On the Global Self-attention Mechanism for Graph Convolutional Networks

Chengyuan Deng
Rutgers University

Chen Wang
Rutgers University

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Global Self-attention Mechanism

GSA in Convolutional Neural Networks

- [ZGMO'18] Self-attention GAN
- Image details generated from global feature locations

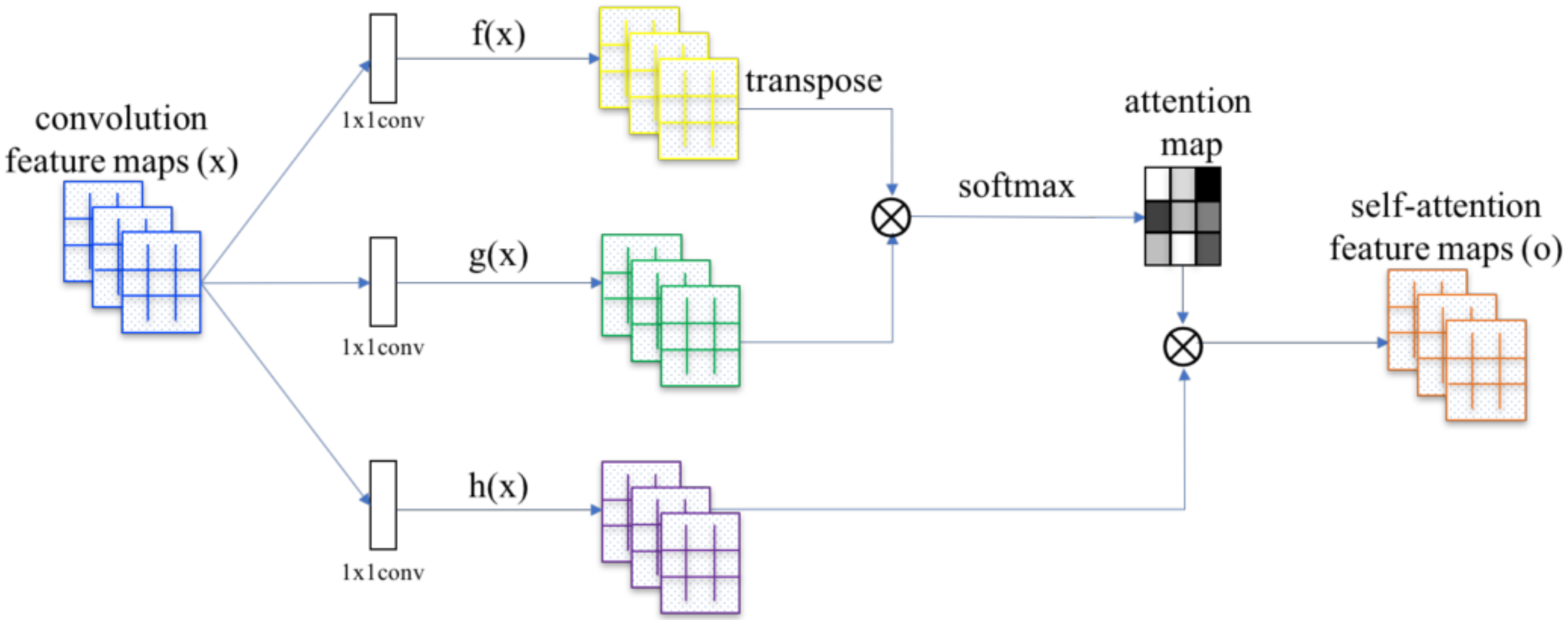
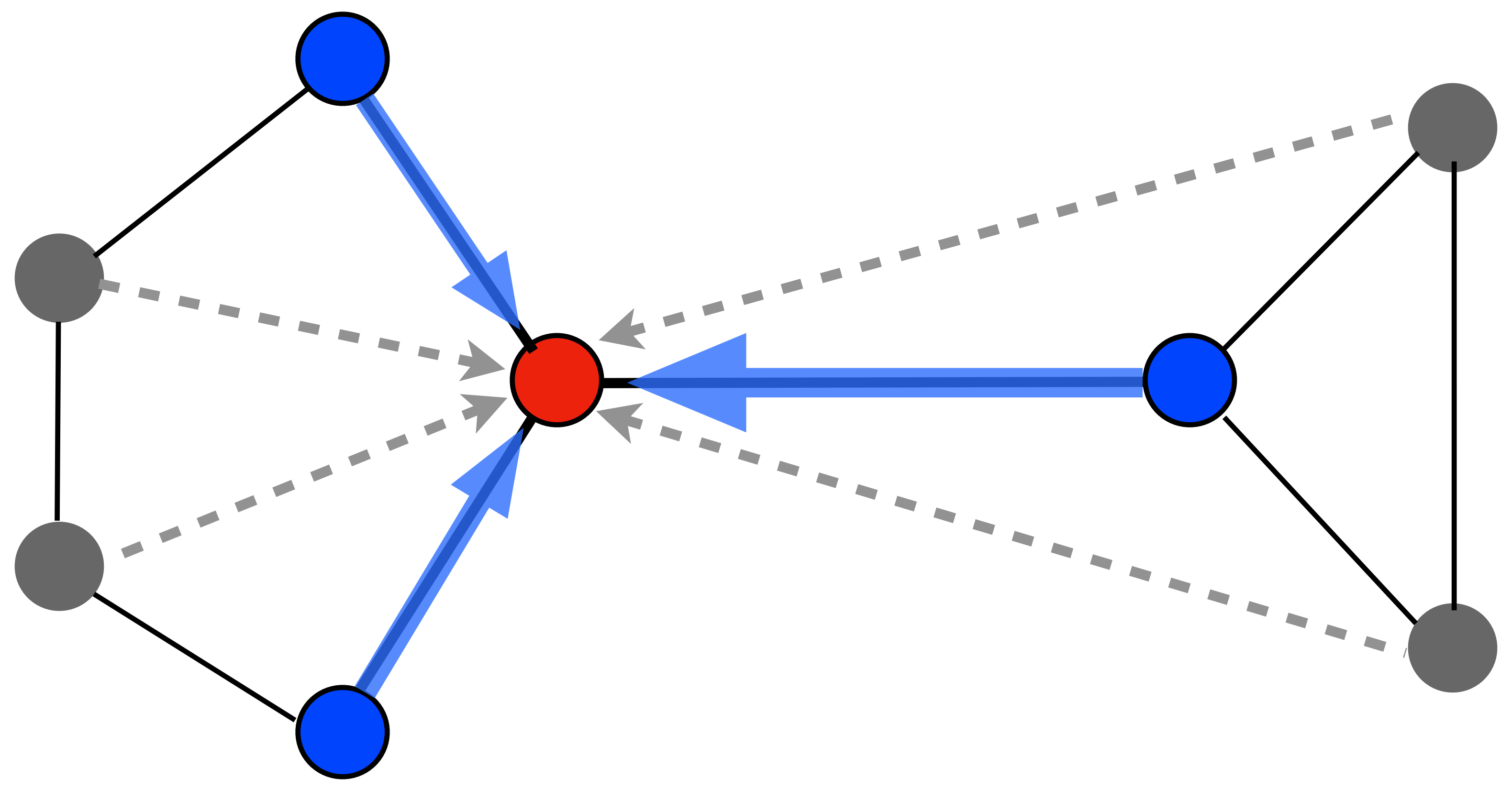


