

Advance Graph Neural Net

Graph Attention Neural Net

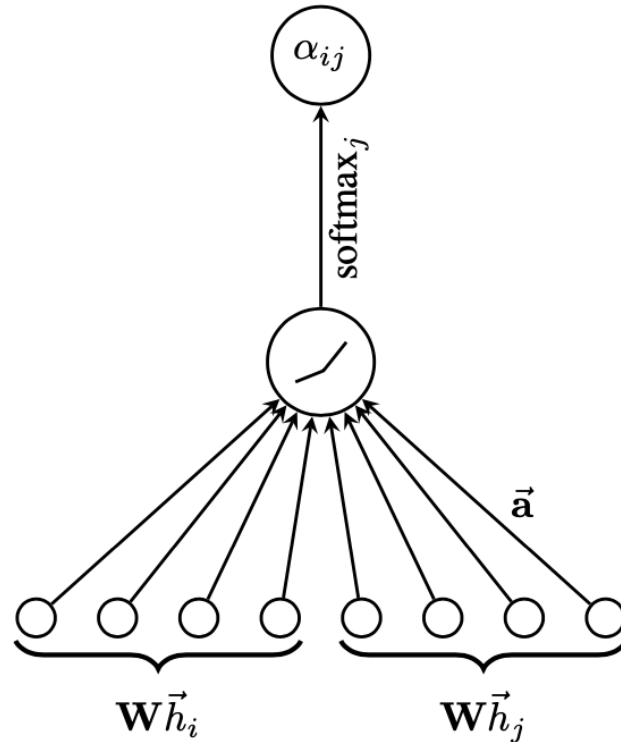
Graph Attention Neural Net

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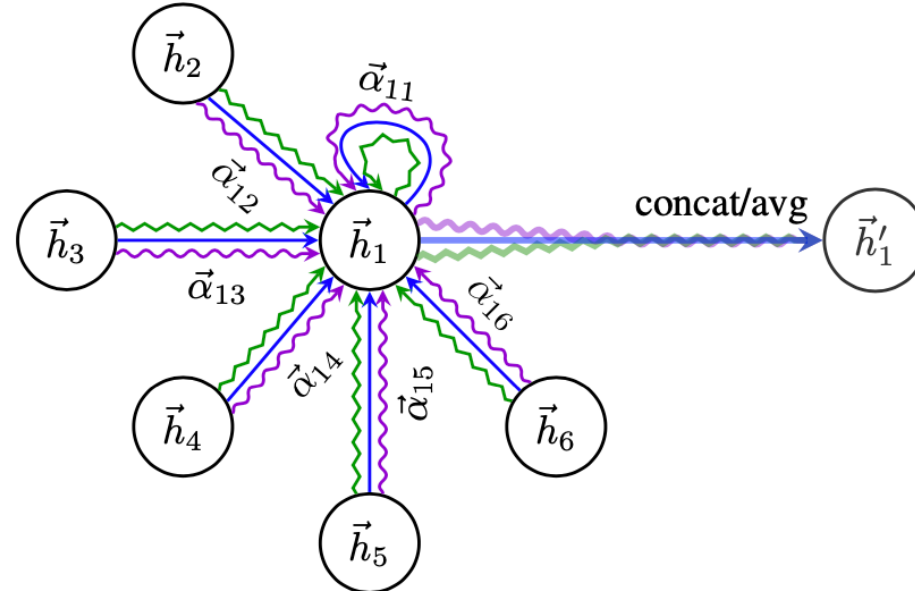
그래프 어텐션 신경망 (Graph Attention Network GAT)

