

Simple and Deep Graph Convolutional Networks

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Problem

- Graph Convolutional Networks are stuck in a shallow architecture due to the over-smoothing issue.
- This paper proposes some modifications to the convolution of the GCNs, enabling a deep architecture.

Variants of GCNs

- Vanilla GCN:

$$\mathbf{H}^{(\ell+1)} = \sigma \left(\tilde{\mathbf{P}} \mathbf{H}^{(\ell)} \mathbf{W}^{(\ell)} \right)$$

- APPNP:

$$\mathbf{H}^{(\ell+1)} = (1 - \alpha) \tilde{\mathbf{P}} \mathbf{H}^{(\ell)} + \alpha \mathbf{H}^{(0)}$$

- JKNet:

$$\text{Aggregate}(\left[\mathbf{H}^{(1)}, \dots, \mathbf{H}^{(K)} \right])$$

- DropEdge:

$$\mathbf{H}^{(\ell+1)} = \sigma \left(\tilde{\mathbf{P}}_{\text{drop}} \mathbf{H}^{(\ell)} \mathbf{W}^{(\ell)} \right)$$

Deep GCNs

- Initial residual connection:

$$(1 - \alpha_\ell) \tilde{\mathbf{P}} \mathbf{H}^{(\ell)} + \alpha_\ell \mathbf{H}^{(0)}$$

- Identity mapping:

$$(1 - \beta_\ell) \mathbf{I}_n + \beta_\ell \mathbf{W}^{(\ell)}$$

- Propagation rule of the deep GCNs:

$$\mathbf{H}^{(\ell+1)} = \sigma \left(\left((1 - \alpha_\ell) \tilde{\mathbf{P}} \mathbf{H}^{(\ell)} + \alpha_\ell \mathbf{H}^{(0)} \right) \left((1 - \beta_\ell) \mathbf{I}_n + \beta_\ell \mathbf{W}^{(\ell)} \right) \right)$$

- α_ℓ is recommended to set to 0.1 or 0.2
- $\beta_\ell = \log(\frac{\lambda}{\ell} + 1) \approx \frac{\lambda}{\ell}$ where λ is a hyper-parameter (they set to 0.5)

Deep GCNs

- Vanilla GCNs simulate a polynomial filter $\left(\sum_{\ell=0}^K \theta_{\ell} \tilde{\mathbf{L}}^{\ell}\right) \mathbf{x}$ of order K with fixed coefficients θ .
- On the other hand, Deep GCNs with K layers are proved to be able to express a K order polynomial filter with arbitrary coefficients.
- The authors attribute this difference to the success of the Deep GCNs.

Results

Table 2. Summary of classification accuracy (%) results on Cora, Citeseer, and Pubmed. The number in parentheses corresponds to the number of layers of the model.

Method	Cora	Citeseer	Pubmed
GCN	81.5	71.1	79.0
GAT	83.1	70.8	78.5
APPNP	83.3	71.8	80.1
JKNet	81.1 (4)	69.8 (16)	78.1 (32)
JKNet(Drop)	83.3 (4)	72.6 (16)	79.2 (32)
Incep(Drop)	83.5 (64)	72.7 (4)	79.5 (4)
GCNII	85.5 \pm 0.5 (64)	73.4 \pm 0.6 (32)	80.2 \pm 0.4 (16)
GCNII*	85.3 \pm 0.2 (64)	73.2 \pm 0.8 (32)	80.3 \pm 0.4 (16)

Results

Table 3. Summary of classification accuracy (%) results with various depths.

Dataset	Method	Layers					
		2	4	8	16	32	64
Cora	GCN	81.1	80.4	69.5	64.9	60.3	28.7
	GCN(Drop)	82.8	82.0	75.8	75.7	62.5	49.5
	JKNet	-	80.2	80.7	80.2	81.1	71.5
	JKNet(Drop)	-	83.3	82.6	83.0	82.5	83.2
	Incep	-	77.6	76.5	81.7	81.7	80.0
	Incep(Drop)	-	82.9	82.5	83.1	83.1	83.5
	GCNII	82.2	82.6	84.2	84.6	85.4	85.5
	GCNII*	80.2	82.3	82.8	83.5	84.9	85.3
Citeseer	GCN	70.8	67.6	30.2	18.3	25.0	20.0
	GCN(Drop)	72.3	70.6	61.4	57.2	41.6	34.4
	JKNet	-	68.7	67.7	69.8	68.2	63.4
	JKNet(Drop)	-	72.6	71.8	72.6	70.8	72.2
	Incep	-	69.3	68.4	70.2	68.0	67.5
	Incep(Drop)	-	72.7	71.4	72.5	72.6	71.0
	GCNII	68.2	68.9	70.6	72.9	73.4	73.4
	GCNII*	66.1	67.9	70.6	72.0	73.2	73.1
Pubmed	GCN	79.0	76.5	61.2	40.9	22.4	35.3
	GCN(Drop)	79.6	79.4	78.1	78.5	77.0	61.5
	JKNet	-	78.0	78.1	72.6	72.4	74.5
	JKNet(Drop)	-	78.7	78.7	79.1	79.2	78.9
	Incep	-	77.7	77.9	74.9	OOM	OOM
	Incep(Drop)	-	79.5	78.6	79.0	OOM	OOM
	GCNII	78.2	78.8	79.3	80.2	79.8	79.7
	GCNII*	77.7	78.2	78.8	80.3	79.8	80.1