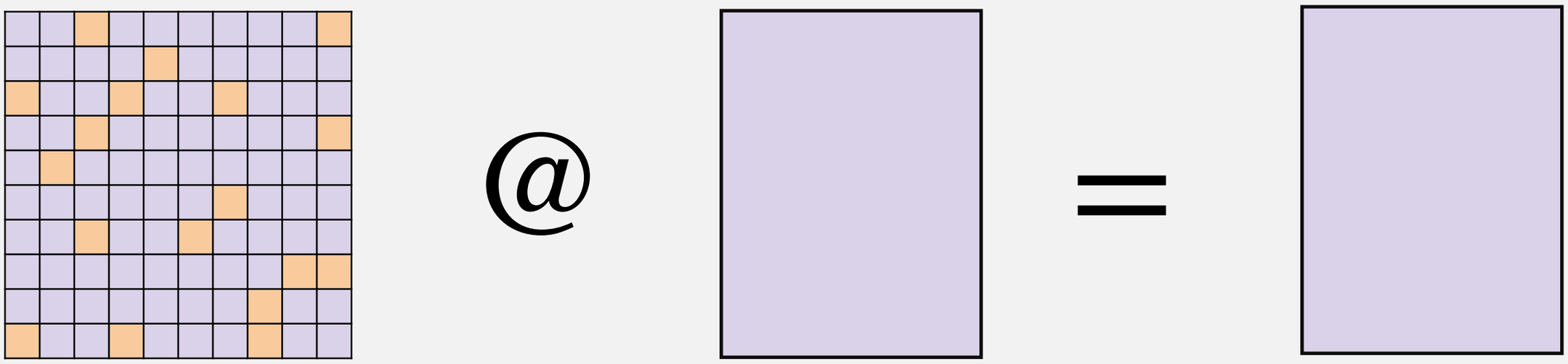
Graph Attention

A Walkthrough



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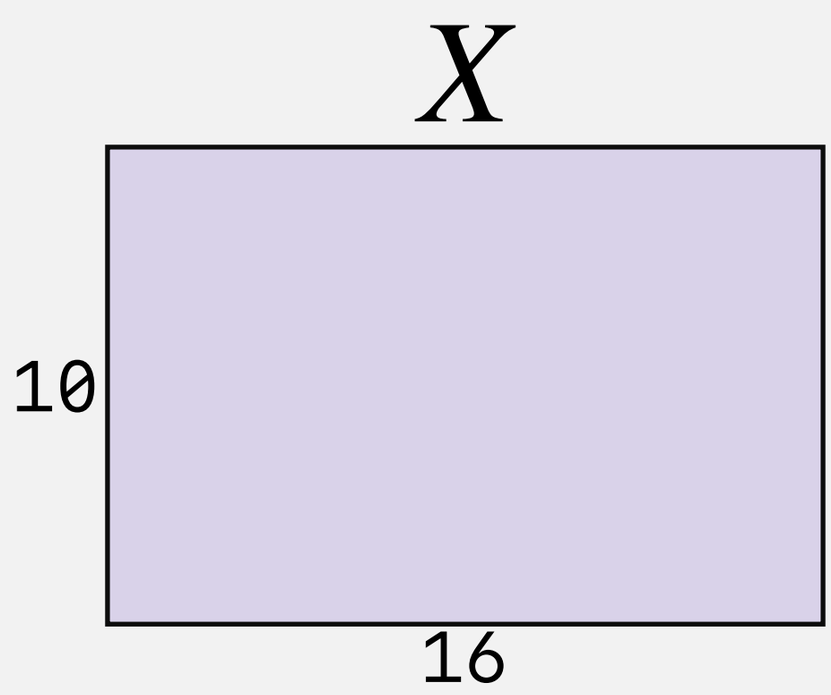
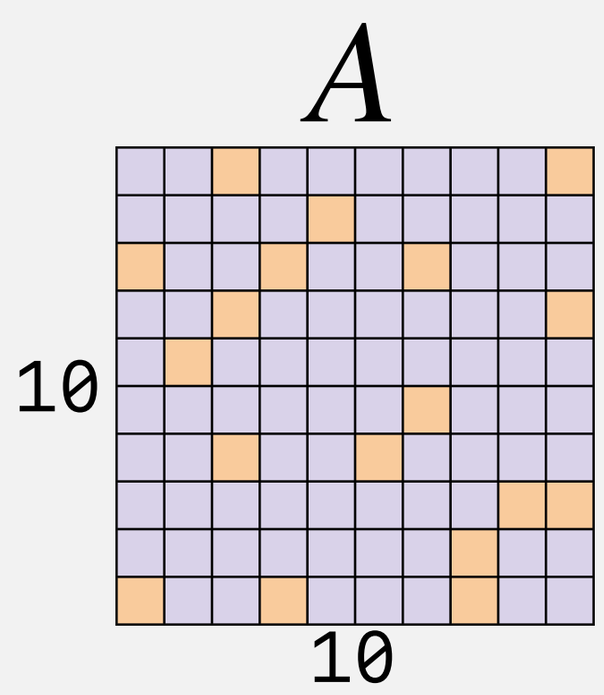
Inputs

```
# hyperparameters
n_nodes          = 10
in_features      = 16
hidden_features = 8
n_classes        = 7
n_heads          = 4
```





