parameters, by applying them to all the input positions.

很多任务的数据结构是：图
eg. 社交网络，电信网络，生物网络，大脑连接体

However, many interesting tasks involve data that can not be represented in a grid-like structure and that instead lies in an irregular domain. This is the case of 3D meshes, social networks, telecommunication networks, biological networks or brain connectomes. Such data can usually be represented in the form of graphs.

There have been several attempts in the literature to extend neural networks to deal with arbitrarily structured graphs. Early work used recursive neural networks to process data represented in graph domains as directed acyclic graphs (Frasconi et al., 1998; Sperduti & Starita, 1997). Graph Neural Networks (GNNs) were introduced in Gori et al. (2005) and Scarselli et al. (2009) as a generalization of recursive neural networks that can directly deal with a more general class of graphs, e.g. cyclic, directed and undirected graphs. GNNs consist of an iterative process, which propagates the node states until equilibrium; followed by a neural network, which produces an output for each node

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早期工作处理任意结构的图：

- 1.递归神经网络将域中表示的数据处理为有向无环图
- 2.图神经网络（GNNs）：GNNs由一个迭代过程组成，这个迭代过程将节点状态传播到平衡状态；接着是一个神经网络，它为每个节点产生一个输出

based on its state. This idea was adopted and improved by Li et al. (2016), which propose to use gated recurrent units (Cho et al., 2014) in the propagation step.

Nevertheless, there is an increasing interest in generalizing convolutions to the graph domain. Advances in this direction are often categorized as spectral approaches and non-spectral approaches.

卷积推广到图领域：

1. 谱方法
2. 非谱方法

1. (2014) 通过计算图拉普拉斯的特征分解在傅里叶域中定义卷积操作，从而将潜在的密集计算和非空间局部化滤波器。
2. (2015) 引入了平滑系数滤波器的参数化，以便其在空间上局部化。
3. (2016) 建议通过图拉普拉斯的切比雪夫展开来近似滤波器，从而无需计算拉普拉斯的特征向量并产生空间局部化滤波器。
4. (2017) 通过限制滤波器在每个节点周围的一步邻域中操作，简化了先前的方法。

On one hand, spectral approaches work with a spectral representation of the graphs and have been successfully applied in the context of node classification. In Bruna et al. (2014), the convolution operation is defined in the Fourier domain by computing the eigendecomposition of the graph Laplacian, resulting in potentially intense computations and non-spatially localized filters. These issues were addressed by subsequent works. Henaff et al. (2015) introduced a parameterization of the spectral filters with smooth coefficients in order to make them spatially localized. Later, Defferrard et al. (2016) proposed to approximate the filters by means of a Chebyshev expansion of the graph Laplacian, removing the need to compute the eigenvectors of the Laplacian and yielding spatially localized filters. Finally, Kipf & Welling (2017) simplified the previous method by restricting the filters to operate in a 1-step neighborhood around each node. However, in all of the aforementioned spectral approaches, the learned filters depend on the Laplacian eigenbasis, which depends on the graph structure. Thus, a model trained on a specific structure can not be directly applied to a graph with a different structure.

谱方法研究进程

On the other hand, we have non-spectral approaches (Duvenaud et al., 2015; Atwood & Towsley, 2016; Hamilton et al., 2017), which define convolutions directly on the graph, operating on groups of spatially close neighbors. One of the challenges of these approaches is to define an operator which works with different sized neighborhoods and maintains the weight sharing property of CNNs. In some cases, this requires learning a specific weight matrix for each node degree (Duvenaud et al., 2015), using the powers of a transition matrix to define the neighborhood while learning weights for each input channel and neighborhood degree (Atwood & Towsley, 2016), or extracting and normalizing neighborhoods containing a fixed number of nodes (Niepert et al., 2016). Monti et al. (2016) presented mixture model CNNs (MoNet), a spatial approach which provides a unified generalization of CNN architectures to graphs. More recently, Hamilton et al. (2017) introduced GraphSAGE, a method for computing node representations in an *inductive* manner. This technique operates by sampling a fixed-size neighborhood of each node, and then performing a specific aggregator over it (such as the mean over all the sampled neighbors' feature vectors, or the result of feeding them through a recurrent neural network). This approach has yielded impressive performance across several large-scale inductive benchmarks.

非谱方法研究进程

Attention mechanisms have become almost a *de facto* standard in many sequence-based tasks (Bahdanau et al., 2015; Gehring et al., 2016). One of the benefits of attention mechanisms is that they allow for dealing with variable sized inputs, focusing on the most relevant parts of the input to make decisions. When an attention mechanism is used to compute a representation of a single sequence, it is commonly referred to as *self-attention* or *intra-attention*. Together with Recurrent Neural Networks (RNNs) or convolutions, self-attention has proven to be useful for tasks such as machine reading (Cheng et al., 2016) and learning sentence representations (Lin et al., 2017). However, Vaswani et al. (2017) showed that not only *self-attention* can improve a method based on RNNs or convolutions, but also that it is sufficient for constructing a powerful model obtaining *state-of-the-art* performance on the machine translation task.

注意力机制已经成为基于序列任务的标准

注意力机制的好处之一是，它们允许处理不同大小的输入，关注输入中最相关的部分来做出决定

当注意力机制用于计算单个序列的表示时，它通常被称为自我注意或内部注意。

与递归神经网络 (RNN) 或卷积一起，自我注意被证明对机器阅读和学习句子表征等任务有用。

研究表明，自我关注不仅可以改进基于RNNs或卷积的方法，而且对于构建一个强大的模型，获得机器翻译任务的最佳性能也是足够的。

Inspired by this recent work, we introduce an attention-based architecture to perform node classification of graph-structured data. The idea is to compute the hidden representations of each node in the graph, by attending over its neighbors, following a *self-attention* strategy. The attention architecture has several interesting properties: (1) the operation is efficient, since it is parallelizable across node-neighbor pairs; (2) it can be applied to graph nodes having different degrees by specifying arbitrary weights to the neighbors; and (3) the model is directly applicable to *inductive* learning problems, including tasks where the model has to generalize to completely unseen graphs. We validate the proposed approach on four challenging benchmarks: *Cora*, *Citeseer* and *Pubmed* citation networks as well as an inductive *protein-protein interaction* dataset, achieving or matching state-of-the-art results that highlight the potential of attention-based models when dealing with arbitrarily structured graphs.

