Lecture 13: Attention

Midterm

Grades will be out in ~1 week

Please do not discuss midterm questions on Piazza

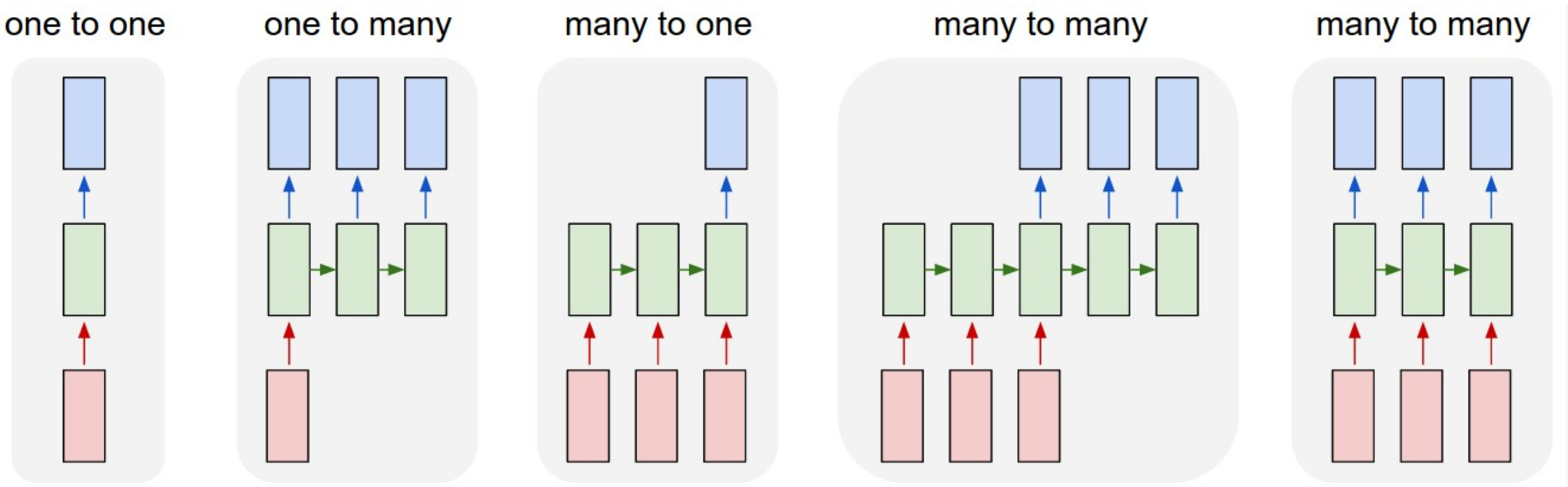
Someone left a waterbottle in exam room – Post on Piazza if it is yours

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

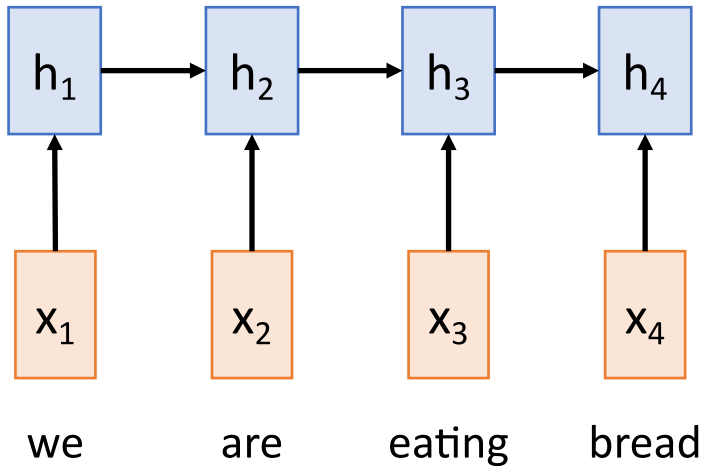


Sequence-to-Sequence with RNNs

Input: Sequence $x_1, \ldots x_T$

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

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



Sutskever et al, "Sequence to sequence learning with neural networks", NeurIPS 2014

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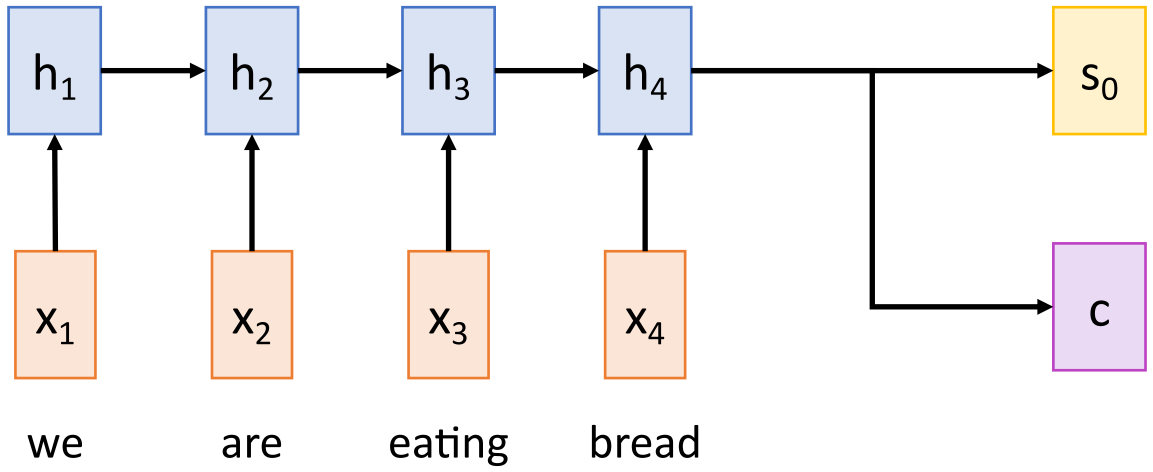
From final hidden state predict:
Initial decoder state s_0
Context vector c (often $c=h_T$)



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Sequence-to-Sequence with RNNs

Input: Sequence $x_1, \dots x_T$

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

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From final hidden state predict:

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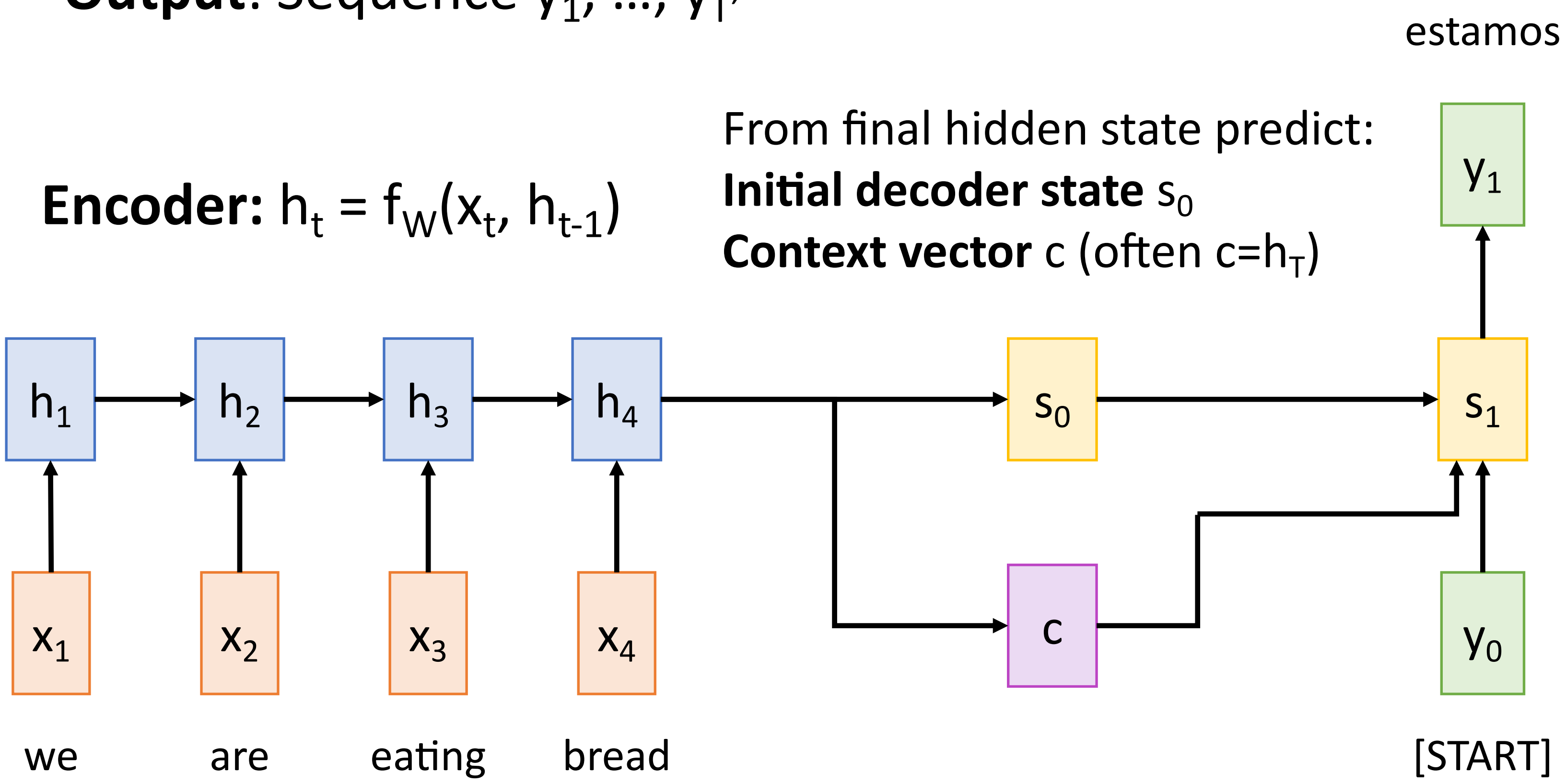

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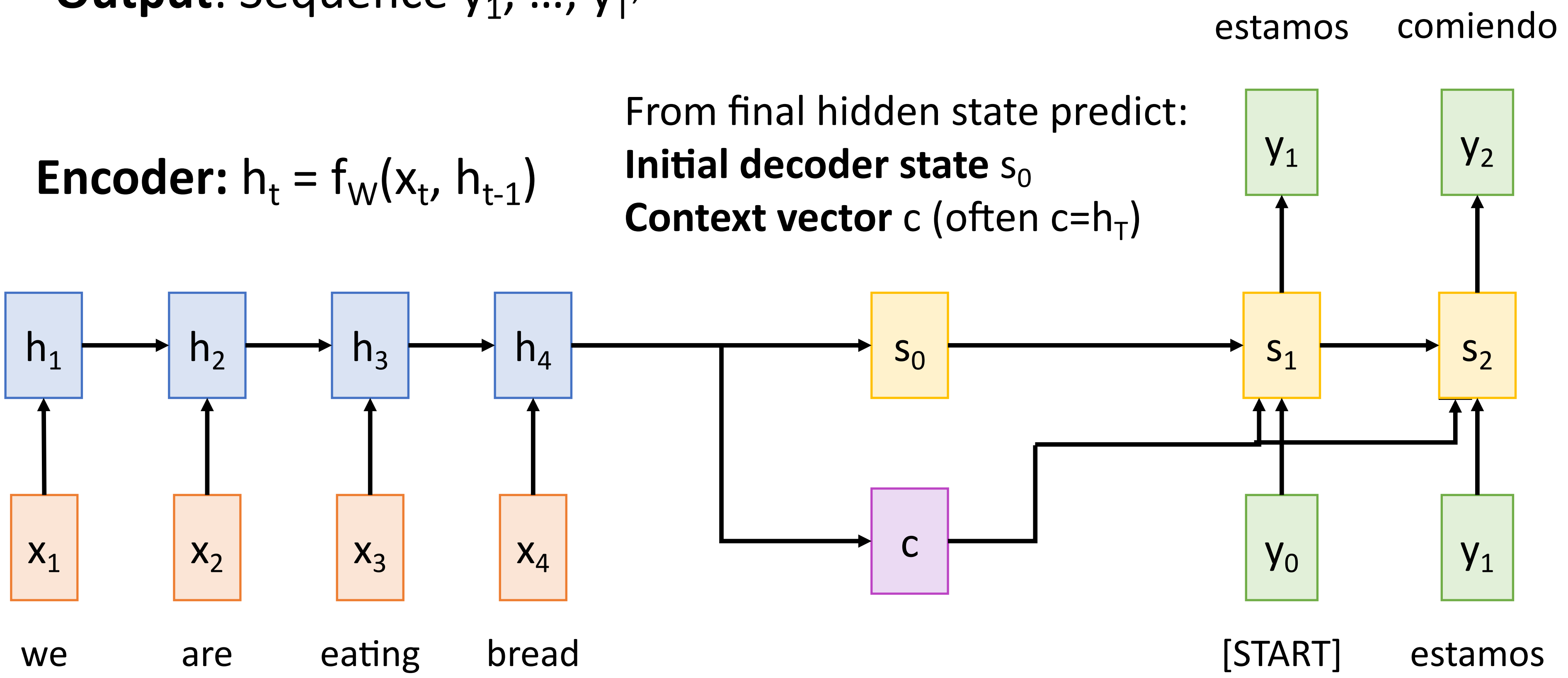

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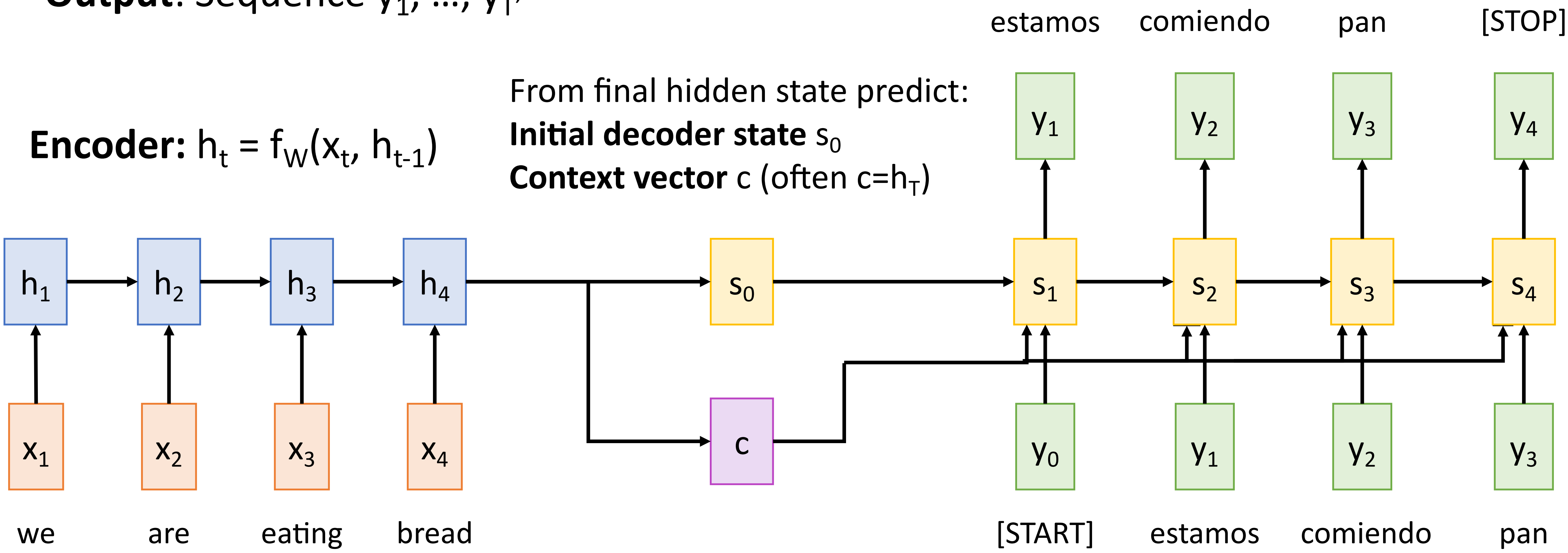

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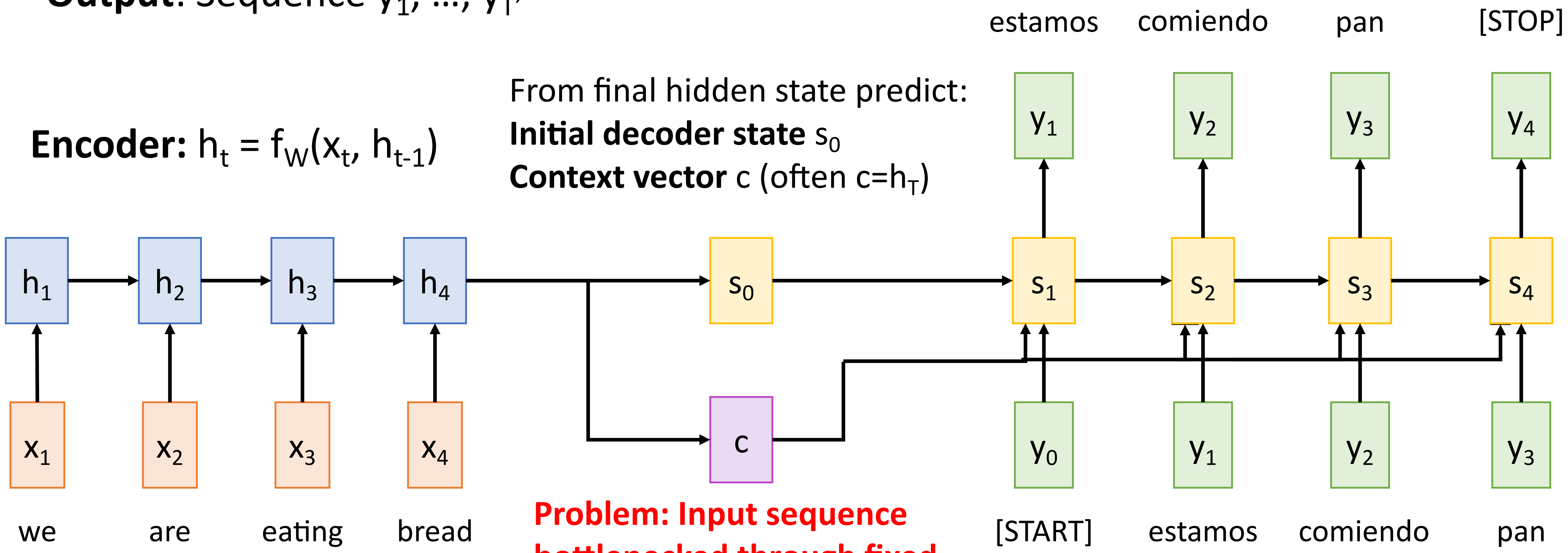

Problem: Input sequence bottlenecked through fixed-sized vector. What if T=1000?

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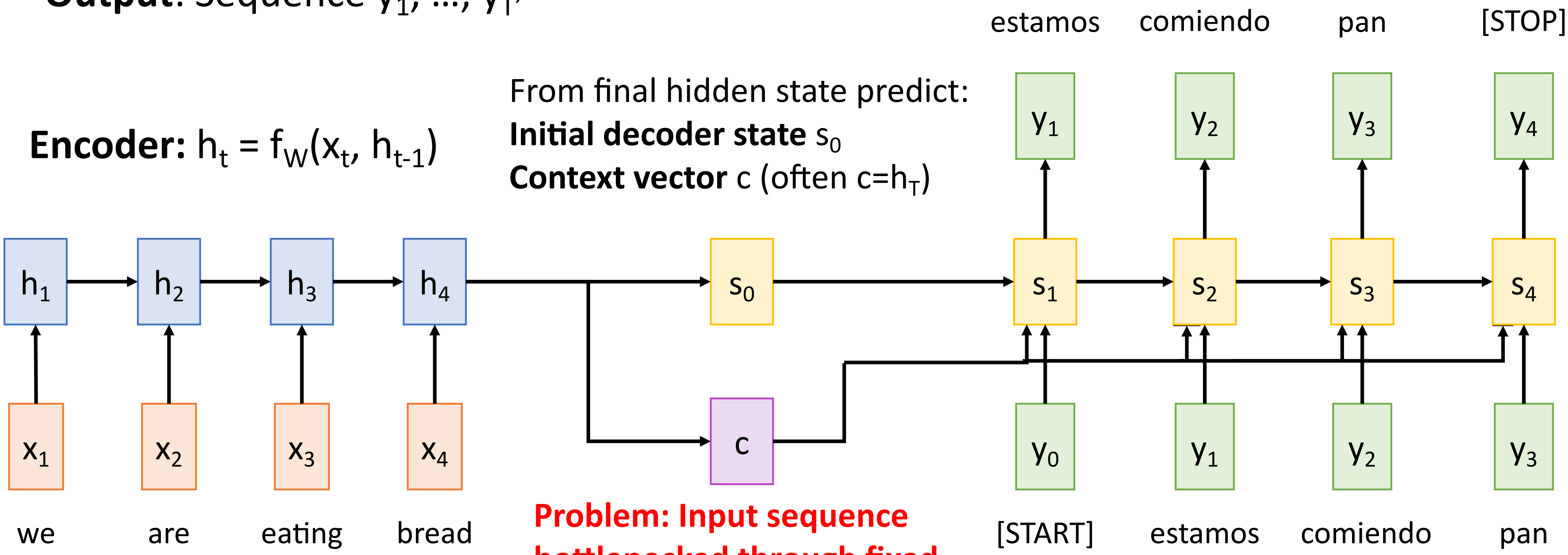

Problem: Input sequence bottlenecked through fixed-sized vector. What if T=1000?

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

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Sequence-to-Sequence with RNNs **and Attention**

Input: Sequence $x_1, \ldots x_T$

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

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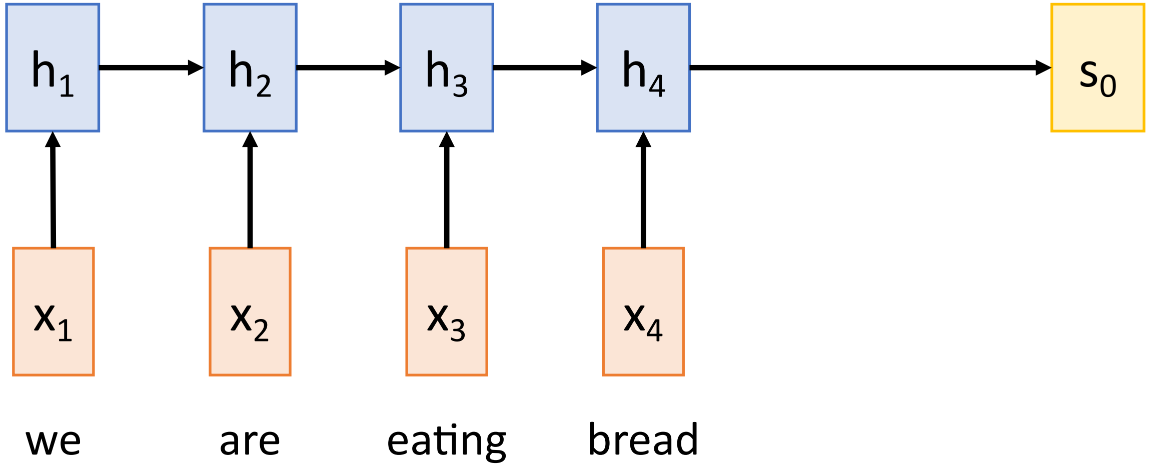
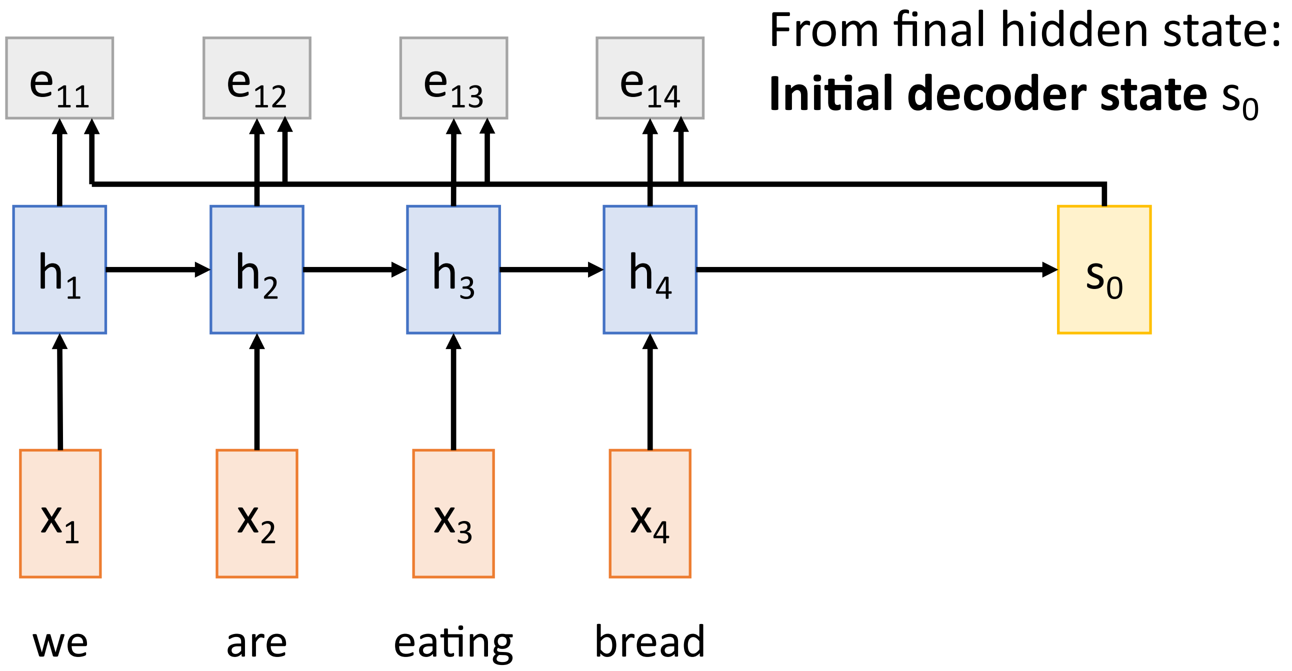


Bahdanau et al, "Neural machine translation by jointly learning to align and translate", ICLR 2015

Sequence-to-Sequence with RNNs **and Attention**

Compute (scalar) **alignment scores**

$e_{t,i} = f_{att}(s_{t-1}, h_i)$ (f_{att} is an MLP)



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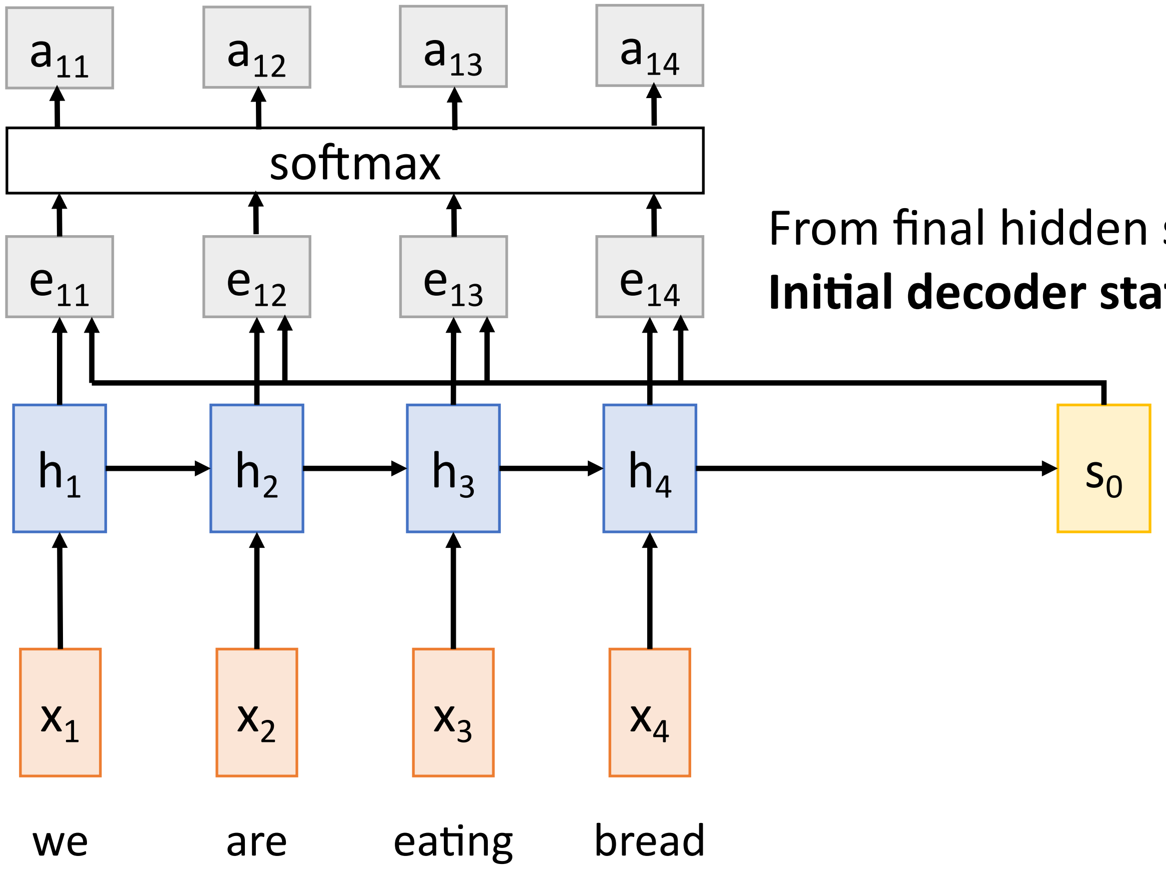

From final hidden state:
Initial decoder state s_0

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

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

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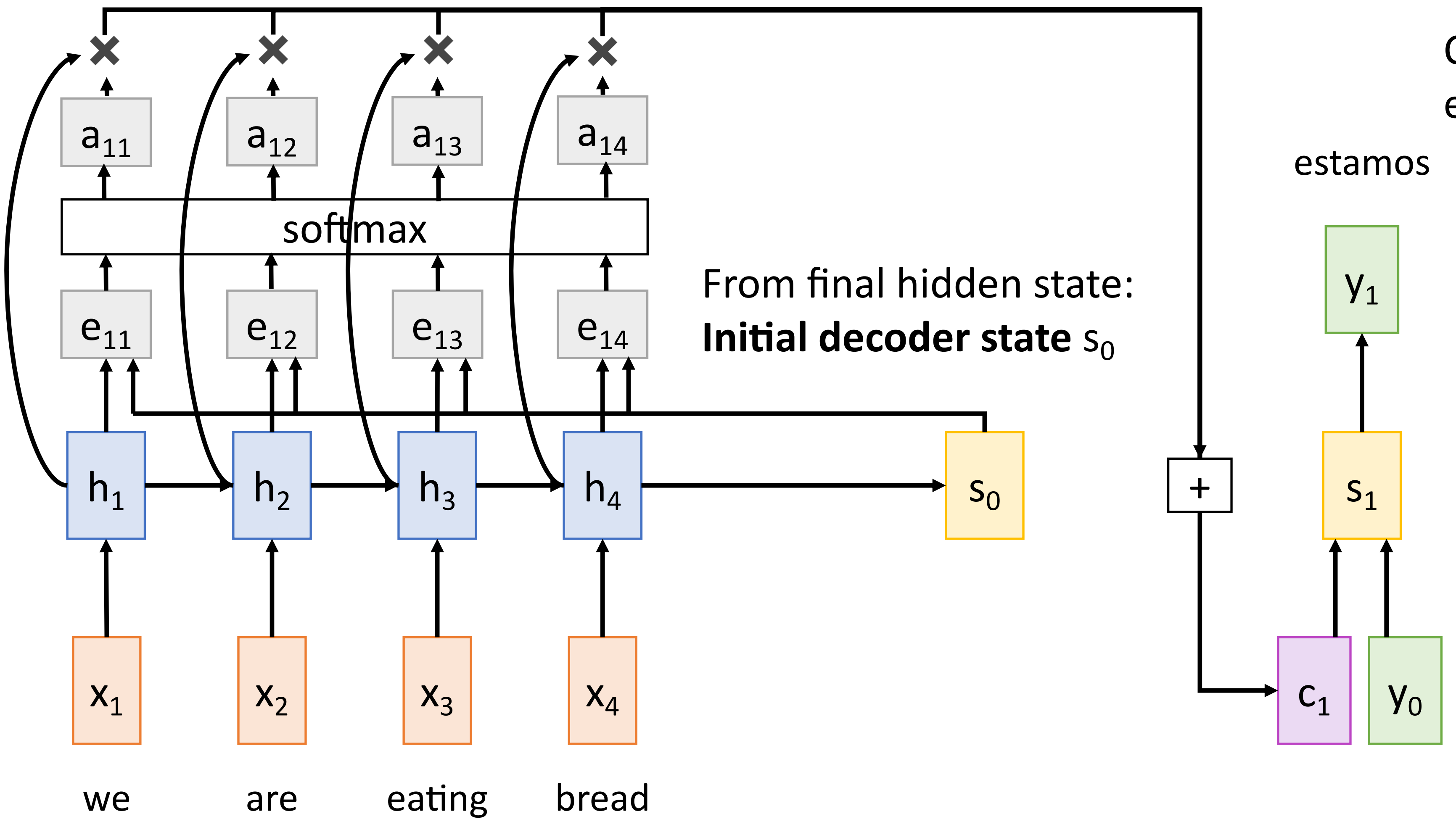
Sequence-to-Sequence with RNNs **and Attention**



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

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

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

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

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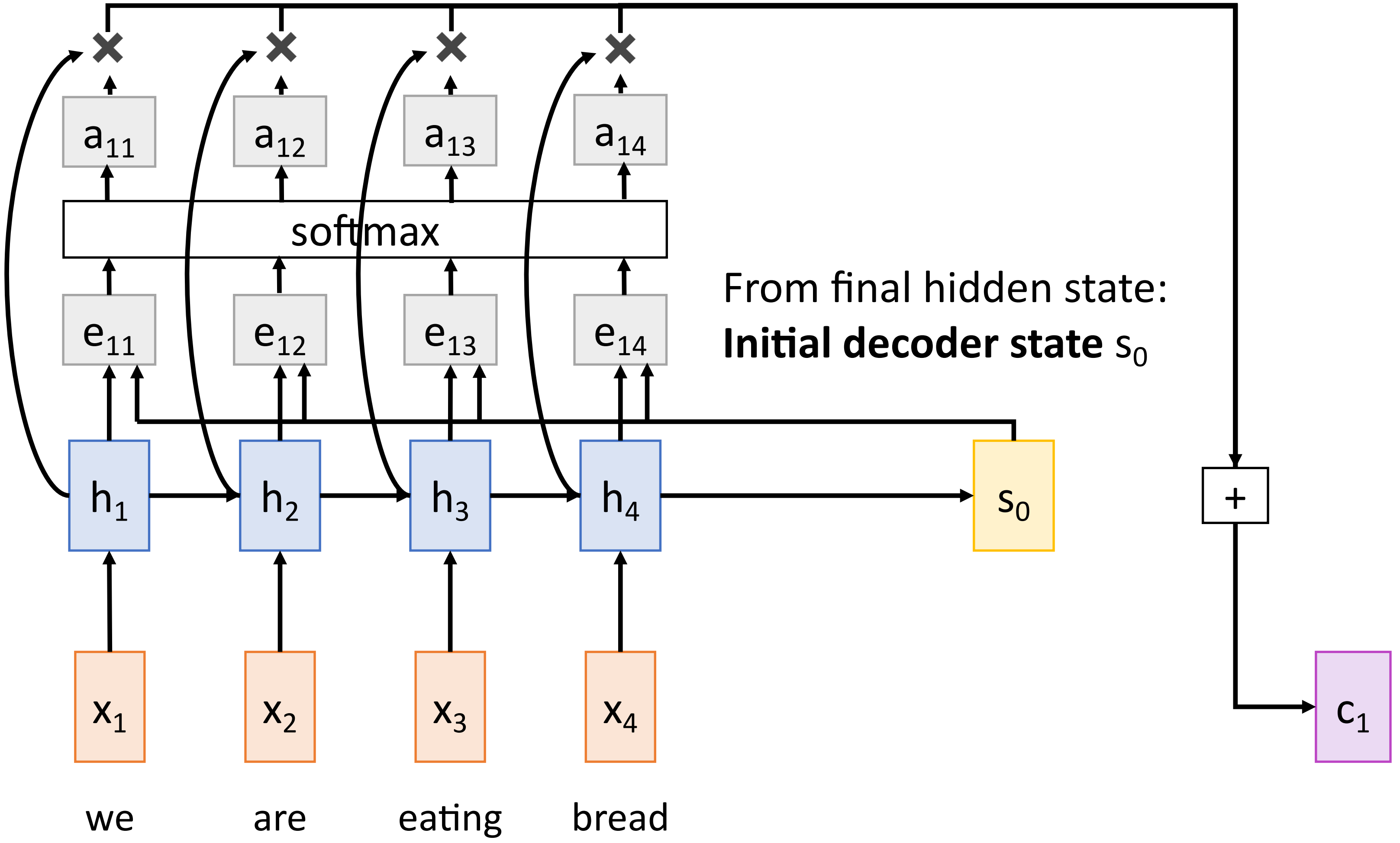
Sequence-to-Sequence with RNNs **and Attention**