Graph + Attention

임베딩된 정점들의 집계 과정을 Attention 방식으로 수행



Self-Attention

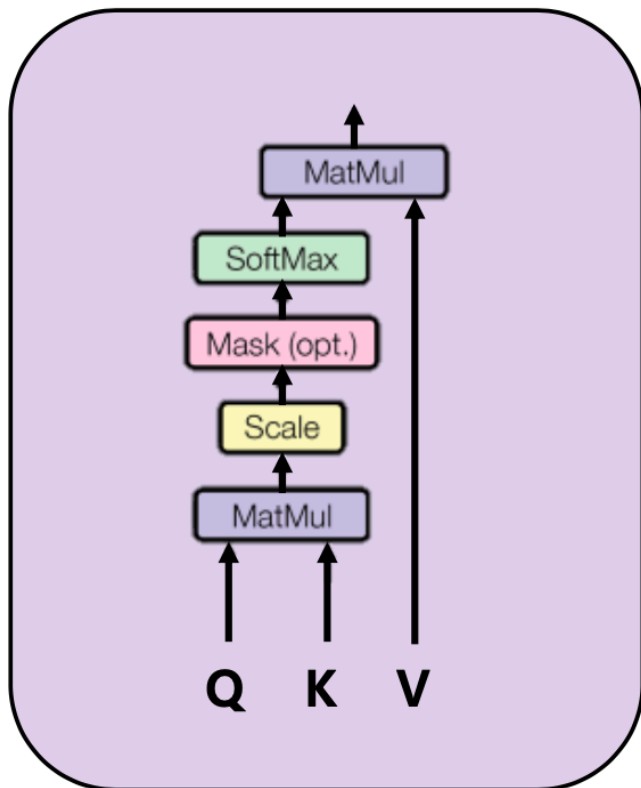


Multi-head Attention

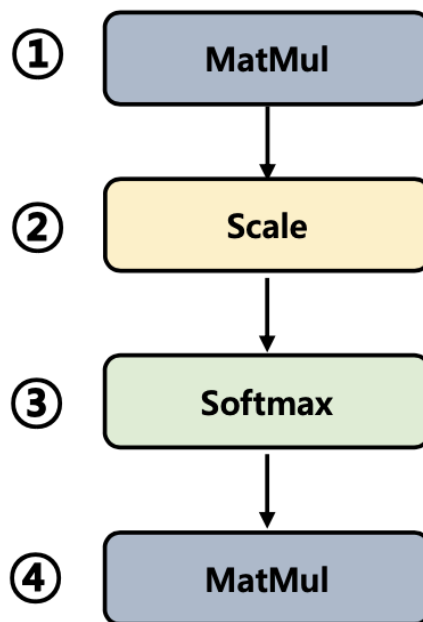
Self-Attention

Graph Attention Neural Net

Self-Attention (Transformer)



Generalized Attention Form



$$A(q, K, V) = \sum_i softmax(f(K, q)) V$$

$$f(K, Q) = QK^T \quad (K = KW^K, Q = QW^Q, V = VW^V)$$

$$\frac{QK^T}{\sqrt{d_k}}$$

$$softmax(\frac{QK^T}{\sqrt{d_k}})$$

$$softmax(\frac{QK^T}{\sqrt{d_k}}) V$$

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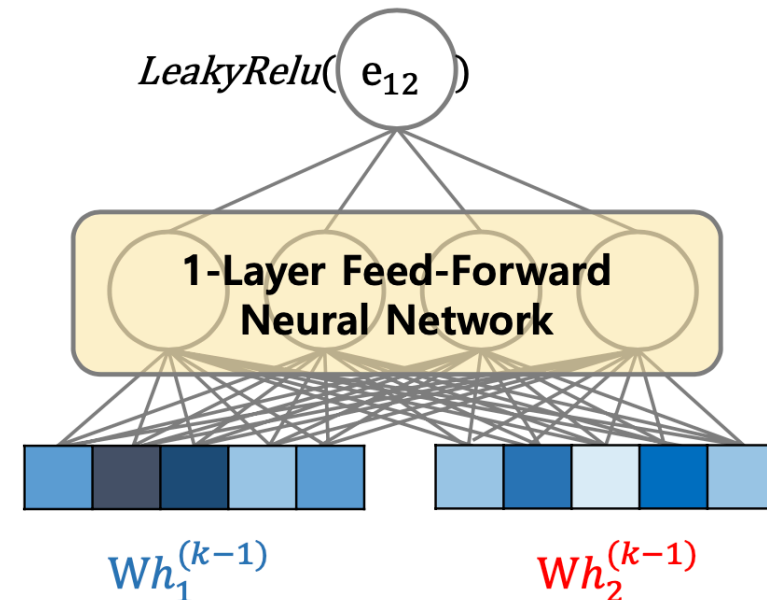
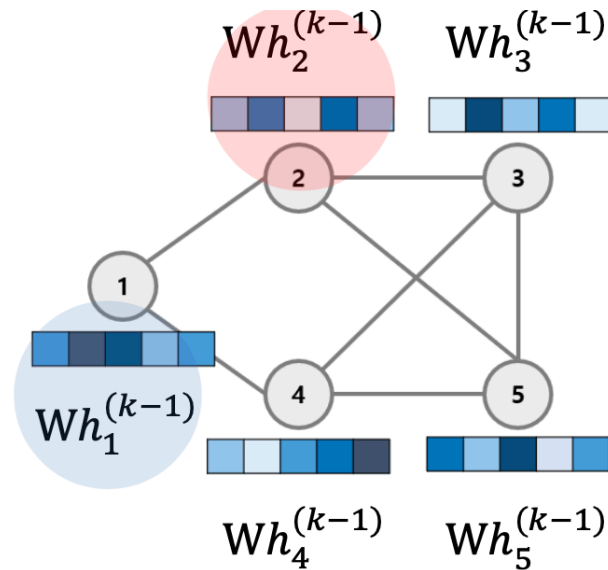
Self-Attention (GAT)

