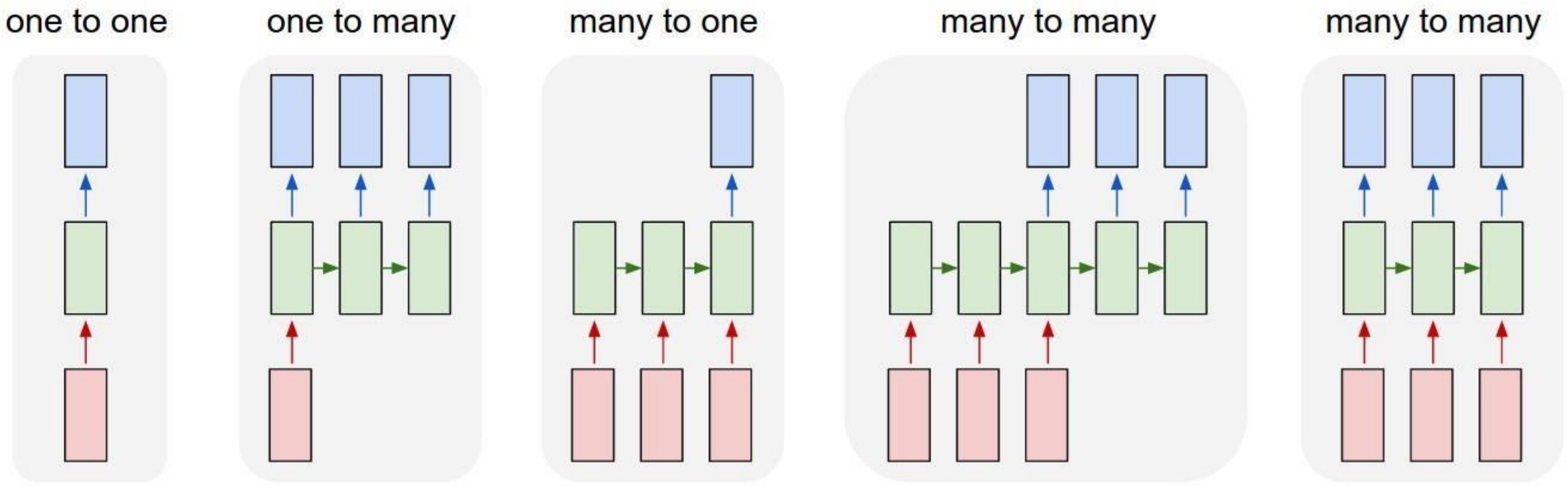
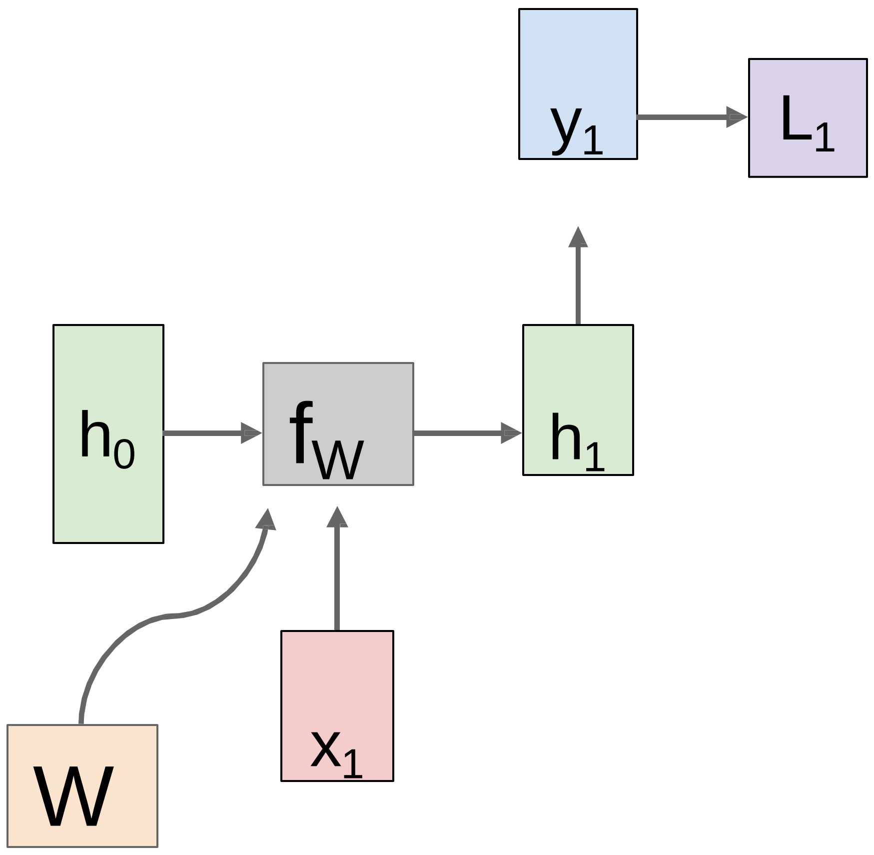
Transformer

Dr. Trần Vũ Hoàng

Last Time: Recurrent Neural Networks



Last Time: Variable length computation graph with shared weights



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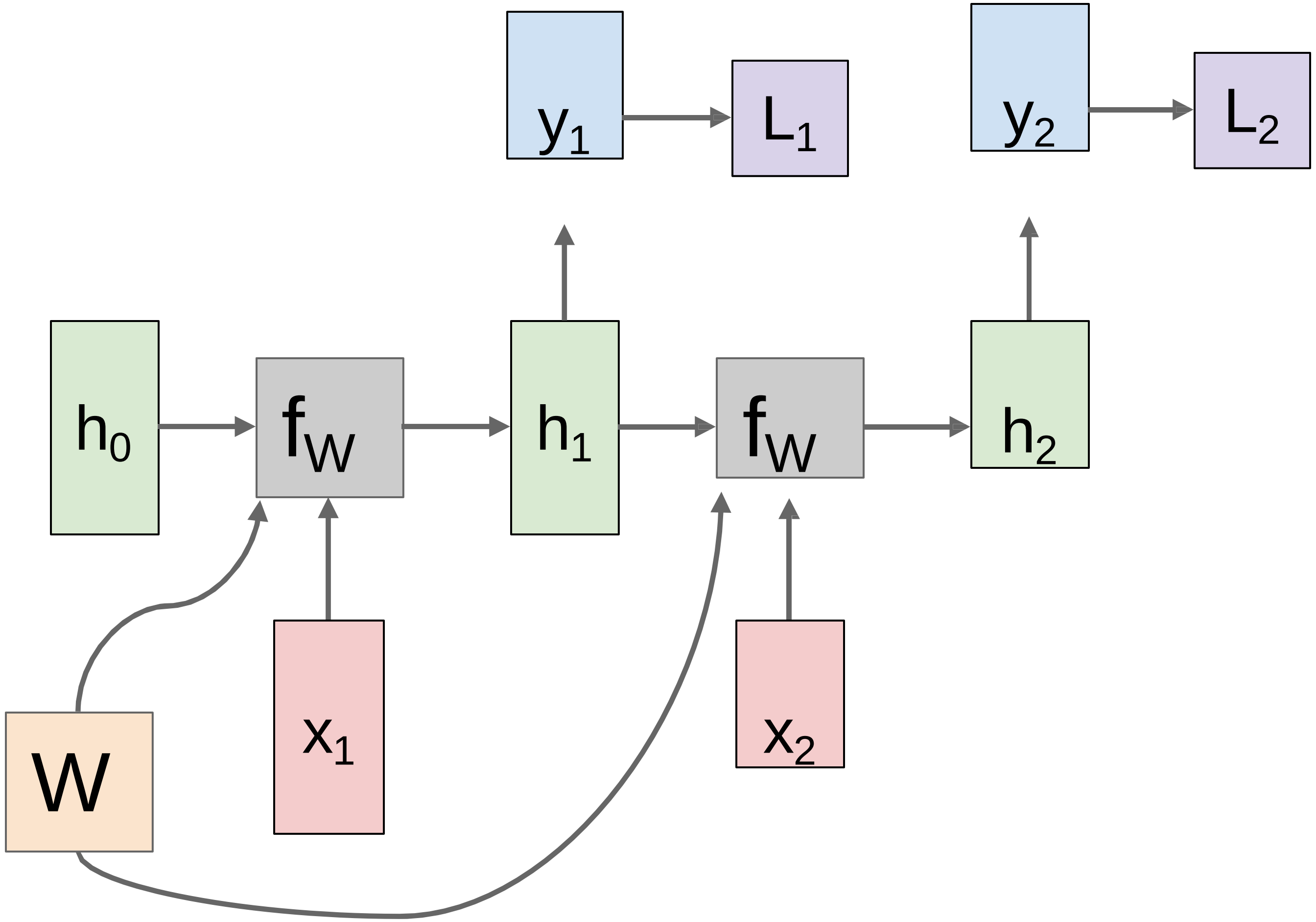
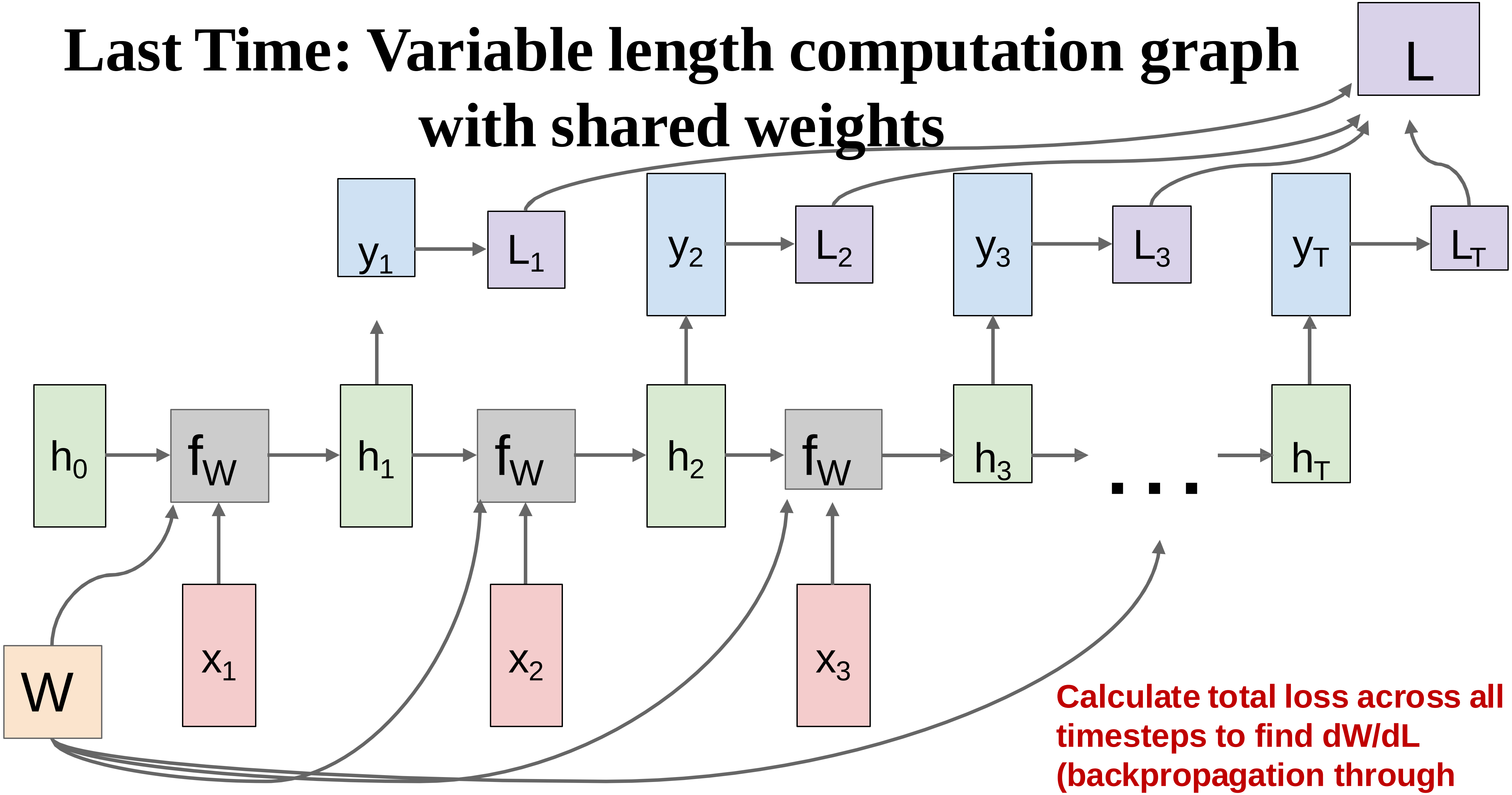


W is reused (recurrently)!

Last Time: Variable length computation graph with shared weights



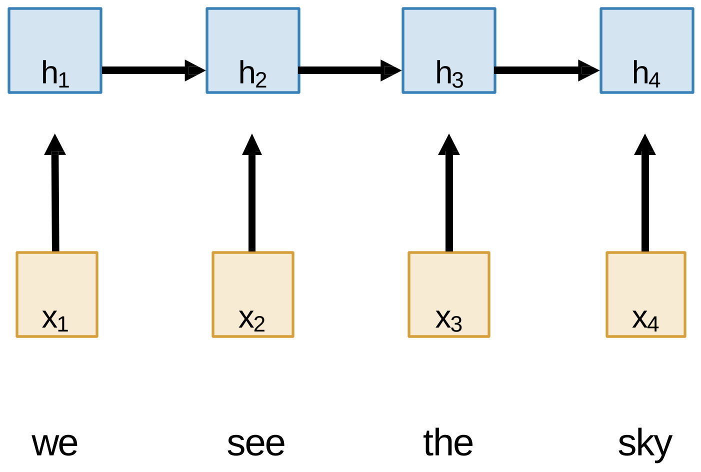
Calculate total loss across all timesteps to find dW/dL (backpropagation through time)!

Sequence to Sequence with RNNs: Encoder - Decoder

Input: Sequence $x_1, \dots x_T$
Output: Sequence $y_1, \dots, y_{T'}$

A motivating example for today's discussion – machine translation! English → Italian

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



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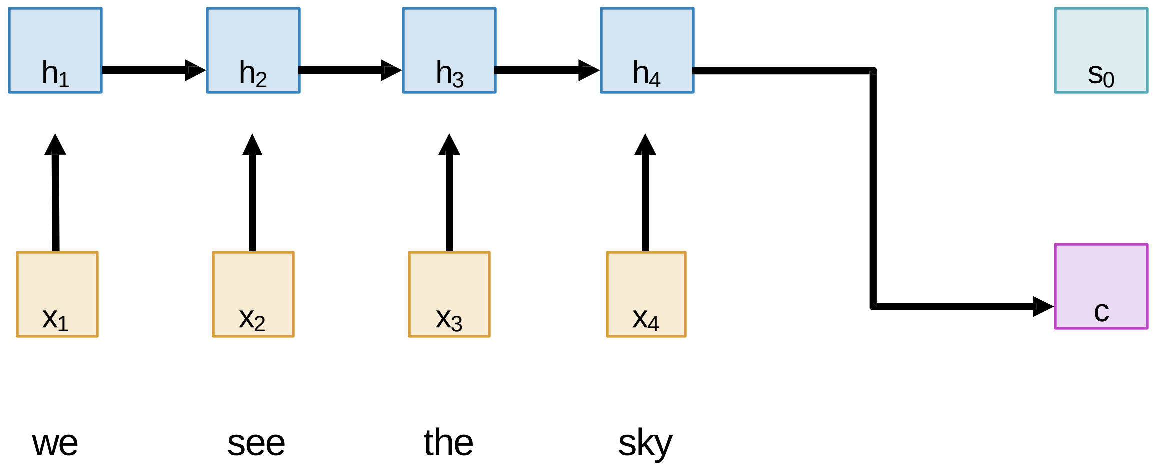
From final hidden state predict:
Initial decoder state s_0
Context vector c (often $c=h_T$)



Sequence to Sequence with RNNs

Input: Sequence $x_1, \ldots x_T$
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Decoder: $s_t = g_U(y_{t-1}, s_{t-1}, c)$

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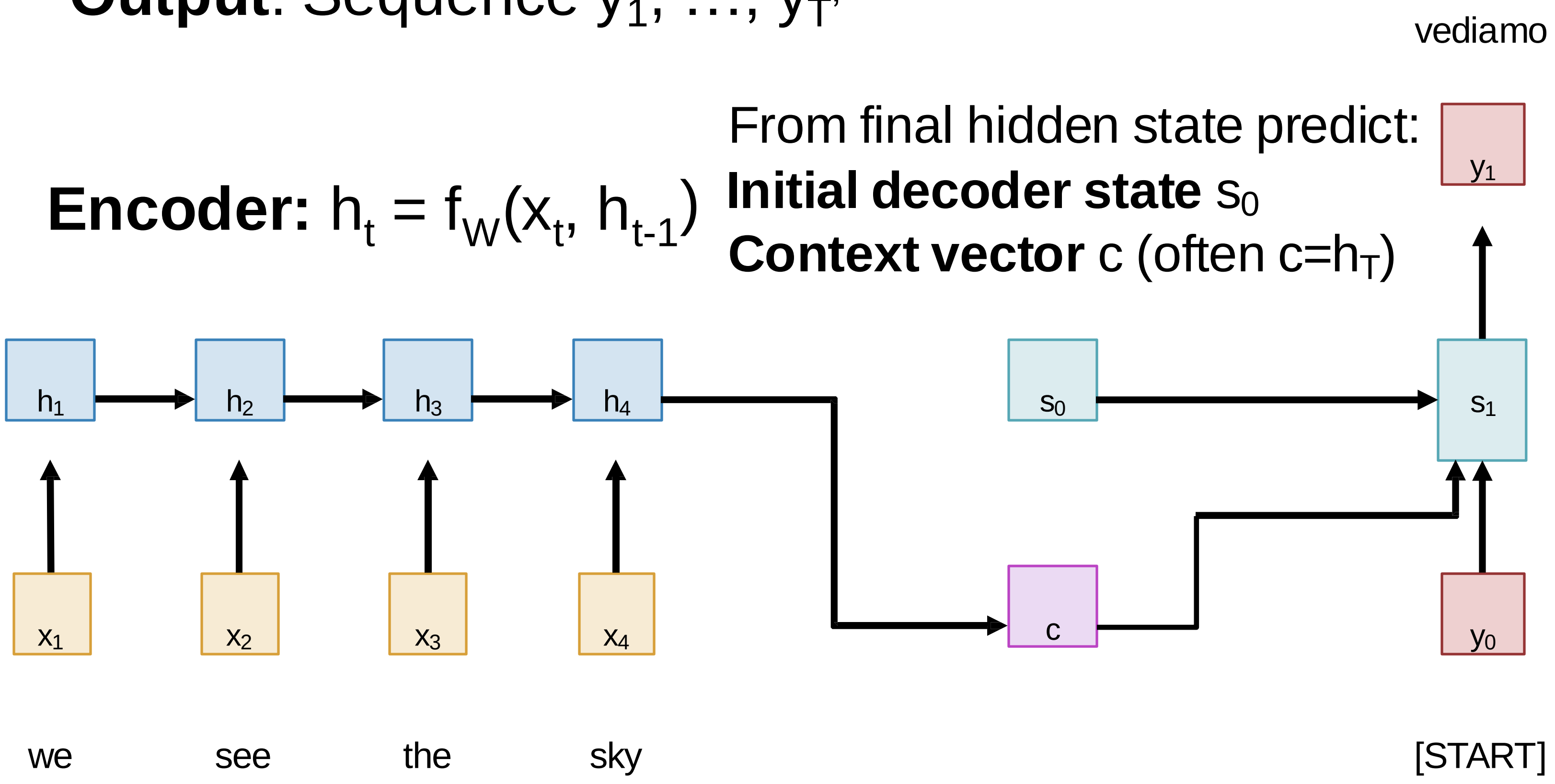

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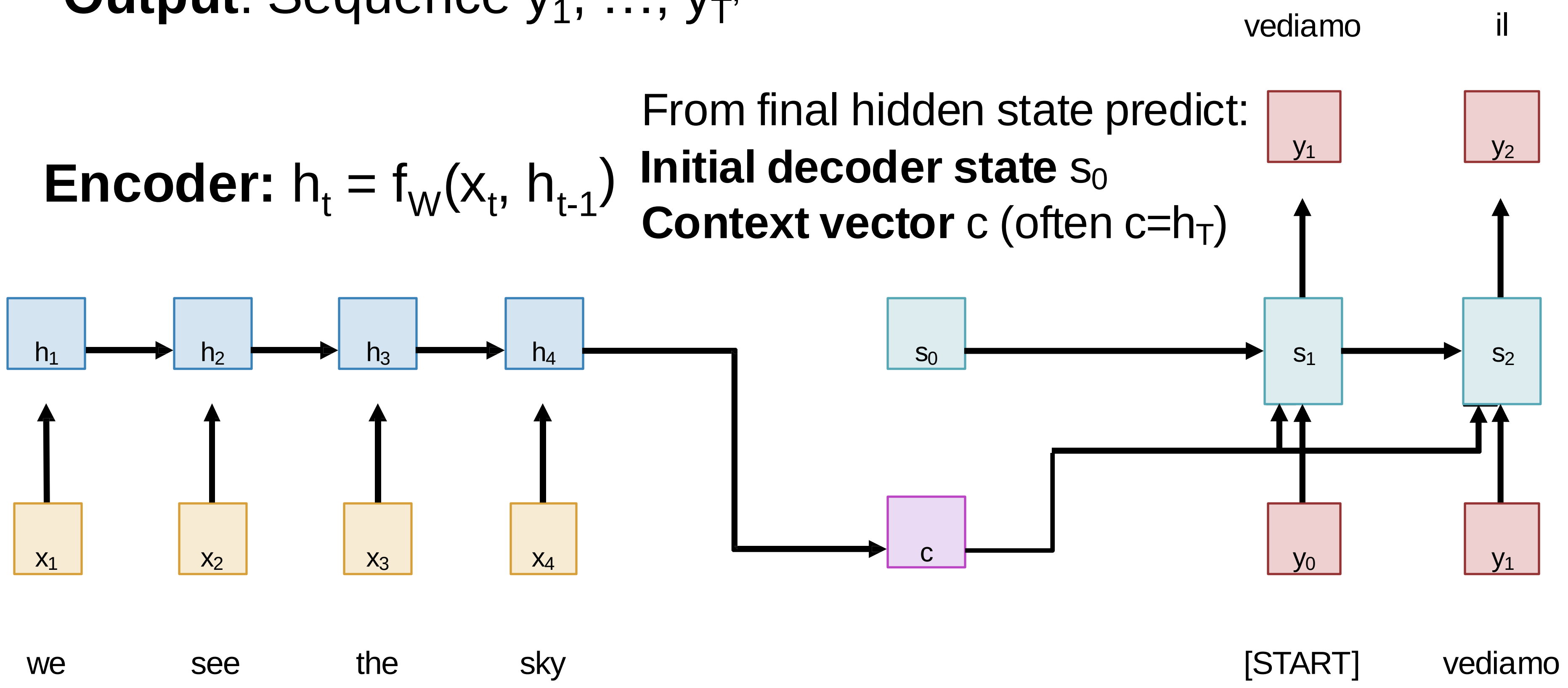

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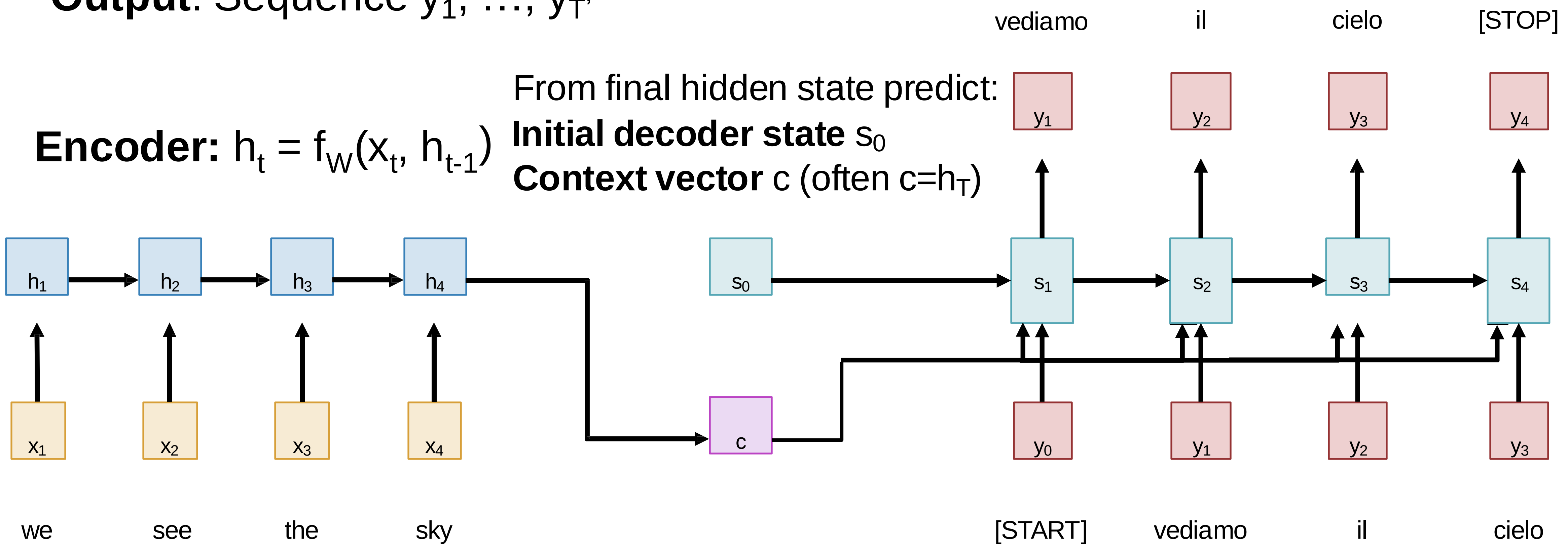


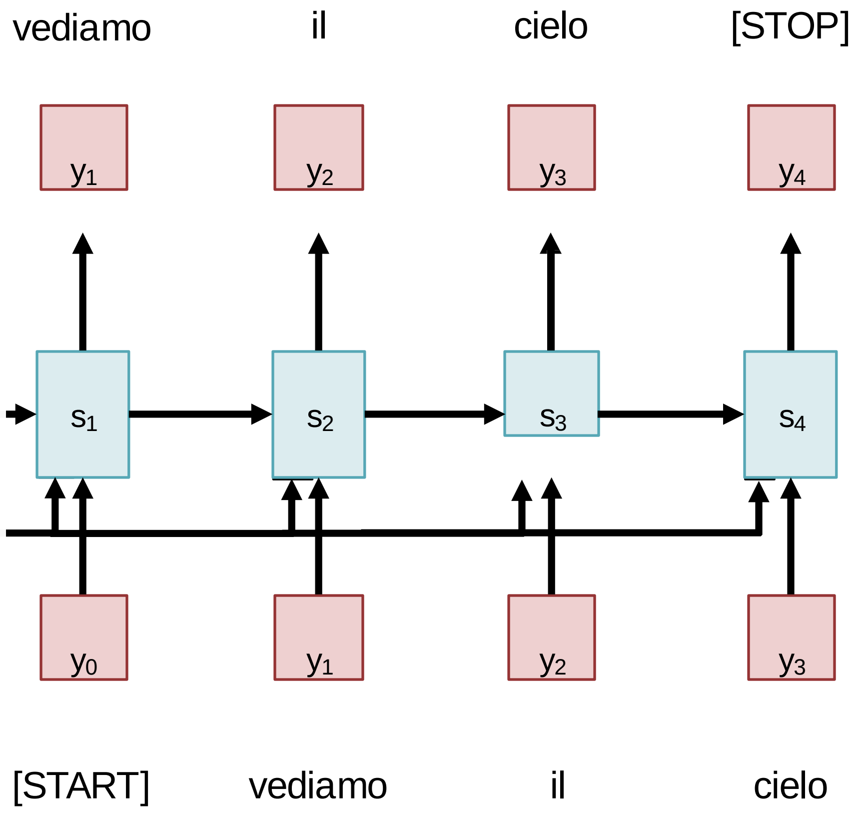
Sequence to Sequence with RNNs

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

Remember:

During Training:
Often, we use the "correct" token even if the model is wrong. Called **teacher forcing**

During Test-time:
We sample from the model's outputs until we sample [STOP]



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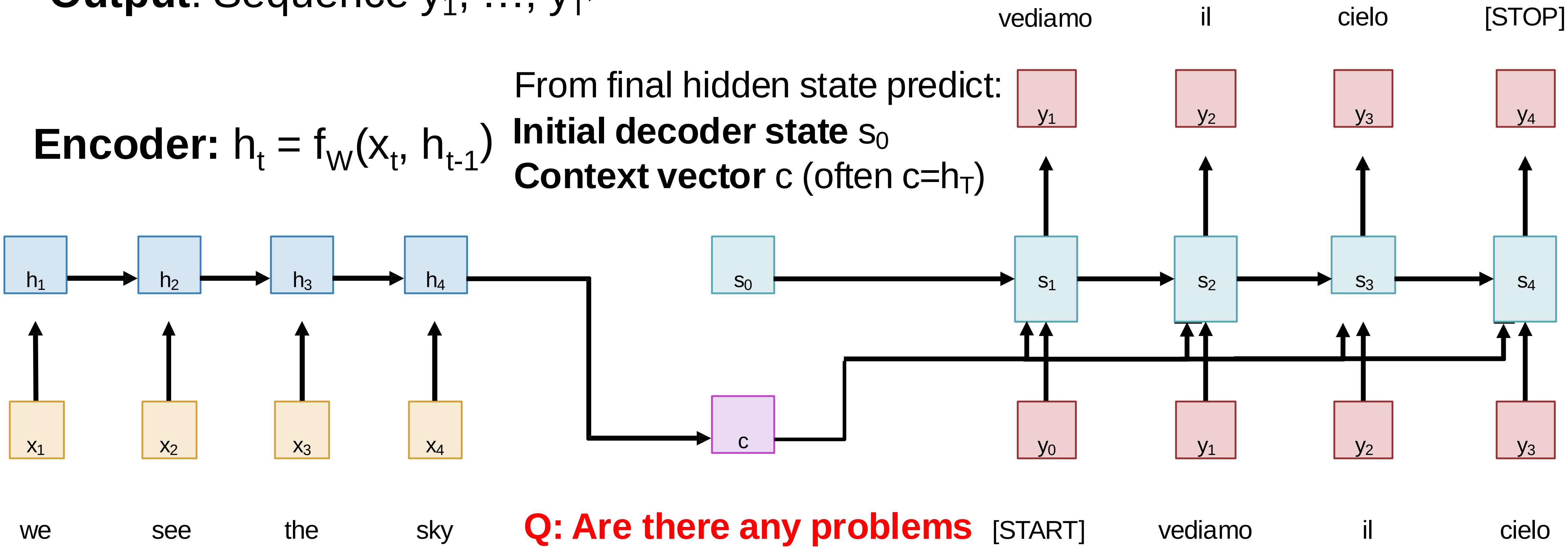

Q: Are there any problems with using C like this??

Sequence to Sequence with RNNs

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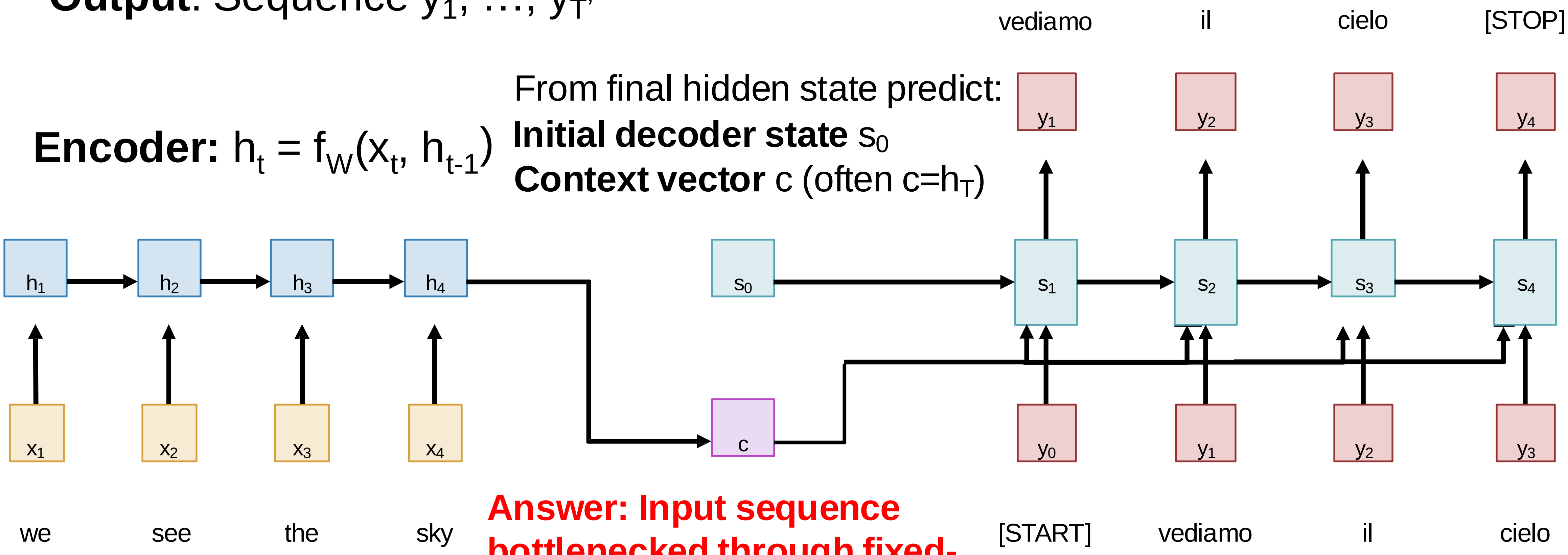

Answer: Input sequence bottlenecked through fixed-sized vector. What if T=1000?

Sequence to Sequence with RNNs

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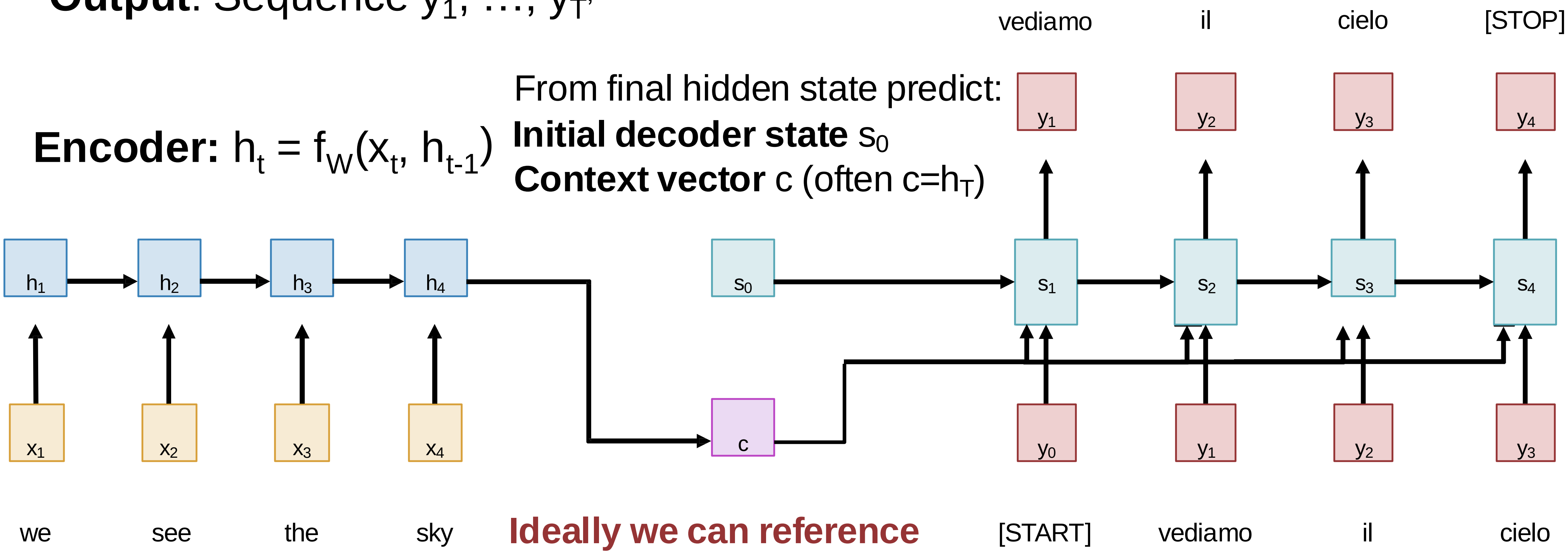

Ideally we can reference the inputs as we decode…

Sequence to Sequence with RNNs and Attention

Input: Sequence $x_1, \ldots x_T$

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

From final hidden state:
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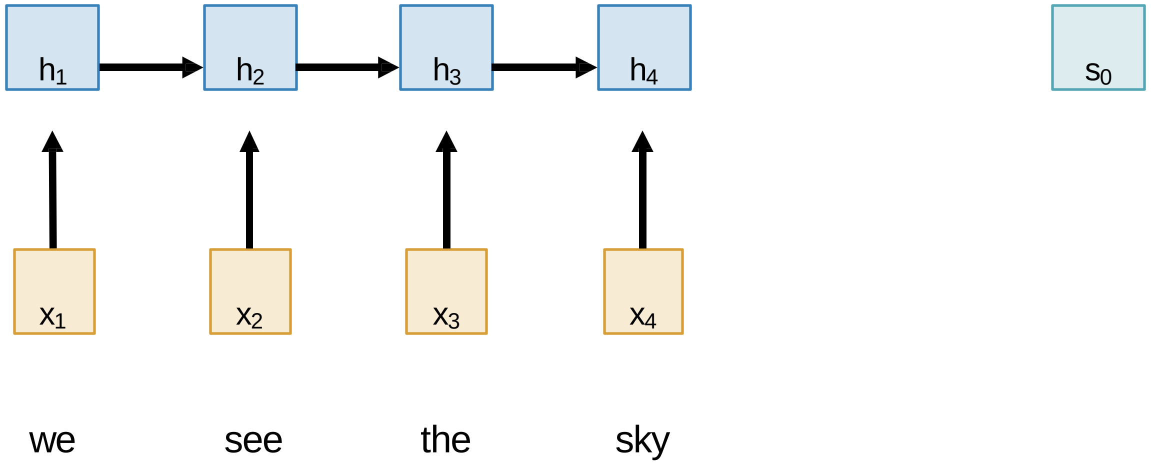
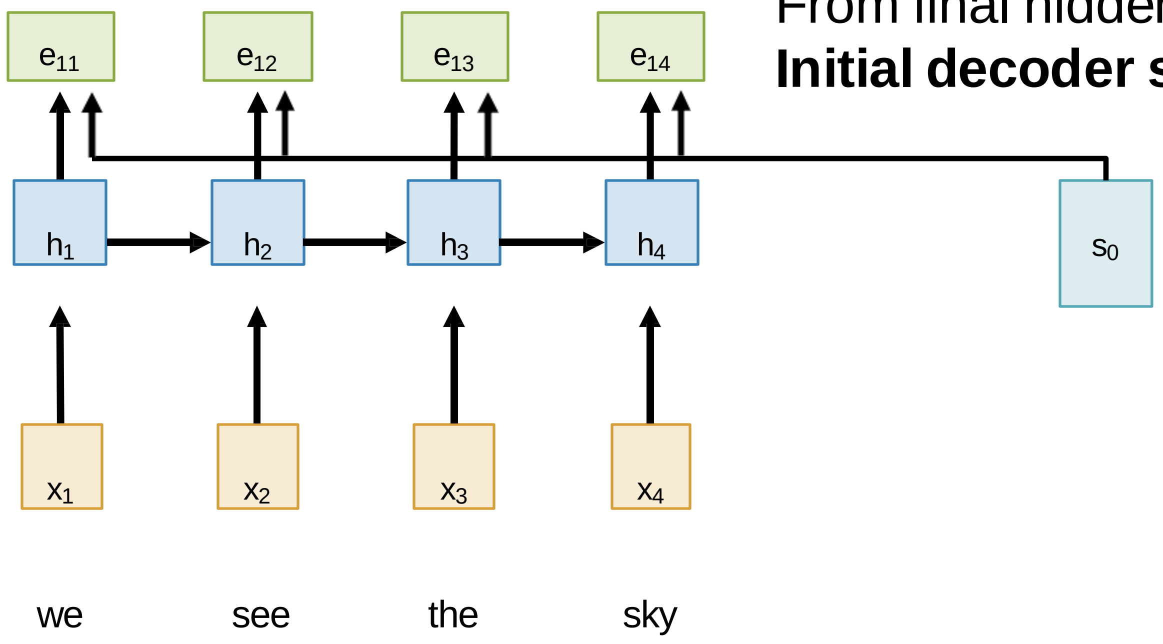


Sequence to Sequence with RNNs and Attention

Compute (scalar) **alignment scores**

$e_{t,i} = f_{att}(s_{t-1}, h_i)$ (f_{att} is a Linear Layer)



