Advance Graph Neural Net

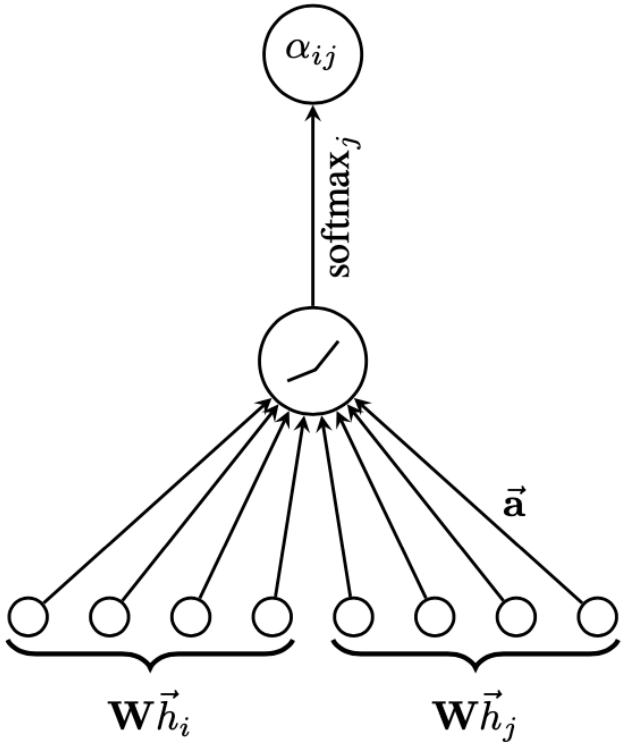
Graph Attention Neural Net

Graph Attention Neural Net

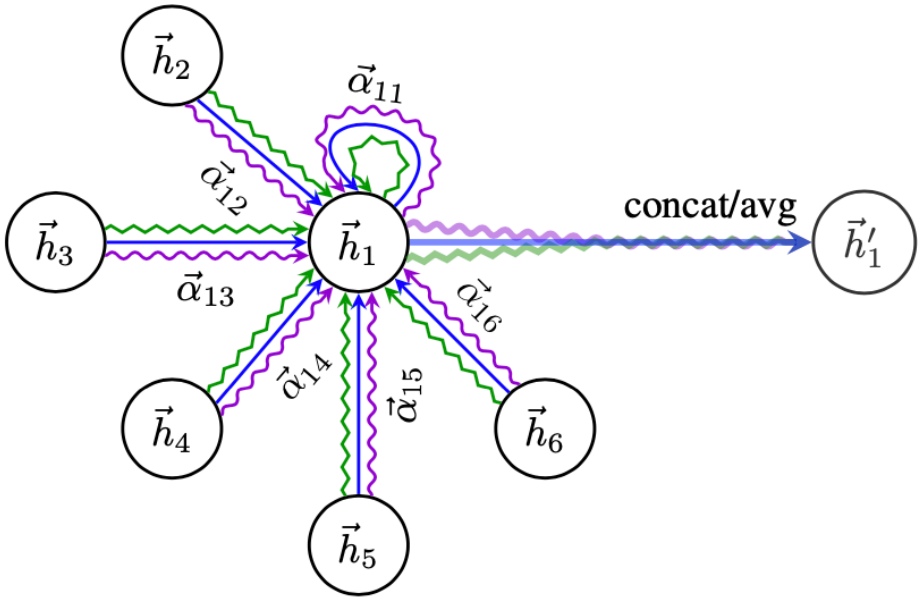
그래프 어텐션 신경망 (Graph Attention Network GAT)