$$A(q, K, V) = \sum_i \text{softmax}(f(K, q))V$$

$$a_v^{k-1} = \text{Attention}(\{h_u^{k-1}, u \in N(v) \cup \{v\}\})$$

$$\text{Key} = \text{Query} = \text{Value} = h_u^{k-1}$$

similarity Function(f) = 1 layer feedword neural net



$$e_{ij} = f(\text{CONCAT}(Wh_i^{k-1}, Wh_j^{k-1}))$$

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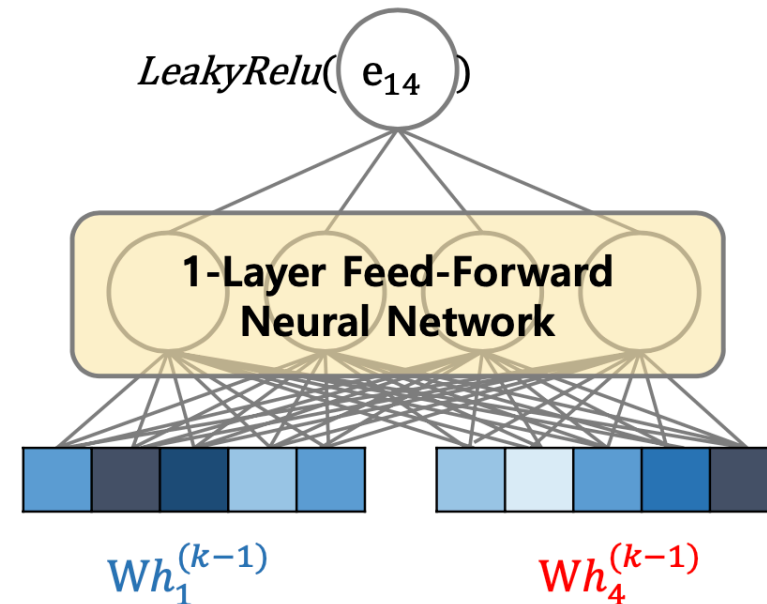
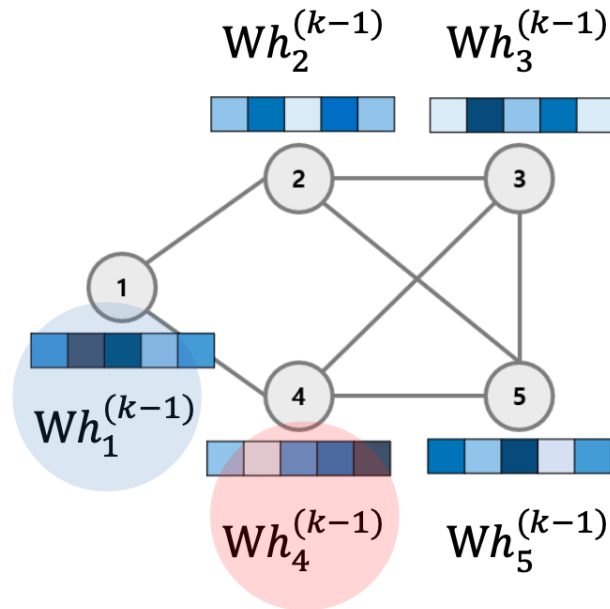
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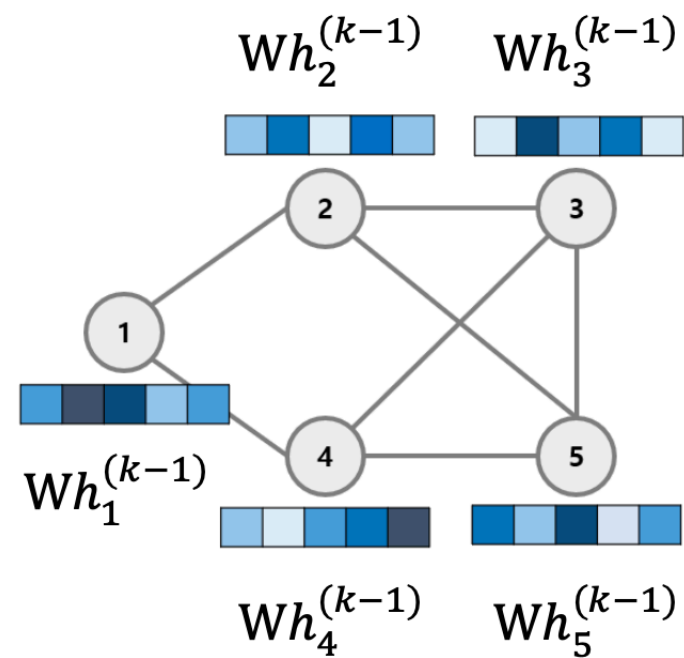
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Self-Attention (GAT)

