PairNorm: Tackling Oversmoothing in GNNS

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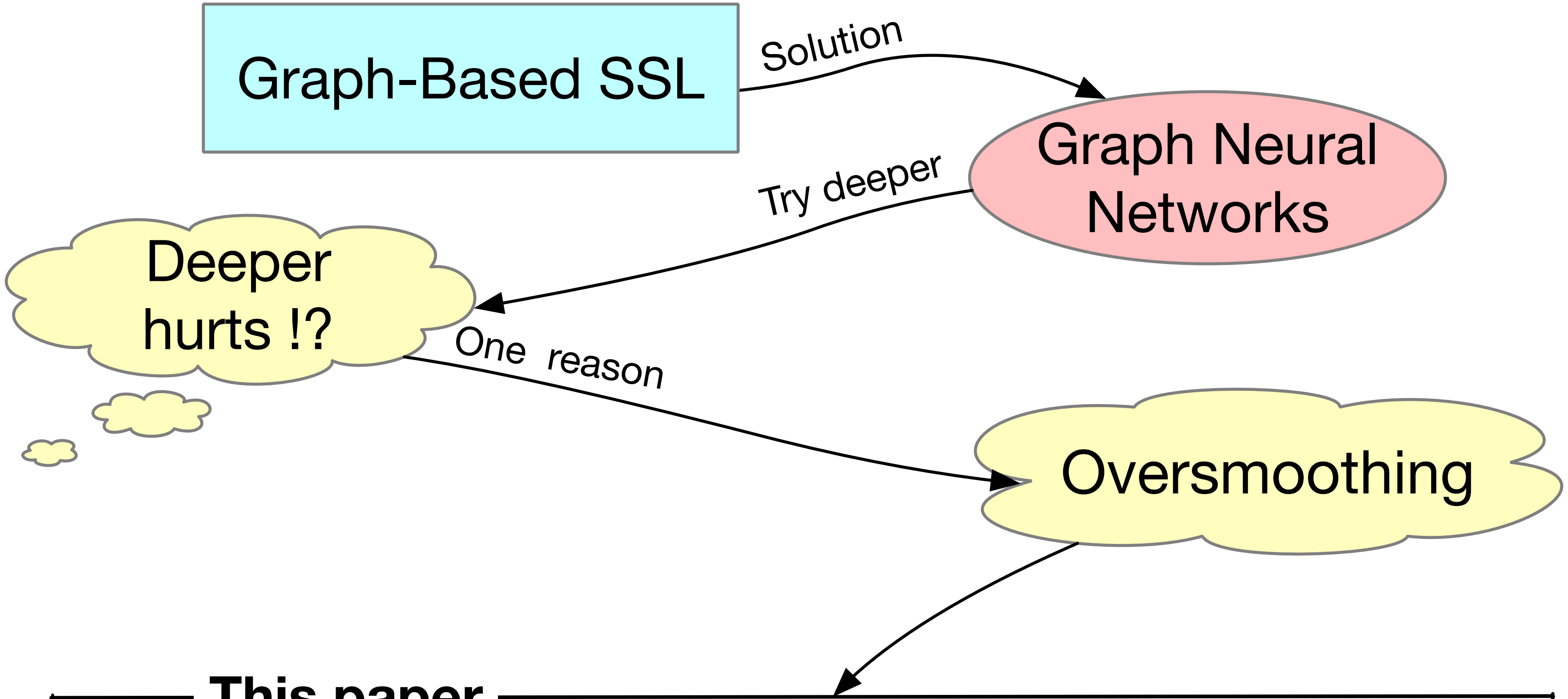
The Big Picture



This paper

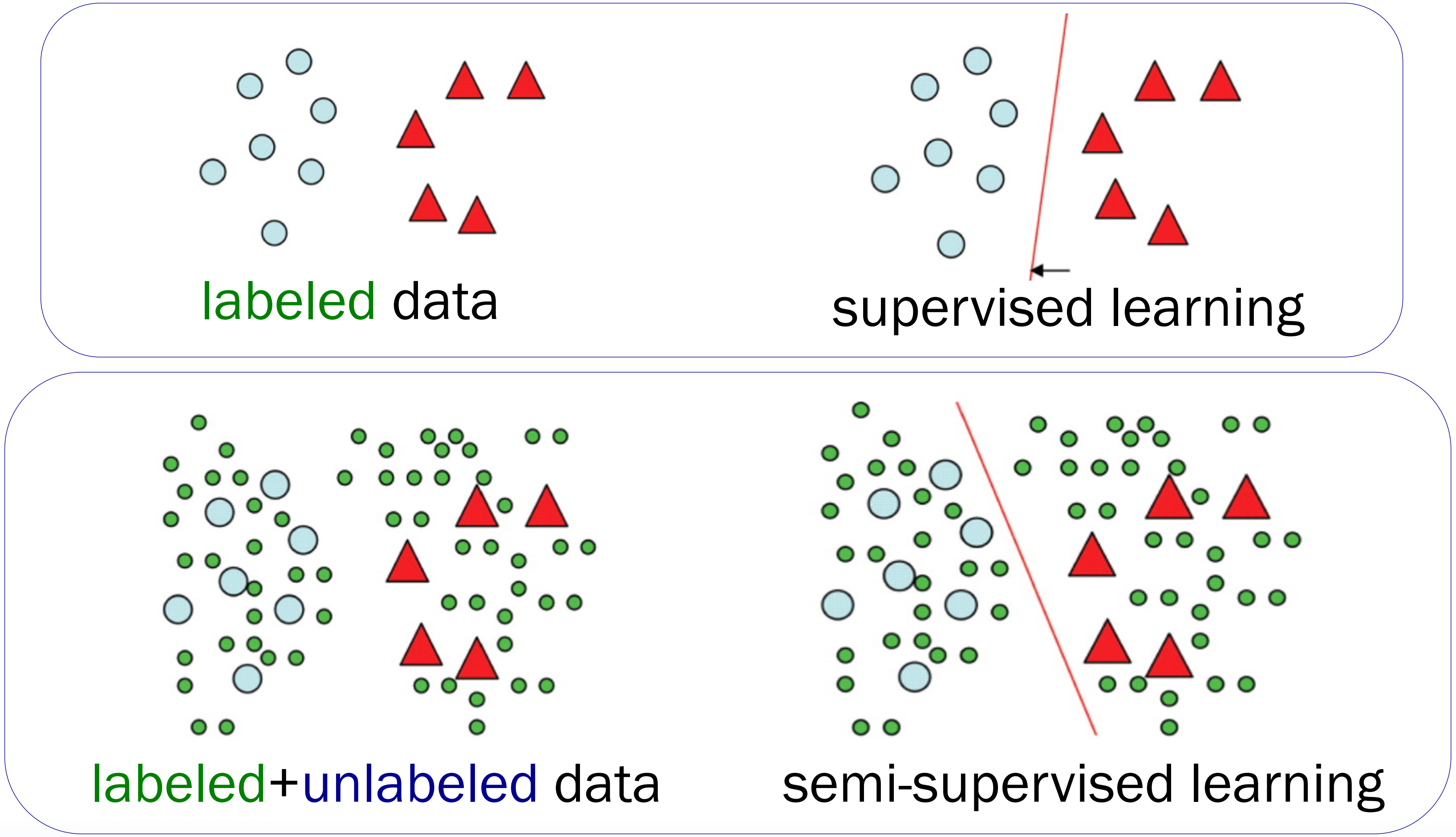
What is over smoothing? Any measures?
How to solve or relieve it for any GNNs?