Image source: https://arxiv.org/abs/1805.08318

Global Self-attention Mechanism

GSA in Graph Convolutional Networks

- Vanilla self-attention: information between neighbors
- [WD'20] Global self-attention: regardless of edge connection



Graph Convolutional Networks

Graph Convolutions [KW '17]

- Message-passing GNN
- First order approximation of spectral convolutions

Layer Update

- $f(H^{(l+1)}, A) = \sigma(\hat{D}^{-\frac{1}{2}}\hat{A}\hat{D}^{-\frac{1}{2}}H^{(l)}W^{(l)})$

  where $\hat{A}$ is a normalized adjacency matrix, and $\hat{D}_{ii} = \sum_j \hat{A}_{ij}$

Motivation

Attention methods in GNNs

- Attention methods in GNNs: [VCCRLB '18] [ZXT '20][ZSXMKY '18]
- [PWCLY '18] Weakness: "lack of the ability to capture long-range dependencies"
- [ZGMO'18] Self-attention GAN remedies the weakness
- Main motivation:
  - Similarity between convolutions on images and graphs
  - Can Global self-attention improves the performance of GCNs?

Motivation

Theoretical Anlaysis on GCNs

- [RHXH '19] and [LMTD '19] Over-smoothing problem of GCNs:
    - Deep GCNs: hard to optimize training loss
- [LHW '19] Why over-smoothing?
    - A special form of Laplacian smoothing
    - Converge to a feature-invariant space as
- [OS '20] Convergence rate:
    - Exponential to the maximum singular value of the convolutional filter

Contributions: Two-Fold

Theoretical Analysis

- Prove: Global Self-attention can alleviate over-fitting and over-smoothing problems

GSA-GCN: A Novel Framework

- Experiments on two classical tasks: node classification and graph classification
- Empirical results corroborate our theoretical analysis

Theoretical Analysis

Main Results on Over-fitting

Assumptions: (1) d-regular graph (2) -1/1 feature influence between vertices

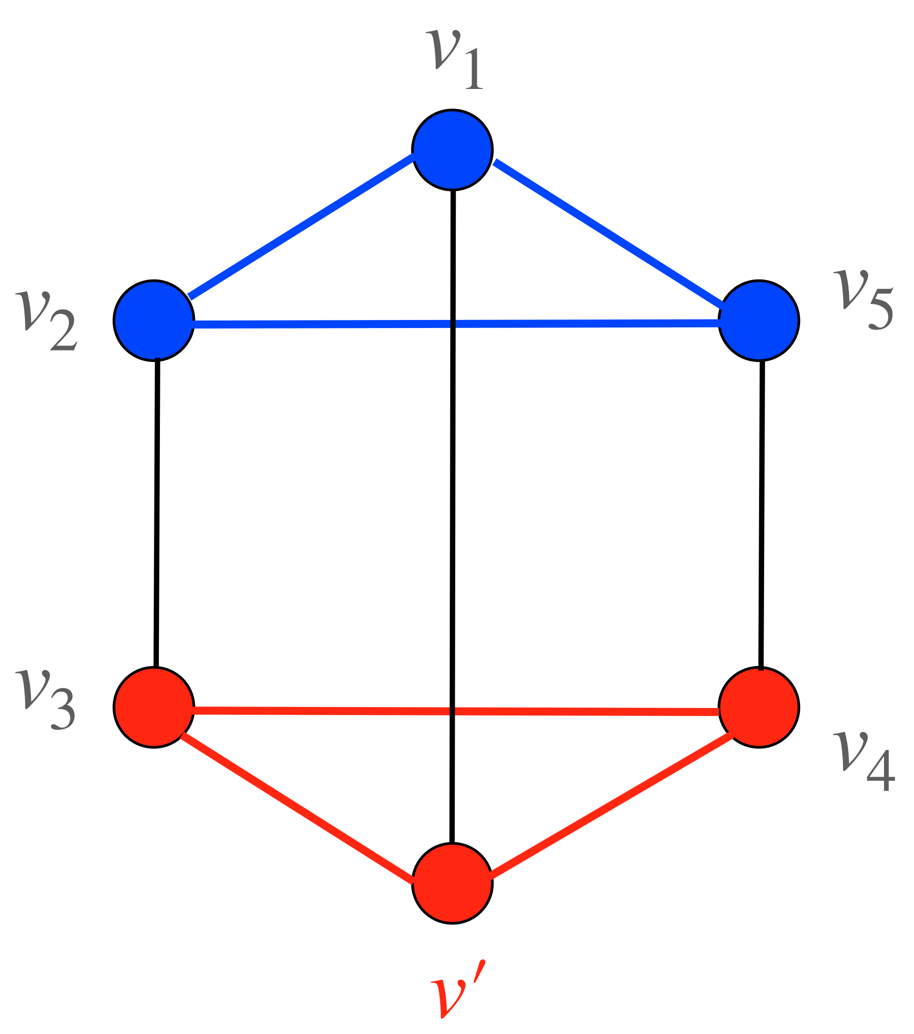
- Key Lemma: There exists a way to arrange the GSA feature relations, such that for at least $\Omega(\frac{n}{4^r})$ $(r < n)$ vertices, the GSA mechanism will eliminate the influence of one vertex in the neighbors
- Proof sketch of the Key Lemma:
  - A natural corollary of Ramsey theorem

