Attention and Transformer

Slides refer to Prof. Fei-Fei Li’s one at Stanford

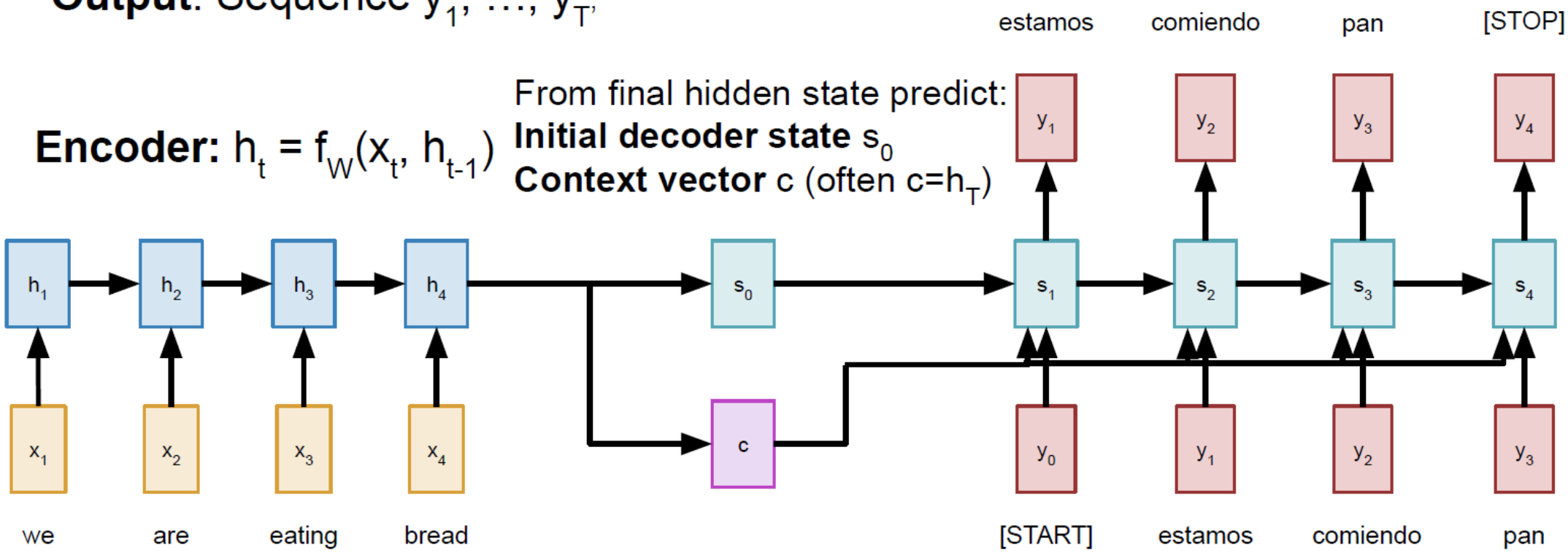
Sequence to Sequence with RNNs

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

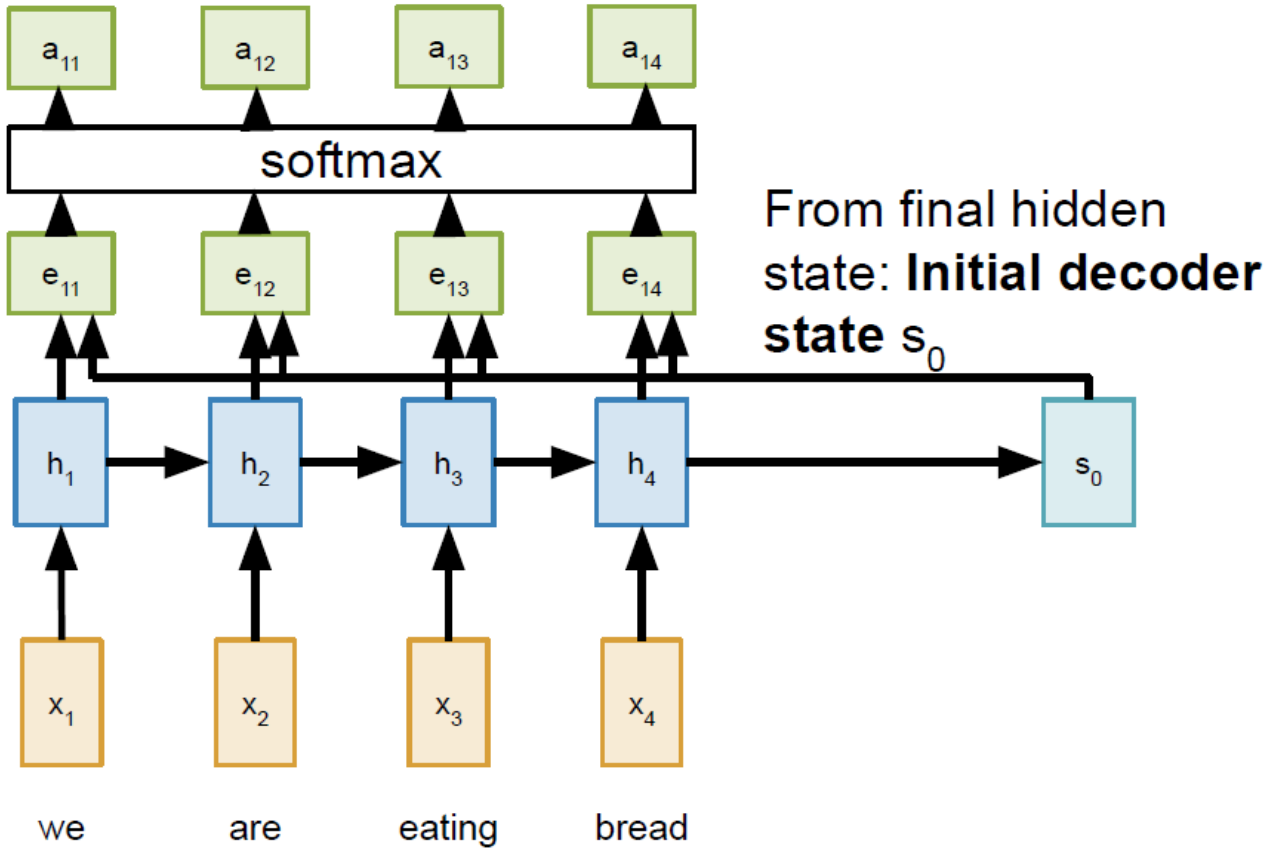
Encoder: $h_t = f_W(x_t, h_{t-1})$

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

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



Sequence to Sequence with RNNs and Attention



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

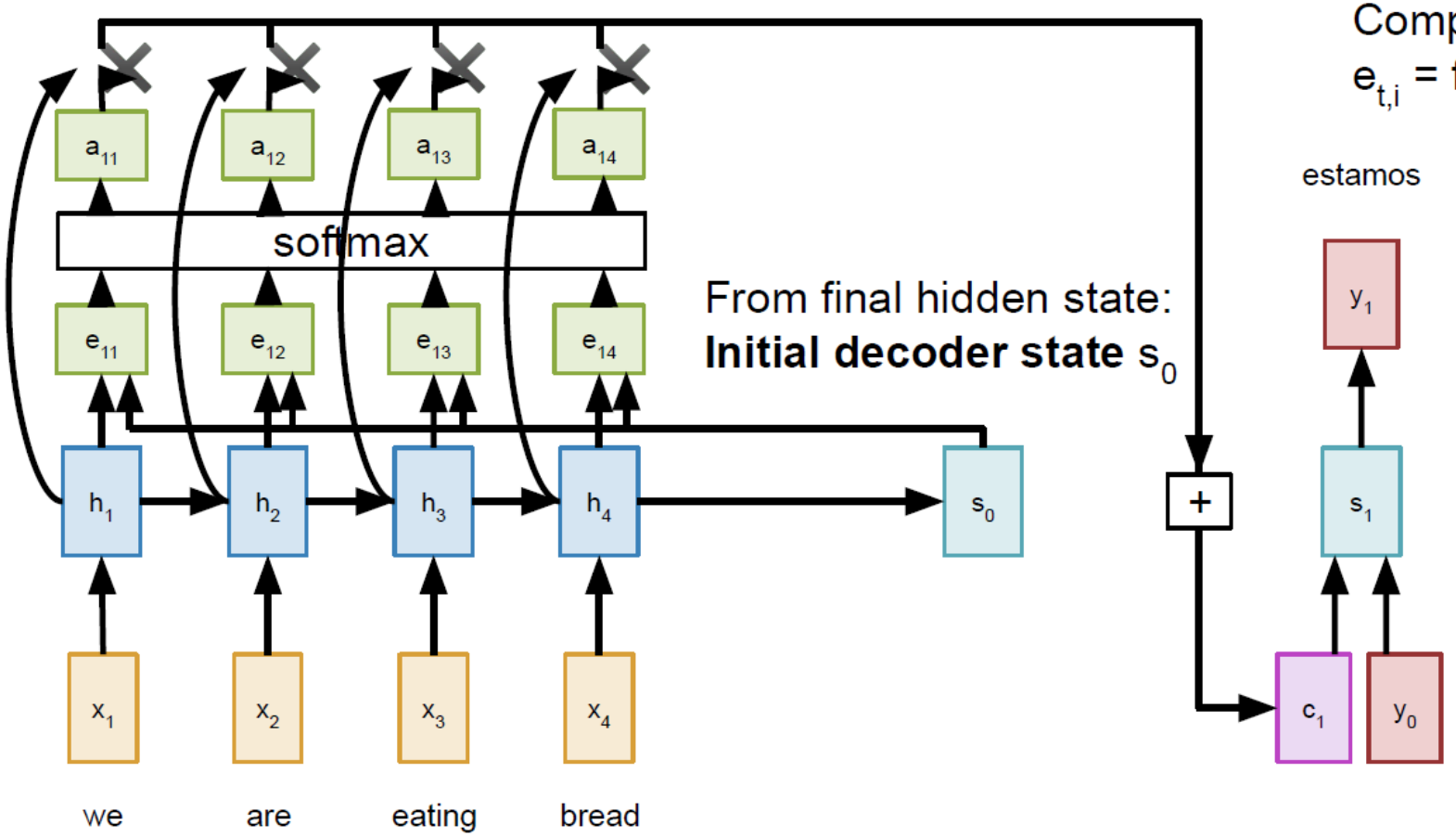
Compute (scalar) **alignment scores**

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

Normalize alignment scores to get **attention weights**

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

Sequence to Sequence with RNNs and Attention



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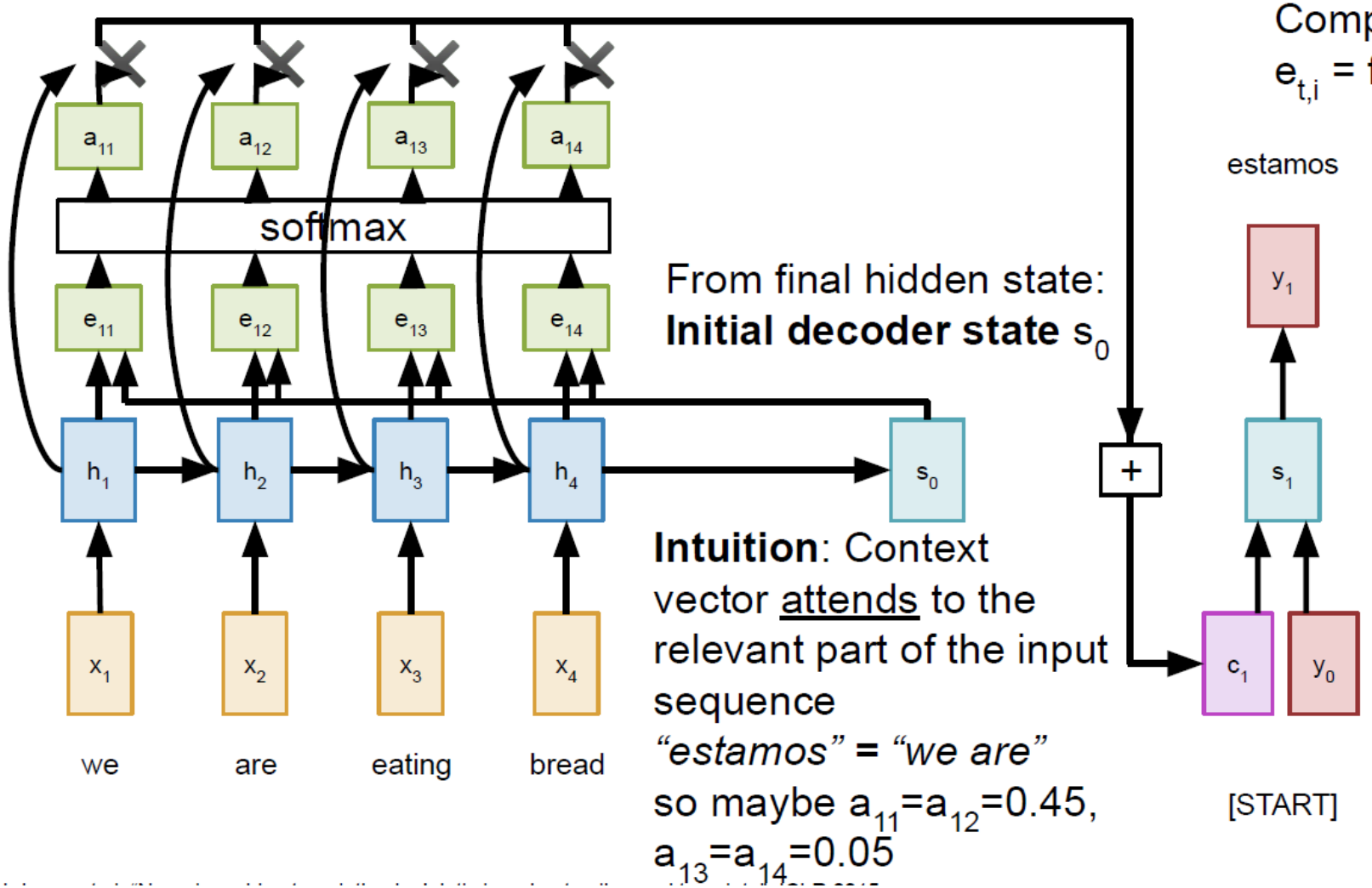
Compute context vector as linear combination of hidden states