我们引入了一个基于注意力的架构来执行图形结构数据的节点分类。其思想是计算图中每个节点的隐藏表示，通过关注它的邻居，遵循自我关注策略。

注意力结构的特性

1. 效率高，因为可以并行访问邻居节点
2. 给每个邻居节点设置一个权重，很容易应用到图上
3. 模型可以直接应用在归纳学习中，包括生成一些完全没见过的图

It is worth noting that, as Kipf & Welling (2017) and Atwood & Towsley (2016), our work can also be reformulated as a particular instance of MoNet (Monti et al., 2016). Moreover, our approach of

sharing a neural network computation across edges is reminiscent of the formulation of relational networks (Santoro et al., 2017) and VAIN (Hoshen, 2017), wherein relations between objects or agents are aggregated pair-wise, by employing a shared mechanism. Similarly, our proposed attention model can be connected to the works by Duan et al. (2017) and Denil et al. (2017), which use a neighborhood attention operation to compute attention coefficients between different objects in an environment. Other related approaches include locally linear embedding (LLE) (Roweis & Saul, 2000) and memory networks (Weston et al., 2014). LLE selects a fixed number of neighbors around each data point, and learns a weight coefficient for each neighbor to reconstruct each point as a weighted sum of its neighbors. A second optimization step extracts the point’s feature embedding. Memory networks also share some connections with our work, in particular, if we interpret the neighborhood of a node as the memory, which is used to compute the node features by attending over its values, and then is updated by storing the new features in the same position.

其他相关方法包括局部线性嵌入(LLE)和内存网络
1. LLE在每个数据点周围选择固定数量的邻居，学习每个邻居的权重系数，将每个点重构为其邻居的加权和。
2. 第二步优化提取点的嵌入特征。
记忆网络也与我们的工作有一些共同之处，特别是，如果我们把一个节点的邻域解释为记忆，它被用来计算节点的特征值，然后通过相同的位置存储新特征来更新。

2 GAT ARCHITECTURE

In this section, we will present the building block layer used to construct arbitrary graph attention networks (through stacking this layer), and directly outline its theoretical and practical benefits and limitations compared to prior work in the domain of neural graph processing.

2.1 GRAPH ATTENTIONAL LAYER 图注意力层

We will start by describing a single *graph attentional layer*, as the sole layer utilized throughout all of the GAT architectures used in our experiments. The particular attentional setup utilized by us closely follows the work of Bahdanau et al. (2015)—but the framework is agnostic to the particular choice of attention mechanism.

The input to our layer is a set of node features, $\mathbf{h} = \{\vec{h}_1, \vec{h}_2, \dots, \vec{h}_N\}, \vec{h}_i \in \mathbb{R}^F$, where N is the number of nodes, and F is the number of features in each node. The layer produces a new set of node features (of potentially different cardinality F'), $\mathbf{h}' = \{\vec{h}'_1, \vec{h}'_2, \dots, \vec{h}'_N\}, \vec{h}'_i \in \mathbb{R}^{F'}$, as its output.

输入：
N为节点的个数
F为feature的个数
这表示输入为N个节点的每个节点的F个feature
输出：
表示对这N个节点的F'个输出，
输出为N个节点的每个节点的F'个feature

In order to obtain sufficient expressive power to transform the input features into higher-level features, at least one learnable linear transformation is required. To that end, as an initial step, a shared linear transformation, parametrized by a *weight matrix*, $\mathbf{W} \in \mathbb{R}^{F' \times F}$, is applied to every node. We then perform *self-attention* on the nodes—a shared *attentional mechanism* $a : \mathbb{R}^{F'} \times \mathbb{R}^{F'} \rightarrow \mathbb{R}$ computes *attention coefficients*.

这个权重矩阵就是
输入F个feature与
输出的F'个feature之间的关系。

注意机制a是一个单层前向神经网络
应用LeakyReLU非线性（负输入斜率 = 0.2） $e_{ij} = a(\mathbf{W}\vec{h}_i, \mathbf{W}\vec{h}_j)$ 这表明了节点j的特征对节点i的重要性。(1)

共享的注意力机制a

that indicate the *importance* of node j ’s features to node i . In its most general formulation, the model allows every node to attend on every other node, *dropping all structural information*. We inject the graph structure into the mechanism by performing *masked attention*—we only compute e_{ij} for nodes $j \in \mathcal{N}_i$, where \mathcal{N}_i is some *neighborhood* of node i in the graph. In all our experiments, these will be exactly the first-order neighbors of i (including i). To make coefficients easily comparable across different nodes, we normalize them across all choices of j using the softmax function:

$$\alpha_{ij} = \text{softmax}_j(e_{ij}) = \frac{\exp(e_{ij})}{\sum_{k \in \mathcal{N}_i} \exp(e_{ik})}.$$

为了使不同节点之间的系数易于比较，
我们使用softmax函数 (2)
对所有j选项中的系数进行规范化：

In our experiments, the attention mechanism a is a single-layer feedforward neural network, parametrized by a weight vector $\vec{a} \in \mathbb{R}^{2F'}$, and applying the LeakyReLU nonlinearity (with negative input slope $\alpha = 0.2$). Fully expanded out, the coefficients computed by the attention mechanism (illustrated by Figure 1 (left)) may then be expressed as:

注意机制计算系数公式：

$$\alpha_{ij} = \frac{\exp\left(\text{LeakyReLU}\left(\vec{a}^T [\mathbf{W}\vec{h}_i \| \mathbf{W}\vec{h}_j]\right)\right)}{\sum_{k \in \mathcal{N}_i} \exp\left(\text{LeakyReLU}\left(\vec{a}^T [\mathbf{W}\vec{h}_i \| \mathbf{W}\vec{h}_k]\right)\right)} \quad (3)$$

where \cdot^T represents transposition and $\|$ is the concatenation operation. T代表转置 ||代表拼接

Once obtained, the normalized attention coefficients are used to compute a linear combination of the features corresponding to them, to serve as the final output features for every node (after potentially

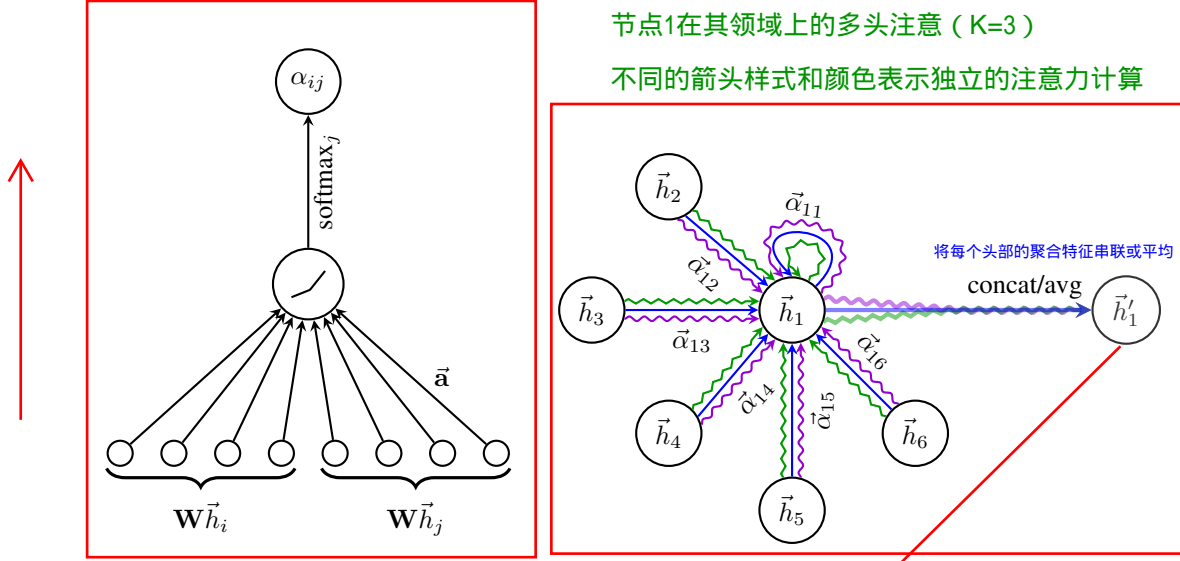


Figure 1: **Left:** The attention mechanism $a(\mathbf{W}\vec{h}_i, \mathbf{W}\vec{h}_j)$ employed by our model, parametrized by a weight vector $\vec{a} \in \mathbb{R}^{2F'}$, applying a LeakyReLU activation. **Right:** An illustration of multi-head attention (with $K = 3$ heads) by node 1 on its neighborhood. Different arrow styles and colors denote independent attention computations. The aggregated features from each head are concatenated or averaged to obtain \vec{h}'_1 .

applying a nonlinearity, σ):

$$\vec{h}'_i = \sigma \left(\sum_{j \in \mathcal{N}_i} \alpha_{ij} \mathbf{W} \vec{h}_j \right). \quad (4)$$

To stabilize the learning process of self-attention, we have found extending our mechanism to employ *multi-head attention* to be beneficial, similarly to Vaswani et al. (2017). Specifically, K independent attention mechanisms execute the transformation of Equation 4, and then their features are concatenated, resulting in the following output feature representation:

具体地说, K 个独立注意机制执行(4)的变换, 然后将它们的特征串联起来, 从而产生以下输出特征表示:

$$\vec{h}'_i = \parallel_{k=1}^K \sigma \left(\sum_{j \in \mathcal{N}_i} \alpha_{ij}^k \mathbf{W}^k \vec{h}_j \right) \quad (5)$$

where \parallel represents concatenation, α_{ij}^k are normalized attention coefficients computed by the k -th attention mechanism (a^k), and \mathbf{W}^k is the corresponding input linear transformation's weight matrix. Note that, in this setting, the final returned output, \vec{h}'_i , will consist of $K F'$ features (rather than F') for each node.

第k个注意机制计算的归一化注意系数

Specially, if we perform multi-head attention on the final (prediction) layer of the network, concatenation is no longer sensible—instead, we employ *averaging*, and delay applying the final nonlinearity (usually a softmax or logistic sigmoid for classification problems) until then:

特别是, 如果我们在网络的最终(预测)层上执行多个头部注意, 则串联不再是明智的, 而是采用平均和延迟应用最终非线性

$$\vec{h}'_i = \sigma \left(\frac{1}{K} \sum_{k=1}^K \sum_{j \in \mathcal{N}_i} \alpha_{ij}^k \mathbf{W}^k \vec{h}_j \right) \quad (6)$$

The aggregation process of a multi-head graph attentional layer is illustrated by Figure 1 (right).

2.2 COMPARISONS TO RELATED WORK 与相关工作比较

图注意层直接解决了以前用神经网络建模图形结构数据的方法存在的问题

The graph attentional layer described in subsection 2.1 directly addresses several issues that were present in prior approaches to modelling graph-structured data with neural networks:

- 1>在计算上是高效的。不需要特征分解或者代价高昂的矩阵运算。各个头部计算是完全独立的, 可以并行化
- Computationally, it is highly efficient: the operation of the self-attentional layer can be parallelized across all edges, and the computation of output features can be parallelized across

all nodes. No eigendecompositions or similar costly matrix operations are required. The time complexity of a single GAT attention head computing F' features may be expressed as $O(|V|FF' + |E|F')$, where F is the number of input features, and $|V|$ and $|E|$ are the numbers of nodes and edges in the graph, respectively. This complexity is on par with the baseline methods such as Graph Convolutional Networks (GCNs) (Kipf & Welling, 2017). Applying multi-head attention multiplies the storage and parameter requirements by a factor of K , while the individual heads' computations are fully independent and can be parallelized.