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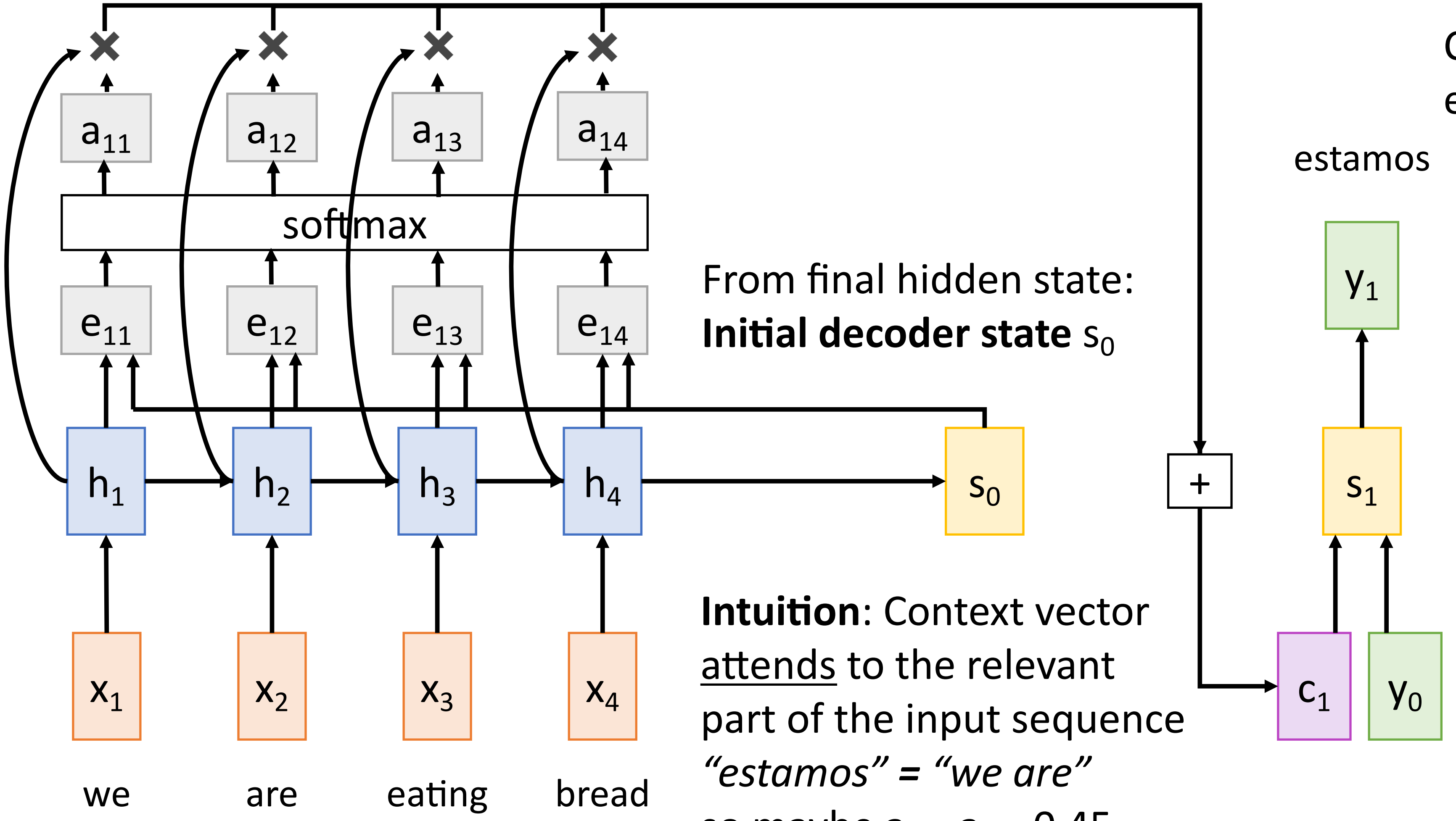


From final hidden state: **Initial decoder state** s_0

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

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

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

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

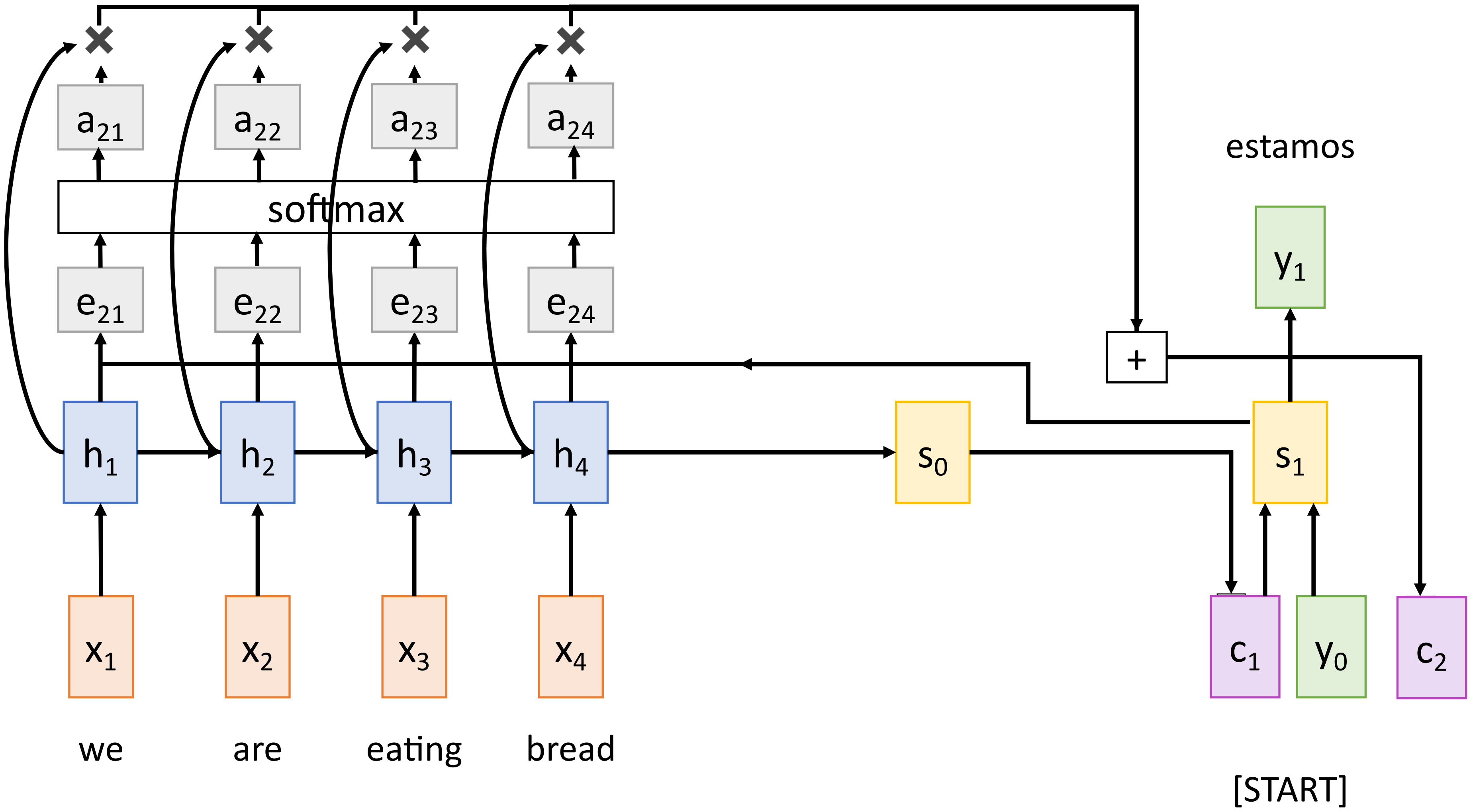
Intuition: Context vector attends to the relevant part of the input sequence
"estamos" = "we are"
so maybe $a_{11}=a_{12}=0.45$, $a_{13}=a_{14}=0.05$

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

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

Sequence-to-Sequence with RNNs

Repeat: Use s_1 to compute new context vector c_2



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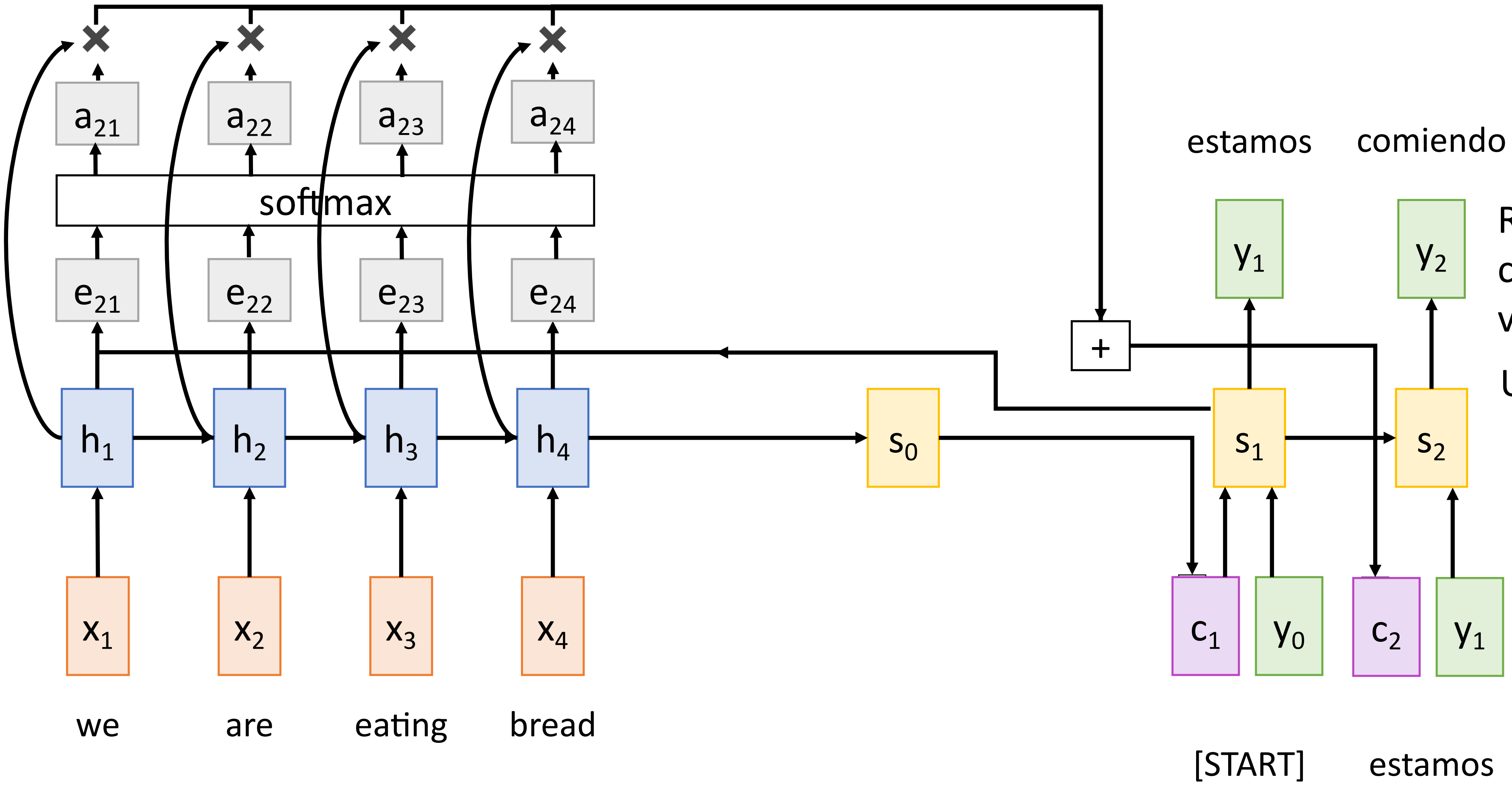
Sequence-to-Sequence with RNNs **and Attention**

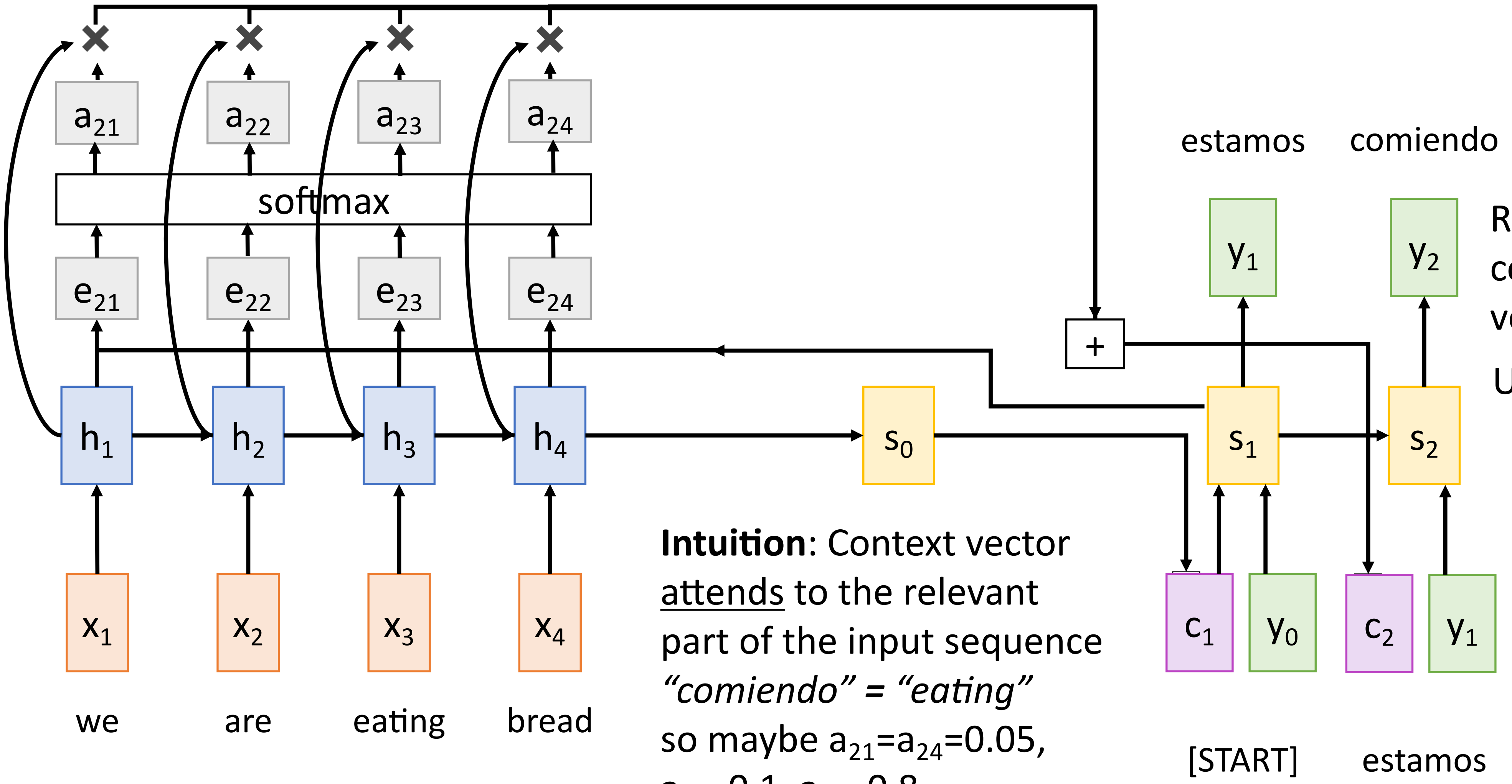


Repeat: Use s_1 to compute new context vector c_2

Use c_2 to compute s_2, y_2

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

Sequence-to-Sequence with RNNs **and Attention**



Repeat: Use s_1 to compute new context vector c_2

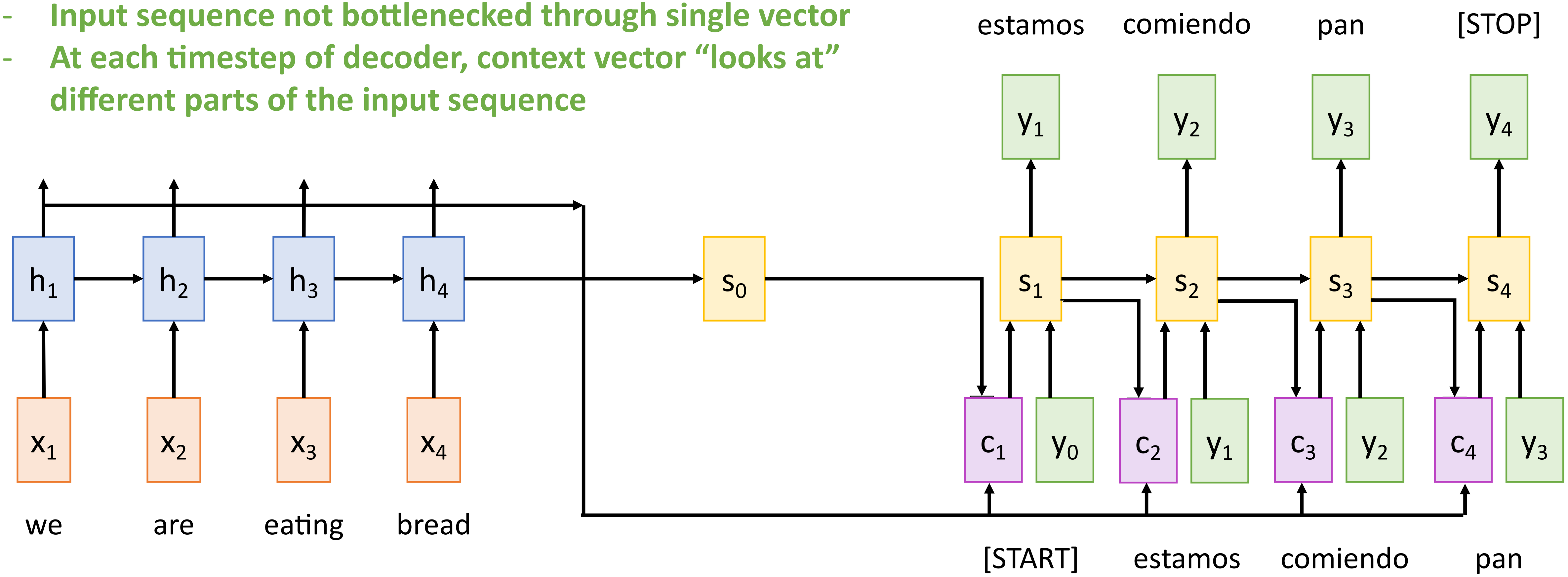
Use c_2 to compute s_2, y_2

Intuition: Context vector <u>attends</u> to the relevant part of the input sequence *"comiendo" = "eating"* so maybe $a_{21}=a_{24}=0.05$, $a_{22}=0.1$, $a_{23}=0.8$

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

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**



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

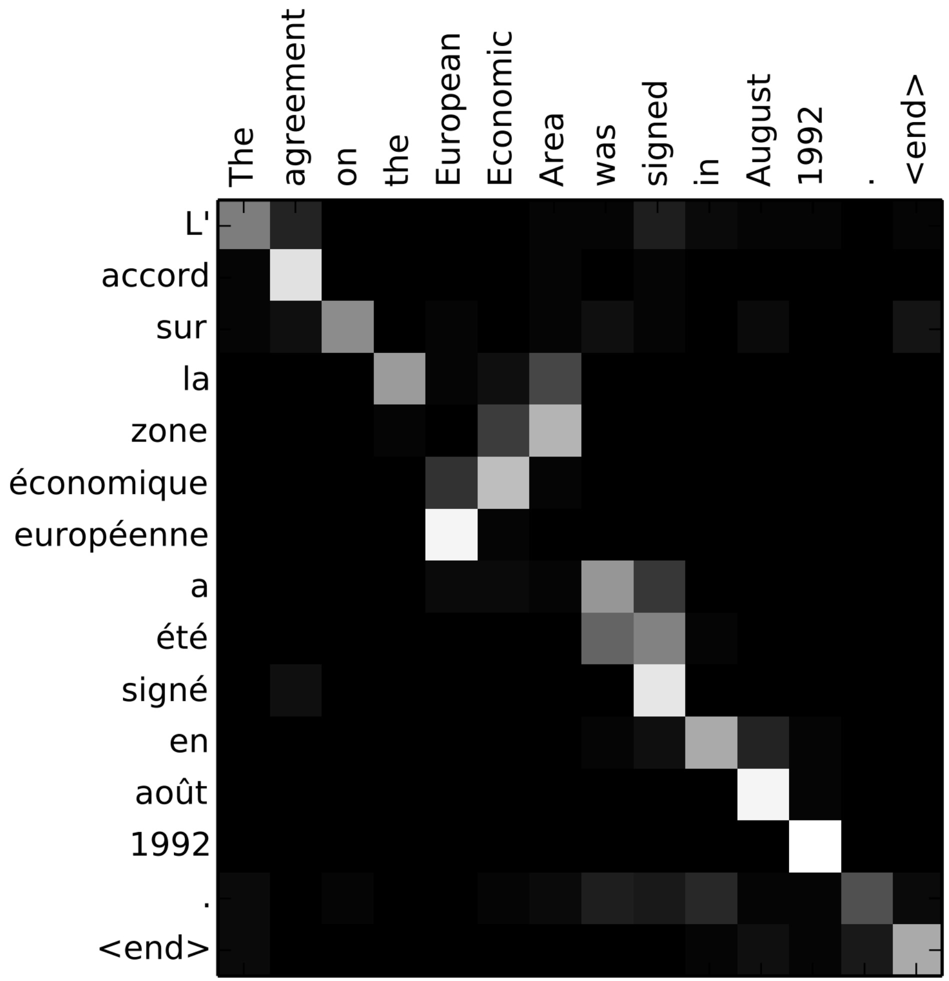
Sequence-to-Sequence with RNNs **and Attention**

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."

Visualize attention weights $a_{t,i}$



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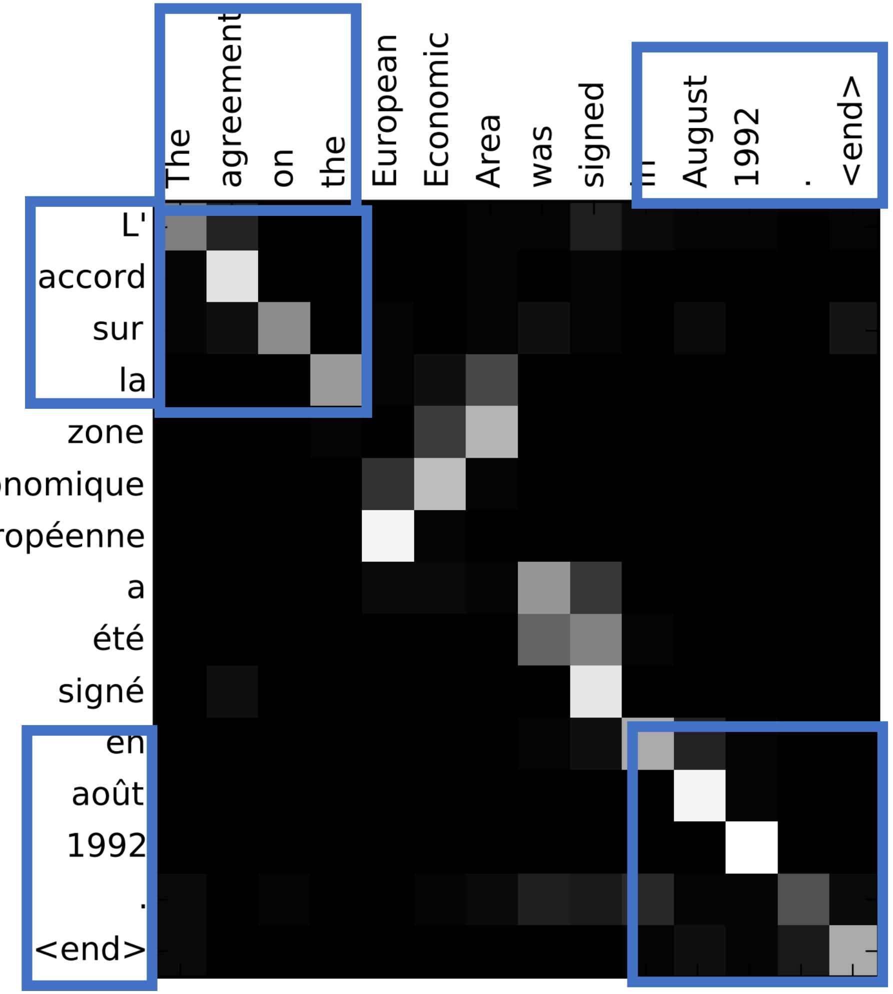
Sequence-to-Sequence with RNNs **and Attention**

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**."

Visualize attention weights $a_{t,i}$



Diagonal attention means words correspond in order

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Sequence-to-Sequence with RNNs **and Attention**

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Example: English to French translation

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

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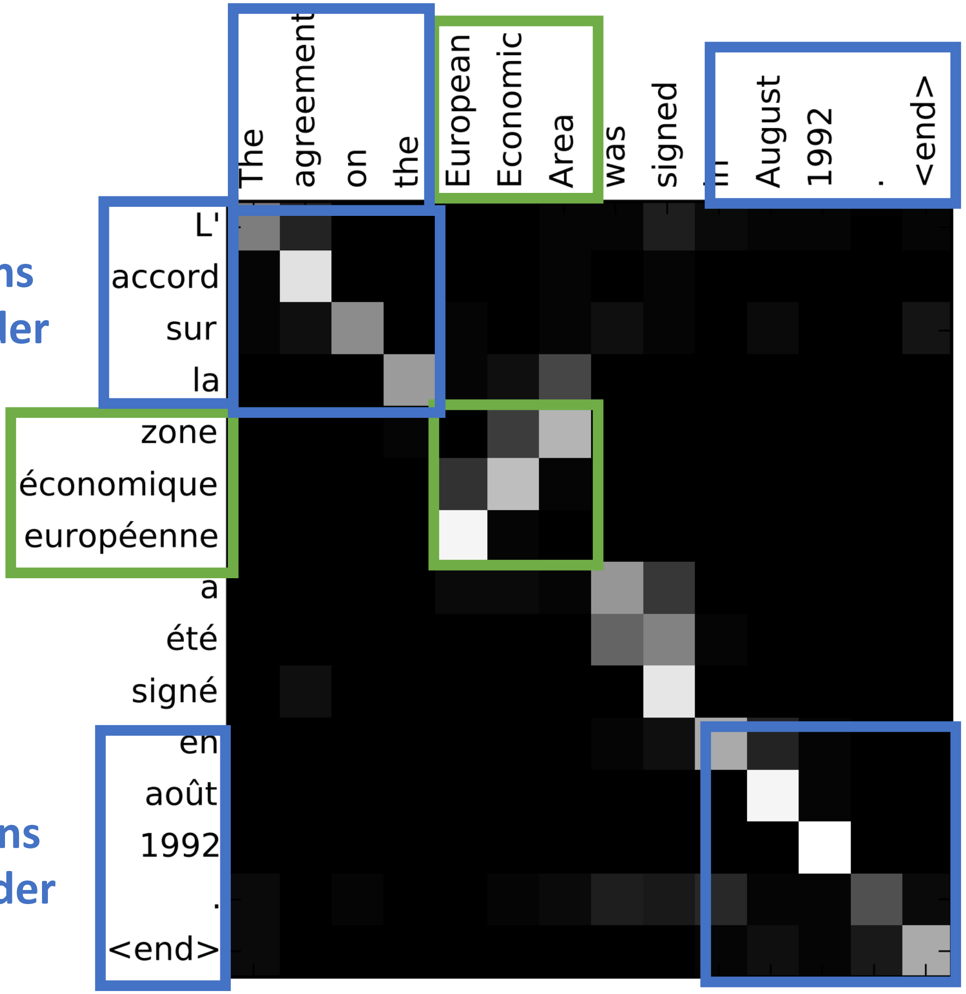
Diagonal attention means words correspond in order

Attention figures out different word orders

Diagonal attention means words correspond in order



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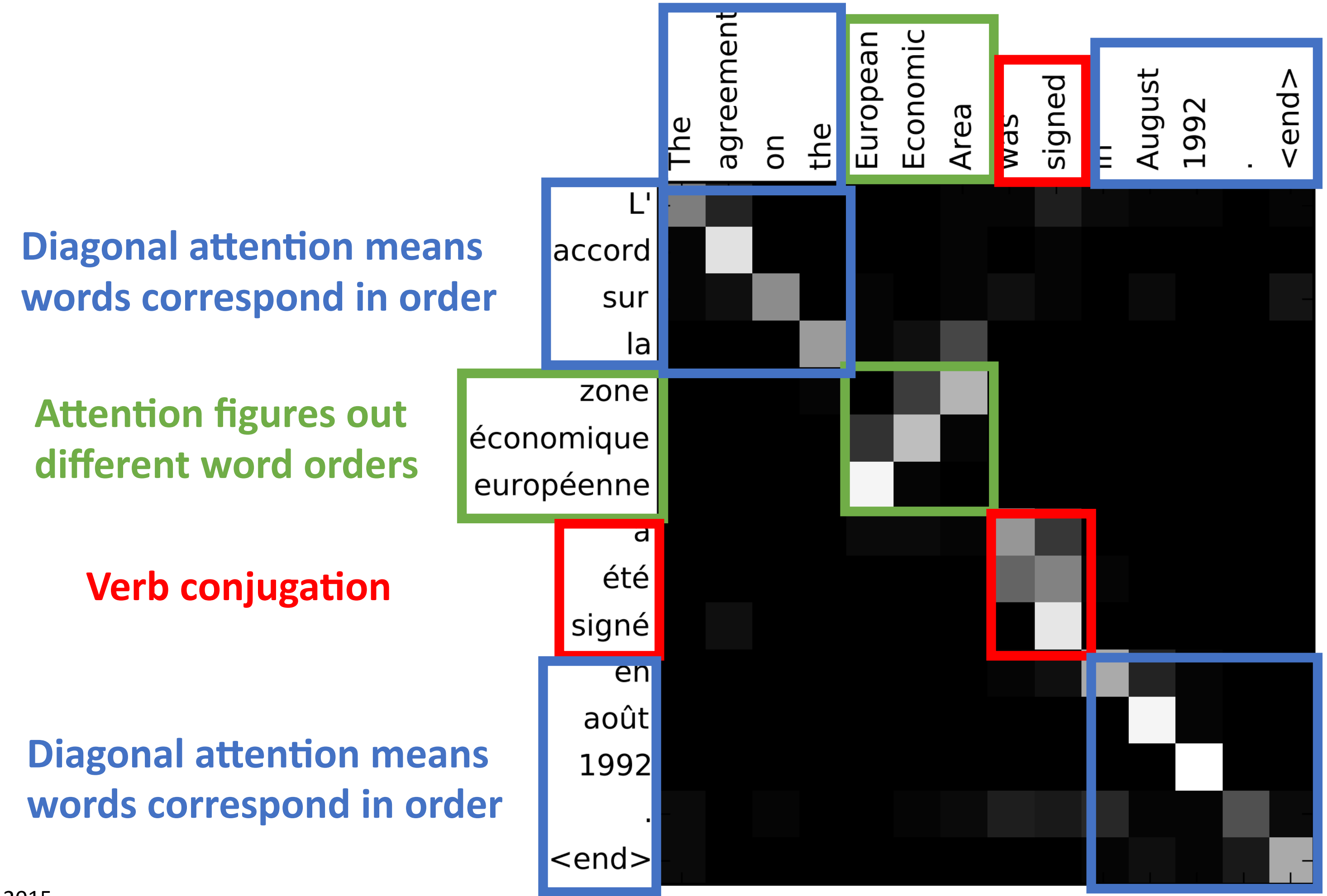

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Sequence-to-Sequence with RNNs **and Attention**

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 $\{h_i\}$!

