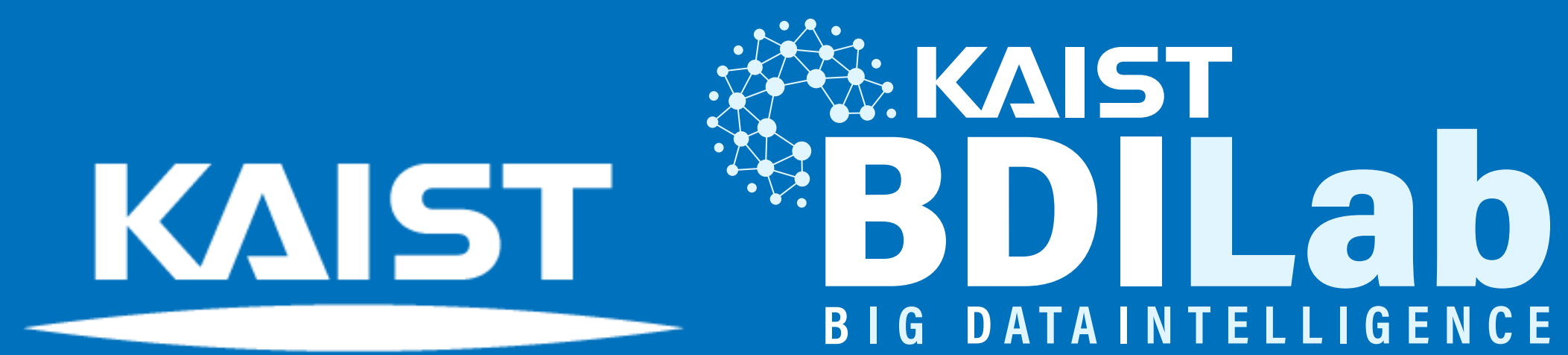


Learn When and Where to Connect: Adaptive Virtual Nodes for Dynamic Message Passing on Graphs

Jaejun Lee¹ and Joyce Jiyoung Whang^{2*}

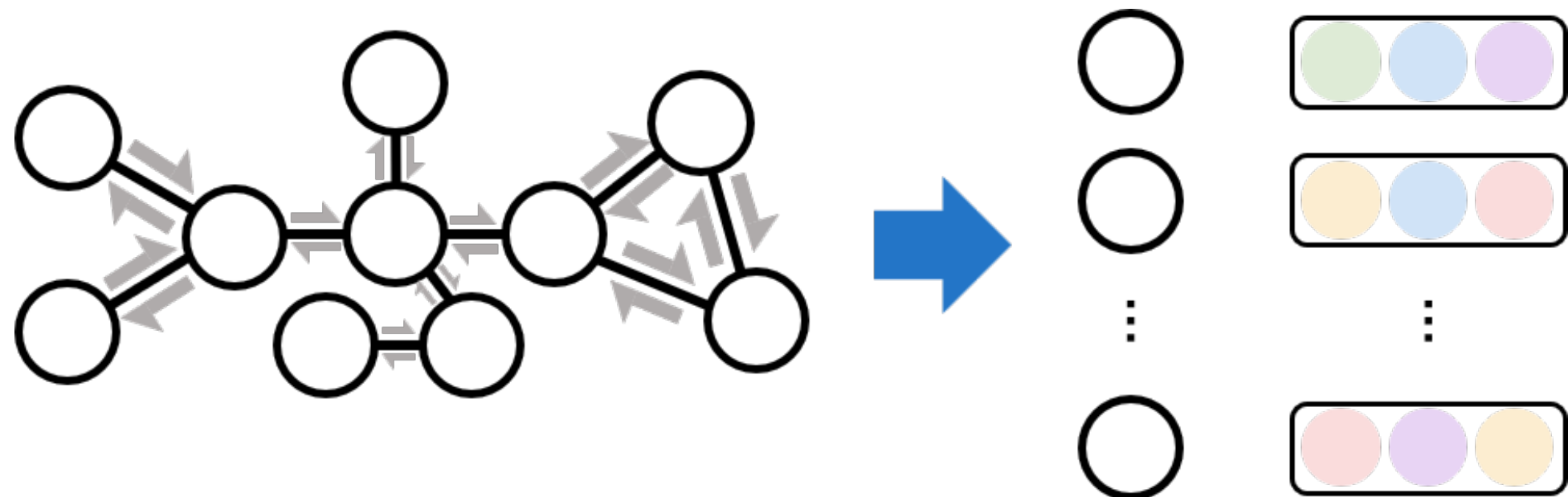
¹School of Computing, KAIST, ²Department of AI Computing, KAIST

