Transformer Model (1/2): Attention without RNN

Shusen Wang

Transformer Model

 Original paper: Vaswani et al. Attention Is All You Need. In NIPS, 2017.

Attention Is All You Need

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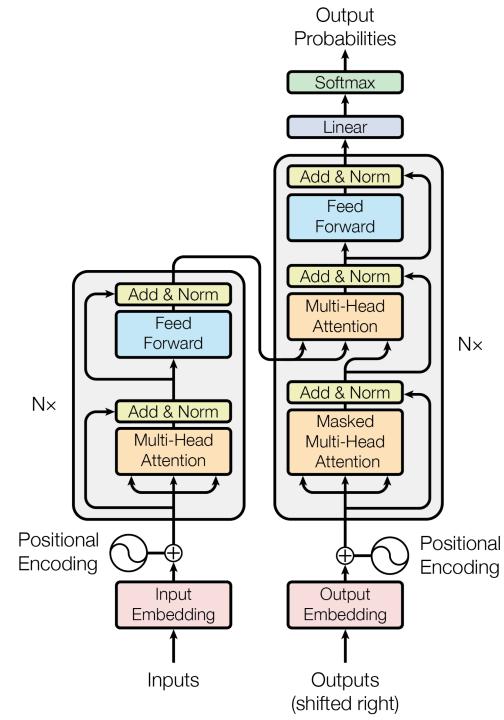
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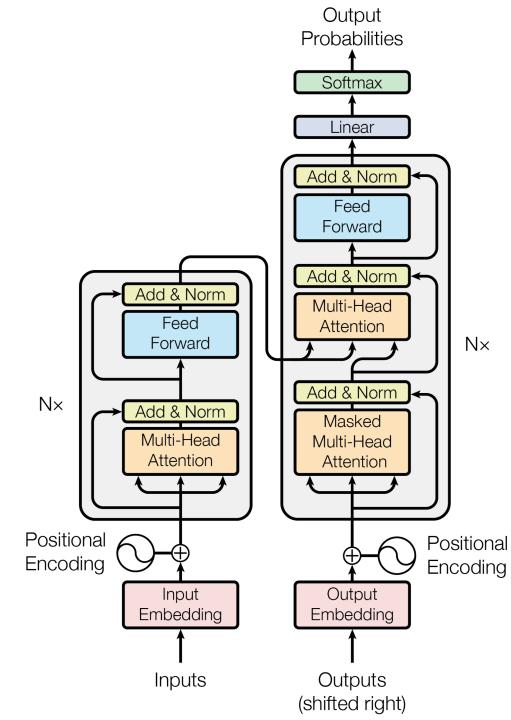
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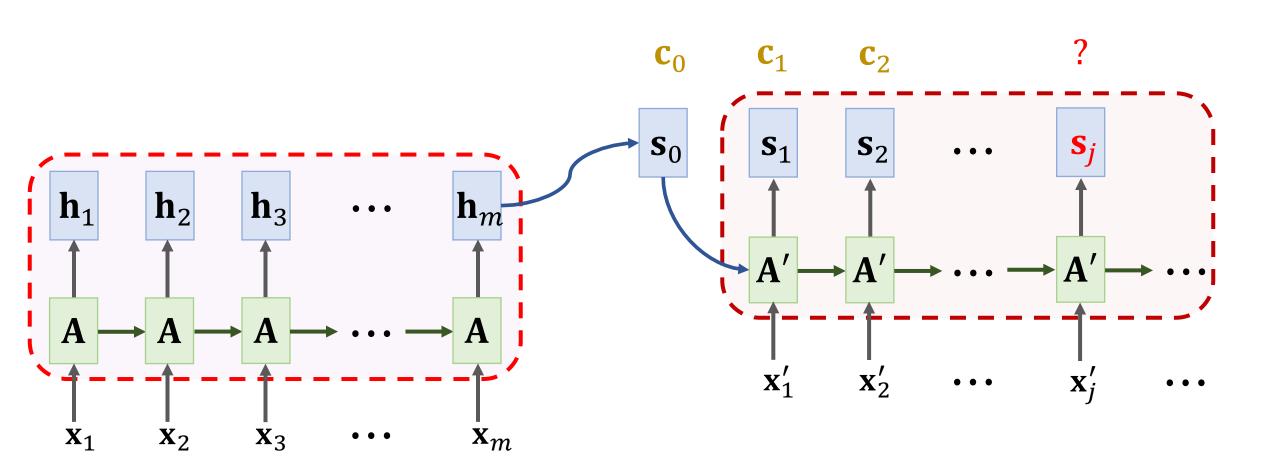
Transformer Model

- Transformer is a Seq2Seq model.
- Transformer is not RNN.
- Purely based attention and dense layers.

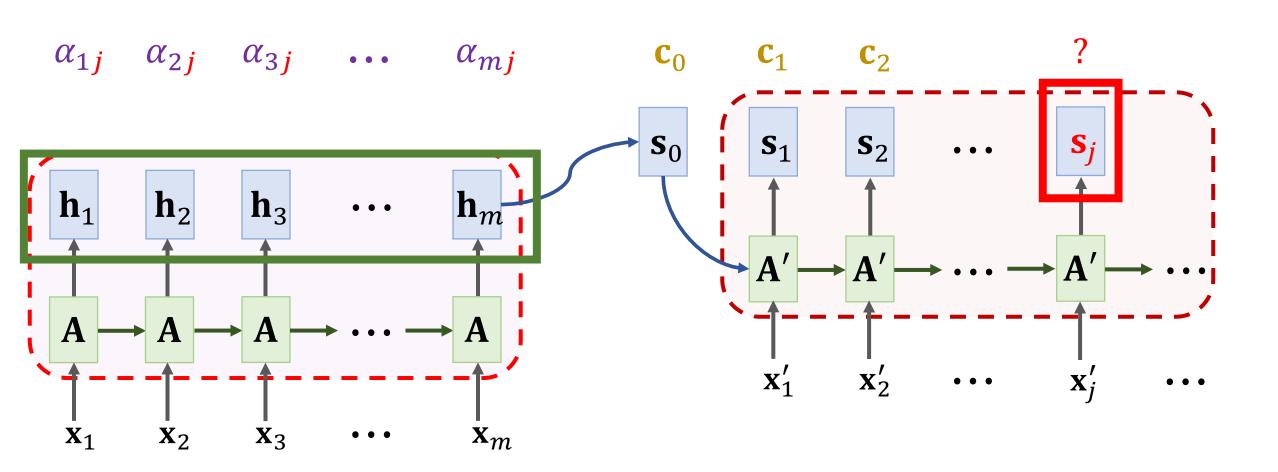
Higher accuracy than RNNs on large datasets.



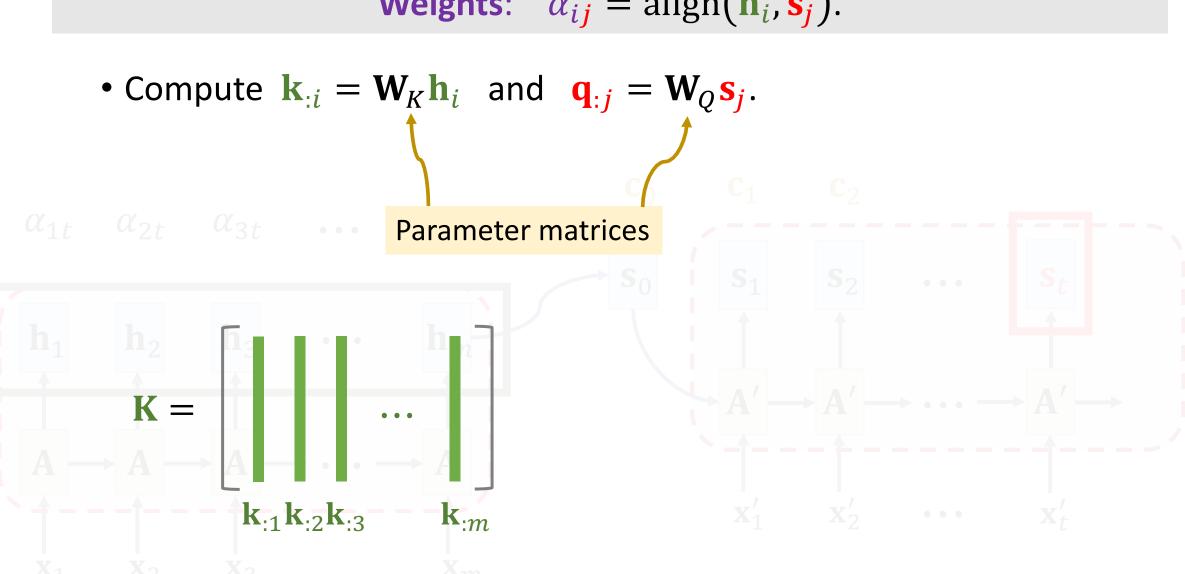
Revisiting Attention for RNN



Weights:
$$\alpha_{ij} = \operatorname{align}(\mathbf{h}_i, \mathbf{s}_j)$$
.