Graph + Attention

임베딩된 정점들의 집계 과정을 Attention 방식으로 수행



Self-Attention

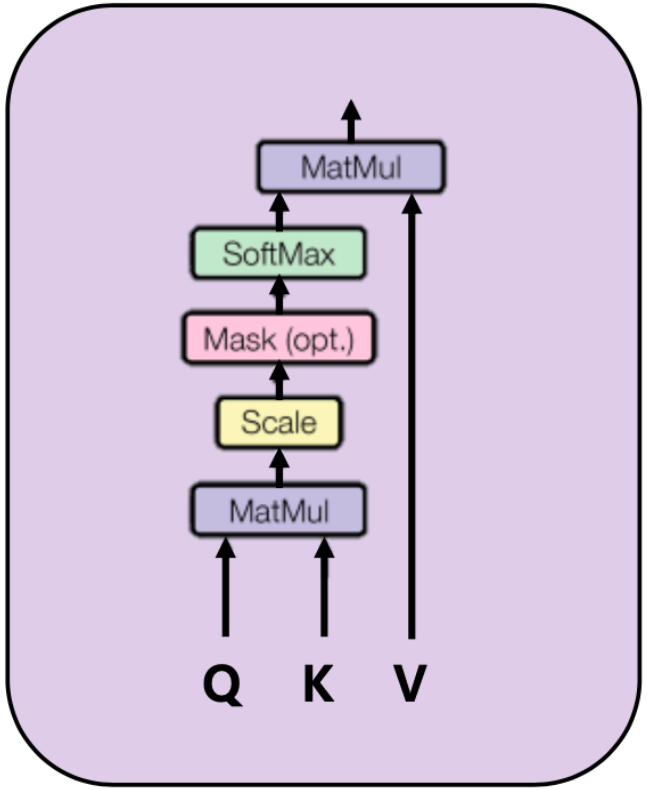


Multi-head Attention

Self-Attention

Graph Attention Neural Net

Self-Attention (Transformer)



Generalized Attention Form

$$A(q, K, V) = \sum_{i} softmax(f(K, q))\, V$$

① MatMul

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

② Scale

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

③ Softmax

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

④ MatMul

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

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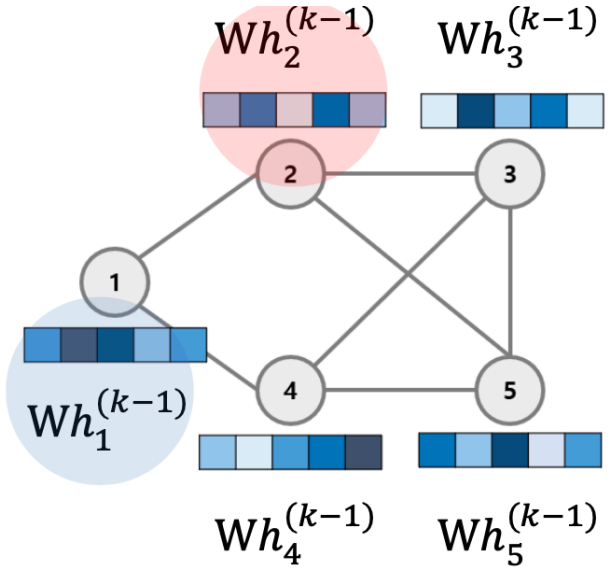
Self-Attention (GAT)

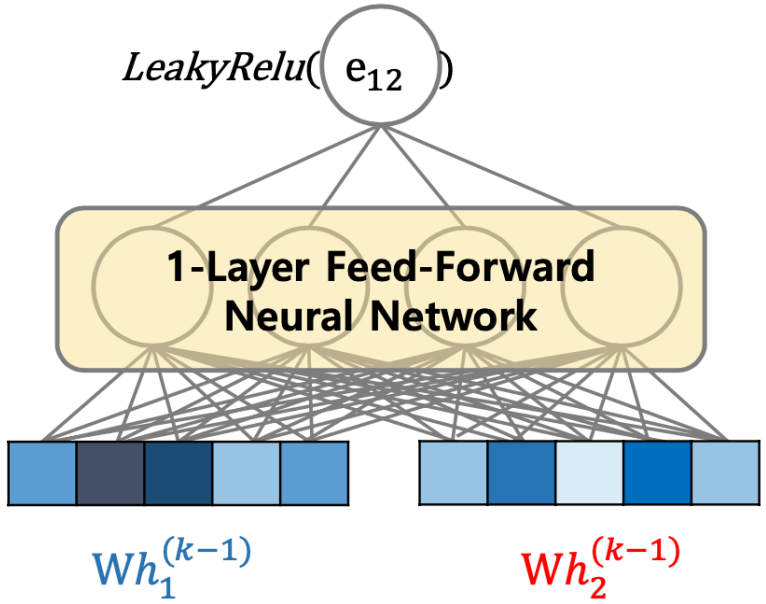
$$A(q, K, V) = \sum_i softmax\big(f(K, q)\big)V$$

