

Lecture 13: Attention

Assignment 4

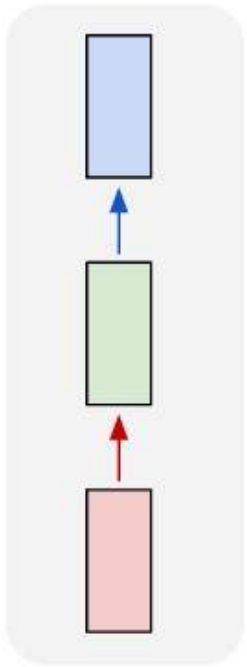
A4 will be released today or tomorrow
Due 2 weeks from the time it is released

Will cover:

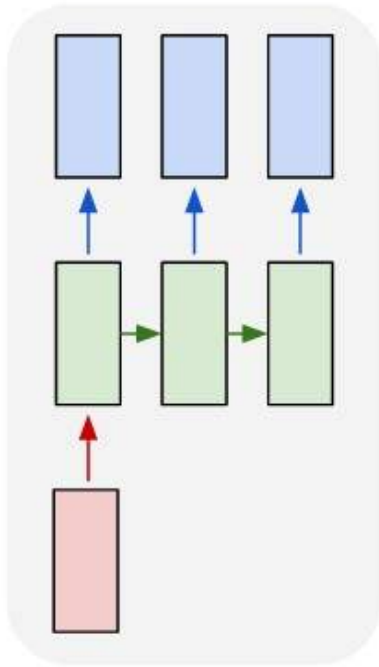
- PyTorch autograd
- Residual networks
- Recurrent neural networks
- Attention
- Feature visualization
- Style transfer
- Adversarial examples

Last Time: Recurrent Neural Networks

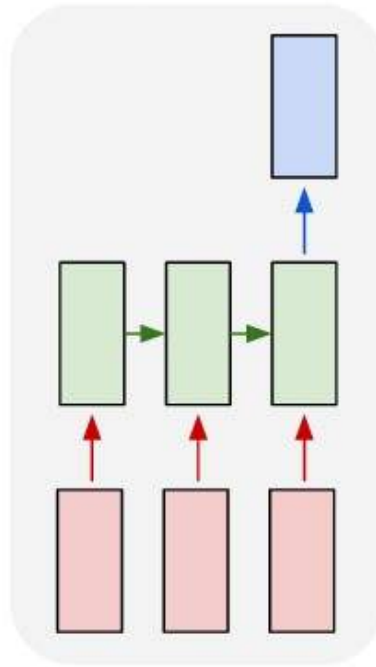
one to one



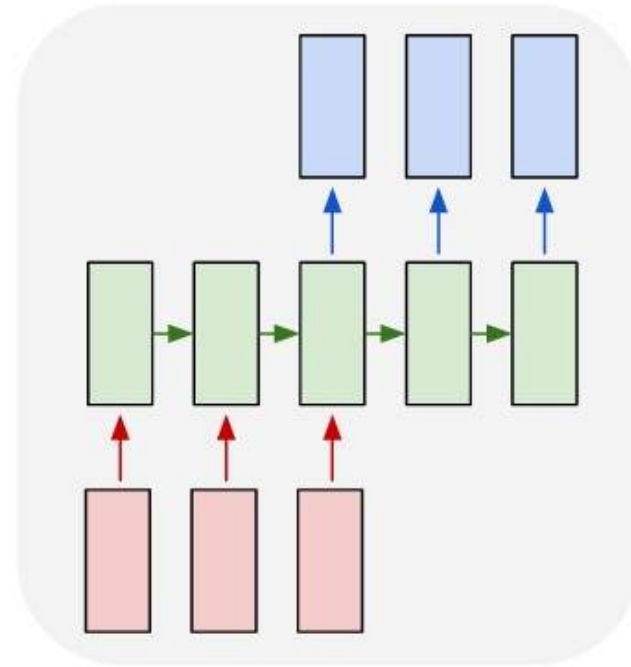
one to many



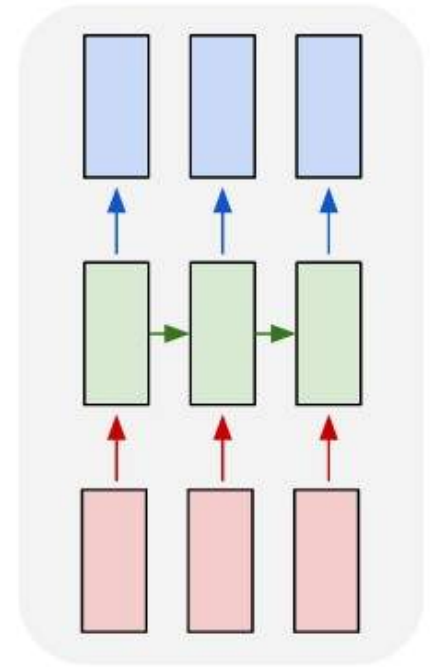
many to one



many to many



many to many

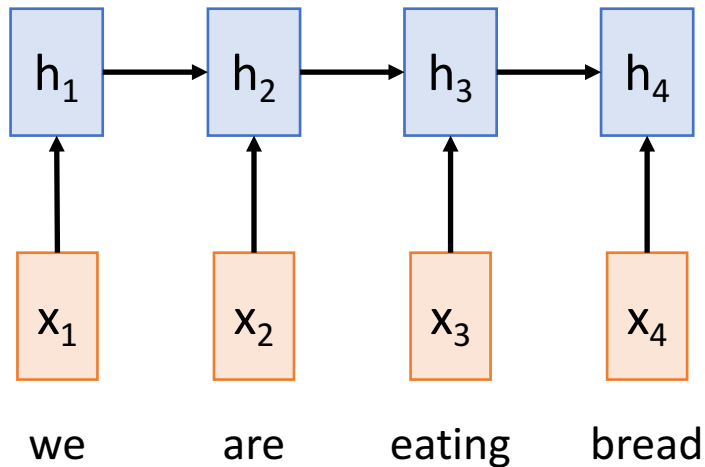


Sequence-to-Sequence with RNNs

Input: Sequence x_1, \dots, x_T

Output: Sequence $y_1, \dots, y_{T'}$

Encoder: $h_t = f_W(x_t, h_{t-1})$



Sequence-to-Sequence with RNNs

Input: Sequence x_1, \dots, x_T

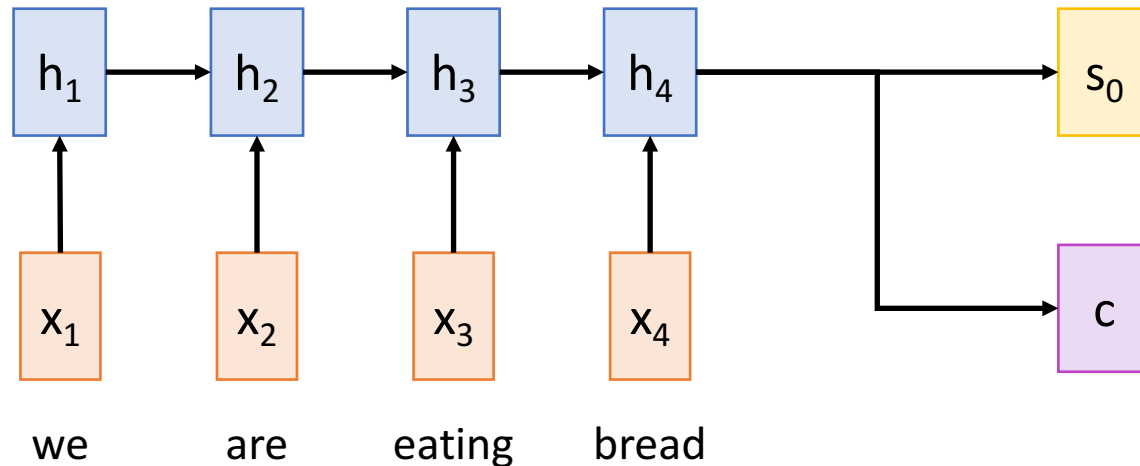
Output: Sequence $y_1, \dots, y_{T'}$

Encoder: $h_t = f_W(x_t, h_{t-1})$

From final hidden state predict:

Initial decoder state s_0

Context vector c (often $c=h_T$)



Sequence-to-Sequence with RNNs

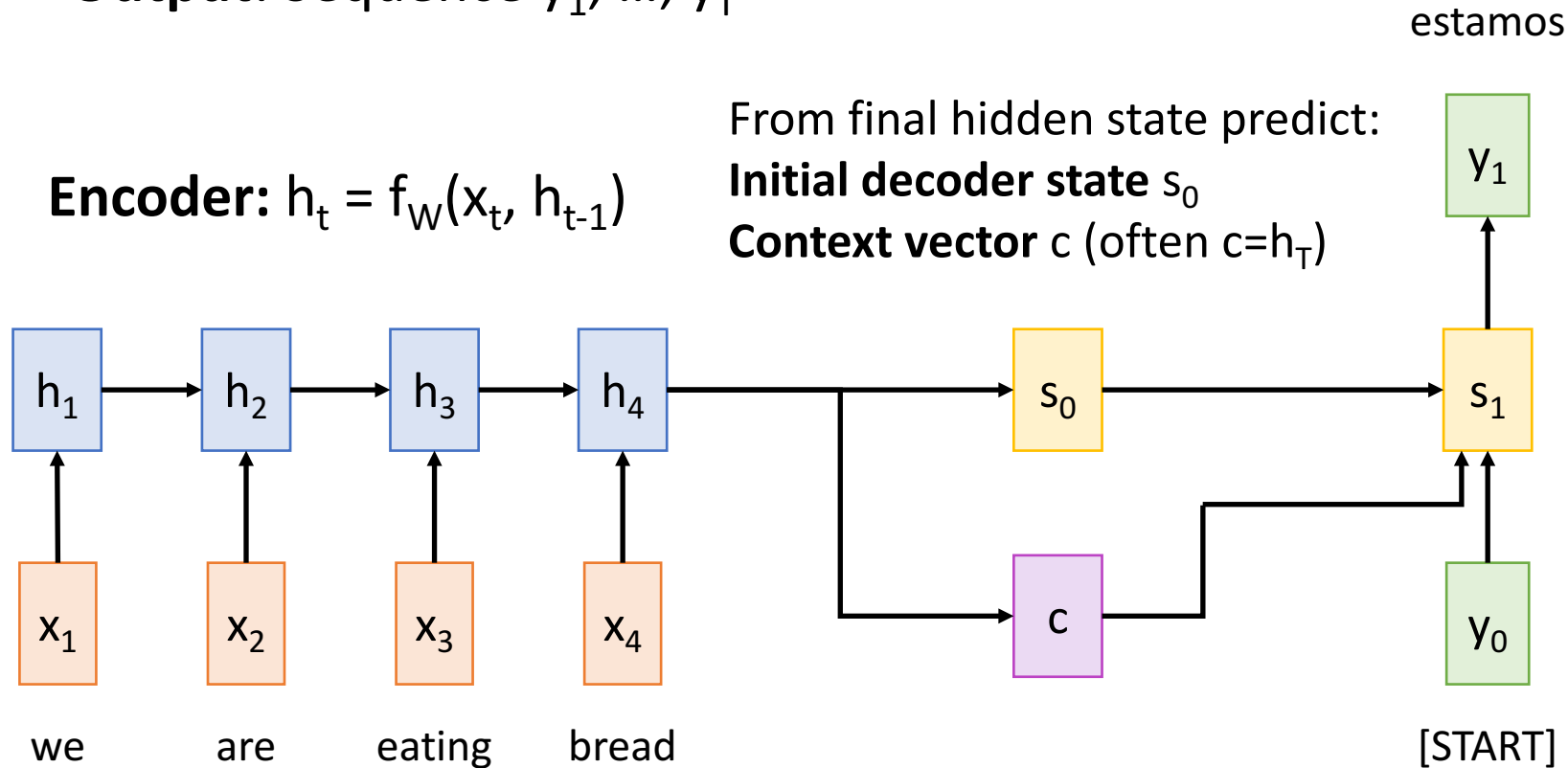
Input: Sequence x_1, \dots, x_T

Output: Sequence y_1, \dots, y_T

Decoder: $s_t = g_U(y_{t-1}, h_{t-1}, c)$

Encoder: $h_t = f_W(x_t, h_{t-1})$

From final hidden state predict:
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Sequence-to-Sequence with RNNs

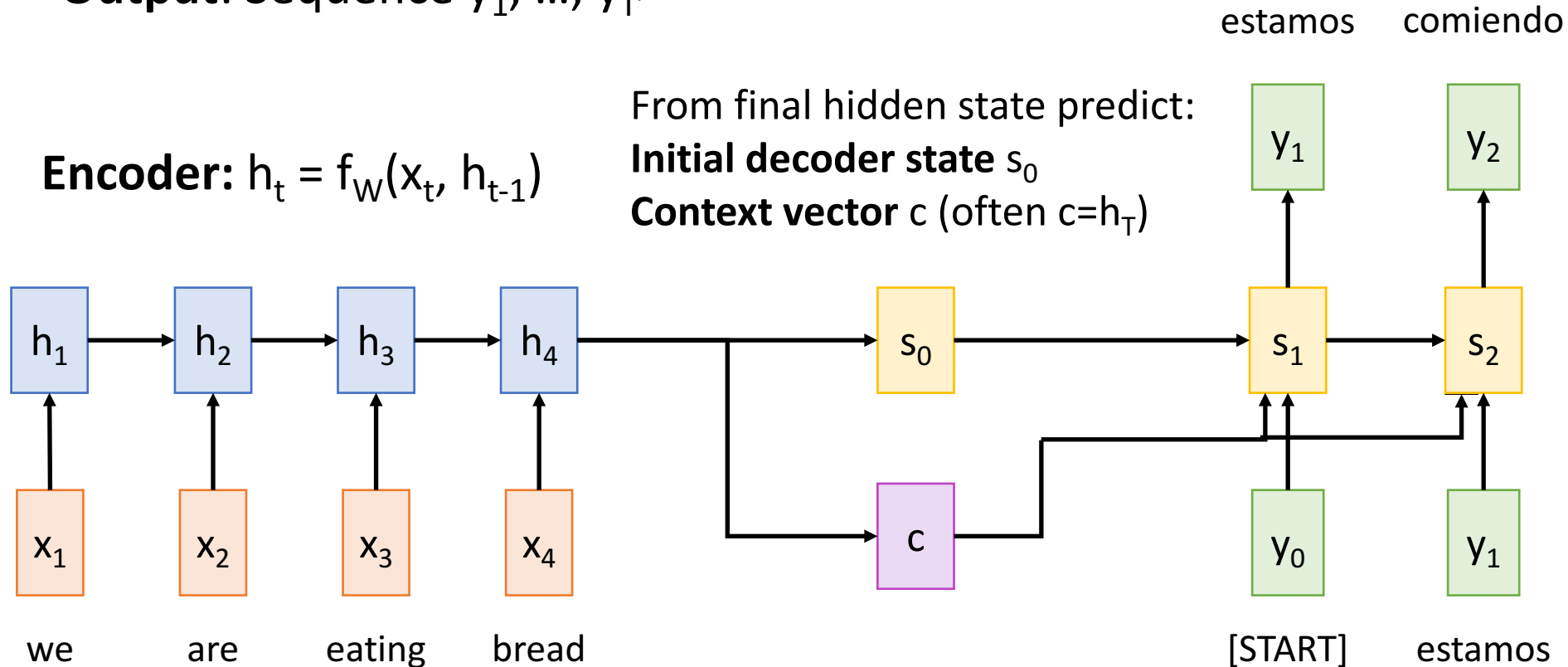
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Sequence-to-Sequence with RNNs

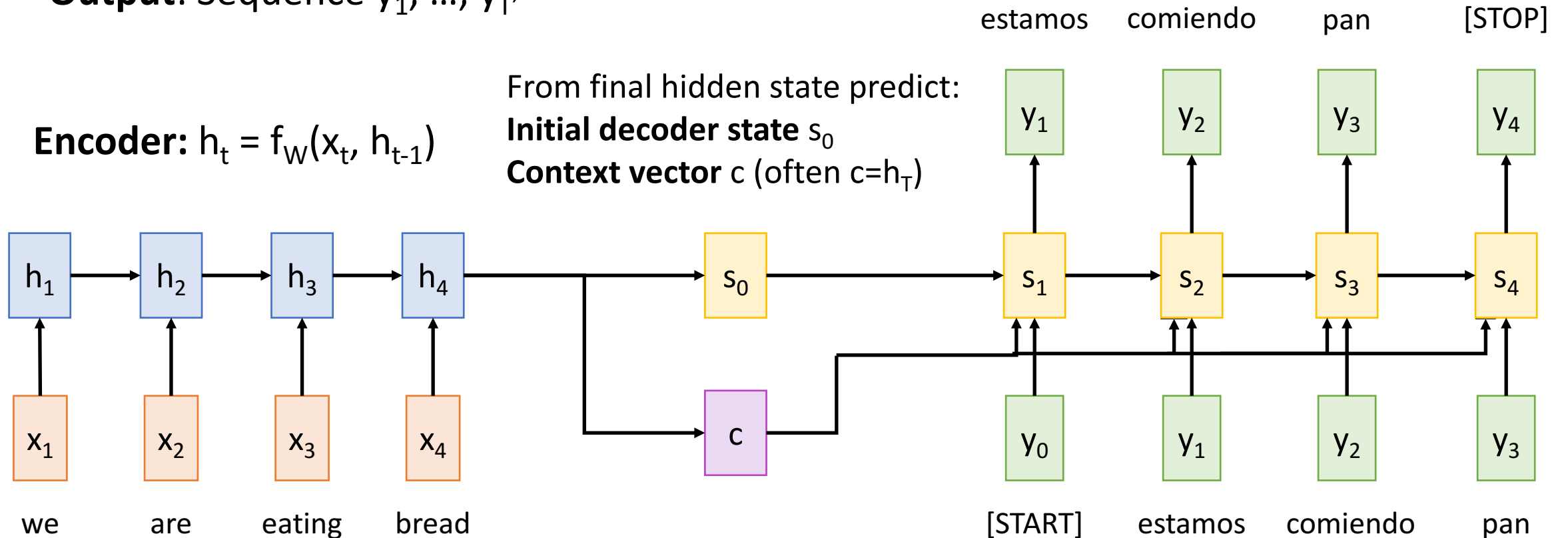
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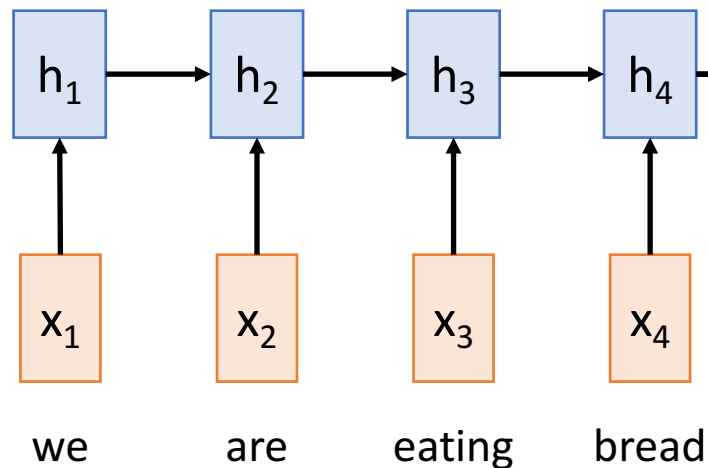
Sequence-to-Sequence with RNNs

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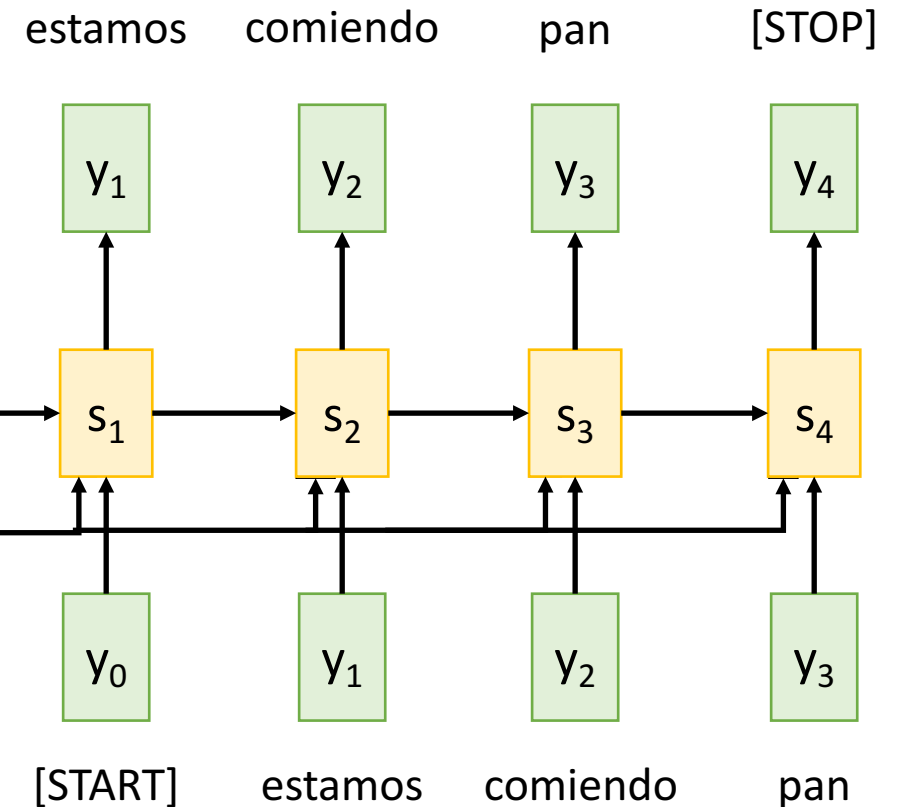
Decoder: $s_t = g_U(y_{t-1}, h_{t-1}, c)$

Encoder: $h_t = f_W(x_t, h_{t-1})$



From final hidden state predict:
Initial decoder state s_0
Context vector c (often $c=h_T$)

Problem: Input sequence bottlenecked through fixed-sized vector. What if $T=1000$?



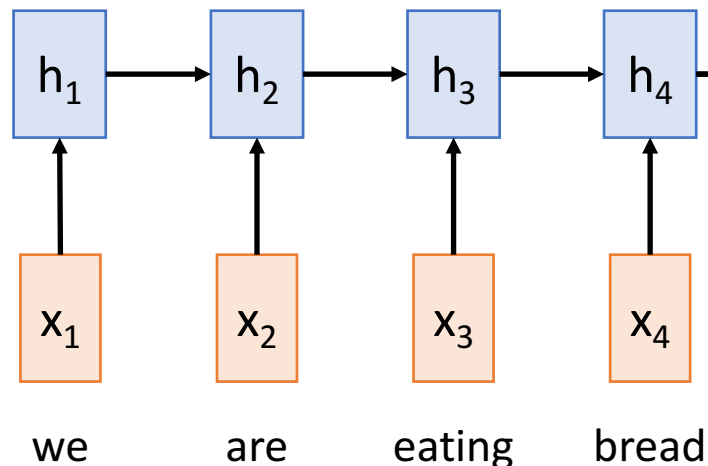
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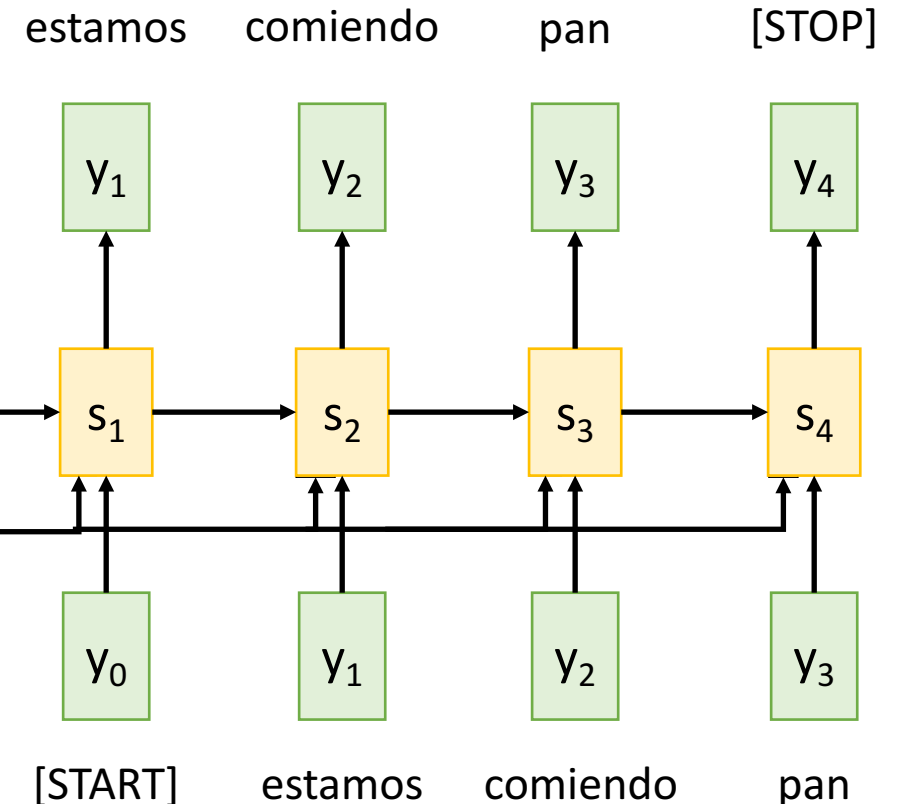
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From final hidden state predict:
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Context vector c (often $c=h_T$)

Problem: Input sequence bottlenecked through fixed-sized vector. What if $T=1000$?



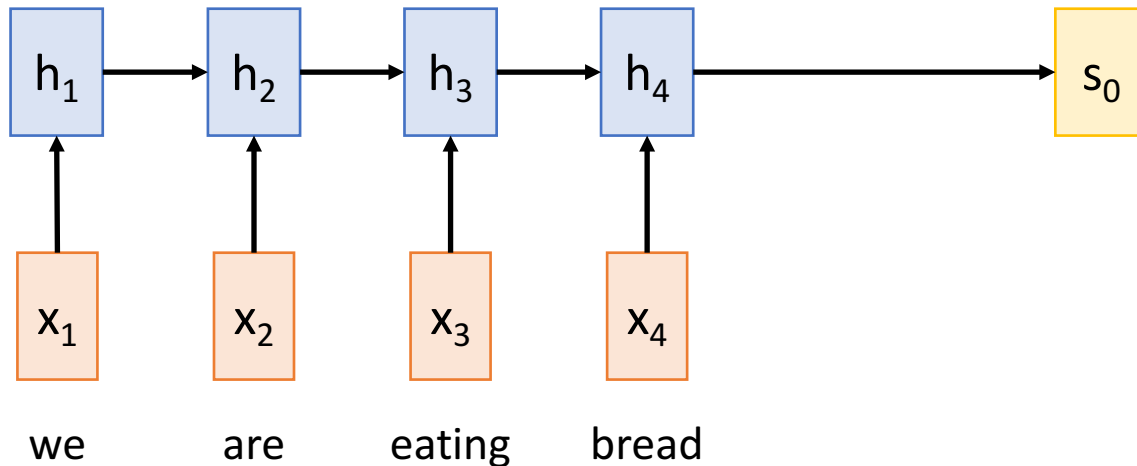
Idea: use new context vector at each step of decoder!

Sequence-to-Sequence with RNNs and Attention

Input: Sequence x_1, \dots, x_T

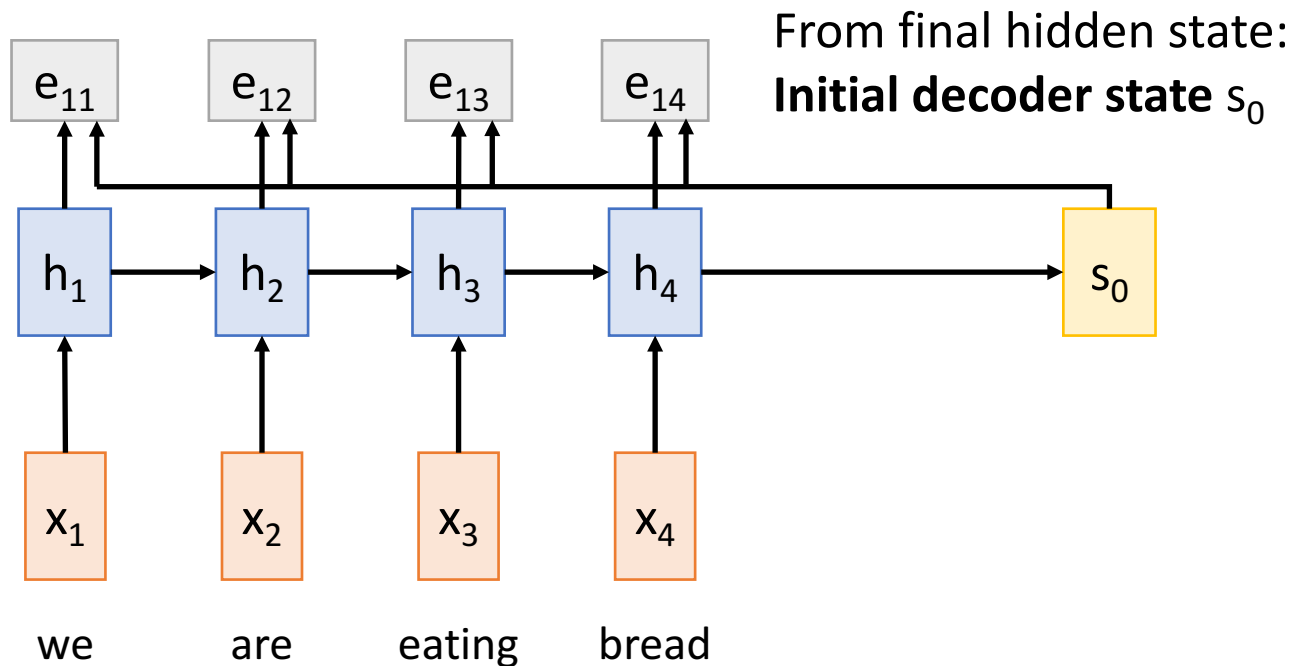
Output: Sequence $y_1, \dots, y_{T'}$

Encoder: $h_t = f_W(x_t, h_{t-1})$ From final hidden state:
Initial decoder state s_0

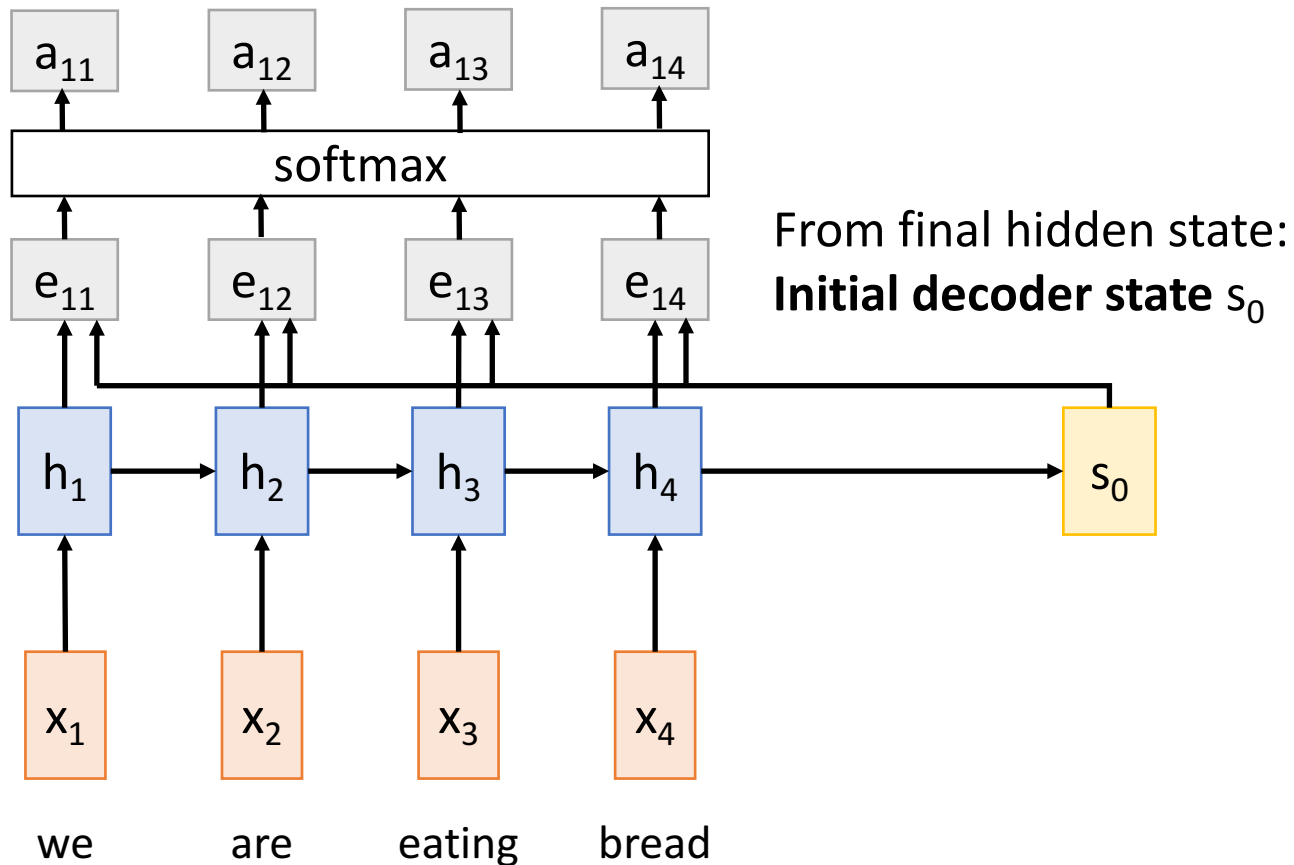


Sequence-to-Sequence with RNNs and Attention

Compute (scalar) **alignment scores**
 $e_{t,i} = f_{\text{att}}(s_{t-1}, h_i)$ (f_{att} is an MLP)



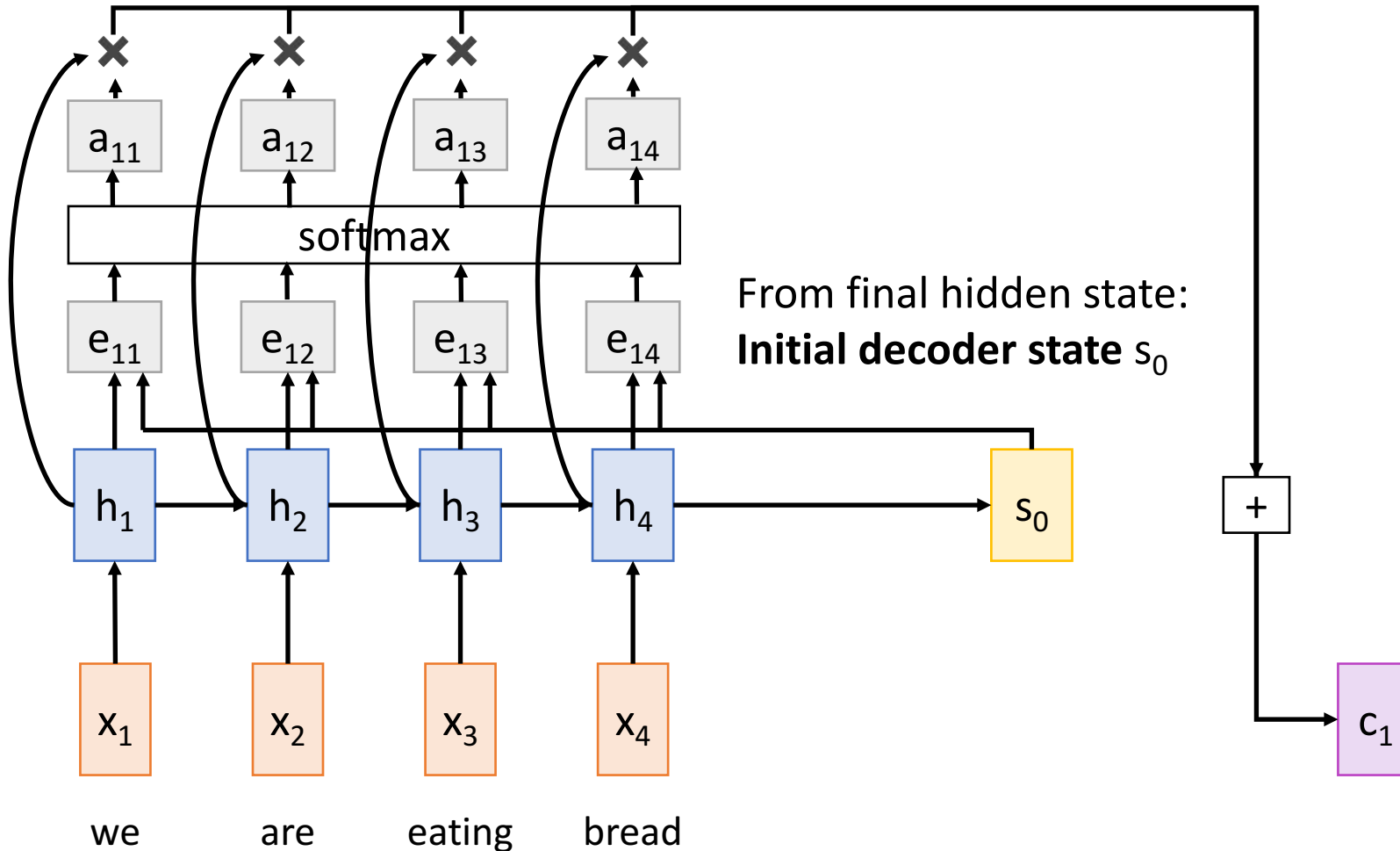
Sequence-to-Sequence with RNNs and Attention