From final hidden state:
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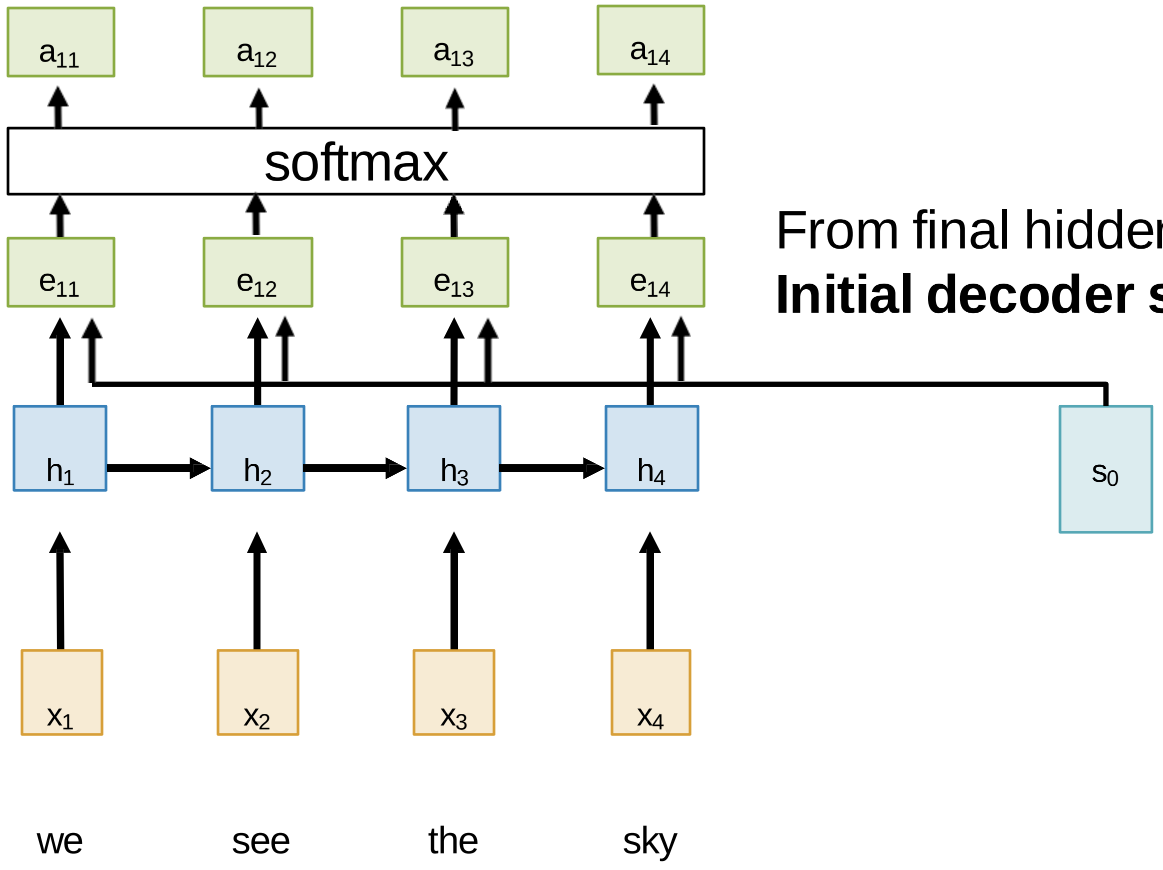
Sequence to Sequence with RNNs and Attention



From final hidden state:
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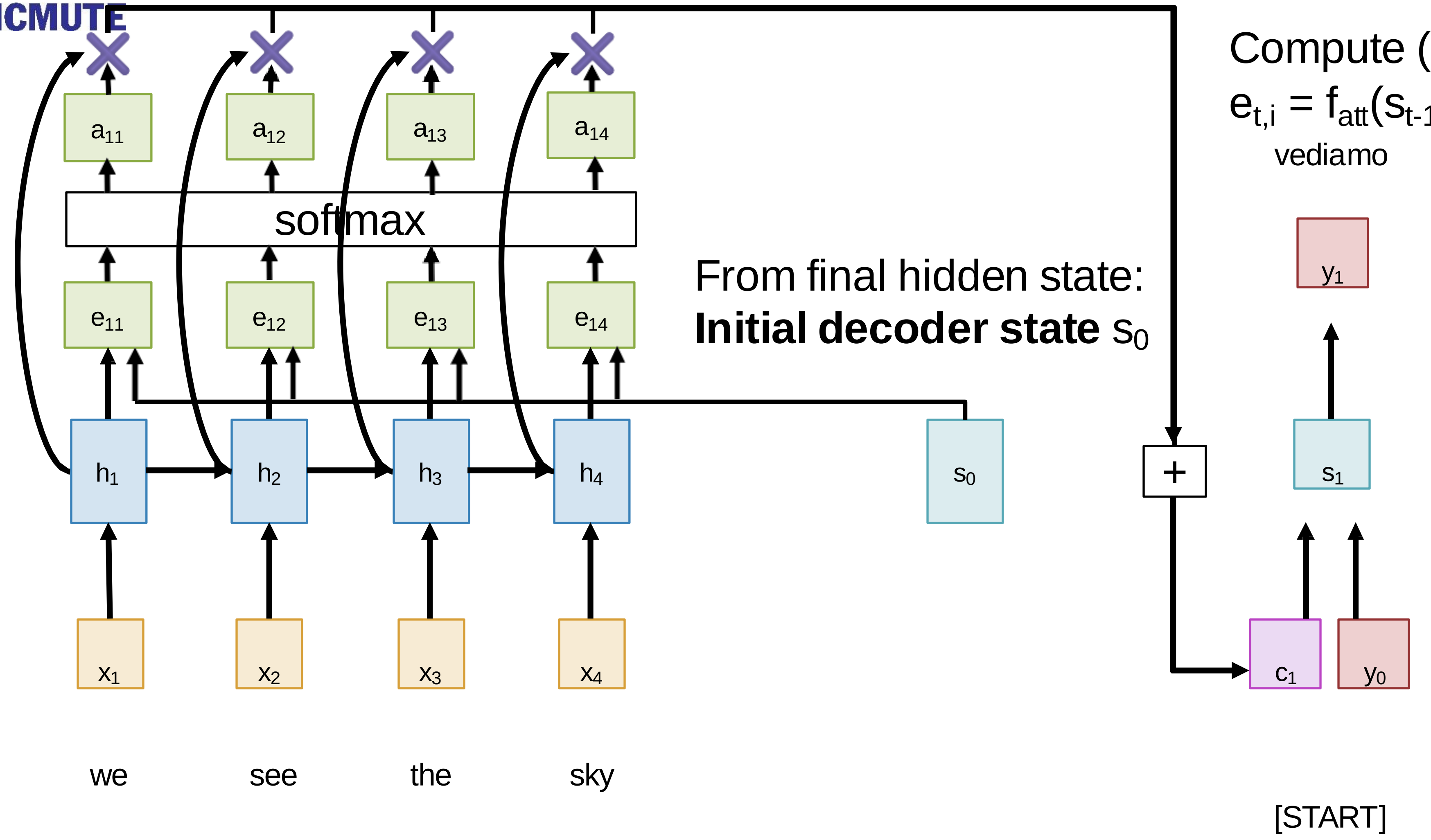
Compute (scalar) **alignment scores**
$e_{t,i} = f_{att}(s_{t-1}, h_i)$ (f_{att} is a Linear Layer)

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

Sequence to Sequence with RNNs and Attention



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

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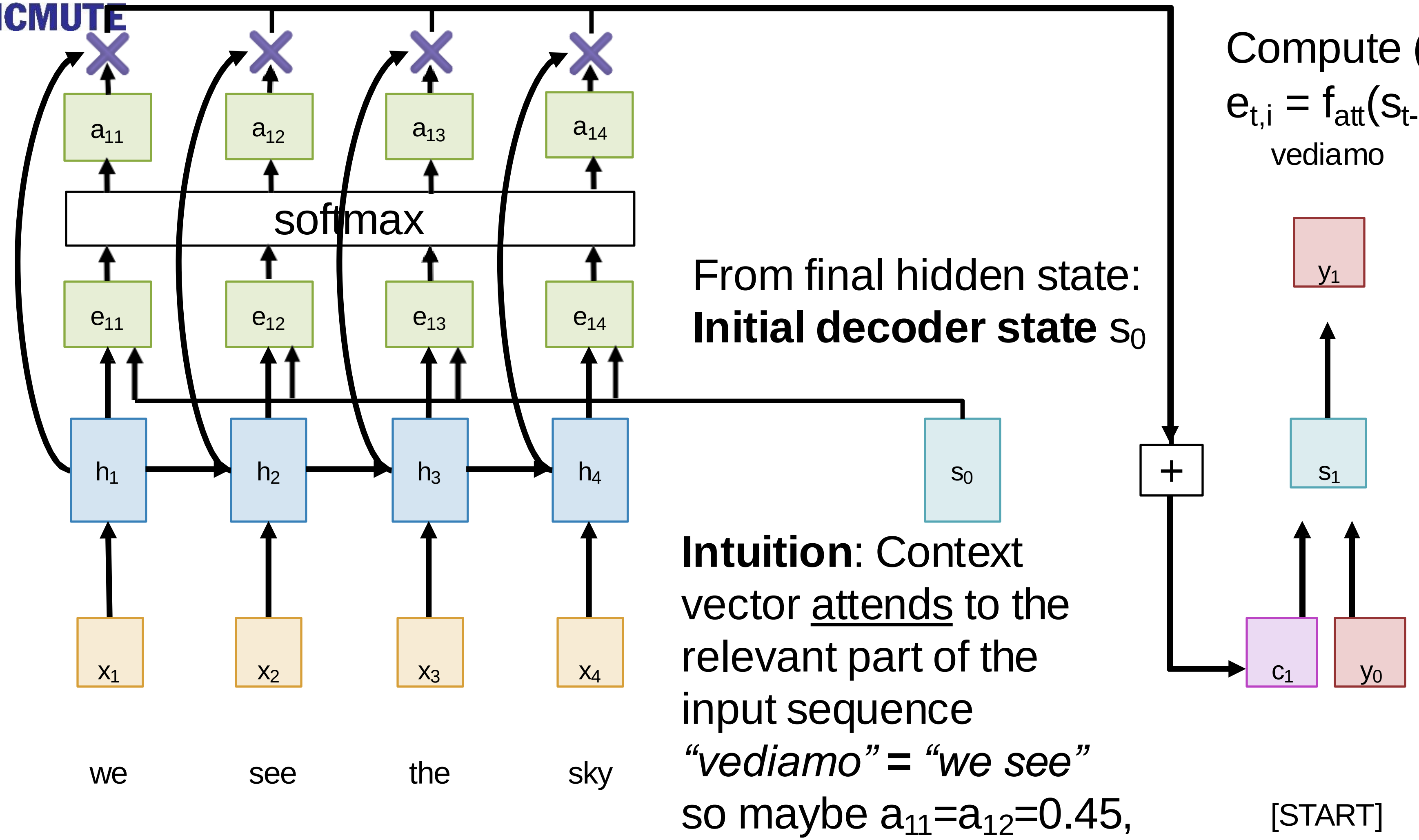
Compute context vector as **weighted sum of hidden states**

$c_t = \sum_i a_{t,i} h_i$

Sequence to Sequence with RNNs and Attention



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

Intuition: Context vector attends to the relevant part of the input sequence

"vediamo" **=** *"we see"*

so maybe $a_{11}=a_{12}=0.45$, $a_{13}=a_{14}=0.05$

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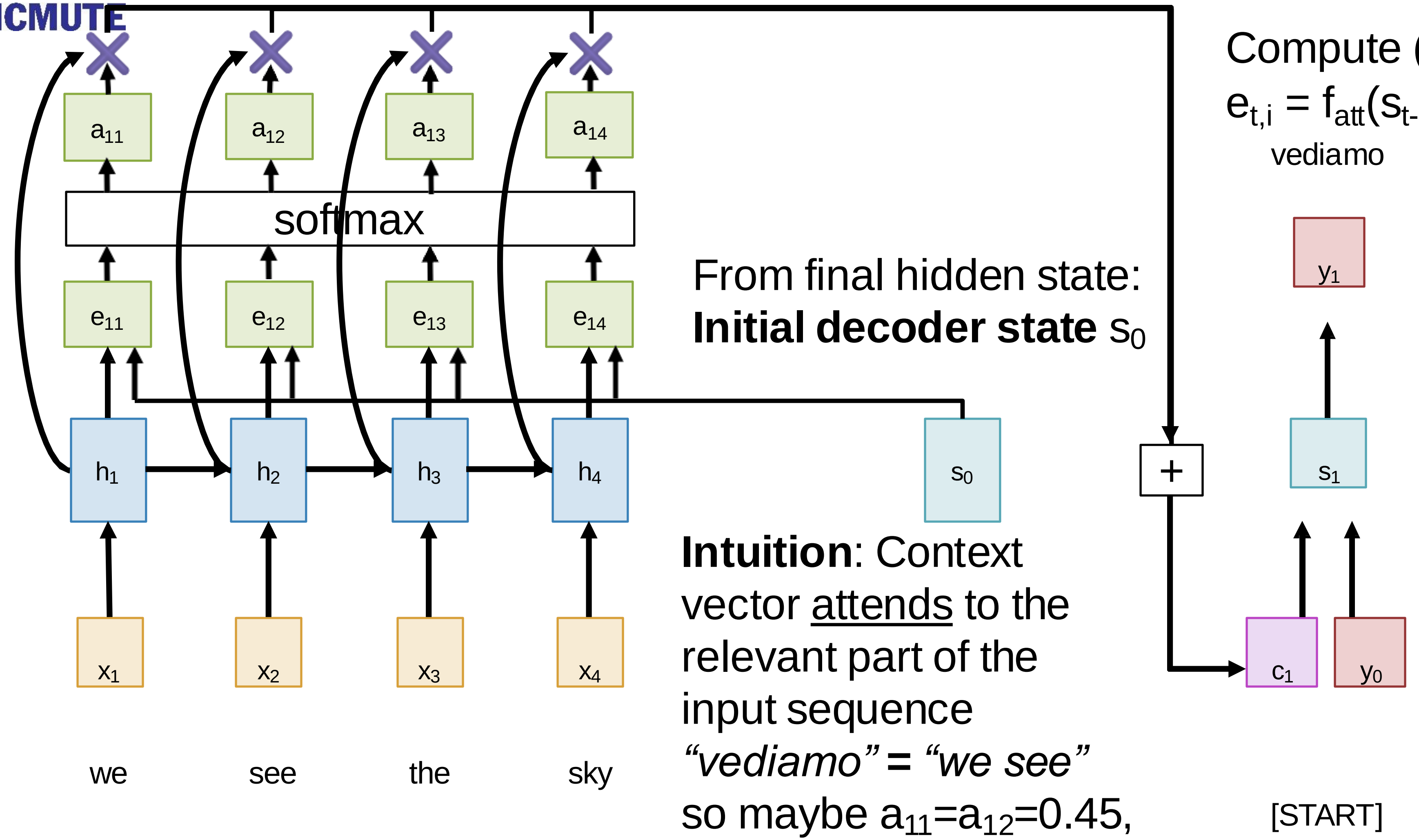
Compute **context vector** as weighted sum of hidden states

$c_t = \sum_i a_{t,i} h_i$

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

Sequence to Sequence with RNNs and Attention



Compute (scalar) **alignment scores**

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

Normalize alignment scores to get **attention weights**

$0 < a_{t,i} < 1$ $\sum_i a_{t,i} = 1$

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$c_t = \sum_i a_{t,i} h_i$

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

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"vediamo" = *"we see"*

so maybe $a_{11}=a_{12}=0.45$, $a_{13}=a_{14}=0.05$

This is all differentiable! No supervision on attention weights – backprop through everything

Sequence to Sequence with RNNs and Attention

Repeat: Use s_1 to compute new context vector c_2

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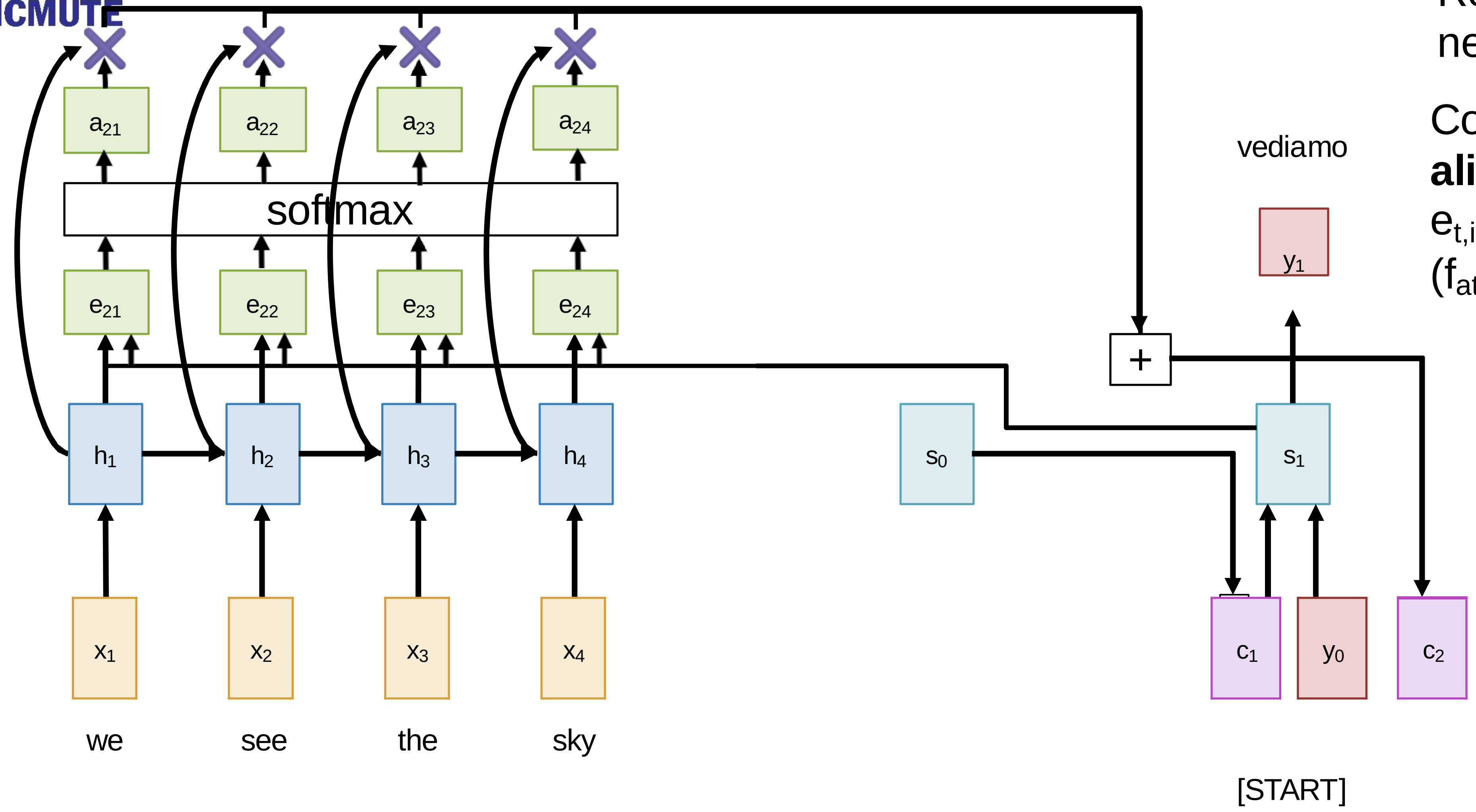

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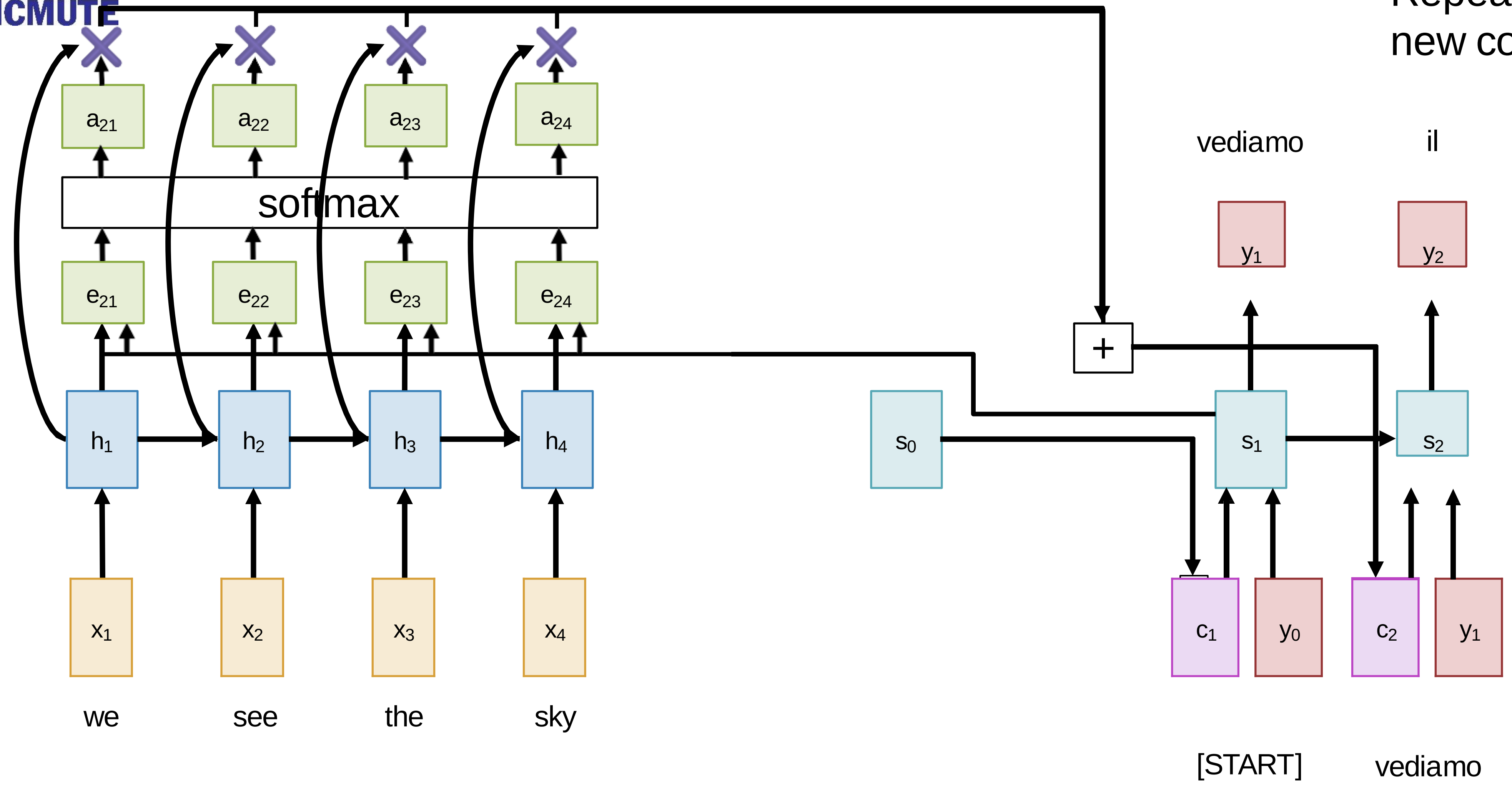

Use context vector in decoder: $s_t = g_U(y_{t-1}, s_{t-1}, c_t)$

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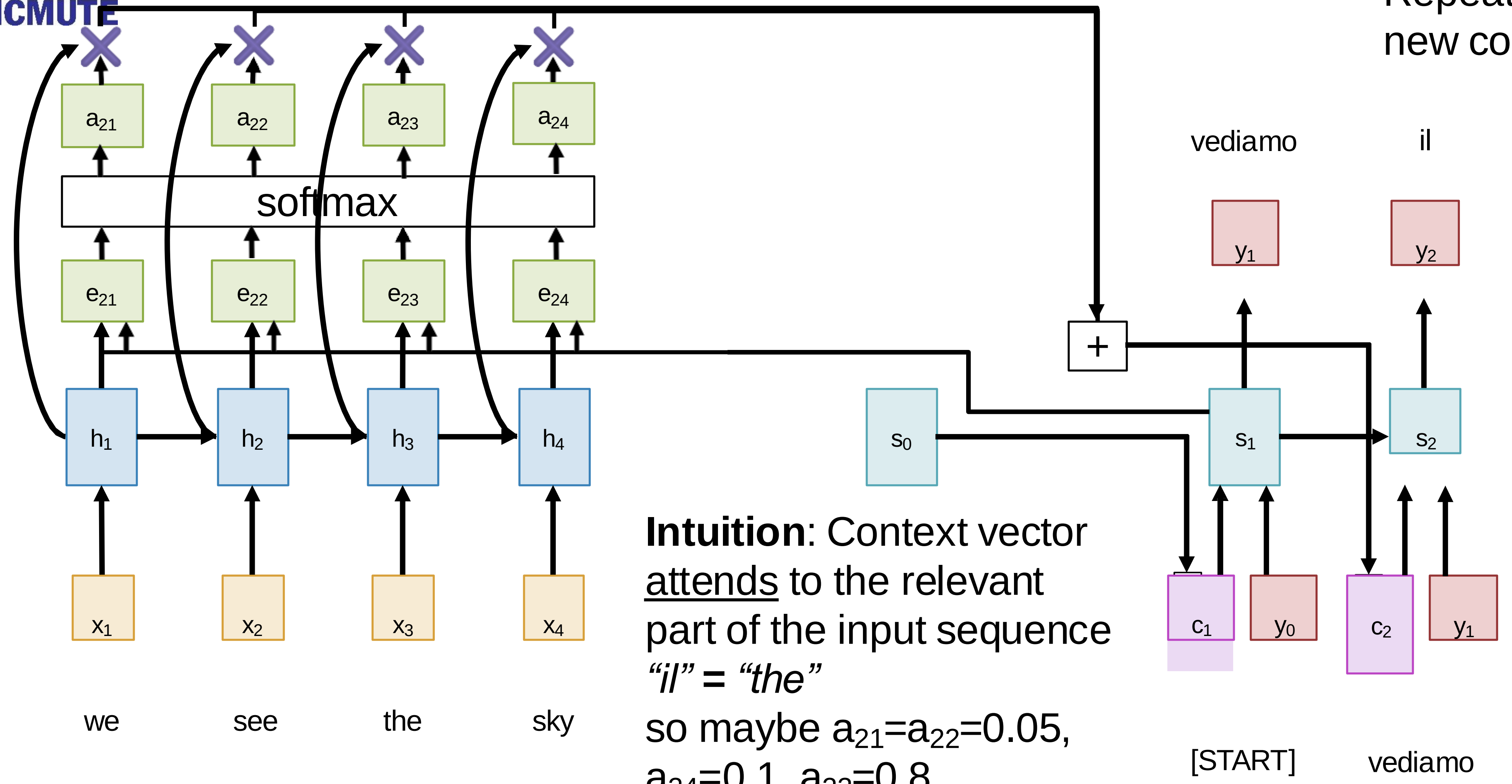

Use context vector in decoder: $s_t = g_U(y_{t-1}, s_{t-1}, c_t)$

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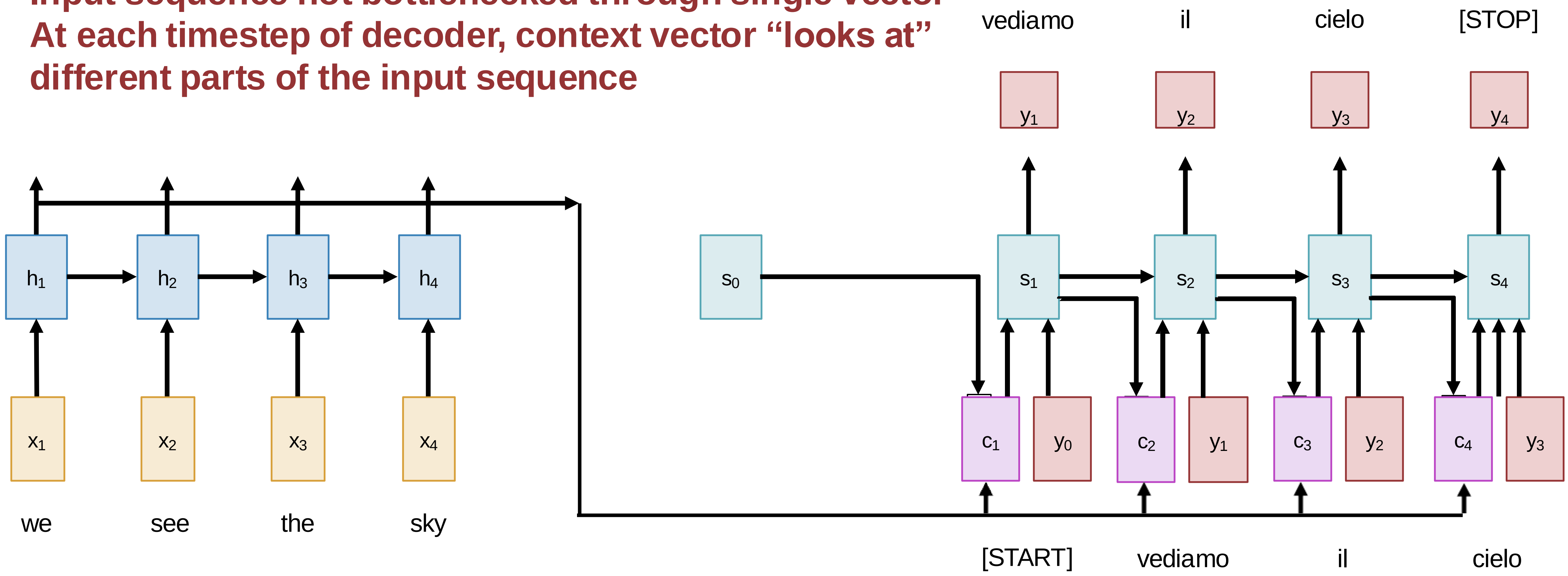
"il" = "the"

so maybe $a_{21}=a_{22}=0.05$, $a_{24}=0.1$, $a_{23}=0.8$

Sequence to Sequence with RNNs and Attention

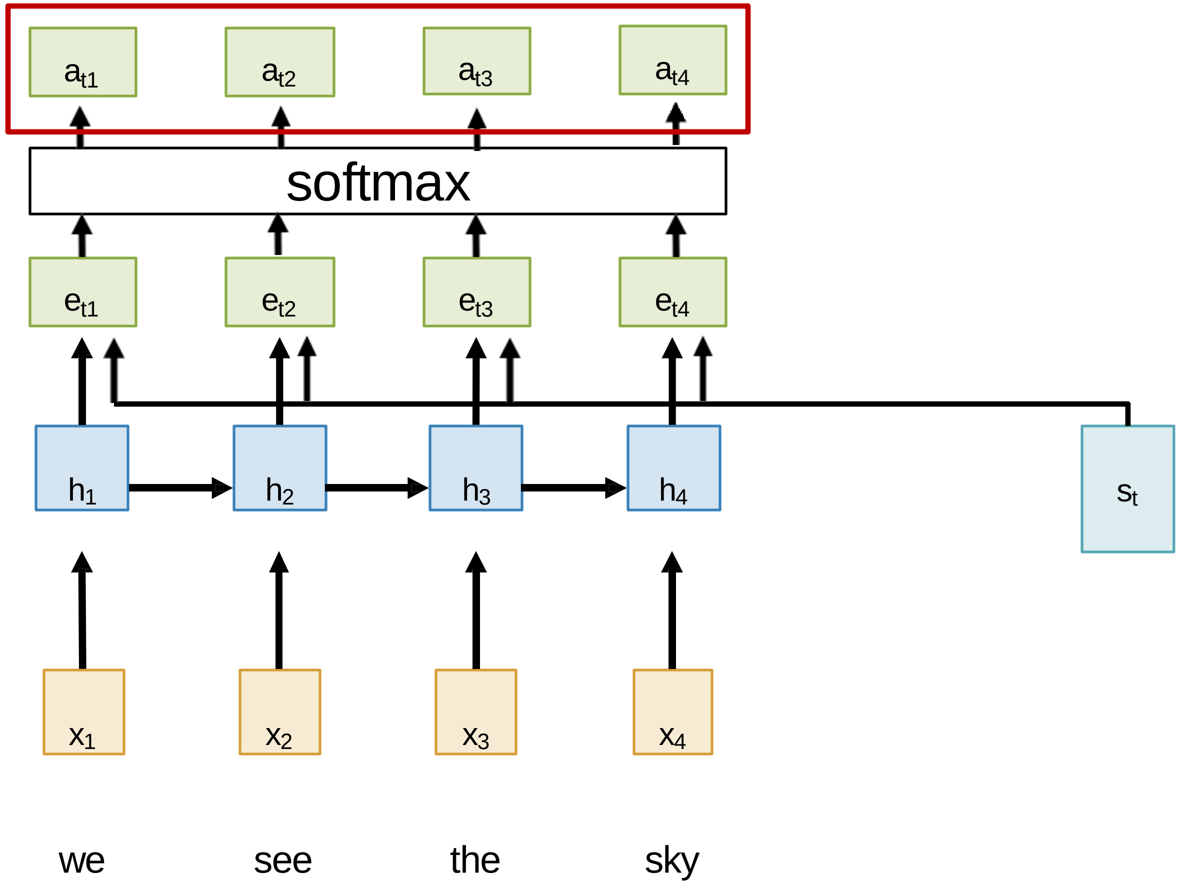
Use a different context vector in each timestep of decoder

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

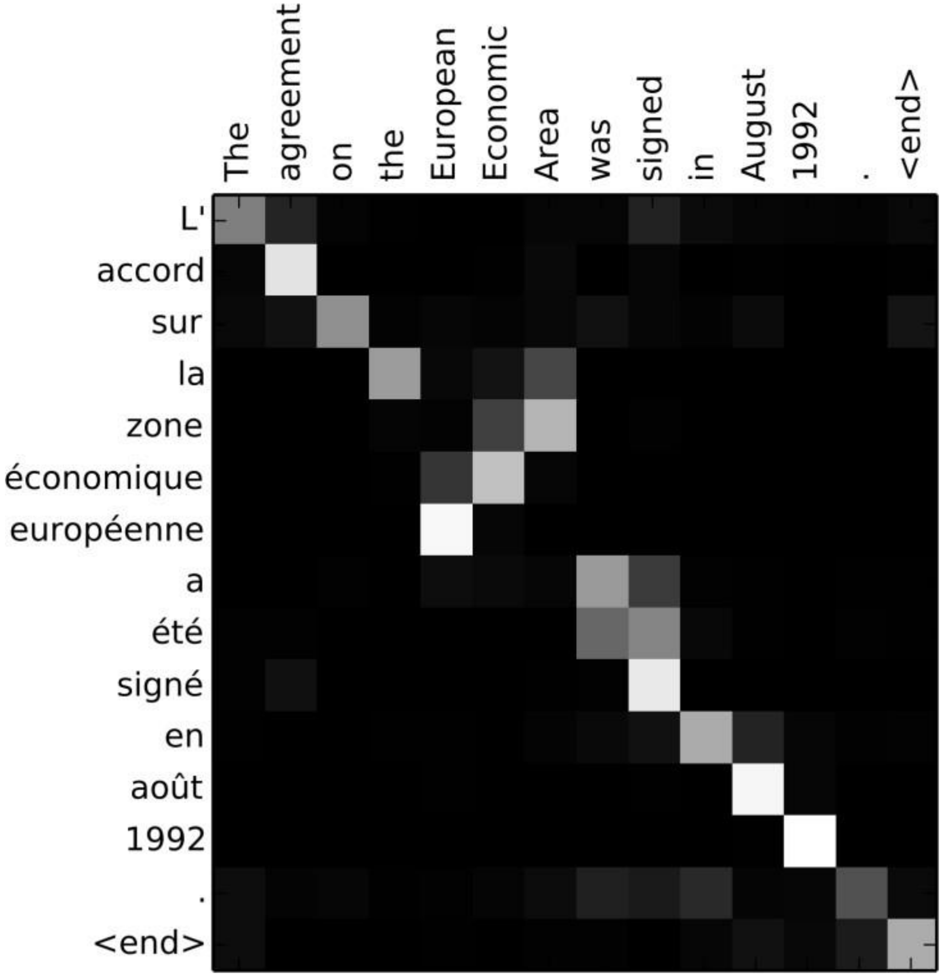


Sequence to Sequence with RNNs and Attention

Example: English to French translation



Visualize attention weights $a_{t,i}$



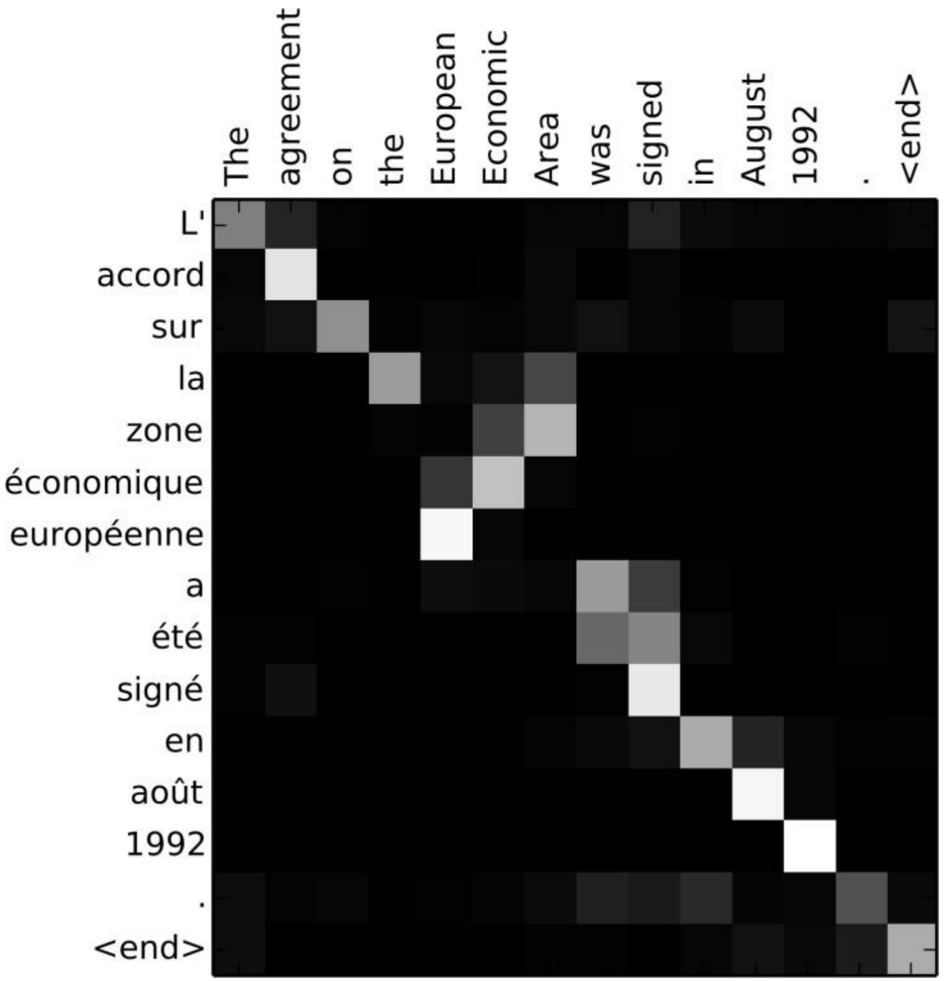
Sequence to Sequence with RNNs and Attention

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.”



