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Graph Attention Networks

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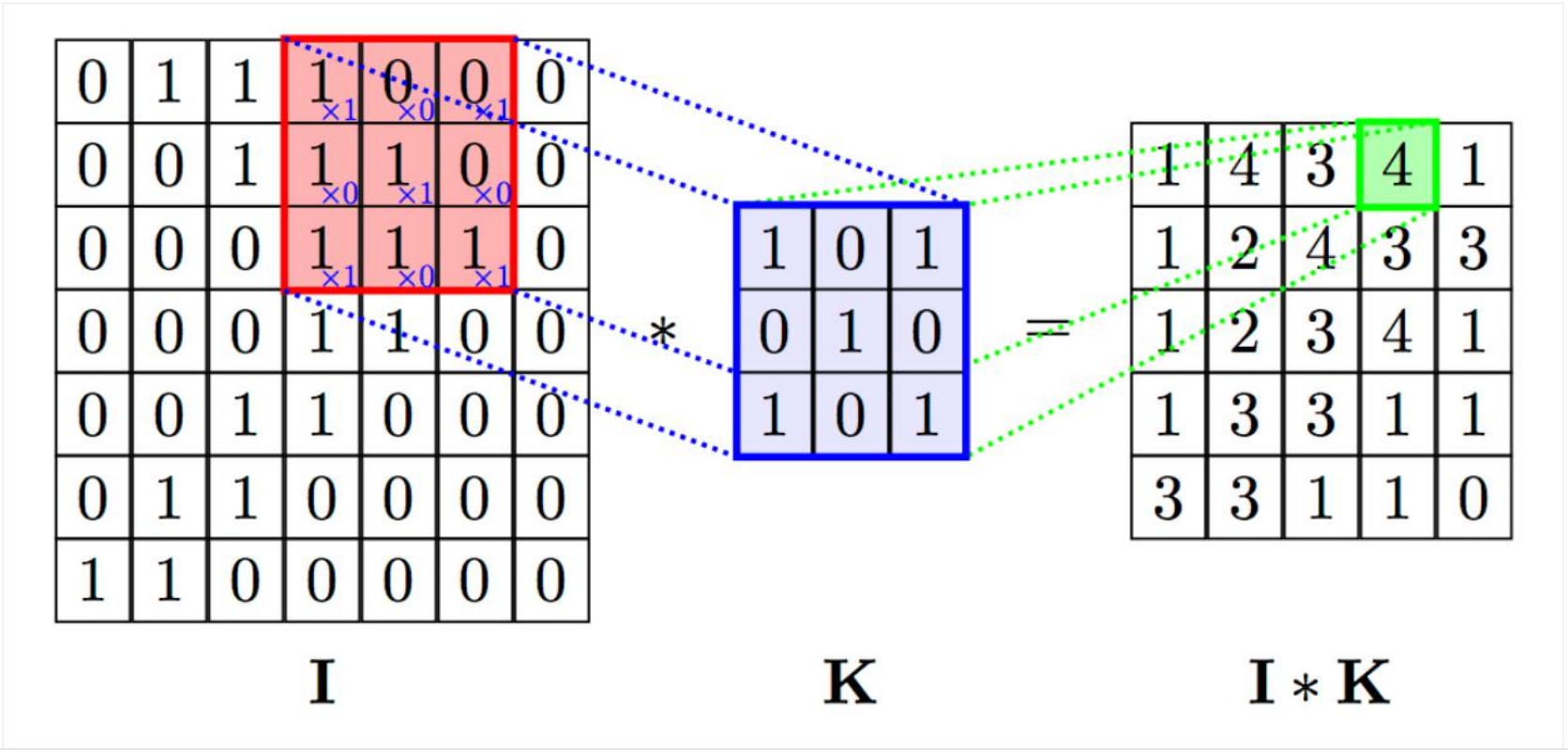
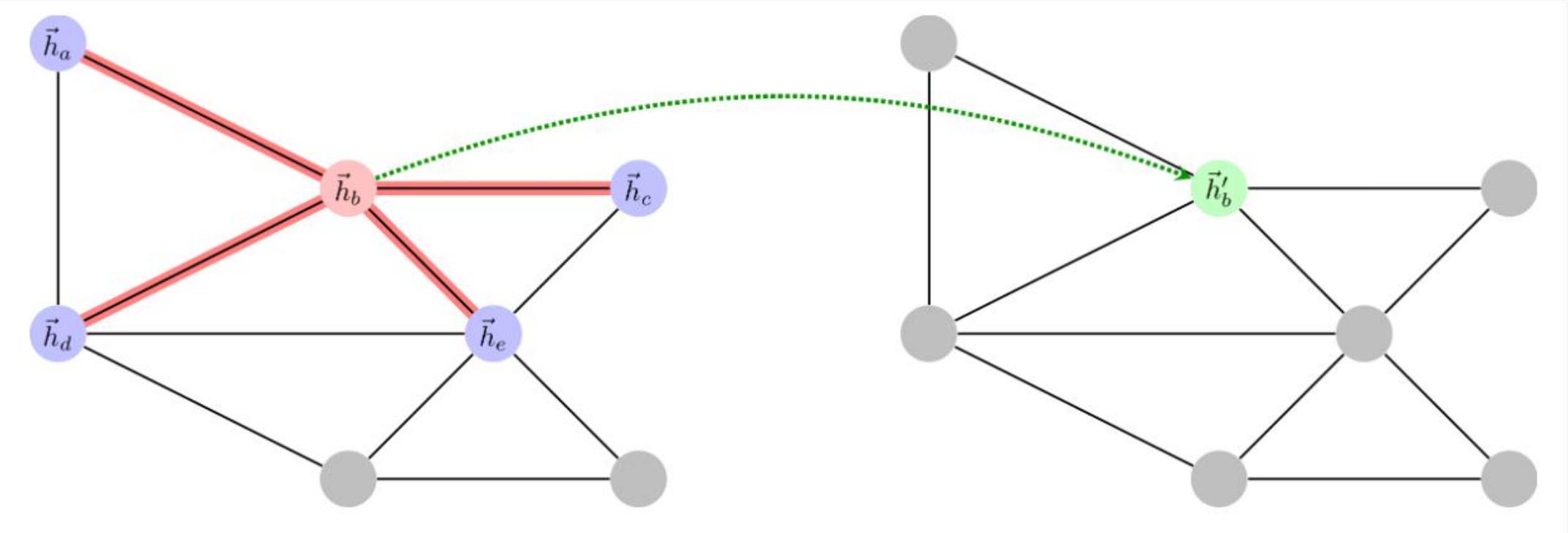
Motivation for graph convolutions

