GRAPH ATTENTION NETWORKS

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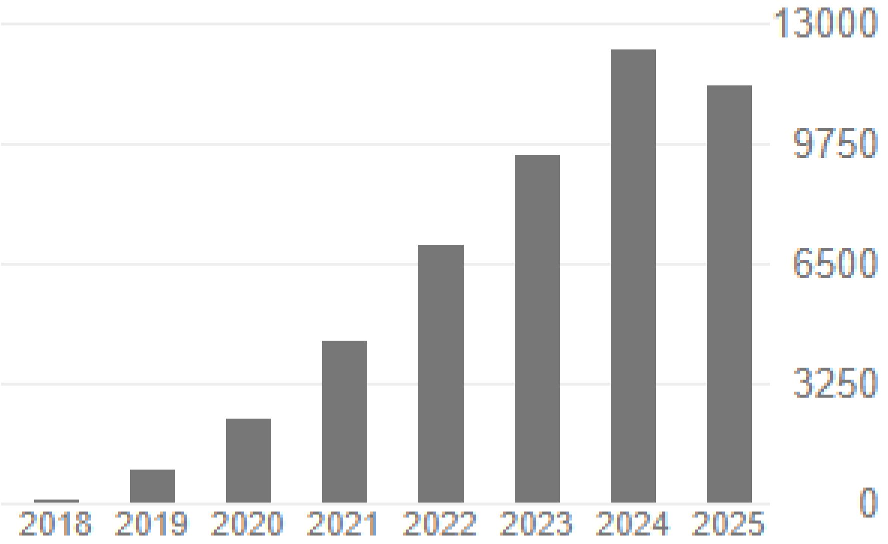
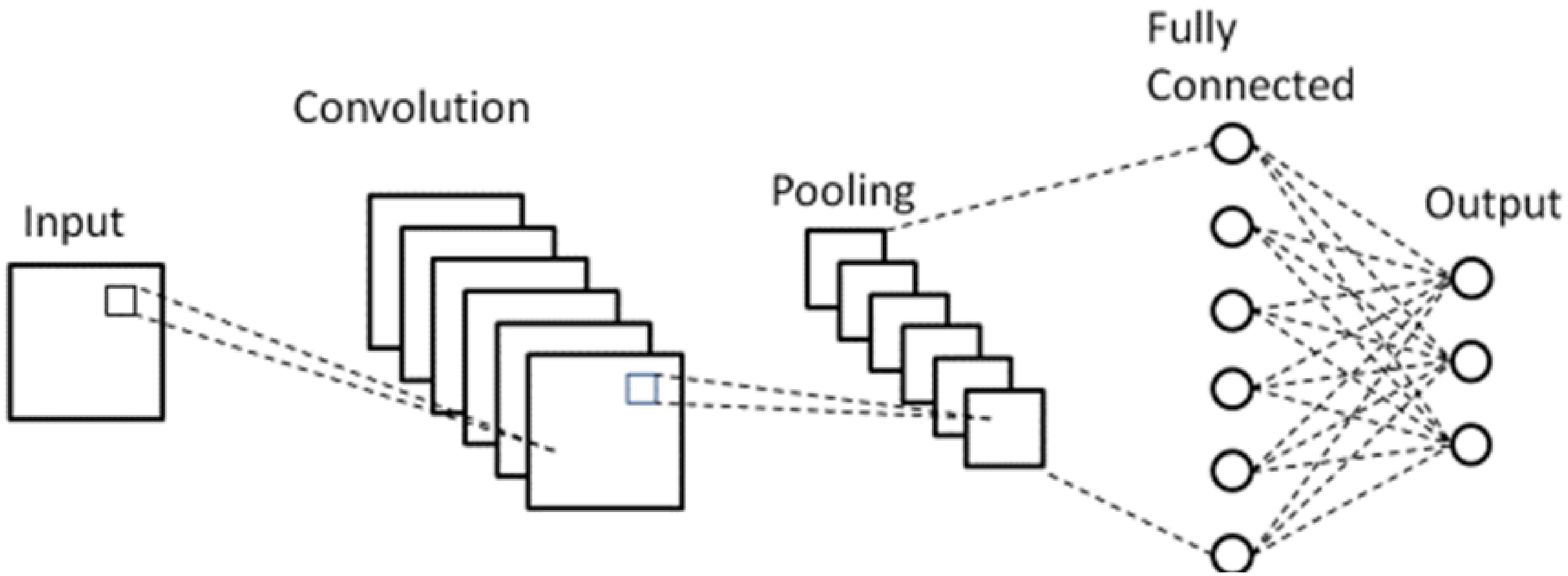


