On the Bottleneck of Graph Neural Networks and its Practical Implications

(ICLR ‘2021)

Uri Alon
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Main Contribution: GNNs suffer from a **bottleneck** that causes **over-squashing** when trying to capture long-range interactions.

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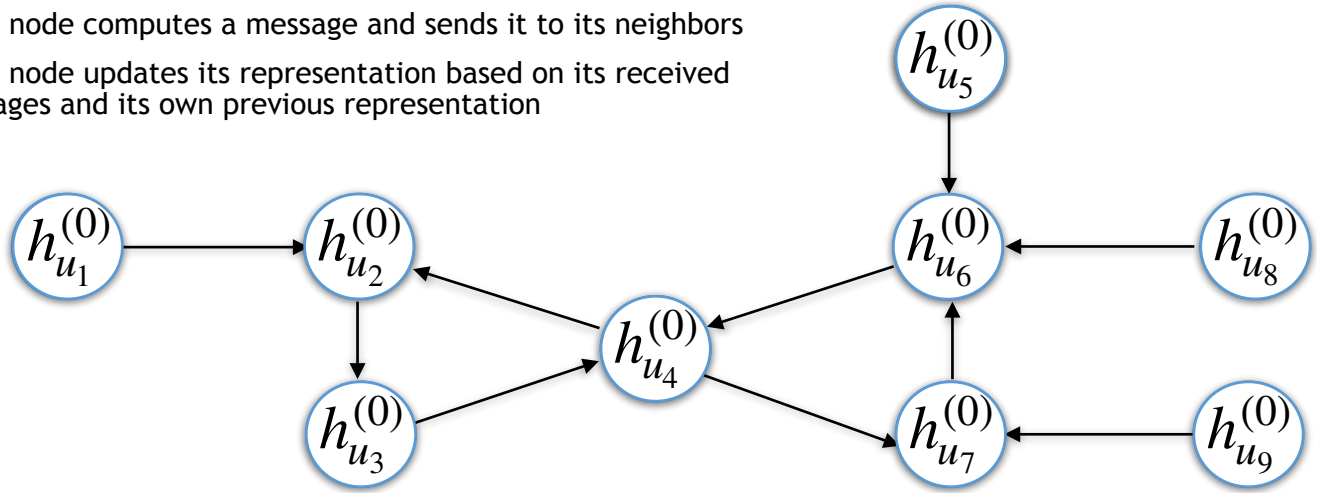
A GNN as a Message Passing Network

[Gilmer, ICML'2017]

- Initial representations are embeddings or features
- At every message passing step (=layer):
  - Every node computes a message and sends it to its neighbors
  - Every node updates its representation based on its received messages and its own previous representation



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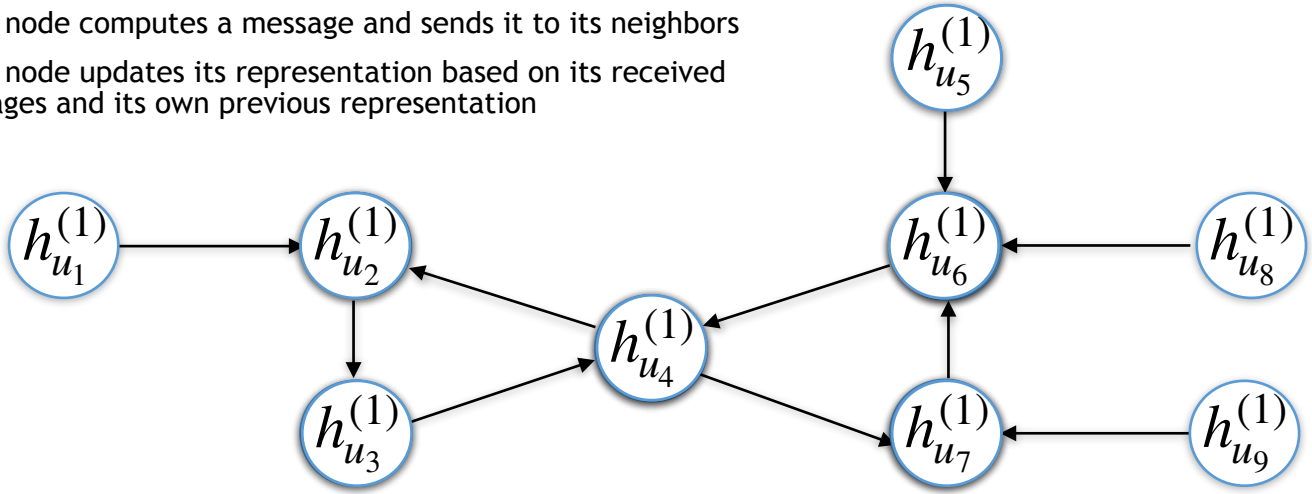

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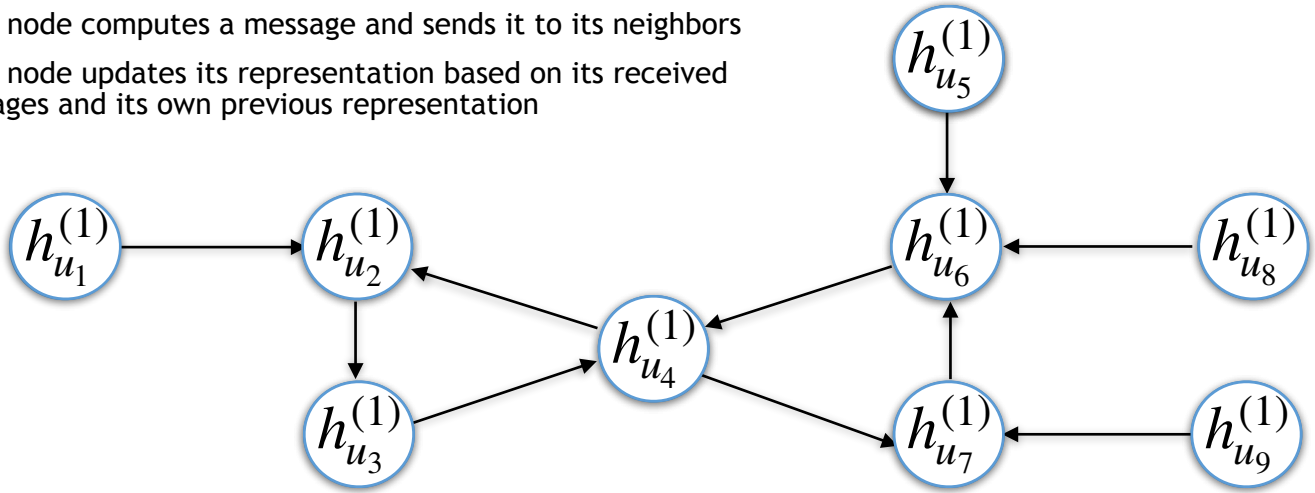

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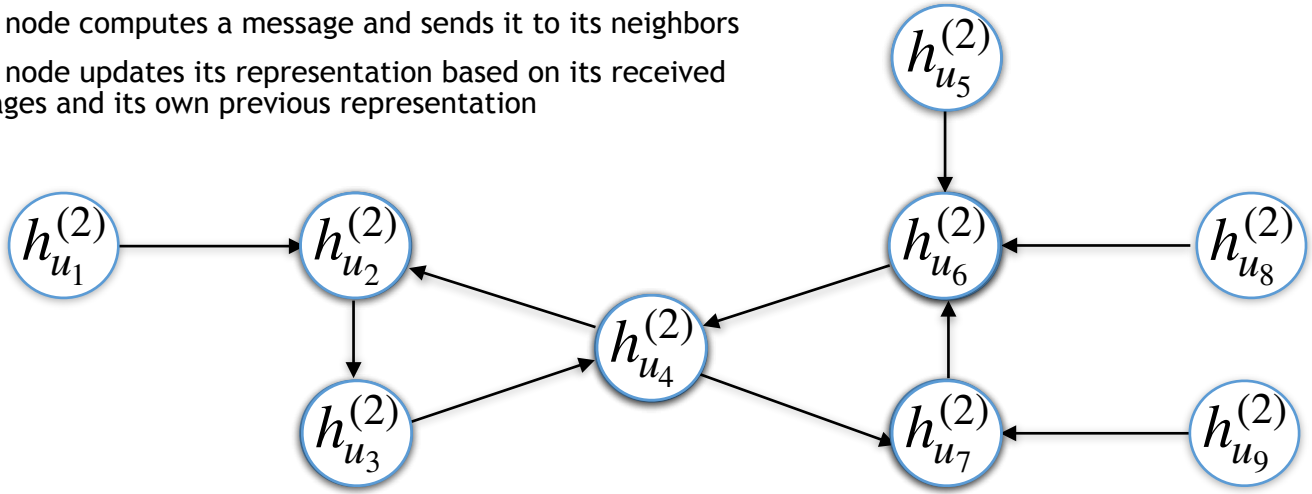

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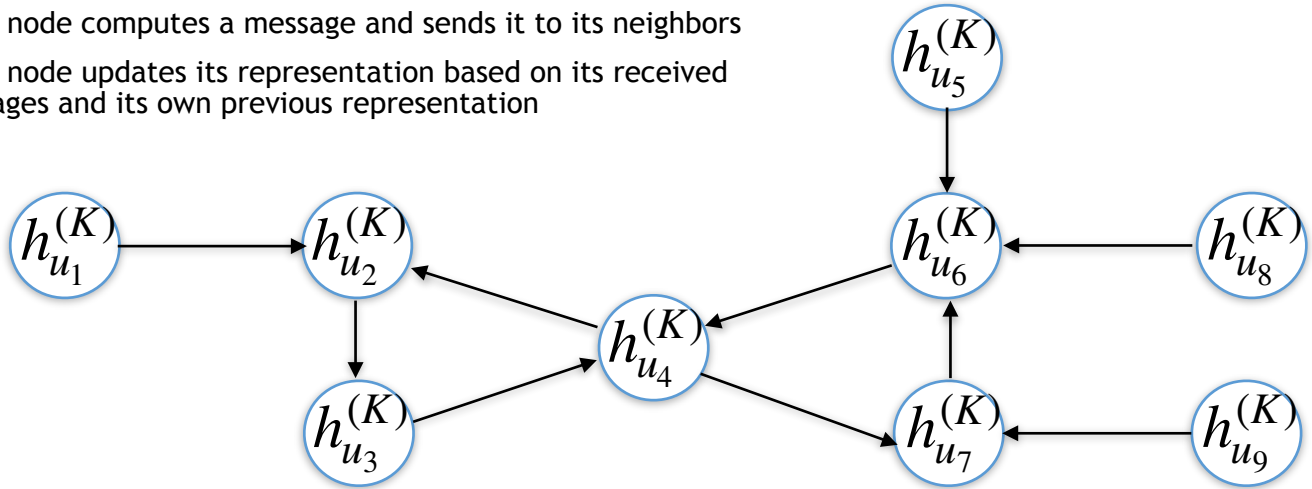

- Given $\{h_u^{(K)} \mid u \in V\}$:
  - Node classification, graph classification, link prediction, sequence generation

GNN Types

- General: $\mathbf{h}_v^{(k)} = f_k\left(\mathbf{h}_v^{(k-1)}, \{\mathbf{h}_u^{(k-1)} \mid u \in \mathcal{N}_v\}\right) \qquad \mathcal{N}_v = \{u \in V \mid (u, v) \in E\}$

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  (Kipf & Welling, ICLR'2017)

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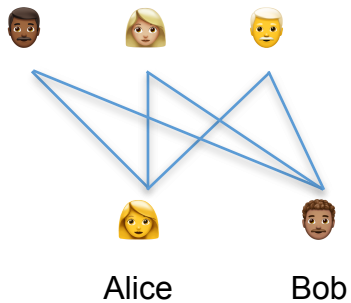

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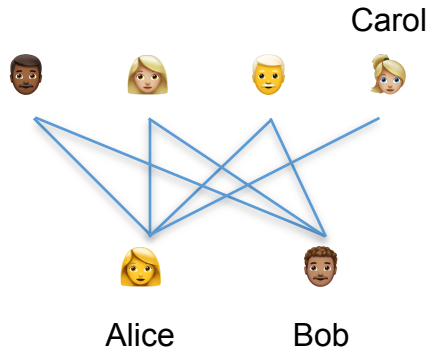

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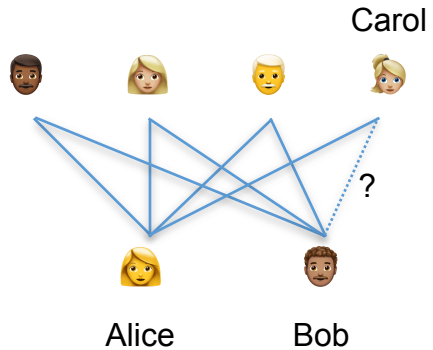

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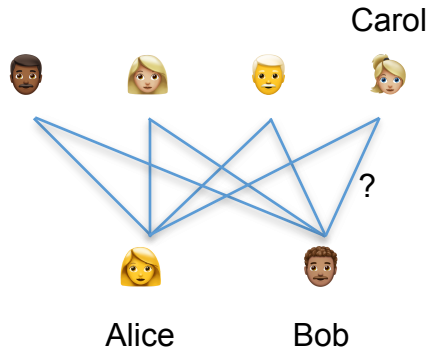

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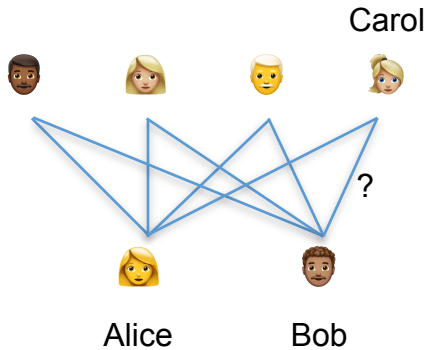

Very local property,

requires only 2-3 message-passing steps

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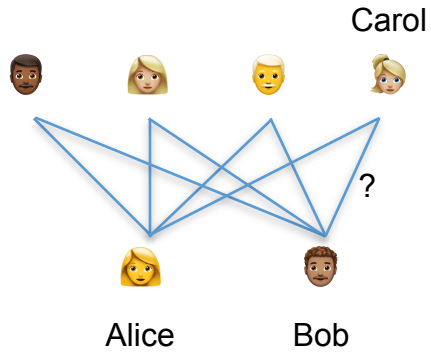

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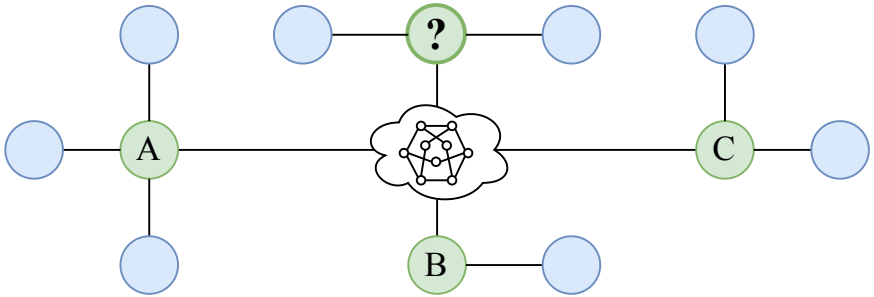
- This work: but not that good for **long-range** tasks (4+ edges away interaction)

The NeighborsMatch problem

- Assume that we wish to predict a label for the target node



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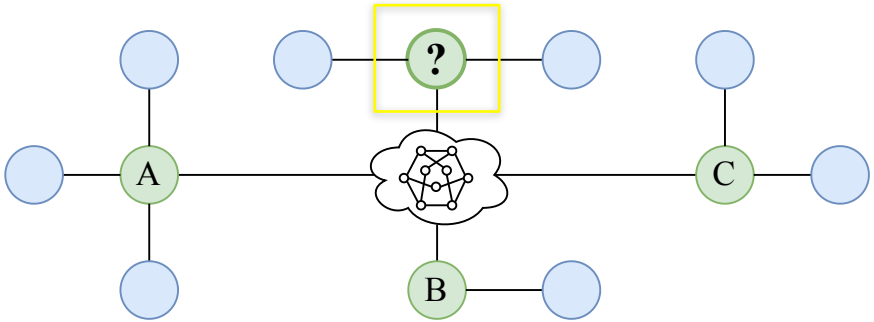

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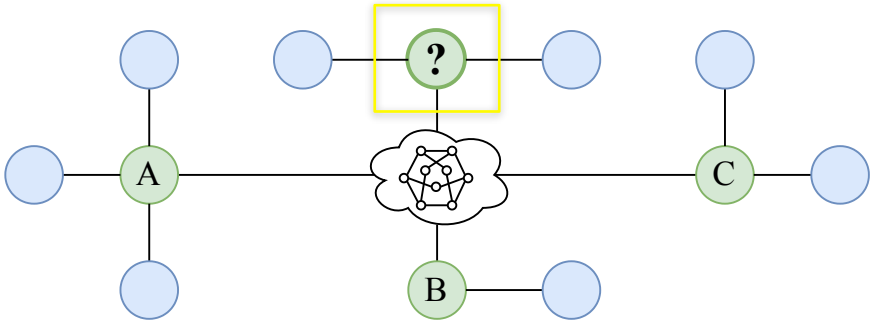
- Assume that we wish to predict a label for the target node
- The correct label is the label of the green node that has the same number of blue neighbors as the target node, in the same graph