Compute (scalar) **alignment scores**
 $e_{t,i} = f_{\text{att}}(s_{t-1}, h_i)$ (f_{att} is an MLP)

Normalize alignment scores
to get **attention weights**
 $0 < a_{t,i} < 1 \quad \sum_i a_{t,i} = 1$

Sequence-to-Sequence with RNNs and Attention

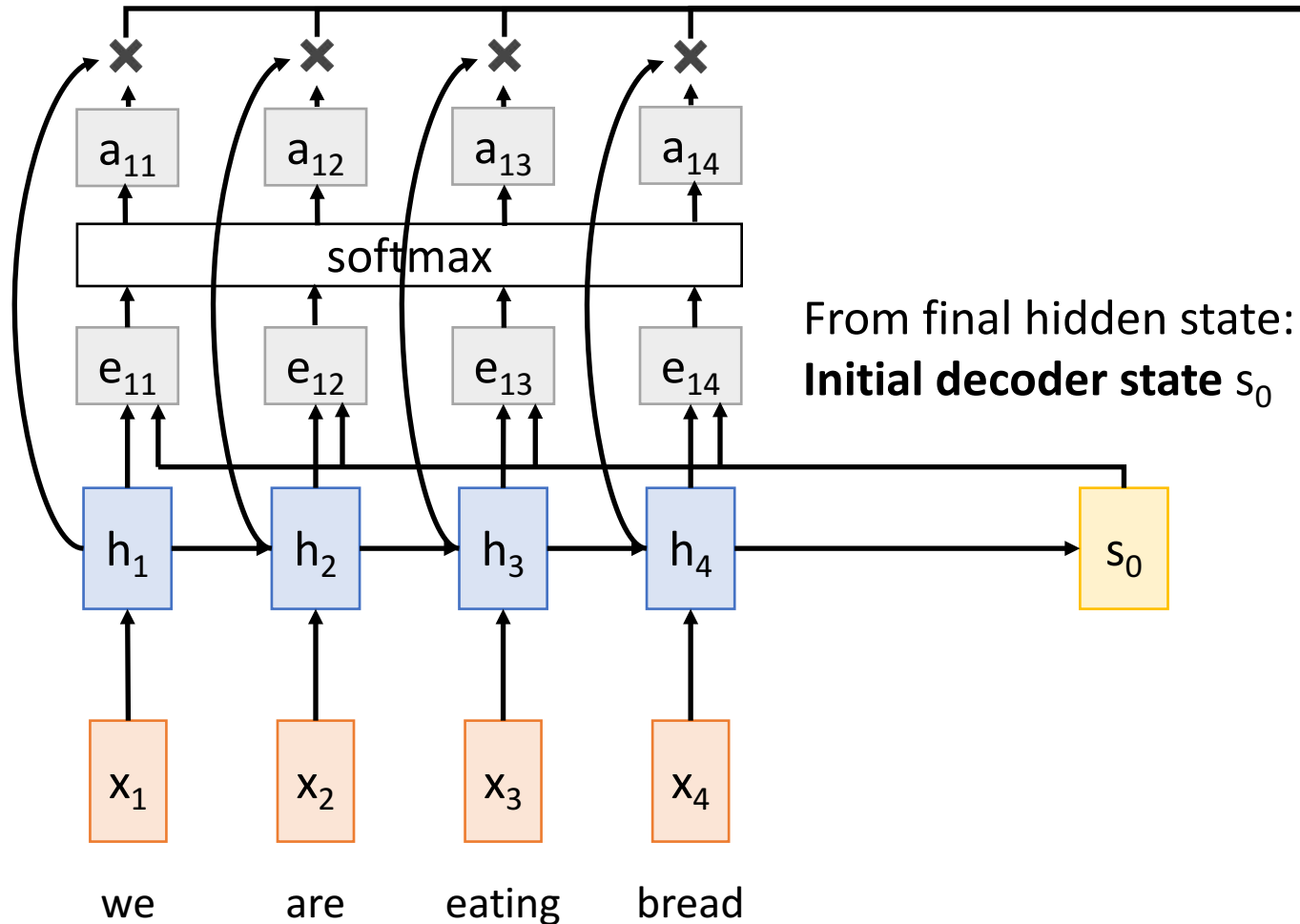


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Compute context vector as linear
combination of hidden states
 $c_t = \sum_i a_{t,i} h_i$

Sequence-to-Sequence with RNNs and Attention



Compute (scalar) **alignment scores**
 $e_{t,i} = f_{\text{att}}(s_{t-1}, h_i)$ (f_{att} is an MLP)

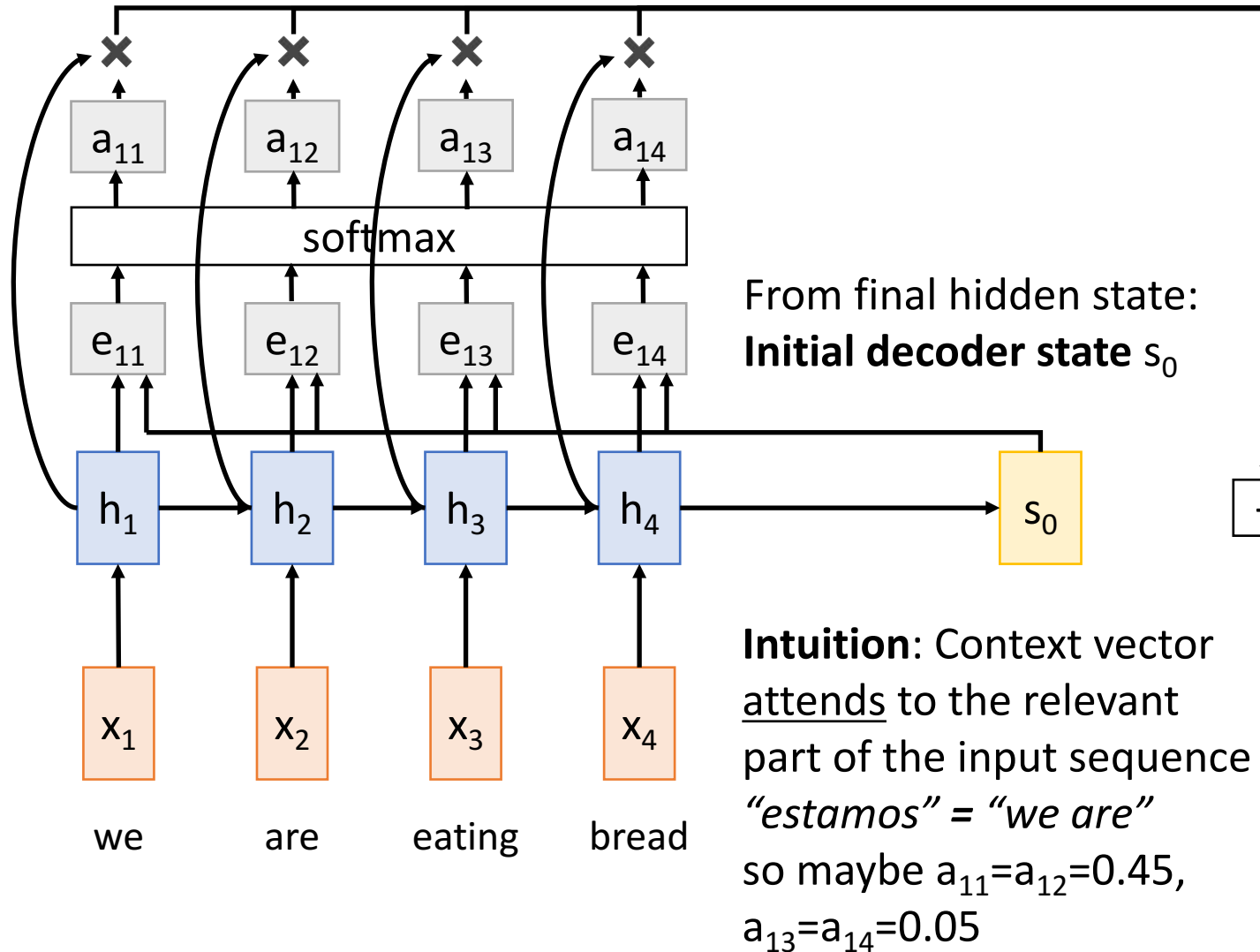
Normalize alignment scores
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 $0 < a_{t,i} < 1 \quad \sum_i a_{t,i} = 1$

Compute context vector as linear
combination of hidden states
 $c_t = \sum_i a_{t,i} h_i$

Use context vector in
decoder: $s_t = g_U(y_{t-1}, h_{t-1}, c_t)$

**This is all differentiable! Do not
supervise attention weights –
backprop through everything**

Sequence-to-Sequence with RNNs and Attention



Compute (scalar) **alignment scores**
 $e_{t,i} = f_{\text{att}}(s_{t-1}, h_i)$ (f_{att} is an MLP)

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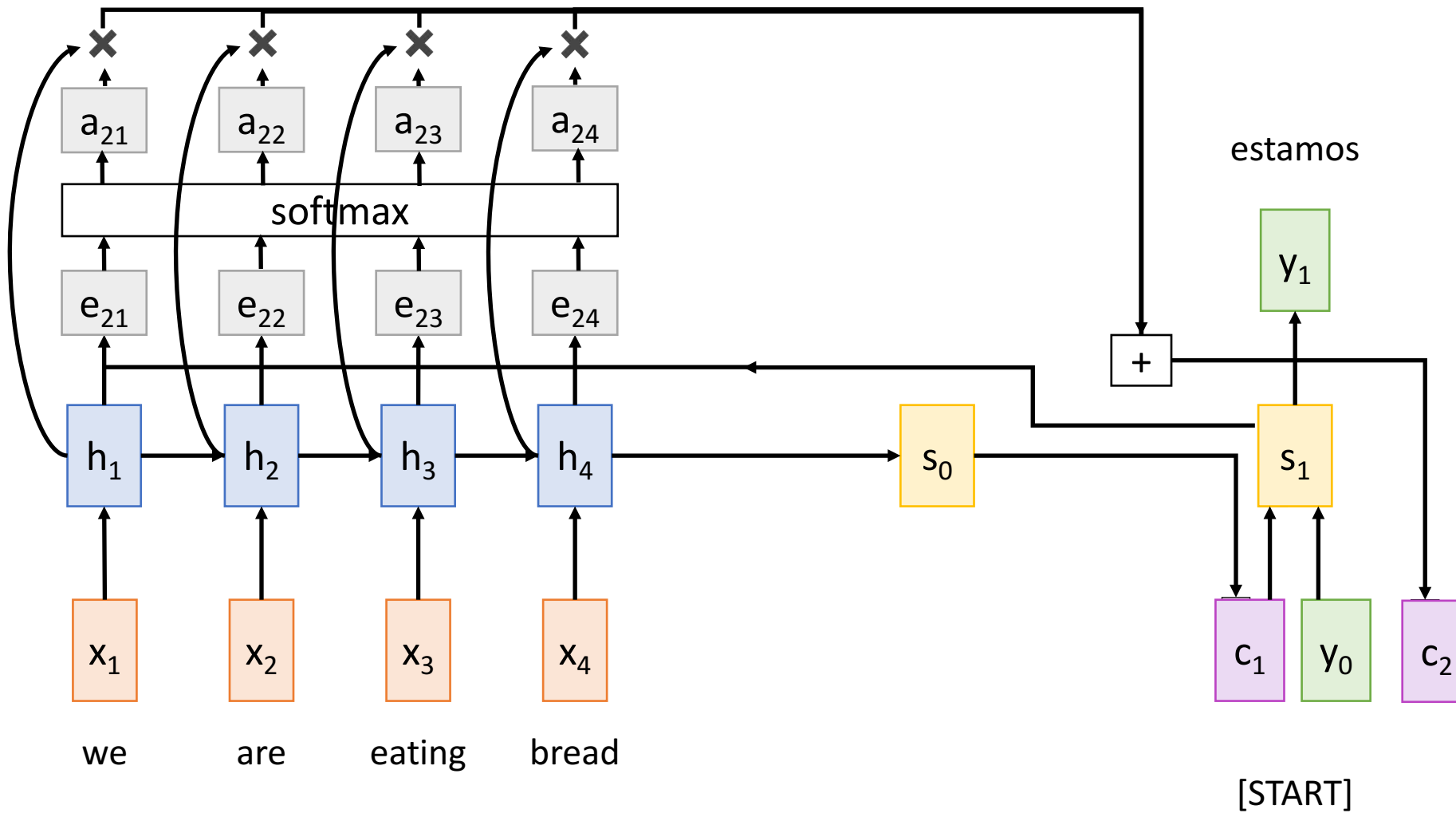
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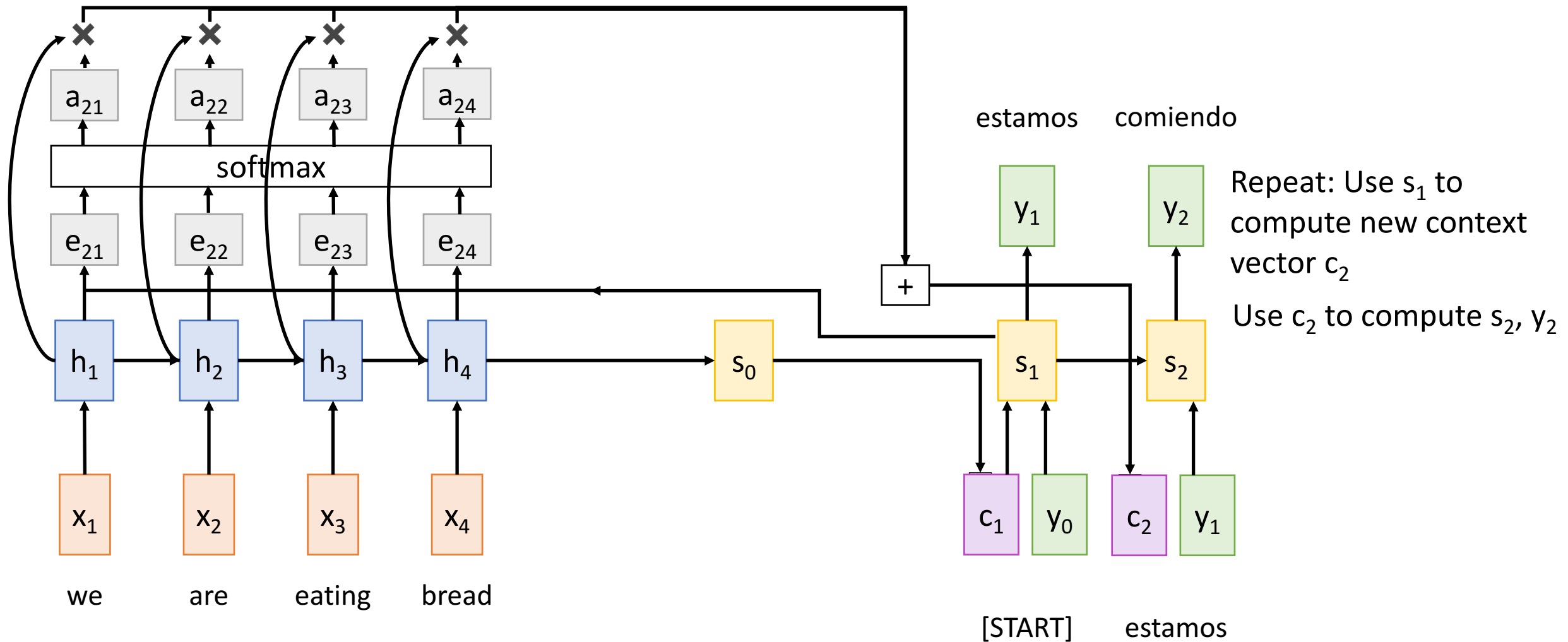
**This is all differentiable! Do not
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Sequence-to-Sequence with RNNs

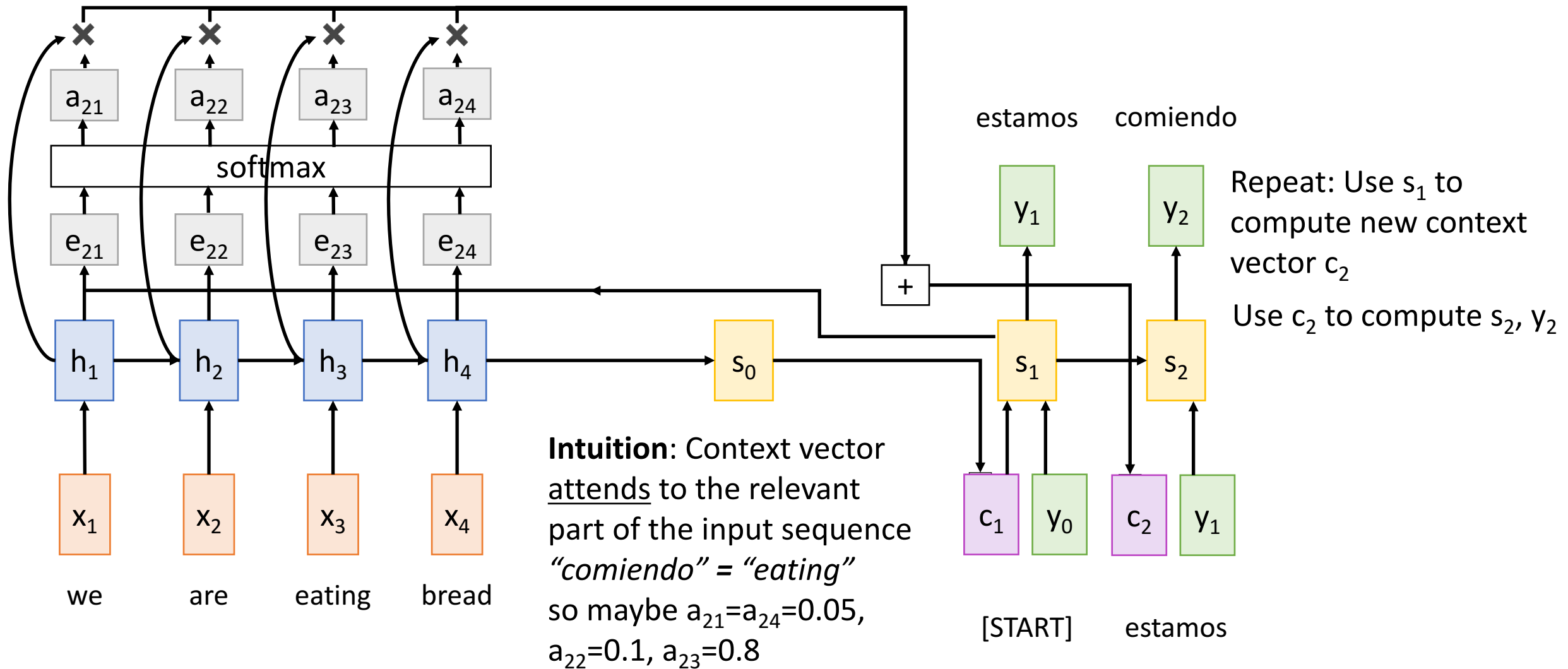
Repeat: Use s_1 to compute new context vector c_2



Sequence-to-Sequence with RNNs and Attention



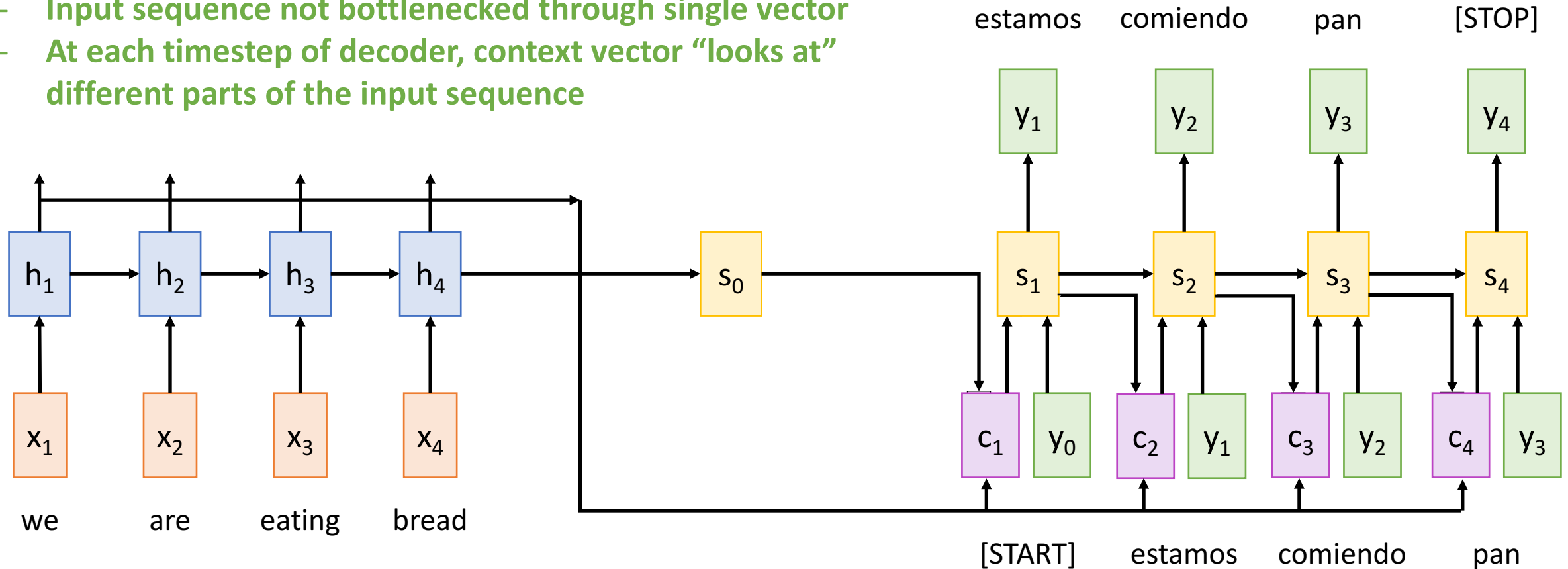
Sequence-to-Sequence with RNNs and Attention



Sequence-to-Sequence with RNNs and Attention

Use a different context vector in each timestep of decoder

- Input sequence not bottlenecked through single vector
- At each timestep of decoder, context vector “looks at” different parts of the input sequence



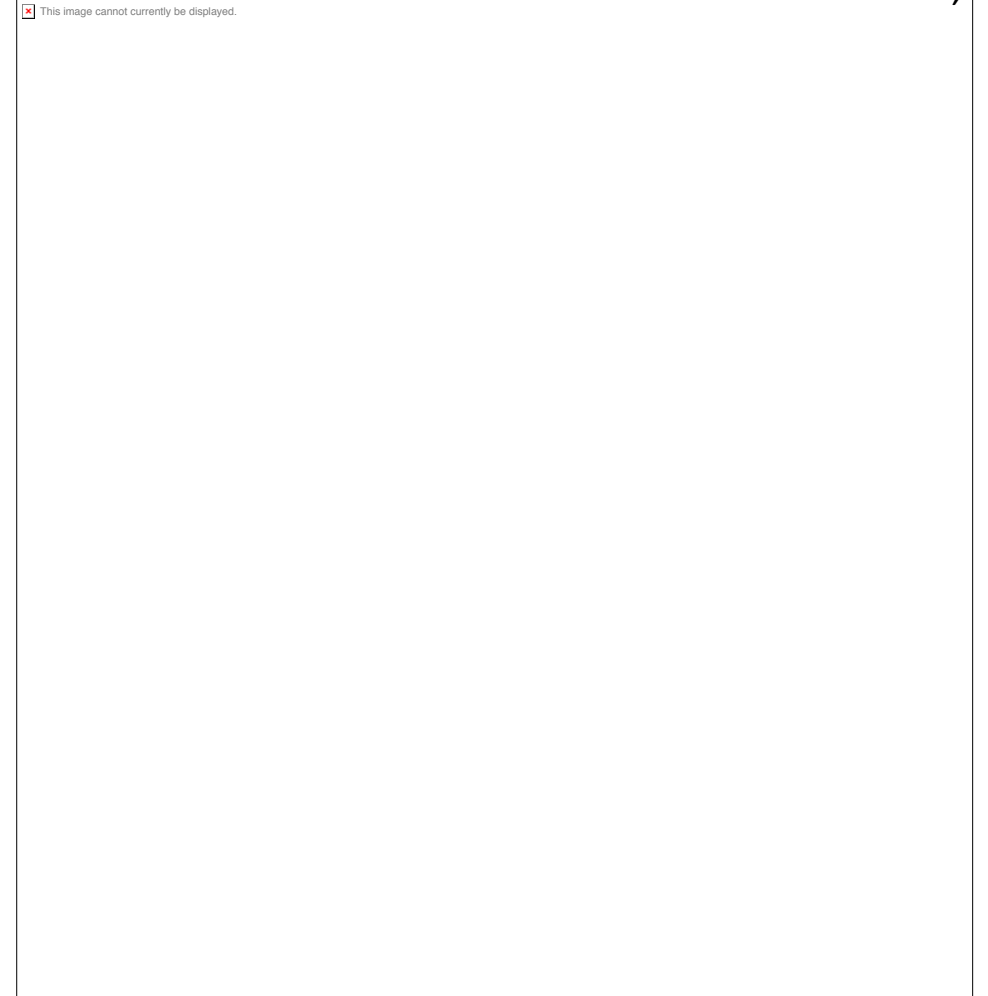
Sequence-to-Sequence with RNNs and Attention

Visualize attention weights $a_{t,i}$

Example: English to French translation

Input: “The agreement on the European Economic Area was signed in August 1992.”

Output: “L’accord sur la zone économique européenne a été signé en août 1992.”



Bahdanau et al, “Neural machine translation by jointly learning to align and translate”, ICLR 2015

Sequence-to-Sequence with RNNs and Attention

Example: English to French translation

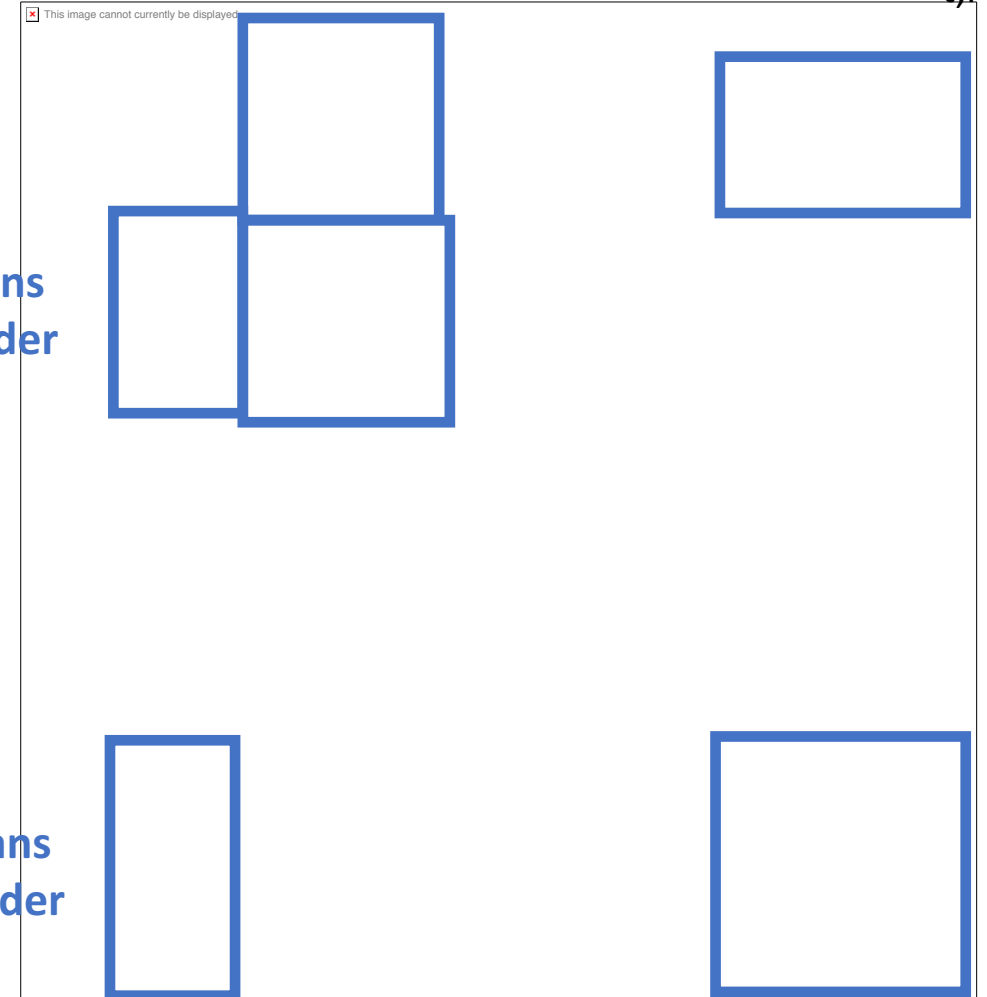
Input: “**The agreement on the** European Economic Area was signed **in August 1992.**”

Output: “**L’accord sur la** zone économique européenne a été signé **en août 1992.**”

Diagonal attention means words correspond in order

Diagonal attention means words correspond in order

Visualize attention weights $a_{t,i}$



Sequence-to-Sequence with RNNs and Attention

Example: English to French translation

Input: “The agreement on the European Economic Area was signed in August 1992.”

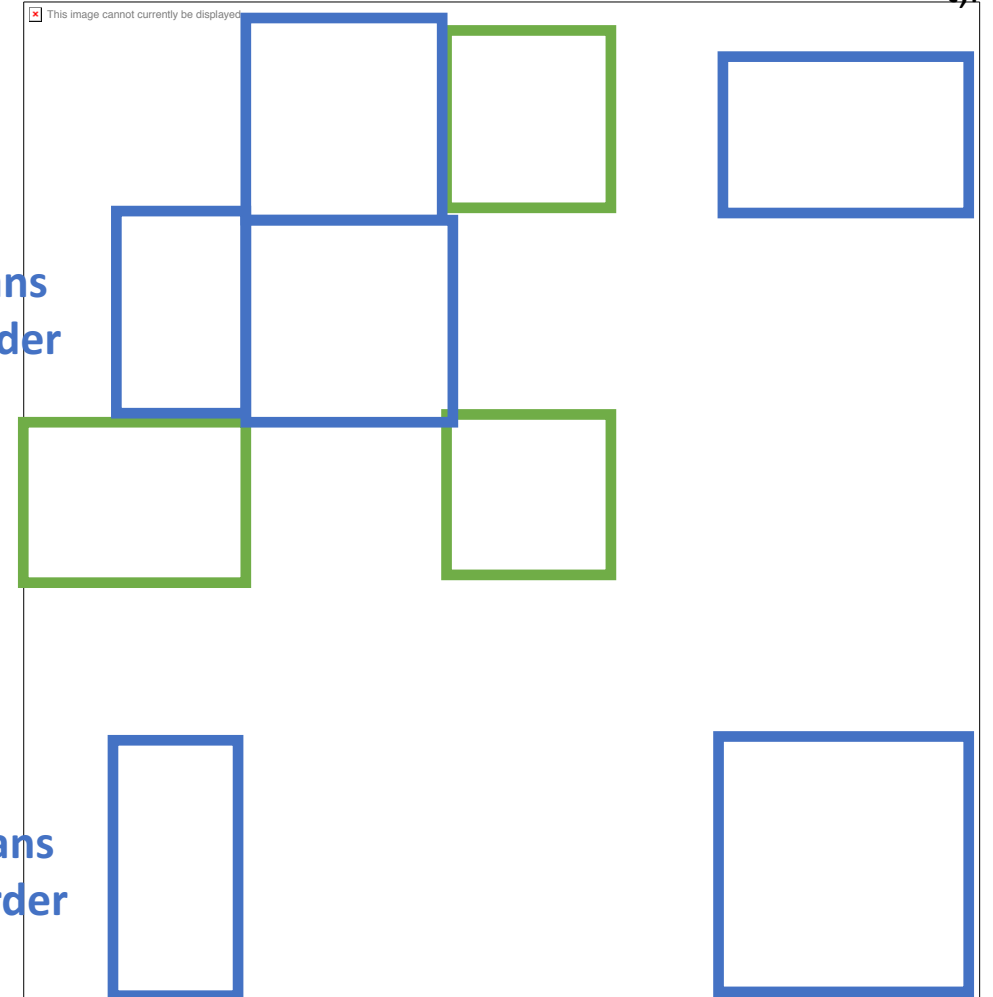
Output: “L’accord sur la zone économique européenne a été signé en août 1992.”

Diagonal attention means words correspond in order

Attention figures out different word orders

Diagonal attention means words correspond in order

Visualize attention weights $a_{t,i}$



Sequence-to-Sequence with RNNs and Attention

Example: English to French translation

Input: “The agreement on the European Economic Area was signed in August 1992.”

Output: “L’accord sur la zone économique européenne a été signé en août 1992.”

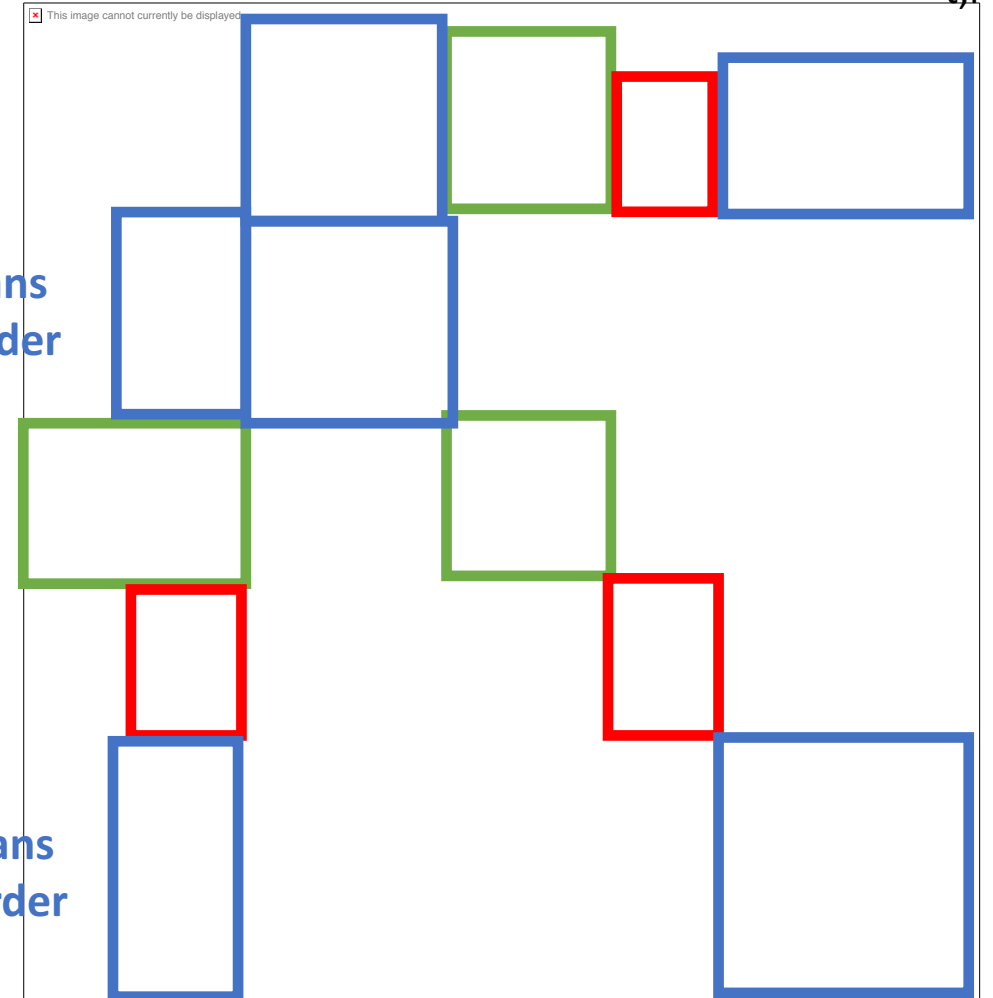
Diagonal attention means words correspond in order

Attention figures out different word orders

Verb conjugation

Diagonal attention means words correspond in order

Visualize attention weights $a_{t,i}$



Sequence-to-Sequence with RNNs and Attention

The decoder doesn't use the fact that h_i form an ordered sequence – it just treats them as an unordered set $\{h_i\}$

Can use similar architecture given any set of input hidden vectors $\{h_i\}$!