TITLE	CITED BY	YEAR
Graph Attention Networks P Veličković, G Cucurull, A Casanova, A Romero, P Liò, Y Bengio 6th International Conference on Learning Representations (ICLR 2018)	32588 *	2018
Deep Graph Infomax P Veličković, W Fedus, WL Hamilton, P Liò, Y Bengio, RD Hjelm 7th International Conference on Learning Representations (ICLR 2019)	3551	2019
Geometric deep learning: Grids, groups, graphs, geodesics, and gauges MM Bronstein, J Bruna, T Cohen, P Veličković arXiv preprint arXiv:2104.13478	2095	2021
Scientific discovery in the age of artificial intelligence H Wang*, T Fu*, Y Du*, W Gao, K Huang, Z Liu, P Chandak, S Liu, ... Nature 620 (7972), 47-60	1642	2023

Background

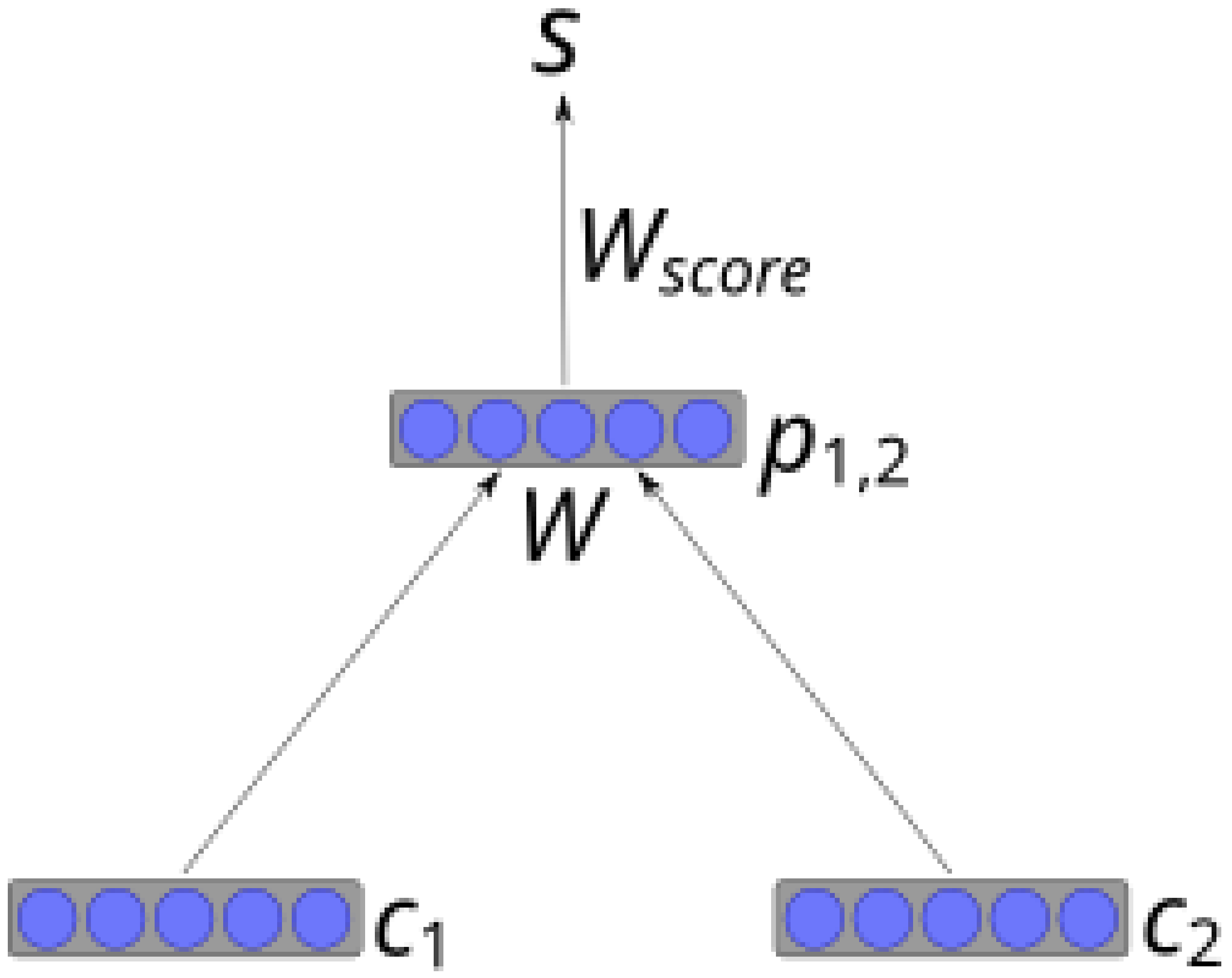
- **Convolutional Neural Networks (CNNs)** have been successfully applied to tackle problems such as image, semantic segmentation or machine translation, where the underlying data representation has a grid-like structure.



