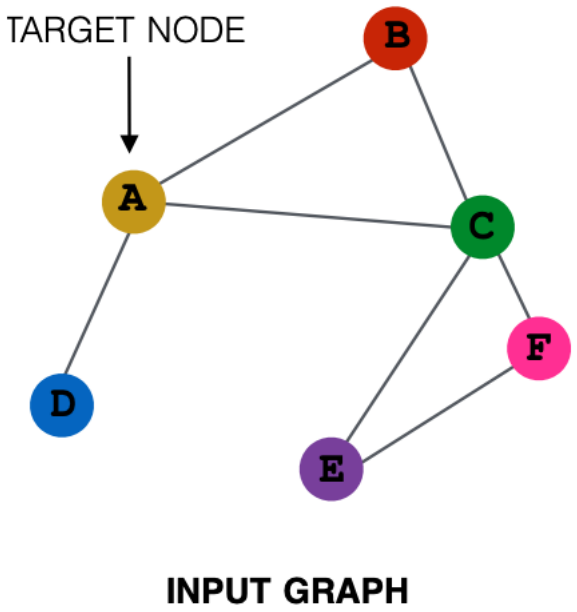
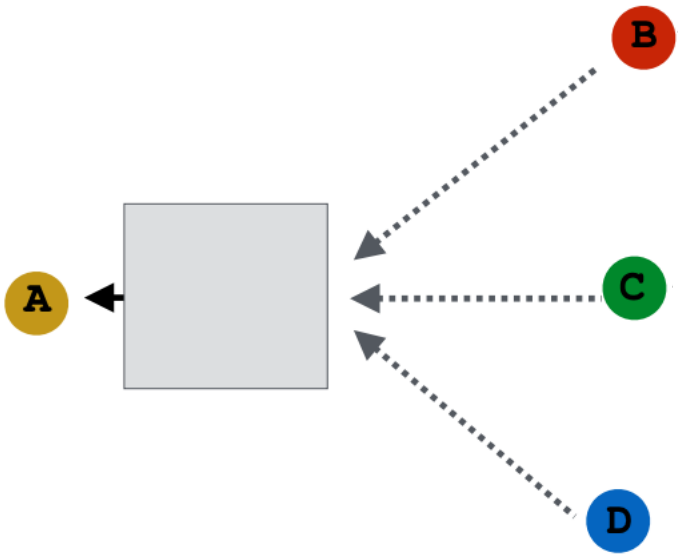
Oversmoothing of GCN

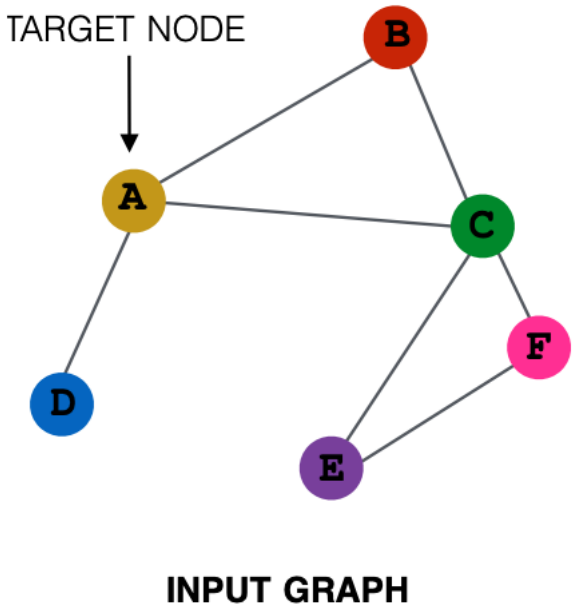
Neural Networks Design And Application

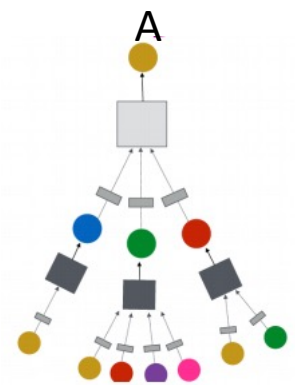
Graph networks: aggregate neighbors

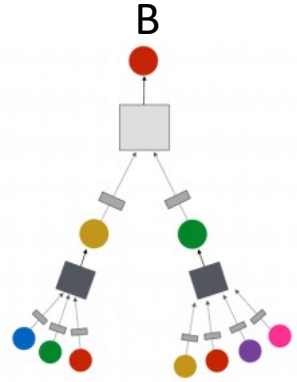


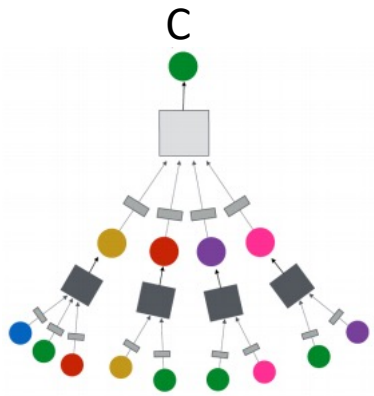


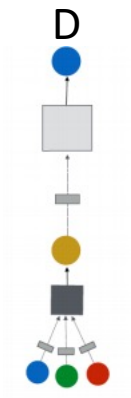
Graph networks: aggregate neighbors

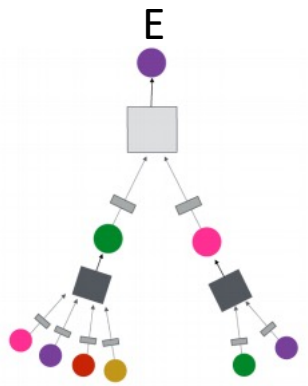


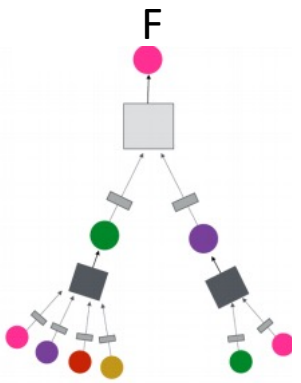




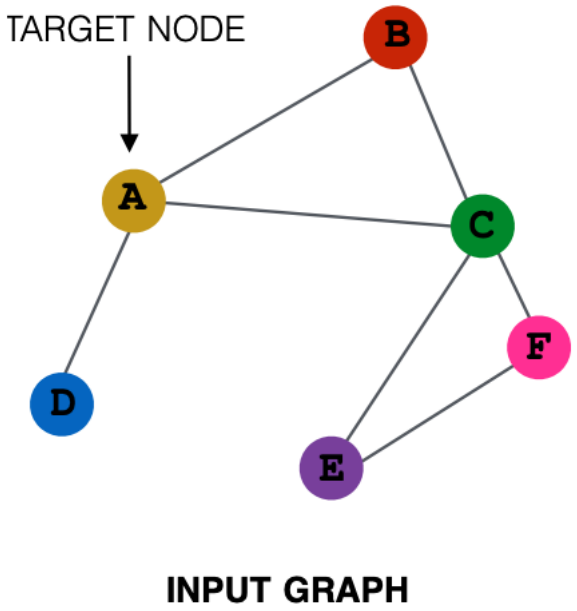


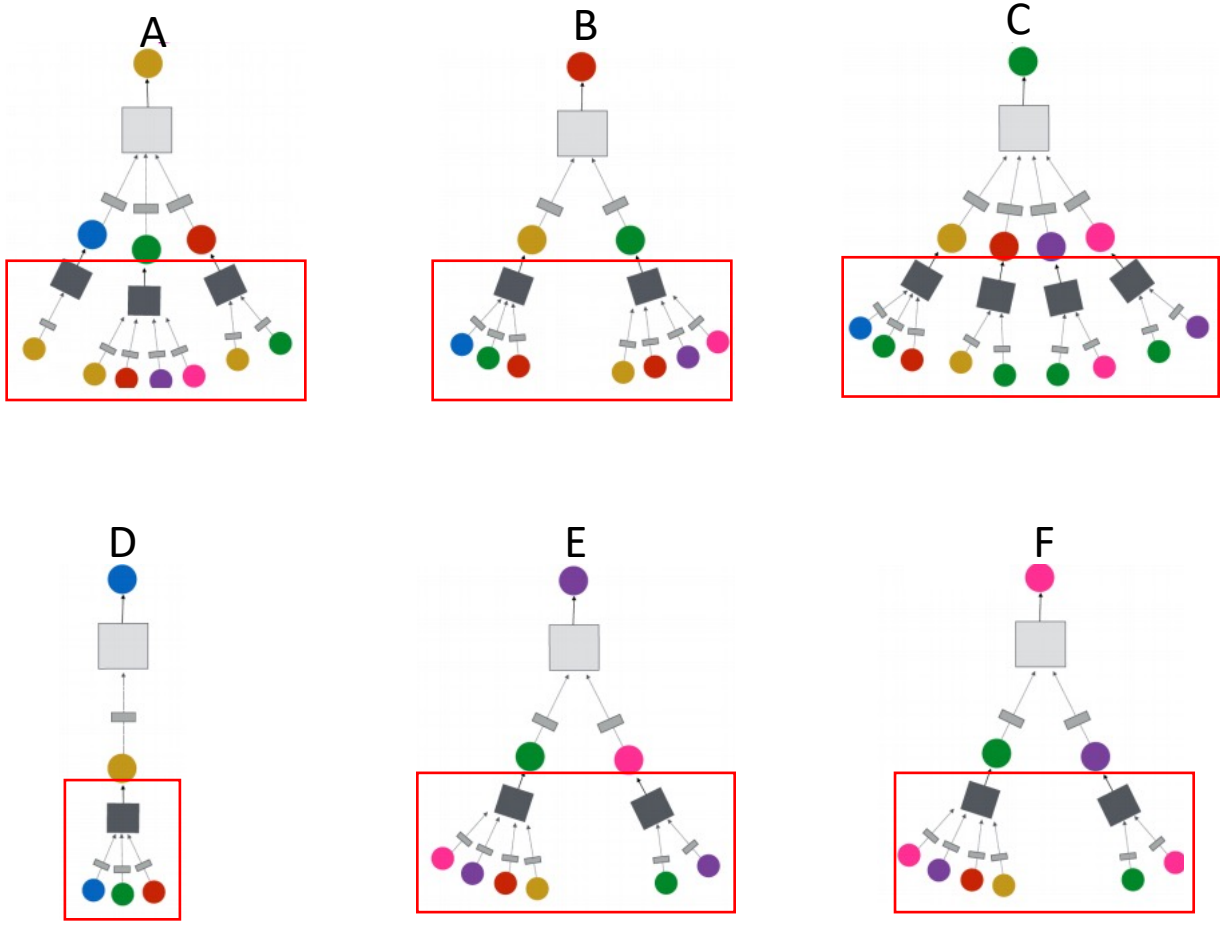






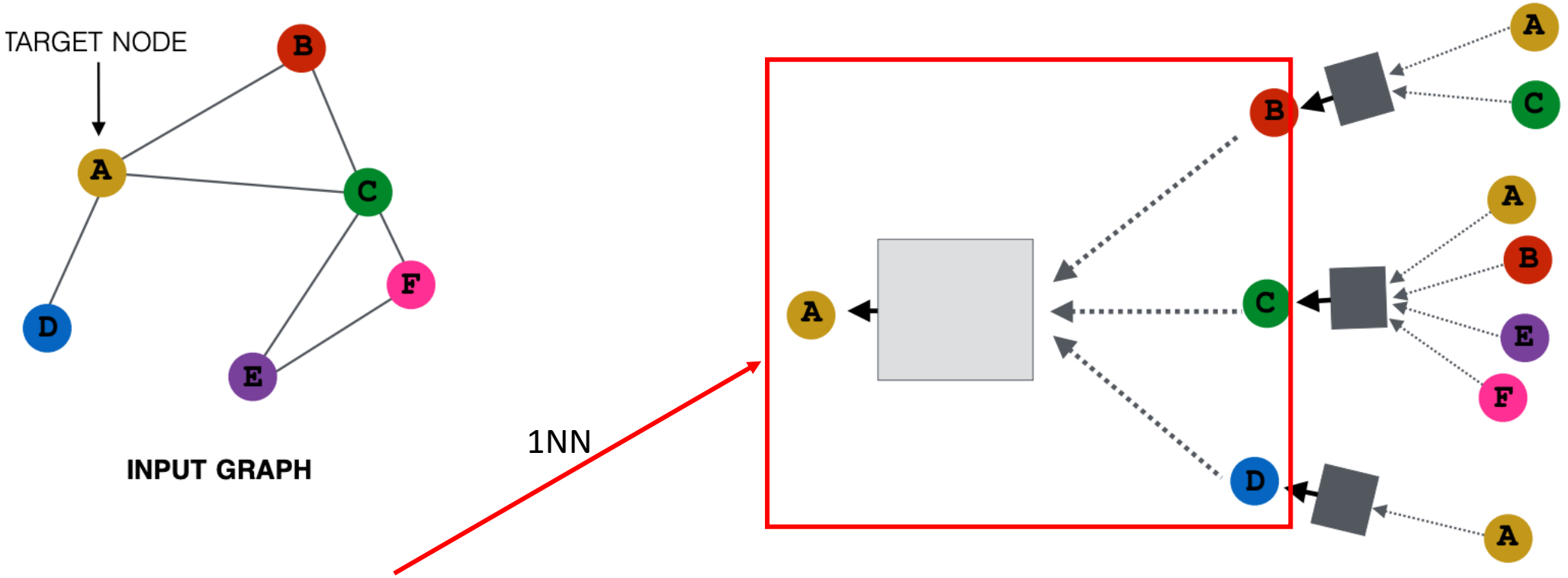
Graph networks: aggregate neighbors





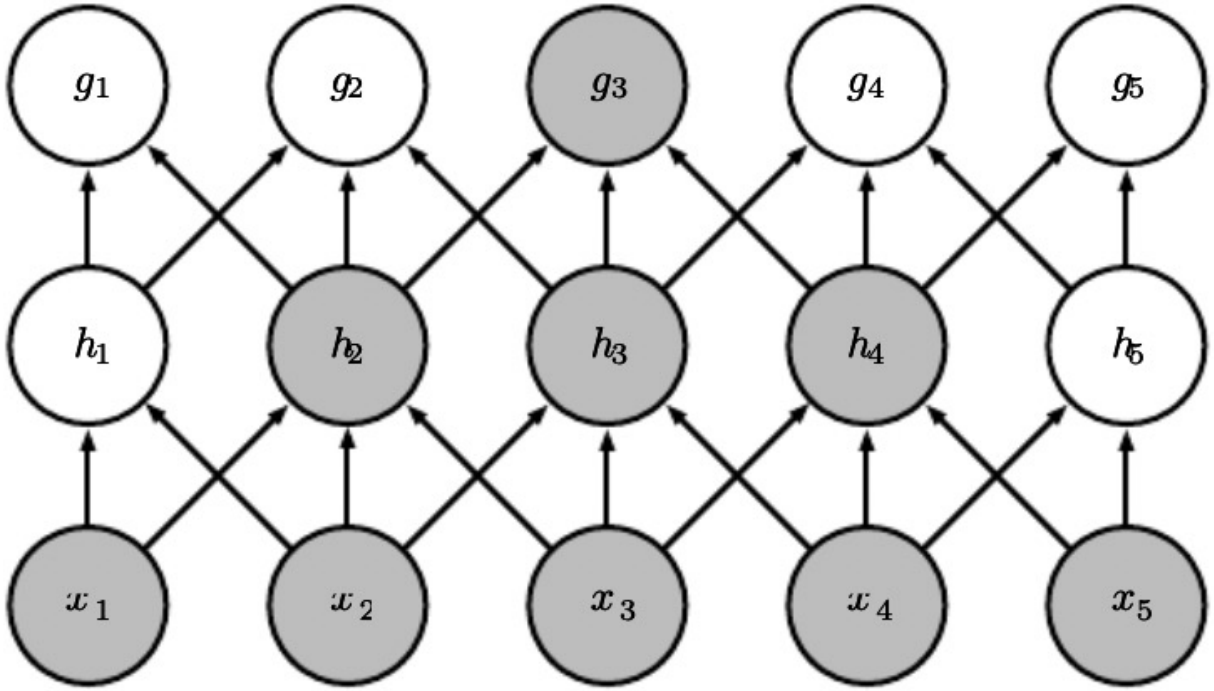
Two hops (two nearest neighbors, 2NN)

Graph networks: aggregate neighbors

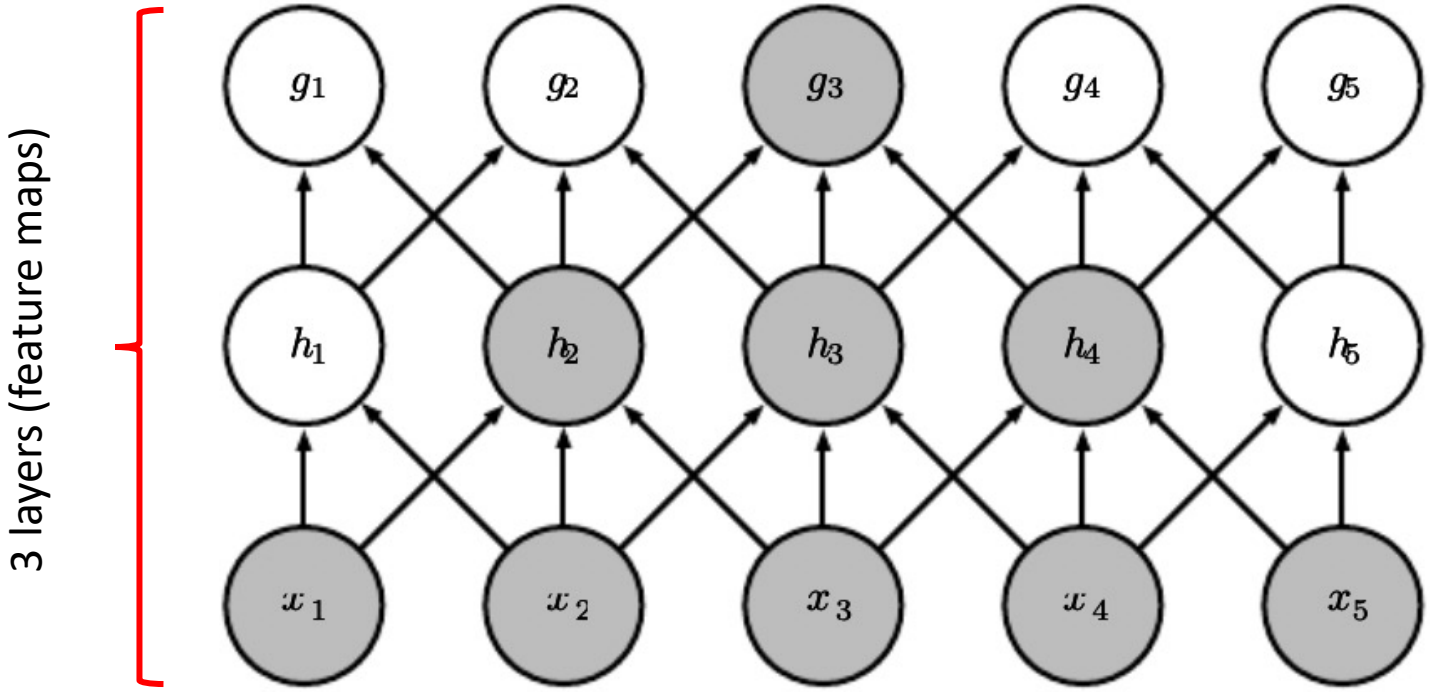


Q: can we add more NNs? → 3NN, 4NN, …
→ it will aggregate/cover all nodes in a graph