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

Sequence to Sequence with RNNs and Attention



From final hidden state:
Initial decoder state s_0

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

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

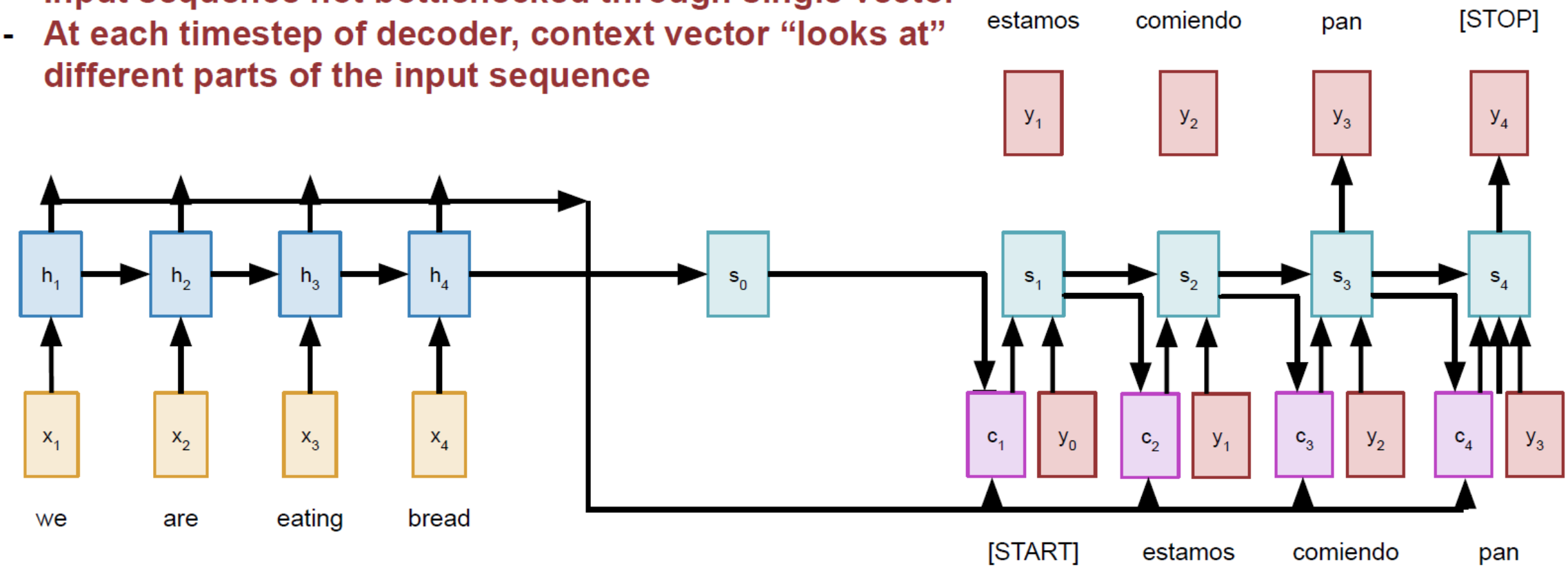
Compute context vector as linear combination of hidden states
$c_t = \sum_i a_{t,i} h_i$

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

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**



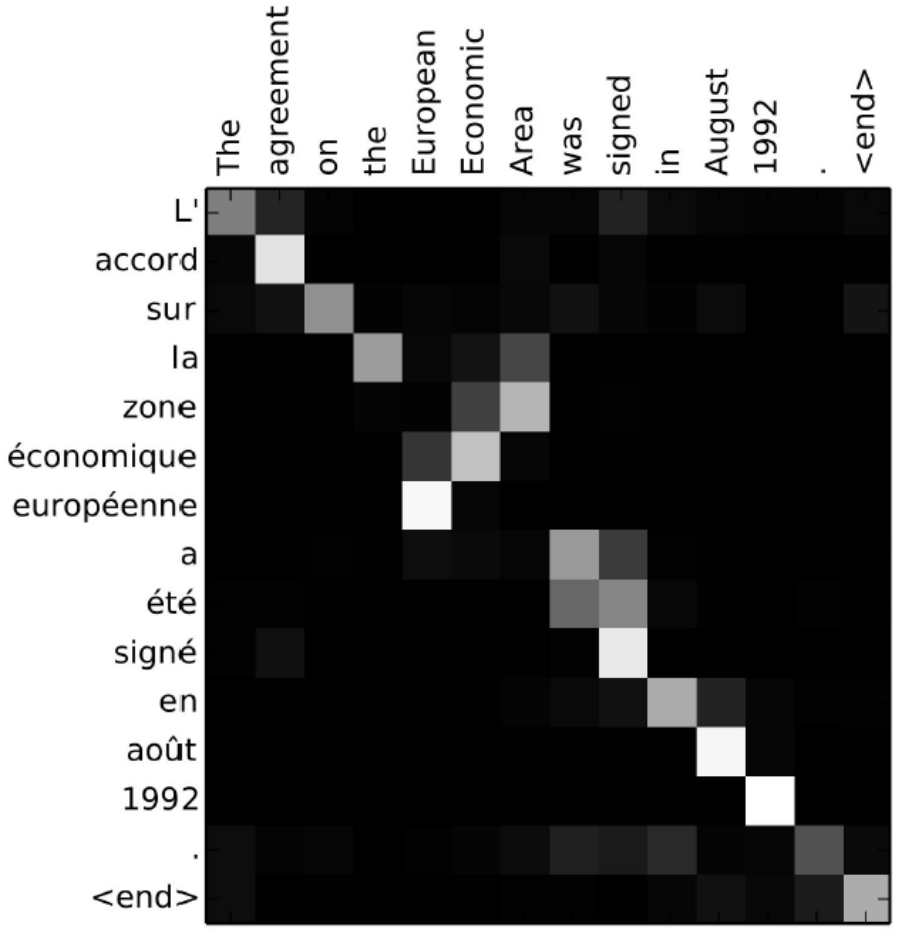
Sequence to Sequence with RNNs and Attention

Example: English to French translation

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 $a_{t,i}$



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

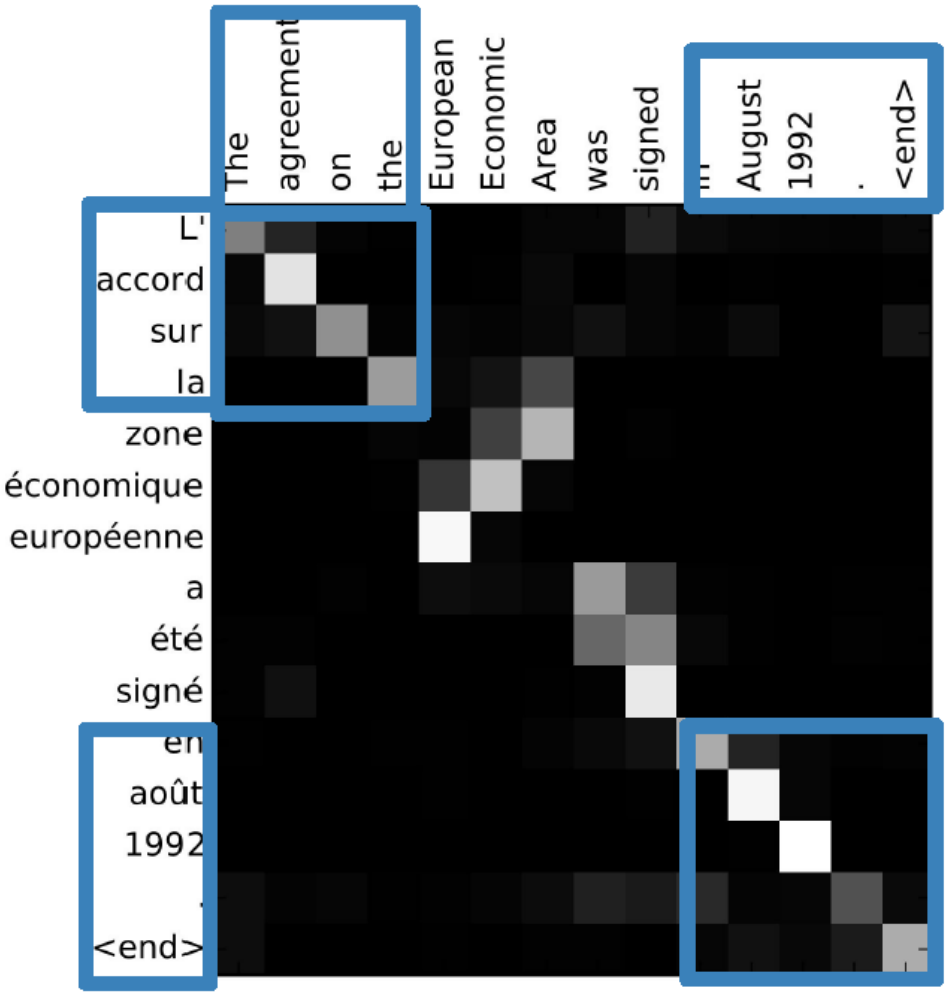
Sequence to Sequence with RNNs and Attention

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 $a_{t,i}$



Diagonal attention means words correspond in order

Diagonal attention means words correspond in order

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

Sequence to Sequence with RNNs and Attention

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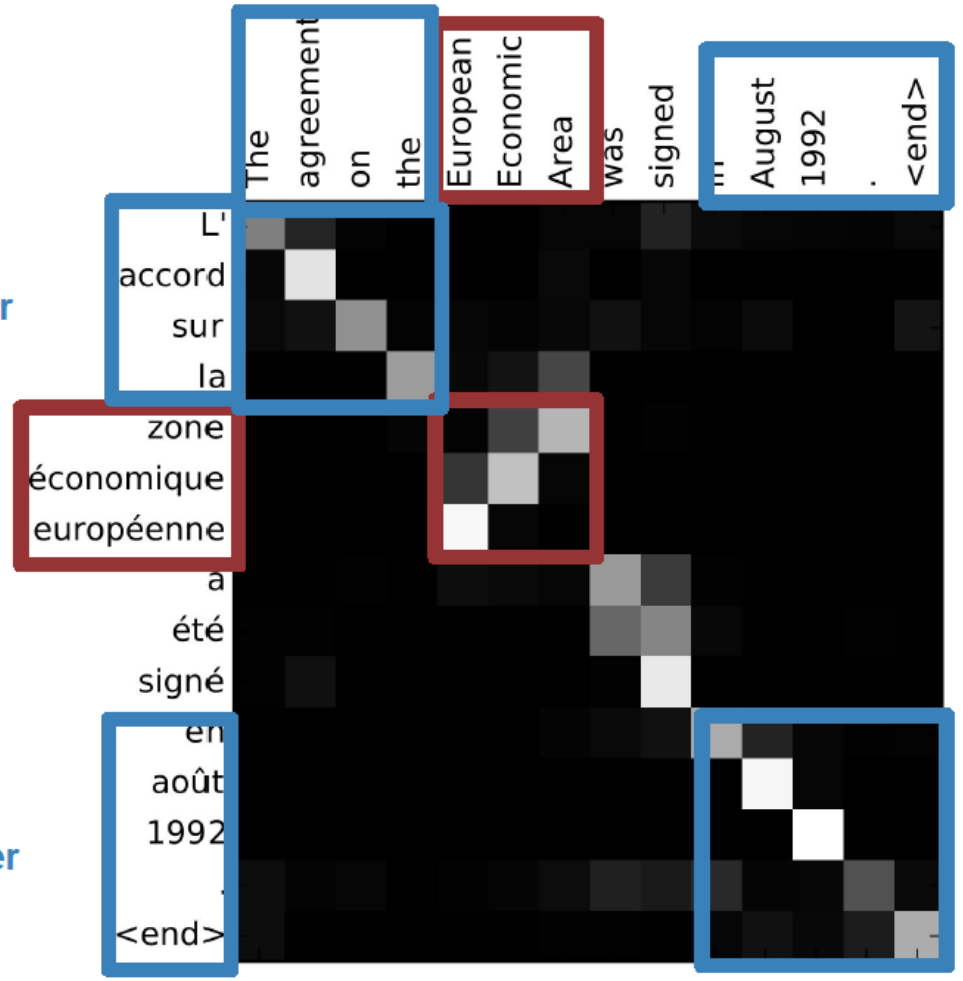


Diagonal attention means words correspond in order

Attention figures out different word orders

Diagonal attention means words correspond in order

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

Sequence to Sequence with RNNs and Attention

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

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

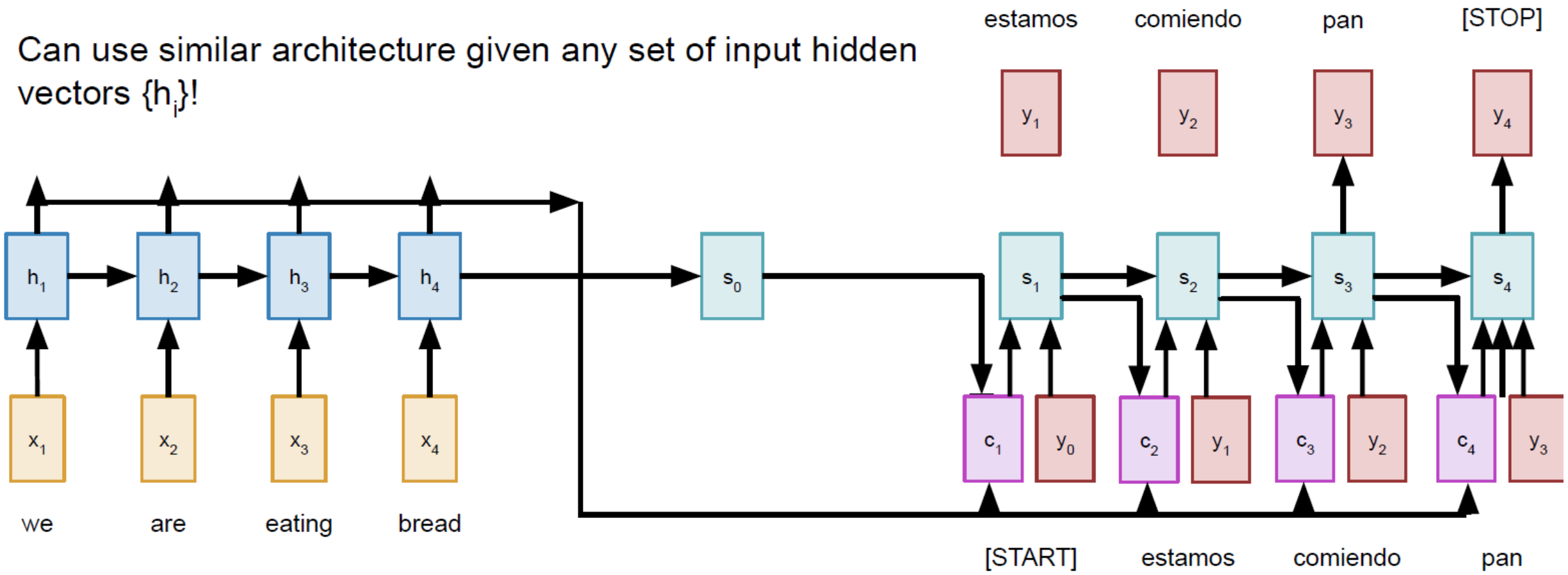
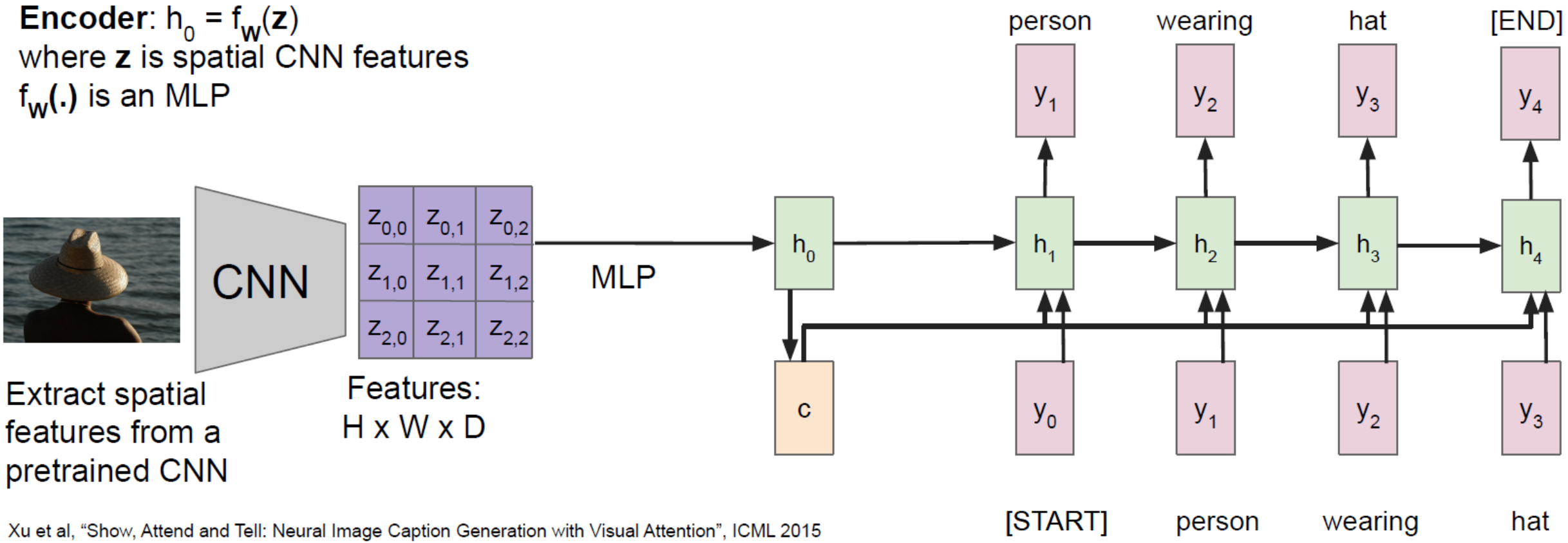