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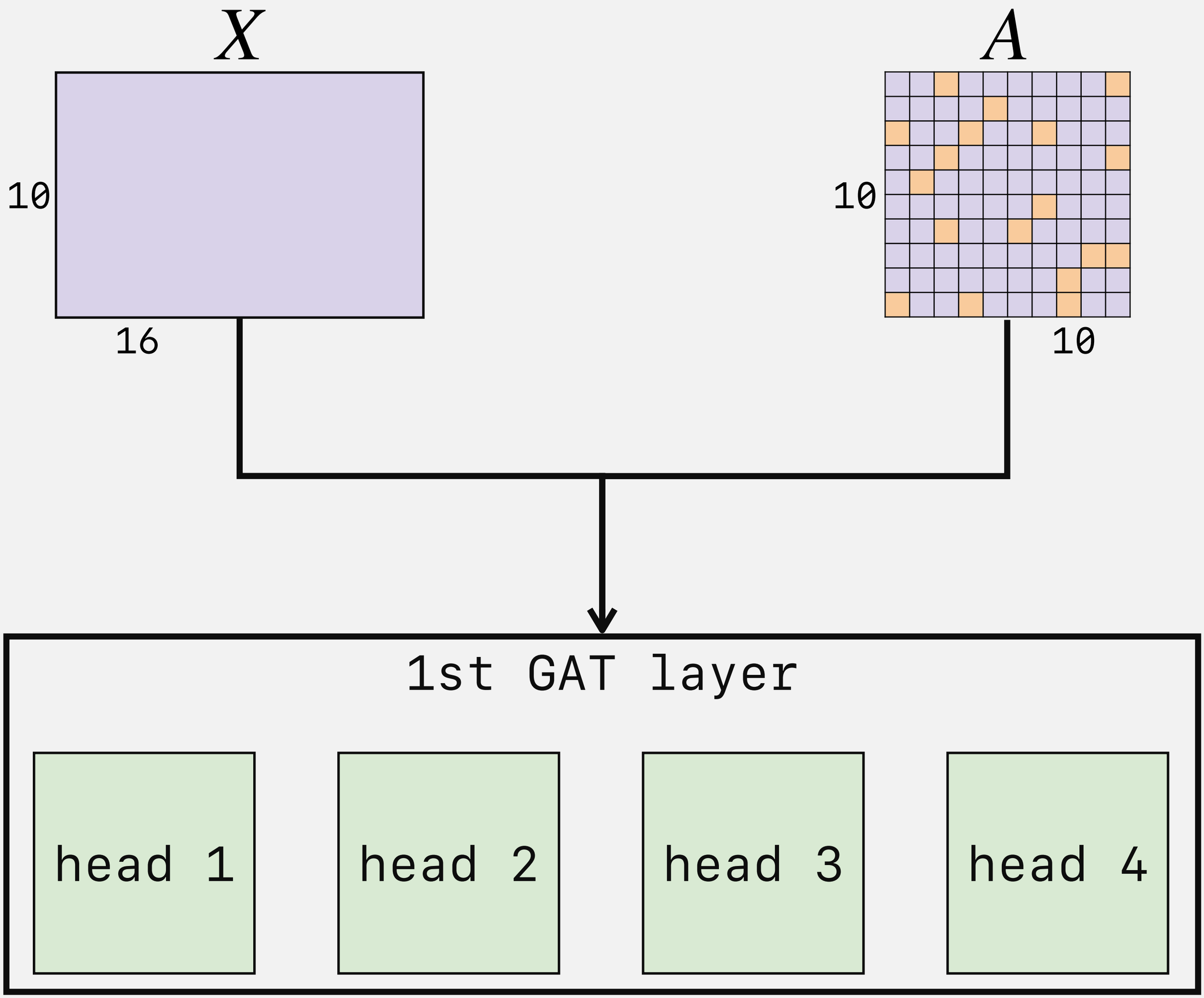
1st GAT layer, input



