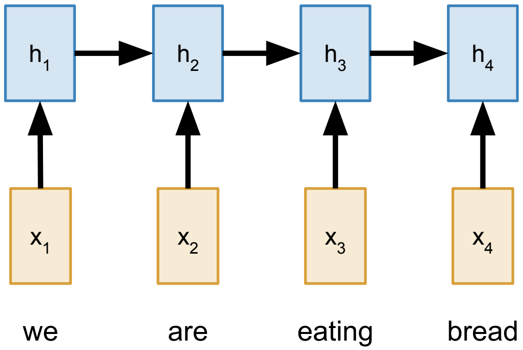
Sequence to Sequence with RNNs

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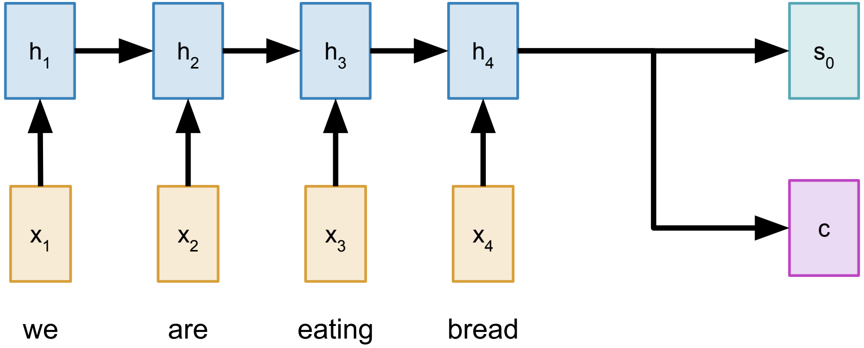
From final hidden state predict:
Initial decoder state s_0
Context vector c (often $c=h_T$)



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Sequence to Sequence with RNNs

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

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

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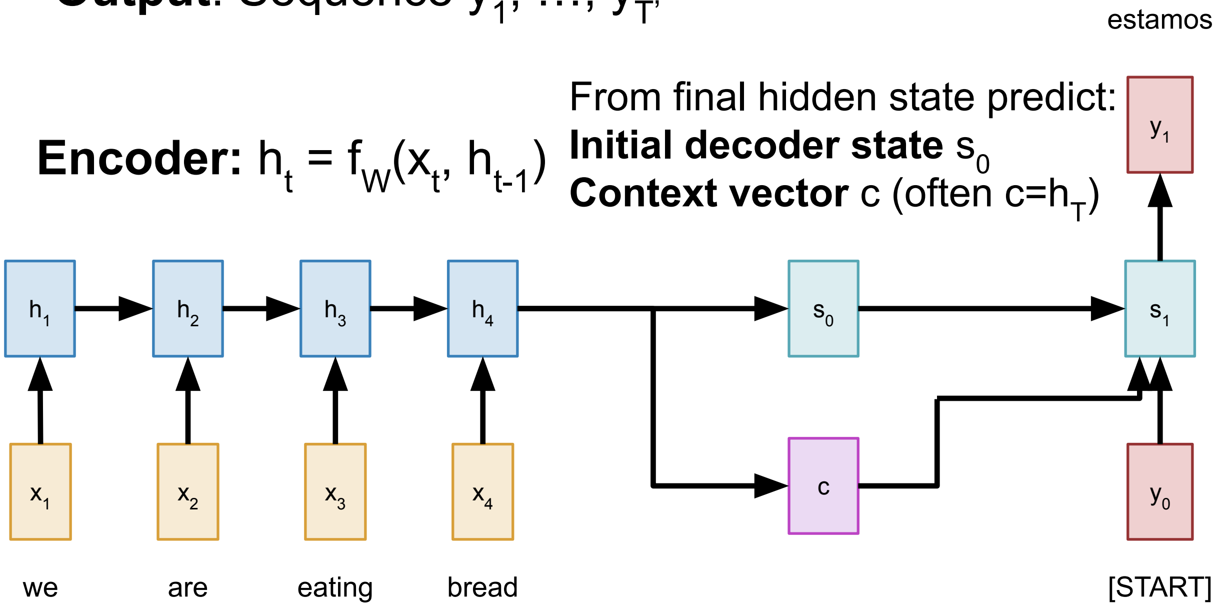