CNNs are a major workforce when it comes to working with image data. They exploit the fact that images have a highly rigid and regular connectivity pattern (each pixel “connected” to its eight neighbouring pixels), making such an operator trivial to deploy (as a small kernel matrix which is slid across the image).



Motivation for graph convolutions

Arbitrary graphs are a **much harder** challenge! Ideally, we would like to aggregate information across each of the nodes' neighbourhoods in a principled manner, but we are no longer guaranteed such rigidity of structure.



A desirable form of a graph convolutional operator.

Enumerating the desirable traits of image convolutions, we arrive at the following properties we would ideally like our graph convolutional layer to have:

- **Computational and storage efficiency** (requiring no more than $O(V + E)$ time and memory);
- **Fixed** number of parameters (independent of input graph size);
- **Localisation** (acting on a *local neighbourhood* of a node);
- Ability to specify **arbitrary importances** to different neighbours;
- Applicability to **inductive problems** (arbitrary, unseen graph structures).

Towards a viable graph convolution

Consider a graph of n nodes, specified as a set of node features, $(\vec{h}_1, \vec{h}_2, \ldots, \vec{h}_n)$, and an adjacency matrix $\mathbf{A}$, such that $\mathbf{A}_{ij} = 1$ if i and j are connected, and 0 otherwise[1]. A **graph convolutional layer** then computes a set of new node features, $(\vec{h}'_1, \vec{h}'_2, \ldots, \vec{h}'_n)$, based on the input features as well as the graph structure.

Every graph convolutional layer starts off with a shared node-wise feature transformation (in order to achieve a higher-level representation), specified by a weight matrix $\mathbf{W}$. This transforms the feature vectors into $\vec{g}_i = \mathbf{W}\vec{h}_i$. After this, the vectors $\vec{g}_i$ are typically recombined in some way at each node.

An attention coefficients αij over neighbourhoods of nodes Ni

$$e_{ij} = a(\mathbf{W}\vec{h}_i, \mathbf{W}\vec{h}_j)$$

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

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

where $\cdot^T$ represents transposition and $\|$ is the concatenation operation.