Agenda

- Background
  - Graph-based semi-supervised learning
  - Modern approach: graph neural networks
  - Oversmoothing problem of GNN
- Understanding oversmoothing
- PairNorm: tackling oversmoothing
- Semi-supervised node classification with missing feature

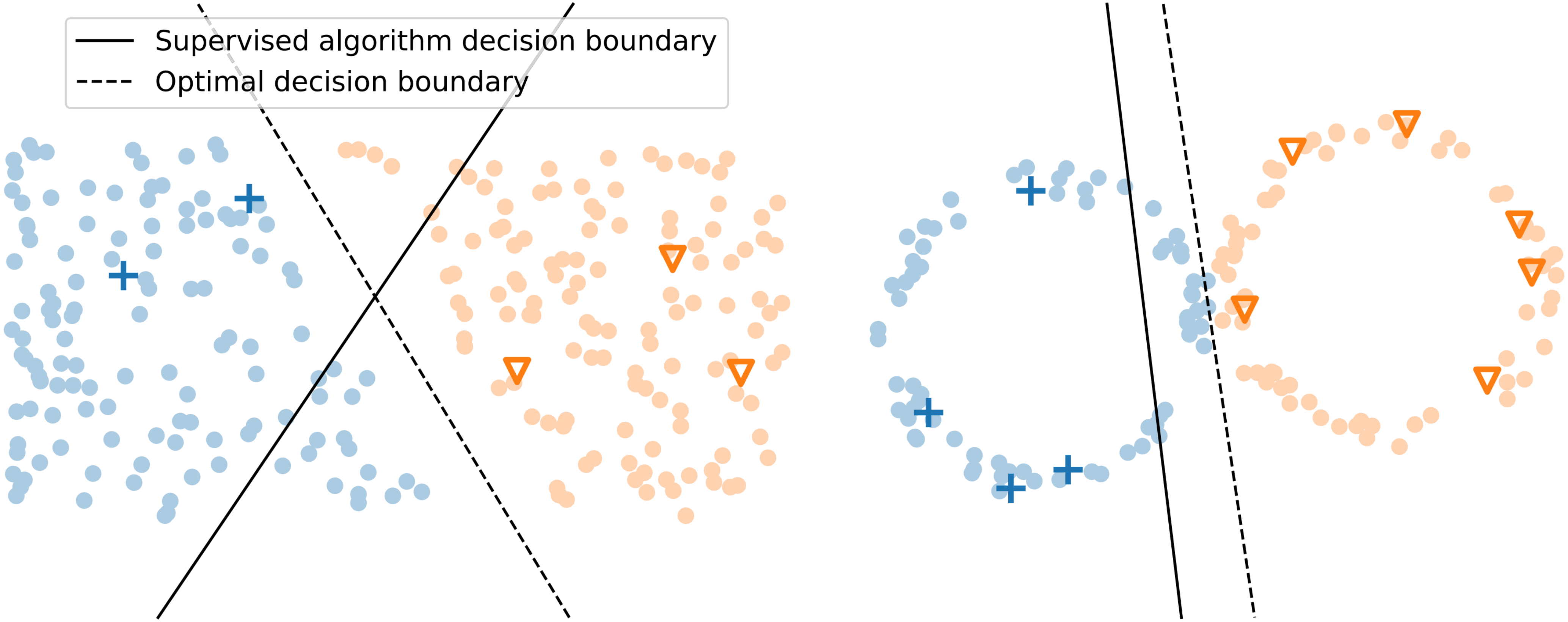
Background: SSL

- Semi Supervised Learning (SSL)



Background: SSL

- **Why SSL works:** assumptions link P(X) and P(Y|X)

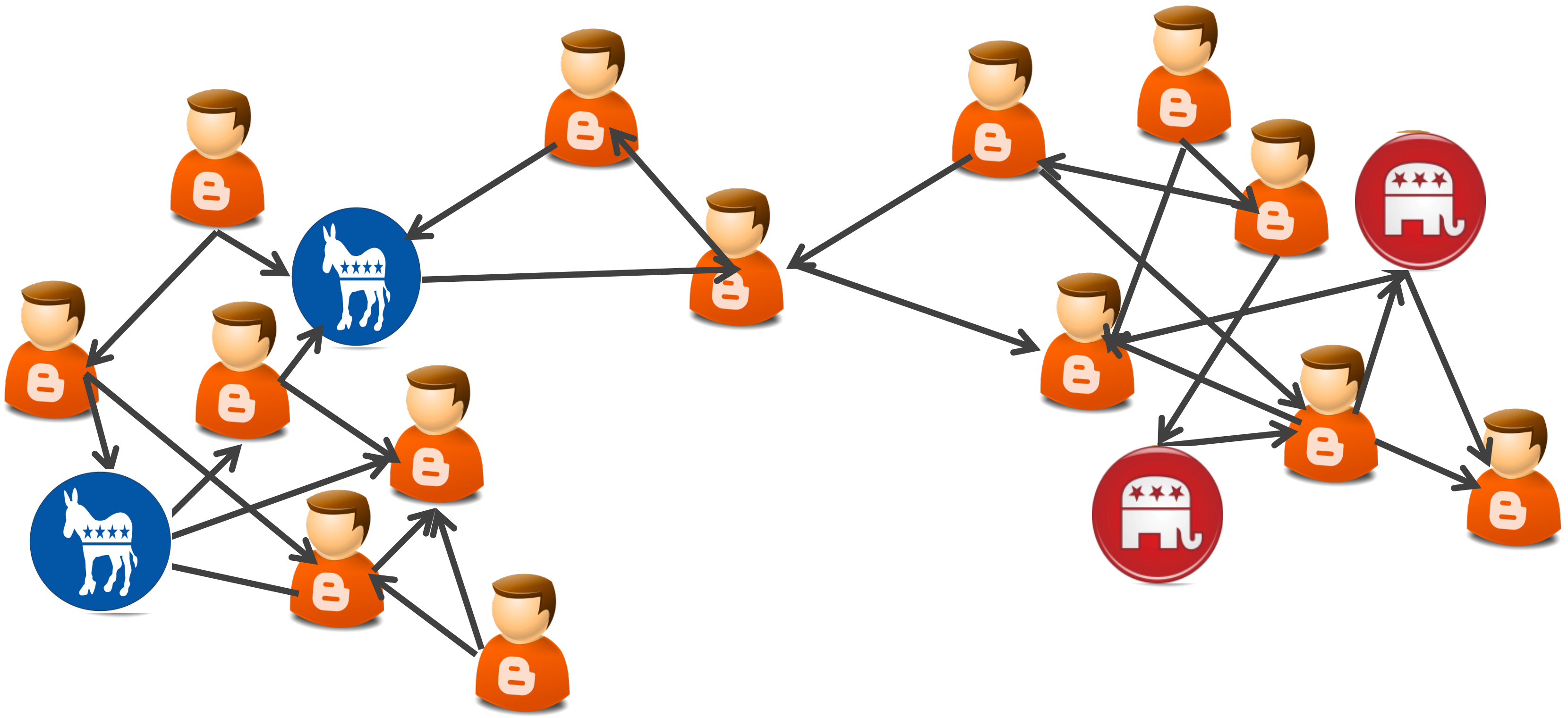


(a) Smoothness and low-density assumptions. **(b)** Manifold assumption.

Borrowed from https://link.springer.com/content/pdf/10.1007/s10994-019-05855-6.pdf