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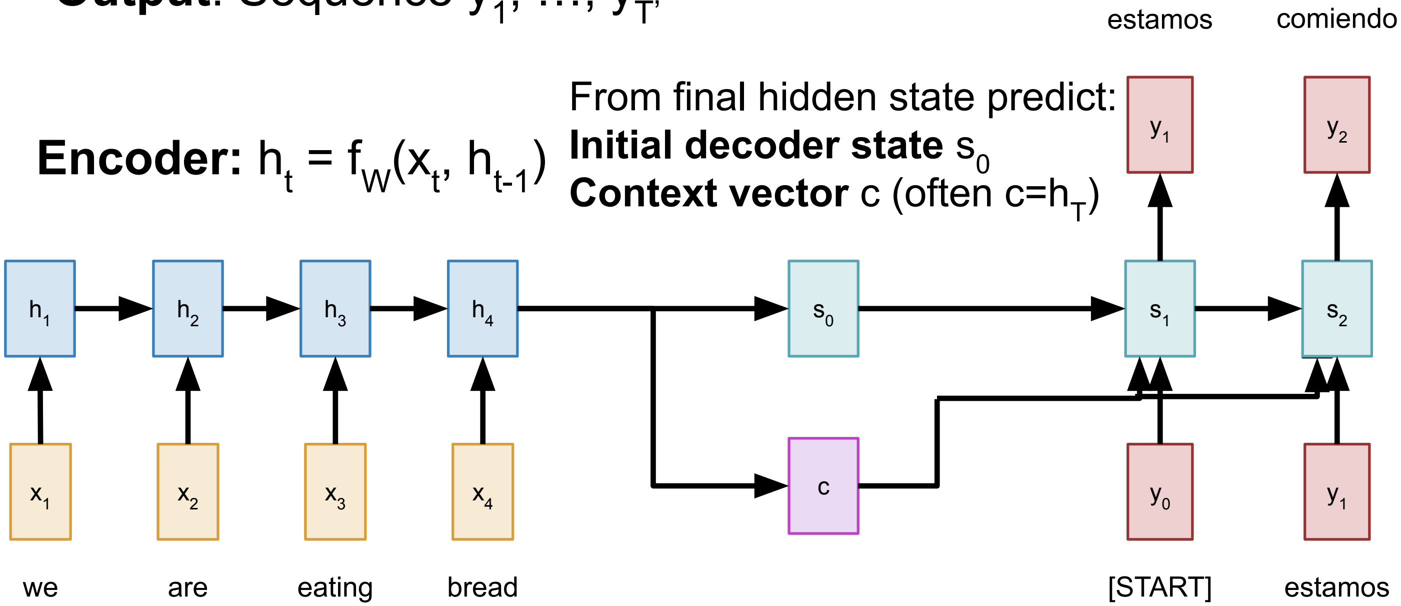

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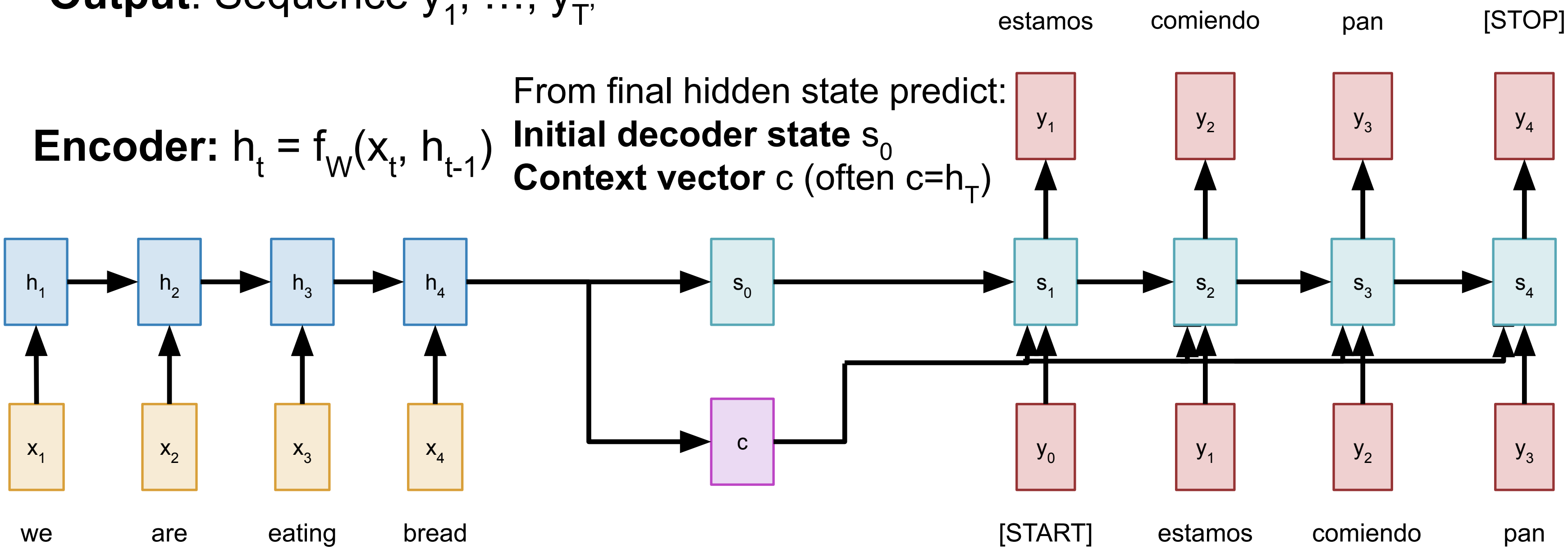