The NeighborsMatch problem

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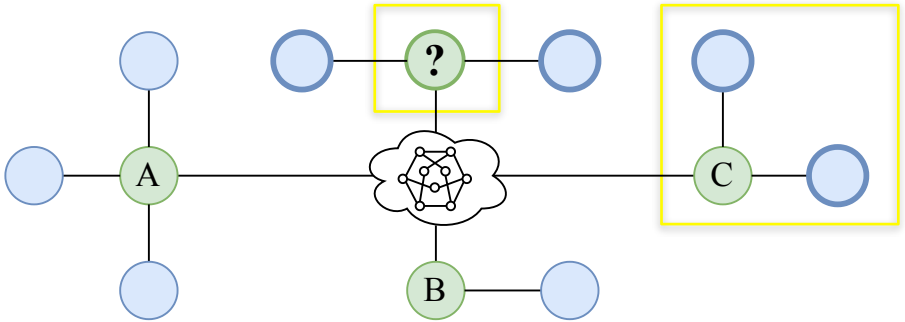
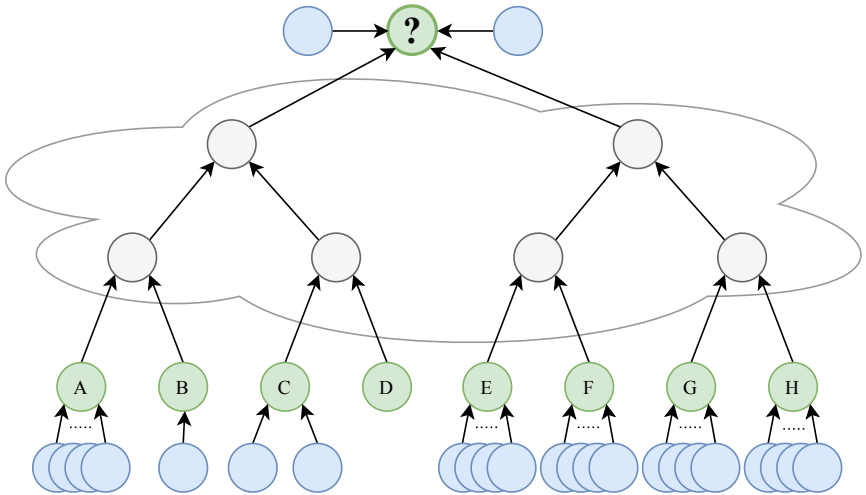
  - In this example – **C**



The GNN Bottleneck

From the perspective of the target node, the rest of the graph may look like a tree, where the target node itself is the root



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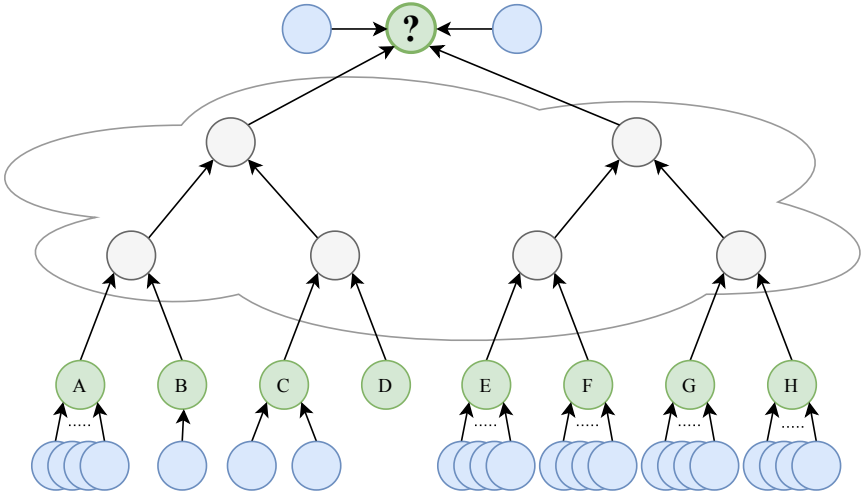

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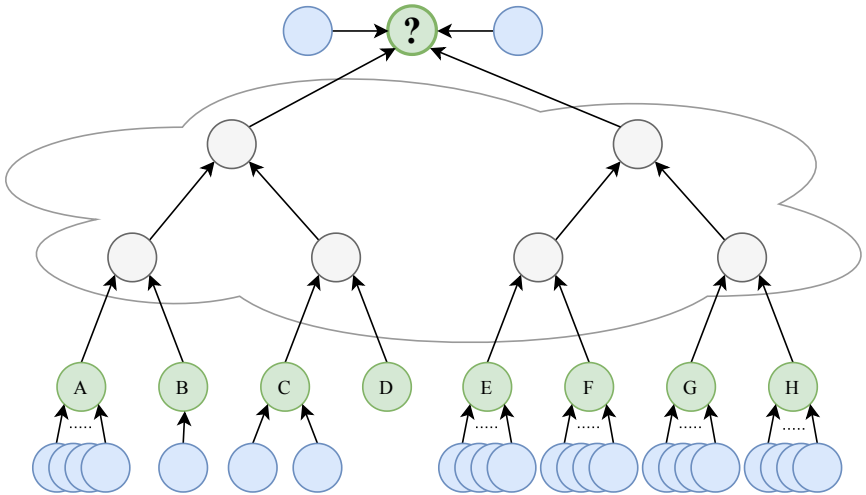

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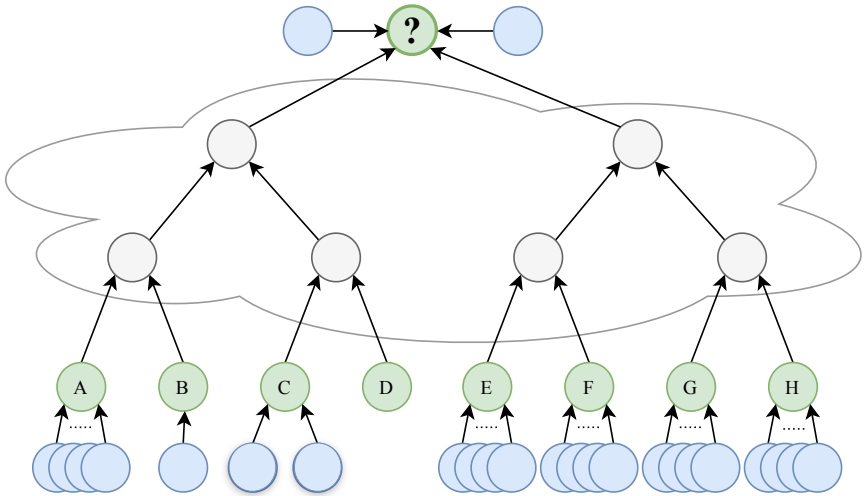

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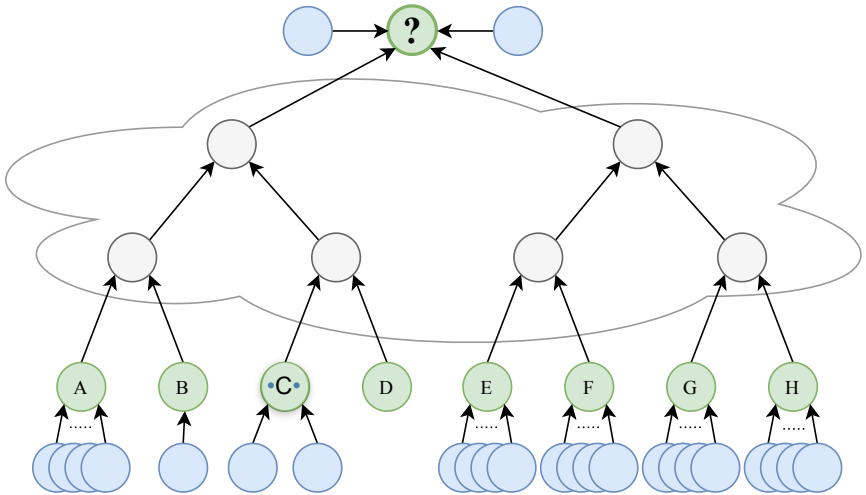

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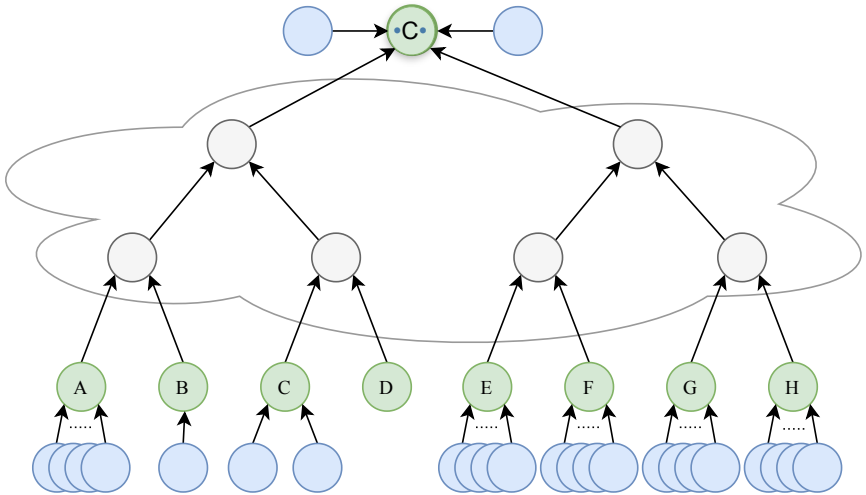

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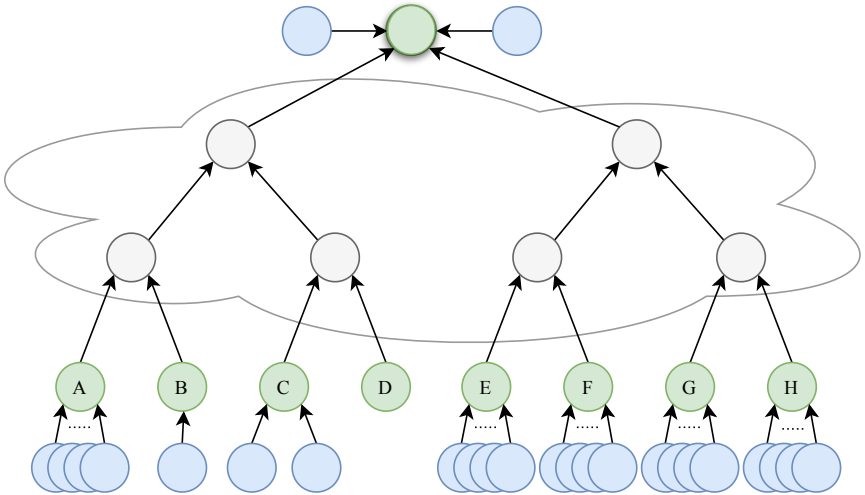

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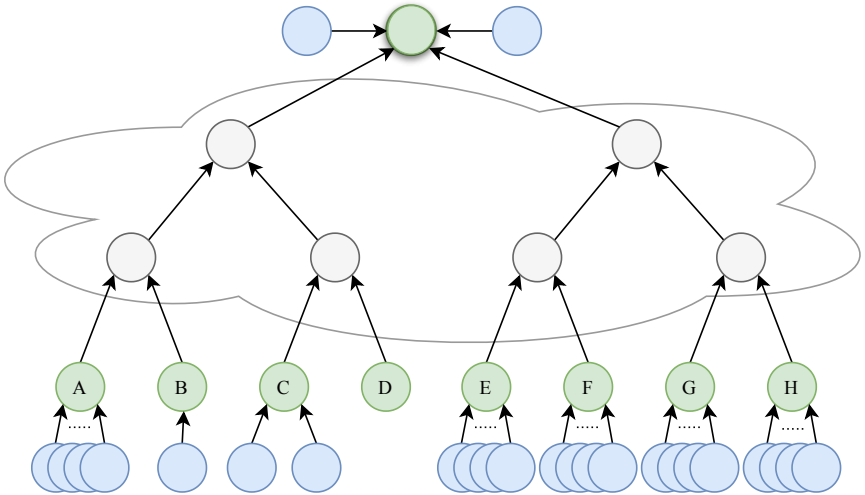

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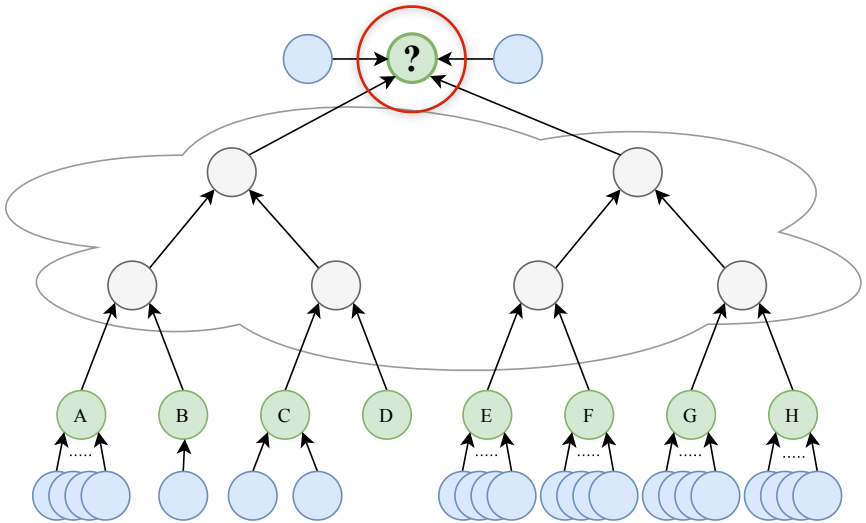

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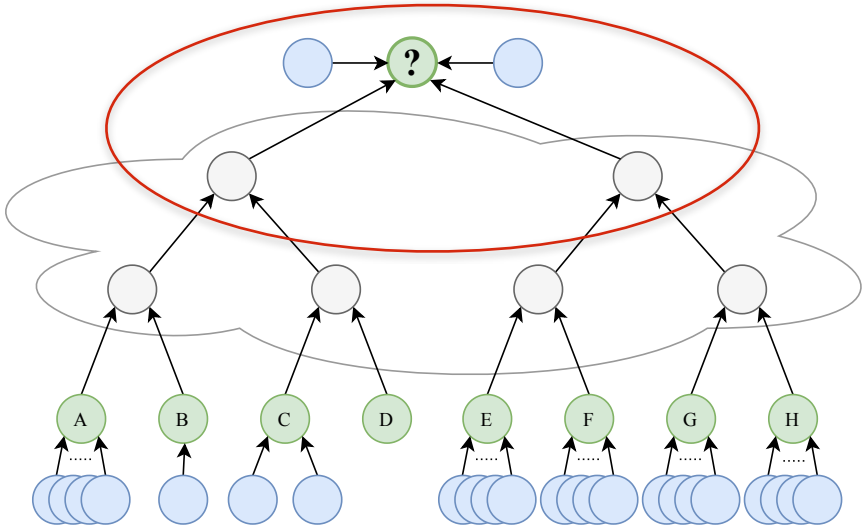

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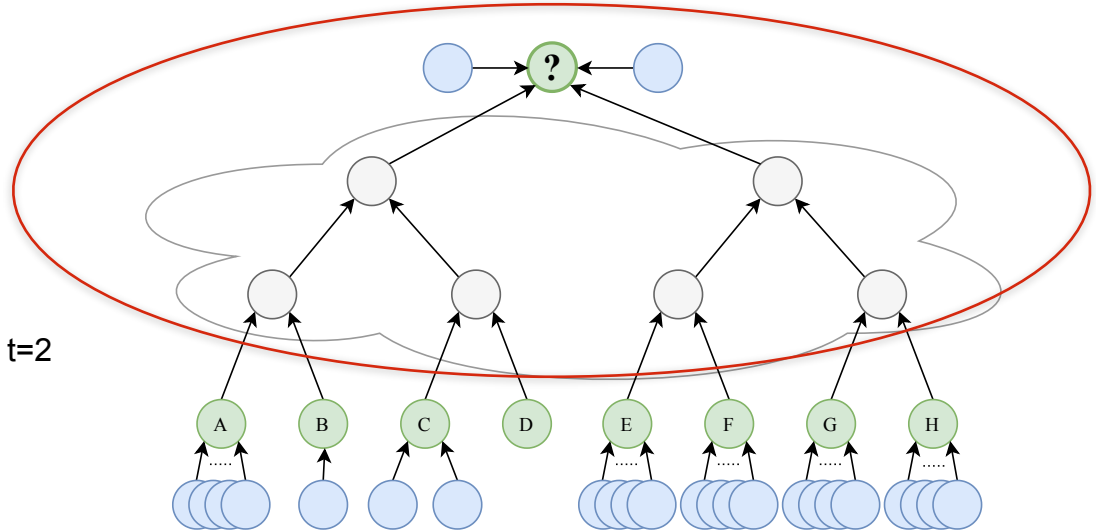