$$A(q,K,V) = \sum_i softmax(\boxed{f(K,q)})V$$

1layer feedforward 를 통해서 Attention score 를 구하고
Adjacency matrix 의 정보를 반영하여 Masked Self-Attention을 수행



e_{11}	e_{12}		e_{14}	
e_{21}	e_{22}	e_{23}		e_{25}
	e_{32}	e_{33}	e_{34}	e_{35}
e_{41}		e_{43}	e_{44}	e_{45}
	e_{25}	e_{53}	e_{54}	e_{55}

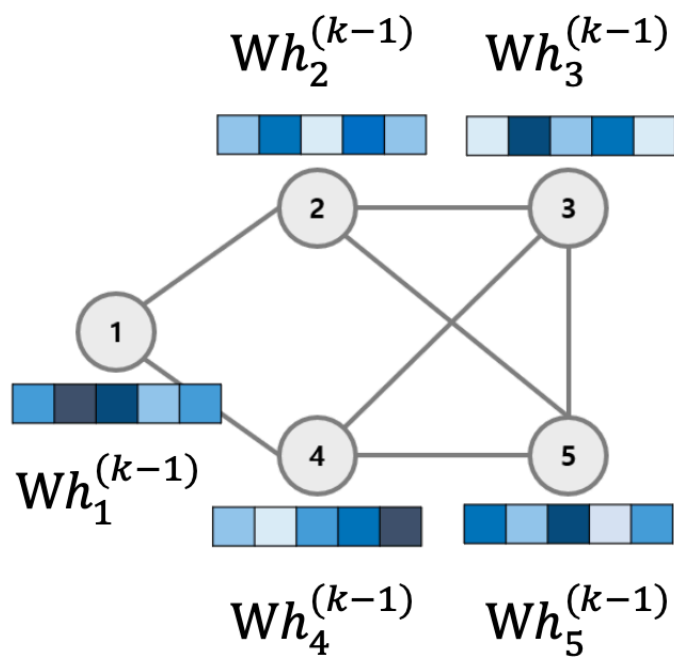
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Score 에 softmax 부여