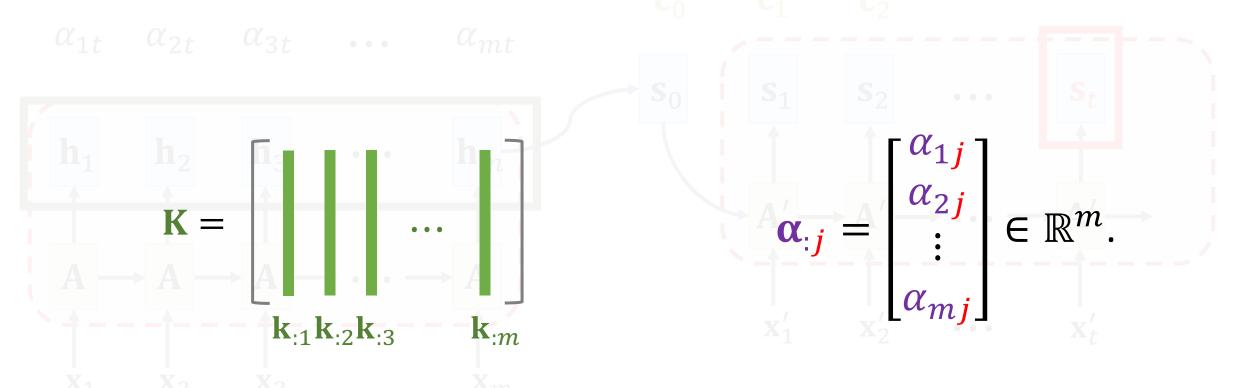


Weights:
$$\alpha_{ij} = \operatorname{align}(\mathbf{h}_i, \mathbf{s}_j)$$
.



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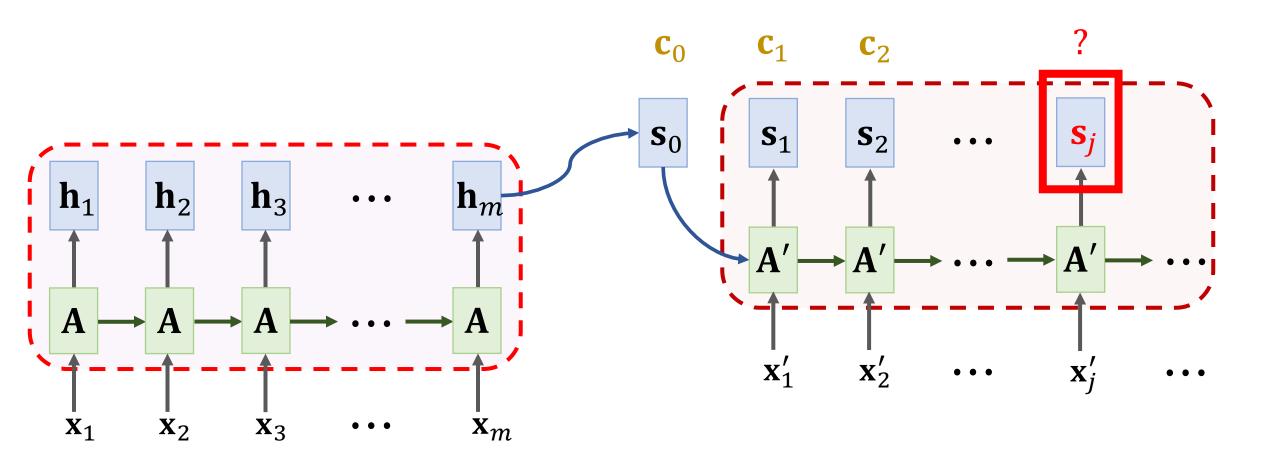
- Compute $\mathbf{k}_{:i} = \mathbf{W}_K \mathbf{h}_i$ and $\mathbf{q}_{:j} = \mathbf{W}_Q \mathbf{s}_j$.
- Compute weights: $\alpha_{:j} = \text{Softmax}(\mathbf{K}^T \mathbf{q}_{:j}) \in \mathbb{R}^m$.



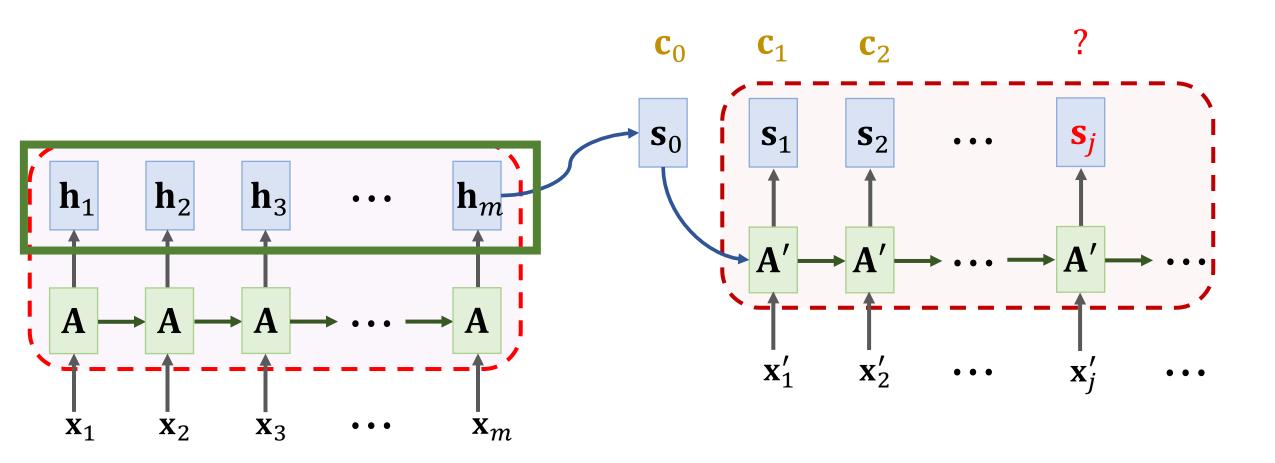
Weights:
$$\alpha_{ij} = \operatorname{align}(\mathbf{h}_i, \mathbf{s}_j)$$
.

- Compute $\mathbf{k}_{:i} = \mathbf{W}_K \mathbf{h}_i$ and $\mathbf{q}_{:j} = \mathbf{W}_Q \mathbf{s}_j$.
- Compute weights: $\alpha_{:j} = \text{Softmax}(\mathbf{K}^T \mathbf{q}_{:j}) \in \mathbb{R}^m$.
- Query: $\mathbf{q}_{:i} = \mathbf{W}_O \mathbf{s}_i$. (To match others.)
- Key: $\mathbf{k}_{:i} = \mathbf{W}_K \mathbf{h}_i$. (To be matched.)
- Value: $\mathbf{v}_{:i} = \mathbf{W}_V \mathbf{h}_i$. (To be weighted averaged.)

Query: $\mathbf{q}_{:j} = \mathbf{W}_Q \mathbf{s}_j$, Key: $\mathbf{k}_{:i} = \mathbf{W}_K \mathbf{h}_i$, Value: $\mathbf{v}_{:i} = \mathbf{W}_V \mathbf{h}_i$.

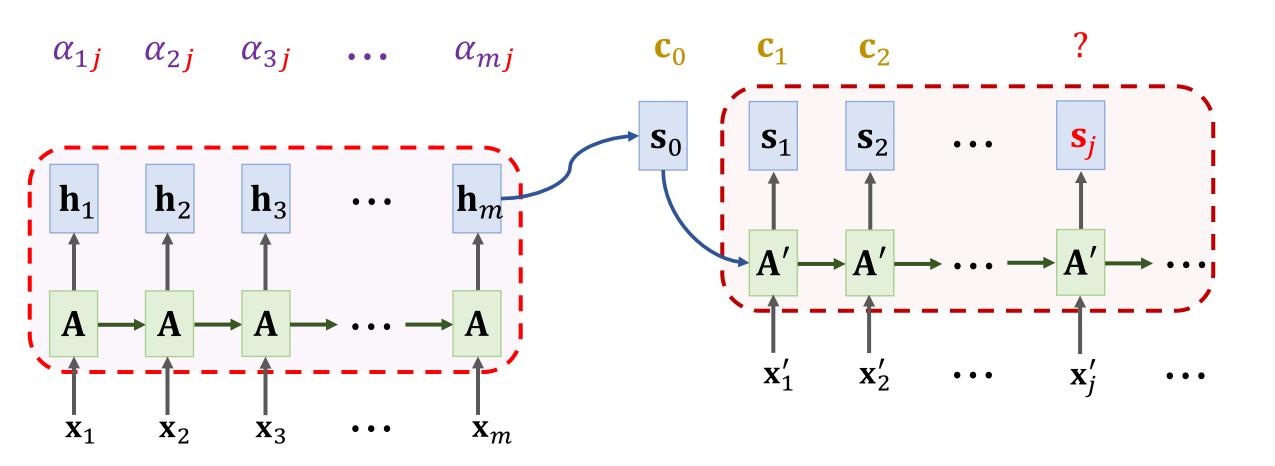


Query: $\mathbf{q}_{:j} = \mathbf{W}_Q \mathbf{s}_j$, Key: $\mathbf{k}_{:i} = \mathbf{W}_K \mathbf{h}_i$, Value: $\mathbf{v}_{:i} = \mathbf{W}_V \mathbf{h}_i$.



