Graph Neural Networks with Adaptive Residual

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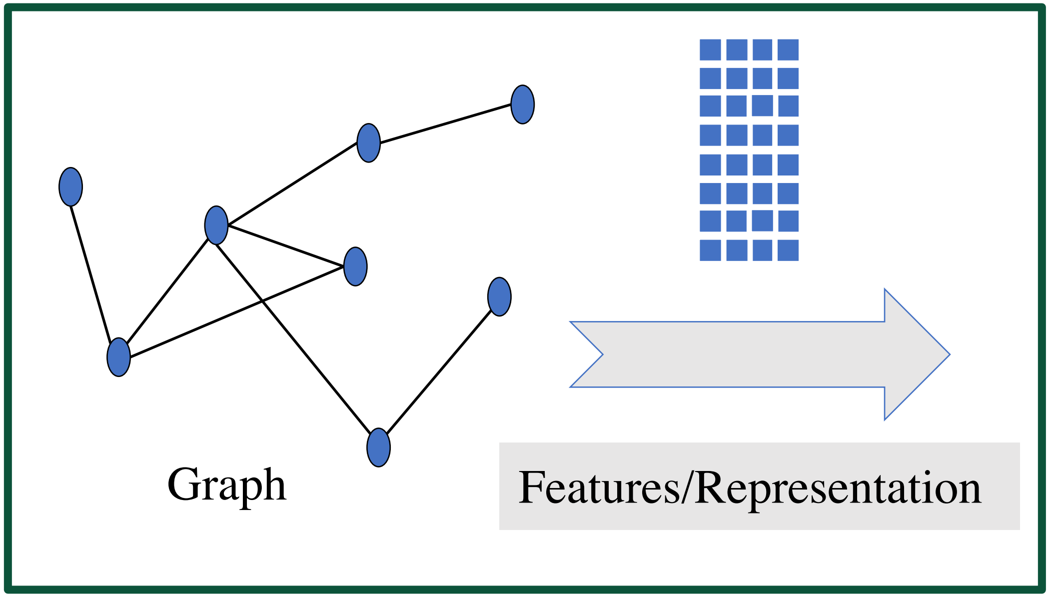
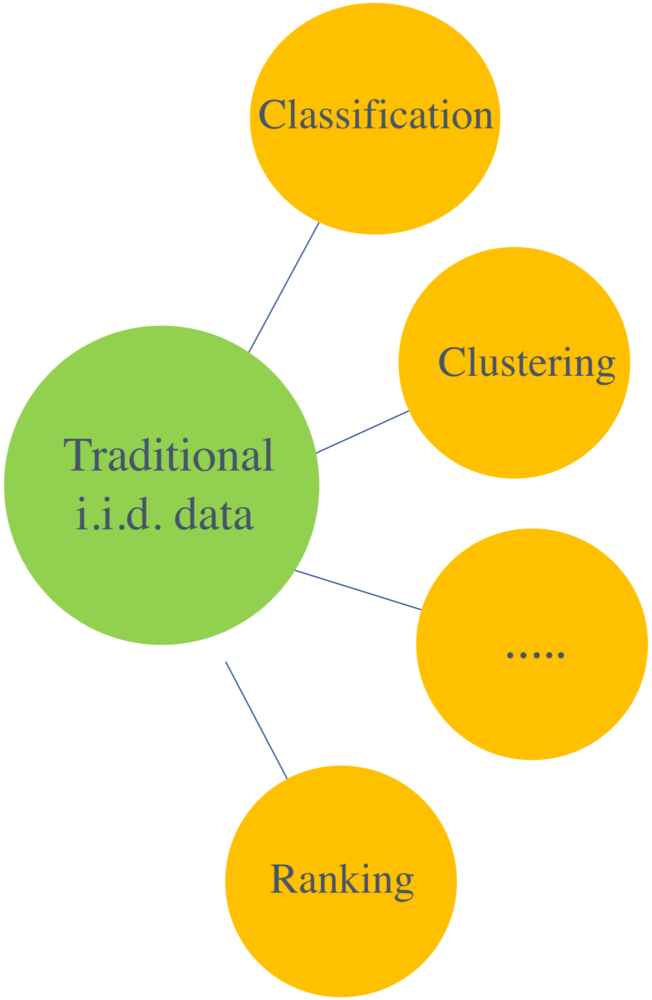
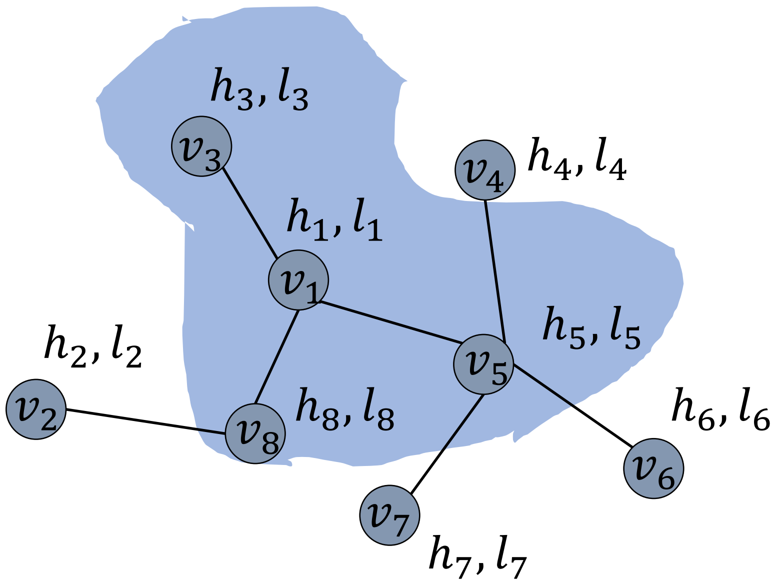
Machine Learning on Graphs