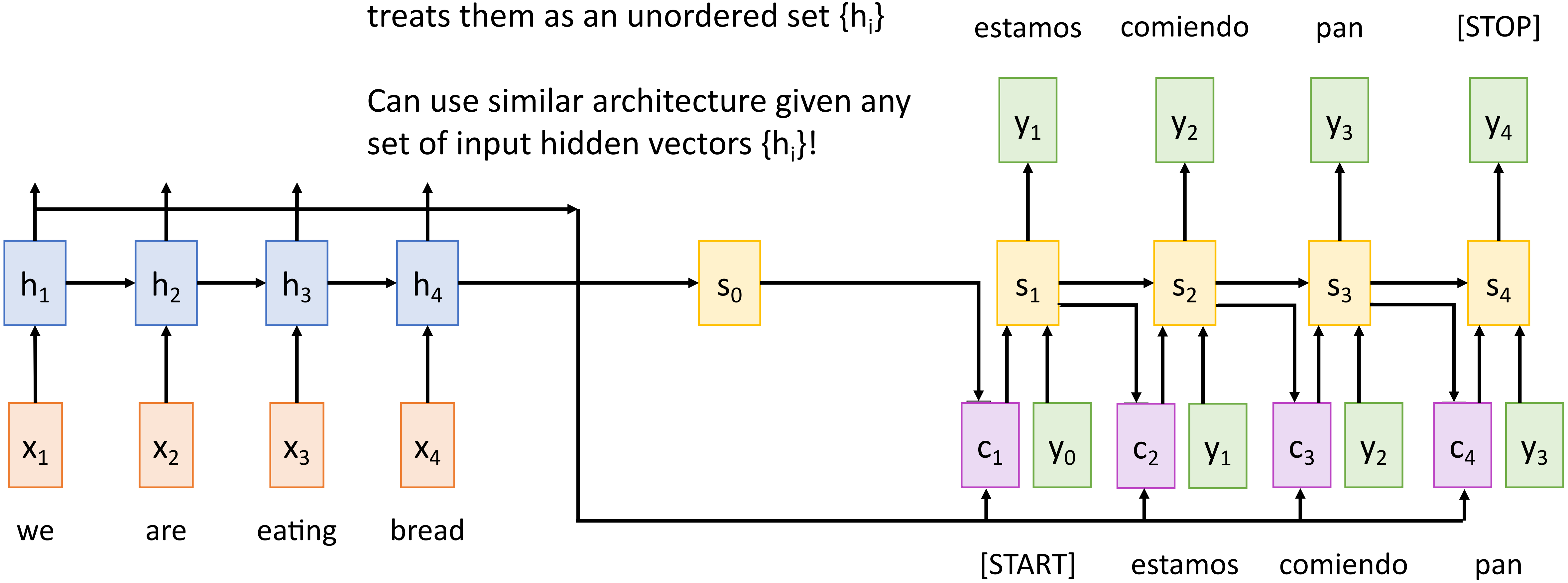

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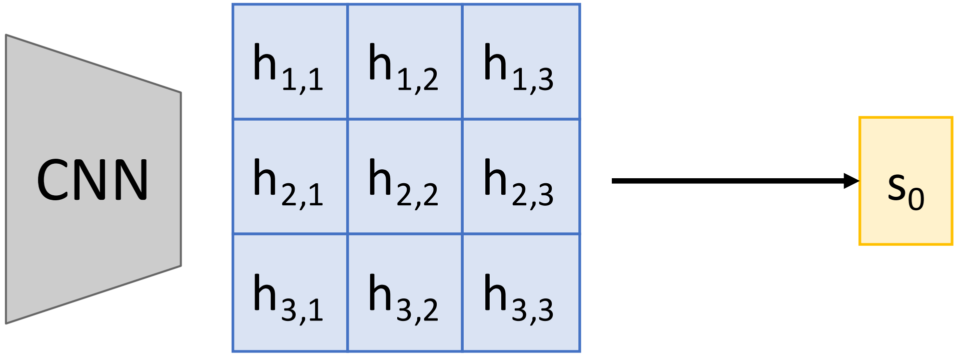
Image Captioning with RNNs and Attention



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

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

Image Captioning with RNNs and Attention

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

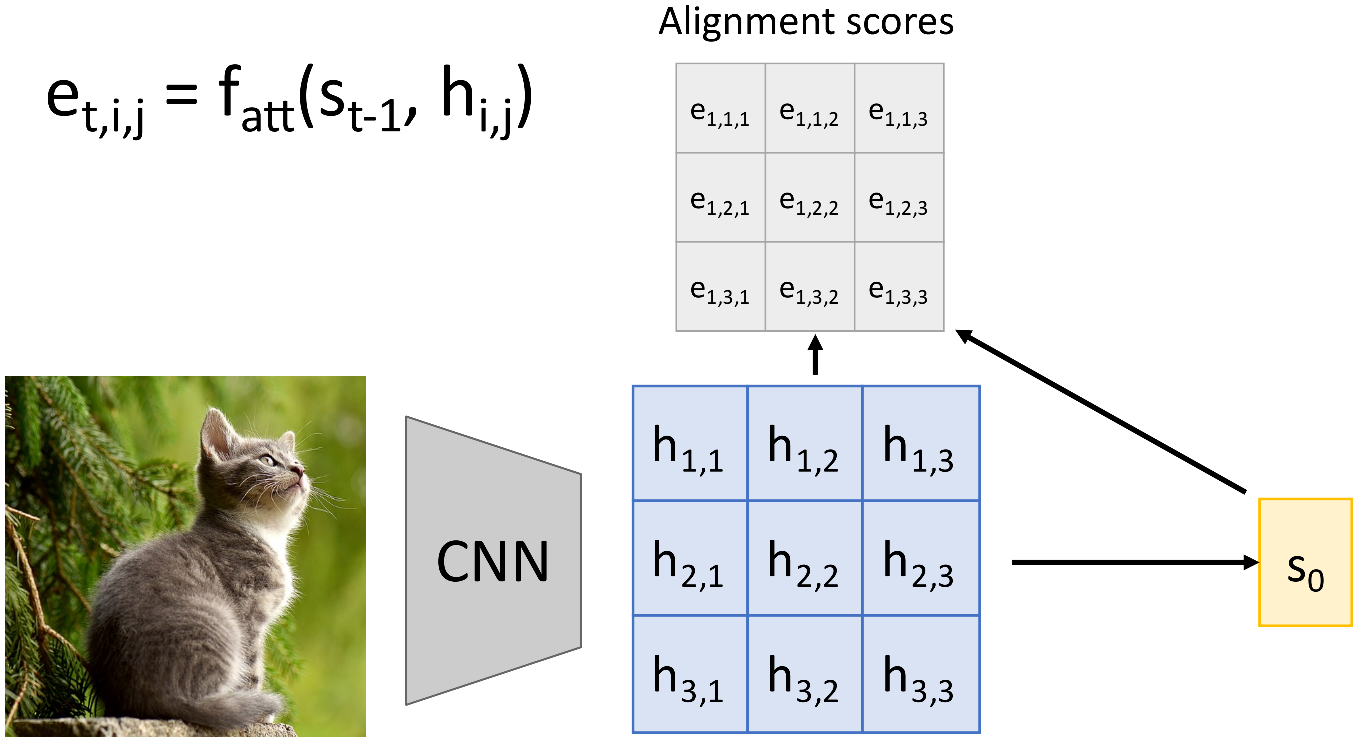


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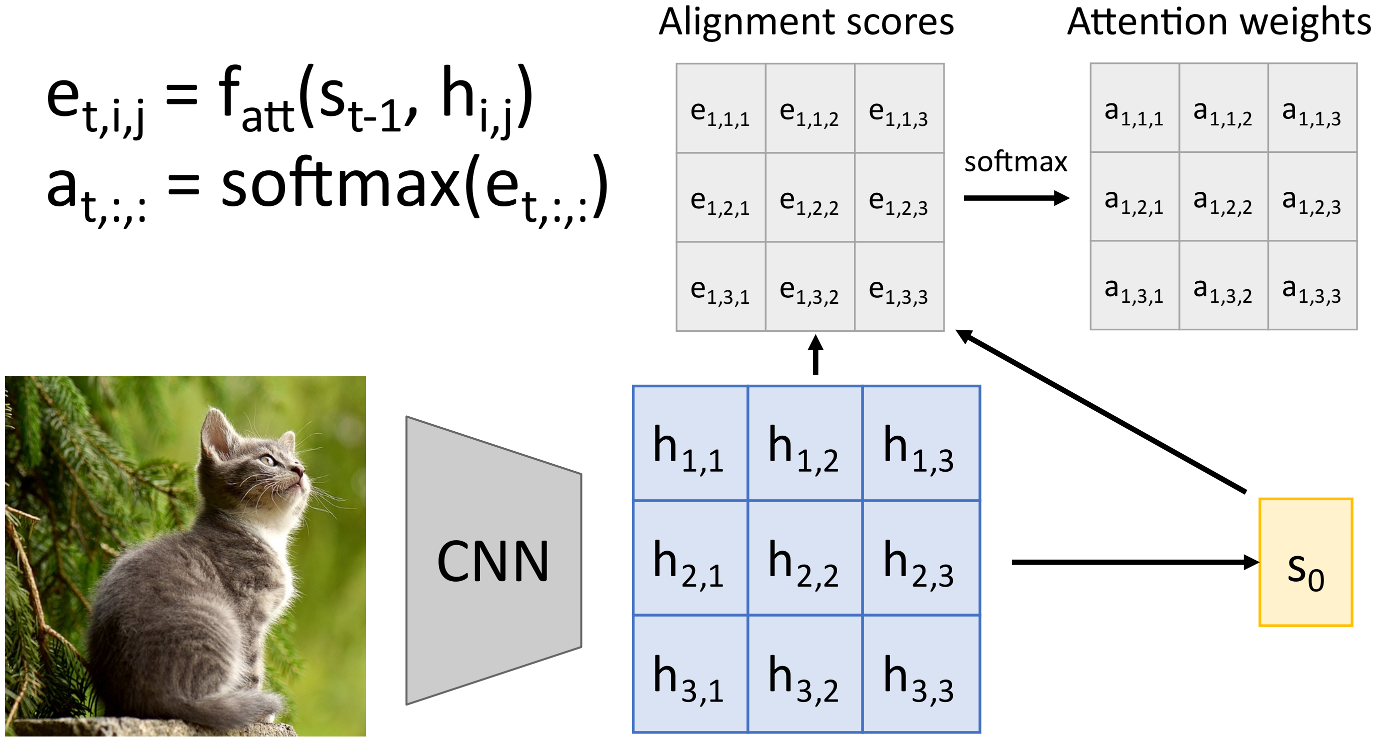
Image Captioning with RNNs and Attention

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

$a_{t,:,:} = \text{softmax}(e_{t,:,:})$



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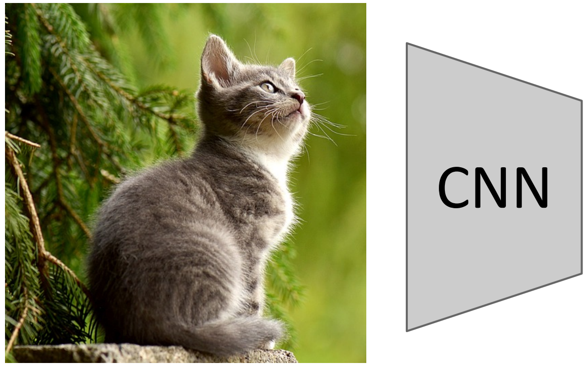

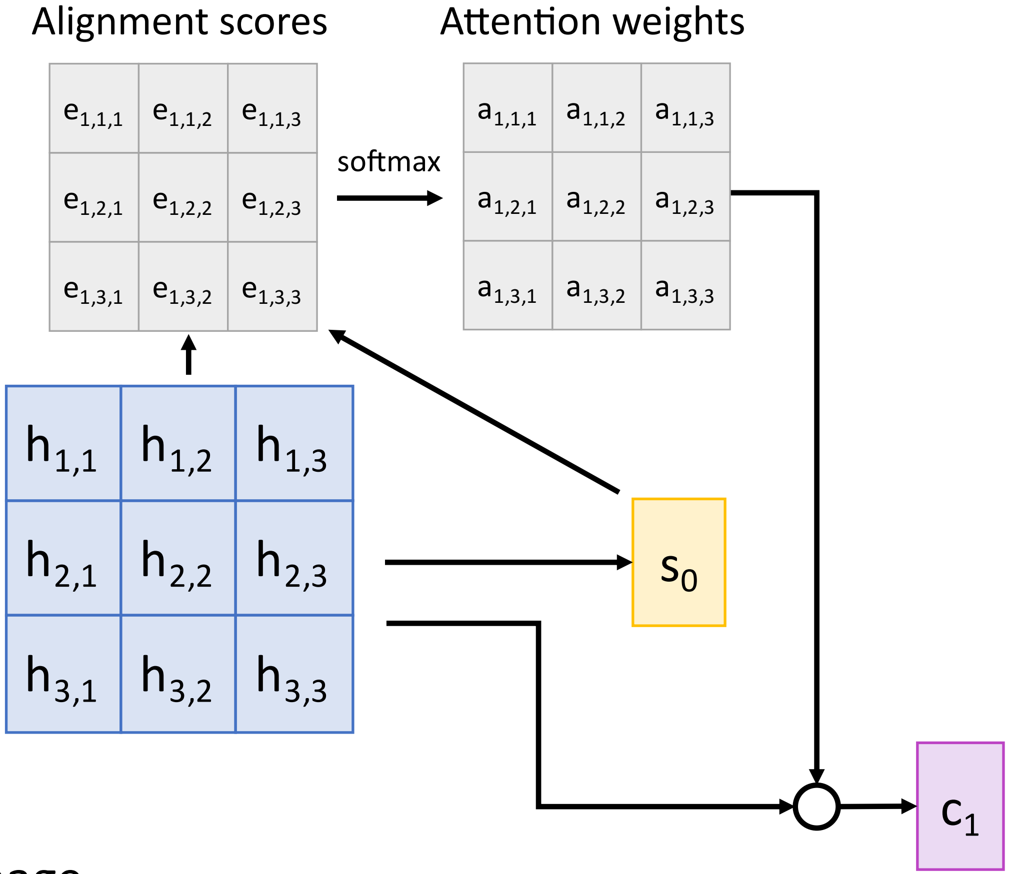

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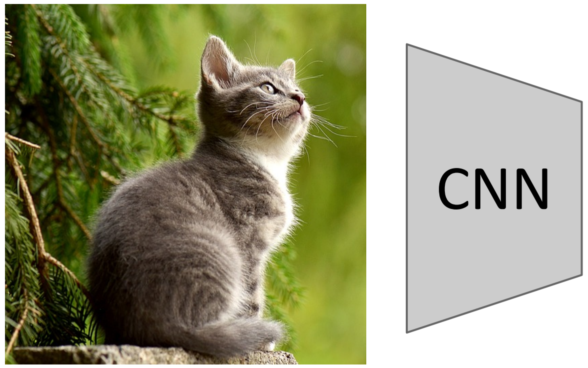

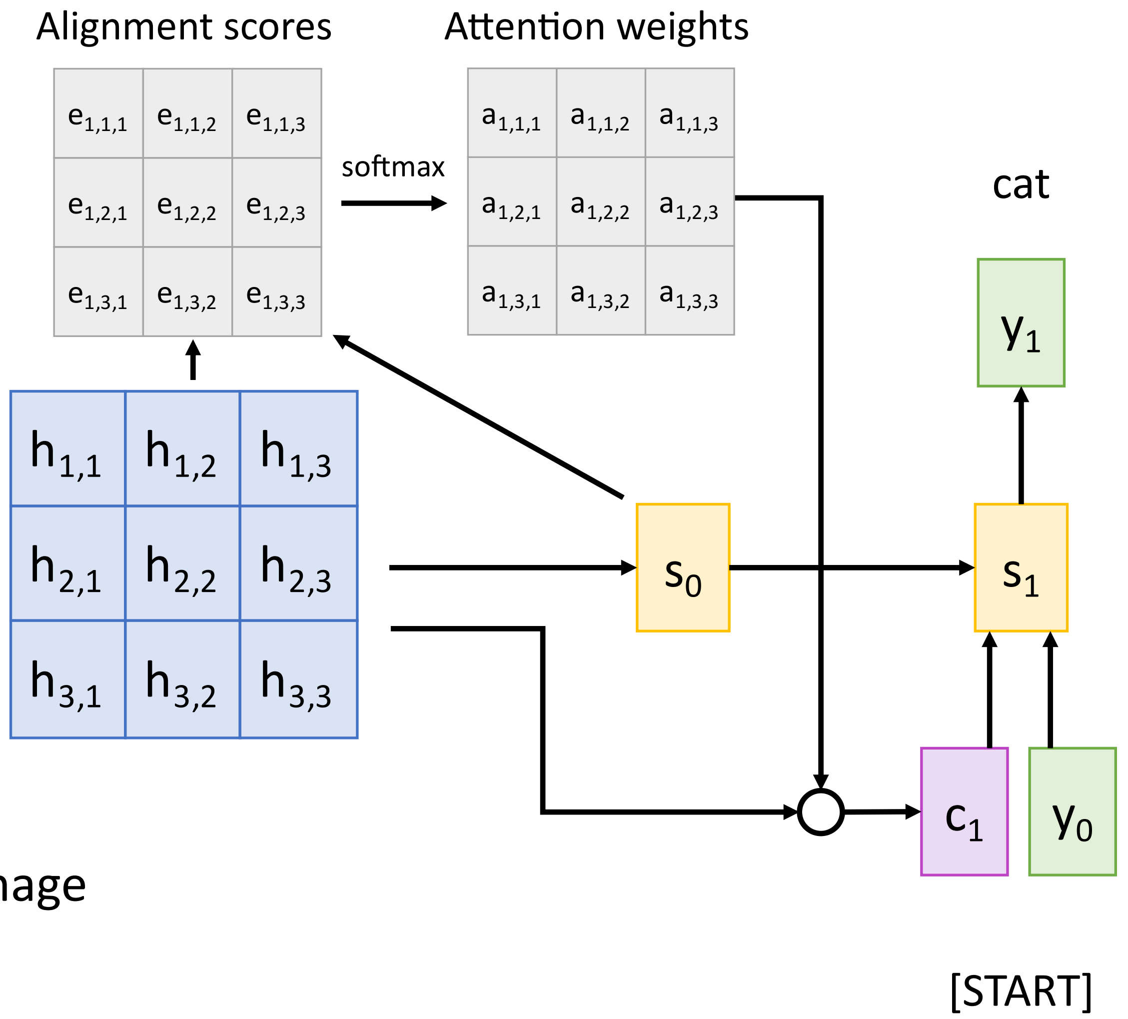

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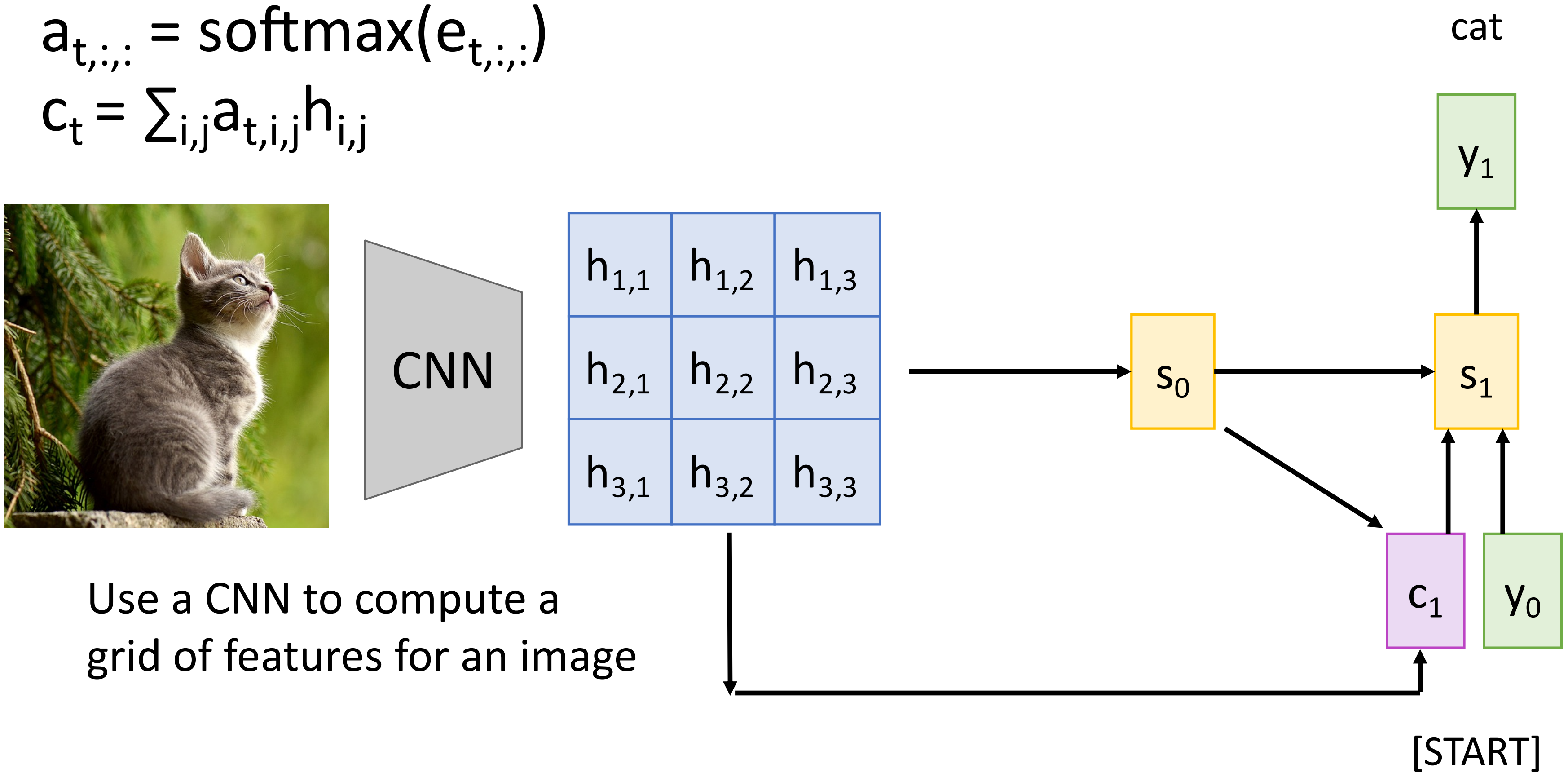

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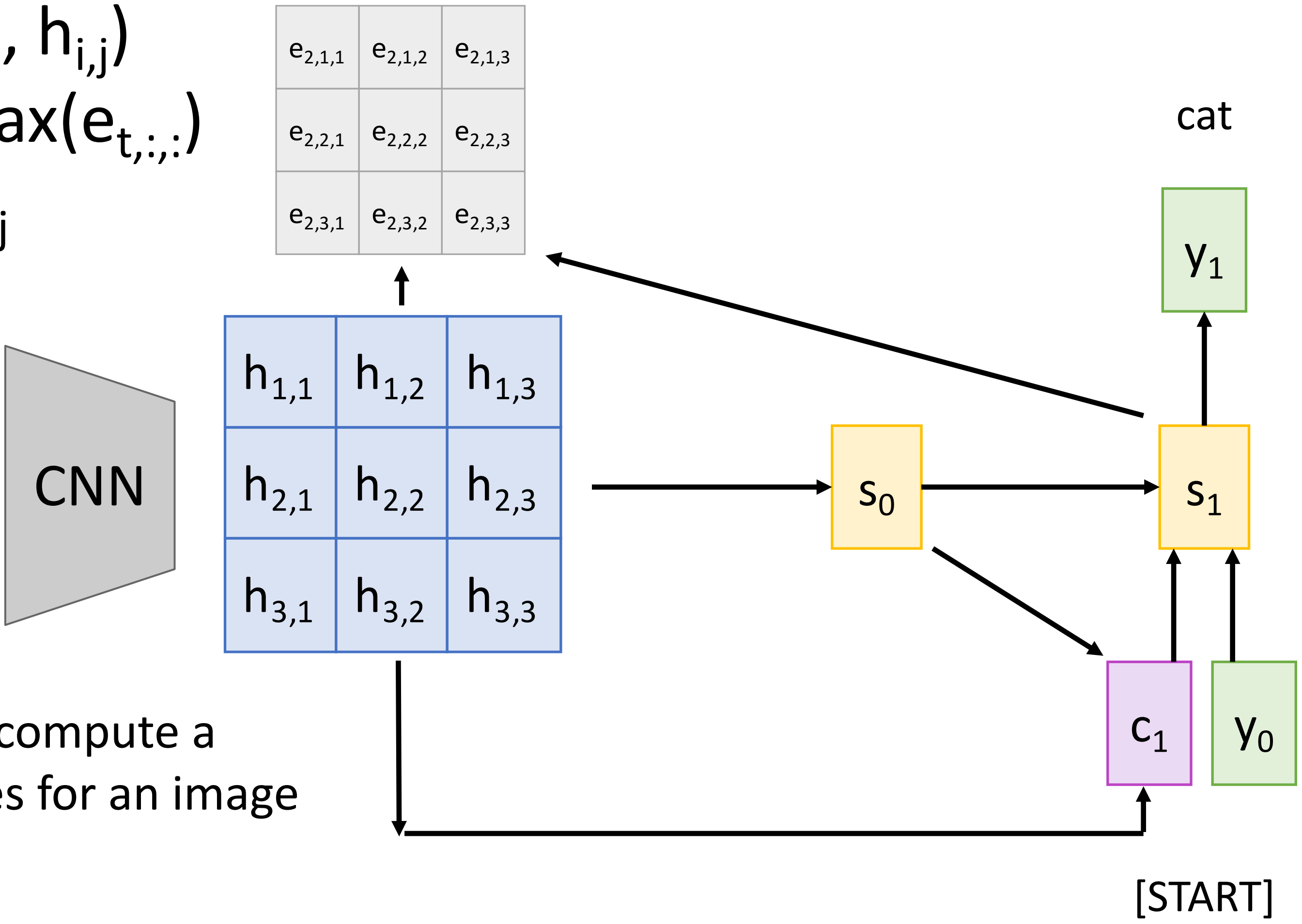

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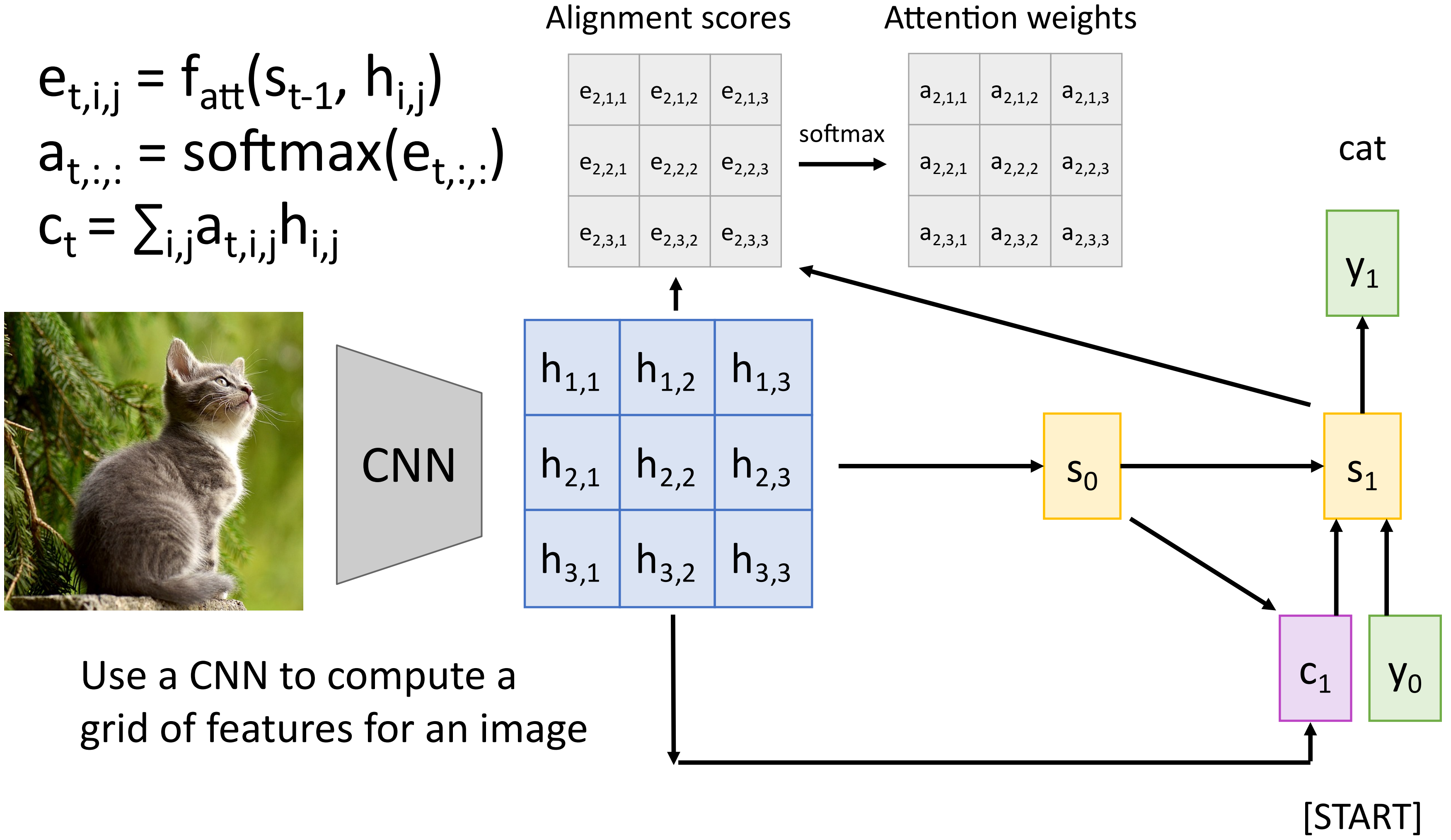

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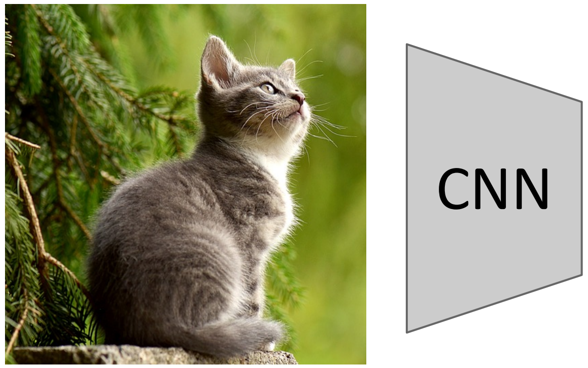

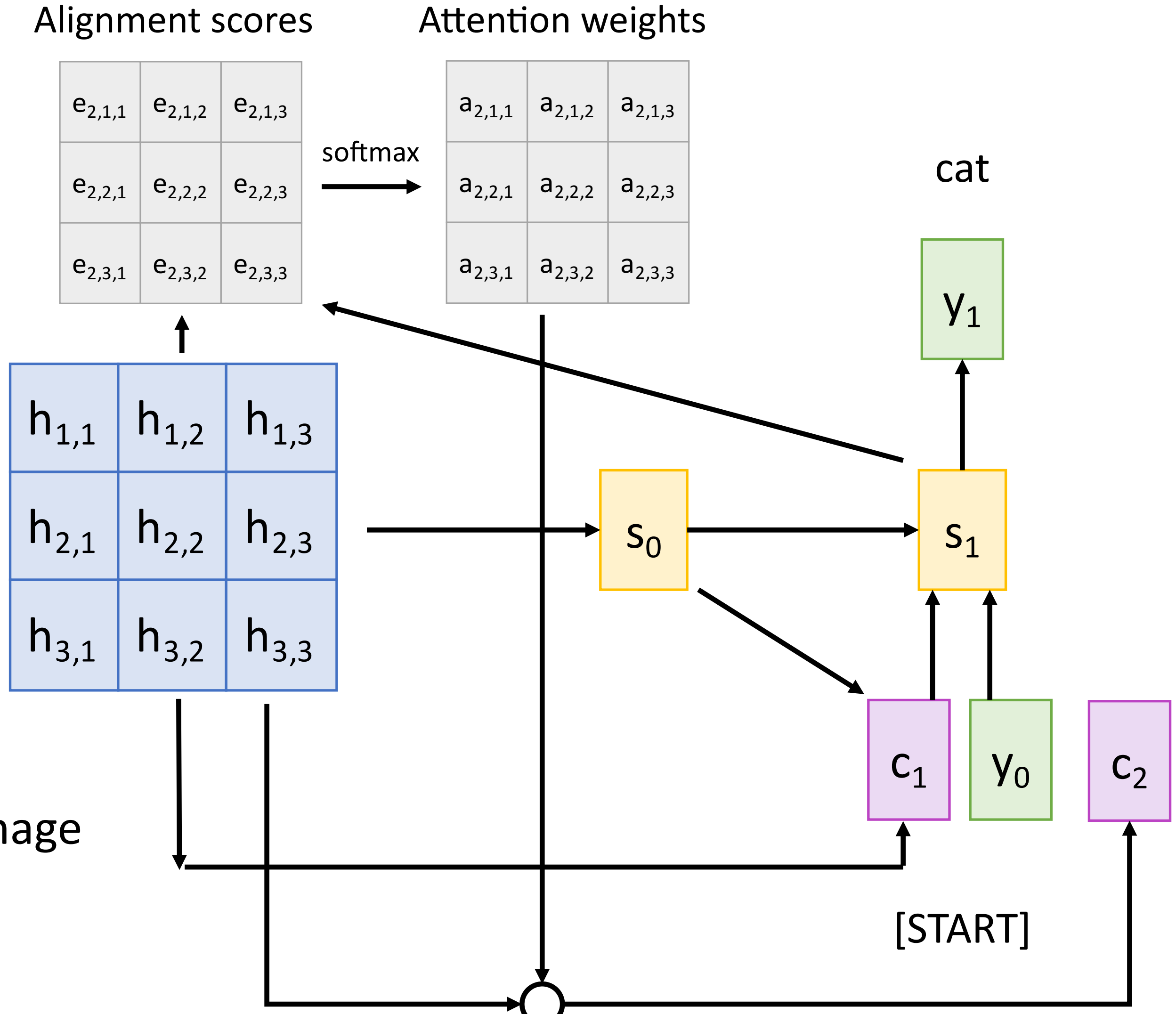

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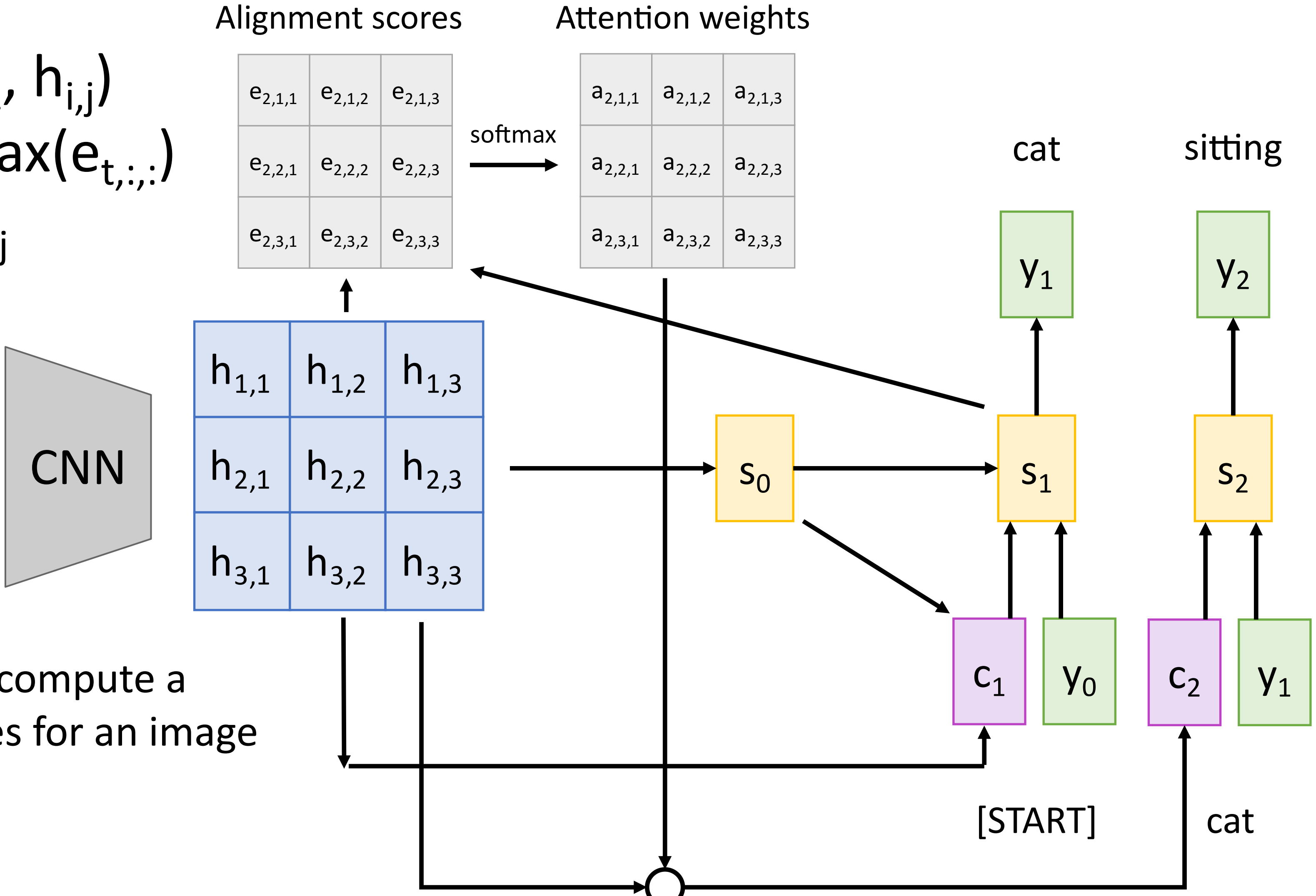