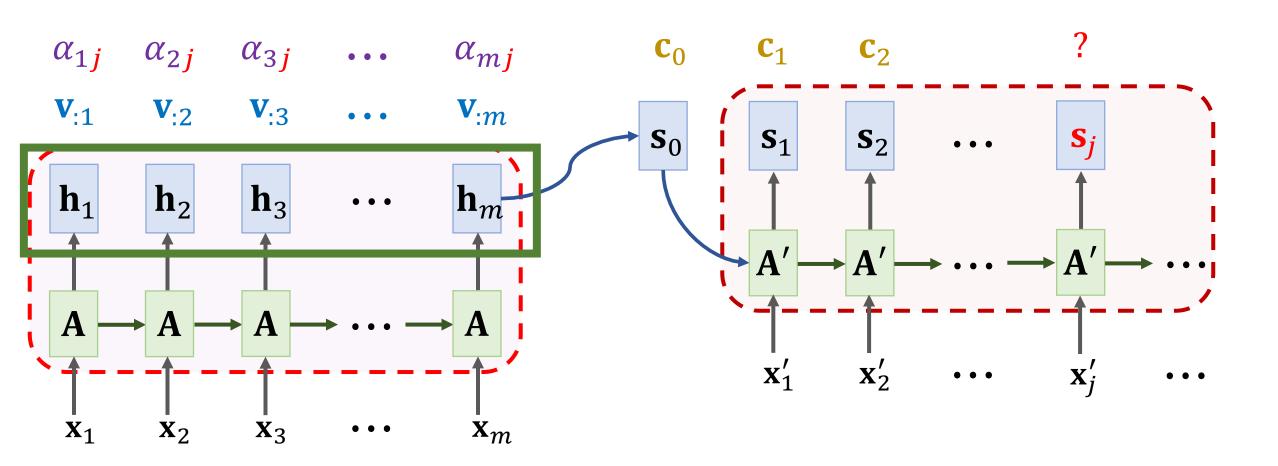
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Query: \mathbf{q}_{:j} = \mathbf{W}_Q \mathbf{s}_j, Key: \mathbf{k}_{:i} = \mathbf{W}_K \mathbf{h}_i, Value: \mathbf{v}_{:i} = \mathbf{W}_V \mathbf{h}_i.

Weights: \alpha_{:j} = \operatorname{Softmax}(\mathbf{K}^T \mathbf{q}_{:j}) \in \mathbb{R}^m.
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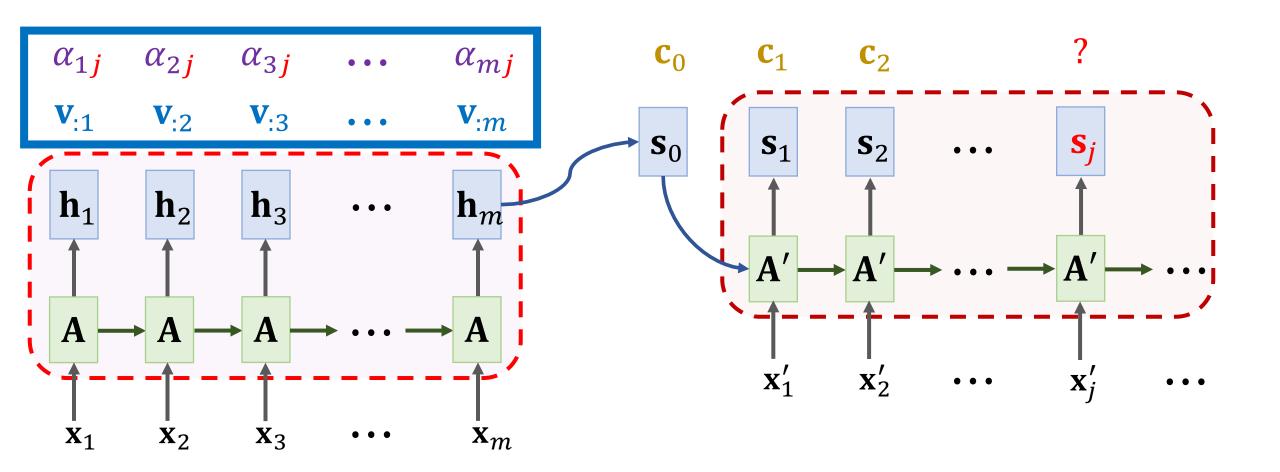
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Query: \mathbf{q}_{:j} = \mathbf{W}_Q \mathbf{s}_j, Key: \mathbf{k}_{:i} = \mathbf{W}_K \mathbf{h}_i, Value: \mathbf{v}_{:i} = \mathbf{W}_V \mathbf{h}_i.

Weights: \alpha_{:j} = \operatorname{Softmax}(\mathbf{K}^T \mathbf{q}_{:j}) \in \mathbb{R}^m.
```



Query:
$$\mathbf{q}_{:j} = \mathbf{W}_Q \mathbf{s}_j$$
, Key: $\mathbf{k}_{:i} = \mathbf{W}_K \mathbf{h}_i$, Value: $\mathbf{v}_{:i} = \mathbf{W}_V \mathbf{h}_i$.

Weights: $\alpha_{:j} = \operatorname{Softmax}(\mathbf{K}^T \mathbf{q}_{:j}) \in \mathbb{R}^m$.



Query:
$$\mathbf{q}_{:j} = \mathbf{W}_{Q}\mathbf{s}_{j}$$
, Key: $\mathbf{k}_{:i} = \mathbf{W}_{K}\mathbf{h}_{i}$, Value: $\mathbf{v}_{:i} = \mathbf{W}_{V}\mathbf{h}_{i}$.

Weights: $\alpha_{:j} = \operatorname{Softmax}(\mathbf{K}^{T}\mathbf{q}_{:j}) \in \mathbb{R}^{m}$.

Context vector: $\mathbf{c}_{j} = \alpha_{1j}\mathbf{v}_{:1} + \cdots + \alpha_{mj}\mathbf{v}_{:m}$.

 $\alpha_{1j} \quad \alpha_{2j} \quad \alpha_{3j} \quad \cdots \quad \alpha_{mj}$
 $\mathbf{v}_{:1} \quad \mathbf{v}_{:2} \quad \mathbf{v}_{:3} \quad \cdots \quad \mathbf{v}_{:m}$
 $\mathbf{s}_{0} \quad \mathbf{s}_{1} \quad \mathbf{s}_{2} \quad \cdots \quad \mathbf{s}_{j}$
 $\mathbf{h}_{1} \quad \mathbf{h}_{2} \quad \mathbf{h}_{3} \quad \cdots \quad \mathbf{h}_{m}$
 $\mathbf{a}_{1} \quad \mathbf{a}_{2} \quad \mathbf{a}_{3} \quad \cdots \quad \mathbf{a}_{mj}$
 $\mathbf{a}_{2} \quad \mathbf{a}_{3} \quad \cdots \quad \mathbf{a}_{mj}$
 $\mathbf{a}_{3} \quad \mathbf{a}_{2} \quad \mathbf{a}_{3} \quad \cdots \quad \mathbf{a}_{mj}$
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 $\mathbf{a}_{2} \quad \cdots \quad \mathbf{a}_{mj}$
 $\mathbf{a}_{3} \quad \cdots \quad \mathbf{a}_{mj}$
 $\mathbf{a}_{4} \quad \cdots \quad \mathbf{a}_{mj}$

```
Query: \mathbf{q}_{:j} = \mathbf{W}_Q \mathbf{s}_j, Key: \mathbf{k}_{:i} = \mathbf{W}_K \mathbf{h}_i, Value: \mathbf{v}_{:i} = \mathbf{W}_V \mathbf{h}_i.

Weights: \alpha_{:j} = \operatorname{Softmax}(\mathbf{K}^T \mathbf{q}_{:j}) \in \mathbb{R}^m.