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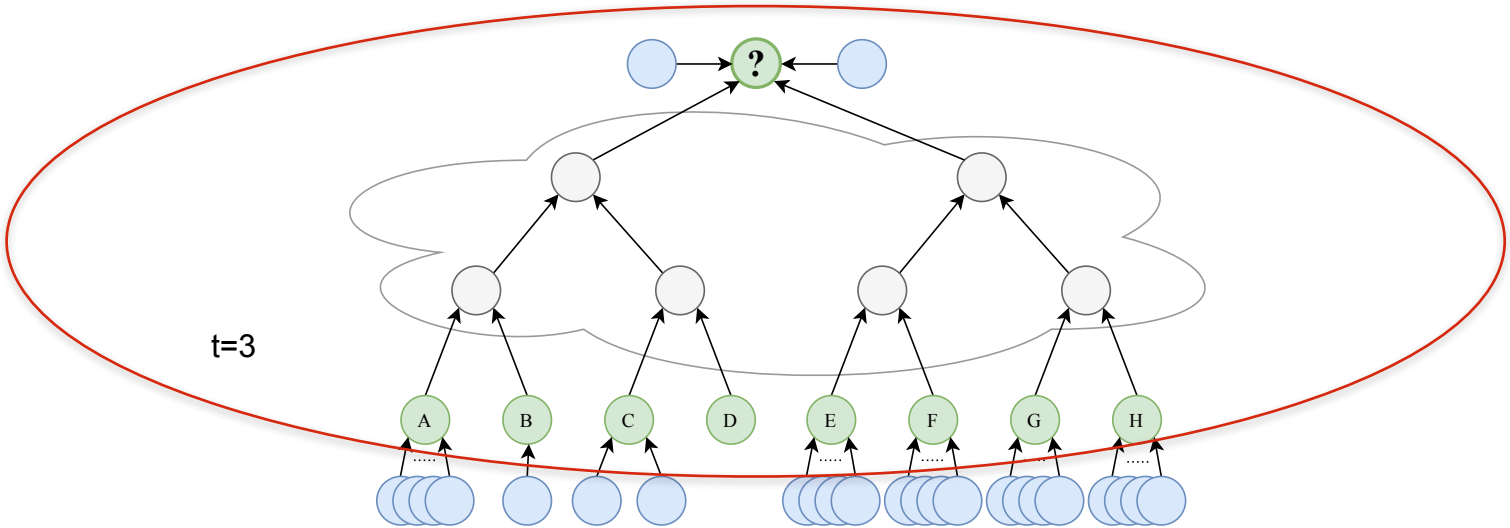

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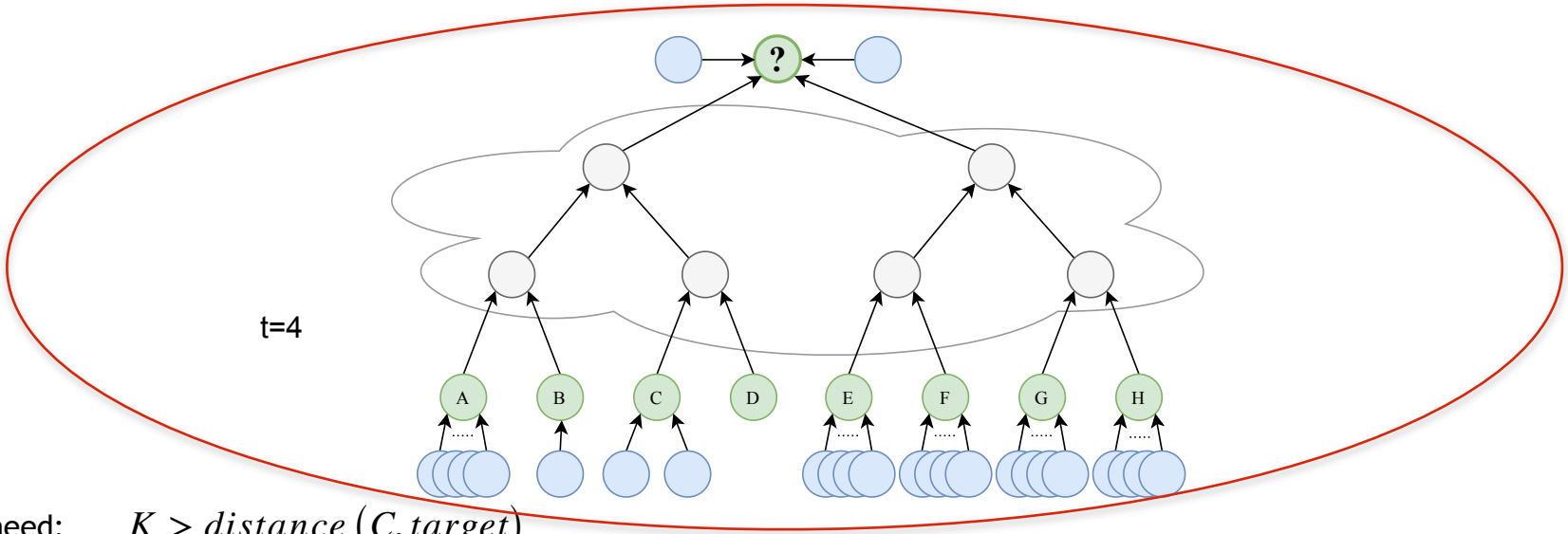

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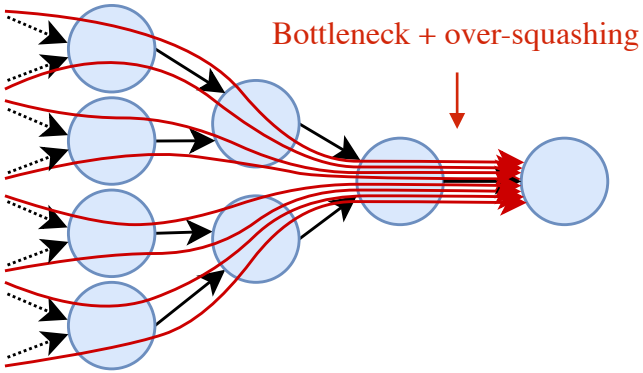

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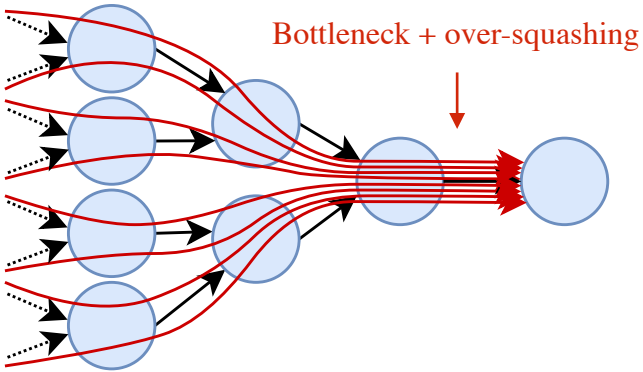
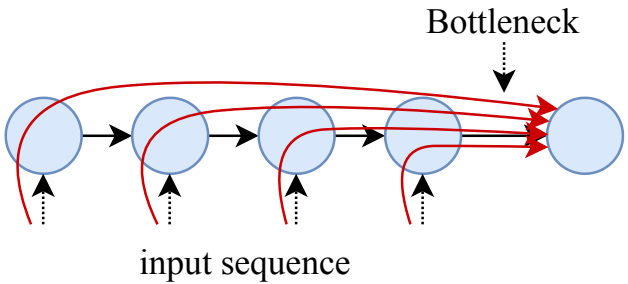


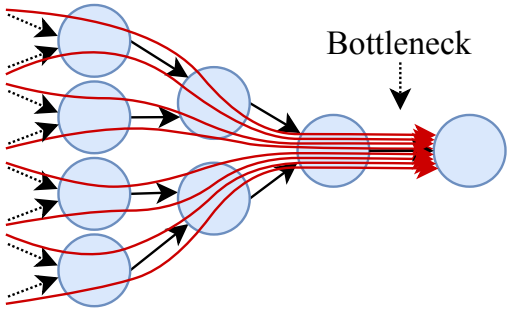
An exponential amount of information is squashed into a fixed-size vector.

Over-squashing

Actually, this is similar to the bottleneck of recurrent sequential models (before attention), except that the receptive field in RNNs grows **linearly**, while in GNNs it grows **exponentially**



RNNs



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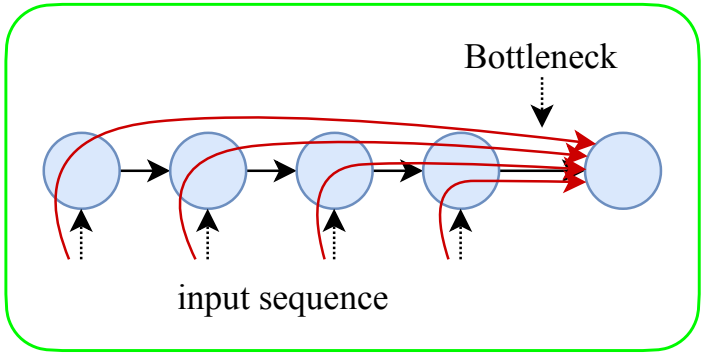

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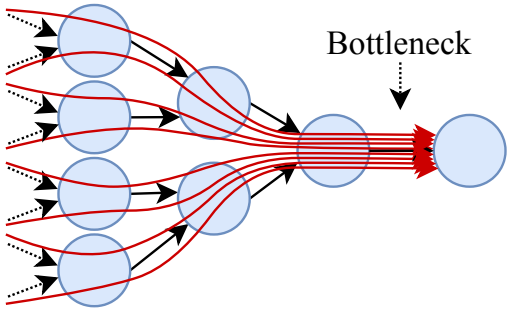

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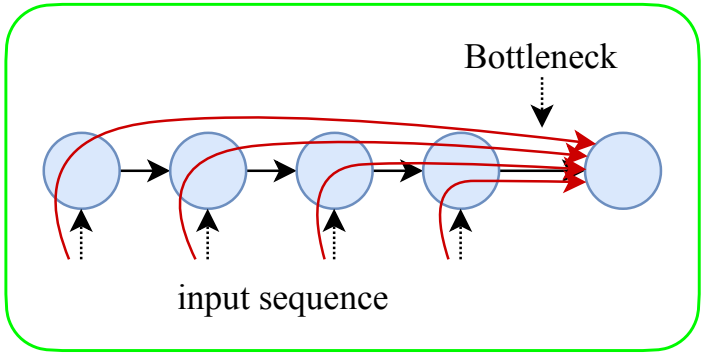

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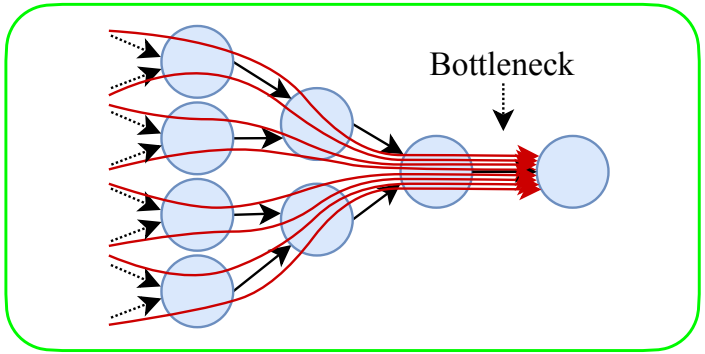

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Over-squashing prevents GNNs from fitting the training data

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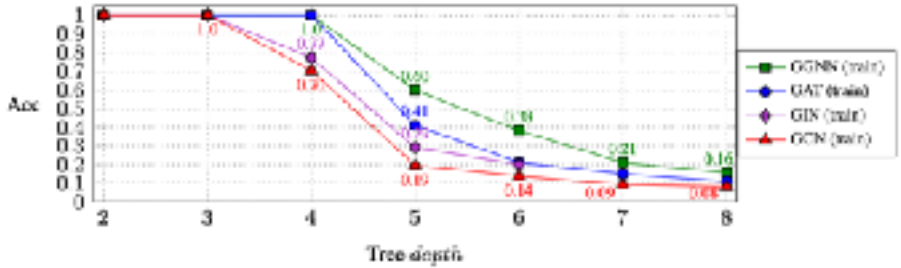

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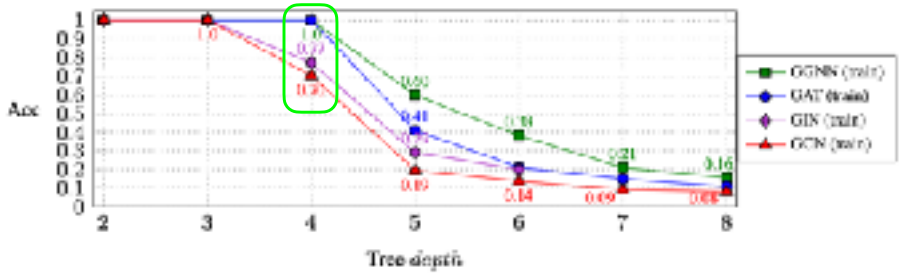

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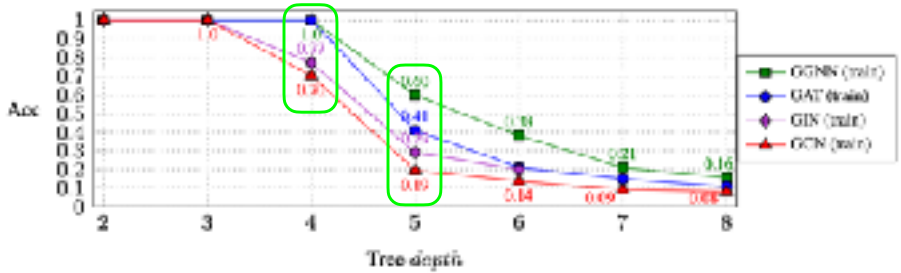

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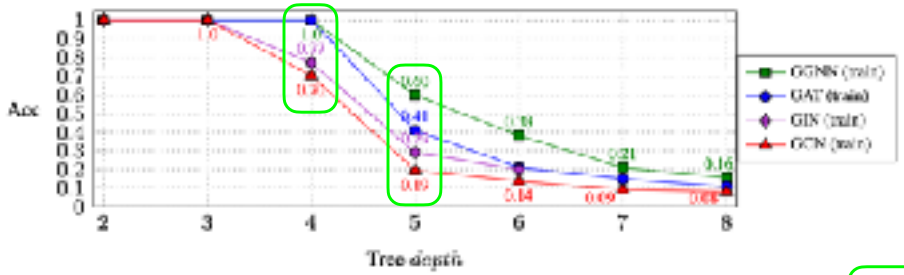

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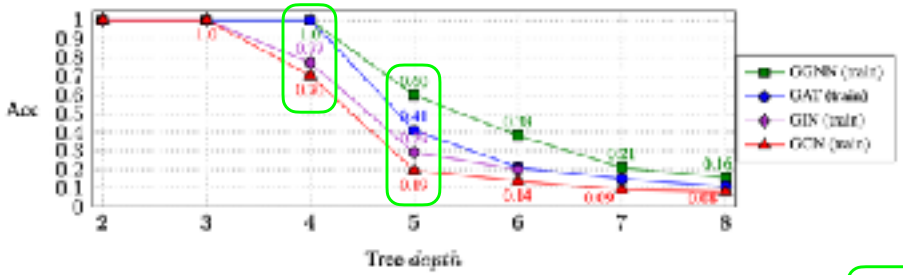

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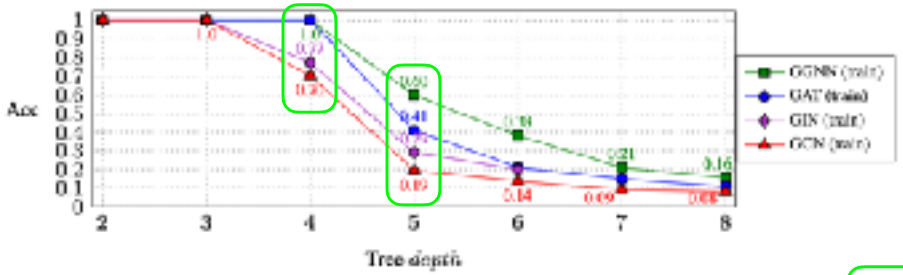

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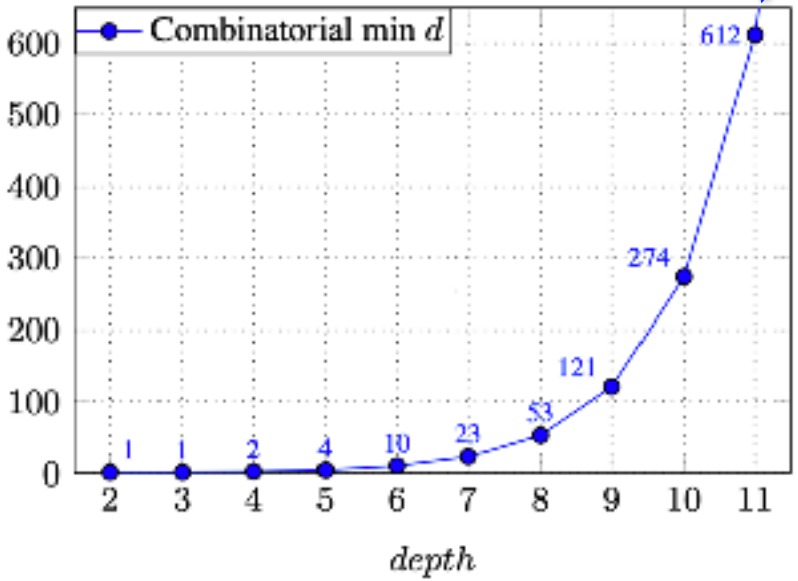

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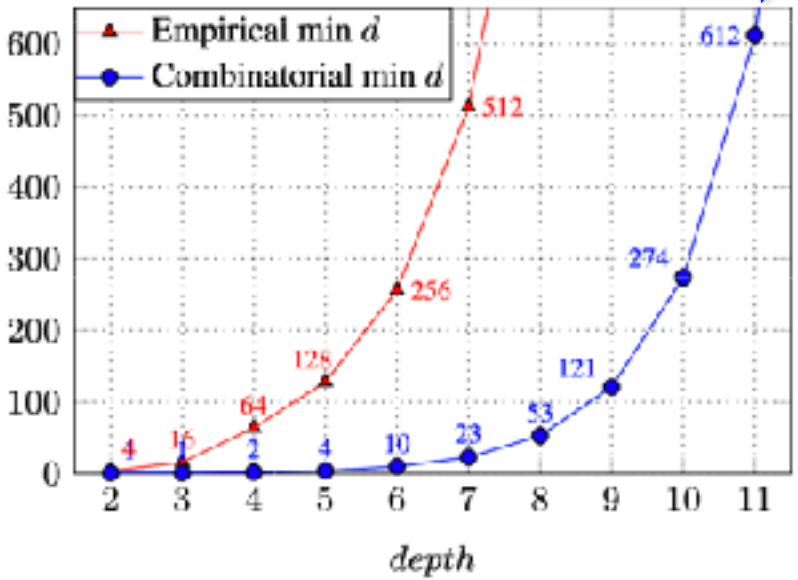