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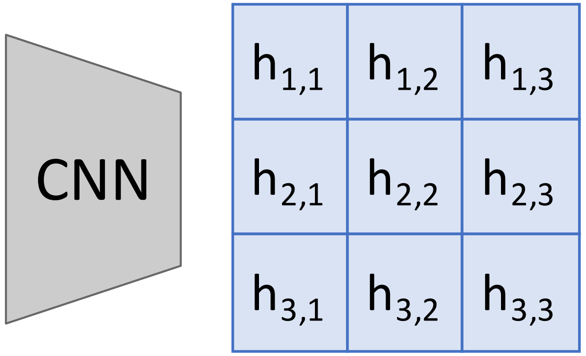
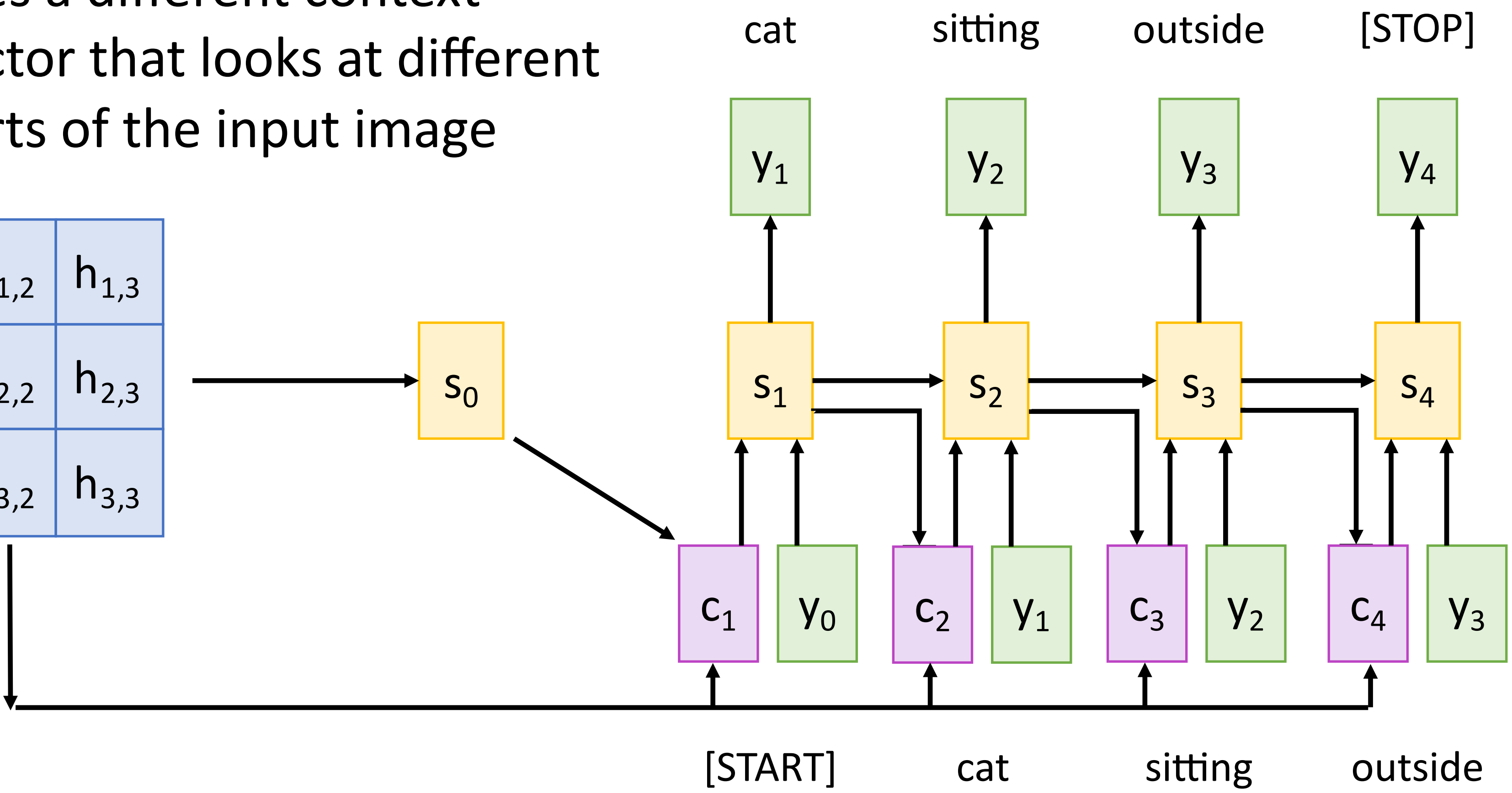
$c_t = \sum_{i,j} a_{t,i,j} h_{i,j}$

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

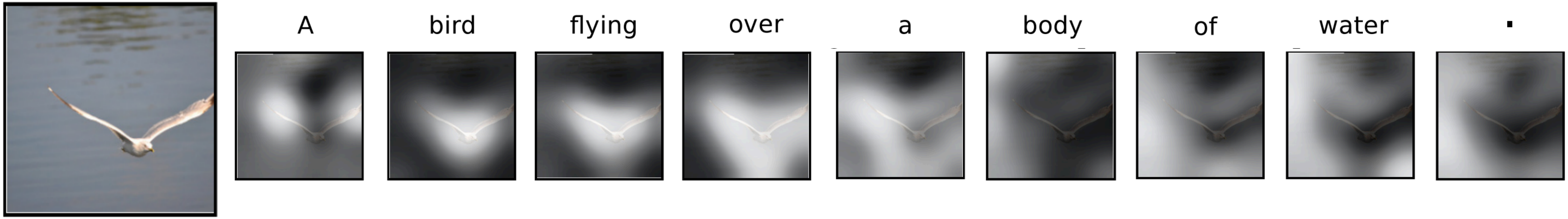


Use a CNN to compute a grid of features for an image



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

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

A dog is standing on a hardwood floor.

A stop sign is on a road with a mountain in the background.

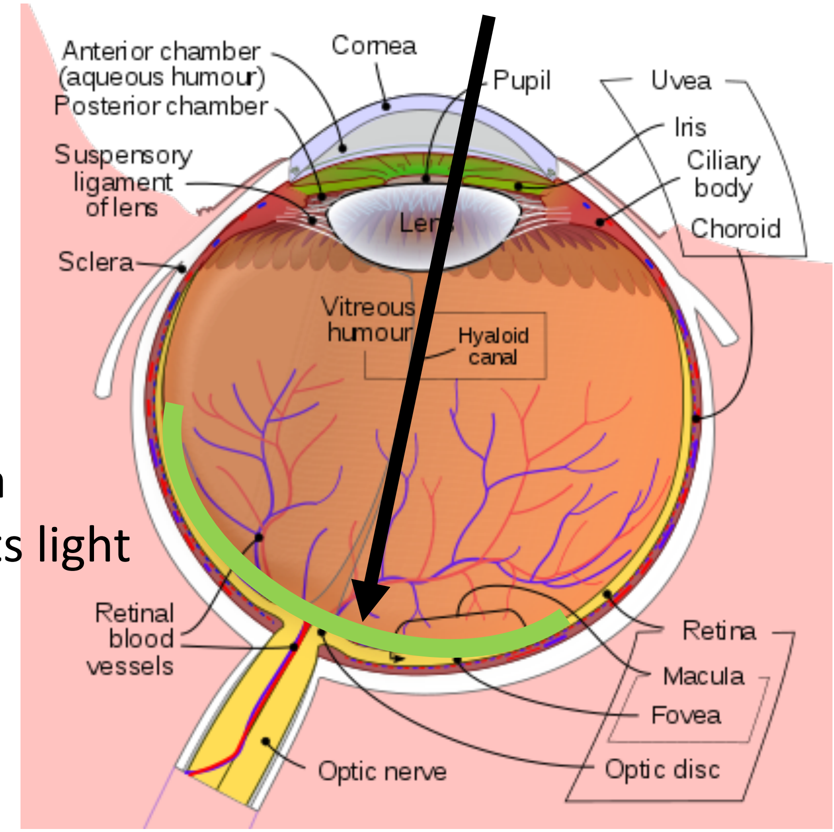
A group of people sitting on a boat in the water.

A giraffe standing in a forest with trees in the background.

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

Human Vision: Fovea

Light enters eye

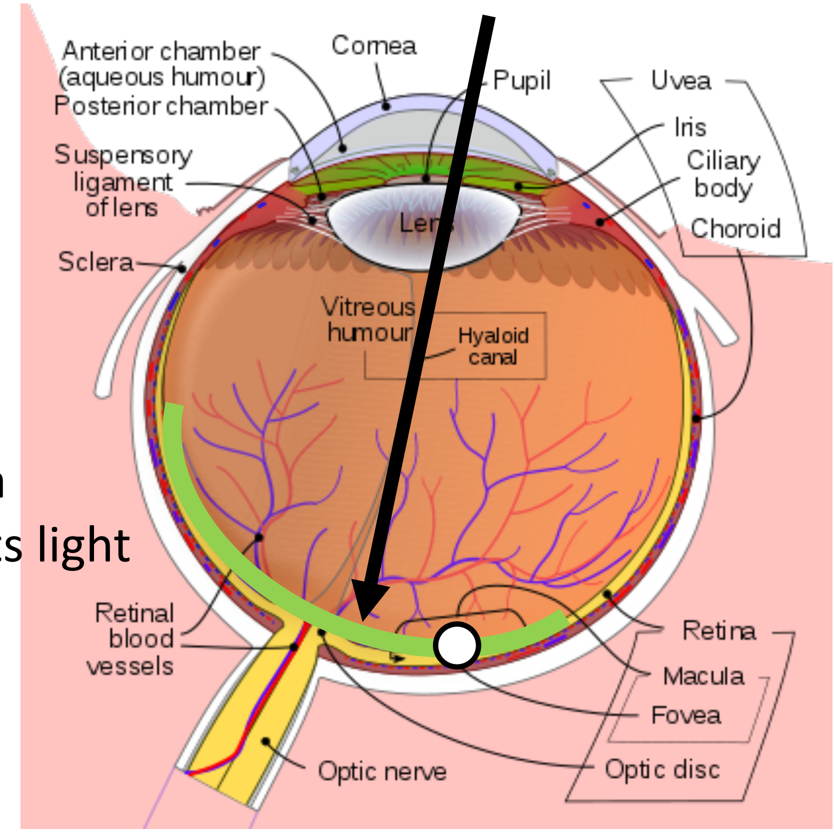


Retina
detects light

Acuity graph is licensed under CC A-SA 3.0 Unported

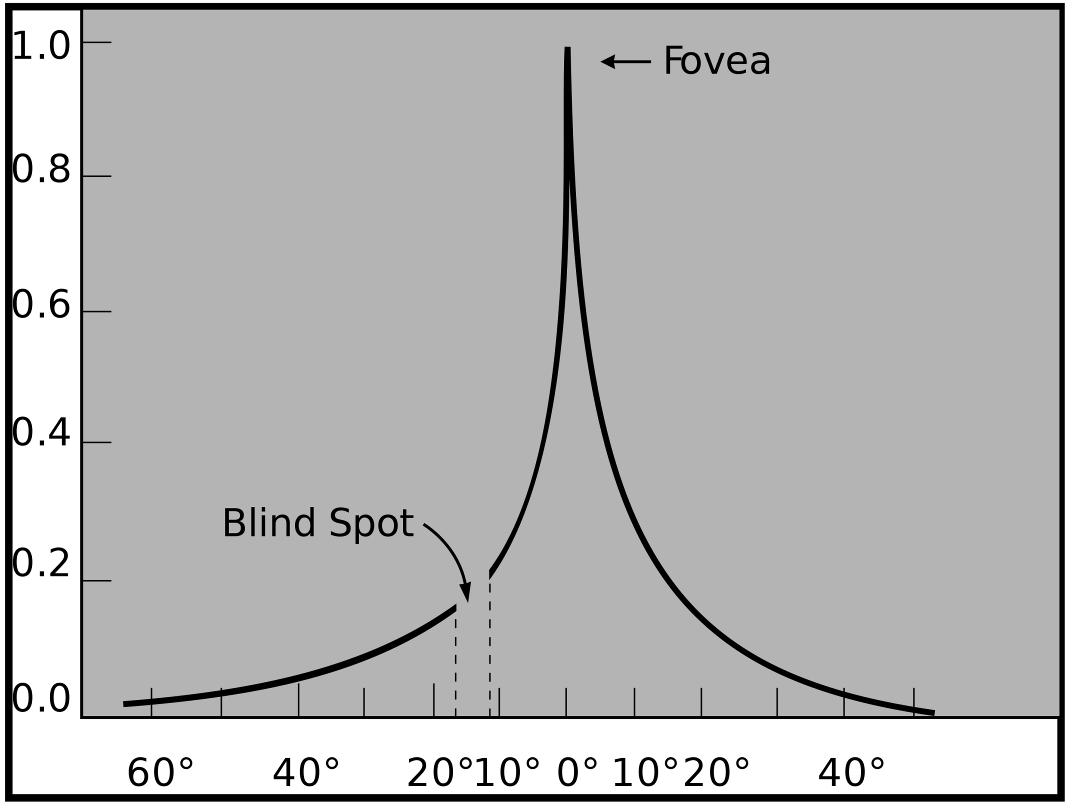
Human Vision: Fovea

Light enters eye



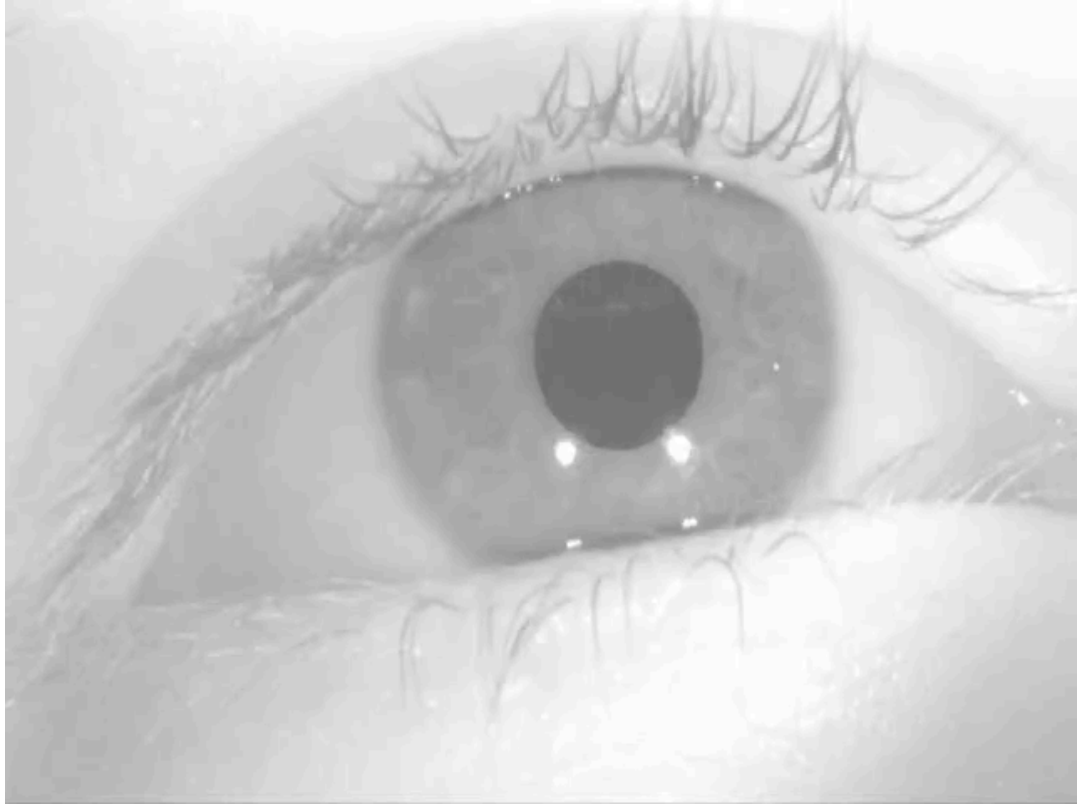
Retina
detects light

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

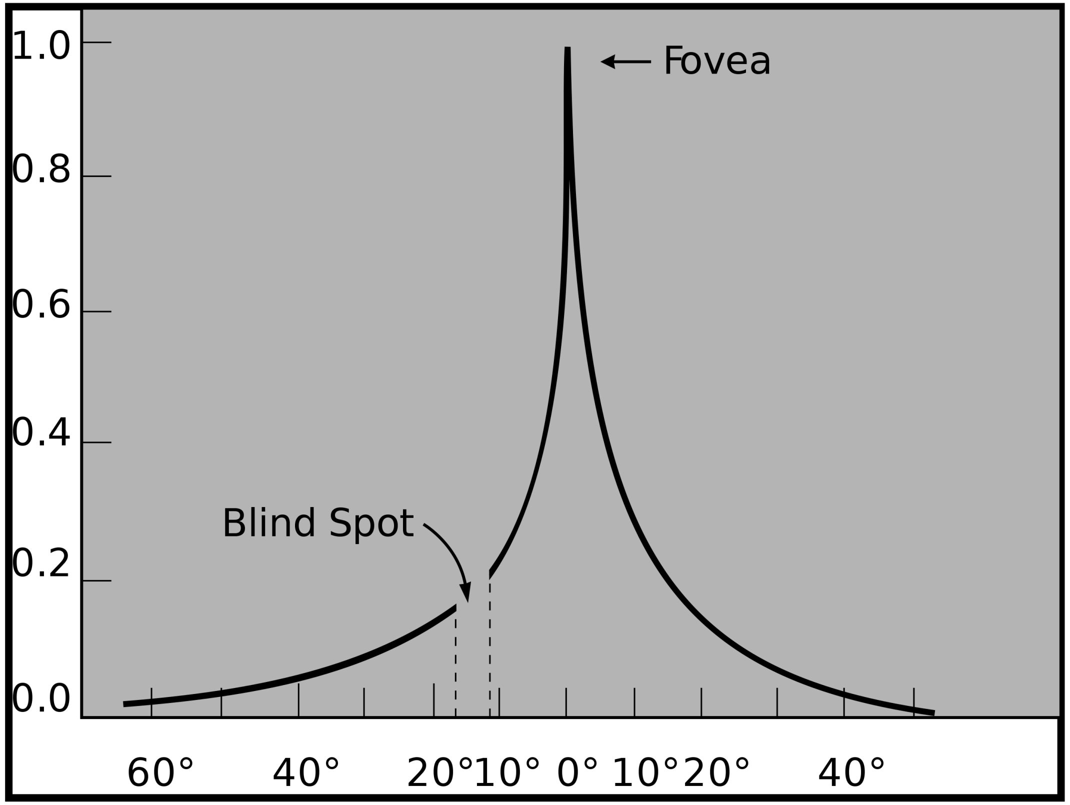
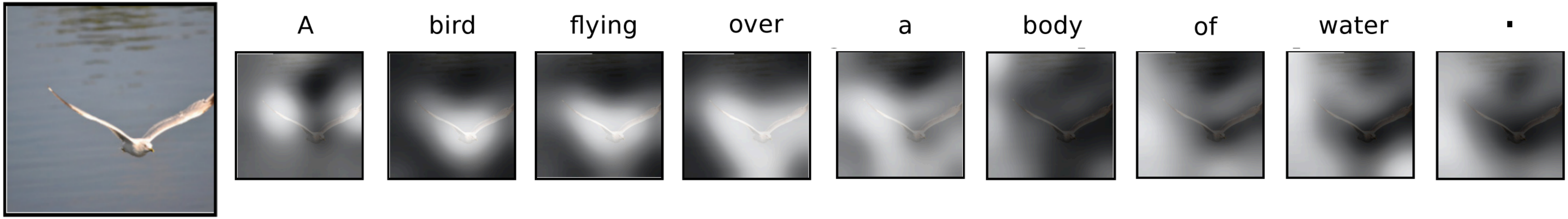
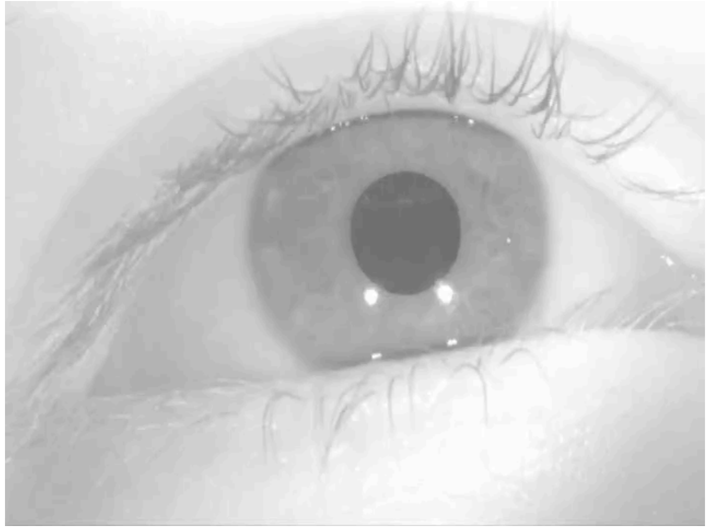


Image Captioning with RNNs and Attention



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



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

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

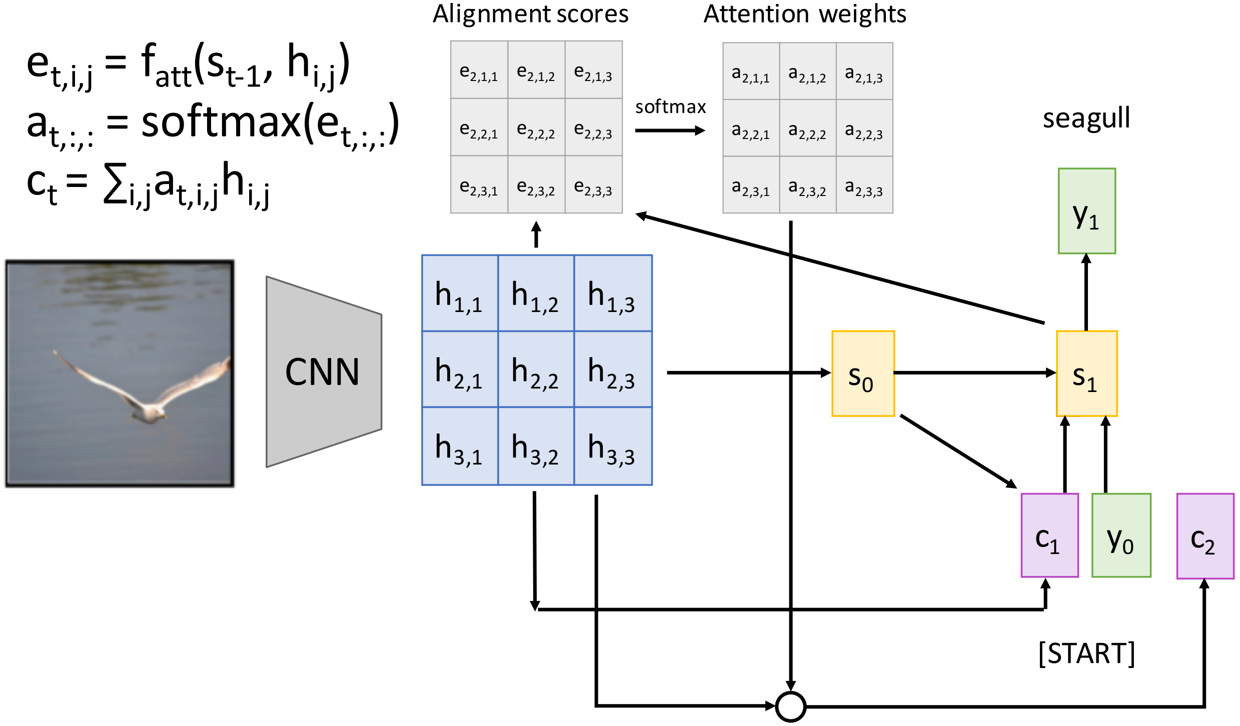
"**Listen, attend, and walk**" *(Mei et al, AAAI 2016)*
Process text, attend to text regions, output navigation commands

"**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

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



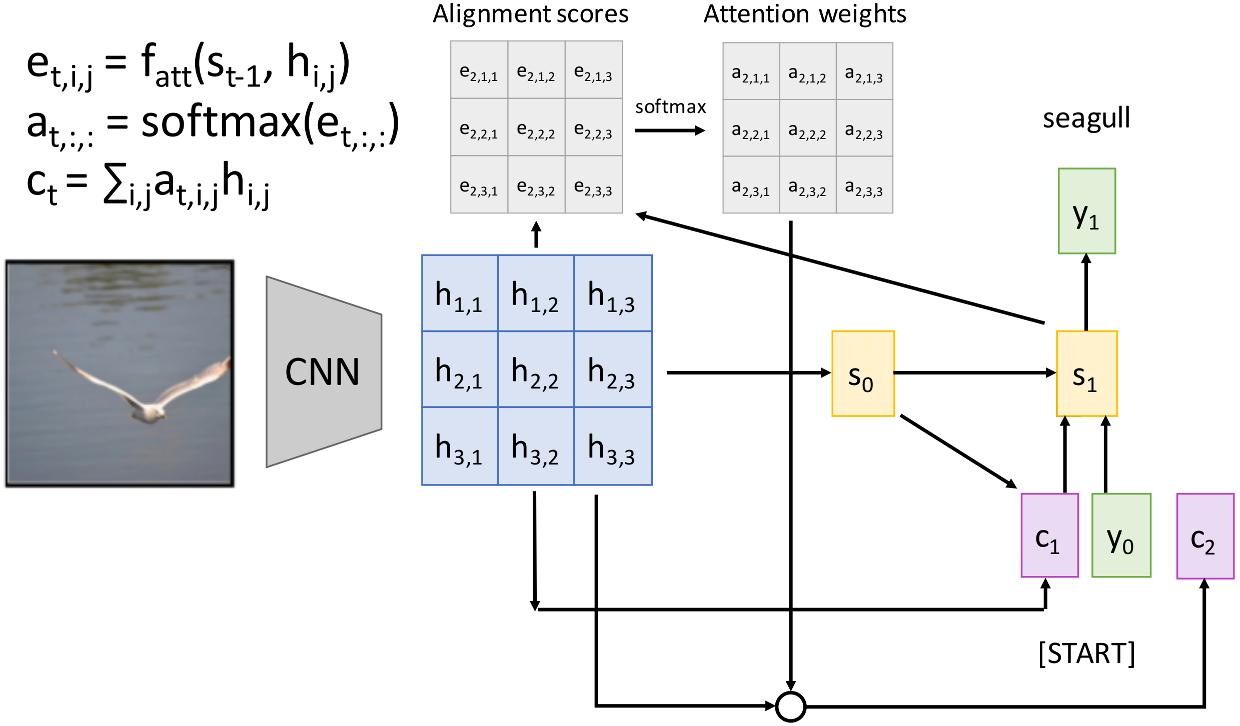
Inputs:
Query vector: **q** (Shape: D_Q)
Input vectors: **X** (Shape: N_X x D_X)
Similarity function: f_{att}

Computation:
Similarities: e (Shape: N_X) $e_i = f_{att}(\mathbf{q}, \mathbf{X}_i)$
Attention weights: a = softmax(e) (Shape: N_X)
Output vector: $y = \sum_i a_i \mathbf{X}_i$ (Shape: D_X)

Attention Layer

Inputs:
Query vector: $\mathbf{q}$ (Shape: D_Q)
Input vectors: $\mathbf{X}$ (Shape: N_X x D_Q)
Similarity function: dot product

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

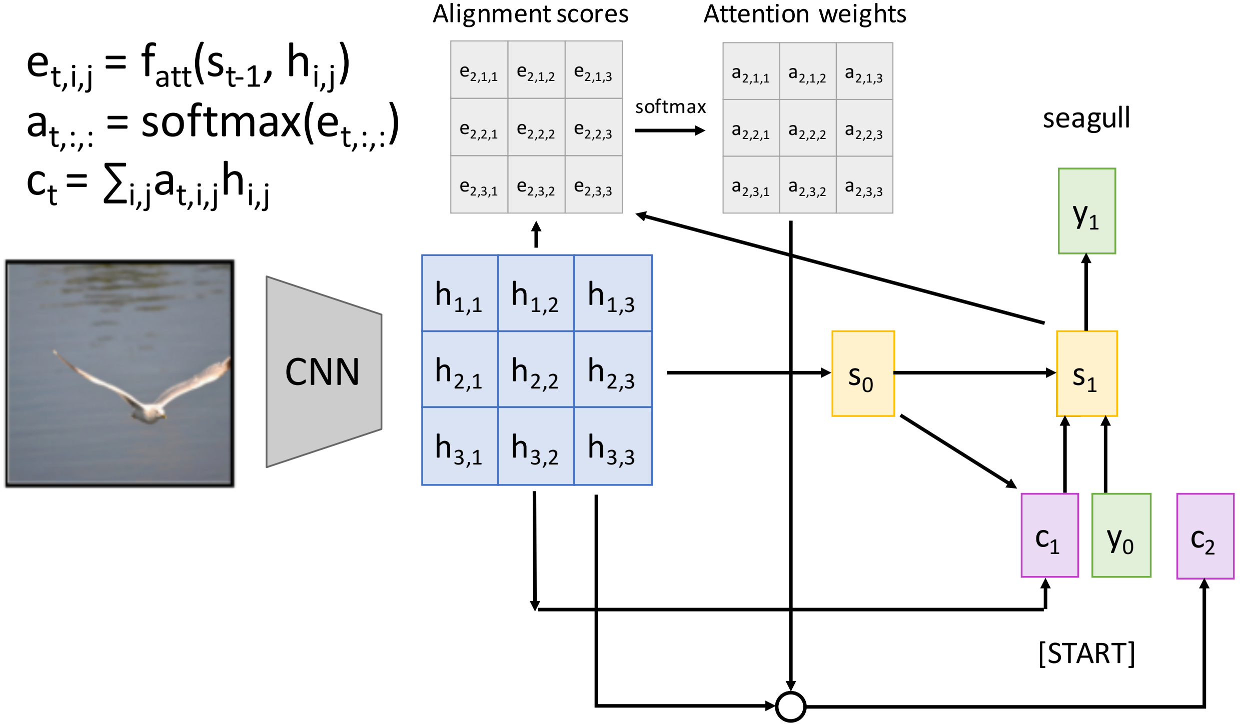


Computation:
Similarities: e (Shape: N_X) $e_i = \mathbf{q} \cdot \mathbf{X}_i$
Attention weights: a = softmax(e) (Shape: N_X)
Output vector: $y = \sum_i a_i \mathbf{X}_i$ (Shape: D_X)

Changes:
- Use dot product for similarity

Attention Layer

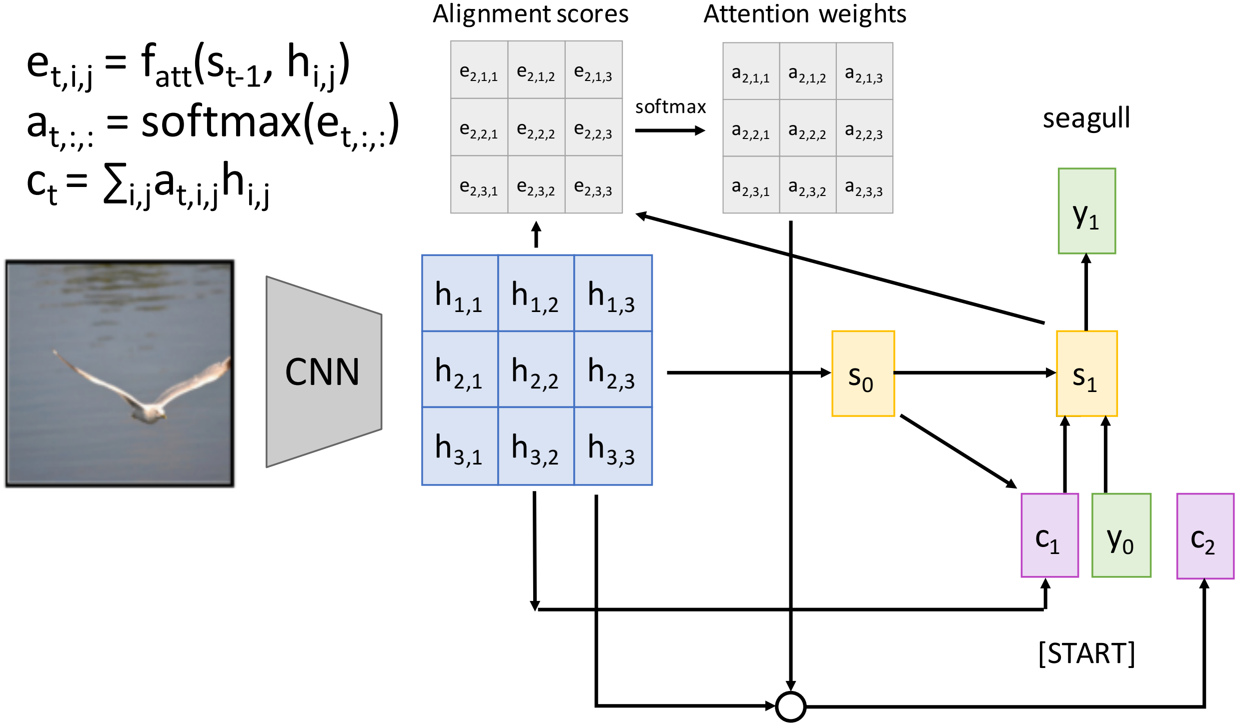
Inputs:
Query vector: **q** (Shape: D_Q)
Input vectors: **X** (Shape: N_X x D_Q)
Similarity function: scaled dot product



Computation:
Similarities: e (Shape: N_X) $e_i = \mathbf{q} \cdot \mathbf{X_i} / \text{sqrt}(D_Q)$
Attention weights: a = softmax(e) (Shape: N_X)
Output vector: $y = \sum_i a_i \mathbf{X_i}$ (Shape: D_X)

Changes:
- Use **scaled** dot product for similarity

Attention Layer



Inputs:
Query vector: **q** (Shape: D_Q)
Input vectors: **X** (Shape: N_X x 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 $|a| = (\sum_i a^2)^{1/2} = a \text{ sqrt}(D)$