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

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

$similarity\ Function(f) = 1\ layer\ feedword\ neural\ net$





$$e_{ij} = f\Big(CONCAT\big(Wh_i^{k-1}, Wh_2^{k-1}\big)\Big)$$

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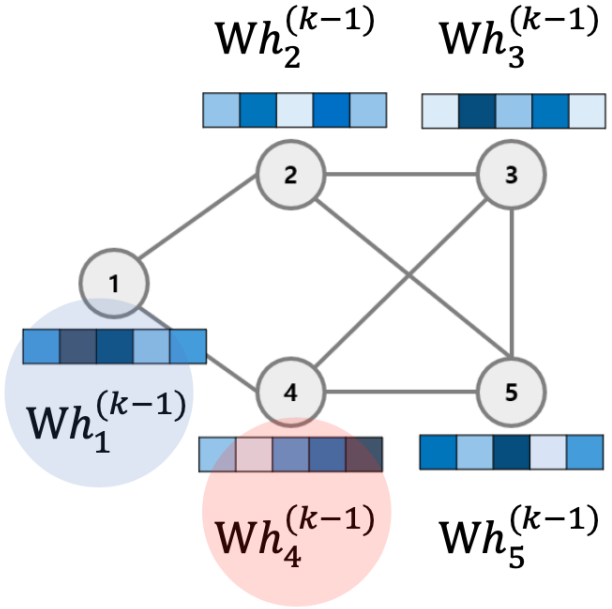

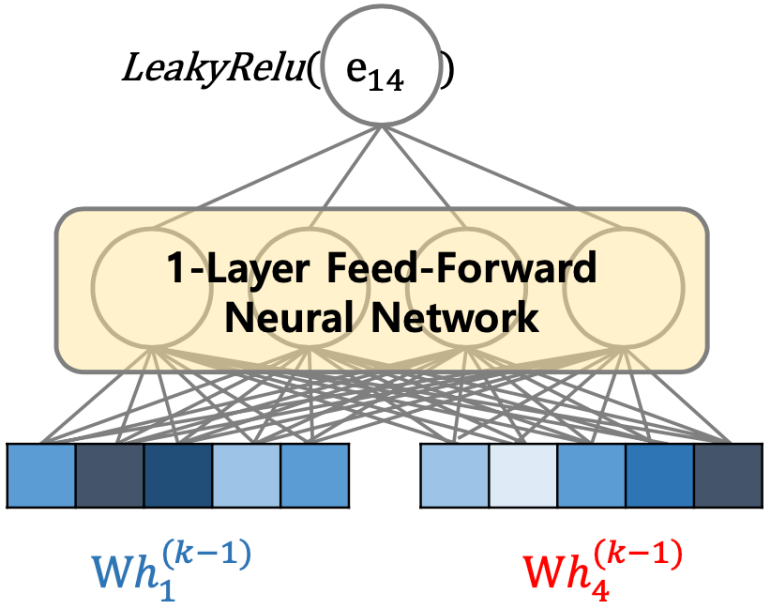

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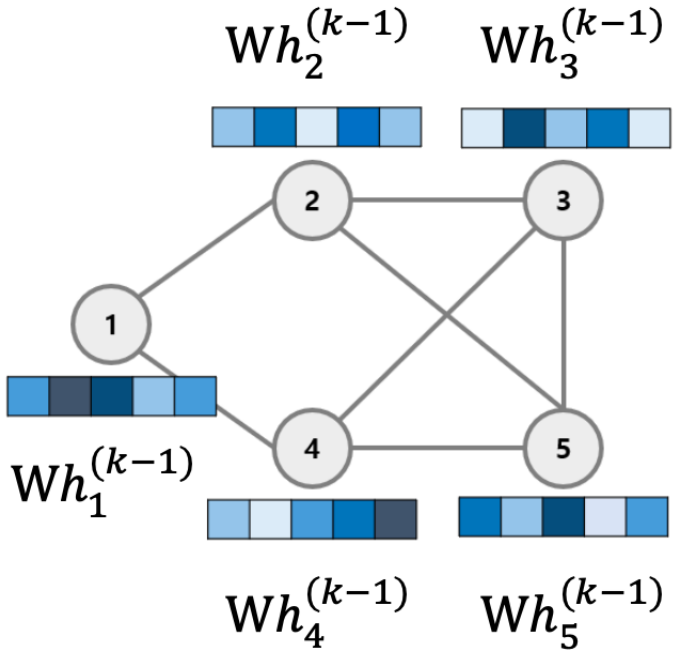
$$A(q, K, V) = \sum_i softmax(f(K, q))V$$