Representation Learning on Graphs



Graph Neural Networks



Message Passing

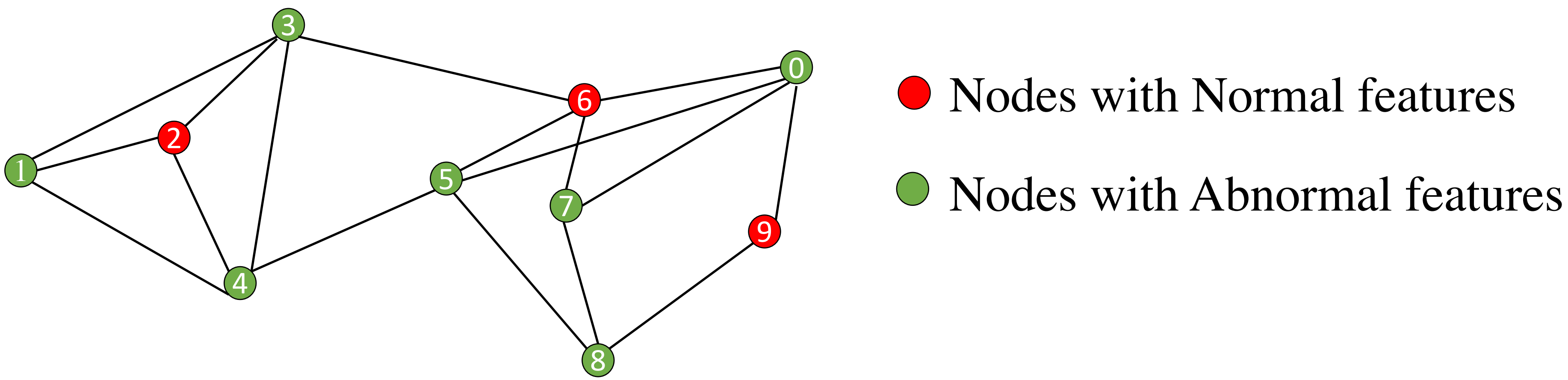
$$m_i^{(k+1)} = \sum_{v_j \in N(v_i)} M_k\left(h_i^{(k)}, h_j^{(k)}, e_{ij}\right)$$