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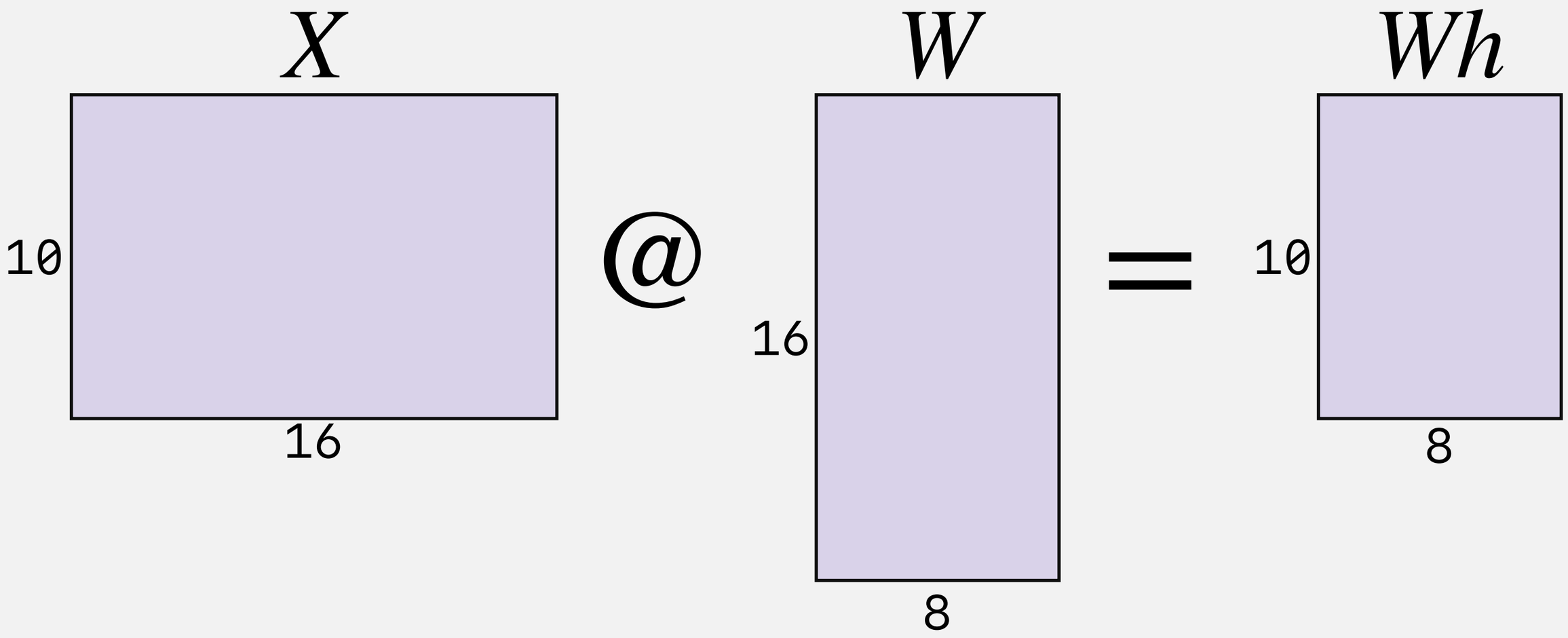
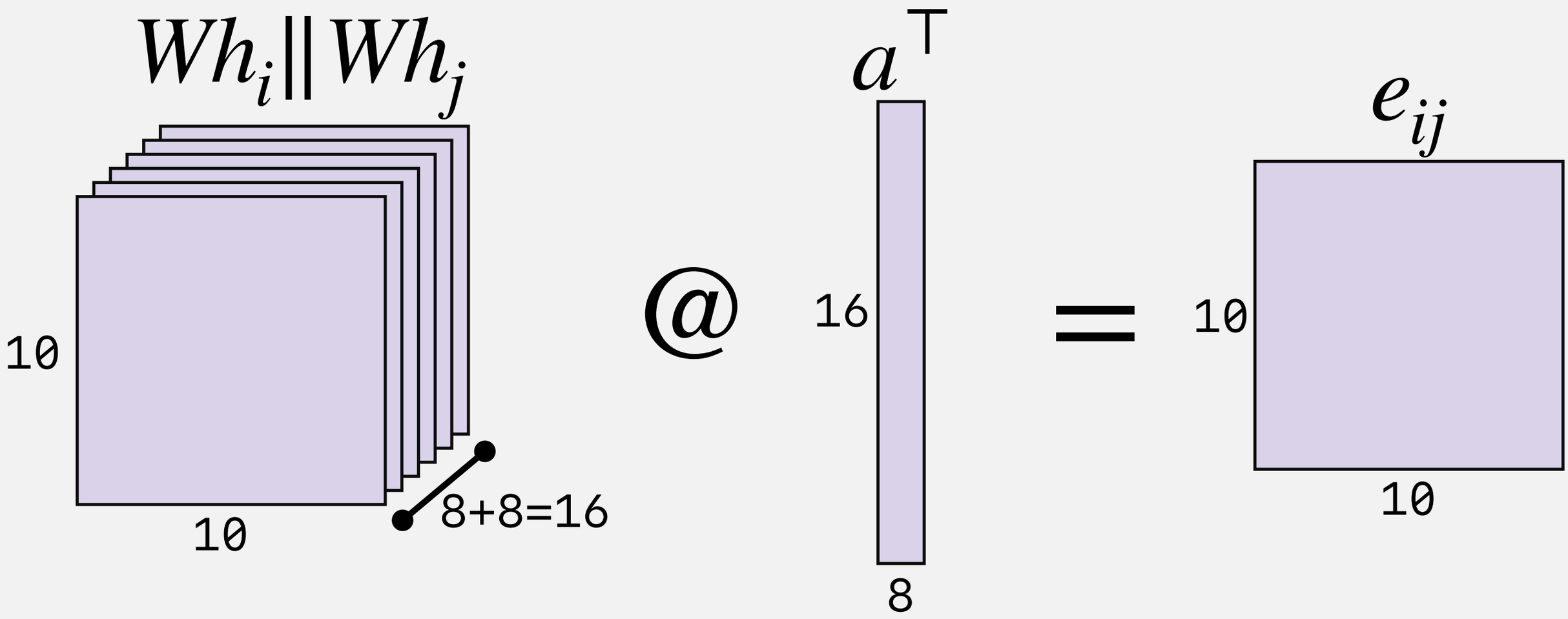
1st GAT layer, head 1