Sequence to Sequence with RNNs and Attention

Example: English to French translation

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Diagonal attention means words correspond in order

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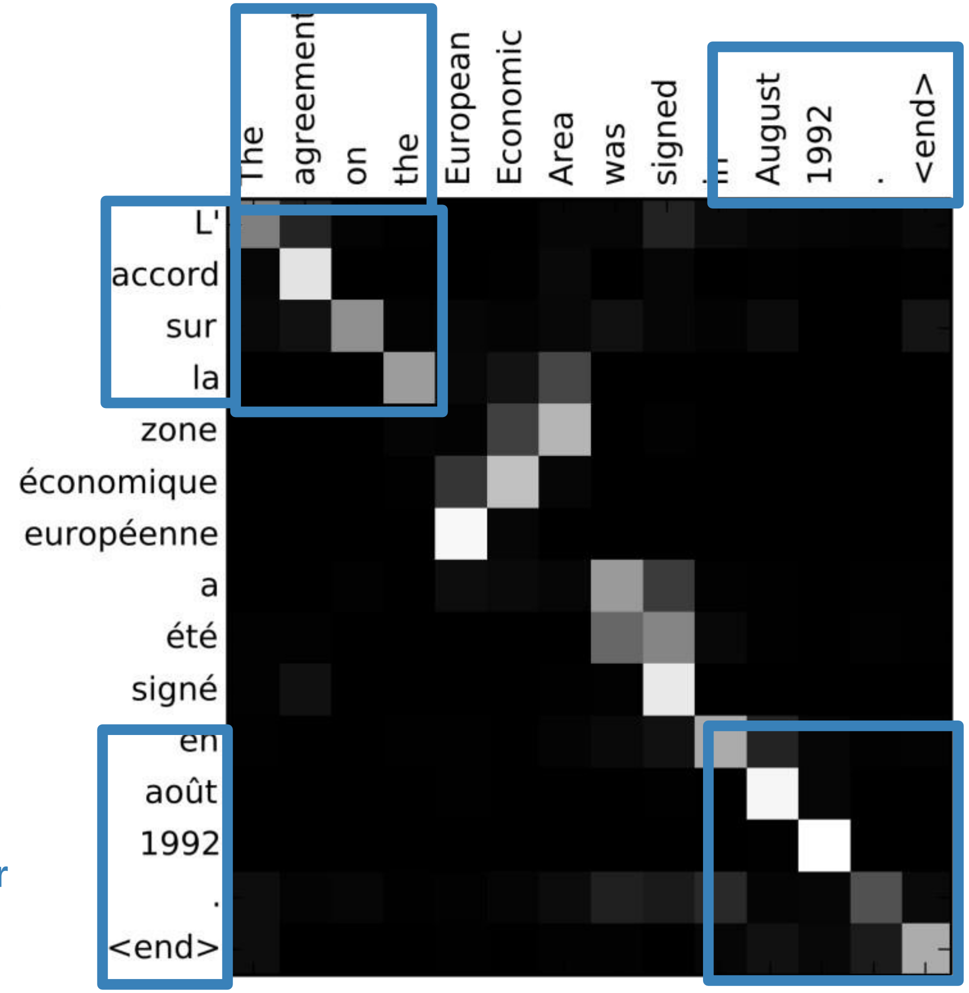

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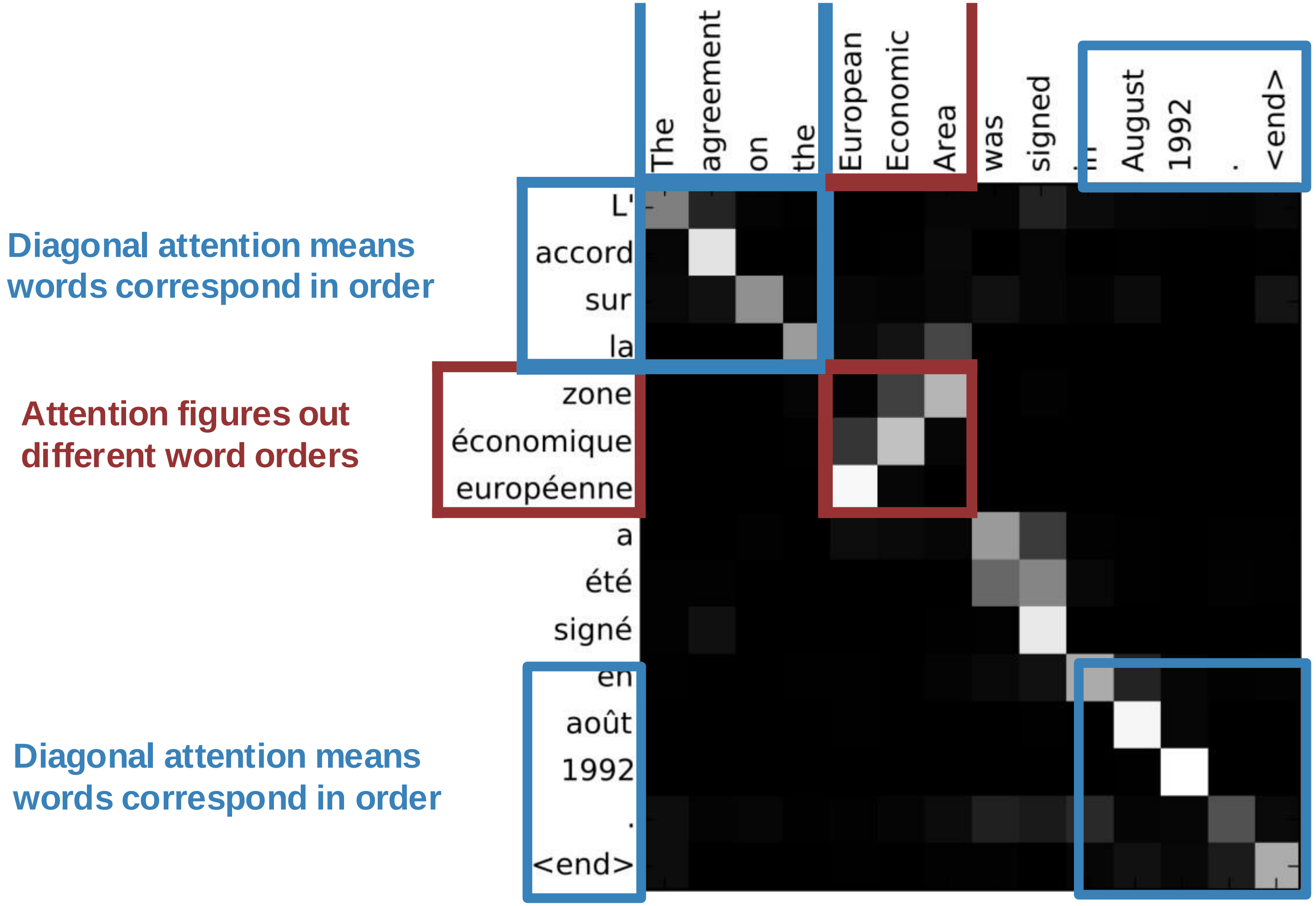


Sequence to Sequence with RNNs and Attention

Context vectors don't use the fact that h_i form an ordered sequence – it just treats them as an unordered set $\{h_i\}$

General architecture + strategy given any set of input hidden vectors $\{h_i\}$! (calculate attention weights + sum)

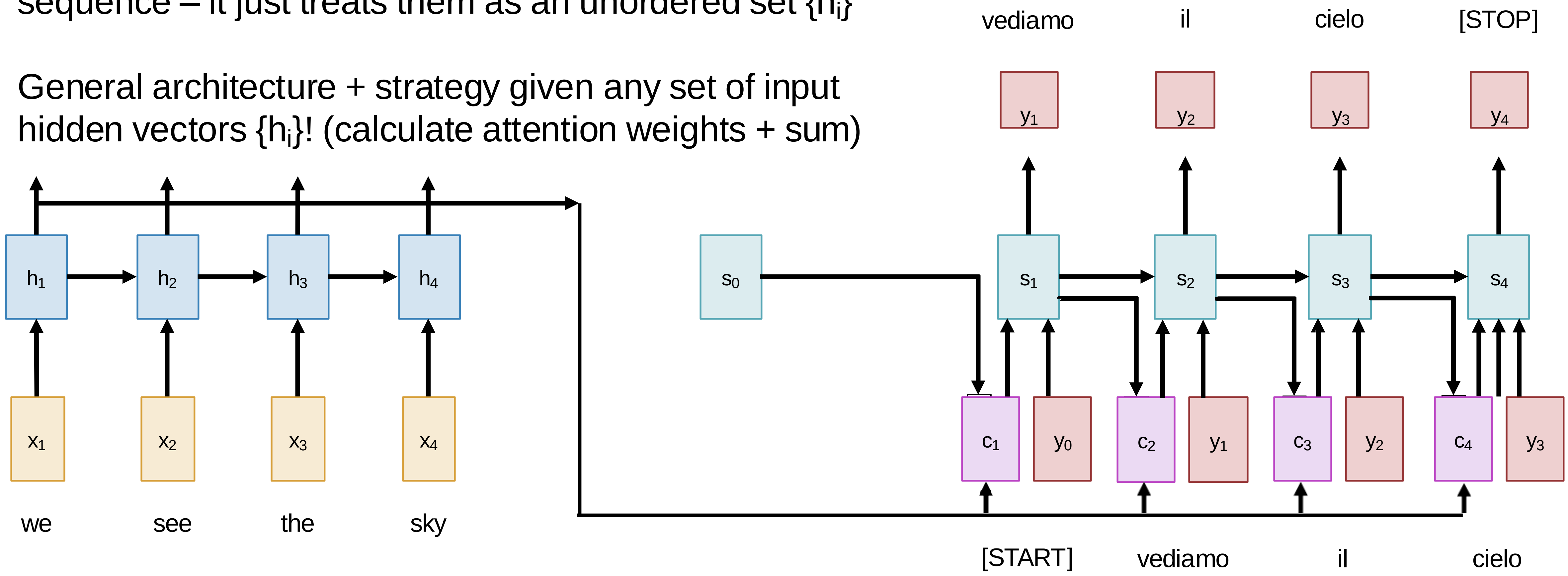
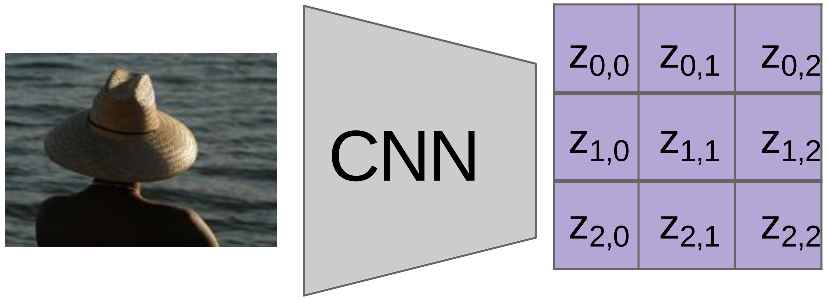


Image Captioning using spatial features

Input: Image **I**
Output: Sequence **y** = $y_1, y_2, \ldots, y_T$

An example network for image captioning **without attention**



Extract spatial features from a pretrained CNN

Features:
H x W x D

Image Captioning using spatial features

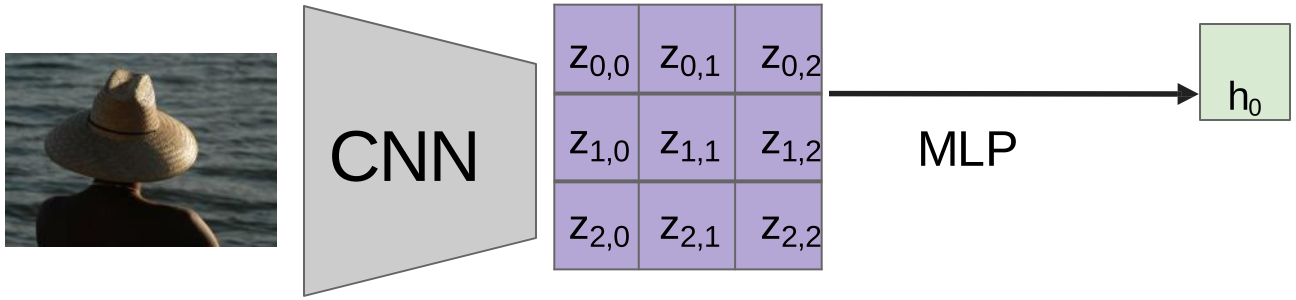
Input: Image **I**

Output: Sequence $\mathbf{y} = y_1, y_2, \ldots, y_T$

Encoder: $h_0 = f_{\mathbf{W}}(\mathbf{z})$

where $\mathbf{z}$ is spatial CNN features

$f_{\mathbf{W}}(.)$ is an MLP



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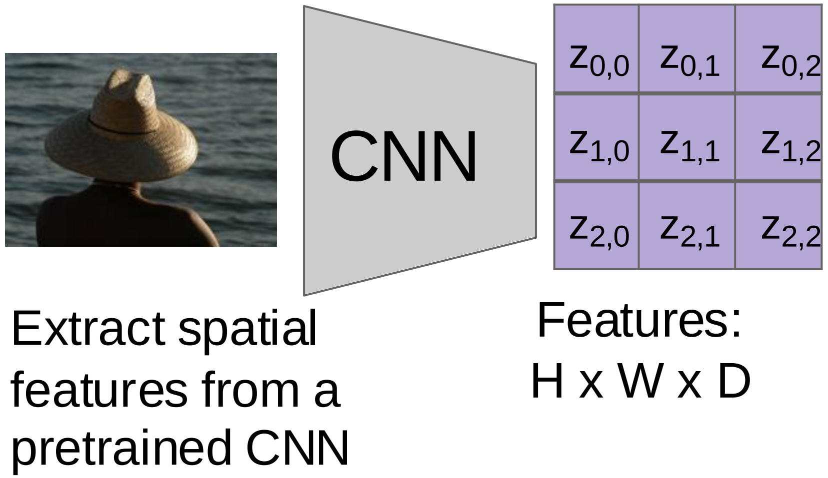

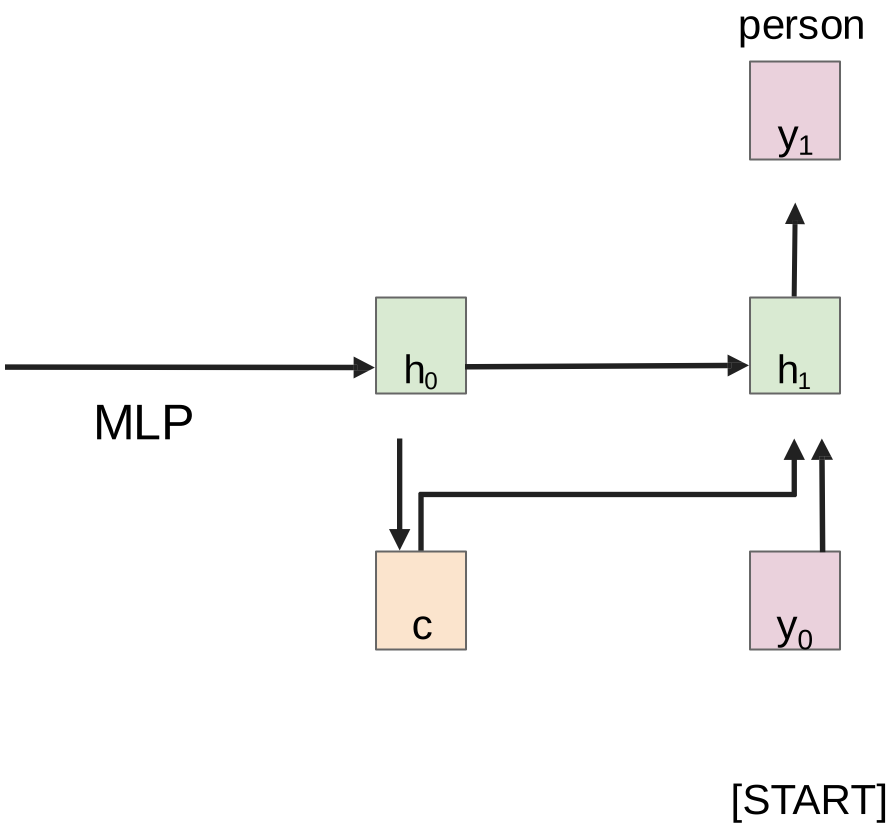

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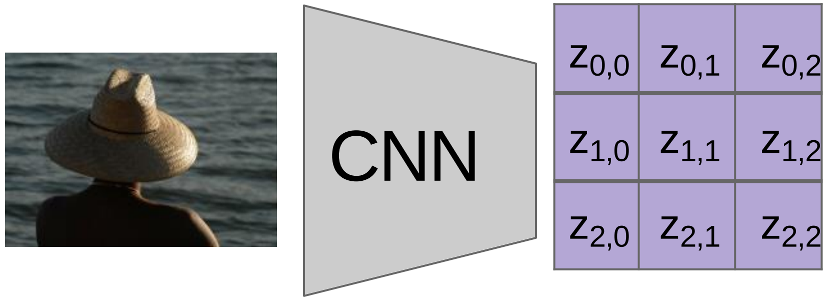

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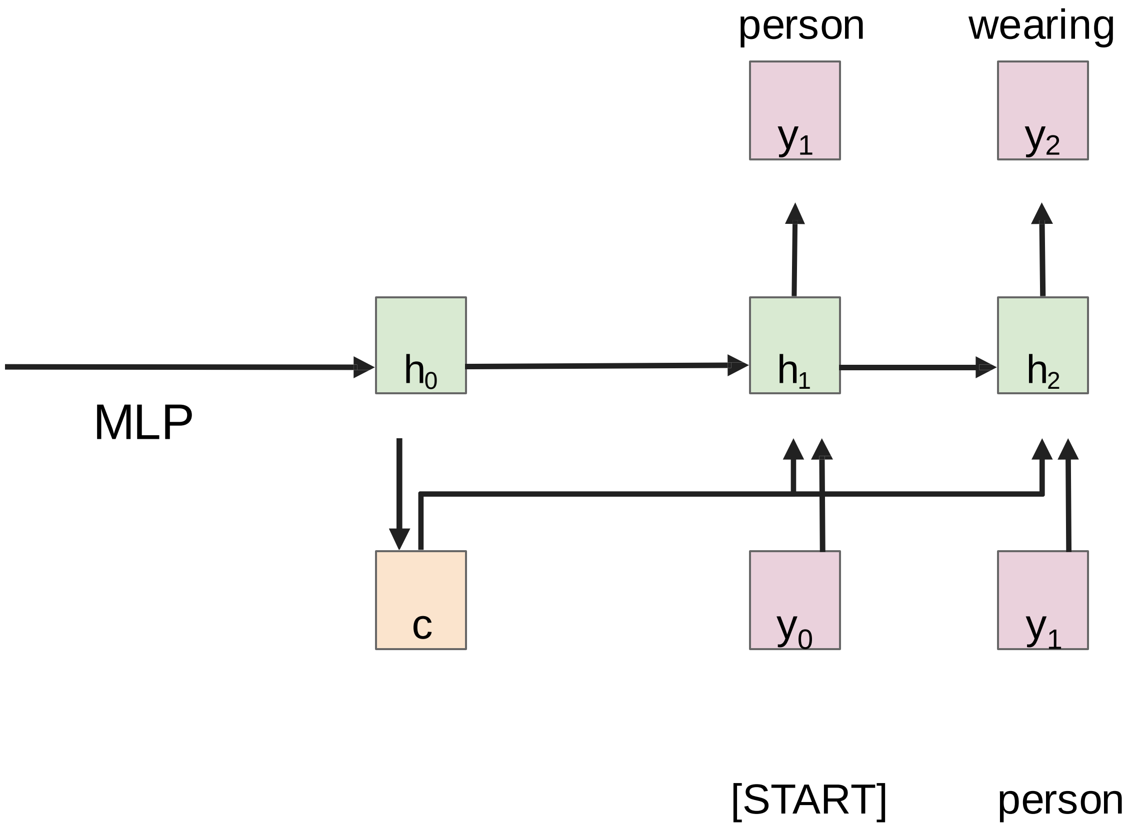

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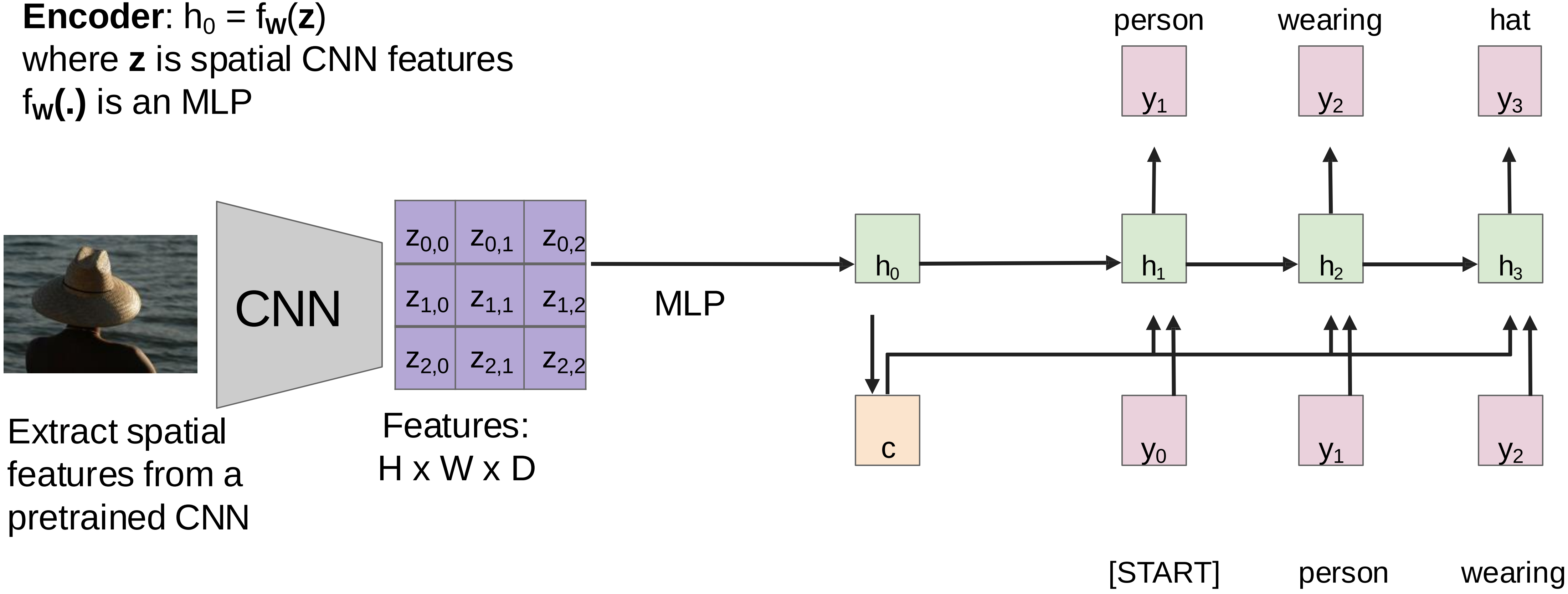

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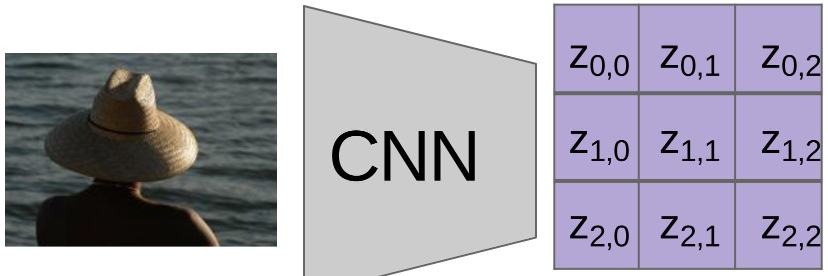

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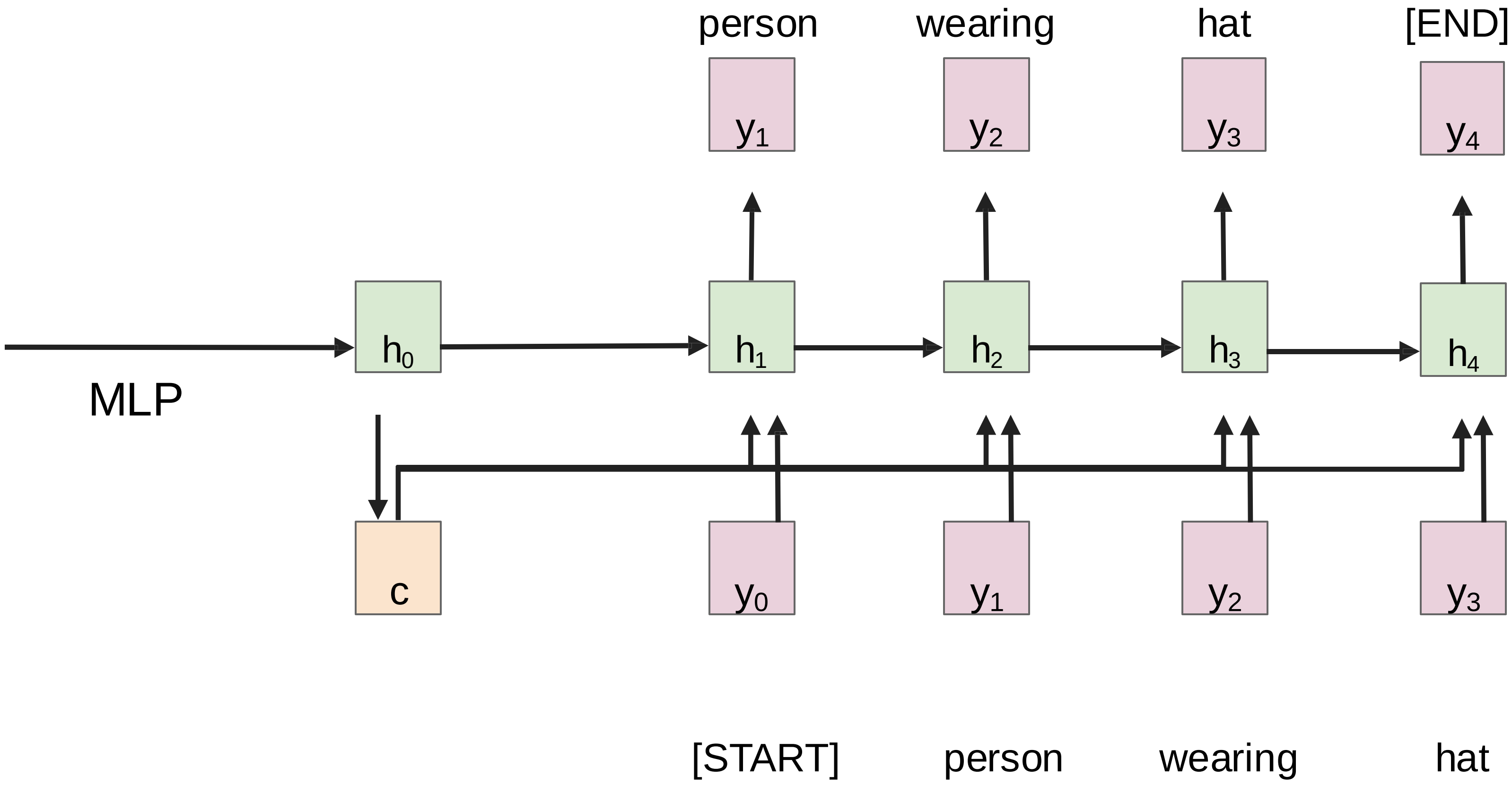
Features: H x W x D



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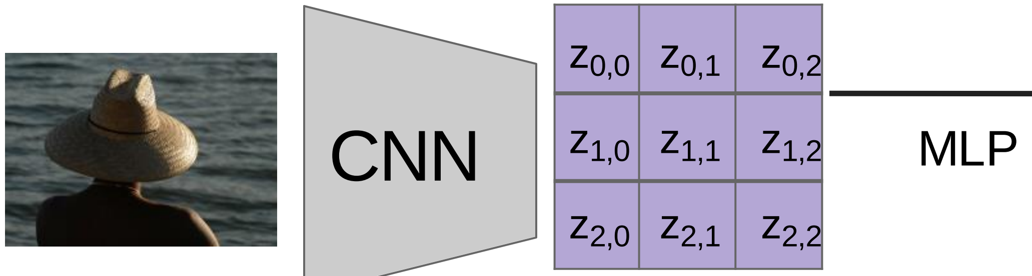
Q: What is the problem with this setup? Think back to last time…



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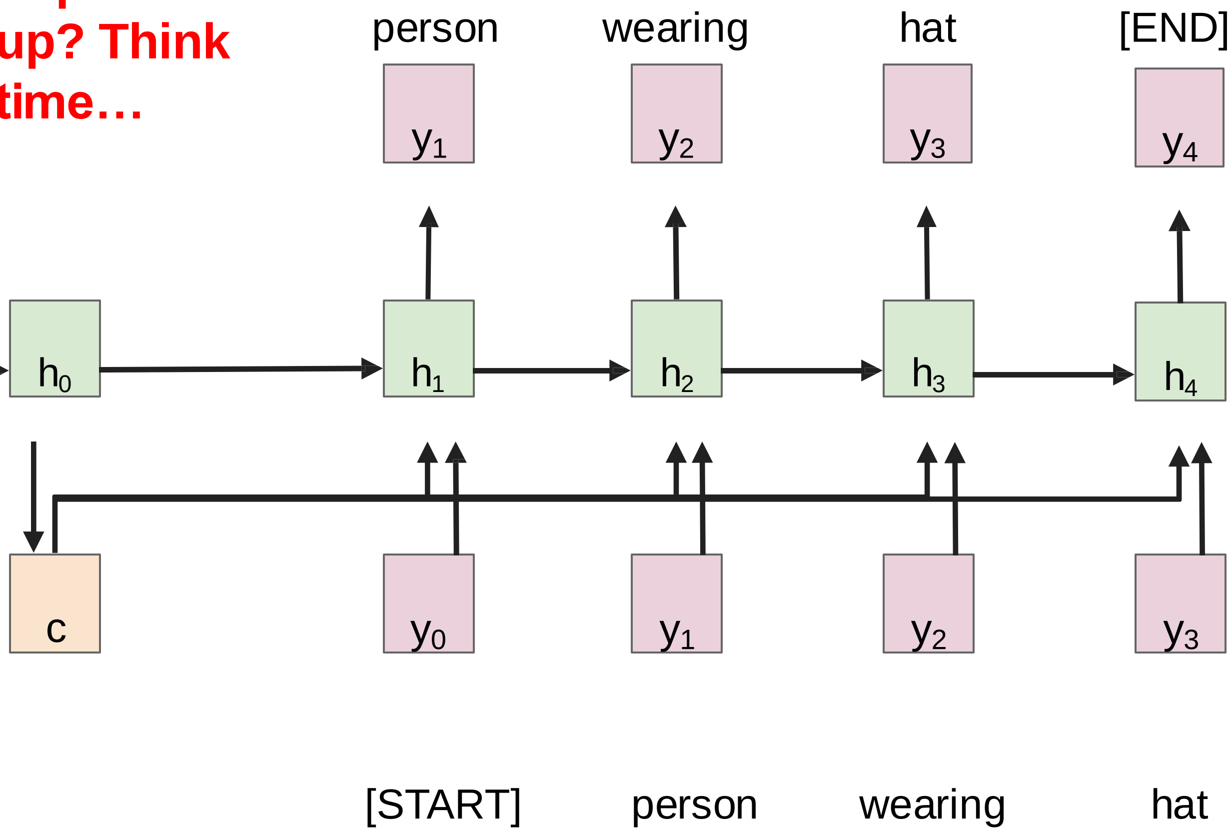
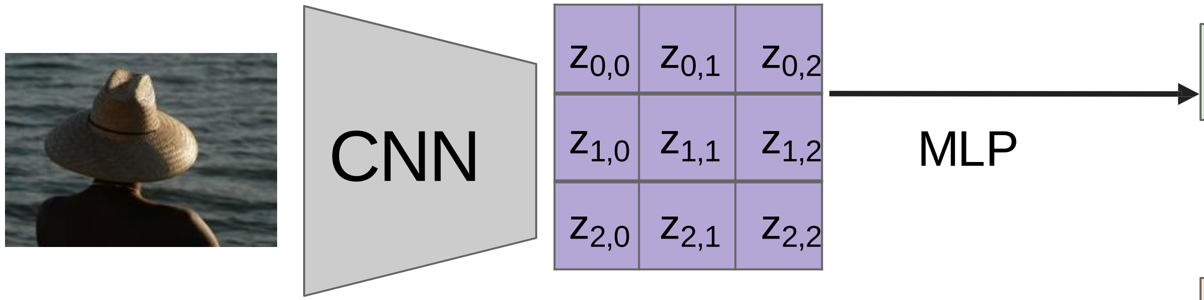


Image Captioning using spatial features

Answer: Input is "bottlenecked" through c

- Model needs to encode everything it wants to say within c

This is a problem if we want to generate really long descriptions? 100s of words long



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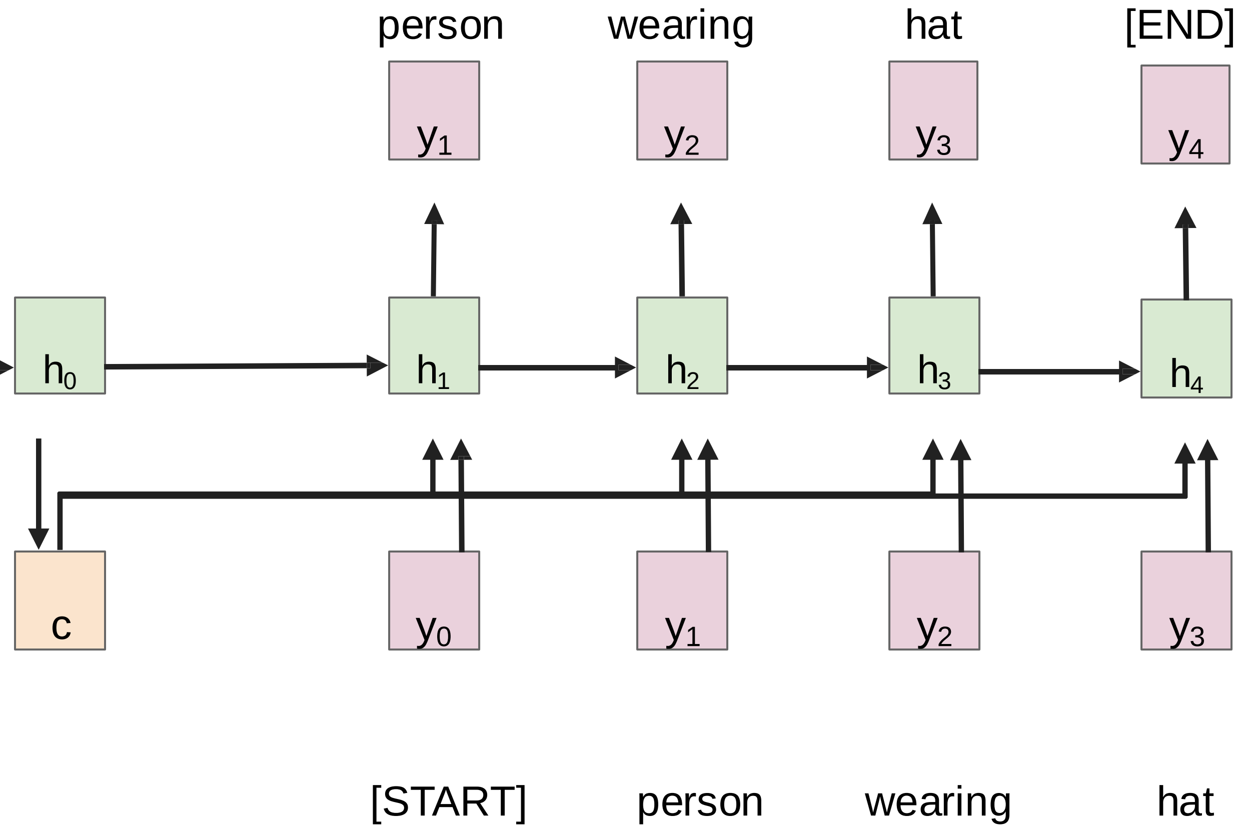
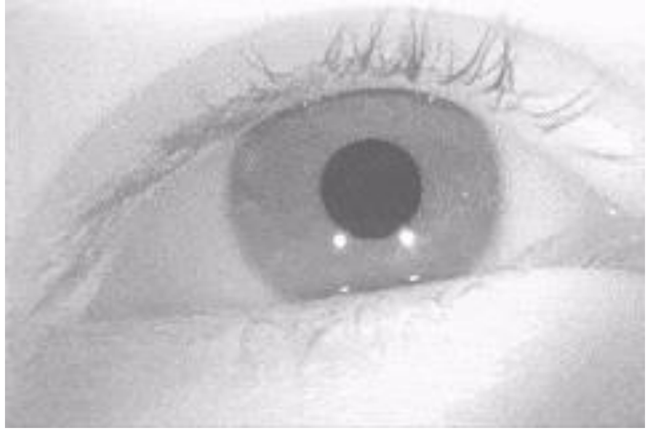


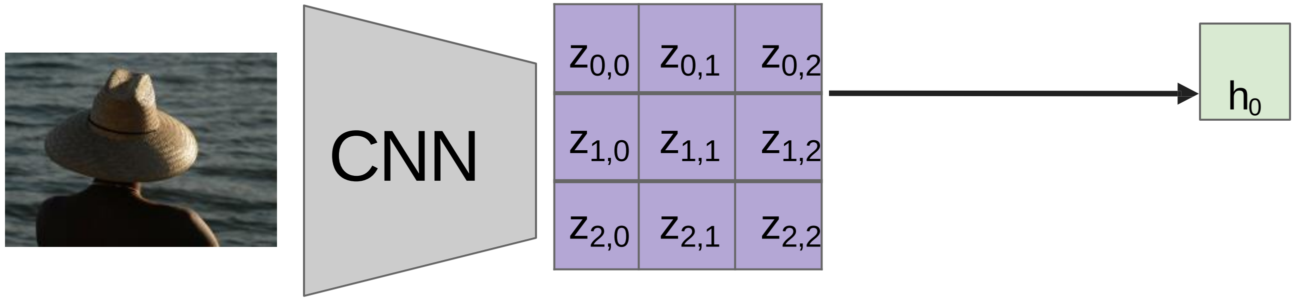
Image Captioning with RNNs and Attention

Attention idea: New context vector at every time step.

Each context vector will attend to different image regions



Attention Saccades in humans



Extract spatial features from a pretrained CNN

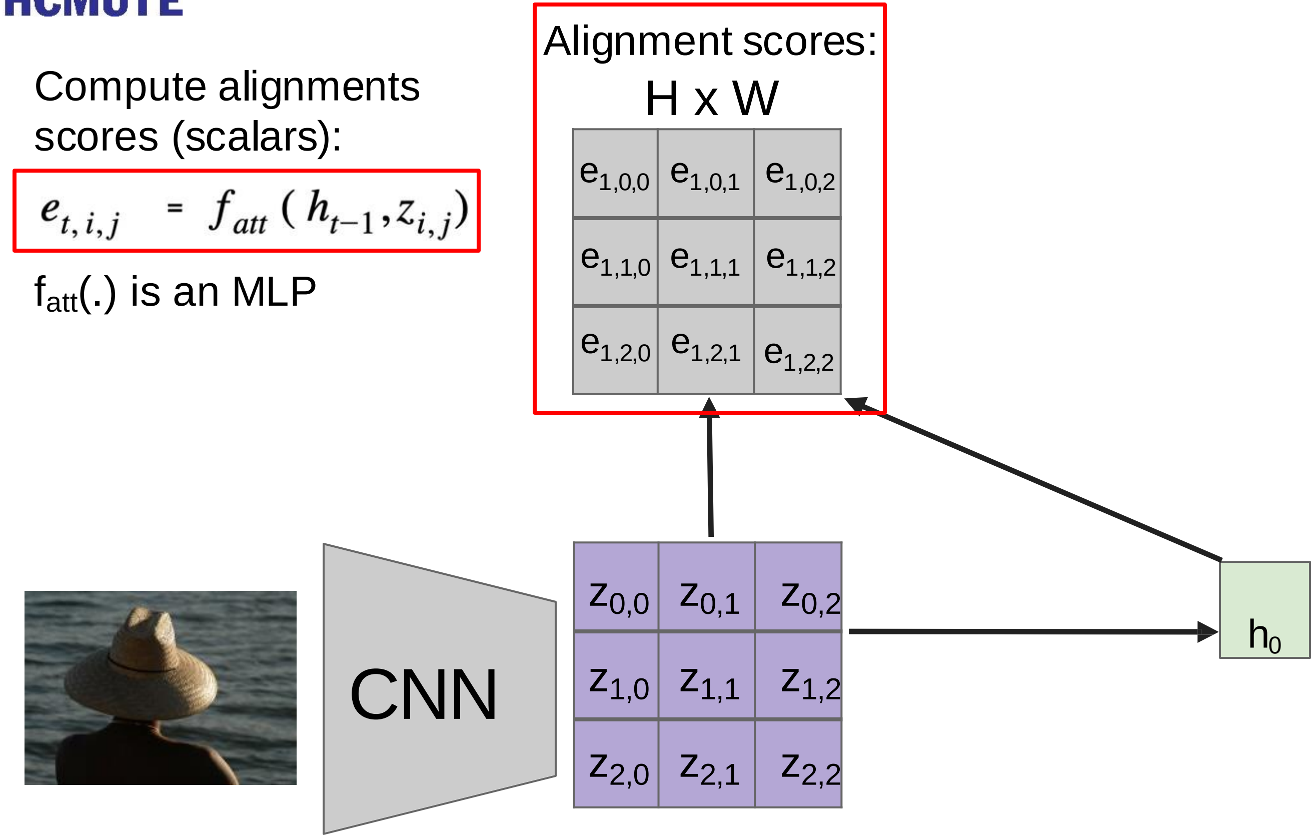
Features: H x W x D

Image Captioning with RNNs and Attention

Compute alignments scores (scalars):

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

$f_{att}(.)$ is an MLP



Extract spatial features from a pretrained CNN

Features:
H x W x D

Image Captioning with RNNs and Attention

Compute alignments scores (scalars):

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

$f_{att}(.)$ is an MLP

Alignment scores:
H x W

$e_{1,0,0}$	$e_{1,0,1}$	$e_{1,0,2}$
$e_{1,1,0}$	$e_{1,1,1}$	$e_{1,1,2}$
$e_{1,2,0}$	$e_{1,2,1}$	$e_{1,2,2}$

Attention:
H x W

$a_{1,0,0}$	$a_{1,0,1}$	$a_{1,0,2}$
$a_{1,1,0}$	$a_{1,1,1}$	$a_{1,1,2}$
$a_{1,2,0}$	$a_{1,2,1}$	$a_{1,2,2}$

Normalize to get attention weights:

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

$0 < a_{t,i,j} < 1$,
attention values sum to 1

CNN

$z_{0,0}$	$z_{0,1}$	$z_{0,2}$
$z_{1,0}$	$z_{1,1}$	$z_{1,2}$
$z_{2,0}$	$z_{2,1}$	$z_{2,2}$

h_0

Extract spatial features from a pretrained CNN

Features:
H x W x D

Image Captioning with RNNs and Attention

Compute alignments scores (scalars):

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

$f_{att}(.)$ is an MLP

Alignment scores: H x W

Attention: H x W

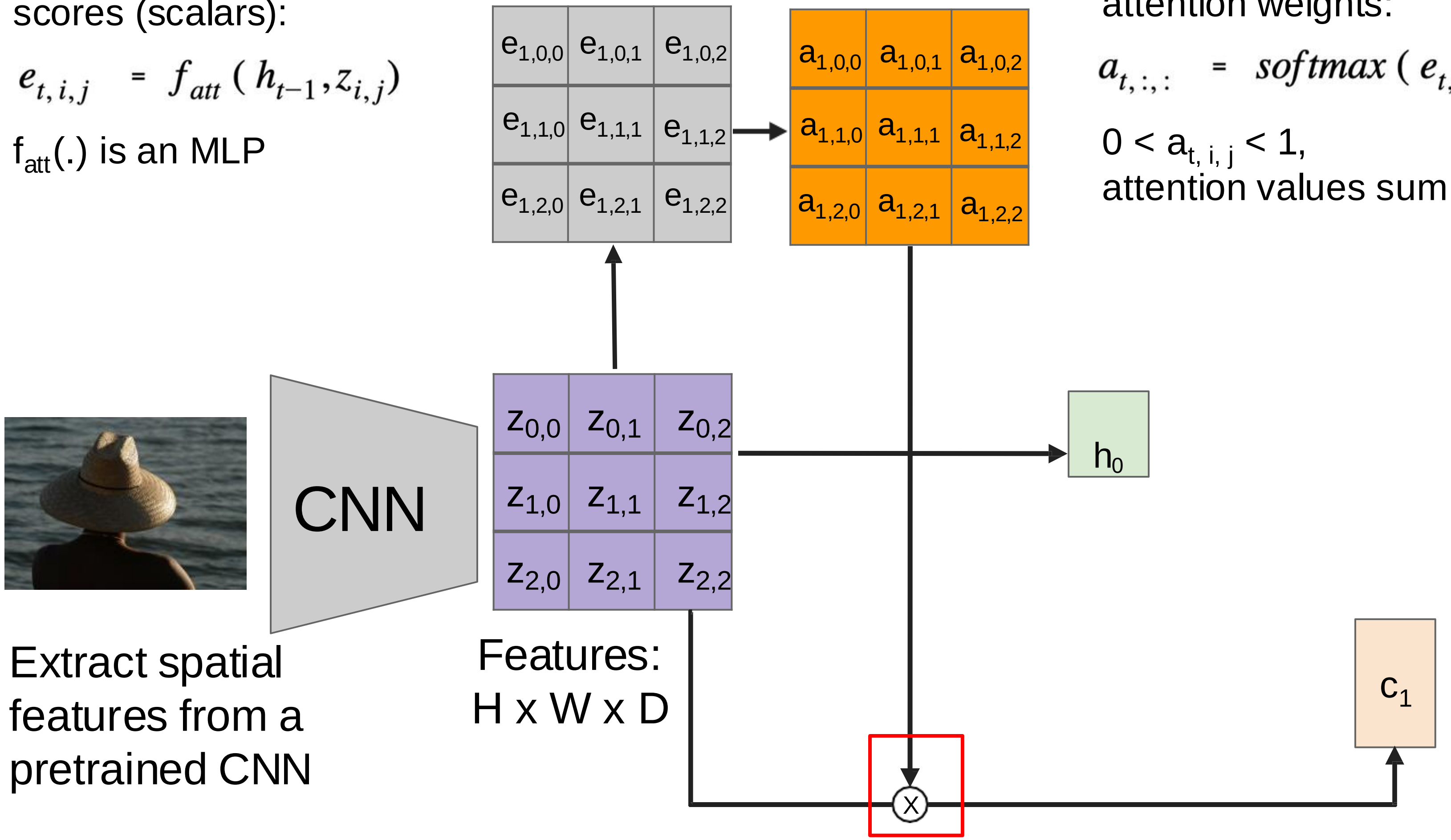
Normalize to get attention weights:

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

$0 < a_{t,i,j} < 1$,
attention values sum to 1

Compute context vector:

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



Extract spatial features from a pretrained CNN

Features: H x W x D

Q: How many context vectors are computed?