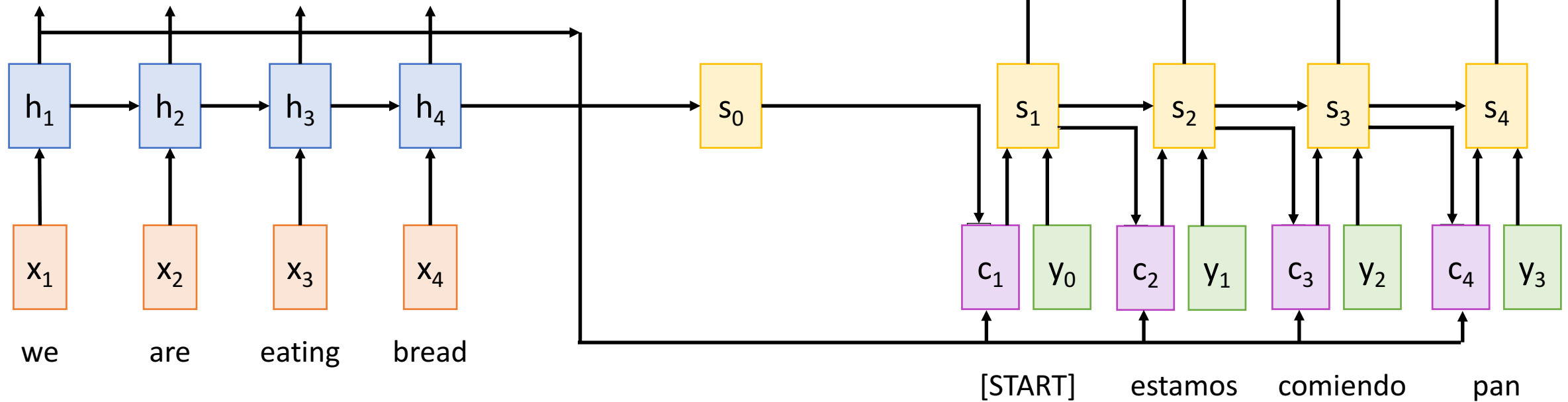
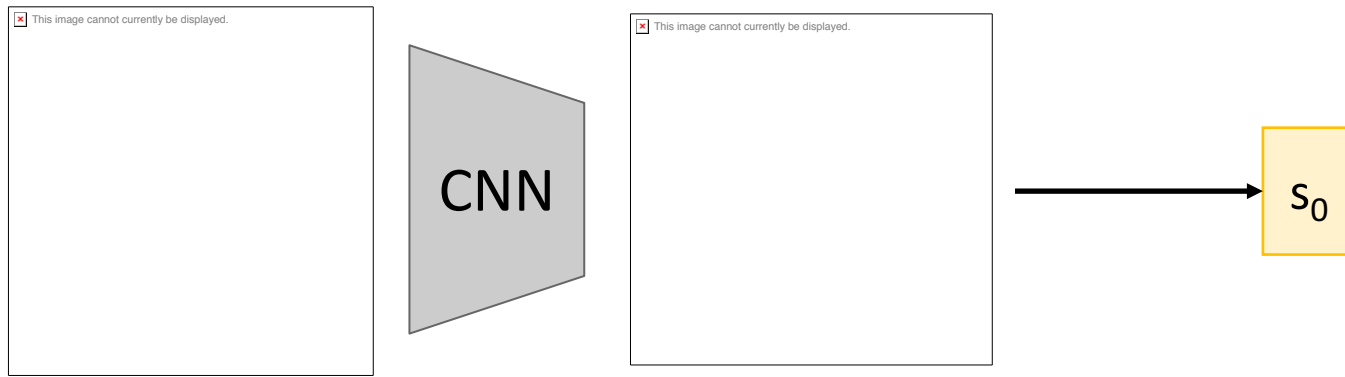


Image Captioning with RNNs and Attention

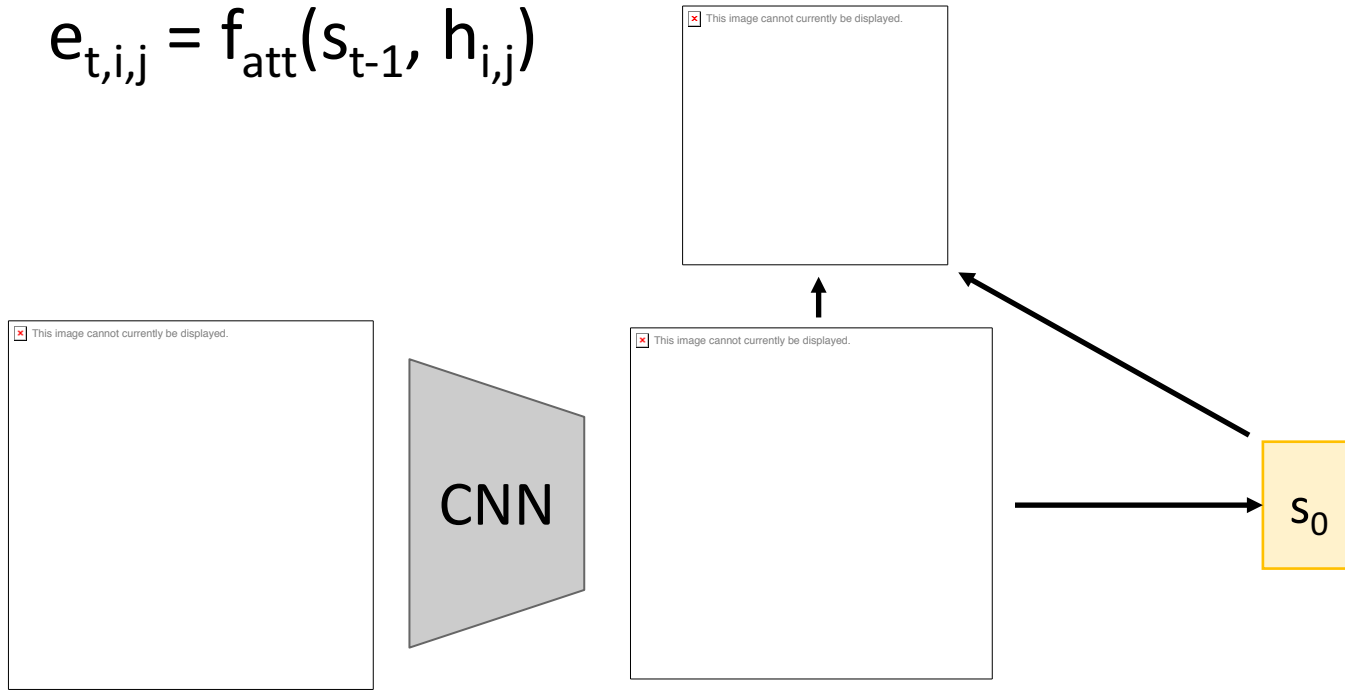


Use a CNN to compute a
grid of features for an image

Image Captioning with RNNs and Attention

$$e_{t,i,j} = f_{\text{att}}(s_{t-1}, h_{i,j})$$

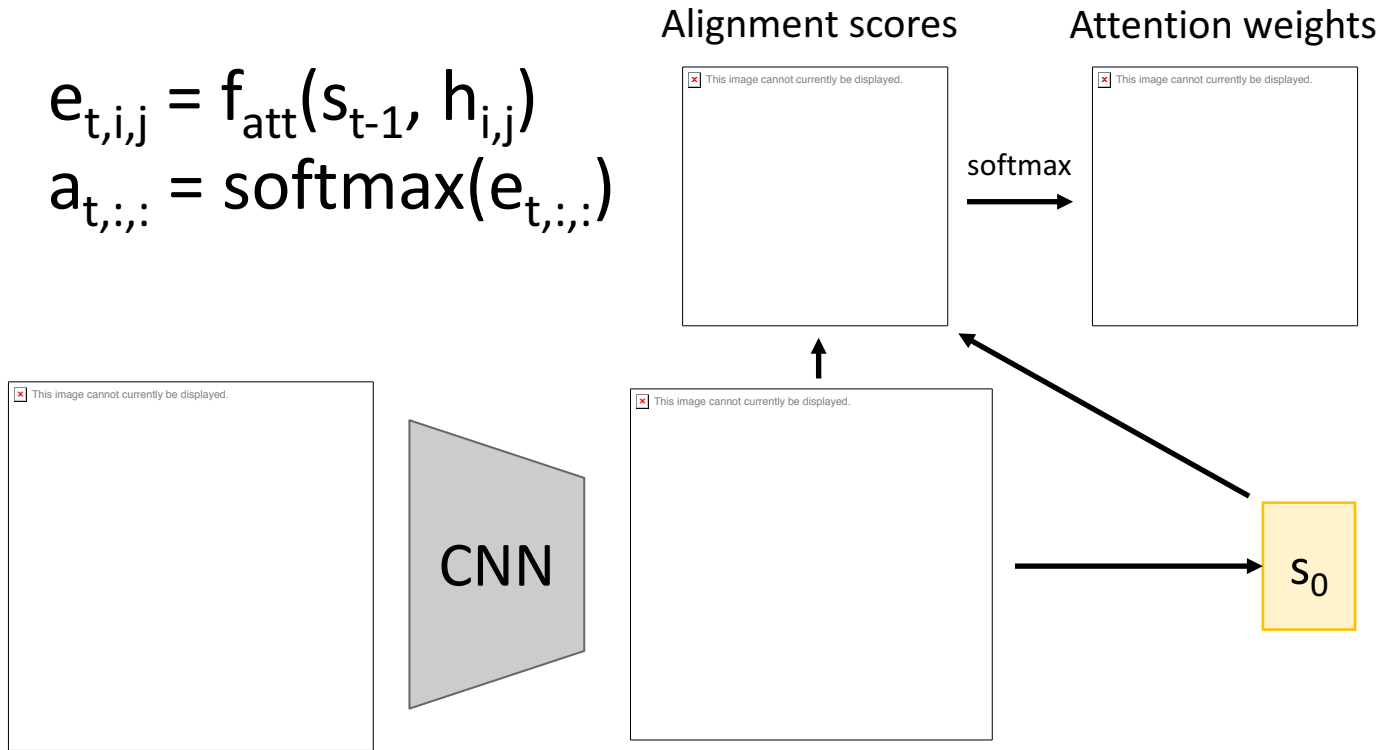
Alignment scores



Use a CNN to compute a
grid of features for an image

Image Captioning with RNNs and Attention

$$e_{t,i,j} = f_{\text{att}}(s_{t-1}, h_{i,j})$$
$$a_{t,:,:} = \text{softmax}(e_{t,:,:})$$



Use a CNN to compute a
grid of features for an image

Image Captioning with RNNs and Attention

$$e_{t,i,j} = f_{\text{att}}(s_{t-1}, h_{i,j})$$
$$a_{t,:} = \text{softmax}(e_{t,:})$$
$$c_t = \sum_{i,j} a_{t,i,j} h_{i,j}$$

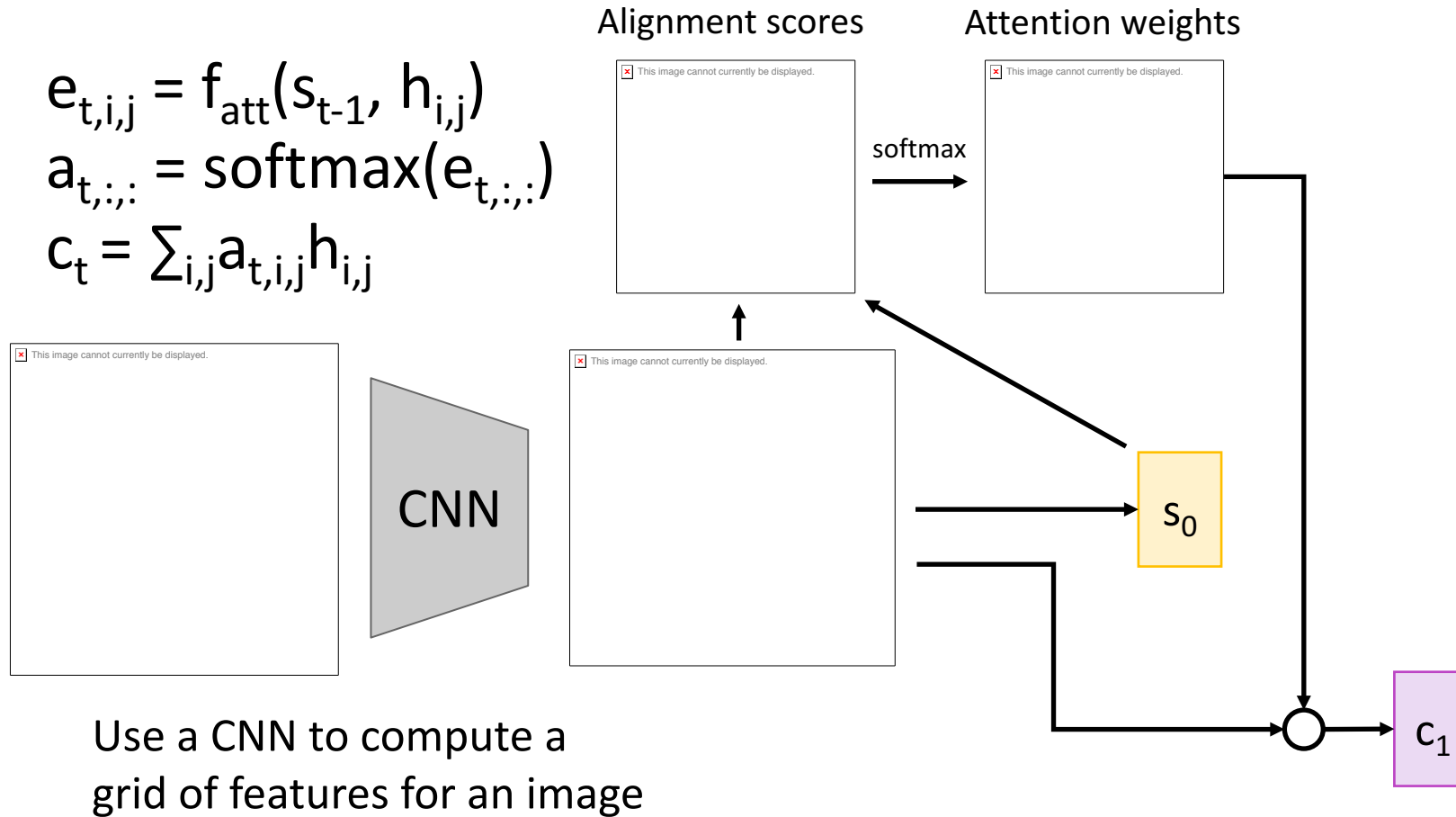


Image Captioning with RNNs and Attention

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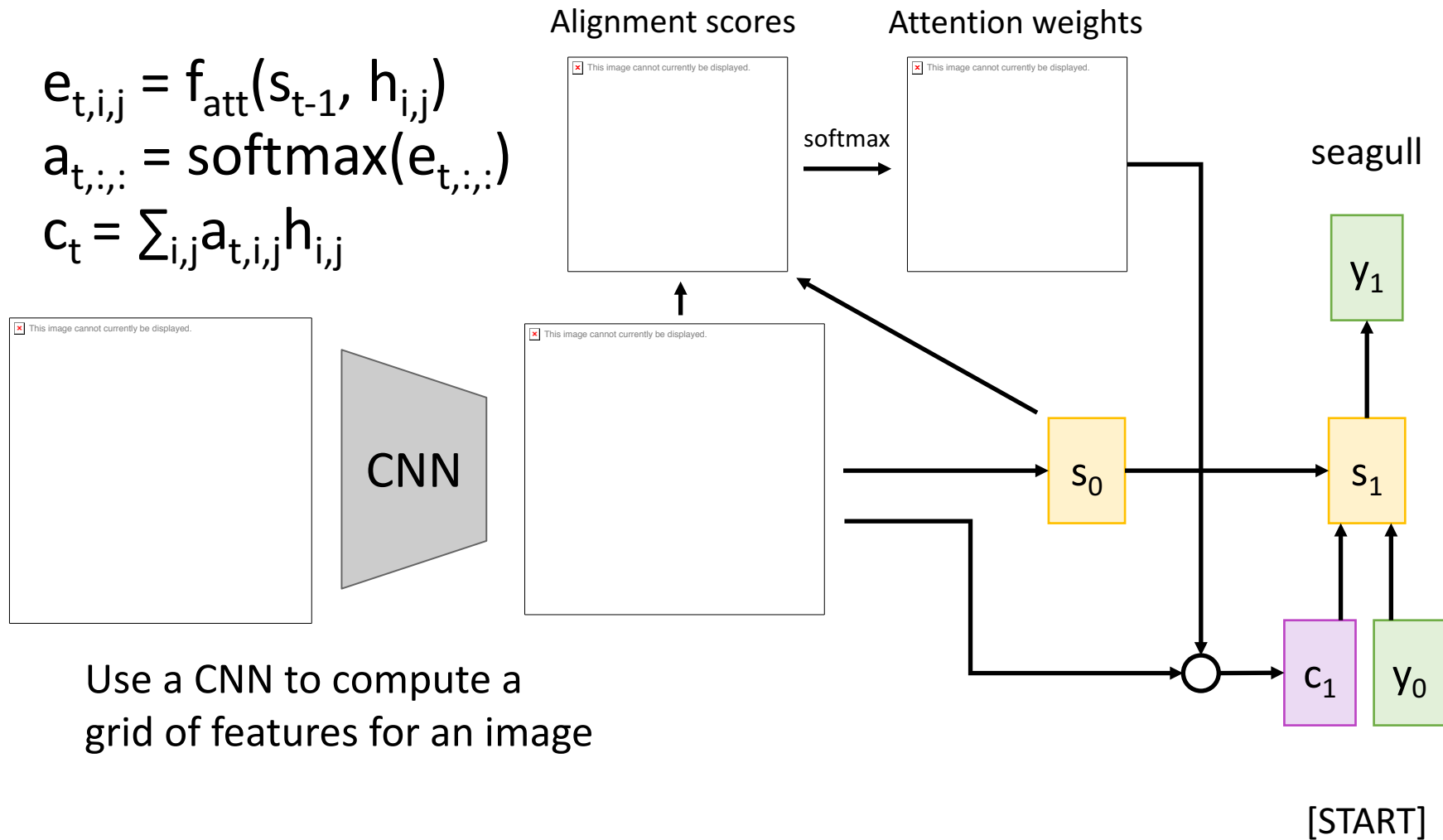


Image Captioning with RNNs and Attention

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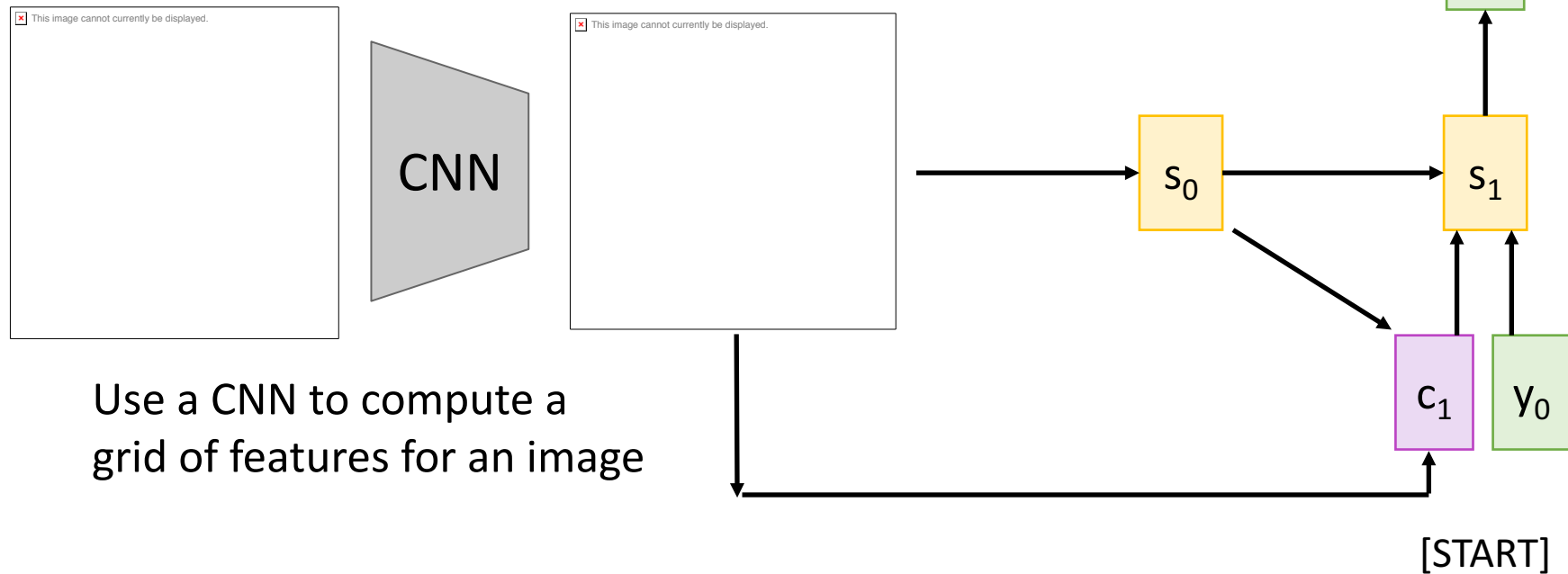
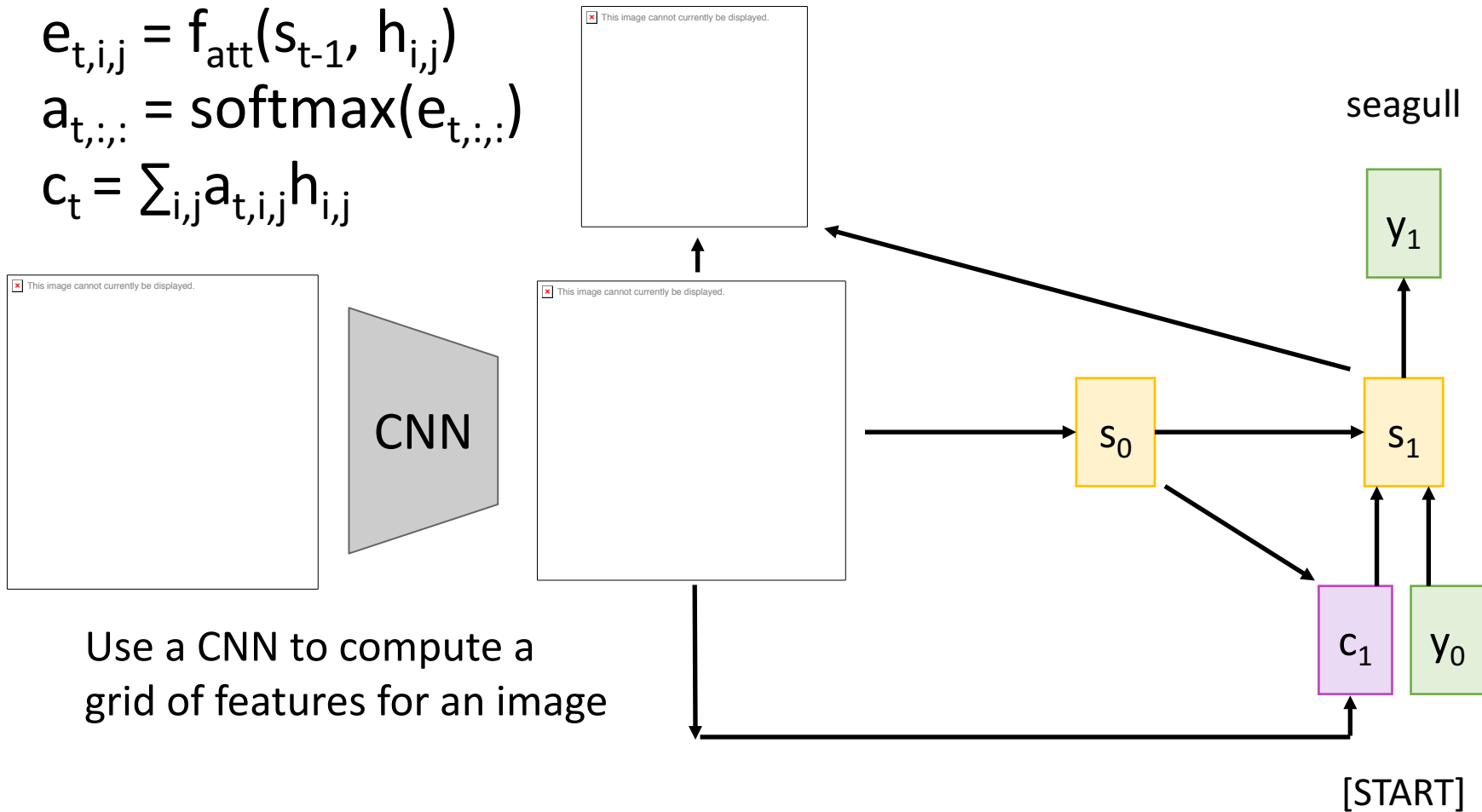


Image Captioning with RNNs and Attention

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Alignment scores



Xu et al, "Show, Attend, and Tell: Neural Image Caption Generation with Visual Attention", ICML 2015

Image Captioning with RNNs and Attention

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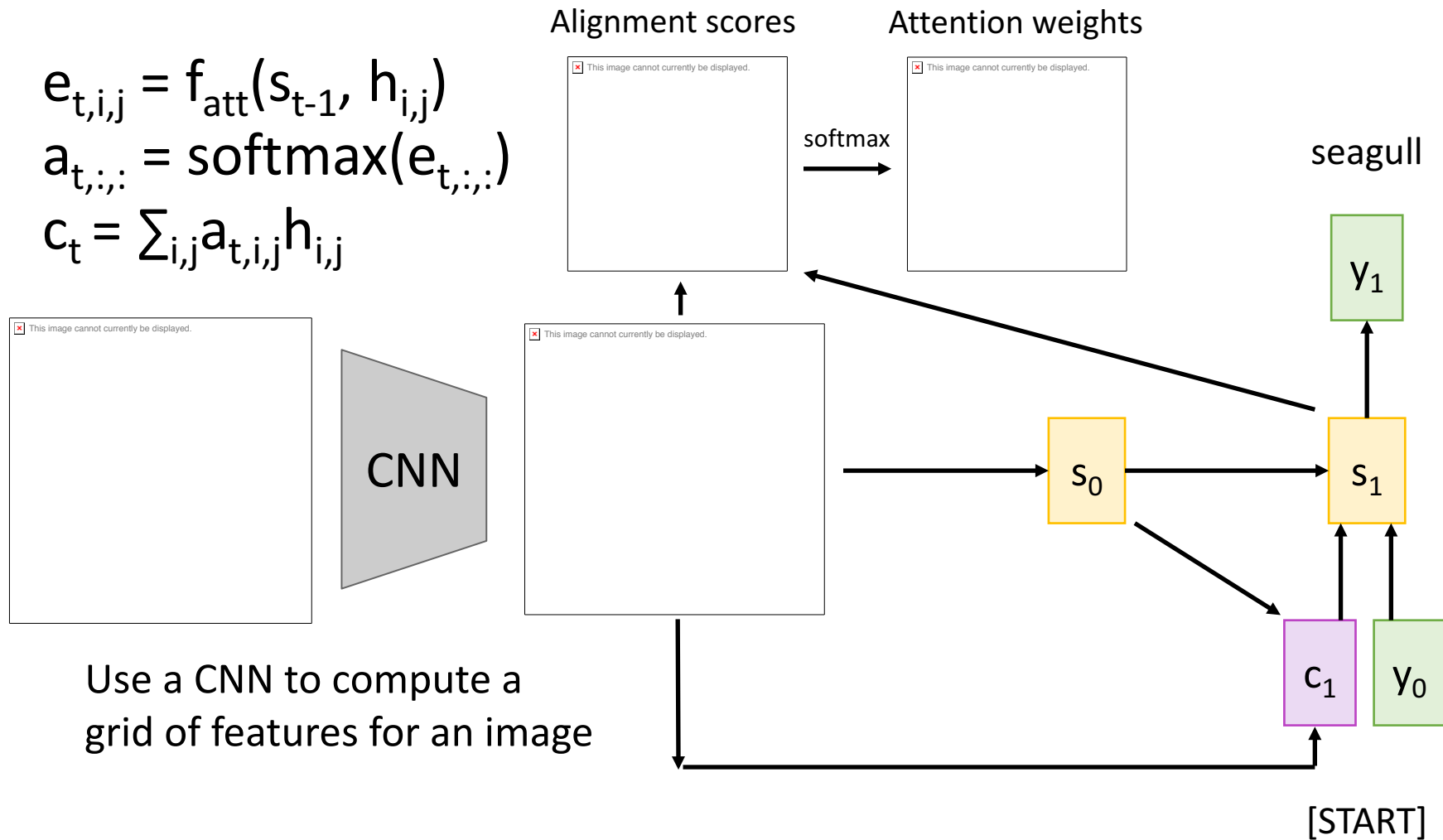
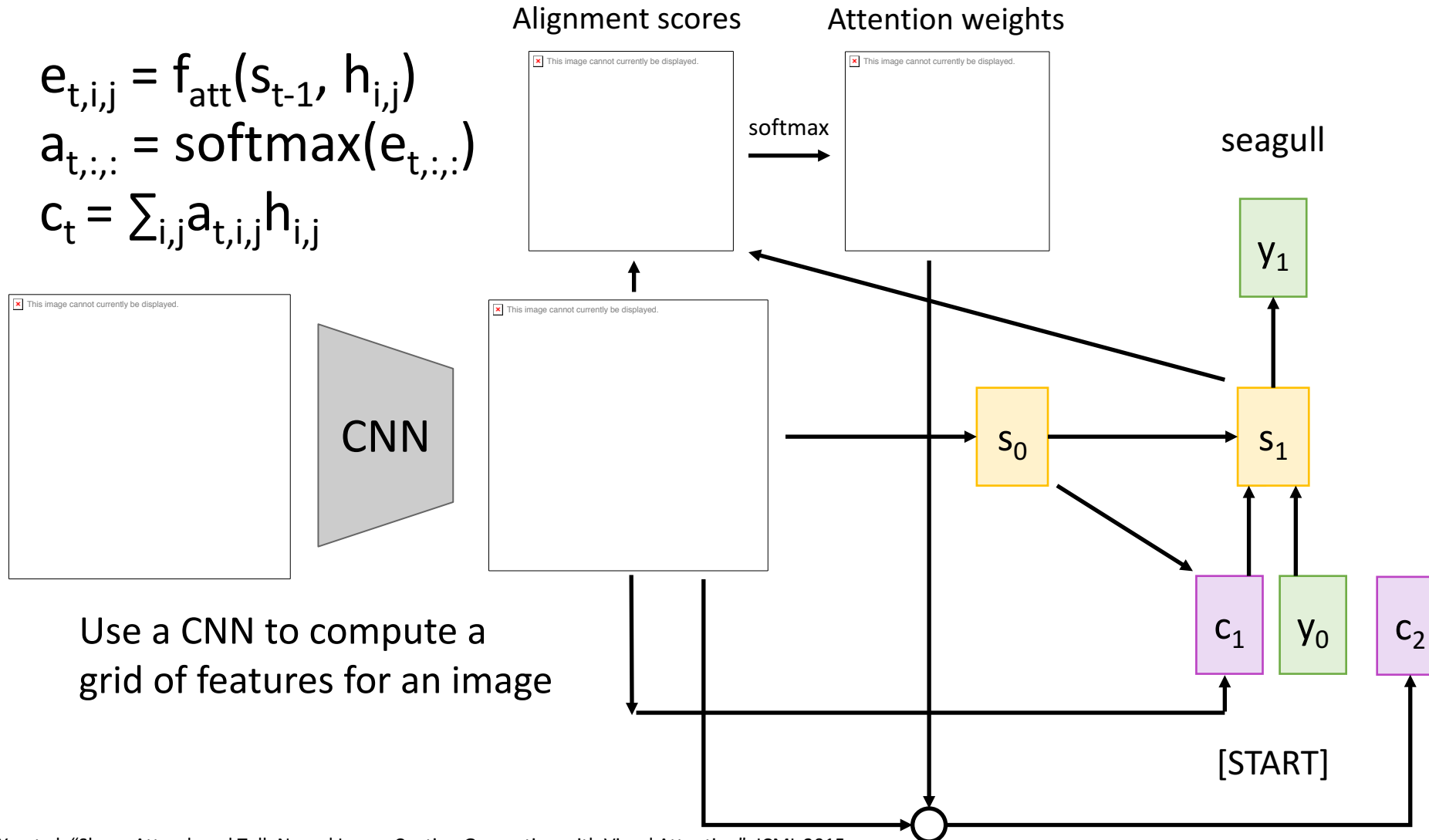


Image Captioning with RNNs and Attention

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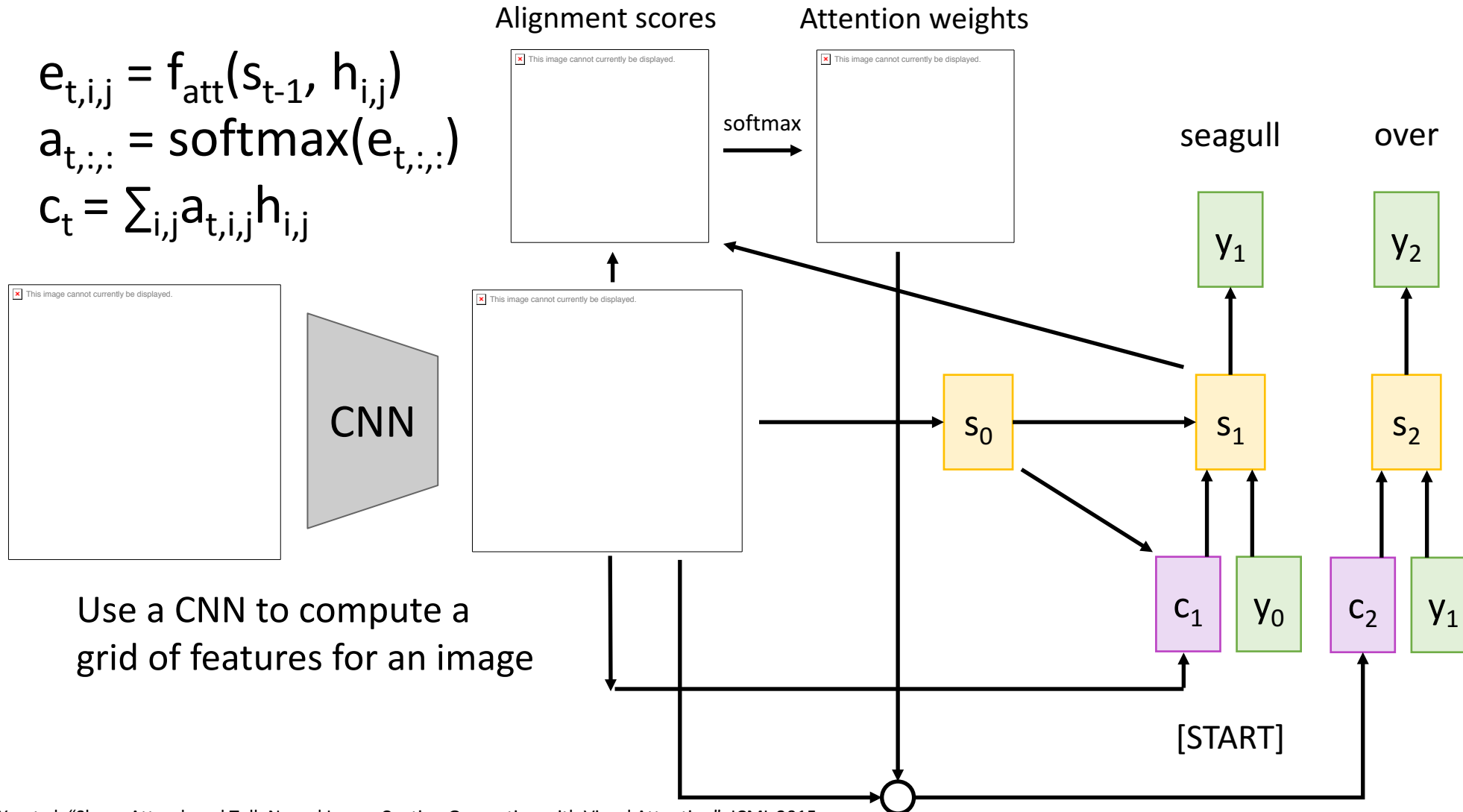
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Image Captioning with RNNs and Attention