Theoretical Analysis

Main Results on Over-fitting

Key Lemma: There exists a way to arrange the GSA feature relations, such that for at least $\Omega(\frac{n}{4^r})$ $(r < n)$ vertices, the GSA mechanism will eliminate the influence of one vertex in the neighbors

- Proof sketch of the Key Lemma:
  - A natural corollary of Ramsey theorem
  - $R(r+1, r+1)$ vertices, there must exist $(r+1)$ vertices with either +1 / -1 influence
  - Normalized GSA influence: +1 / -1, pick $\gamma = \frac{1}{d}$
  - GSA influence: $+\frac{1}{d}$ or $-\frac{1}{d}$
  - Eliminate the influence from one $v_i \in N(v')$



Theoretical Analysis

Main Results on Over-smoothing

The convergence rate to the feature-invariant subspace of GSA-GCN is slower than that of plain GCNs

- Key lemma: Applying GSA is equivalent to substituting convolution weight matrices with a larger maximum singular value
- High-level proof of the key lemma:
  - GSA matrix: Hermitian and Positive Definite $PW = (I + \gamma \cdot Q)W$
  - [KT '01] Minimum eigenvalue larger than 1 $\lambda_{min}(P) \geq \lambda_{min}(I) + \lambda_{min}(Q) > 1$
  - 2-norm connects singular value and above results

$$\tilde{s}^l = ||\tilde{W}^l|| = ||(I + \gamma \cdot Q)W^l|| \geq \lambda_{min}(P)||W^l|| > ||W^l|| = s^l$$

GSA-GCN: Framework

Layer Update of GSA-GCN:

$$H^{(l+1)} = \sigma((\tilde{A}H^{(l)} + \gamma O^{(l)})W^{(l)})$$

where $O^{(l)}$ is the output of the GSA layer, γ is a non-negative trainable parameter and $W^{(l)}$ is the convolution matrix of layer l

GSA-GCN: Experiments

Node Classification: Inductive

- We strictly follow the experimental setup in the literature [KW'17]
- Two-layer GCN backbone is considered as baseline

Table 2: Semi-supervised Node Classification Accuracy(%)

Model	Cora	Citeseer	Pubmed
GCN	81.5	70.3	79.0
GAT	83.0	72.5	79.0
JK-Net (4)	80.2	68.7	78.0
DropEdge-GCN	82.8	72.3	79.6
GSA-GCN	**83.3**	**72.9**	**80.1**