After applying the weight matrix W, the resulting node representations are denoted as Wh. For any two nodes i and j, the concatenation $Wh_i || Wh_j$ combines their feature vectors along the feature dimension.



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1st GAT layer, head 1

$$\texttt{LeakyReLU}\left(\begin{array}{c} e_{ij} \\ \texttt{10} \\ \\ \texttt{10} \end{array}\right)$$

```
# masked attention
torch.where(adj > 0, e, zero_vec)
```

Masked attention must be applied before the `softmax` function. Reversing this order leads to `softmax` being calculated over incorrect values.

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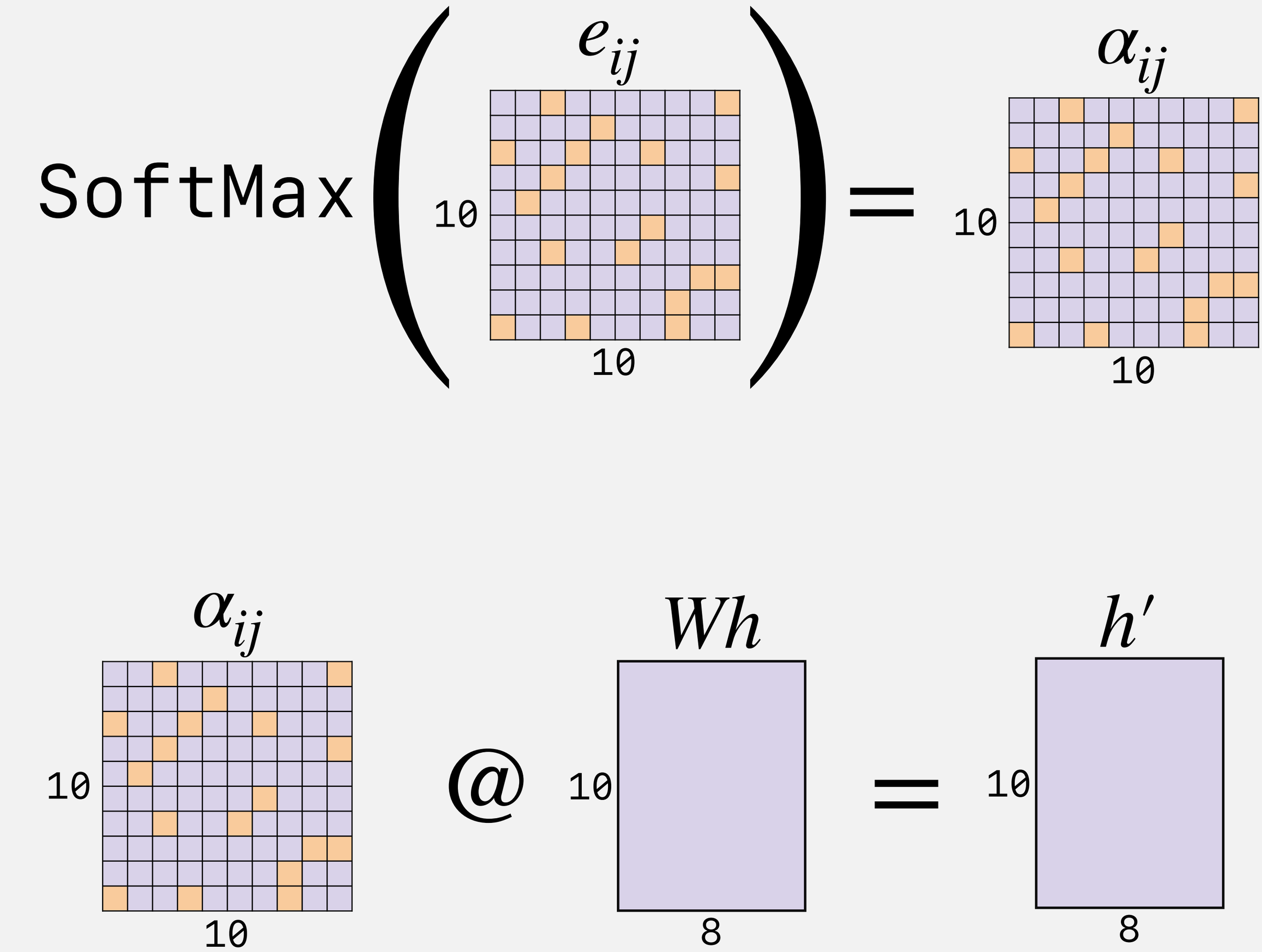
1st GAT layer, head 1