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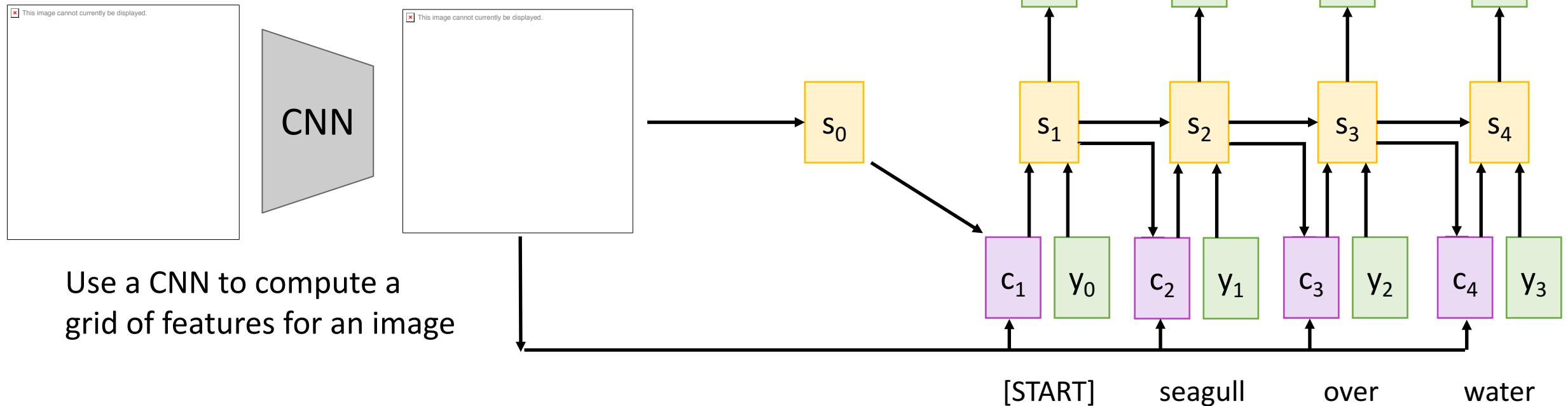


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Image Captioning with RNNs and Attention

$$e_{t,i,j} = f_{\text{att}}(s_{t-1}, h_{i,j})$$
$$a_{t,:} = \text{softmax}(e_{t,:})$$
$$c_t = \sum_{i,j} a_{t,i,j} h_{i,j}$$

Each timestep of decoder uses a different context vector that looks at different parts of the input image



$h_{1,1}$	$h_{1,2}$	$h_{1,3}$
$h_{2,1}$	$h_{2,2}$	$h_{2,3}$
$h_{3,1}$	$h_{3,2}$	$h_{3,3}$

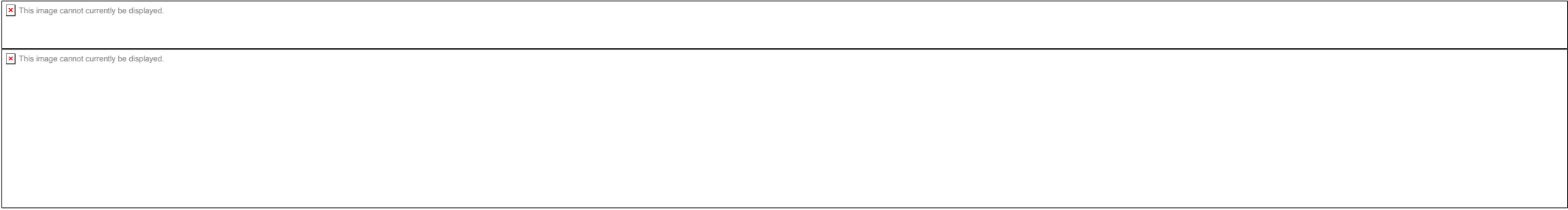
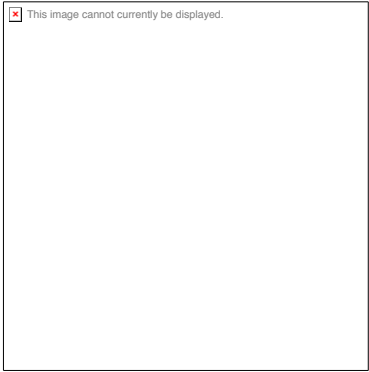
$e_{1,1,1}$	$e_{1,1,2}$	$e_{1,1,3}$
$e_{1,2,1}$	$e_{1,2,2}$	$e_{1,2,3}$
$e_{1,3,1}$	$e_{1,3,2}$	$e_{1,3,3}$

$a_{1,1,1}$	$a_{1,1,2}$	$a_{1,1,3}$
$a_{1,2,1}$	$a_{1,2,2}$	$a_{1,2,3}$
$a_{1,3,1}$	$a_{1,3,2}$	$a_{1,3,3}$

$e_{2,1,1}$	$e_{2,1,2}$	$e_{2,1,3}$
$e_{2,2,1}$	$e_{2,2,2}$	$e_{2,2,3}$
$e_{2,3,1}$	$e_{2,3,2}$	$e_{2,3,3}$


$a_{2,1,1}$	$a_{2,1,2}$	$a_{2,1,3}$
$a_{2,2,1}$	$a_{2,2,2}$	$a_{2,2,3}$
$a_{2,3,1}$	$a_{2,3,2}$	$a_{2,3,3}$

Image Captioning with RNNs and Attention



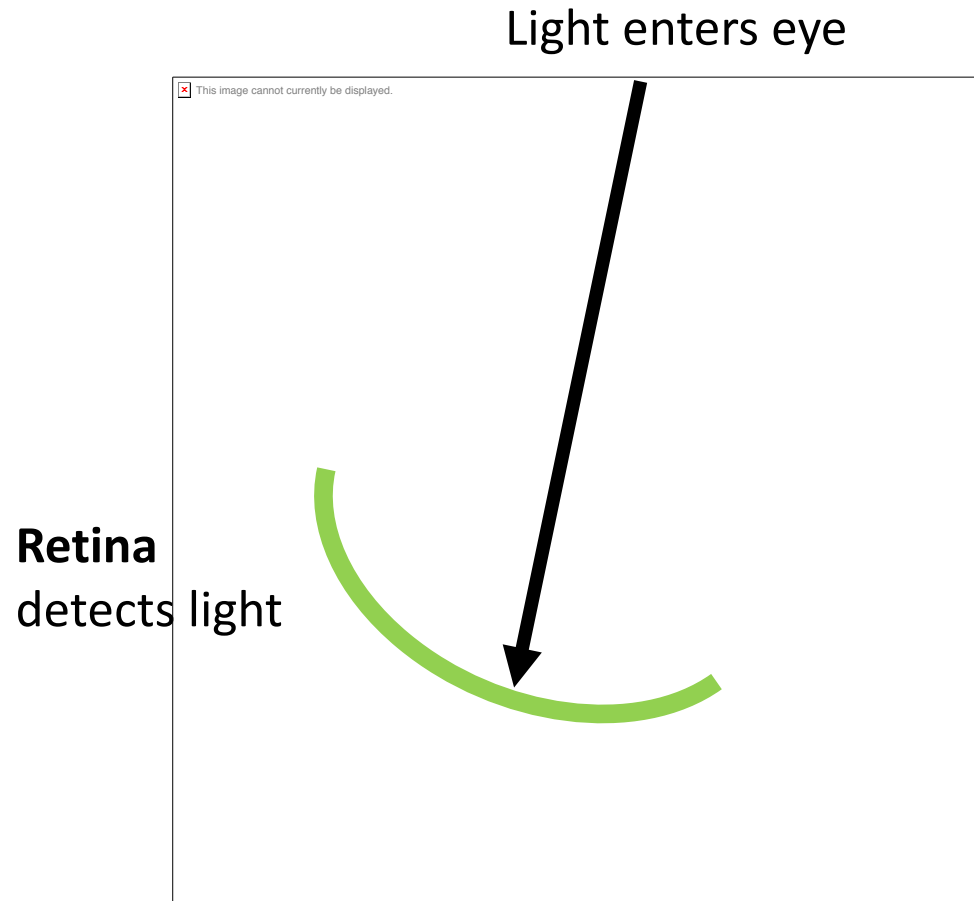
Xu et al, "Show, Attend, and Tell: Neural Image Caption Generation with Visual Attention", ICML 2015

Image Captioning with RNNs and Attention

 This image cannot currently be displayed.

Xu et al, "Show, Attend, and Tell: Neural Image Caption Generation with Visual Attention", ICML 2015

Human Vision: Fovea



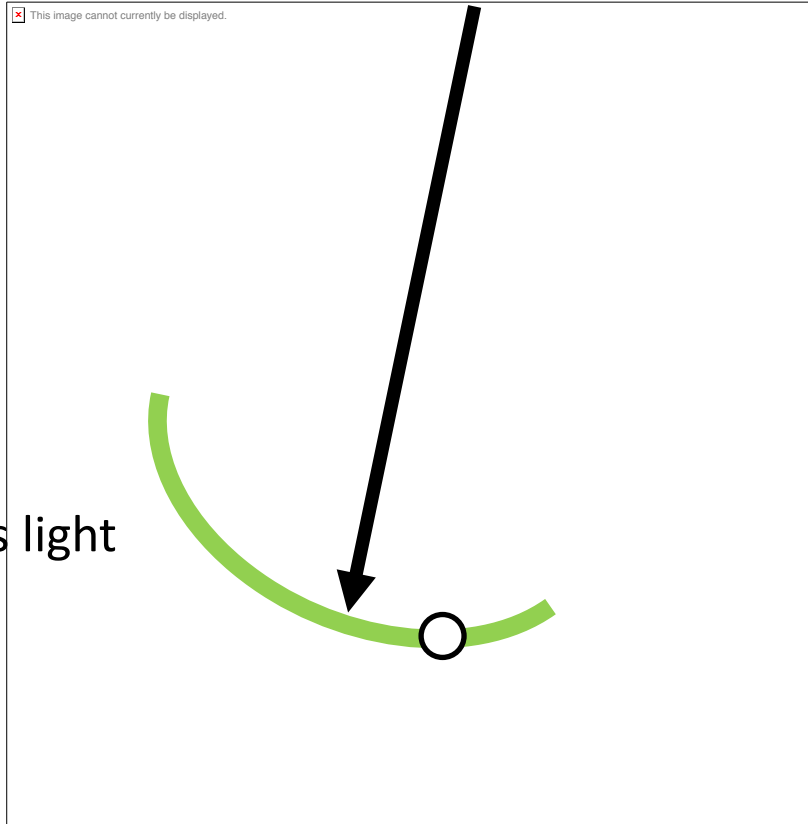
[Eye image](#) is licensed under [CC A-SA 3.0 Unported](#) (added black arrow and green arc)

[Acuity graph](#) is licensed under [CC A-SA 3.0 Unported](#)

Human Vision: Fovea

Light enters eye

Retina
detects light



The **fovea** is a tiny region of the retina that can see with high acuity



Human Vision: Saccades

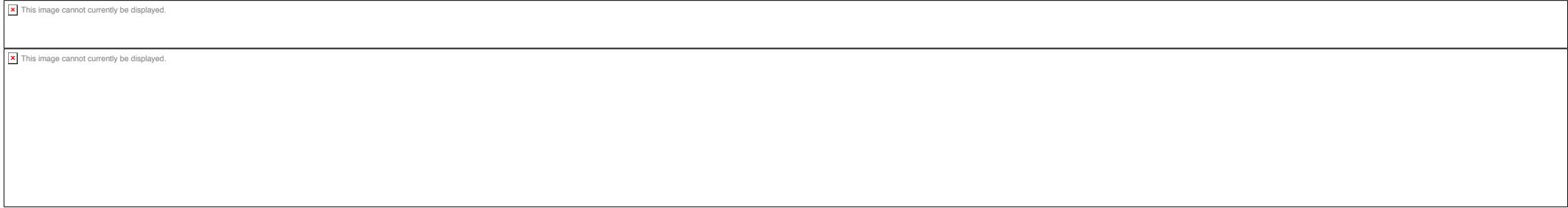
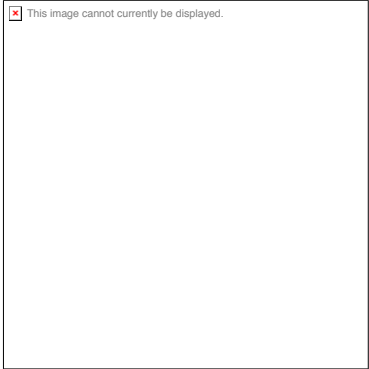
Human eyes are constantly moving so we don't notice



The **fovea** is a tiny region of the retina that can see with high acuity



Image Captioning with RNNs and Attention



Attention weights at each
timestep kind of like
saccades of human eye



X, Attend, and Y

“Show, attend, and tell” (*Xu et al, ICML 2015*)

Look at image, attend to image regions, produce question

“Ask, attend, and answer” (*Xu and Saenko, ECCV 2016*)

“Show, ask, attend, and answer” (*Kazemi and Elqursh, 2017*)

Read text of question, attend to image regions, produce answer

“Listen, attend, and spell” (*Chan et al, ICASSP 2016*)

Process raw audio, attend to audio regions while producing text

“Listen, attend, and walk” (*Mei et al, AAAI 2016*)

Process text, attend to text regions, output navigation commands

“Show, attend, and interact” (*Qureshi et al, ICRA 2017*)

Process image, attend to image regions, output robot control commands

“Show, attend, and read” (*Li et al, AAAI 2019*)

Process image, attend to image regions, output text

Attention Layer

Inputs:

Query vector: \mathbf{q} (Shape: D_Q)

Input vectors: \mathbf{X} (Shape: $N_X \times D_X$)

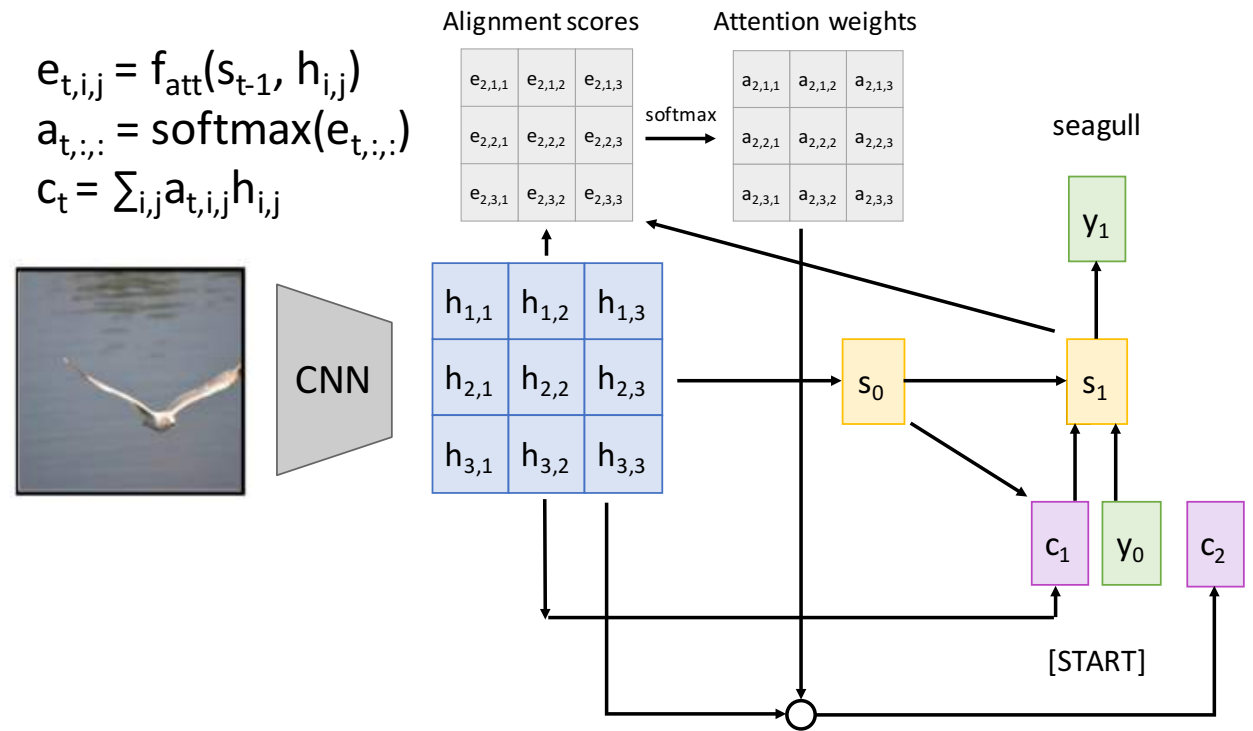
Similarity function: f_{att}

Computation:

Similarities: \mathbf{e} (Shape: N_X) $e_i = f_{\text{att}}(\mathbf{q}, \mathbf{X}_i)$

Attention weights: $\mathbf{a} = \text{softmax}(\mathbf{e})$ (Shape: N_X)

Output vector: $\mathbf{y} = \sum_i a_i \mathbf{X}_i$ (Shape: D_X)



Attention Layer

Inputs:

Query vector: \mathbf{q} (Shape: D_Q)

Input vectors: \mathbf{X} (Shape: $N_X \times D_Q$)

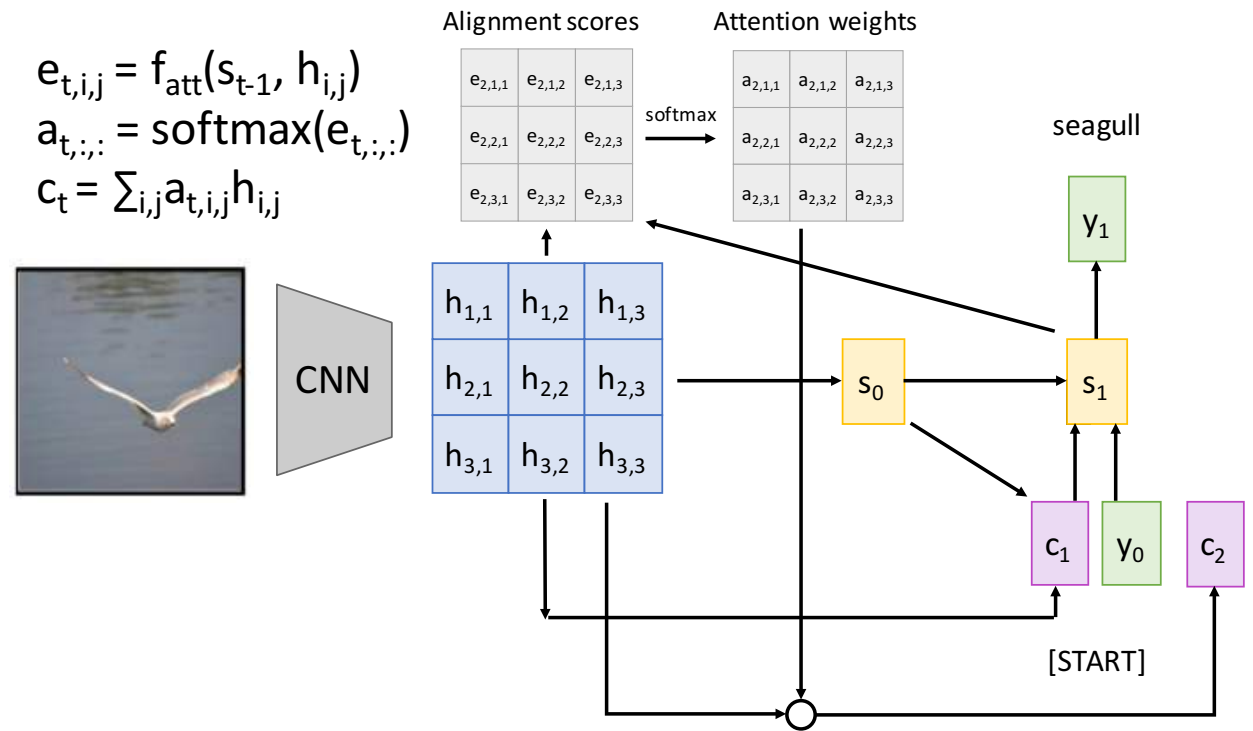
Similarity function: dot product

Computation:

Similarities: \mathbf{e} (Shape: N_X) $\mathbf{e}_i = \mathbf{q} \cdot \mathbf{X}_i$

Attention weights: $\mathbf{a} = \text{softmax}(\mathbf{e})$ (Shape: N_X)

Output vector: $\mathbf{y} = \sum_i \mathbf{a}_i \mathbf{X}_i$ (Shape: D_X)



Changes:

- Use dot product for similarity

Attention Layer

Inputs:

Query vector: \mathbf{q} (Shape: D_Q)

Input vectors: \mathbf{X} (Shape: $N_X \times D_Q$)

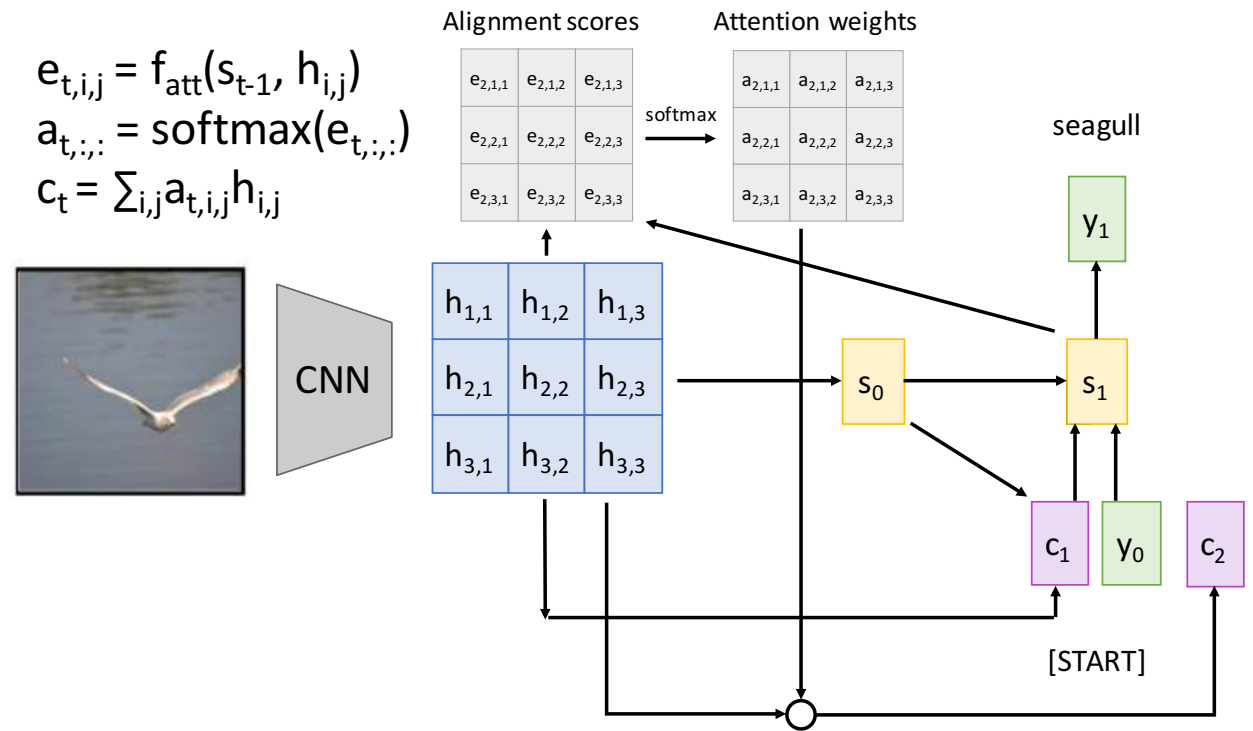
Similarity function: scaled dot product

Computation:

Similarities: \mathbf{e} (Shape: N_X) $e_i = \mathbf{q} \cdot \mathbf{X}_i / \sqrt{D_Q}$

Attention weights: $\mathbf{a} = \text{softmax}(\mathbf{e})$ (Shape: N_X)

Output vector: $\mathbf{y} = \sum_i a_i \mathbf{X}_i$ (Shape: D_X)



Changes:

- Use **scaled** dot product for similarity

Attention Layer

Inputs:

Query vector: \mathbf{q} (Shape: D_Q)

Input vectors: \mathbf{X} (Shape: $N_X \times D_Q$)

Similarity function: scaled dot product

Large similarities will cause softmax to saturate and give vanishing gradients

Recall $a \cdot b = |a| |b| \cos(\text{angle})$

Suppose that a and b are constant vectors of dimension D

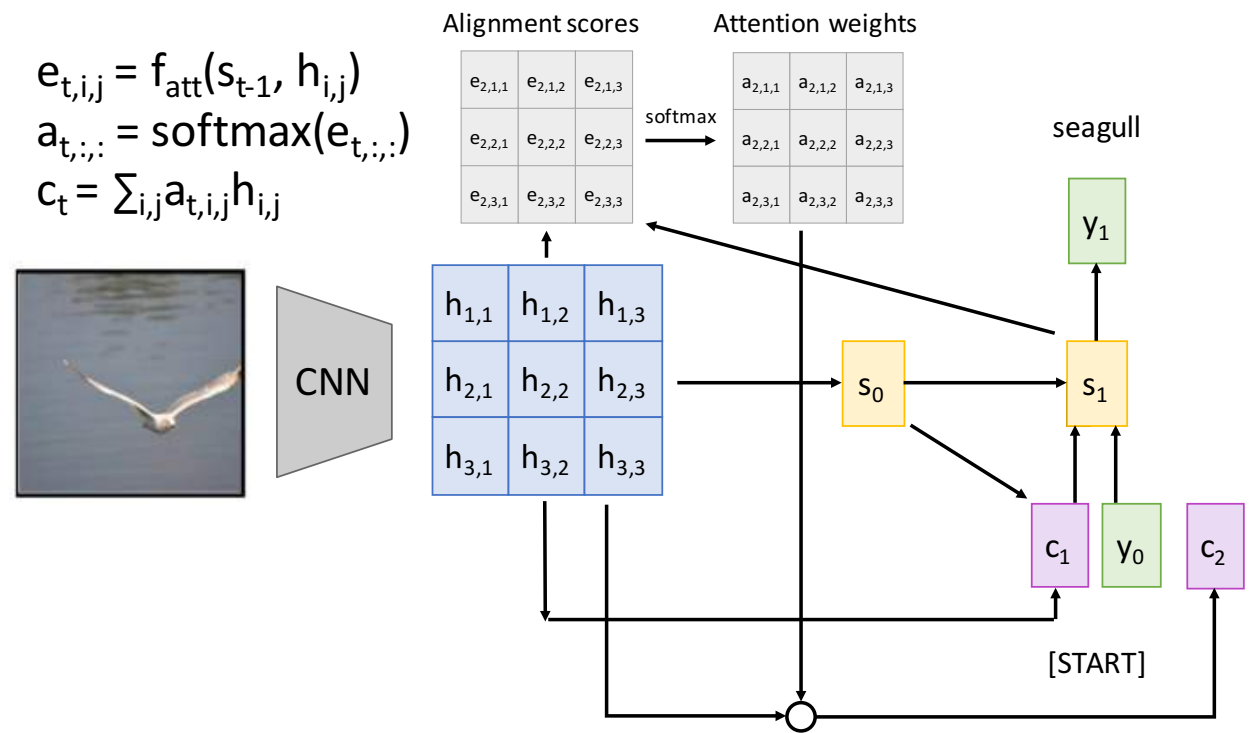
Then $|a| = (\sum_i a_i^2)^{1/2} = a \text{ sqrt}(D)$

Computation:

Similarities: e (Shape: N_X) $e_i = \mathbf{q} \cdot \mathbf{X}_i / \text{sqrt}(D_Q)$

Attention weights: $a = \text{softmax}(e)$ (Shape: N_X)

Output vector: $\mathbf{y} = \sum_i a_i \mathbf{X}_i$ (Shape: D_X)



Changes:

- Use **scaled** dot product for similarity

Attention Layer

Inputs:

Query vectors: **Q** (Shape: $N_Q \times D_Q$)

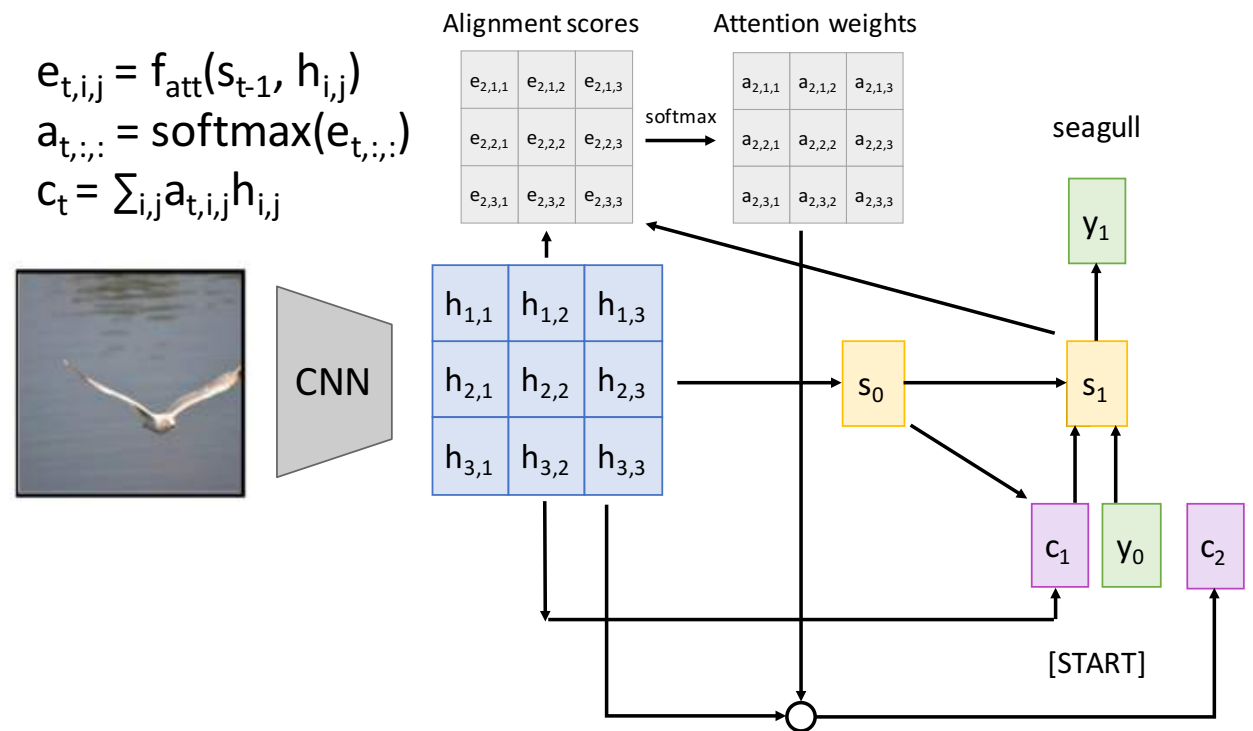
Input vectors: **X** (Shape: $N_X \times D_Q$)

Computation:

Similarities: $E = QX^T$ (Shape: $N_Q \times N_X$) $E_{i,j} = Q_i \cdot X_j / \sqrt{D_Q}$

Attention weights: $A = \text{softmax}(E, \text{dim}=1)$ (Shape: $N_Q \times N_X$)

Output vectors: $Y = AX$ (Shape: $N_Q \times D_X$) $Y_i = \sum_j A_{i,j} X_j$



Changes:

- Use dot product for similarity
- Multiple **query** vectors

Attention Layer

Inputs:

Query vectors: **Q** (Shape: $N_Q \times D_Q$)

Input vectors: **X** (Shape: $N_X \times D_X$)

Key matrix: **W_K** (Shape: $D_X \times D_Q$)

Value matrix: **W_V** (Shape: $D_X \times D_V$)

Computation:

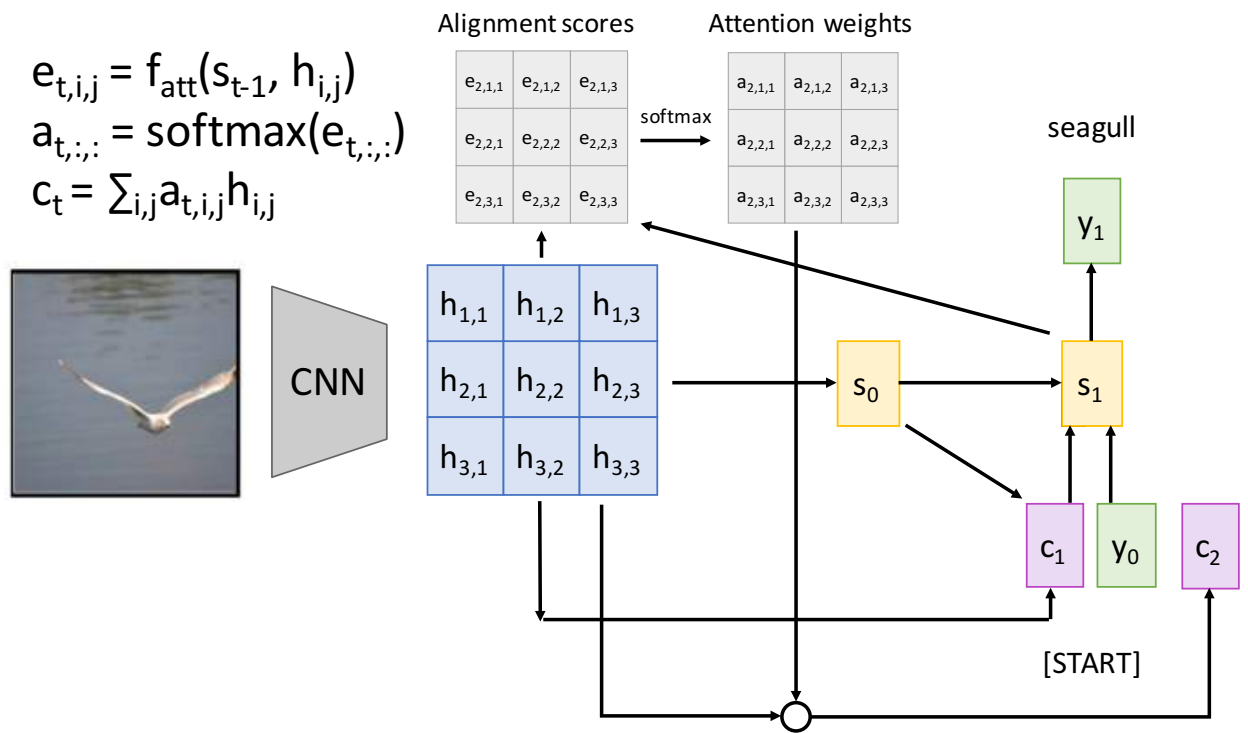
Key vectors: **K** = **X** **W_K** (Shape: $N_X \times D_Q$)

Value Vectors: **V** = **X** **W_V** (Shape: $N_X \times D_V$)

Similarities: **E** = **QK^T** (Shape: $N_Q \times N_X$) $E_{i,j} = \mathbf{Q}_i \cdot \mathbf{K}_j / \text{sqrt}(D_Q)$