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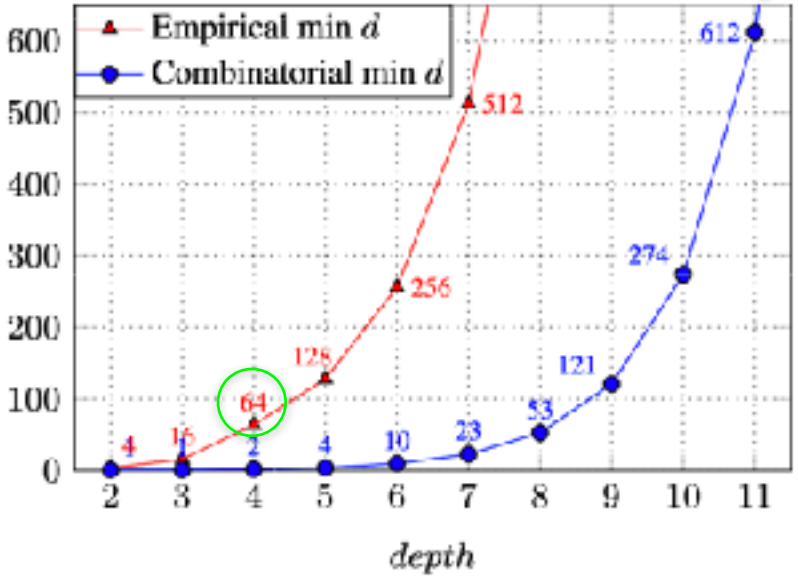

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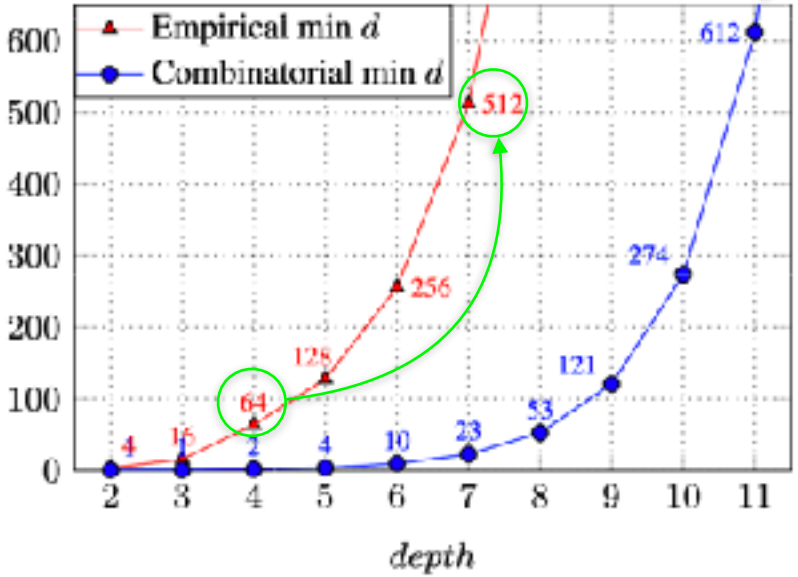

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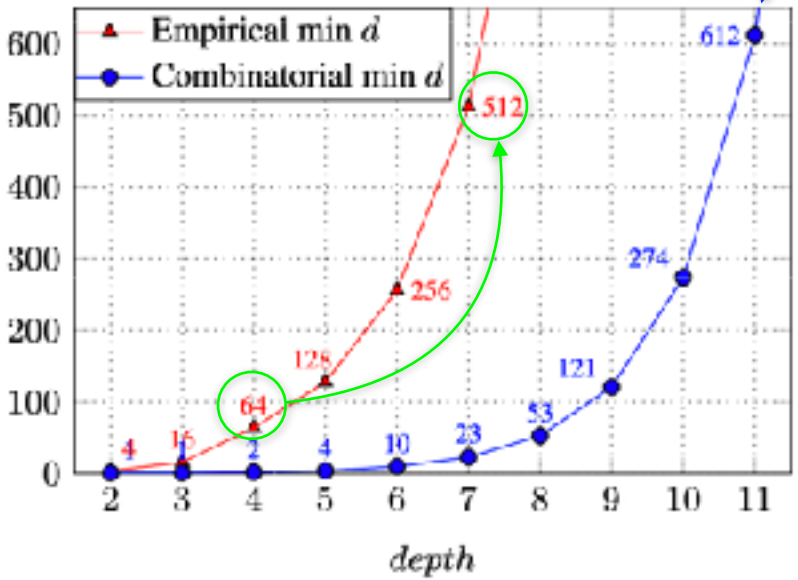

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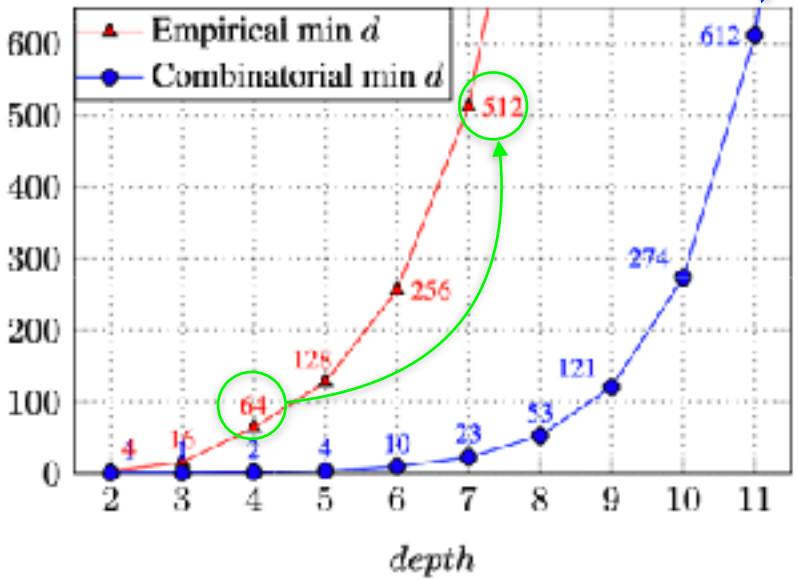

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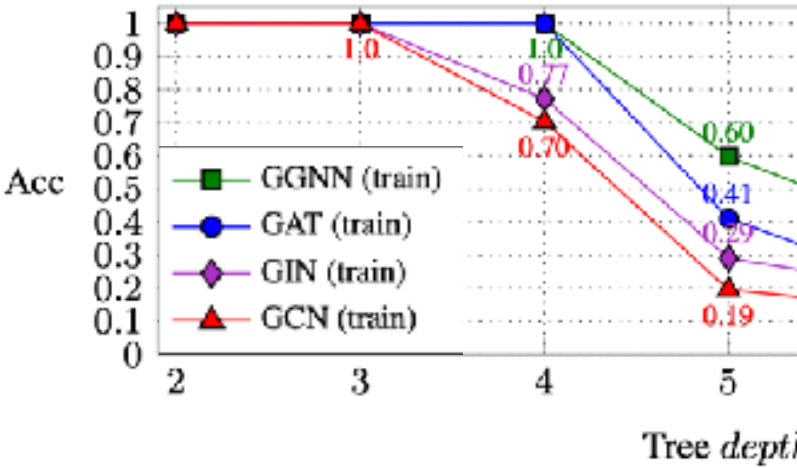
Over-squashing is only partially treatable by increasing dimensions

Different GNNs are affected by the bottleneck differently

- **GCN** and **GIN** suffer from over-squashing **more** than **GAT** and **GGNN**.



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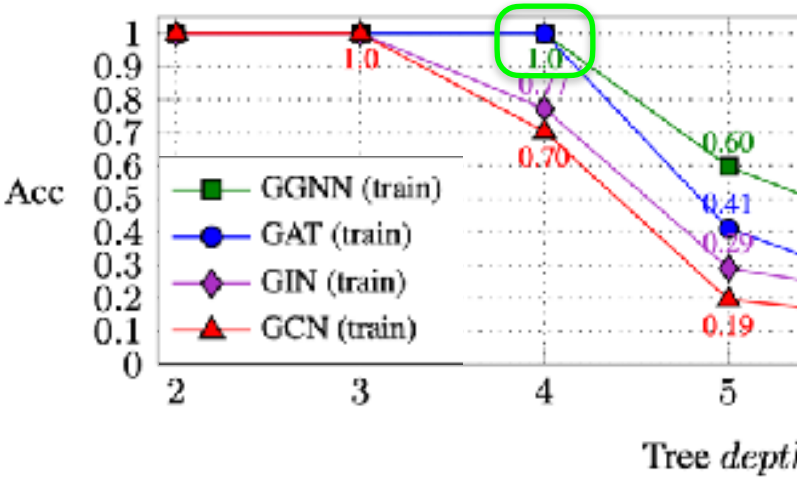

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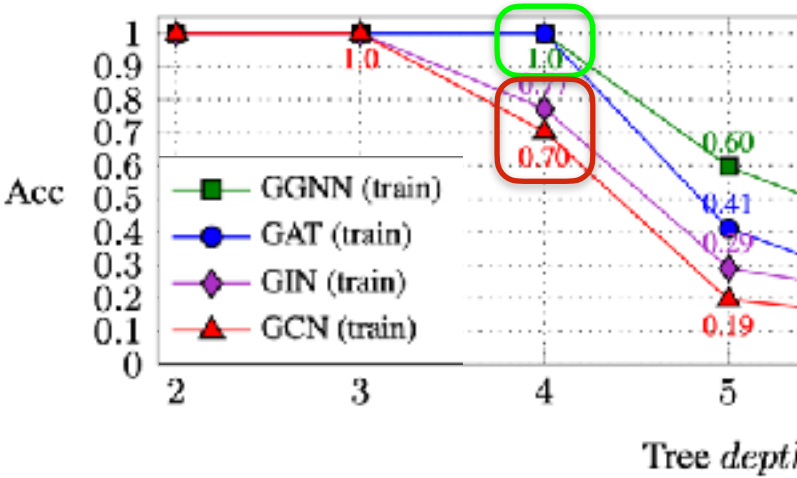

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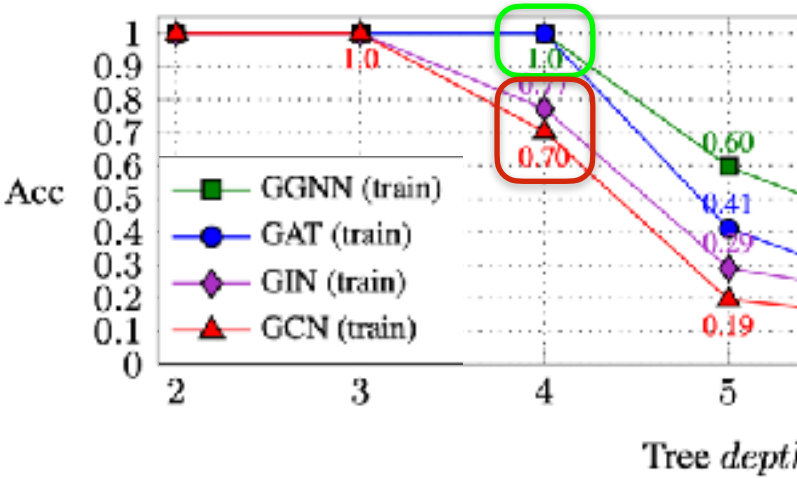

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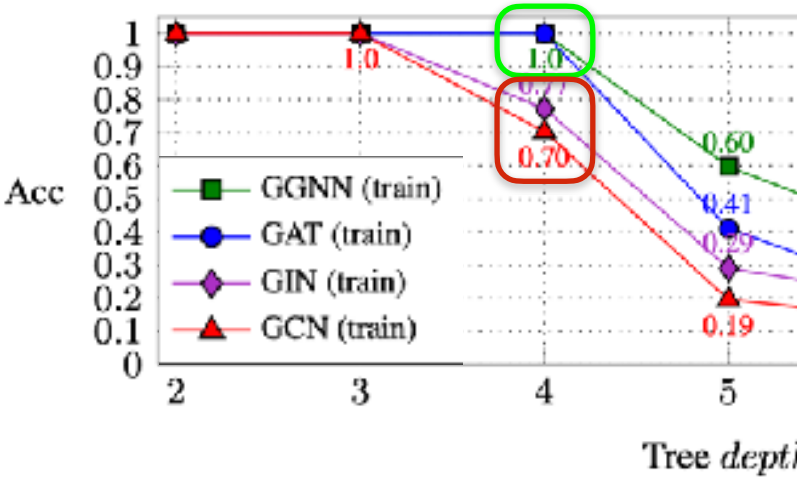

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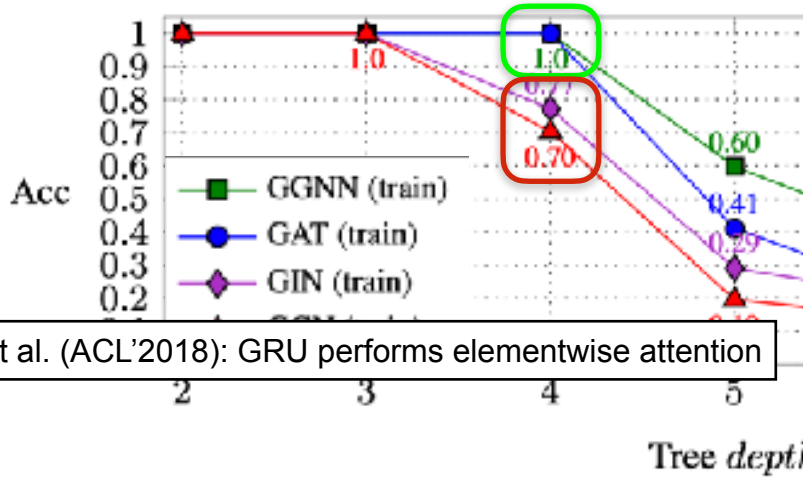

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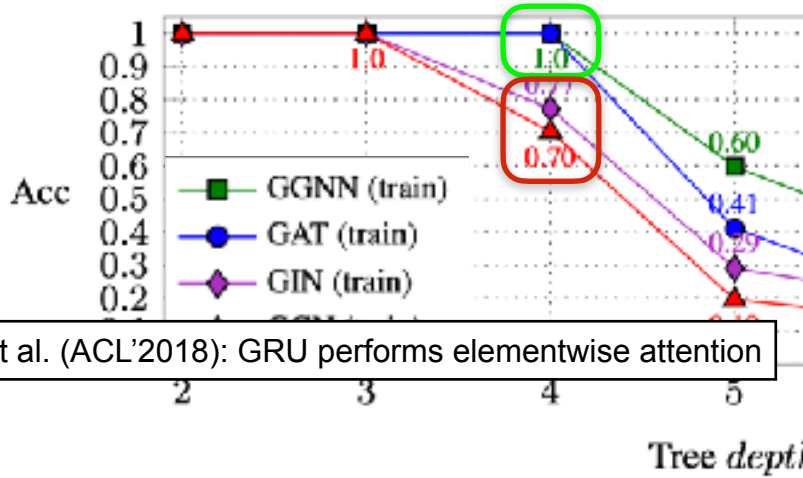

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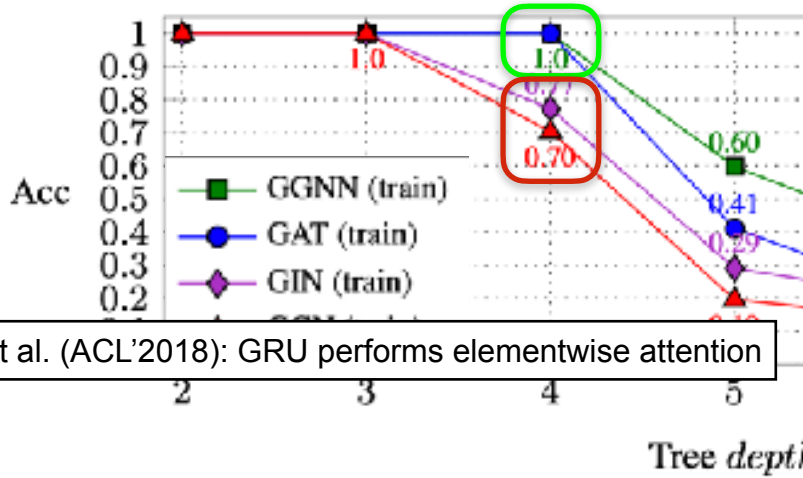

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The reason is the multihead, not the attention
("How Attentive are Graph Attention Networks?", 2021)