Image Captioning with RNNs and Attention

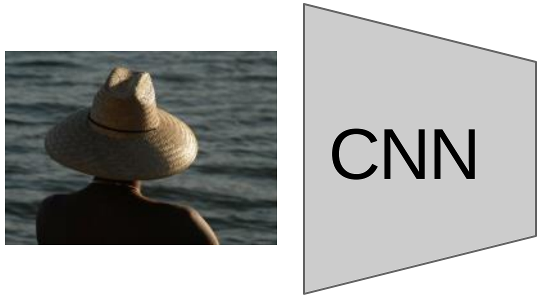
Decoder: $y_t = g_V(y_{t-1}, h_{t-1}, c_t)$
New context vector at every time step

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

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

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

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



Extract spatial features from a pretrained CNN

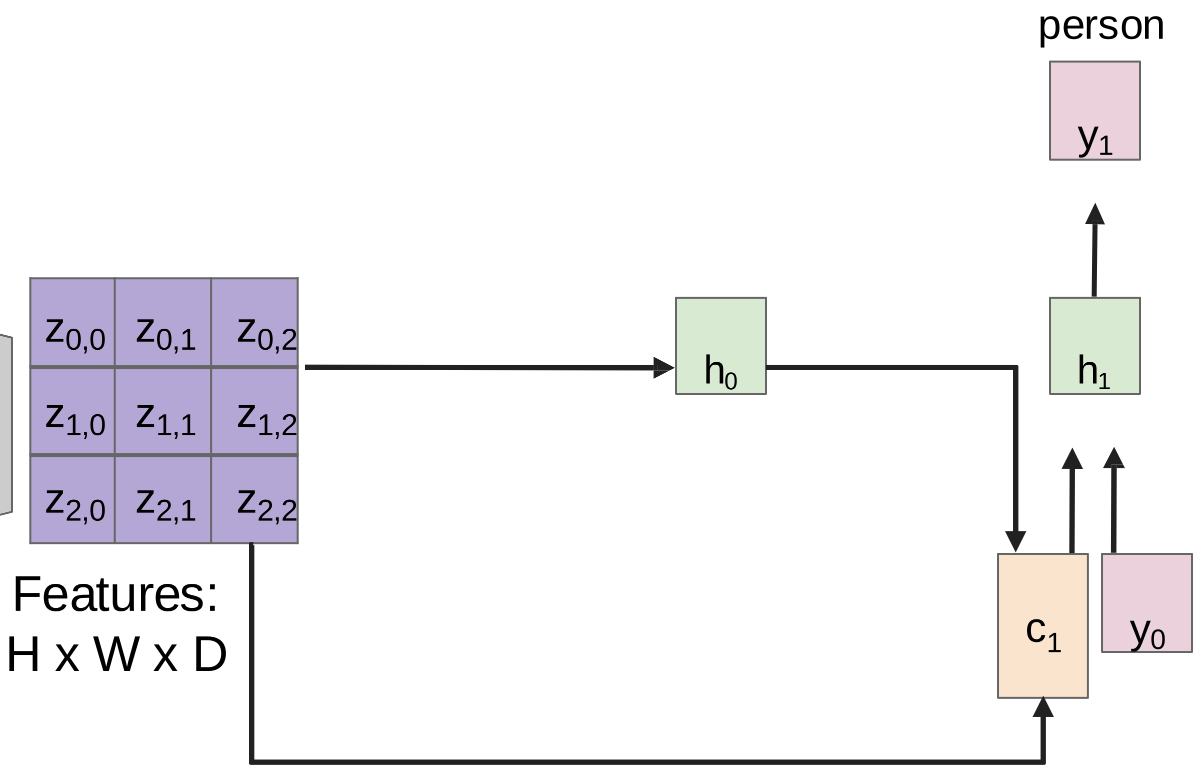


Image Captioning with RNNs and Attention

Decoder: $y_t = g_V(y_{t-1}, h_{t-1}, c_t)$
New context vector at every time step

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

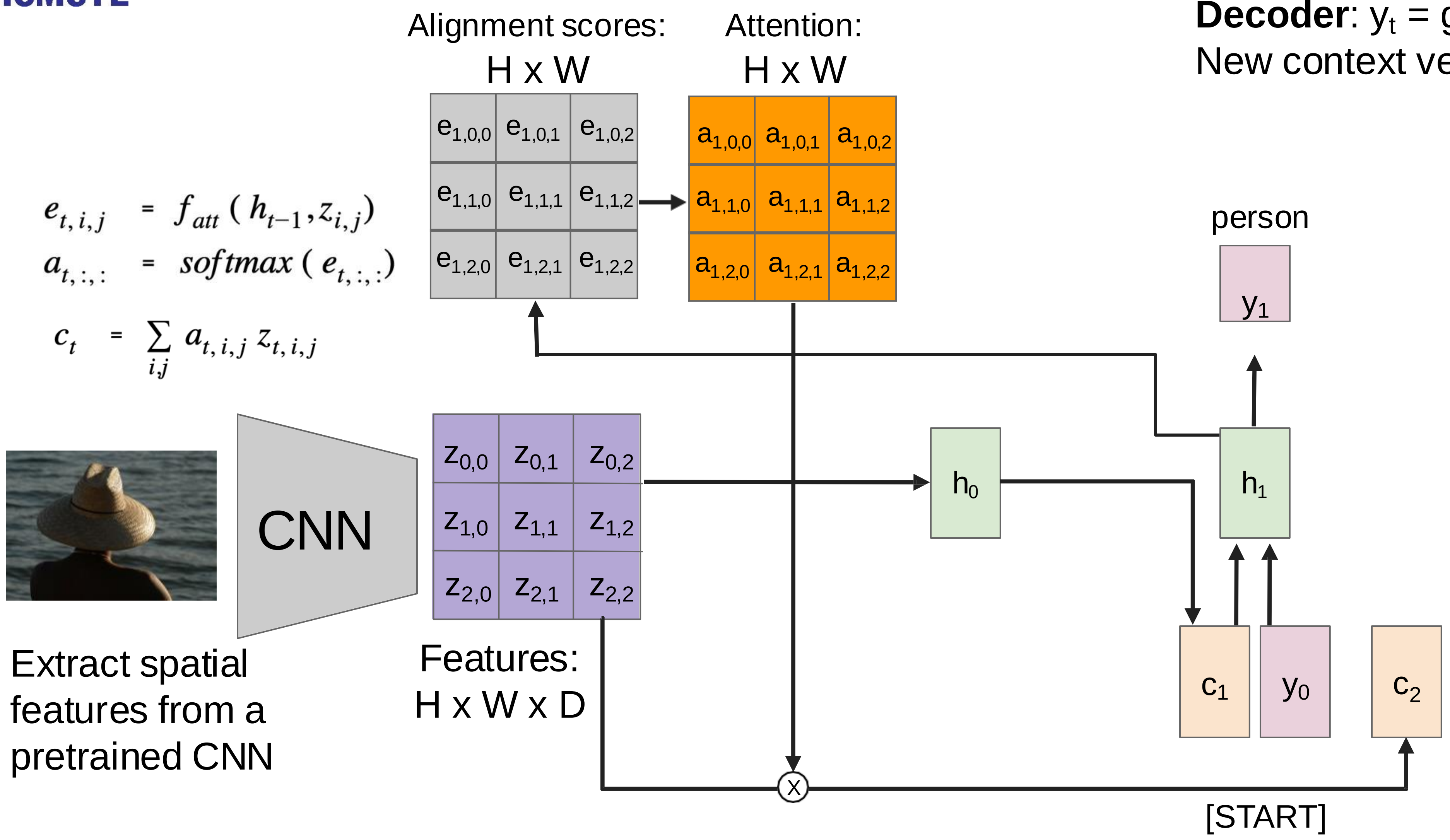
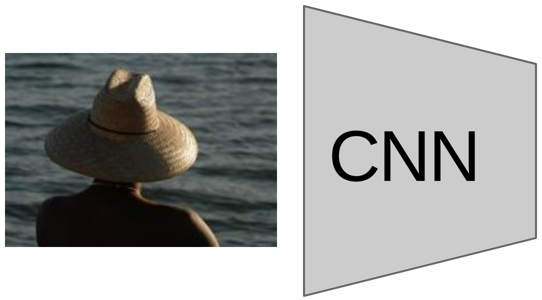


Image Captioning with RNNs and Attention

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

Decoder: $y_t = g_V(y_{t-1}, h_{t-1}, c_t)$
New context vector at every time step

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



Extract spatial features from a pretrained CNN

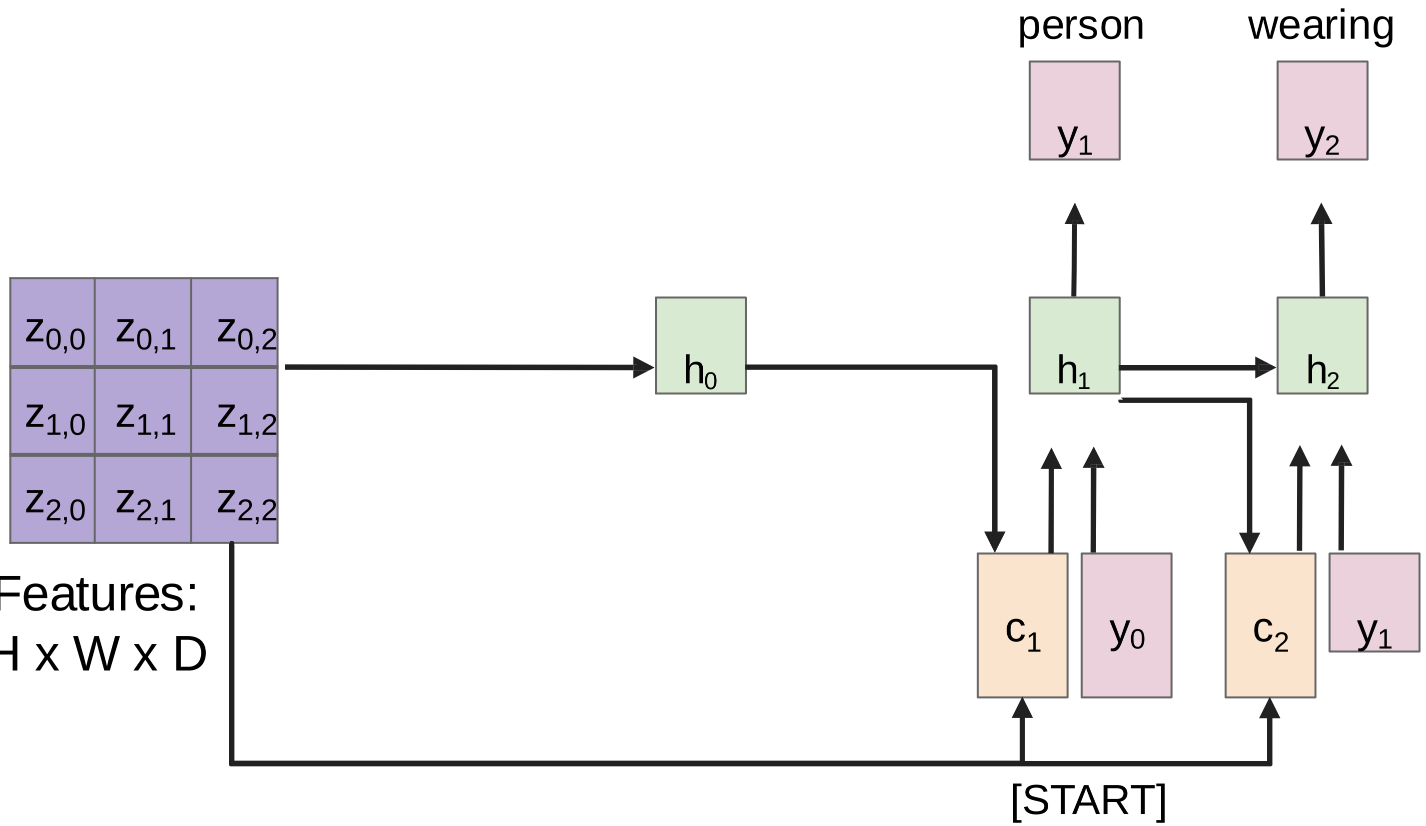
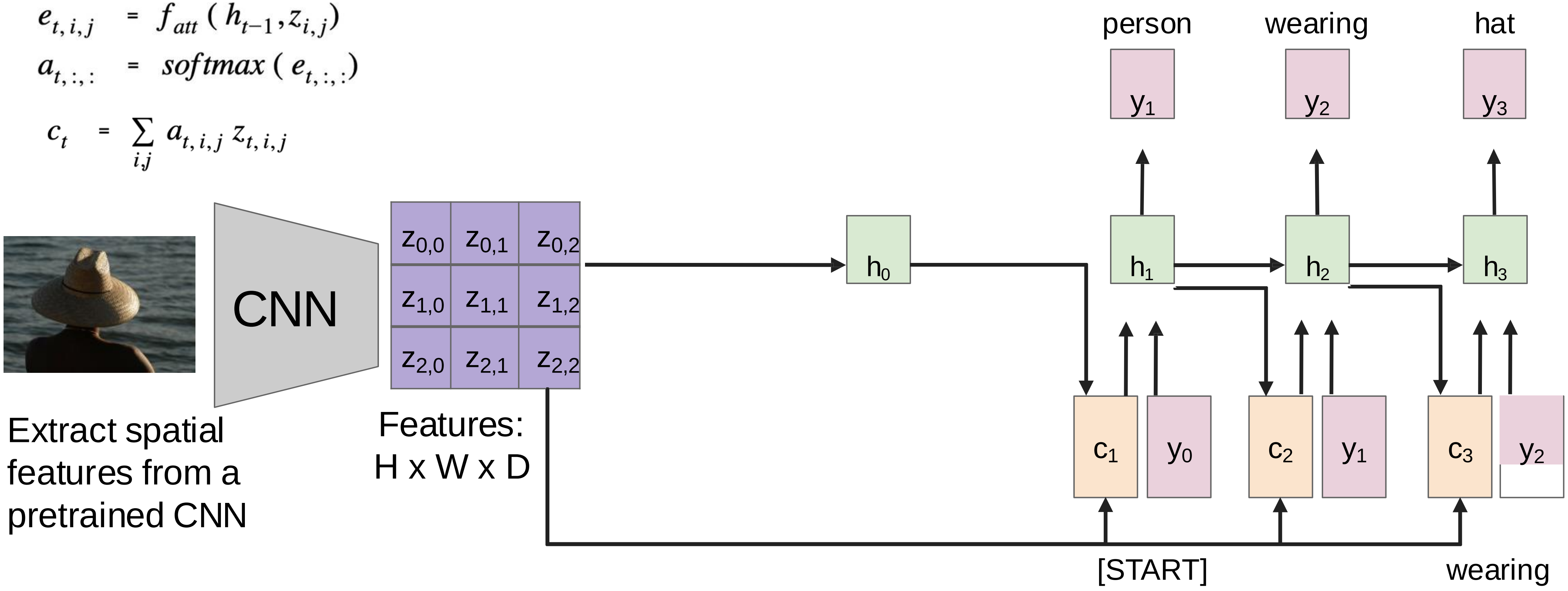


Image Captioning with RNNs and Attention

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

Decoder: $y_t = g_V(y_{t-1}, h_{t-1}, c_t)$
New context vector at every time step

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



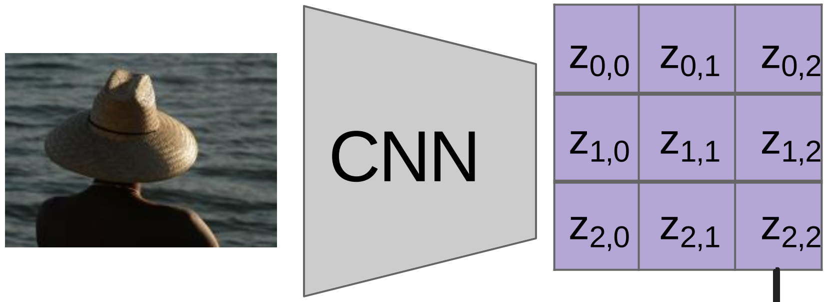
Extract spatial features from a pretrained CNN

Image Captioning with RNNs and Attention

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

Decoder: $y_t = g_V(y_{t-1}, h_{t-1}, c_t)$
New context vector at every time step

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



Extract spatial features from a pretrained CNN

Features: H x W x D

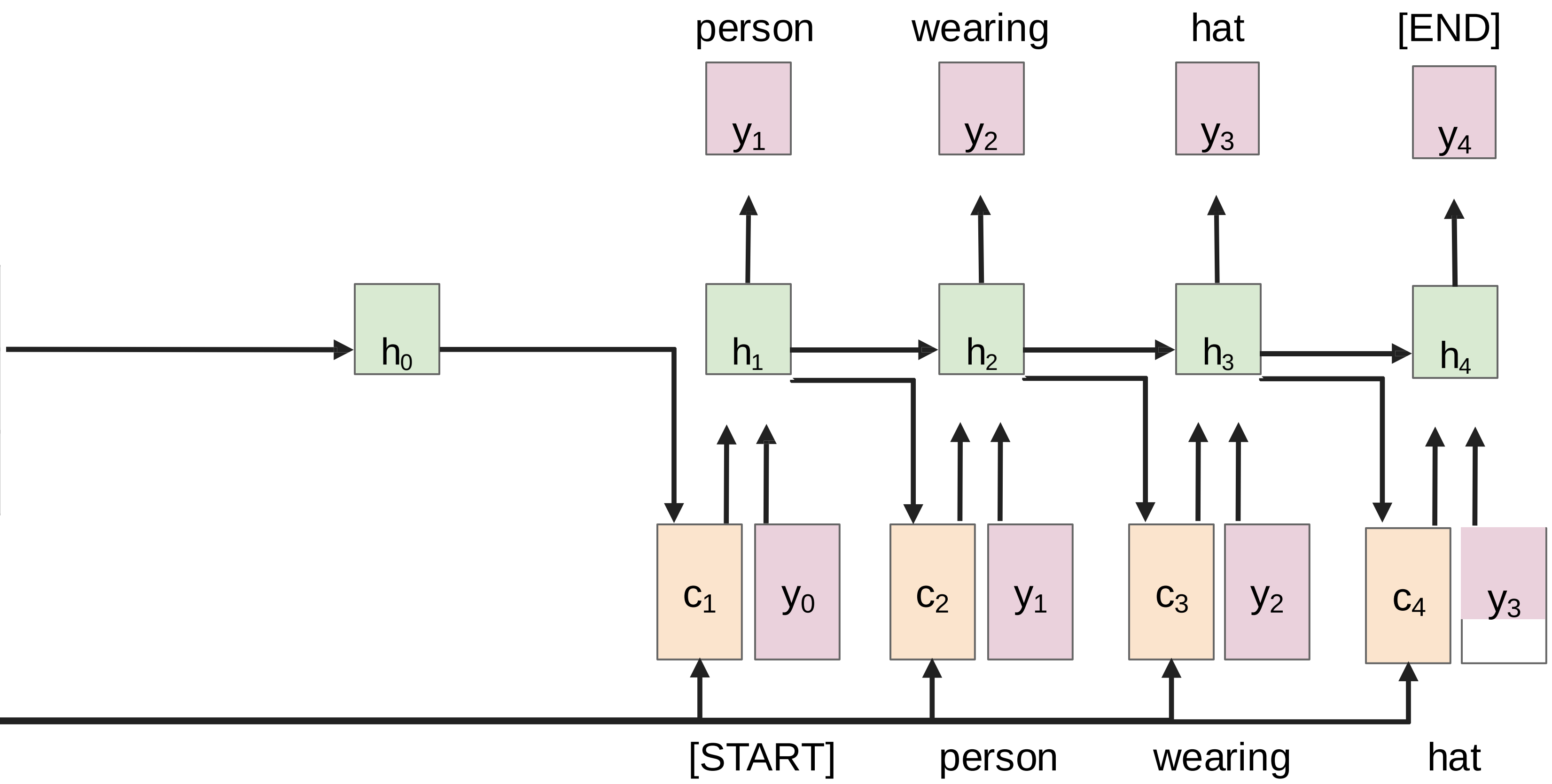


Image Captioning with RNNs and Attention

This entire process is differentiable.

- model chooses its own attention weights. No attention supervision is required

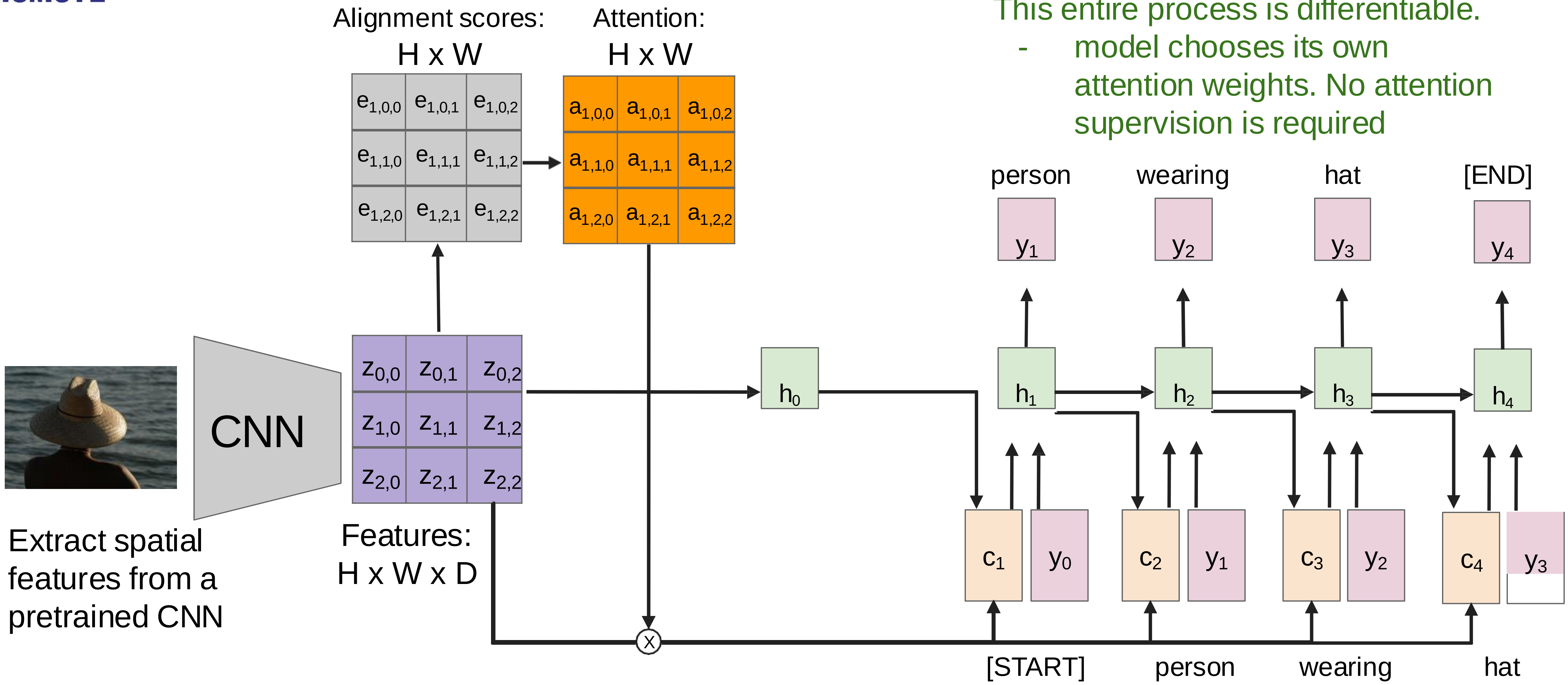
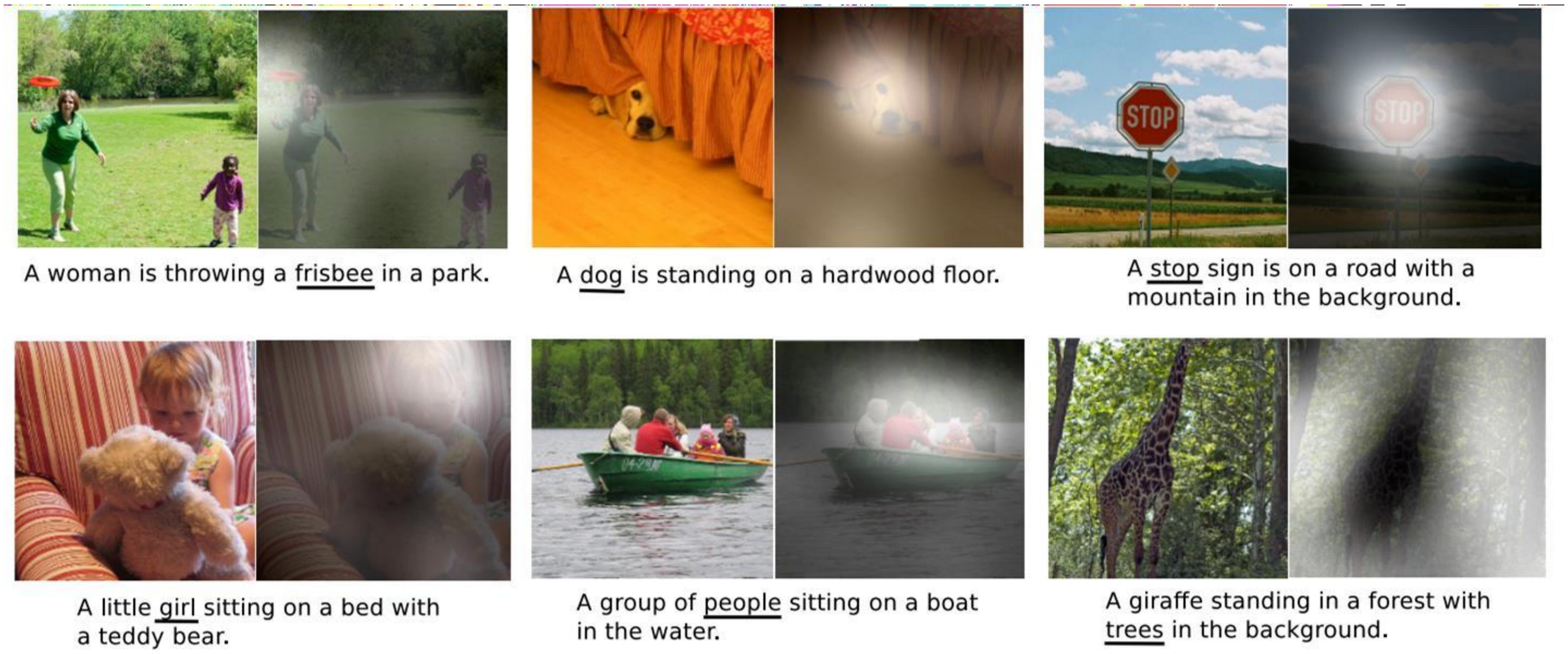


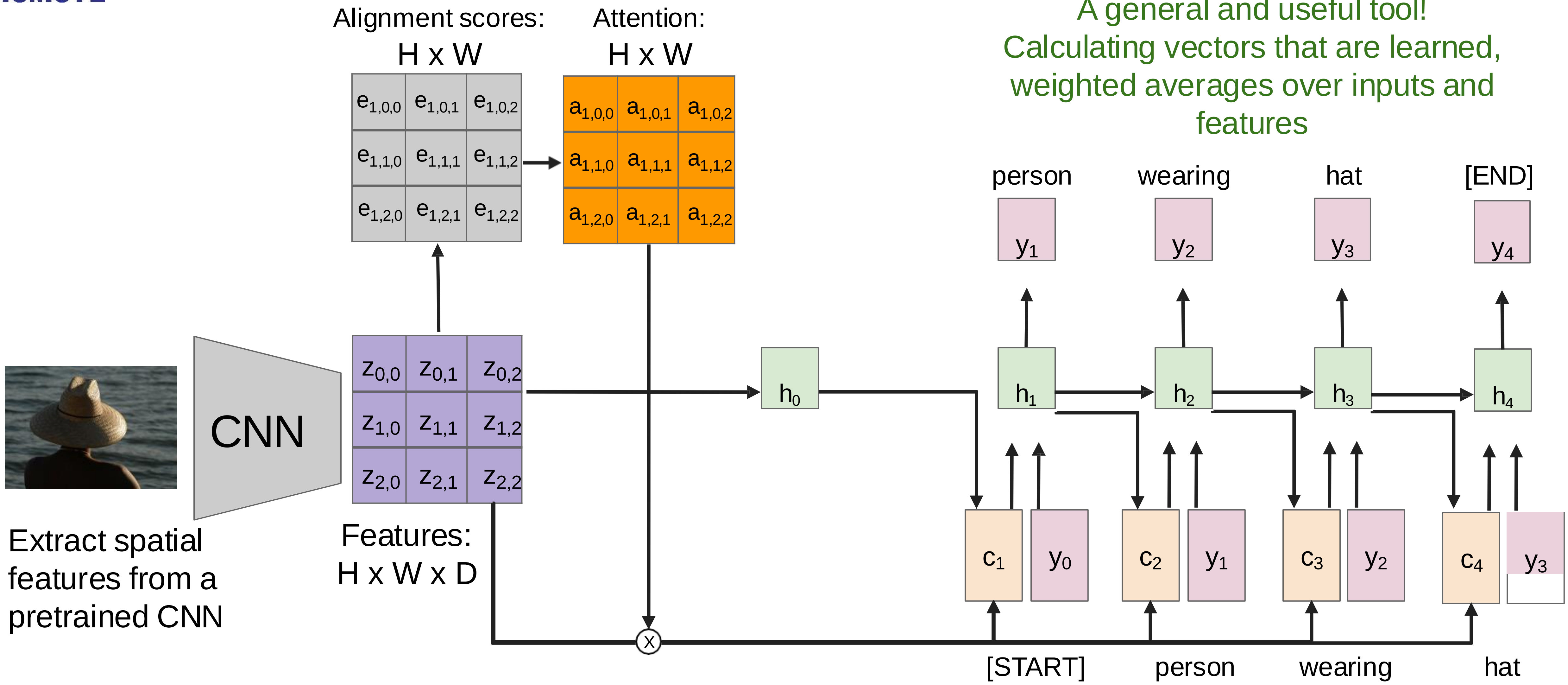
Image Captioning with Attention



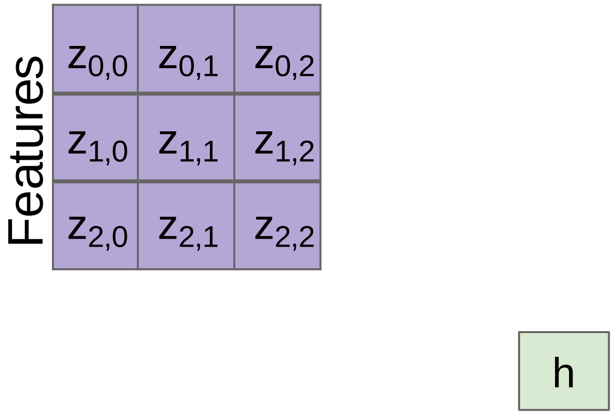
Xu et al, "Show, Attend, and Tell: Neural Image Caption Generation with Visual Attention", ICML 2015

Image Captioning with RNNs and Attention

A general and useful tool!
Calculating vectors that are learned, weighted averages over inputs and features



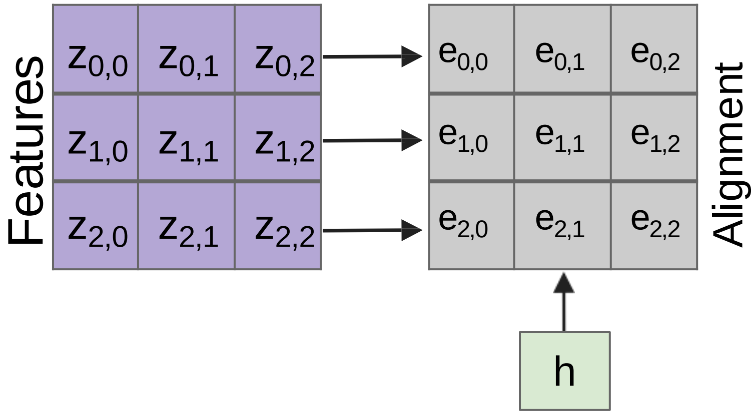
Attention we just saw in image captioning



Inputs:
Features: **z** (shape: H x W x D)
Query: **h** (shape: D) ← “query” refers to a vector used to calculate a corresponding context vector.

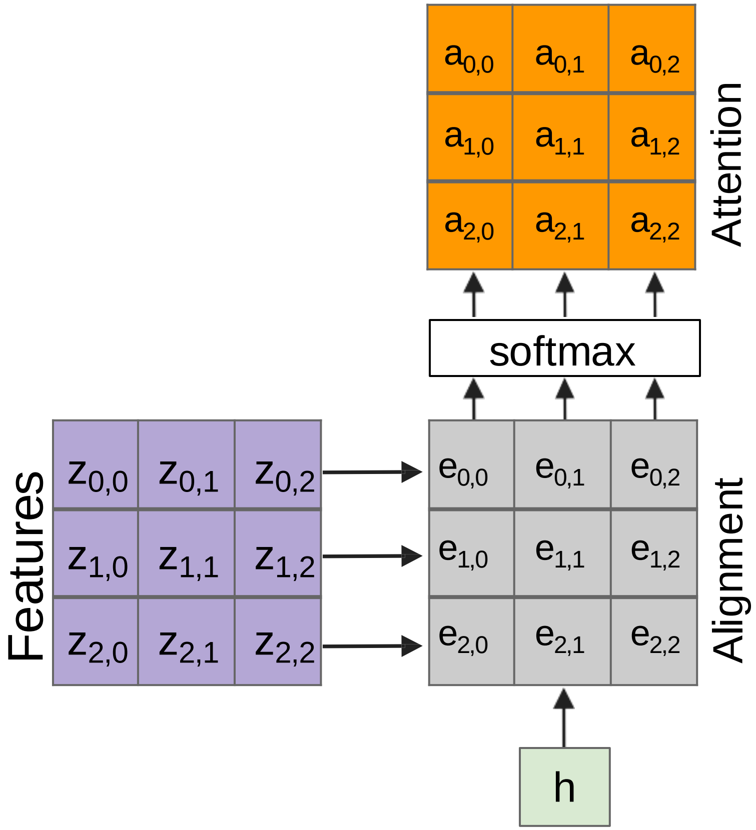
Attention we just saw in image captioning

Operations:
Alignment: $e_{i,j} = f_{att}(h, z_{i,j})$



Inputs:
Features: **z** (shape: H x W x D)
Query: **h** (shape: D)

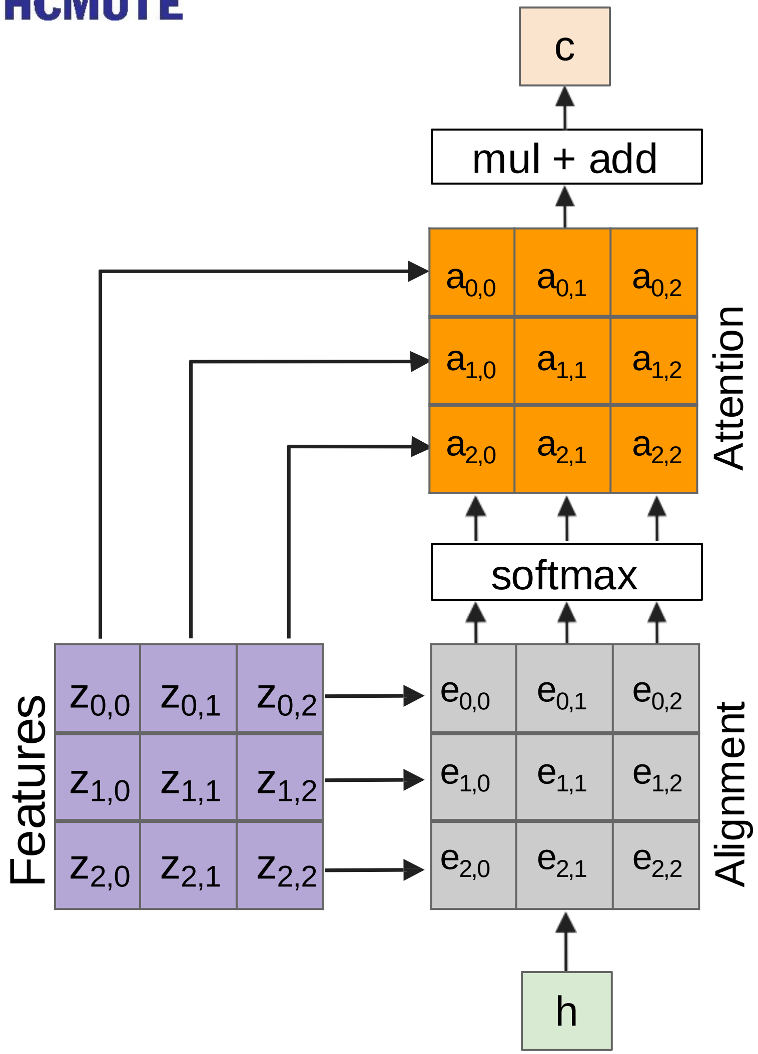
Attention we just saw in image captioning



Operations:
Alignment: $e_{i,j} = f_{att}(h, z_{i,j})$
Attention: $\mathbf{a} = \text{softmax}(\mathbf{e})$

Inputs:
Features: **z** (shape: H x W x D)
Query: **h** (shape: D)

Attention we just saw in image captioning

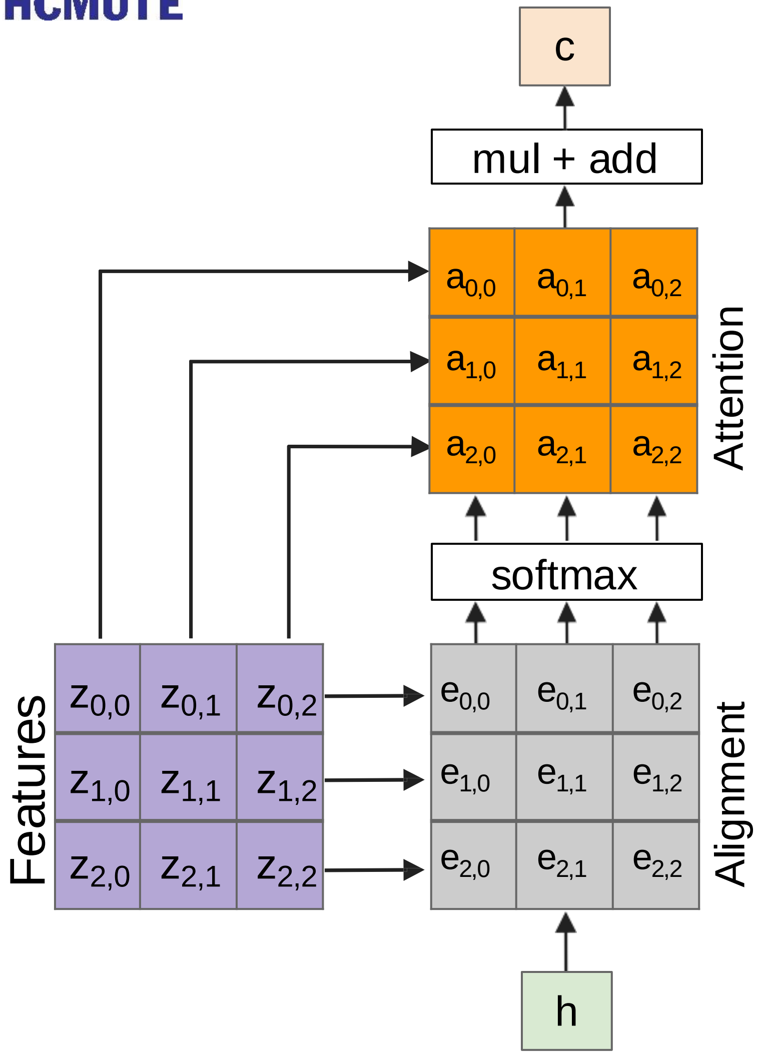


Outputs:
context vector: **c** (shape: D)

Operations:
Alignment: $e_{i,j} = f_{att}(h, z_{i,j})$
Attention: $\mathbf{a} = \text{softmax}(\mathbf{e})$
Output: $\mathbf{c} = \sum_{i,j} a_{i,j} z_{i,j}$

Inputs:
Features: **z** (shape: H x W x D)
Query: **h** (shape: D)

Attention we just saw in image captioning



Outputs:
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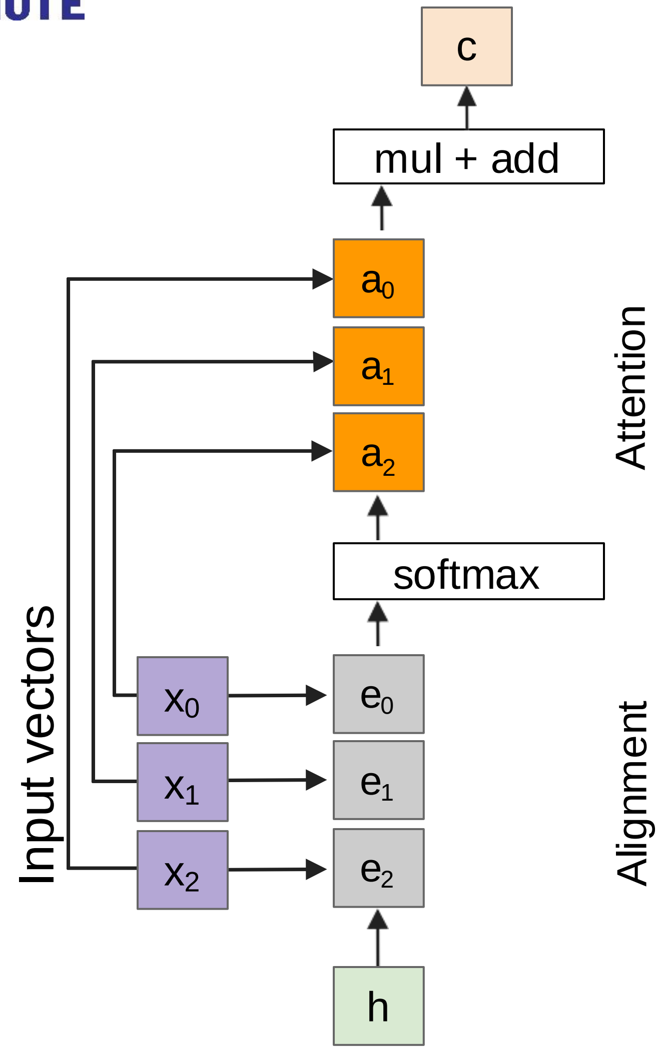
Alignment: $e_{i,j} = f_{att}(h, z_{i,j})$
Attention: $\mathbf{a} = \text{softmax}(\mathbf{e})$
Output: $\mathbf{c} = \sum_{i,j} a_{i,j} z_{i,j}$

Inputs:
Features: **z** (shape: H x W x D)
Query: **h** (shape: D)

How is this different from the attention mechanism in transformers?