2>我们设计的模型允许隐式地为同一个邻居节点分配不同的重要性。分析学习到的注意权重有助于提高解释能力

- As opposed to GCNs, our model allows for (implicitly) assigning *different importances* to nodes of a same neighborhood, enabling a leap in model capacity. Furthermore, analyzing the learned attentional weights may lead to benefits in interpretability, as was the case in the machine translation domain (e.g. the qualitative analysis of Bahdanau et al. (2015)).

3>注意机制以共享的方式应用于图中的所有边，不依赖对全局图结构

- The attention mechanism is applied in a shared manner to all edges in the graph, and therefore it does not depend on upfront access to the global graph structure or (features of) all of its nodes (a limitation of many prior techniques). This has several desirable implications:

- The graph is not required to be undirected (we may simply leave out computing α_{ij} if edge $j \rightarrow i$ is not present). 图不需要是无向的

- It makes our technique directly applicable to *inductive* learning—including tasks where the model is evaluated on graphs that are *completely unseen* during training.

它使我们的技术直接适用于归纳学习，包括在训练过程中完全看不见的图形上评估模型的任务。

4>比LSTM更强

- The recently published inductive method of Hamilton et al. (2017) samples a *fixed-size neighborhood* of each node, in order to keep its computational footprint consistent; this does not allow it access to the entirety of the neighborhood while performing inference. Moreover, this technique achieved some of its strongest results when an LSTM (Hochreiter & Schmidhuber, 1997)-based neighborhood aggregator is used. This assumes the existence of a consistent sequential node ordering across neighborhoods, and the authors have rectified it by consistently feeding randomly-ordered sequences to the LSTM. Our technique does not suffer from either of these issues—it works with the entirety of the neighborhood (at the expense of a variable computational footprint, which is still on-par with methods like the GCN), and does not assume any ordering within it.

5>与MoNet相比

- As mentioned in Section 1, GAT can be reformulated as a particular instance of MoNet (Monti et al., 2016). More specifically, setting the pseudo-coordinate function to be $u(x, y) = f(x) \| f(y)$, where $f(x)$ represent (potentially MLP-transformed) features of node x and $\|$ is concatenation; and the weight function to be $w_j(u) = \text{softmax}(\text{MLP}(u))$ (with the softmax performed over the entire neighborhood of a node) would make MoNet's patch operator similar to ours. Nevertheless, one should note that, in comparison to previously considered MoNet instances, our model uses node features for similarity computations, rather than the node's structural properties (which would assume knowing the graph structure upfront).

We were able to produce a version of the GAT layer that leverages *sparse* matrix operations, reducing the storage complexity to linear in the number of nodes and edges and enabling the execution of GAT models on larger graph datasets. However, the tensor manipulation framework we used only supports sparse matrix multiplication for rank-2 tensors, which limits the batching capabilities of the layer as it is currently implemented (especially for datasets with multiple graphs). Appropriately addressing this constraint is an important direction for future work. Depending on the regularity of the graph structure in place, GPUs may not be able to offer major performance benefits compared to CPUs in these sparse scenarios. It should also be noted that the size of the “receptive field” of our model is upper-bounded by the depth of the network (similarly as for GCN and similar models). Techniques such as skip connections (He et al., 2016) could be readily applied for appropriately extending the depth, however. Lastly, parallelization across all the graph edges, especially in a distributed manner, may involve a lot of redundant computation, as the neighborhoods will often highly overlap in graphs of interest.

3 EVALUATION 评估

We have performed comparative evaluation of GAT models against a wide variety of strong baselines and previous approaches, on four established graph-based benchmark tasks (transductive as

Table 1: Summary of the datasets used in our experiments.

	Cora	Citeseer	Pubmed	PPI
Task	Transductive	Transductive	Transductive	Inductive
# Nodes	2708 (1 graph)	3327 (1 graph)	19717 (1 graph)	56944 (24 graphs)
# Edges	5429	4732	44338	818716
# Features/Node	1433	3703	500	50
# Classes	7	6	3	121 (multilabel)
# Training Nodes	140	120	60	44906 (20 graphs)
# Validation Nodes	500	500	500	6514 (2 graphs)
# Test Nodes	1000	1000	1000	5524 (2 graphs)

well as inductive), achieving or matching state-of-the-art performance across all of them. This section summarizes our experimental setup, results, and a brief qualitative analysis of a GAT model’s extracted feature representations.

3.1 DATASETS

Transductive learning We utilize three standard citation network benchmark datasets—Cora, Citeseer and Pubmed (Sen et al., 2008)—and closely follow the transductive experimental setup of Yang et al. (2016). In all of these datasets, nodes correspond to documents and edges to (undirected) citations. Node features correspond to elements of a bag-of-words representation of a document. Each node has a class label. We allow for only 20 nodes per class to be used for training—however, honoring the transductive setup, the training algorithm has access to all of the nodes’ feature vectors. The predictive power of the trained models is evaluated on 1000 test nodes, and we use 500 additional nodes for validation purposes (the same ones as used by Kipf & Welling (2017)). The Cora dataset contains 2708 nodes, 5429 edges, 7 classes and 1433 features per node. The Citeseer dataset contains 3327 nodes, 4732 edges, 6 classes and 3703 features per node. The Pubmed dataset contains 19717 nodes, 44338 edges, 3 classes and 500 features per node.