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Message Passing Neural Networks (MPNNs)

- A class of neural networks for processing graph-structured data



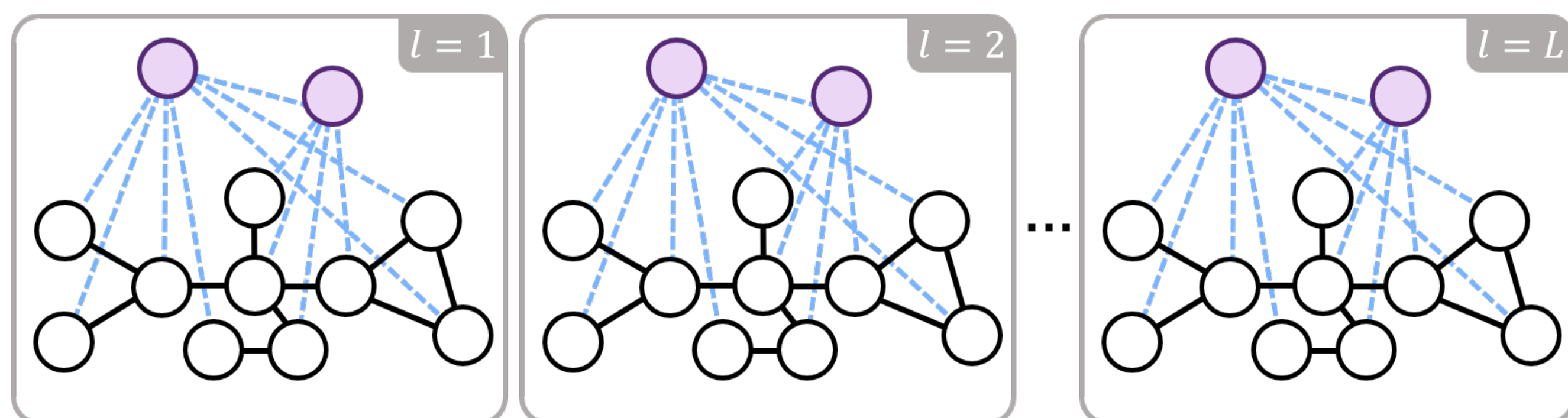
- Limitations of MPNNs

- Under-reaching**: insufficiently deep layers cause MPNNs to fail to capture long-range dependencies appropriately
- Over-smoothing**: excessively deep layers can lead to overly similar receptive fields, making representations indistinguishable
- Over-squashing**: fixed-size vectors may struggle to encode information from extensive receptive fields

