GRAPH ATTENTION NETWORKS

Petar Velickovic´, Guillem Cucurull, Arantxa Casanova, Adriana Romero, Pietro Lio, Yoshua Bengio

Presented by: Tawkat

Why Graph Neural Net

- CNN can tackle problem when the underlying data representation is a grid-like structure.

- Not in the case of social networks, 3D-Mesh, biological networks

- We need to represent them with graph structure

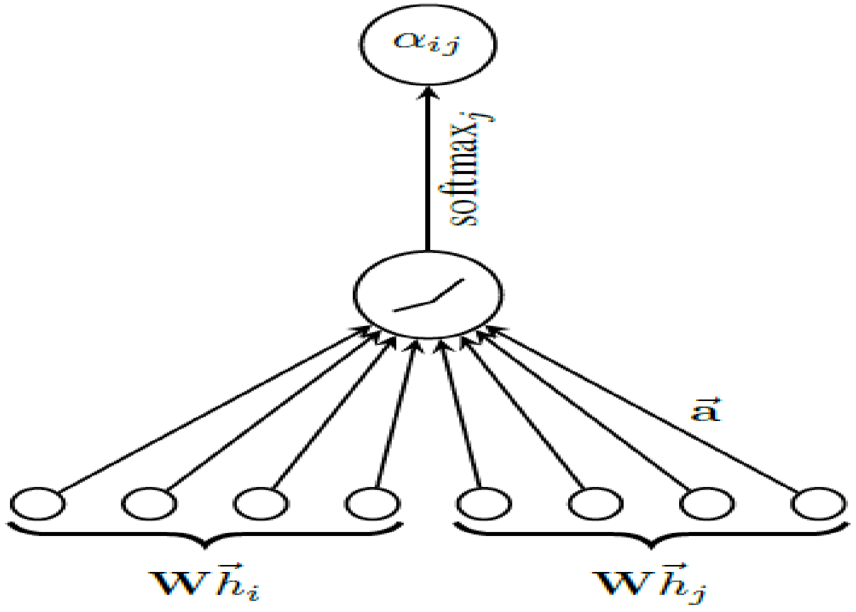
Why Graph Attn Net

- Traditional GNN assigns same weights to all nodes within a neighborhood, whereas GAT assigns weights to the nodes depending on their contributions.

- GAT enables better interpretability

- GAT applies attention mechanism to all the edges, so it does not depend on the global graph structure.

Graph Attn Net



- Input node features: $h = \{h_1, h_2, \ldots, h_N\} \in R^F$
- Output node features: $h' = \{h'_1, h'_2, \ldots, h'_N\} \in R^{F'}$
- Weight Matrix: $W \in R^{F \times F'}$
- $eij = a(Wh_i, Wh_j)$; where a: $R^{2 \times F'}$ is attention coeff. that indicate the importance of node j's features to node i.

Graph Attn Net

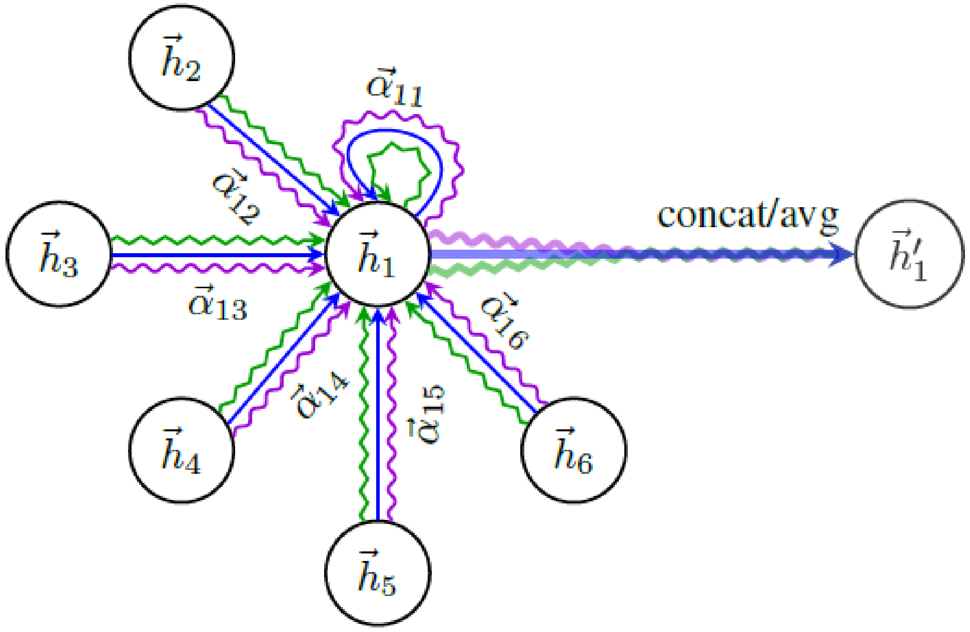
$$e_{ij} = a(\mathbf{W}\vec{h}_i, \mathbf{W}\vec{h}_j)$$

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

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

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

Graph Attn Net-Multi-Head



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

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

Experimental Results

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%

Experimental Results

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)	$\mathbf{0.973} \pm 0.002$

Future Works

- Analysis on better interpretability.
- Graph classification instead of node classification.
- Including edge features instead of treating edges just as boolean variables