Image Captioning using spatial features

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

Decoder: $y_t = g_V(y_{t-1}, h_{t-1}, c)$
where context vector c is often $c = h_0$

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



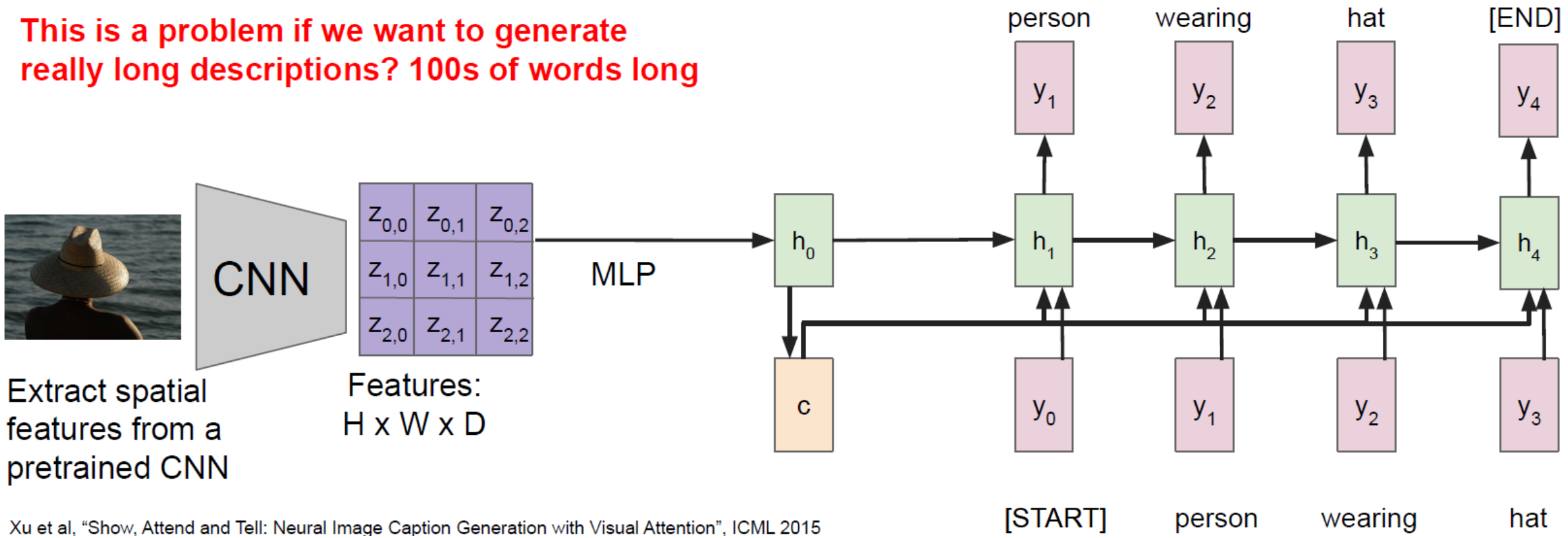
Xu et al, "Show, Attend and Tell: Neural Image Caption Generation with Visual Attention", ICML 2015

Image Captioning using spatial features

Problem: 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



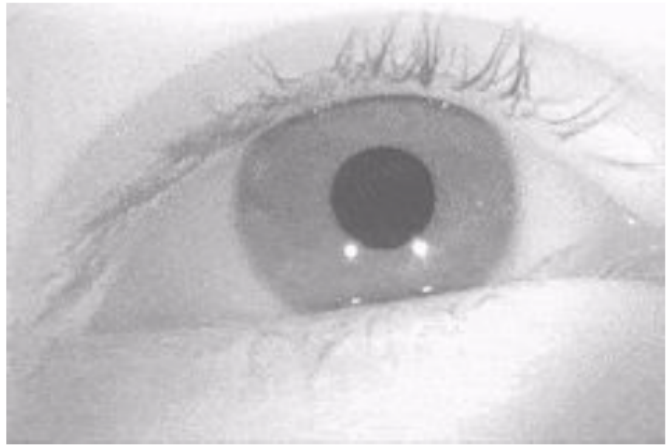
Extract spatial features from a pretrained CNN

Features: H x W x D

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

Image Captioning with RNNs and Attention

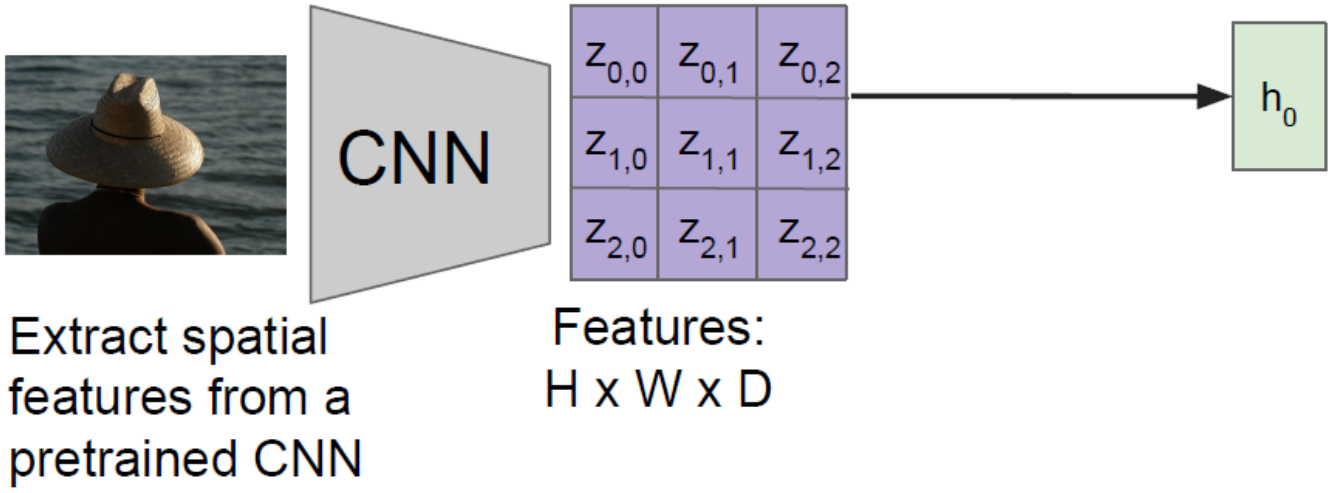
gif source



Attention Saccades in humans

Attention idea: New context vector at every time step.

Each context vector will attend to different image regions



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

Image Captioning with RNNs and Attention

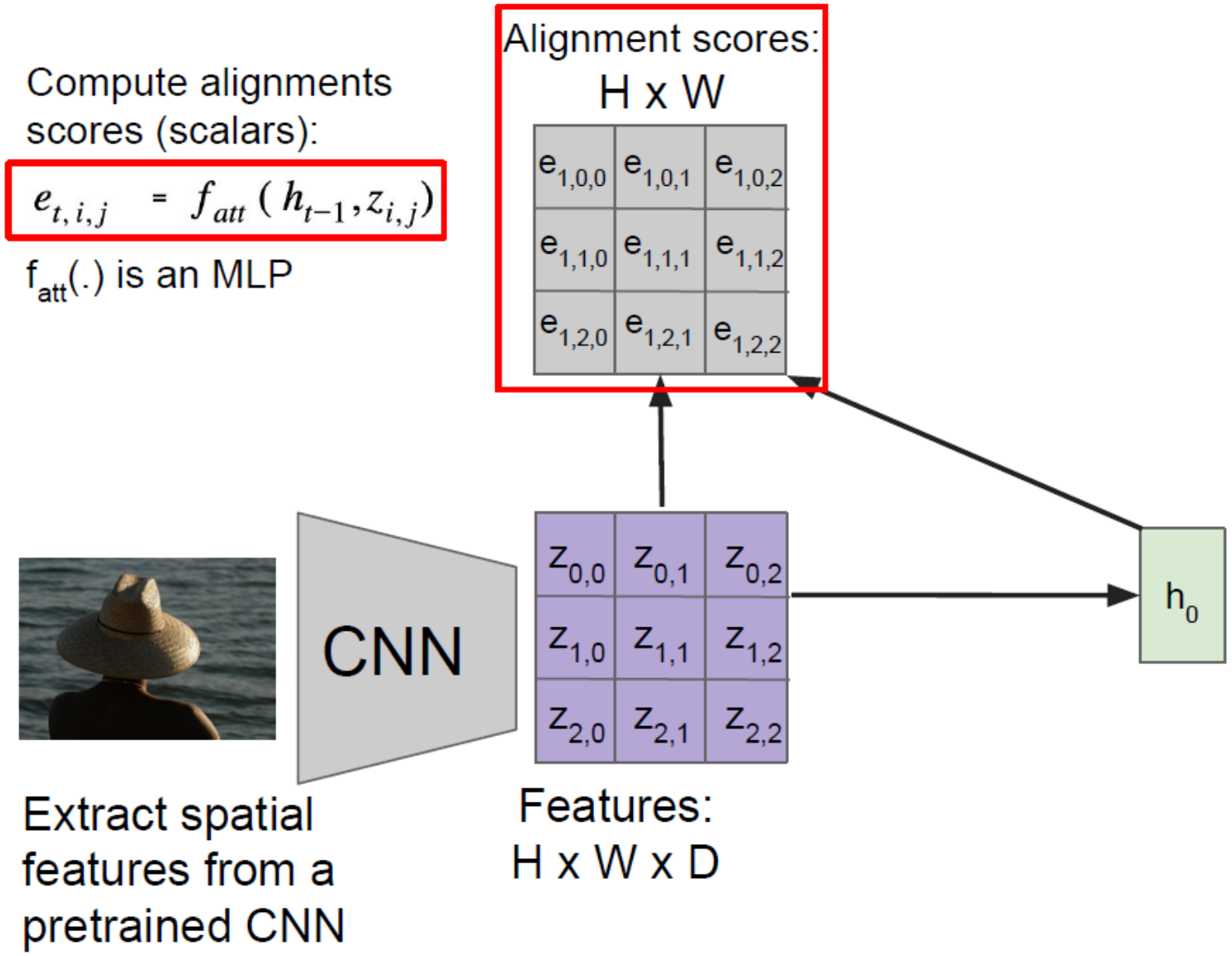


Image Captioning with RNNs and Attention

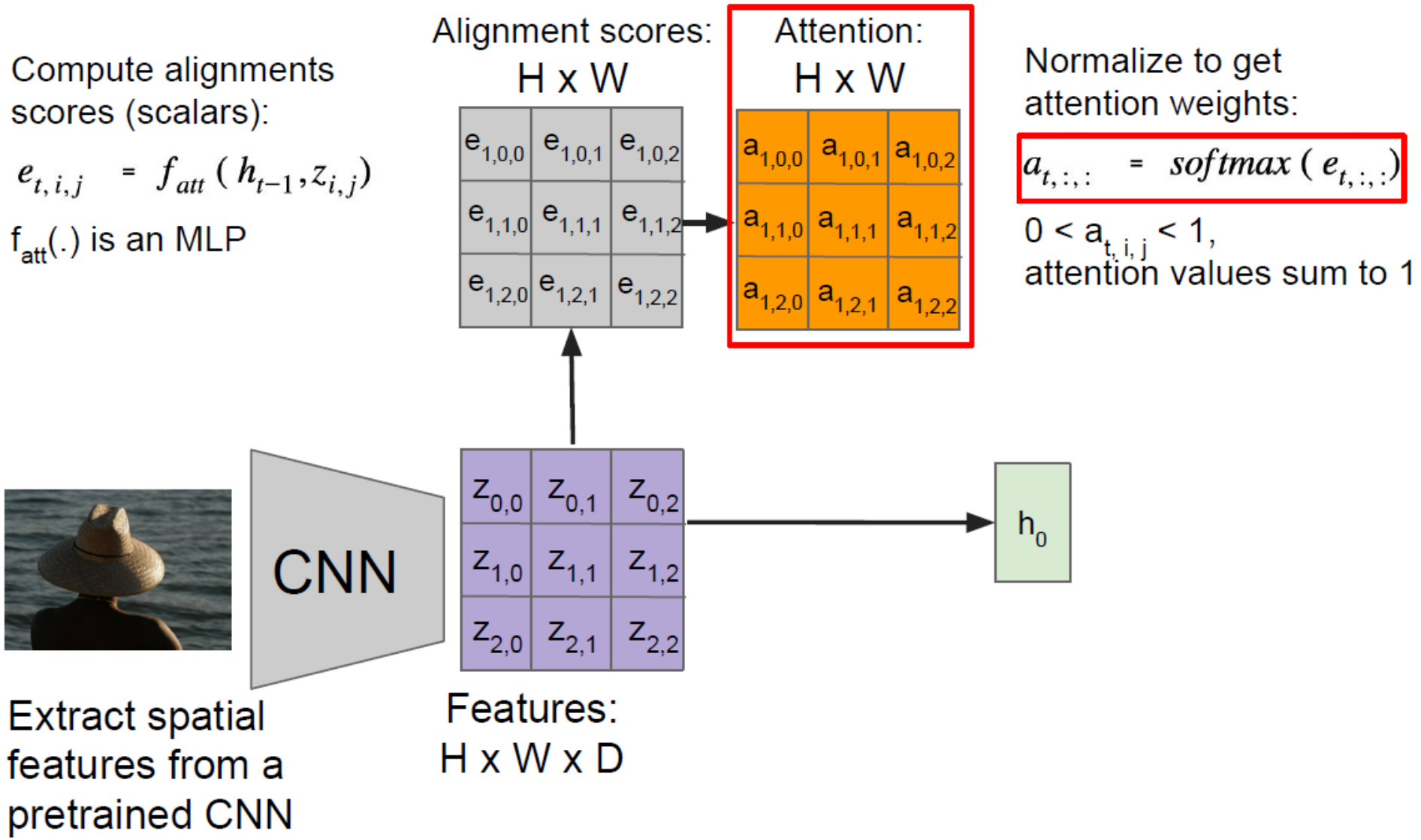


Image Captioning with RNNs and Attention

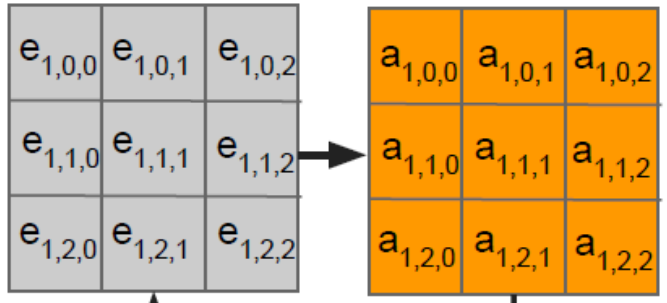
Compute alignments scores (scalars):