Inductive learning We make use of a protein-protein interaction (PPI) dataset that consists of graphs corresponding to different human tissues (Zitnik & Leskovec, 2017). The dataset contains 20 graphs for training, 2 for validation and 2 for testing. Critically, testing graphs remain *completely unobserved* during training. To construct the graphs, we used the preprocessed data provided by Hamilton et al. (2017). The average number of nodes per graph is 2372. Each node has 50 features that are composed of positional gene sets, motif gene sets and immunological signatures. There are 121 labels for each node set from gene ontology, collected from the Molecular Signatures Database (Subramanian et al., 2005), and a node can possess several labels simultaneously.

An overview of the interesting characteristics of the datasets is given in Table 1.

3.2 STATE-OF-THE-ART METHODS 最先进的方法

Transductive learning For transductive learning tasks, we compare against the same strong baselines and state-of-the-art approaches as specified in Kipf & Welling (2017). This includes label propagation (LP) (Zhu et al., 2003), semi-supervised embedding (SemiEmb) (Weston et al., 2012), manifold regularization (ManiReg) (Belkin et al., 2006), skip-gram based graph embeddings (DeepWalk) (Perozzi et al., 2014), the iterative classification algorithm (ICA) (Lu & Getoor, 2003) and Planetoid (Yang et al., 2016). We also directly compare our model against GCNs (Kipf & Welling, 2017), as well as graph convolutional models utilising higher-order Chebyshev filters (Defferrard et al., 2016), and the MoNet model presented in Monti et al. (2016).

Inductive learning For the inductive learning task, we compare against the four different supervised GraphSAGE inductive methods presented in Hamilton et al. (2017). These provide a variety of approaches to aggregating features within a sampled neighborhood: GraphSAGE-GCN (which extends a graph convolution-style operation to the inductive setting), GraphSAGE-mean (taking

the elementwise mean value of feature vectors), GraphSAGE-LSTM (aggregating by feeding the neighborhood features into an LSTM) and GraphSAGE-pool (taking the elementwise maximization operation of feature vectors transformed by a shared nonlinear multilayer perceptron). The other transductive approaches are either completely inappropriate in an inductive setting or assume that nodes are incrementally added to a single graph, making them unusable for the setup where test graphs are completely unseen during training (such as the PPI dataset).

Additionally, for both tasks we provide the performance of a per-node shared multilayer perceptron (MLP) classifier (that does not incorporate graph structure at all).

3.3 EXPERIMENTAL SETUP

Transductive learning For the transductive learning tasks, we apply a two-layer GAT model. Its architectural hyperparameters have been optimized on the Cora dataset and are then reused for Citeseer. The first layer consists of $K = 8$ attention heads computing $F' = 8$ features each (for a total of 64 features), followed by an exponential linear unit (ELU) (Clevert et al., 2016) nonlinearity. The second layer is used for classification: a single attention head that computes C features (where C is the number of classes), followed by a softmax activation. For coping with the small training set sizes, regularization is liberally applied within the model. During training, we apply L_2 regularization with $\lambda = 0.0005$. Furthermore, dropout (Srivastava et al., 2014) with $p = 0.6$ is applied to both layers’ inputs, as well as to the *normalized attention coefficients* (critically, this means that at each training iteration, each node is exposed to a stochastically sampled neighborhood). Similarly as observed by Monti et al. (2016), we found that Pubmed’s training set size (60 examples) required slight changes to the GAT architecture: we have applied $K = 8$ output attention heads (instead of one), and strengthened the L_2 regularization to $\lambda = 0.001$. Otherwise, the architecture matches the one used for Cora and Citeseer.

Inductive learning For the inductive learning task, we apply a three-layer GAT model. Both of the first two layers consist of $K = 4$ attention heads computing $F' = 256$ features (for a total of 1024 features), followed by an ELU nonlinearity. The final layer is used for (multi-label) classification: $K = 6$ attention heads computing 121 features each, that are averaged and followed by a logistic sigmoid activation. The training sets for this task are sufficiently large and we found no need to apply L_2 regularization or dropout—we have, however, successfully employed skip connections (He et al., 2016) across the intermediate attentional layer. We utilize a batch size of 2 graphs during training. To strictly evaluate the benefits of applying an attention mechanism in this setting (i.e. comparing with a near GCN-equivalent model), we also provide the results when a *constant attention mechanism*, $a(x, y) = 1$, is used, with the same architecture—this will assign the same weight to every neighbor.

Both models are initialized using Glorot initialization (Glorot & Bengio, 2010) and trained to minimize cross-entropy on the training nodes using the Adam SGD optimizer (Kingma & Ba, 2014) with an initial learning rate of 0.01 for Pubmed, and 0.005 for all other datasets. In both cases we use an early stopping strategy on both the cross-entropy loss and accuracy (transductive) or micro- F_1 (inductive) score on the validation nodes, with a patience of 100 epochs¹.

3.4 RESULTS

The results of our comparative evaluation experiments are summarized in Tables 2 and 3.

For the transductive tasks, we report the mean classification accuracy (with standard deviation) on the test nodes of our method after 100 runs, and reuse the metrics already reported in Kipf & Welling (2017) and Monti et al. (2016) for state-of-the-art techniques. Specifically, for the Chebyshev filter-based approach (Defferrard et al., 2016), we provide the maximum reported performance for filters of orders $K = 2$ and $K = 3$. In order to fairly assess the benefits of the attention mechanism, we further evaluate a GCN model that computes 64 hidden features, attempting both the ReLU and ELU activation, and reporting (as GCN-64*) the better result after 100 runs (which was the ReLU in all three cases).

For the inductive task, we report the micro-averaged F_1 score on the nodes of the two unseen test graphs, averaged after 10 runs, and reuse the metrics already reported in Hamilton et al. (2017) for

¹Our implementation of the GAT layer may be found at: <https://github.com/PetarV-/GAT>.

Table 2: Summary of results in terms of classification accuracies, for Cora, Citeseer and Pubmed. GCN-64* corresponds to the best GCN result computing 64 hidden features (using ReLU or ELU).