Recall: receptive field of CNN

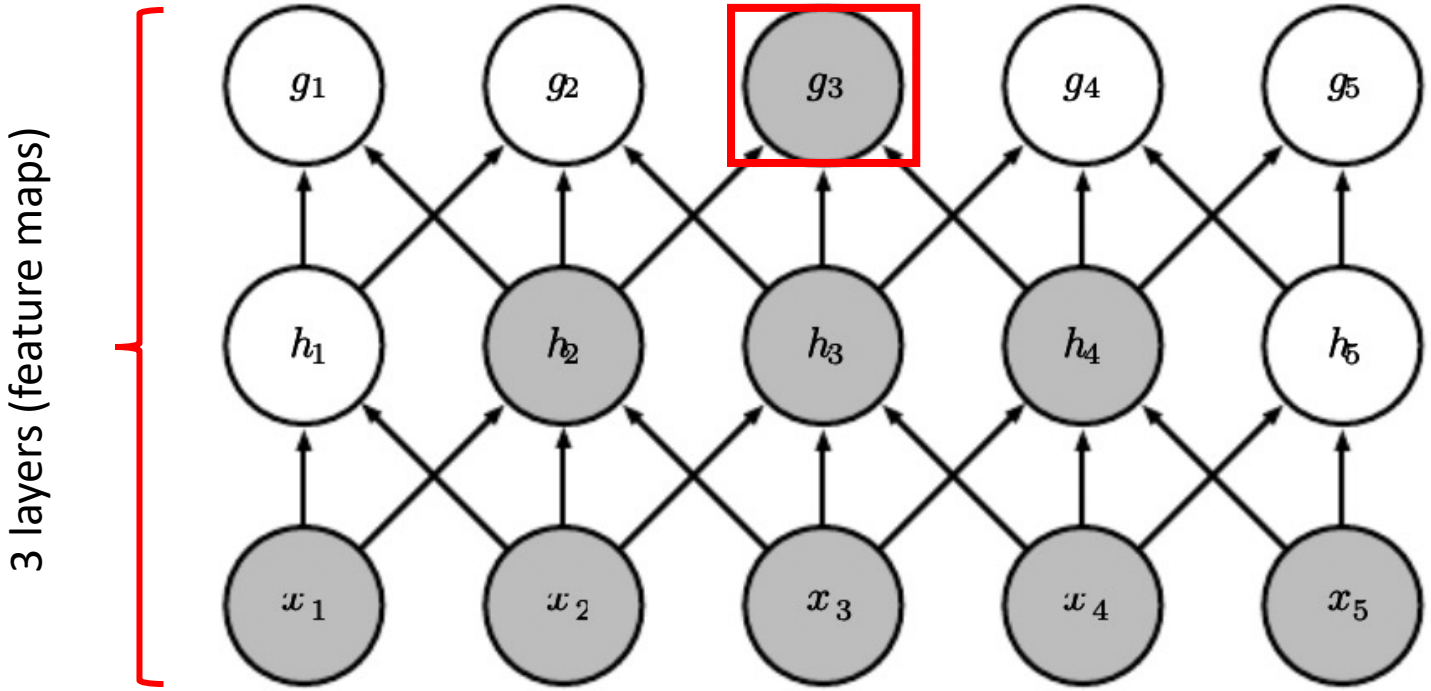


Recall: receptive field of CNN

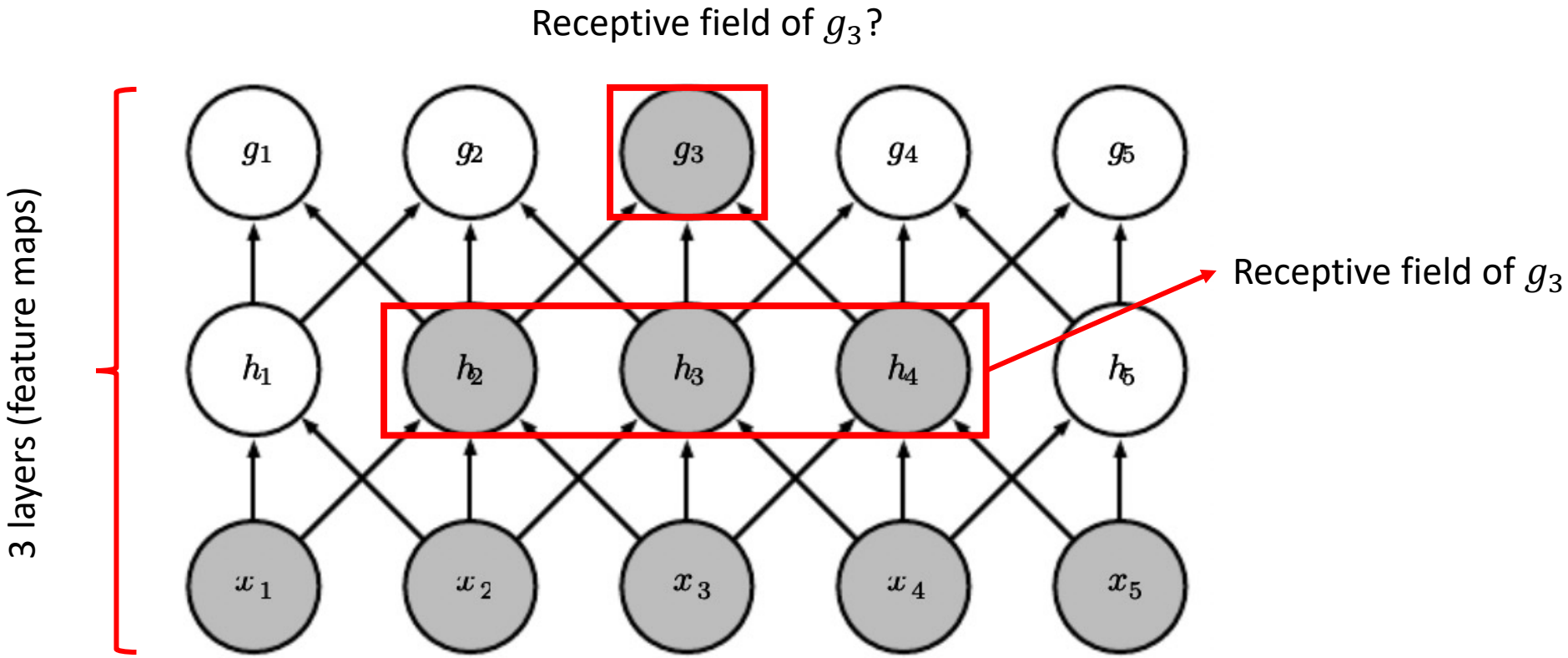


Recall: receptive field of CNN

Receptive field of g_3?

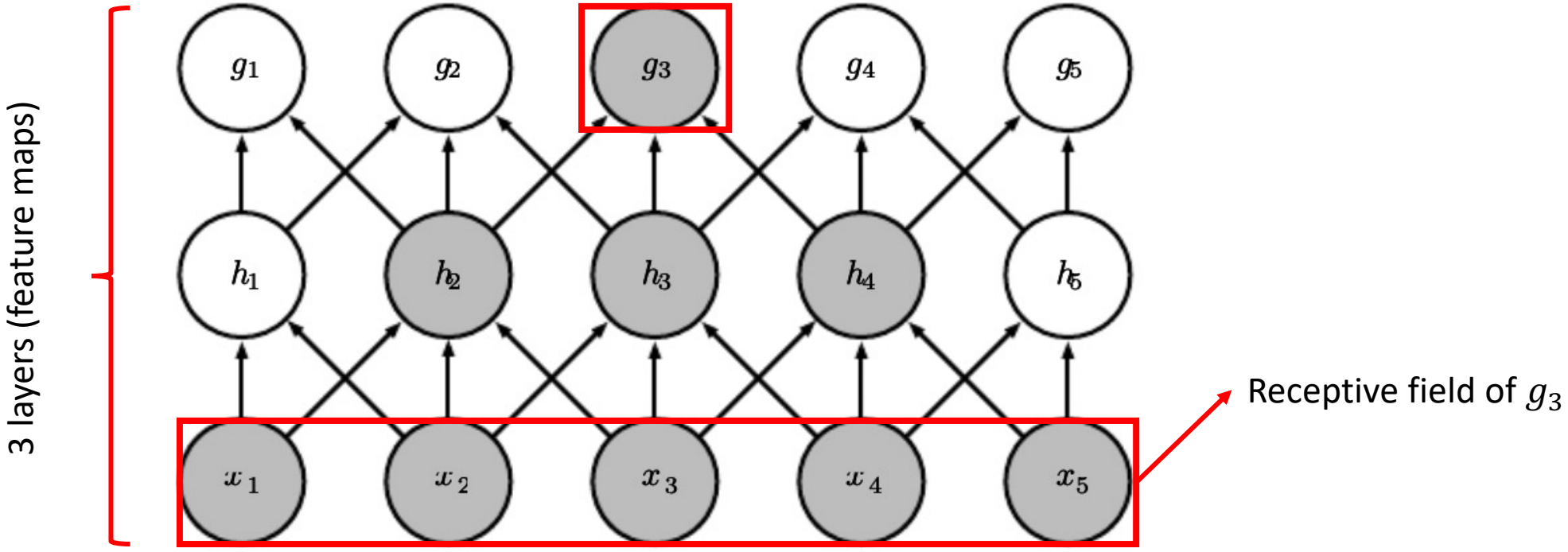


Recall: receptive field of CNN



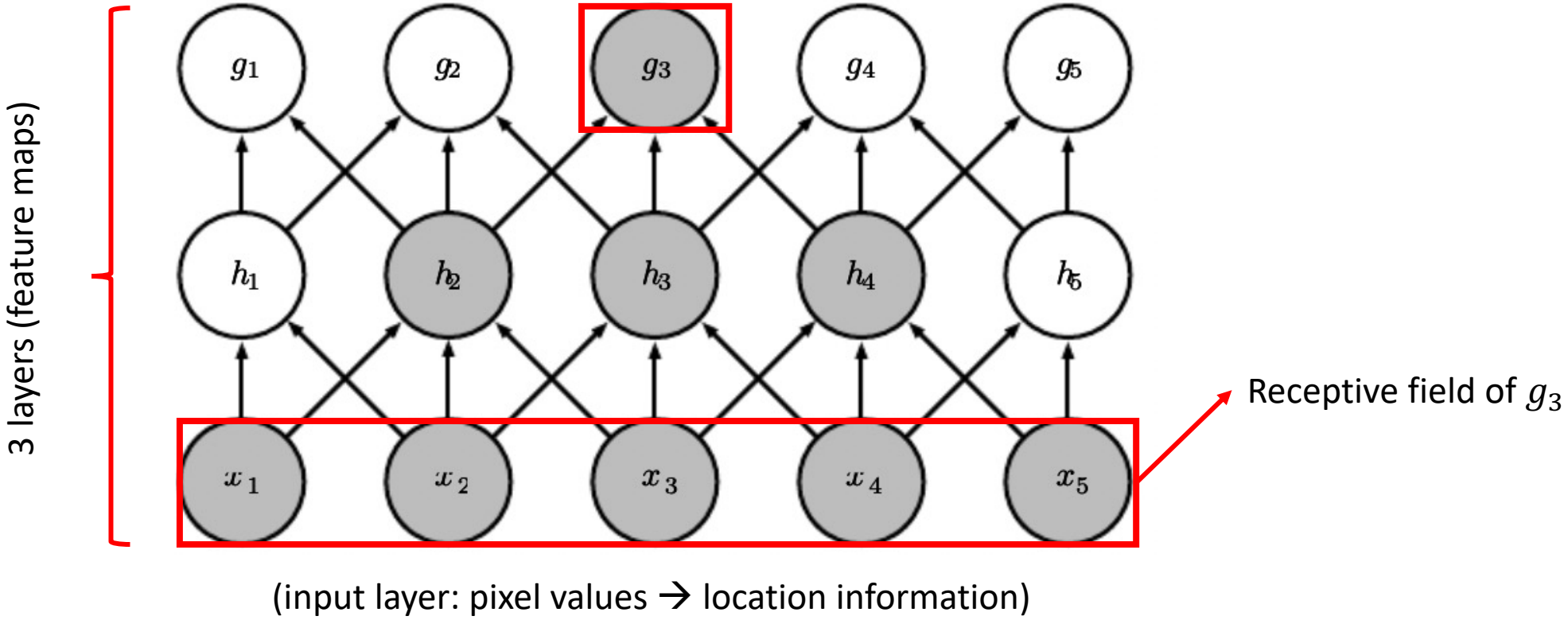
Recall: receptive field of CNN

Receptive field of g_3?



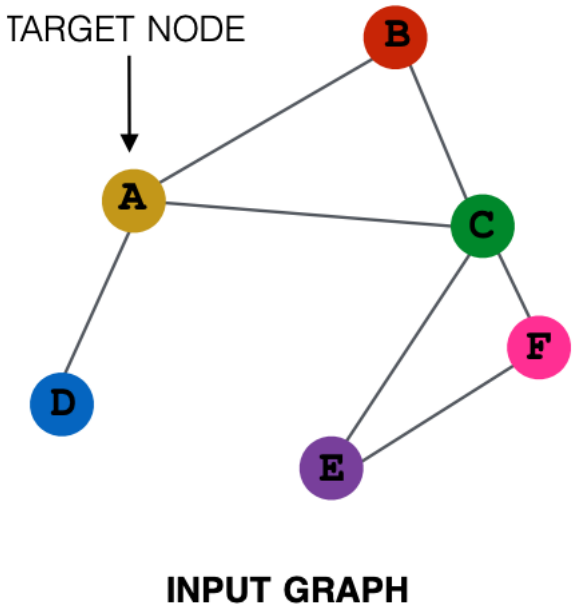
Recall: receptive field of CNN

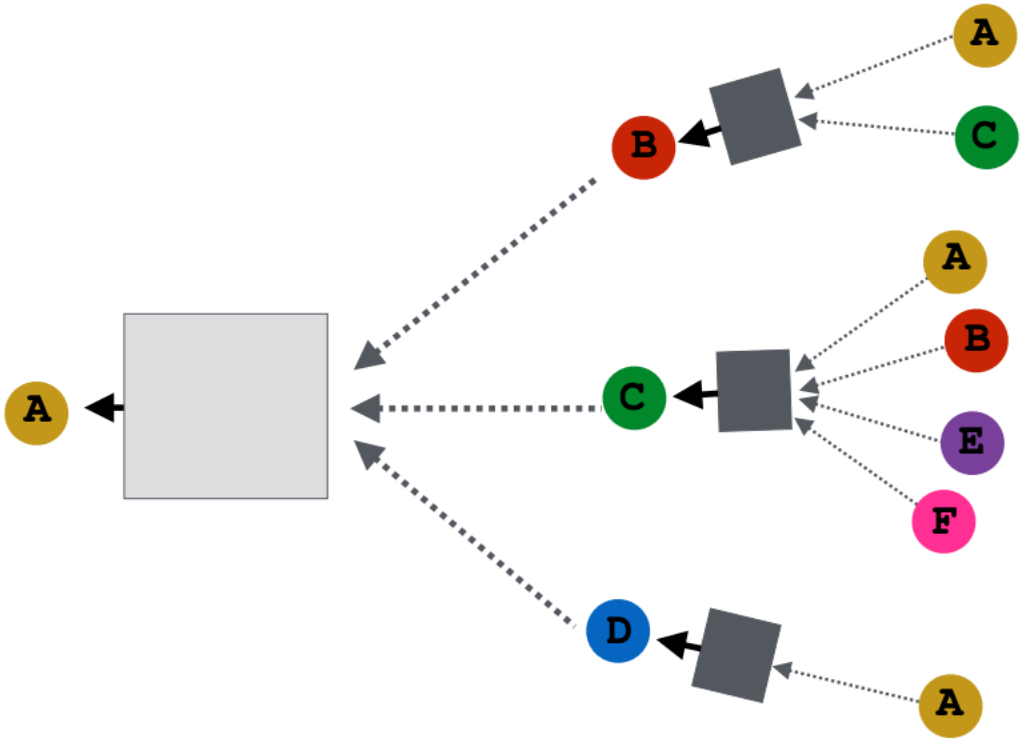
Receptive field of g_3?



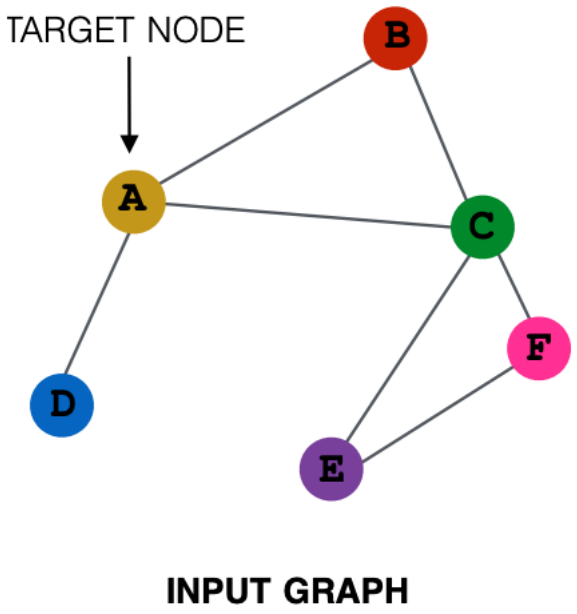
(input layer: pixel values → location information)