Adaptive Virtual Nodes (VNs) for MPNNs

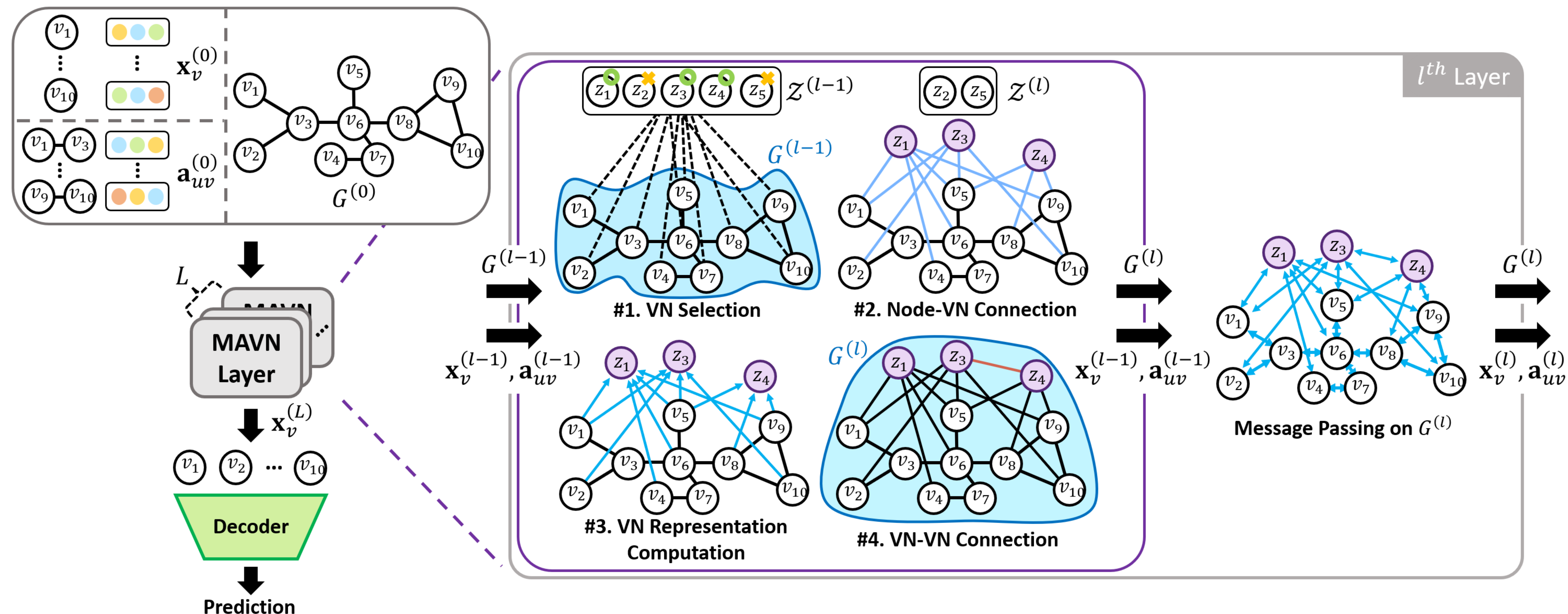
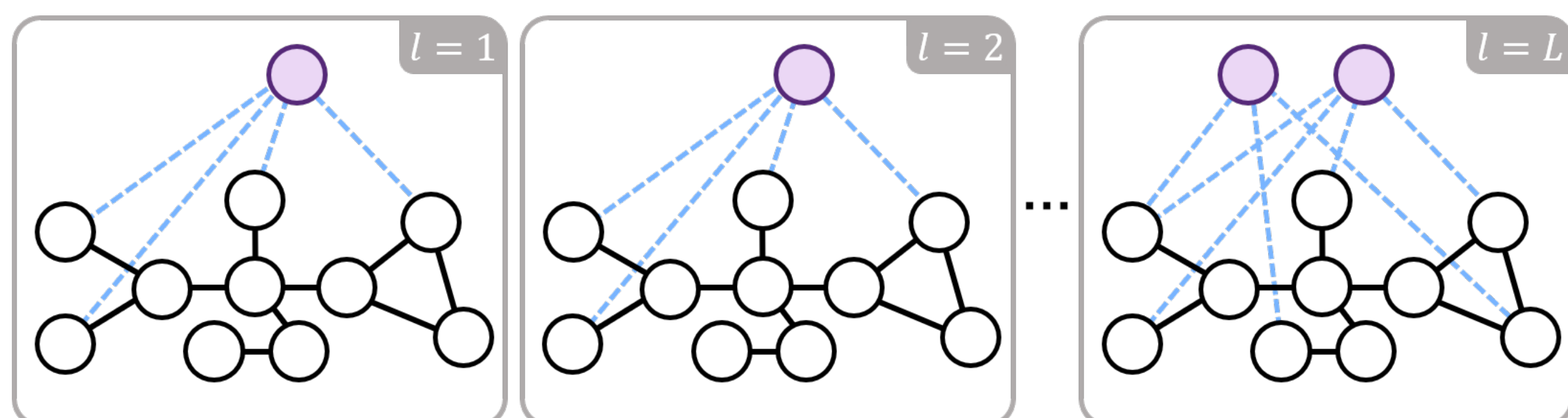
- VNs: Often utilized to mitigate the limitations of MPNNs
- Limitations of Existing VN-based Methods

- Equal number of connected VNs** per node
- Independently** establish node-VN connections
- Connections are fixed** before applying VNs



- Motivations of Adaptive VNs for MPNNs

- Individual nodes may require a **varying number of connections**
- A node-VN connection should **account for the other nodes connecting to that VN**
- Additional VNs may **need to be introduced at specific layers**