Feature Updating

$$h_i^{(k+1)} = U_k\left(h_i^{(k)}, m_i^{(k+1)}\right)$$

Neural Message Passing for Quantum Chemistry, Justin Gilmer et al**,** ICML 2017

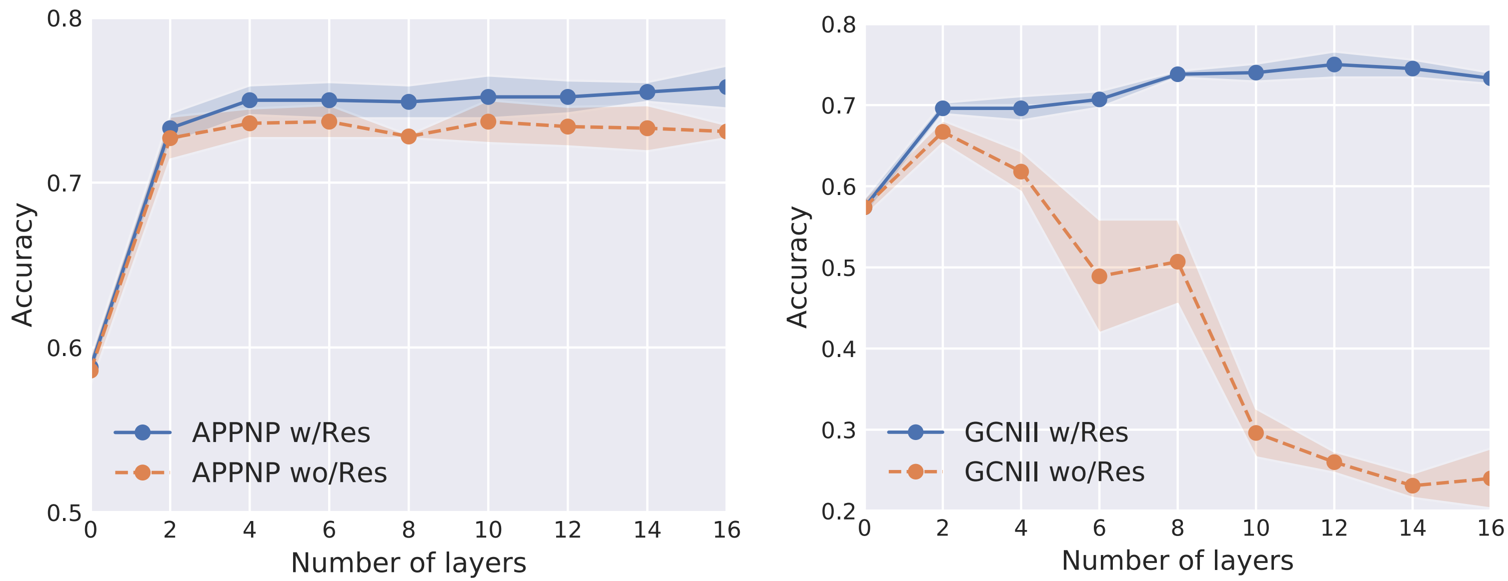
A Practical Scenario



Examples of abnormal features

- **Missing feature**: new users in social networks
- **Noisy feature**: uncertainty and dynamics in traffic information
- **Adversarial features**: node attributes are maliciously manipulated

An Interesting Discovery



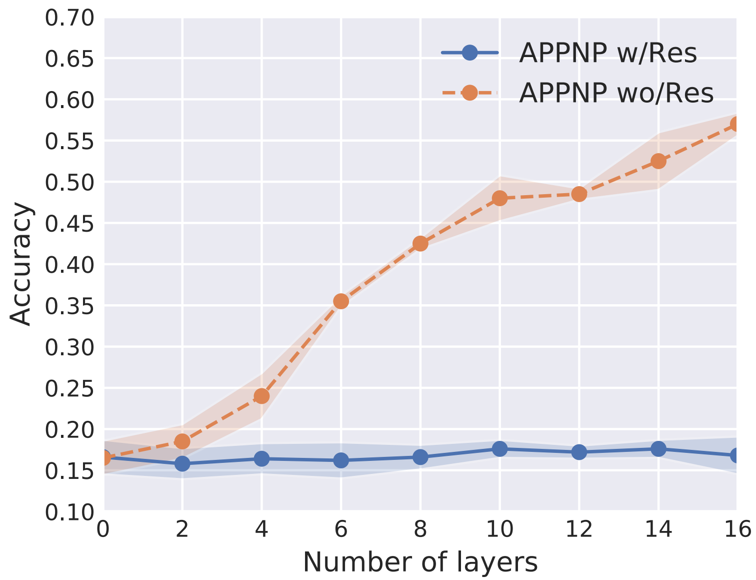
Node classification accuracy for nodes with normal features
(with 10% noisy nodes in Cora)

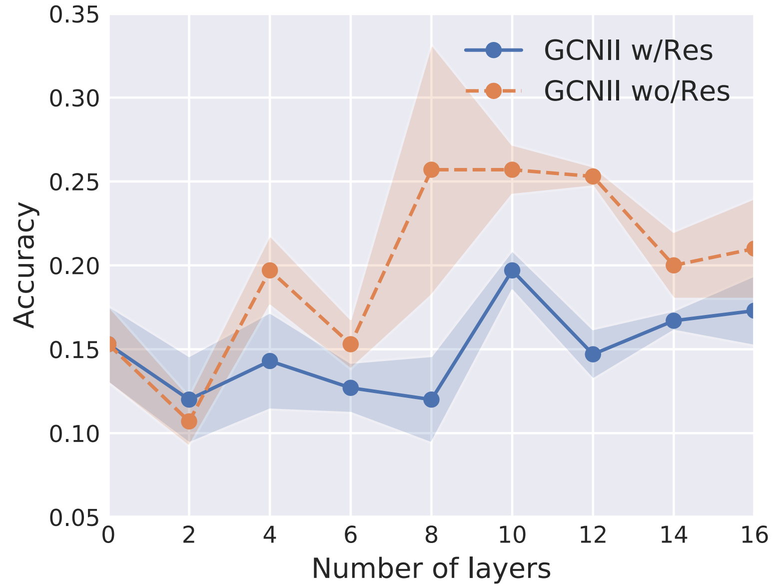
Finding I: (necessity of residual)

(1) Residual connection helps GNNs benefit from more layers;

(2) Without residual, too many aggregations could hurt the performance.