Receptive field of GCN

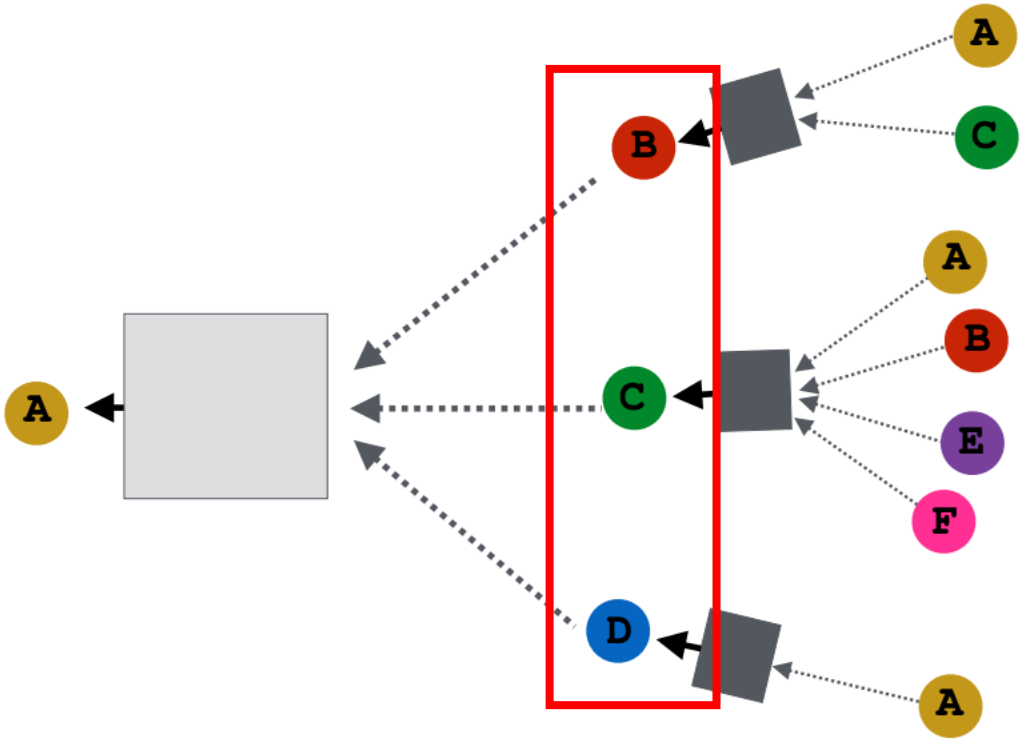




Receptive field of GCN

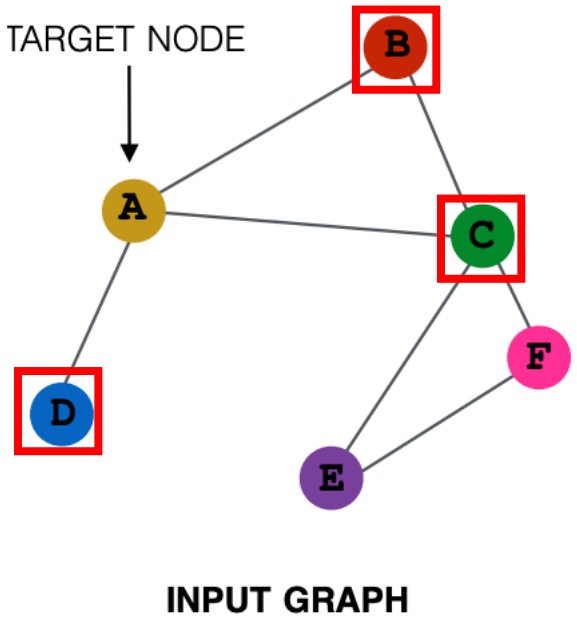


INPUT GRAPH

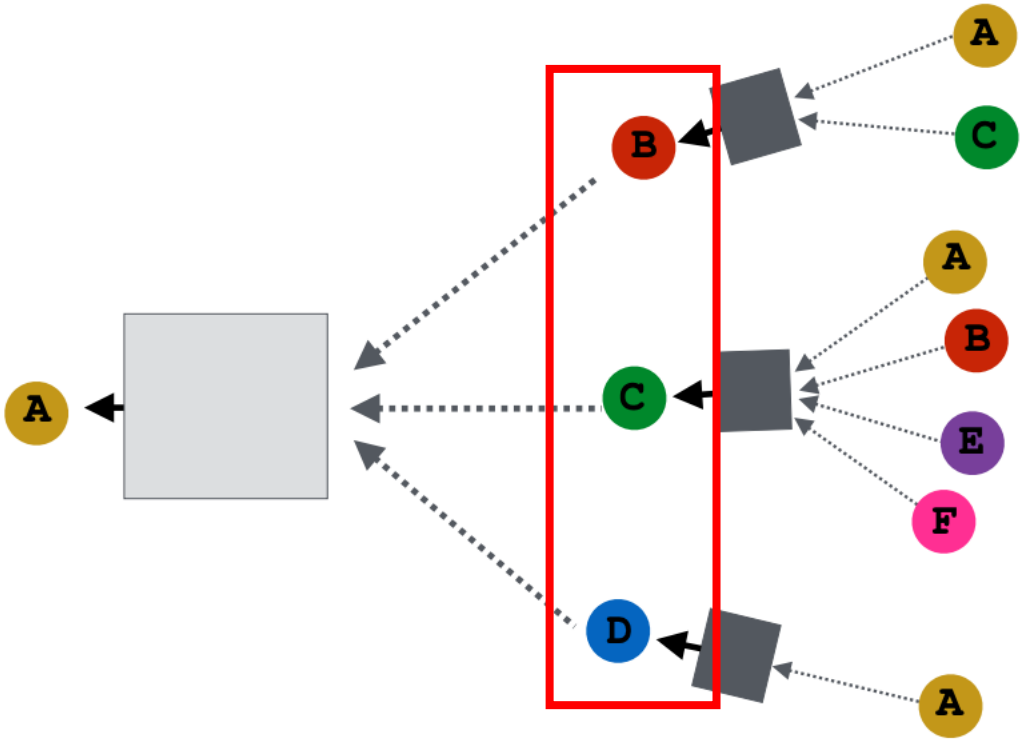


B, C, D

Receptive field of GCN

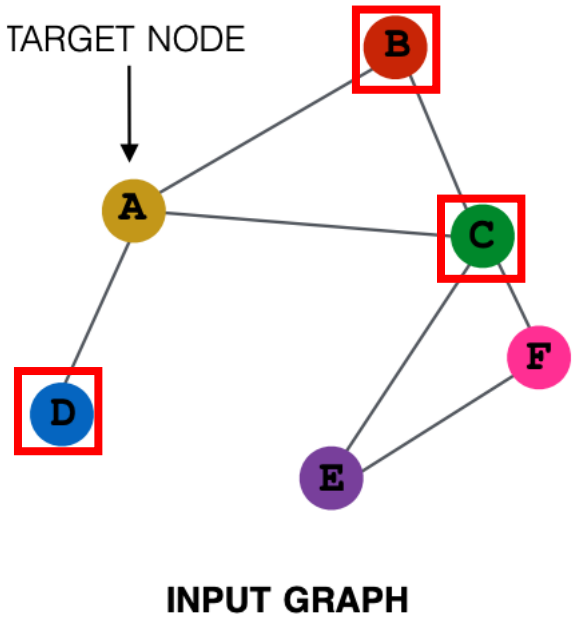


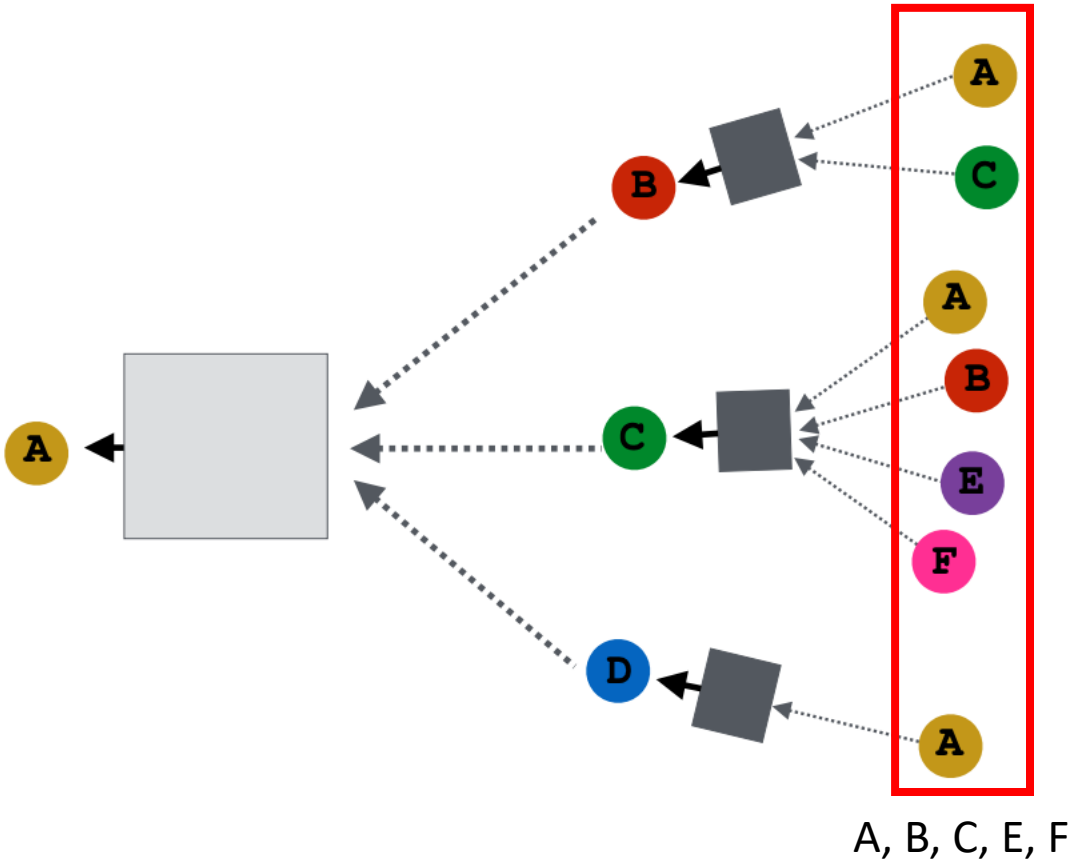
INPUT GRAPH



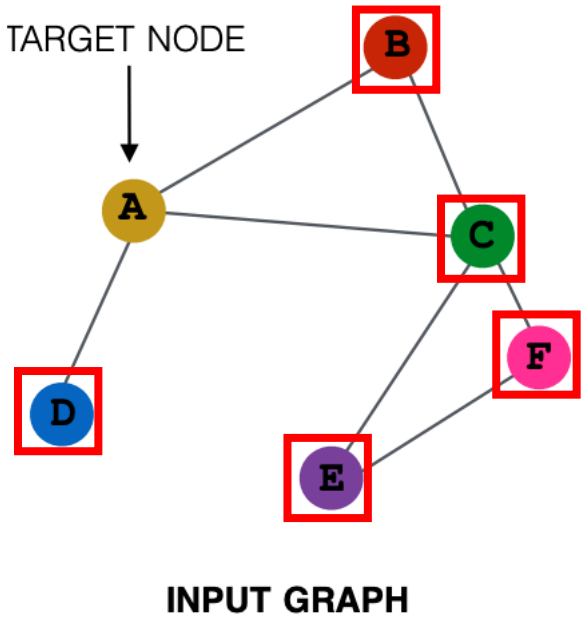
B, C, D

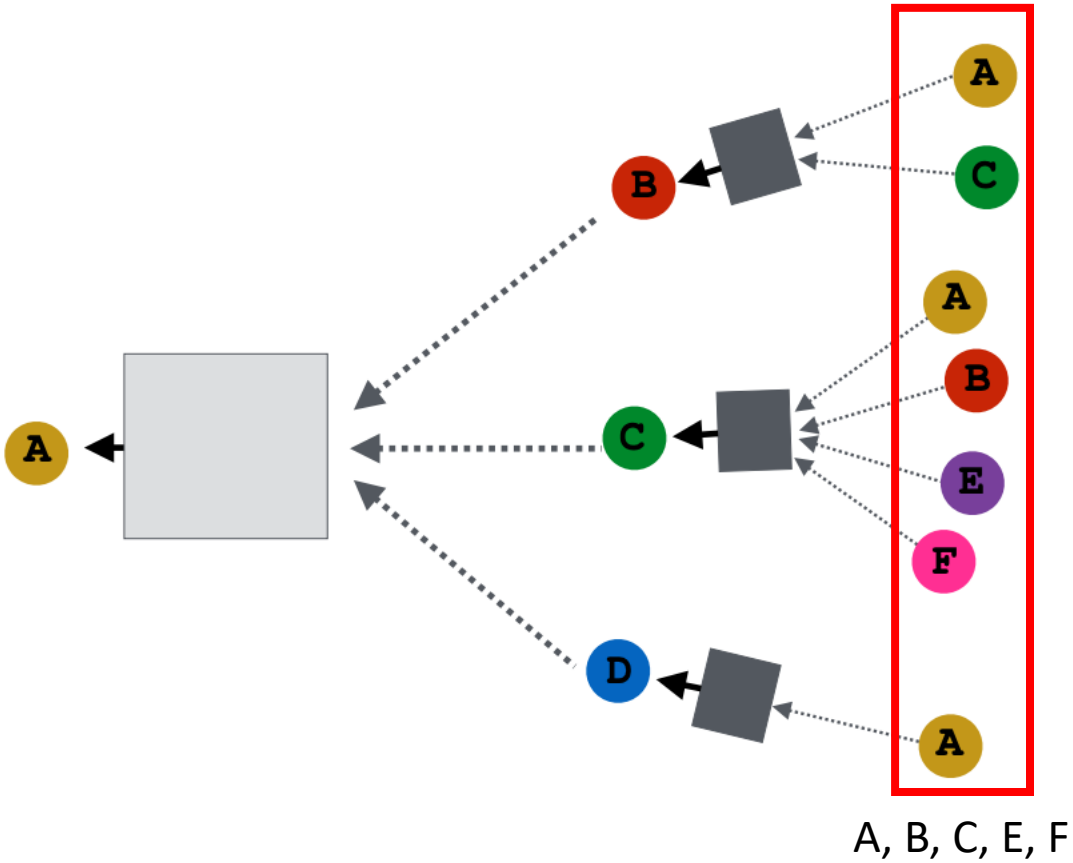
Receptive field of GCN



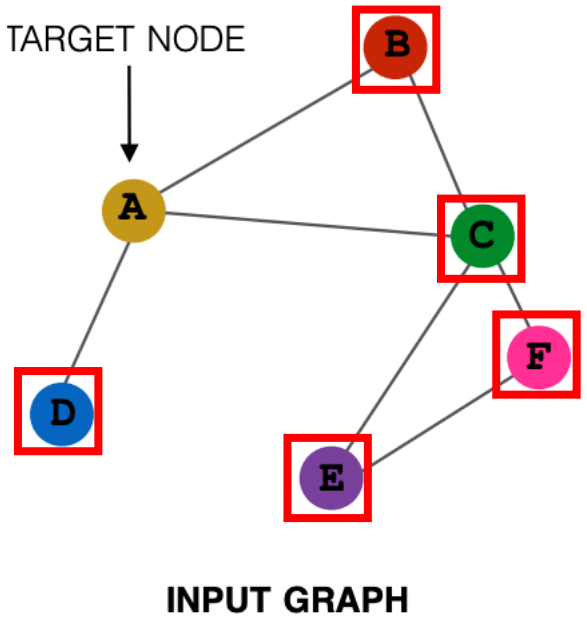


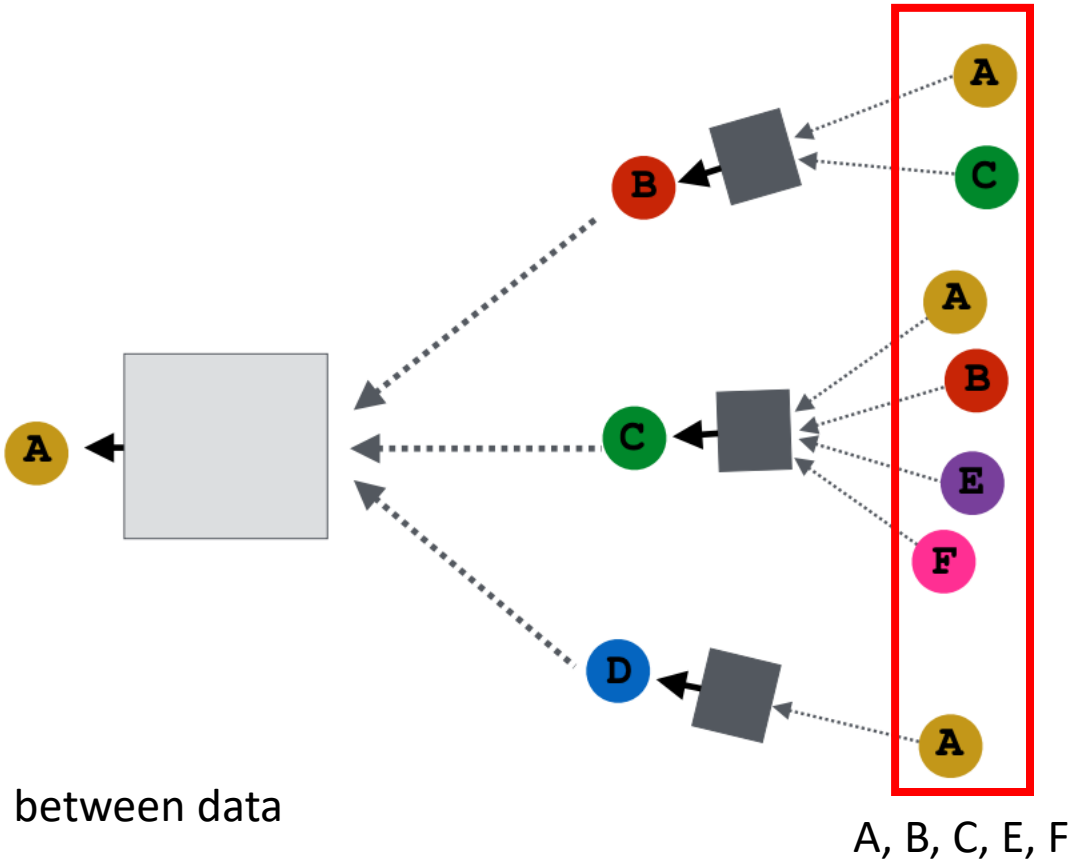
Receptive field of GCN





Receptive field of GCN



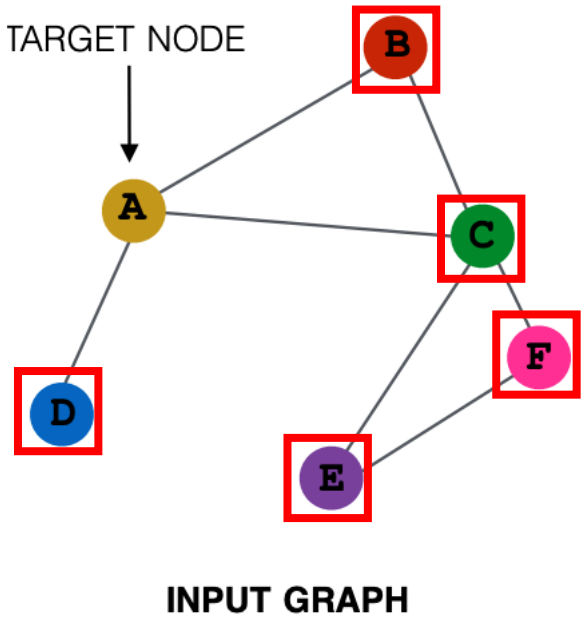


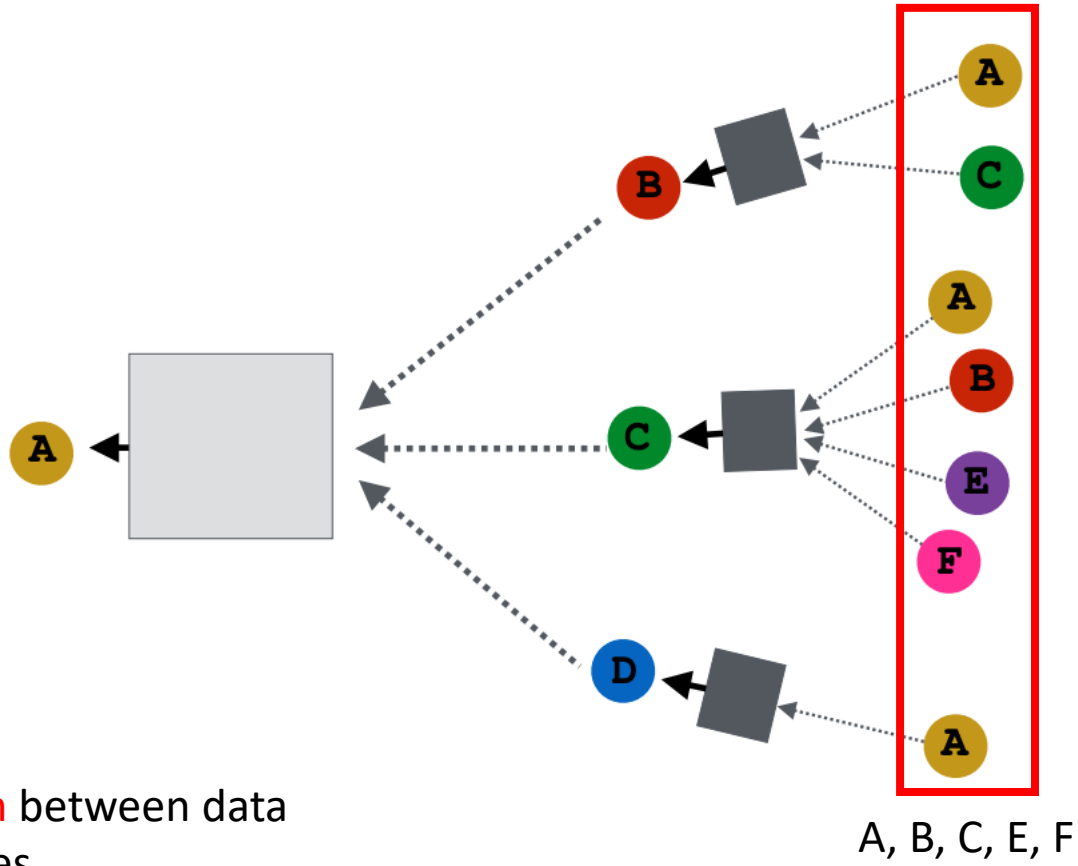
Cover the entire graph

GCN: learn representation/feature capturing the correlation between data

A, B, C, E, F

Receptive field of GCN



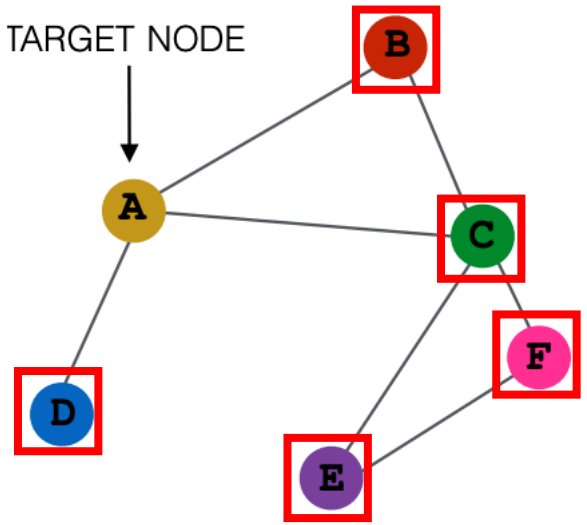


Cover the entire graph

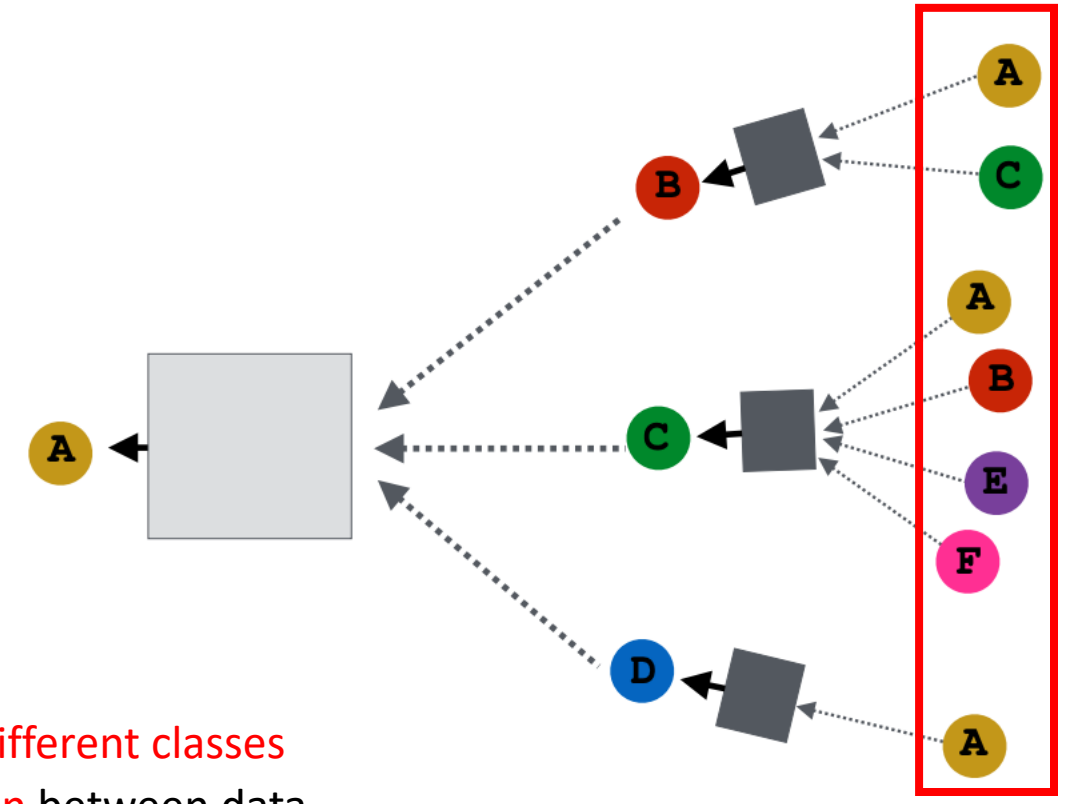
GCN: learn representation/feature capturing the correlation between data

Node classification: differentiate nodes from different classes

Receptive field of GCN



INPUT GRAPH



A, B, C, E, F

Cover the entire graph → correlation between different classes ?