Background: Graph-Based SSL

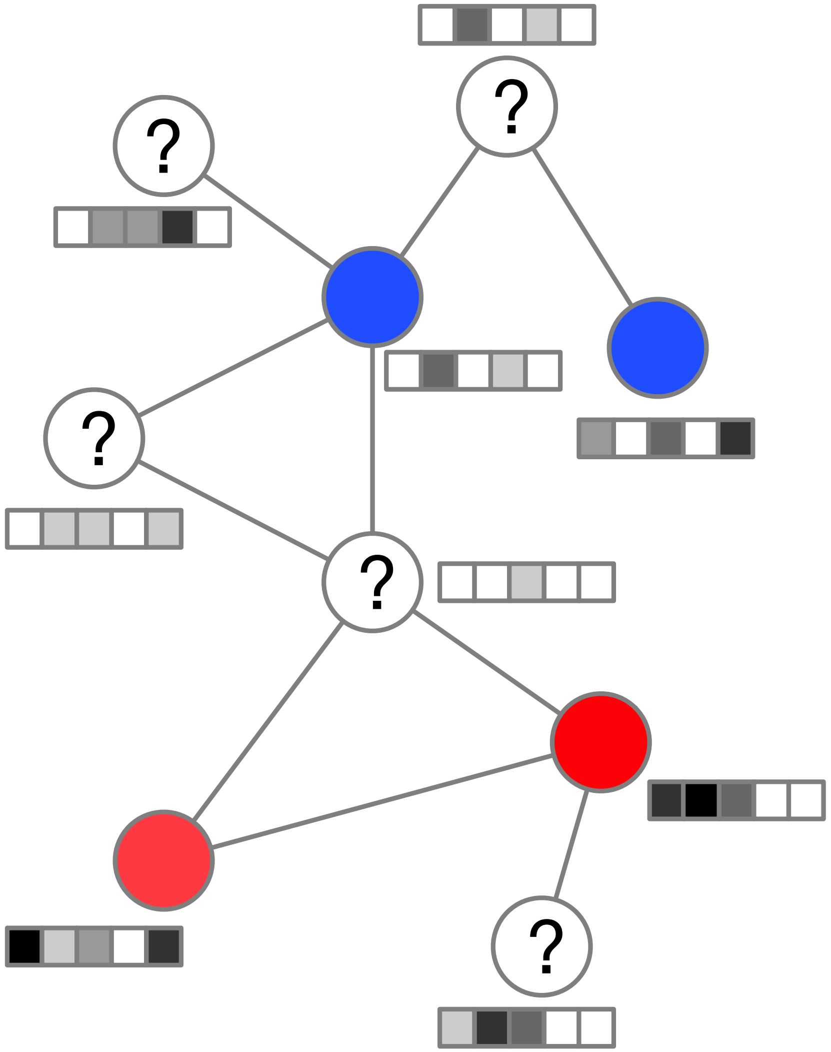
- Additional information: Graph



- Example: Political blog citations

Background: Graph-Based SSL

- Given
  - Set L of labeled nodes with attributes
  - Set U of unlabeled nodes with attributes
  - A graph A of all nodes
- Goal
  - Assign label Y to all unlabeled nodes in U
- Old approaches
  - Label Propagation [Zhu 03]
  - Deep Walk [Perozzi 14]
  - Iterative Classification [Lu 03]
  - ....



Modern Solution: Graph Convolutional Network

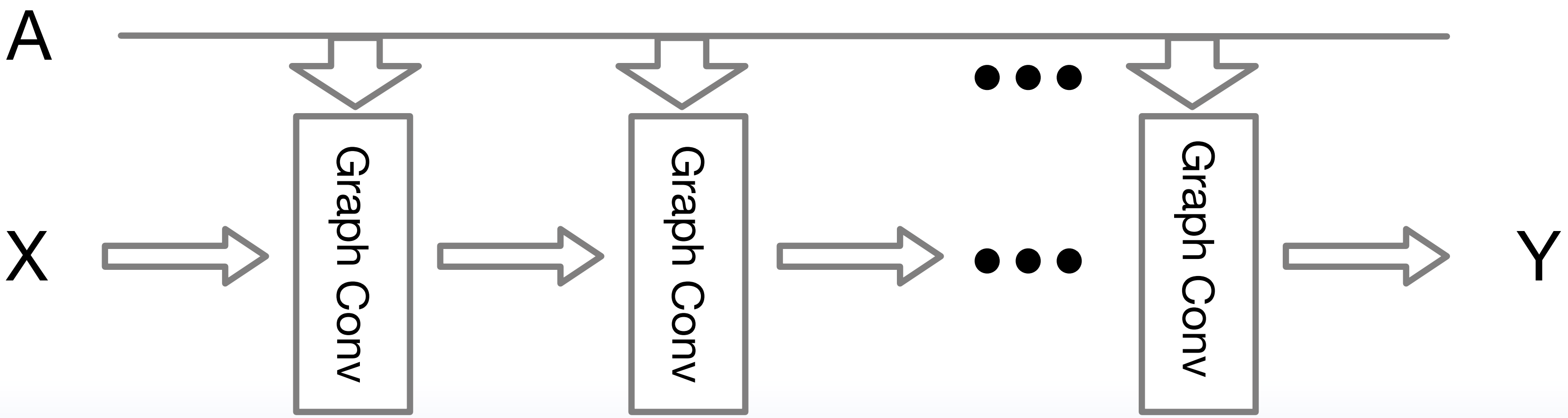
- Neural Network
  - Stacking of linear layer followed by nonlinear activation

$$H^{(t+1)} = \sigma(H^{(t)}W^{(t)} + b^{(t)})$$

[W, b are Params]

- Graph Convolutional Neural Network (GCN) [Kipf 17]
  - Stacking of GraphConv layer followed by nonlinear activation

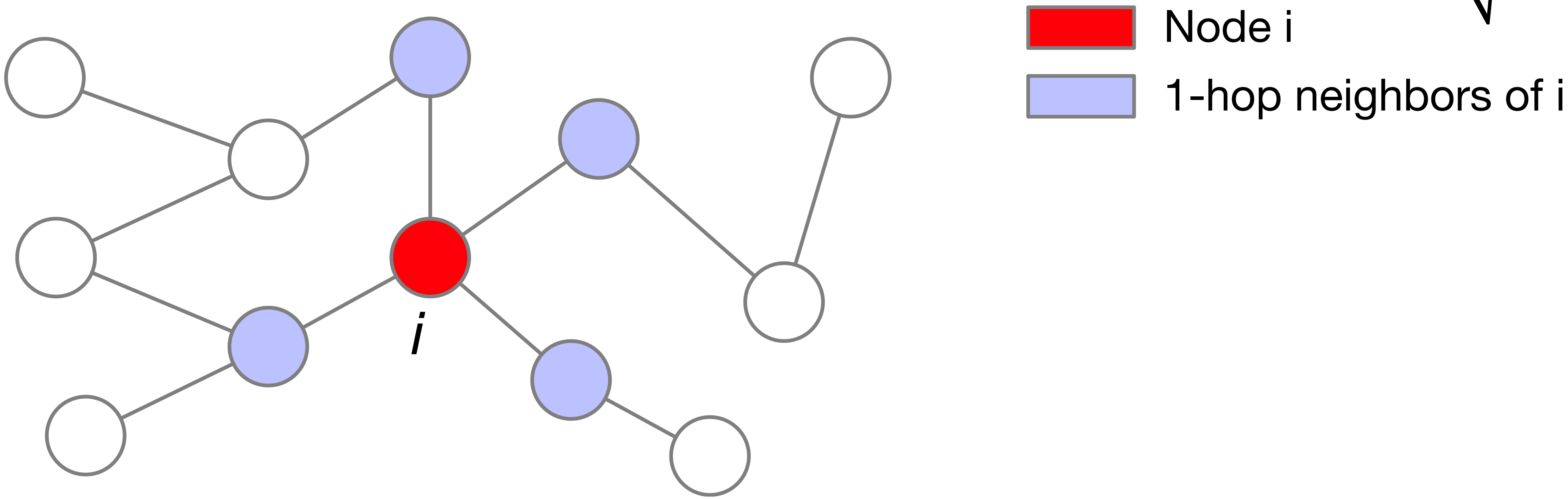
$$H^{(t+1)} = \sigma(\tilde{A}H^{(t)}W^{(t)} + b^{(t)})$$



Modern Solution: Graph Convolutional Network

- GraphConv: Micro Perspective

$$H^{(t+1)} = \sigma(\tilde{A}H^{(t)}W^{(t)} + b^{(t)}) \Rightarrow h_i^{(t+1)} = \sigma(W^{(t)} \sum_{j \in N_i \cup \{i\}} \frac{h_j^{(t+1)}}{\sqrt{|N_i||N_j|}})$$



- Stacking k layers expand the receptive field to k-hop neighbors!