- However, many … grid-like structure
  and that instead

Background

- 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.
- A recursive neural network is created by **applying the same set of weights recursively** over a structured input, to produce a structured prediction over variable-size input structures, by traversing a given structure **in topological order**.
- In the simplest architecture, nodes are combined into parents using a weight matrix and a non-linearity such as the tanh hyperbolic function.



$$p_{1,2} = \tanh(W[c_1; c_2])$$

Background

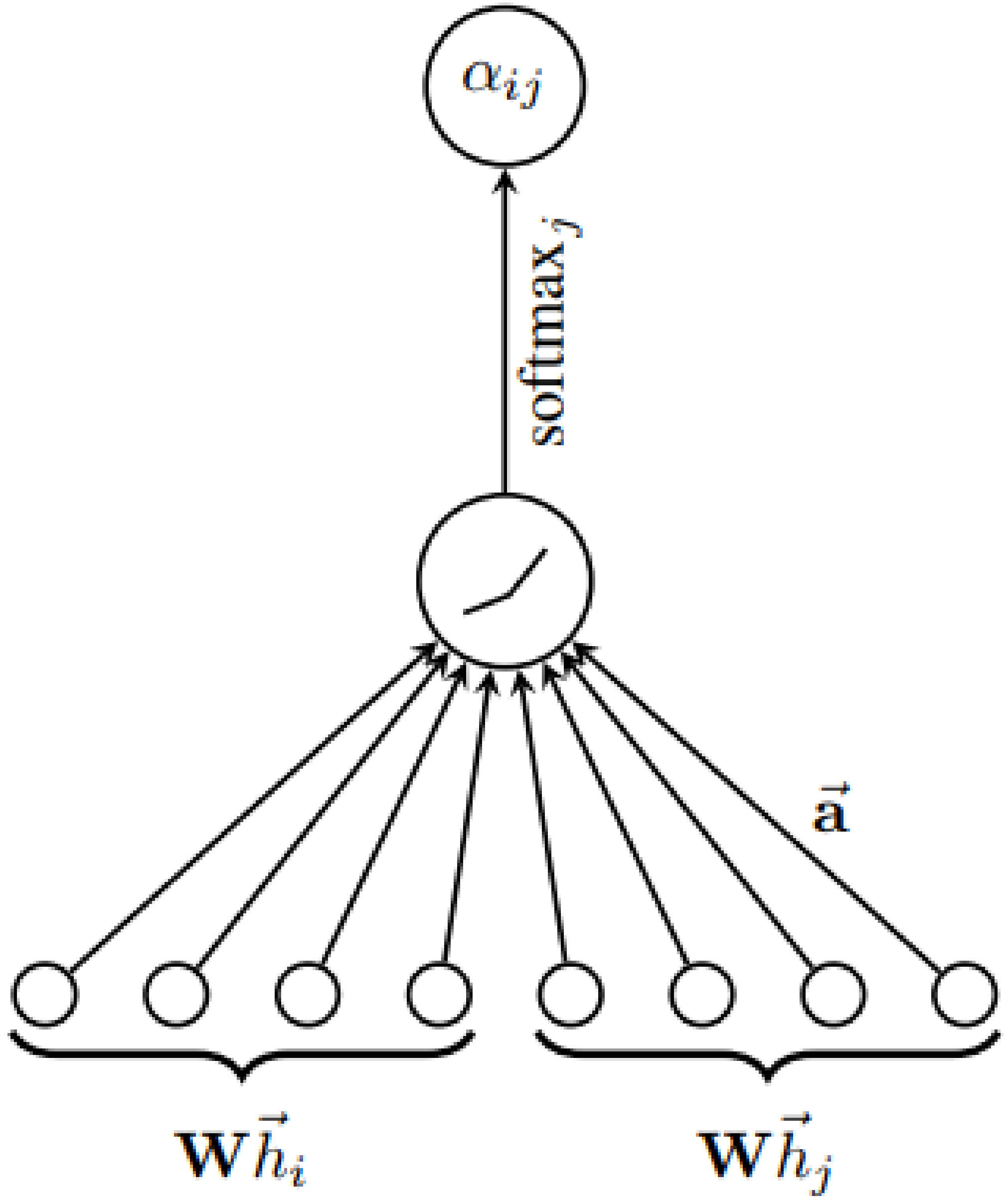
- A **Graph Convolutional Network (GCN)** extends the idea of convolution from regular grids (like images) to graph-structured data.
- Input Representation: Each node v has a feature vector x. The graph is defined by an adjacency matrix A.
- Neighborhood Aggregation (Message Passing): Each node updates its representation by aggregating features from its neighbors (and often itself).