GCN: learn representation/feature capturing the correlation between data

Node classification: differentiate nodes from different classes

Receptive field of GCN

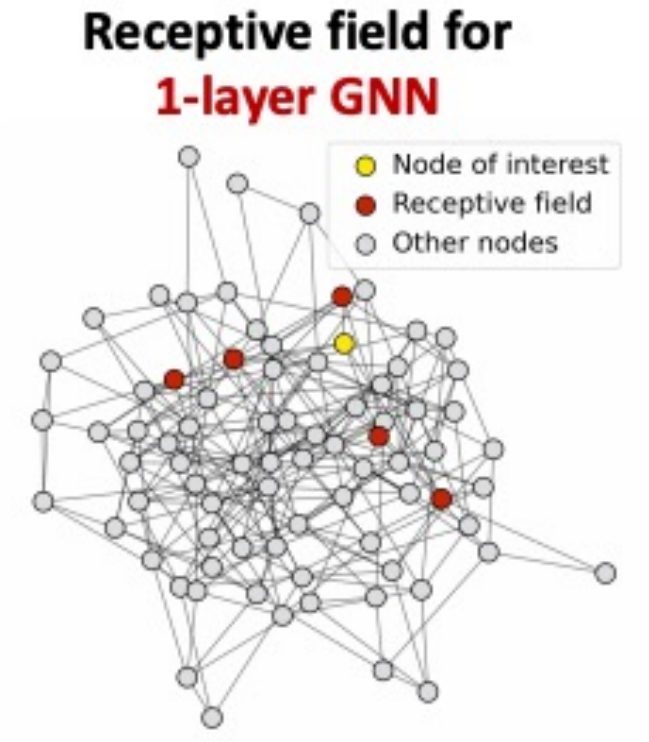
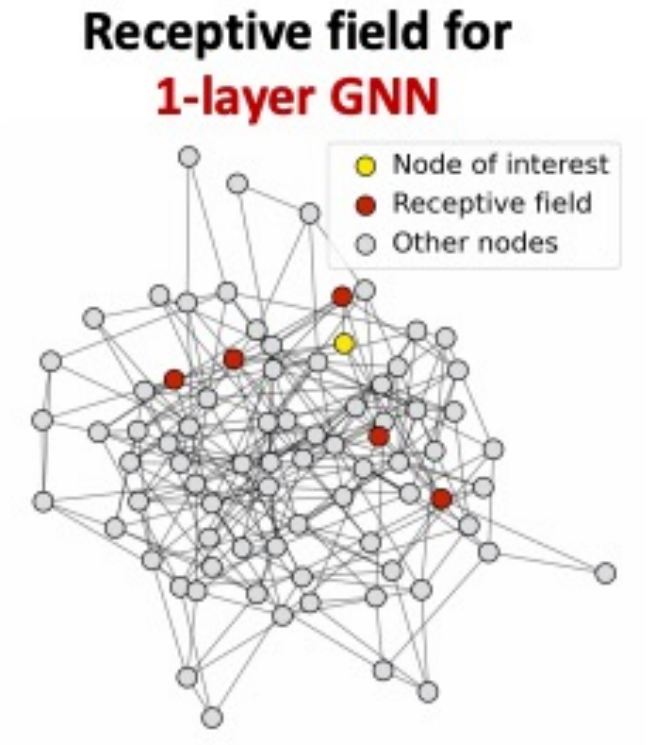


Image credit http://web.stanford.edu/class/cs224w/slides/07-GNN2.pdf

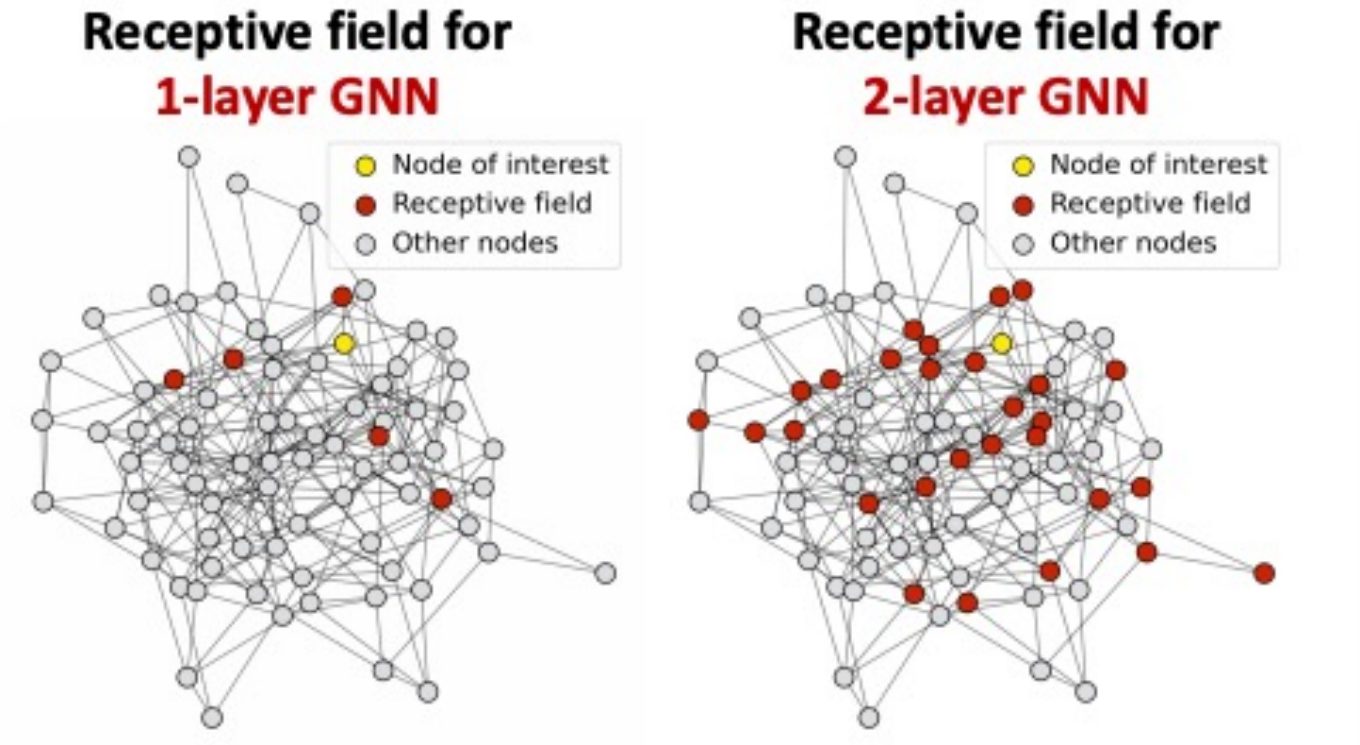
Receptive field of GCN



Only 5 nearest neighbors

Image credit http://web.stanford.edu/class/cs224w/slides/07-GNN2.pdf

Receptive field of GCN



Only 5 nearest neighbors

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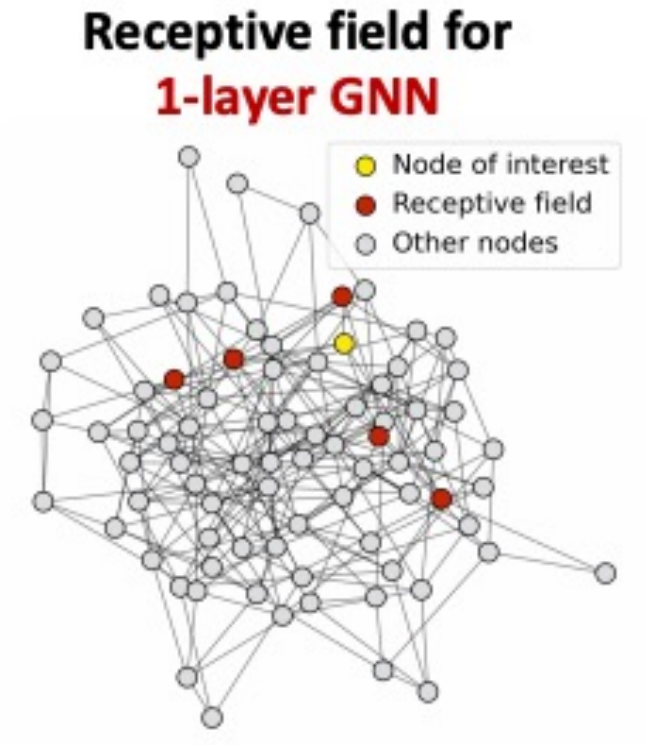
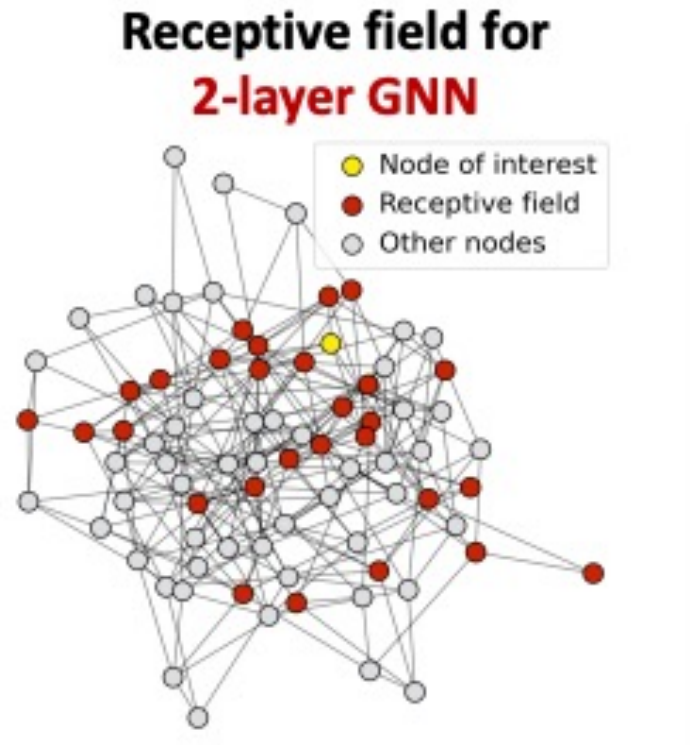
Receptive field of GCN



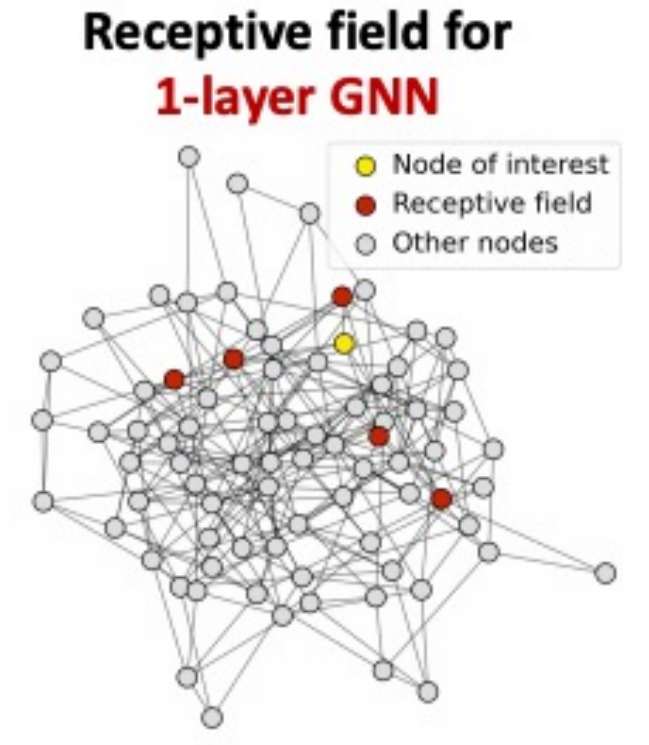
Only 5 nearest neighbors



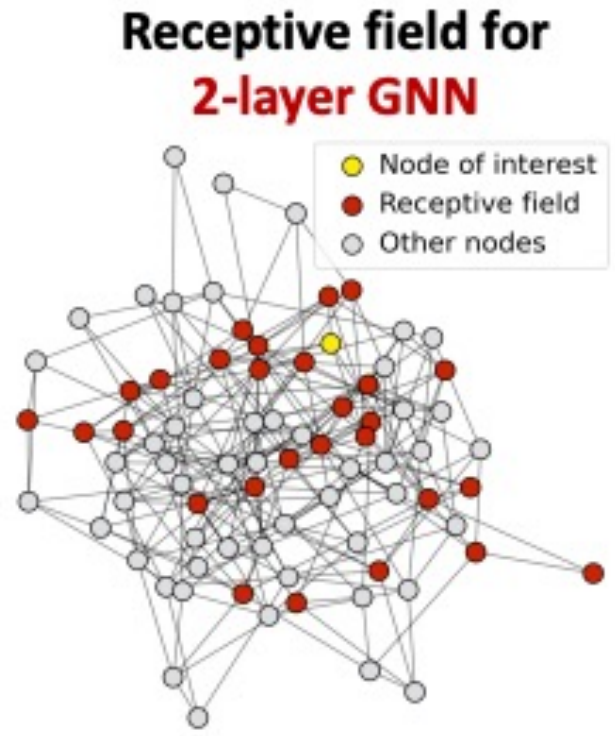
Over 20 nodes

Image credit http://web.stanford.edu/class/cs224w/slides/07-GNN2.pdf

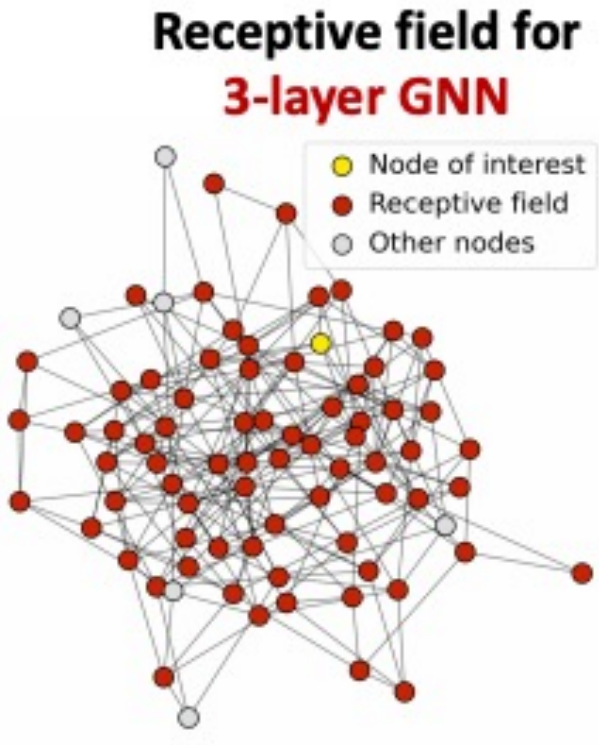
Receptive field of GCN



Only 5 nearest neighbors



Over 20 nodes



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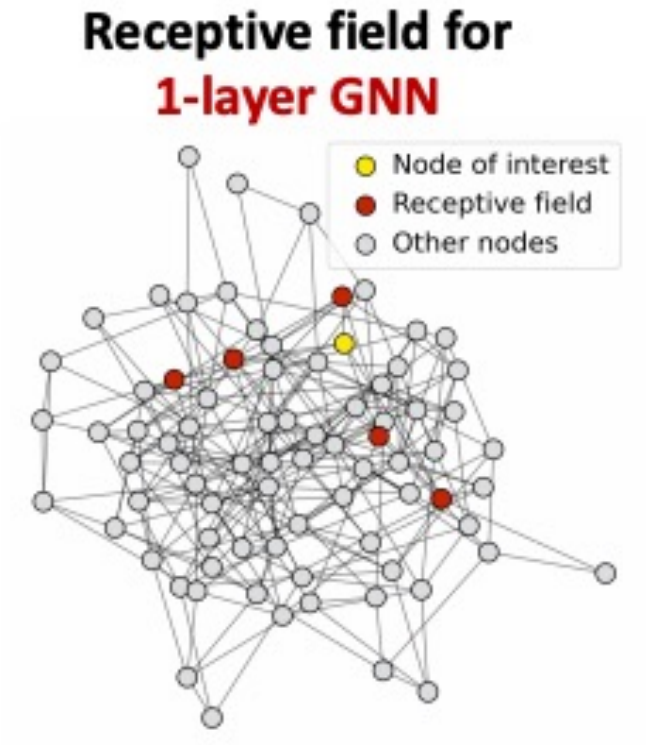
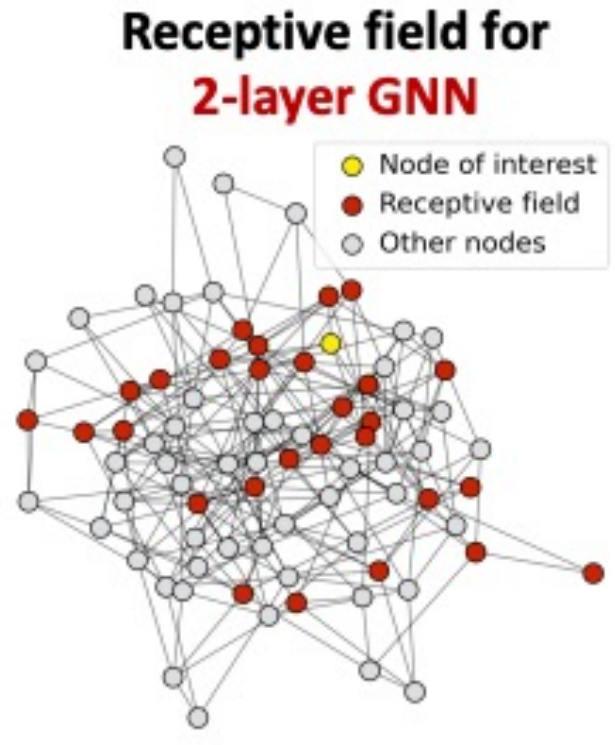
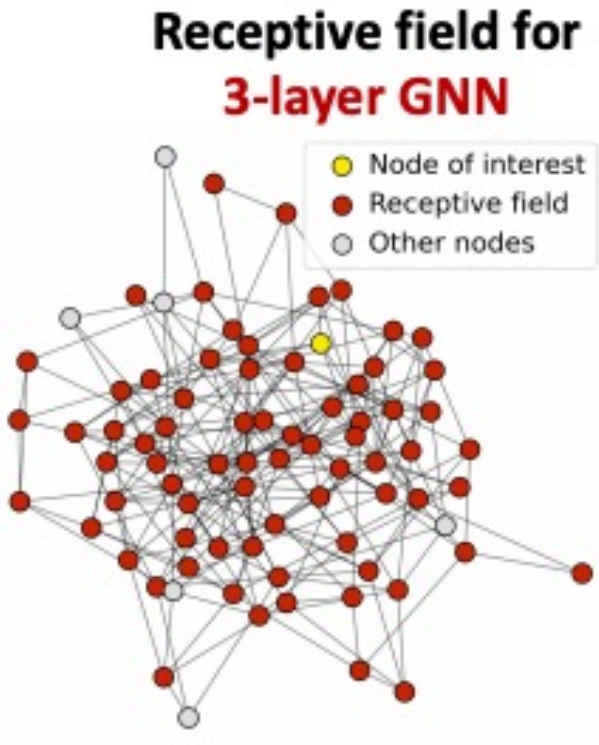
Receptive field of GCN