Other variants of GNN

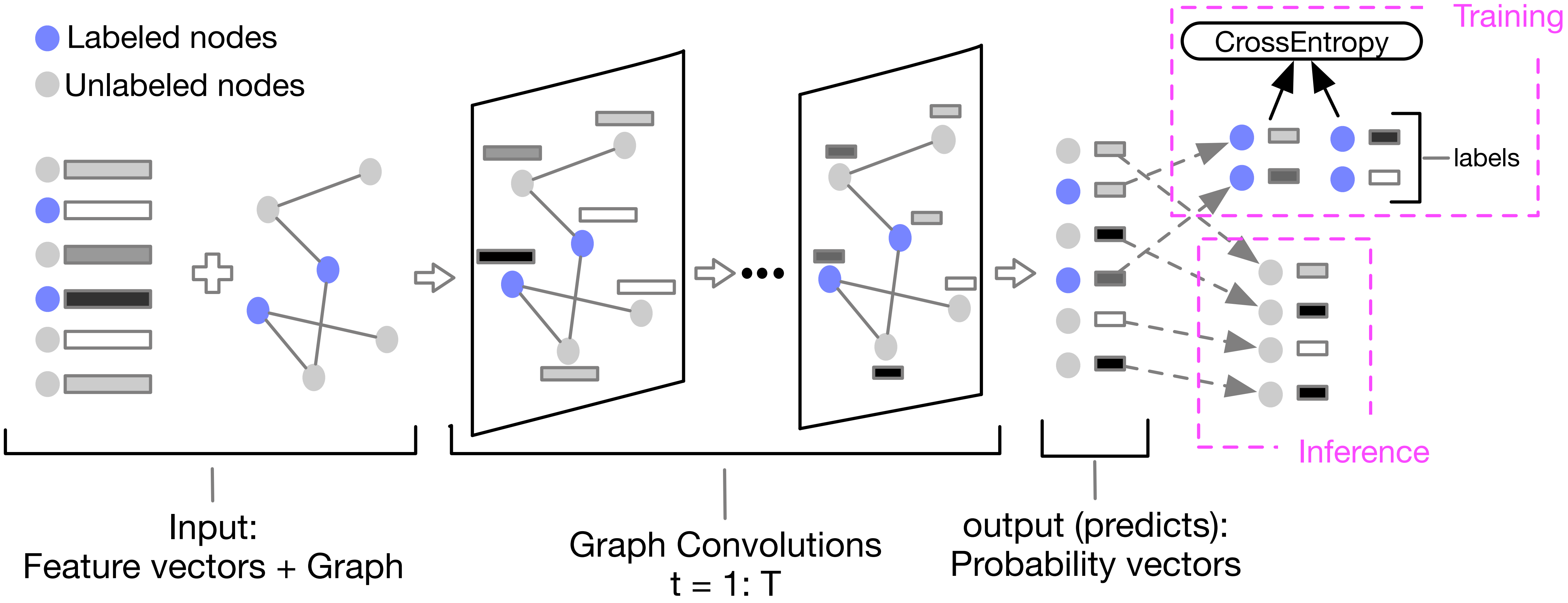
- Graph Attention Network [Velickovic et al., 2018]
- GraphSAGE [Hamilton et al., 2017]
- Deep graph infomax [Velickovic et al., 2019]
- Graph Markov Neural Networks [Qu et al., 2019]
- …

Refer to a good survey of GNN:

Wu, Zonghan et al., *arXiv preprint arXiv:1901.00596* (2019).

A comprehensive survey on graph neural networks.

Apply GCN to SSL



Oversmoothing problem: view 1

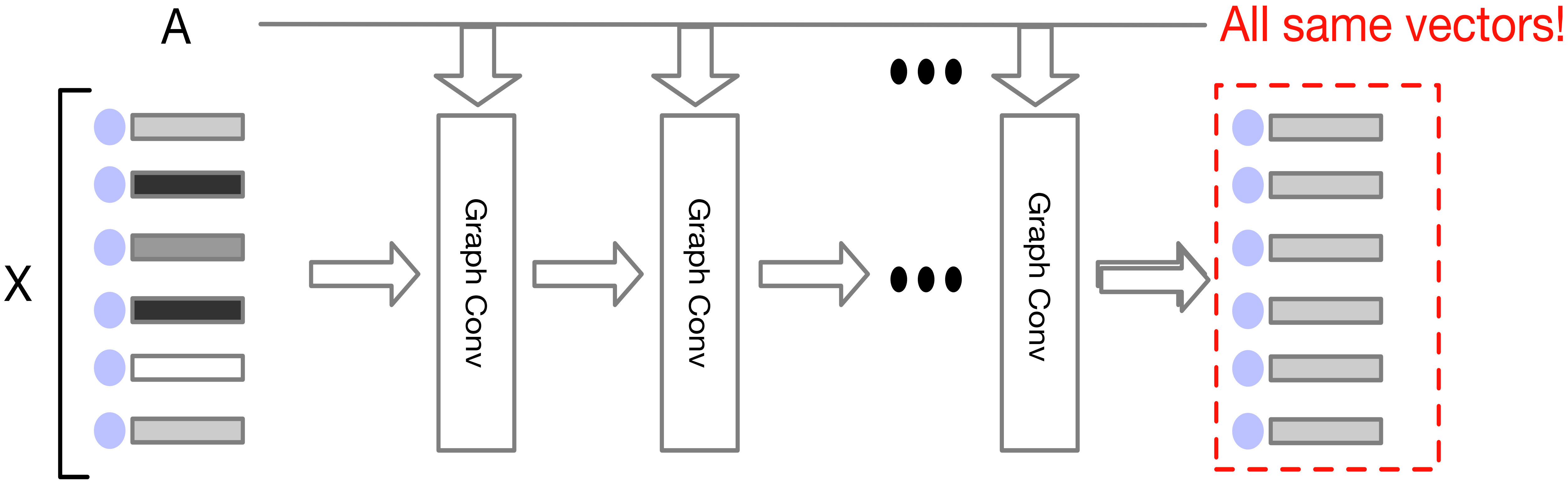
- **Intuition:** More layers => larger receptive fields => more information
- **Observation:** hurt the performance (after more than 2~3 layers)?
- **Why?**
    1. More parameters => overfitting
    2. More layers => vanishing gradient => hard to train
    3. Oversmoothing of graph convolution operation [our focus]
- Recall that in GCN:

$$\boldsymbol{h}_i^{l+1} = \boldsymbol{\sigma}\left(\boldsymbol{W}^l \sum_{j \in N_i \cup \{i\}} \frac{\boldsymbol{h}_j^l}{\sqrt{|N_i||N_j|}}\right)$$

Intuitively, keeping aggregating information from neighbors can make all nodes **indistinguishable**!

Node-wise oversmoothing

Node-wise oversmoothing



Oversmoothing problem: view 2

- Different view from matrix form (ignoring parameters)

$$H^{l+1} = \widetilde{A}_{sym} H^{l}$$

$$\Longrightarrow \quad H^{N} = \widetilde{A}_{sym}^{N} H^{0} = \widetilde{A}_{sym}^{N} X$$

- There is a stationary distribution for $\widetilde{A}_{sym}$, if viewing it as transition matrix of random walk.