We'll go into that next, any questions?

General attention layer – used in LLMs + beyond



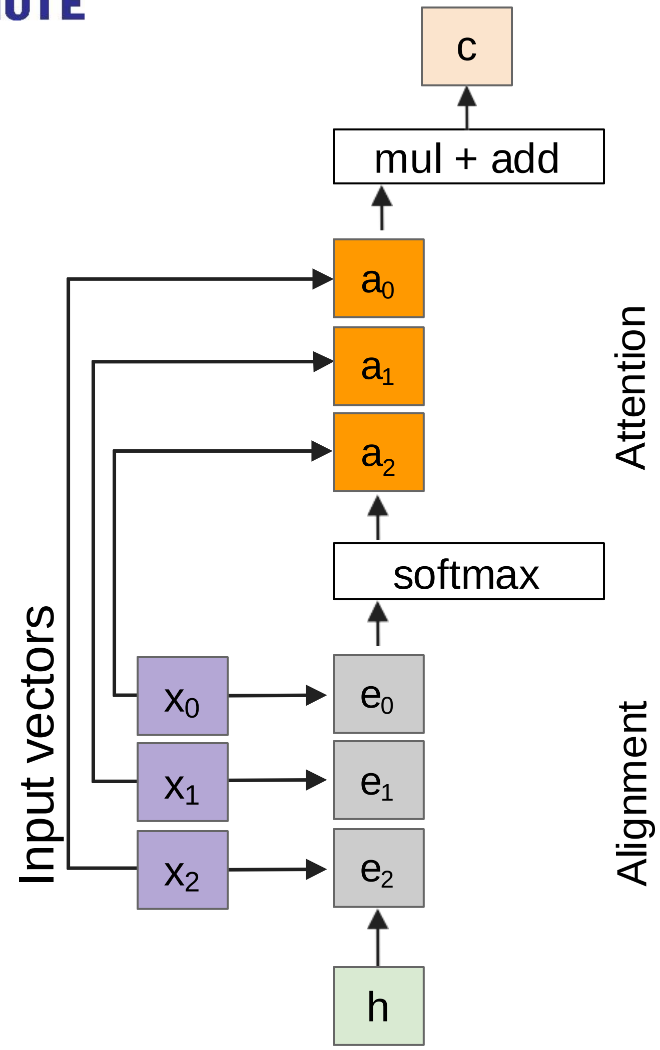
Outputs:
context vector: **c** (shape: D)

Operations:
Alignment: $e_i = f_{att}(h, x_i)$
Attention: $\mathbf{a} = \text{softmax}(\mathbf{e})$
Output: $\mathbf{c} = \sum_i a_i x_i$

Inputs:
Input vectors: **x** (shape: N x D)
Query: **h** (shape: D)

Attention operation is **permutation invariant.**
- Doesn't care about ordering of the features
- Stretch into **N = H x W** vectors

General attention layer



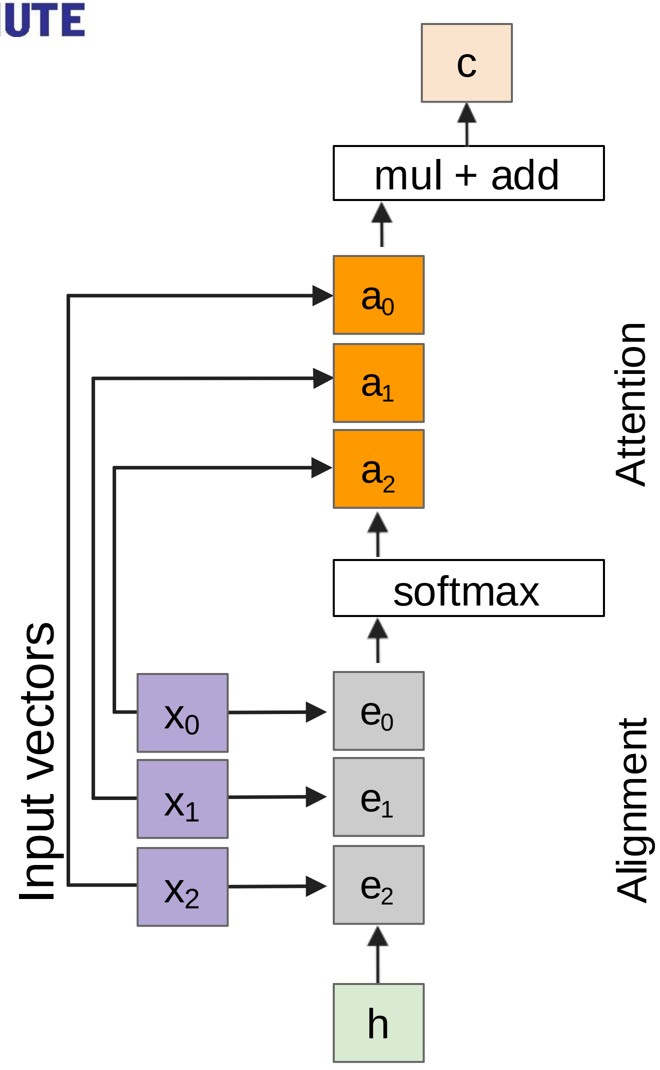
Outputs:
context vector: **c** (shape: D)

Operations:
$\boxed{\text{Alignment: } e_i = h \cdot x_i}$
Attention: **a** = softmax(**e**)
Output: **c** = $\sum_i a_i x_i$

Change $f_{att}(.)$ to a dot product, this actually can work well in practice, but a simple dot product can have some issues…

Inputs:
Input vectors: **x** (shape: N x D)
Query: **h** (shape: D)

General attention layer



Outputs:
context vector: **c** (shape: D)

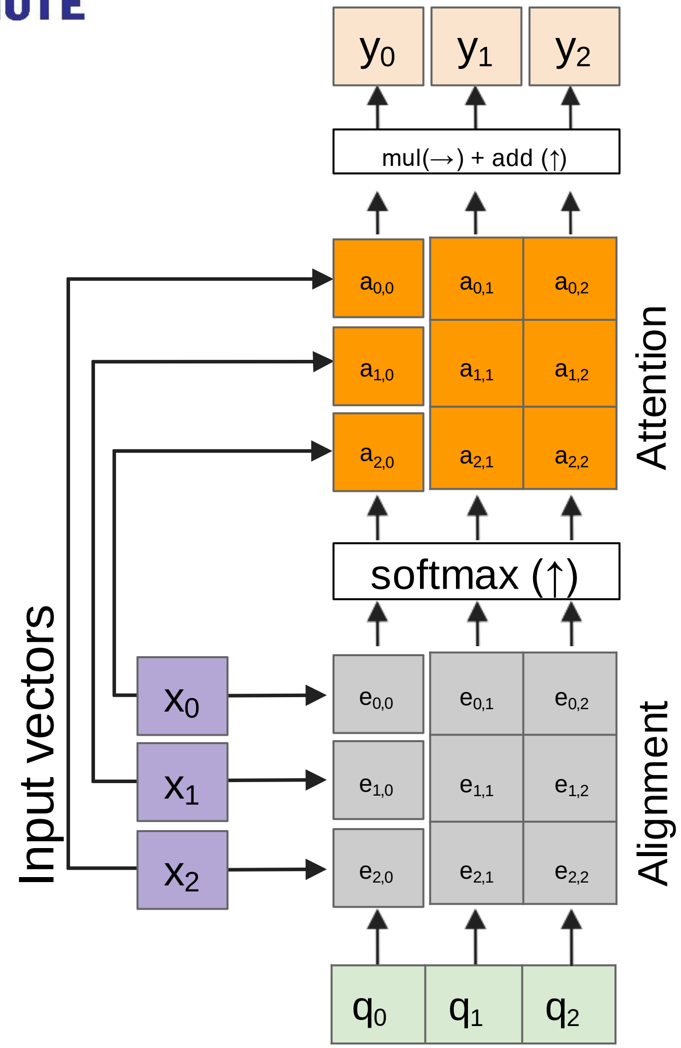
Operations:
Alignment: $e_i = h \cdot x_i / \sqrt{D}$
Attention: $\mathbf{a} = \text{softmax}(\mathbf{e})$
Output: $\mathbf{c} = \sum_i a_i x_i$

Inputs:
Input vectors: **x** (shape: N x D)
Query: **h** (shape: D)

Change $f_{att}(.)$ to a scaled simple dot product

- Larger dimensions means more terms in the dot product sum.
- So, the variance of the logits is higher. Large magnitude vectors will produce much higher logits.
- So, the post-softmax distribution has lower- entropy
- Ultimately, these large magnitude vectors will cause softmax to peak and assign very little weight to all others
- Divide by $\sqrt{D}$ to reduce effect of large magnitude vectors

General attention layer



Outputs:
context vectors: **y** (shape: D)

Multiple query vectors
- each query creates a new, corresponding output context vector

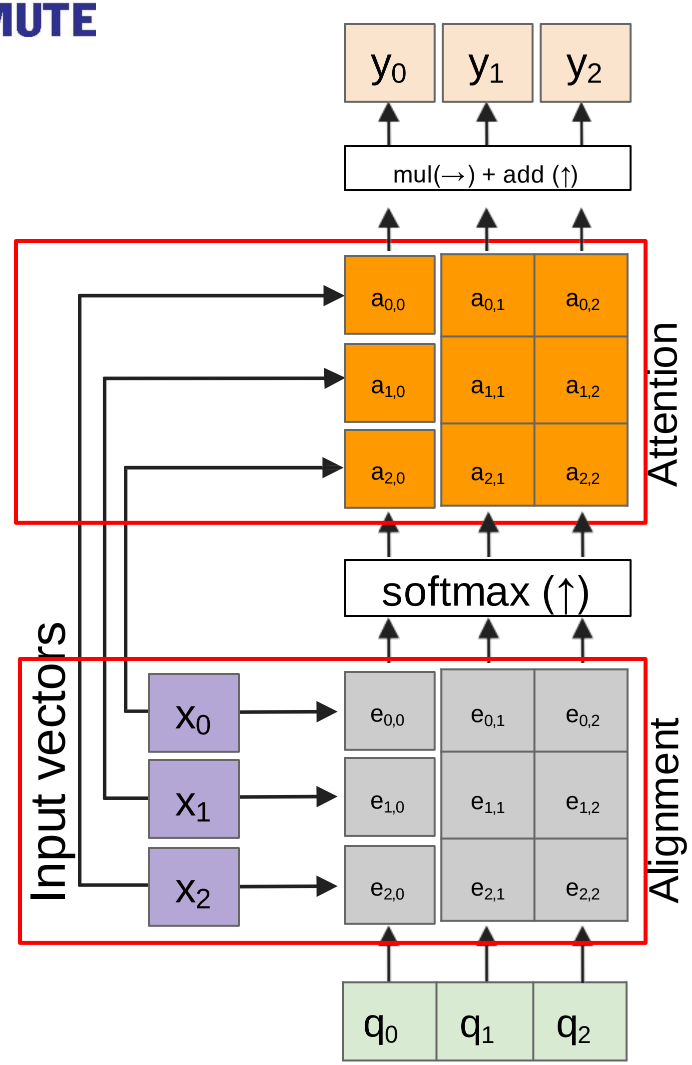
Operations:
Alignment: $e_{i,j} = q_j \cdot x_i / \sqrt{D}$
Attention: **a** = softmax(**e**)
Output: $y_j = \sum_i a_{i,j} x_i$

Allows us to compute multiple attention context vectors at once
Will go into more details in future slides, but this allows us to compute context vectors for multiple timesteps in parallel

Inputs:
Input vectors: **x** (shape: N x D)
Queries: **q** (shape: M x D)

Multiple query vectors

General attention layer



Outputs:
context vectors: **y** (shape: D)

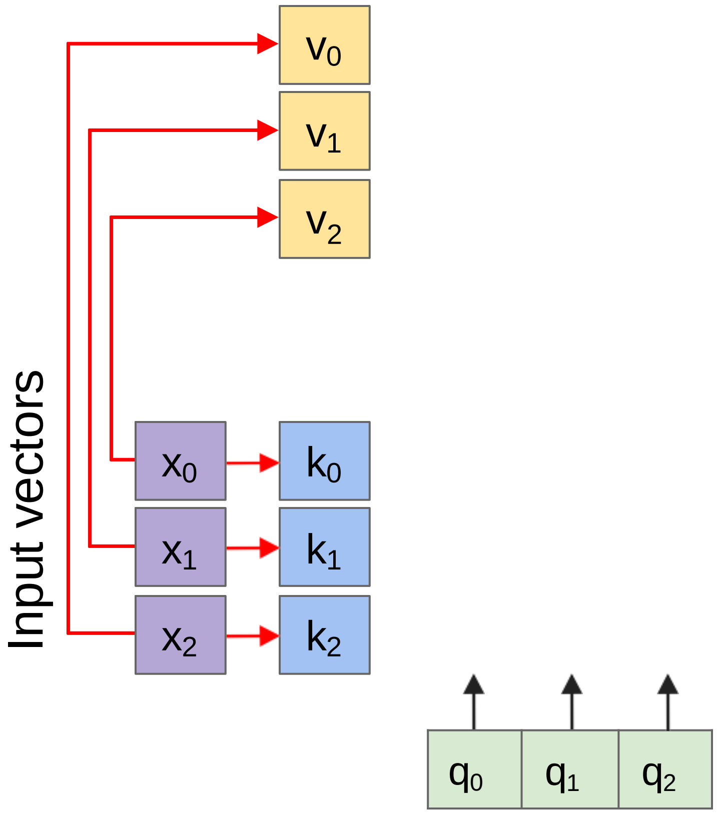
Operations:
Alignment: $e_{i,j} = q_j \cdot x_i / \sqrt{D}$
Attention: **a** = softmax(**e**)
Output: $y_j = \sum_i a_{i,j} x_i$

Inputs:
Input vectors: **x** (shape: N x D)
Queries: **q** (shape: M x D)

Notice that the input vectors are used for **both the alignment as well as the attention** calculations.

- We can add more expressivity to the layer by adding a different FC layer before each of the two steps.

General attention layer



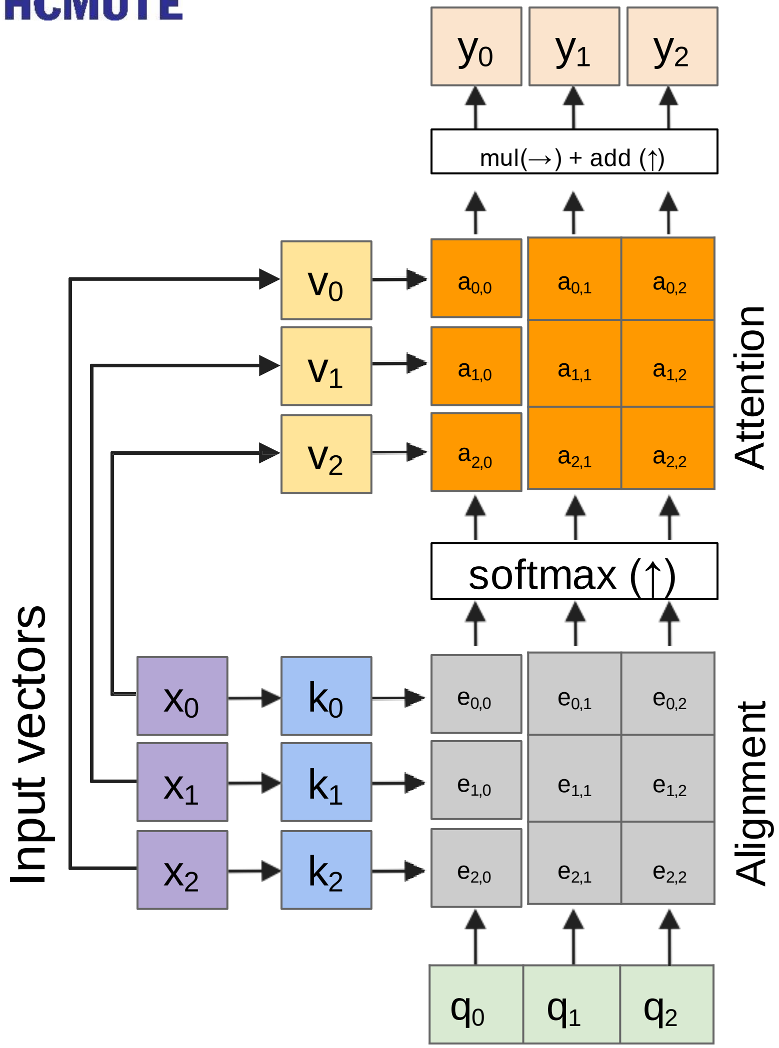
Operations:
Key vectors: $\mathbf{k} = \mathbf{x}W_k$
Value vectors: $\mathbf{v} = \mathbf{x}W_v$

Notice that the input vectors are used for both the alignment as well as the attention calculations.

- We can add more expressivity to the layer by adding a different FC layer before each of the two steps.

Inputs:
Input vectors: **x** (shape: N x D)
Queries: **q** (shape: M x D_k)

General attention layer



Outputs:
context vectors: **y** (shape: $\boxed{D_v}$)

The input and output dimensions can now change depending on the key and value FC layers

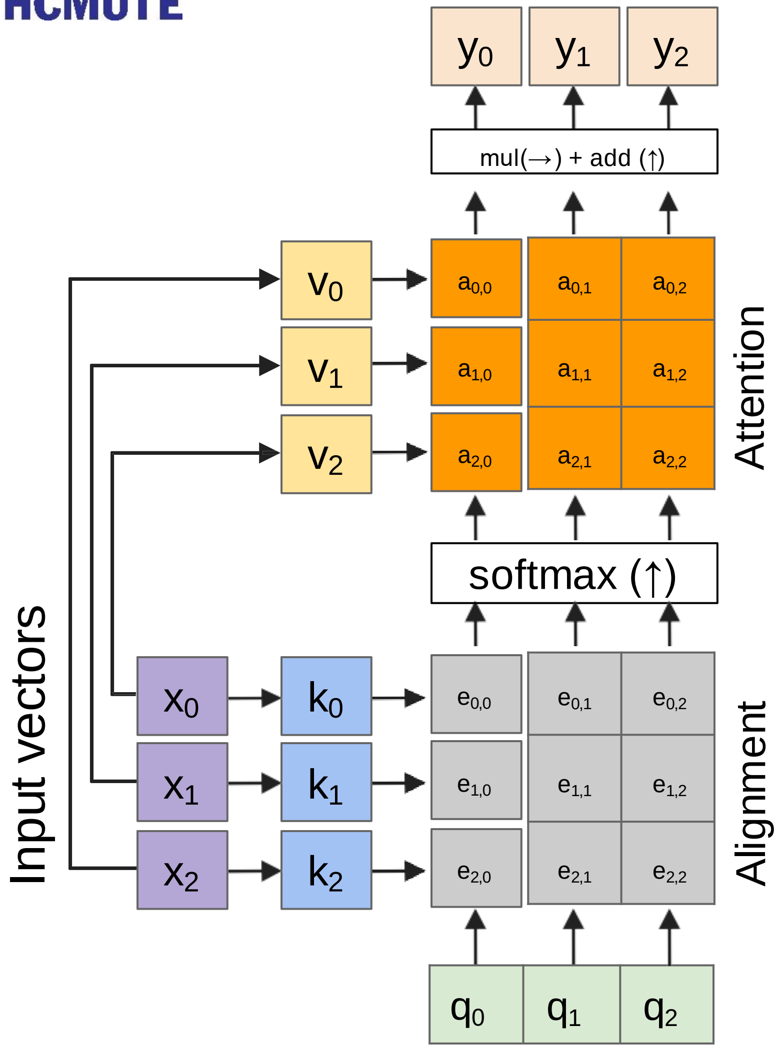
Operations:
Key vectors: $\mathbf{k} = \mathbf{x}\mathbf{W_k}$
Value vectors: $\mathbf{v} = \mathbf{x}\mathbf{W_v}$
Alignment: $e_{i,j} = q_j \cdot k_i / \sqrt{D}$
Attention: $\mathbf{a} = \text{softmax}(\mathbf{e})$
Output: $y_j = \sum_i a_{i,j} v_i$

Since the alignment scores are just scalars, the value vectors can be any dimension we want

Inputs:
Input vectors: **x** (shape: N x D)
Queries: **q** (shape: M x $\boxed{D_k}$)

General attention layer

This is a working example of how we could use an attention layer + CNN encoder for image captioning



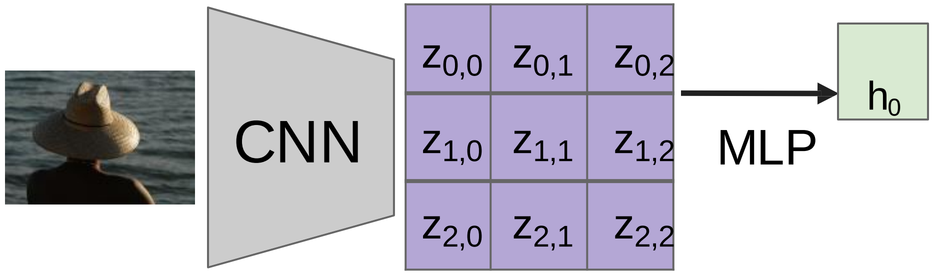
Outputs:
context vectors: **y** (shape: D_v)

Operations:
Key vectors: $\mathbf{k} = \mathbf{x}\mathbf{W_k}$
Value vectors: $\mathbf{v} = \mathbf{x}\mathbf{W_v}$
Alignment: $e_{i,j} = q_j \cdot k_i / \sqrt{D}$
Attention: $\mathbf{a} = \text{softmax}(\mathbf{e})$
Output: $y_j = \sum_i a_{i,j} v_i$

Inputs:
Input vectors: **x** (shape: N x D)
Queries: **q** (shape: M x D_k)

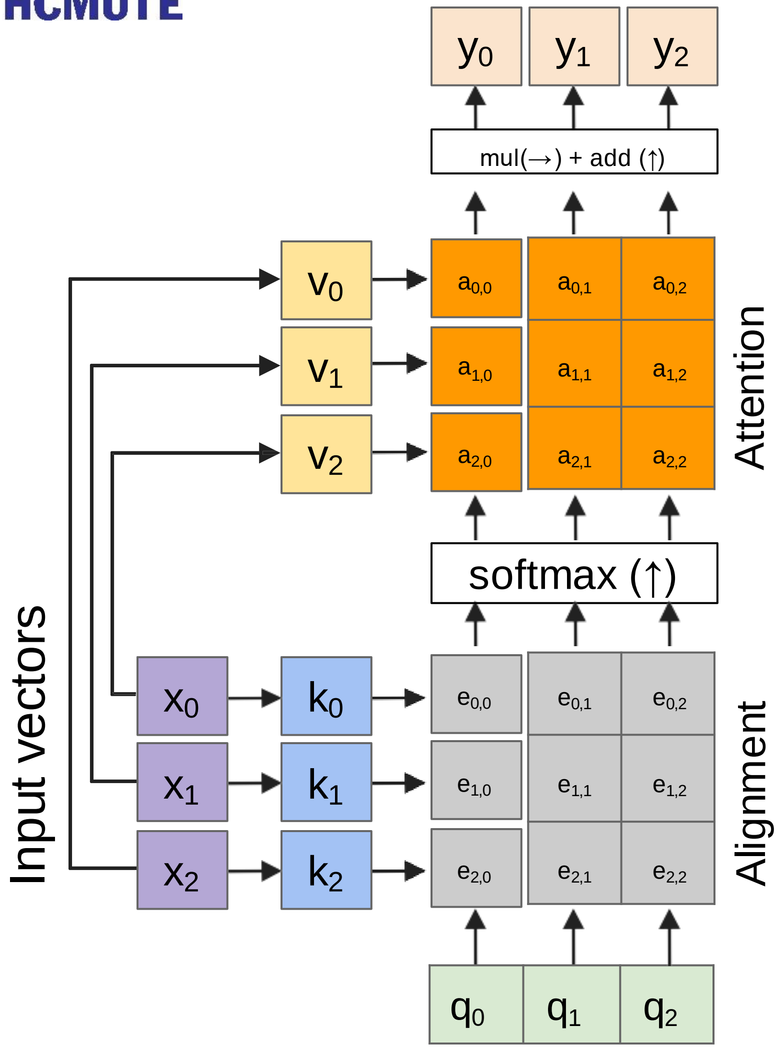
Recall that the query vector was a function of the input vectors

Encoder: $h_0 = f_{\mathbf{W}}(\mathbf{z})$
where **z** is spatial CNN features
$f_{\mathbf{W}}(.)$ is an MLP



We used h_0 as q_0 previously

Next: The Self-attention Layer



Outputs:
context vectors: **y** (shape: D_v)

Operations:
Key vectors: $\mathbf{k} = \mathbf{x}\mathbf{W_k}$
Value vectors: $\mathbf{v} = \mathbf{x}\mathbf{W_v}$
Alignment: $e_{i,j} = q_j \cdot k_i / \sqrt{D}$
Attention: $\mathbf{a} = \text{softmax}(\mathbf{e})$
Output: $y_j = \sum_i a_{i,j} v_i$

Inputs:
Input vectors: **x** (shape: N x D)
Queries: **q** (shape: M x D_k)

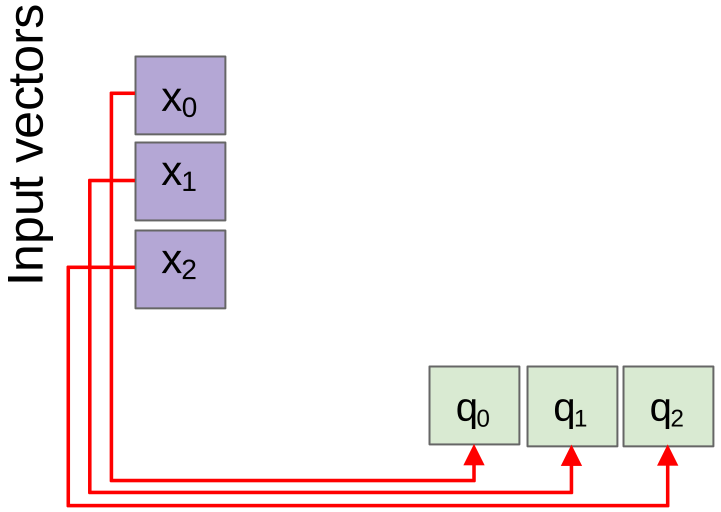
Idea: leverages the strengths of attention layers without the need for separate query vectors.

Self attention layer

We can calculate the query vectors from the input vectors, therefore, defining a "self-attention" layer.

Operations:
Key vectors: $\mathbf{k} = \mathbf{x}\mathbf{W_k}$
Value vectors: $\mathbf{v} = \mathbf{x}\mathbf{W_v}$
$\boxed{\begin{array}{l}\text{Query vectors: } \mathbf{q} = \mathbf{x}\mathbf{W_q} \\ \text{Alignment: } e_{i,j} = q_j \cdot k_i / \sqrt{D}\end{array}}$
Attention: $\mathbf{a} = \text{softmax}(\mathbf{e})$
Output: $y_j = \sum_i a_{i,j} v_i$

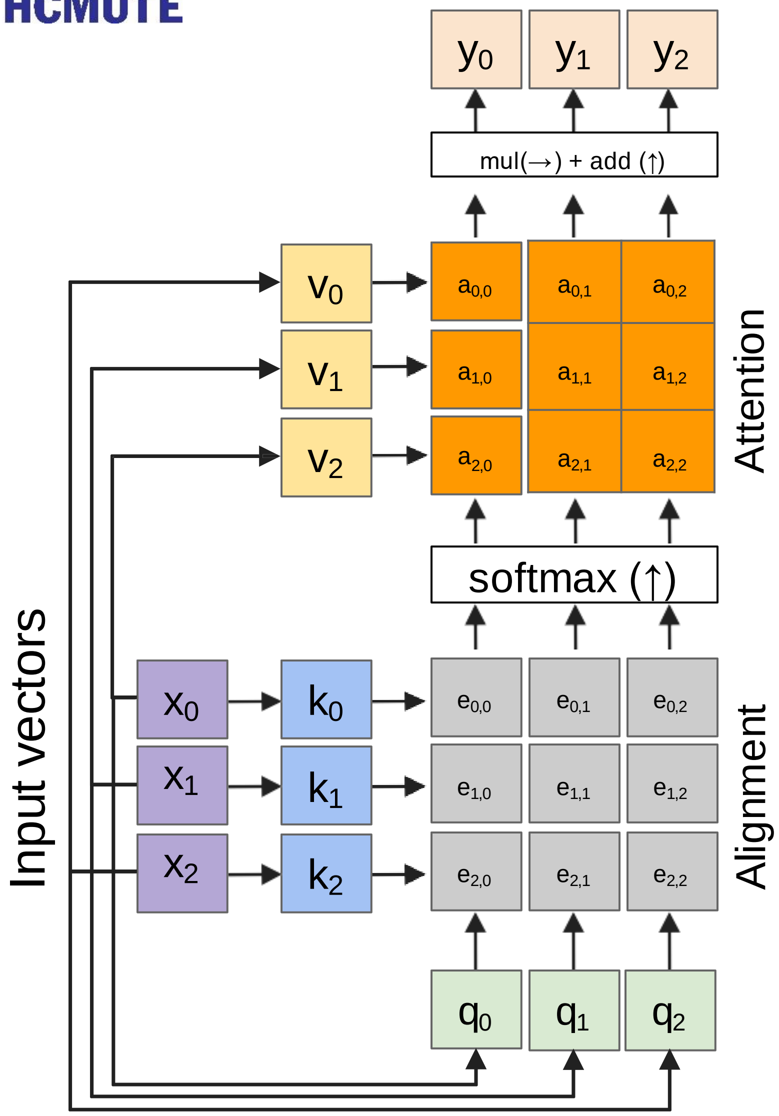
Instead, query vectors are calculated using a FC layer.



No input query vectors anymore

Inputs:
Input vectors: $\mathbf{x}$ (shape: N x D)
$\boxed{\cancel{\text{Queries: } \mathbf{q} \text{ (shape: M x } D_k)}}$

Self attention layer

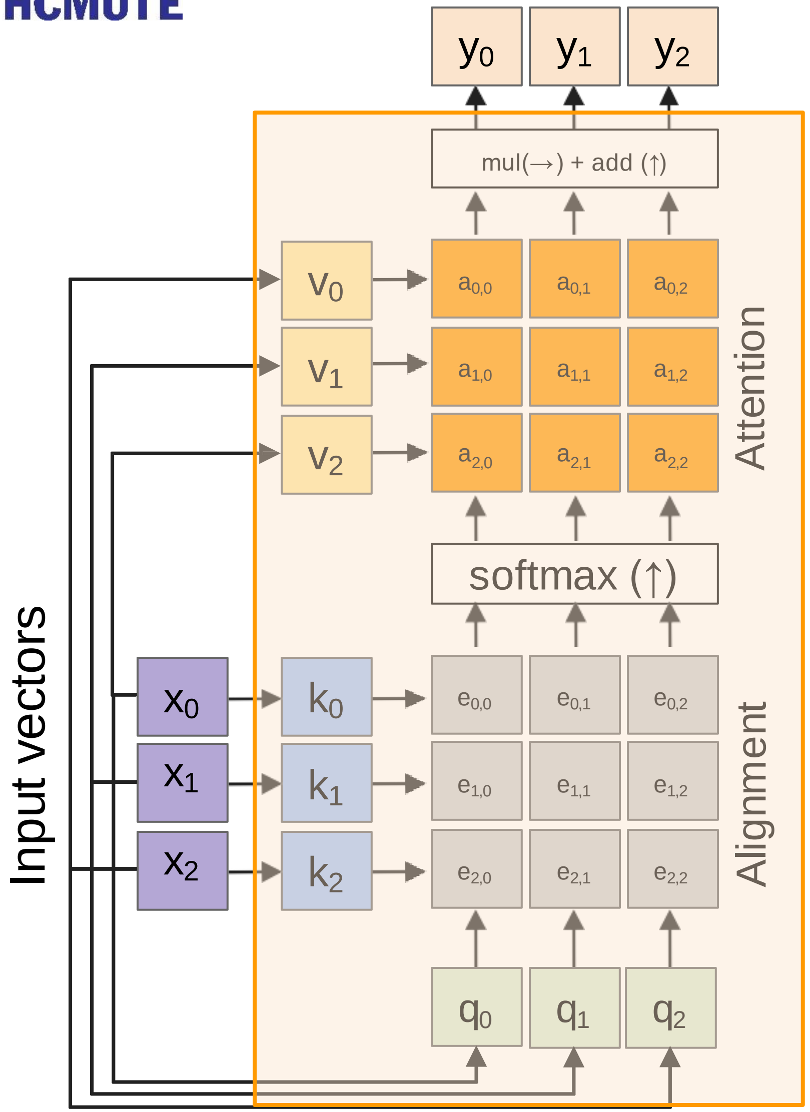


Outputs:
context vectors: **y** (shape: D_v)

Operations:
Key vectors: $\mathbf{k} = \mathbf{x}\mathbf{W_k}$
Value vectors: $\mathbf{v} = \mathbf{x}\mathbf{W_v}$
Query vectors: $\mathbf{q} = \mathbf{x}\mathbf{W_q}$
Alignment: $e_{i,j} = q_j \cdot k_i / \sqrt{D}$
Attention: $\mathbf{a} = \text{softmax}(\mathbf{e})$
Output: $y_j = \sum_i a_{i,j} v_i$

Inputs:
Input vectors: **x** (shape: N x D)

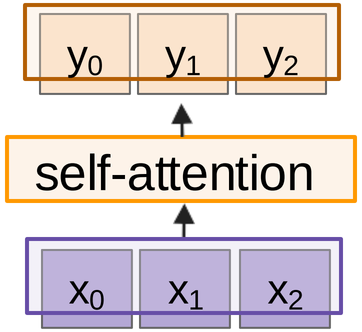
Self attention layer - attends over sets of inputs



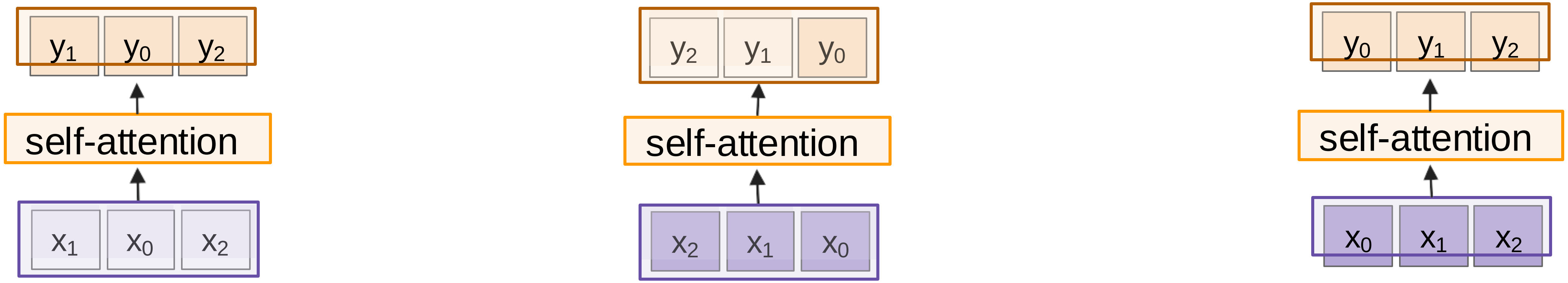
Outputs:
context vectors: **y** (shape: D_v)

Operations:
Key vectors: $\mathbf{k} = \mathbf{x}\mathbf{W_k}$
Value vectors: $\mathbf{v} = \mathbf{x}\mathbf{W_v}$
Query vectors: $\mathbf{q} = \mathbf{x}\mathbf{W_q}$
Alignment: $e_{i,j} = q_j \cdot k_i / \sqrt{D}$
Attention: $\mathbf{a} = \text{softmax}(\mathbf{e})$
Output: $y_j = \sum_i a_{i,j} v_i$

Inputs:
Input vectors: **x** (shape: N x D)



Self attention layer - attends over sets of inputs

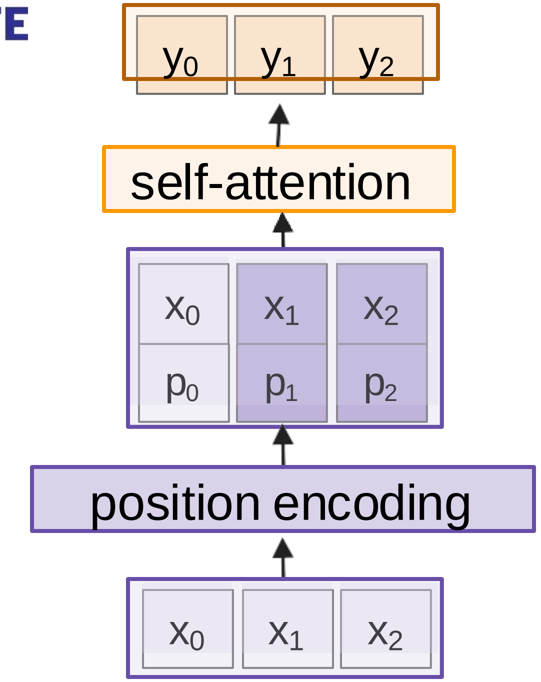


Permutation equivariant

Self-attention layer doesn’t care about the orders of the inputs!

Problem: How can we encode ordered sequences like language or spatially ordered image features?

Positional encoding



Concatenate or **add** special positional encoding p_j to each input vector x_j

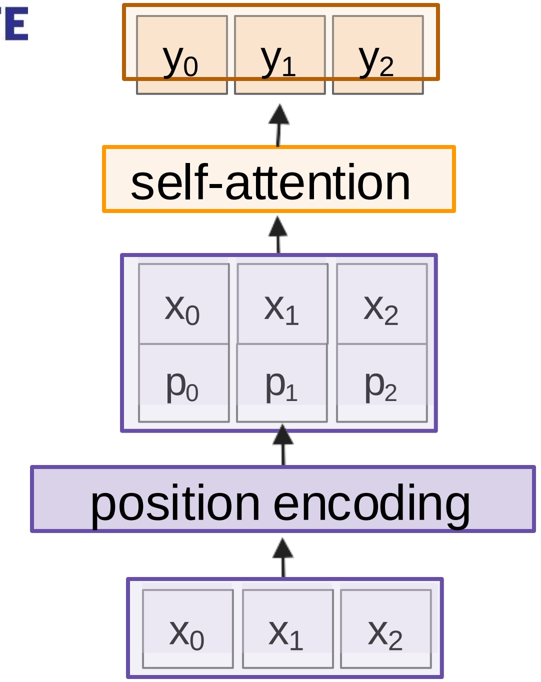
We use a function *pos*: $\mathbb{N} \rightarrow \mathbb{R}^d$ to process the position j of the vector into a d-dimensional vector

So, $p_j = pos(j)$

Possible desirable properties of *pos*(.) :

1. It should output a **unique** encoding for each time-step (word's position in a sentence)
2. **Distance** between any two time-steps should be consistent across sentences with different lengths.
3. Our model should generalize to **longer** sentences without any efforts. Its values should be bounded.
4. It must be **deterministic**.

Positional encoding



Concatenate special positional encoding p_j to each input vector x_j

We use a function *pos*: $N \rightarrow R^d$ to process the position j of the vector into a d-dimensional vector

So, $p_j = pos(j)$

Options for *pos*(.)

1. Learn a lookup table:
   - Learn parameters to use for *pos*(t) for t ε [0, T)
   - Lookup table contains T x d parameters.