An Interesting Discovery (Cont.)





Node classification accuracy for nodes with noisy features
(with 10% noisy nodes in Cora)

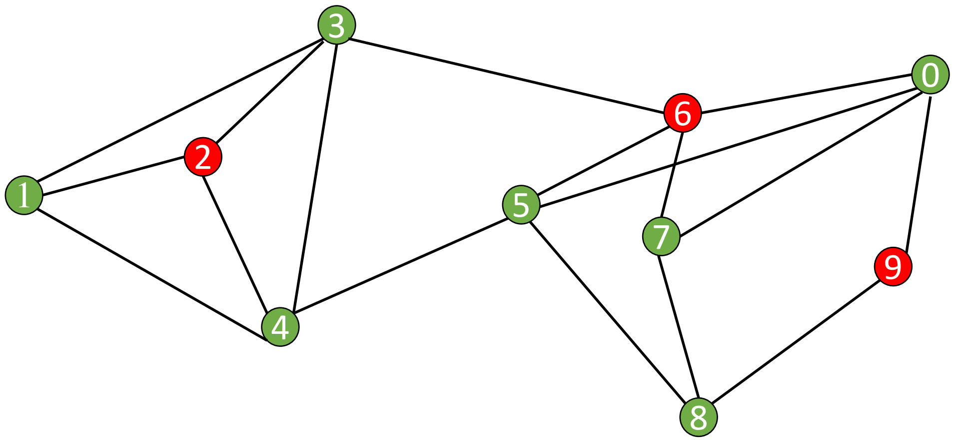
Finding II: (necessity of aggregation)

(1) Feature aggregations can boost the performance for noisy nodes;

(2) Residual connection makes GNNs more fragile to noisy node features.

An Interesting Discovery (Cont.)

A practical scenario



Nodes with Normal features

Nodes with Abnormal features

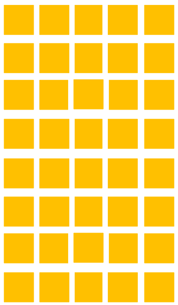
The dilemma:

(1) Normal features need residual connections to avoid over-smoothing

(2) Residual connections hurt the performance for nodes with abnormal features

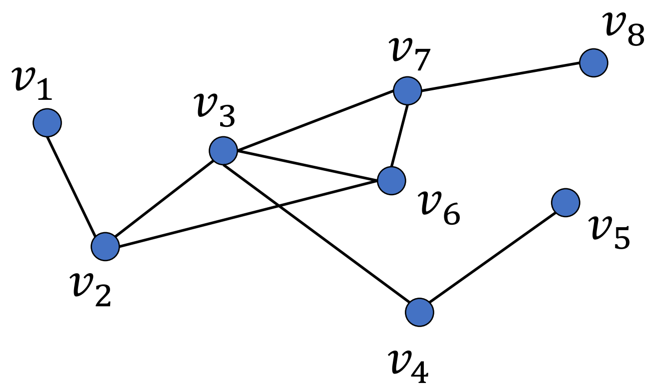
Understanding from GSP

"Noisy Signal"

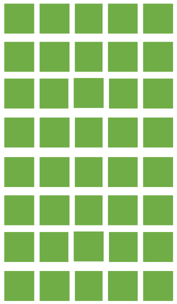


$\mathbf{X}_{\mathrm{in}}$

Graph



"Clean Signal"



$\mathbf{F}$

"Nodes are similar as their neighbors"

$$\arg\min_{\mathbf{X}\in\mathbb{R}^{n\times d}} \mathcal{L}(\mathbf{X}) := \frac{\alpha}{2(1-\alpha)}\|\mathbf{X}-\mathbf{X}_{\mathrm{in}}\|_F^2 + \frac{1}{2}\mathrm{tr}\Big(\mathbf{X}^\top(\mathbf{I}-\tilde{\mathbf{A}})\mathbf{X}\Big)$$

Proximity to the input **Smoothness prior**

A unified view on graph neural networks as graph signal denoising, Yao Ma, Xiaorui Liu et al, 2020