GSA-GCN: Experiments

Node Classification: Transductive

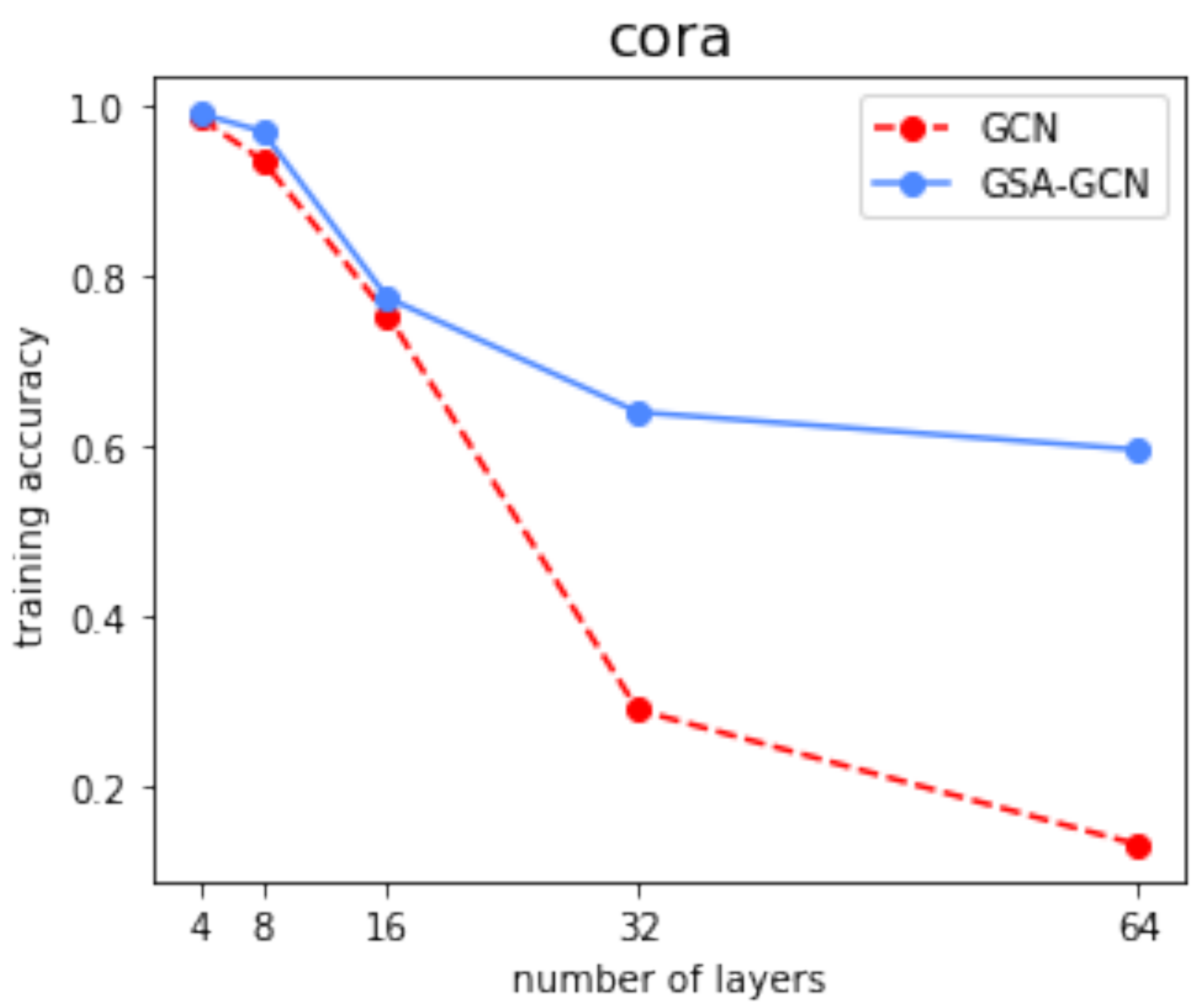
Table 3: Full-supervised Node Classification Accuracy(%)