Only 5 nearest neighbors



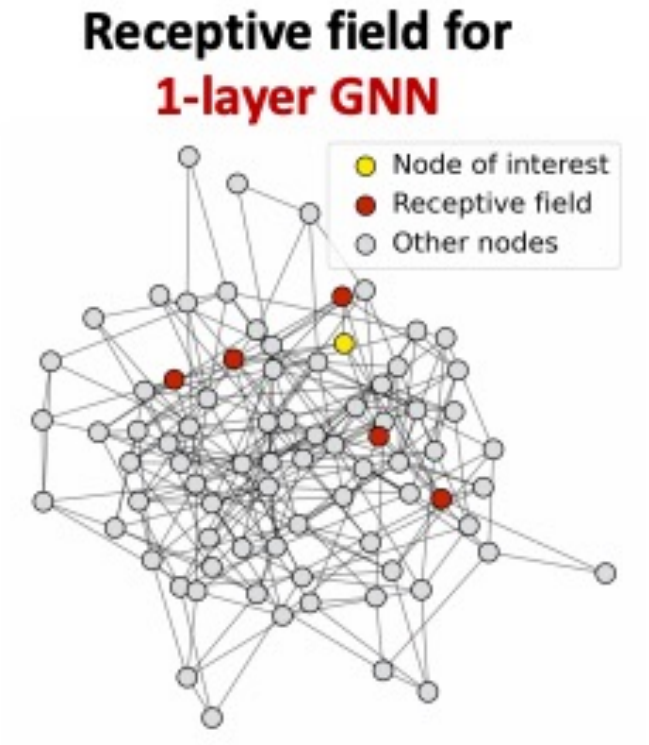
Over 20 nodes



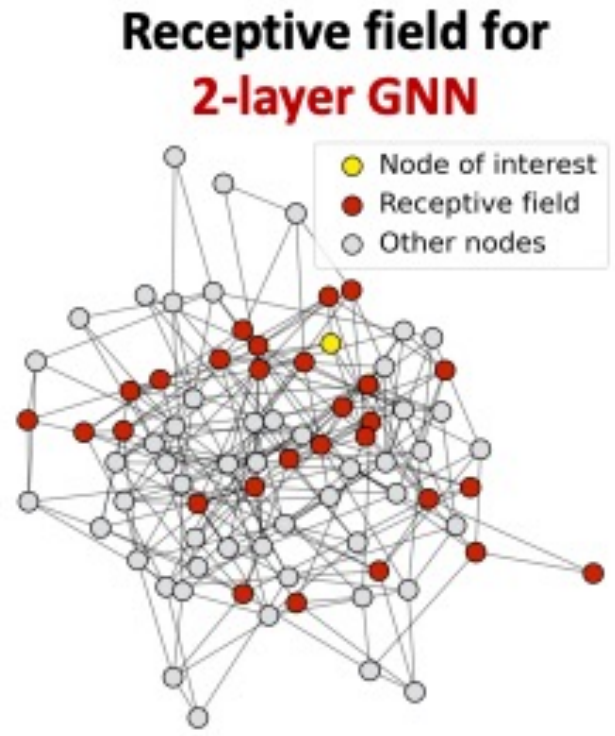
Almost all nodes

Image credit http://web.stanford.edu/class/cs224w/slides/07-GNN2.pdf

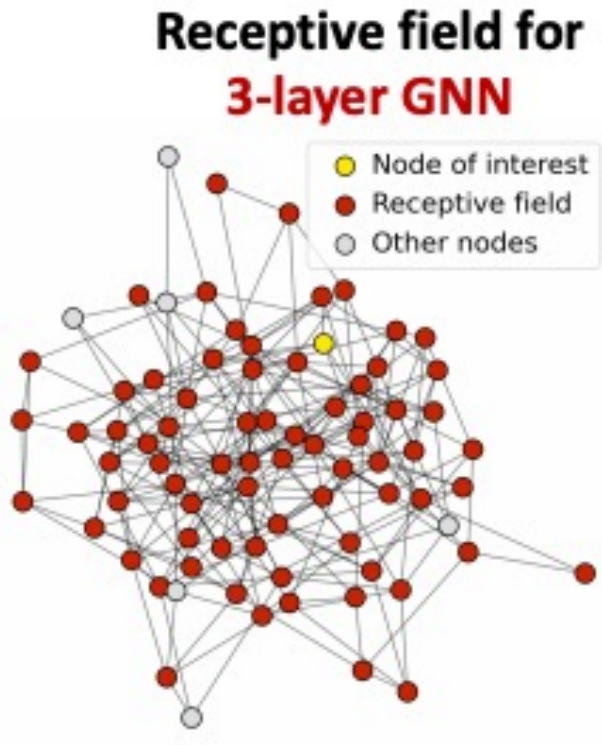
Receptive field of GCN



Only 5 nearest neighbors



Over 20 nodes



Almost all nodes
Aggregate node features regardless the clusters (communities)

Image credit http://web.stanford.edu/class/cs224w/slides/07-GNN2.pdf

Smooth a curve

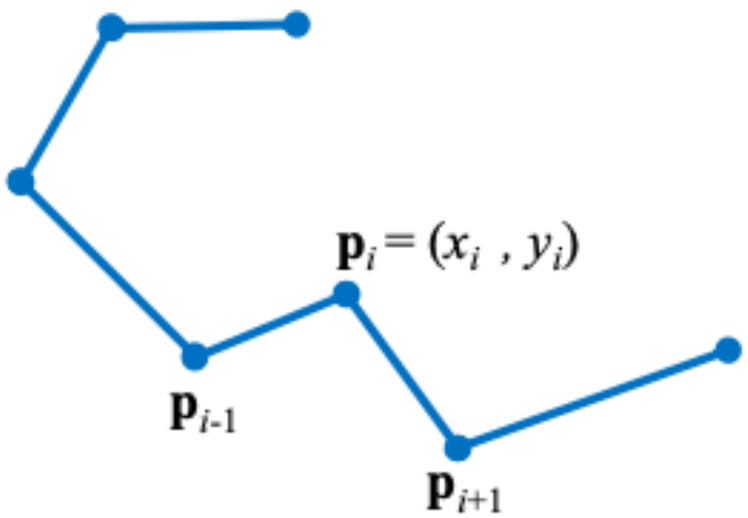


Image credit https://graphics.stanford.edu/courses/cs468-12-spring/LectureSlides/06_smoothing.pdf

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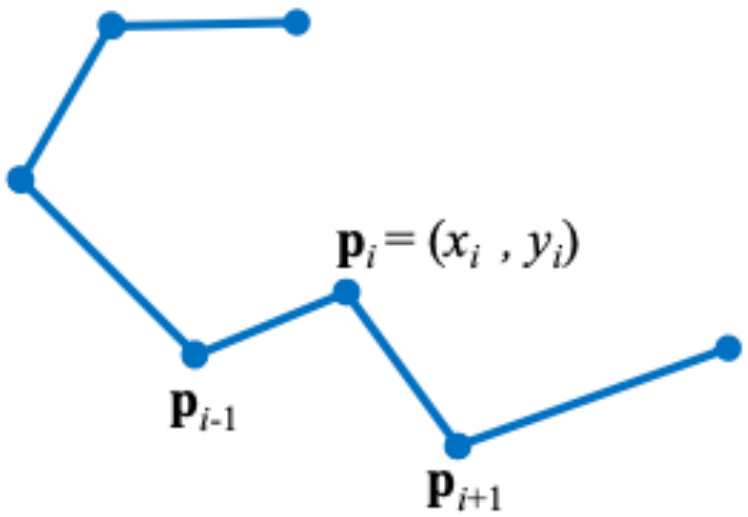
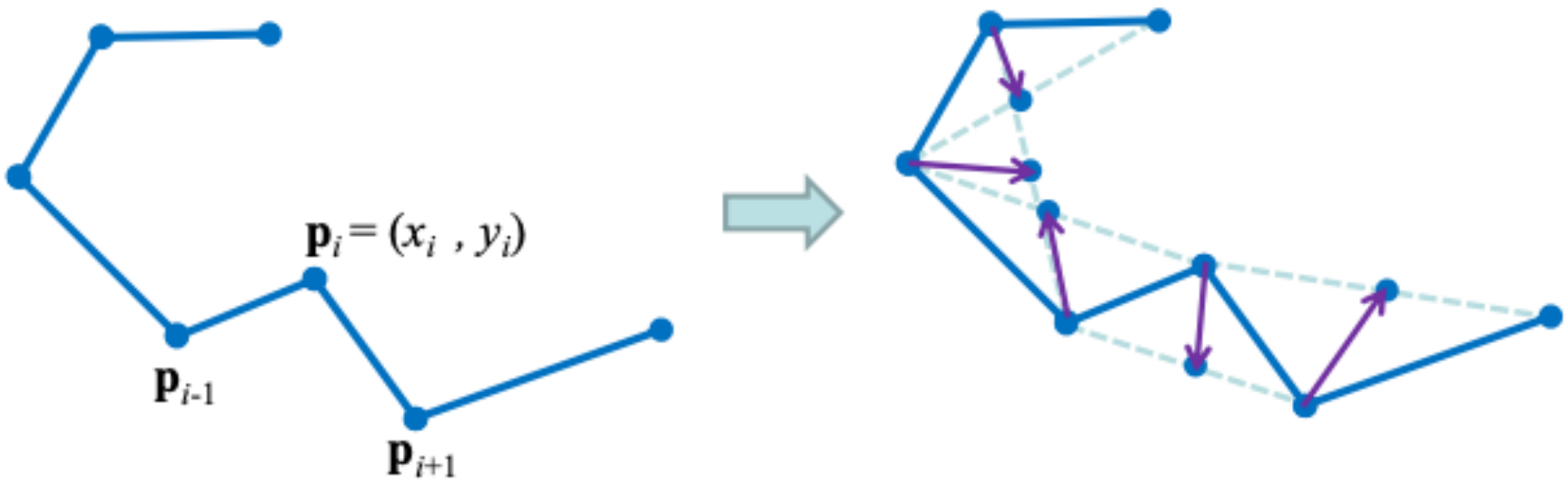


Q: how can we smooth this curve to be more like a straight line?

Image credit https://graphics.stanford.edu/courses/cs468-12-spring/LectureSlides/06_smoothing.pdf

Smooth a curve

Laplacian smoothing



Q: how can we smooth this curve to be more like a straight line?

$$(\mathbf{p}_{i-1} + \mathbf{p}_{i+1})/2 - \mathbf{p}_i$$

$$L(\mathbf{p}_i) = \frac{1}{2}(\mathbf{p}_{i+1} - \mathbf{p}_i) + \frac{1}{2}(\mathbf{p}_{i-1} - \mathbf{p}_i)$$

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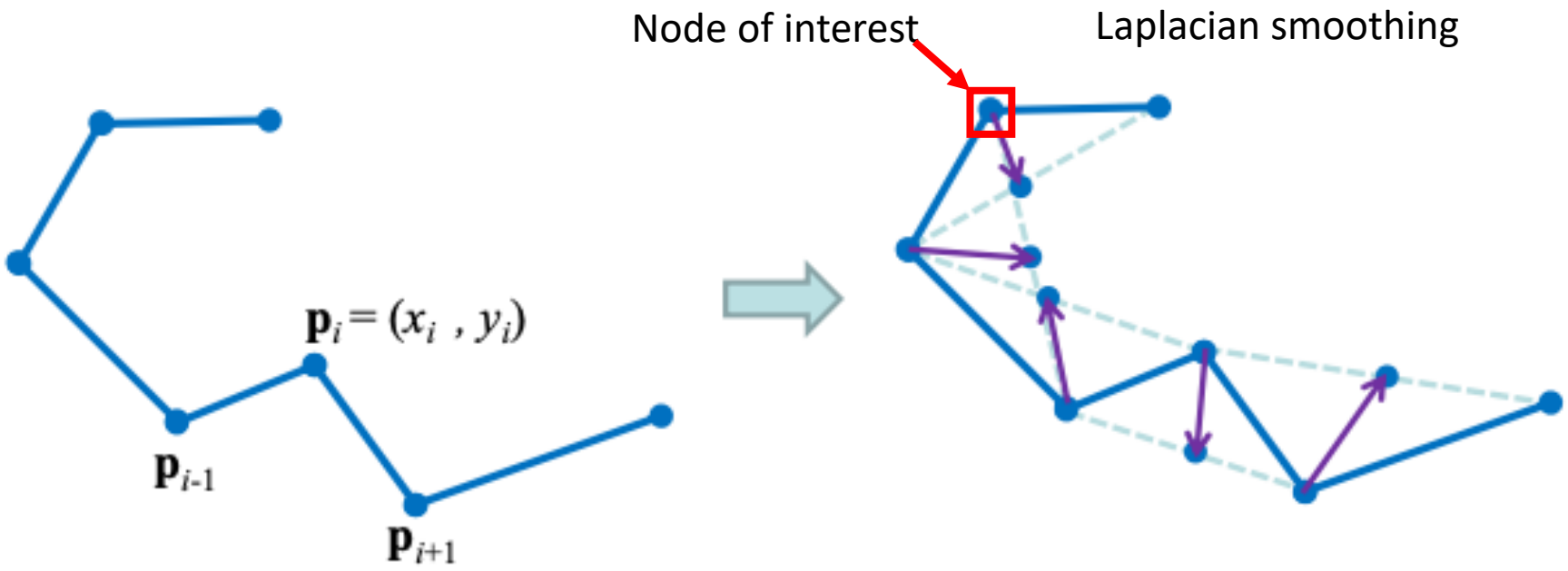
Smooth a curve



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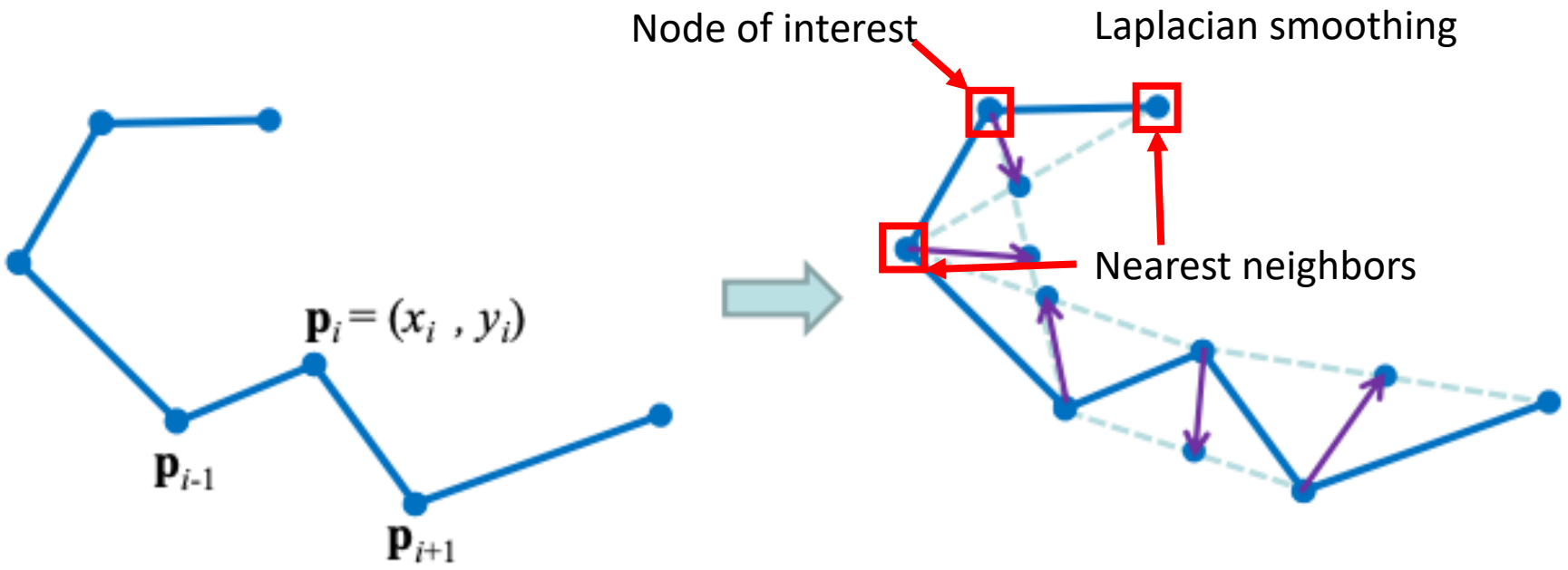

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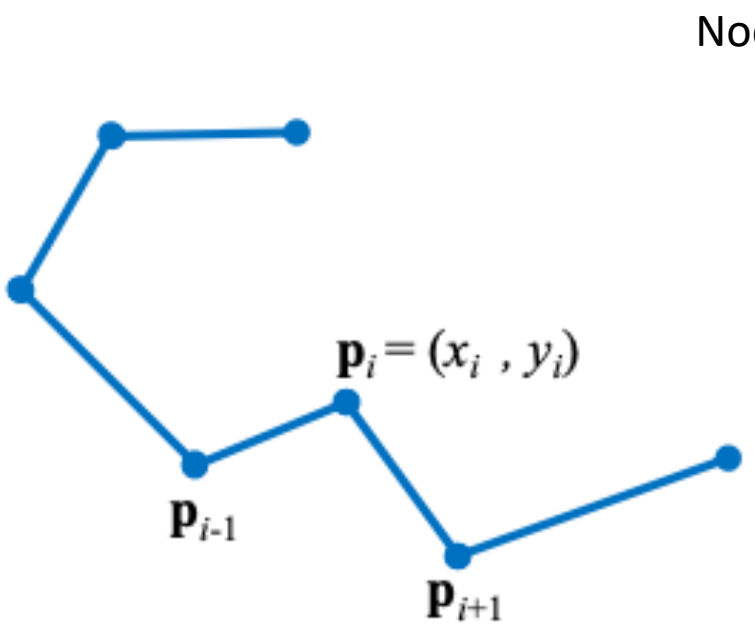

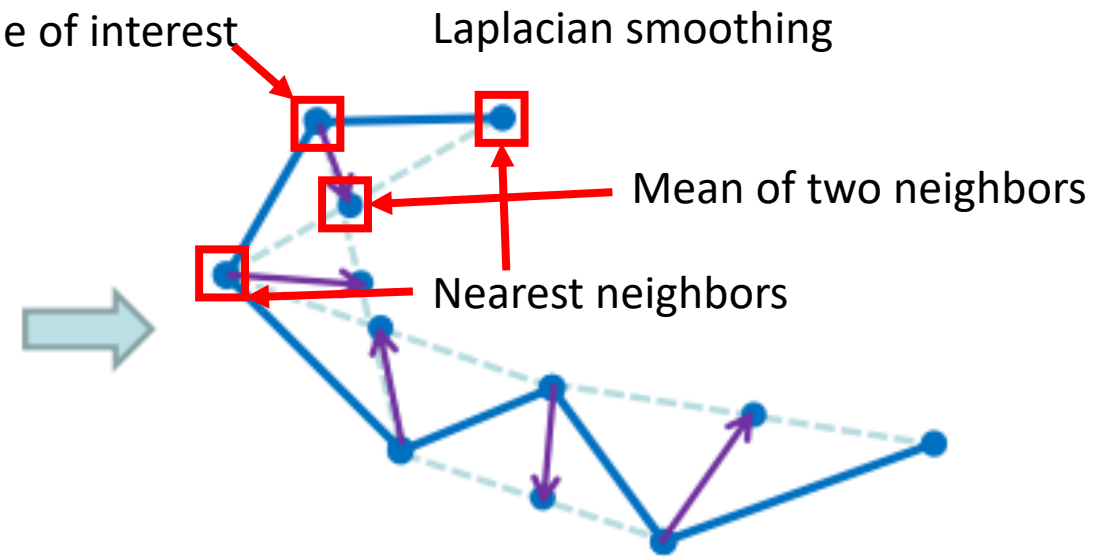

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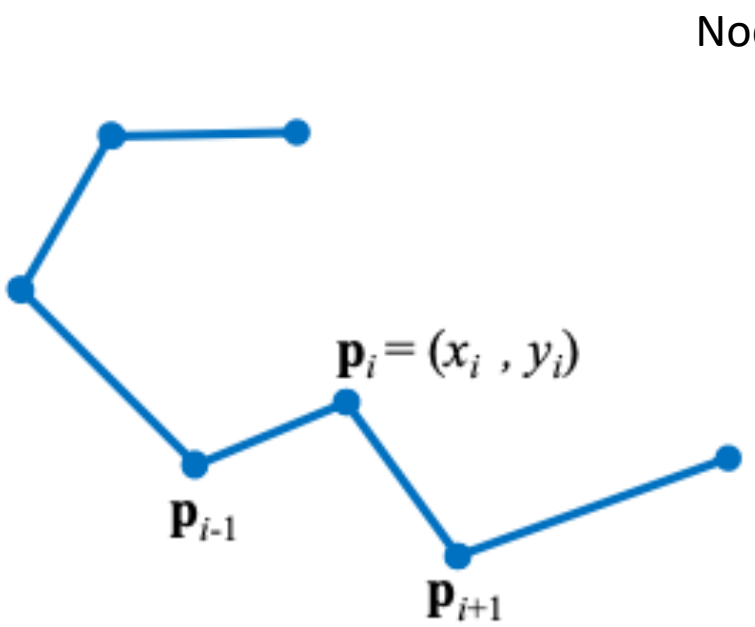