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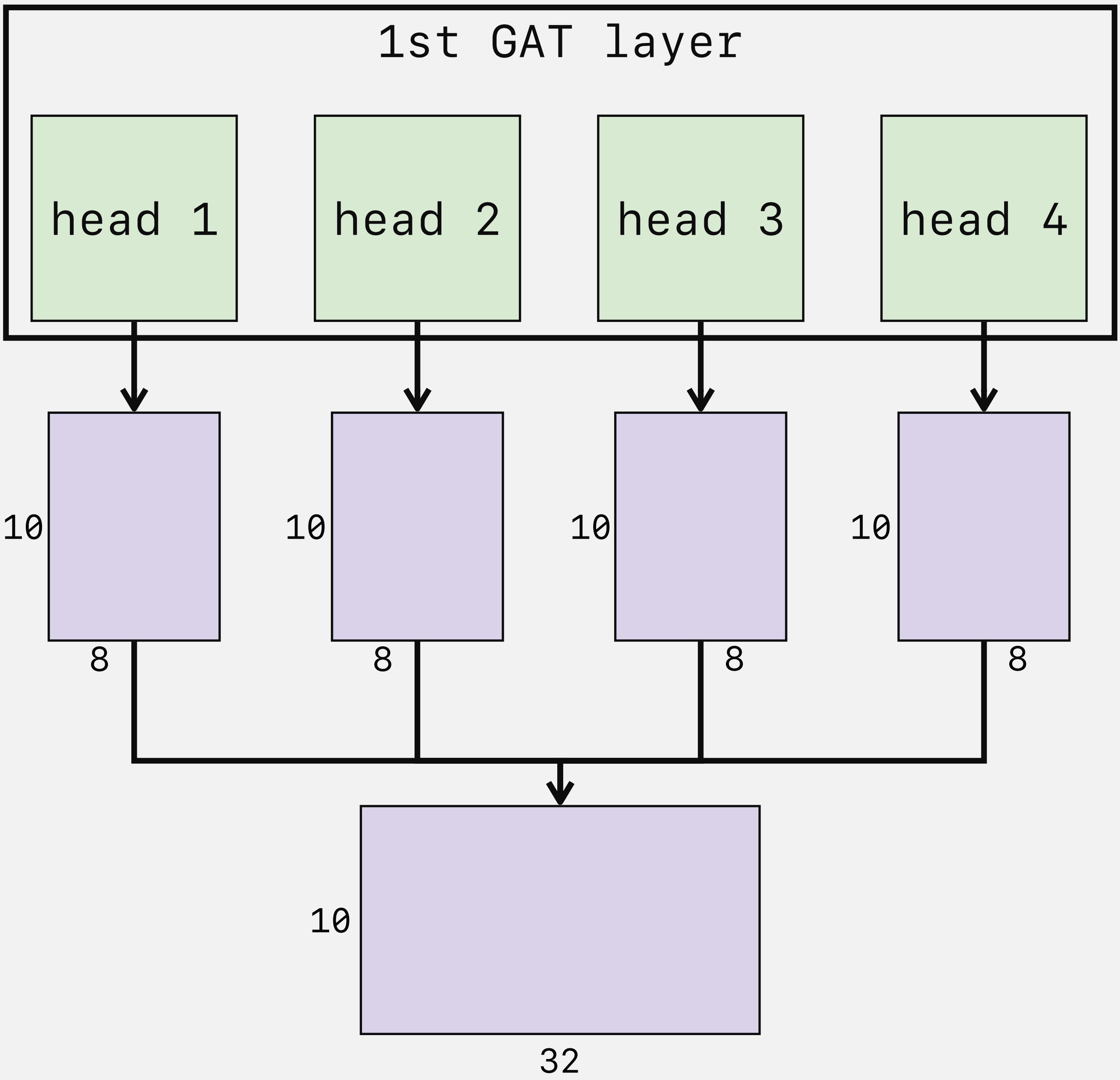
1st GAT layer, output