Feature-wise oversmoothing

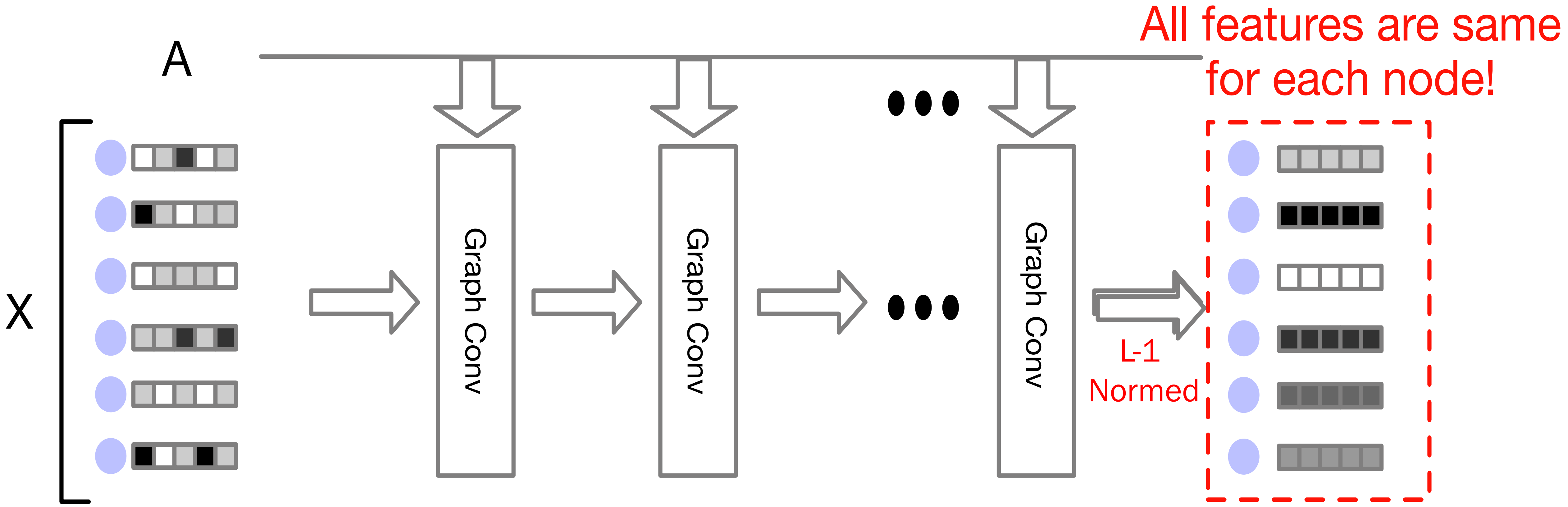
Let $\mathbf{x}_{\cdot j} \in \mathbb{R}^n$ denote the j-th column of $\mathbf{X}$. Then, for *any* $\mathbf{x}_{\cdot j} \in \mathbb{R}^n$:

$$\lim_{k \to \infty} \tilde{\mathbf{A}}_{\text{sym}}^{k} \mathbf{x}_{\cdot j} = \boldsymbol{\pi}_j \quad \text{and} \quad \frac{\boldsymbol{\pi}_j}{\|\boldsymbol{\pi}_j\|_1} = \boldsymbol{\pi} \,,$$

$\boldsymbol{\pi} \in \mathbb{R}^n$ satisfies $\boldsymbol{\pi}_i = \frac{\sqrt{deg_i}}{\sum_i \sqrt{deg_i}}$ for all $i \in [n]$.

Typo: $x_{\cdot j} \in \mathbb{R}^{+n}$

Feature-wise oversmoothing



Overswmoothing washes away the original features!

Agenda

- Background
- Understanding oversmoothing
  - Focusing on oversmoothing: via SGC
  - Measures: row-diff and col-diff
  - Results for semi-supervised node classification(**SSNC**) problem
- PairNorm: tackling oversmoothing
- Semi-supervised node classification with missing feature

Simplified graph convolutional network (SGC)

- SGC [Wu et al., 2019]

Graph convolution: $\boldsymbol{H}^{l+1} = \widetilde{\boldsymbol{A}}_{\boldsymbol{sym}}\boldsymbol{H}^{l}$

Readout: $\boldsymbol{O} = Softmax(\boldsymbol{H}^{N}\boldsymbol{W}^{N})$

- Removing parameters and activation functions of GCN
  Add a linear transformation in readout

- Achieve similar result as GCN for SSL

Focusing on oversmoothing: via SGC

- Recall reasons:
  1. More parameters => overfitting
  2. More layers => vanishing gradient => hard to train
  3. Oversmoothing of graph convolution operation

- To decouple oversmoothing from other factors, we study the oversmoothing problem using SGC model. [Wu et al., 2019]

$$\widehat{\boldsymbol{Y}} = \mathrm{softmax}(\tilde{\mathbf{A}}_{\mathrm{sym}}^{K}\ \mathbf{X}\ \mathbf{W})$$

  i. **No effect of overfiiting:** fixed number of parameters
  ii. **No effect of vanishing gradient:** not a ”deep” model

Measures: row-diff and col-diff

- **Row-diff**: measuring node-wise oversmoothing

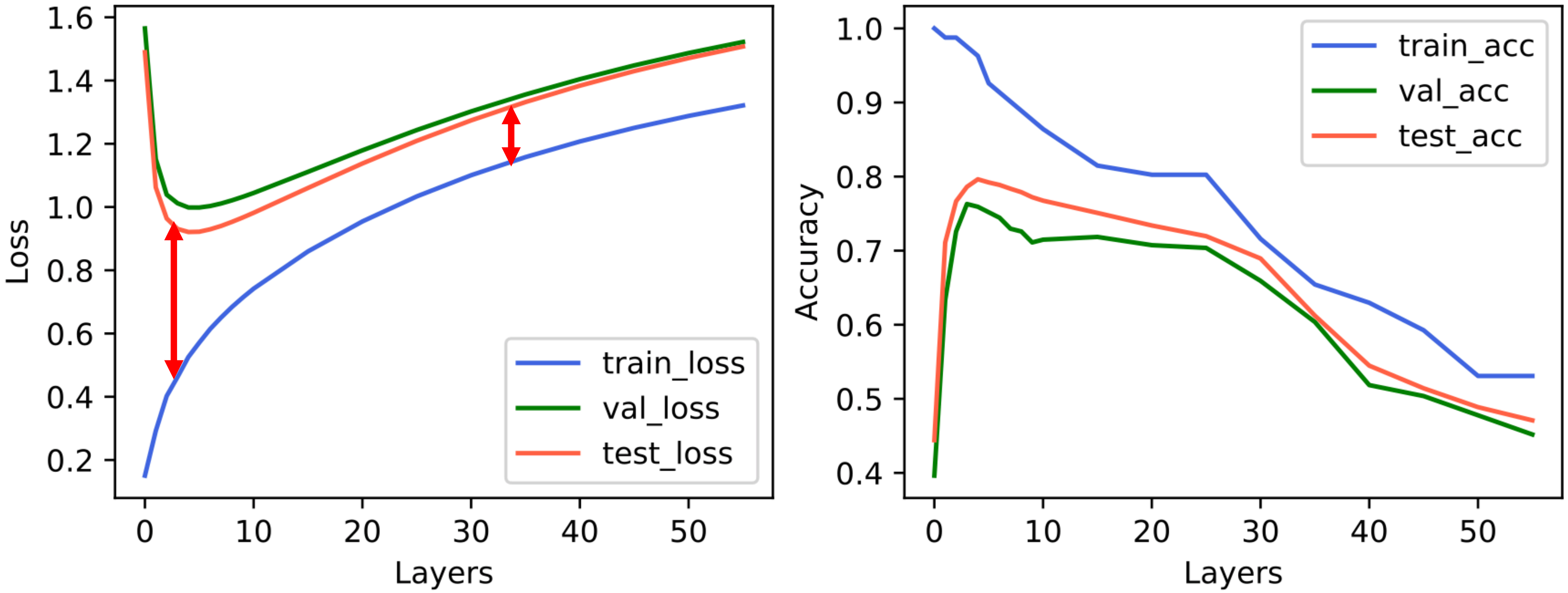
$$\text{row-diff}(\mathbf{H}^{(k)}) = \frac{1}{n^2} \sum_{i,j \in [n]} \left\| \mathbf{h}_i^{(k)} - \mathbf{h}_j^{(k)} \right\|_2$$

- **Col-diff**: measuring feature-wise oversmoothing

$$\text{col-diff}(\mathbf{H}^{(k)}) = \frac{1}{d^2} \sum_{i,j \in [d]} \left\| \mathbf{h}_{\cdot i}^{(k)} / \|\mathbf{h}_{\cdot i}^{(k)}\|_1 - \mathbf{h}_{\cdot j}^{(k)} / \|\mathbf{h}_{\cdot j}^{(k)}\|_1 \right\|_2$$