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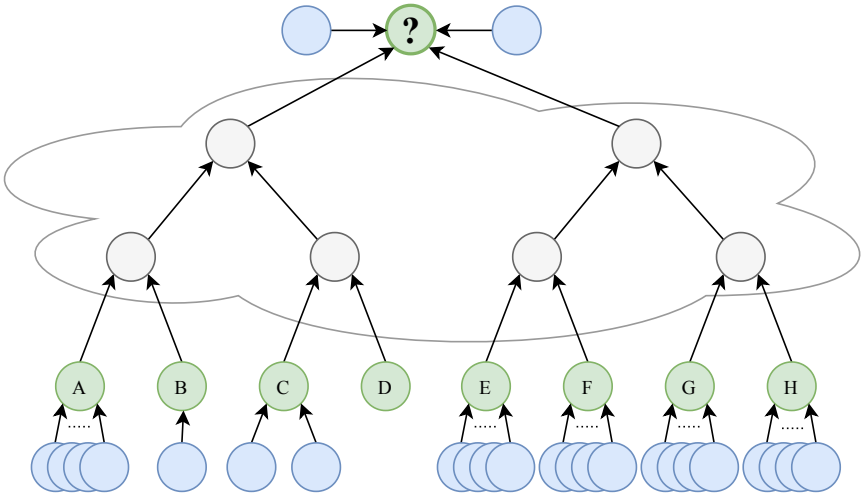

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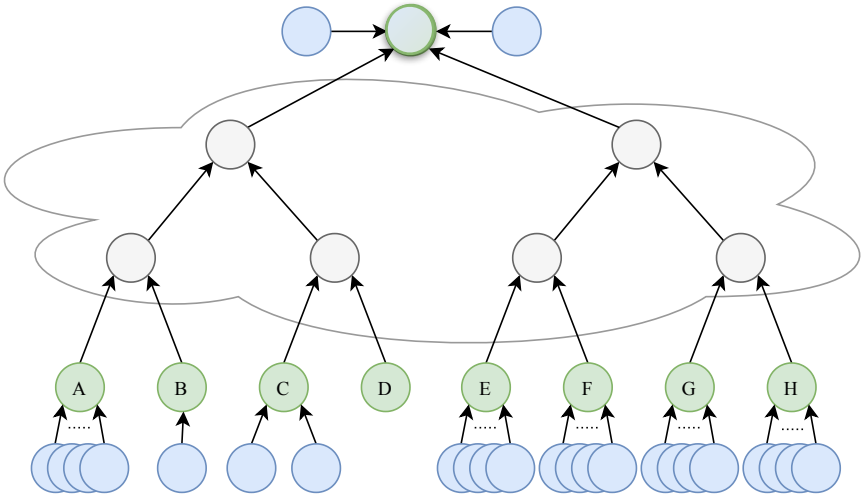

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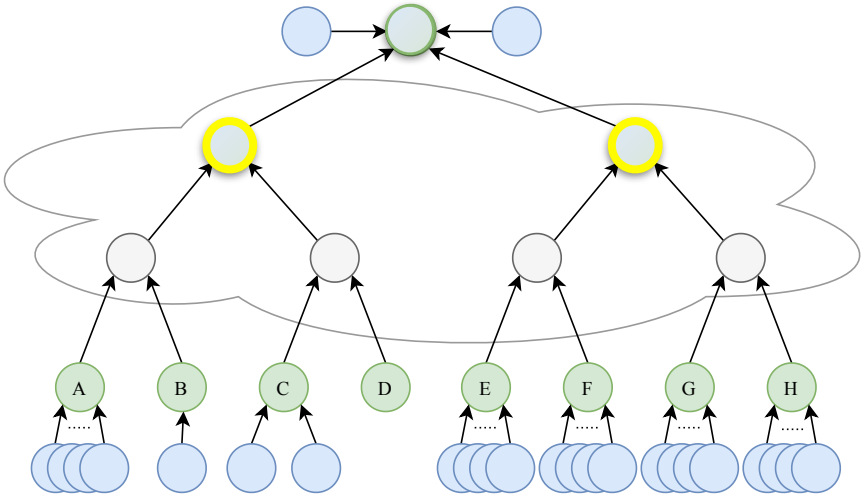

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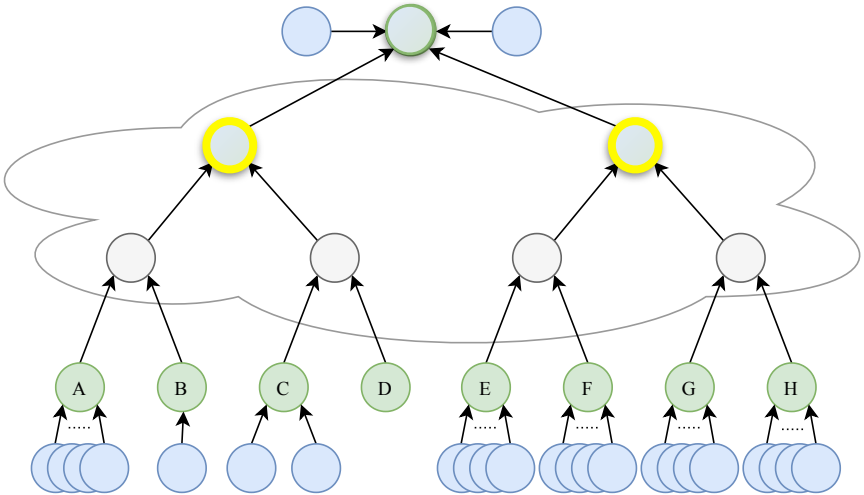

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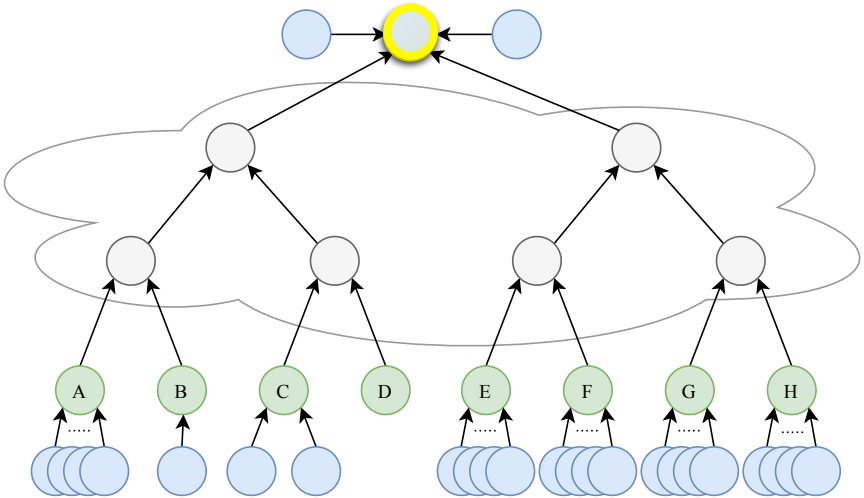

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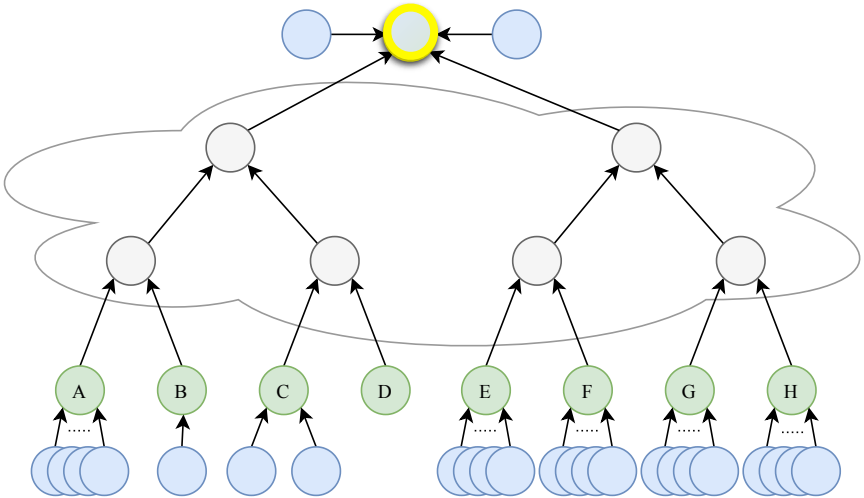

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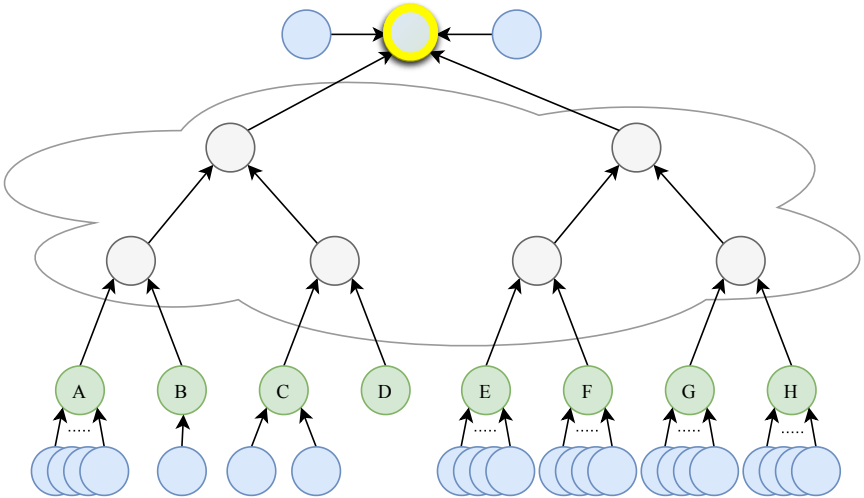

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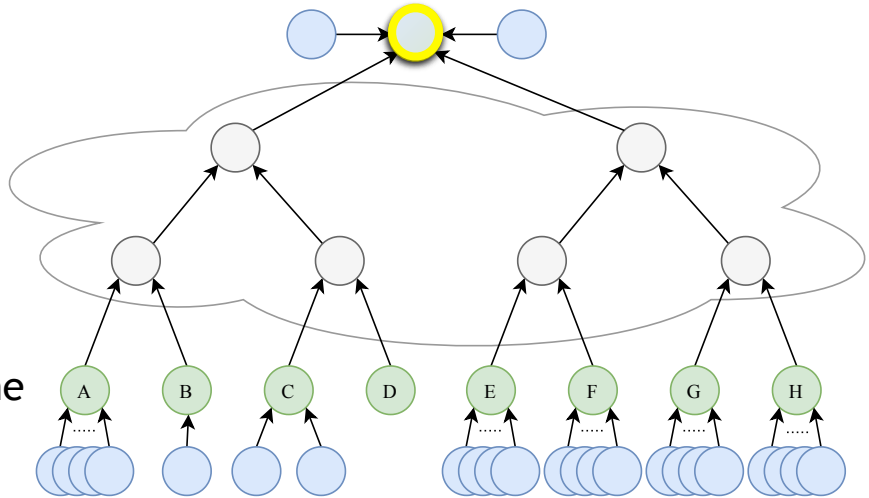

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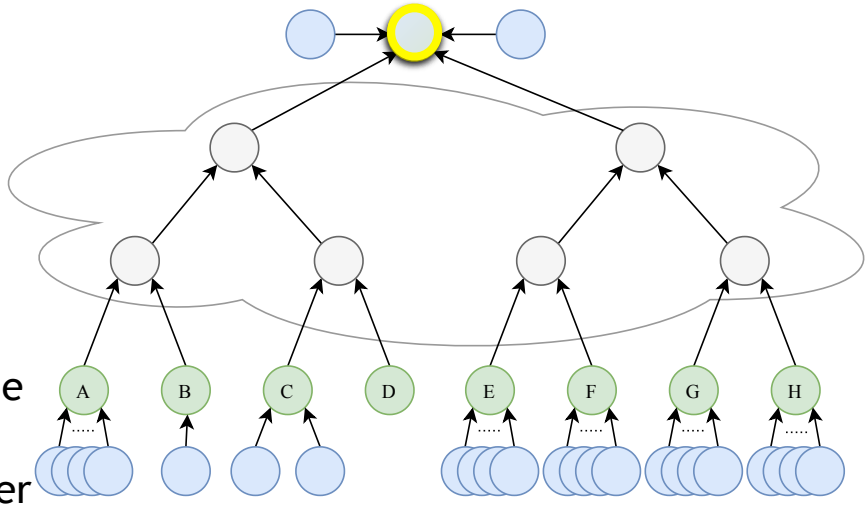

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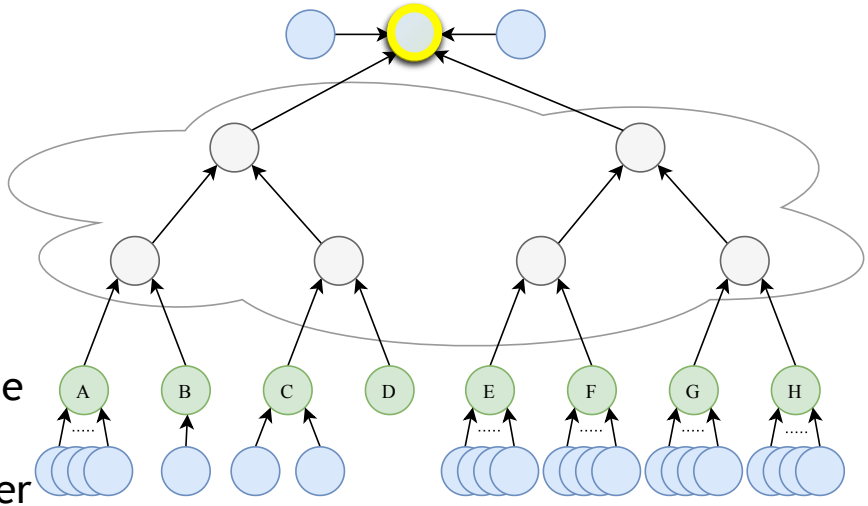

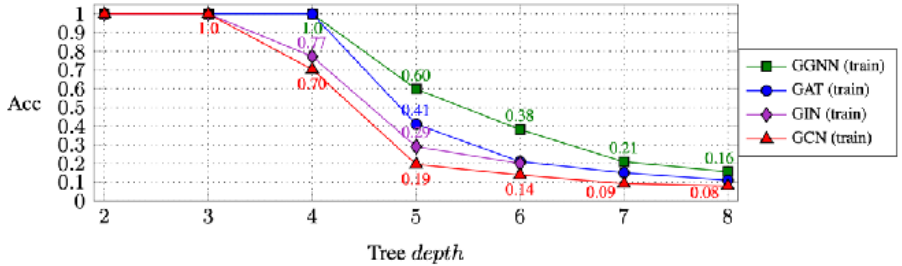

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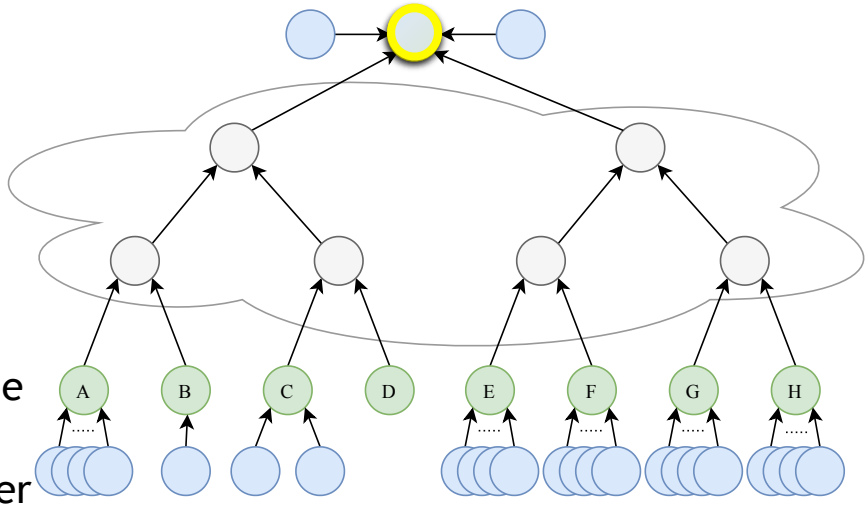

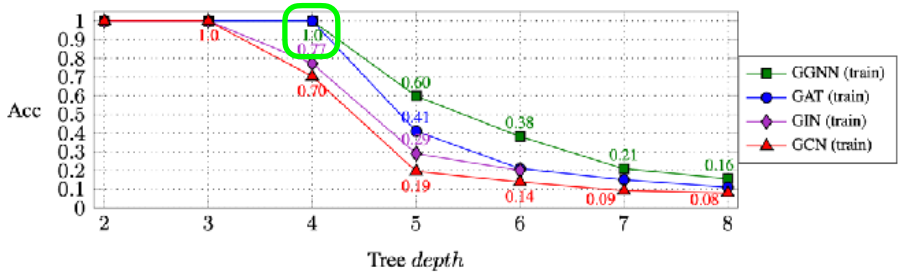

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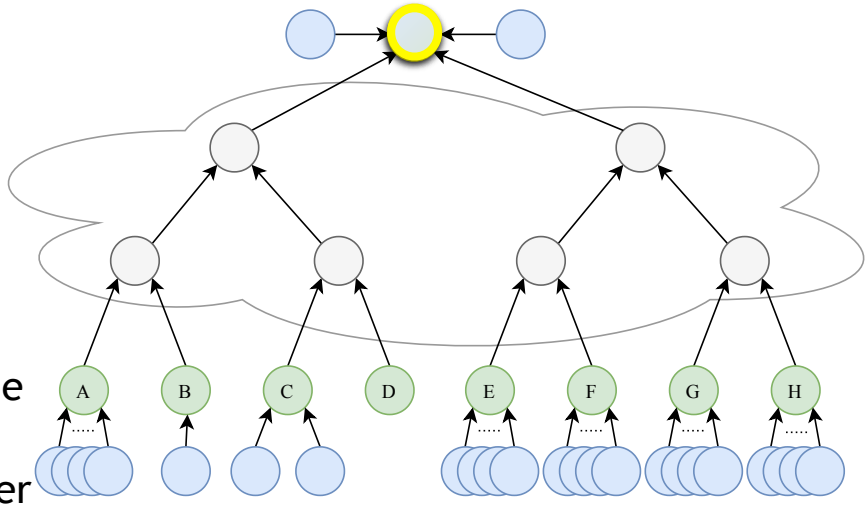