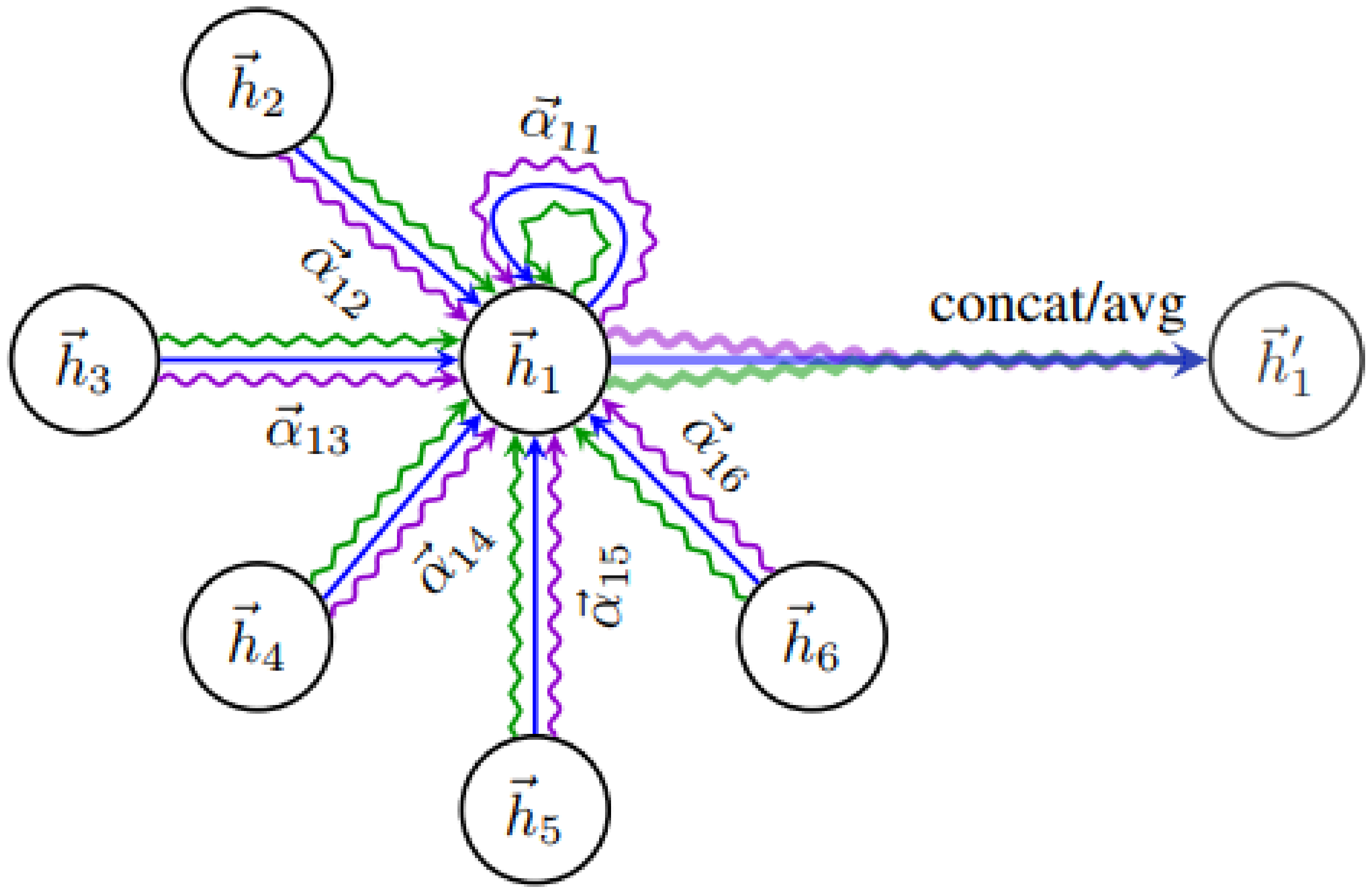
- There is an increasing interest in generalizing convolutions to the graph domain. **However, the learned filters depends** n a specific structure can not be directly applied t