Attention weights: **A** = $\text{softmax}(\mathbf{E}, \text{dim}=1)$ (Shape: $N_Q \times N_X$)

Output vectors: **Y** = **AV** (Shape: $N_Q \times D_V$) $Y_i = \sum_j A_{i,j} \mathbf{V}_j$



Changes:

- Use dot product for similarity
- Multiple **query** vectors
- Separate **key** and **value**

Attention Layer

Inputs:

Query vectors: \mathbf{Q} (Shape: $N_Q \times D_Q$)

Input vectors: \mathbf{X} (Shape: $N_X \times D_X$)

Key matrix: \mathbf{W}_K (Shape: $D_X \times D_Q$)

Value matrix: \mathbf{W}_V (Shape: $D_X \times D_V$)

Computation:

Key vectors: $\mathbf{K} = \mathbf{XW}_K$ (Shape: $N_X \times D_Q$)

Value Vectors: $\mathbf{V} = \mathbf{XW}_V$ (Shape: $N_X \times D_V$)

Similarities: $E = \mathbf{QK}^T$ (Shape: $N_Q \times N_X$) $E_{i,j} = \mathbf{Q}_i \cdot \mathbf{K}_j / \text{sqrt}(D_Q)$

Attention weights: $A = \text{softmax}(E, \text{dim}=1)$ (Shape: $N_Q \times N_X$)

Output vectors: $Y = AV$ (Shape: $N_Q \times D_V$) $Y_i = \sum_j A_{i,j} \mathbf{V}_j$

X_1

X_2

X_3

Q_1

Q_2

Q_3

Q_4

Attention Layer

Inputs:

Query vectors: \mathbf{Q} (Shape: $N_Q \times D_Q$)

Input vectors: \mathbf{X} (Shape: $N_X \times D_X$)

Key matrix: \mathbf{W}_K (Shape: $D_X \times D_Q$)

Value matrix: \mathbf{W}_V (Shape: $D_X \times D_V$)

Computation:

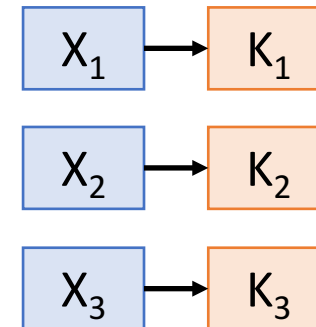
Key vectors: $\mathbf{K} = \mathbf{XW}_K$ (Shape: $N_X \times D_Q$)

Value Vectors: $\mathbf{V} = \mathbf{XW}_V$ (Shape: $N_X \times D_V$)

Similarities: $\mathbf{E} = \mathbf{QK}^T$ (Shape: $N_Q \times N_X$) $E_{i,j} = \mathbf{Q}_i \cdot \mathbf{K}_j / \sqrt{D_Q}$

Attention weights: $\mathbf{A} = \text{softmax}(\mathbf{E}, \text{dim}=1)$ (Shape: $N_Q \times N_X$)

Output vectors: $\mathbf{Y} = \mathbf{AV}$ (Shape: $N_Q \times D_V$) $Y_i = \sum_j A_{i,j} \mathbf{V}_j$



Attention Layer

Inputs:

Query vectors: \mathbf{Q} (Shape: $N_Q \times D_Q$)

Input vectors: \mathbf{X} (Shape: $N_X \times D_X$)

Key matrix: \mathbf{W}_K (Shape: $D_X \times D_Q$)

Value matrix: \mathbf{W}_V (Shape: $D_X \times D_V$)

Computation:

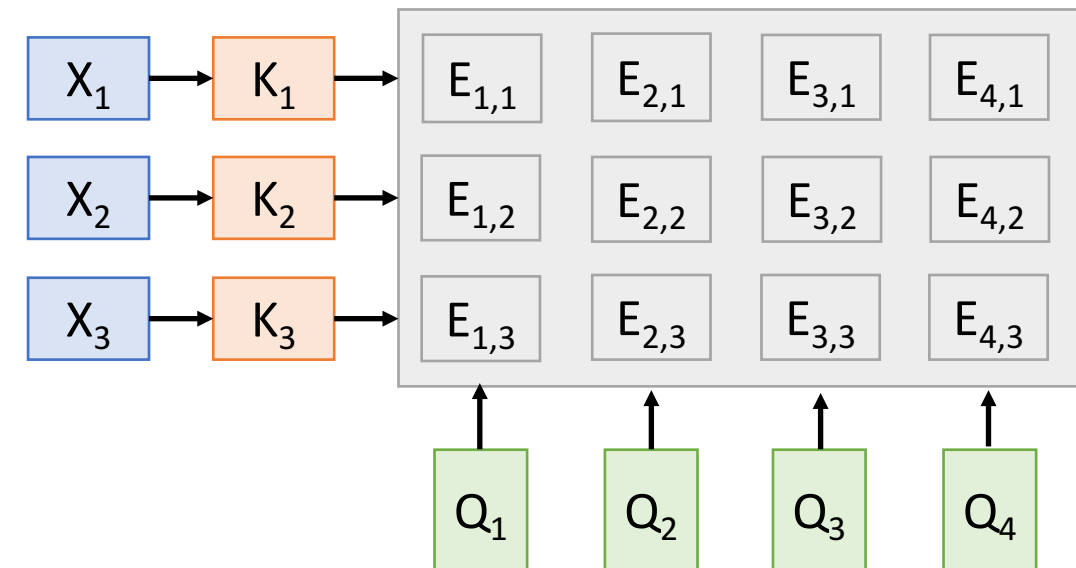
Key vectors: $\mathbf{K} = \mathbf{XW}_K$ (Shape: $N_X \times D_Q$)

Value Vectors: $\mathbf{V} = \mathbf{XW}_V$ (Shape: $N_X \times D_V$)

Similarities: $\mathbf{E} = \mathbf{QK}^T$ (Shape: $N_Q \times N_X$) $E_{i,j} = \mathbf{Q}_i \cdot \mathbf{K}_j / \text{sqrt}(D_Q)$

Attention weights: $\mathbf{A} = \text{softmax}(\mathbf{E}, \text{dim}=1)$ (Shape: $N_Q \times N_X$)

Output vectors: $\mathbf{Y} = \mathbf{AV}$ (Shape: $N_Q \times D_V$) $Y_i = \sum_j A_{i,j} \mathbf{V}_j$



Attention Layer

Inputs:

Query vectors: \mathbf{Q} (Shape: $N_Q \times D_Q$)

Input vectors: \mathbf{X} (Shape: $N_X \times D_X$)

Key matrix: \mathbf{W}_K (Shape: $D_X \times D_Q$)

Value matrix: \mathbf{W}_V (Shape: $D_X \times D_V$)

Computation:

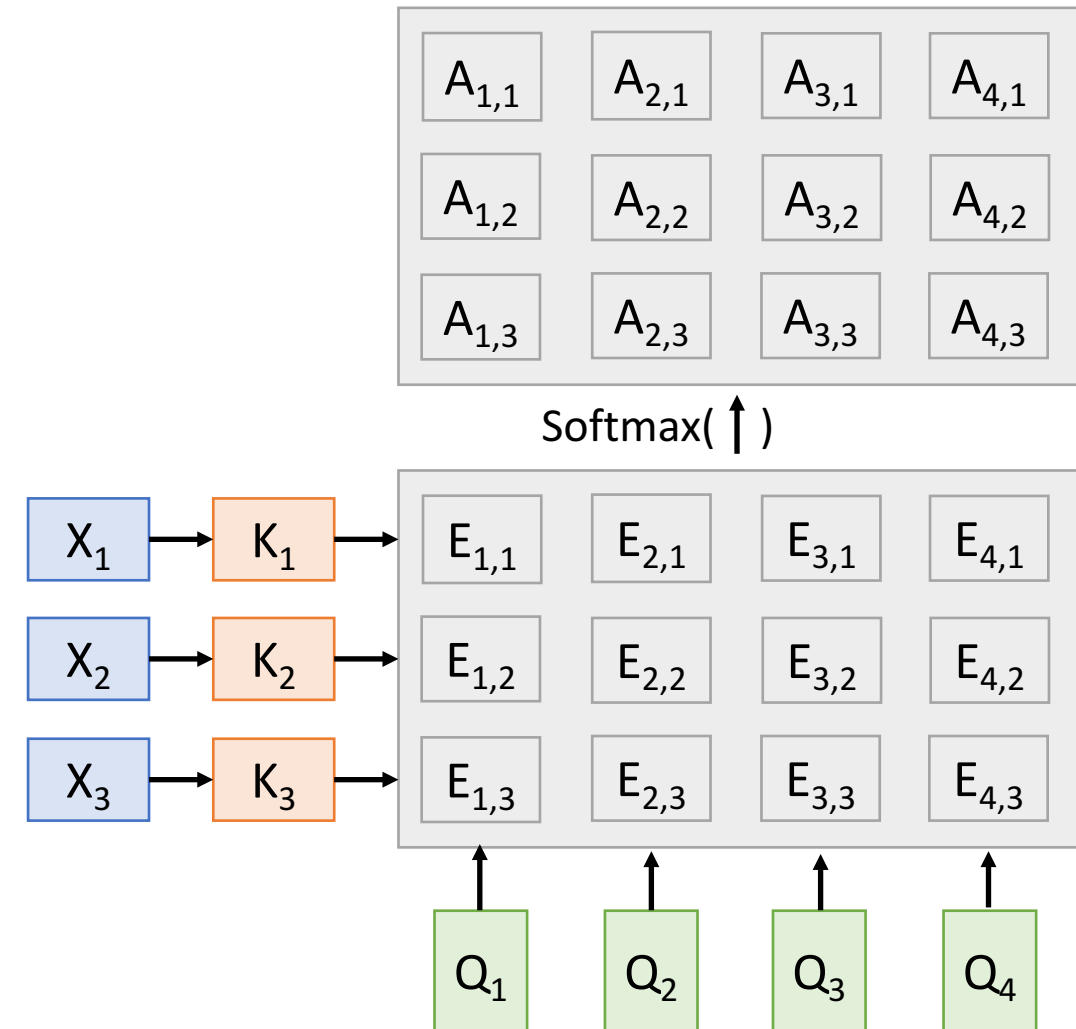
Key vectors: $\mathbf{K} = \mathbf{XW}_K$ (Shape: $N_X \times D_Q$)

Value Vectors: $\mathbf{V} = \mathbf{XW}_V$ (Shape: $N_X \times D_V$)

Similarities: $\mathbf{E} = \mathbf{QK}^T$ (Shape: $N_Q \times N_X$) $E_{i,j} = \mathbf{Q}_i \cdot \mathbf{K}_j / \text{sqrt}(D_Q)$

Attention weights: $\mathbf{A} = \text{softmax}(\mathbf{E}, \text{dim}=1)$ (Shape: $N_Q \times N_X$)

Output vectors: $\mathbf{Y} = \mathbf{AV}$ (Shape: $N_Q \times D_V$) $Y_i = \sum_j A_{i,j} \mathbf{V}_j$



Attention Layer

Inputs:

Query vectors: **Q** (Shape: $N_Q \times D_Q$)

Input vectors: **X** (Shape: $N_X \times D_X$)

Key matrix: **W_K** (Shape: $D_X \times D_Q$)

Value matrix: **W_V** (Shape: $D_X \times D_V$)

Computation:

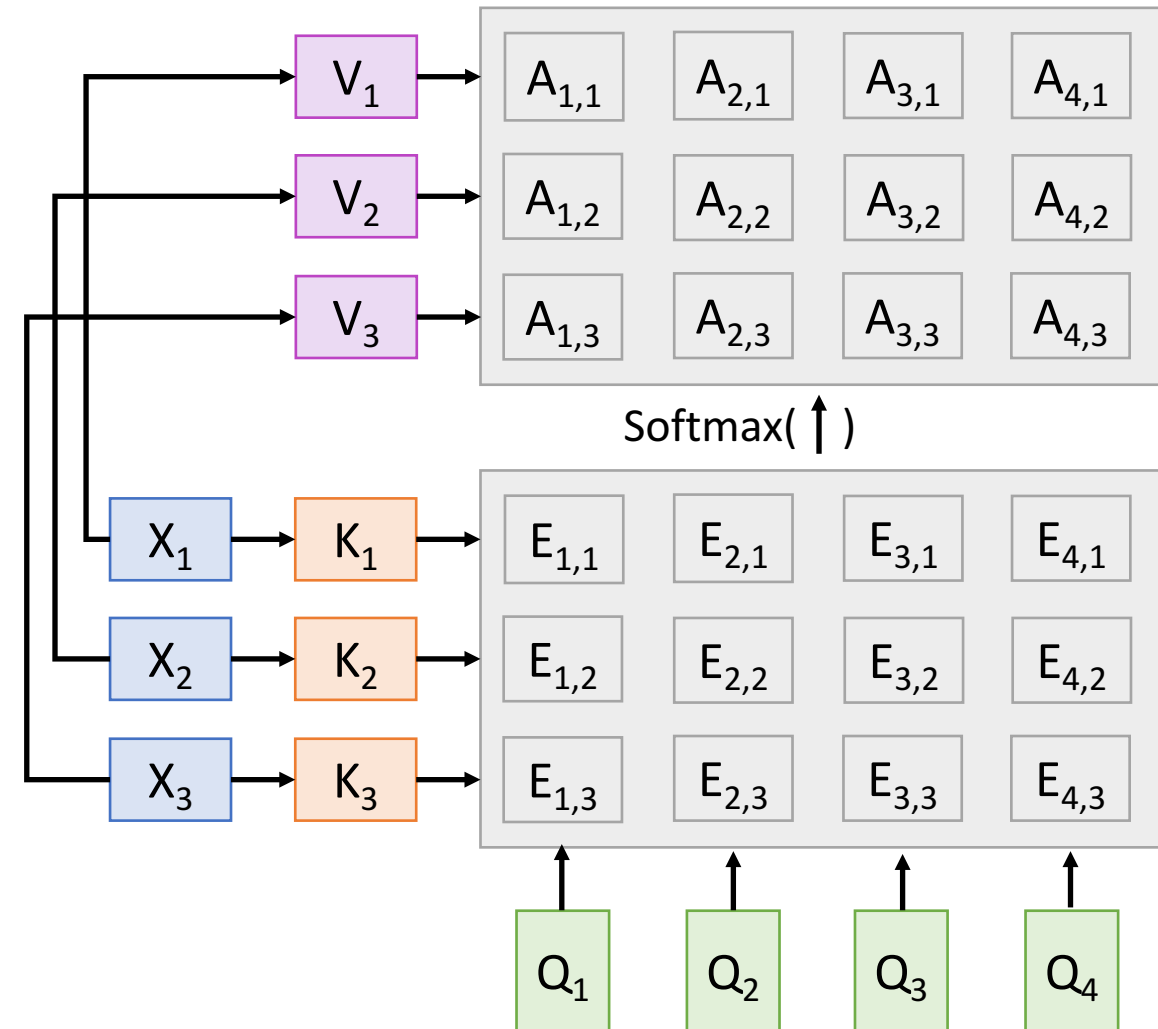
Key vectors: **K** = **XW_K** (Shape: $N_X \times D_Q$)

Value Vectors: **V** = **XW_V** (Shape: $N_X \times D_V$)

Similarities: **E** = **QK^T** (Shape: $N_Q \times N_X$) $E_{i,j} = \mathbf{Q}_i \cdot \mathbf{K}_j / \text{sqrt}(D_Q)$

Attention weights: **A** = softmax(**E**, dim=1) (Shape: $N_Q \times N_X$)

Output vectors: **Y** = **AV** (Shape: $N_Q \times D_V$) $Y_i = \sum_j A_{i,j} \mathbf{V}_j$



Attention Layer

Inputs:

Query vectors: \mathbf{Q} (Shape: $N_Q \times D_Q$)

Input vectors: \mathbf{X} (Shape: $N_X \times D_X$)

Key matrix: \mathbf{W}_K (Shape: $D_X \times D_Q$)

Value matrix: \mathbf{W}_V (Shape: $D_X \times D_V$)

Computation:

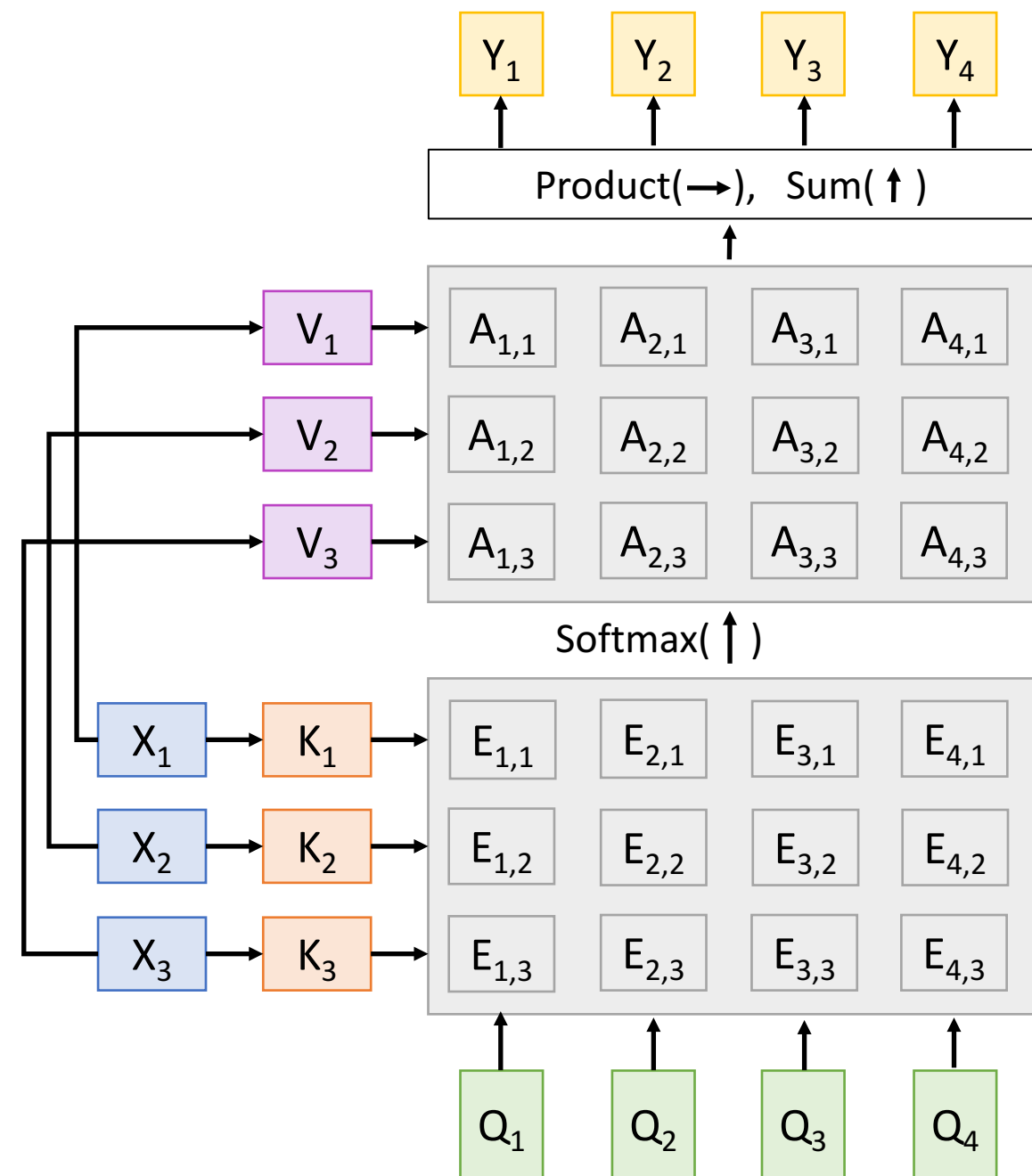
Key vectors: $\mathbf{K} = \mathbf{XW}_K$ (Shape: $N_X \times D_Q$)

Value Vectors: $\mathbf{V} = \mathbf{XW}_V$ (Shape: $N_X \times D_V$)

Similarities: $\mathbf{E} = \mathbf{QK}^T$ (Shape: $N_Q \times N_X$) $E_{i,j} = \mathbf{Q}_i \cdot \mathbf{K}_j / \text{sqrt}(D_Q)$

Attention weights: $\mathbf{A} = \text{softmax}(\mathbf{E}, \text{dim}=1)$ (Shape: $N_Q \times N_X$)

Output vectors: $\mathbf{Y} = \mathbf{AV}$ (Shape: $N_Q \times D_V$) $Y_i = \sum_j A_{i,j} \mathbf{V}_j$



$e_{1,1,1}$	$e_{1,1,2}$	$e_{1,1,3}$
$e_{1,2,1}$	$e_{1,2,2}$	$e_{1,2,3}$
$e_{1,3,1}$	$e_{1,3,2}$	$e_{1,3,3}$

$a_{1,1,1}$	$a_{1,1,2}$	$a_{1,1,3}$
$a_{1,2,1}$	$a_{1,2,2}$	$a_{1,2,3}$
$a_{1,3,1}$	$a_{1,3,2}$	$a_{1,3,3}$

$E_{1,1}$	$E_{2,1}$	$E_{3,1}$	$E_{4,1}$
$E_{1,2}$	$E_{2,2}$	$E_{3,2}$	$E_{4,2}$
$E_{1,3}$	$E_{2,3}$	$E_{3,3}$	$E_{4,3}$

$A_{1,1}$	$A_{2,1}$	$A_{3,1}$	$A_{4,1}$
$A_{1,2}$	$A_{2,2}$	$A_{3,2}$	$A_{4,2}$
$A_{1,3}$	$A_{2,3}$	$A_{3,3}$	$A_{4,3}$

Self-Attention Layer

One **query** per **input vector**

Inputs:

Input vectors: \mathbf{X} (Shape: $N_x \times D_x$)

Key matrix: \mathbf{W}_K (Shape: $D_x \times D_Q$)

Value matrix: \mathbf{W}_V (Shape: $D_x \times D_V$)

Query matrix: \mathbf{W}_Q (Shape: $D_x \times D_Q$)

Computation:

Query vectors: $\mathbf{Q} = \mathbf{XW}_Q$

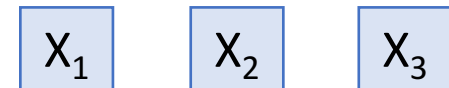
Key vectors: $\mathbf{K} = \mathbf{XW}_K$ (Shape: $N_x \times D_Q$)

Value Vectors: $\mathbf{V} = \mathbf{XW}_V$ (Shape: $N_x \times D_V$)

Similarities: $\mathbf{E} = \mathbf{QK}^T$ (Shape: $N_x \times N_x$) $E_{i,j} = \mathbf{Q}_i \cdot \mathbf{K}_j / \text{sqrt}(D_Q)$

Attention weights: $\mathbf{A} = \text{softmax}(\mathbf{E}, \text{dim}=1)$ (Shape: $N_Q \times N_x$)

Output vectors: $\mathbf{Y} = \mathbf{AV}$ (Shape: $N_x \times D_V$) $Y_i = \sum_j A_{i,j} \mathbf{V}_j$



Self-Attention Layer

One **query** per **input vector**

Inputs:

Input vectors: \mathbf{X} (Shape: $N_x \times D_x$)

Key matrix: \mathbf{W}_K (Shape: $D_x \times D_Q$)

Value matrix: \mathbf{W}_V (Shape: $D_x \times D_V$)

Query matrix: \mathbf{W}_Q (Shape: $D_x \times D_Q$)

Computation:

Query vectors: $\mathbf{Q} = \mathbf{XW}_Q$

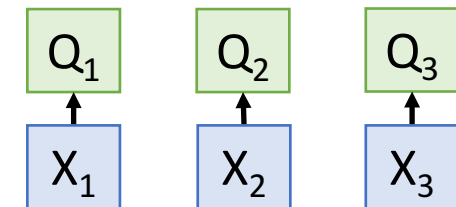
Key vectors: $\mathbf{K} = \mathbf{XW}_K$ (Shape: $N_x \times D_Q$)

Value Vectors: $\mathbf{V} = \mathbf{XW}_V$ (Shape: $N_x \times D_V$)

Similarities: $\mathbf{E} = \mathbf{QK}^T$ (Shape: $N_x \times N_x$) $E_{i,j} = \mathbf{Q}_i \cdot \mathbf{K}_j / \text{sqrt}(D_Q)$

Attention weights: $\mathbf{A} = \text{softmax}(\mathbf{E}, \text{dim}=1)$ (Shape: $N_Q \times N_x$)

Output vectors: $\mathbf{Y} = \mathbf{AV}$ (Shape: $N_x \times D_V$) $Y_i = \sum_j A_{i,j} \mathbf{V}_j$



Self-Attention Layer

One **query** per **input vector**

Inputs:

Input vectors: \mathbf{X} (Shape: $N_x \times D_x$)

Key matrix: \mathbf{W}_k (Shape: $D_x \times D_Q$)

Value matrix: \mathbf{W}_v (Shape: $D_x \times D_V$)

Query matrix: \mathbf{W}_Q (Shape: $D_x \times D_Q$)

Computation:

Query vectors: $\mathbf{Q} = \mathbf{XW}_Q$

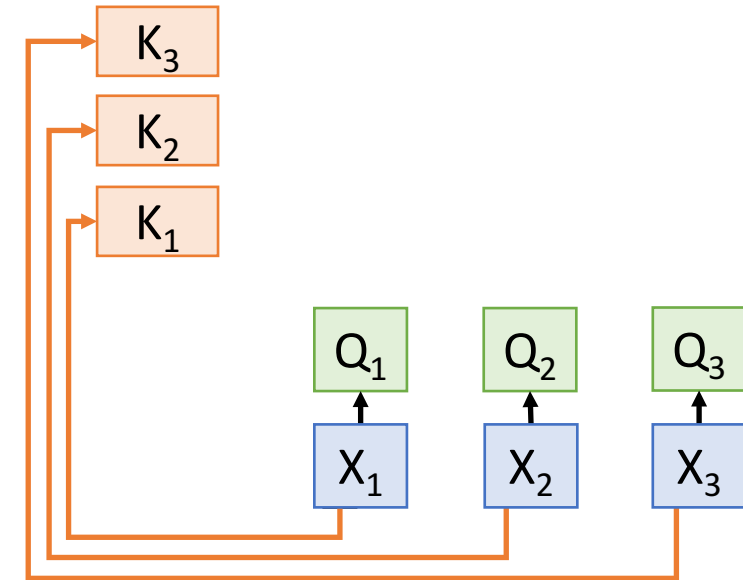
Key vectors: $\mathbf{K} = \mathbf{XW}_k$ (Shape: $N_x \times D_Q$)

Value Vectors: $\mathbf{V} = \mathbf{XW}_v$ (Shape: $N_x \times D_V$)

Similarities: $\mathbf{E} = \mathbf{QK}^T$ (Shape: $N_x \times N_x$) $E_{i,j} = \mathbf{Q}_i \cdot \mathbf{K}_j / \text{sqrt}(D_Q)$

Attention weights: $\mathbf{A} = \text{softmax}(\mathbf{E}, \text{dim}=1)$ (Shape: $N_Q \times N_x$)

Output vectors: $\mathbf{Y} = \mathbf{AV}$ (Shape: $N_x \times D_V$) $Y_i = \sum_j A_{i,j} \mathbf{V}_j$



Self-Attention Layer

One **query** per **input vector**

Inputs:

Input vectors: \mathbf{X} (Shape: $N_x \times D_x$)

Key matrix: \mathbf{W}_K (Shape: $D_x \times D_Q$)

Value matrix: \mathbf{W}_V (Shape: $D_x \times D_V$)

Query matrix: \mathbf{W}_Q (Shape: $D_x \times D_Q$)

Computation:

Query vectors: $\mathbf{Q} = \mathbf{XW}_Q$

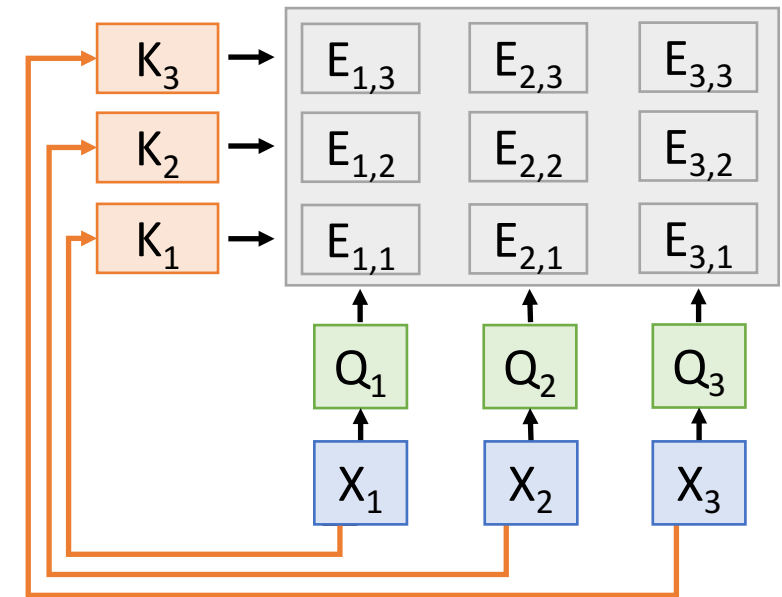
Key vectors: $\mathbf{K} = \mathbf{XW}_K$ (Shape: $N_x \times D_Q$)

Value Vectors: $\mathbf{V} = \mathbf{XW}_V$ (Shape: $N_x \times D_V$)

Similarities: $\mathbf{E} = \mathbf{QK}^T$ (Shape: $N_x \times N_x$) $E_{i,j} = \mathbf{Q}_i \cdot \mathbf{K}_j / \text{sqrt}(D_Q)$

Attention weights: $\mathbf{A} = \text{softmax}(\mathbf{E}, \text{dim}=1)$ (Shape: $N_Q \times N_x$)

Output vectors: $\mathbf{Y} = \mathbf{AV}$ (Shape: $N_x \times D_V$) $Y_i = \sum_j A_{i,j} \mathbf{V}_j$



Self-Attention Layer

One **query** per **input vector**

Inputs:

Input vectors: \mathbf{X} (Shape: $N_x \times D_x$)

Key matrix: \mathbf{W}_K (Shape: $D_x \times D_Q$)

Value matrix: \mathbf{W}_V (Shape: $D_x \times D_V$)

Query matrix: \mathbf{W}_Q (Shape: $D_x \times D_Q$)

Computation:

Query vectors: $\mathbf{Q} = \mathbf{XW}_Q$

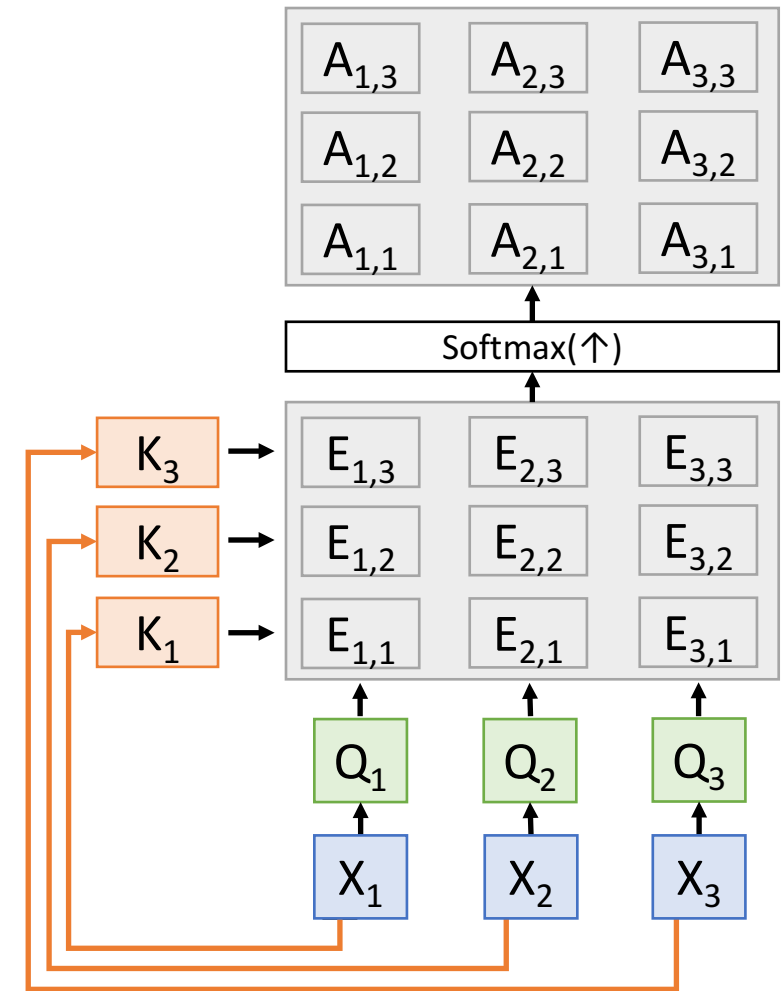
Key vectors: $\mathbf{K} = \mathbf{XW}_K$ (Shape: $N_x \times D_Q$)

Value Vectors: $\mathbf{V} = \mathbf{XW}_V$ (Shape: $N_x \times D_V$)

Similarities: $\mathbf{E} = \mathbf{QK}^T$ (Shape: $N_x \times N_x$) $E_{i,j} = \mathbf{Q}_i \cdot \mathbf{K}_j / \text{sqrt}(D_Q)$

Attention weights: $\mathbf{A} = \text{softmax}(\mathbf{E}, \text{dim}=1)$ (Shape: $N_Q \times N_x$)

Output vectors: $\mathbf{Y} = \mathbf{AV}$ (Shape: $N_x \times D_V$) $Y_i = \sum_j A_{i,j} \mathbf{V}_j$



Self-Attention Layer

One **query** per **input vector**

Inputs:

Input vectors: \mathbf{X} (Shape: $N_x \times D_x$)

Key matrix: \mathbf{W}_K (Shape: $D_x \times D_Q$)

Value matrix: \mathbf{W}_V (Shape: $D_x \times D_V$)

Query matrix: \mathbf{W}_Q (Shape: $D_x \times D_Q$)

Computation:

Query vectors: $\mathbf{Q} = \mathbf{XW}_Q$

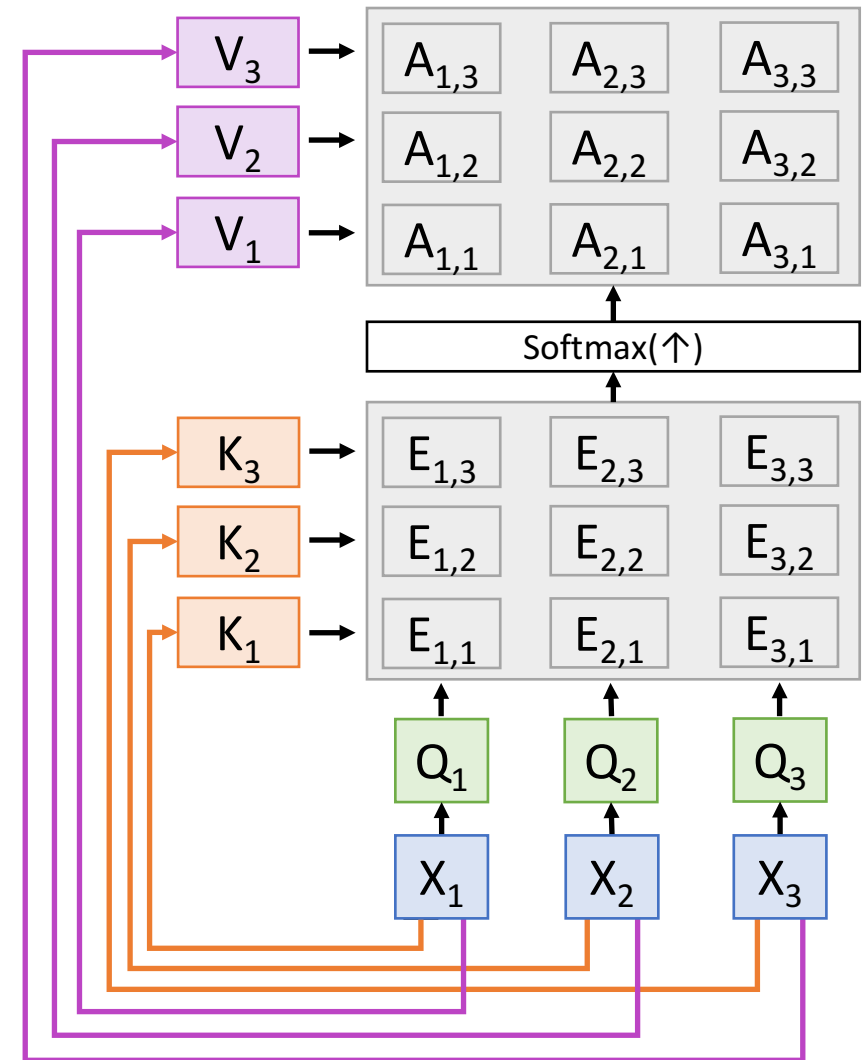
Key vectors: $\mathbf{K} = \mathbf{XW}_K$ (Shape: $N_x \times D_Q$)