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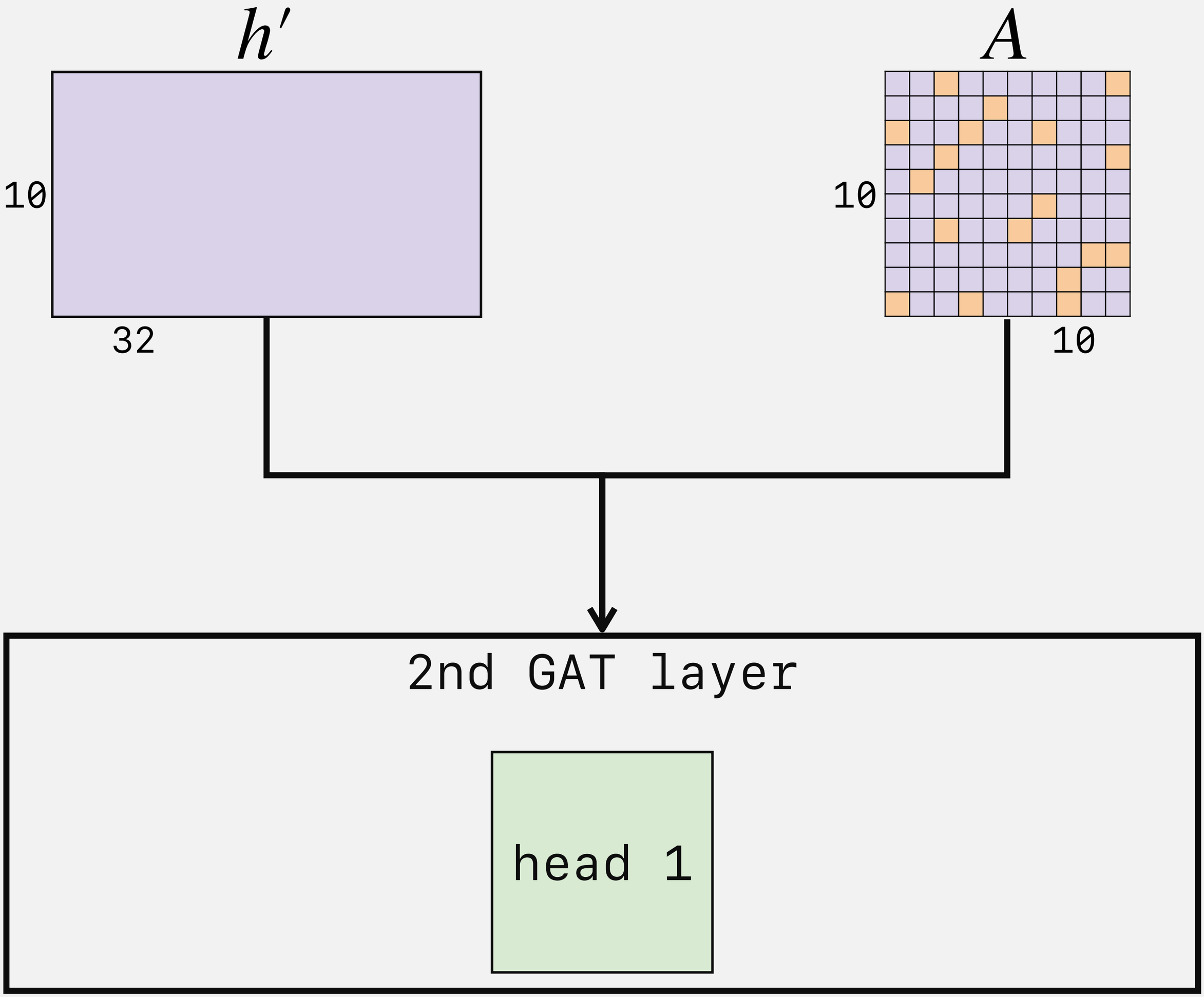
2nd GAT layer, input