<i>Transductive</i>			
Method	Cora	Citeseer	Pubmed
MLP	55.1%	46.5%	71.4%
ManiReg (Belkin et al., 2006)	59.5%	60.1%	70.7%
SemiEmb (Weston et al., 2012)	59.0%	59.6%	71.7%
LP (Zhu et al., 2003)	68.0%	45.3%	63.0%
DeepWalk (Perozzi et al., 2014)	67.2%	43.2%	65.3%
ICA (Lu & Getoor, 2003)	75.1%	69.1%	73.9%
Planetoid (Yang et al., 2016)	75.7%	64.7%	77.2%
Chebyshev (Defferrard et al., 2016)	81.2%	69.8%	74.4%
GCN (Kipf & Welling, 2017)	81.5%	70.3%	79.0%
MoNet (Monti et al., 2016)	81.7 \pm 0.5%	—	78.8 \pm 0.3%
GCN-64*	81.4 \pm 0.5%	70.9 \pm 0.5%	79.0 \pm 0.3%
GAT (ours)	83.0 \pm 0.7%	72.5 \pm 0.7%	79.0 \pm 0.3%

Table 3: Summary of results in terms of micro-averaged F_1 scores, for the PPI dataset. GraphSAGE* corresponds to the best GraphSAGE result we were able to obtain by just modifying its architecture. Const-GAT corresponds to a model with the same architecture as GAT, but with a constant attention mechanism (assigning same importance to each neighbor; GCN-like inductive operator).

<i>Inductive</i>	
Method	PPI
Random	0.396
MLP	0.422
GraphSAGE-GCN (Hamilton et al., 2017)	0.500
GraphSAGE-mean (Hamilton et al., 2017)	0.598
GraphSAGE-LSTM (Hamilton et al., 2017)	0.612
GraphSAGE-pool (Hamilton et al., 2017)	0.600
GraphSAGE*	0.768
Const-GAT (ours)	0.934 \pm 0.006
GAT (ours)	0.973 \pm 0.002

the other techniques. Specifically, as our setup is supervised, we compare against the supervised GraphSAGE approaches. To evaluate the benefits of aggregating across the entire neighborhood, we further provide (as GraphSAGE*) the best result we were able to achieve with GraphSAGE by just modifying its architecture (this was with a three-layer GraphSAGE-LSTM with [512, 512, 726] features computed in each layer and 128 features used for aggregating neighborhoods). Finally, we report the 10-run result of our constant attention GAT model (as Const-GAT), to fairly evaluate the benefits of the attention mechanism against a GCN-like aggregation scheme (with the same architecture).

Our results successfully demonstrate state-of-the-art performance being achieved or matched across all four datasets—in concordance with our expectations, as per the discussion in Section 2.2. More specifically, we are able to improve upon GCNs by a margin of 1.5% and 1.6% on Cora and Citeseer, respectively, suggesting that assigning different weights to nodes of a same neighborhood may be beneficial. It is worth noting the improvements achieved on the PPI dataset: Our GAT model improves by 20.5% w.r.t. the best GraphSAGE result we were able to obtain, demonstrating that our model has the potential to be applied in inductive settings, and that larger predictive power can be leveraged by observing the entire neighborhood. Furthermore, it improves by 3.9% w.r.t. Const-GAT (the identical architecture with constant attention mechanism), once again directly demonstrating the significance of being able to assign different weights to different neighbors.

The effectiveness of the learned feature representations may also be investigated qualitatively—and for this purpose we provide a visualization of the t-SNE (Maaten & Hinton, 2008)-transformed feature representations extracted by the first layer of a GAT model pre-trained on the Cora dataset (Figure 2). The representation exhibits discernible clustering in the projected 2D space. Note that these clusters correspond to the seven labels of the dataset, verifying the model’s discriminative power across the seven topic classes of Cora. Additionally, we visualize the relative strengths of the normalized attention coefficients (averaged across all eight attention heads). Properly interpreting these coefficients (as performed by e.g. Bahdanau et al. (2015)) will require further domain knowledge about the dataset under study, and is left for future work.

4 CONCLUSIONS

We have presented graph attention networks (GATs), novel convolution-style neural networks that operate on graph-structured data, leveraging masked self-attentional layers. The graph attentional layer utilized throughout these networks is computationally efficient (does not require costly matrix operations, and is parallelizable across all nodes in the graph), allows for (implicitly) assigning different importances to different nodes within a neighborhood while dealing with different sized neighborhoods, and does not depend on knowing the entire graph structure upfront—thus addressing many of the theoretical issues with previous spectral-based approaches. Our models leveraging attention have successfully achieved or matched state-of-the-art performance across four well-established node classification benchmarks, both transductive and inductive (especially, with completely unseen graphs used for testing).

There are several potential improvements and extensions to graph attention networks that could be addressed as future work, such as overcoming the practical problems described in subsection 2.2 to be able to handle larger batch sizes. A particularly interesting research direction would be taking advantage of the attention mechanism to perform a thorough analysis on the model interpretability. Moreover, extending the method to perform graph classification instead of node classification would also be relevant from the application perspective. Finally, extending the model to incorporate edge features (possibly indicating relationship among nodes) would allow us to tackle a larger variety of problems.