Possible desirable properties of *pos*(.) :

1. It should output a **unique** encoding for each time-step (word's position in a sentence)
2. **Distance** between any two time-steps should be consistent across sentences with different lengths.
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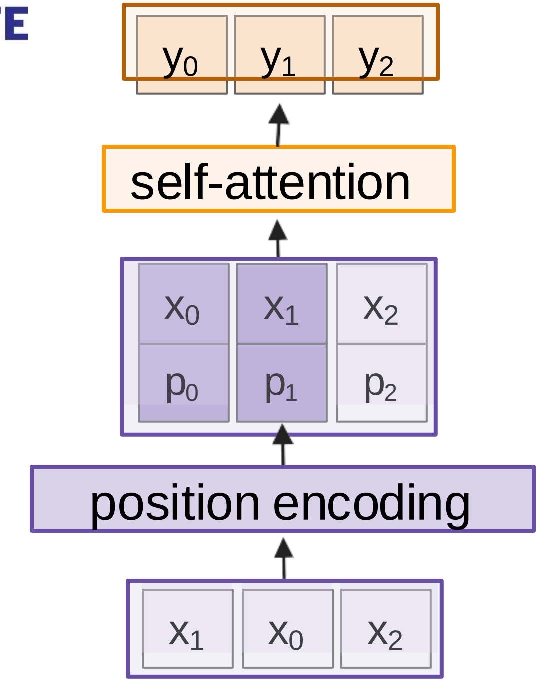
4. It must be **deterministic**.

Positional encoding

Options for *pos*(.)



Concatenate special positional encoding p_j to each input vector x_j

We use a function *pos*: $N \rightarrow R^d$ to process the position j of the vector into a d-dimensional vector

So, $p_j = pos(j)$

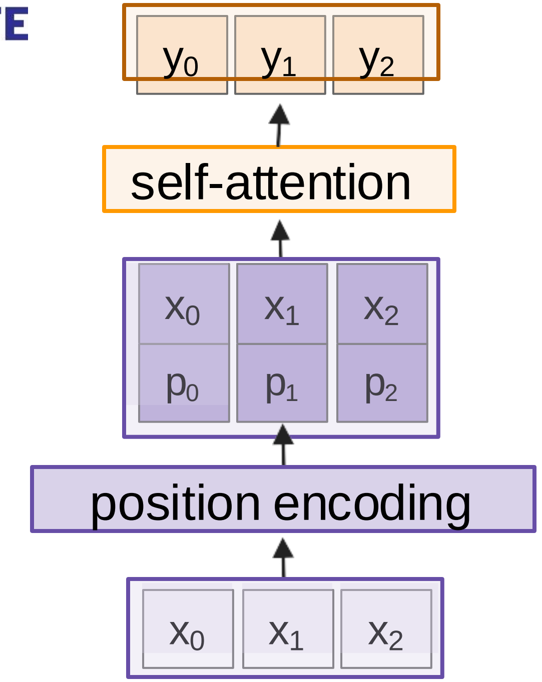
1. Learn a lookup table:
   - Learn parameters to use for *pos*(t) for t ε [0, T)
   - Lookup table contains T x d parameters.

2. Design a fixed function with the desired properties

$$\mathbf{p(t)} = \begin{bmatrix} \sin(\omega_1 . t) \\ \cos(\omega_1 . t) \\ \\ \sin(\omega_2 . t) \\ \cos(\omega_2 . t) \\ \\ \vdots \\ \\ \sin(\omega_{d/2} . t) \\ \cos(\omega_{d/2} . t) \end{bmatrix}_d$$

where $\omega_k = \frac{1}{10000^{2k/d}}$

Positional encoding



Concatenate special positional encoding p_j to each input vector x_j

We use a function $pos: N \rightarrow R^d$ to process the position j of the vector into a d-dimensional vector

So, $p_j = pos(j)$

Options for $pos(.)$

1. Learn a lookup table:
   - Learn parameters to use for $pos(t)$ for $t \in [0, T)$
   - Lookup table contains T x d parameters.

2. Design a fixed function with the desired properties

$$\mathbf{p(t)} = \begin{bmatrix} \sin(\omega_1 . t) \\ \cos(\omega_1 . t) \\ \\ \sin(\omega_2 . t) \\ \cos(\omega_2 . t) \\ \\ \vdots \\ \\ \sin(\omega_{d/2} . t) \\ \cos(\omega_{d/2} . t) \end{bmatrix}_d$$

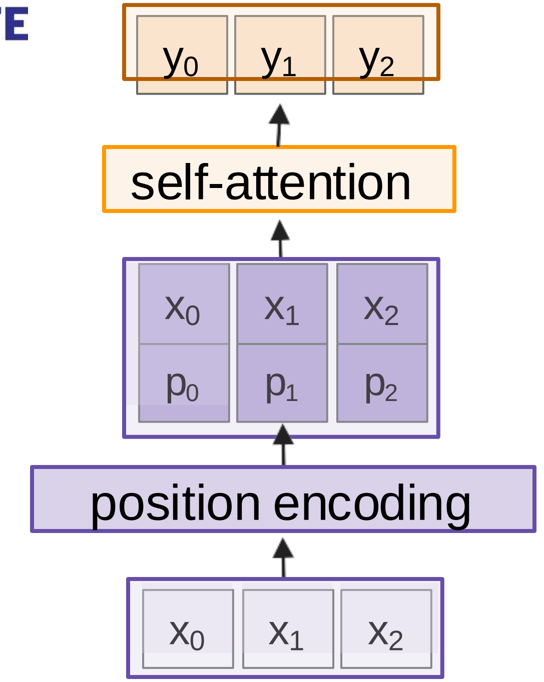
Intuition:

0 :	0 0 0 0	8 :	1 0 0 0
1 :	0 0 0 1	9 :	1 0 0 1
2 :	0 0 1 0	10 :	1 0 1 0
3 :	0 0 1 1	11 :	1 0 1 1
4 :	0 1 0 0	12 :	1 1 0 0
5 :	0 1 0 1	13 :	1 1 0 1
6 :	0 1 1 0	14 :	1 1 1 0
7 :	0 1 1 1	15 :	1 1 1 1

where $\omega_k = \dfrac{1}{10000^{2k/d}}$

Positional encoding

Options for *pos*(.)



Concatenate special positional encoding p_j to each input vector x_j

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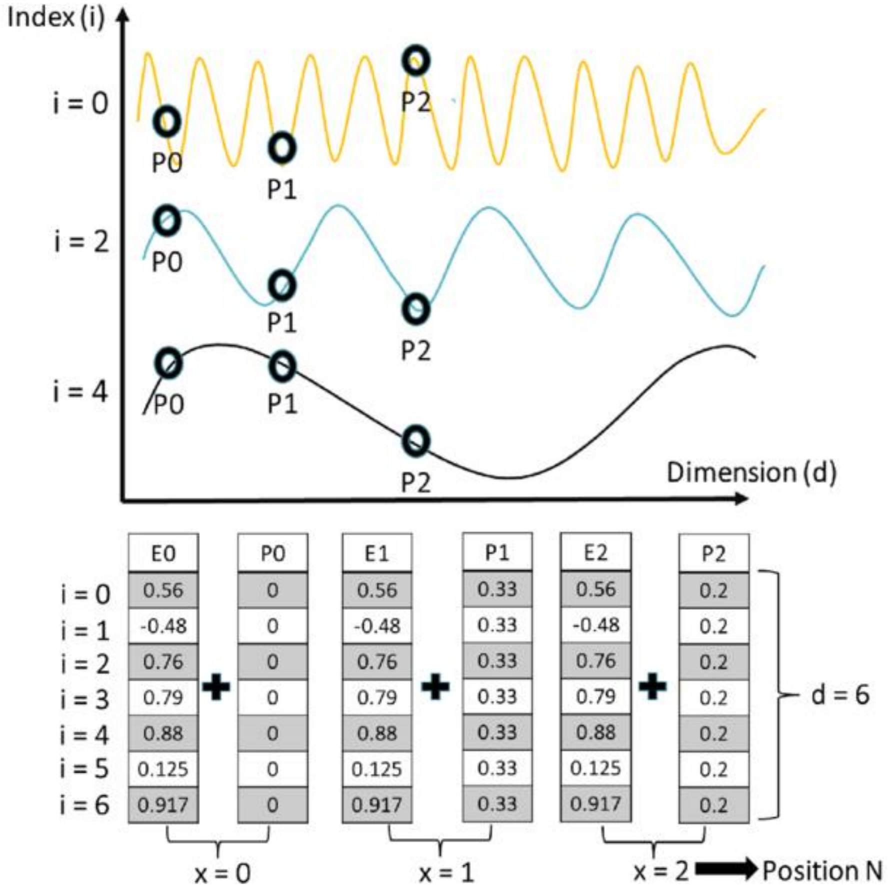
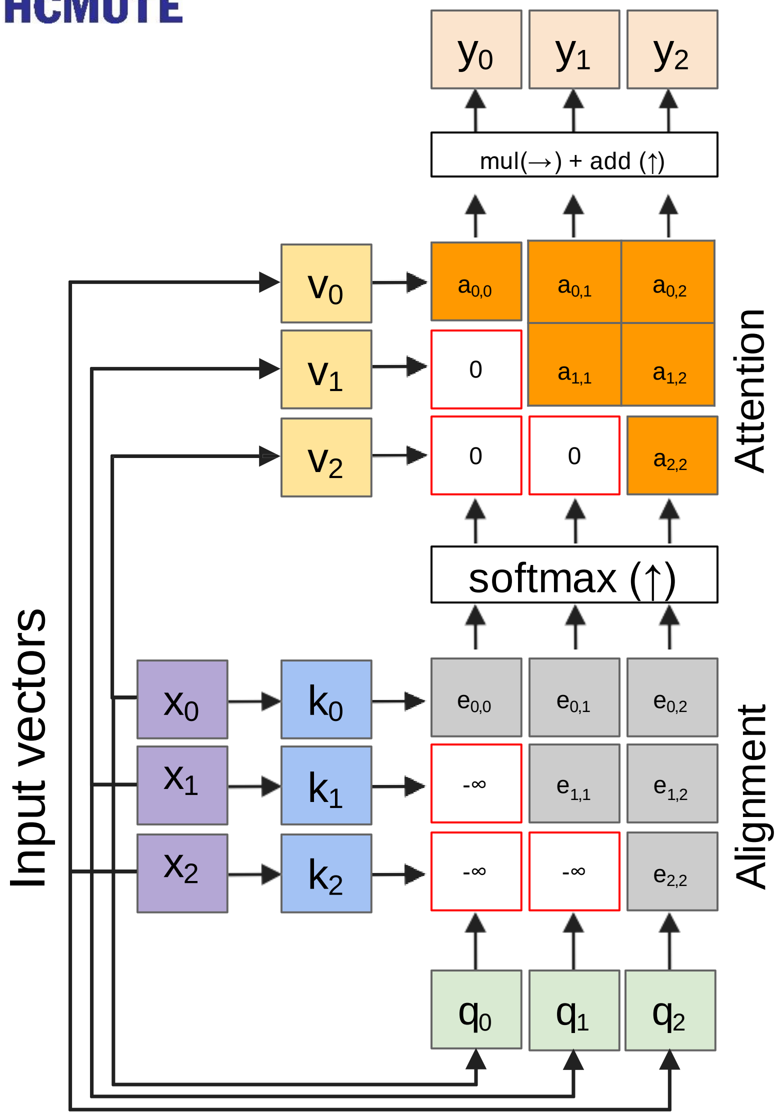


Masked self-attention layer



Outputs:
context vectors: **y** (shape: D_v)

Operations:
Key vectors: $\mathbf{k} = \mathbf{x}\mathbf{W_k}$
Value vectors: $\mathbf{v} = \mathbf{x}\mathbf{W_v}$
Query vectors: $\mathbf{q} = \mathbf{x}\mathbf{W_q}$
Alignment: $e_{i,j} = q_j \cdot k_i / \sqrt{D}$
Attention: $\mathbf{a} = \text{softmax}(\mathbf{e})$
Output: $y_j = \sum_i a_{i,j} v_i$

Inputs:
Input vectors: **x** (shape: N x D)

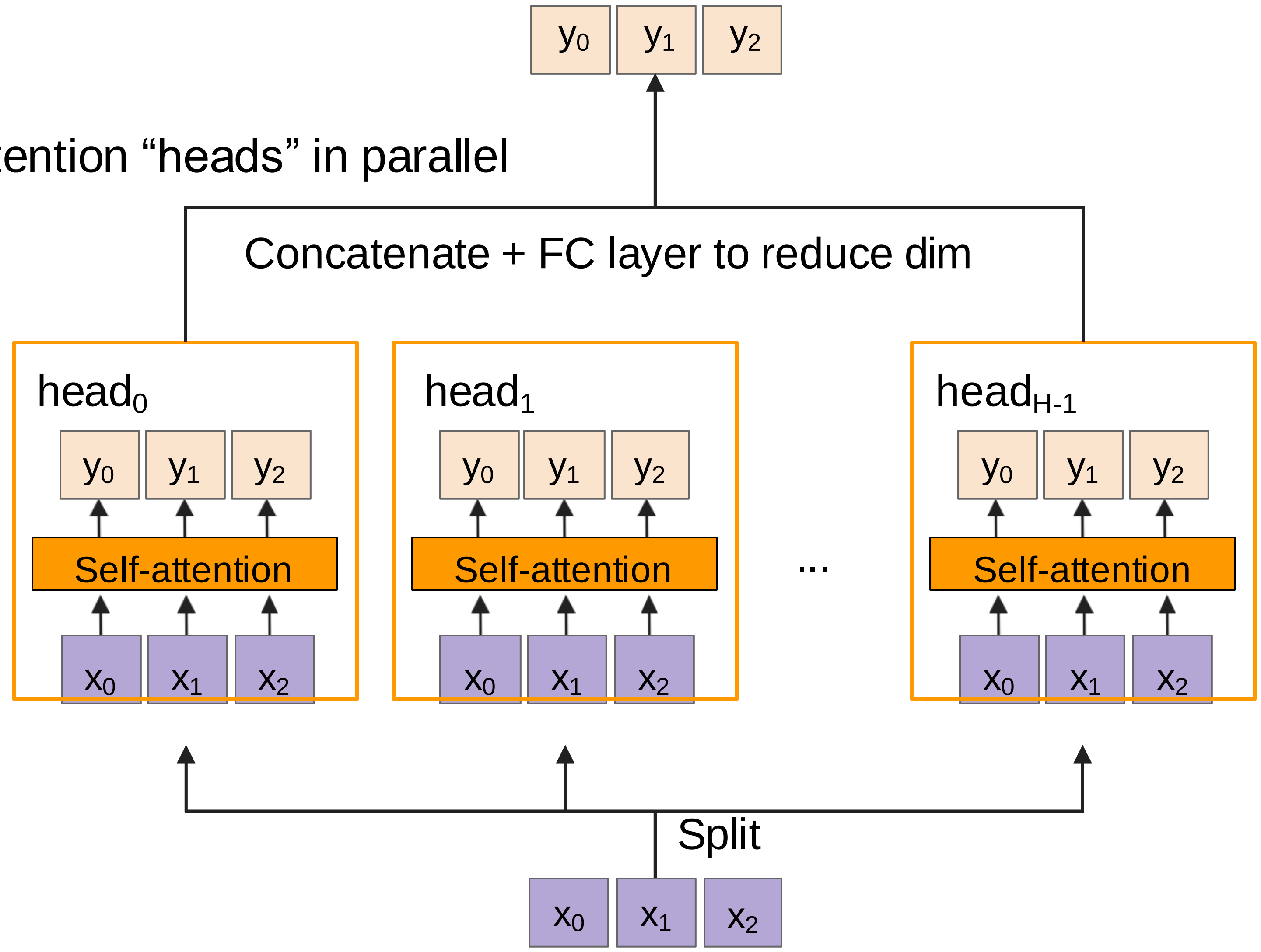
- Allows us to parallelize attention across time
- Don’t need to calculate the context vectors from the previous timestep first!

- Prevent vectors from looking at future vectors.
- Manually set alignment scores to –infinity (-nan)

Multi-head self-attention layer

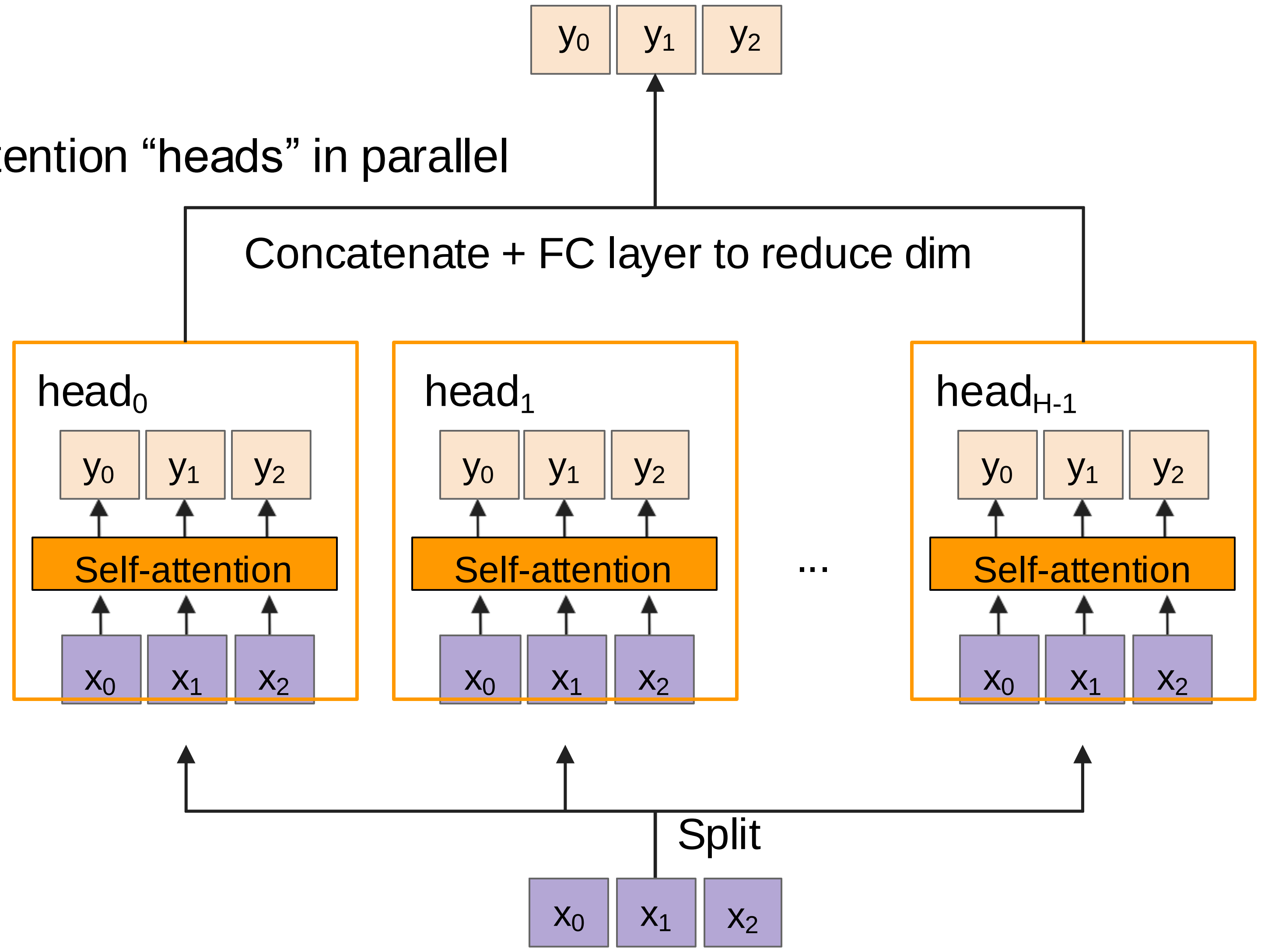
Multiple self-attention “heads” in parallel

Q: Why do this?



Multi-head self-attention layer

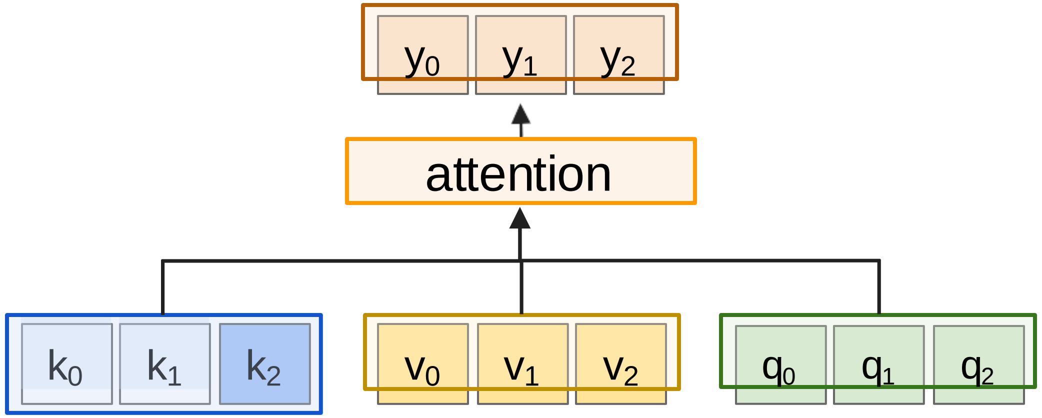
Multiple self-attention “heads” in parallel

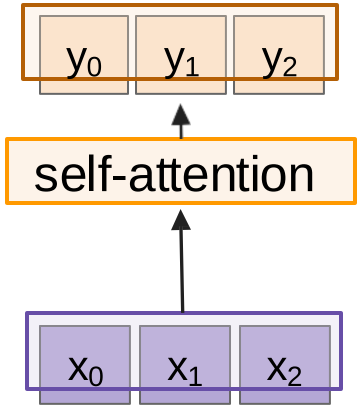


A: We may want to have multiple sets of queries/keys/values calculated in the layer. This is a similar idea to having multiple conv filters learned in a layer

General attention versus self-attention

Transformer models rely on many, stacked self-attention layers





Comparing RNNs to Transformer

- RNNs

(+) LSTMs work reasonably well for long sequences.

(-) Expects an ordered sequences of inputs

(-) Sequential computation: subsequent hidden states can only be computed after the previous ones are done.

- Transformer:

(+) Good at long sequences. Each attention calculation looks at all inputs.
(+) Can operate over unordered sets or ordered sequences with positional encodings.

(+) Parallel computation: All alignment and attention scores for all inputs can be done in parallel.

(-) Requires a lot of memory: N x M alignment and attention scalers need to be calculated and stored for a single self-attention head. (but GPUs are getting bigger and better)

Attention Is All You Need

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"ImageNet Moment for Natural Language Processing"

Pretraining:
Download a lot of text from the internet

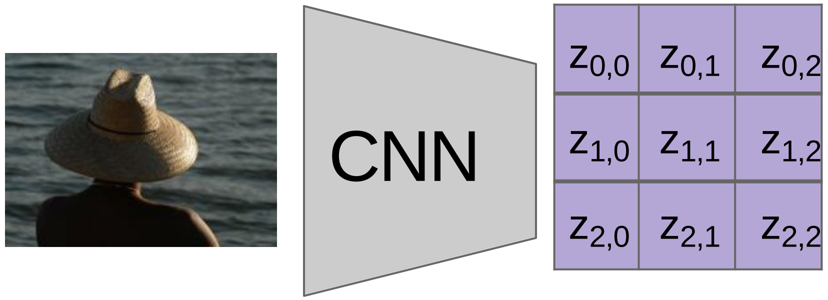
Train a giant Transformer model for language modeling

Finetuning:
Fine-tune the Transformer on your own NLP task

Image Captioning using Transformers

Input: Image **I**

Output: Sequence $\mathbf{y} = y_1, y_2, \ldots, y_T$



Extract spatial features from a pretrained CNN

Features: H x W x D

Image Captioning using Transformers

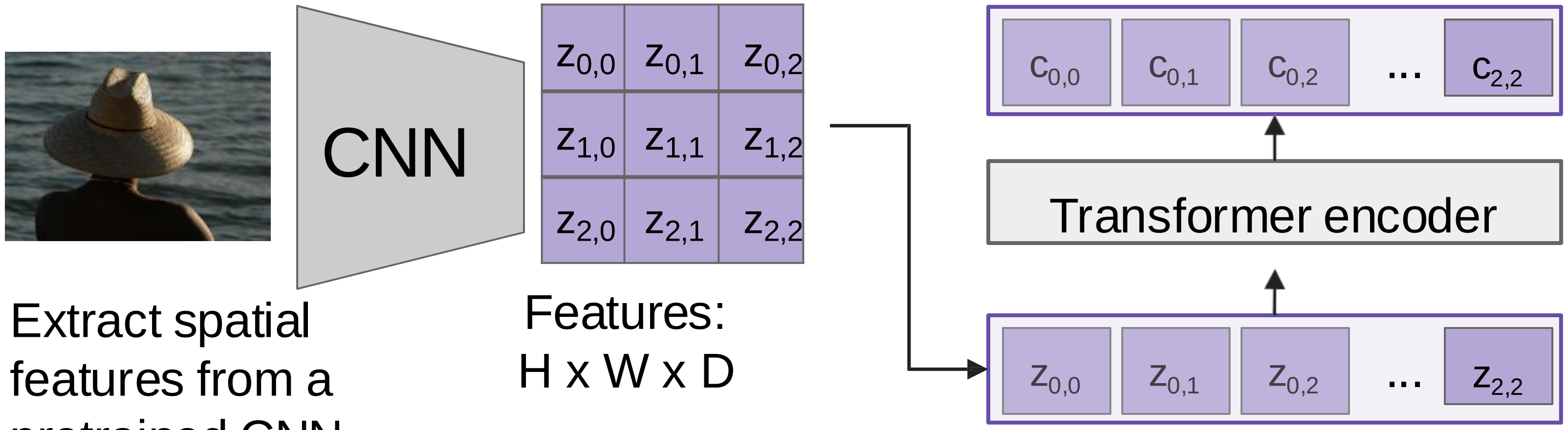
Input: Image **I**

Output: Sequence $\mathbf{y} = y_1, y_2, \ldots, y_T$

Encoder: $\mathbf{c} = T_W(\mathbf{z})$

where $\mathbf{z}$ is spatial CNN features

$T_W(\mathbf{.})$ is the transformer encoder



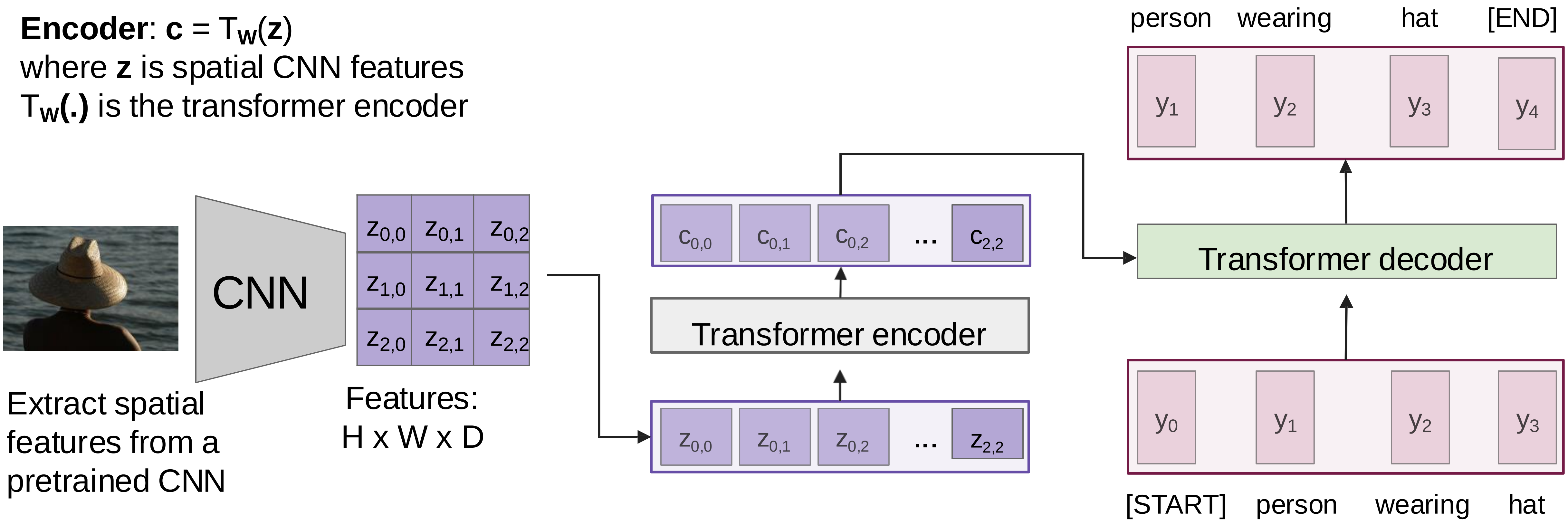
Extract spatial features from a pretrained CNN

Image Captioning using Transformers

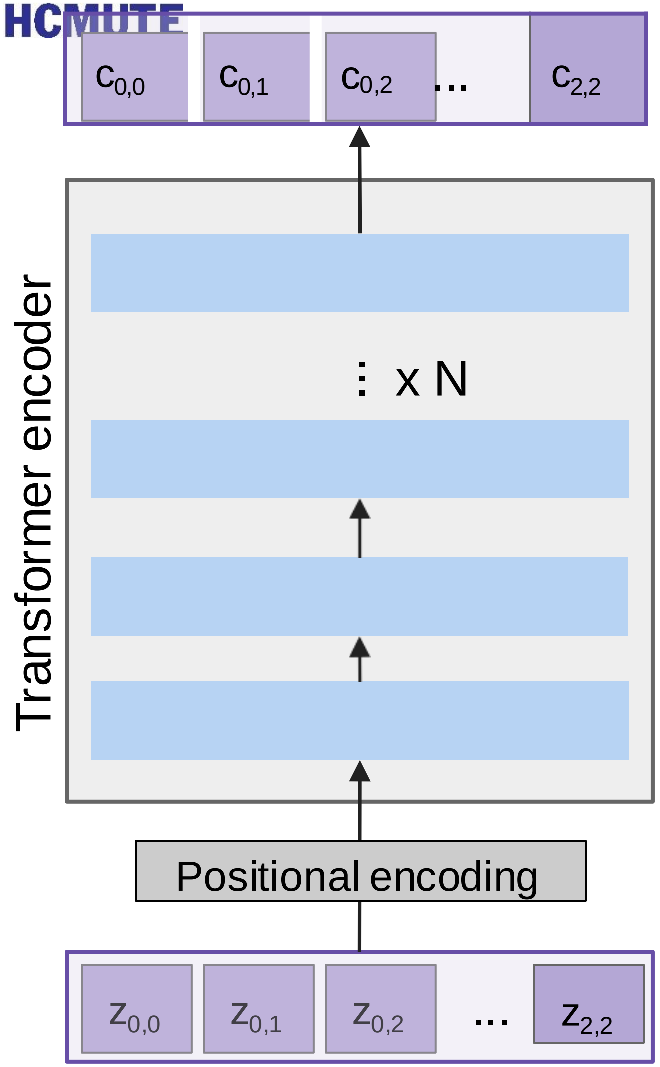
Input: Image **I**
Output: Sequence $\mathbf{y} = y_1, y_2, \ldots, y_T$

Decoder: $y_t = T_D(\mathbf{y}_{0:t-1}, \mathbf{c})$
where $T_D(.)$ is the transformer decoder

Encoder: $\mathbf{c} = T_W(\mathbf{z})$
where **z** is spatial CNN features
$T_W(.)$ is the transformer encoder



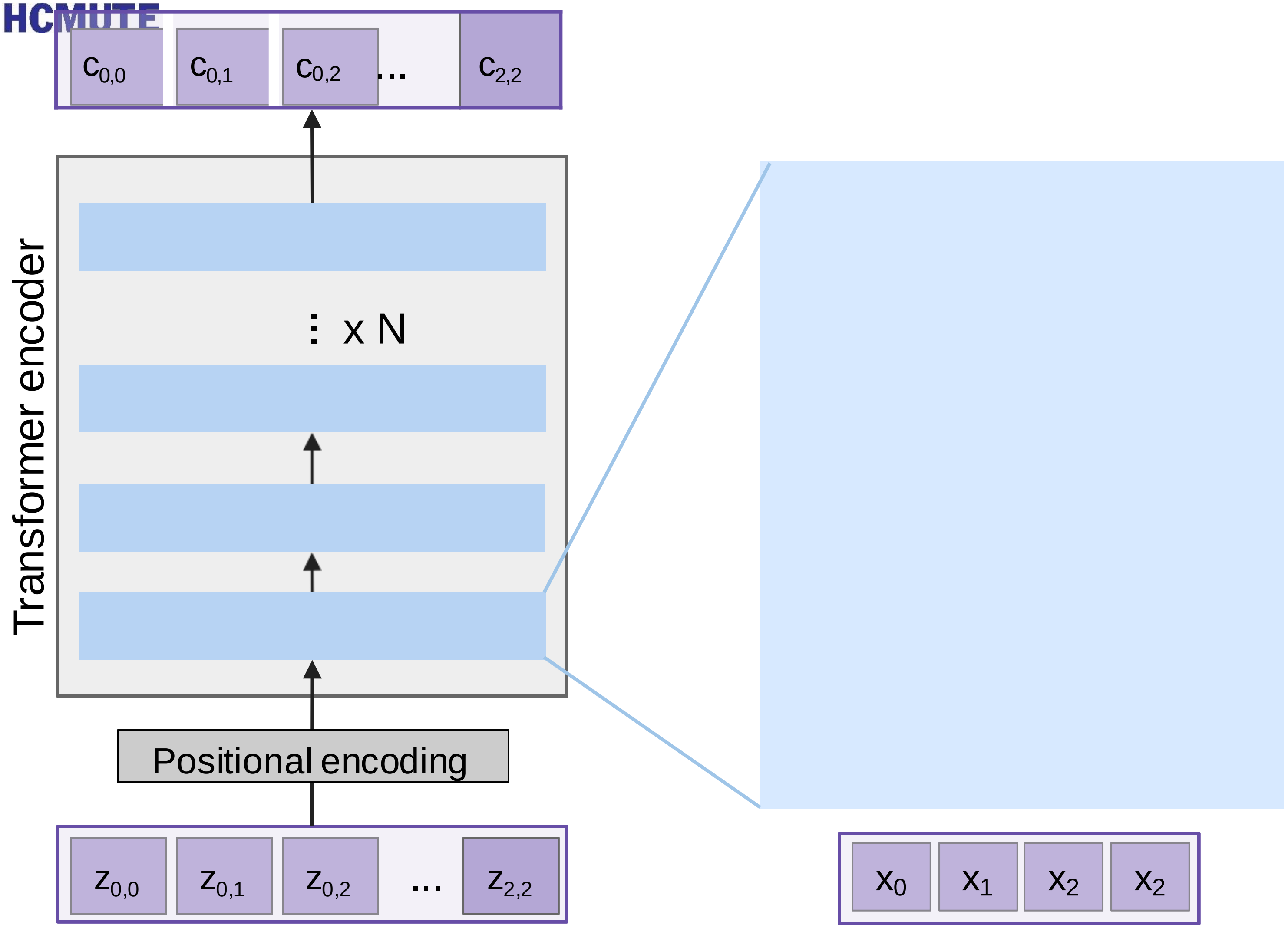
The Transformer encoder block



Made up of N encoder blocks.