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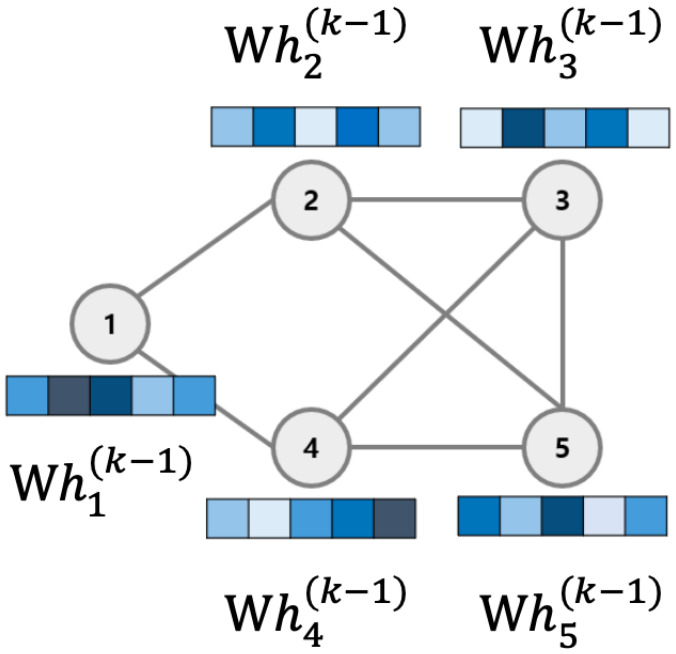
$$A(q, K, V) = \sum_i softmax\big(f(K, q)\big)V$$

Score 에 softmax 부여



e_{11}	e_{12} Softmax		e_{14}	
e_{21}	e_{22} Softmax			e_{25}
	e_{32} Softmax		e_{34}	e_{35}
e_{41}	Softmax		e_{44}	e_{45}
	e_{25} Softmax		e_{54}	e_{55}

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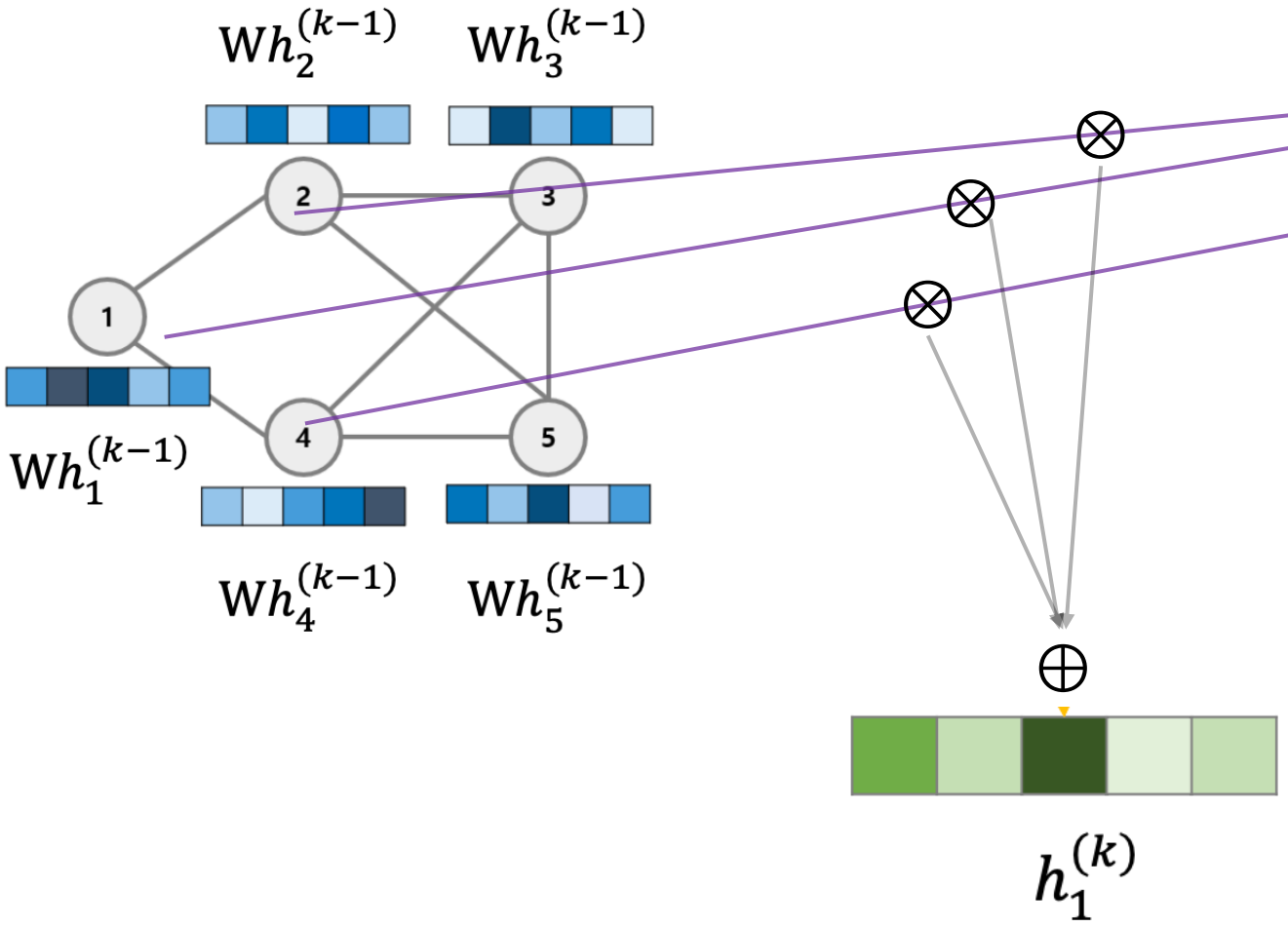