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

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

Alignment scores: H x W

Attention: H x W



Normalize to get attention weights:

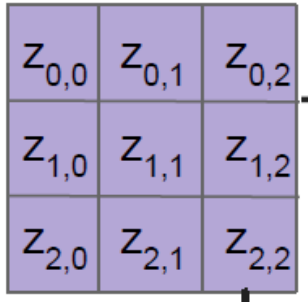
$a_{t,:,:} = softmax(e_{t,:,:})$

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

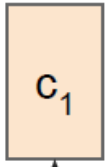
Compute context vector:

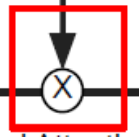
$$c_t = \sum_{i,j} a_{t,i,j} z_{t,i,j}$$

CNN



Features: H x W x D





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

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

CNN

Extract spatial features from a pretrained CNN

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

Features: H x W x D

h_0

person

y_1

h_1

c_1 y_0

Image Captioning with RNNs and Attention

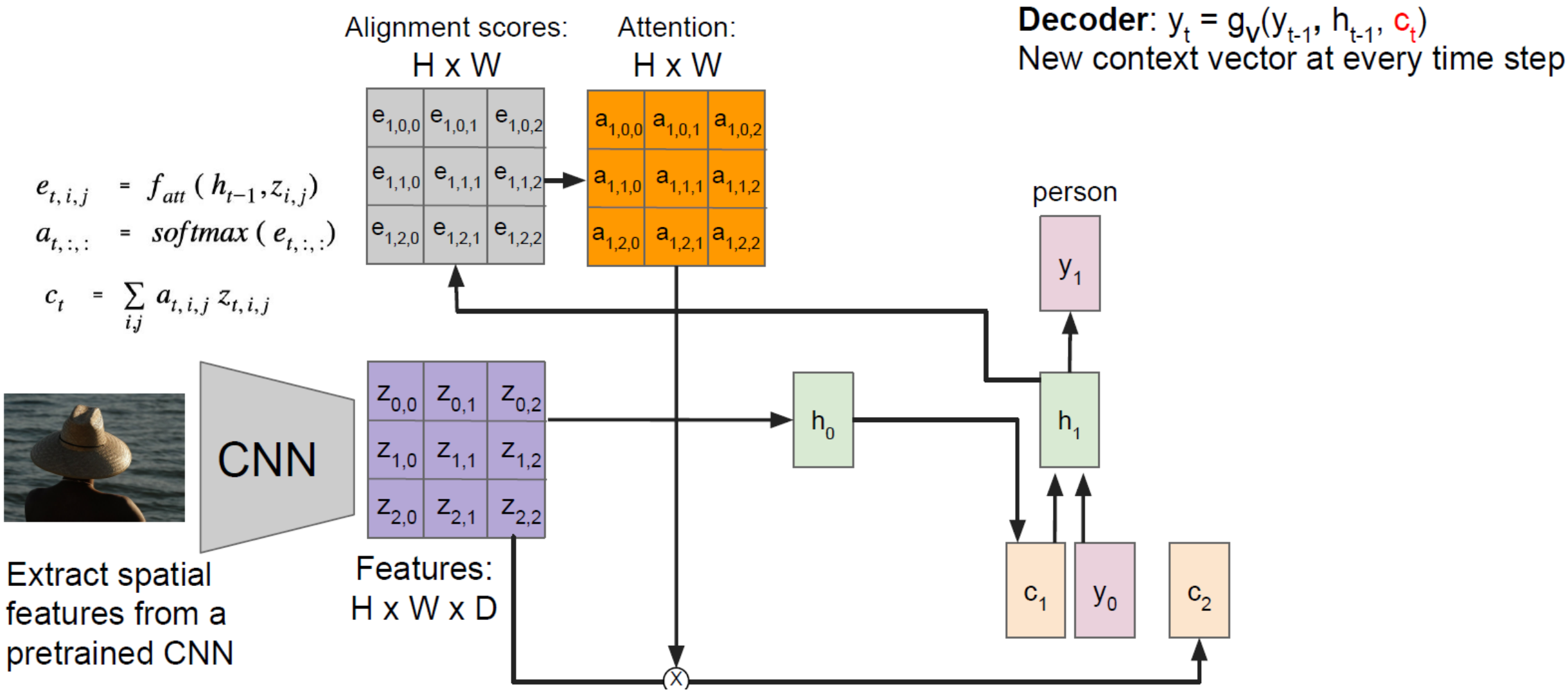


Image Captioning with RNNs and Attention

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

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

CNN

Extract spatial features from a pretrained CNN

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

Features: H x W x D

h_0 h_1 h_2 h_3 h_4

c_1 y_0 c_2 y_1 c_3 y_2 c_4 y_3

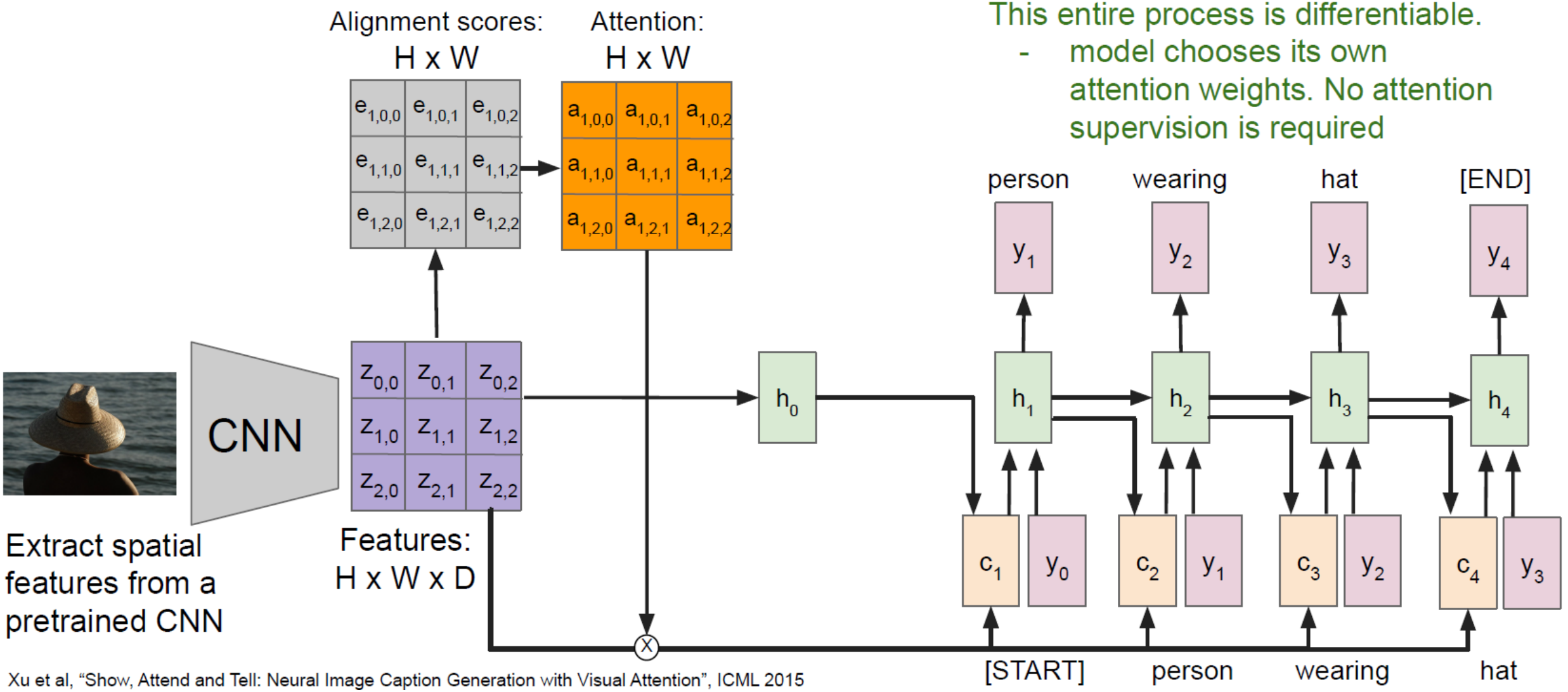
y_1 y_2 y_3 y_4

person wearing hat [END]

[START] person wearing hat

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 Attention

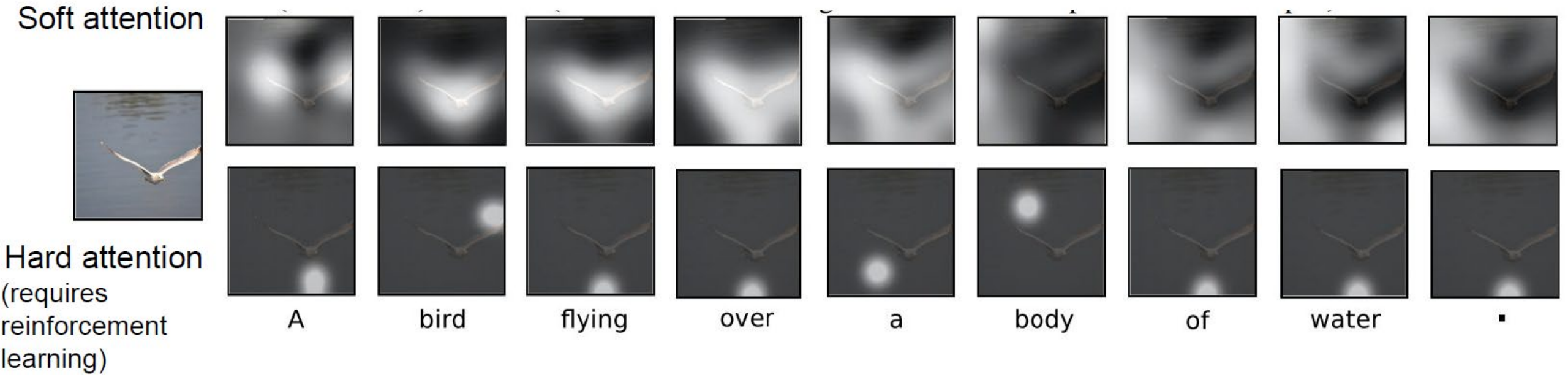


Image Captioning with Attention

A woman is throwing a frisbee in a park.

A dog is standing on a hardwood floor.

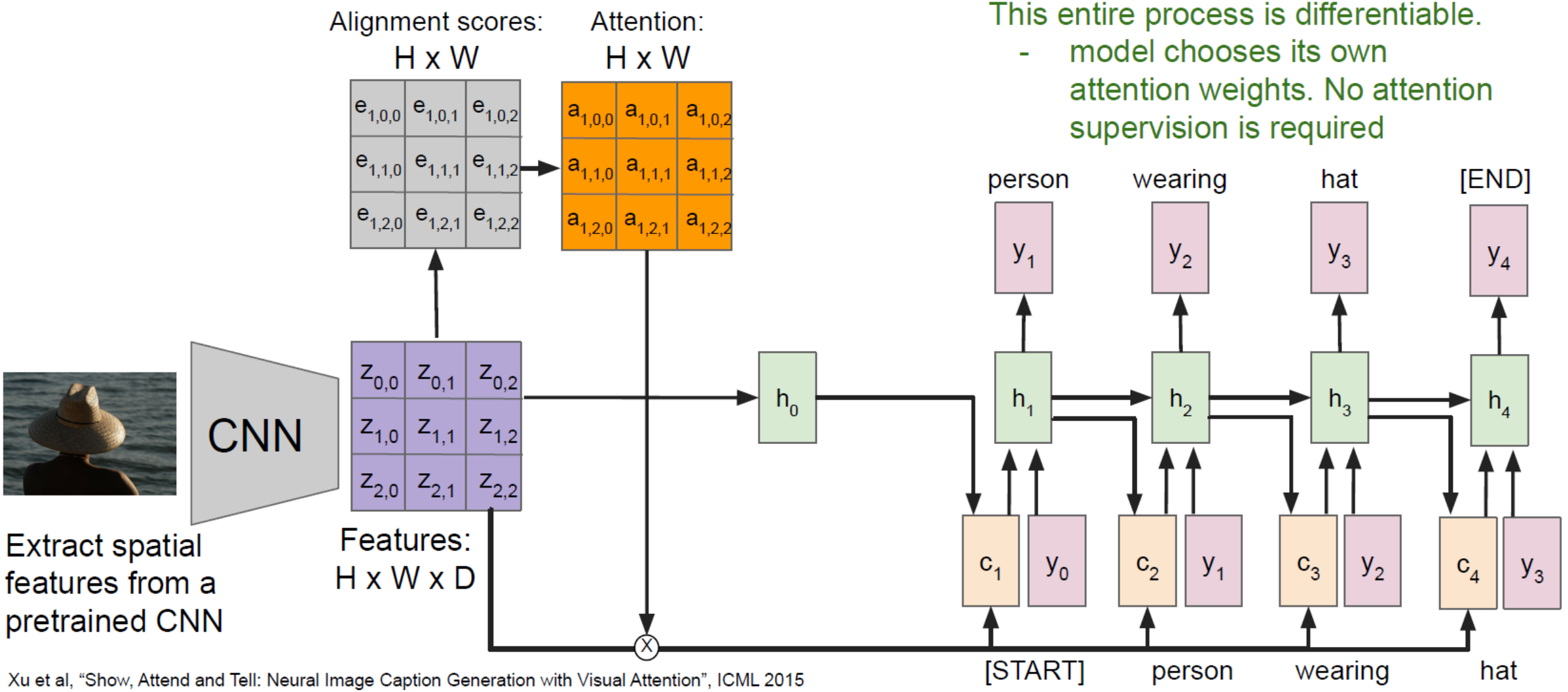
A stop sign is on a road with a mountain in the background.

A little girl sitting on a bed with a teddy bear.