Value Vectors: $\mathbf{V} = \mathbf{XW}_V$ (Shape: $N_x \times D_V$)

Similarities: $\mathbf{E} = \mathbf{QK}^T$ (Shape: $N_x \times N_x$) $E_{i,j} = \mathbf{Q}_i \cdot \mathbf{K}_j / \text{sqrt}(D_Q)$

Attention weights: $\mathbf{A} = \text{softmax}(\mathbf{E}, \text{dim}=1)$ (Shape: $N_Q \times N_x$)

Output vectors: $\mathbf{Y} = \mathbf{AV}$ (Shape: $N_x \times D_V$) $Y_i = \sum_j A_{i,j} \mathbf{V}_j$



Self-Attention Layer

One **query** per **input vector**

Inputs:

Input vectors: \mathbf{X} (Shape: $N_x \times D_x$)

Key matrix: \mathbf{W}_K (Shape: $D_x \times D_Q$)

Value matrix: \mathbf{W}_V (Shape: $D_x \times D_V$)

Query matrix: \mathbf{W}_Q (Shape: $D_x \times D_Q$)

Computation:

Query vectors: $\mathbf{Q} = \mathbf{XW}_Q$

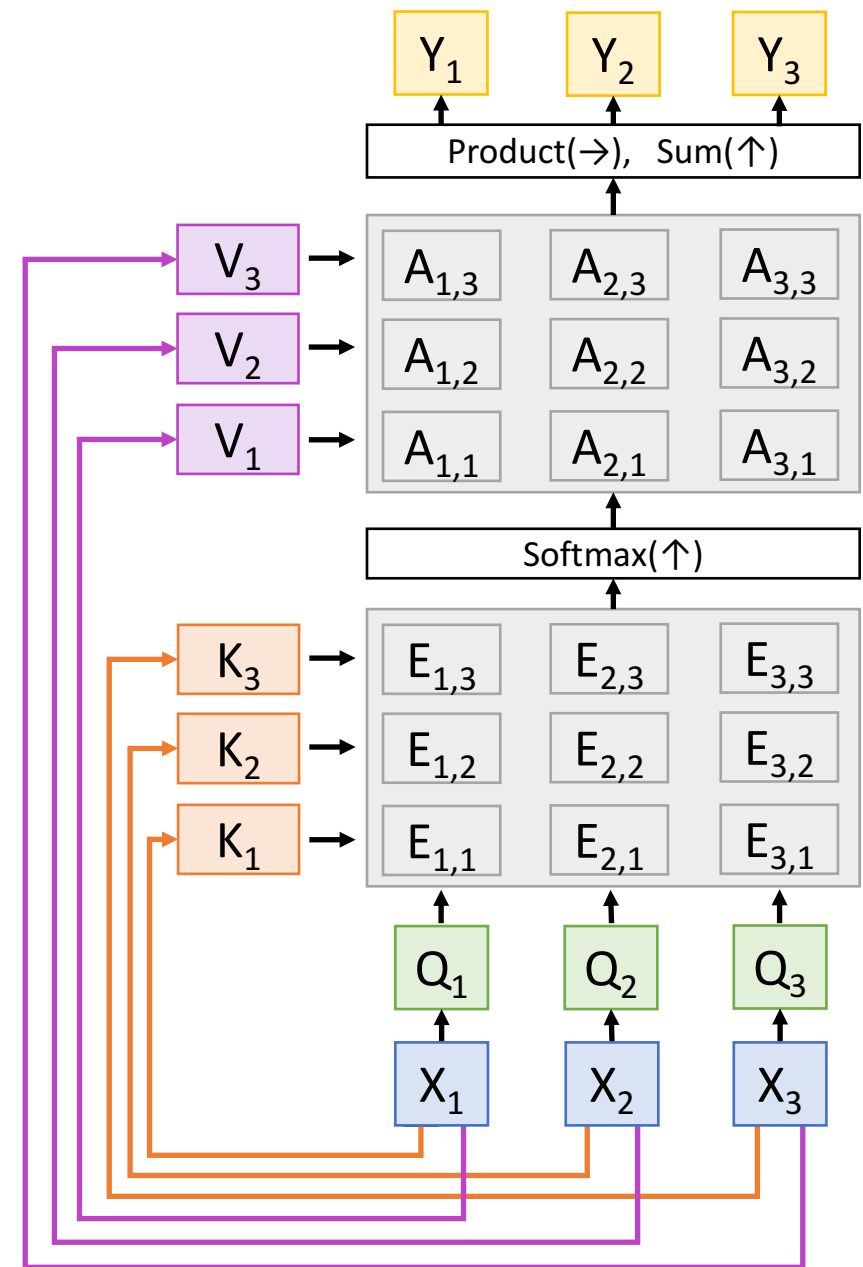
Key vectors: $\mathbf{K} = \mathbf{XW}_K$ (Shape: $N_x \times D_Q$)

Value Vectors: $\mathbf{V} = \mathbf{XW}_V$ (Shape: $N_x \times D_V$)

Similarities: $\mathbf{E} = \mathbf{QK}^T$ (Shape: $N_x \times N_x$) $E_{i,j} = \mathbf{Q}_i \cdot \mathbf{K}_j / \text{sqrt}(D_Q)$

Attention weights: $\mathbf{A} = \text{softmax}(\mathbf{E}, \text{dim}=1)$ (Shape: $N_Q \times N_x$)

Output vectors: $\mathbf{Y} = \mathbf{AV}$ (Shape: $N_x \times D_V$) $Y_i = \sum_j A_{i,j} \mathbf{V}_j$



Self-Attention Layer

Inputs:

Input vectors: \mathbf{X} (Shape: $N_x \times D_x$)

Key matrix: \mathbf{W}_K (Shape: $D_x \times D_Q$)

Value matrix: \mathbf{W}_V (Shape: $D_x \times D_V$)

Query matrix: \mathbf{W}_Q (Shape: $D_x \times D_Q$)

Computation:

Query vectors: $\mathbf{Q} = \mathbf{XW}_Q$

Key vectors: $\mathbf{K} = \mathbf{XW}_K$ (Shape: $N_x \times D_Q$)

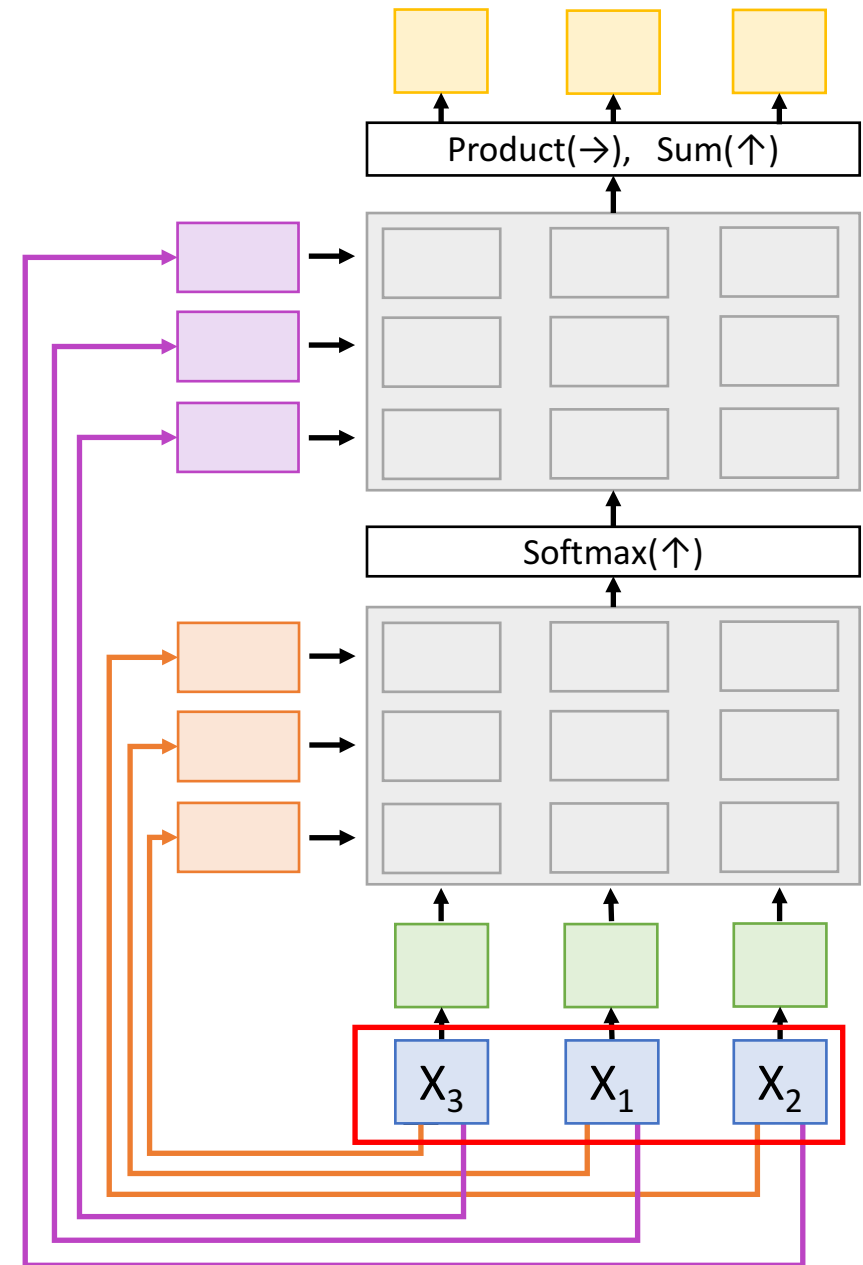
Value Vectors: $\mathbf{V} = \mathbf{XW}_V$ (Shape: $N_x \times D_V$)

Similarities: $\mathbf{E} = \mathbf{QK}^T$ (Shape: $N_x \times N_x$) $E_{i,j} = \mathbf{Q}_i \cdot \mathbf{K}_j / \text{sqrt}(D_Q)$

Attention weights: $\mathbf{A} = \text{softmax}(\mathbf{E}, \text{dim}=1)$ (Shape: $N_Q \times N_x$)

Output vectors: $\mathbf{Y} = \mathbf{AV}$ (Shape: $N_x \times D_V$) $Y_i = \sum_j A_{i,j} \mathbf{V}_j$

Consider **permuting**
the input vectors:



Self-Attention Layer

Inputs:

Input vectors: \mathbf{X} (Shape: $N_x \times D_x$)

Key matrix: \mathbf{W}_K (Shape: $D_x \times D_Q$)

Value matrix: \mathbf{W}_V (Shape: $D_x \times D_V$)

Query matrix: \mathbf{W}_Q (Shape: $D_x \times D_Q$)

Computation:

Query vectors: $\mathbf{Q} = \mathbf{XW}_Q$

Key vectors: $\mathbf{K} = \mathbf{XW}_K$ (Shape: $N_x \times D_Q$)

Value Vectors: $\mathbf{V} = \mathbf{XW}_V$ (Shape: $N_x \times D_V$)

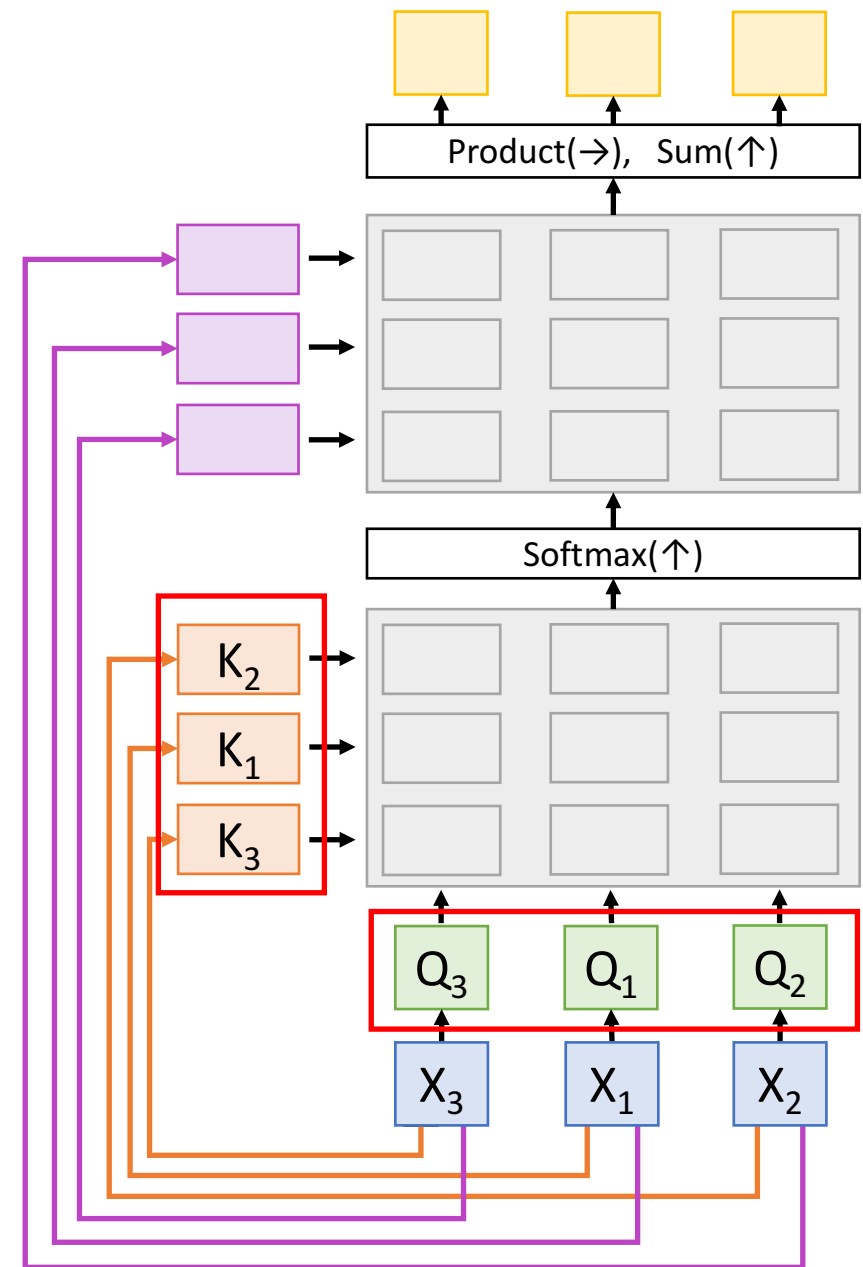
Similarities: $\mathbf{E} = \mathbf{QK}^T$ (Shape: $N_x \times N_x$) $E_{i,j} = \mathbf{Q}_i \cdot \mathbf{K}_j / \text{sqrt}(D_Q)$

Attention weights: $\mathbf{A} = \text{softmax}(\mathbf{E}, \text{dim}=1)$ (Shape: $N_Q \times N_x$)

Output vectors: $\mathbf{Y} = \mathbf{AV}$ (Shape: $N_x \times D_V$) $Y_i = \sum_j A_{i,j} \mathbf{V}_j$

Consider **permuting**
the input vectors:

Queries and Keys will be
the same, but permuted



Self-Attention Layer

Inputs:

Input vectors: \mathbf{X} (Shape: $N_x \times D_x$)

Key matrix: \mathbf{W}_K (Shape: $D_x \times D_Q$)

Value matrix: \mathbf{W}_V (Shape: $D_x \times D_V$)

Query matrix: \mathbf{W}_Q (Shape: $D_x \times D_Q$)

Computation:

Query vectors: $\mathbf{Q} = \mathbf{XW}_Q$

Key vectors: $\mathbf{K} = \mathbf{XW}_K$ (Shape: $N_x \times D_Q$)

Value Vectors: $\mathbf{V} = \mathbf{XW}_V$ (Shape: $N_x \times D_V$)

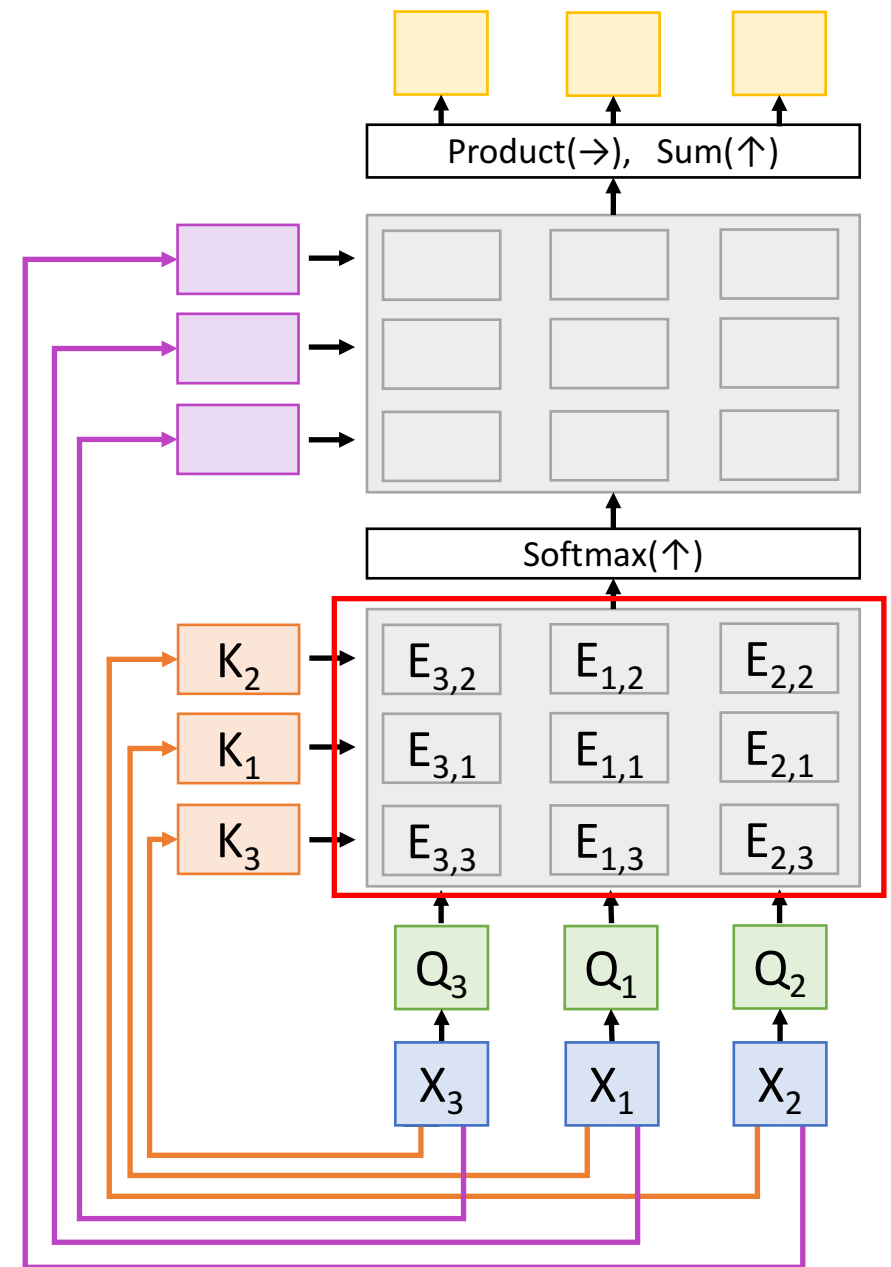
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Attention weights: $\mathbf{A} = \text{softmax}(\mathbf{E}, \text{dim}=1)$ (Shape: $N_Q \times N_x$)

Output vectors: $\mathbf{Y} = \mathbf{AV}$ (Shape: $N_x \times D_V$) $Y_i = \sum_j A_{i,j} \mathbf{V}_j$

Consider **permuting**
the input vectors:

Similarities will be the
same, but permuted



Self-Attention Layer

Inputs:

Input vectors: \mathbf{X} (Shape: $N_x \times D_x$)

Key matrix: \mathbf{W}_K (Shape: $D_x \times D_Q$)

Value matrix: \mathbf{W}_V (Shape: $D_x \times D_V$)

Query matrix: \mathbf{W}_Q (Shape: $D_x \times D_Q$)

Computation:

Query vectors: $\mathbf{Q} = \mathbf{XW}_Q$

Key vectors: $\mathbf{K} = \mathbf{XW}_K$ (Shape: $N_x \times D_Q$)

Value Vectors: $\mathbf{V} = \mathbf{XW}_V$ (Shape: $N_x \times D_V$)

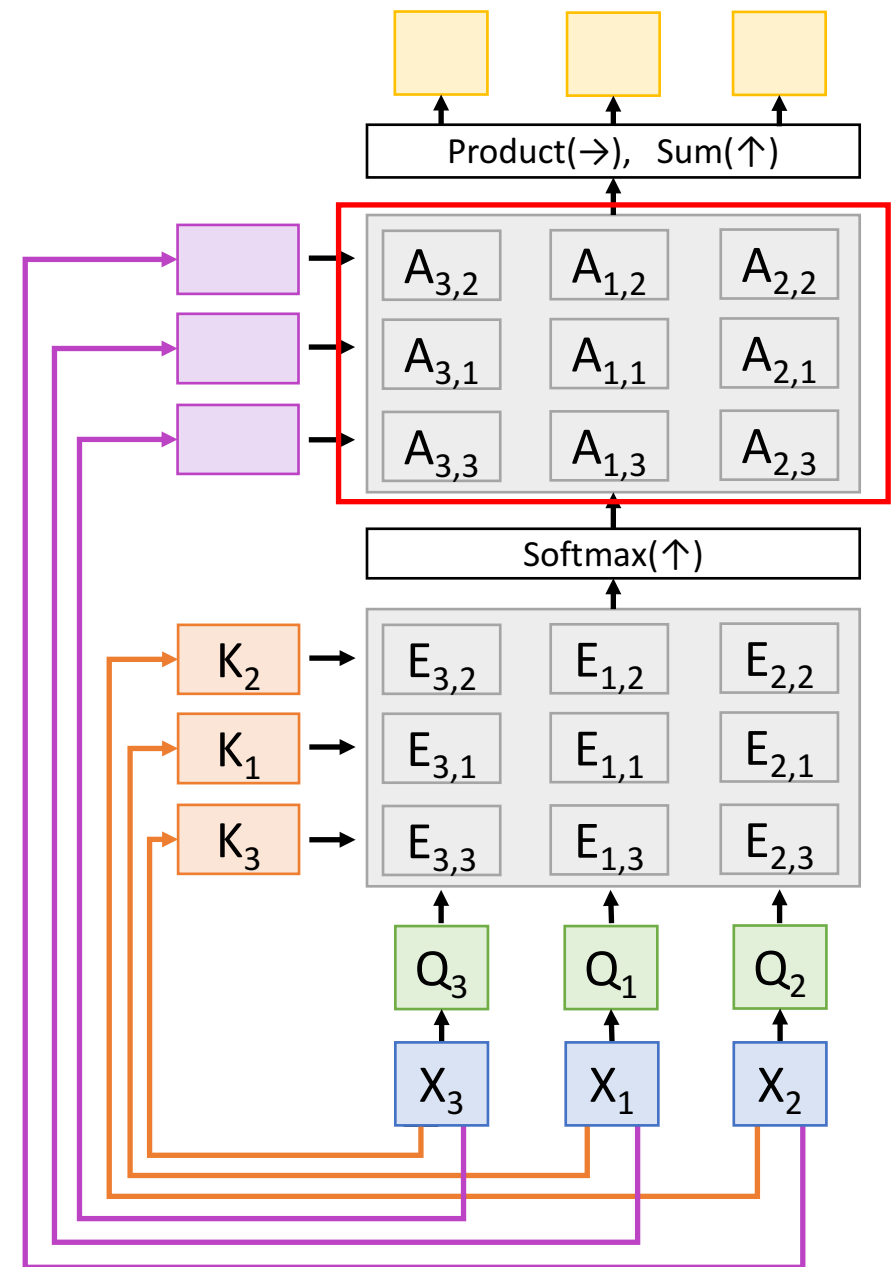
Similarities: $\mathbf{E} = \mathbf{QK}^T$ (Shape: $N_x \times N_x$) $E_{i,j} = \mathbf{Q}_i \cdot \mathbf{K}_j / \text{sqrt}(D_Q)$

Attention weights: $\mathbf{A} = \text{softmax}(\mathbf{E}, \text{dim}=1)$ (Shape: $N_Q \times N_x$)

Output vectors: $\mathbf{Y} = \mathbf{AV}$ (Shape: $N_x \times D_V$) $Y_i = \sum_j A_{i,j} \mathbf{V}_j$

Consider **permuting**
the input vectors:

Attention weights will be
the same, but permuted



Self-Attention Layer

Inputs:

Input vectors: \mathbf{X} (Shape: $N_x \times D_x$)

Key matrix: \mathbf{W}_K (Shape: $D_x \times D_Q$)

Value matrix: \mathbf{W}_V (Shape: $D_x \times D_V$)

Query matrix: \mathbf{W}_Q (Shape: $D_x \times D_Q$)

Computation:

Query vectors: $\mathbf{Q} = \mathbf{XW}_Q$

Key vectors: $\mathbf{K} = \mathbf{XW}_K$ (Shape: $N_x \times D_Q$)

Value Vectors: $\mathbf{V} = \mathbf{XW}_V$ (Shape: $N_x \times D_V$)

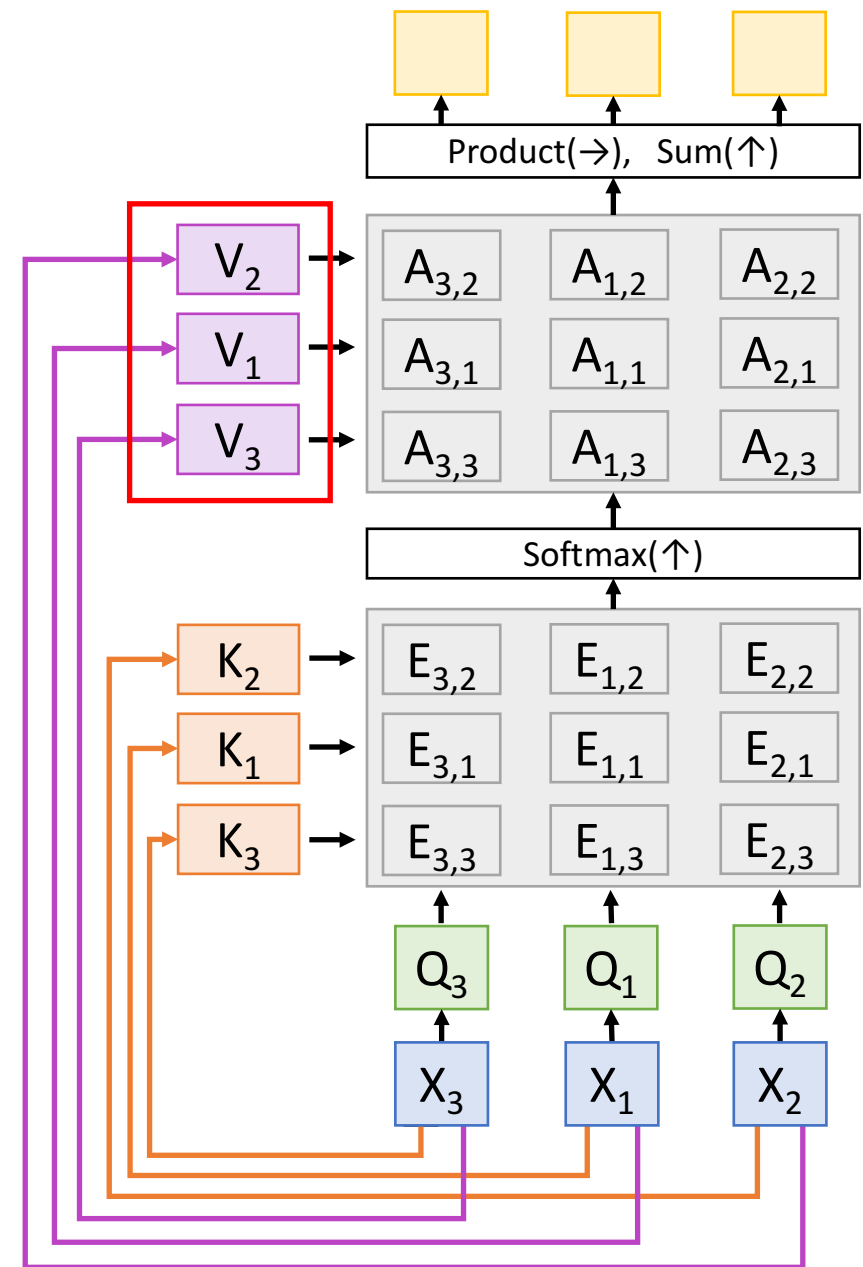
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Attention weights: $\mathbf{A} = \text{softmax}(\mathbf{E}, \text{dim}=1)$ (Shape: $N_Q \times N_x$)

Output vectors: $\mathbf{Y} = \mathbf{AV}$ (Shape: $N_x \times D_V$) $Y_i = \sum_j A_{i,j} \mathbf{V}_j$

Consider **permuting**
the input vectors:

Values will be the
same, but permuted



Self-Attention Layer

Inputs:

Input vectors: \mathbf{X} (Shape: $N_x \times D_x$)

Key matrix: \mathbf{W}_K (Shape: $D_x \times D_Q$)

Value matrix: \mathbf{W}_V (Shape: $D_x \times D_V$)

Query matrix: \mathbf{W}_Q (Shape: $D_x \times D_Q$)

Computation:

Query vectors: $\mathbf{Q} = \mathbf{XW}_Q$

Key vectors: $\mathbf{K} = \mathbf{XW}_K$ (Shape: $N_x \times D_Q$)

Value Vectors: $\mathbf{V} = \mathbf{XW}_V$ (Shape: $N_x \times D_V$)

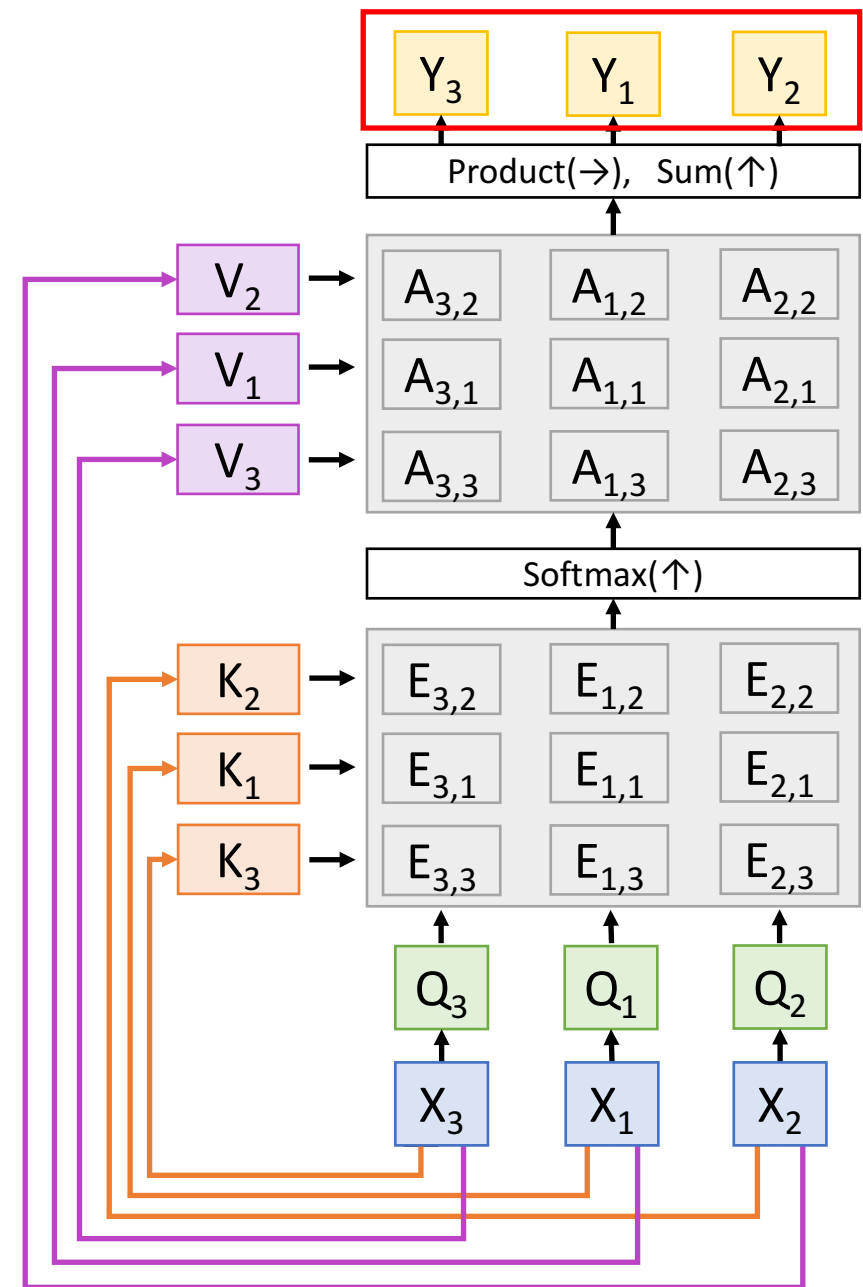
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Attention weights: $\mathbf{A} = \text{softmax}(\mathbf{E}, \text{dim}=1)$ (Shape: $N_Q \times N_x$)

Output vectors: $\mathbf{Y} = \mathbf{AV}$ (Shape: $N_x \times D_V$) $Y_i = \sum_j A_{i,j} \mathbf{V}_j$

Consider **permuting**
the input vectors:

Outputs will be the
same, but **permuted**



Self-Attention Layer

Inputs:

Input vectors: \mathbf{X} (Shape: $N_X \times D_X$)

Key matrix: \mathbf{W}_K (Shape: $D_X \times D_Q$)

Value matrix: \mathbf{W}_V (Shape: $D_X \times D_V$)

Query matrix: \mathbf{W}_Q (Shape: $D_X \times D_Q$)

Computation:

Query vectors: $\mathbf{Q} = \mathbf{XW}_Q$

Key vectors: $\mathbf{K} = \mathbf{XW}_K$ (Shape: $N_X \times D_Q$)

Value Vectors: $\mathbf{V} = \mathbf{XW}_V$ (Shape: $N_X \times D_V$)

Similarities: $\mathbf{E} = \mathbf{QK}^T$ (Shape: $N_X \times N_X$) $E_{i,j} = \mathbf{Q}_i \cdot \mathbf{K}_j / \text{sqrt}(D_Q)$

Attention weights: $\mathbf{A} = \text{softmax}(\mathbf{E}, \text{dim}=1)$ (Shape: $N_Q \times N_X$)