Understanding from GSP

$$\arg\min_{\mathbf{X}\in\mathbb{R}^{n\times d}} \mathcal{L}(\mathbf{X}) := \frac{\alpha}{2(1-\alpha)}\|\mathbf{X}-\mathbf{X}_{\text{in}}\|_F^2 + \frac{1}{2}\operatorname{tr}\left(\mathbf{X}^\top(\mathbf{I}-\tilde{\mathbf{A}})\mathbf{X}\right)$$

Proximity to the input **Smoothness prior**

Define Prior ⇨ Optimization Solver ⇨ Message Passing

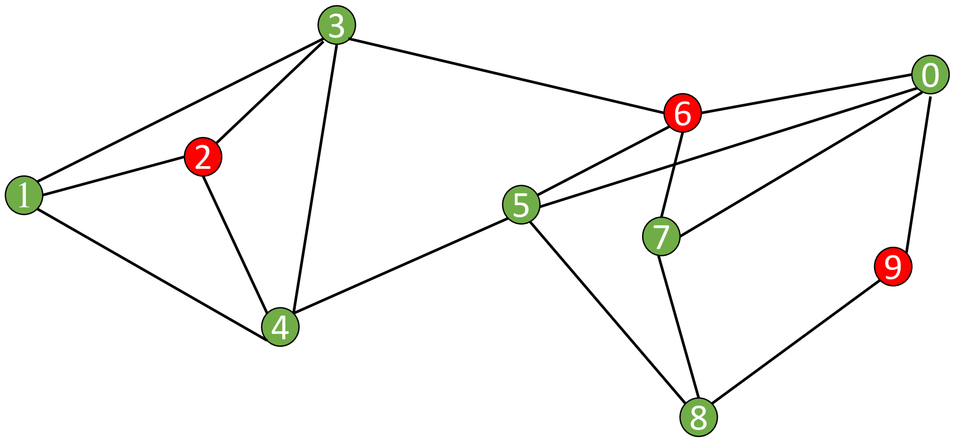
GCN $\mathbf{X}_{\text{out}} = \tilde{\mathbf{A}}\mathbf{X}_{\text{in}}$ APPNP/GCNII $\mathbf{X}^{(k+1)} = (1-\alpha)\tilde{\mathbf{A}}\mathbf{X}^{(k)} + \alpha\mathbf{X}_{\text{in}}$

- **Feature aggregation**: correct abnormal features by smoothing
- **Residual connection**: reduce feature over-smoothing by maintaining feature proximity but carry undesirable abnormal features

A unified view on graph neural networks as graph signal denoising, Yao Ma, Xiaorui Liu et al, 2020

Motivation

A practical scenario



- Nodes with Normal features
- Nodes with Abnormal features

Can we design a message passing with node-wise adaptive feature aggregation and residual connection to achieve good performance on both types of nodes?

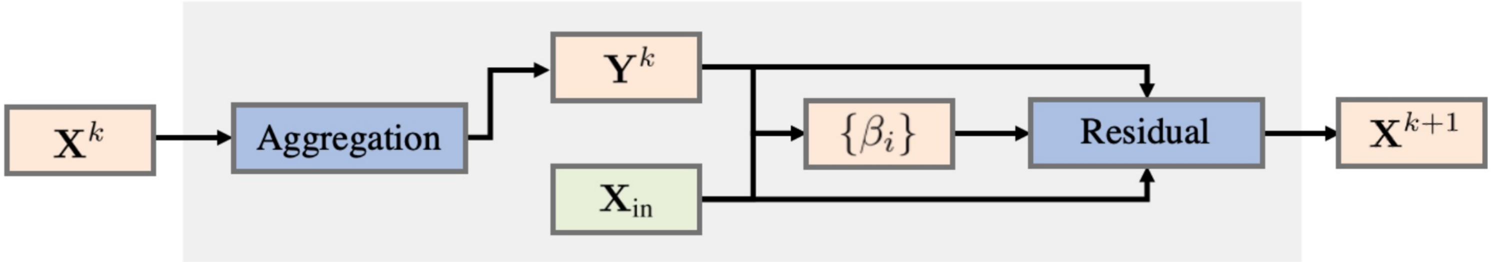
Motivation

$$\underset{\mathbf{X}\in\mathbb{R}^{n\times d}}{\arg\min} \quad \mathcal{L}(\mathbf{X}) := \lambda\|\mathbf{X}-\mathbf{X}_{\text{in}}\|_{21} + (1-\lambda)\mathrm{tr}(\mathbf{X}^\top(\mathbf{I}-\tilde{\mathbf{A}})\mathbf{X})$$

$$\|\mathbf{X}-\mathbf{X}_{\text{in}}\|_{21} := \sum_{i=1}^{n}\|\mathbf{X}_i-(\mathbf{X}_{\text{in}})_i\|_2$$