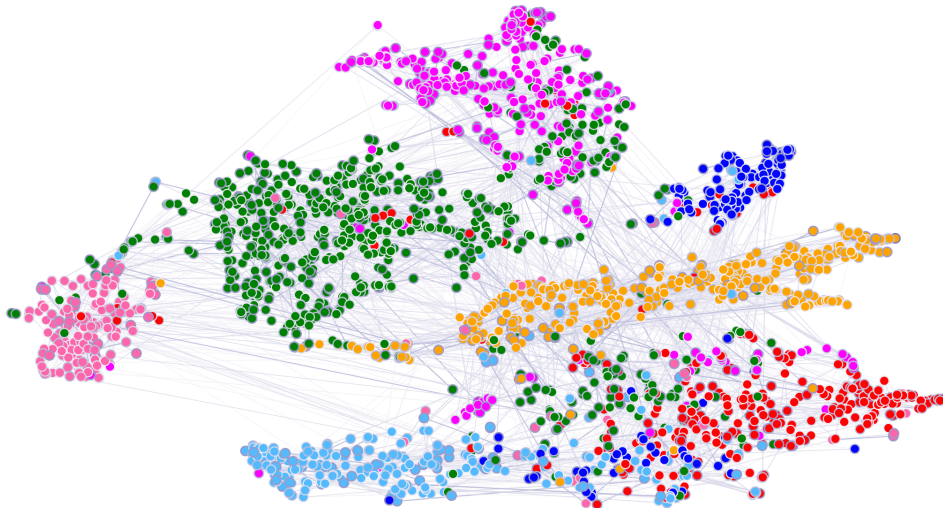


Figure 2: A t-SNE plot of the computed feature representations of a pre-trained GAT model’s first hidden layer on the Cora dataset. Node colors denote classes. Edge thickness indicates aggregated normalized attention coefficients between nodes i and j , across all eight attention heads ($\sum_{k=1}^K \alpha_{ij}^k + \alpha_{ji}^k$).

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REFERENCES 参考文献

- Martín Abadi, Ashish Agarwal, Paul Barham, Eugene Brevdo, Zhifeng Chen, Craig Citro, Greg S. Corrado, Andy Davis, Jeffrey Dean, Matthieu Devin, Sanjay Ghemawat, Ian Goodfellow, Andrew Harp, Geoffrey Irving, Michael Isard, Yangqing Jia, Rafal Jozefowicz, Lukasz Kaiser, Manjunath Kudlur, Josh Levenberg, Dan Mané, Rajat Monga, Sherry Moore, Derek Murray, Chris Olah, Mike Schuster, Jonathon Shlens, Benoit Steiner, Ilya Sutskever, Kunal Talwar, Paul Tucker, Vincent Vanhoucke, Vijay Vasudevan, Fernanda Viégas, Oriol Vinyals, Pete Warden, Martin Wattenberg, Martin Wicke, Yuan Yu, and Xiaoqiang Zheng. TensorFlow: Large-scale machine learning on heterogeneous systems, 2015. URL <https://www.tensorflow.org/>. Software available from tensorflow.org.
- James Atwood and Don Towsley. Diffusion-convolutional neural networks. In *Advances in Neural Information Processing Systems*, pp. 1993–2001, 2016.
- Dzmitry Bahdanau, Kyunghyun Cho, and Yoshua Bengio. Neural machine translation by jointly learning to align and translate. *International Conference on Learning Representations (ICLR)*, 2015.
- Mikhail Belkin, Partha Niyogi, and Vikas Sindhwani. Manifold regularization: A geometric framework for learning from labeled and unlabeled examples. *Journal of machine learning research*, 7 (Nov):2399–2434, 2006.
- Joan Bruna, Wojciech Zaremba, Arthur Szlam, and Yann LeCun. Spectral networks and locally connected networks on graphs. *International Conference on Learning Representations (ICLR)*, 2014.
- Jianpeng Cheng, Li Dong, and Mirella Lapata. Long short-term memory-networks for machine reading. *arXiv preprint arXiv:1601.06733*, 2016.
- Kyunghyun Cho, Bart Van Merriënboer, Caglar Gulcehre, Dzmitry Bahdanau, Fethi Bougares, Holger Schwenk, and Yoshua Bengio. Learning phrase representations using rnn encoder-decoder for statistical machine translation. *arXiv preprint arXiv:1406.1078*, 2014.
- Djork-Arné Clevert, Thomas Unterthiner, and Sepp Hochreiter. Fast and accurate deep network learning by exponential linear units (elus). *International Conference on Learning Representations (ICLR)*, 2016.
- Michaël Defferrard, Xavier Bresson, and Pierre Vandergheynst. Convolutional neural networks on graphs with fast localized spectral filtering. In *Advances in Neural Information Processing Systems*, pp. 3844–3852, 2016.
- Misha Denil, Sergio Gómez Colmenarejo, Serkan Cabi, David Saxton, and Nando de Freitas. Programmable agents. *arXiv preprint arXiv:1706.06383*, 2017.
- Yan Duan, Marcin Andrychowicz, Bradly Stadie, Jonathan Ho, Jonas Schneider, Ilya Sutskever, Pieter Abbeel, and Wojciech Zaremba. One-shot imitation learning. *arXiv preprint arXiv:1703.07326*, 2017.
- David K Duvenaud, Dougal Maclaurin, Jorge Iparraguirre, Rafael Bombarell, Timothy Hirzel, Alán Aspuru-Guzik, and Ryan P Adams. Convolutional networks on graphs for learning molecular fingerprints. In *Advances in neural information processing systems*, pp. 2224–2232, 2015.