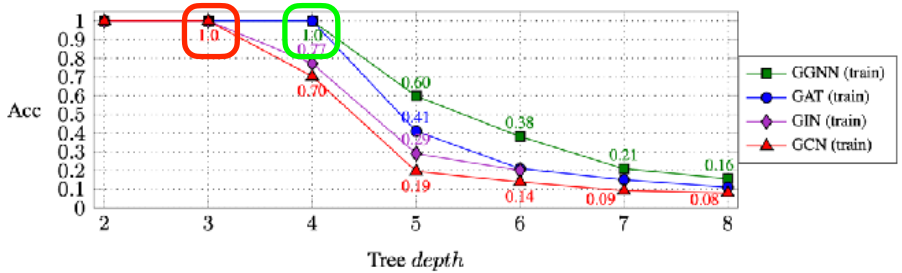

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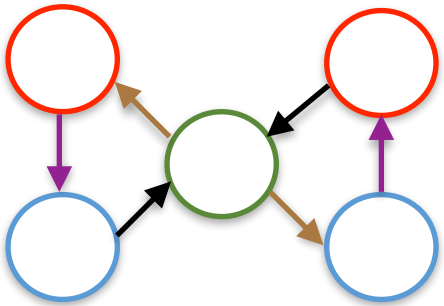
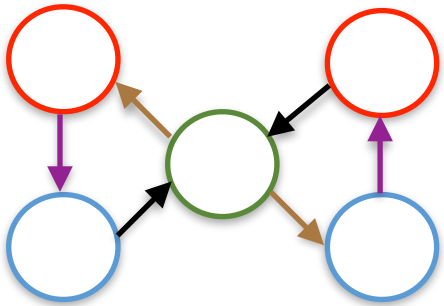


t=0



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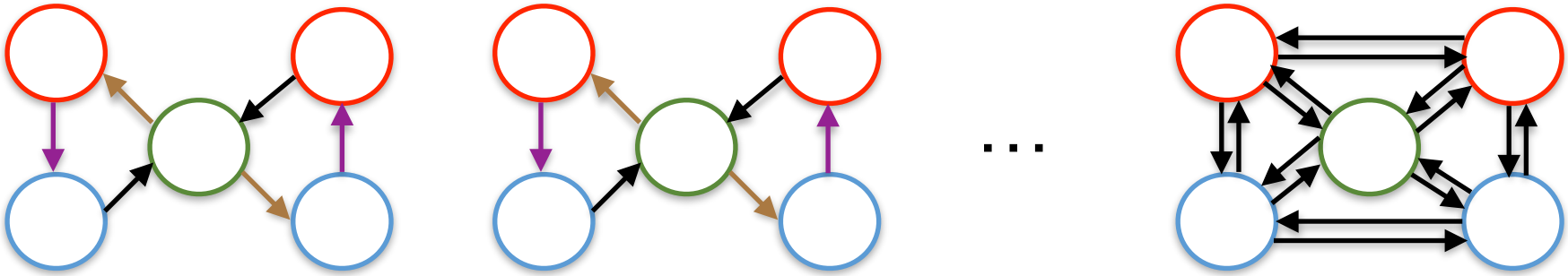

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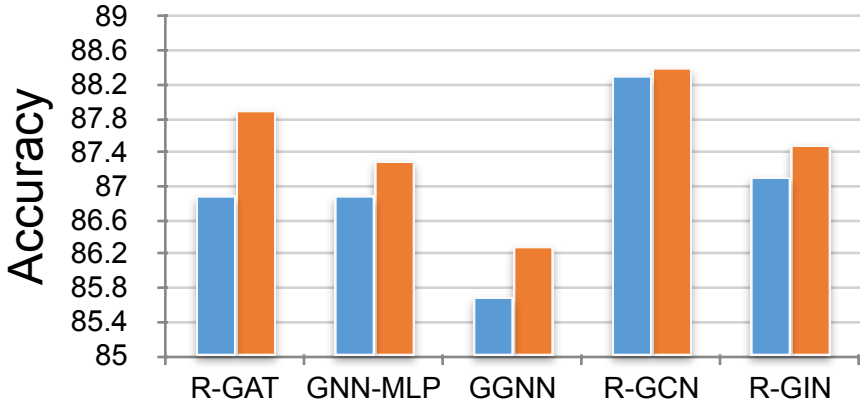
SeenProj test set



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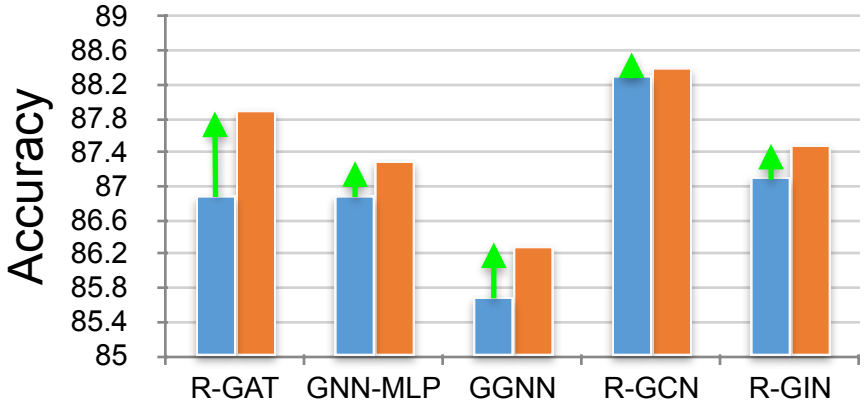

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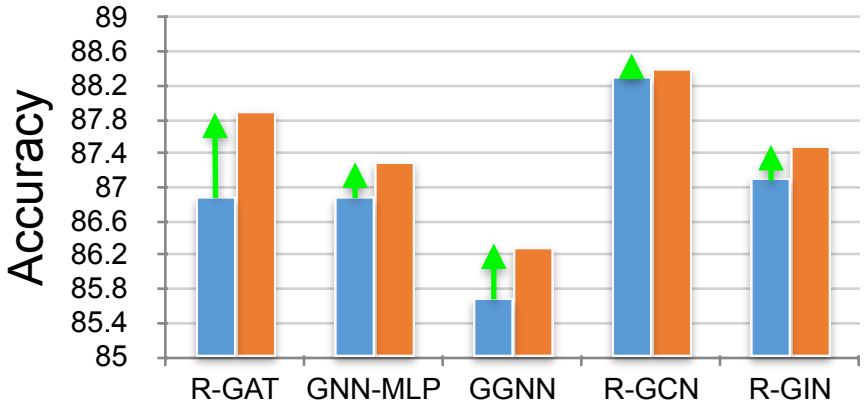

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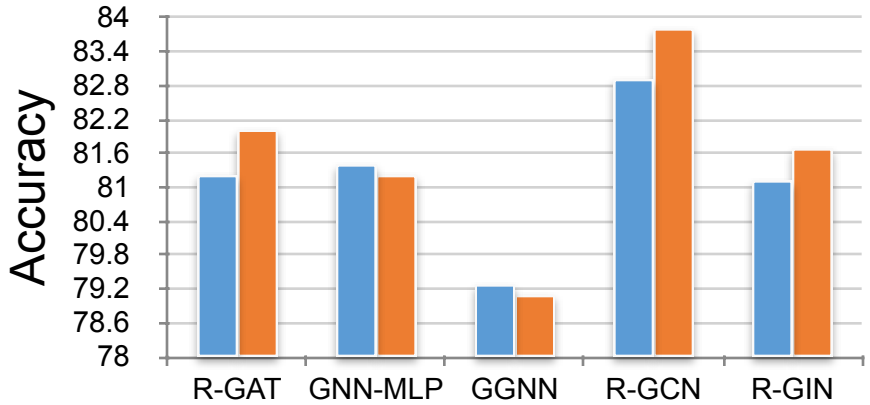

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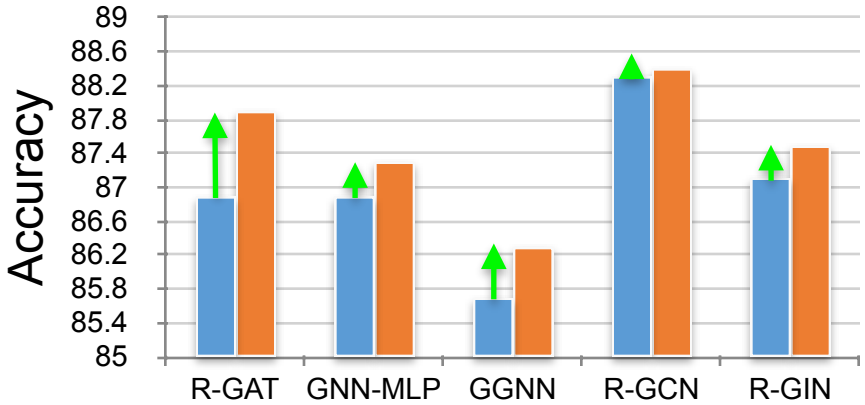

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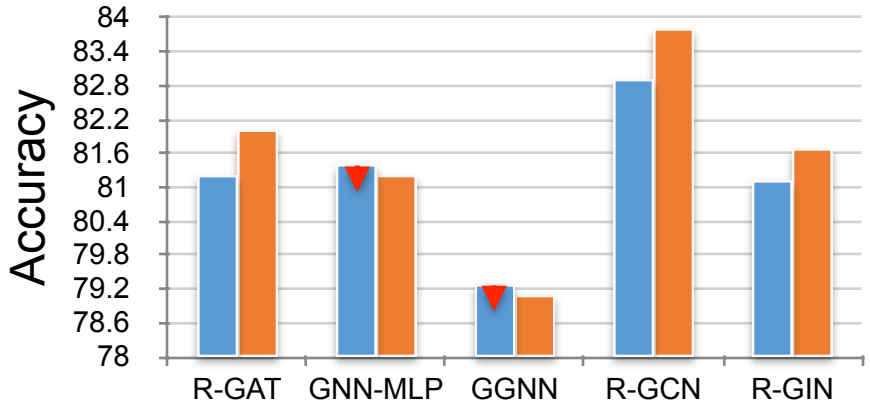

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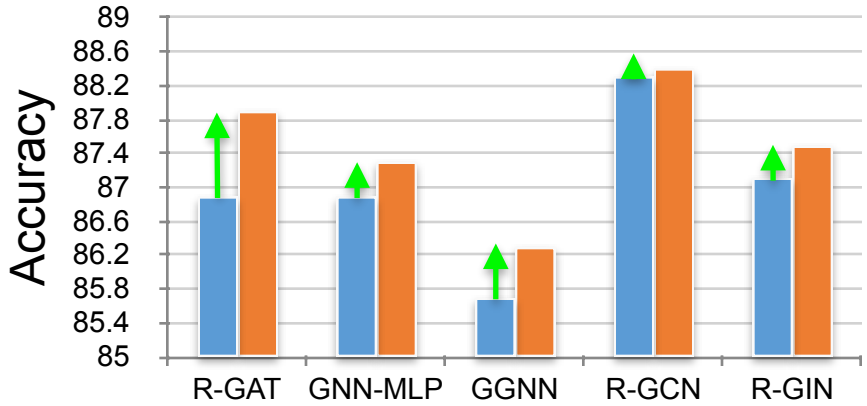

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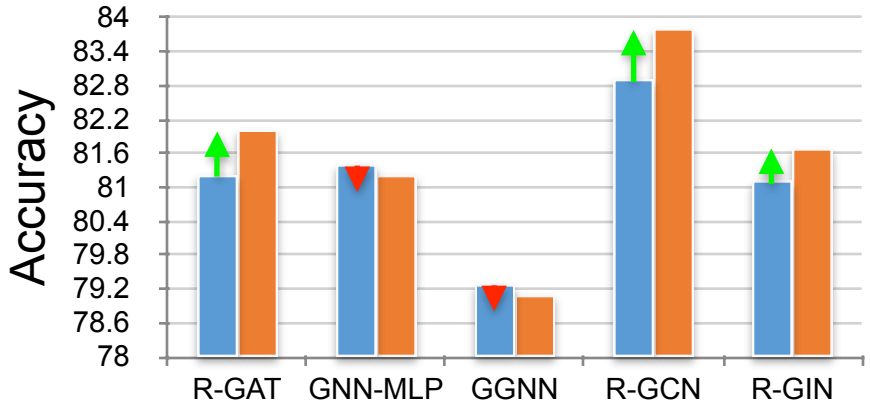

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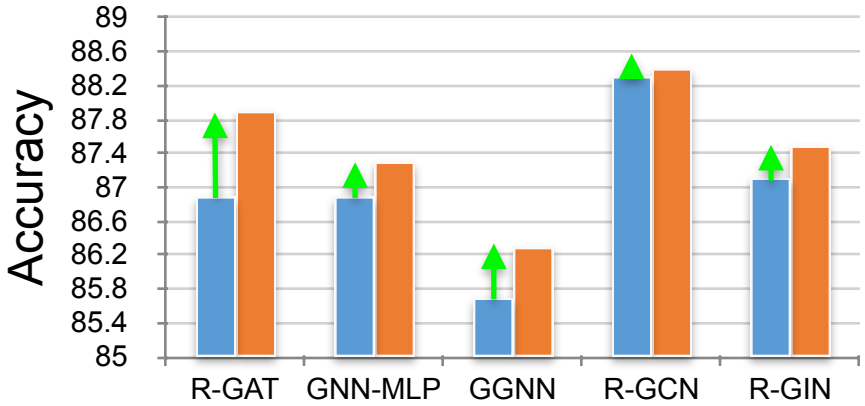

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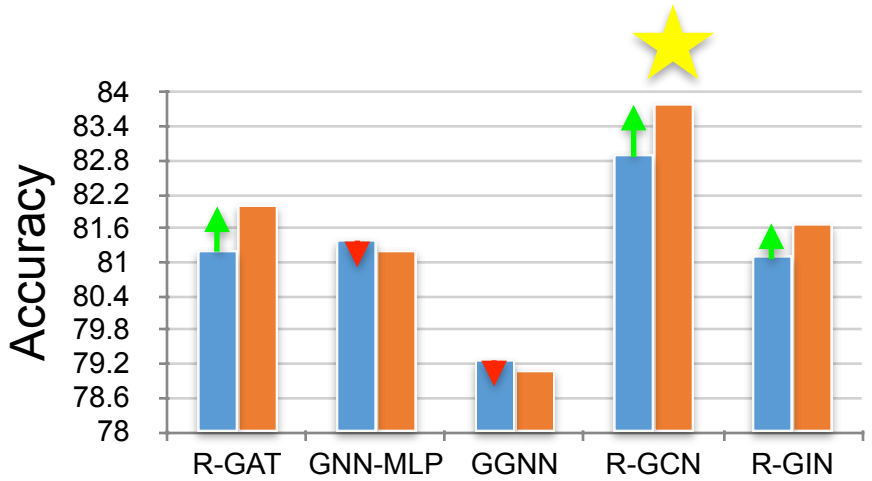
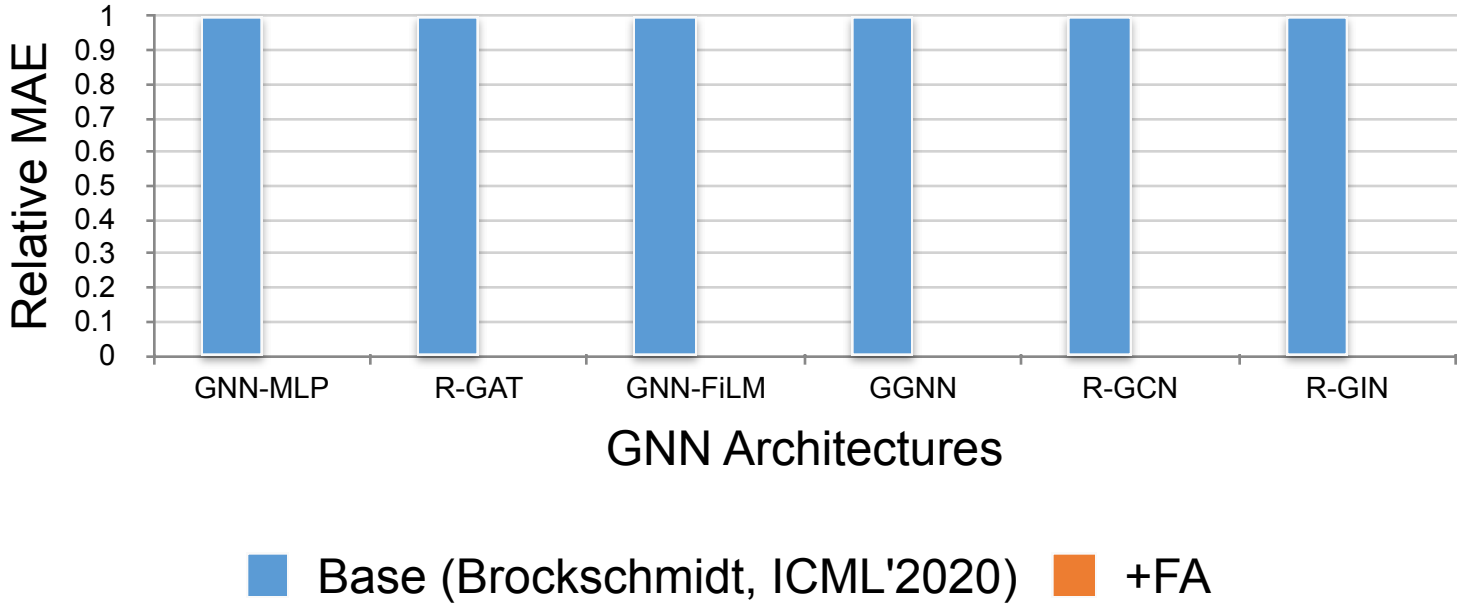