Measuring oversmoothing effect

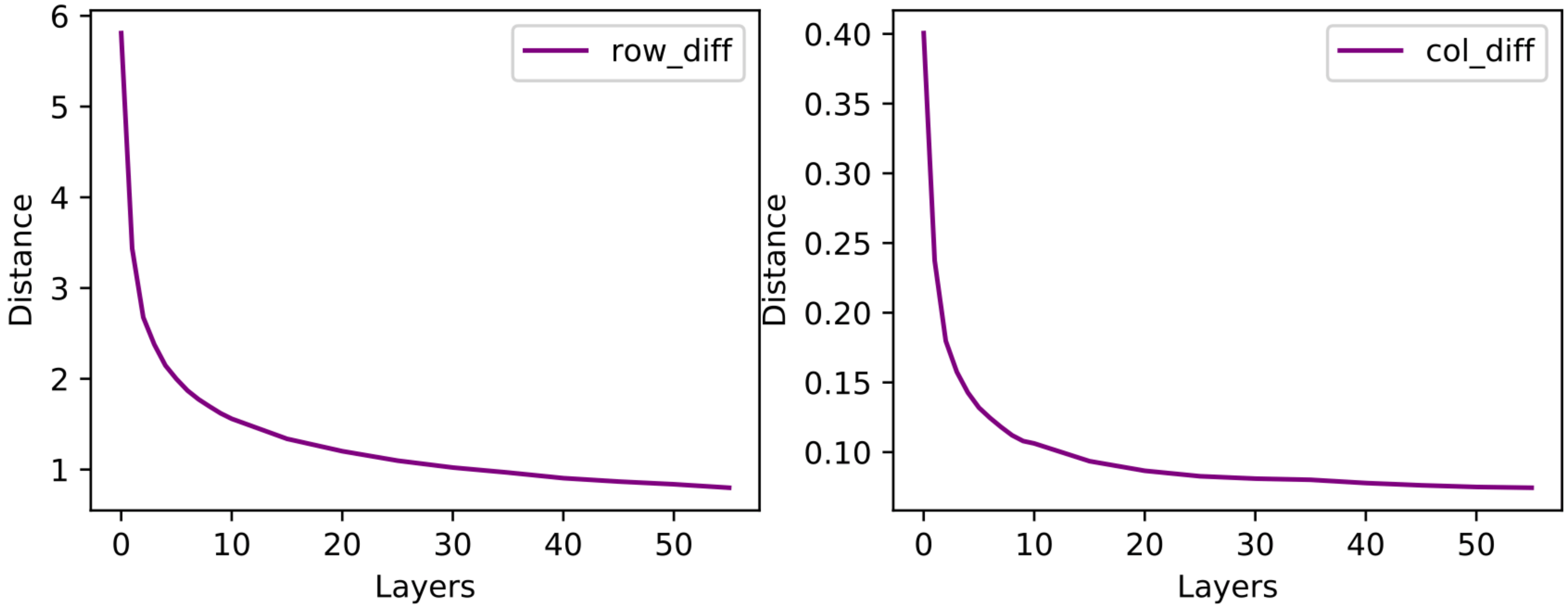
- Data: Cora, random split with 3%train, 10%valiation, 87% test
- Model: SGC



- Learning harder materials makes you perform better in exam! But can not be too hard!   [Human learning perspective]

Measuring oversmoothing level

- Cora dataset: random split with 3%train, 10%valiation, 87% test



- Both node-wise and feature-wise oversmoothing are happening

Agenda

- Background
- Understanding oversmoothing
- **PairNorm: tackling oversmoothing**
  - PairNorm: normalizing total pairwise distance
  - Effective of SGC+PairNorm over SSNC problem
- Semi-supervised node classification with missing feature

PairNorm: normalizing pairwise squared distance

- **Design:** Normalization layer after GraphConv
- **Intuition:** keep total pairwise squared distance (TPSD) constant across layers to prevent node-wise oversmoothing. Combining with GraphConv can push away pairs that are not connected.
- **Notation:**

  $\mathbf{X}$: input of GraphConv
  $\tilde{\mathbf{X}}$: input of PairNorm, also the output of GraphConv
  $\dot{\mathbf{X}}$: output of PairNorm

  $\text{TPSD}(\dot{\mathbf{X}}) := \sum_{i,j\in[n]} \|\dot{\mathbf{x}}_i - \dot{\mathbf{x}}_j\|_2^2$

- **Goal:**

$$\text{TPSD}(\mathbf{X}) = \text{TPSD}(\dot{\mathbf{X}})$$

PairNorm: normalizing pairwise squared distance

- TPSD pairwise calculation: $\mathcal{O}(n^2 d)$ complexity.

- Notice that TPSD can be rewritten as:

$$\operatorname{TPSD}(\tilde{\mathbf{X}}) = \sum_{i,j \in [n]} \|\tilde{\mathbf{x}}_i - \tilde{\mathbf{x}}_j\|_2^2 = 2n^2 \left(\frac{1}{n} \sum_{i=1}^{n} \|\tilde{\mathbf{x}}_i\|_2^2 - \|\frac{1}{n} \sum_{i=1}^{n} \tilde{\mathbf{x}}_i\|_2^2 \right)$$

- First term: the mean squared length of node representations

- Second term: the squared length of node representations

PairNorm

- Operations of PairNorm: Center-and-Scale

$$\tilde{\mathbf{x}}_i^c = \tilde{\mathbf{x}}_i - \frac{1}{n}\sum_{i=1}^{n}\tilde{\mathbf{x}}_i \qquad \text{(Center)}$$

$$\dot{\mathbf{x}}_i = s \cdot \frac{\tilde{\mathbf{x}}_i^c}{\sqrt{\frac{1}{n}\sum_{i=1}^{n}\|\tilde{\mathbf{x}}_i^c\|_2^2}} = s\sqrt{n} \cdot \frac{\tilde{\mathbf{x}}_i^c}{\sqrt{\|\tilde{\mathbf{X}}^c\|_F^2}} \qquad \text{(Scale)}$$

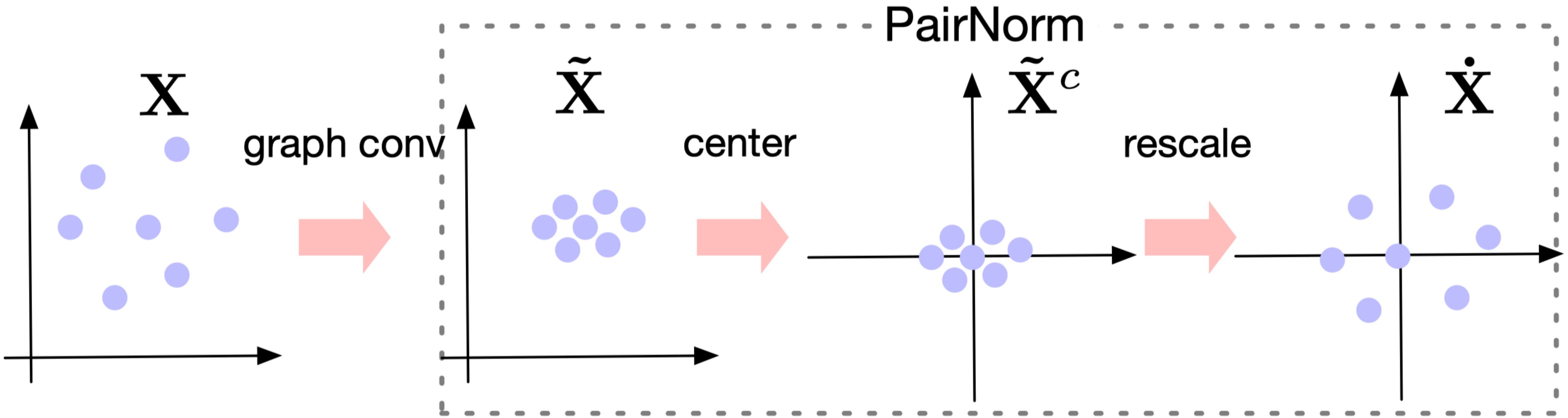
- After PairNorm:

$\dot{\mathbf{X}} := \textsc{PairNorm}(\tilde{\mathbf{X}})$ has row-wise mean $\mathbf{0}$ (i.e., is centered)

And $\text{TPSD}(\dot{\mathbf{X}}) = 2n\|\dot{\mathbf{X}}\|_F^2 = 2n^2s^2$, where **s** is a hyperparameter.