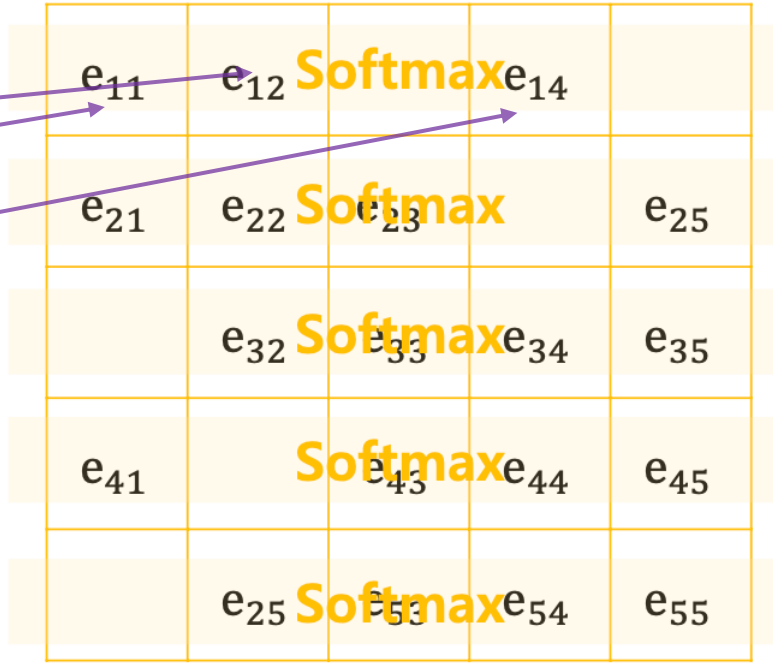

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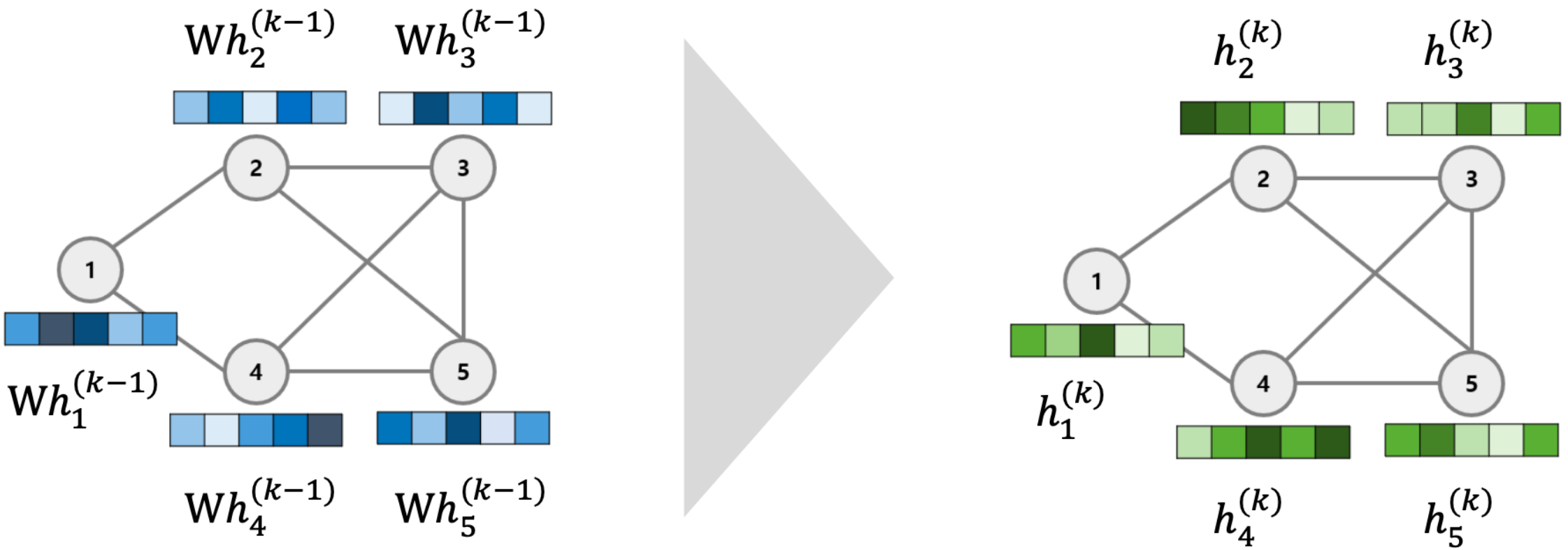
$$A(q, K, V) = \sum_i softmax\big(f(K, q)\big)V$$



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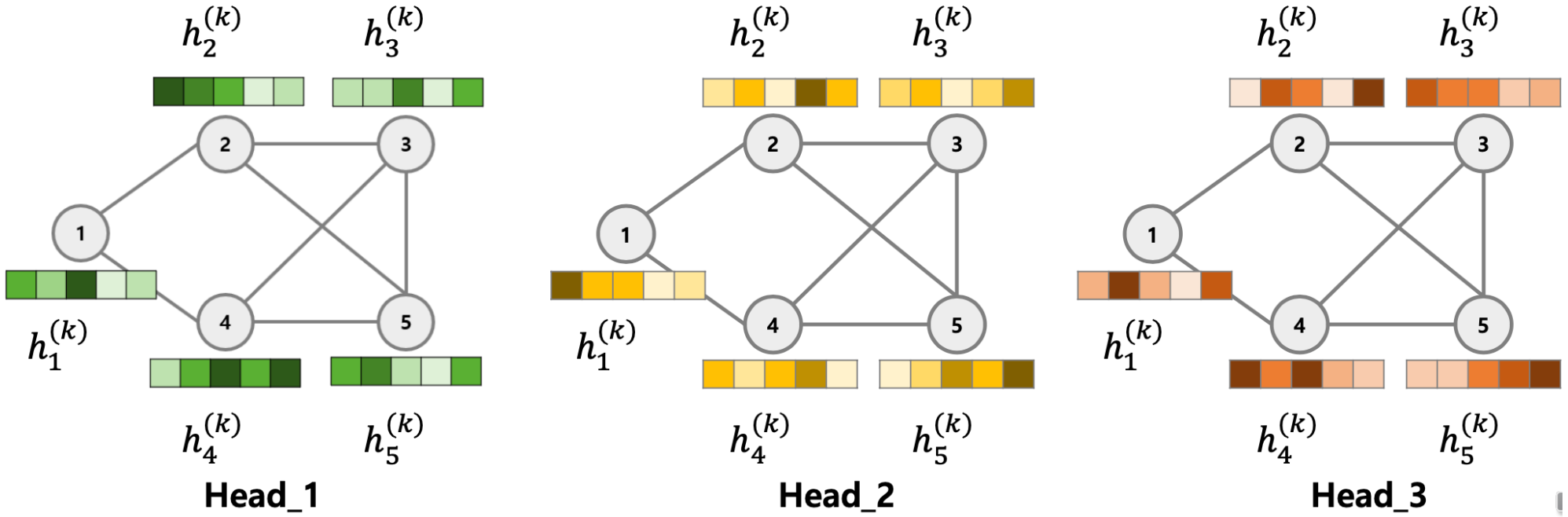
Multi-head Attention (GAT)

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



출처

Graph Attention Neural Net

DMQA

https://www.youtube.com/watch?v=NSjpECvEf0Y

Graph Attention Networks – Petar Velicˇkovicć … ICLR 2018

https://arxiv.org/abs/1710.10903