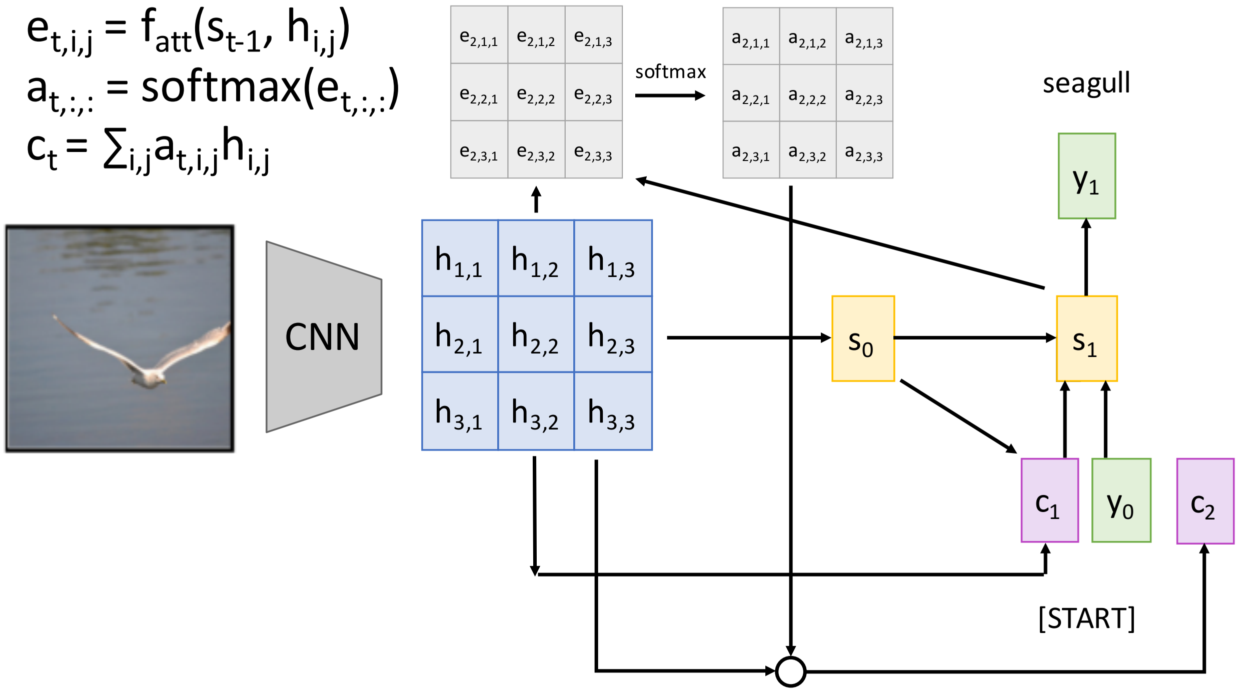
Computation:
Similarities: e (Shape: N_X) $e_i = \mathbf{q} \cdot \mathbf{X}_i / \text{sqrt}(D_Q)$
Attention weights: a = softmax(e) (Shape: N_X)
Output vector: $y = \sum_i a_i \mathbf{X}_i$ (Shape: D_X)

Changes:
- Use **scaled** dot product for similarity

Attention Layer

Inputs:
Query vectors: **Q** (Shape: N_Q x D_Q)
Input vectors: **X** (Shape: N_X x D_Q)

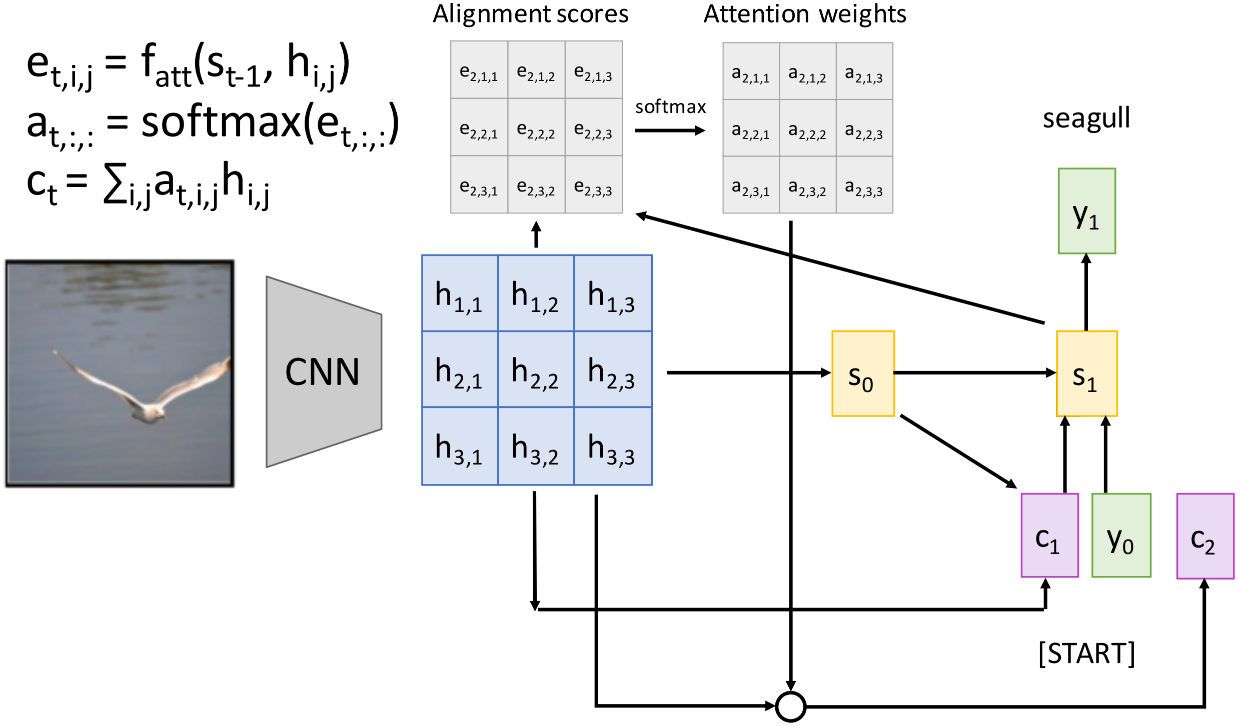
$e_{t,i,j} = f_{att}(s_{t-1}, h_{i,j})$
$a_{t,:,:} = \text{softmax}(e_{t,:,:})$
$c_t = \sum_{i,j} a_{t,i,j} h_{i,j}$



Computation:
Similarities: E = **QX**^{T} (Shape: N_Q x N_X) $E_{i,j} = Q_i \cdot X_j / \text{sqrt}(D_Q)$
Attention weights: A = softmax(E, dim=1) (Shape: N_Q x N_X)
Output vectors: Y = A**X** (Shape: N_Q x 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 x D_Q)

Input vectors: **X** (Shape: N_X x D_X)

Key matrix: **W_K** (Shape: D_X x D_Q)

Value matrix: **W_V** (Shape: D_X x D_V)

Computation:

Key vectors: **K** = **XW_K** (Shape: N_X x D_Q)

Value Vectors: **V** = **XW_V** (Shape: N_X x D_V)

Similarities: E = **QK^T** (Shape: N_Q x N_X) $E_{i,j} = Q_i \cdot K_j / \text{sqrt}(D_Q)$

Attention weights: A = softmax(E, dim=1) (Shape: N_Q x N_X)

Output vectors: Y = A**V** (Shape: N_Q x D_V) $Y_i = \sum_j A_{i,j} V_j$

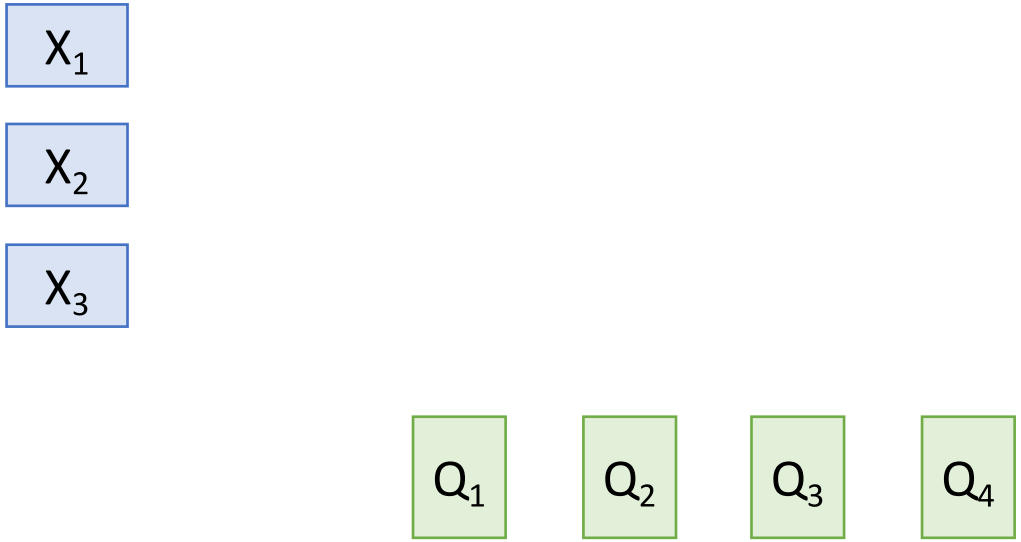
Changes:

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

Attention Layer

Inputs:
Query vectors: **Q** (Shape: N_Q x D_Q)
Input vectors: **X** (Shape: N_X x D_X)
Key matrix: $\mathbf{W_K}$ (Shape: D_X x D_Q)
Value matrix: $\mathbf{W_V}$ (Shape: D_X x D_V)

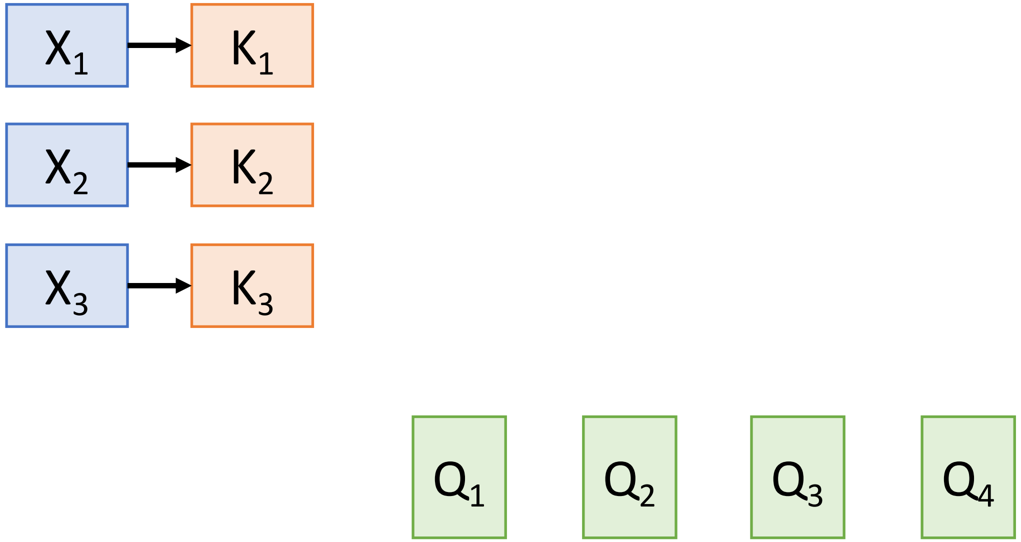
Computation:
Key vectors: $\mathbf{K} = \mathbf{XW_K}$ (Shape: N_X x D_Q)
Value Vectors: $\mathbf{V} = \mathbf{XW_V}$ (Shape: N_X x D_V)
Similarities: $E = \mathbf{QK}^T$ (Shape: N_Q x N_X) $E_{i,j} = \mathbf{Q_i} \cdot \mathbf{K_j} / \mathrm{sqrt}(D_Q)$
Attention weights: A = softmax(E, dim=1) (Shape: N_Q x N_X)
Output vectors: $Y = A\mathbf{V}$ (Shape: N_Q x D_V) $Y_i = \sum_j A_{i,j}\mathbf{V_j}$



Attention Layer

Inputs:
Query vectors: **Q** (Shape: N_Q x D_Q)
Input vectors: **X** (Shape: N_X x D_X)
Key matrix: $\mathbf{W_K}$ (Shape: D_X x D_Q)
Value matrix: $\mathbf{W_V}$ (Shape: D_X x D_V)

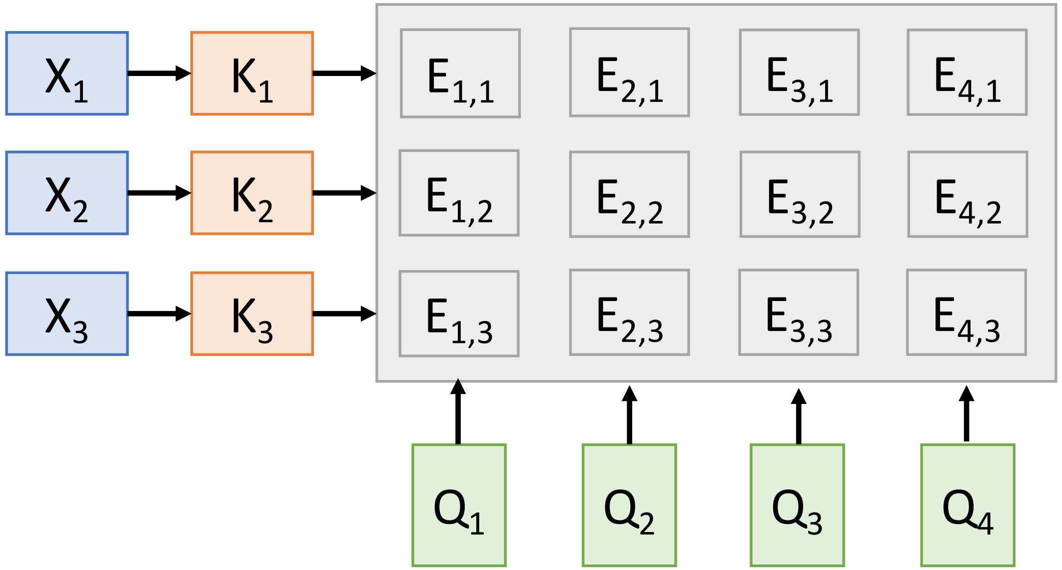
Computation:
Key vectors: **K** = $\mathbf{XW_K}$ (Shape: N_X x D_Q)
Value Vectors: **V** = $\mathbf{XW_V}$ (Shape: N_X x D_V)
Similarities: E = $\mathbf{QK^T}$ (Shape: N_Q x N_X) $E_{i,j} = \mathbf{Q_i} \cdot \mathbf{K_j} / \text{sqrt}(D_Q)$
Attention weights: A = softmax(E, dim=1) (Shape: N_Q x N_X)
Output vectors: Y = A**V** (Shape: N_Q x D_V) $Y_i = \sum_j A_{i,j}\mathbf{V_j}$



Attention Layer

Inputs:
Query vectors: Q (Shape: N_Q x D_Q)
Input vectors: X (Shape: N_X x D_X)
Key matrix: W_K (Shape: D_X x D_Q)
Value matrix: W_V (Shape: D_X x D_V)

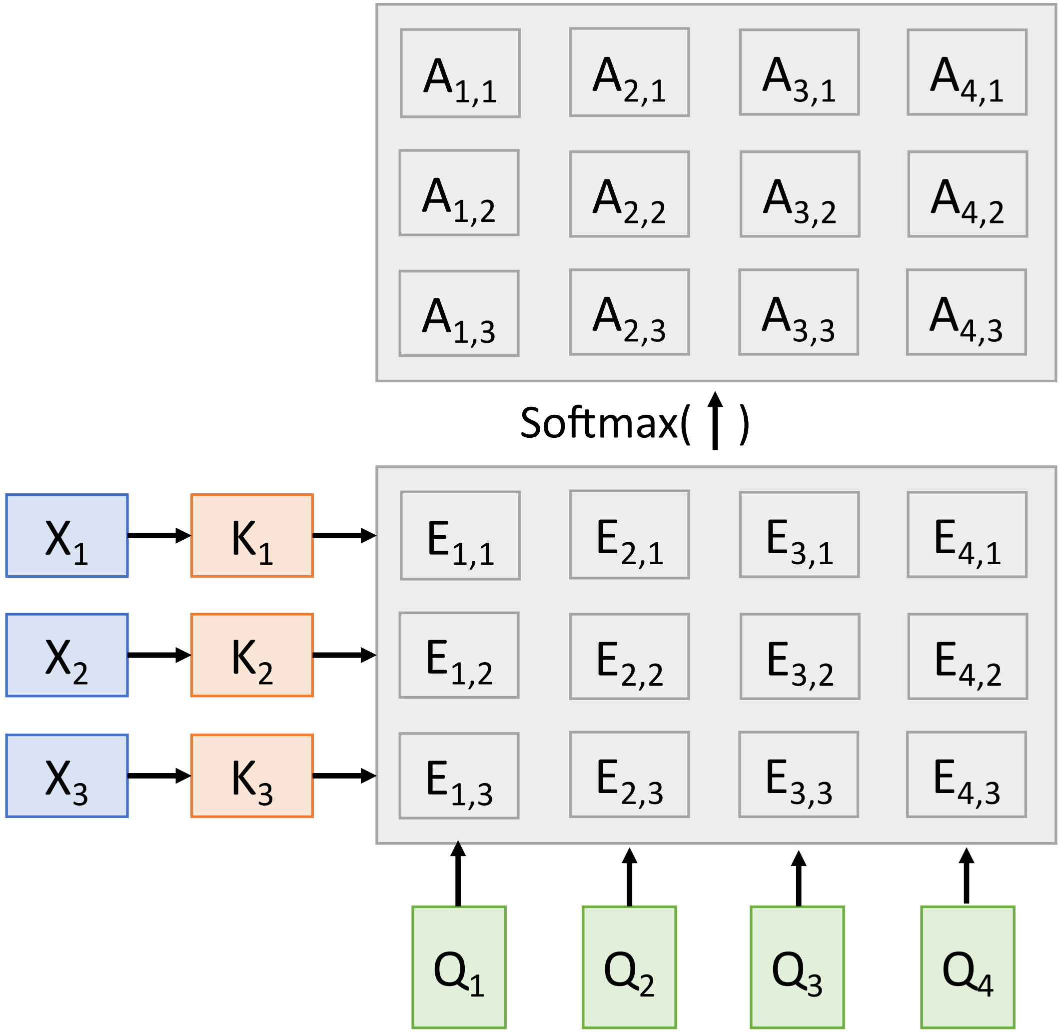
Computation:
Key vectors: $K = XW_K$ (Shape: N_X x D_Q)
Value Vectors: $V = XW_V$ (Shape: N_X x D_V)
Similarities: $E = QK^T$ (Shape: N_Q x N_X) $E_{i,j} = Q_i \cdot K_j / \text{sqrt}(D_Q)$
Attention weights: $A = \text{softmax}(E, \text{dim}=1)$ (Shape: N_Q x N_X)
Output vectors: $Y = AV$ (Shape: N_Q x D_V) $Y_i = \sum_j A_{i,j} V_j$



Attention Layer

Inputs:
Query vectors: **Q** (Shape: N_Q x D_Q)
Input vectors: **X** (Shape: N_X x D_X)
Key matrix: **W_K** (Shape: D_X x D_Q)
Value matrix: **W_V** (Shape: D_X x D_V)

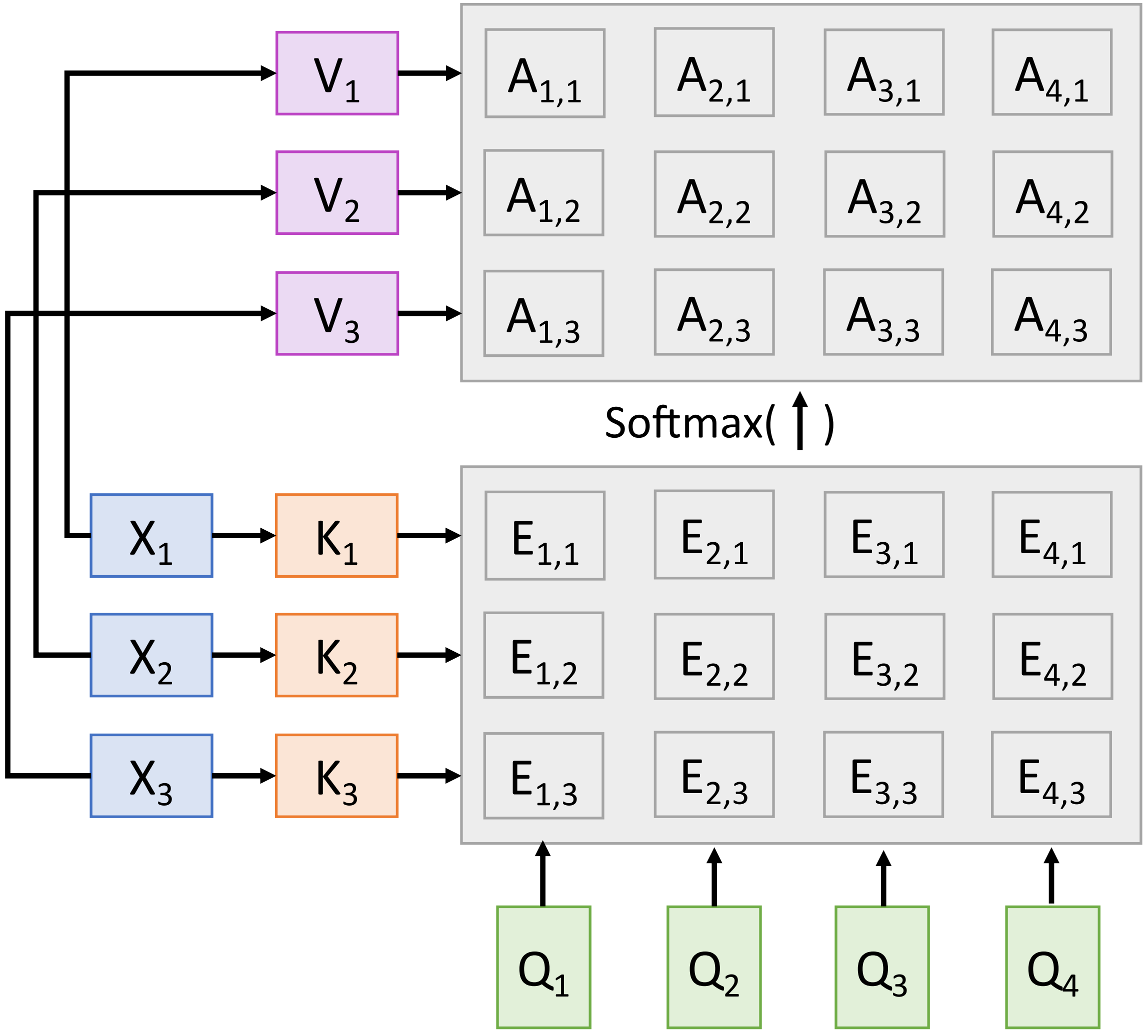
Computation:
Key vectors: **K** = **XW_K** (Shape: N_X x D_Q)
Value Vectors: **V** = **XW_V** (Shape: N_X x D_V)
Similarities: E = QK^T (Shape: N_Q x N_X) $E_{i,j} = Q_i \cdot K_j / \mathrm{sqrt}(D_Q)$
Attention weights: A = softmax(E, dim=1) (Shape: N_Q x N_X)
Output vectors: Y = AV (Shape: N_Q x D_V) $Y_i = \sum_j A_{i,j} V_j$



Attention Layer

Inputs:
Query vectors: **Q** (Shape: N_Q x D_Q)
Input vectors: **X** (Shape: N_X x D_X)
Key matrix: **W_K** (Shape: D_X x D_Q)
Value matrix: **W_V** (Shape: D_X x D_V)

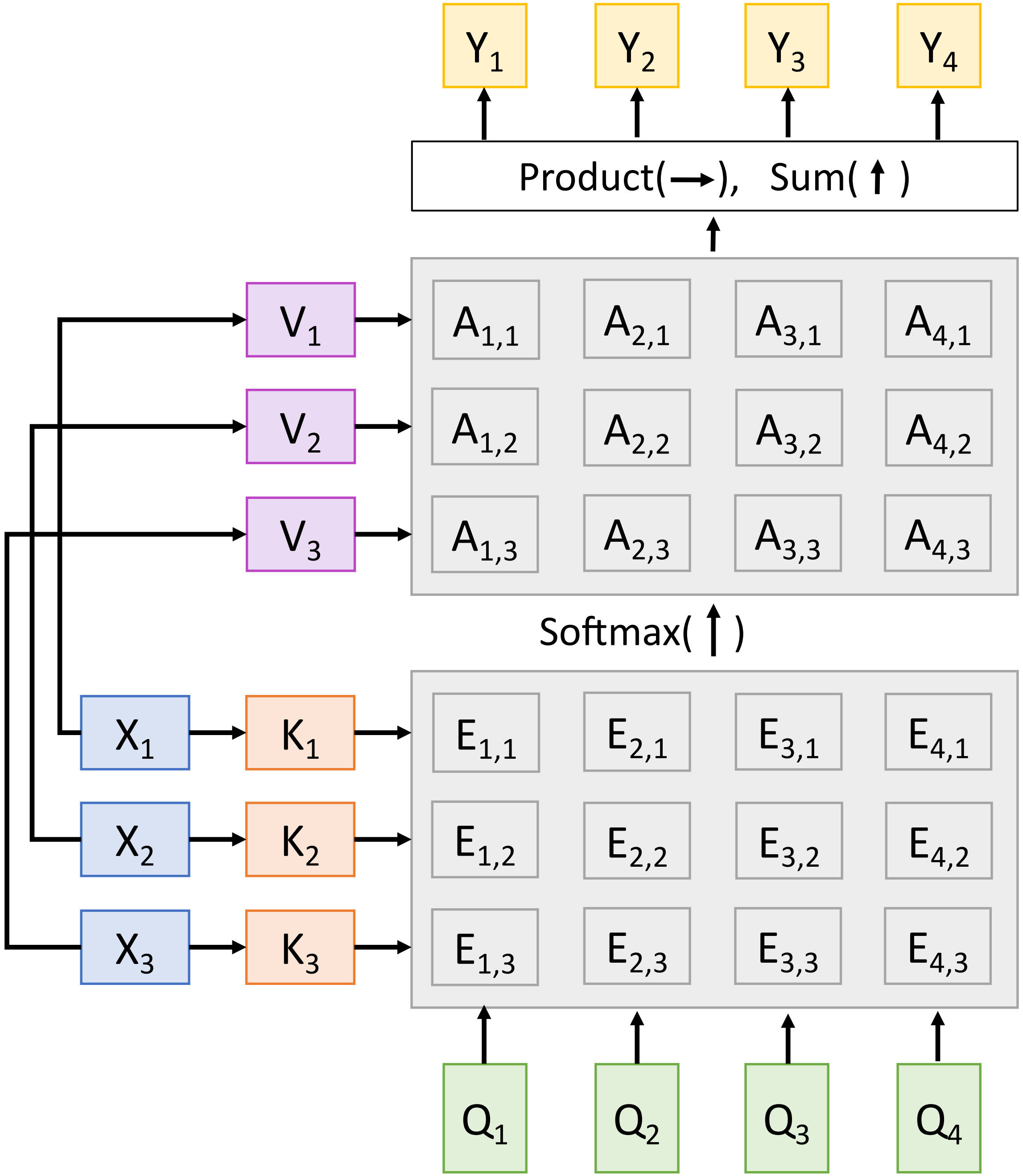
Computation:
Key vectors: **K** = **XW_K** (Shape: N_X x D_Q)
Value Vectors: **V** = **XW_V** (Shape: N_X x D_V)
Similarities: E = **QK^T** (Shape: N_Q x N_X) $E_{i,j} = Q_i \cdot K_j / \text{sqrt}(D_Q)$
Attention weights: A = softmax(E, dim=1) (Shape: N_Q x N_X)
Output vectors: Y = AV (Shape: N_Q x D_V) $Y_i = \sum_j A_{i,j} V_j$



Attention Layer

Inputs:
Query vectors: **Q** (Shape: N_Q x D_Q)
Input vectors: **X** (Shape: N_X x D_X)
Key matrix: $\mathbf{W_K}$ (Shape: D_X x D_Q)
Value matrix: $\mathbf{W_V}$ (Shape: D_X x D_V)

Computation:
Key vectors: **K** = $\mathbf{XW_K}$ (Shape: N_X x D_Q)
Value Vectors: **V** = $\mathbf{XW_V}$ (Shape: N_X x D_V)
Similarities: E = $\mathbf{QK^T}$ (Shape: N_Q x 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 x N_X)
Output vectors: Y = A**V** (Shape: N_Q x D_V) $Y_i = \sum_j A_{i,j} \mathbf{V_j}$

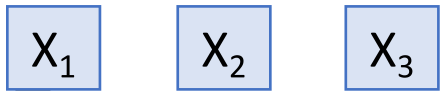


Self-Attention Layer

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

Inputs:
Input vectors: $\mathbf{X}$ (Shape: N_X x D_X)
Key matrix: $\mathbf{W_K}$ (Shape: D_X x D_Q)
Value matrix: $\mathbf{W_V}$ (Shape: D_X x D_V)
Query matrix: $\mathbf{W_Q}$ (Shape: D_X x D_Q)

Computation:
Query vectors: $\mathbf{Q} = \mathbf{XW_Q}$
Key vectors: $\mathbf{K} = \mathbf{XW_K}$ (Shape: N_X x D_Q)
Value Vectors: $\mathbf{V} = \mathbf{XW_V}$ (Shape: N_X x D_V)
Similarities: $E = \mathbf{QK}^T$ (Shape: N_X x N_X) $E_{i,j} = \mathbf{Q_i} \cdot \mathbf{K_j} / \mathrm{sqrt}(D_Q)$
Attention weights: $A = \mathrm{softmax}(E, \mathrm{dim}=1)$ (Shape: N_X x N_X)
Output vectors: $Y = A\mathbf{V}$ (Shape: N_X x D_V) $Y_i = \sum_j A_{i,j}\mathbf{V_j}$

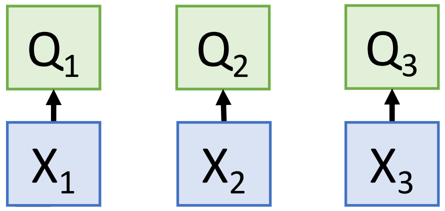


Self-Attention Layer

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

Inputs:
Input vectors: **X** (Shape: N_X x D_X)
Key matrix: $\mathbf{W_K}$ (Shape: D_X x D_Q)
Value matrix: $\mathbf{W_V}$ (Shape: D_X x D_V)
Query matrix: $\mathbf{W_Q}$ (Shape: D_X x D_Q)

Computation:
Query vectors: $\mathbf{Q} = \mathbf{XW_Q}$
Key vectors: $\mathbf{K} = \mathbf{XW_K}$ (Shape: N_X x D_Q)
Value Vectors: $\mathbf{V} = \mathbf{XW_V}$ (Shape: N_X x D_V)
Similarities: $E = \mathbf{QK}^T$ (Shape: N_X x N_X) $E_{i,j} = \mathbf{Q_i} \cdot \mathbf{K_j} / \mathrm{sqrt}(D_Q)$
Attention weights: A = softmax(E, dim=1) (Shape: N_X x N_X)
Output vectors: $Y = A\mathbf{V}$ (Shape: N_X x D_V) $Y_i = \sum_j A_{i,j}\mathbf{V_j}$

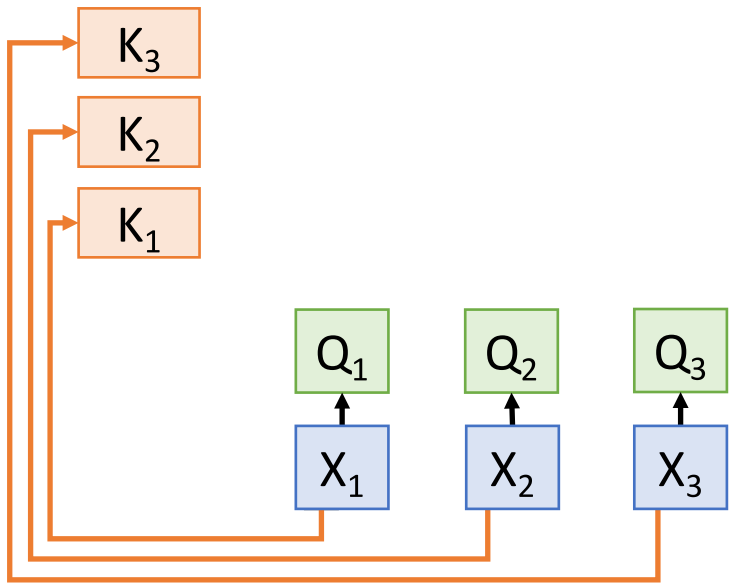


Self-Attention Layer

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: $E = \mathbf{QK}^T$ (Shape: $N_X \times N_X$) $E_{i,j} = \mathbf{Q_i} \cdot \mathbf{K_j} / \text{sqrt}(D_Q)$
Attention weights: $A = \text{softmax}(E, \text{dim}=1)$ (Shape: $N_X \times N_X$)
Output vectors: $Y = A\mathbf{V}$ (Shape: $N_X \times D_V$) $Y_i = \sum_j A_{i,j}\mathbf{V_j}$



Self-Attention Layer

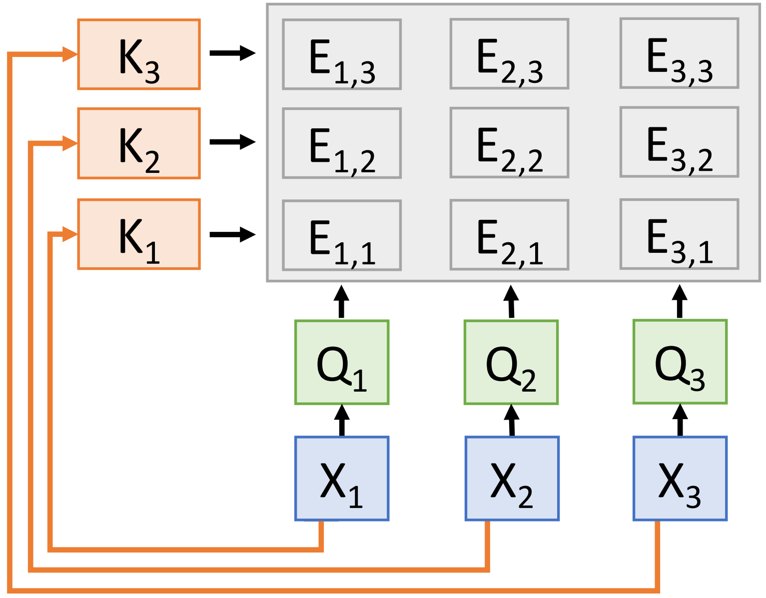
One **query** per **input vector**

<u>**Inputs**</u>:

Input vectors: **X** (Shape: N_X x D_X)
Key matrix: $\mathbf{W_K}$ (Shape: D_X x D_Q)
Value matrix: $\mathbf{W_V}$ (Shape: D_X x D_V)
Query matrix: $\mathbf{W_Q}$ (Shape: D_X x D_Q)

<u>**Computation**</u>:

Query vectors: $\mathbf{Q} = \mathbf{XW_Q}$
Key vectors: $\mathbf{K} = \mathbf{XW_K}$ (Shape: N_X x D_Q)
Value Vectors: $\mathbf{V} = \mathbf{XW_V}$ (Shape: N_X x D_V)
Similarities: $E = \mathbf{QK}^T$ (Shape: N_X x 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_X x N_X)
Output vectors: $Y = A\mathbf{V}$ (Shape: N_X x D_V) $Y_i = \sum_j A_{i,j}\mathbf{V_j}$

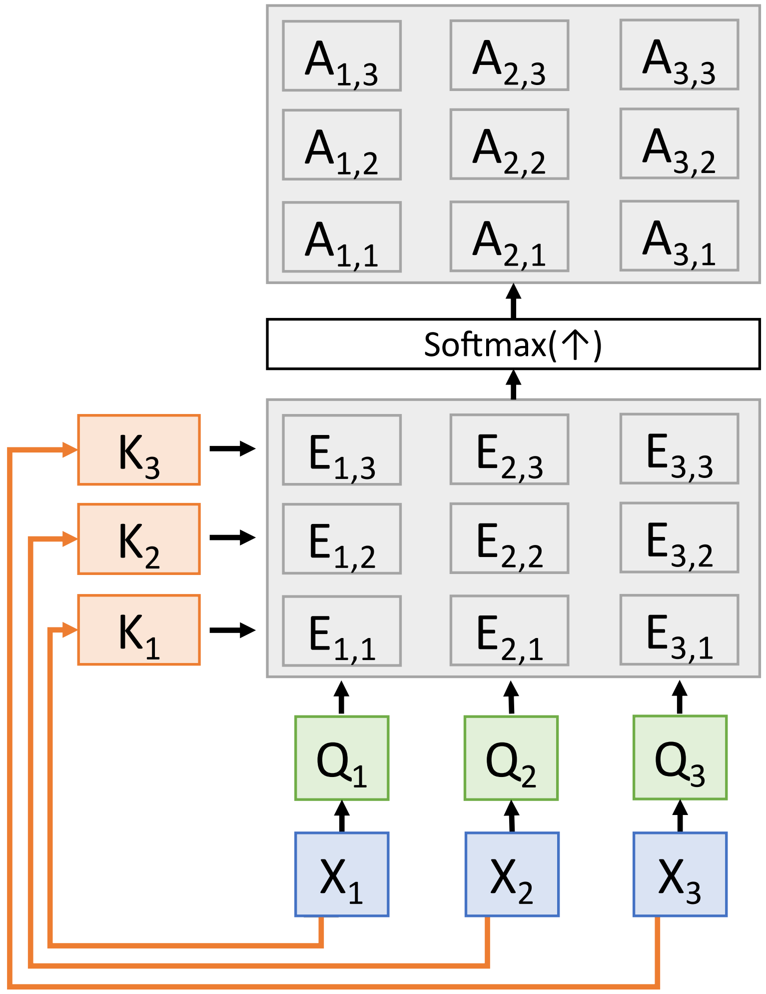


Self-Attention Layer

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

<u>Inputs</u>:
Input vectors: **X** (Shape: N_X x D_X)
Key matrix: **W_K** (Shape: D_X x D_Q)
Value matrix: **W_V** (Shape: D_X x D_V)
Query matrix: **W_Q** (Shape: D_X x D_Q)

<u>Computation</u>:
Query vectors: **$Q = XW_Q$**
Key vectors: **$K = XW_K$** (Shape: N_X x D_Q)
Value Vectors: **$V = XW_V$** (Shape: N_X x D_V)
Similarities: $E = QK^T$ (Shape: N_X x N_X) $E_{i,j} = Q_i \cdot K_j / \text{sqrt}(D_Q)$
Attention weights: $A = \text{softmax}(E, \text{dim}=1)$ (Shape: N_X x N_X)
Output vectors: $Y = AV$ (Shape: N_X x D_V) $Y_i = \sum_j A_{i,j} V_j$

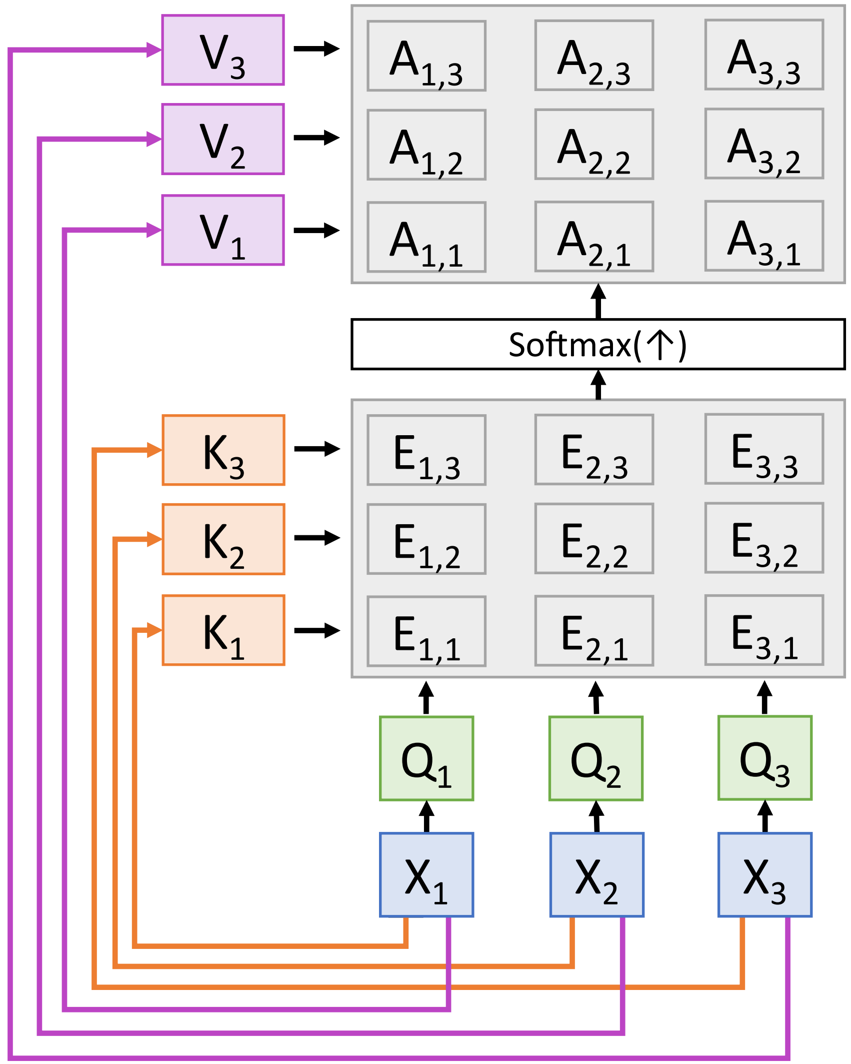


Self-Attention Layer

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

Inputs:
Input vectors: **X** (Shape: N_X x D_X)
Key matrix: $\mathbf{W_K}$ (Shape: D_X x D_Q)
Value matrix: $\mathbf{W_V}$ (Shape: D_X x D_V)
Query matrix: $\mathbf{W_Q}$ (Shape: D_X x D_Q)

Computation:
Query vectors: $\mathbf{Q} = \mathbf{XW_Q}$
Key vectors: $\mathbf{K} = \mathbf{XW_K}$ (Shape: N_X x D_Q)
Value Vectors: $\mathbf{V} = \mathbf{XW_V}$ (Shape: N_X x D_V)
Similarities: $E = \mathbf{QK}^T$ (Shape: N_X x 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_X x N_X)
Output vectors: $Y = A\mathbf{V}$ (Shape: N_X x D_V) $Y_i = \sum_j A_{i,j}\mathbf{V_j}$

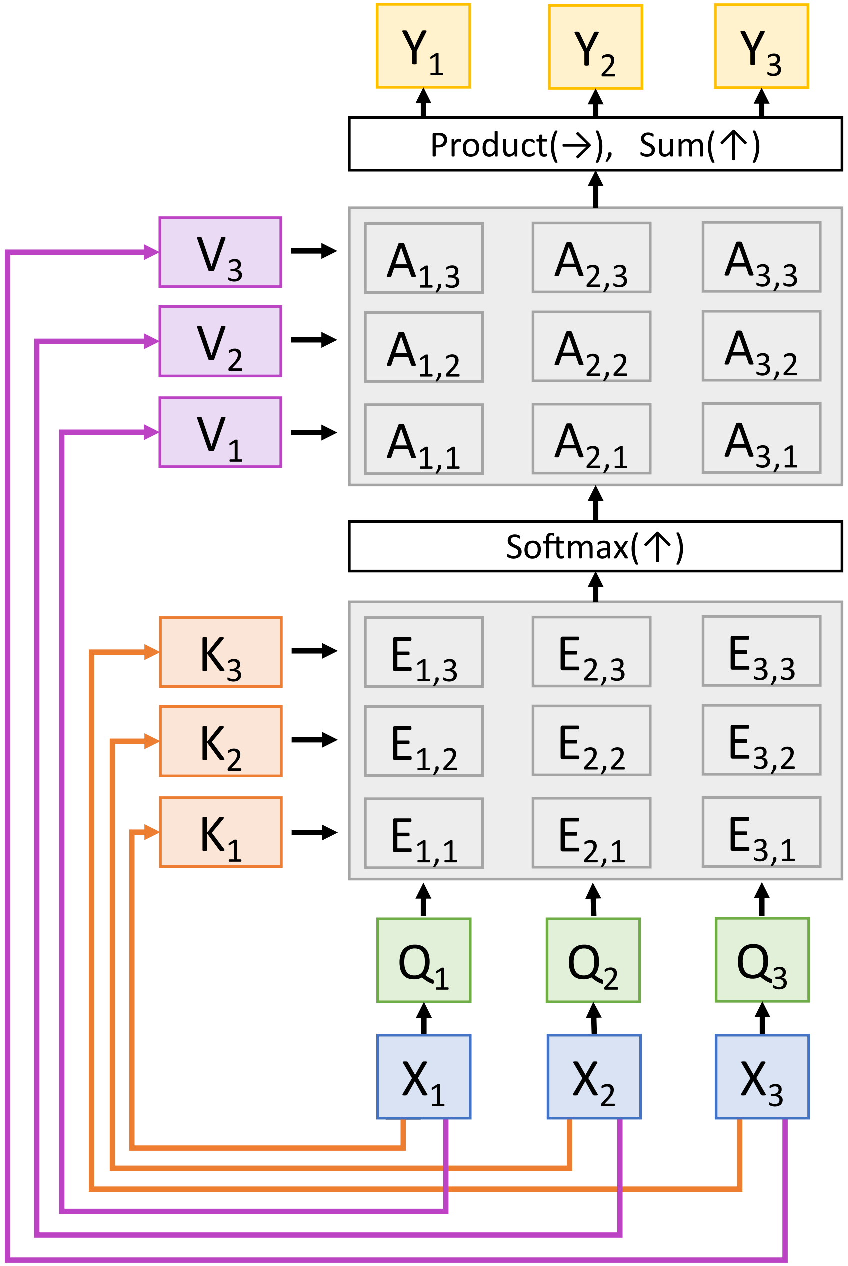


Self-Attention Layer

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

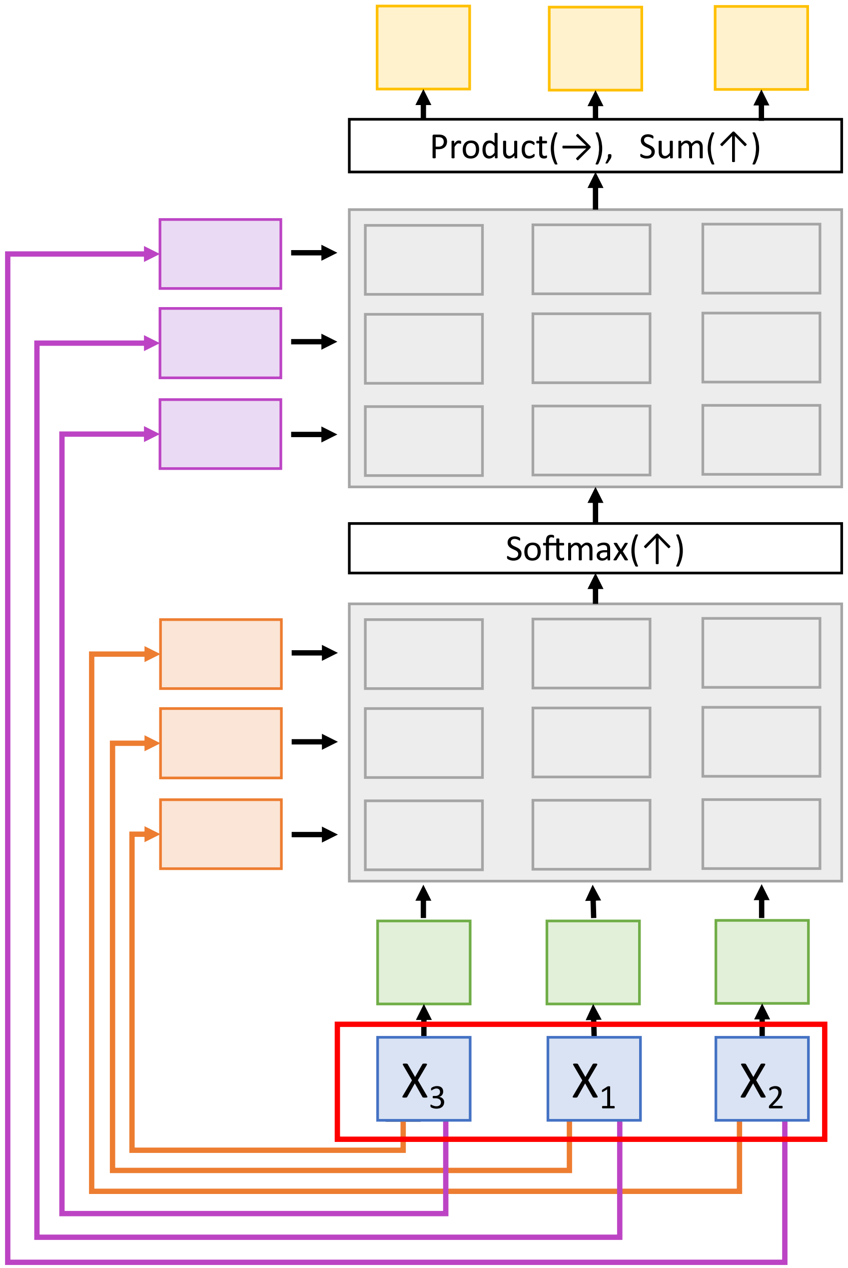
Inputs:
Input vectors: **X** (Shape: N_X x D_X)
Key matrix: $\mathbf{W_K}$ (Shape: D_X x D_Q)
Value matrix: $\mathbf{W_V}$ (Shape: D_X x D_V)
Query matrix: $\mathbf{W_Q}$ (Shape: D_X x D_Q)

Computation:
Query vectors: $\mathbf{Q} = \mathbf{XW_Q}$
Key vectors: $\mathbf{K} = \mathbf{XW_K}$ (Shape: N_X x D_Q)
Value Vectors: $\mathbf{V} = \mathbf{XW_V}$ (Shape: N_X x D_V)
Similarities: $E = \mathbf{QK^T}$ (Shape: N_X x 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_X x N_X)
Output vectors: $Y = A\mathbf{V}$ (Shape: N_X x D_V) $Y_i = \sum_j A_{i,j}\mathbf{V_j}$



Self-Attention Layer

Consider **permuting** the input vectors:



Inputs:
Input vectors: X (Shape: N_X x D_X)
Key matrix: W_K (Shape: D_X x D_Q)
Value matrix: W_V (Shape: D_X x D_V)
Query matrix: W_Q (Shape: D_X x D_Q)

Computation:
Query vectors: $Q = XW_Q$
Key vectors: $K = XW_K$ (Shape: N_X x D_Q)
Value Vectors: $V = XW_V$ (Shape: N_X x D_V)
Similarities: $E = QK^T$ (Shape: N_X x N_X) $E_{i,j} = Q_i \cdot K_j / \text{sqrt}(D_Q)$
Attention weights: $A = \text{softmax}(E, \text{dim}=1)$ (Shape: N_X x N_X)
Output vectors: $Y = AV$ (Shape: N_X x D_V) $Y_i = \sum_j A_{i,j} V_j$

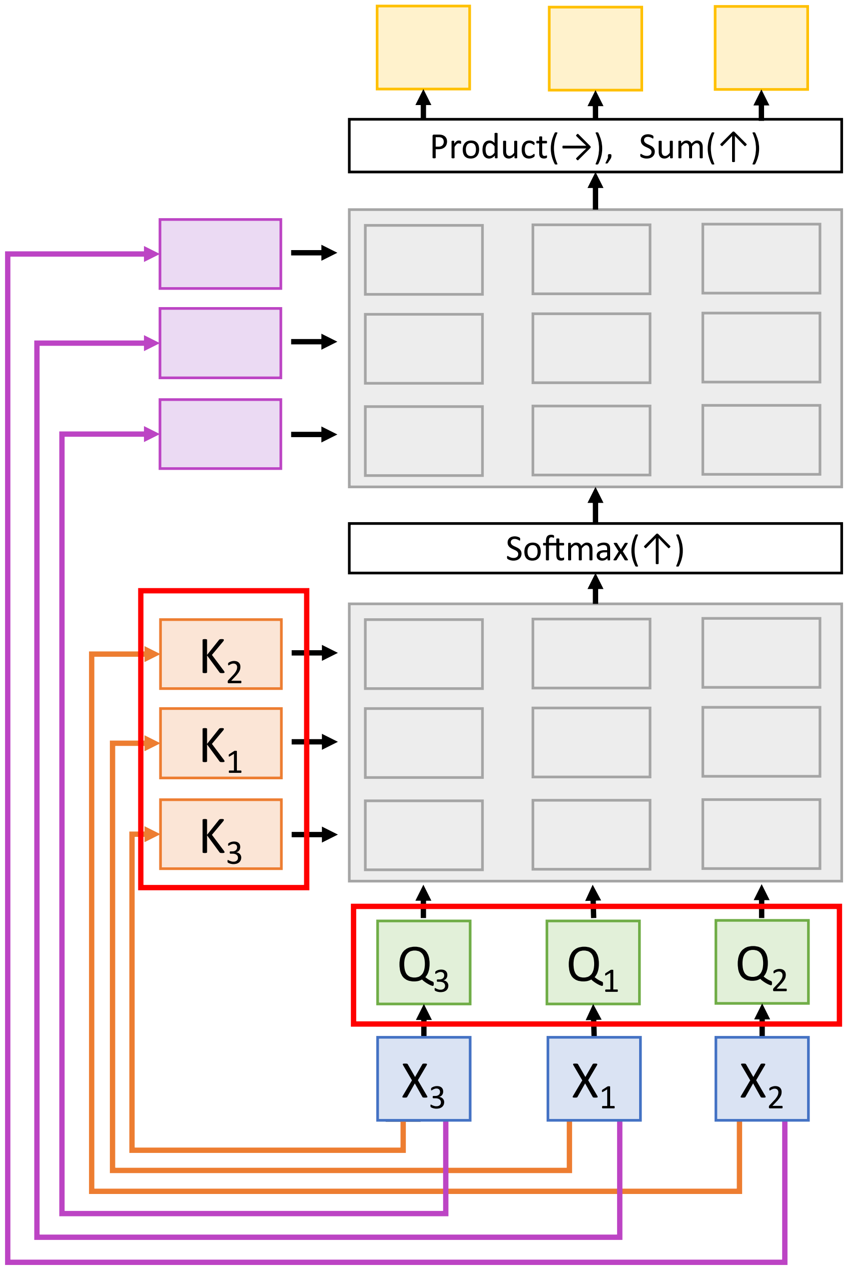
Self-Attention Layer

Inputs:
Input vectors: **X** (Shape: N_X x D_X)
Key matrix: $\mathbf{W_K}$ (Shape: D_X x D_Q)
Value matrix: $\mathbf{W_V}$ (Shape: D_X x D_V)
Query matrix: $\mathbf{W_Q}$ (Shape: D_X x D_Q)

Computation:
Query vectors: $\mathbf{Q} = \mathbf{XW_Q}$
Key vectors: $\mathbf{K} = \mathbf{XW_K}$ (Shape: N_X x D_Q)
Value Vectors: $\mathbf{V} = \mathbf{XW_V}$ (Shape: N_X x D_V)
Similarities: $E = \mathbf{QK}^T$ (Shape: N_X x 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_X x N_X)
Output vectors: $Y = A\mathbf{V}$ (Shape: N_X x D_V) $Y_i = \sum_j A_{i,j} \mathbf{V_j}$

Consider **permuting** the input vectors:

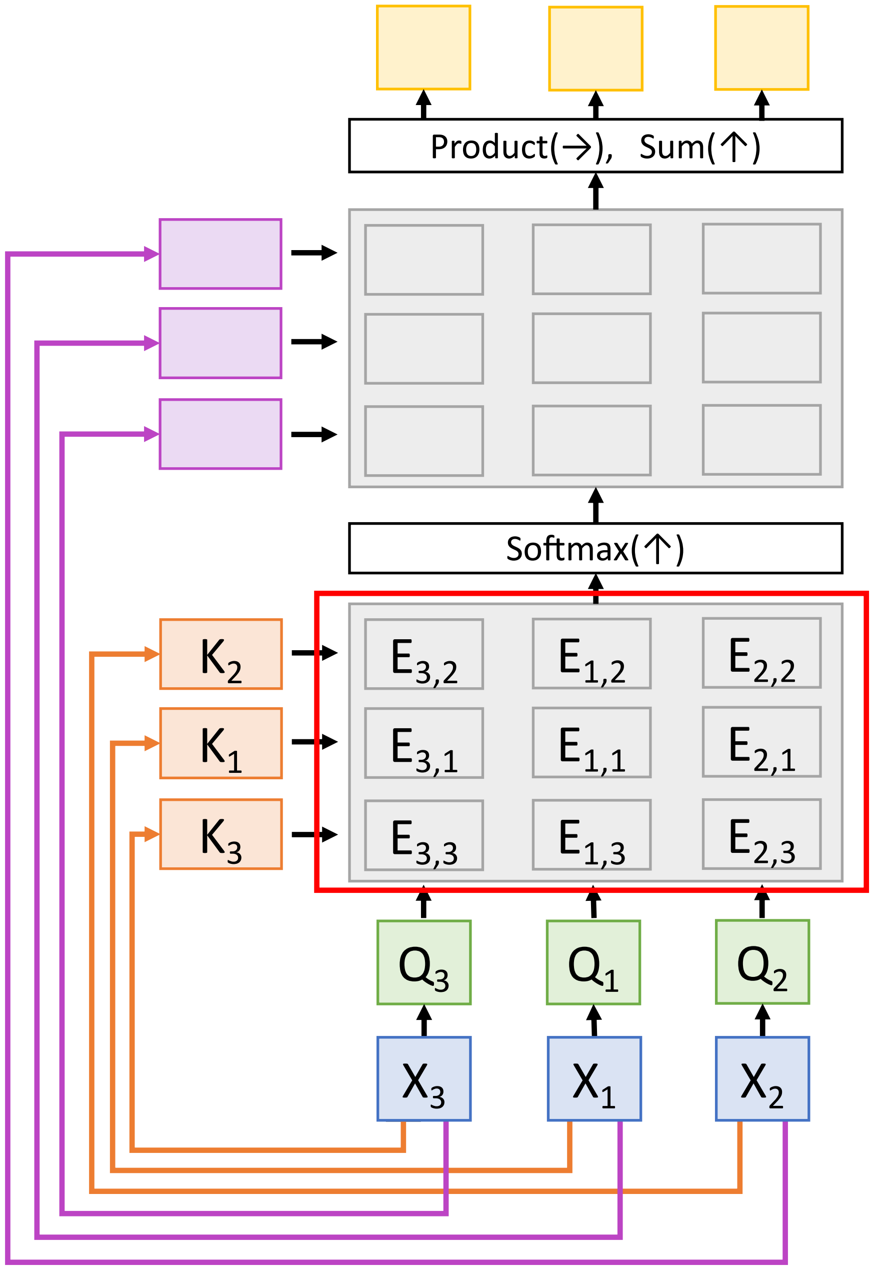
Queries and Keys will be the same, but permuted



Self-Attention Layer

Consider **permuting** the input vectors:

Similarities will be the same, but permuted



Inputs:

Input vectors: **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: $E = \mathbf{QK}^T$ (Shape: $N_X \times N_X$) $E_{i,j} = \mathbf{Q_i} \cdot \mathbf{K_j} / \text{sqrt}(D_Q)$

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

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

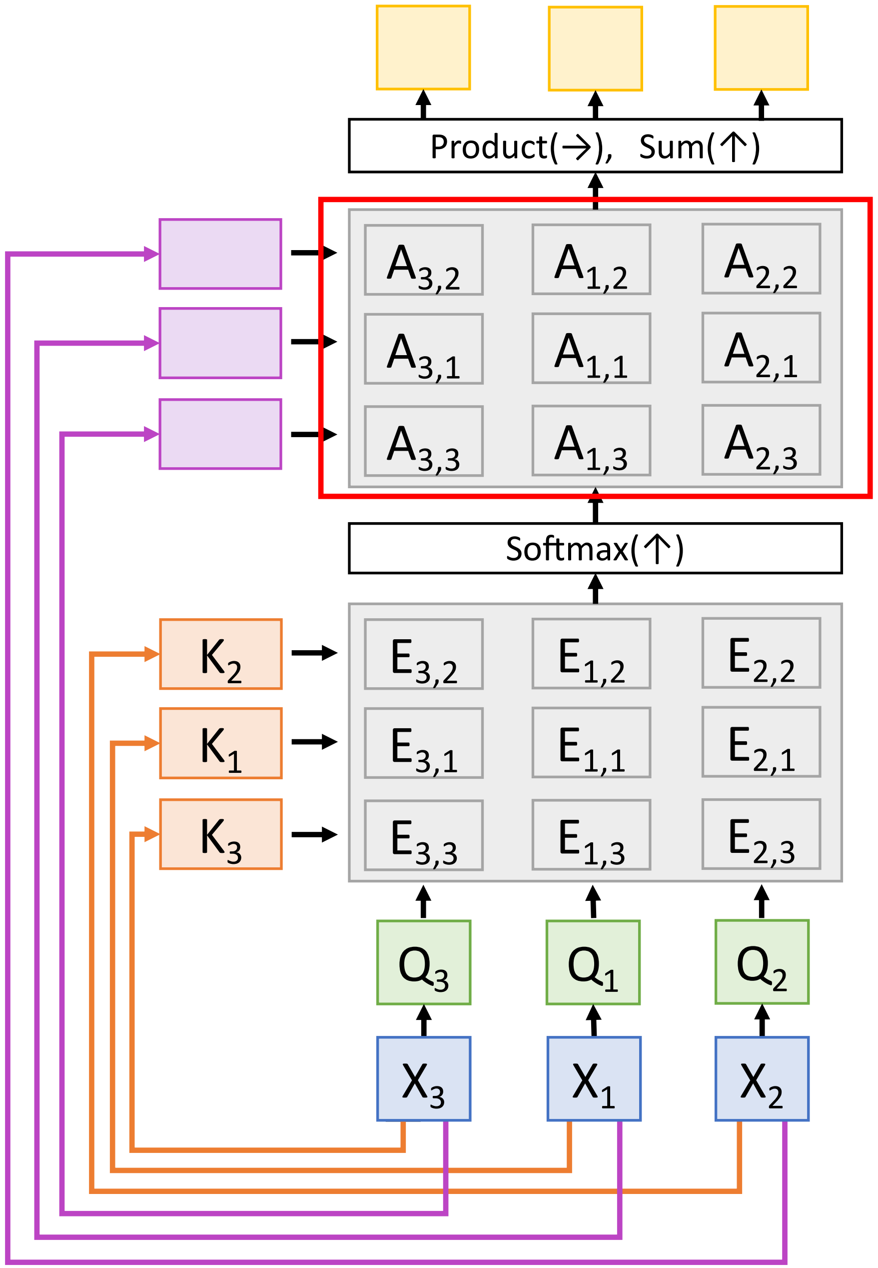
Self-Attention Layer

Consider **permuting** the input vectors:

Attention weights will be the same, but permuted

Inputs:
Input vectors: **X** (Shape: $N_X \times D_X$)
Key matrix: W_K (Shape: $D_X \times D_Q$)
Value matrix: W_V (Shape: $D_X \times D_V$)
Query matrix: W_Q (Shape: $D_X \times D_Q$)

Computation:
Query vectors: $Q = XW_Q$
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: $N_X \times N_X$) $E_{i,j} = Q_i \cdot K_j / \text{sqrt}(D_Q)$
Attention weights: A = softmax(E, dim=1) (Shape: $N_X \times N_X$)
Output vectors: $Y = AV$ (Shape: $N_X \times D_V$) $Y_i = \sum_j A_{i,j} V_j$



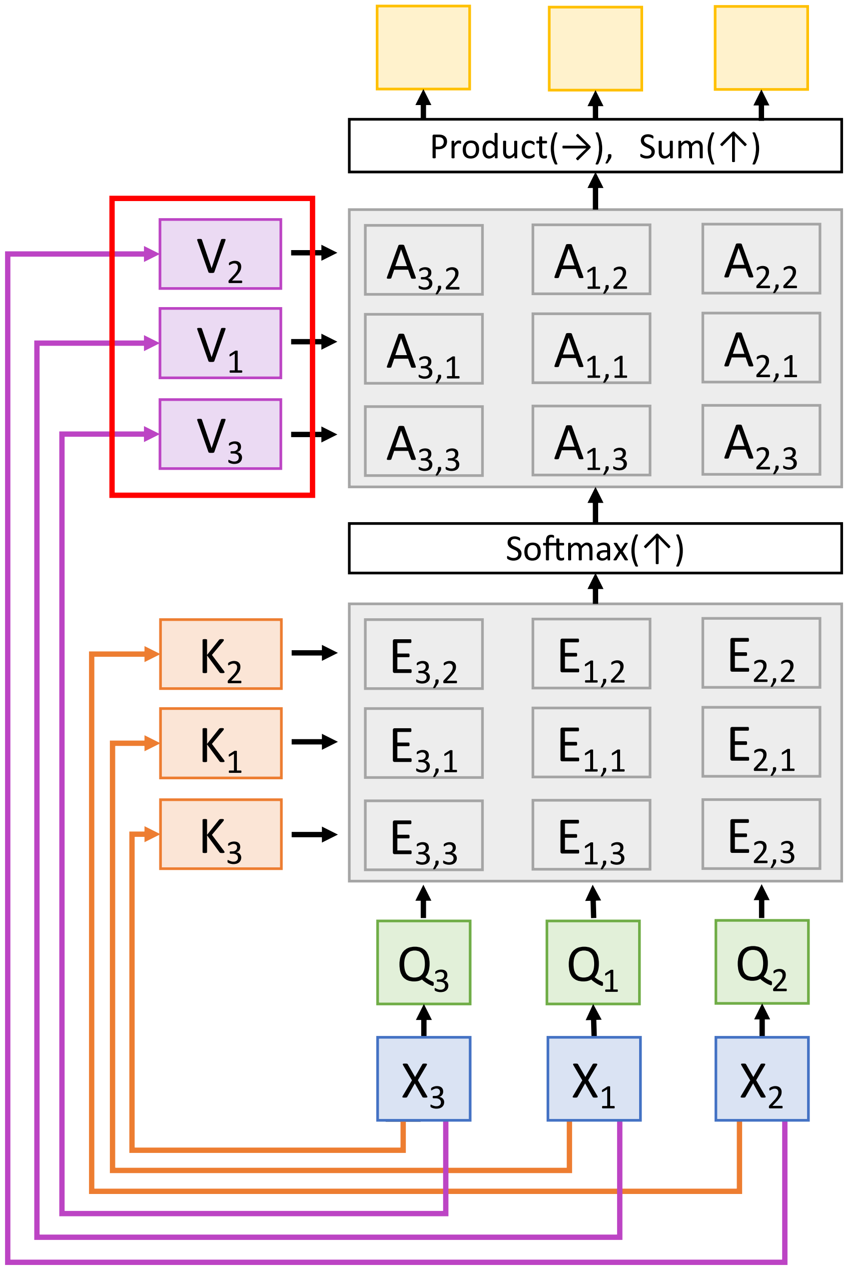
Self-Attention Layer

Consider **permuting** the input vectors:

Values will be the same, but permuted

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: $E = \mathbf{QK}^T$ (Shape: $N_X \times N_X$) $E_{i,j} = \mathbf{Q_i} \cdot \mathbf{K_j} / \mathrm{sqrt}(D_Q)$
Attention weights: $A = \mathrm{softmax}(E, \mathrm{dim}=1)$ (Shape: $N_X \times N_X$)
Output vectors: $Y = A\mathbf{V}$ (Shape: $N_X \times D_V$) $Y_i = \sum_j A_{i,j}\mathbf{V_j}$



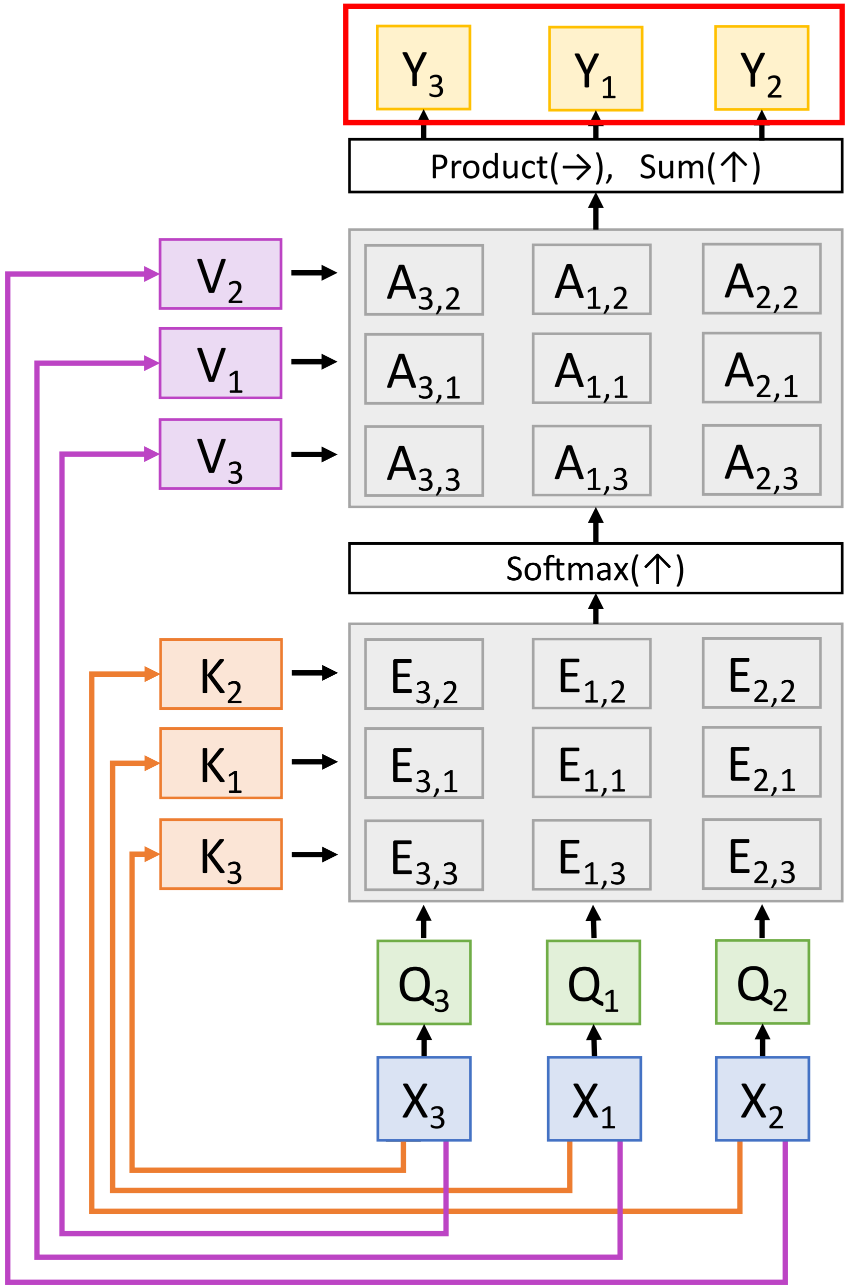
Self-Attention Layer

Consider **permuting** the input vectors:

Outputs will be the same, but permuted

Inputs:
Input vectors: **X** (Shape: N_X x D_X)
Key matrix: $\mathbf{W_K}$ (Shape: D_X x D_Q)
Value matrix: $\mathbf{W_V}$ (Shape: D_X x D_V)
Query matrix: $\mathbf{W_Q}$ (Shape: D_X x D_Q)

Computation:
Query vectors: $\mathbf{Q} = \mathbf{XW_Q}$
Key vectors: $\mathbf{K} = \mathbf{XW_K}$ (Shape: N_X x D_Q)
Value Vectors: $\mathbf{V} = \mathbf{XW_V}$ (Shape: N_X x D_V)
Similarities: $E = \mathbf{QK}^T$ (Shape: N_X x 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_X x N_X)
Output vectors: $Y = A\mathbf{V}$ (Shape: N_X x D_V) $Y_i = \sum_j A_{i,j}\mathbf{V_j}$



Self-Attention Layer

Inputs:
Input vectors: X (Shape: N_X x D_X)
Key matrix: W_K (Shape: D_X x D_Q)
Value matrix: W_V (Shape: D_X x D_V)
Query matrix: W_Q (Shape: D_X x D_Q)

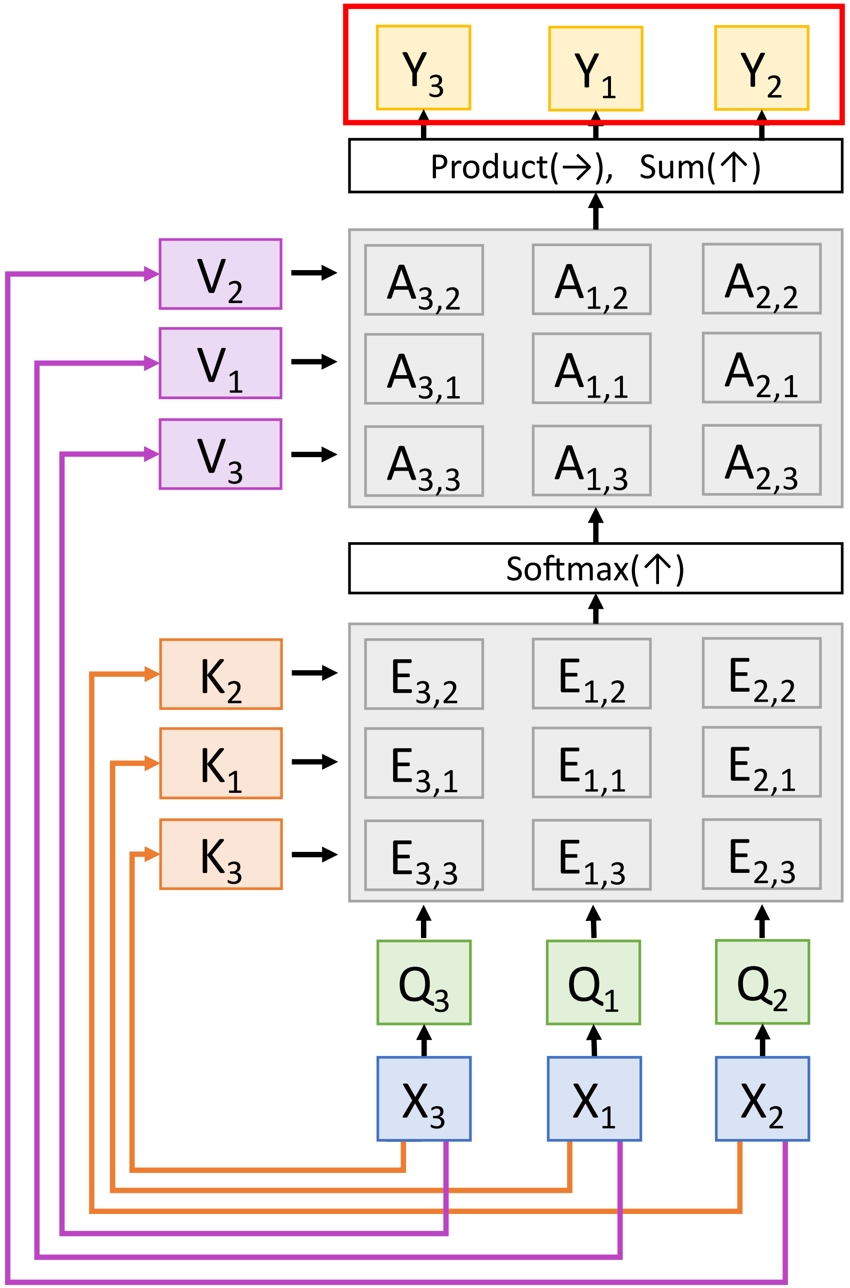
Computation:
Query vectors: $Q = XW_Q$
Key vectors: $K = XW_K$ (Shape: N_X x D_Q)
Value Vectors: $V = XW_V$ (Shape: N_X x D_V)
Similarities: $E = QK^T$ (Shape: N_X x N_X) $E_{i,j} = Q_i \cdot K_j / \mathrm{sqrt}(D_Q)$
Attention weights: $A = \mathrm{softmax}(E, \mathrm{dim}=1)$ (Shape: N_X x N_X)
Output vectors: $Y = AV$ (Shape: N_X x D_V) $Y_i = \sum_j A_{i,j} V_j$

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

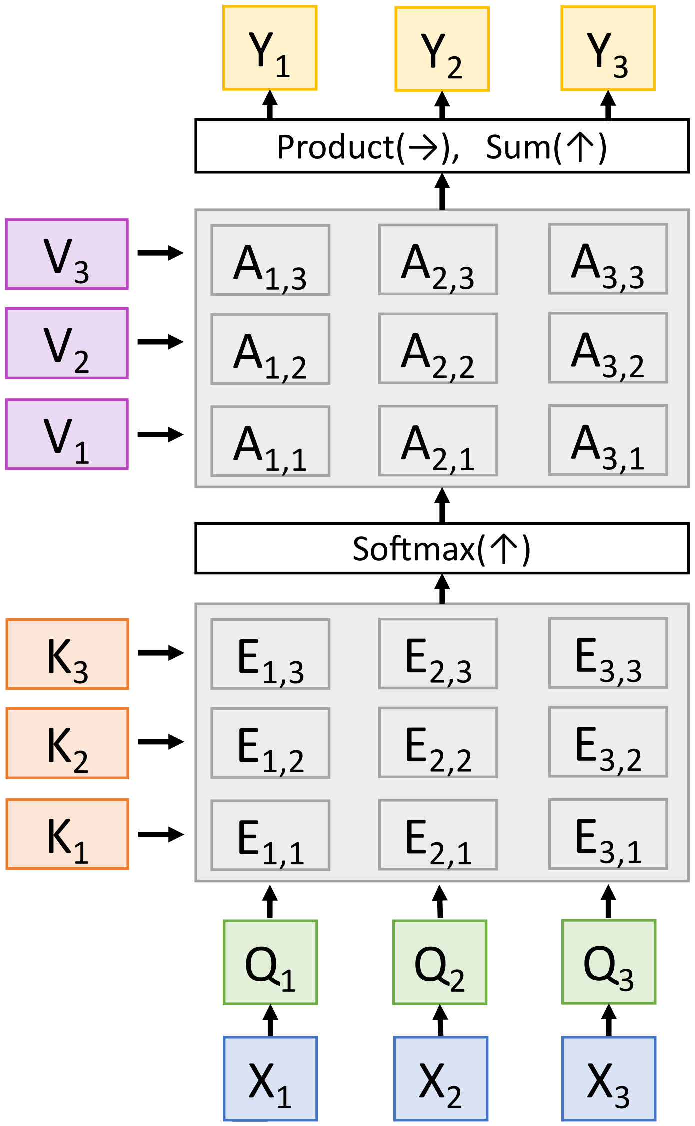


Self-Attention Layer

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

Inputs:
Input vectors: X (Shape: $N_X \times D_X$)
Key matrix: W_K (Shape: $D_X \times D_Q$)
Value matrix: W_V (Shape: $D_X \times D_V$)
Query matrix: W_Q (Shape: $D_X \times D_Q$)

Computation:
Query vectors: $Q = XW_Q$
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: $N_X \times N_X$) $E_{i,j} = Q_i \cdot K_j / \text{sqrt}(D_Q)$
Attention weights: $A = \text{softmax}(E, \text{dim}=1)$ (Shape: $N_X \times N_X$)
Output vectors: $Y = AV$ (Shape: $N_X \times D_V$) $Y_i = \sum_j A_{i,j} V_j$



Self-Attention Layer

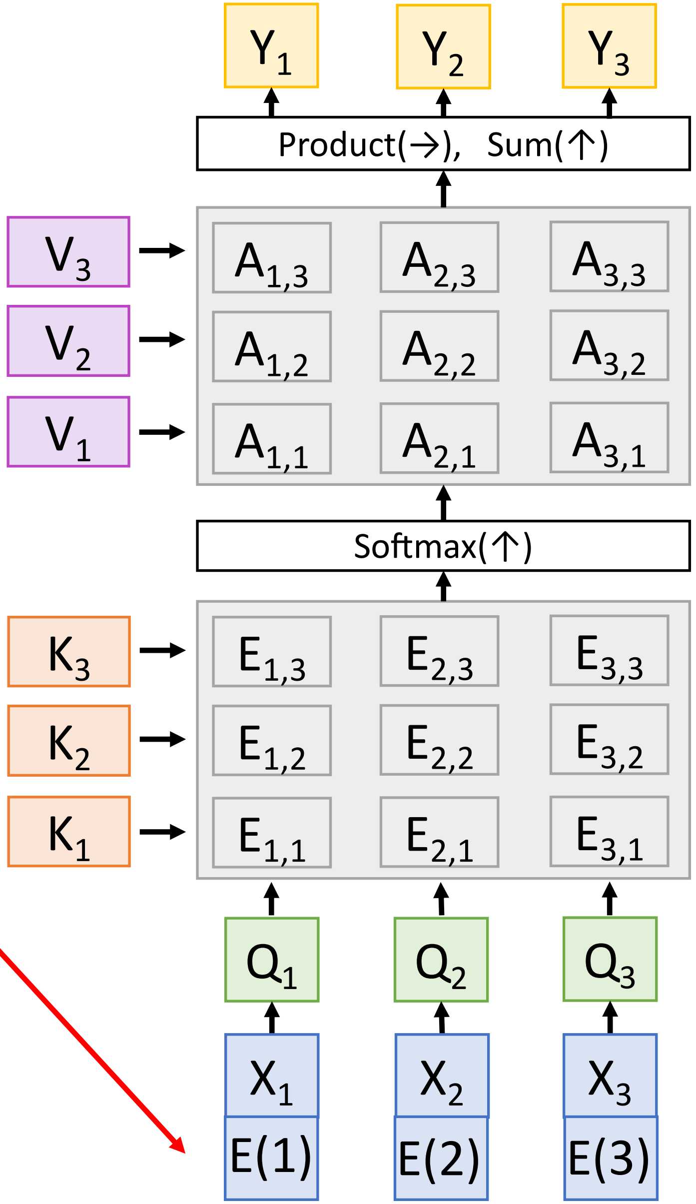
Inputs:
Input vectors: **X** (Shape: N_X x D_X)
Key matrix: W_K (Shape: D_X x D_Q)
Value matrix: W_V (Shape: D_X x D_V)
Query matrix: W_Q (Shape: D_X x D_Q)

Computation:
Query vectors: $Q = XW_Q$
Key vectors: $K = XW_K$ (Shape: N_X x D_Q)
Value Vectors: $V = XW_V$ (Shape: N_X x D_V)
Similarities: $E = QK^T$ (Shape: N_X x N_X) $E_{i,j} = Q_i \cdot K_j / \text{sqrt}(D_Q)$
Attention weights: $A = \text{softmax}(E, \text{dim}=1)$ (Shape: N_X x N_X)
Output vectors: $Y = AV$ (Shape: N_X x D_V) $Y_i = \sum_j A_{i,j} V_j$

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

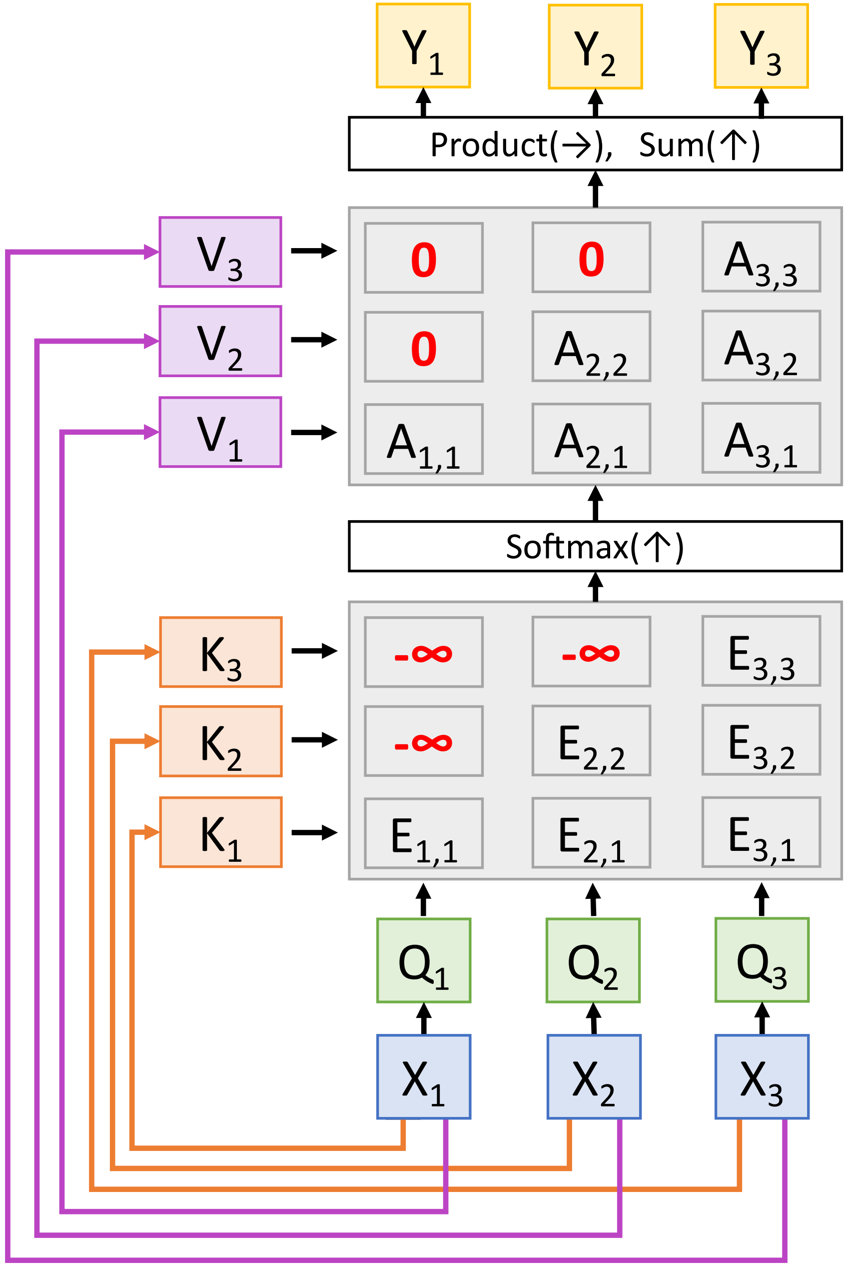


Masked Self-Attention Layer

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

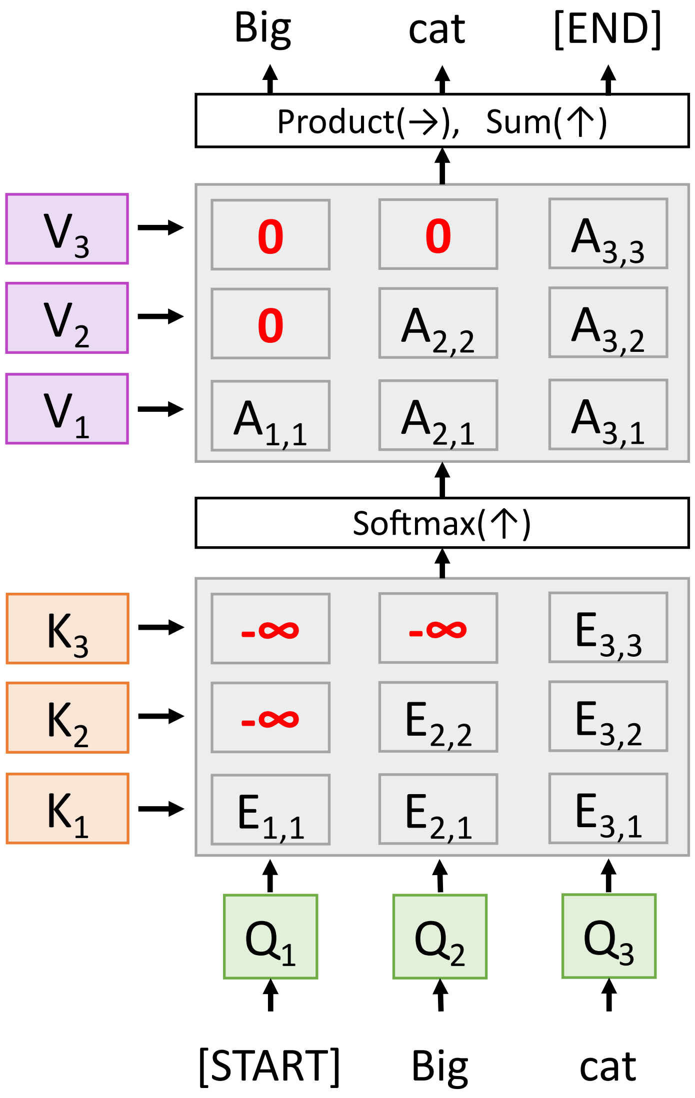
Inputs:
Input vectors: X (Shape: $N_X \times D_X$)
Key matrix: W_K (Shape: $D_X \times D_Q$)
Value matrix: W_V (Shape: $D_X \times D_V$)
Query matrix: W_Q (Shape: $D_X \times D_Q$)

Computation:
Query vectors: $Q = XW_Q$
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: $N_X \times N_X$) $E_{i,j} = Q_i \cdot K_j / \text{sqrt}(D_Q)$
Attention weights: $A = \text{softmax}(E, \text{dim}=1)$ (Shape: $N_X \times N_X$)
Output vectors: $Y = AV$ (Shape: $N_X \times D_V$) $Y_i = \sum_j A_{i,j} V_j$



Masked Self-Attention Layer

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

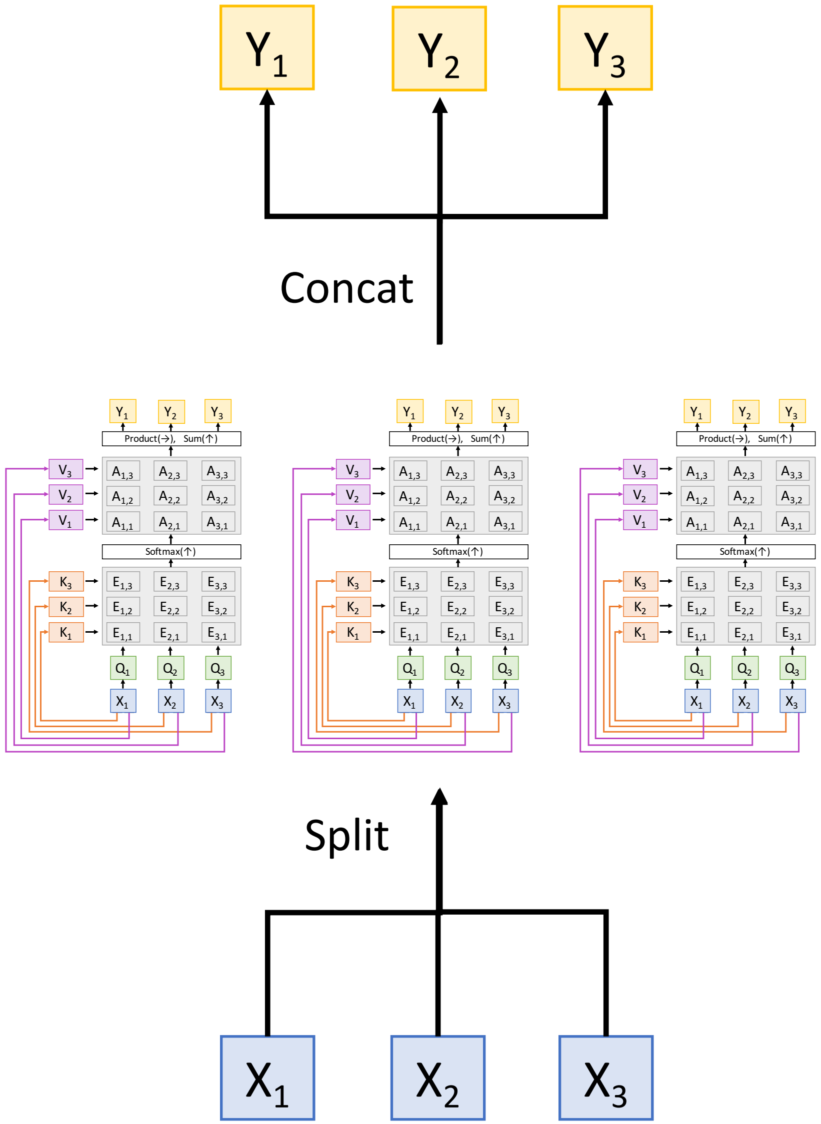


Inputs:
Input vectors: **X** (Shape: N_X x D_X)
Key matrix: **W_K** (Shape: D_X x D_Q)
Value matrix: **W_V** (Shape: D_X x D_V)
Query matrix: **W_Q** (Shape: D_X x D_Q)

Computation:
Query vectors: **Q** = **XW_Q**
Key vectors: **K** = **XW_K** (Shape: N_X x D_Q)
Value Vectors: **V** = **XW_V** (Shape: N_X x D_V)
Similarities: E = **QK^T** (Shape: N_X x N_X) $E_{i,j} = Q_i \cdot K_j / \text{sqrt}(D_Q)$
Attention weights: A = softmax(E, dim=1) (Shape: N_X x N_X)
Output vectors: Y = A**V** (Shape: N_X x D_V) $Y_i = \sum_j A_{i,j} V_j$

Multihead Self-Attention Layer

Use H independent
"Attention Heads" in parallel

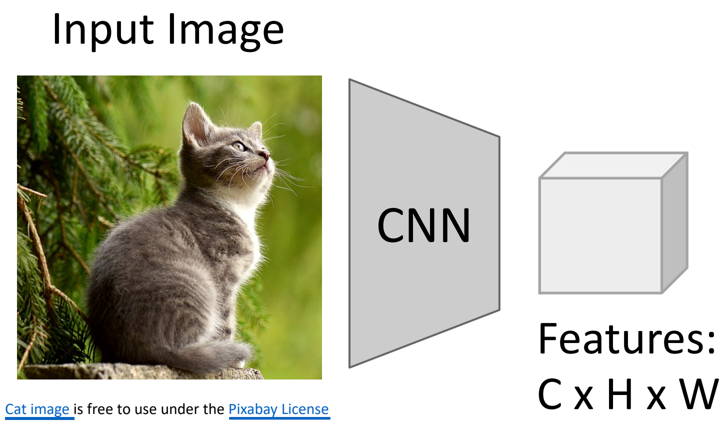


Inputs:
Input vectors: **X** (Shape: N_X x D_X)
Key matrix: W_K (Shape: D_X x D_Q)
Value matrix: W_V (Shape: D_X x D_V)
Query matrix: W_Q (Shape: D_X x D_Q)

Computation:
Query vectors: $Q = XW_Q$
Key vectors: $K = XW_K$ (Shape: N_X x D_Q)
Value Vectors: $V = XW_V$ (Shape: N_X x D_V)
Similarities: $E = QK^T$ (Shape: N_X x N_X) $E_{i,j} = Q_i \cdot K_j / \text{sqrt}(D_Q)$
Attention weights: A = softmax(E, dim=1) (Shape: N_X x N_X)
Output vectors: $Y = AV$ (Shape: N_X x D_V) $Y_i = \sum_j A_{i,j} V_j$

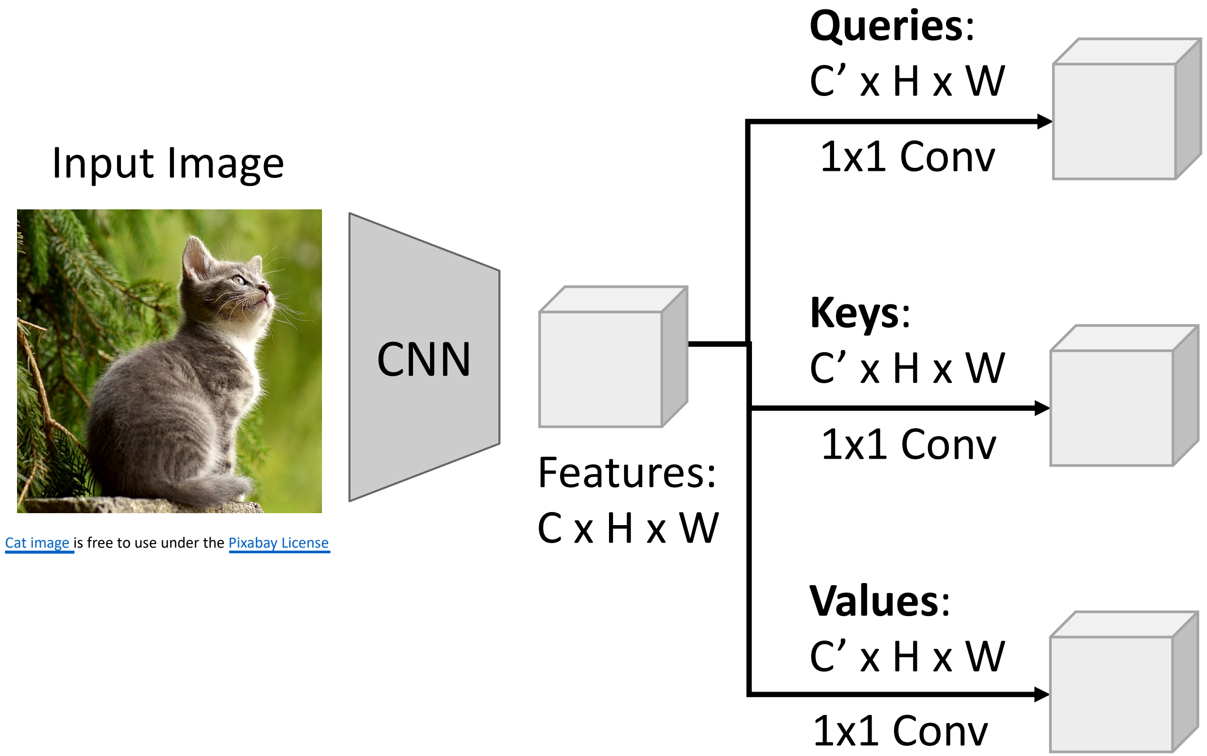
Hyperparameters:
Query dimension D_Q
Number of heads H

Example: CNN with Self-Attention



Zhang et al, "Self-Attention Generative Adversarial Networks", ICML 2018

Example: CNN with Self-Attention

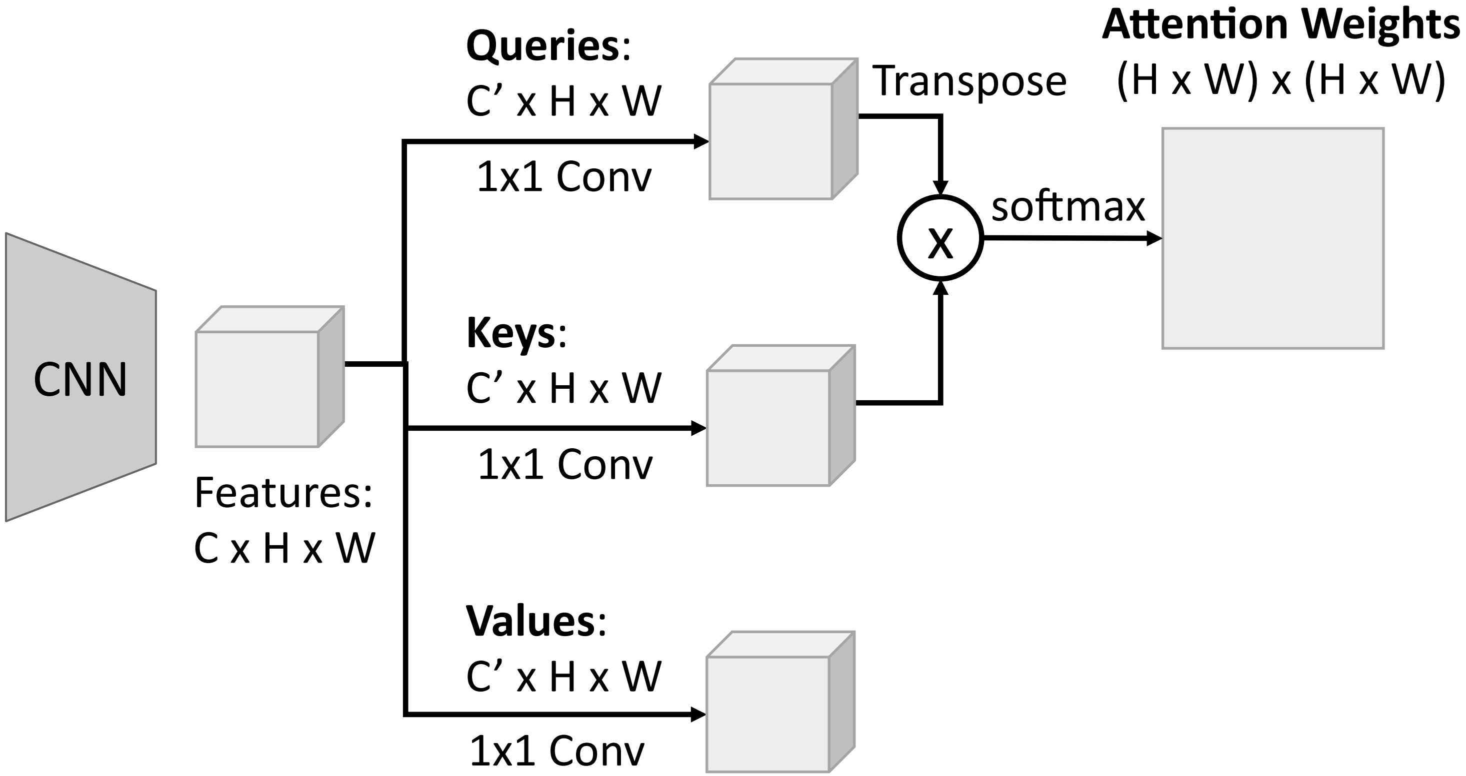


Zhang et al, “Self-Attention Generative Adversarial Networks”, ICML 2018

Example: CNN with Self-Attention

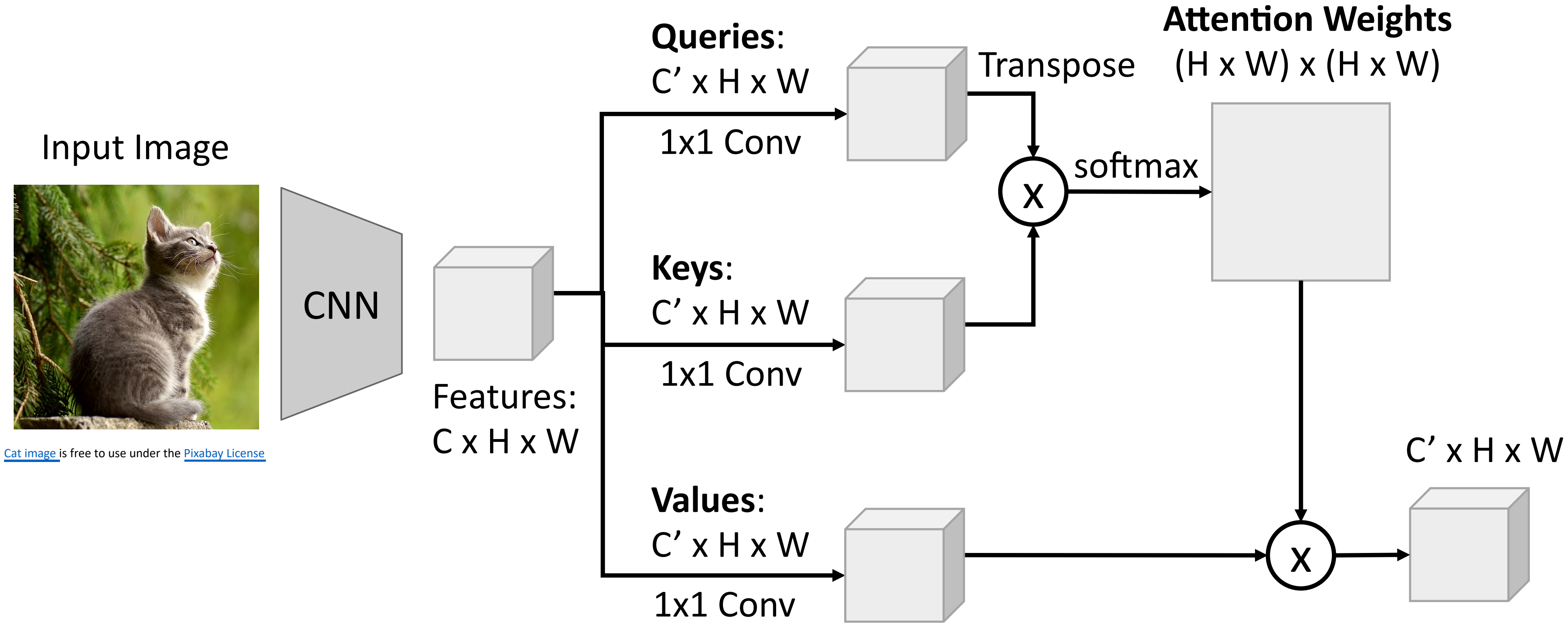
Input Image

Cat image is free to use under the Pixabay License



Zhang et al, "Self-Attention Generative Adversarial Networks", ICML 2018

Example: CNN with Self-Attention



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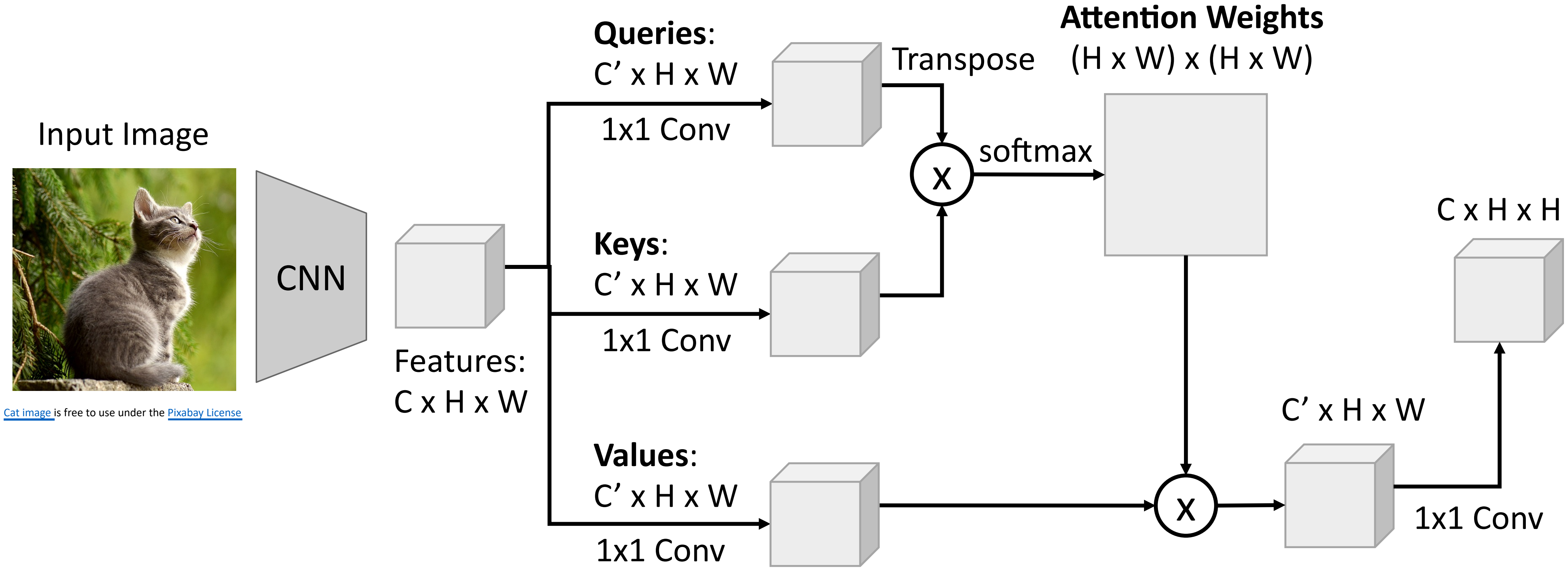
Zhang et al, "Self-Attention Generative Adversarial Networks", ICML 2018