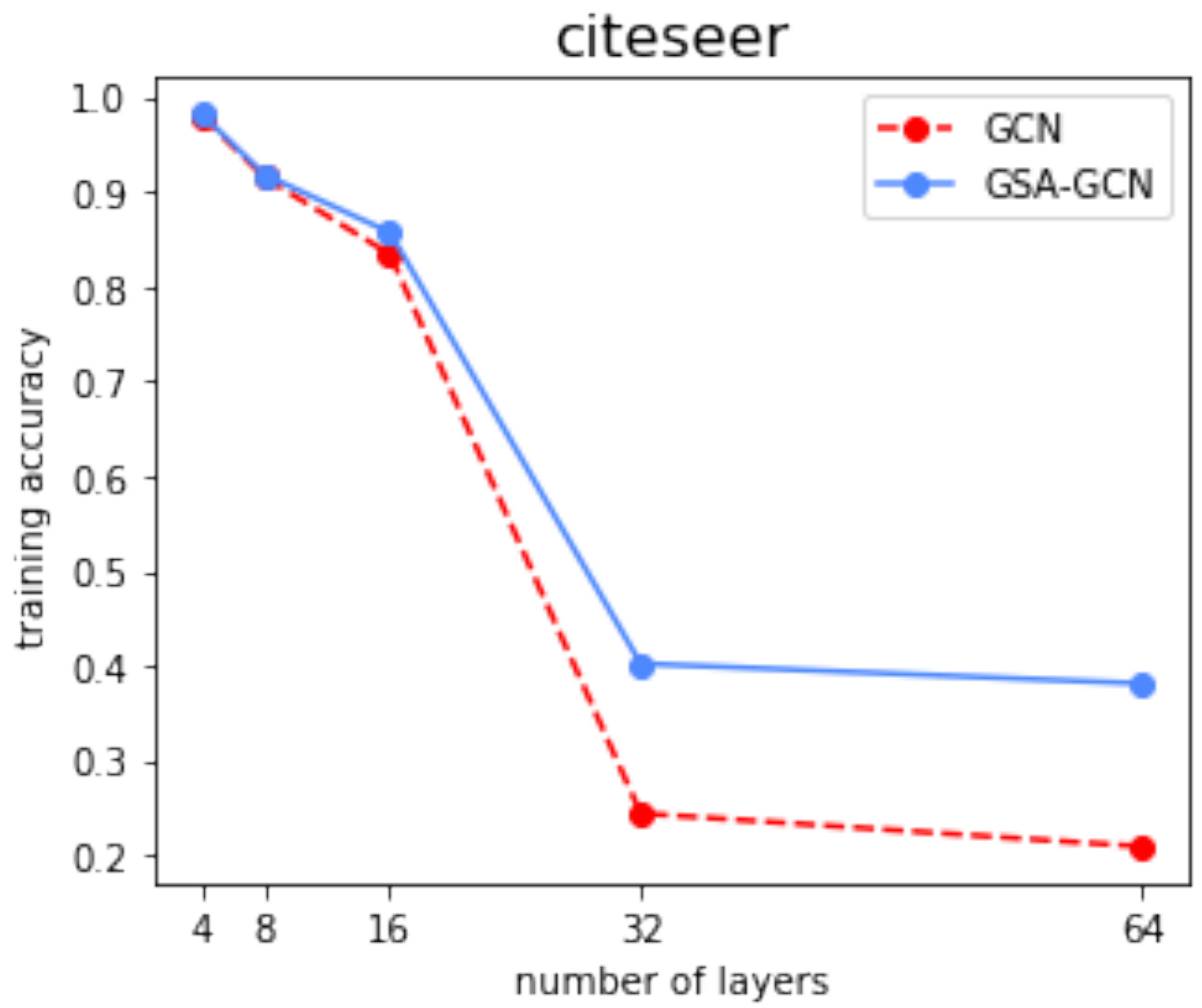
Model	Cora	Citeseer	Pubmed
GCN	86.1	75.9	90.2
GAT	86.4	76.6	OOM
JK-Net	86.9	78.3	90.5
DropEdge-GCN	86.5	78.7	**91.2**
GSA-GCN	**88.2**	**79.1**	89.4

- GSA-GCN performs competitively to the state-of-the-art

GSA-GCN: Experiments

Alleviate Over-smoothing





- As the layers go deeper, the gap between GSA-GCN and plain GCN becomes more significant

Conclusions

- Global Self-attention:
  - Propagate global node features with soft-max
  - Remedy the over-fitting and over-smoothing problem of GCNs
  - Competitive experimental results corroborate

Open Questions

- Remove the assumptions
- Geometry-independent self-attention
  - Explicitly find the fraction of vertices that have impacts
  - (Potentially) Substitute GSA with an efficient algorithm

Main References

[WD'20] On the Global Self-attention Mechanism for GraphConvolutional Networks

[KW'17] Semi-supervised classification with graph convolutional networks

[VCCRLB '18] Graph Attention Networks

[ZXT '20] Context aware graph convolution for skeleton-based action recognition

[ZSXMKY '18] Gaan: Gated attention networks for learning on large and spatiotemporal graphs

[ZGMO'18] Self-attention Generative Adversarial Networks

[PWCLY '18] Geom-gcn: Geometric graph convolutional networks

[RHXH '19] Dropedge: Towards deep graph convolutional networks on node classification

[LMTD '19] Deepgcns: Can GCNs go as deep as CNNs?

[LHW '19] Deeper insights into graph convolutional networks for semisupervised learning

[OS '20] Graph neural networks exponentially lose expressive power for node classification

[KT '01] Honeycombs and Sums of Hermitian Matrices