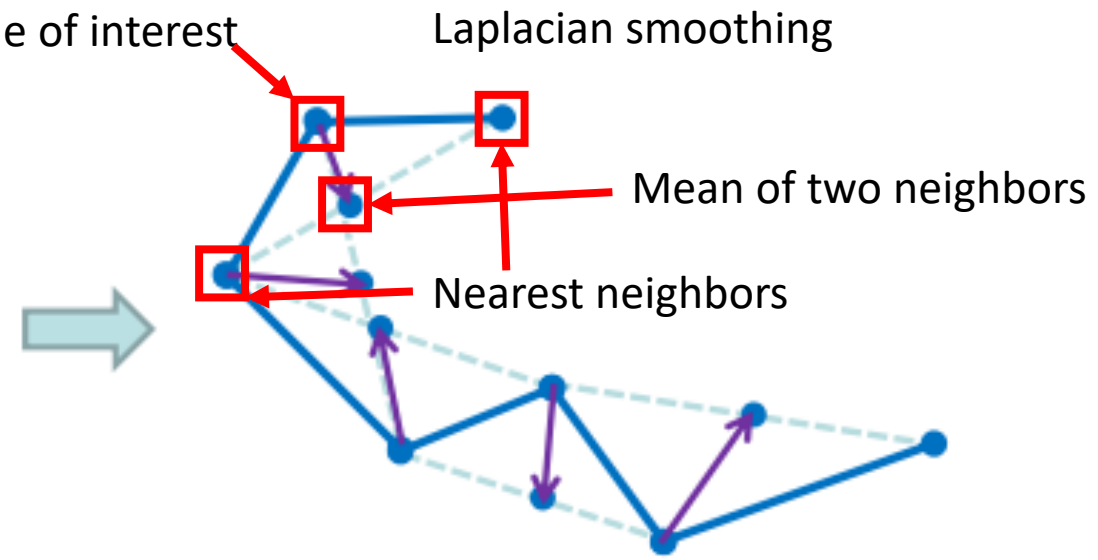

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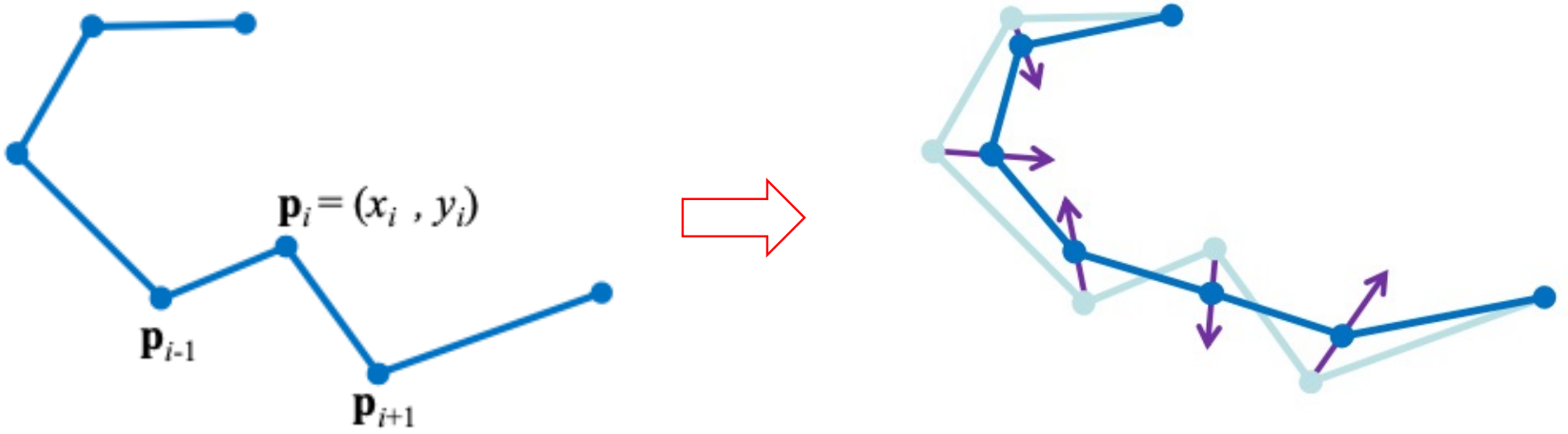

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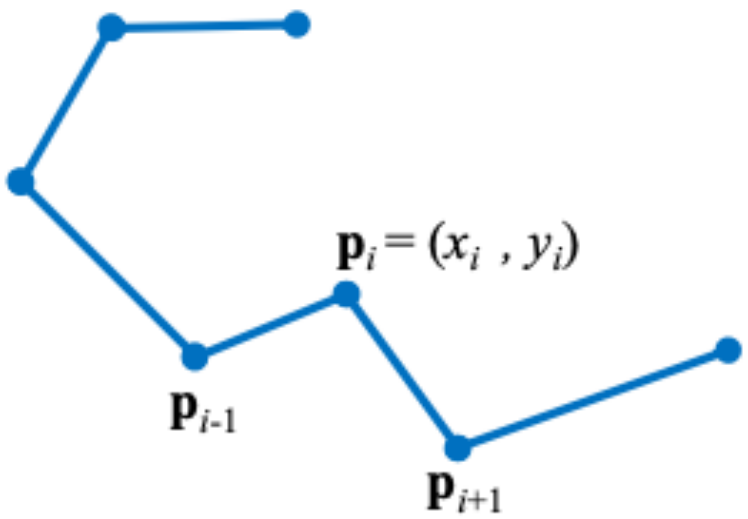
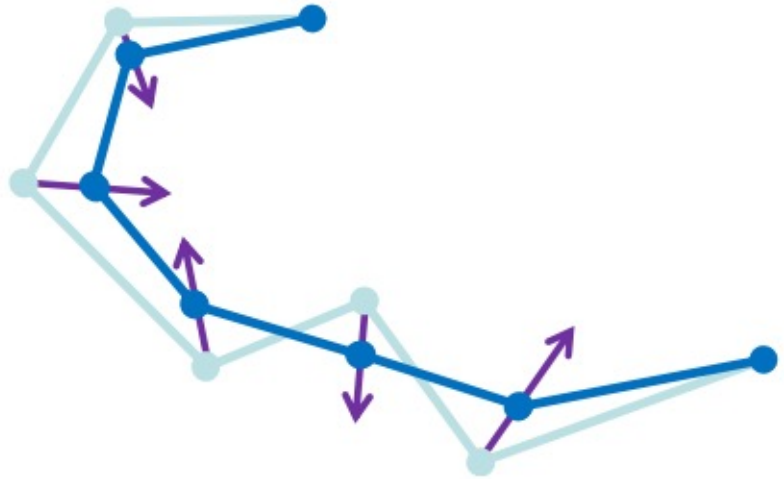


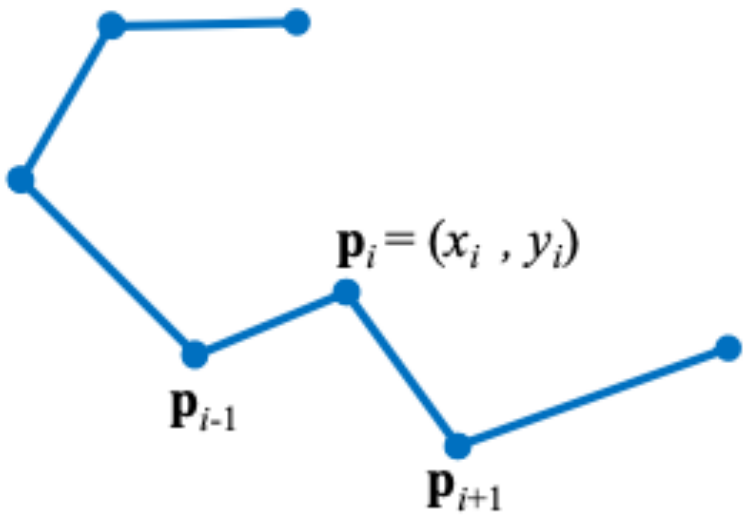


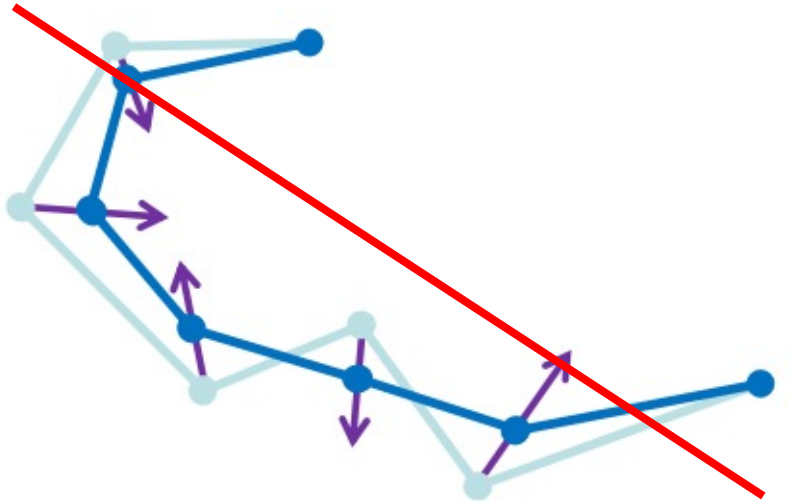
Q: what if we repeat for many times?

Q: how can we smooth this curve to be more like a straight line?

Image credit https://graphics.stanford.edu/courses/cs468-12-spring/LectureSlides/06_smoothing.pdf

Smooth a curve



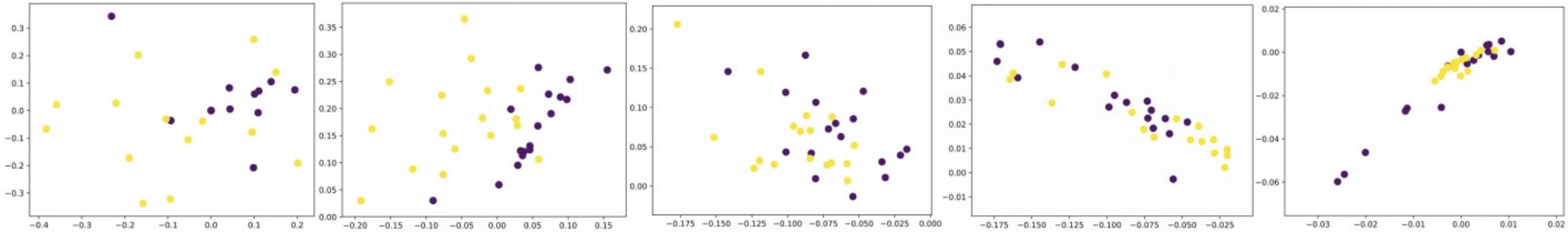


Q: what if we repeat for many times?
Converge to a straight line?

Q: how can we smooth this curve to be more like a straight line?

Image credit https://graphics.stanford.edu/courses/cs468-12-spring/LectureSlides/06_smoothing.pdf

Oversmoothing of GCN

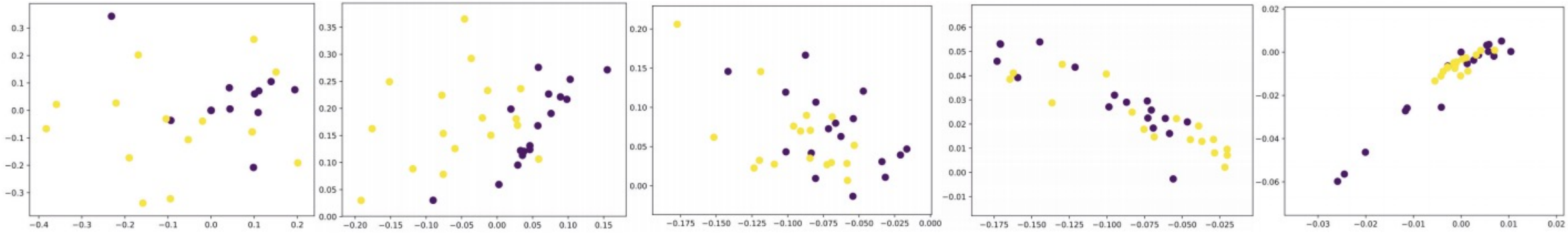


(a) 1-layer (b) 2-layer (c) 3-layer (d) 4-layer (e) 5-layer

Figure 2: Vertex embeddings of Zachary's karate club network with GCNs with 1,2,3,4,5 layers.

Image credit https://arxiv.org/pdf/1801.07606.pdf.
Deeper Insights into Graph Convolutional Networks for Semi-Supervised Learning. In AAAI 2018.

Oversmoothing of GCN



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34 vertices of two classes and 78 edges

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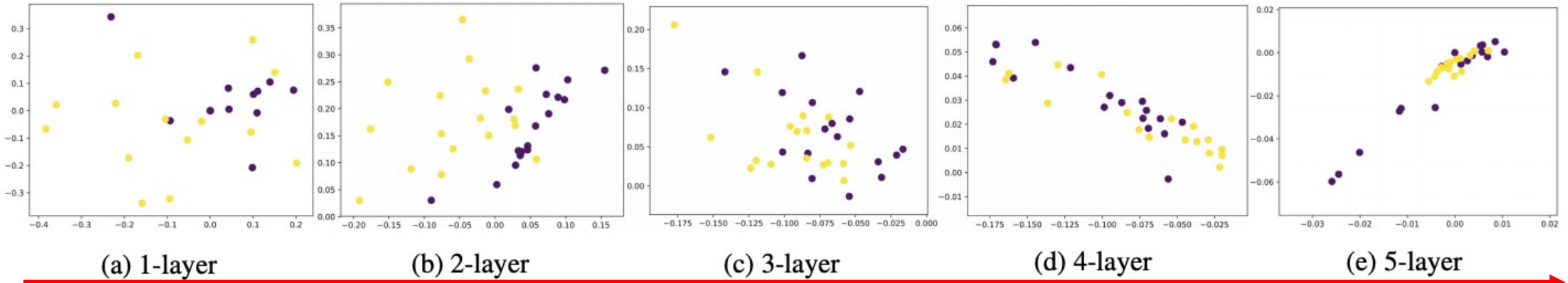

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Larger receptive field

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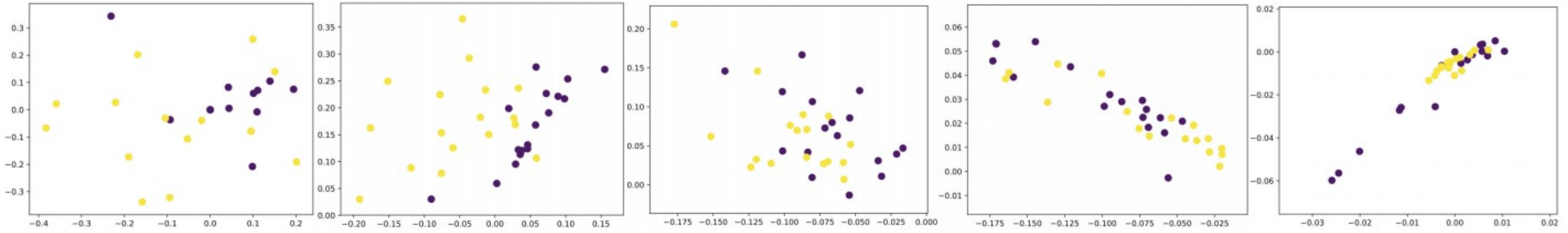
Oversmoothing of GCN

Two classes: yellow vs. blue



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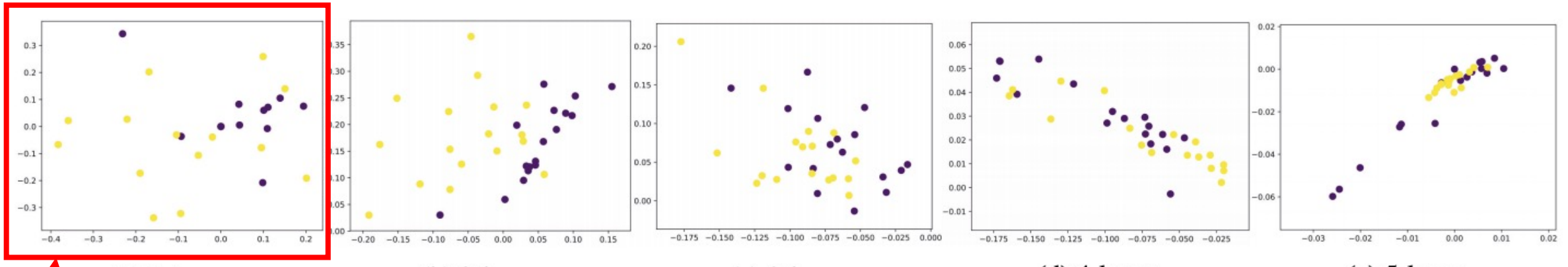

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Q: is it linearly separable (can we use a straight line to separate two classes well)?