Context vector: \mathbf{c}_j = \alpha_{1j} \mathbf{v}_{:1} + \dots + \alpha_{mj} \mathbf{v}_{:m}.
```

Question: How to remove RNN while keeping attention?

Attention without RNN

- We study Seq2Seq model (encoder + decoder).
- Encoder's inputs are vectors $\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_m$.
- Decoder's inputs are vectors $\mathbf{x}'_1, \mathbf{x}'_2, \cdots, \mathbf{x}'_t$.

Encoder's inputs:

Decoder's inputs:

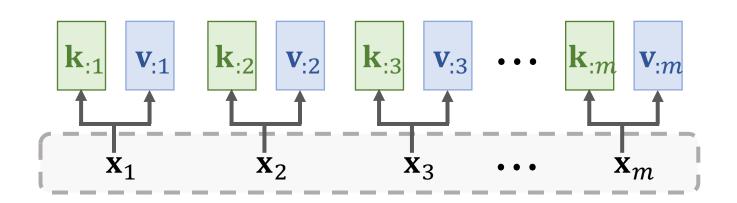
 \mathbf{x}_1 \mathbf{x}_2 \mathbf{x}_3 ••• \mathbf{x}_m



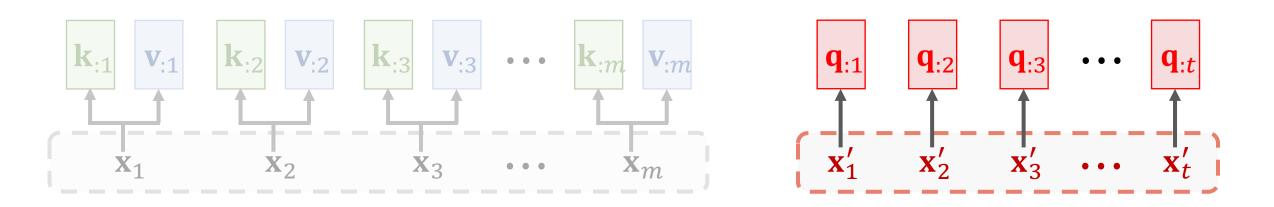
• Keys and values are based on encoder's inputs x_1, x_2, \dots, x_m .

• Key: $\mathbf{k}_{:i} = \mathbf{W}_K \mathbf{x}_i$.

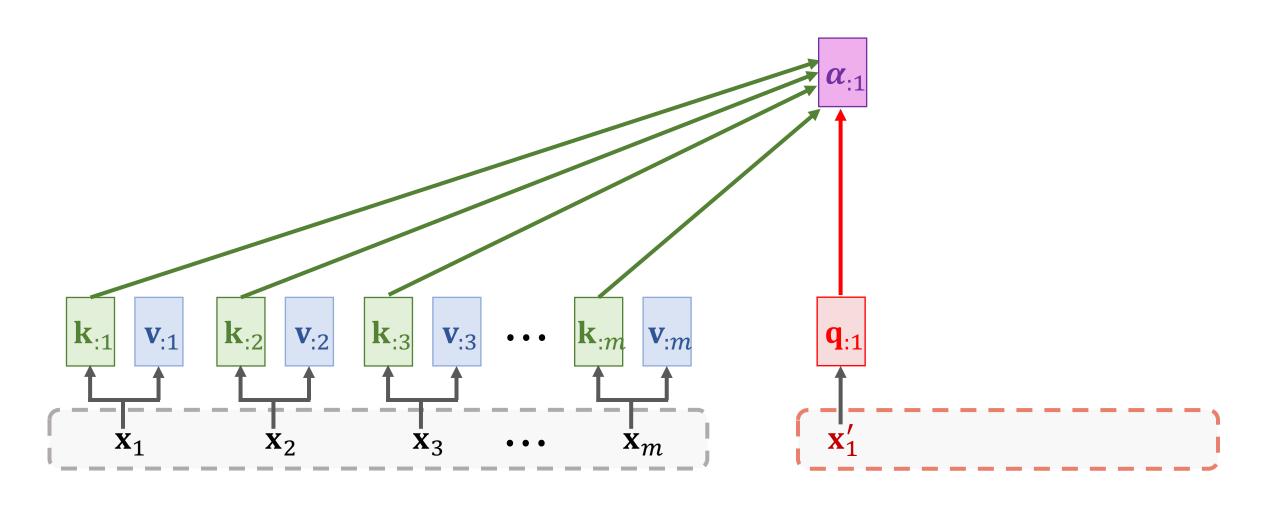
• Value: $\mathbf{v}_{:i} = \mathbf{W}_V \mathbf{x}_i$.



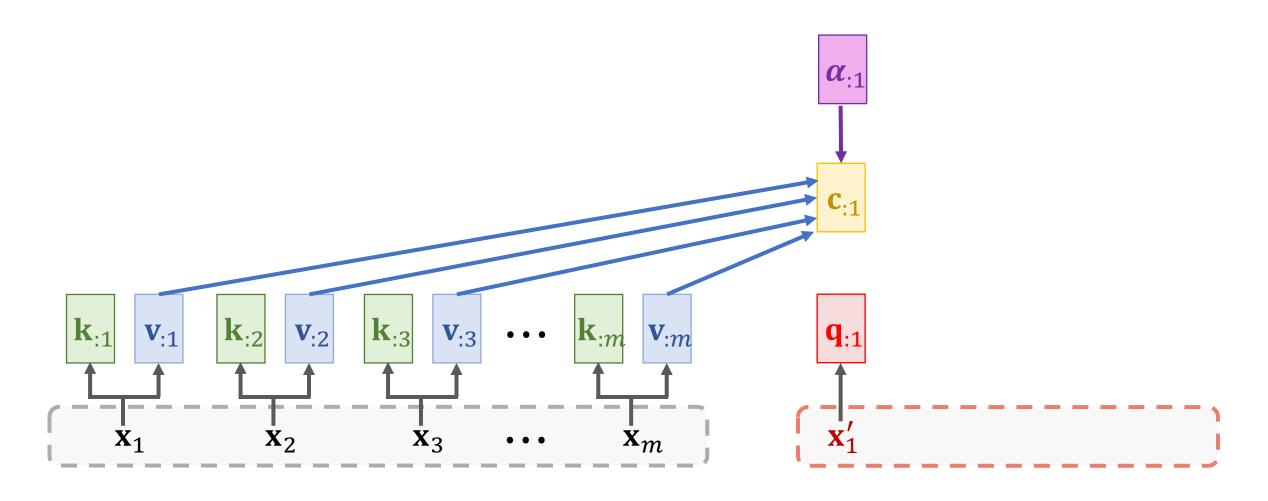
- Keys and values are based on encoder's inputs x_1, x_2, \dots, x_m .
- Key: $\mathbf{k}_{:i} = \mathbf{W}_K \mathbf{x}_i$.
- Value: $\mathbf{v}_{:i} = \mathbf{W}_V \mathbf{x}_i$.
- Queries are based on decoder's inputs $\mathbf{x}_1', \mathbf{x}_2', \cdots, \mathbf{x}_t'$.
- Query: $\mathbf{q}_{:j} = \mathbf{W}_Q \mathbf{x}'_j$.



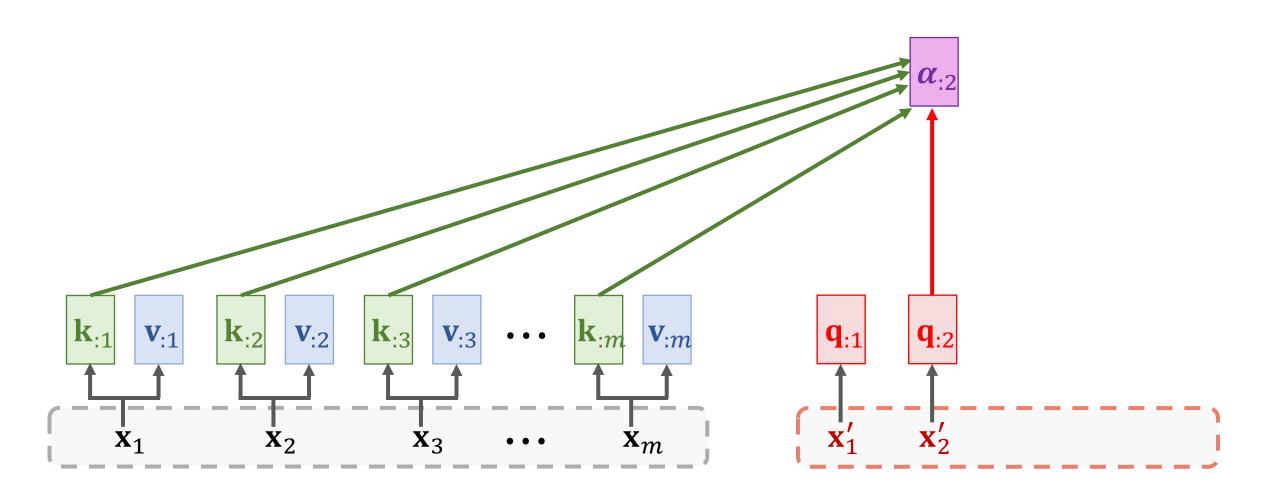
• Compute weights: $\alpha_{:1} = \text{Softmax}(\mathbf{K}^T \mathbf{q}_{:1}) \in \mathbb{R}^m$.