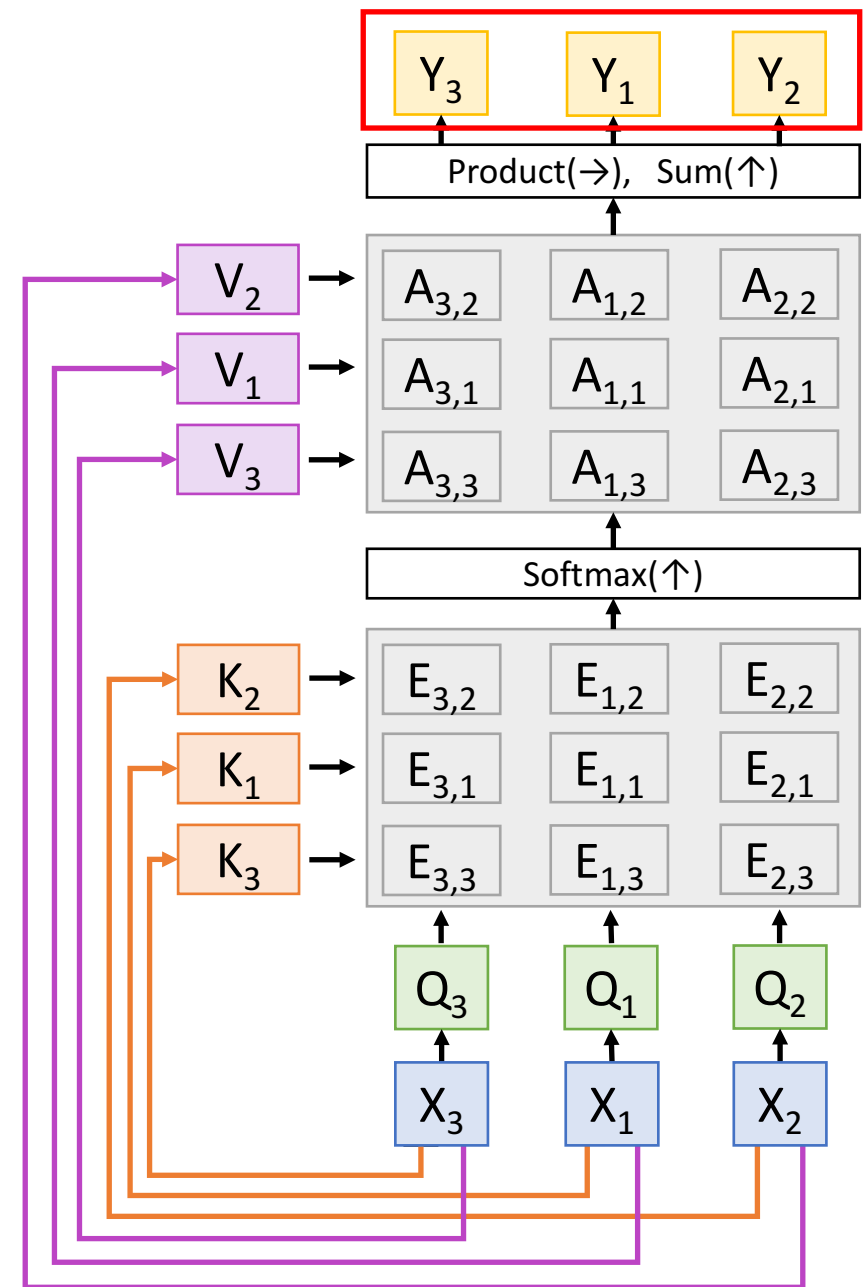
Output vectors: $\mathbf{Y} = \mathbf{AV}$ (Shape: $N_X \times D_V$) $Y_i = \sum_j A_{i,j} \mathbf{V}_j$

Consider **permuting**
the input vectors:

Outputs will be the
same, but **permuted**

Self-attention layer is
Permutation Equivariant
 $f(s(x)) = s(f(x))$

Self-Attention layer works
on **sets** of vectors



Self-Attention Layer

Inputs:

Input vectors: \mathbf{X} (Shape: $N_x \times D_x$)

Key matrix: \mathbf{W}_K (Shape: $D_x \times D_Q$)

Value matrix: \mathbf{W}_V (Shape: $D_x \times D_V$)

Query matrix: \mathbf{W}_Q (Shape: $D_x \times D_Q$)

Computation:

Query vectors: $\mathbf{Q} = \mathbf{XW}_Q$

Key vectors: $\mathbf{K} = \mathbf{XW}_K$ (Shape: $N_x \times D_Q$)

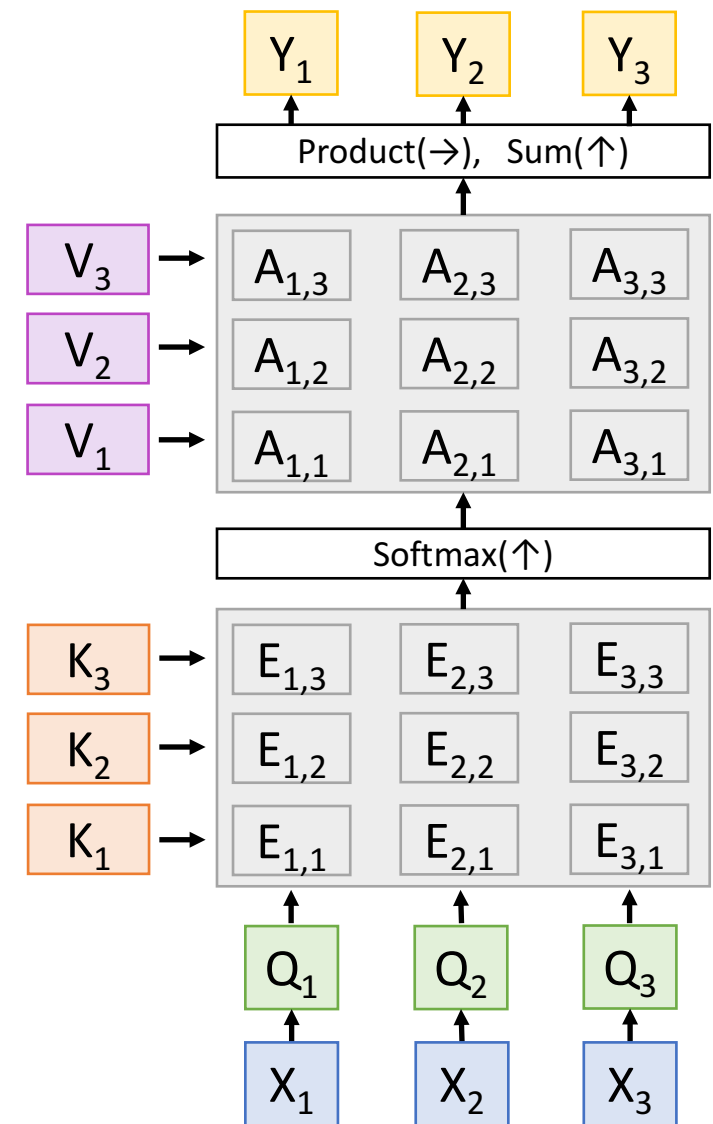
Value Vectors: $\mathbf{V} = \mathbf{XW}_V$ (Shape: $N_x \times D_V$)

Similarities: $\mathbf{E} = \mathbf{QK}^T$ (Shape: $N_x \times N_x$) $E_{i,j} = \mathbf{Q}_i \cdot \mathbf{K}_j / \text{sqrt}(D_Q)$

Attention weights: $\mathbf{A} = \text{softmax}(\mathbf{E}, \text{dim}=1)$ (Shape: $N_Q \times N_x$)

Output vectors: $\mathbf{Y} = \mathbf{AV}$ (Shape: $N_x \times D_V$) $Y_i = \sum_j A_{i,j} \mathbf{V}_j$

Self attention doesn't
"know" the order of the
vectors it is processing!



Self-Attention Layer

Inputs:

Input vectors: \mathbf{X} (Shape: $N_x \times D_x$)

Key matrix: \mathbf{W}_K (Shape: $D_x \times D_Q$)

Value matrix: \mathbf{W}_V (Shape: $D_x \times D_V$)

Query matrix: \mathbf{W}_Q (Shape: $D_x \times D_Q$)

Computation:

Query vectors: $\mathbf{Q} = \mathbf{XW}_Q$

Key vectors: $\mathbf{K} = \mathbf{XW}_K$ (Shape: $N_x \times D_Q$)

Value Vectors: $\mathbf{V} = \mathbf{XW}_V$ (Shape: $N_x \times D_V$)

Similarities: $\mathbf{E} = \mathbf{QK}^T$ (Shape: $N_x \times N_x$) $E_{i,j} = \mathbf{Q}_i \cdot \mathbf{K}_j / \text{sqrt}(D_Q)$

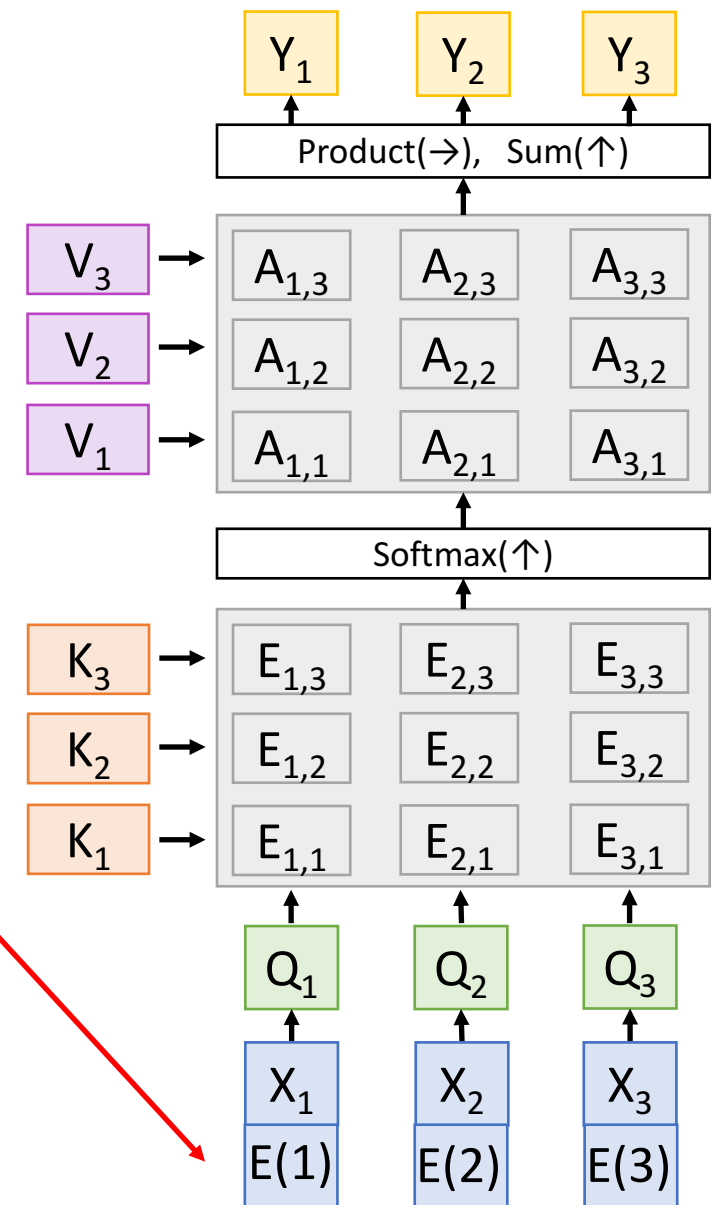
Attention weights: $\mathbf{A} = \text{softmax}(\mathbf{E}, \text{dim}=1)$ (Shape: $N_Q \times N_x$)

Output vectors: $\mathbf{Y} = \mathbf{AV}$ (Shape: $N_x \times D_V$) $Y_i = \sum_j A_{i,j} \mathbf{V}_j$

Self attention doesn't
"know" the order of the
vectors it is processing!

In order to make
processing position-
aware, concatenate input
with **positional encoding**

E can be learned lookup
table, or fixed function



Masked Self-Attention Layer

Don't let vectors "look ahead" in the sequence

Inputs:

Input vectors: \mathbf{X} (Shape: $N_x \times D_x$)

Key matrix: \mathbf{W}_K (Shape: $D_x \times D_Q$)

Value matrix: \mathbf{W}_V (Shape: $D_x \times D_V$)

Query matrix: \mathbf{W}_Q (Shape: $D_x \times D_Q$)

Computation:

Query vectors: $\mathbf{Q} = \mathbf{XW}_Q$

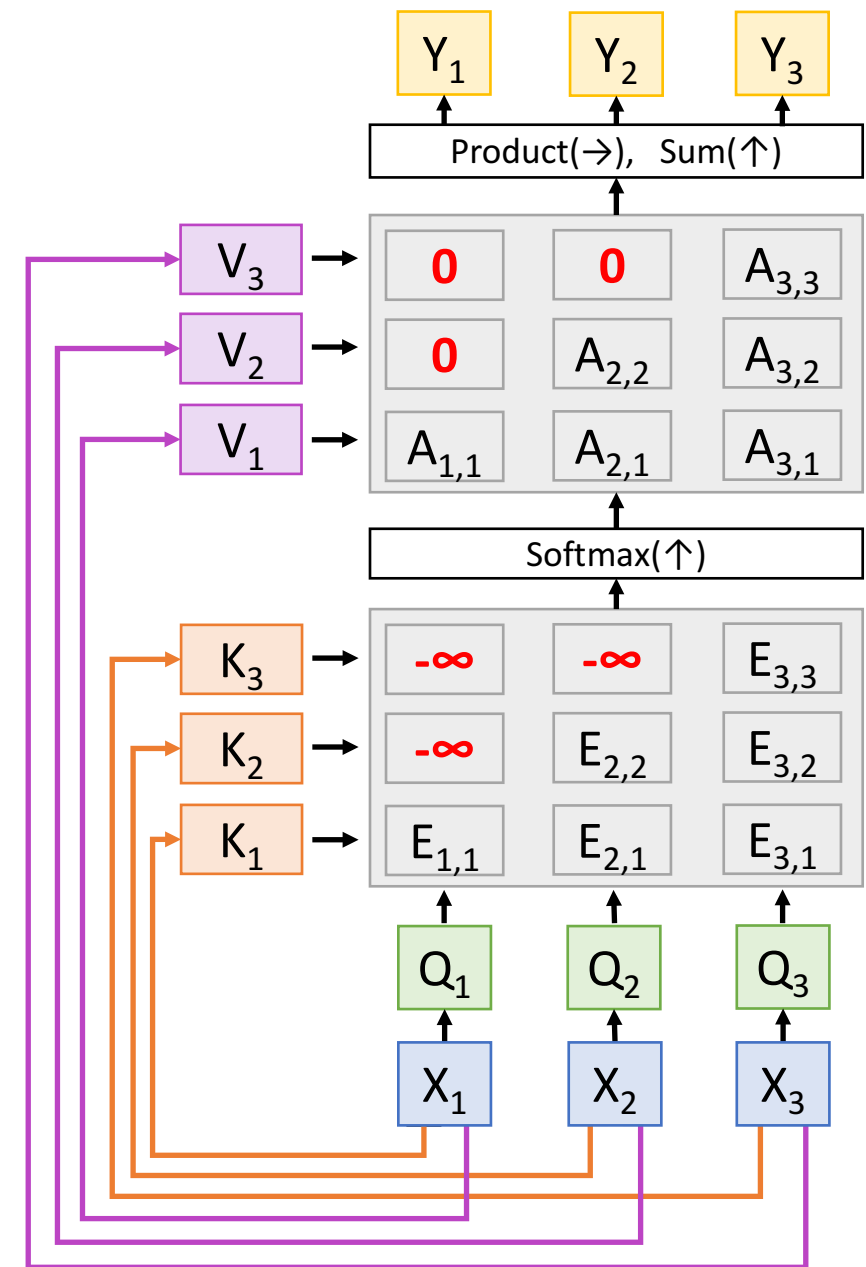
Key vectors: $\mathbf{K} = \mathbf{XW}_K$ (Shape: $N_x \times D_Q$)

Value Vectors: $\mathbf{V} = \mathbf{XW}_V$ (Shape: $N_x \times D_V$)

Similarities: $\mathbf{E} = \mathbf{QK}^T$ (Shape: $N_x \times N_x$) $E_{i,j} = \mathbf{Q}_i \cdot \mathbf{K}_j / \text{sqrt}(D_Q)$

Attention weights: $\mathbf{A} = \text{softmax}(\mathbf{E}, \text{dim}=1)$ (Shape: $N_Q \times N_x$)

Output vectors: $\mathbf{Y} = \mathbf{AV}$ (Shape: $N_x \times D_V$) $Y_i = \sum_j A_{i,j} \mathbf{V}_j$



Masked Self-Attention Layer

Don't let vectors "look ahead" in the sequence
Used for language modeling (predict next word)

Inputs:

Input vectors: \mathbf{X} (Shape: $N_x \times D_x$)

Key matrix: \mathbf{W}_K (Shape: $D_x \times D_Q$)

Value matrix: \mathbf{W}_V (Shape: $D_x \times D_V$)

Query matrix: \mathbf{W}_Q (Shape: $D_x \times D_Q$)

Computation:

Query vectors: $\mathbf{Q} = \mathbf{XW}_Q$

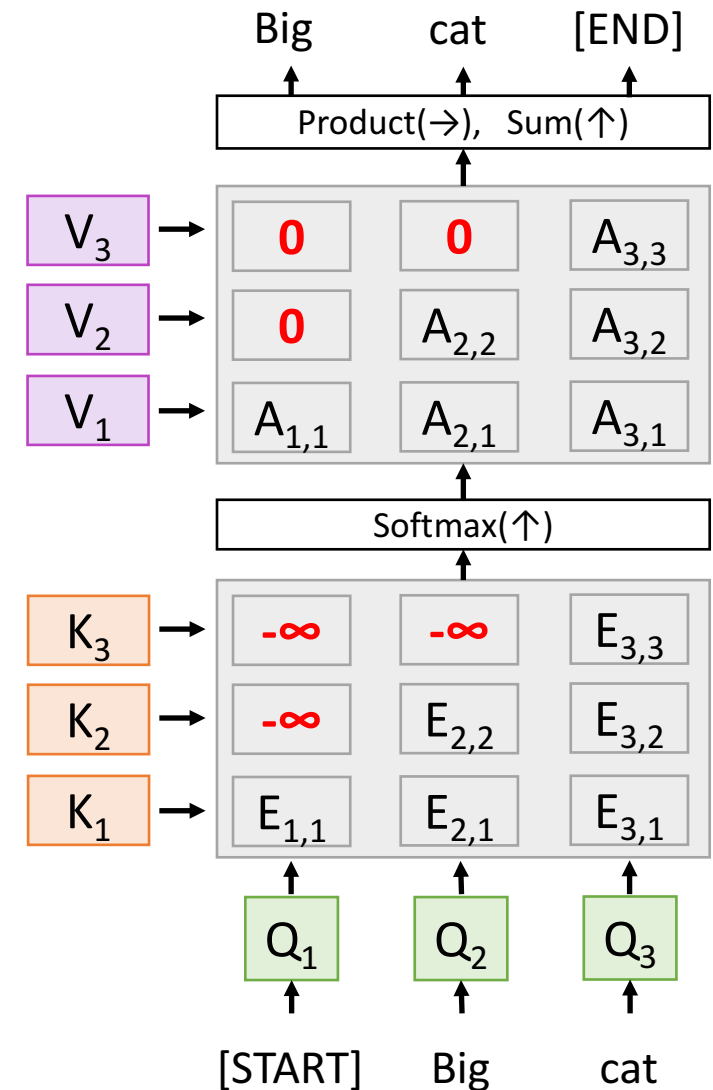
Key vectors: $\mathbf{K} = \mathbf{XW}_K$ (Shape: $N_x \times D_Q$)

Value Vectors: $\mathbf{V} = \mathbf{XW}_V$ (Shape: $N_x \times D_V$)

Similarities: $\mathbf{E} = \mathbf{QK}^T$ (Shape: $N_x \times N_x$) $E_{i,j} = \mathbf{Q}_i \cdot \mathbf{K}_j / \text{sqrt}(D_Q)$

Attention weights: $\mathbf{A} = \text{softmax}(\mathbf{E}, \text{dim}=1)$ (Shape: $N_Q \times N_x$)

Output vectors: $\mathbf{Y} = \mathbf{AV}$ (Shape: $N_x \times D_V$) $Y_i = \sum_j A_{i,j} \mathbf{V}_j$



Multihead Self-Attention Layer

Use H independent
“Attention Heads” in parallel

Inputs:

Input vectors: \mathbf{X} (Shape: $N_X \times D_X$)

Key matrix: \mathbf{W}_K (Shape: $D_X \times D_Q$)

Value matrix: \mathbf{W}_V (Shape: $D_X \times D_V$)

Query matrix: \mathbf{W}_Q (Shape: $D_X \times D_Q$)

Computation:

Query vectors: $\mathbf{Q} = \mathbf{XW}_Q$

Key vectors: $\mathbf{K} = \mathbf{XW}_K$ (Shape: $N_X \times D_Q$)

Value Vectors: $\mathbf{V} = \mathbf{XW}_V$ (Shape: $N_X \times D_V$)

Similarities: $\mathbf{E} = \mathbf{QK}^T$ (Shape: $N_X \times N_X$) $E_{i,j} = \mathbf{Q}_i \cdot \mathbf{K}_j / \text{sqrt}(D_Q)$

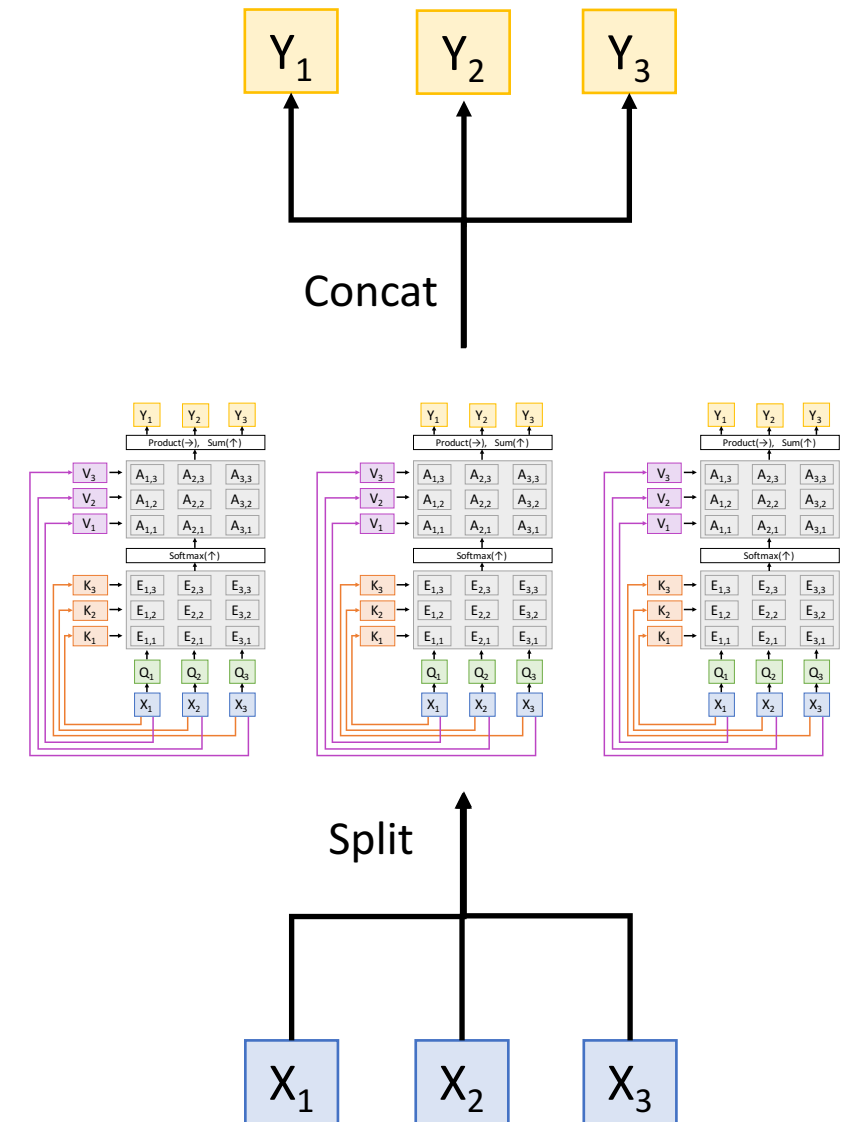
Attention weights: $\mathbf{A} = \text{softmax}(\mathbf{E}, \text{dim}=1)$ (Shape: $N_Q \times N_X$)

Output vectors: $\mathbf{Y} = \mathbf{AV}$ (Shape: $N_X \times D_V$) $Y_i = \sum_j A_{i,j} \mathbf{V}_j$

Hyperparameters:

Query dimension D_Q

Number of heads H

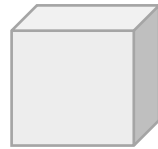
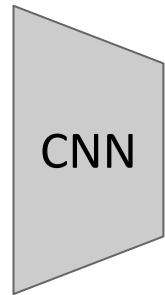


Example: CNN with Self-Attention

Input Image

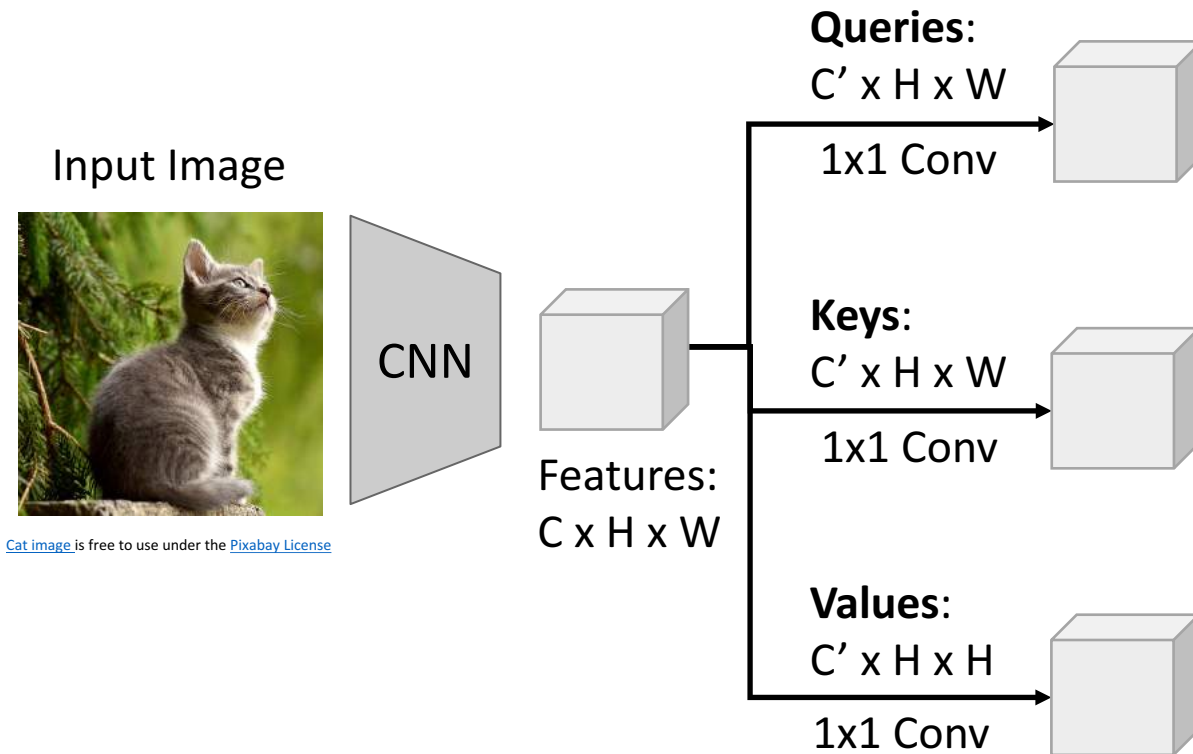


[Cat image](#) is free to use under the [Pixabay License](#)

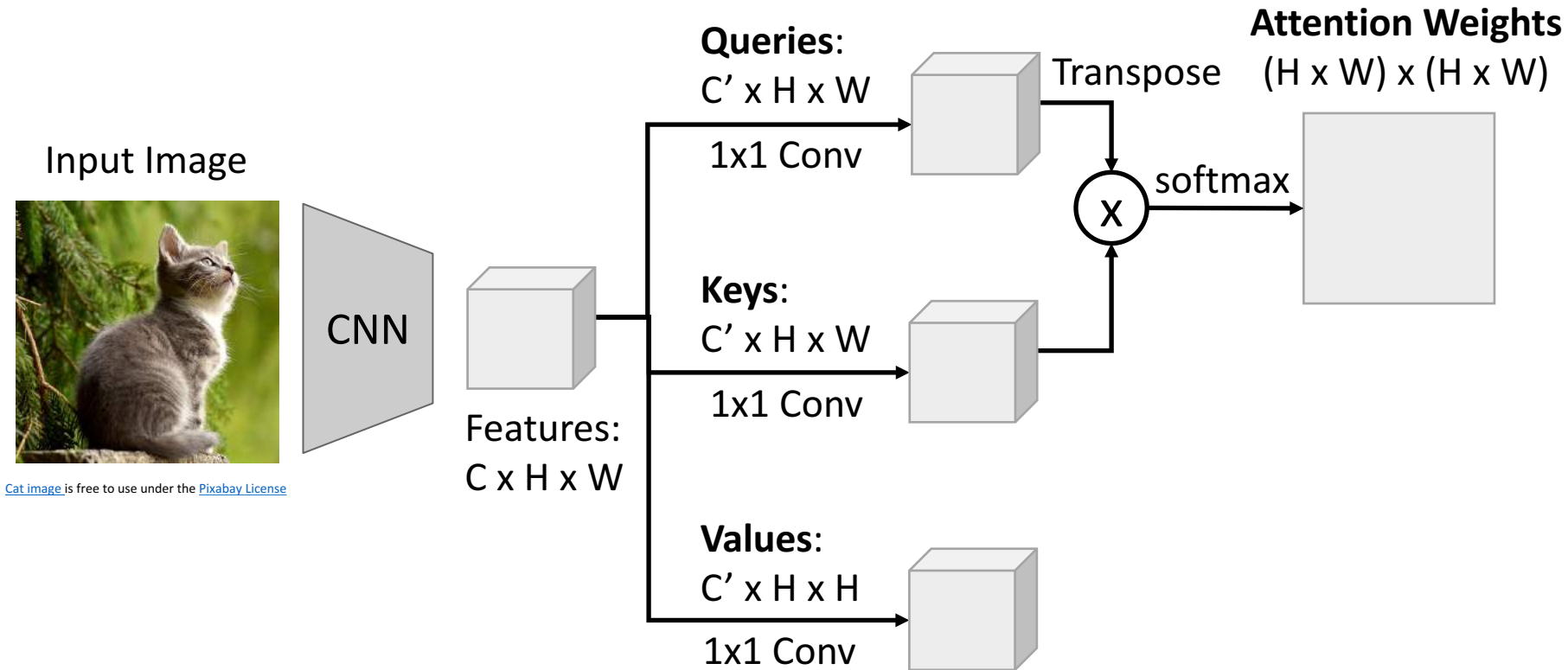


Features:
 $C \times H \times W$

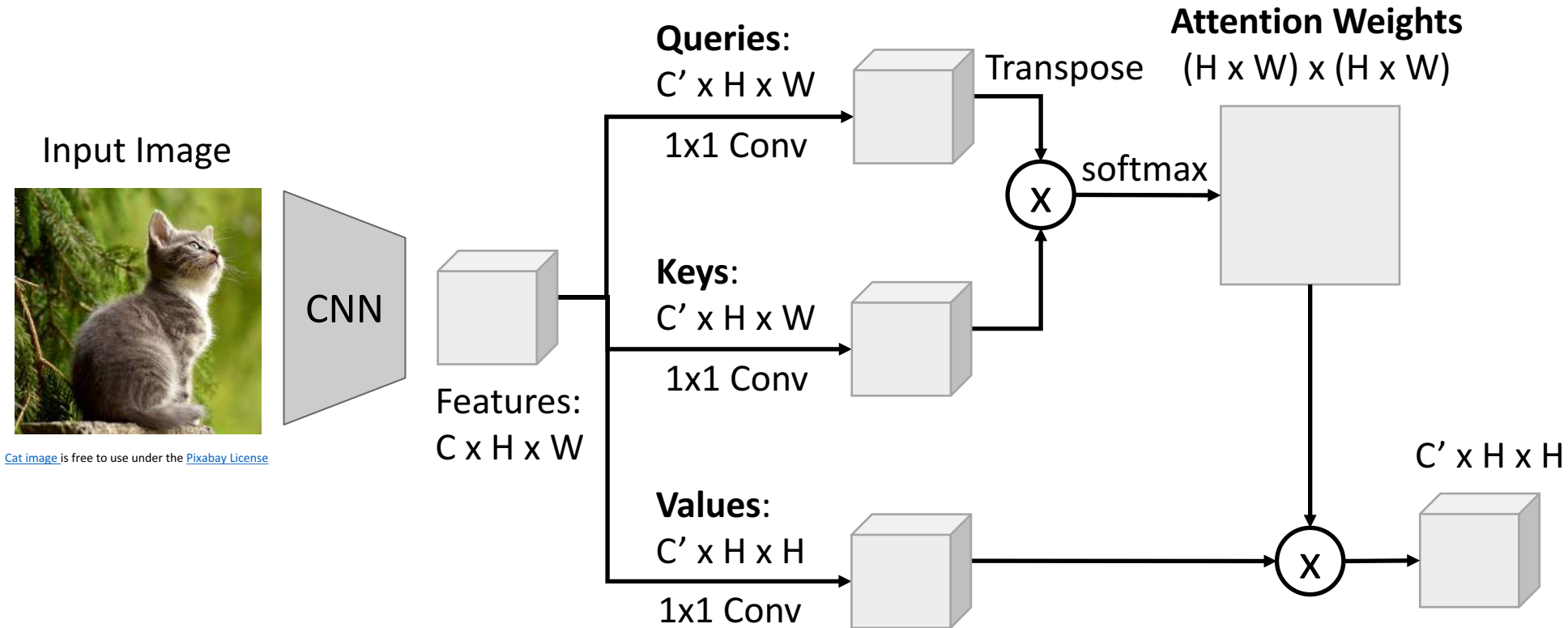
Example: CNN with Self-Attention



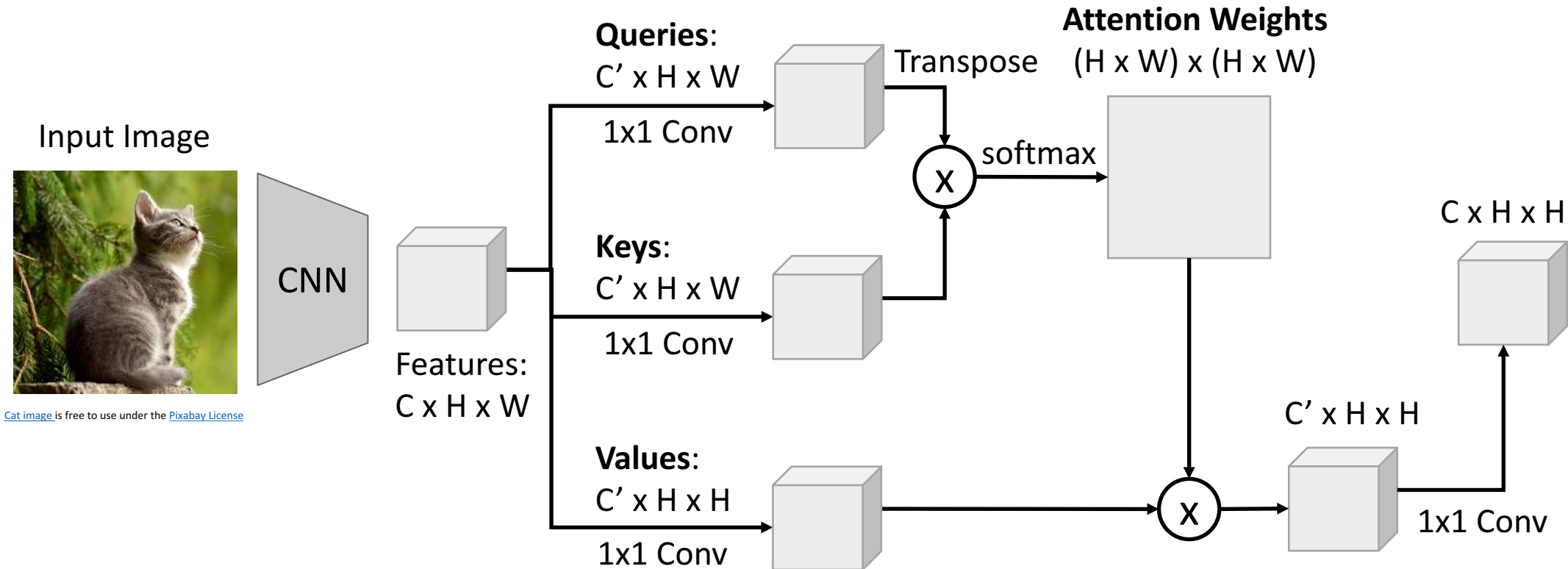
Example: CNN with Self-Attention



Example: CNN with Self-Attention



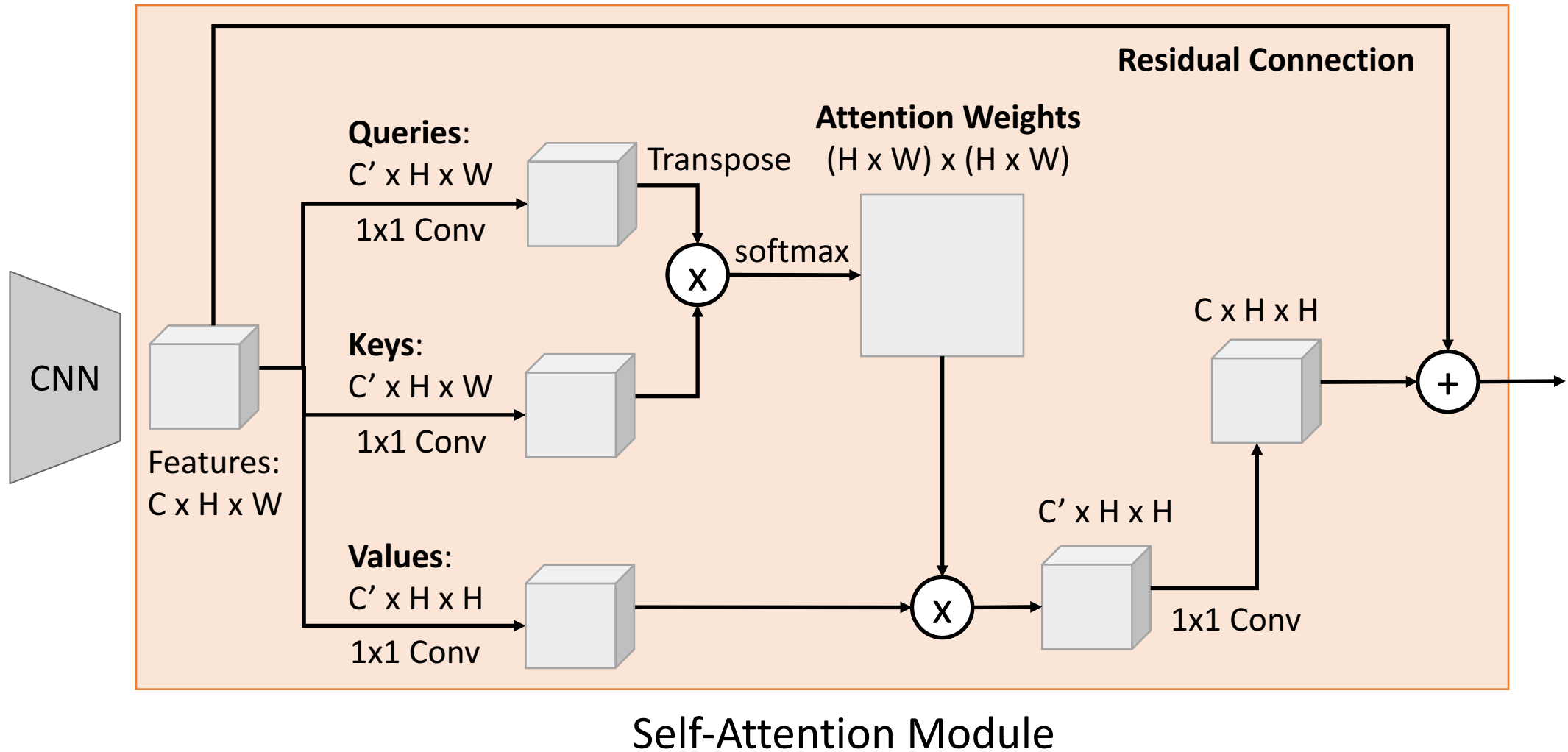
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Example: CNN with Self-Attention