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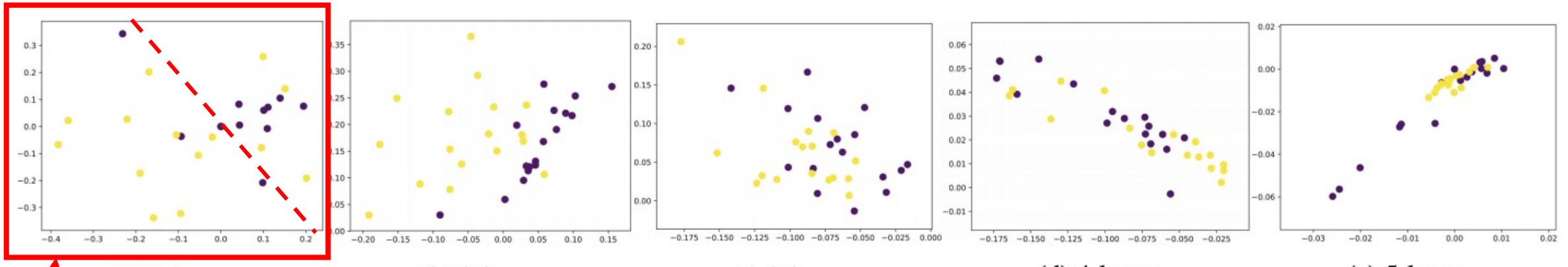

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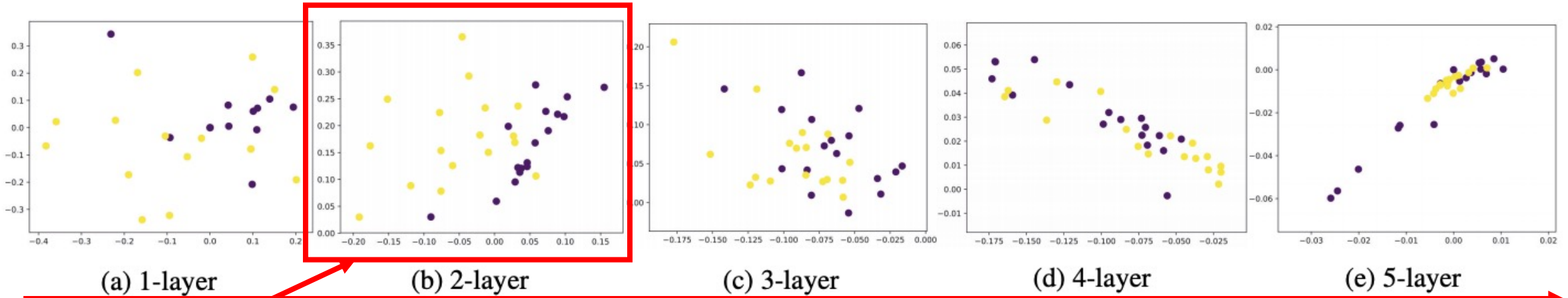

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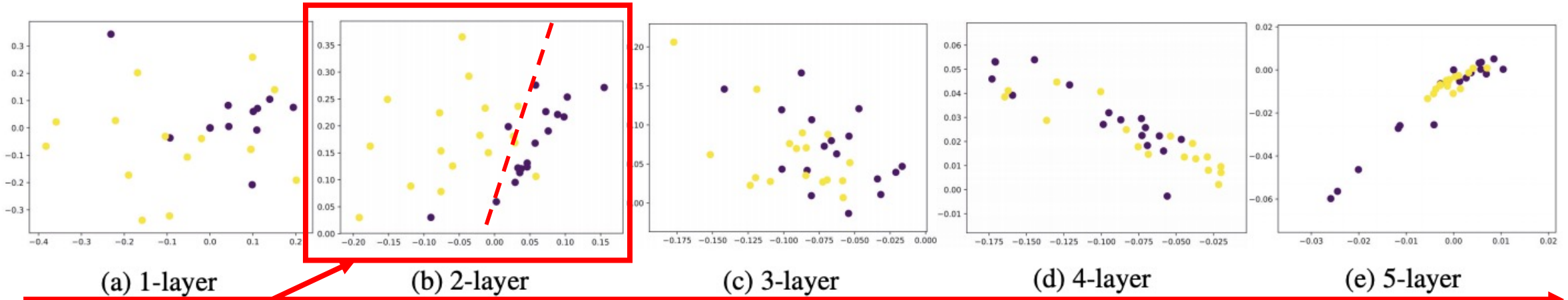

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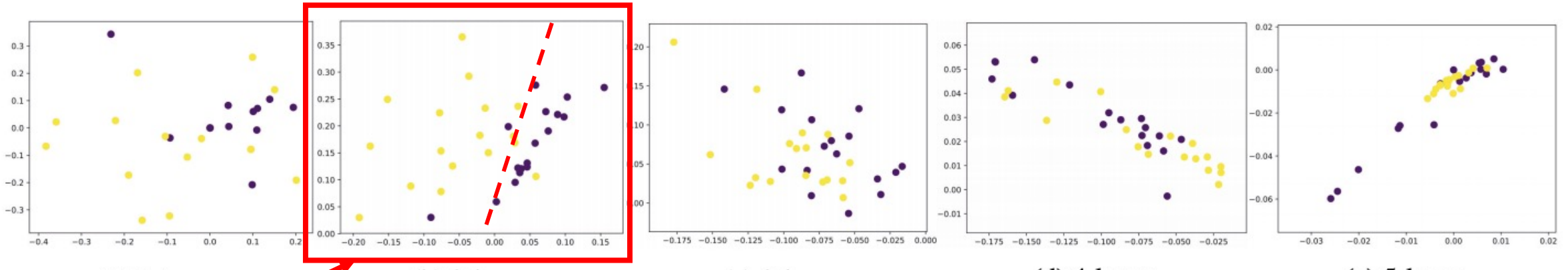
A bit better



Larger receptive field

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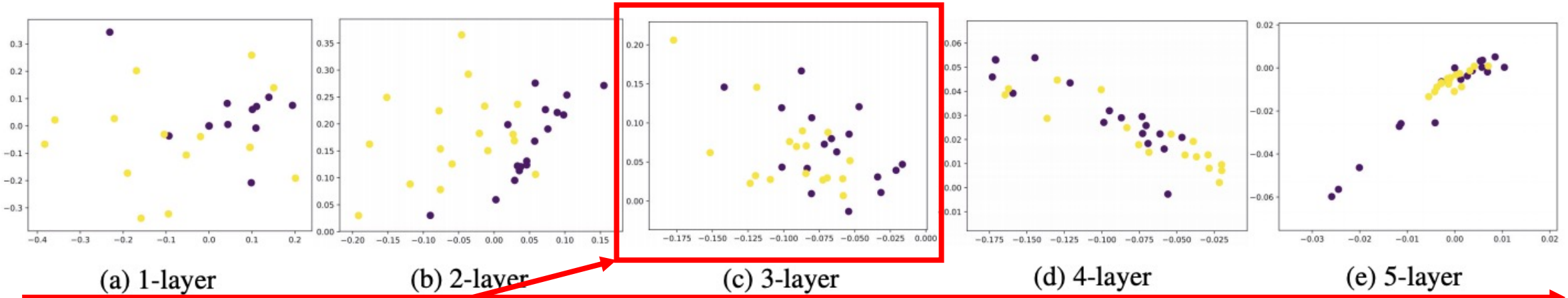

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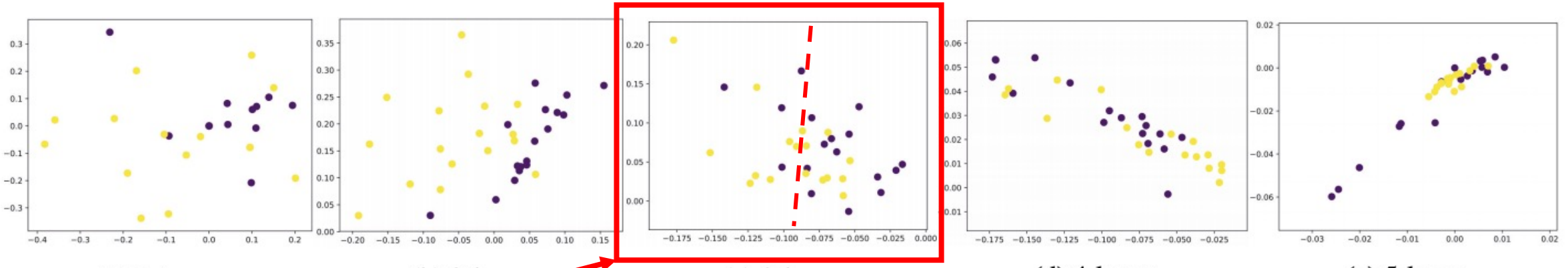

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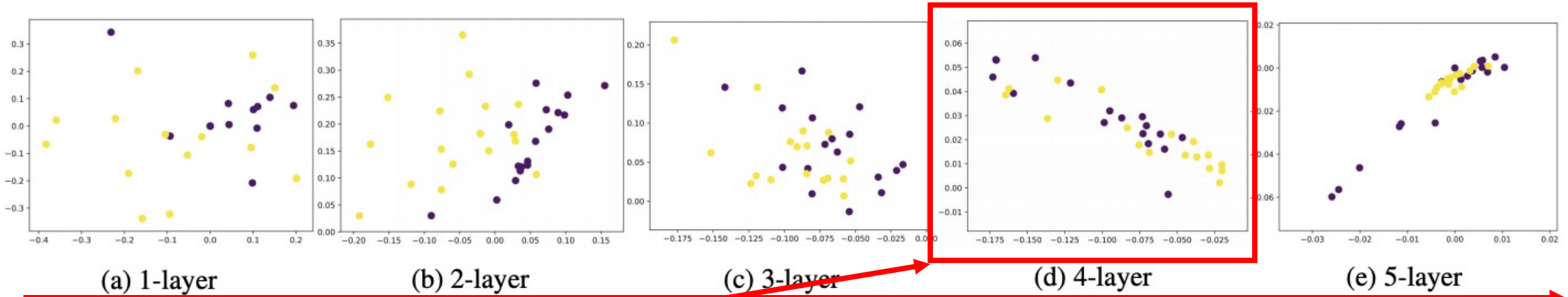

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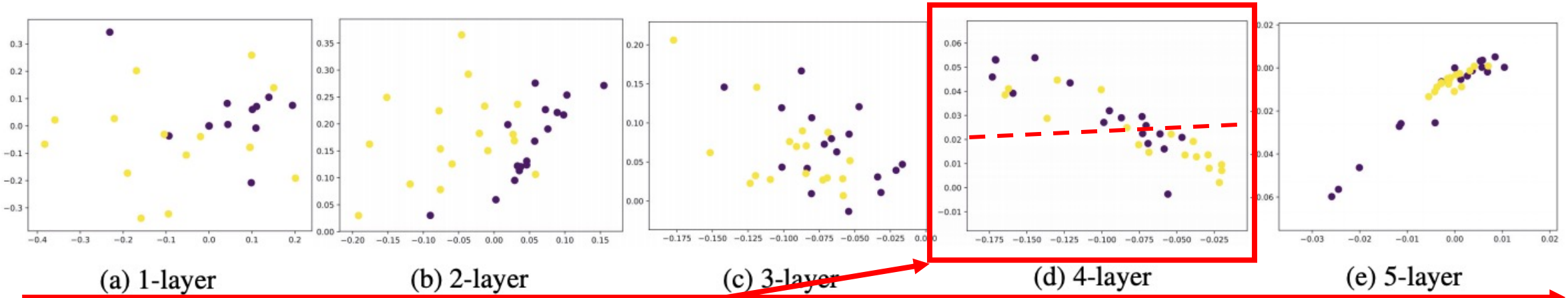

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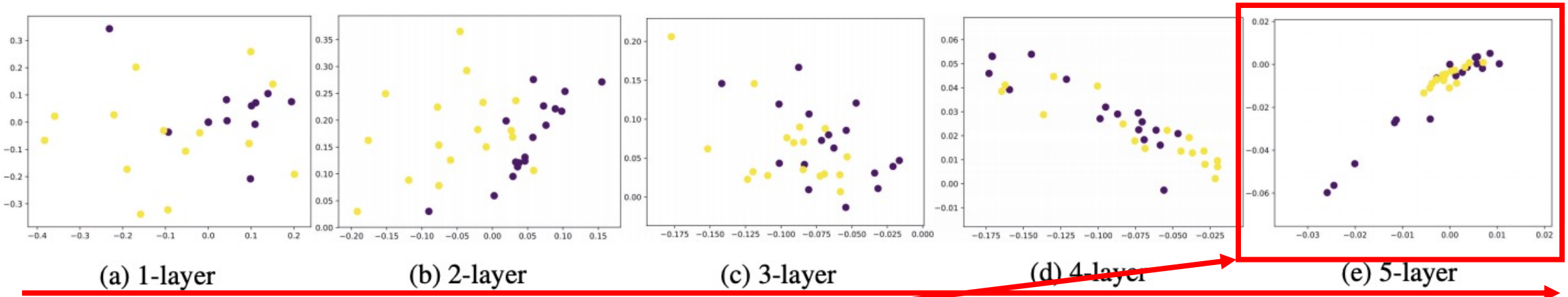

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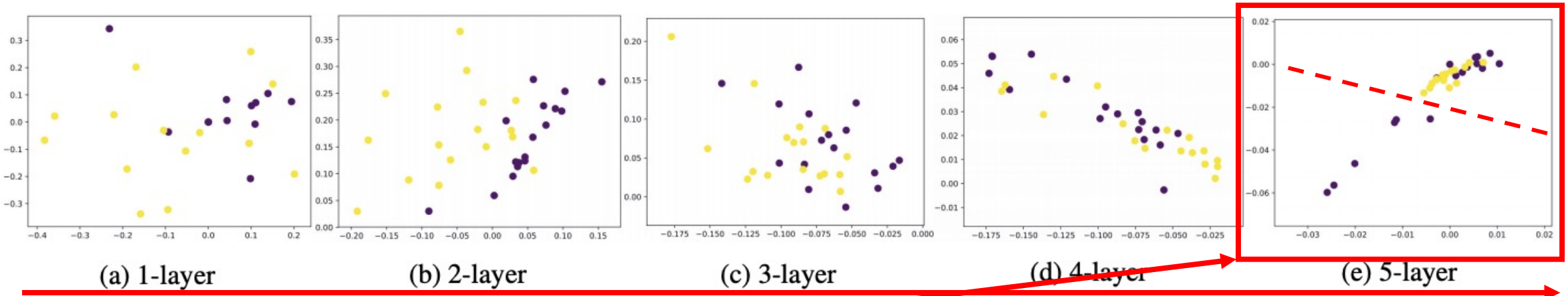

(a) 1-layer (b) 2-layer (c) 3-layer (d) 4-layer (e) 5-layer

Larger receptive field

Figure 2: Vertex embeddings of Zachary's karate club network with GCNs with 1,2,3,4,5 layers.

34 vertices of two classes and 78 edges

Q: is it linearly separable (can we use a straight line to separate two classes well)?

Image credit https://arxiv.org/pdf/1801.07606.pdf.
Deeper Insights into Graph Convolutional Networks for Semi-Supervised Learning. In AAAI 2018.

Oversmoothing of GCN

Two classes: yellow vs. blue

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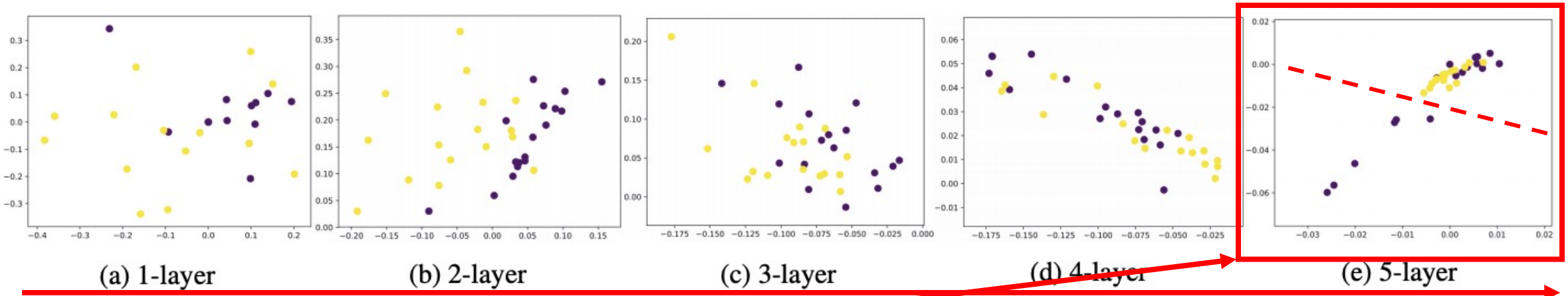

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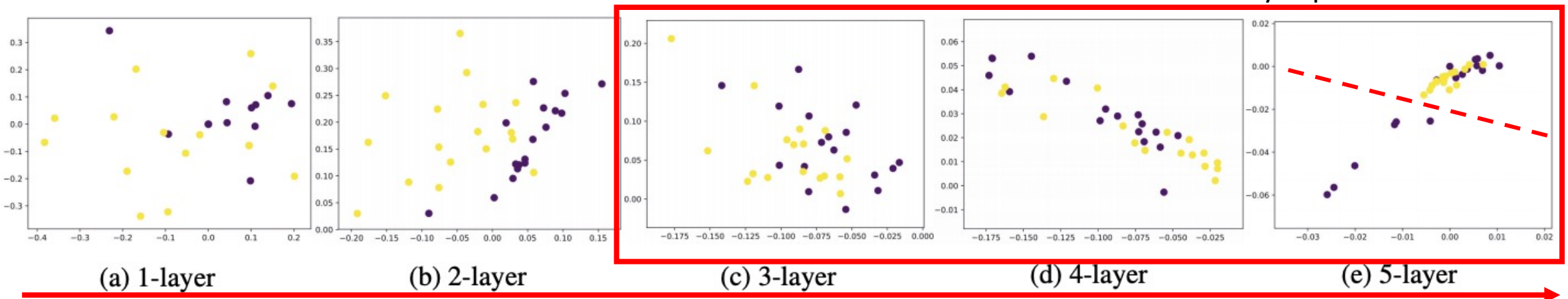
Nodes features are not linearly separable



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Solutions to oversmoothing of GCN

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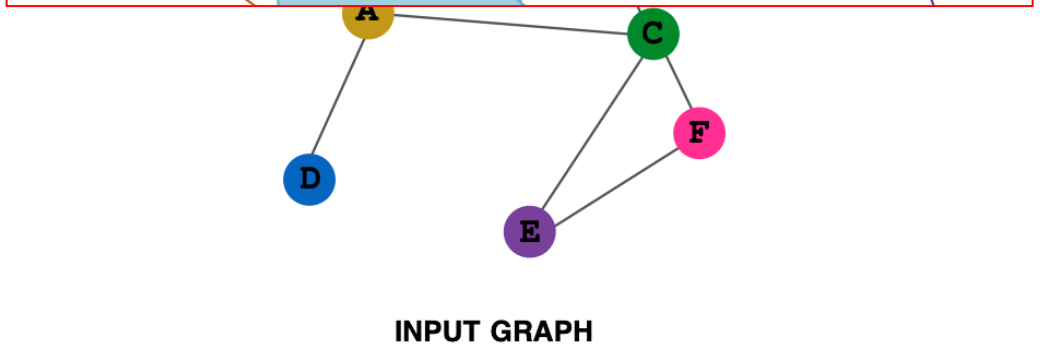
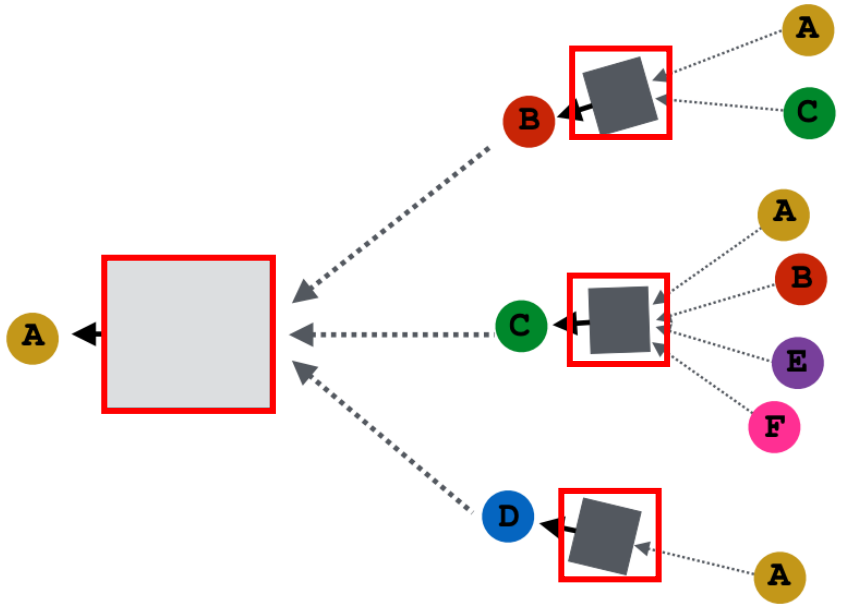


INPUT GRAPH



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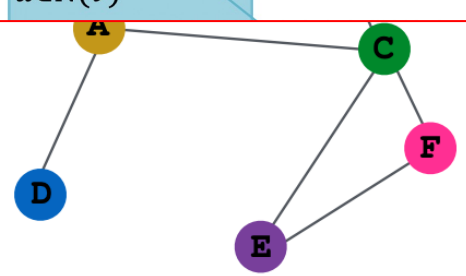

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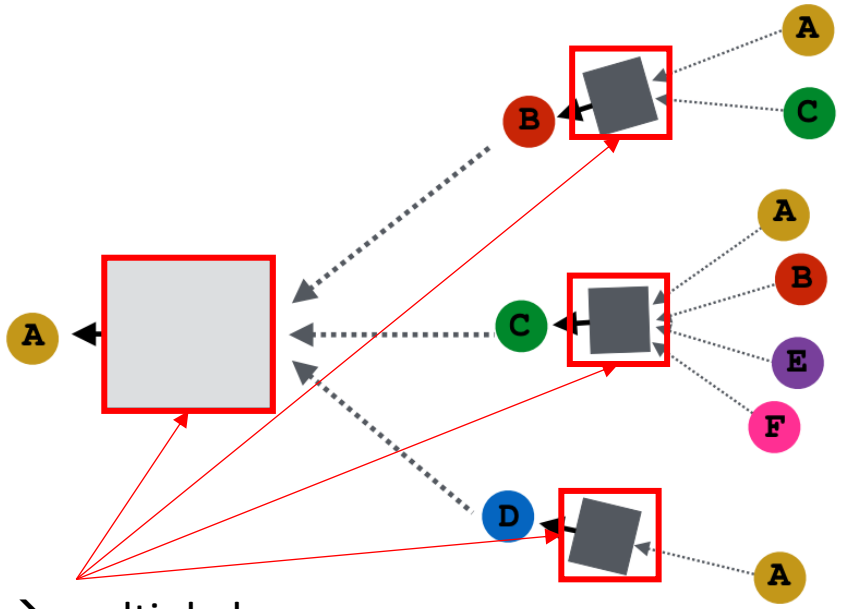