Base (Brockschmidt, ICML'2020)
+FA

QM9 Dataset (molecules regression)

(mean absolute error, lower = better)



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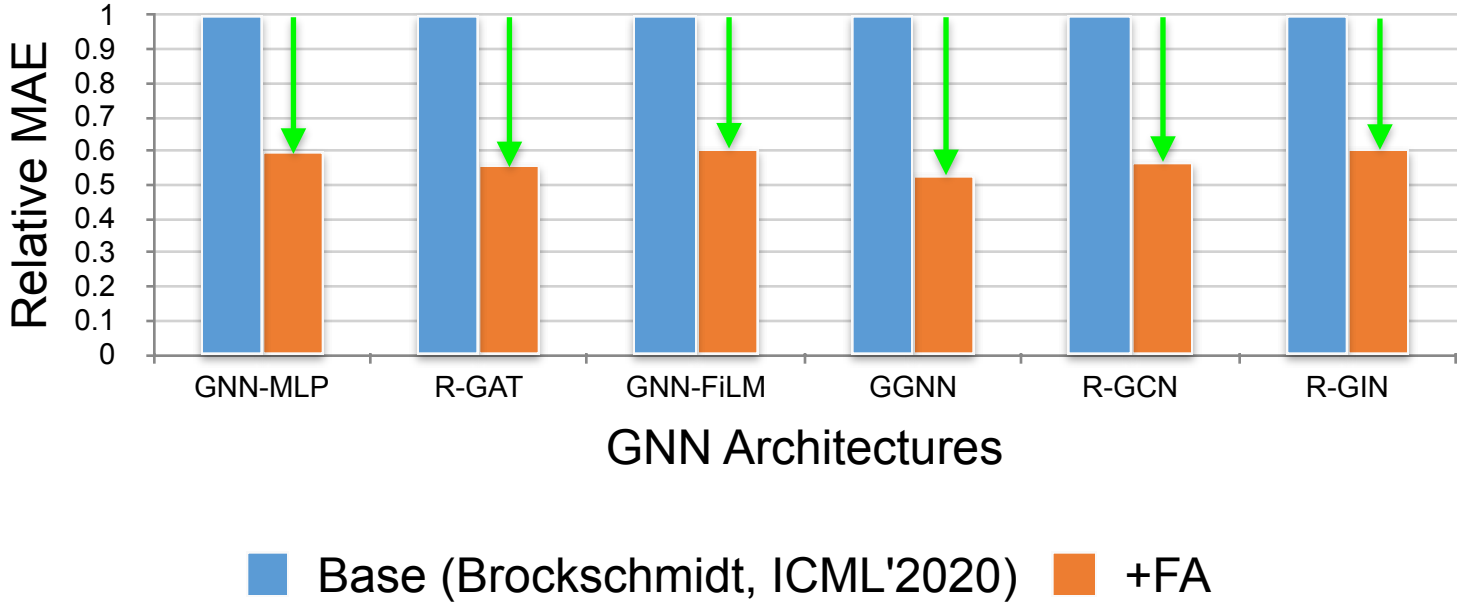
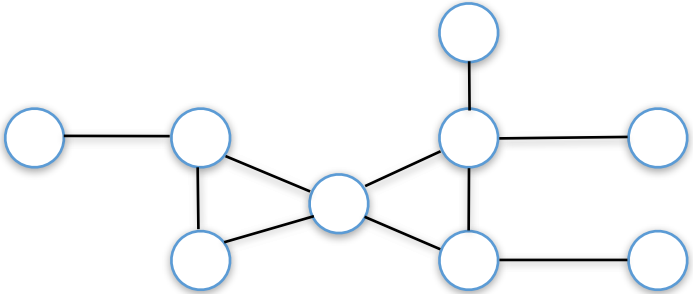


Maybe the number of layers simply wasn't enough?



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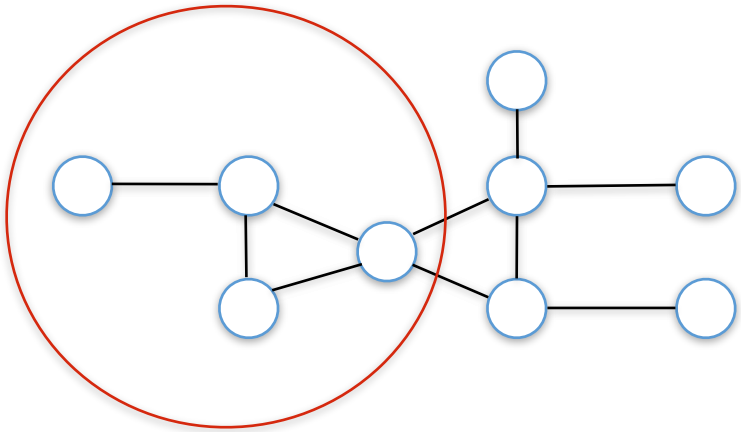

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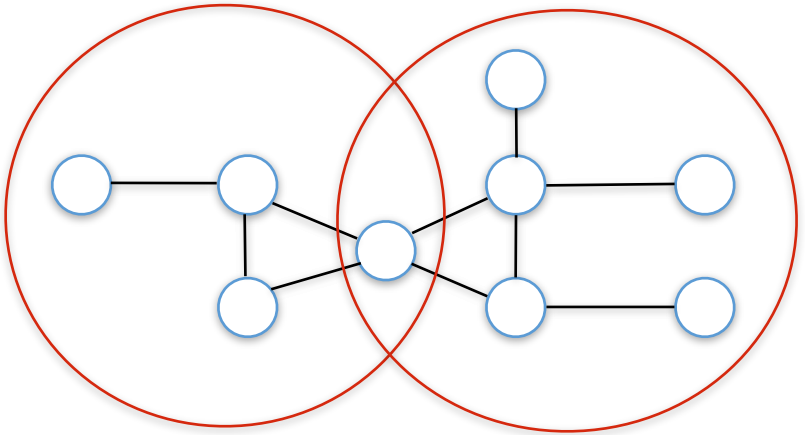
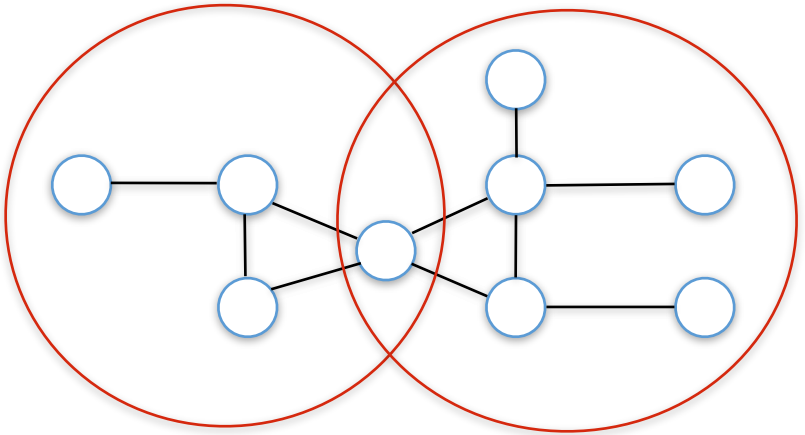


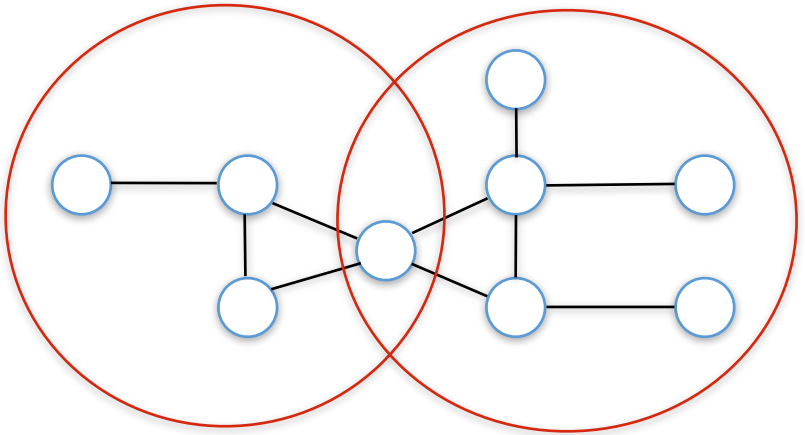
Maybe the number of layers simply wasn't enough?

- "Under-reaching": $K < diameter$



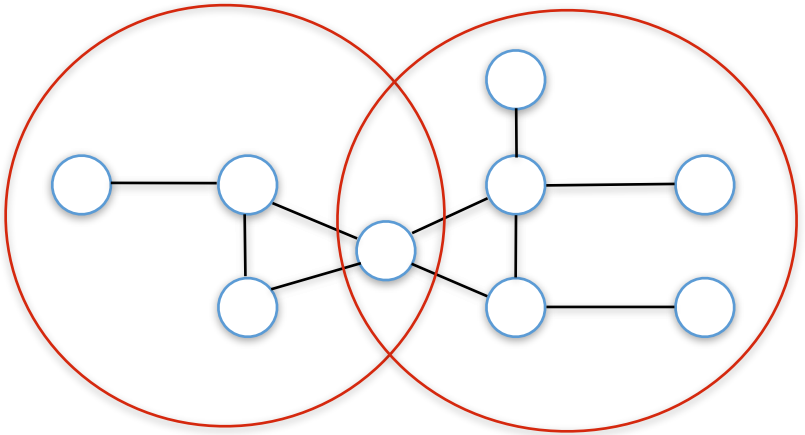
Maybe the number of layers simply wasn't enough?

- "Under-reaching": $K < diameter$
- In QM9:
  - $K = 8$



Maybe the number of layers simply wasn't enough?

- "Under-reaching": $K < diameter$
- In QM9:
  - $K = 8$
  - $diameter = 10$ (max)



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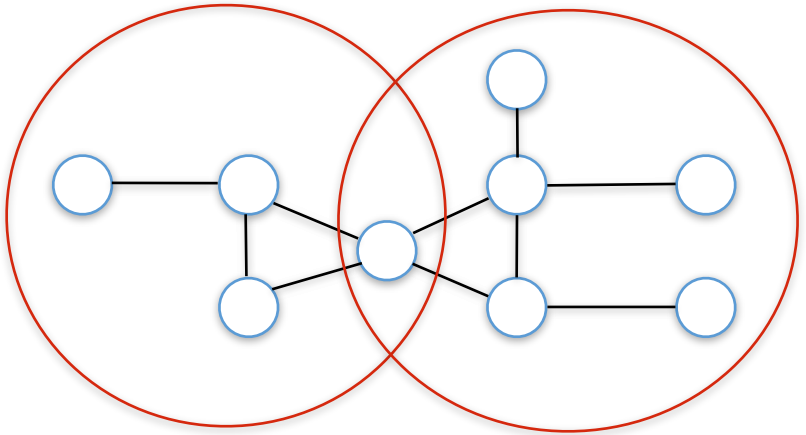
- "Under-reaching": $K < diameter$
- In QM9:
  - $K = 8$
  - $diameter = 10$ (max)
  - $diameter = 6$ (average)



Maybe the number of layers simply wasn't enough?

- "Under-reaching": $K < diameter$
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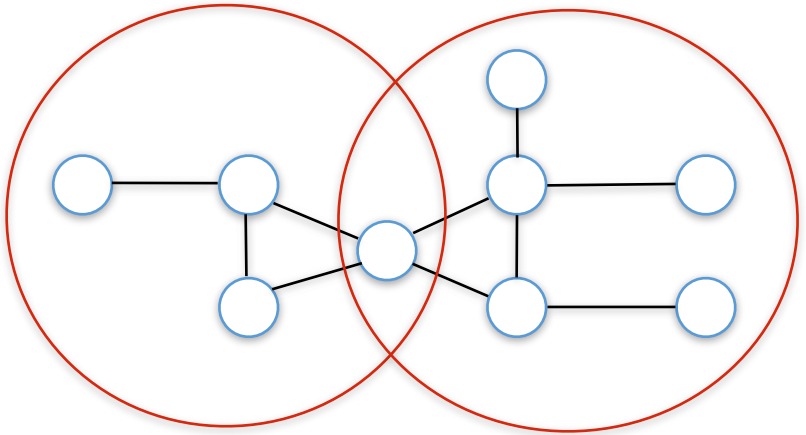
  - $diameter = 6$ (average)
  - $diameter = 8$ (90'th percentile)



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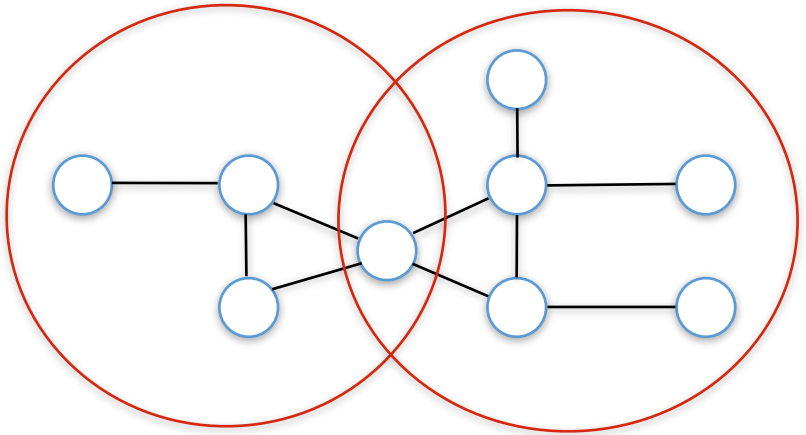
- In QM9:
  - $K = 8$
  - $diameter = 10$ (max)
  - $diameter = 6$ (average)
  - $diameter = 8$ (90'th percentile)
- Setting $K = 10$ didn't help



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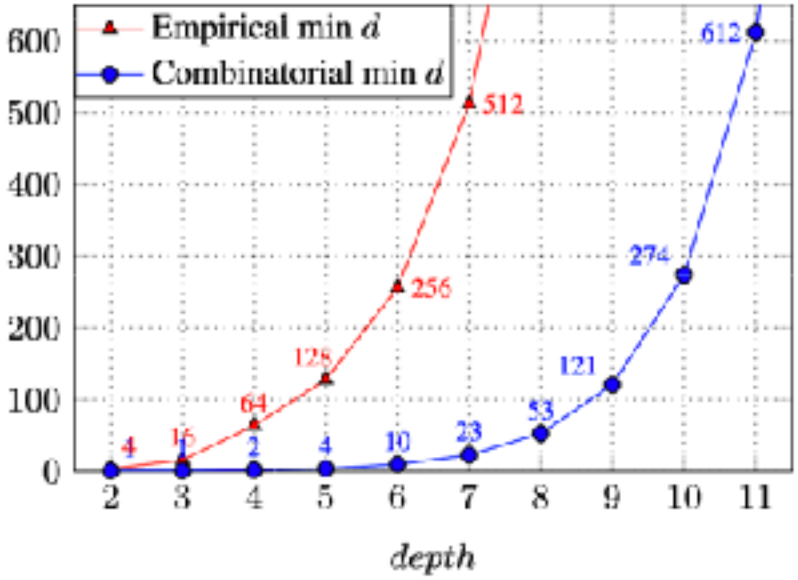

Breaking the Bottleneck in Previous Work

Some previous work implicitly avoided over-squashing:

Breaking the Bottleneck in Previous Work

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“Supersource edges”

[Scarselli, ’2008]

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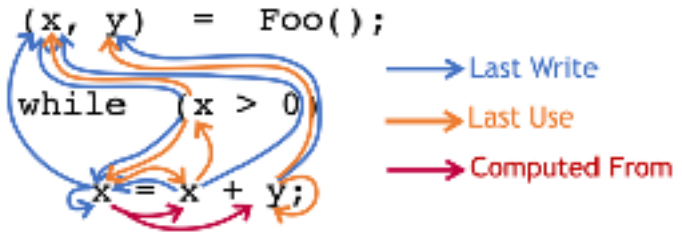

[Allamanis, ICLR’2018] [Brockschmidt, ICLR’2019]

Slide from Marc Brockschmidt

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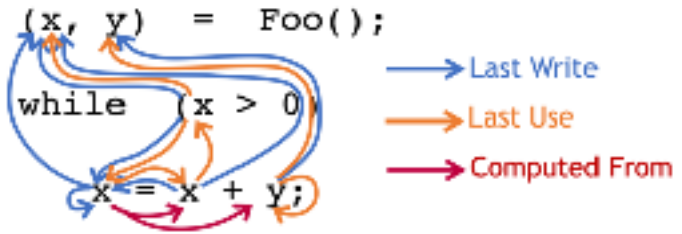

[Allamanis, ICLR’2018] [Brockschmidt, ICLR’2019]

Slide from Marc Brockschmidt

Ad-hoc solutions, none of them explicitly highlighted the bottleneck, explained it, and measured its effects

Over-squashing vs. Over-smoothing

Over-squashing vs. Over-smoothing

r - the problem radius (the required range of interaction between nodes)

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$K >> r$

Over-squashing vs. Over-smoothing

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Over-smoothing

$K >> r$

$r = 1$

$K >> 1$

Over-squashing vs. Over-smoothing

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Nodes will go indistinguishable