- Laplacian smoothing with the robust feature proximity
- Tolerate large deviations due to the less aggressive penalty on large values
- Potential removal of abnormal features

Adaptive Message Passing



$$\begin{cases} \mathbf{Y}^k & = \big(1-2\gamma(1-\lambda)\big)\mathbf{X}^k + 2\gamma(1-\lambda)\tilde{\mathbf{A}}\mathbf{X}^k \\ \beta_i & = \max(1-\dfrac{\gamma\lambda}{\|\mathbf{Y}_i^k-(\mathbf{X}_{\text{in}})_i\|_2},0) \quad \forall i\in[n] \\ \mathbf{X}_i^{k+1} & = (1-\beta_i)(\mathbf{X}_{\text{in}})_i+\beta_i\mathbf{Y}_i^k \qquad \forall i\in[n] \end{cases}$$

Node-wise adaptive message passing

Adaptive Message Passing

$$\begin{cases} \mathbf{Y}^k &= \big(1 - 2\gamma(1-\lambda)\big)\mathbf{X}^k + 2\gamma(1-\lambda)\tilde{\mathbf{A}}\mathbf{X}^k \\ \beta_i &= \max(1 - \dfrac{\gamma\lambda}{\|\mathbf{Y}_i^k - (\mathbf{X}_{\text{in}})_i\|_2}, 0) \quad \forall i \in [n] \\ \mathbf{X}_i^{k+1} &= (1-\beta_i)(\mathbf{X}_{\text{in}})_i + \beta_i \mathbf{Y}_i^k \qquad \forall i \in [n] \end{cases}$$

Node-wise adaptive message passing

Interpretation as feature selection

- Small residual ($\beta_i \to 1$): if $(\mathbf{X}_{\text{in}})_\text{i}$ is significantly inconsistent with local neighbors;
- Large residual ($\beta_i \to 0$): if $(\mathbf{X}_{\text{in}})_\text{i}$ is very consistent with local neighbors;
- β_i provides a natural transition from 0 to 1 modulated by λ

AirGNN

- Adaptive message passing (AMP) can be used as a building block in many GNN architecture

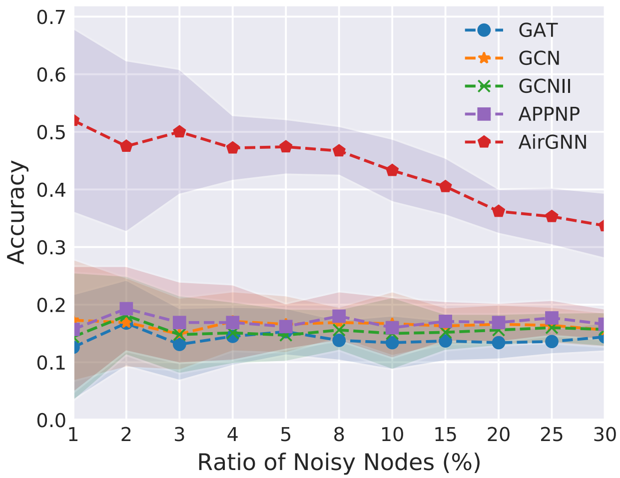
- In this work, we follow the decoupled architecture as APPNP

$$\mathbf{X}_{\text{in}} = h_\theta(\mathbf{X}_{\text{fea}})$$
$$\mathbf{Y}_{\text{pre}} = \mathbf{AMP}\left(\mathbf{X}_{\text{in}}, K, \lambda\right)$$

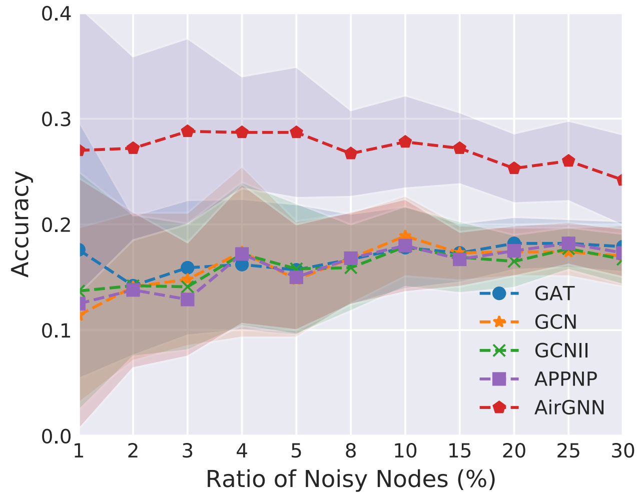
- Parameters θ are trained by the cross-entropy loss defined on labeled data through back propagation