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

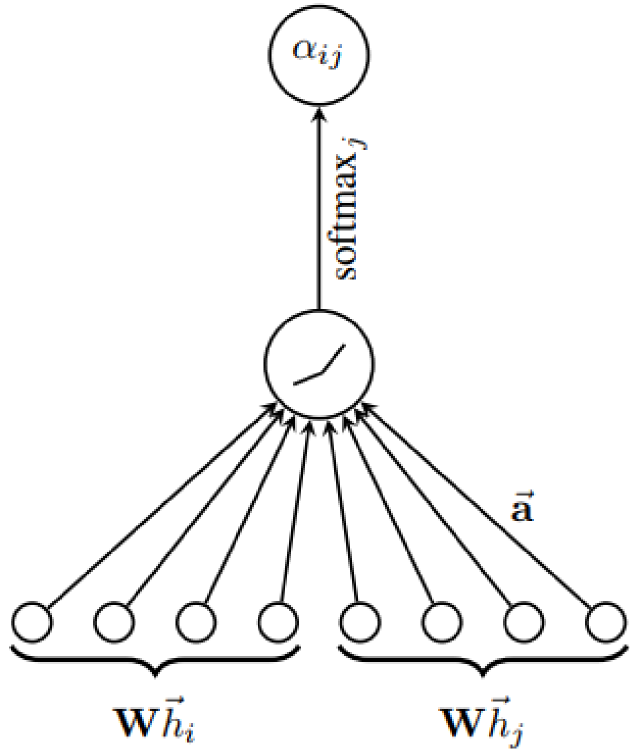
Graph Attention Network

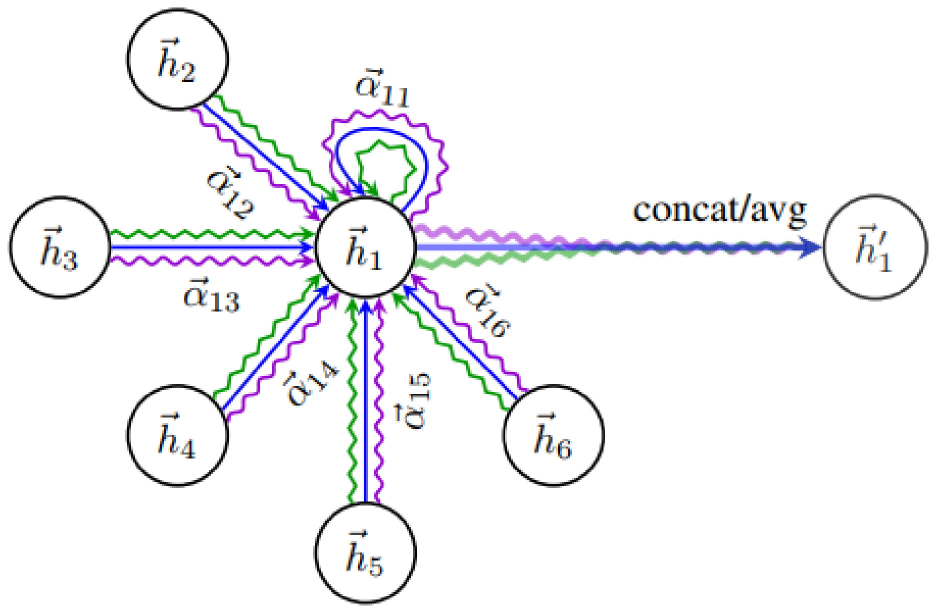
- The input to the layer is a set of **h** nodes with **F** features in each node. The layer produces a new set of node features (of potentially different cardinality **F'**), as its output.
- In order to obtain sufficient expressive power to transform the input features into higher-level features, a shared linear transformation, parametrized by a weight matrix, **W**, is applied to every node.