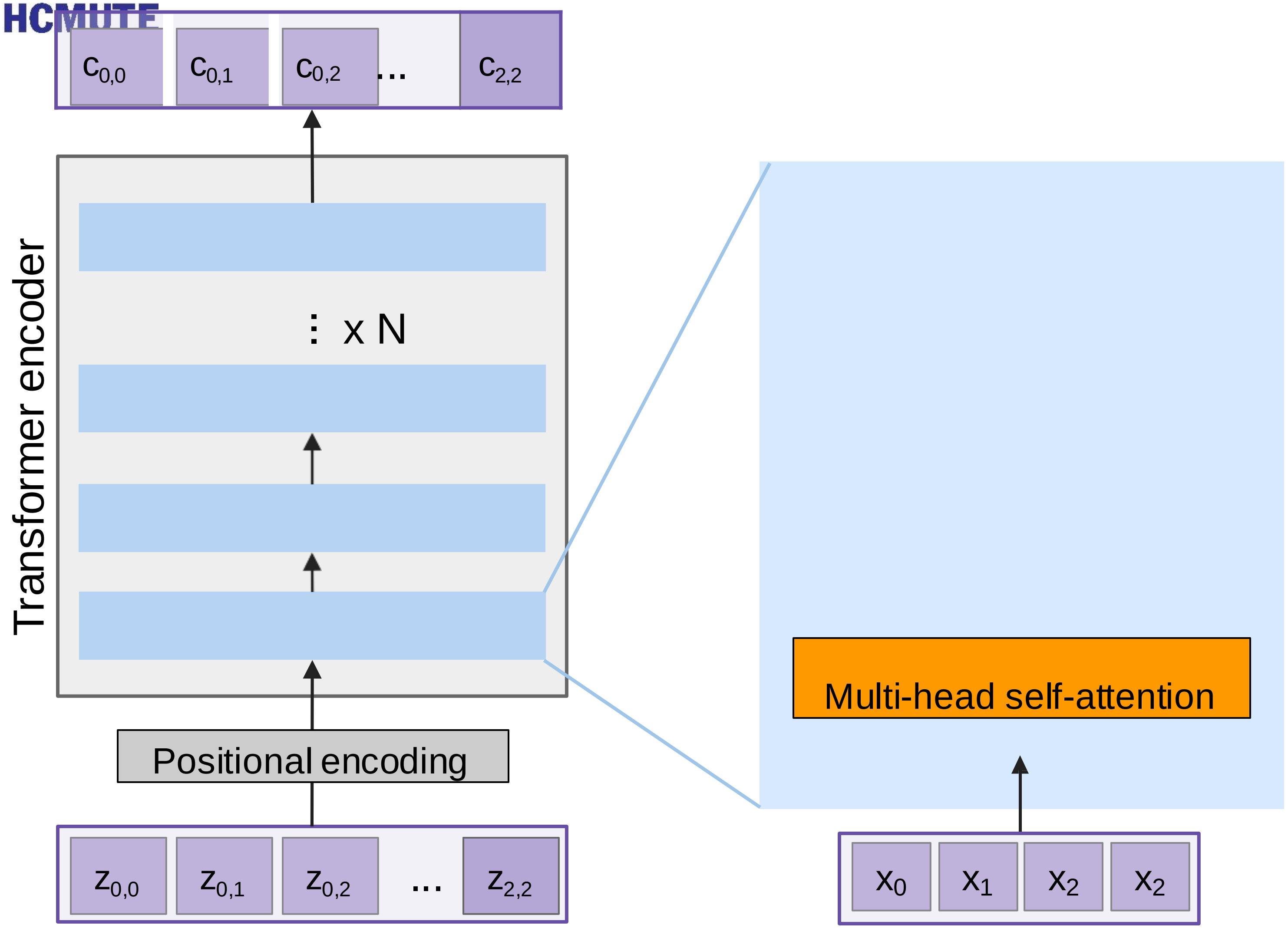
In vaswani et al. N = 6, D_q= 512

The Transformer encoder block



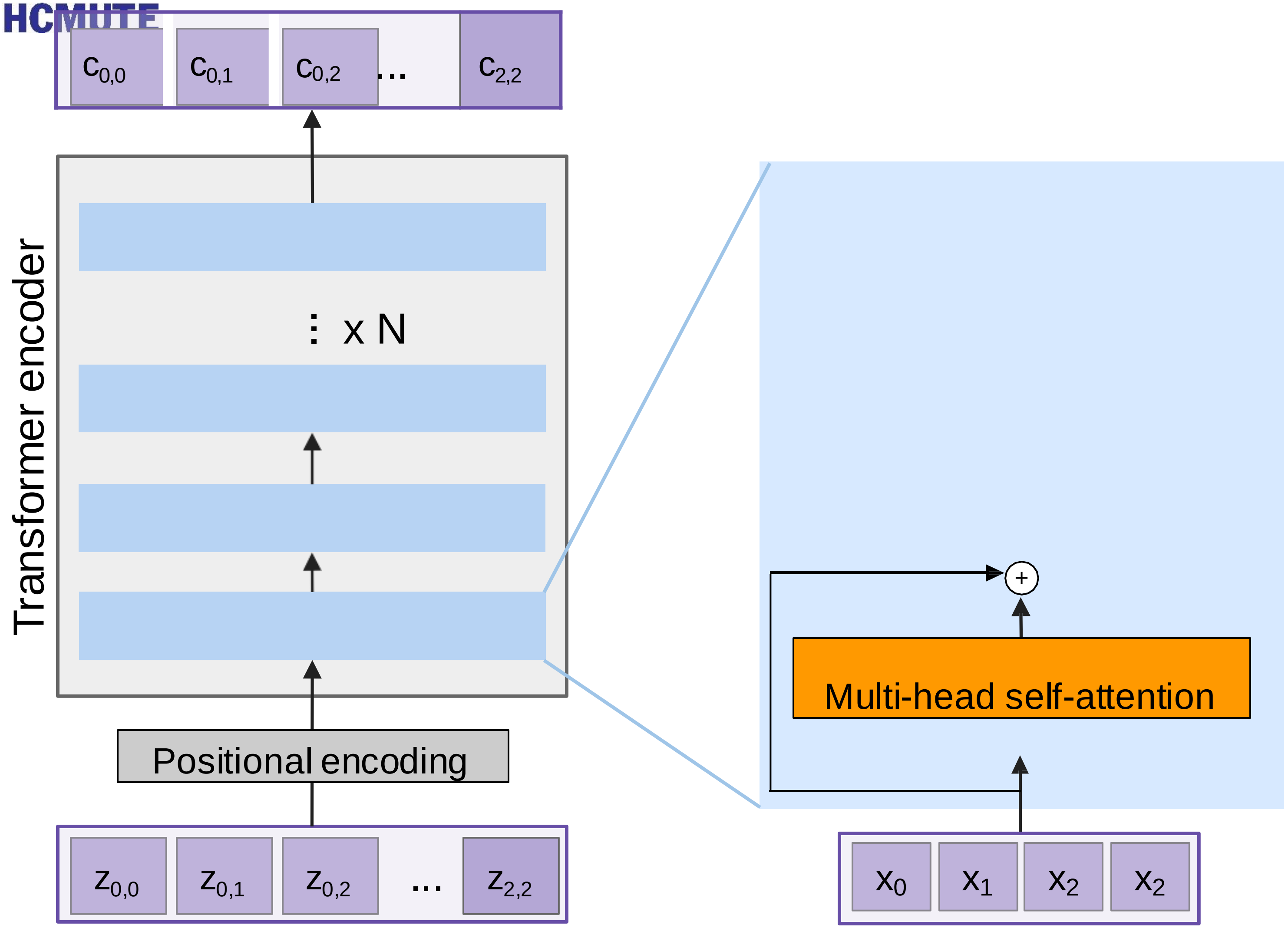
Let's dive into one encoder block

The Transformer encoder block



Attention attends over all the vectors

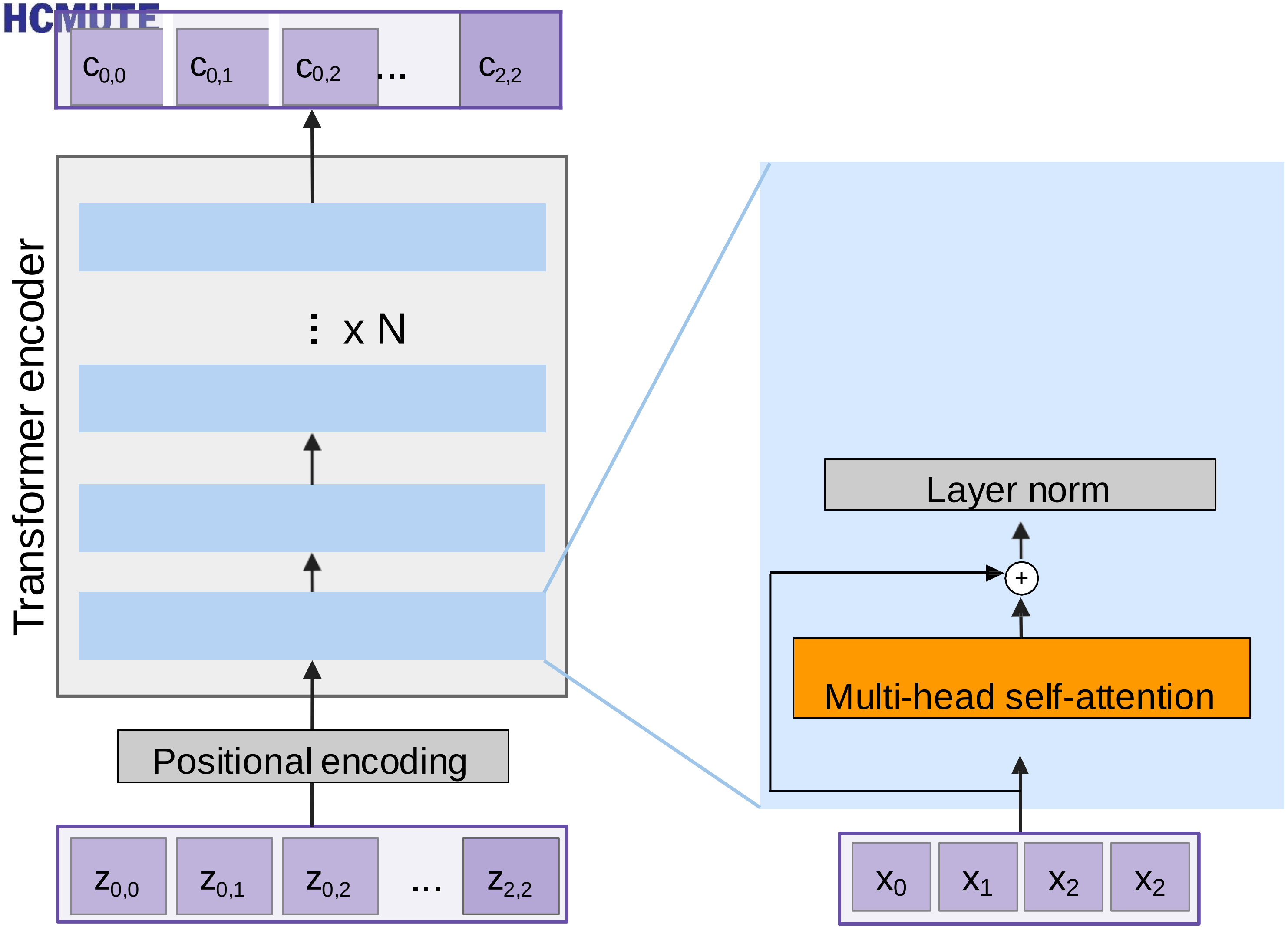
The Transformer encoder block



Residual connection

Attention attends over all the vectors

The Transformer encoder block

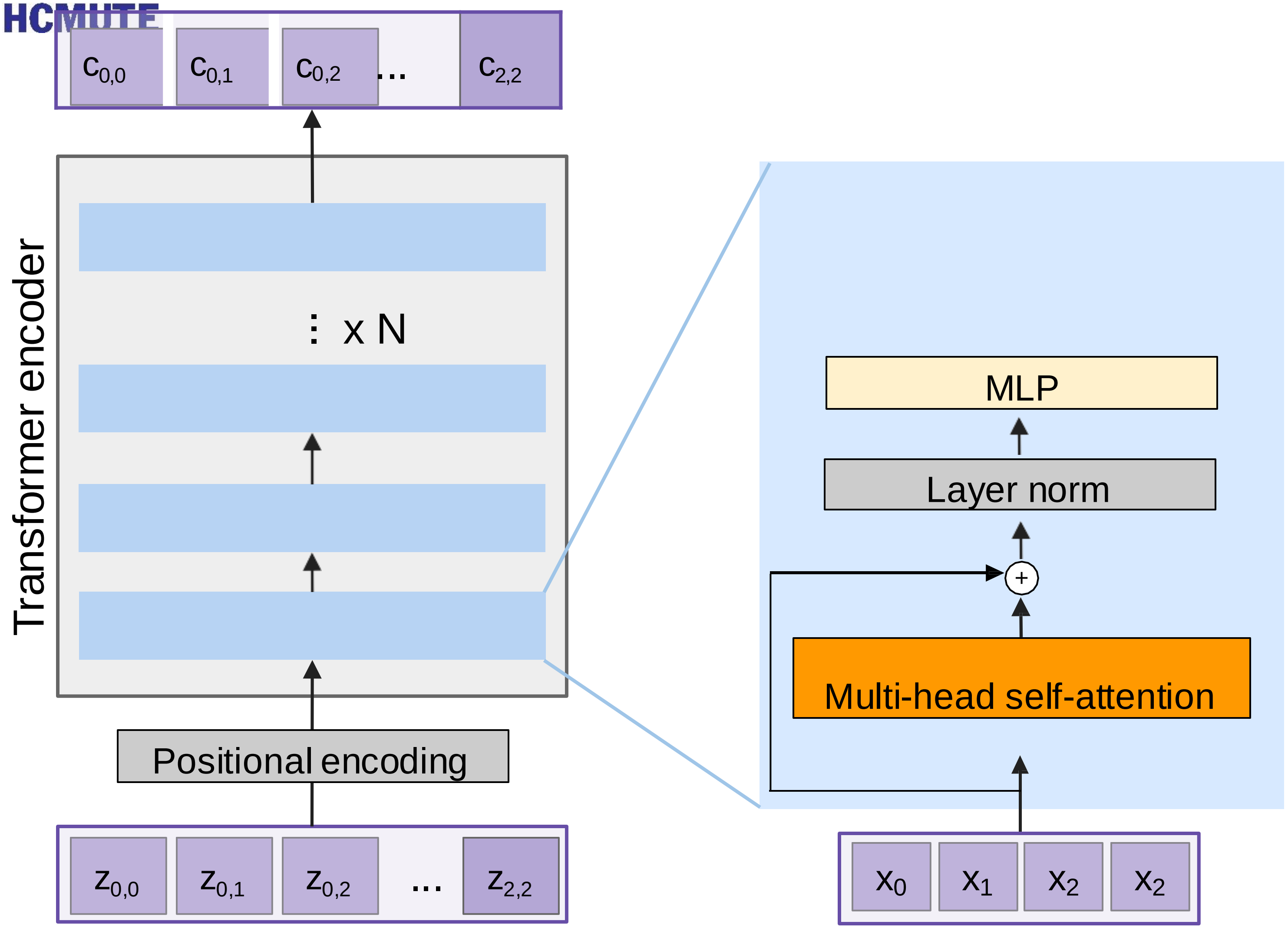


LayerNorm over each vector individually

Residual connection

Attention attends over all the vectors

The Transformer encoder block



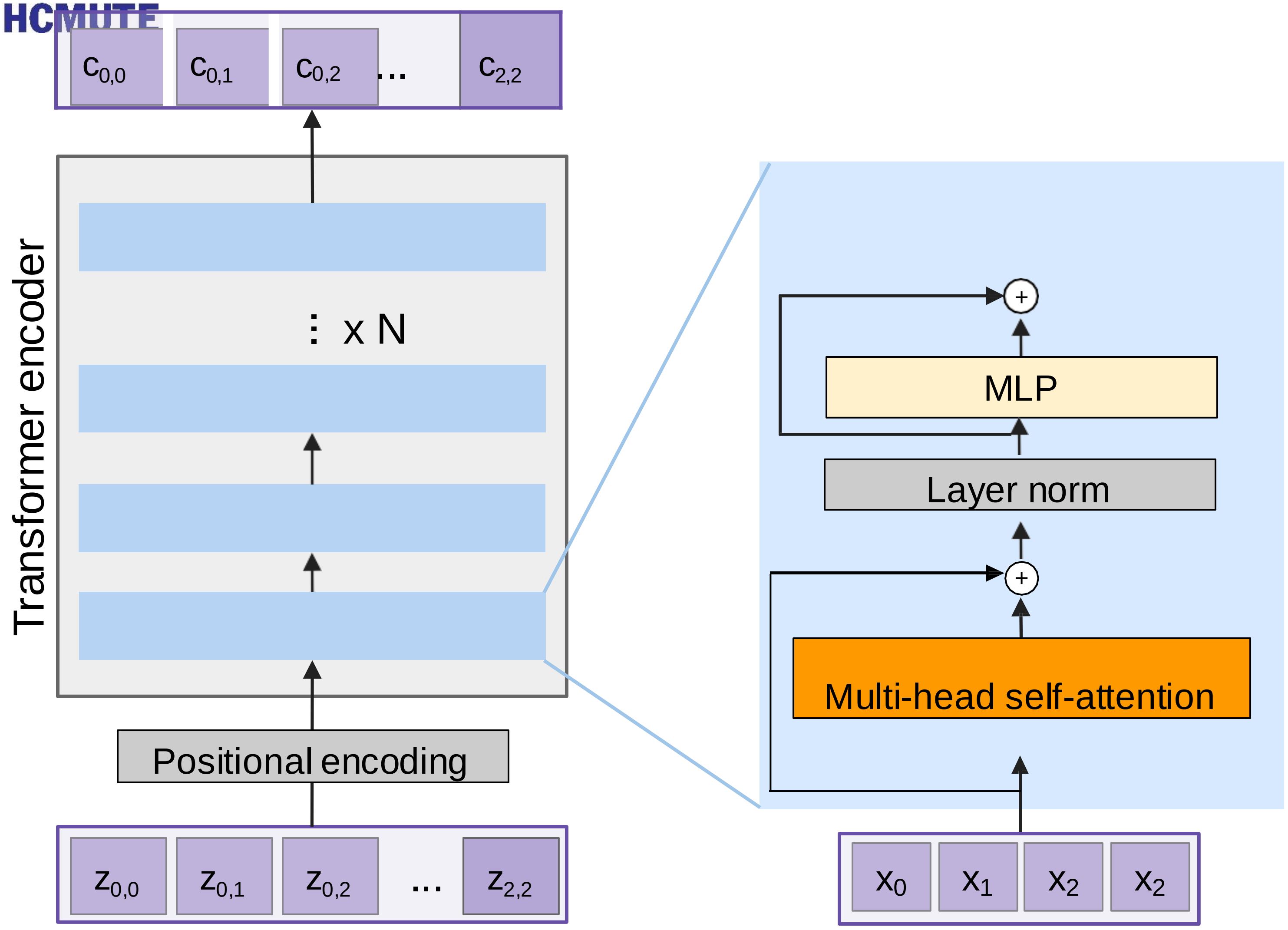
MLP over each vector individually

LayerNorm over each vector individually

Residual connection

Attention attends over all the vectors

The Transformer encoder block



Residual connection

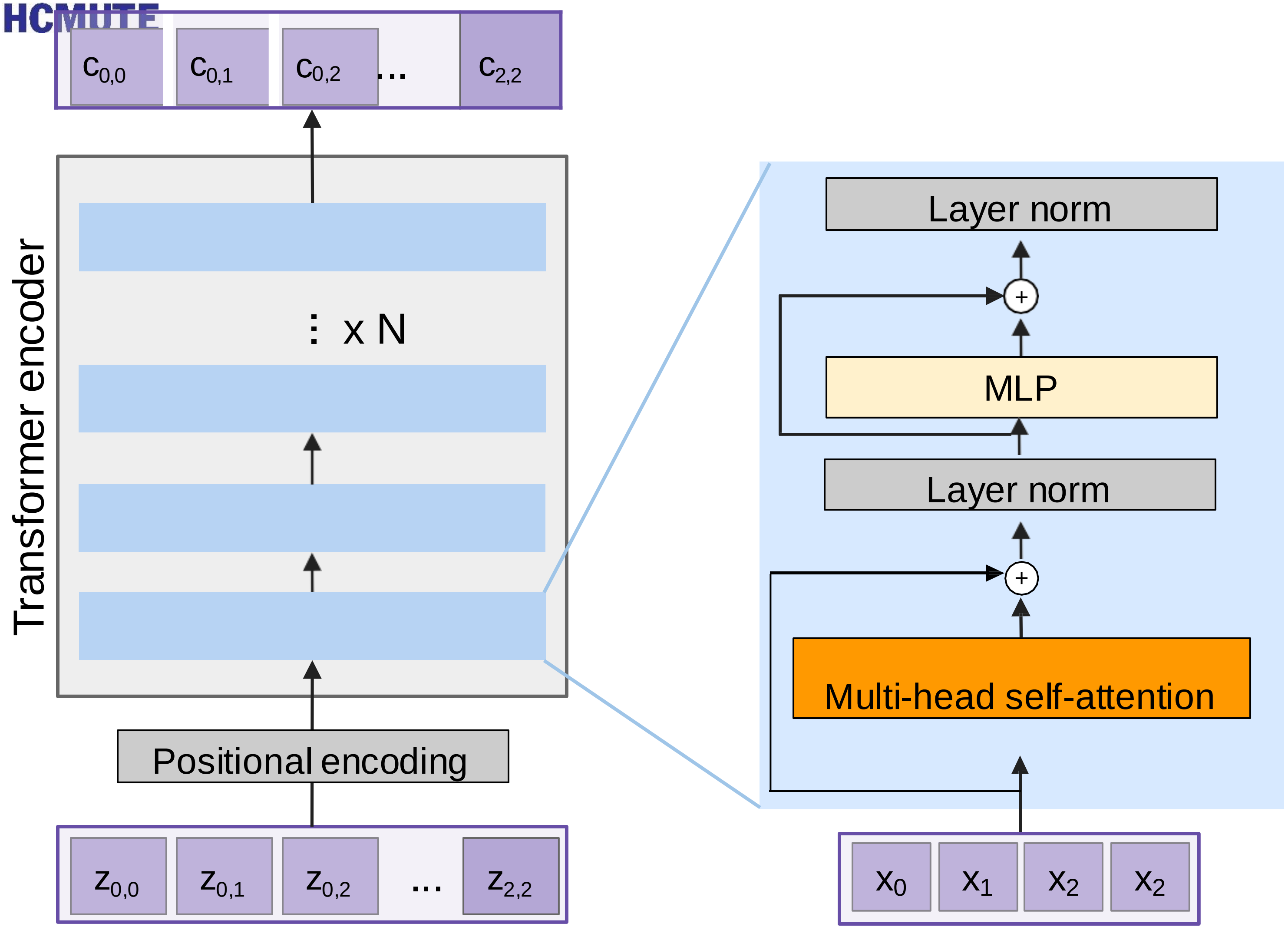
MLP over each vector individually

LayerNorm over each vector individually

Residual connection

Attention attends over all the vectors

The Transformer encoder block



LayerNorm over each vector individually

Residual connection

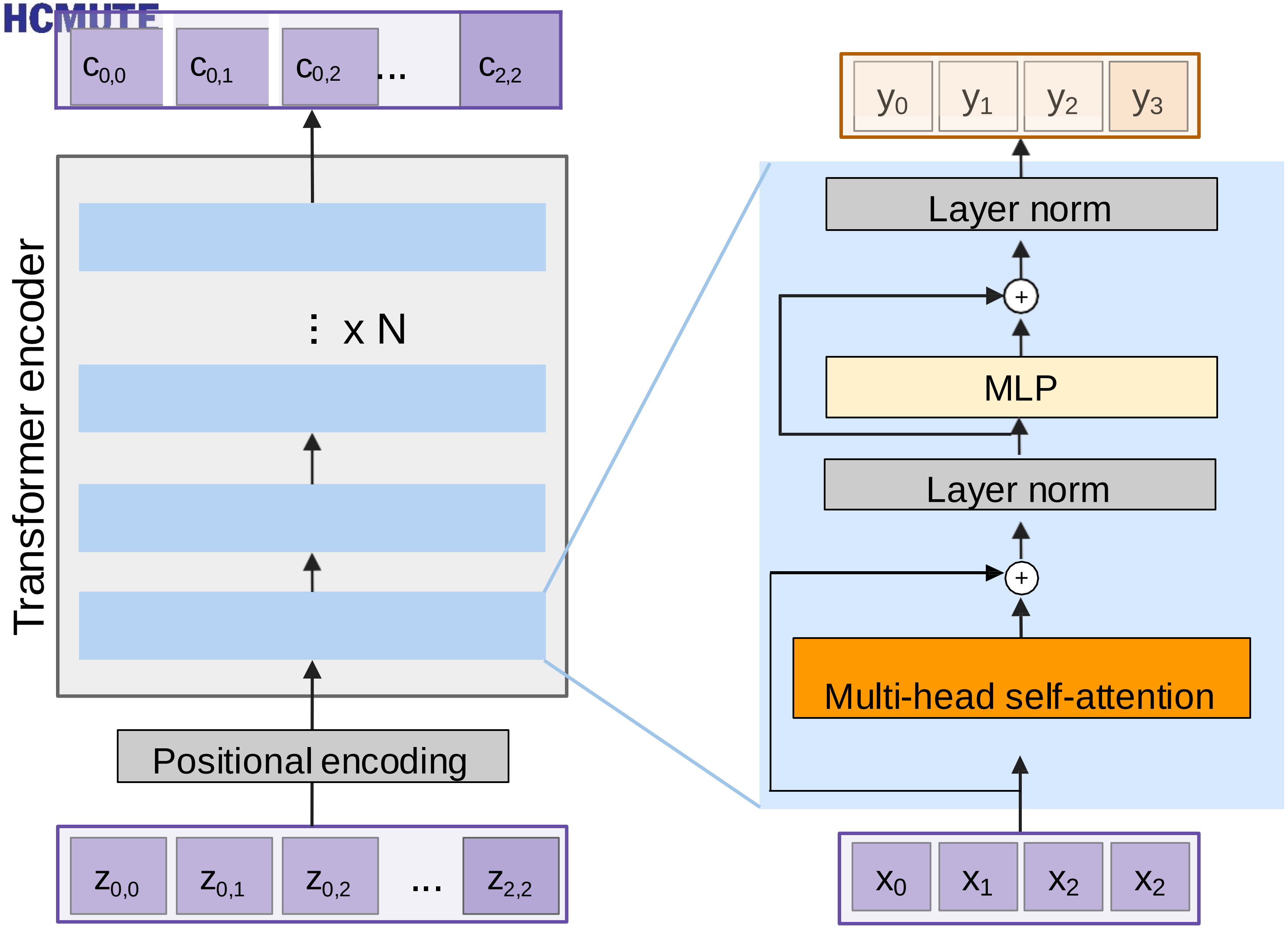
MLP over each vector individually

LayerNorm over each vector individually

Residual connection

Attention attends over all the vectors

The Transformer encoder block



Transformer Encoder Block:

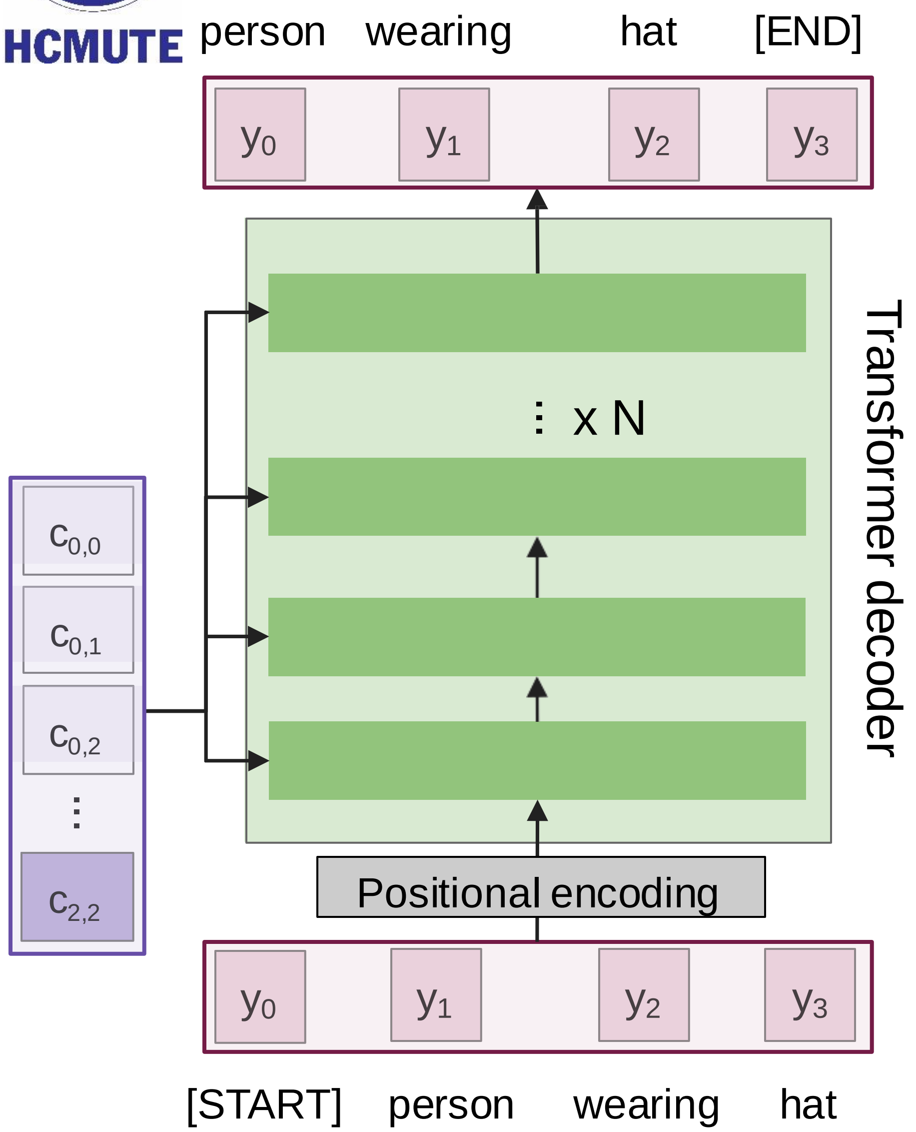
Inputs: Set of vectors **x**
Outputs: Set of vectors **y**

Self-attention is the only interaction between vectors.

Layer norm and MLP operate independently per vector.

Highly scalable, highly parallelizable, but high memory usage.

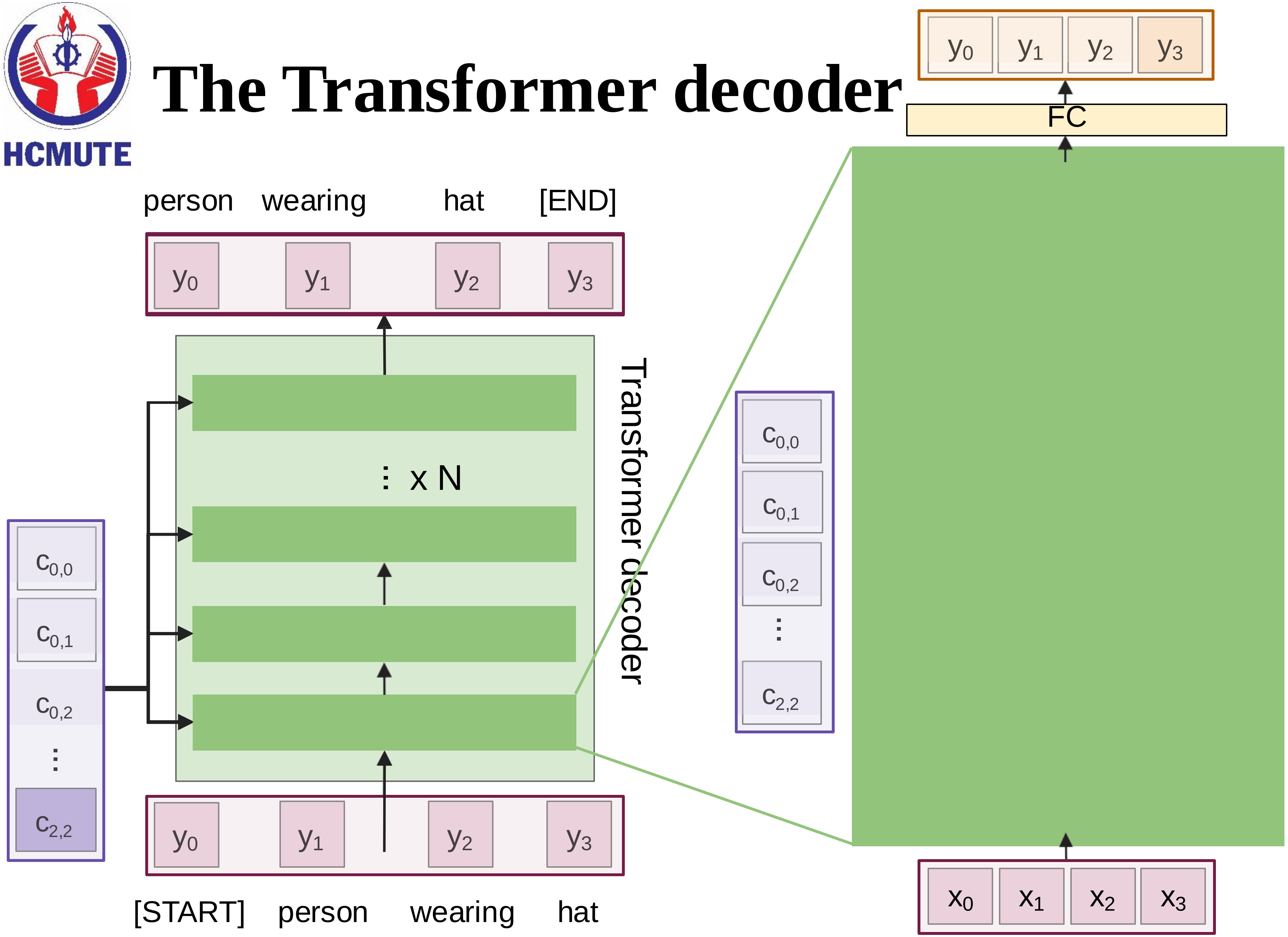
The Transformer decoder



Made up of N decoder blocks.

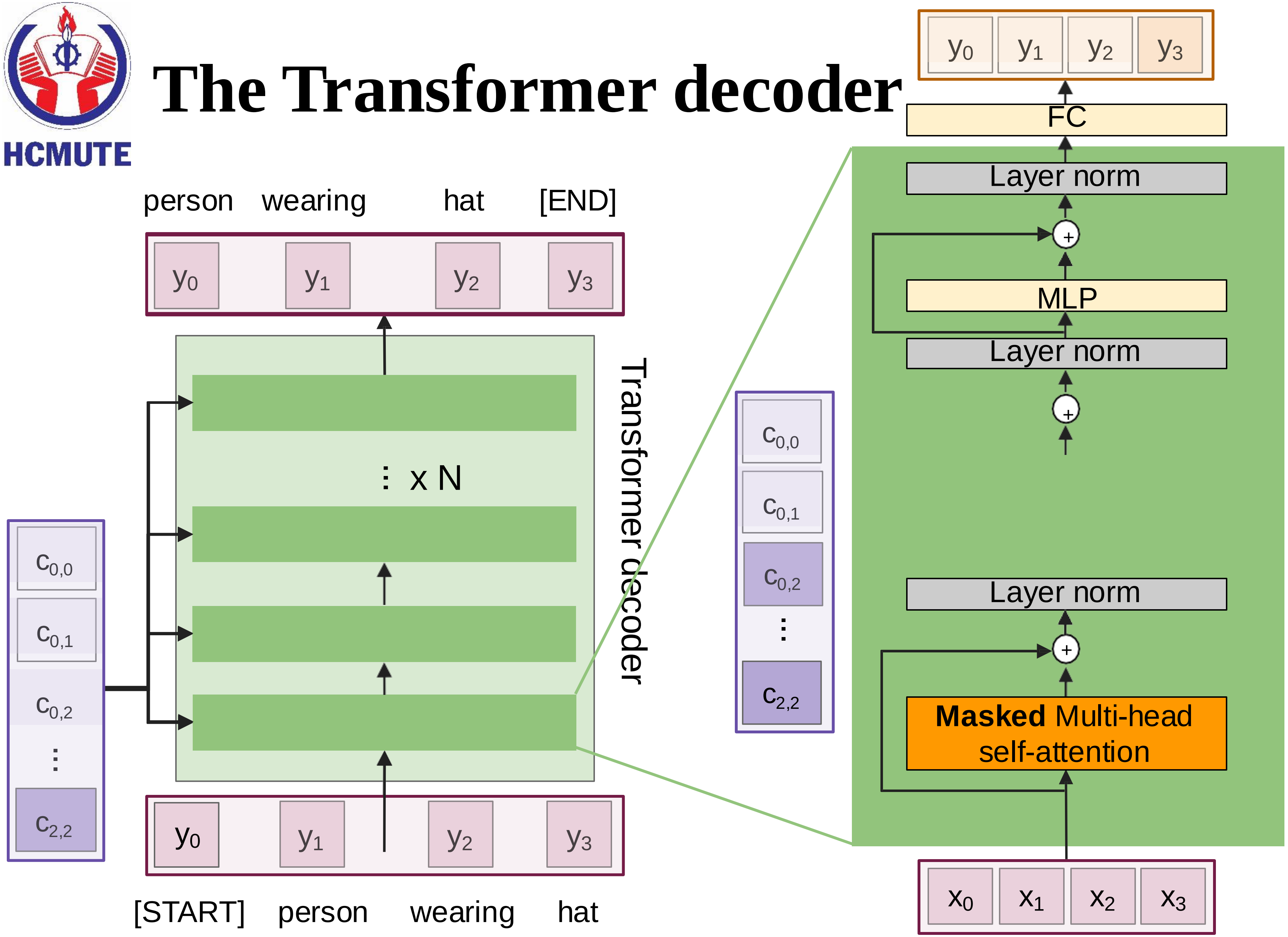
In vaswani et al. N = 6, D_q= 512

The Transformer decoder



Let's dive into the transformer decoder block

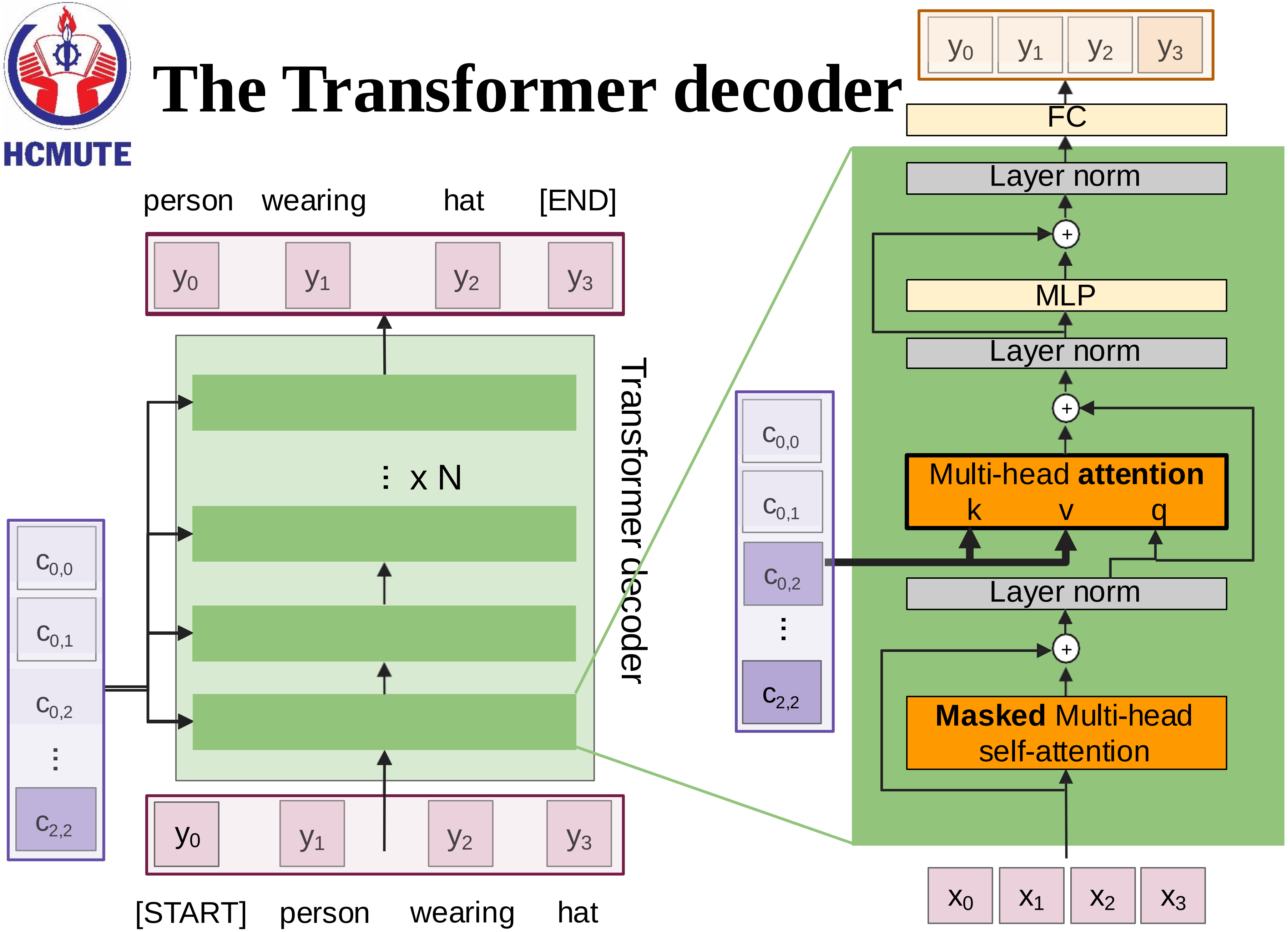
The Transformer decoder



Most of the network is the same the transformer encoder.

Ensures we only look at the previous tokens (teacher forcing during training)

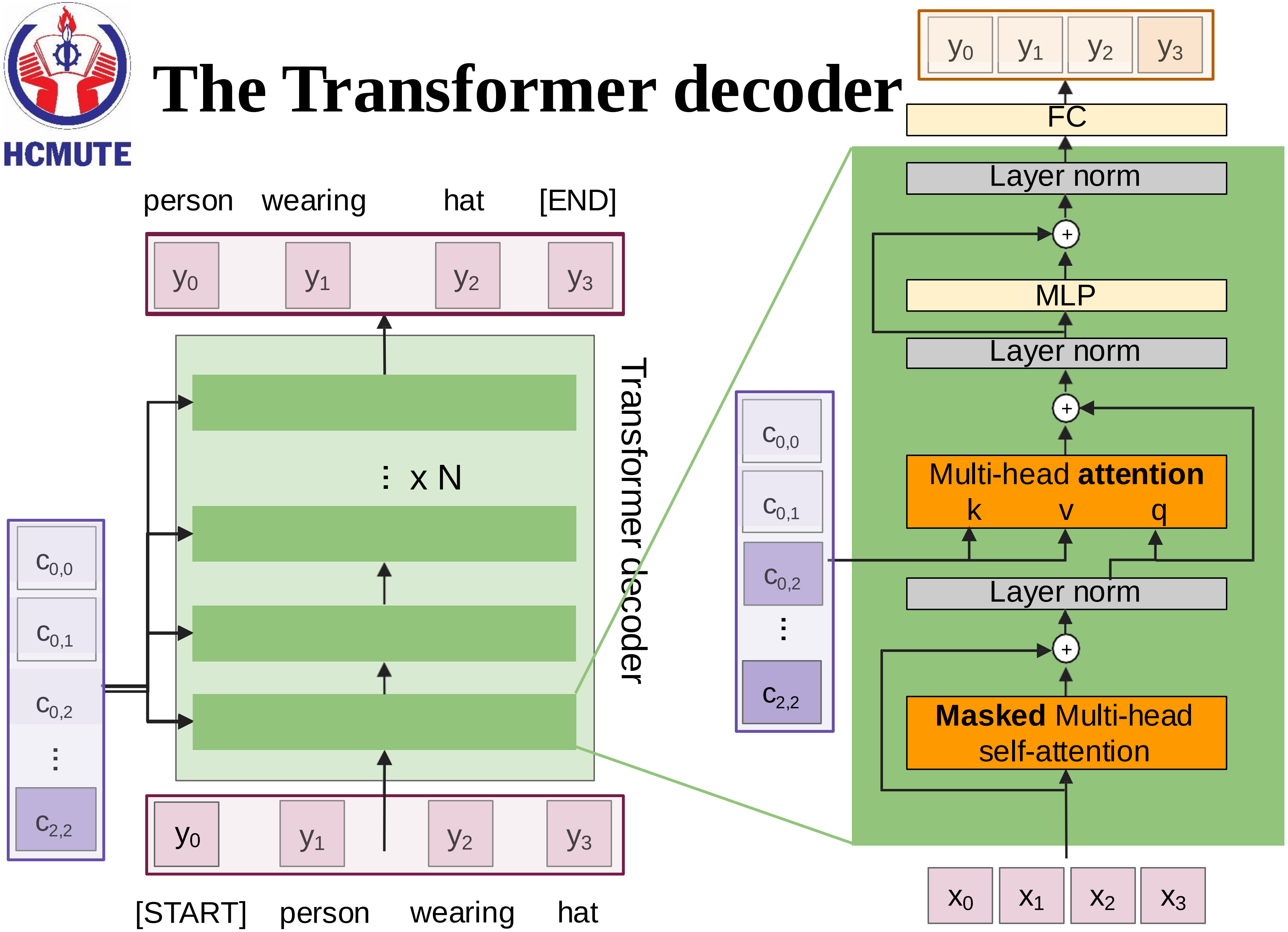
The Transformer decoder



Multi-head attention block attends over the transformer encoder outputs.

For image captioning, this is how we inject image features into the decoder.

The Transformer decoder



Transformer Decoder Block:

Inputs: Set of vectors **x** and Set of context vectors **c.**
Outputs: Set of vectors **y.**

Masked Self-attention only interacts with past inputs.

Multi-head attention block is NOT self-attention. It attends over encoder outputs.

Highly scalable, highly parallelizable, but high memory usage.