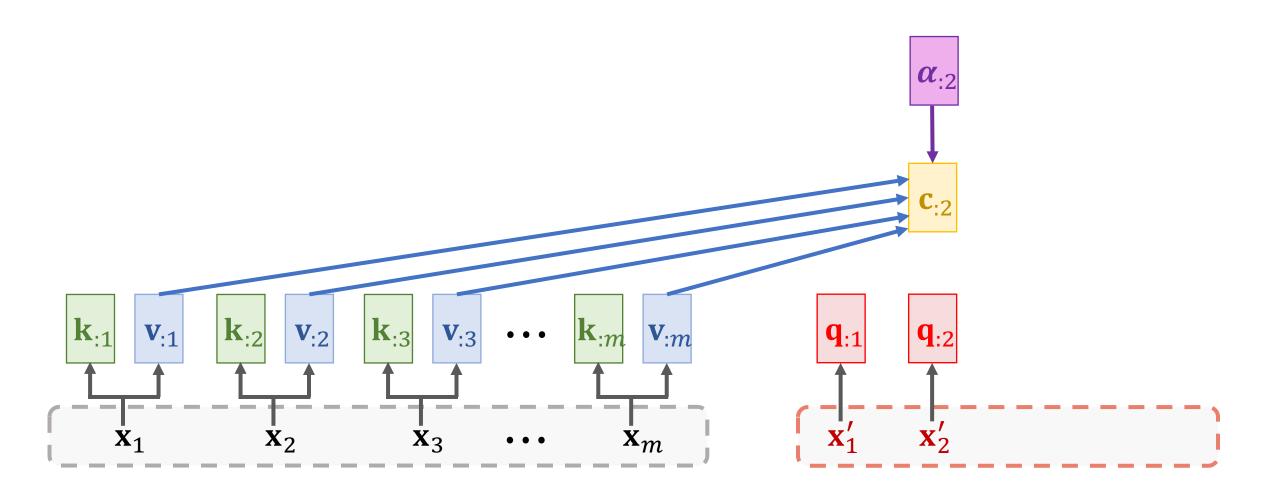
• Compute context vector: $\mathbf{c}_{:1} = \alpha_{11}\mathbf{v}_{:1} + \cdots + \alpha_{m1}\mathbf{v}_{:m} = \mathbf{V}\alpha_{:1}$.



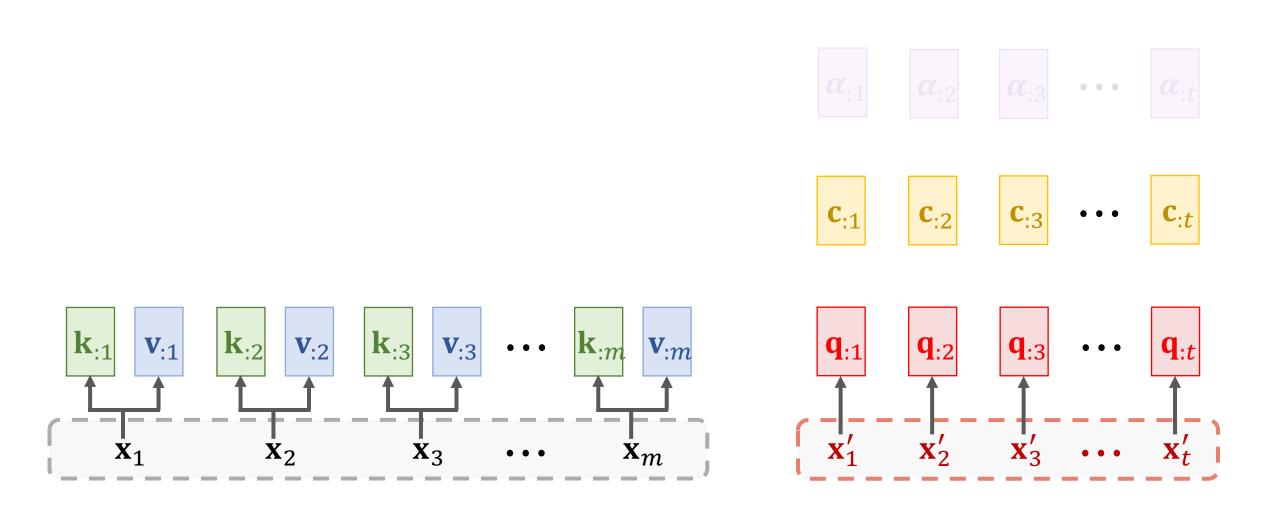
• Compute weights: $\alpha_{:2} = \text{Softmax}(\mathbf{K}^T \mathbf{q}_{:2}) \in \mathbb{R}^m$.



• Compute context vector: $\mathbf{c}_{:2} = \alpha_{12}\mathbf{v}_{:1} + \cdots + \alpha_{m2}\mathbf{v}_{:m} = \mathbf{V}\alpha_{:2}$.

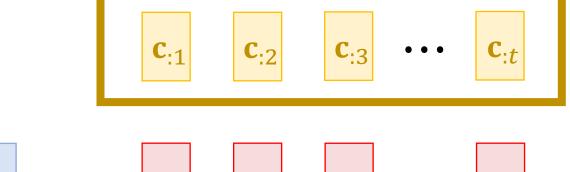


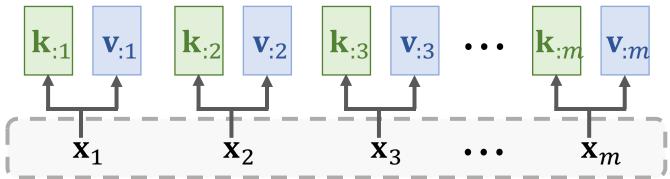
• Compute context vector: $\mathbf{c}_{:j} = \alpha_{1j} \mathbf{v}_{:1} + \cdots + \alpha_{mj} \mathbf{v}_{:m} = \mathbf{V} \alpha_{:j}$.

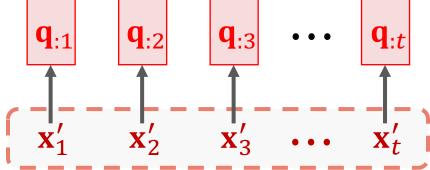


- Output of attention layer: $\mathbf{C} = [\mathbf{c}_{:1}, \mathbf{c}_{:2}, \mathbf{c}_{:3}, \cdots, \mathbf{c}_{:t}].$
- Here, $\mathbf{c}_{:i} = \mathbf{V} \cdot \operatorname{Softmax}(\mathbf{K}^T \mathbf{q}_{:i})$.
- Thus, $\mathbf{c}_{:j}$ is a function of \mathbf{x}'_j and $[\mathbf{x}_1, \dots, \mathbf{x}_m]$.

Output of attention layer:



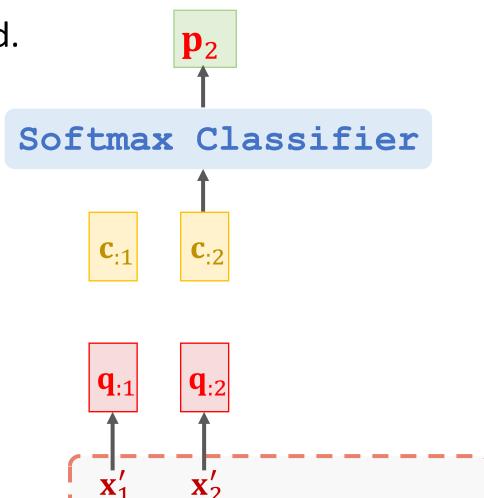


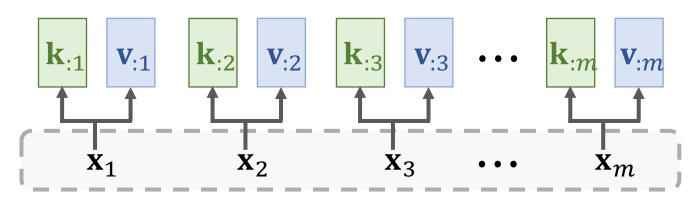


Attention Layer for Machine Translation

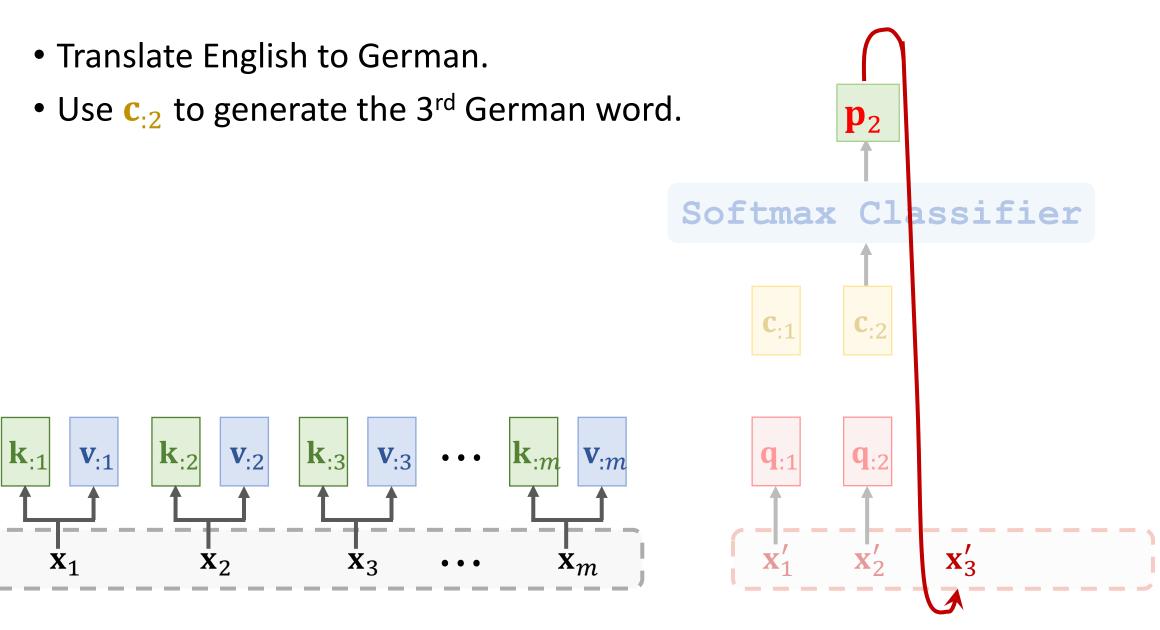