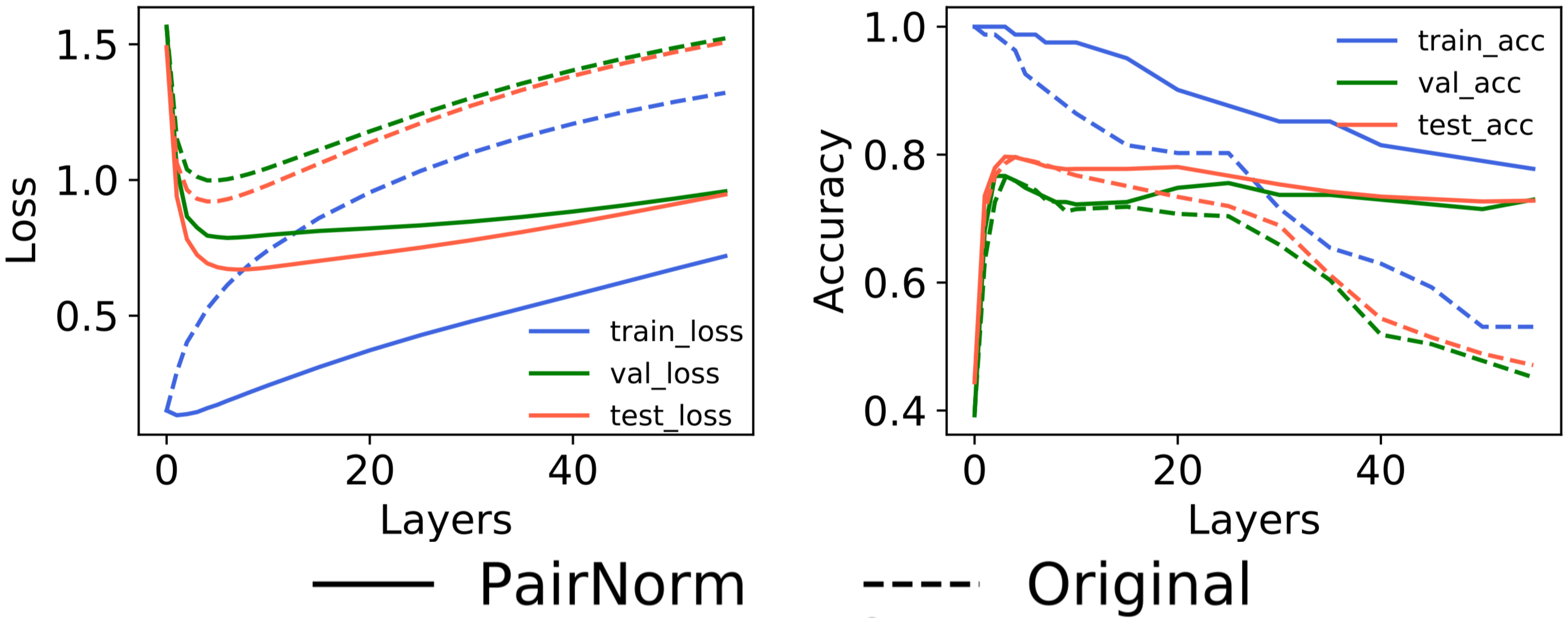
PairNorm

- Visualizing the procedure of PairNorm:



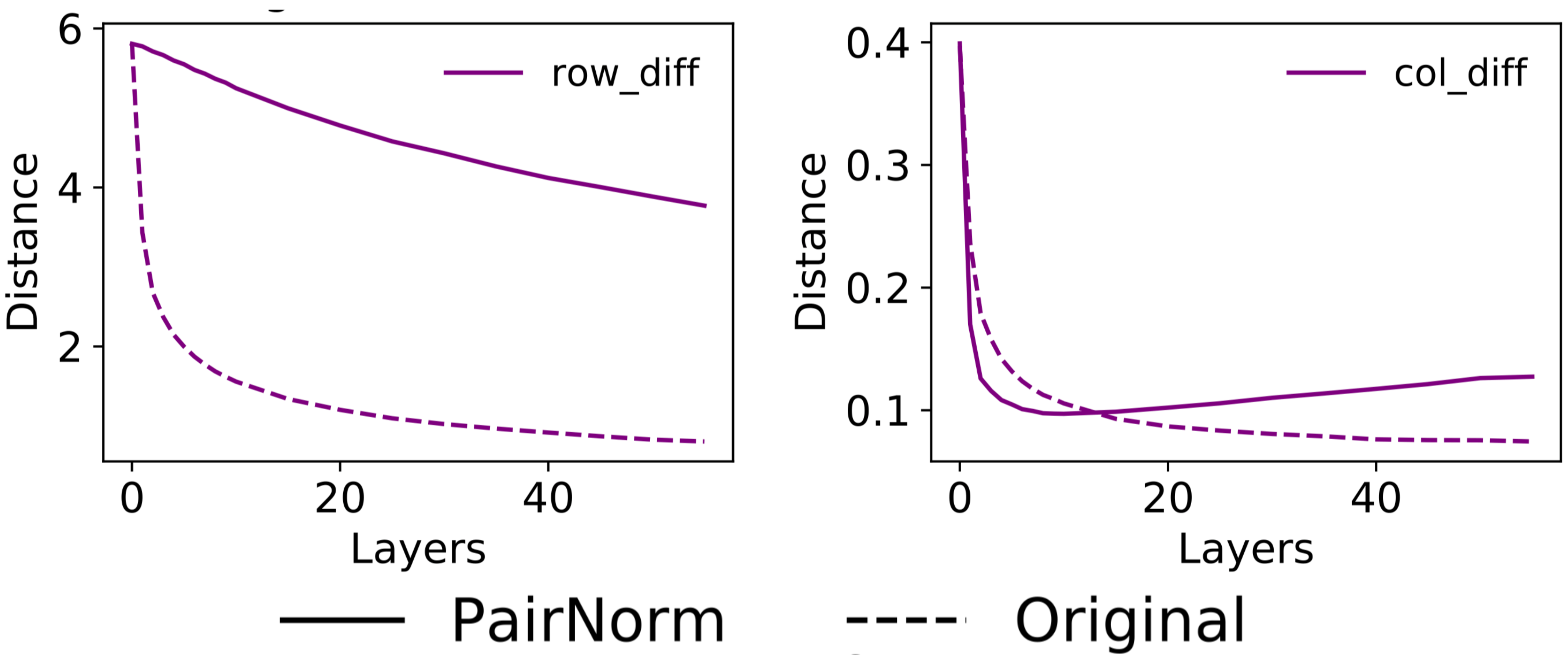
Effective of SGC+PairNorm over SSNC problem