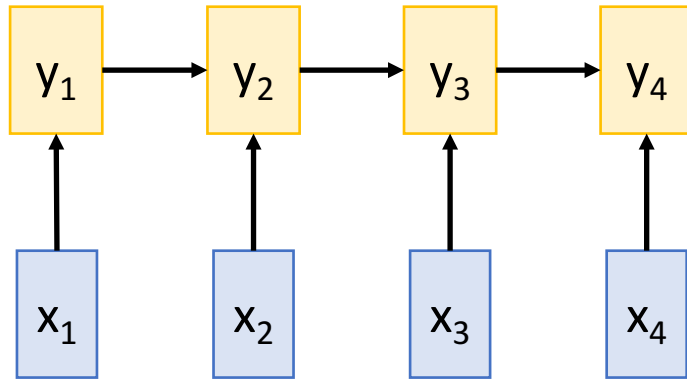


[Cat image](#) is free to use under the [Pixabay License](#)



Three Ways of Processing Sequences

Recurrent Neural Network



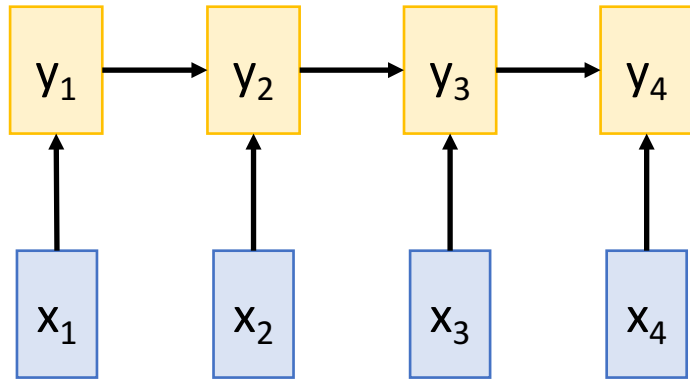
Works on **Ordered Sequences**

(+) **Good at long sequences:** After one RNN layer, h_T "sees" the whole sequence

(-) **Not parallelizable:** need to compute hidden states sequentially

Three Ways of Processing Sequences

Recurrent Neural Network

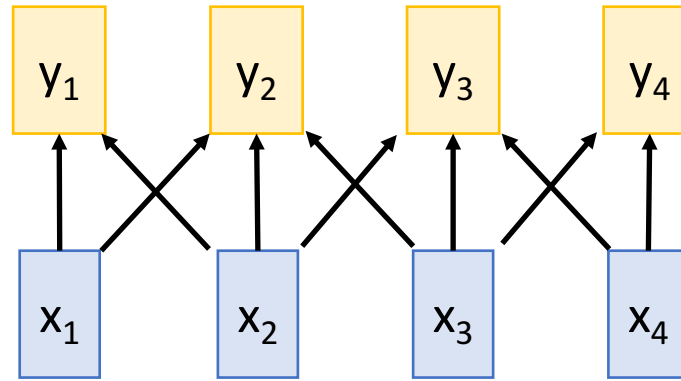


Works on **Ordered Sequences**

(+) **Good at long sequences:** After one RNN layer, h_T "sees" the whole sequence

(-) **Not parallelizable:** need to compute hidden states sequentially

1D Convolution



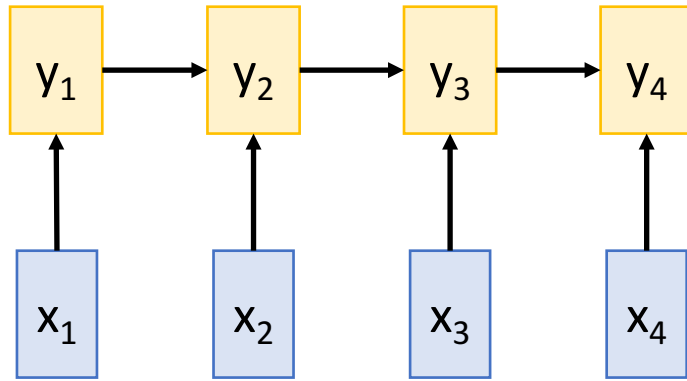
Works on **Multidimensional Grids**

(-) **Bad at long sequences:** Need to stack many conv layers for outputs to "see" the whole sequence

(+) **Highly parallel:** Each output can be computed in parallel

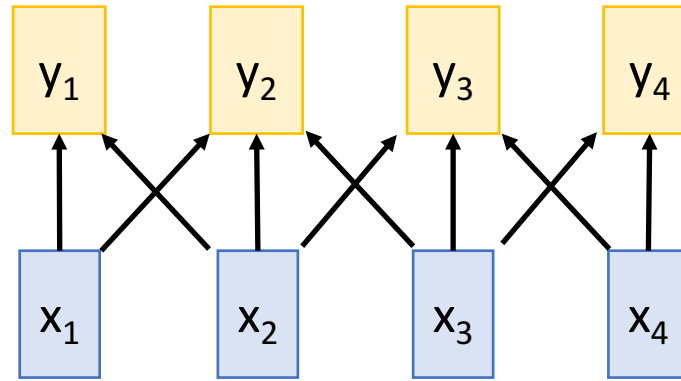
Three Ways of Processing Sequences

Recurrent Neural Network



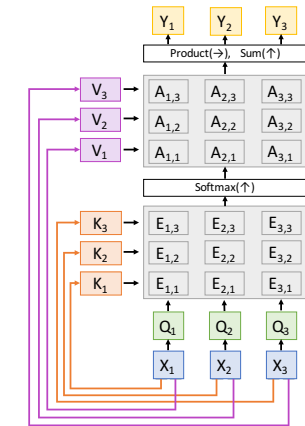
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1D Convolution



Works on **Multidimensional Grids**
(-) **Bad at long sequences:** Need to stack many conv layers for outputs to "see" the whole sequence
(+) **Highly parallel:** Each output can be computed in parallel

Self-Attention



Works on **Sets of Vectors**
(-) **Good at long sequences:** after one self-attention layer, each output "sees" all inputs!
(+) **Highly parallel:** Each output can be computed in parallel
(-) **Very memory intensive**

Three Ways of Processing Sequences

Recurrent Neural Network

1D Convolution

Self-Attention

Attention is all you need

Vaswani et al, NeurIPS 2017

Works on **Ordered Sequences**

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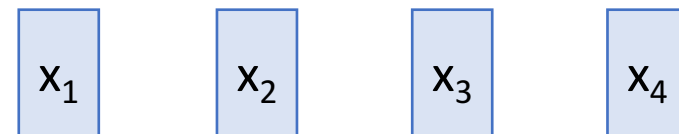
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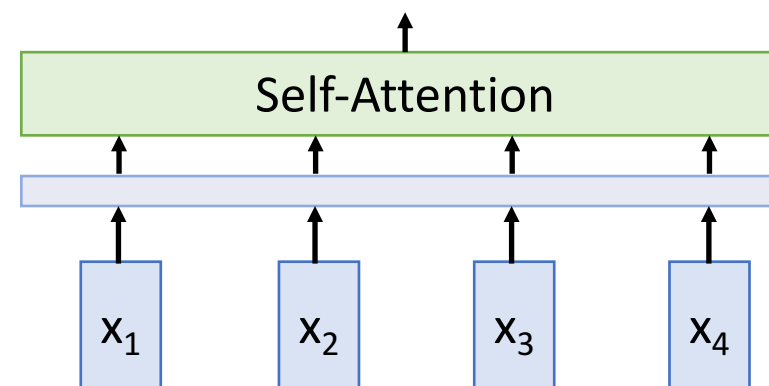
The Transformer



Vaswani et al, "Attention is all you need", NeurIPS 2017

The Transformer

All vectors interact
with each other

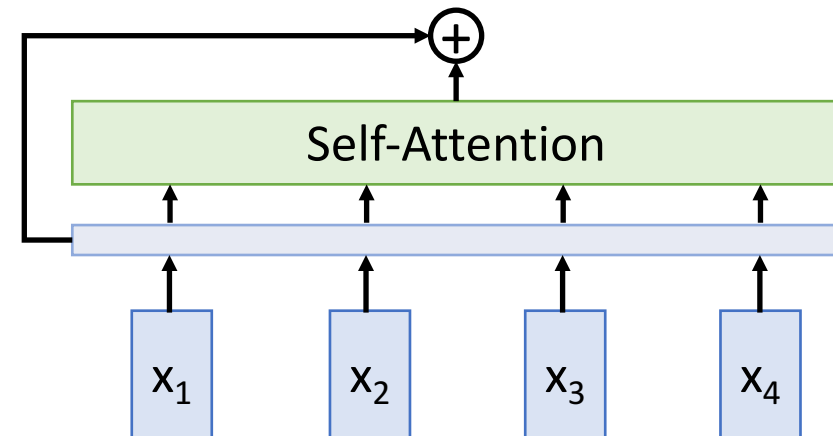


Vaswani et al, "Attention is all you need", NeurIPS 2017

The Transformer

Residual connection

All vectors interact
with each other



The Transformer

Recall **Layer Normalization**:

Given h_1, \dots, h_N (Shape: D)

scale: γ (Shape: D)

Shift: β (Shape: D)

$\mu_i = (1/D) \sum_j h_{i,j}$ (scalar)

$\sigma_i = (\sum_j (h_{i,j} - \mu_i)^2)^{1/2}$ (scalar)

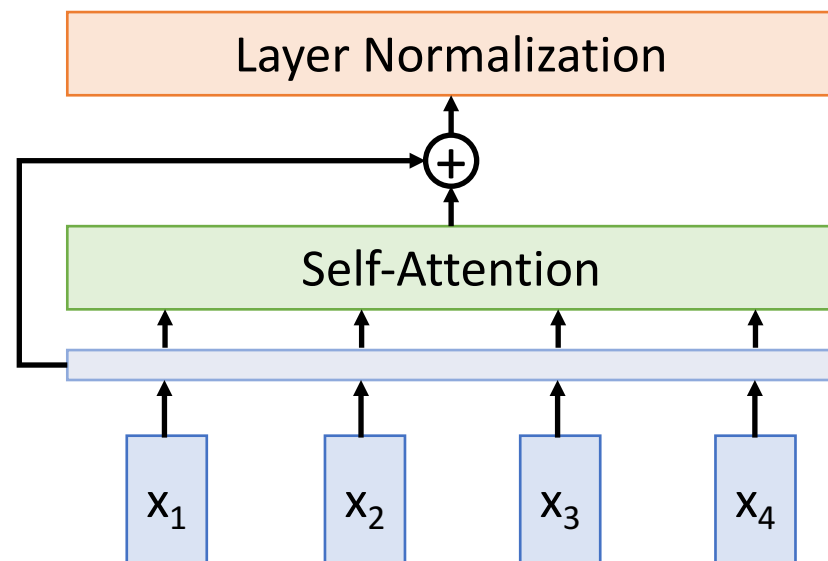
$z_i = (h_i - \mu_i) / \sigma_i$

$y_i = \gamma * z_i + \beta$

Ba et al, 2016

Residual connection

All vectors interact
with each other



Vaswani et al, "Attention is all you need", NeurIPS 2017

The Transformer

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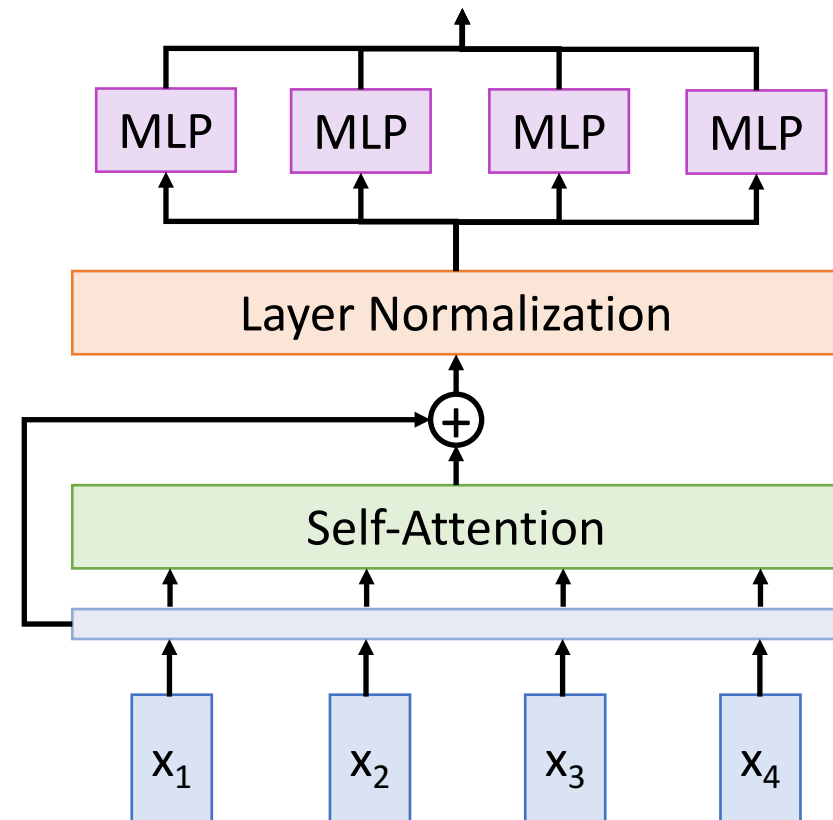
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Ba et al, 2016

MLP independently
on each vector

Residual connection

All vectors interact
with each other



Vaswani et al, "Attention is all you need", NeurIPS 2017

The Transformer

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$y_i = \gamma * z_i + \beta$

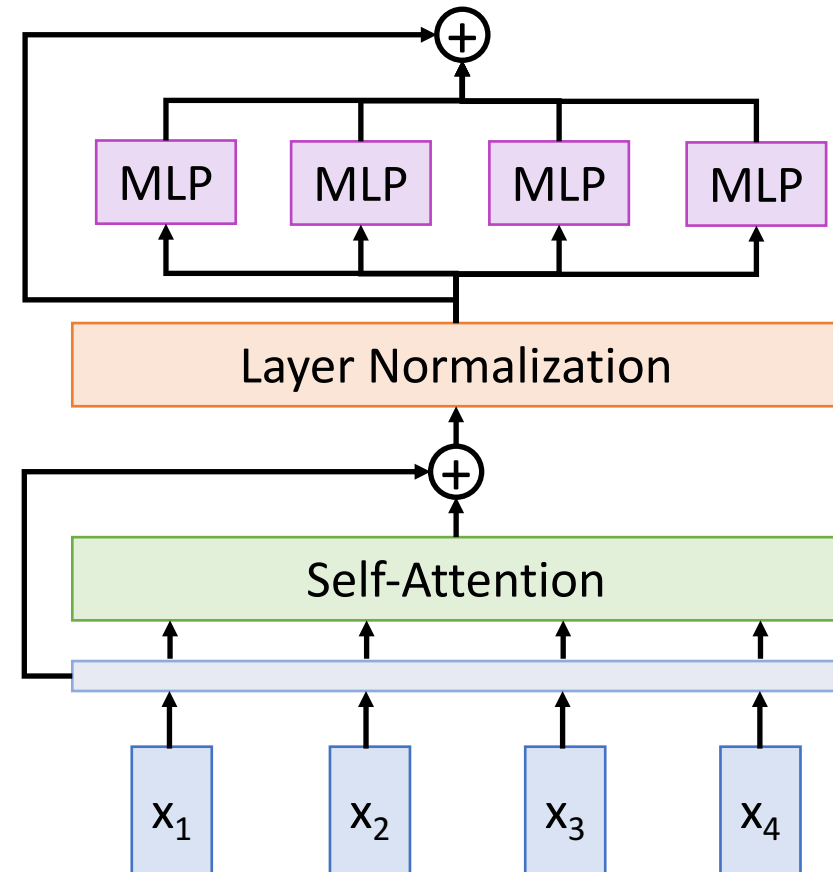
Ba et al, 2016

Residual connection

MLP independently
on each vector

Residual connection

All vectors interact
with each other



Vaswani et al, "Attention is all you need", NeurIPS 2017

The Transformer

Recall **Layer Normalization**:

Given h_1, \dots, h_N (Shape: D)

scale: γ (Shape: D)

Shift: β (Shape: D)

$\mu_i = (1/D) \sum_j h_{i,j}$ (scalar)

$\sigma_i = (\sum_j (h_{i,j} - \mu_i)^2)^{1/2}$ (scalar)

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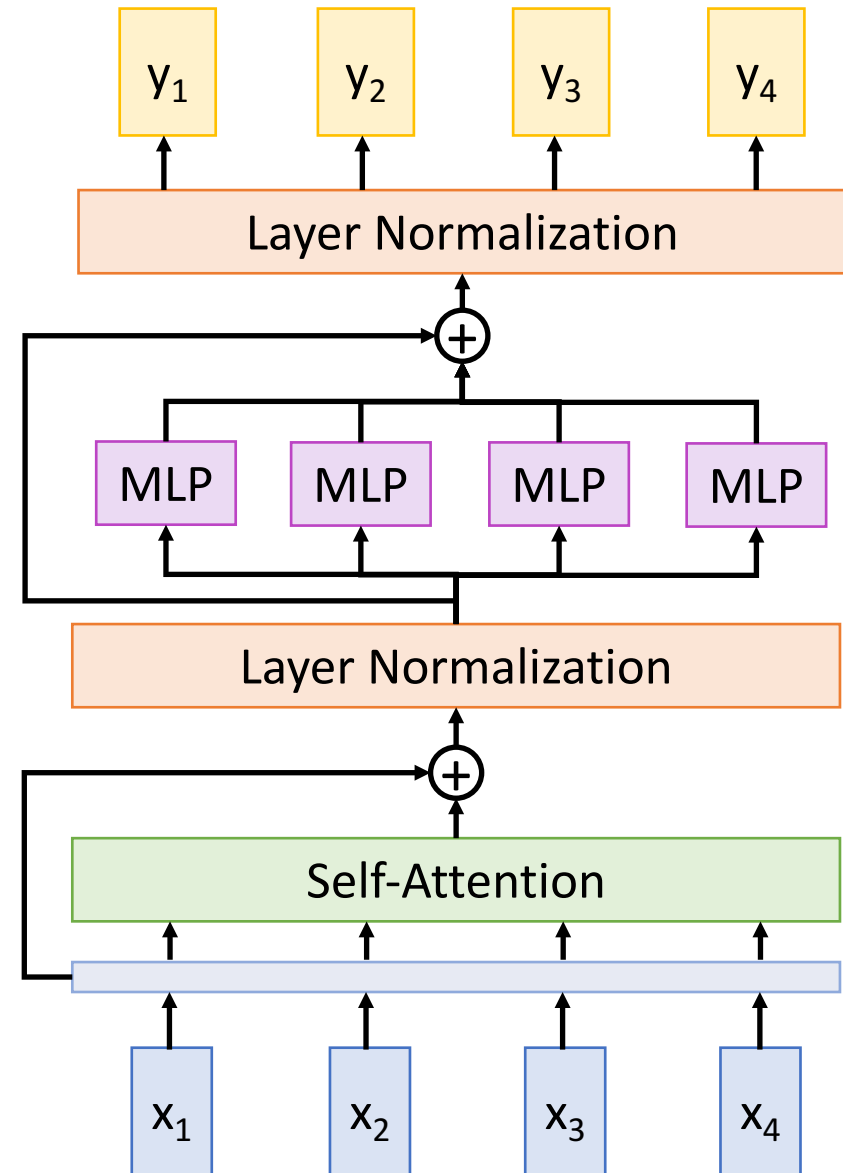
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The Transformer

Transformer Block:

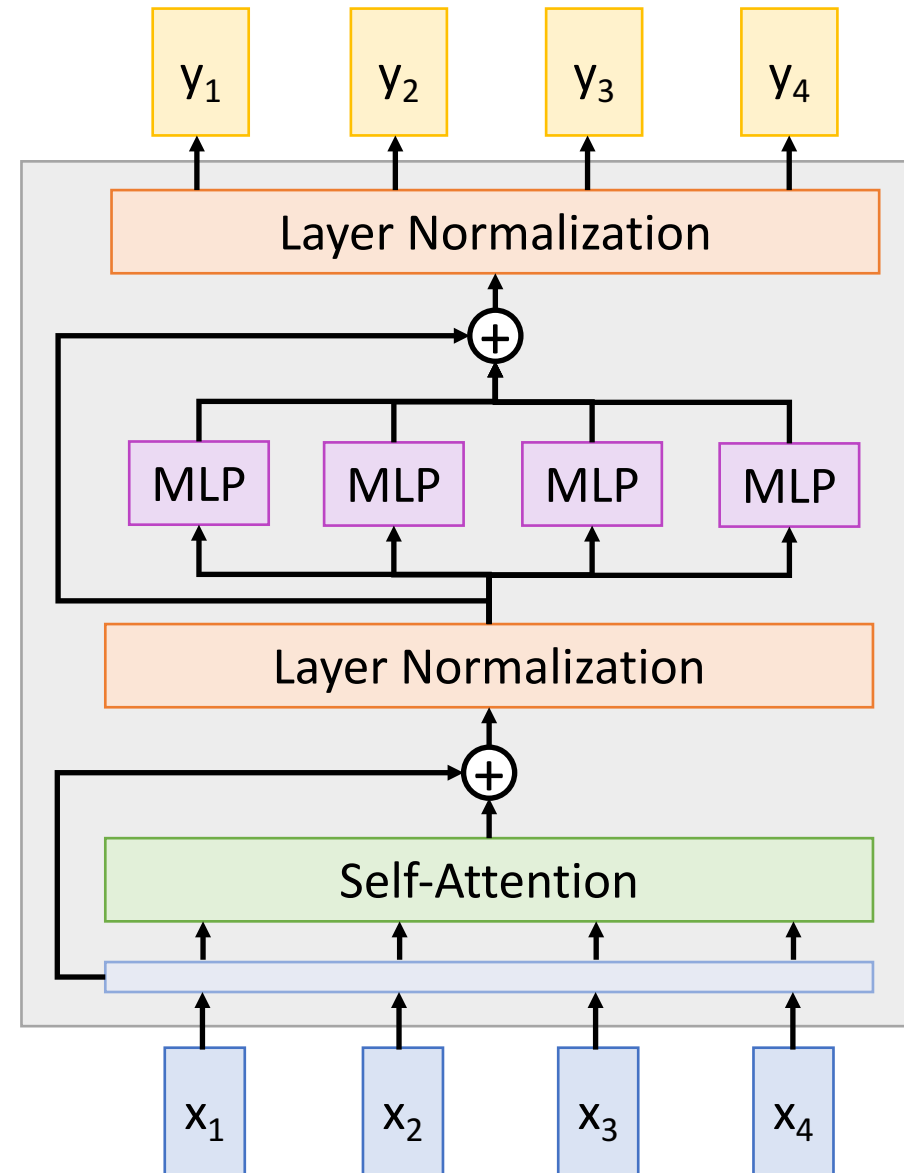
Input: Set of vectors x

Output: Set of vectors y

Self-attention is the only interaction between vectors!

Layer norm and MLP work independently per vector

Highly scalable, highly parallelizable



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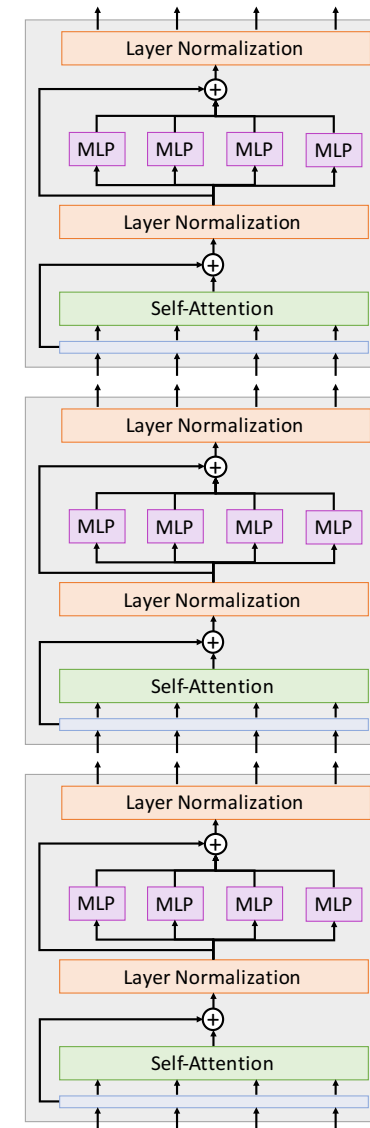
Highly scalable, highly parallelizable

A **Transformer** is a sequence of transformer blocks

Vaswani et al:

Encoder: 6 blocks, $D=512$, 6 heads

Decoder: 6 blocks, $D=512$, 6 heads



The Transformer: Transfer Learning

“ImageNet Moment for Natural Language Processing”

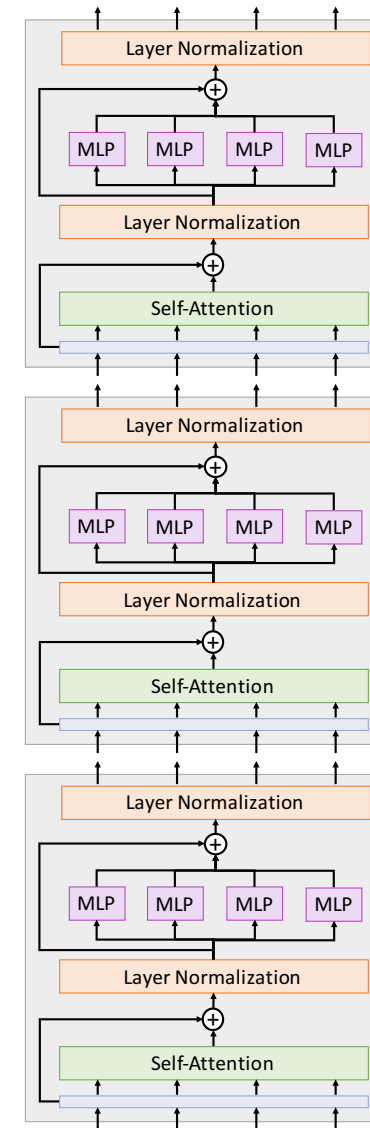
Pretraining:

Download a lot of text from the internet

Train a giant Transformer model for language modeling

Finetuning:

Fine-tune the Transformer on your own NLP task



Scaling up Transformers

Model	Layers	Width	Heads	Params	Data	Training
Transformer-Base	12	512	8	65M		8x P100 (12 hours)
Transformer-Large	12	1024	16	213M		8x P100 (3.5 days)

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Devlin et al, "BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding", EMNLP 2018

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Yang et al, XLNet: Generalized Autoregressive Pretraining for Language Understanding", 2019
Liu et al, "RoBERTa: A Robustly Optimized BERT Pretraining Approach", 2019

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Radford et al, "Language models are unsupervised multitask learners", 2019

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Shoeybi et al, "Megatron-LM: Training Multi-Billion Parameter Language Models using Model Parallelism", 2019

Scaling up Transformers

~\$430,000 on Amazon AWS!

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Now, after almost two centuries, the mystery of what sparked this odd phenomenon is finally solved.

Dr. Jorge Pérez, an evolutionary biologist from the University of La Paz, and several companions, were exploring the Andes Mountains when they found a small valley, with no other animals or humans. Pérez noticed that the valley had what appeared to be a natural fountain, surrounded by two peaks of rock and silver snow.

Pérez and the others then ventured further into the valley. "By the time we reached the top of one peak, the water looked blue, with some crystals on top," said Pérez.

Pérez and his friends were astonished to see the unicorn herd. These creatures could be seen from the air without having to move too much to see them – they were so close they could touch their horns.

While examining these bizarre creatures the scientists discovered that the creatures also spoke some fairly regular English. Pérez stated, "We can see, for example, that they have a common 'language,' something like a dialect or dialectic."

Dr. Pérez believes that the unicorns may have originated in Argentina, where the animals were believed to be descendants of a lost race of people who lived there before the arrival of humans in those parts of South America.

While their origins are still unclear, some believe that perhaps the creatures were created when a human and a unicorn met each other in a time before human civilization. According to Pérez, "In South America, such incidents seem to be quite common."

However, Pérez also pointed out that it is likely that the only way of knowing for sure if unicorns are indeed the descendants of a lost alien race is through DNA. "But they seem to be able to communicate in English quite well, which I believe is a sign of evolution, or at least a change in social organization," said the scientist.

OpenAI, "Better Language Models and their Implications", 2019, <https://openai.com/blog/better-language-models/>

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Try it yourself:

<https://talktotransformer.com>

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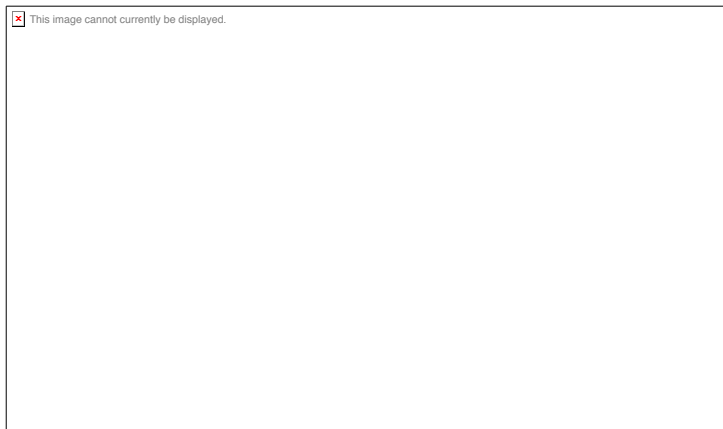
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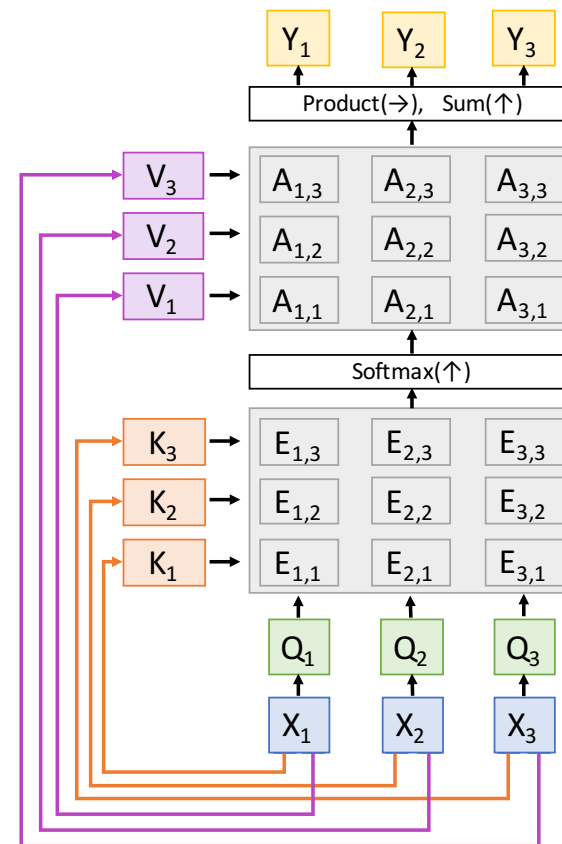
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Summary

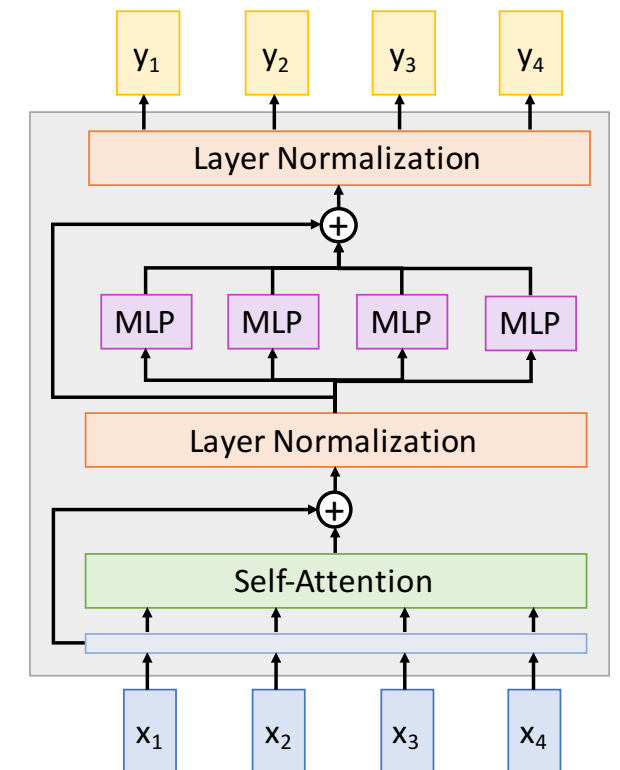
Adding **Attention** to RNN models lets them look at different parts of the input at each timestep



Generalized **Self-Attention** is new, powerful neural network primitive



Transformers are a new neural network model that only uses attention



Next Week: Guest Lectures



Monday 10/28
Luowei Zhou
Vision and Language



Wednesday 10/30
Prof. Atul Prakash
Adversarial Machine Learning