AirGNN: GNN with Adaptive Residual

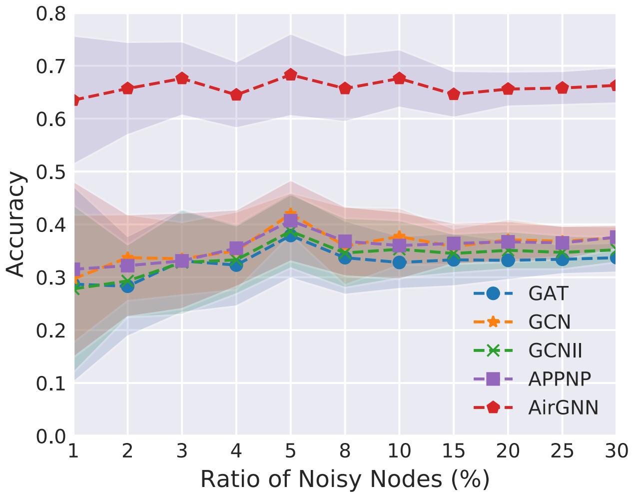
Experiment in Noise Setting



Cora



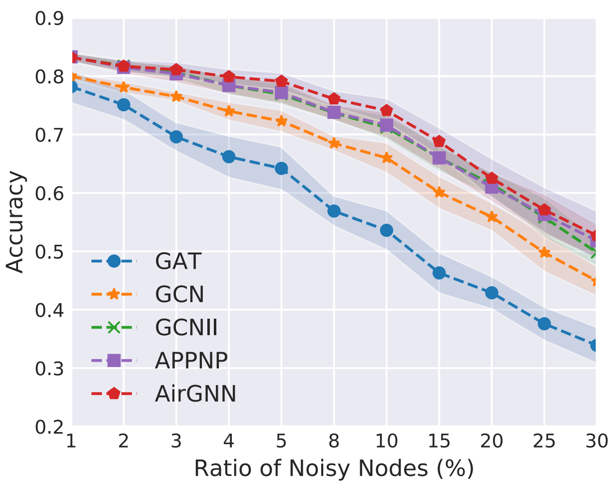
Citeseer



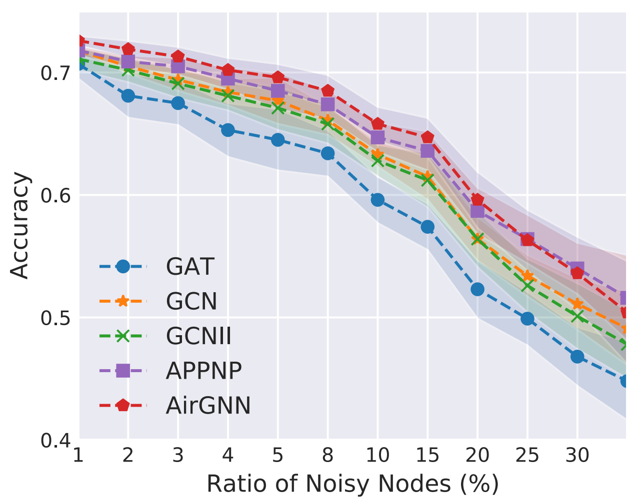
PubMed

Node classification performance on nodes with noisy features

Experiment in Noise Settings



Cora



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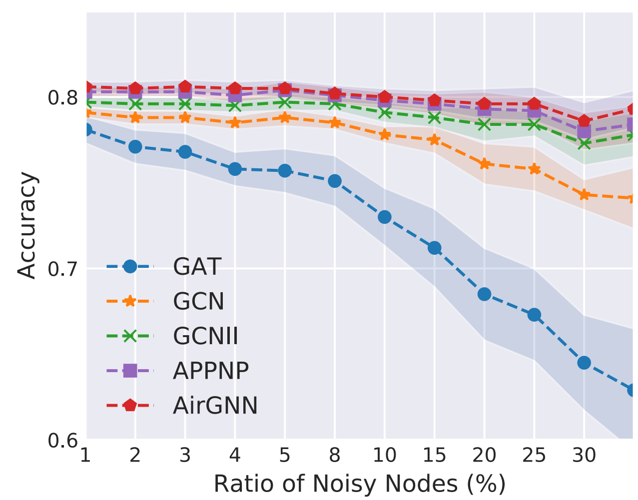