• Translate English to German.

• Use C:2 to generate the 3rd German word.

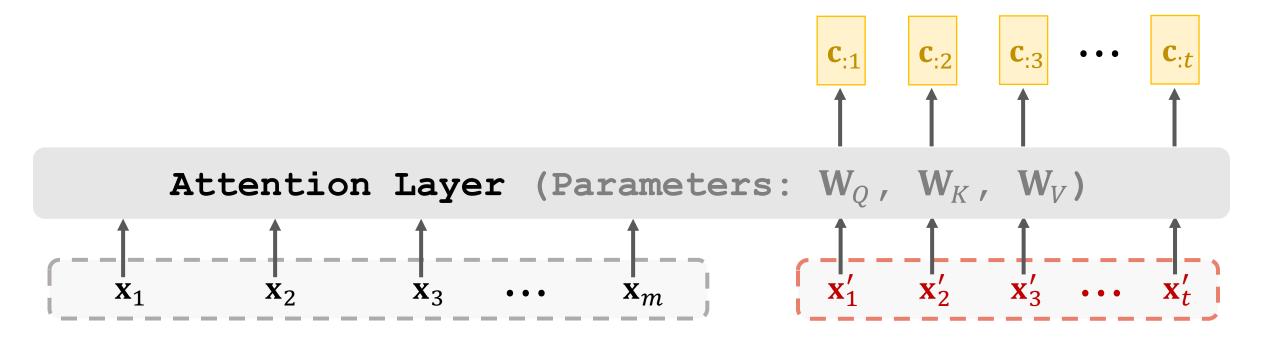




Attention Layer for Machine Translation

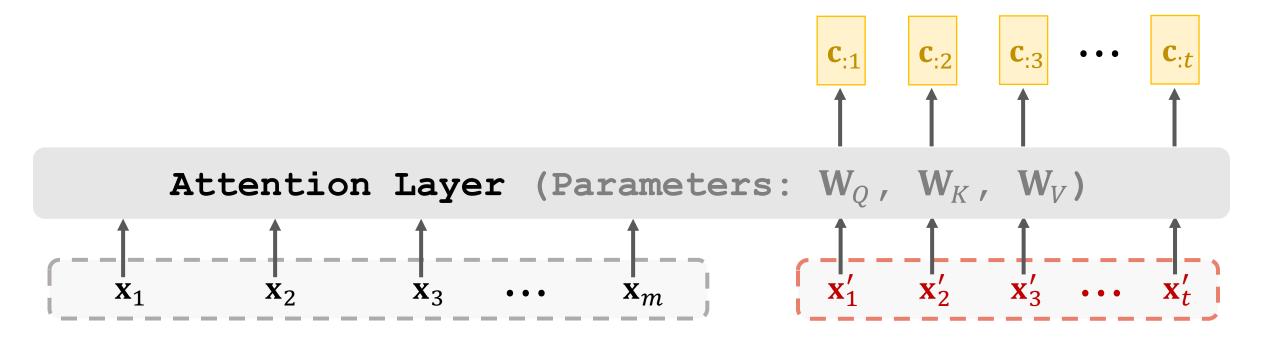


- Attention layer: C = Attn(X, X').
 - Encoder's inputs: $\mathbf{X} = [\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_m]$.
 - Decoder's inputs: $\mathbf{X}' = [\mathbf{x}'_1, \mathbf{x}'_2, \cdots, \mathbf{x}'_t]$.
 - Parameters: \mathbf{W}_Q , \mathbf{W}_K , \mathbf{W}_V .

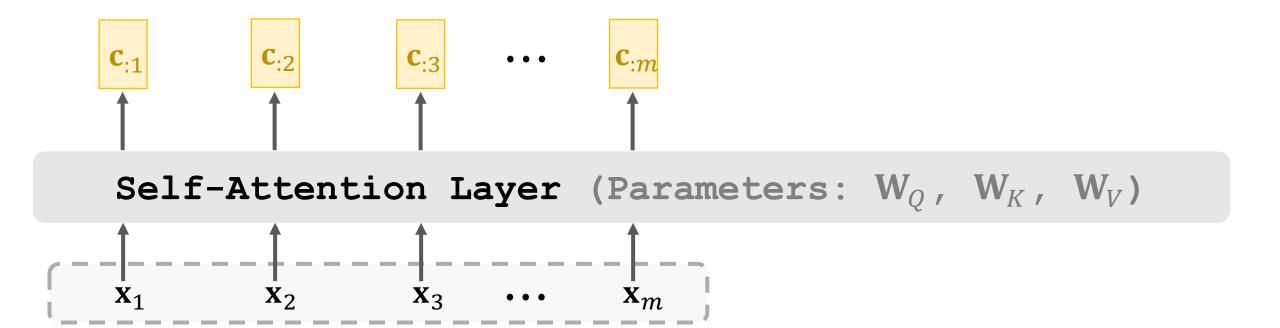


Self-Attention without RNN

- Attention layer: C = Attn(X, X').
 - Encoder's inputs: $\mathbf{X} = [\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_m]$.
 - Decoder's inputs: $\mathbf{X}' = [\mathbf{x}'_1, \mathbf{x}'_2, \cdots, \mathbf{x}'_m]$.
 - Parameters: \mathbf{W}_Q , \mathbf{W}_K , \mathbf{W}_V .



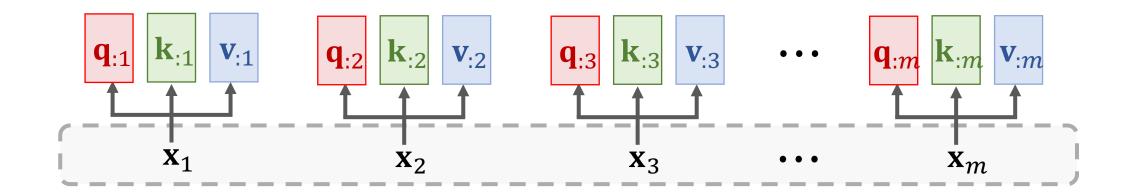
- Self-attention layer: C = Attn(X, X).
 - Inputs: $\mathbf{X} = [\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_m].$
 - Parameters: \mathbf{W}_O , \mathbf{W}_K , \mathbf{W}_V .



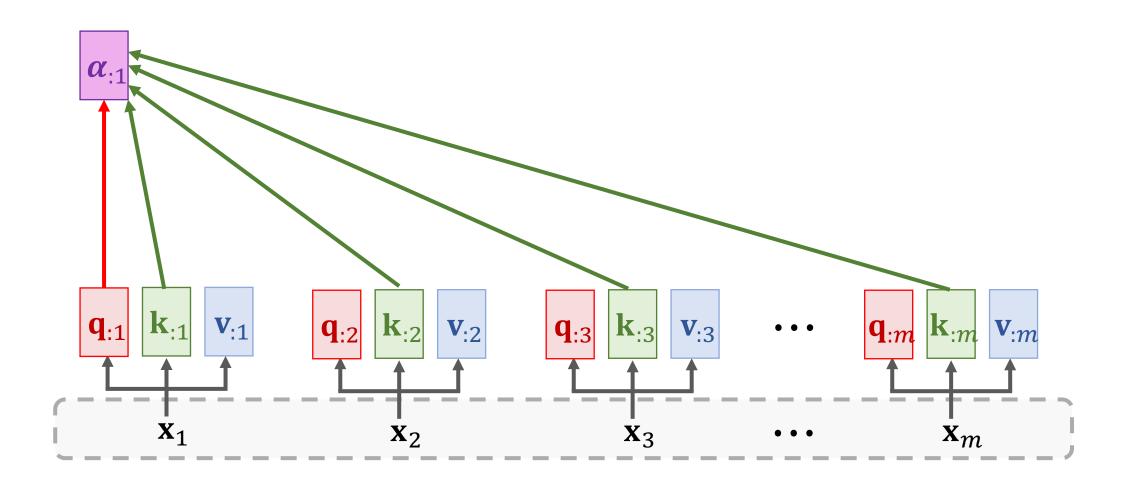
Inputs:



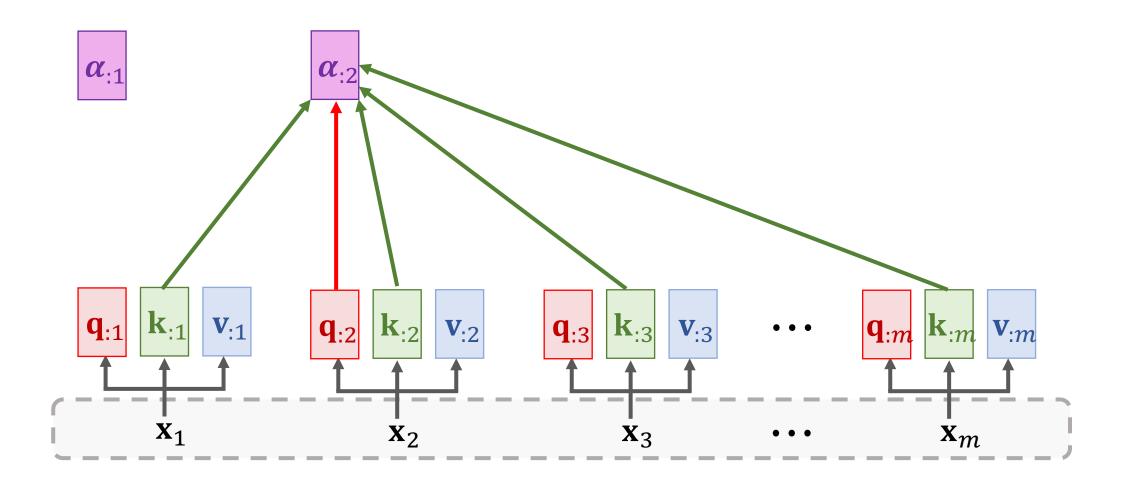
Query: $\mathbf{q}_{:i} = \mathbf{W}_Q \mathbf{x}_i$, Key: $\mathbf{k}_{:i} = \mathbf{W}_K \mathbf{x}_i$, Value: $\mathbf{v}_{:i} = \mathbf{W}_V \mathbf{x}_i$.