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

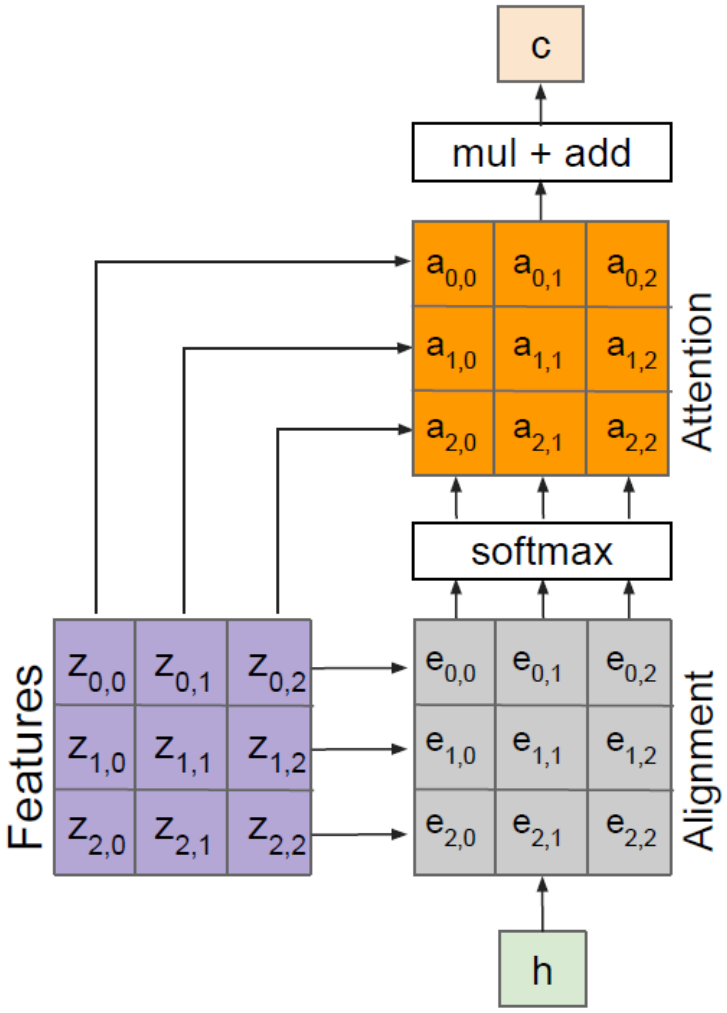
A giraffe standing in a forest with trees in the background.

Image Captioning with RNNs and Attention



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

Attention we just saw in image captioning

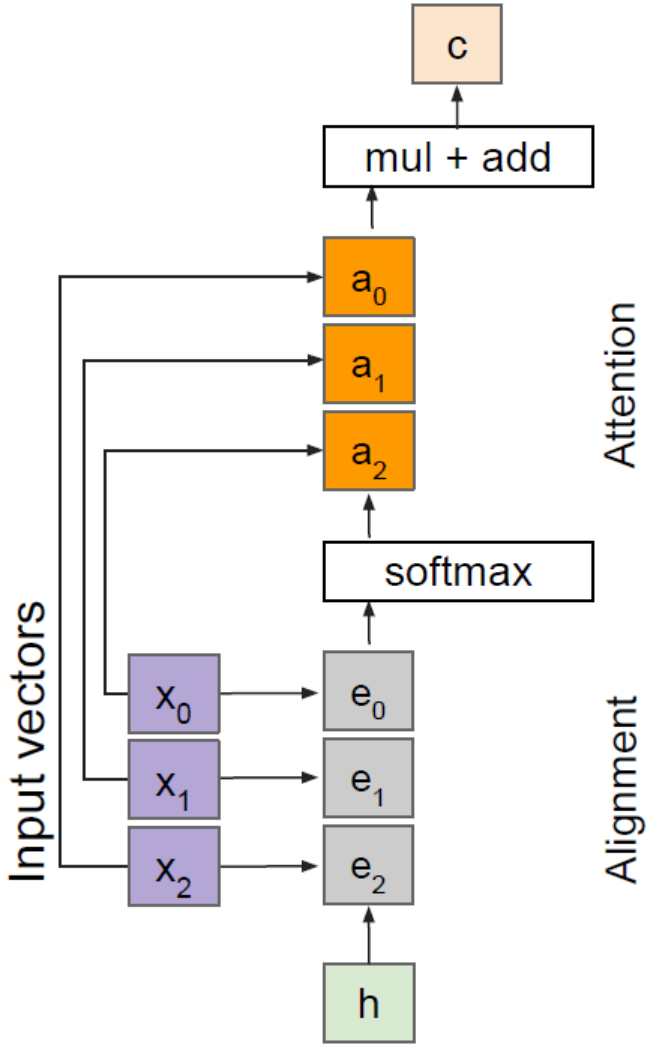


Outputs:
context vector: **c** (shape: D)

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)

General attention layer



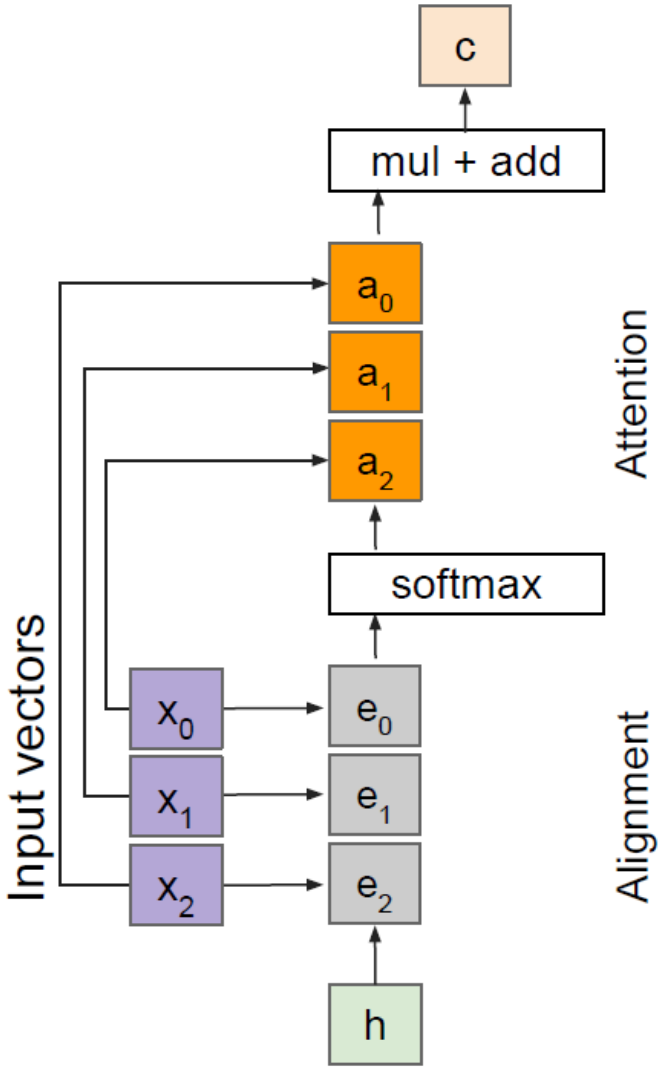
Outputs:
context vector: **c** (shape: D)

Operations:
Alignment: $e_i = f_{att}(h, x_i)$
Attention: **a** = softmax(**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 H x W = N into N vectors

General attention layer



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

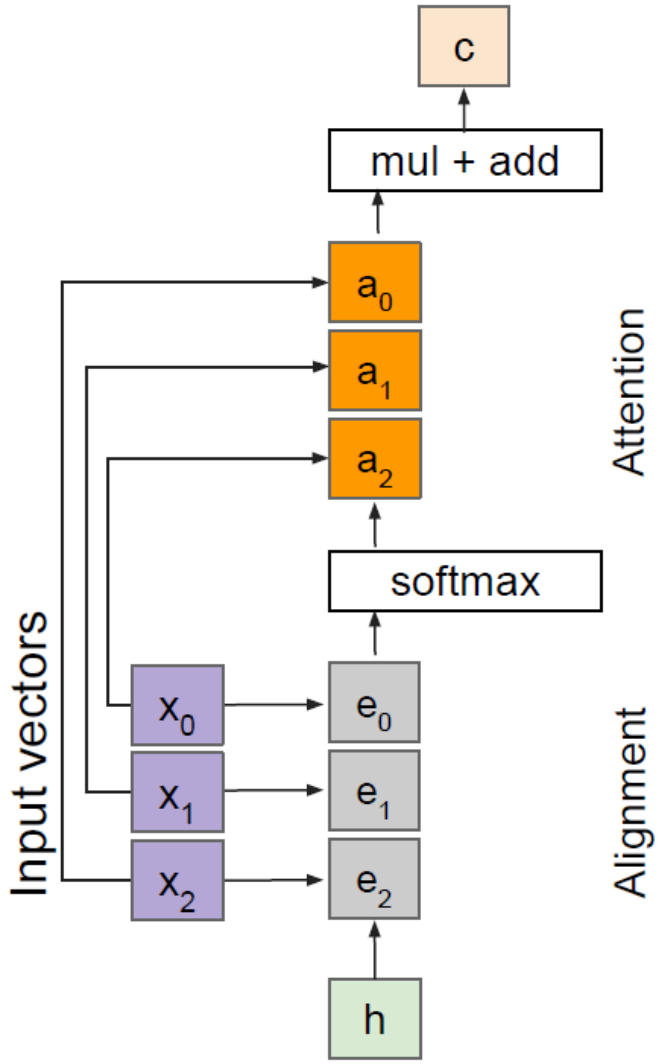
Operations:
Alignment: $e_i = h \cdot x_i$
Attention: **a** = softmax(**e**)
Output: $\mathbf{c} = \sum_i a_i x_i$

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

- only works well with key & value transformation trick (will mention in a few slides)

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

General attention layer



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

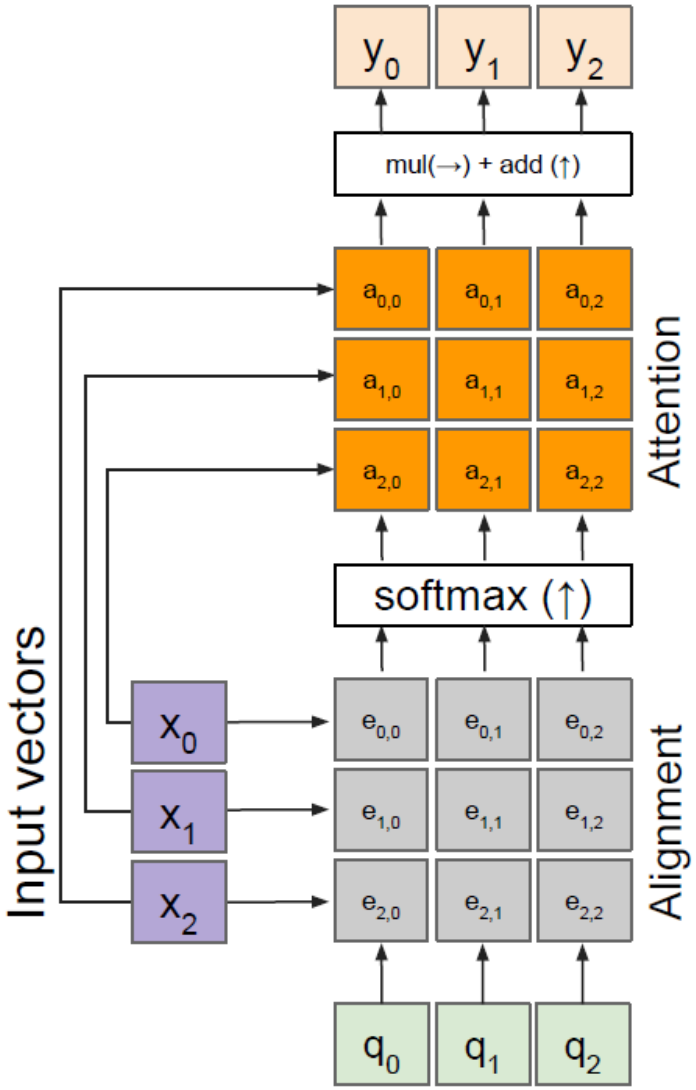
Operations:
Alignment: $e_i = h \cdot x_i / \sqrt{D}$
Attention: **a** = softmax(**e**)
Output: $\mathbf{c} = \sum_i a_i x_i$

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, assuming logits are IID.
- 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)

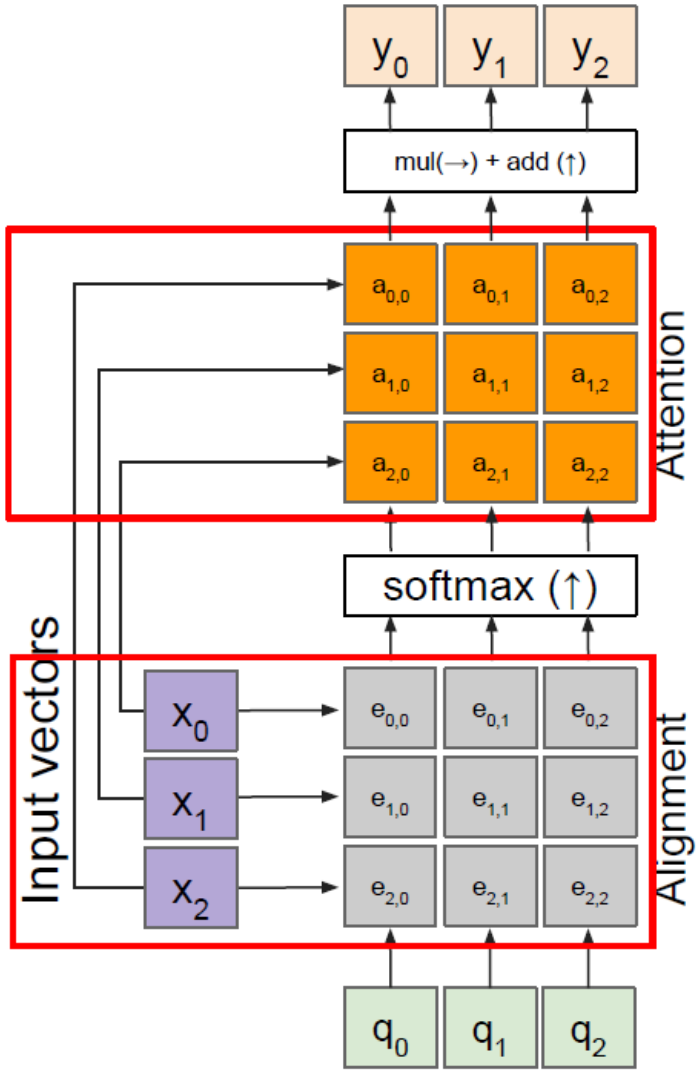
Multiple query vectors
- each query creates a new output context vector