Image Captioning using transformers

- **No recurrence at all**

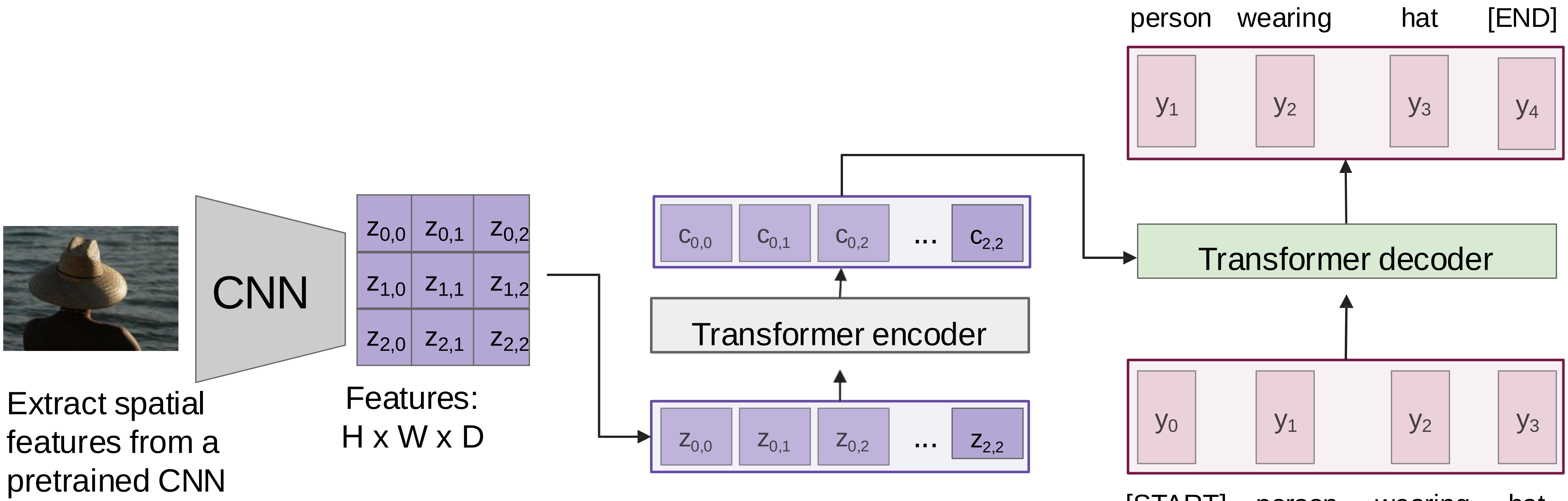


Image Captioning using transformers

- **Perhaps we don't need convolutions at all?**

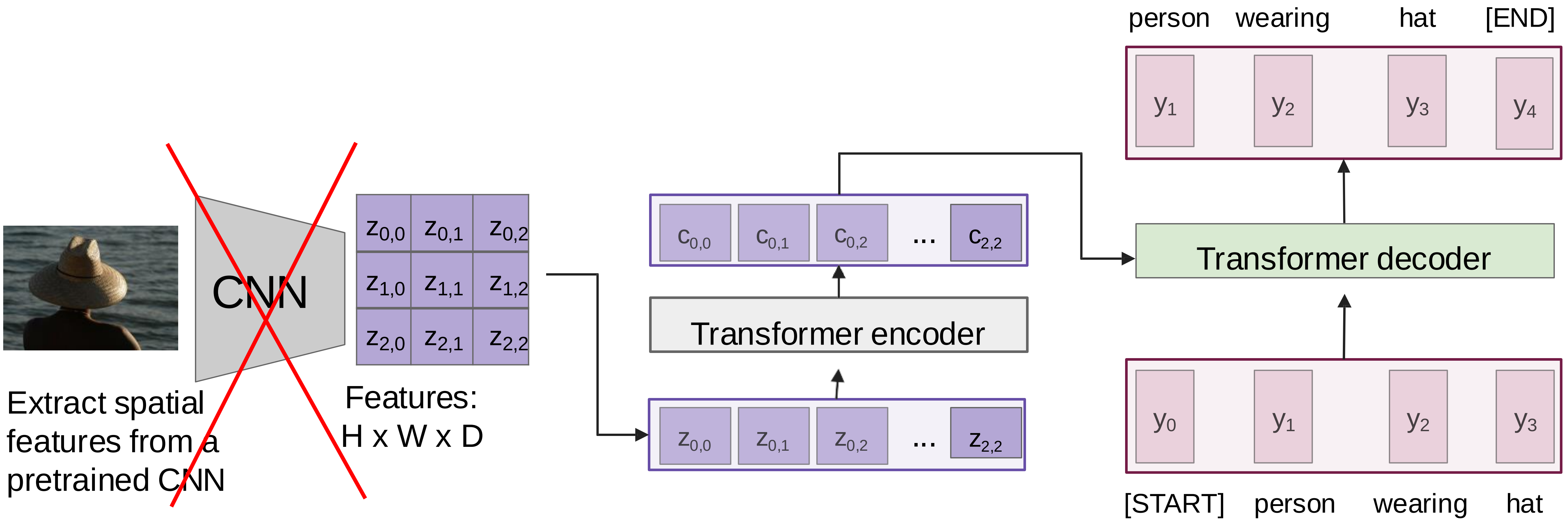
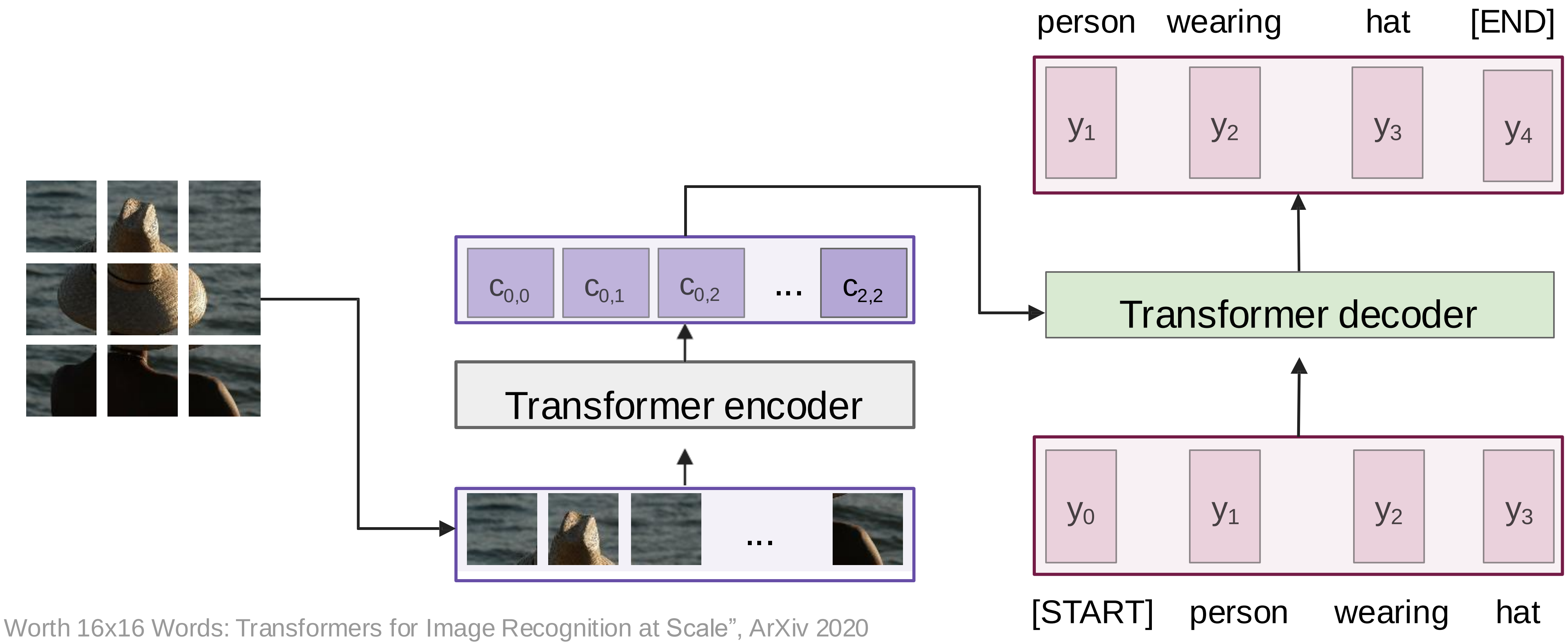


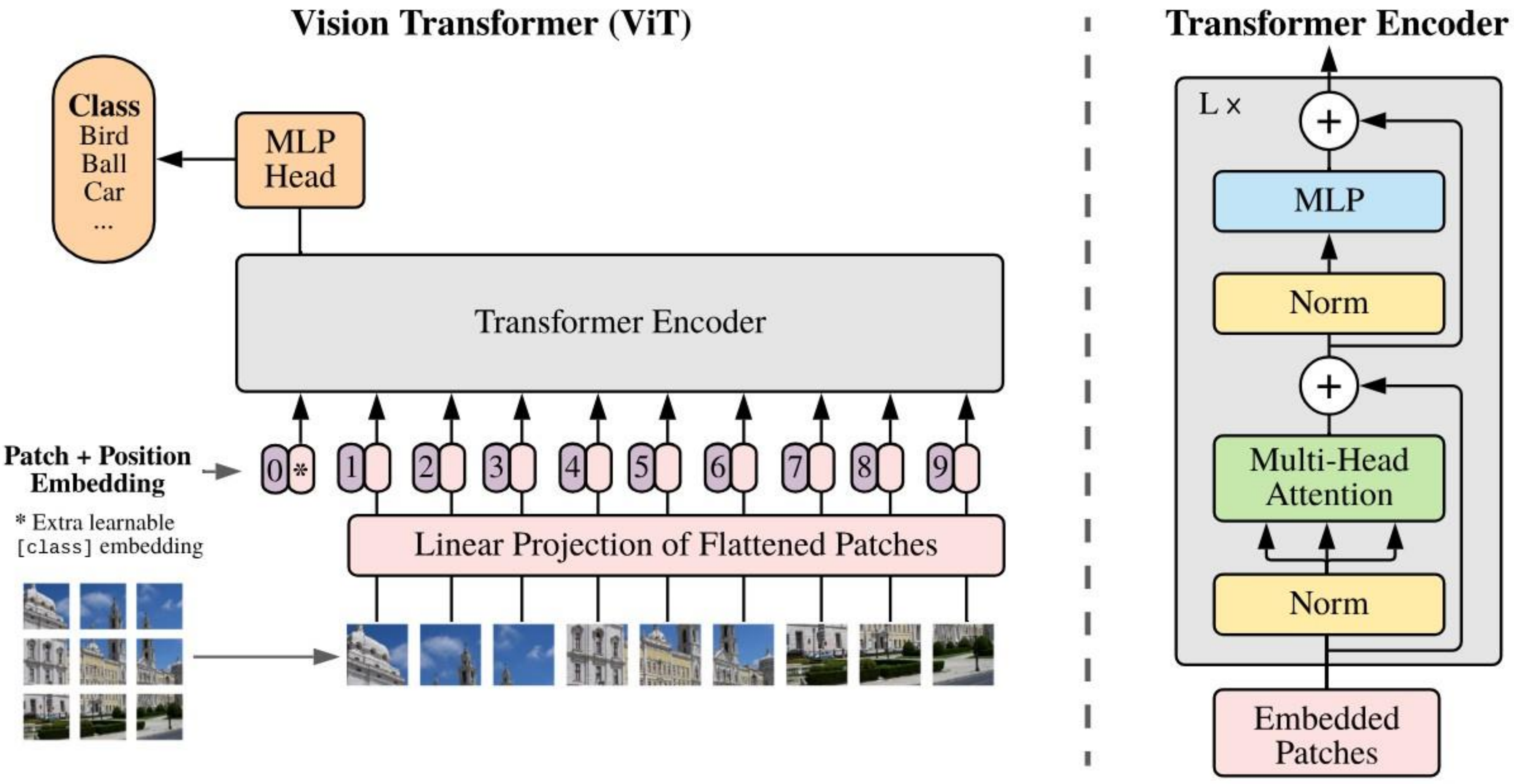
Image Captioning using ONLY transformers

- **Transformers from pixels to language**



Dosovitskiy et al, "An Image is Worth 16x16 Words: Transformers for Image Recognition at Scale", ArXiv 2020

ViTs – Vision Transformers



Dosovitskiy et al, "An Image is Worth 16x16 Words: Transformers for Image Recognition at Scale", ArXiv 2020

Vision Transformers vs. ResNets

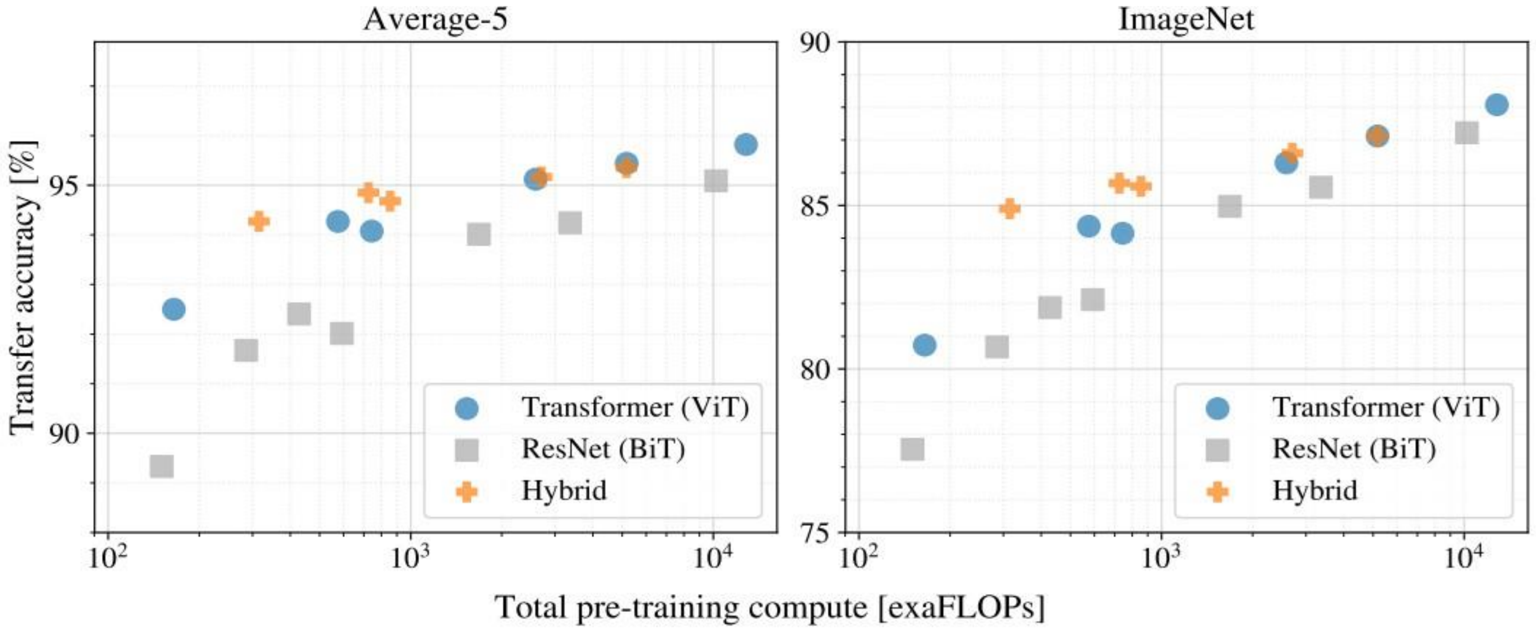
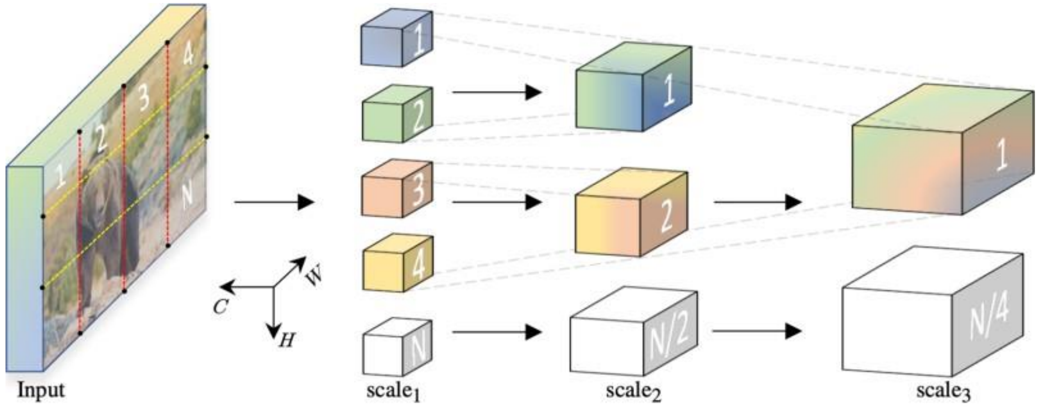


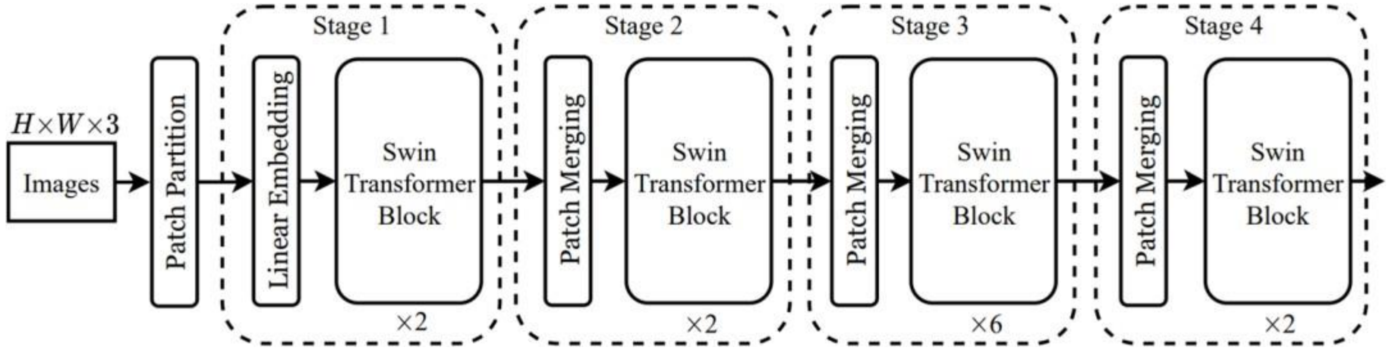
Figure 5: Performance versus cost for different architectures: Vision Transformers, ResNets, and hybrids. Vision Transformers generally outperform ResNets with the same computational budget. Hybrids improve upon pure Transformers for smaller model sizes, but the gap vanishes for larger models.

Dosovitskiy et al, “An Image is Worth 16x16 Words: Transformers for Image Recognition at Scale”, ArXiv 2020

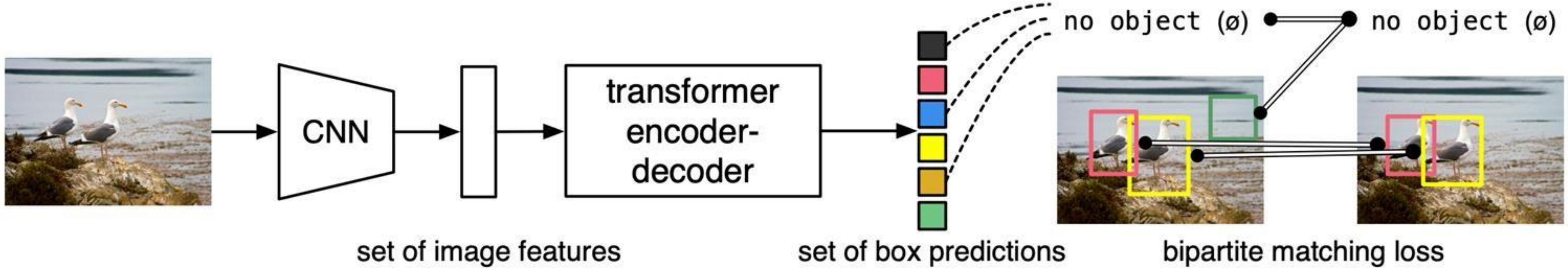
Vision Transformers



Fan et al, "Multiscale Vision Transformers", ICCV 2021

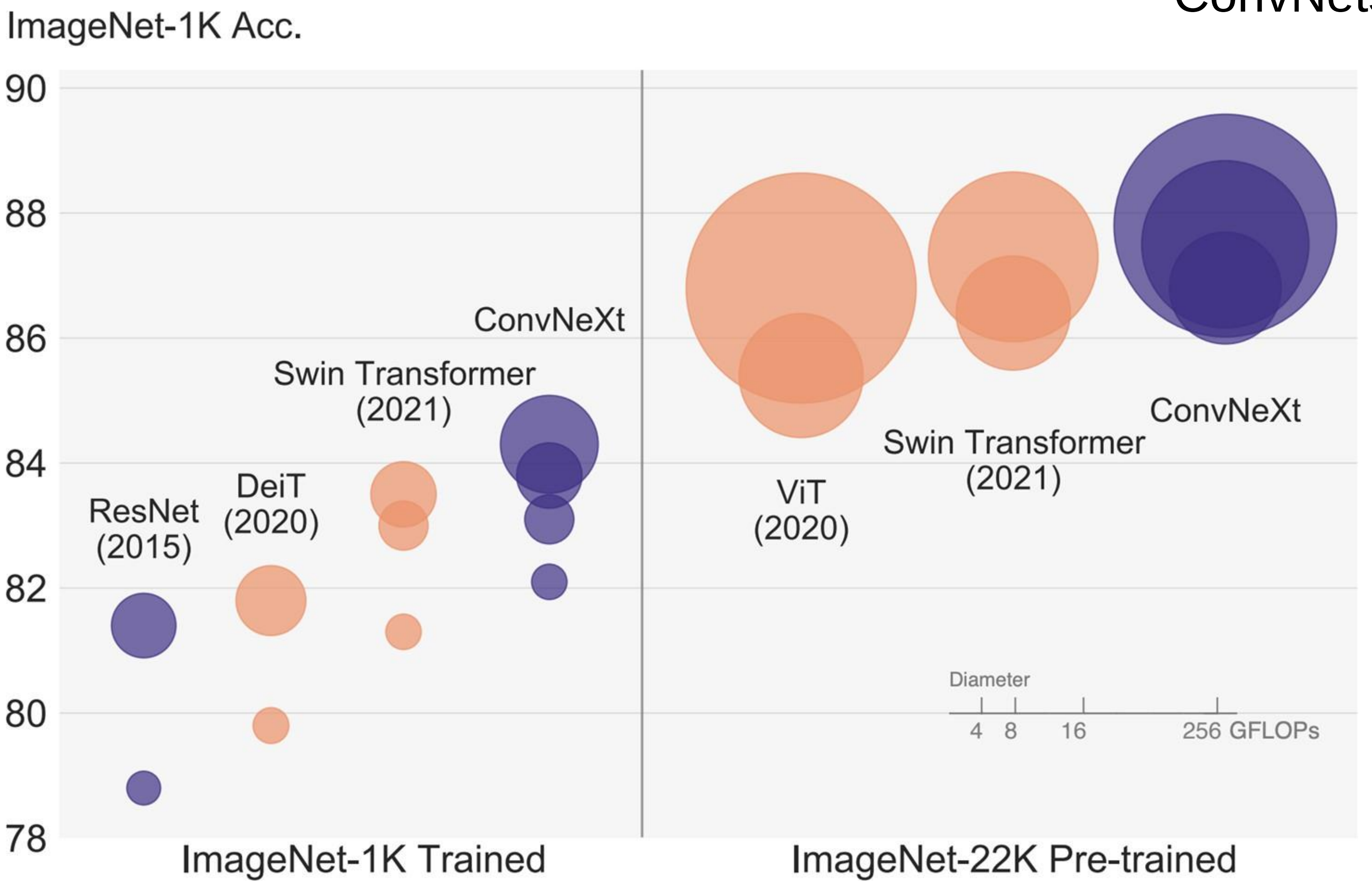


Liu et al, "Swin Transformer: Hierarchical Vision Transformer using Shifted Windows", CVPR 2021



Carion et al, "End-to-End Object Detection with Transformers", ECCV 2020

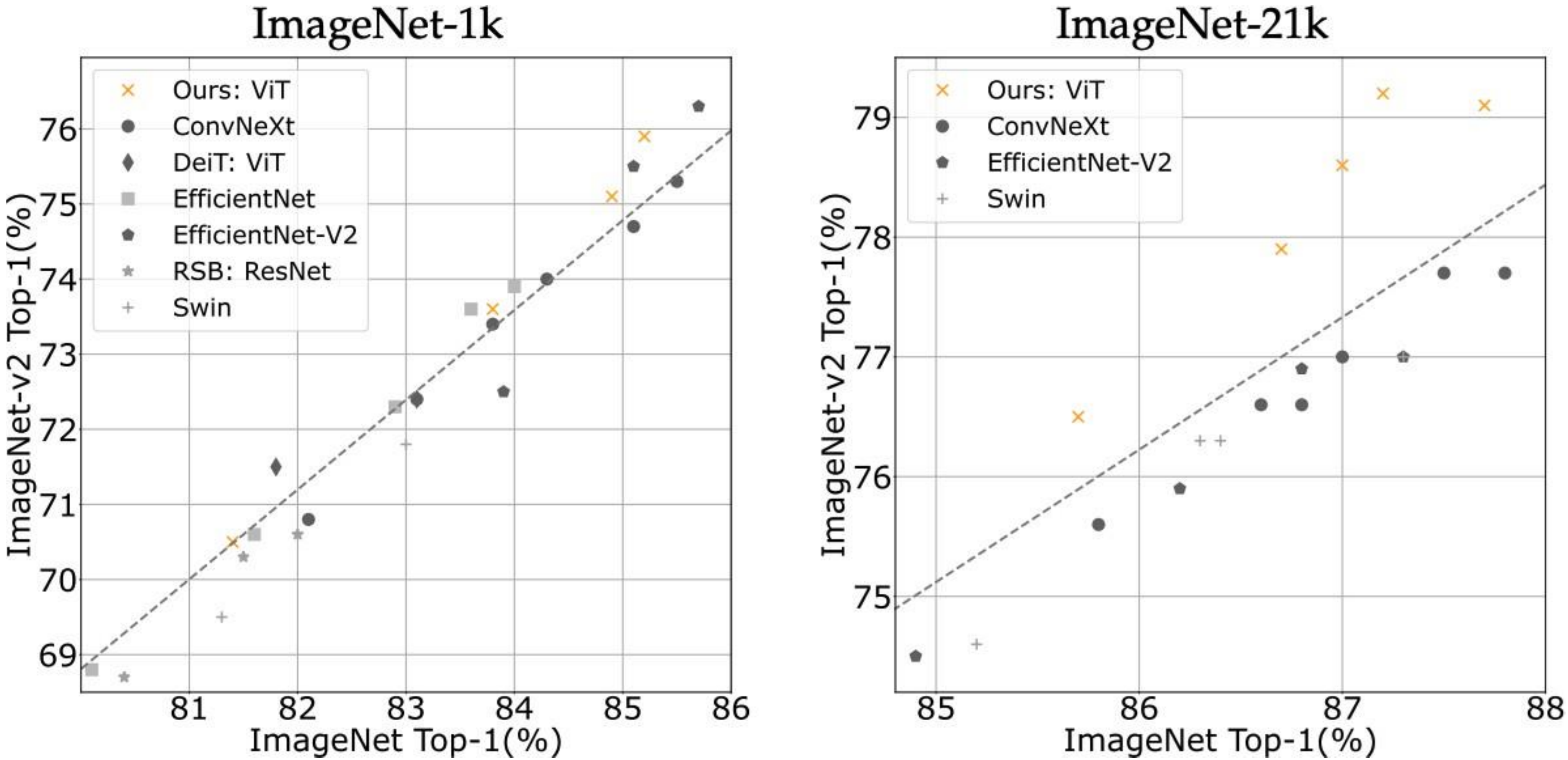
ConvNets strike back!



A ConvNet for the 2020s. Liu et al. CVPR 2022

DeiT III: Revenge of the ViT

Hugo Touvron[*,†] Matthieu Cord[†] Hervé Jégou[*]



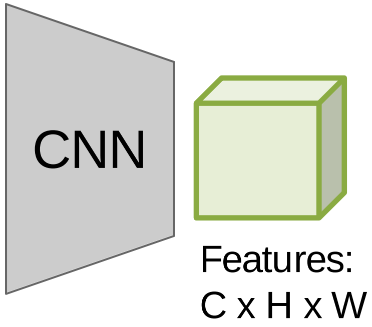
Summary

- Adding **attention** to RNNs allows them to "attend" to different parts of the input at every time step
- The **general attention layer** is a new type of layer that can be used to design new neural network architectures
- **Transformers** are a type of layer that uses **self-attention** and layer norm.
    - It is highly **scalable** and highly **parallelizable**
    - **Faster** training, **larger** models, **better** performance across vision and language tasks
    - They are quickly replacing RNNs, LSTMs, and may(?) even replace convolutions.

Example: CNN with Self-Attention

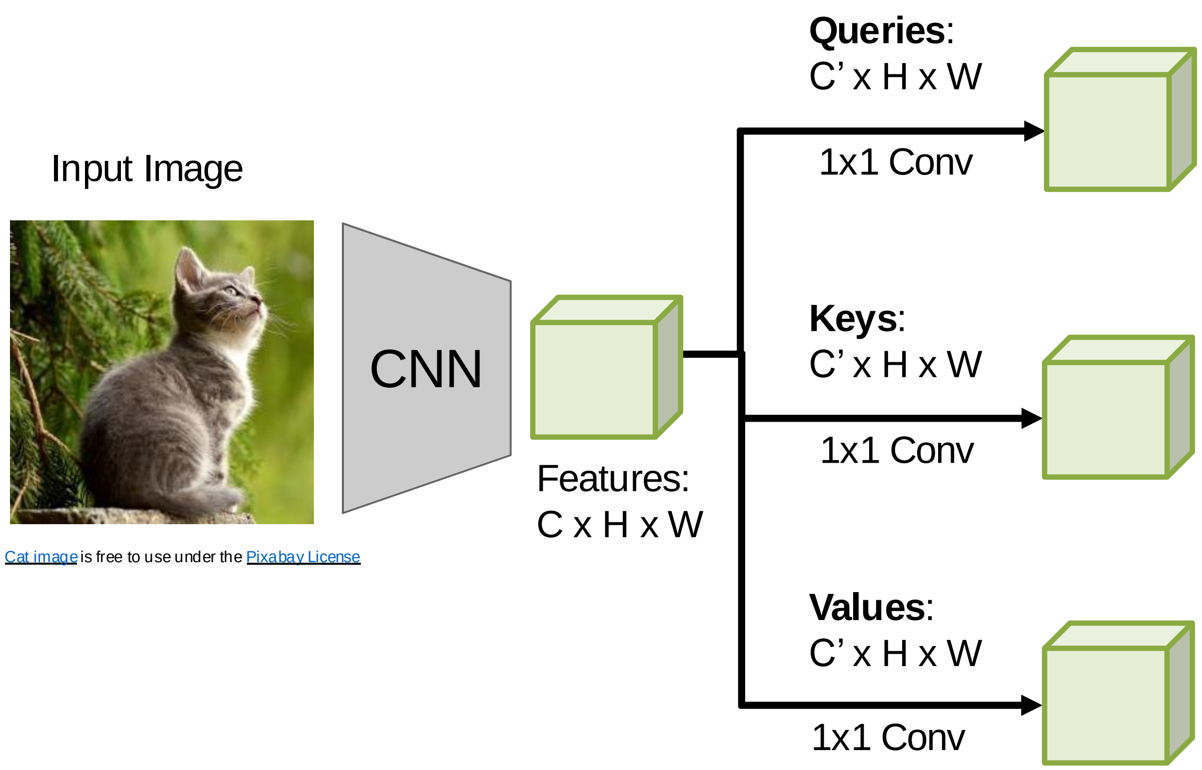
Input Image

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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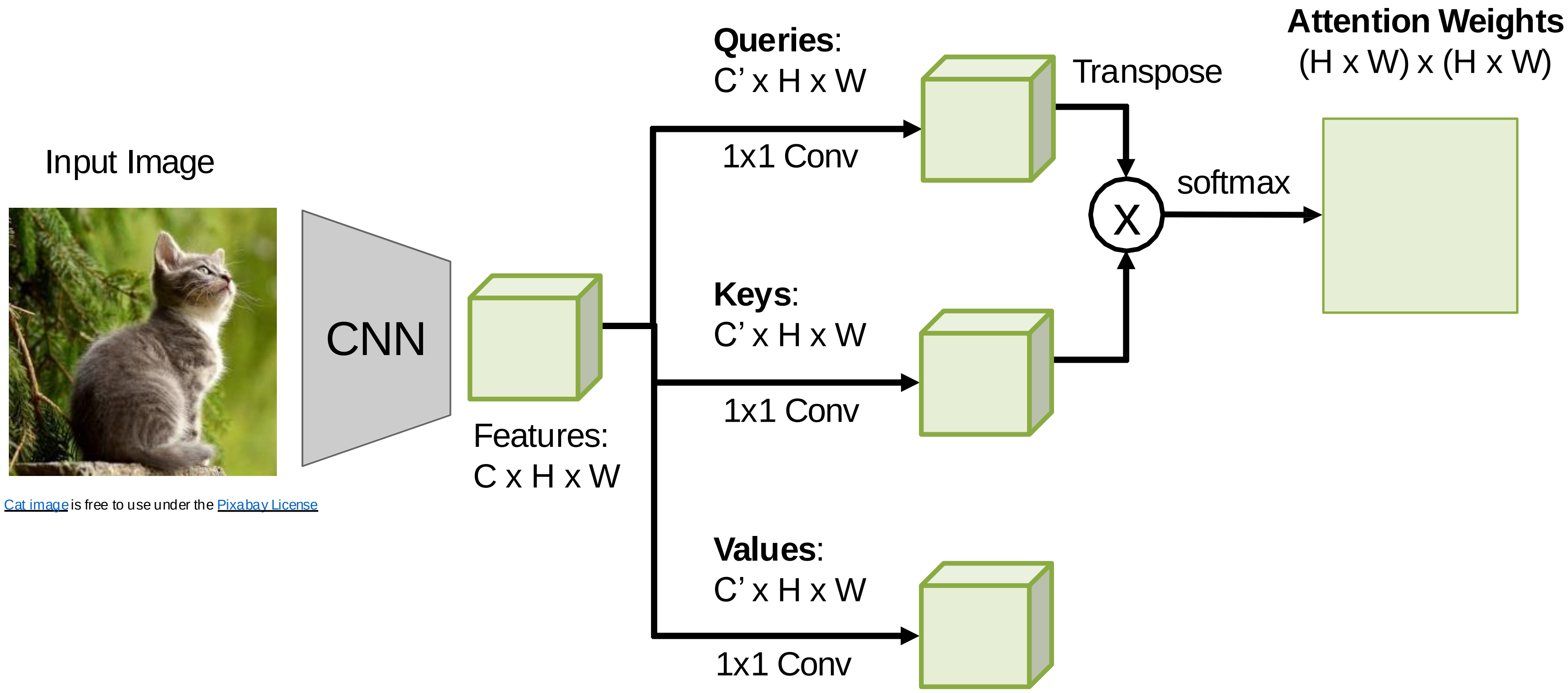
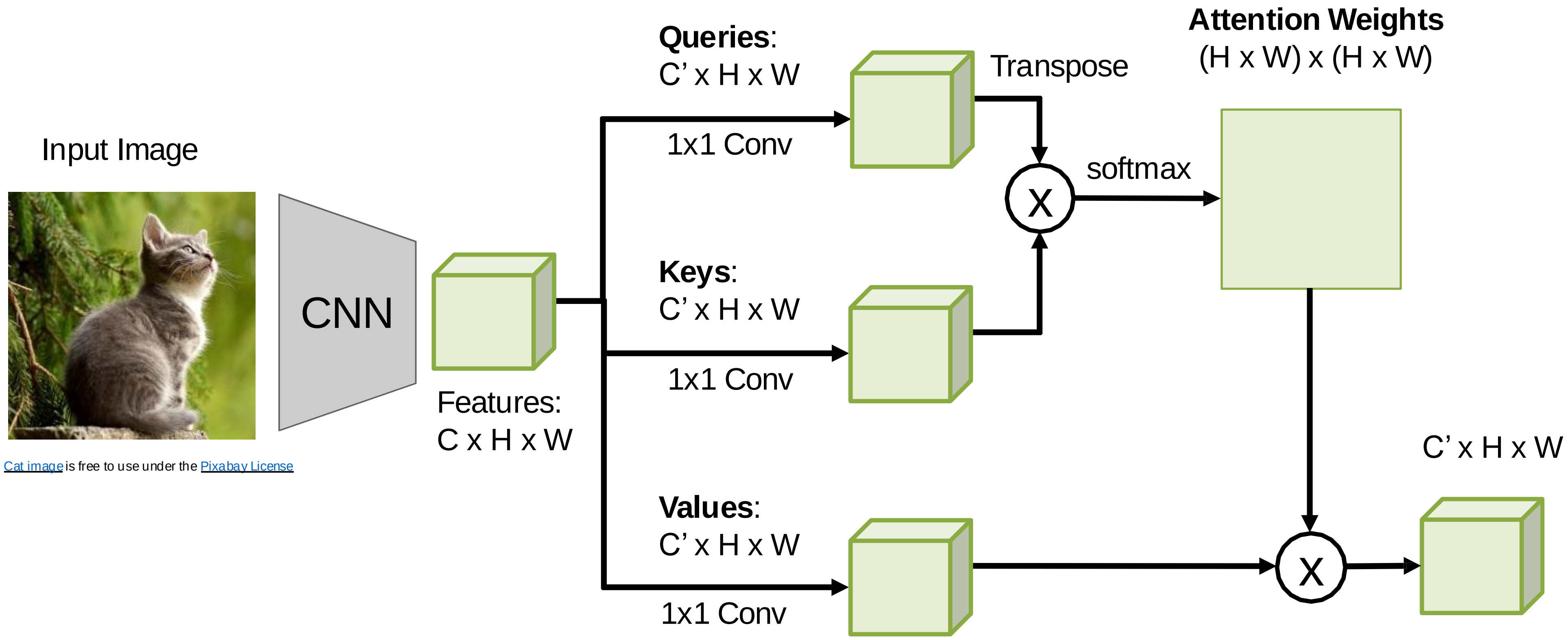
Example: CNN with Self-Attention



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

Example: CNN with Self-Attention



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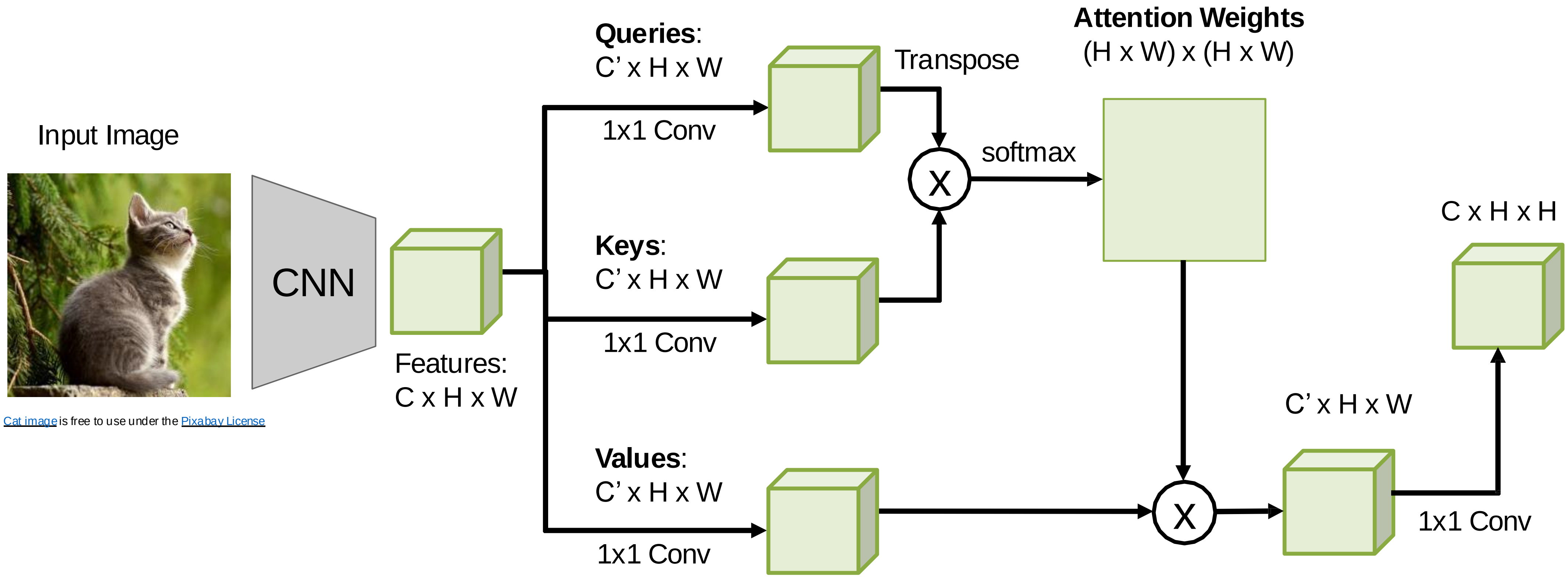
Zhang et al, "Self-Attention Generative Adversarial Networks", ICML 2018

Example: CNN with Self-Attention



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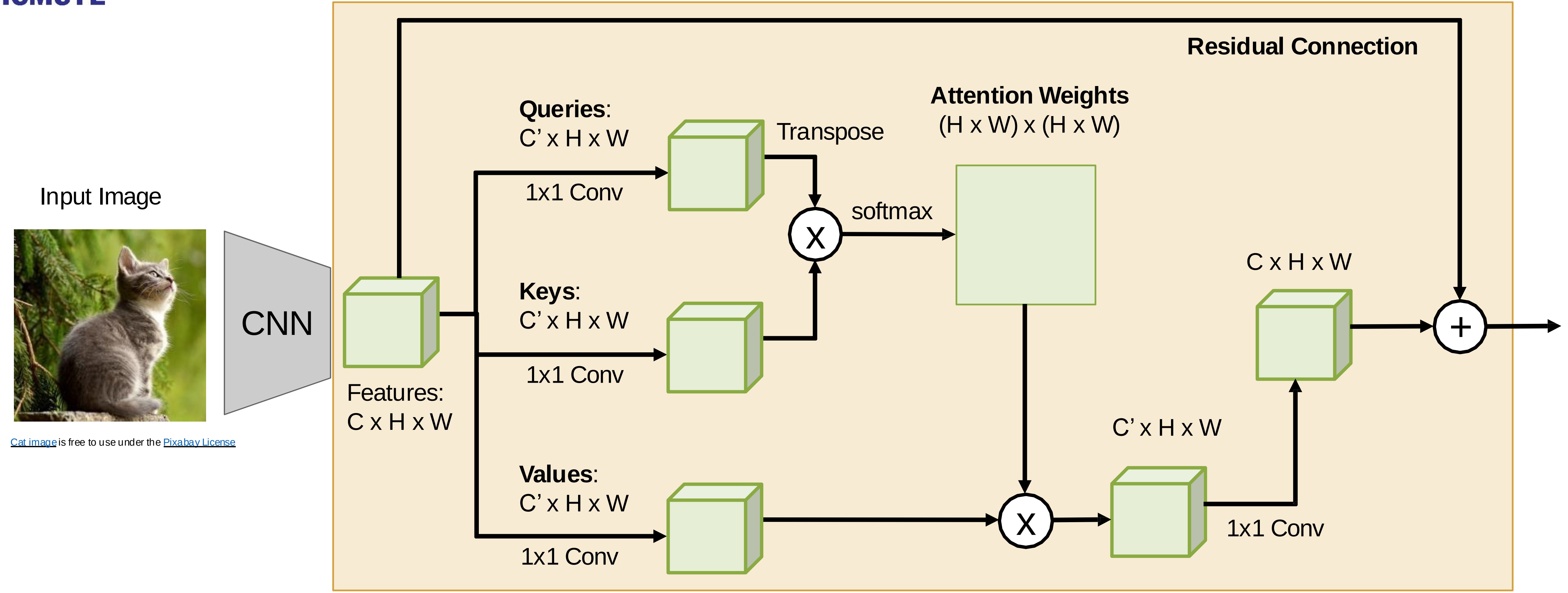
Zhang et al, "Self-Attention Generative Adversarial Networks", ICML 2018

Example: CNN with Self-Attention



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Self-Attention Module

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