Weights:
$$\alpha_{:j} = \operatorname{Softmax}(\mathbf{K}^T \mathbf{q}_{:j}) \in \mathbb{R}^m$$
.

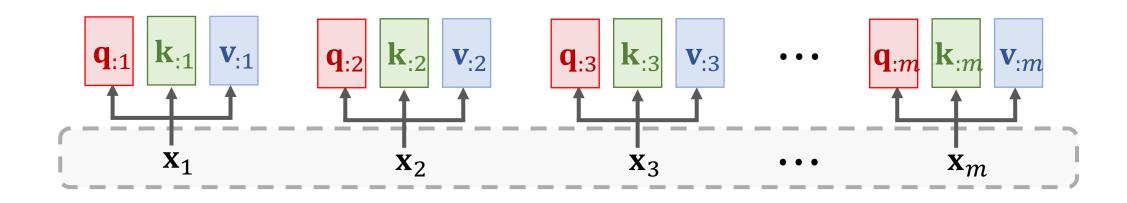


Weights:
$$\alpha_{:j} = \operatorname{Softmax}(\mathbf{K}^T \mathbf{q}_{:j}) \in \mathbb{R}^m$$
.

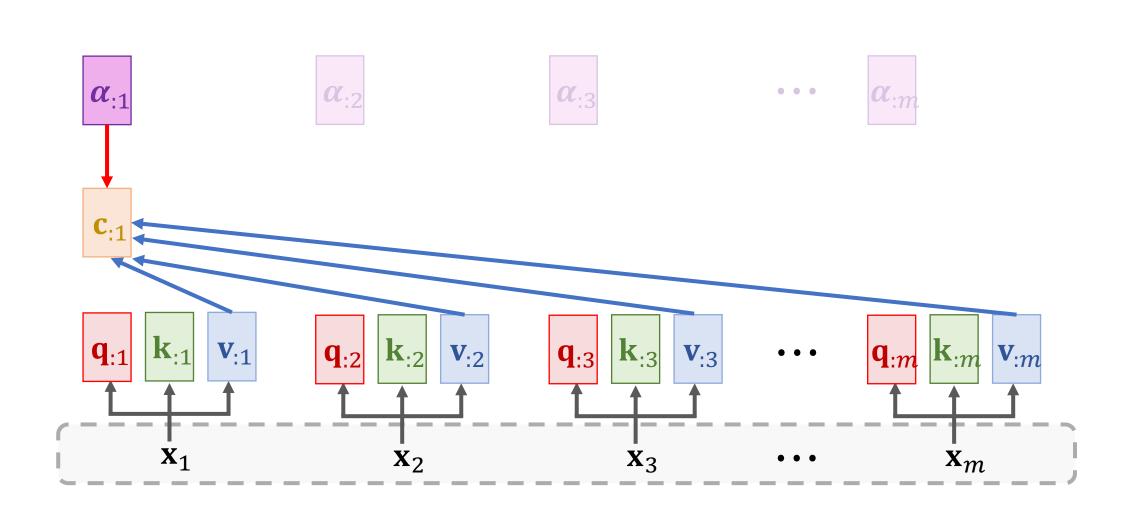


Weights:
$$\alpha_{:j} = \operatorname{Softmax}(\mathbf{K}^T \mathbf{q}_{:j}) \in \mathbb{R}^m$$
.

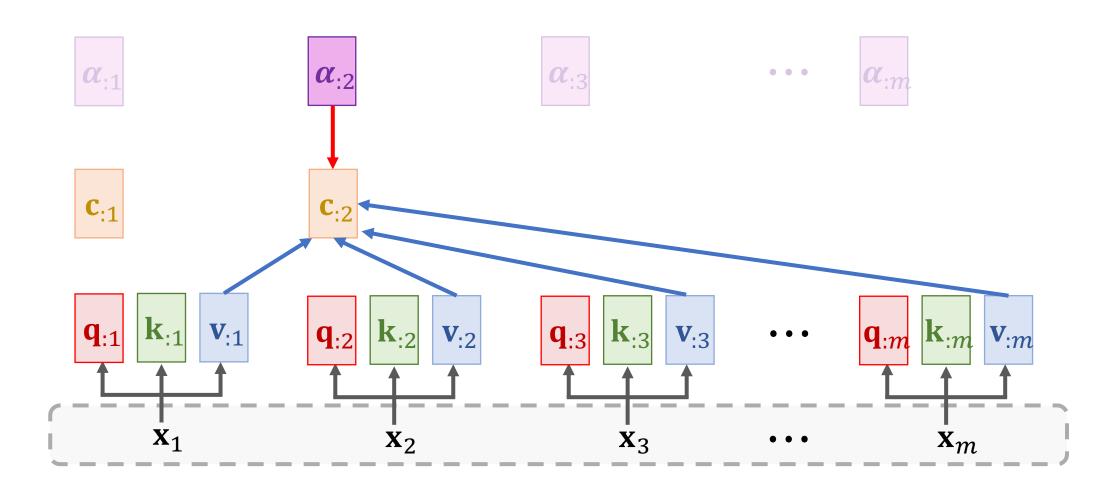
$$|\alpha_{:1}|$$
 $|\alpha_{:2}|$ $|\alpha_{:m}|$



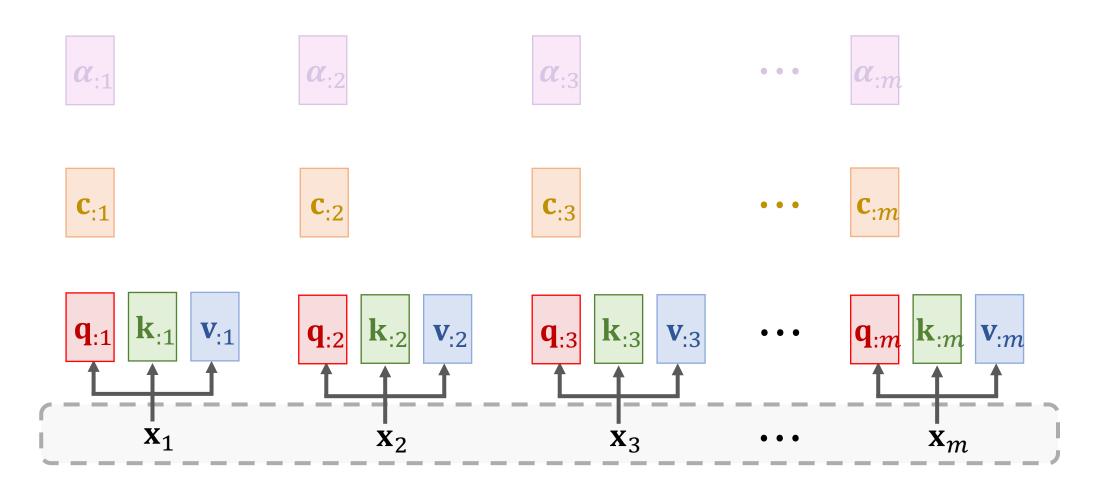
Context vector: $\mathbf{c}_{:1} = \alpha_{11}\mathbf{v}_{:1} + \cdots + \alpha_{m1}\mathbf{v}_{:m} = \mathbf{V}\alpha_{:1}$.



Context vector: $\mathbf{c}_{:2} = \alpha_{12}\mathbf{v}_{:1} + \cdots + \alpha_{m2}\mathbf{v}_{:m} = \mathbf{V}\boldsymbol{\alpha}_{:2}$.

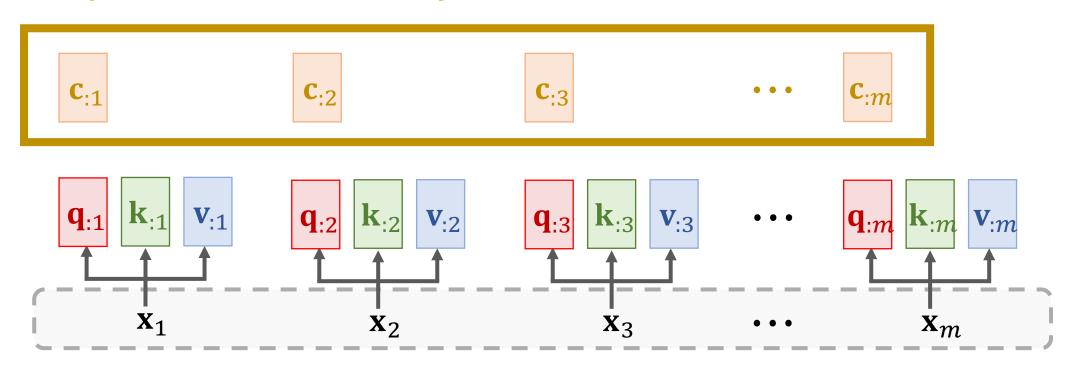


Context vector: $\mathbf{c}_{:j} = \alpha_{1j}\mathbf{v}_{:1} + \cdots + \alpha_{mj}\mathbf{v}_{:m} = \mathbf{V}\alpha_{:j}$.

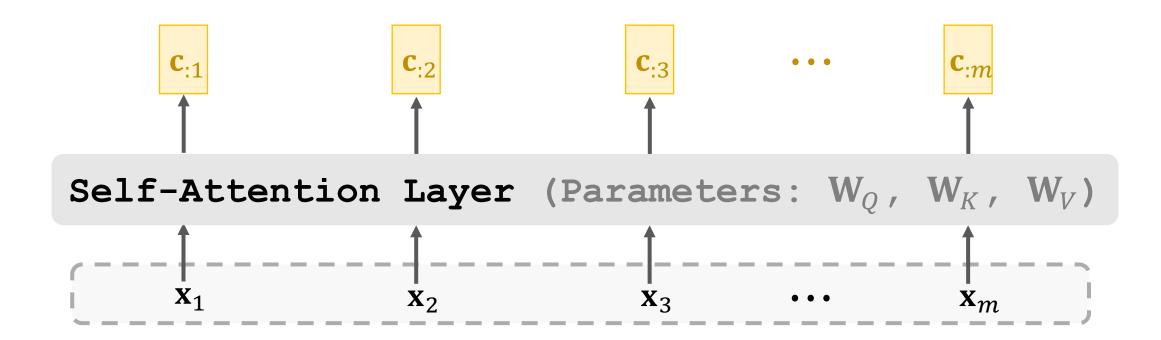


- Here, $\mathbf{c}_{:j} = \mathbf{V} \cdot \operatorname{Softmax}(\mathbf{K}^T \mathbf{q}_{:j})$.
- Thus, $\mathbf{c}_{:j}$ is a function of all the m vectors $\mathbf{x}_1, \cdots, \mathbf{x}_m$.

Output of self-attention layer:



- Self-attention layer: C = Attn(X, X).
 - Inputs: $\mathbf{X} = [\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_m]$.
 - Parameters: \mathbf{W}_Q , \mathbf{W}_K , \mathbf{W}_V .



Summary

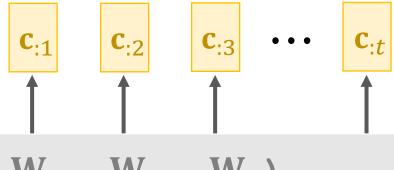
Summary

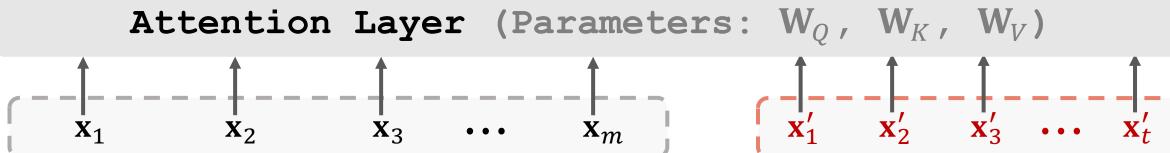
- Attention was originally developed for Seq2Seq RNN models [1].
- Self-attention: attention for all the RNN models (not necessarily Seq2Seq models [2].
- Attention can be used without RNN [3].
- We learned how to build attention layer and self-attention layer.

Reference:

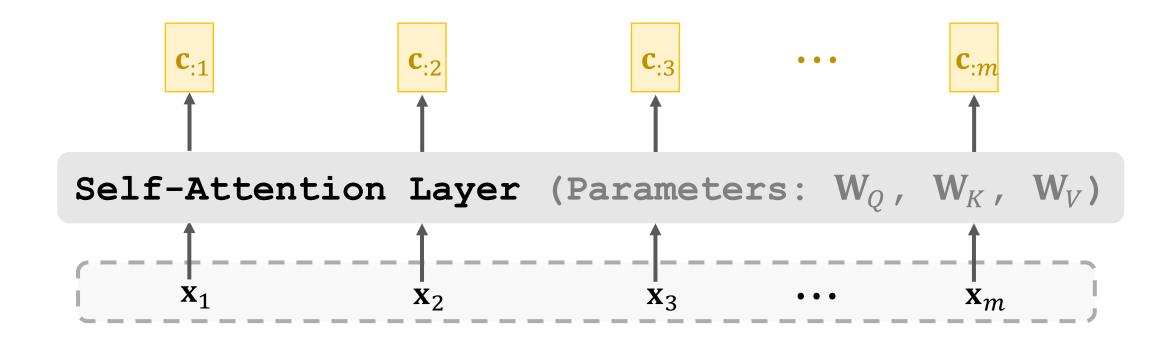
- 1. Bahdanau, Cho, & Bengio. Neural machine translation by jointly learning to align and translate. In *ICLR*, 2015.
- 2. Cheng, Dong, & Lapata. Long Short-Term Memory-Networks for Machine Reading. In *EMNLP*, 2016.
- 3. Vaswani et al. Attention Is All You Need. In NIPS, 2017.

- Attention layer: C = Attn(X, X').
 - Query: $\mathbf{q}_{:j} = \mathbf{W}_Q \mathbf{x}'_j$,
 - Key: $\mathbf{k}_{:i} = \mathbf{W}_K \mathbf{x}_i$,
 - Value: $\mathbf{v}_{:i} = \mathbf{W}_V \mathbf{x}_i$.
 - Output: $\mathbf{c}_{:j} = \mathbf{V} \cdot \operatorname{Softmax}(\mathbf{K}^T \mathbf{q}_{:j})$.





- Attention layer: C = Attn(X, X').
- Self-Attention layer: C = Attn(X, X).



Thank you!