Over-squashing vs. Over-smoothing

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Over-smoothing $K >> r$	Under-reaching $K < r$
$r = 1$ $K >> 1$ 	
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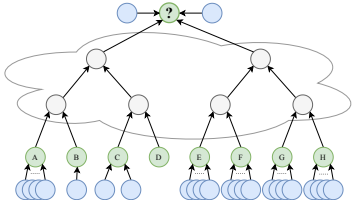
Over-smoothing $K >> r$	Under-reaching $K < r$
$r = 1$ $K >> 1$ 	$r = 4$ $K < 4$ 
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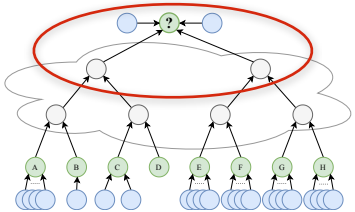
$r = 1$ $K >> 1$ 	$r = 4$ $K < 4$ 
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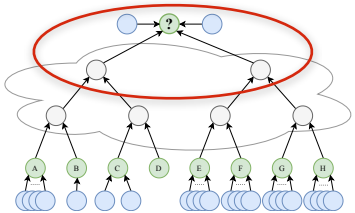
$r = 1$ $K >> 1$ 	$r = 4$ $K < 4$ 
Nodes will go indistinguishable	The GNN cannot fit long-range patterns

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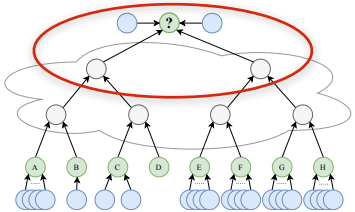
Over-smoothing $K >> r$	Under-reaching $K < r$	Over-squashing $K = r >> 1$
$r = 1$ $K >> 1$ 	$r = 4$ $K < 4$ 	
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Over-squashing vs. Over-smoothing

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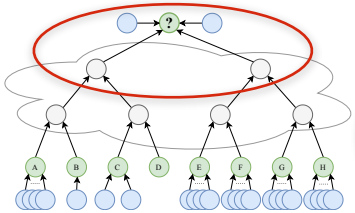
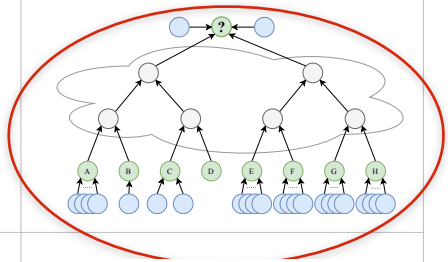
Over-smoothing $K >> r$	Under-reaching $K < r$	Over-squashing $K = r >> 1$
$r = 1$ $K >> 1$ 	$r = 4$ $K < 4$ 	$r = 4$ $K = 4$ 
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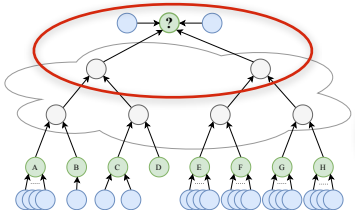
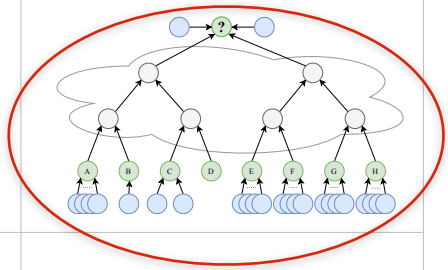
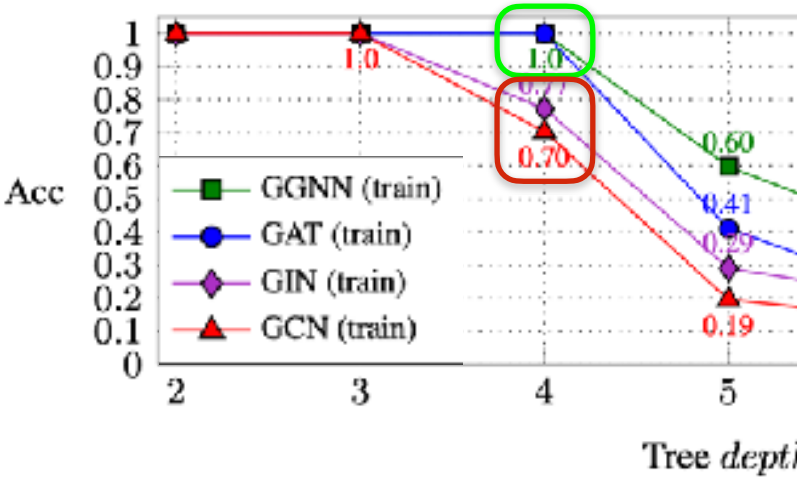
$r = 1$ $K >> 1$ 	$r = 4$ $K < 4$ 	$r = 4$ $K = 4$ 
Nodes will go indistinguishable	The GNN cannot fit long-range patterns	The GNN *fails to* fit long-range patterns

Different GNNs are affected by the bottleneck differently

- **GCN** and **GIN** suffer from over-squashing **more** than **GAT** and **GGNN**.

- **GCN** $\mathbf{h}_v^{(k)} = ReLU\left(W^{(k)}\left(\frac{1}{c_v}\mathbf{h}_v^{(k-1)} + \sum_{u\in\mathcal{N}_v}\frac{1}{c_{v,u}}\mathbf{h}_u^{(k-1)}\right)\right)$
- **GIN** $\mathbf{h}_v^{(k)} = MLP^{(k)}\left(\left(1+\epsilon^{(k)}\right)\mathbf{h}_v^{(k-1)} + \sum_{u\in\mathcal{N}_v}\mathbf{h}_u^{(k-1)}\right)$
- **GGNN** $\mathbf{h}_v^{(k)} = GRU\left(\mathbf{h}_v^{(k-1)}, \sum_{u\in\mathcal{N}_v} W_{neighbor}\mathbf{h}_u^{(k-1)}\right)$
- **GAT** $\mathbf{h}_v^{(k)} = ReLU\left(MultiHeadAttention\left(\mathcal{N}_v \mid \mathbf{h}_v^{(k-1)}\right)\right)$



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How Attentive are Graph Neural Networks?



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How Attentive are Graph Neural Networks?



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q0
q1
q2
q3
q4
q5
q6
q7
q8
q9

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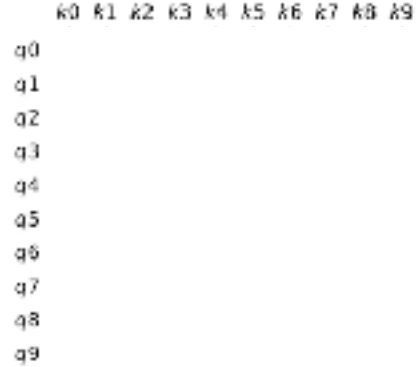

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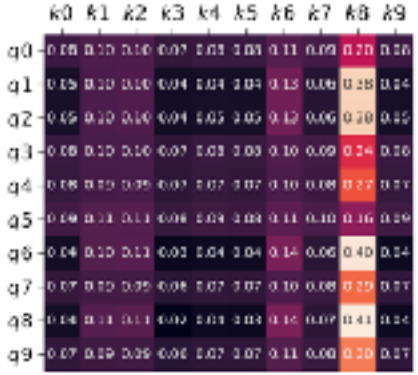

(a) Attention in standard GAT (Veličković et al. (2018))



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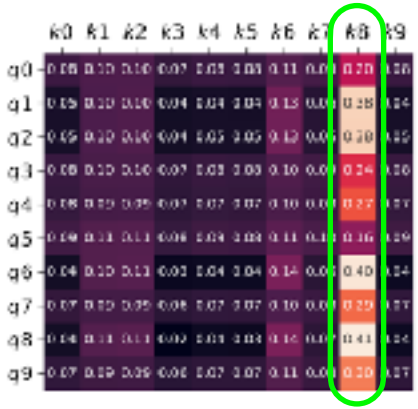

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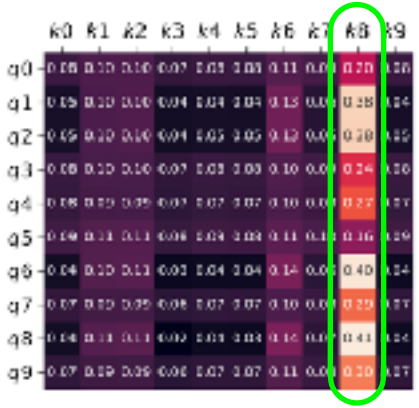

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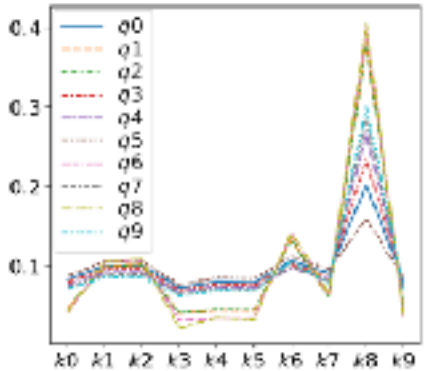



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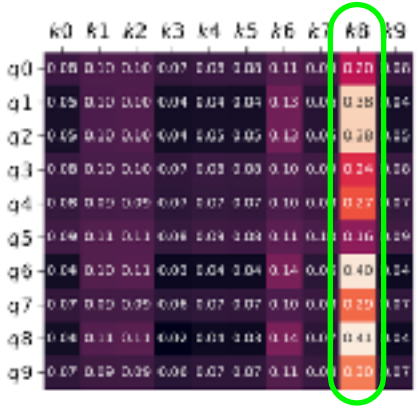
How Attentive are Graph Neural Networks?



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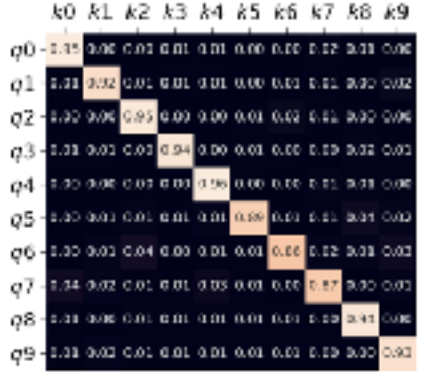
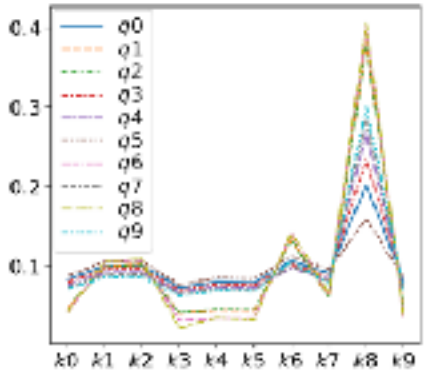
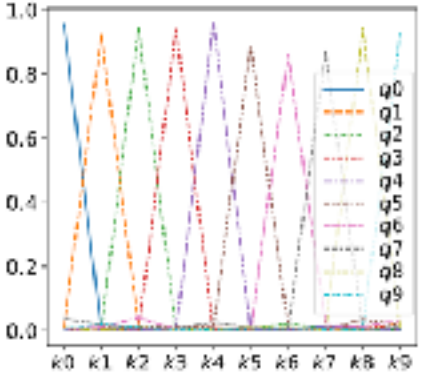


(b) Attention in GATv2, our fixed version of GAT







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How Attentive are Graph Neural Networks?



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How Attentive are Graph Neural Networks?



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Static attention (GAT, Veličković et al., 2018):

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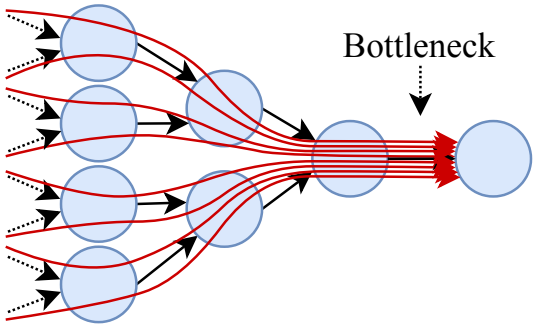
- Theoretically **much** more expressive
- Practically better across **11** benchmarks

Available in PyTorch Geometric:

from torch_geometric.nn.conv.gatv2_conv **import** GATv2Conv

Summary

- To pass long-range messages - we need many GNN layers



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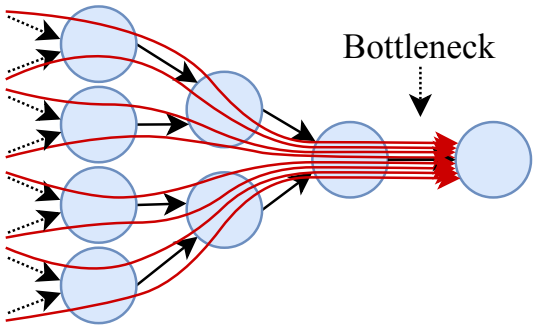

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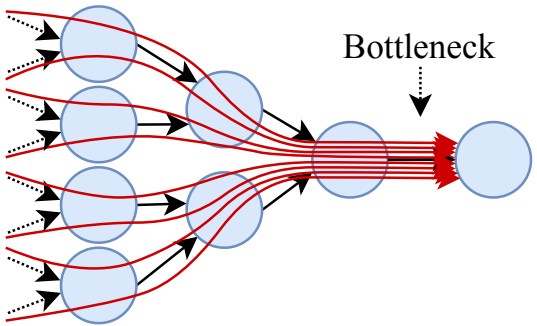

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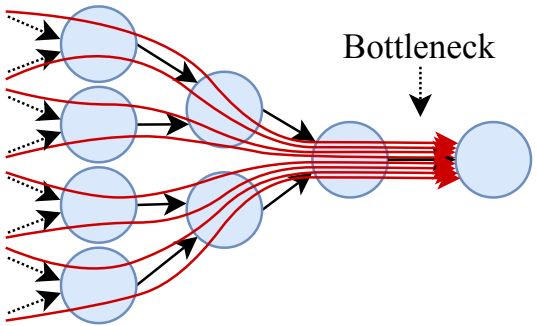

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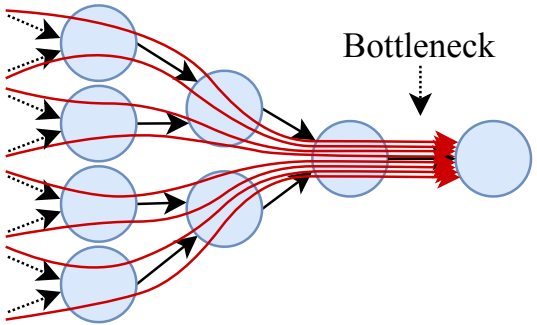

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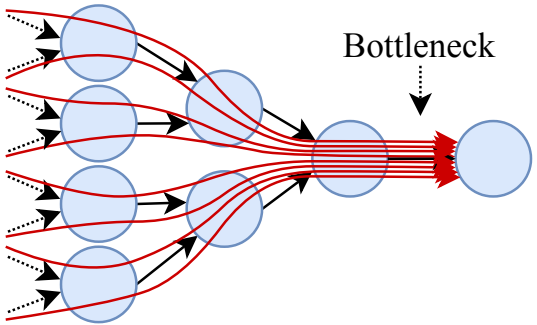

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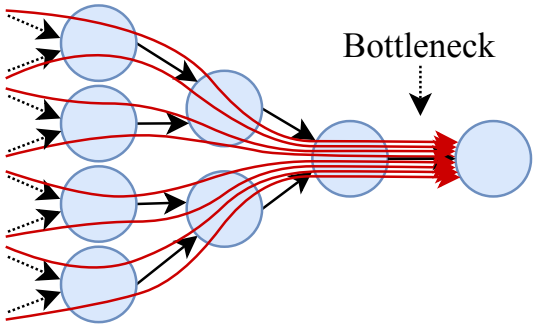

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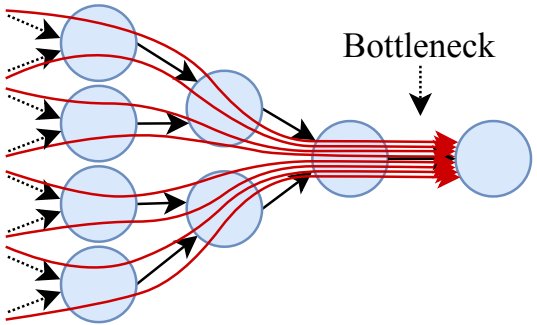


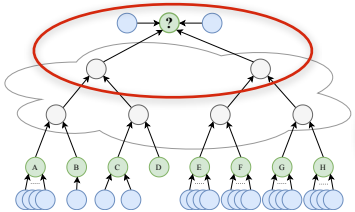
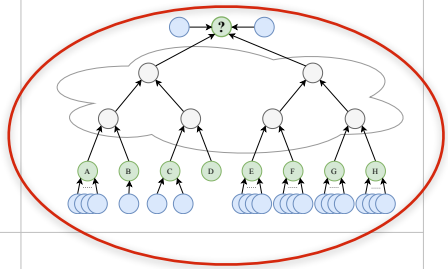
ualon@cs.cmu.edu

http://urialon.ml

Over-squashing vs. Over-smoothing

r - the problem radius (the required range of interaction between nodes)

K - the number of GNN layers

Over-smoothing $K >> r$	Under-reaching $K < r$	Over-squashing $K = r >> 1$
$r = 1$ $K >> 1$ 	$r = 4$ $K < 4$ 	$r = 4$ $K = 4$ 
Nodes will go indistinguishable	The GNN cannot fit long-range patterns	The GNN *fails to* fit long-range patterns