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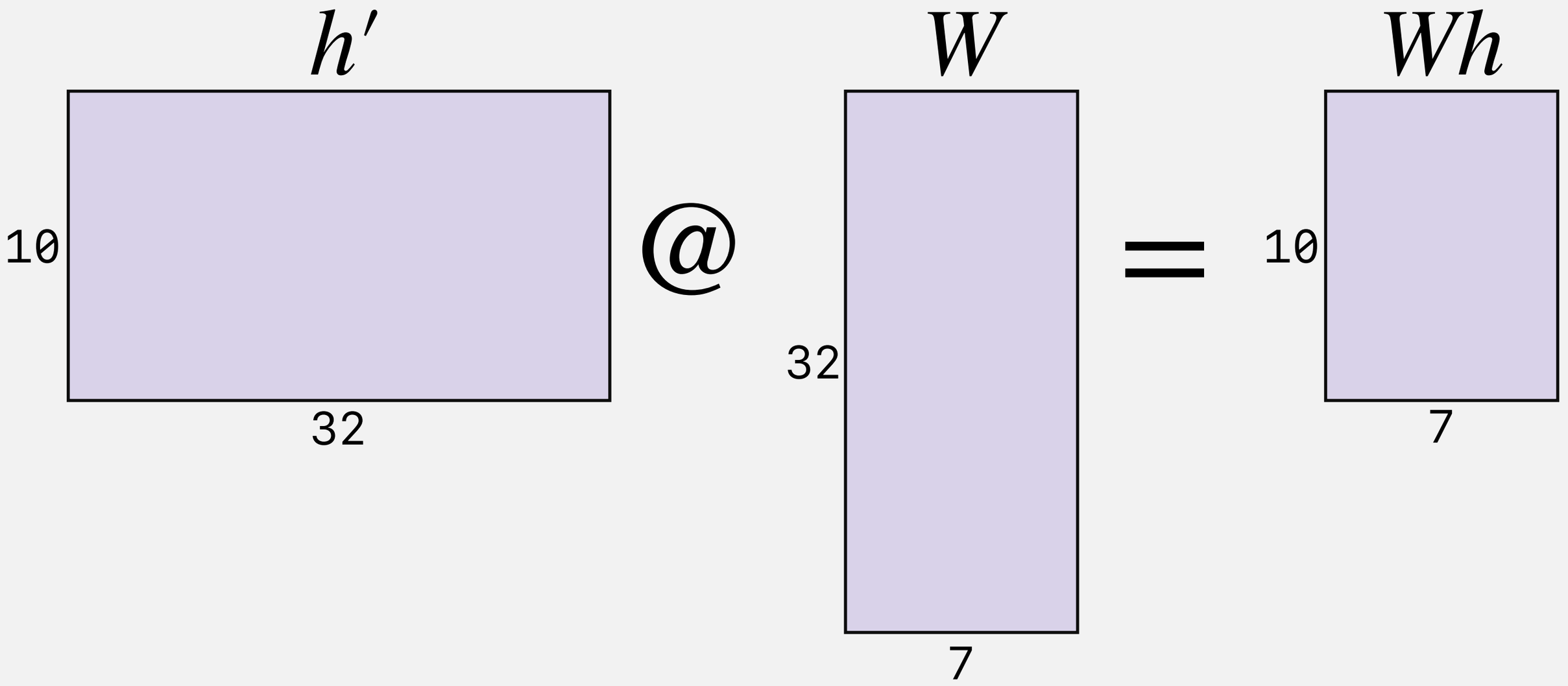
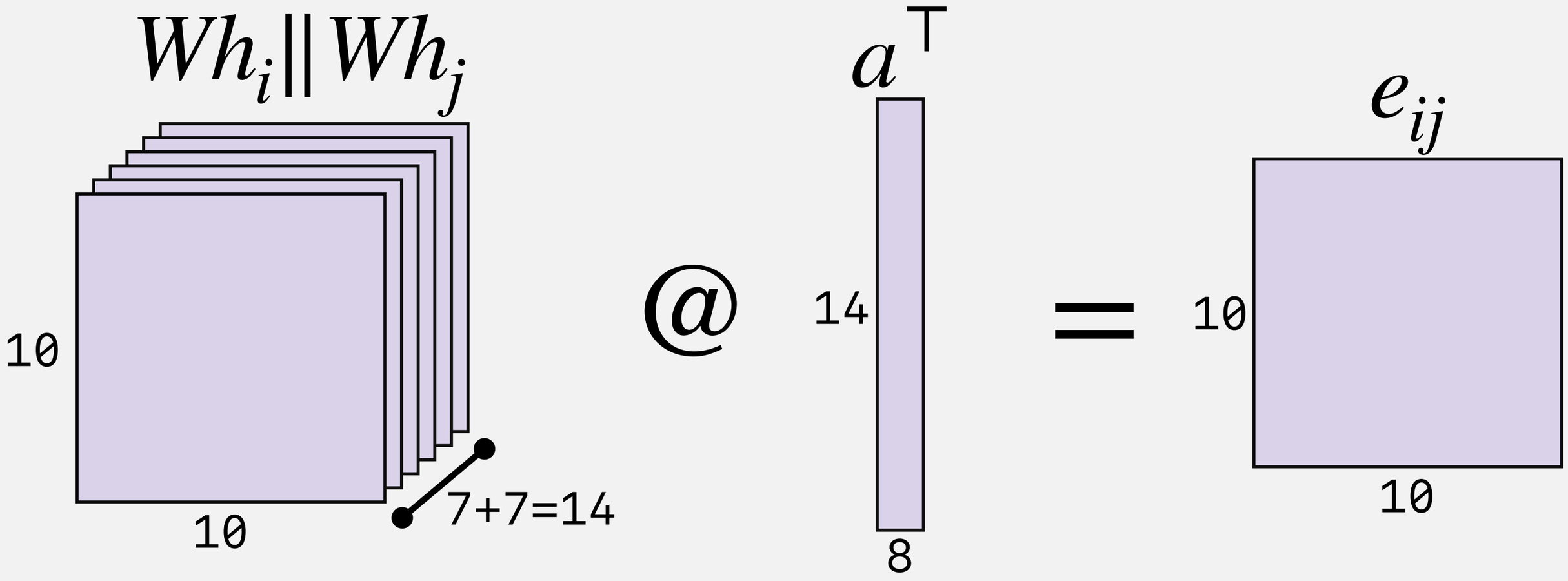
2nd GAT layer, head 1