- Cora dataset: random split with 3%train, 10%valiation, 87% test



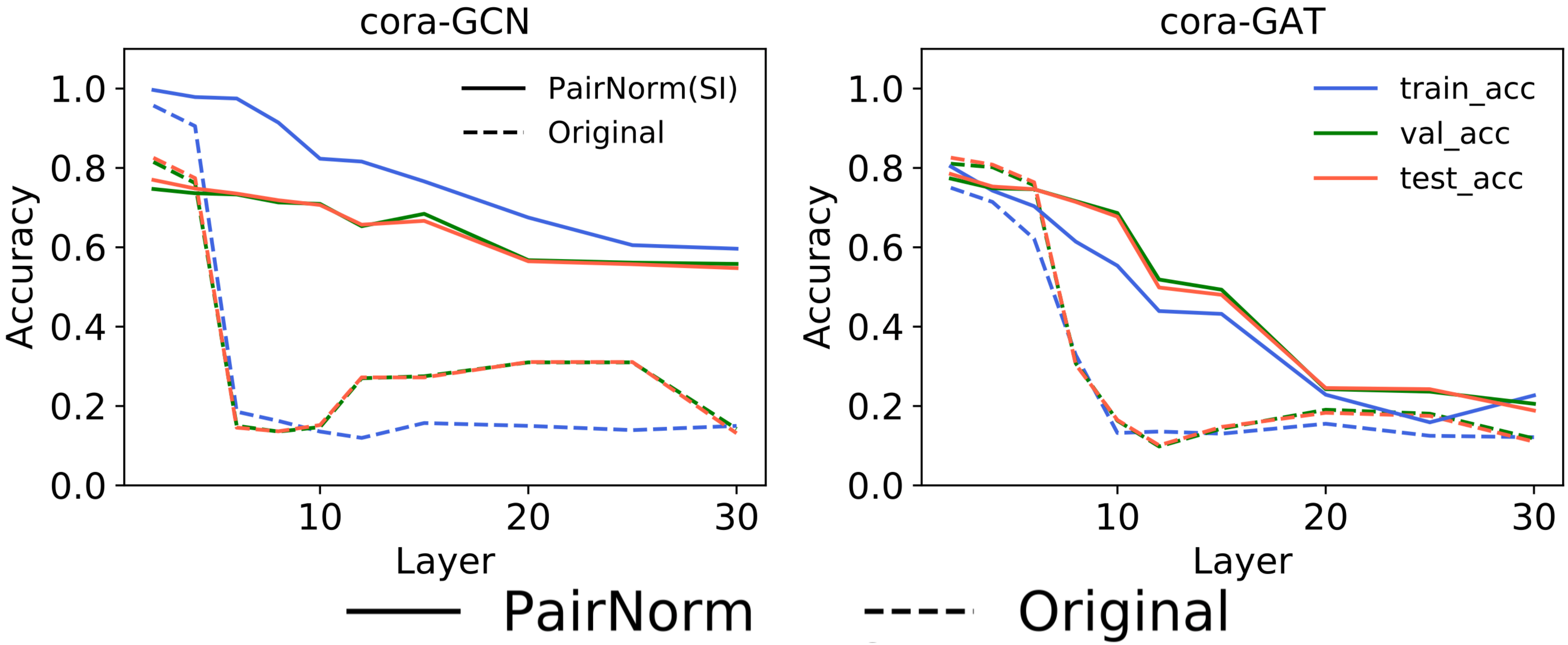
Effective of SGC+PairNorm over SSNC problem

- Cora dataset: random split with 3%train, 10%valiation, 87% test



Effective of GCN/GAT+PairNorm

- Cora dataset: **original** split with 5%train, 10%valiation, 85% test



Agenda

- Background
- Understanding oversmoothing
- PairNorm: tackling oversmoothing
- **Semi-supervised node classification with missing feature**
  - Definition and real-world applications
  - Effective of SGC+PairNorm over SSNC with missing feature

SSNC with missing feature

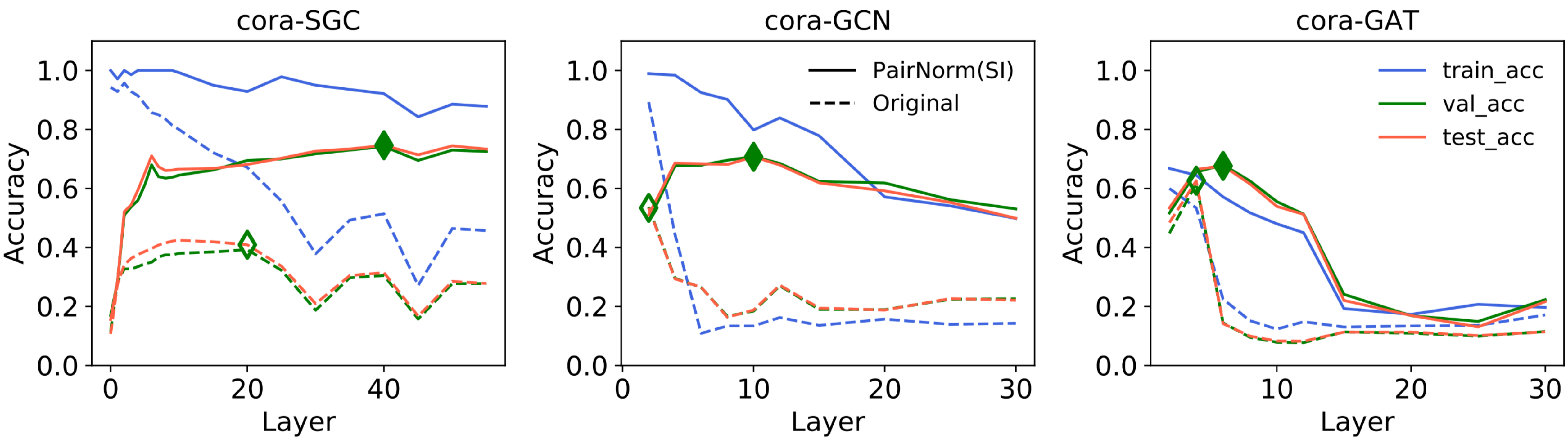
- GNN achieves best performance for SSNC problem with only 2~3 layers, where **overSmoothing** is not really happened.
- The ceiling performance of GNN over SSNC problem is not affected by oversmoothing problem.
- To demonstrate the ability of PairNorm, we investigate a new setting: SSNC with missing feature
- Assume that a certain percentage **(randomly)** of nodes don't have feature – their features are missing due to **privacy protection** or **limited records.**

SSNC with missing feature (SSNC-MF)

- Real-world applications
  1. Credit lending problem of identifying low- vs high-risk customers.
  2. Cold-start problem for graph structured data
  3. Privacy protection: company can only reveals a small fraction of data.
  4. ....
- To our knowledge, this is the first work to study SSNC with missing feature using GNN models.

Effective of SGC/GAT/GCN+PairNorm over SSNC-MF

- Cora dataset, original split. 100% missing of validation and test set.



The green diamond represent where we get highest validation accuracy

More results of SGC+PairNorm

Table 1: Comparison of 'vanilla' vs. PairNorm-enhanced SGC performance in `Cora`, `Citeseer`, `Pubmed`, and `CoauthorCS` for SSNC-MV problem, with missing rate ranging from 0% to 100%. Showing test accuracy at $\#L$ (K in Eq. 4) layers, at which model achieves best validation accuracy.

Missing Percentage		0%		20%		40%		60%		80%		100%	
Dataset	Method	Acc	#L	Acc	#L	Acc	#L	Acc	#L	Acc	#L	Acc	#L
`Cora`	SGC	**0.815**	4	**0.806**	5	0.786	3	0.742	4	0.733	3	0.423	15
	SGC-PN	0.811	7	0.799	7	**0.797**	7	**0.783**	20	**0.780**	25	**0.745**	40
`Citeseer`	SGC	0.689	10	0.684	6	**0.668**	8	**0.657**	9	0.565	8	0.290	2
	SGC-PN	**0.706**	3	**0.695**	3	0.653	4	0.641	5	**0.590**	50	**0.486**	50
`Pubmed`	SGC	0.754	1	0.748	1	0.723	4	0.746	2	0.659	3	0.399	35
	SGC-PN	**0.782**	9	**0.781**	7	**0.778**	60	**0.782**	7	**0.772**	60	**0.719**	40
`CoauthorCS`	SGC	0.914	1	0.898	2	0.877	2	0.824	2	0.751	4	0.318	2
	SGC-PN	**0.915**	2	**0.909**	2	**0.899**	3	**0.891**	4	**0.880**	8	**0.860**	20

Summary

Thank you!

- Defined and measured oversmoothing effect
- A better understanding of GNNs (still immature area)
- Proposed solution: **PairNorm**
  - Solid **theoretical analysis** over SGC
  - **General** ”patch” for any GNN layers
  - **First** normalization layer designed for GNN
- First one to investigate a new scenario, SSL with missing feature, in GNN area.