- Paolo Frasconi, Marco Gori, and Alessandro Sperduti. A general framework for adaptive processing of data structures. *IEEE transactions on Neural Networks*, 9(5):768–786, 1998.
- Jonas Gehring, Michael Auli, David Grangier, and Yann N. Dauphin. A convolutional encoder model for neural machine translation. *CoRR*, abs/1611.02344, 2016. URL <http://arxiv.org/abs/1611.02344>.
- Xavier Glorot and Yoshua Bengio. Understanding the difficulty of training deep feedforward neural networks. In *Proceedings of the Thirteenth International Conference on Artificial Intelligence and Statistics*, pp. 249–256, 2010.
- Marco Gori, Gabriele Monfardini, and Franco Scarselli. A new model for learning in graph domains. In *IEEE International Joint Conference on Neural Networks*, pp. 729734, 2005.
- William L Hamilton, Rex Ying, and Jure Leskovec. Inductive representation learning on large graphs. *Neural Information Processing Systems (NIPS)*, 2017.
- Kaiming He, Xiangyu Zhang, Shaoqing Ren, and Jian Sun. Deep residual learning for image recognition. In *Proceedings of the IEEE conference on computer vision and pattern recognition*, pp. 770–778, 2016.
- Mikael Henaff, Joan Bruna, and Yann LeCun. Deep convolutional networks on graph-structured data. *arXiv preprint arXiv:1506.05163*, 2015.
- Sepp Hochreiter and Jürgen Schmidhuber. Long short-term memory. *Neural computation*, 9(8): 1735–1780, 1997.
- Yedid Hoshen. Vain: Attentional multi-agent predictive modeling. In I. Guyon, U. V. Luxburg, S. Bengio, H. Wallach, R. Fergus, S. Vishwanathan, and R. Garnett (eds.), *Advances in Neural Information Processing Systems 30*, pp. 2698–2708. Curran Associates, Inc., 2017. URL <http://papers.nips.cc/paper/6863-vain-attentional-multi-agent-predictive-modeling.pdf>.
- Simon Jégou, Michal Drozdal, David Vázquez, Adriana Romero, and Yoshua Bengio. The one hundred layers tiramisu: Fully convolutional densenets for semantic segmentation. In *Workshop on Computer Vision in Vehicle Technology CVPRW*, 2017.
- Diederik Kingma and Jimmy Ba. Adam: A method for stochastic optimization. *arXiv preprint arXiv:1412.6980*, 2014.
- Thomas N Kipf and Max Welling. Semi-supervised classification with graph convolutional networks. *International Conference on Learning Representations (ICLR)*, 2017.
- Yujia Li, Daniel Tarlow, Marc Brockschmidt, and Richard Zemel. Gated graph sequence neural networks. *International Conference on Learning Representations (ICLR)*, 2016.
- Zhouhan Lin, Minwei Feng, Cicero Nogueira dos Santos, Mo Yu, Bing Xiang, Bowen Zhou, and Yoshua Bengio. A structured self-attentive sentence embedding. *arXiv preprint arXiv:1703.03130*, 2017.
- Qing Lu and Lise Getoor. Link-based classification. In *Proceedings of the 20th International Conference on Machine Learning (ICML-03)*, pp. 496–503, 2003.
- Laurens van der Maaten and Geoffrey Hinton. Visualizing data using t-sne. *Journal of Machine Learning Research*, 9(Nov):2579–2605, 2008.
- Federico Monti, Davide Boscaini, Jonathan Masci, Emanuele Rodolà, Jan Svoboda, and Michael M Bronstein. Geometric deep learning on graphs and manifolds using mixture model cnns. *arXiv preprint arXiv:1611.08402*, 2016.
- Mathias Niepert, Mohamed Ahmed, and Konstantin Kutskov. Learning convolutional neural networks for graphs. In *Proceedings of The 33rd International Conference on Machine Learning*, volume 48, pp. 2014–2023, 2016.

- Bryan Perozzi, Rami Al-Rfou, and Steven Skiena. Deepwalk: Online learning of social representations. In *Proceedings of the 20th ACM SIGKDD international conference on Knowledge discovery and data mining*, pp. 701–710. ACM, 2014.
- Sam T. Roweis and Lawrence K. Saul. Nonlinear dimensionality reduction by locally linear embedding. *Science*, 290:2323–2326, 2000.
- Adam Santoro, David Raposo, David GT Barrett, Mateusz Malinowski, Razvan Pascanu, Peter Battaglia, and Timothy Lillicrap. A simple neural network module for relational reasoning. *arXiv preprint arXiv:1706.01427*, 2017.
- Franco Scarselli, Marco Gori, Ah Chung Tsoi, Markus Hagenbuchner, and Gabriele Monfardini. The graph neural network model. *IEEE Transactions on Neural Networks*, 20(1):61–80, 2009.
- Prithviraj Sen, Galileo Namata, Mustafa Bilgic, Lise Getoor, Brian Galligher, and Tina Eliassi-Rad. Collective classification in network data. *AI magazine*, 29(3):93, 2008.
- A. Sperduti and A. Starita. Supervised neural networks for the classification of structures. *Trans. Neur. Netw.*, 8(3):714–735, May 1997. ISSN 1045-9227. doi: 10.1109/72.572108.
- Nitish Srivastava, Geoffrey E Hinton, Alex Krizhevsky, Ilya Sutskever, and Ruslan Salakhutdinov. Dropout: a simple way to prevent neural networks from overfitting. *Journal of machine learning research*, 15(1):1929–1958, 2014.
- Aravind Subramanian, Pablo Tamayo, Vamsi K Mootha, Sayan Mukherjee, Benjamin L Ebert, Michael A Gillette, Amanda Paulovich, Scott L Pomeroy, Todd R Golub, Eric S Lander, et al. Gene set enrichment analysis: a knowledge-based approach for interpreting genome-wide expression profiles. *Proceedings of the National Academy of Sciences*, 102(43):15545–15550, 2005.
- Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N Gomez, Lukasz Kaiser, and Illia Polosukhin. Attention is all you need. *arXiv preprint arXiv:1706.03762*, 2017.
- Jason Weston, Frédéric Ratle, Hossein Mobahi, and Ronan Collobert. Deep learning via semi-supervised embedding. In *Neural Networks: Tricks of the Trade*, pp. 639–655. Springer, 2012.
- Jason Weston, Sumit Chopra, and Antoine Bordes. Memory networks. *CoRR*, abs/1410.3916, 2014. URL <http://arxiv.org/abs/1410.3916>.
- Zhilin Yang, William Cohen, and Ruslan Salakhutdinov. Revisiting semi-supervised learning with graph embeddings. In *International Conference on Machine Learning*, pp. 40–48, 2016.
- Xiaojin Zhu, Zoubin Ghahramani, and John D Lafferty. Semi-supervised learning using gaussian fields and harmonic functions. In *Proceedings of the 20th International conference on Machine learning (ICML-03)*, pp. 912–919, 2003.
- Marinka Zitnik and Jure Leskovec. Predicting multicellular function through multi-layer tissue networks. *Bioinformatics*, 33(14):i190–i198, 2017.