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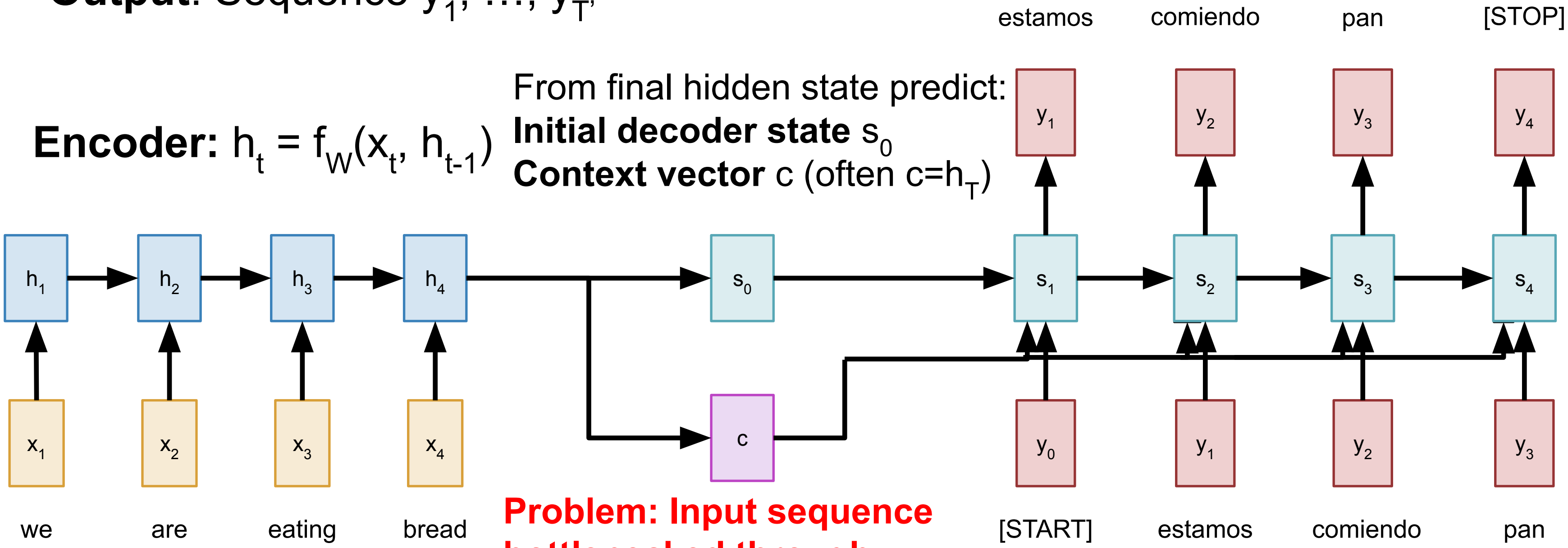

Problem: Input sequence bottlenecked through fixed-sized vector. What if T=1000?