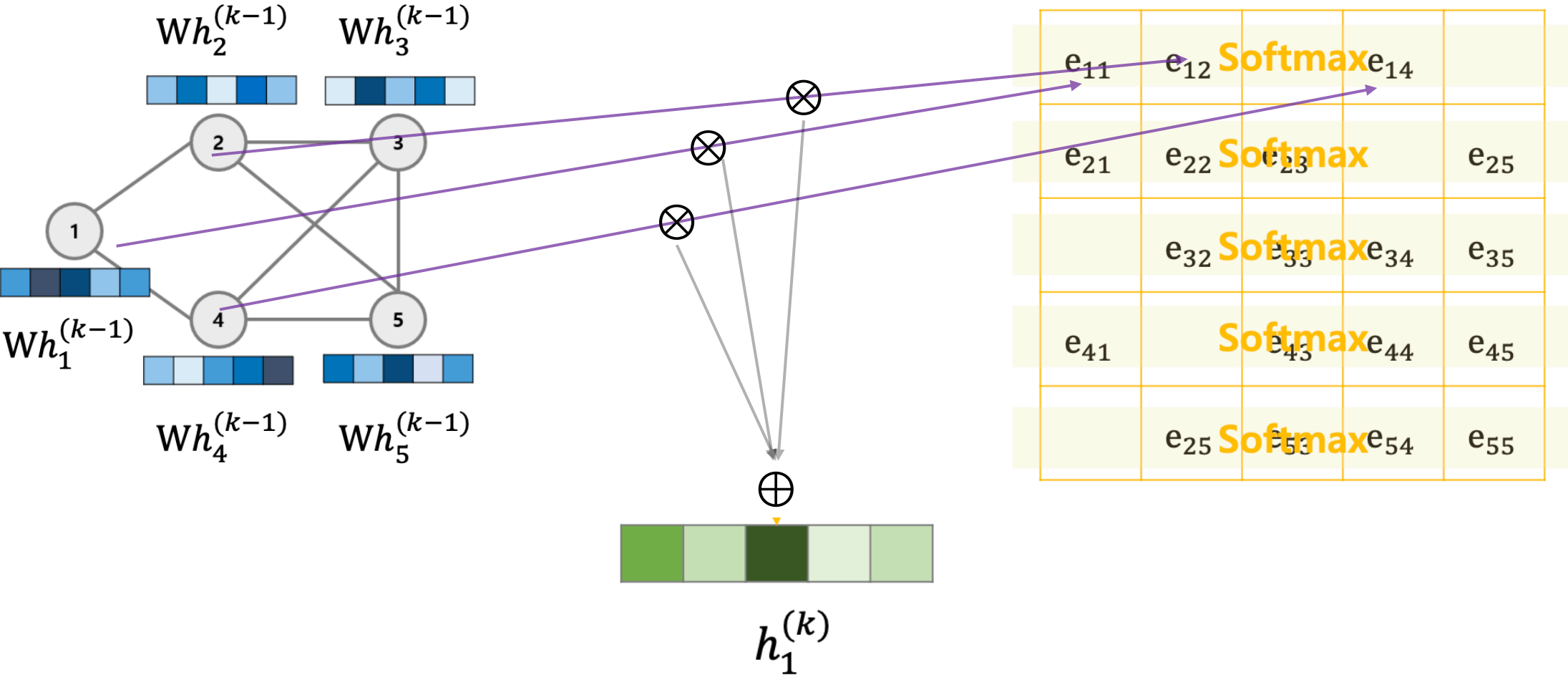
e ₁₁	e ₁₂	Softmax	e ₁₄	
e ₂₁	e ₂₂	Softmax	e ₂₃	e ₂₅
	e ₃₂	Softmax	e ₃₃	e ₃₄
e ₄₁		Softmax	e ₄₃	e ₄₄
	e ₅₂	Softmax	e ₅₃	e ₅₄
				e ₅₅