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

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

For stability, we employ *multi-head attention*—parallelising this process across K independent *attention heads*:

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

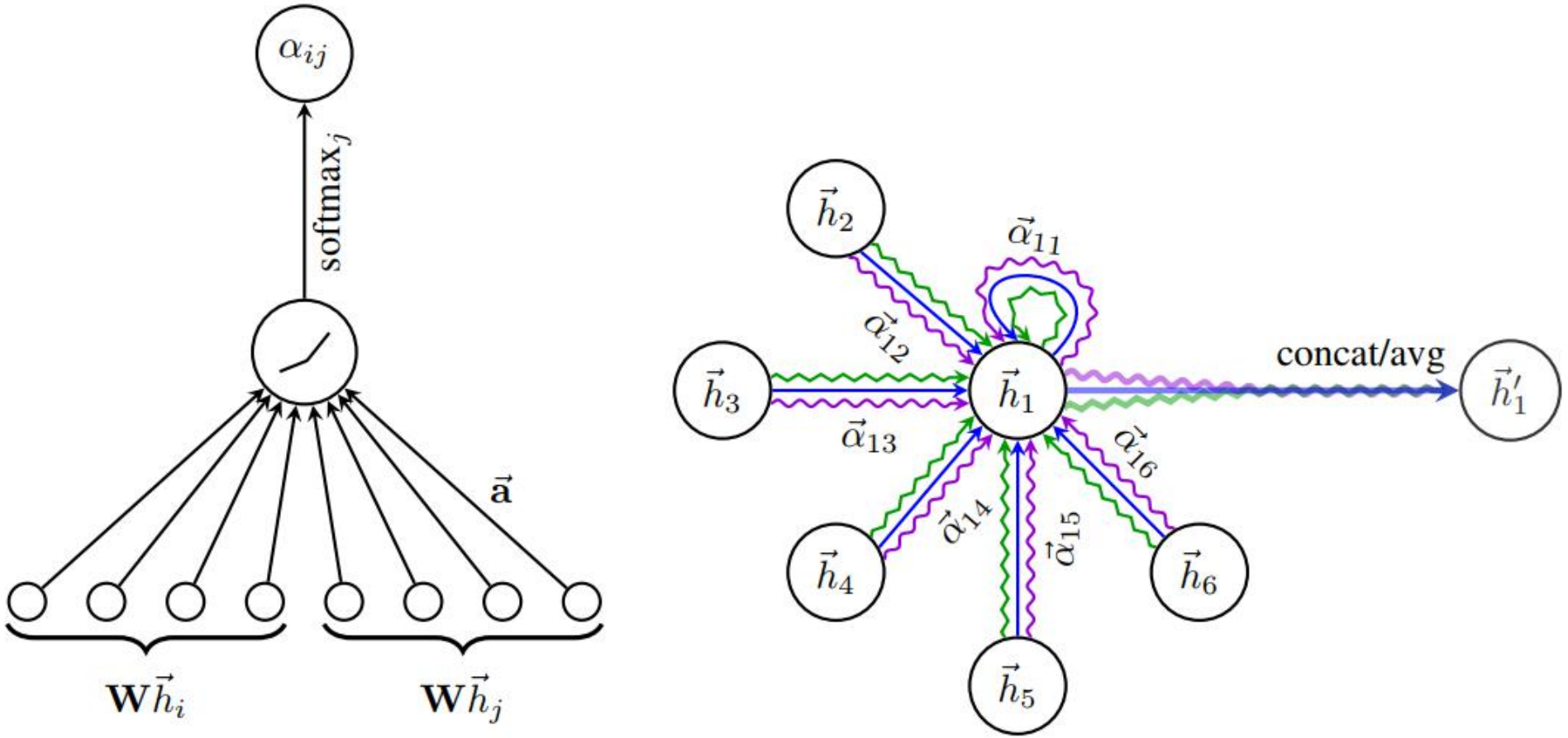


Figure 1: **Left:** The attention mechanism $a(\mathbf{W}\vec{h}_i, \mathbf{W}\vec{h}_j)$ employed by our model, parametrized by a weight vector $\vec{\mathbf{a}} \in \mathbb{R}^{2F'}$, applying a LeakyReLU activation. **Right:** An illustration of multi-head attention (with $K = 3$ heads) by node 1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

Properties

Computationally efficient: attention computation can be parallelised across all edges of the graph, and aggregation across all nodes!

Storage efficient—a sparse version does not require storing more than $O(V + E)$ entries anywhere;

Fixed number of parameters (dependent only on the desirable feature count, not on the node count);

Trivially **localised** (as we aggregate only over neighbourhoods);

Allows for (implicitly) specifying **different importances** to **different neighbours**, through its attentional mechanism;

Readily applicable to **inductive problems** (as it is a shared *edge-wise* mechanism that does not depend on the global graph structure)!

Satisfies all of the major requirements for a *graph convolutional layer* simultaneously.