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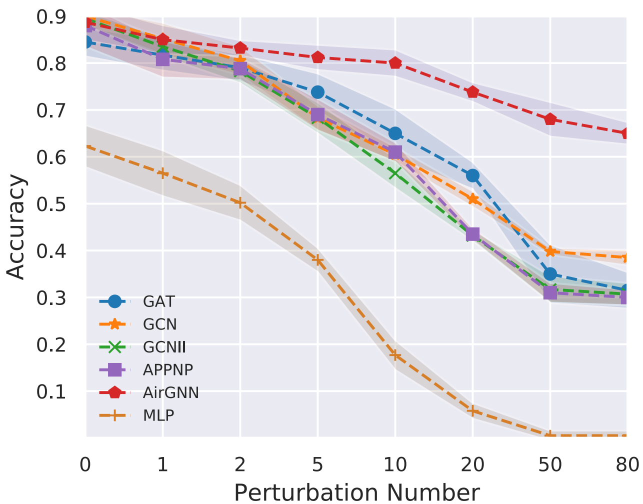
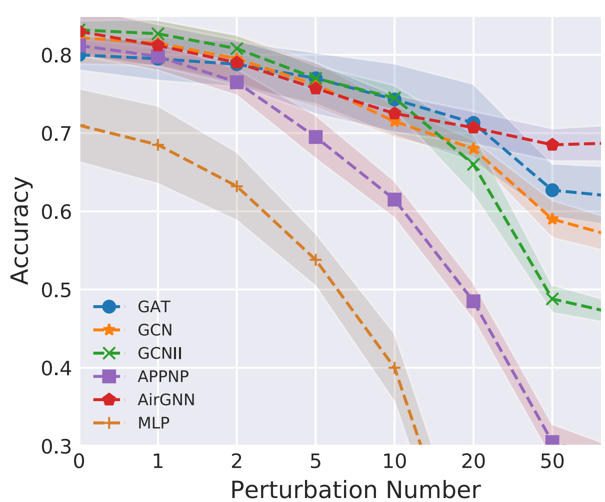
Node classification performance on normal nodes

Experiment in Adversarial Settings



Cora



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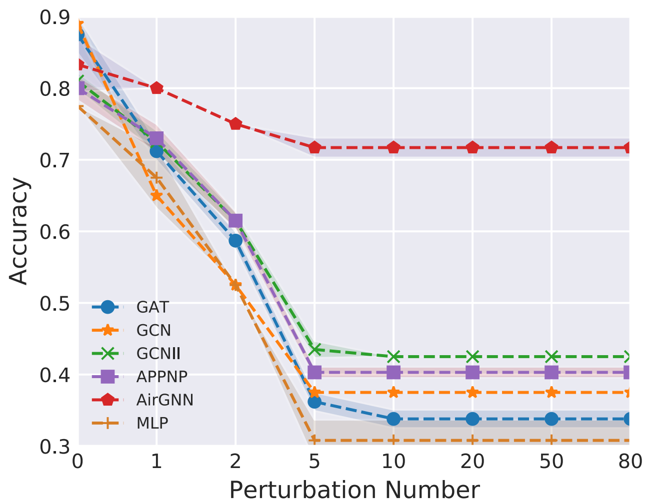

PubMed

Node classification performance on adversarially perturbed nodes

Adaptive Residual

Table 1: Average adaptive score (β) and residual weight ($1-\beta$) in the noisy feature scenario.

Measure	**Cora**	**CiteSeer**	**PubMed**
Average adaptive score for abnormal nodes	0.998 ± 0.000	0.988 ± 0.000	0.996 ± 0.000
Average adaptive score for normal nodes	0.924 ± 0.002	0.807 ± 0.005	0.869 ± 0.006
Average residual weight for abnormal nodes	0.002 ± 0.000	0.012 ± 0.000	0.004 ± 0.000
Average residual weight for normal nodes	0.076 ± 0.002	0.193 ± 0.005	0.131 ± 0.006

Table 2: Average adaptive score (β) and residual weight ($1-\beta$) in the adversarial feature scenario.

Measure	**Cora**	**CiteSeer**	**PubMed**
Average adaptive score for abnormal nodes	0.987 ± 0.000	0.930 ± 0.007	0.959 ± 0.005
Average adaptive score for normal nodes	0.922 ± 0.004	0.689 ± 0.024	0.826 ± 0.016
Average residual weight for abnormal nodes	0.013 ± 0.000	0.070 ± 0.007	0.041 ± 0.005
Average residual weight for normal nodes	0.078 ± 0.004	0.311 ± 0.024	0.174 ± 0.016

Conclusion

Summary

- Discover the intrinsic tension between feature aggregation and residual connection in GNNs
- Design a simple and effective adaptive message passing scheme that can be used a building block to improve the robustness against abnormal features
- Design AirGNN that achieves impressive performance improvement in multiple abnormal settings
- Verify that the adaptive residual is a good indicator of abnormal features in ablation study

Code: https://github.com/lxiaorui/AirGNN