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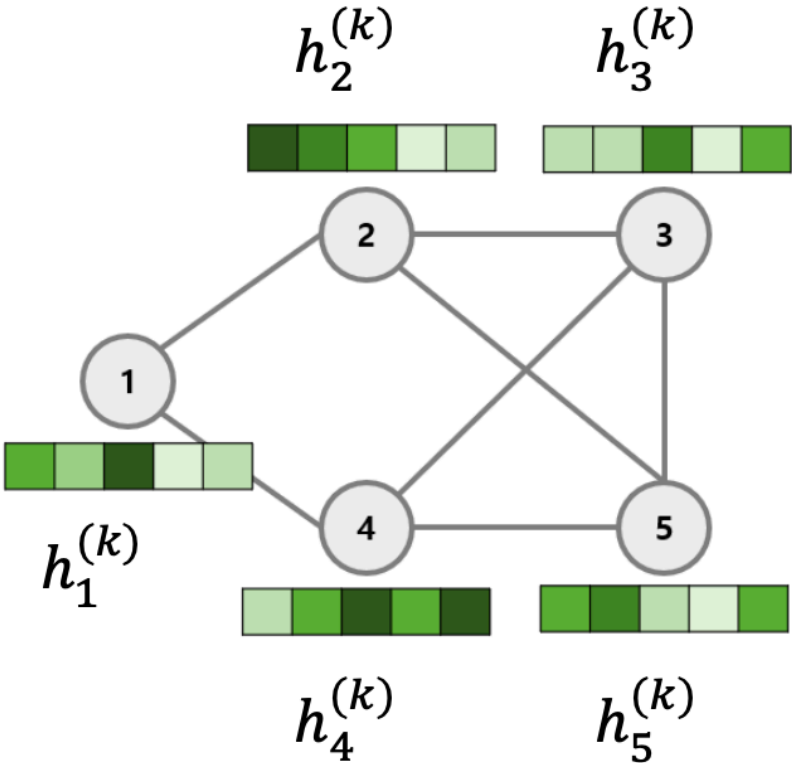
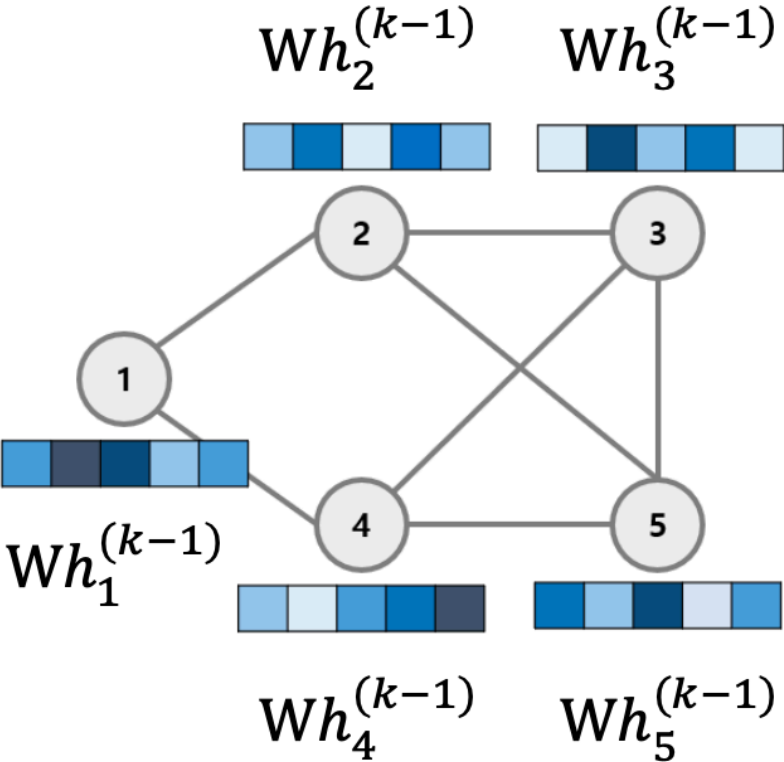


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Self-Attention (GAT)

$$A(q,K,V) = \sum_i softmax(f(K,q))V$$



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Multi-head Attention (GAT)

$$A(q, K, V) = \sum_i \text{softmax}(f(K, q))V$$