Graph Attention Network





- Self-attention is then performed on the nodes—a shared attentional mechanism $a : \mathbb{R}^{F'} \times \mathbb{R}^{F'} \rightarrow \mathbb{R}$ computes attention coefficients:

$$e_{ij} = a(\mathbf{W}\vec{h}_i, \mathbf{W}\vec{h}_j) \qquad \alpha_{ij} = \mathrm{softmax}_j(e_{ij}) = \frac{\exp(e_{ij})}{\sum_{k\in\mathcal{N}_i}\exp(e_{ik})}$$

$$\alpha_{ij} = \frac{\exp\left(\mathrm{LeakyReLU}\left(\vec{\mathbf{a}}^T[\mathbf{W}\vec{h}_i\|\mathbf{W}\vec{h}_j]\right)\right)}{\sum_{k\in\mathcal{N}_i}\exp\left(\mathrm{LeakyReLU}\left(\vec{\mathbf{a}}^T[\mathbf{W}\vec{h}_i\|\mathbf{W}\vec{h}_k]\right)\right)} \qquad \vec{h}'_i = \sigma\left(\sum_{j\in\mathcal{N}_i}\alpha_{ij}\mathbf{W}\vec{h}_j\right)$$

Transductive Learning

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)

- Utilize three standard citation network benchmark datasets—Cora, Citeseer and Pubmed. In all 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.
- Following the transductive setup, the training algorithm has access to all of the nodes' feature vectors.

Inductive Learning

- Make use of a protein-protein interaction (PPI) dataset that consists of graphs corresponding to different human tissues.
- The dataset contains 20 graphs for training, 2 for validation and 2 for testing. Critically, testing graphs remain completely unobserved during training.
- 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.

Experimental Setup

- For the **transductive learning** tasks, a **two-layer GAT** model was applied. The first layer consists of 8 attention heads computing, F', 8 features each (for a total of 64 features), followed by an exponential linear unit (ELU) 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 the **inductive learning** tasks, a **three-layer GAT** model was applied. Both first 2 layers consist of 4 attention heads computing, F', 256 features each (for a total of 1024 features), followed by an ELU nonlinearity.
- The final layer is used for (multi-label) classification with 6 attention heads computing 121 features each, that are averaged and followed by a logistic sigmoid activation.

Results

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).

Transductive

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*	$81.4 \pm 0.5\%$	$70.9 \pm 0.5\%$	$\mathbf{79.0} \pm 0.3\%$
GAT (ours)	$\mathbf{83.0} \pm 0.7\%$	$\mathbf{72.5} \pm 0.7\%$	$\mathbf{79.0} \pm 0.3\%$

Results

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).

Inductive

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 ± 0.006
GAT (ours)	$\mathbf{0.973} \pm 0.002$

Conclusion

- The graph attention networks (GATs) operate on graph-structured data.
- The graph attentional layer utilized throughout these networks is **computationally efficient**, **allows for assigning different importances to different nodes** within a neighborhood, and does not depend on knowing the entire graph structure upfront.
- Potential improvements: able to handle larger batch sizes, extending the method to perform graph classification instead of node classification, extending the model to incorporate edge features would allow us to tackle a larger variety of problems.