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

Multiple query vectors

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

General attention layer



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

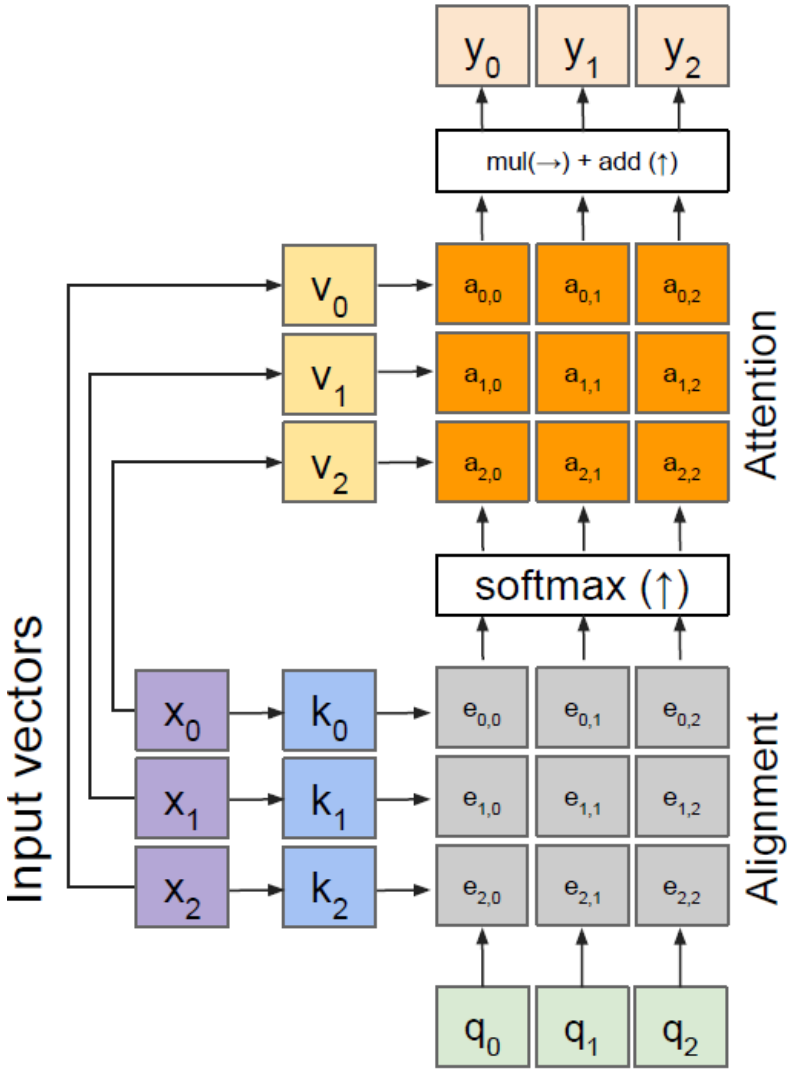
Operations:
Alignment: $e_{i,j} = q_j \cdot x_i / \sqrt{D}$
Attention: **a** = softmax(**e**)
Output: $y_j = \sum_i a_{i,j} x_i$

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



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

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

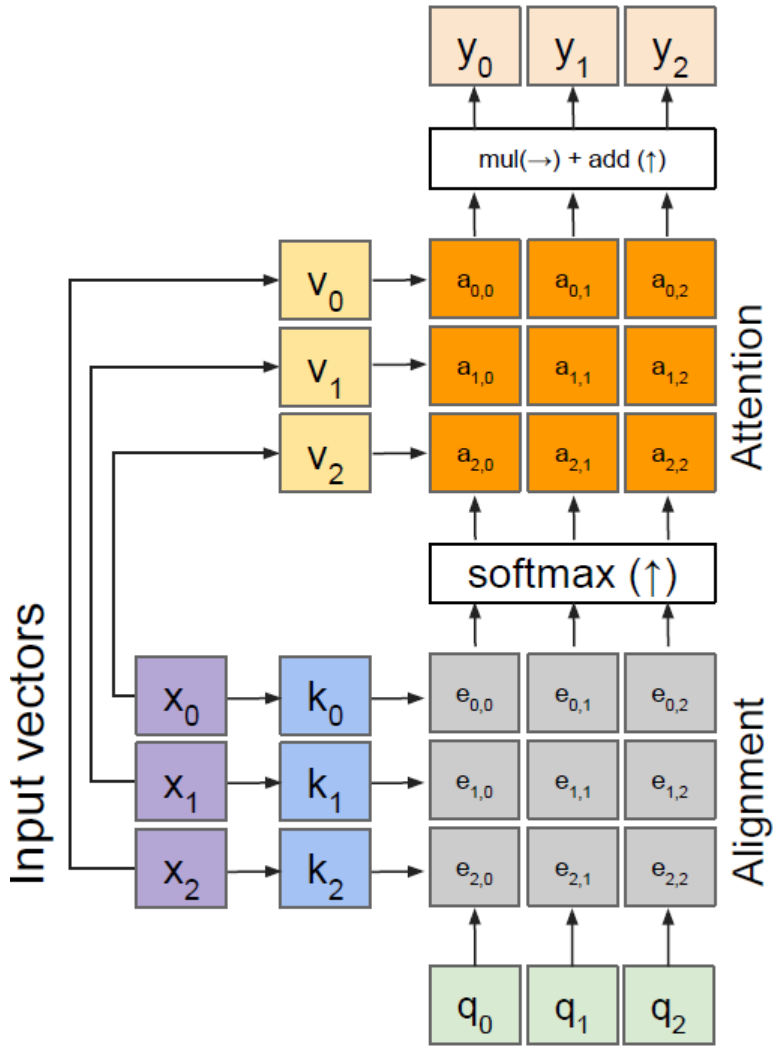
Inputs:
Input vectors: **x** (shape: N x D)
Queries: **q** (shape: M x D_k)

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

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



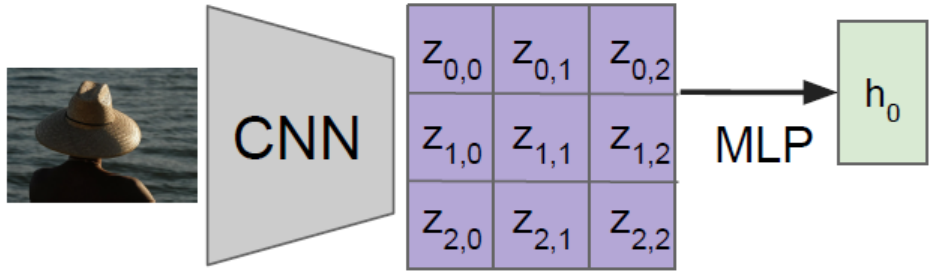
Outputs:
context vectors: **y** (shape: D_v)

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

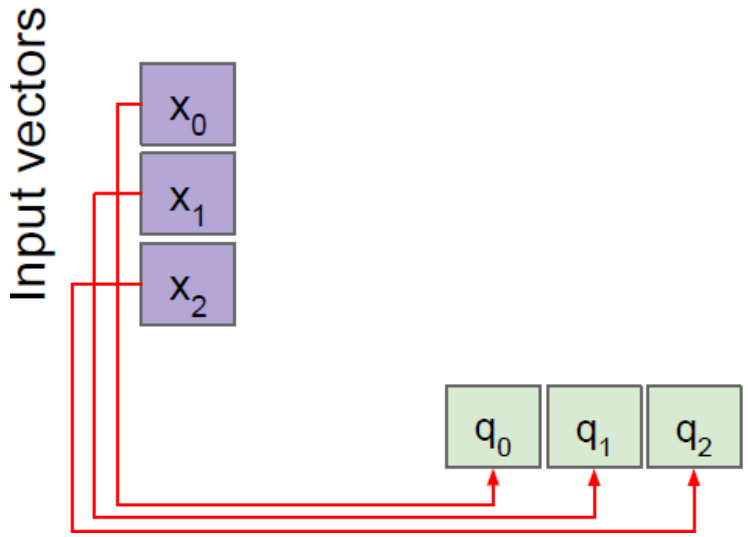
Inputs:
Input vectors: **x** (shape: N x D)
Queries: **q** (shape: M x D_k)

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

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



Self attention layer



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

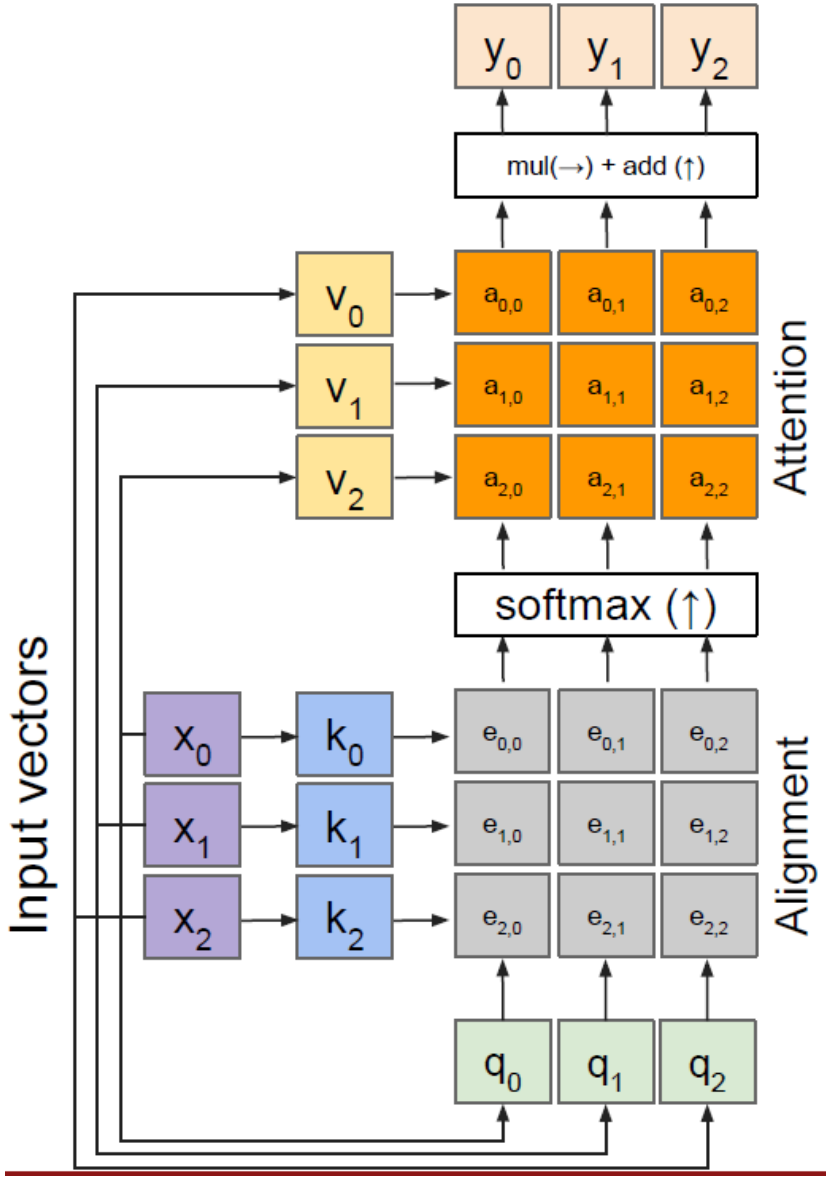
We can calculate the query vectors from the input vectors, therefore, defining a "self-attention" layer.

Instead, query vectors are calculated using a FC layer.

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

No input query vectors anymore

Self attention layer

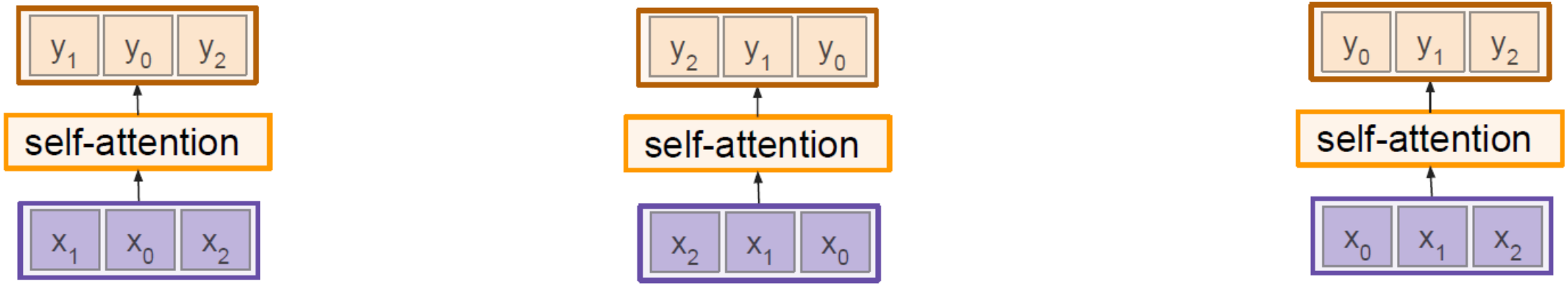


Outputs:
context vectors: **y** (shape: D_v)

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

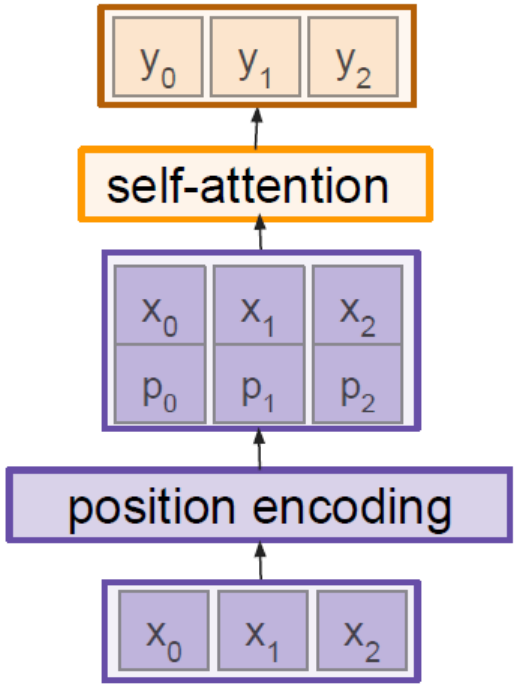


Permutation equivariant

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/add special positional encoding p_j to each input vector x_j

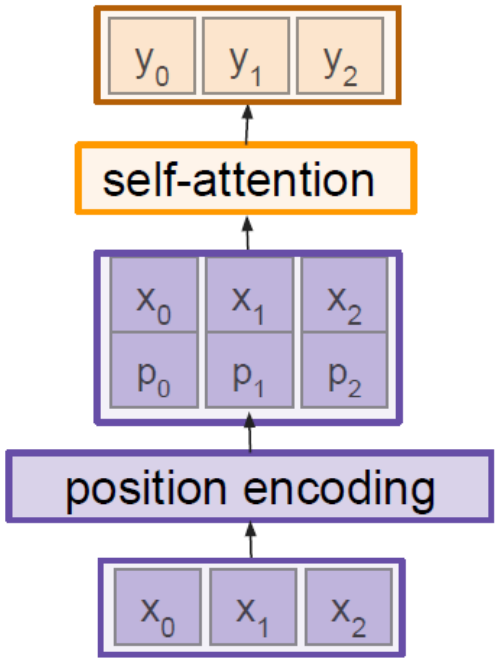
We use a function *pos*: $N \rightarrow R^d$ to process the position j of the vector into a d-dimensional vector

So, $p_j = pos(j)$

Desiderata 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, $p_i = pos(j)$

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.
2. Design a fixed function with the desiderata

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

Intuition:

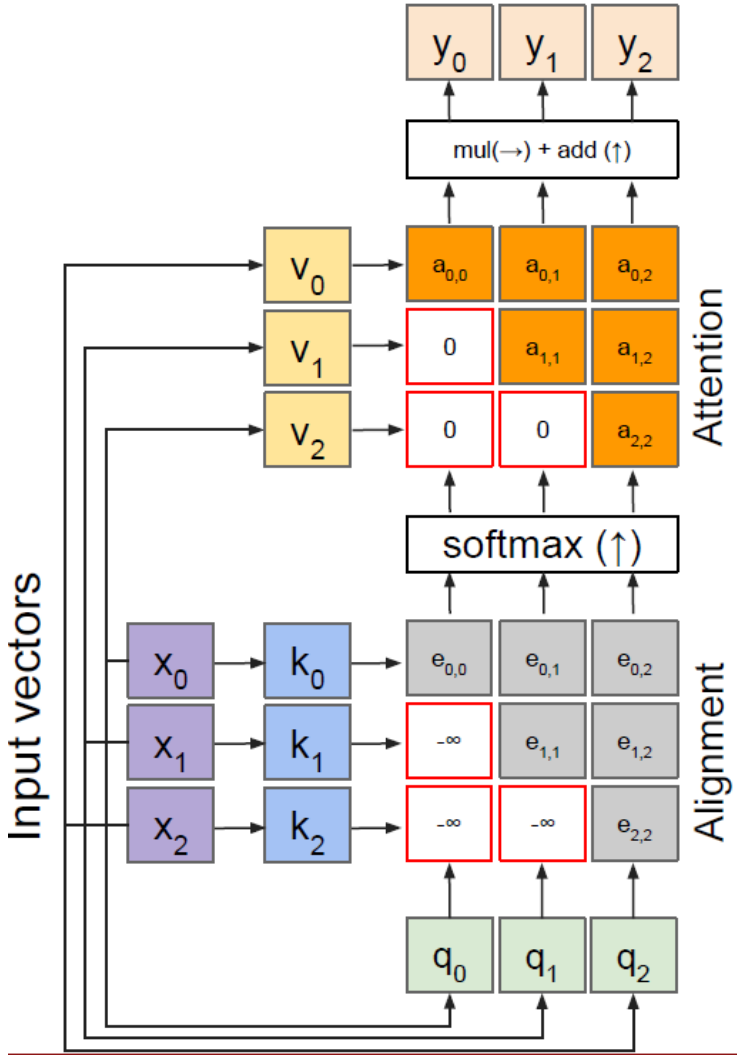
0 :	0	0	0	0	8 :	1	0	0	0
1 :	0	0	0	1	9 :	1	0	0	1
2 :	0	0	1	0	10 :	1	0	1	0
3 :	0	0	1	1	11 :	1	0	1	1
4 :	0	1	0	0	12 :	1	1	0	0
5 :	0	1	0	1	13 :	1	1	0	1
6 :	0	1	1	0	14 :	1	1	1	0
7 :	0	1	1	1	15 :	1	1	1	1

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

image source

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

Masked self-attention layer



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

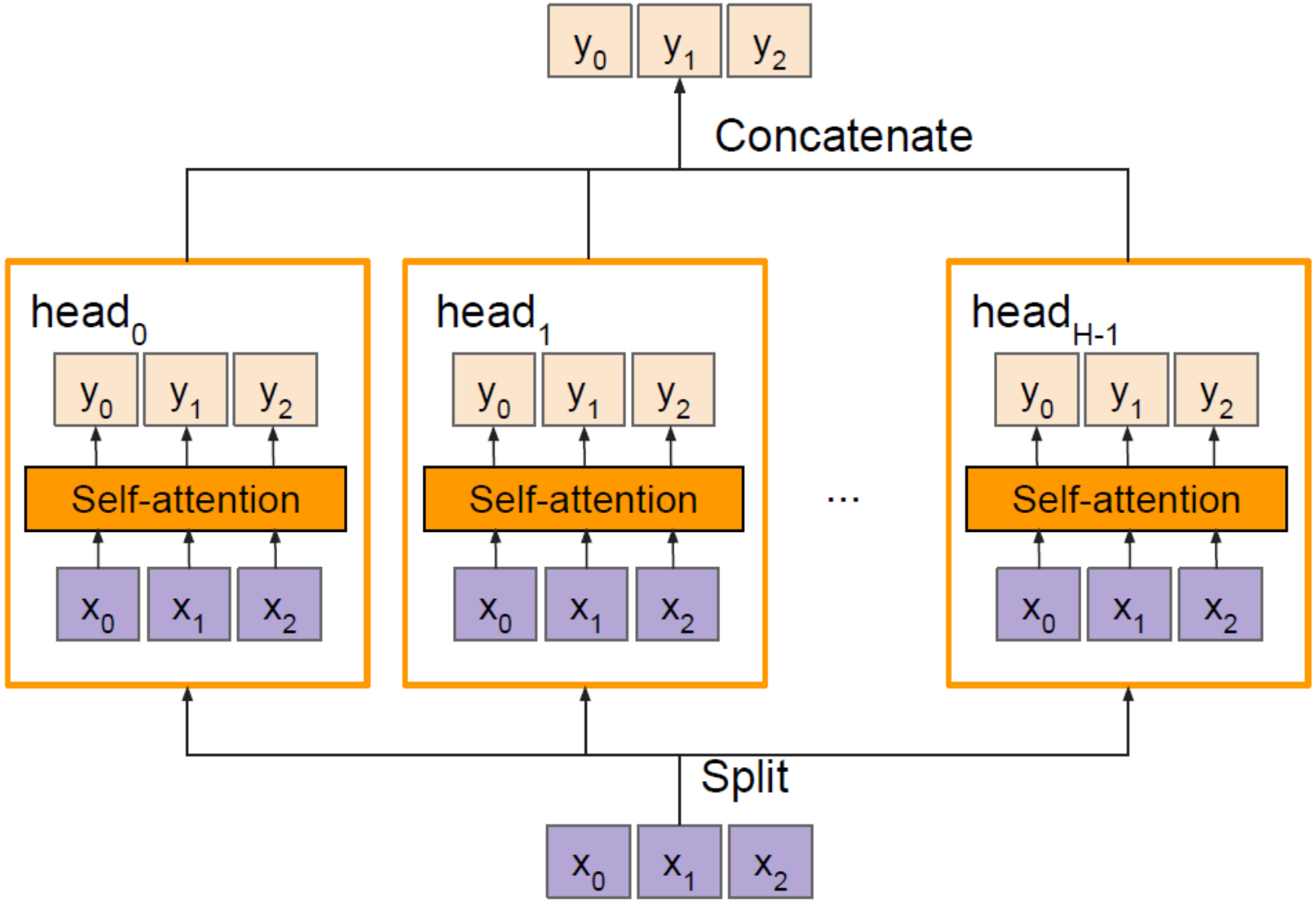
Operations:
Key vectors: $\mathbf{k} = \mathbf{x}W_k$
Value vectors: $\mathbf{v} = \mathbf{x}W_v$
Query vectors: $\mathbf{q} = \mathbf{x}W_q$
Alignment: $e_{i,j} = q_j \cdot k_i / \sqrt{D}$
Attention: $\mathbf{a} = \text{softmax}(\mathbf{e})$
Output: $y_j = \sum_i a_{i,j} v_i$

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

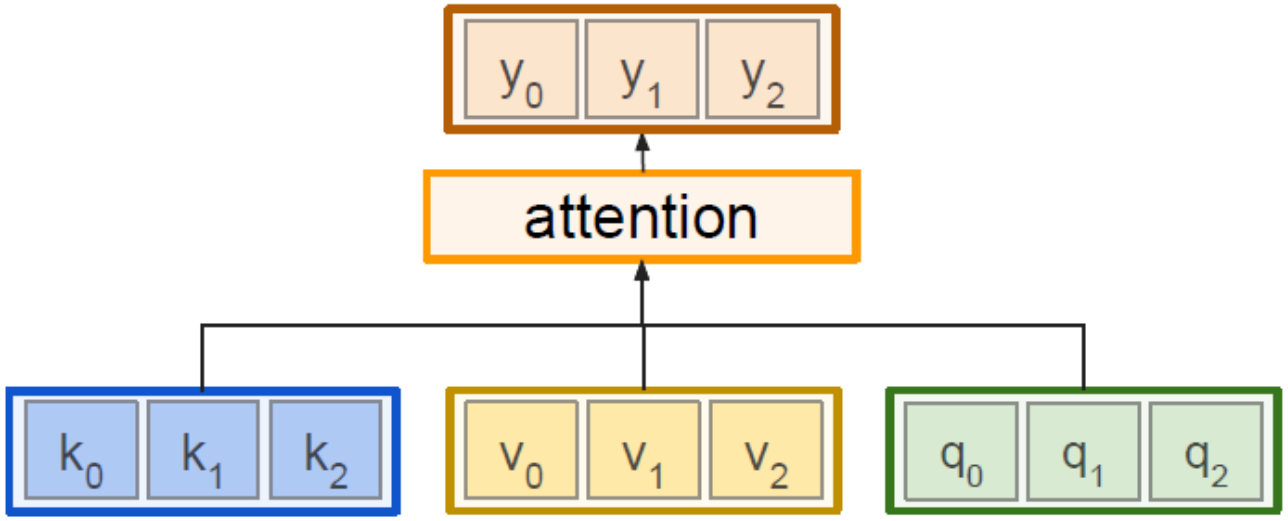
- Prevent vectors from looking at future vectors.
- Manually set alignment scores to -infinity

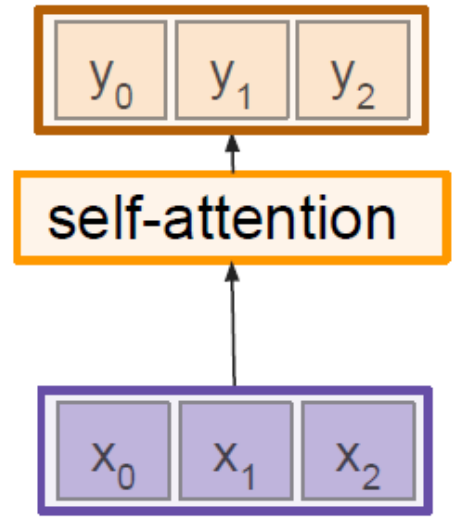
Multi-head self attention layer

- Multiple self-attention heads in parallel

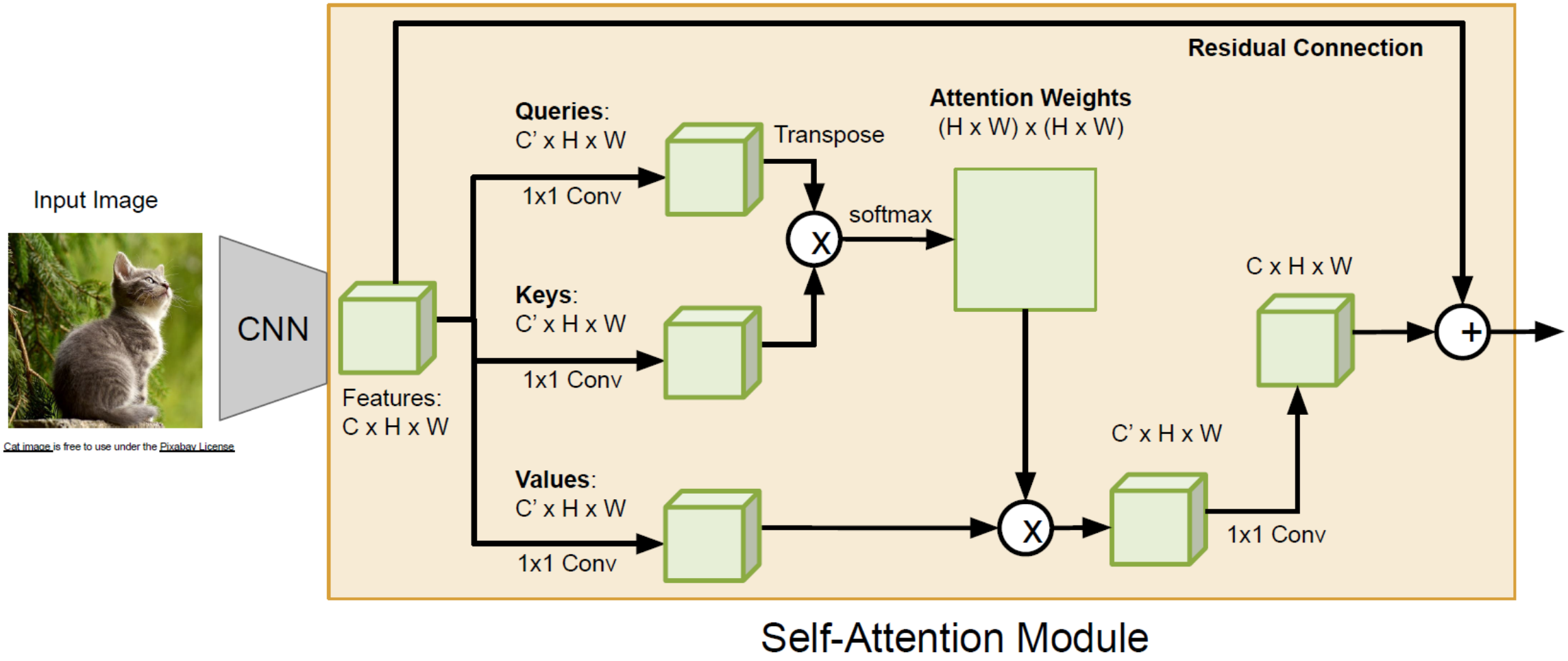


General attention versus self-attention





Example: CNN with Self-Attention



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.