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2nd GAT layer, head 1

$$\texttt{LeakyReLU}\left(\begin{array}{c} e_{ij} \\ \boxed{\begin{array}{c}10\end{array}} \\ 10 \end{array}\right)$$

```
# masked attention
torch.where(adj > 0, e, zero_vec)
```

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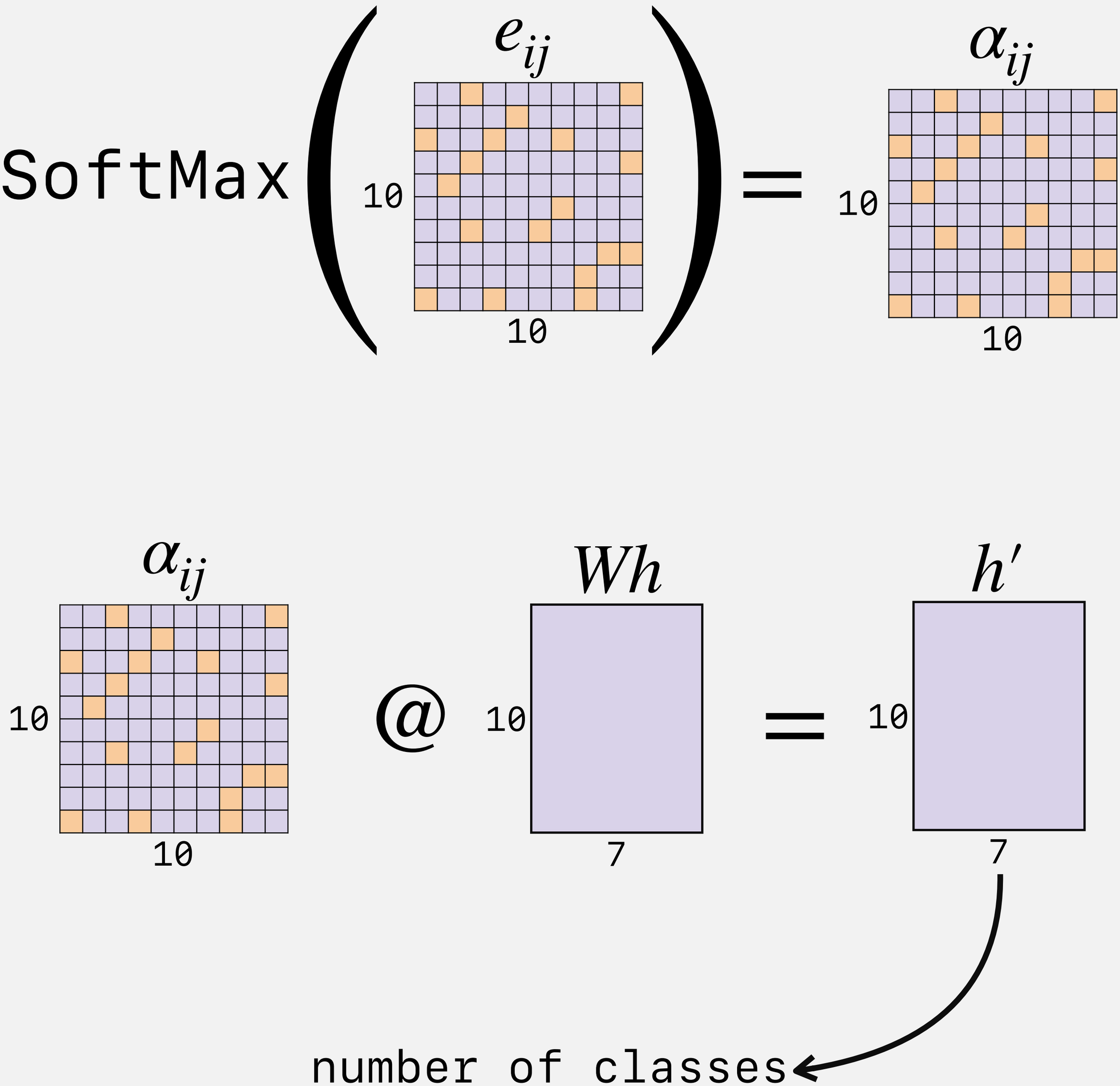
2nd GAT layer, head 1



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