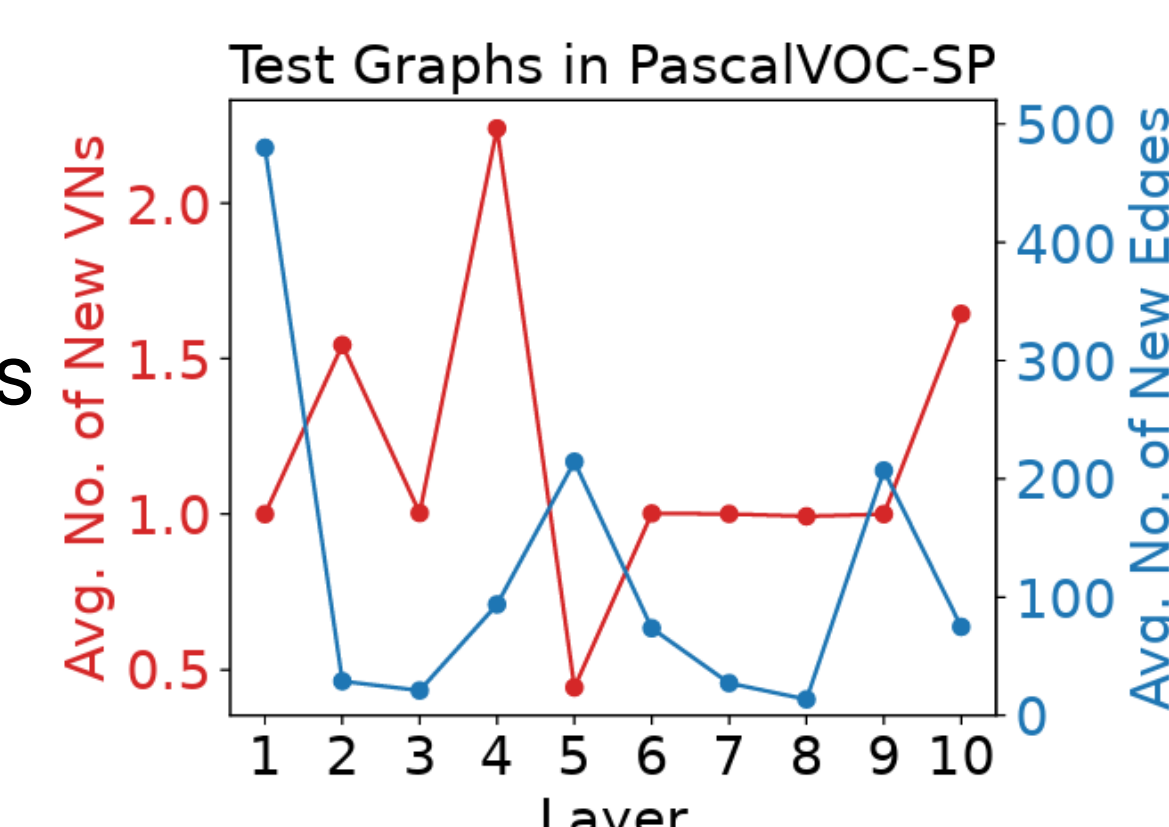


MAVN: Dynamic Message Passing with Adaptive VNs

- Computes the relevance score for each node-VN pair
 - $s_{vz}^{(l)} = \text{MLP}^{(l)}(\mathbf{x}_v^{(l-1)}) \cdot k_z^{(l)} / \sqrt{d_{\text{dot}}}, z \in \mathcal{Z}^{(l-1)}, v \in \mathcal{V}^{(l-1)}$
- Relevance scores are adjusted based on their **relative importance across all candidates**
 - Logsoftmax values over the candidate set is used for adjustment

Analyses of MAVN

- Theoretical Analysis: Flexibility of Message Passing Path Generation
 - For any graph structure augmented by connecting VNs to nodes, there exists a **single-layer MAVN** that constructs the same structure
 - MAVN can simulate graph structures of **existing VN-based methods**
- Qualitative Analysis
 - The number of new VNs and their connectivity patterns vary across layers
 - MAVN **adaptively introduces VNs** and **flexibly forms connections**



Experimental Results

- Consistently improves the performance of backbone MPNNs

		GCN	GINE	GatedGCN
Peptides-func	Backbone	68.60	66.21	67.65
	MAVN+Backbone	72.38 (+5.5%)	68.97 (+4.1%)	70.70 (+4.5%)
PascalVOC-SP	Backbone	20.78	27.18	38.80
	MAVN+Backbone	30.44 (+46.5%)	35.94 (+32.2%)	48.28 (+24.4%)
		GCN	GAT	GraphSAGE
roman-empire	Backbone	90.81	90.39	89.81
	MAVN+Backbone	91.64 (+0.9%)	92.30 (+2.1%)	91.03 (+1.4%)
tolokers	Backbone	86.30	85.66	84.82
	MAVN+Backbone	86.64 (+0.4%)	86.73 (+1.2%)	85.59 (+0.9%)

Conclusion

- Propose MAVN, a novel framework **that learns to determine when and where to introduce and connect VNs**
- MAVN **makes no assumptions about the backbone** and **relies solely on node representations** to dynamically update message passing paths
- Theoretically, for **any node-VN connectivity pattern**, there exists a set of parameters of MAVN that can simulate the pattern
- Experimental results show that **MAVN consistently improves the backbone MPNN's performance**