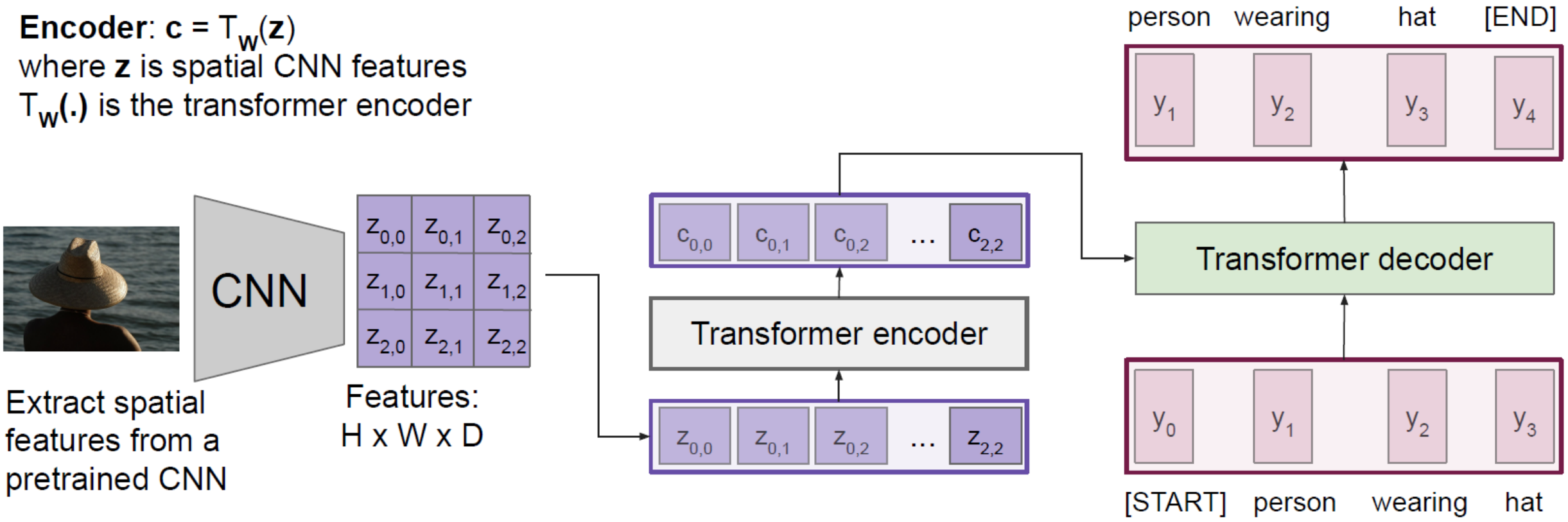
Transformer:
(+) Good at long sequences. Each attention calculation looks at all inputs.
(+) Can operate over unordered sets or ordered sequences with positional encodings.
(+) Parallel computation: All alignment and attention scores for all inputs can be done in parallel.
(-) Requires a lot of memory: 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)

Image Captioning using Transformers

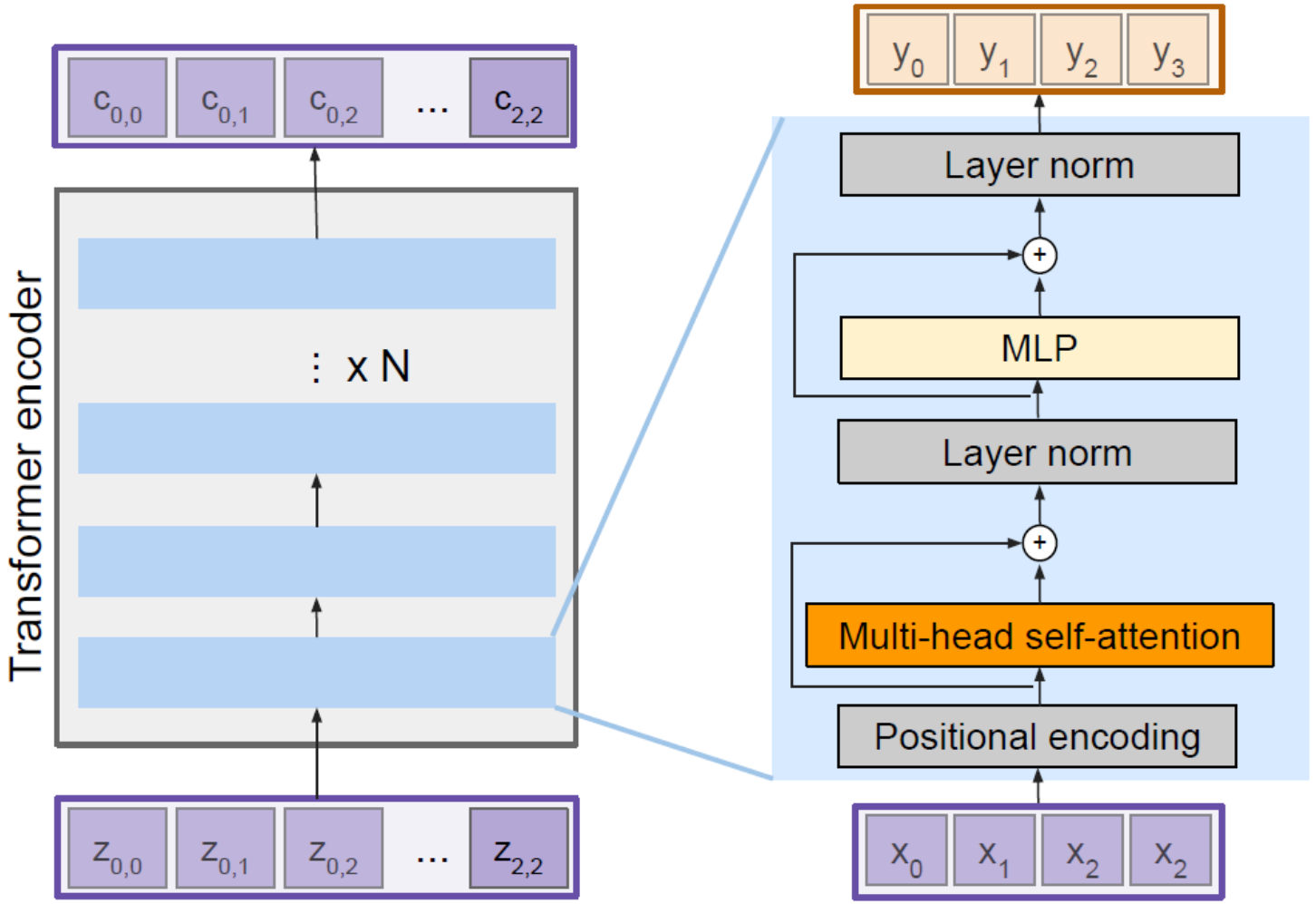
Input: Image **I**
Output: Sequence **y** = $y_1, y_2, \ldots, y_T$

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

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



The Transformer encoder block



Transformer Encoder Block:

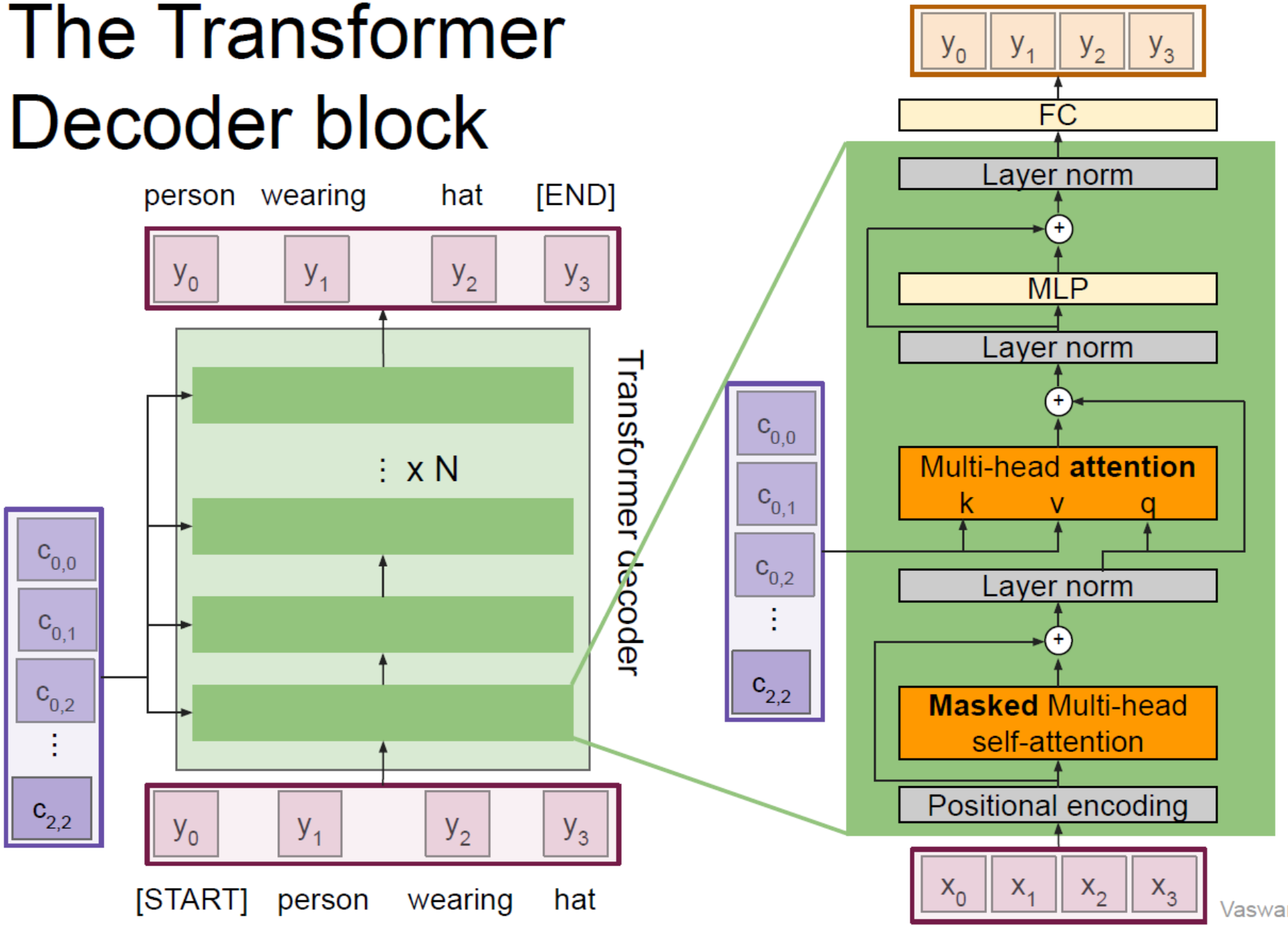
Inputs: Set of vectors **x**
Outputs: Set of vectors **y**

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 block



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.

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

Image Captioning using transformers

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

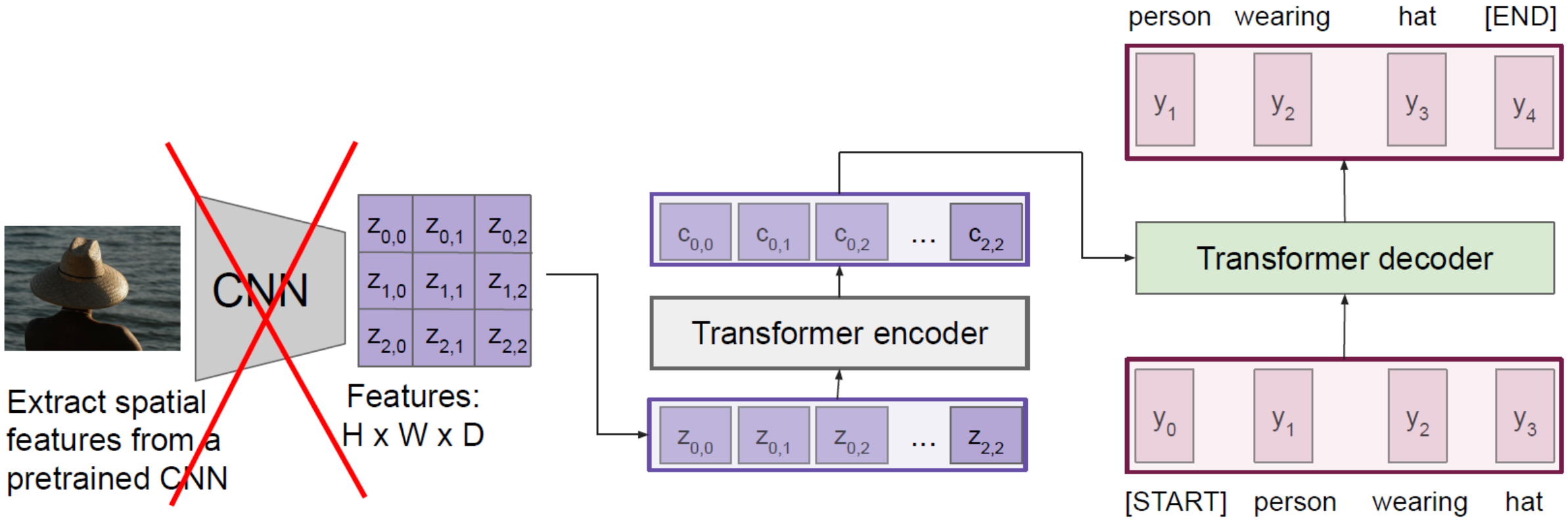
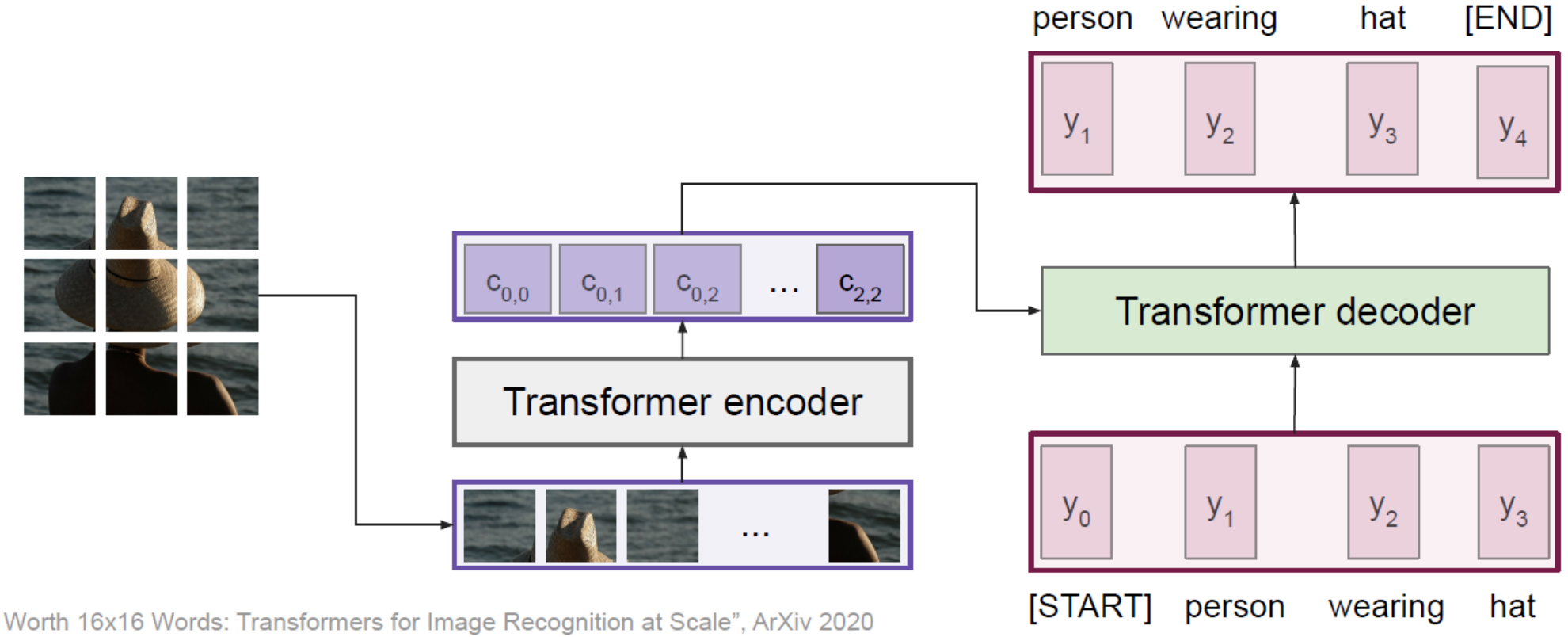


Image Captioning using ONLY transformers

- **Transformers from pixels to language**



Dosovitskiy et al, "An Image is Worth 16x16 Words: Transformers for Image Recognition at Scale", ArXiv 2020
Colab link to an implementation of vision transformers