Example: CNN with Self-Attention

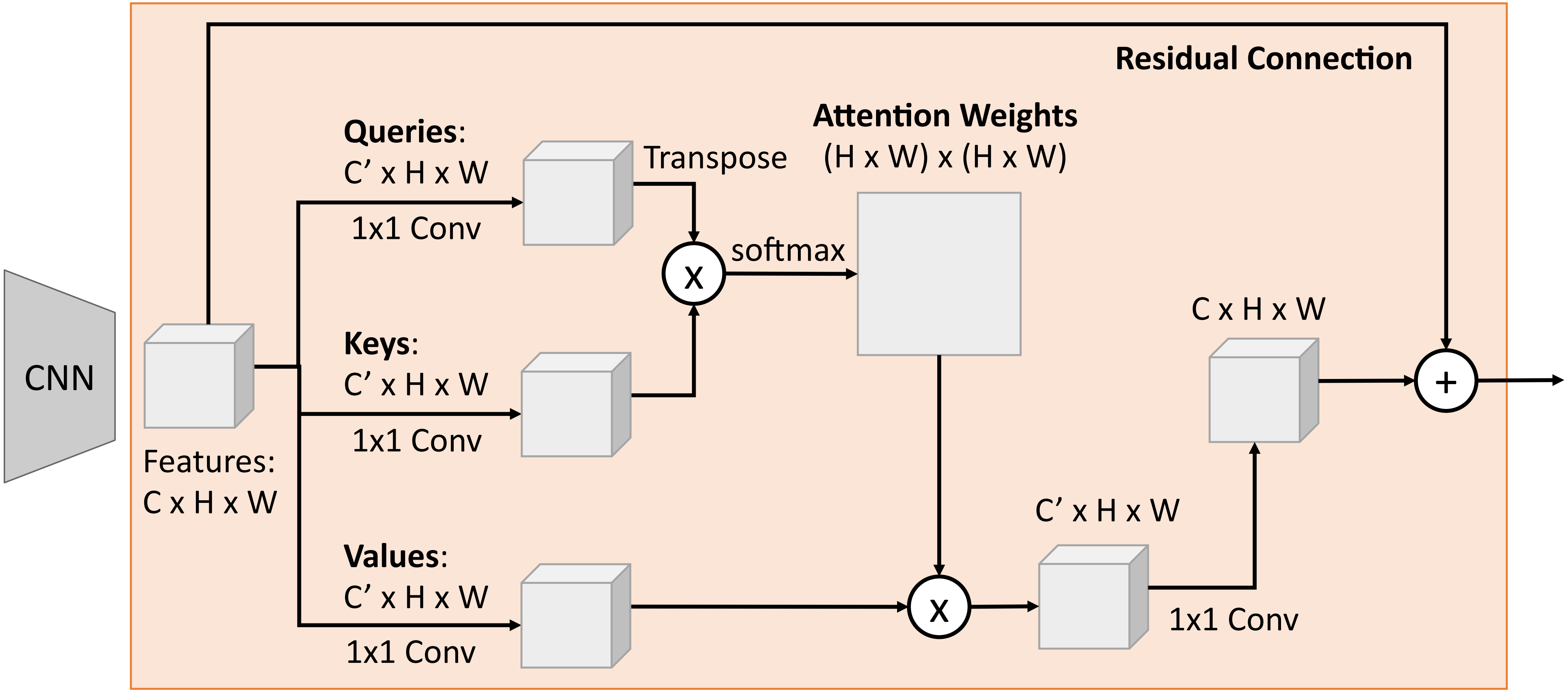


Zhang et al, “Self-Attention Generative Adversarial Networks”, ICML 2018

Example: CNN with Self-Attention

Input Image

Cat image is free to use under the Pixabay License

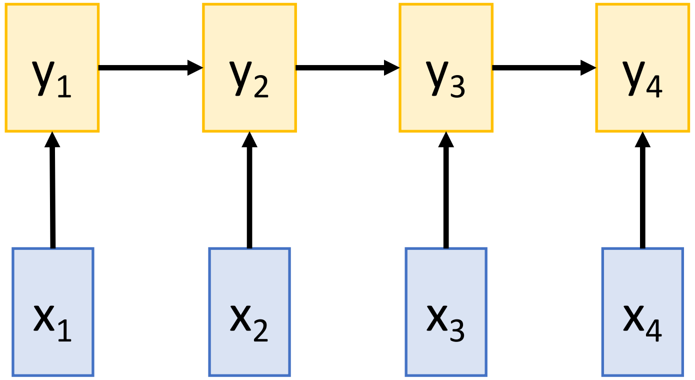


Self-Attention Module

Zhang et al, "Self-Attention Generative Adversarial Networks", ICML 2018

Three Ways of Processing Sequences

Recurrent Neural Network



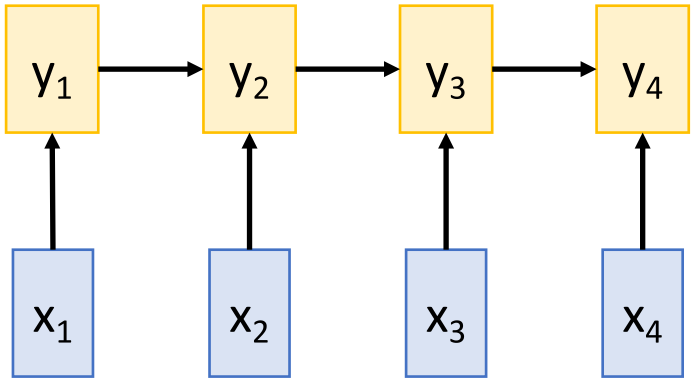
Works on **Ordered Sequences**

(+) 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

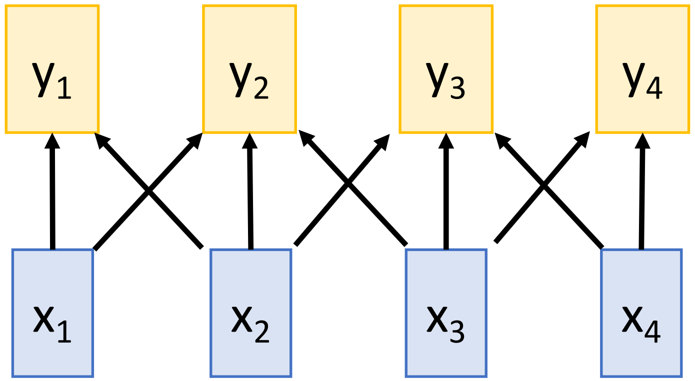


Works on **Ordered Sequences**

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

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

1D Convolution



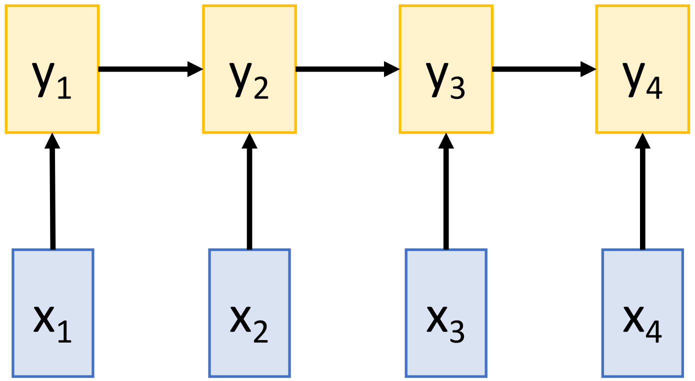
Works on **Multidimensional Grids**

(-) 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



Works on **Ordered Sequences**

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

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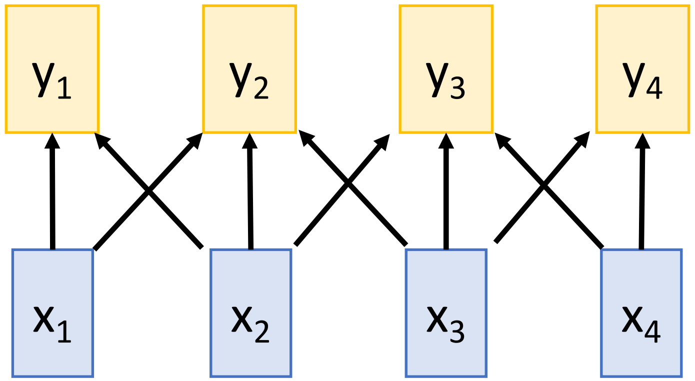
1D Convolution

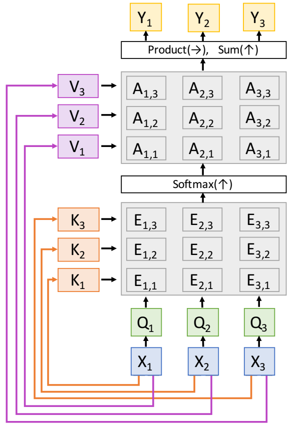


Works on **Multidimensional Grids**

(-) 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

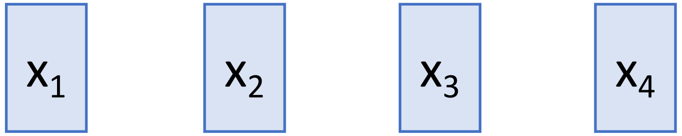
Vaswani et al, NeurIPS 2017

Works on **Ordered Sequences**
(+) Good at long sequences: After one RNN layer, h_T "sees" the whole sequence
(-) Not parallelizable: need to compute hidden states sequentially

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

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

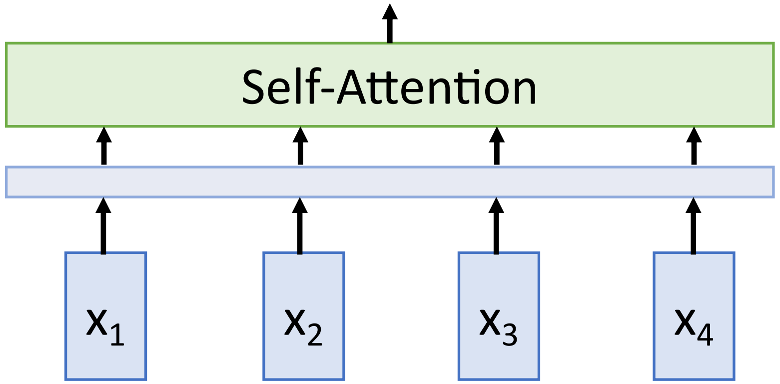
The Transformer



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

The Transformer

All vectors interact with each other

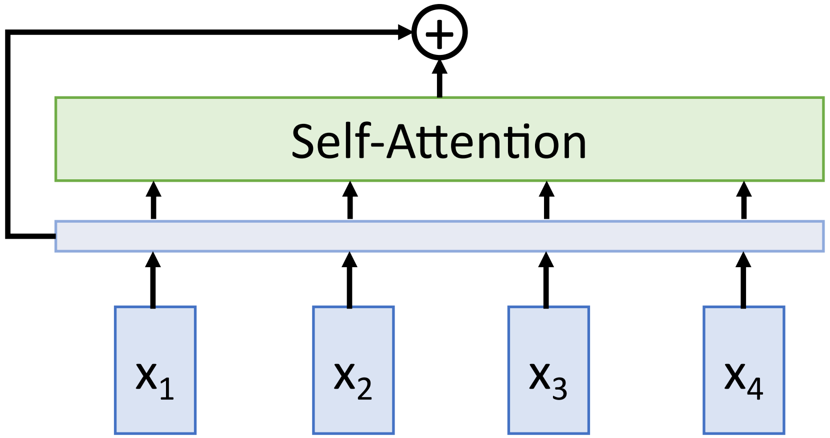


Vaswani et al, "Attention is all you need", NeurIPS 2017

The Transformer

Residual connection

All vectors interact with each other



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

The Transformer

Recall **Layer Normalization**:

Given $h_1, \ldots, h_N$ (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)

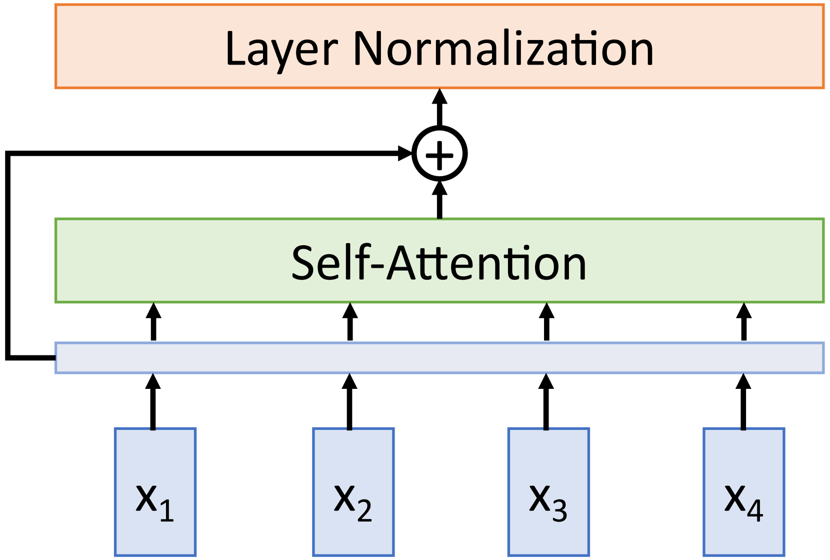
$z_i = (h_i - \mu_i) / \sigma_i$

$y_i = \gamma * z_i + \beta$

Ba et al, 2016

Residual connection

All vectors interact with each other



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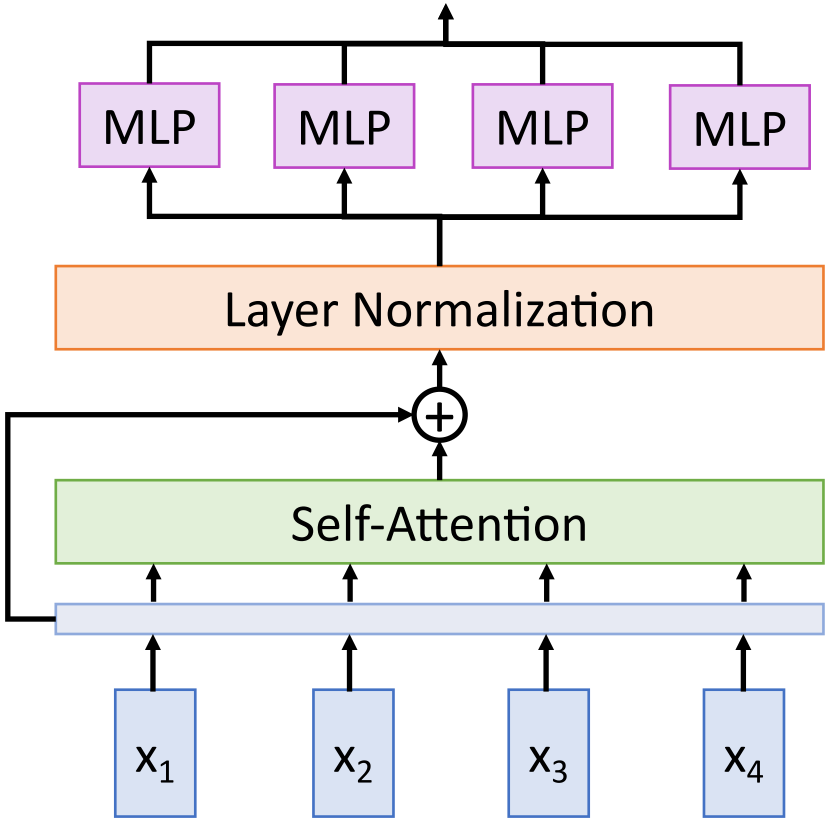
Ba et al, 2016

MLP independently on each vector

Residual connection

All vectors interact with each other



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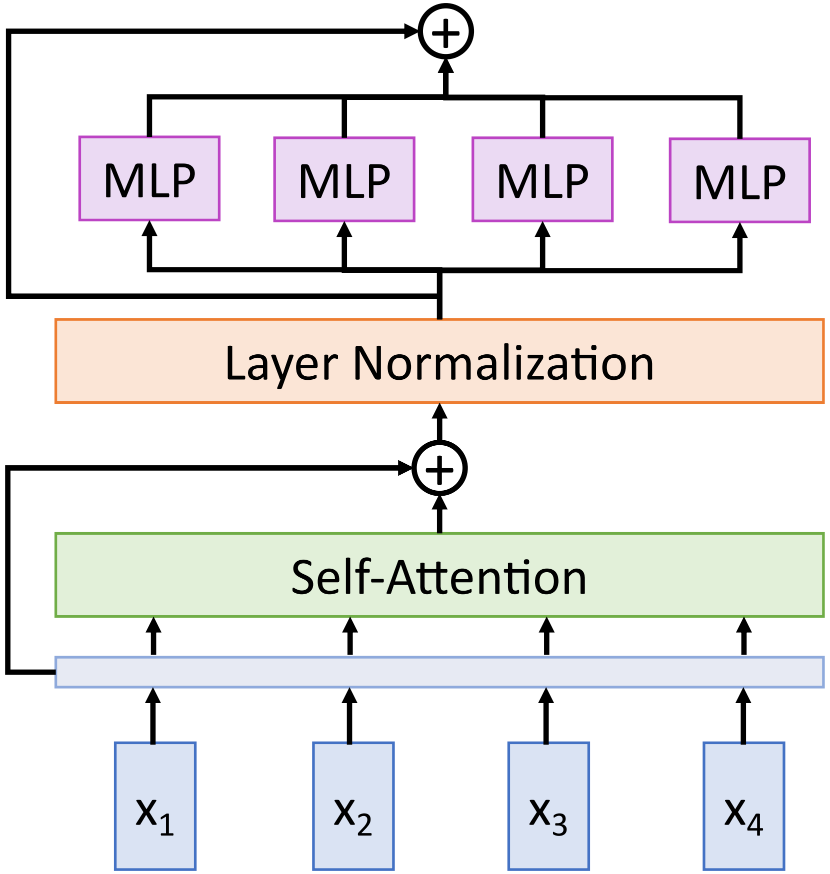

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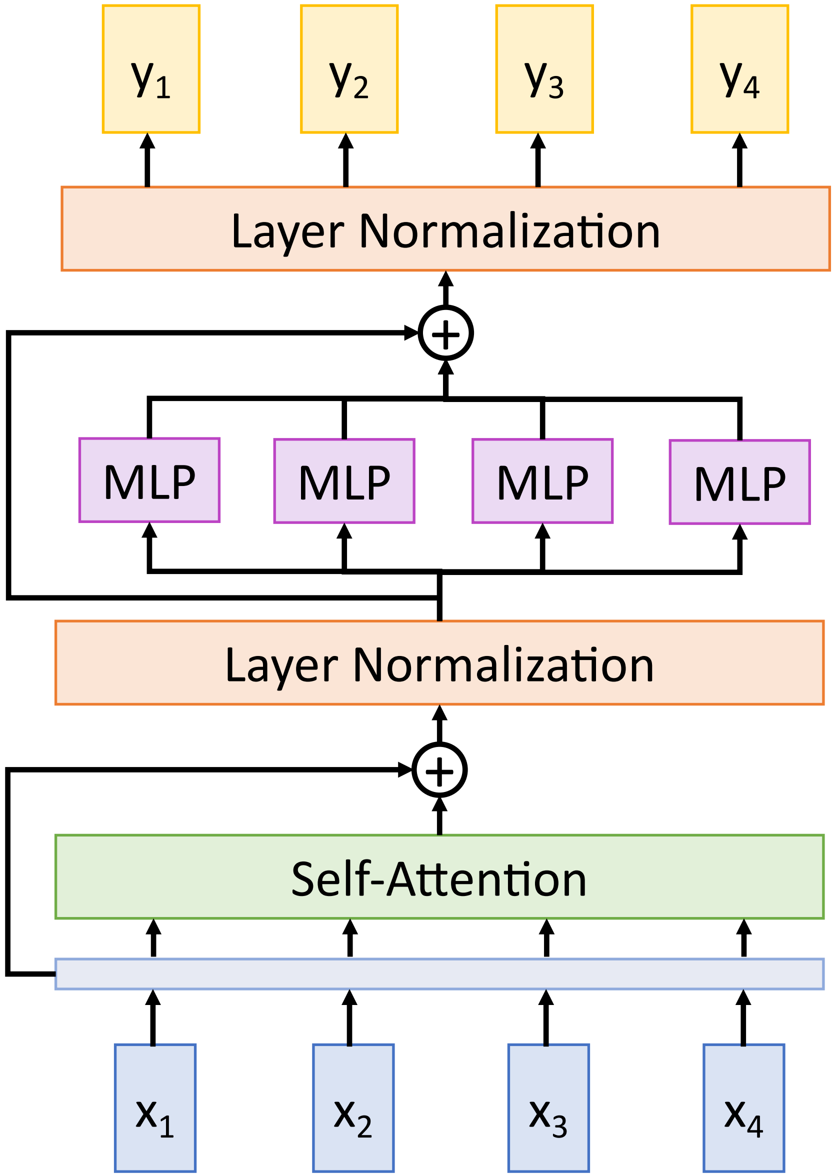


Vaswani et al, "Attention is all you need", NeurIPS 2017

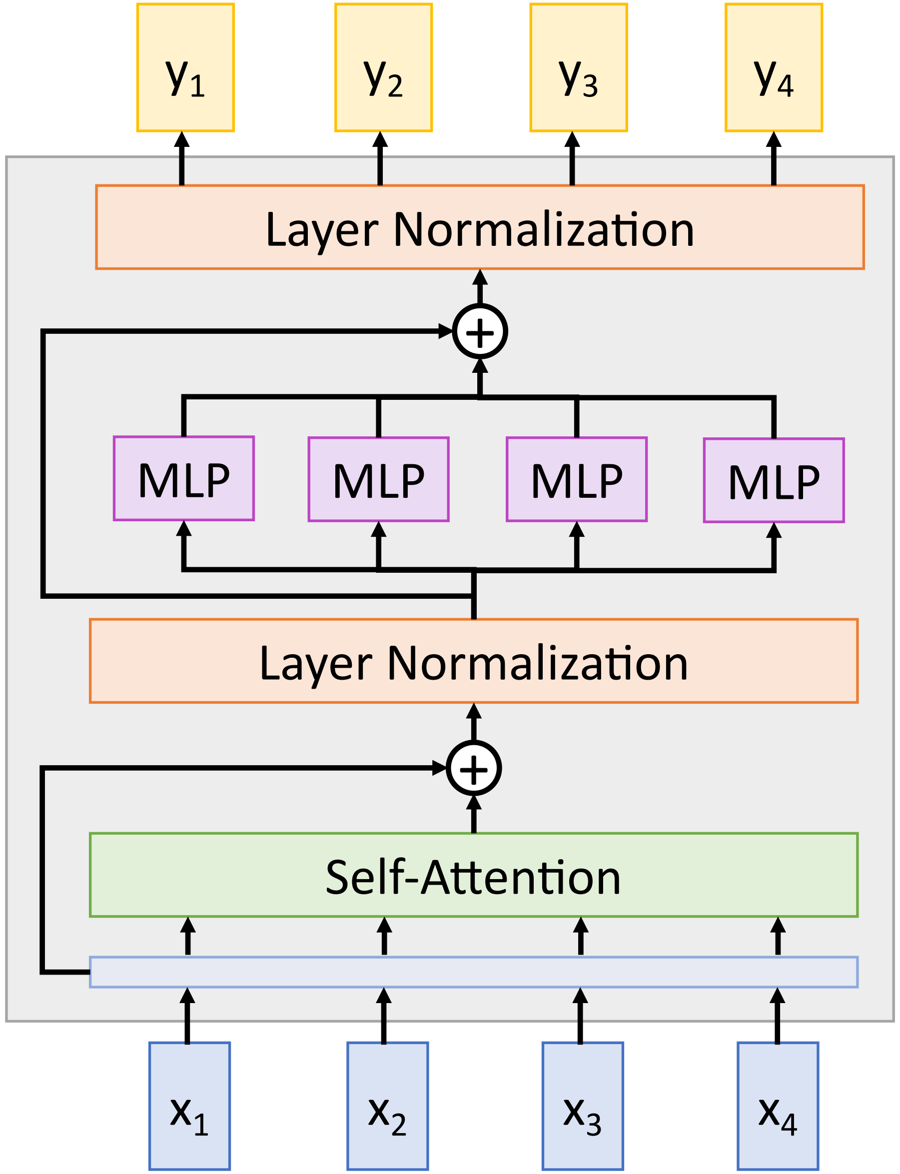
The Transformer

<u>**Transformer Block**</u>:
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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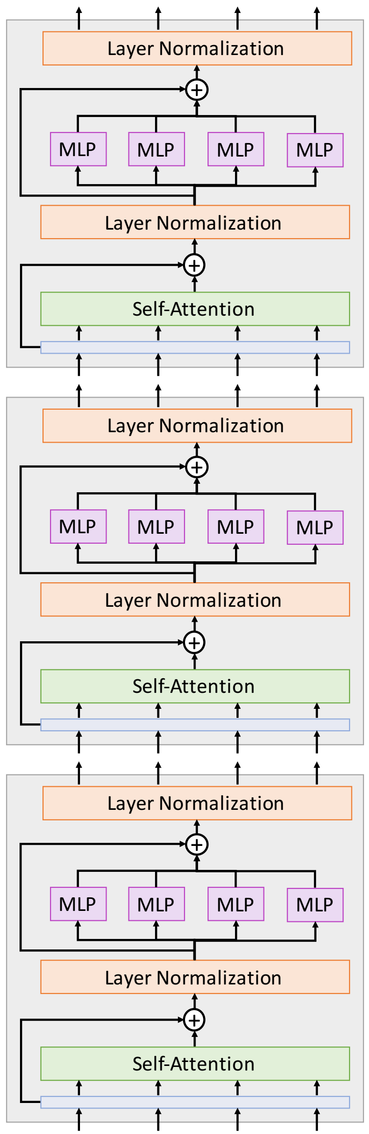
A **Transformer** is a sequence of transformer blocks

Vaswani et al:
12 blocks, D_Q=512, 6 heads



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

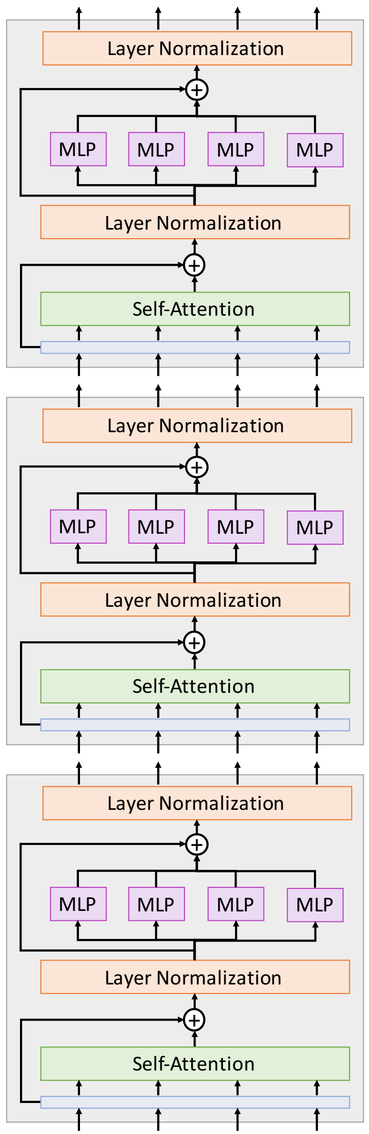
The Transformer: Transfer Learning

"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



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

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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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 Languge Models using Model Parallelism", 2019

Scaling up Transformers

~$430,000 on Amazon AWS!

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

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COMPLETION (Transformer-written): The scientist named the population, after their distinctive horn, Ovid's Unicorn. These four-horned, silver-white unicorns were previously unknown to science.

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.

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Try it yourself:

https://talktotransformer.com

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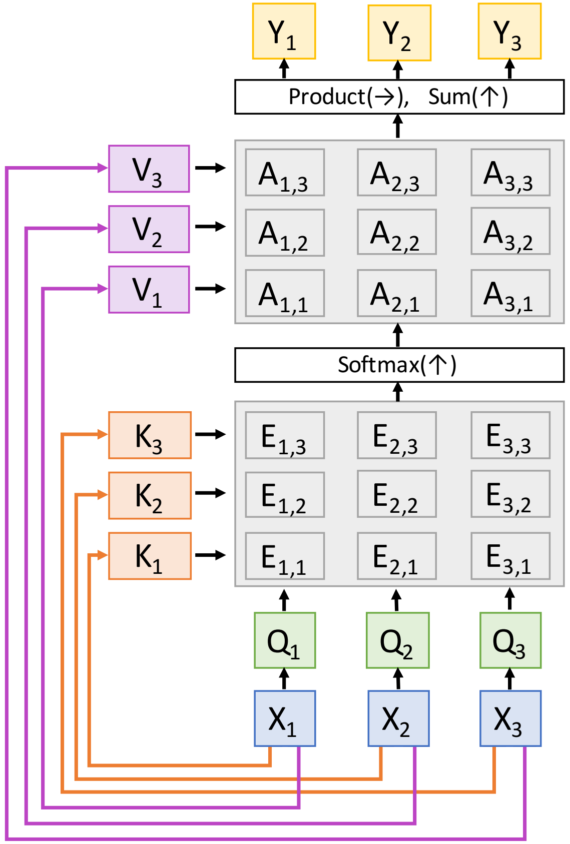
Summary

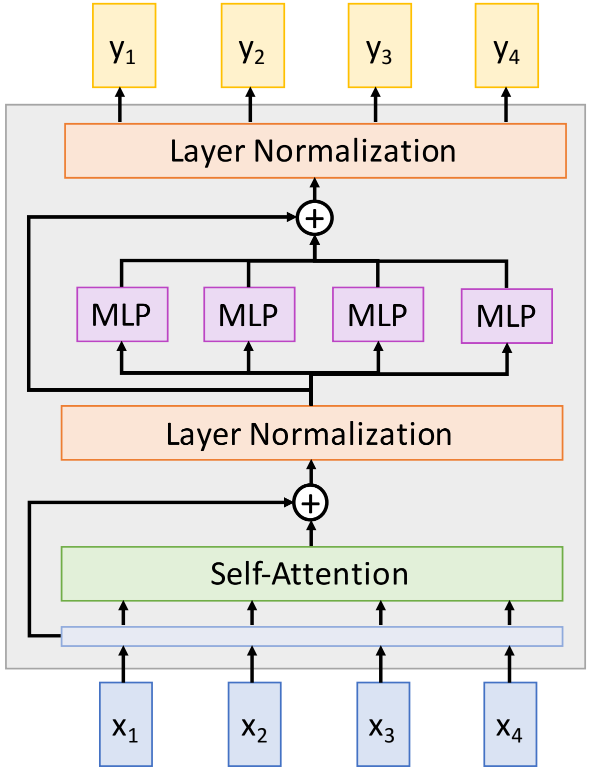
Adding **Attention** to RNN models lets them look at different parts of the input at each timestep

A dog is standing on a hardwood floor.

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



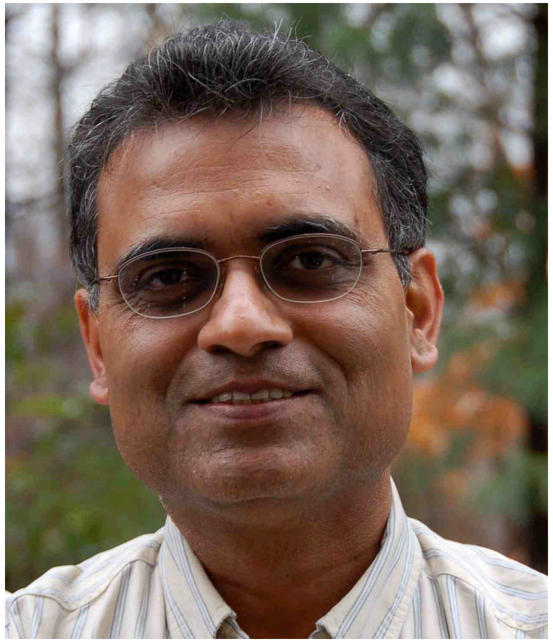
Transformers are a new neural network model that only uses attention



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

Next Week: Guest Lectures

Monday 10/28
Luowei Zhou
Vision and Language



Wednesday 10/30
Prof. Atul Prakash
Adversarial Machine Learning