One layer → multiple layers

Solutions to oversmoothing of GCN

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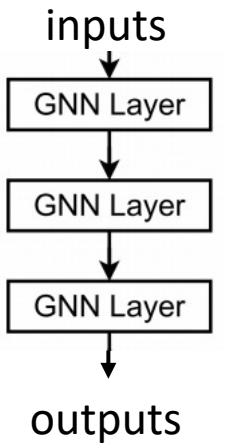

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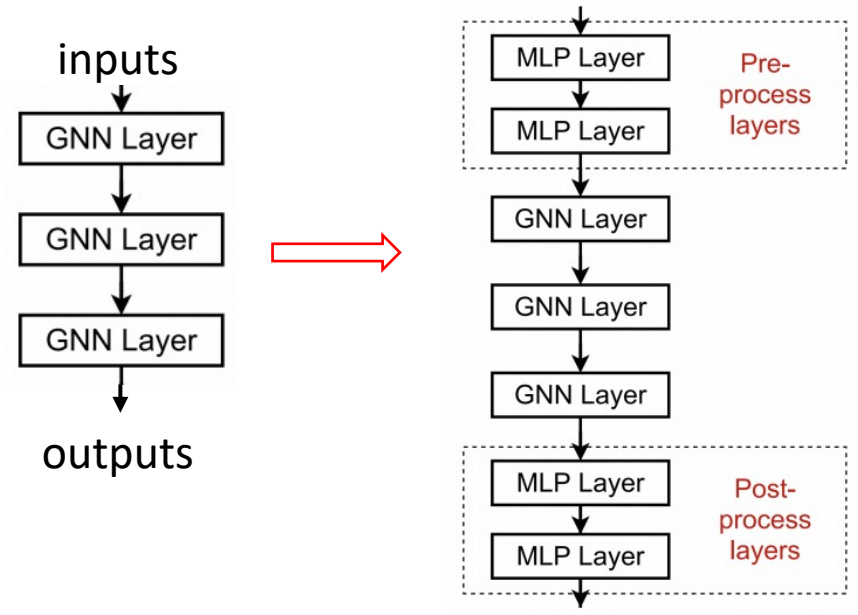

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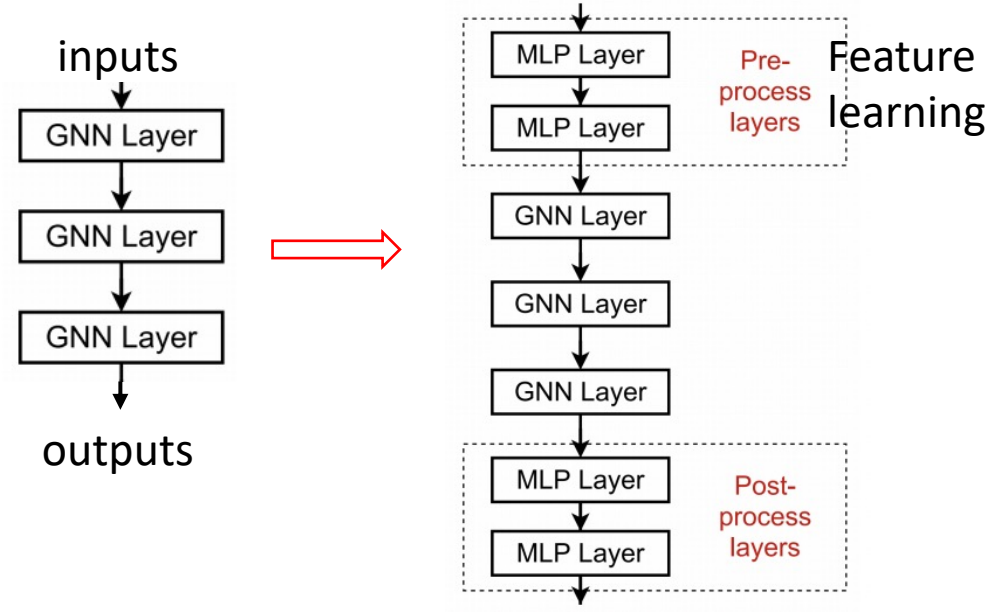

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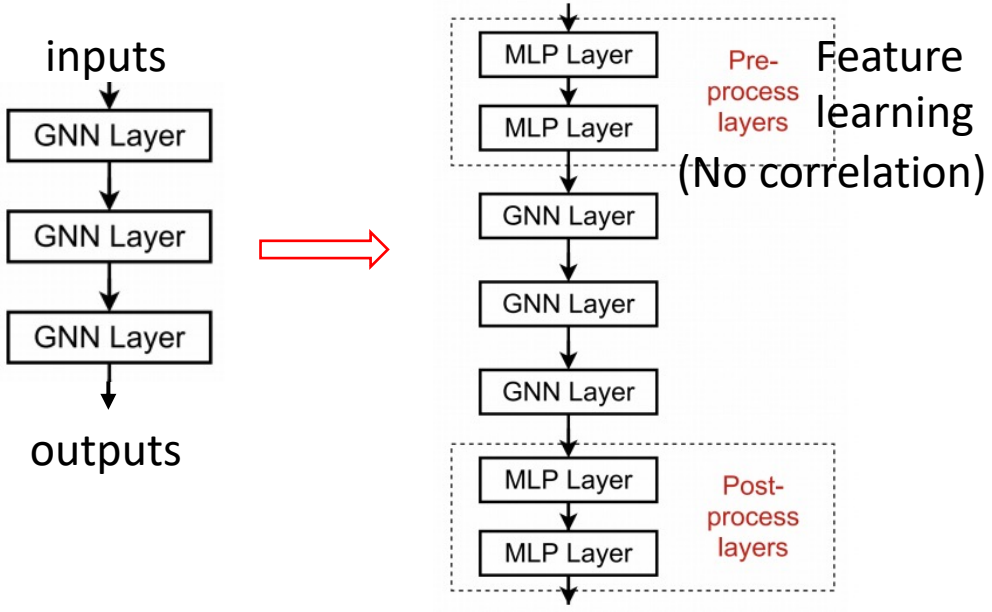

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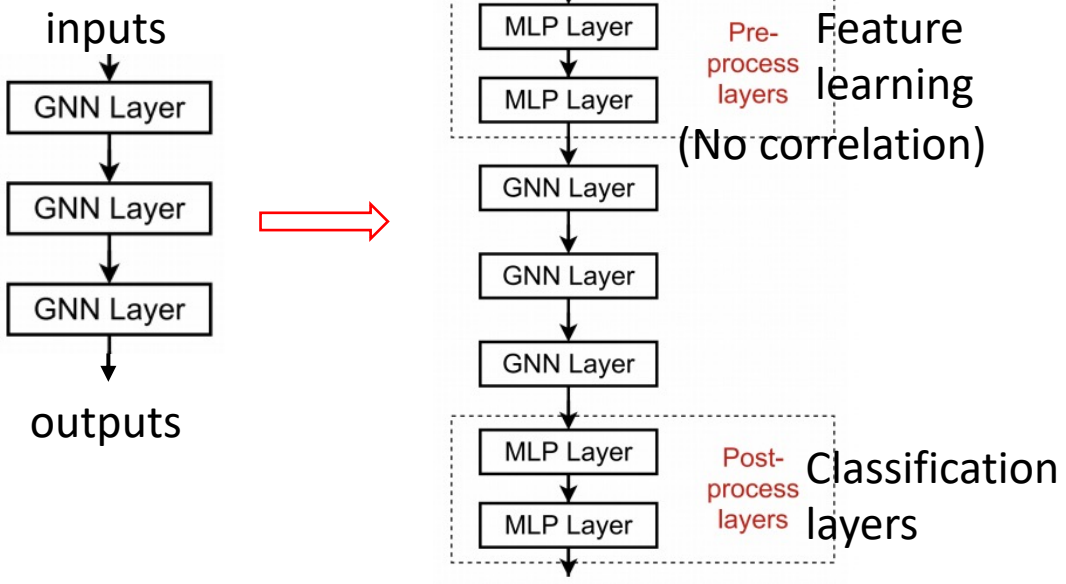

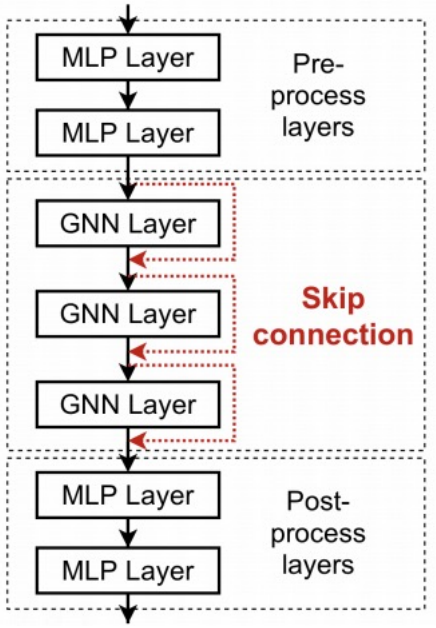

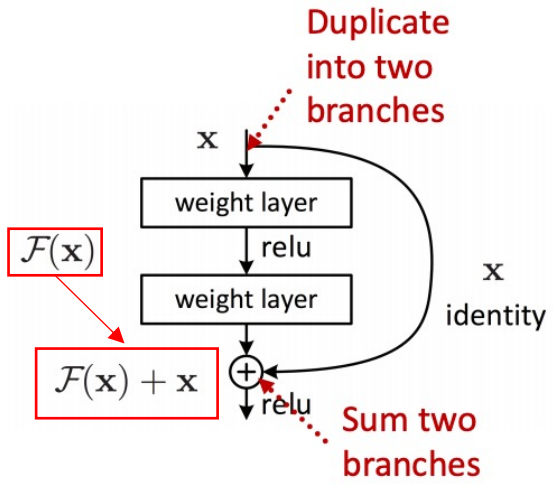

Why skip connection works?

discriminative features

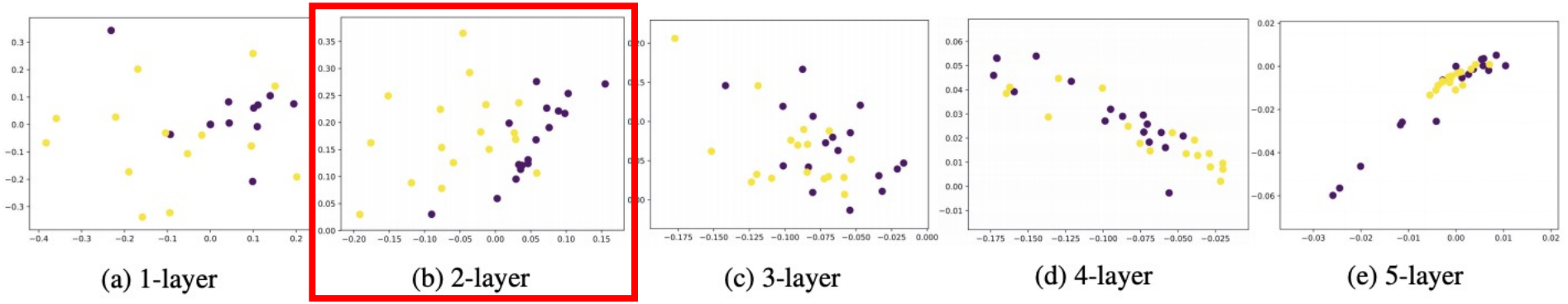

Figure 2: Vertex embeddings of Zachary's karate club network with GCNs with 1,2,3,4,5 layers.

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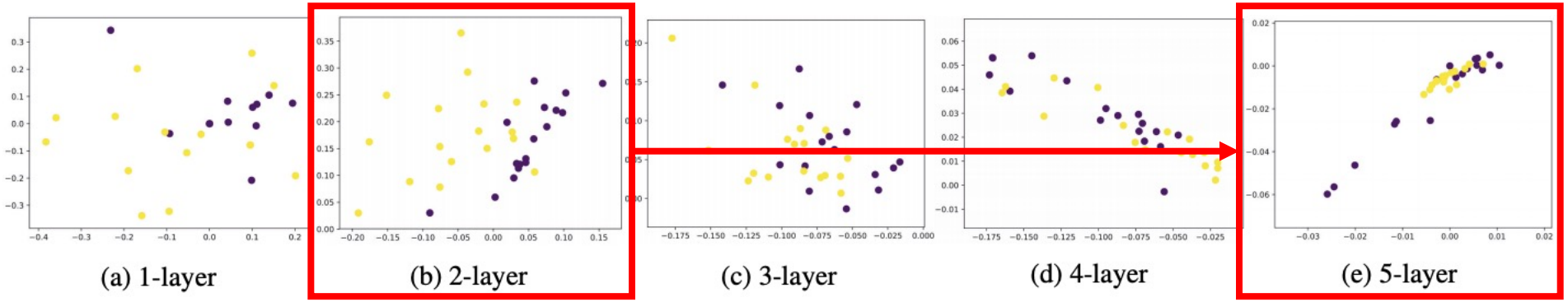

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- **A standard GCN layer**
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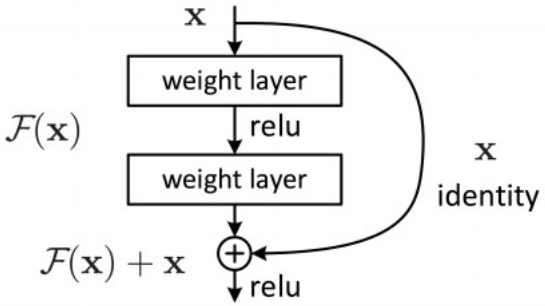

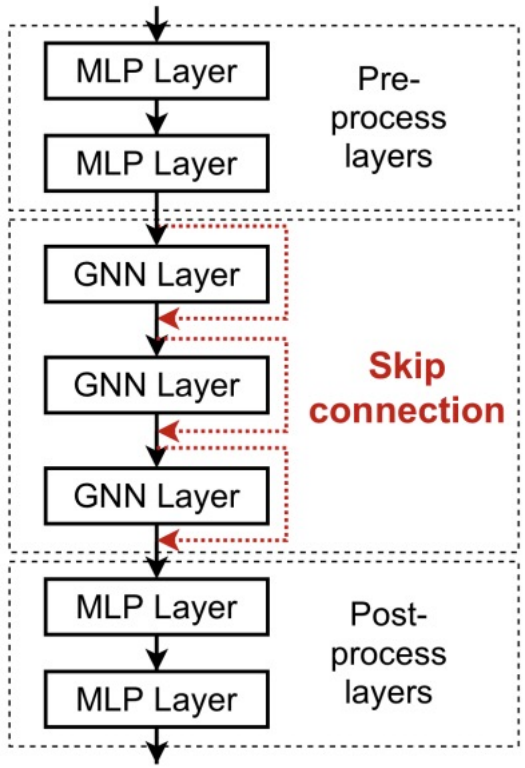

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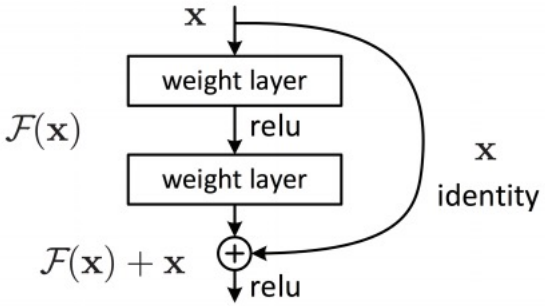
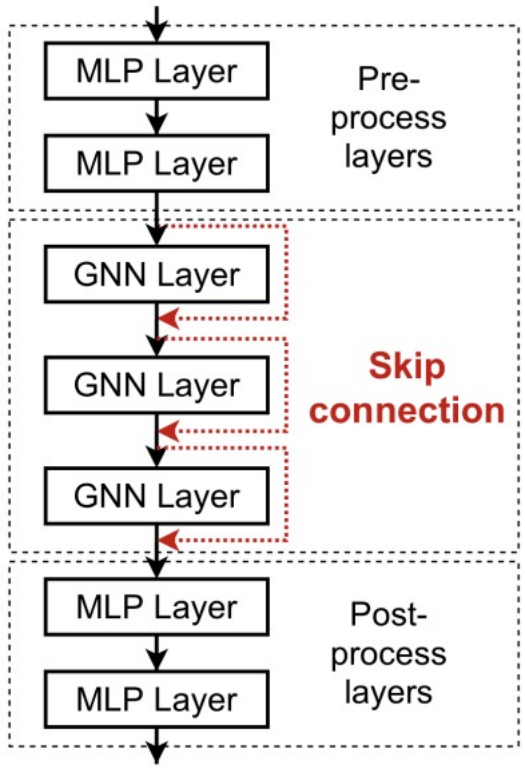
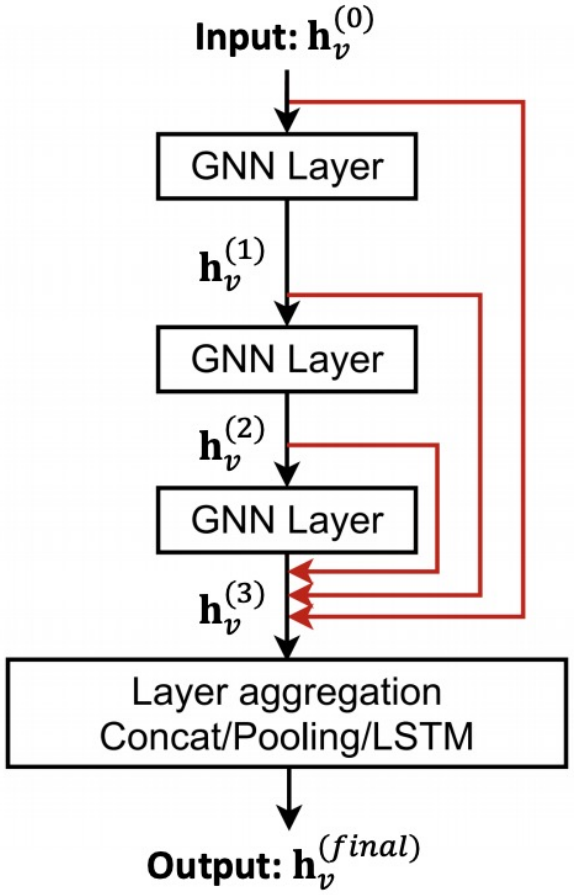
- **A GCN layer with skip connection**
- $\mathbf{h}_v^{(l)} = \sigma\left(\sum_{u \in N(v)} \mathbf{W}^{(l)} \frac{\mathbf{h}_u^{(l-1)}}{|N(v)|} + \mathbf{h}_v^{(l-1)}\right)$

$F(\mathbf{x})$ + $\mathbf{x}$





Other ways to add skip connections



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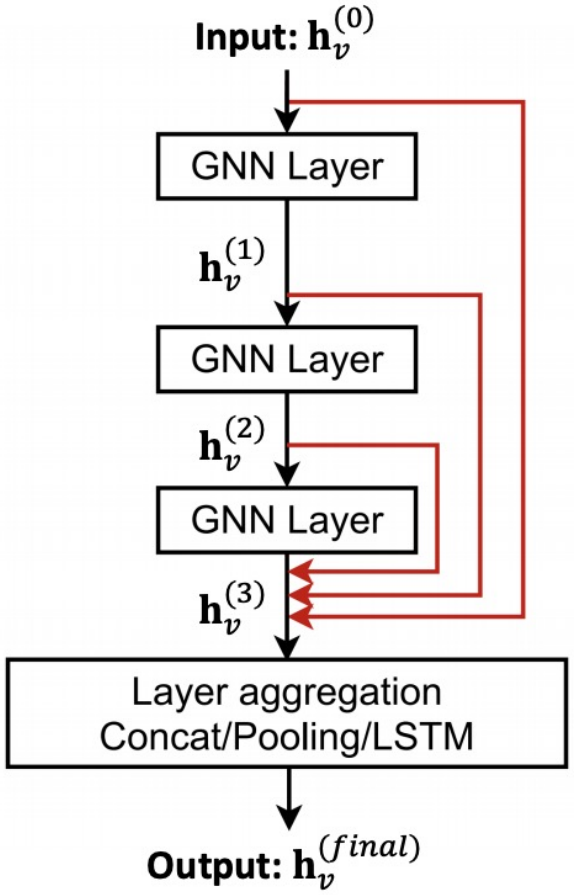

Oversmoothing is still an open problem