Experiment

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 ± 0.5%	—	78.8 ± 0.3%
GCN-64*	81.4 ± 0.5%	70.9 ± 0.5%	**79.0** ± 0.3%
GAT (ours)	**83.0** ± 0.7%	**72.5** ± 0.7%	**79.0** ± 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).

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)	$\mathbf{0.973} \pm 0.002$

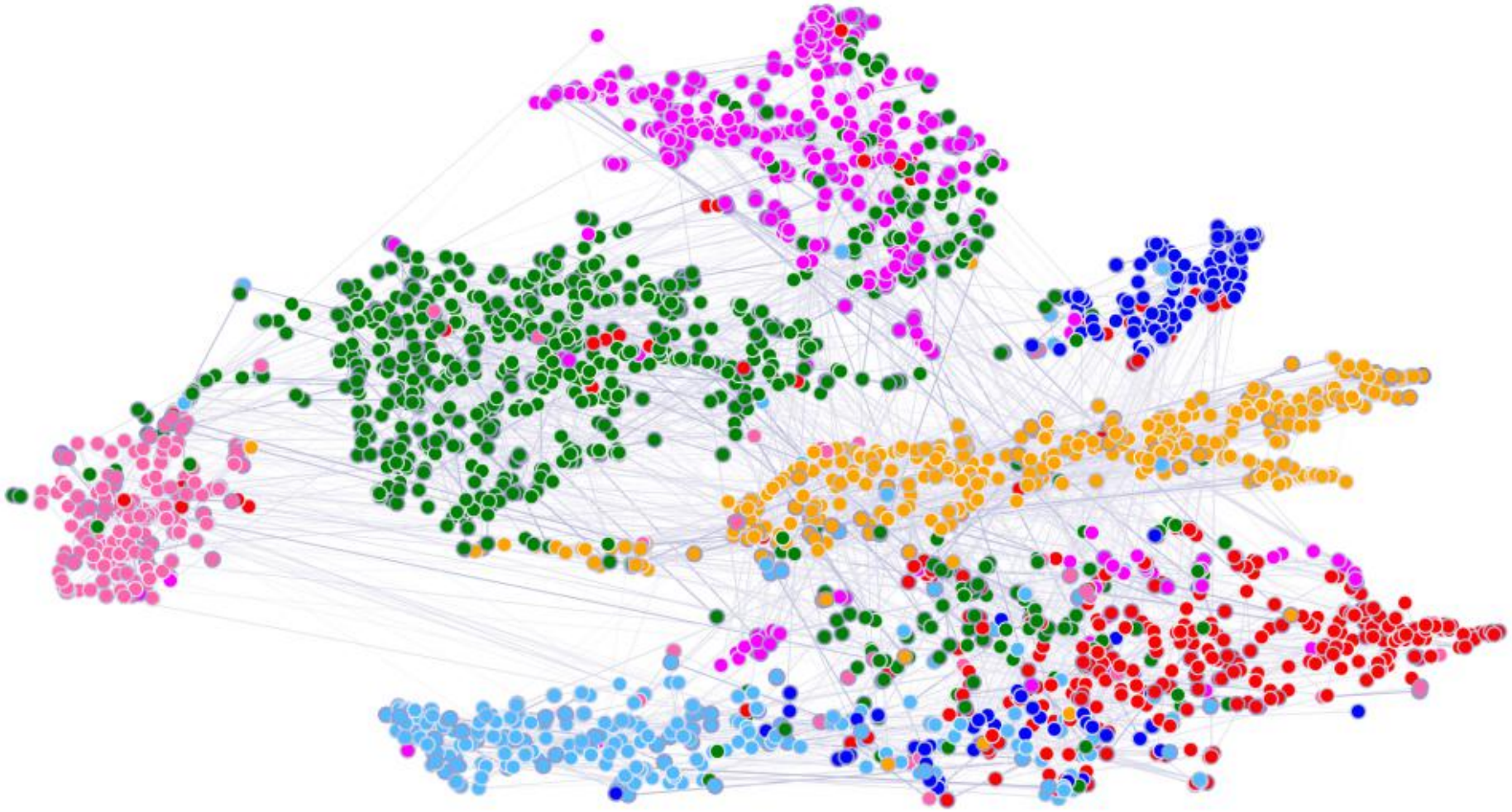


Figure 2: A t-SNE plot of the computed feature representations of a pre-trained GAT model's first hidden layer on the Cora dataset. Node colors denote classes. Edge thickness indicates aggregated normalized attention coefficients between nodes i and j, across all eight attention heads ($\sum_{k=1}^{K}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