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

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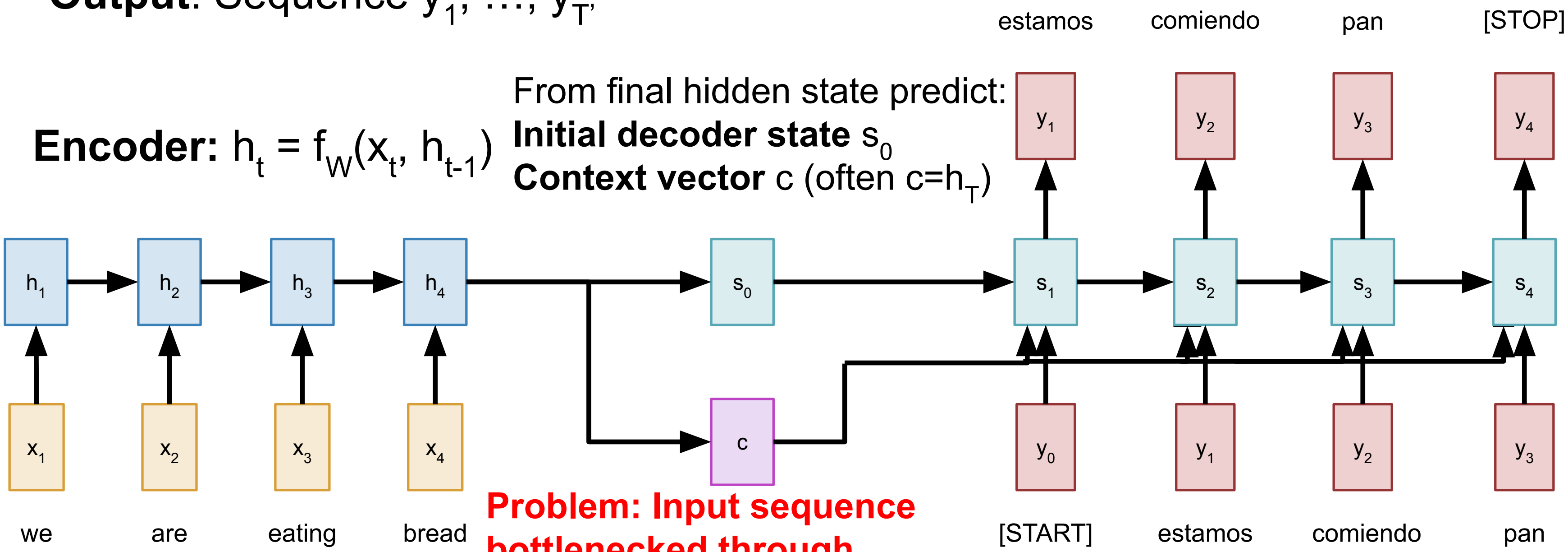


Problem: Input sequence bottlenecked through fixed-sized vector. What if T=1000?

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

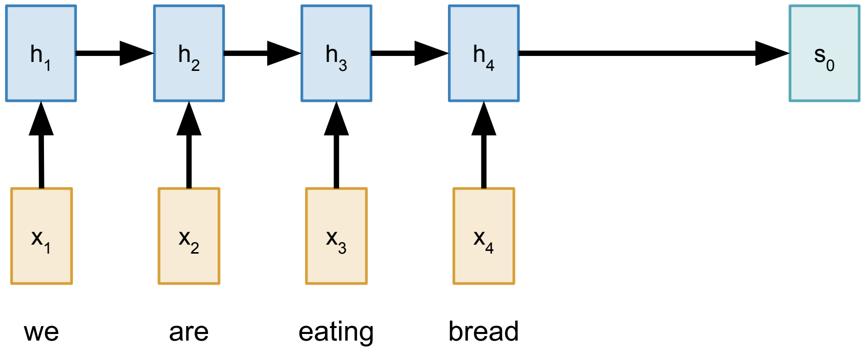
Sutskever et al, "Sequence to sequence learning with neural networks", NeurIPS 2014

Sequence to Sequence with RNNs and Attention

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

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

From final hidden state:
Initial decoder state s_0

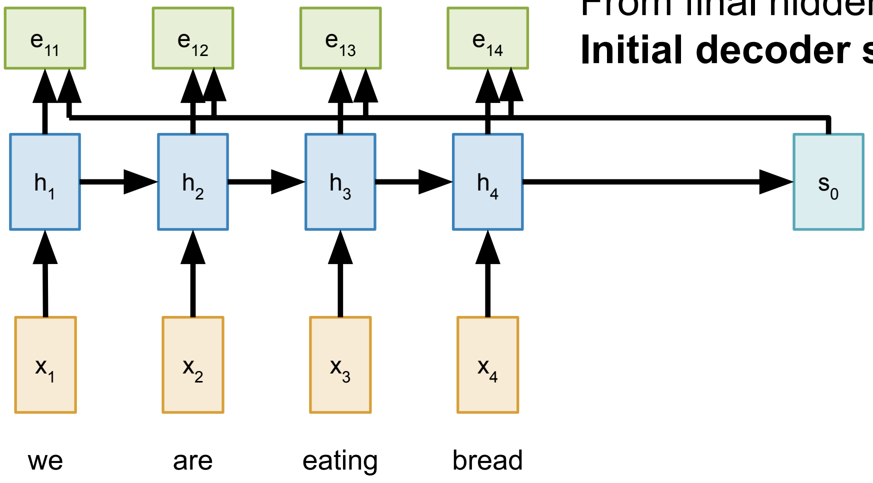


Bahdanau et al, "Neural machine translation by jointly learning to align and translate", ICLR 2015

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)

From final hidden state:
Initial decoder state s_0



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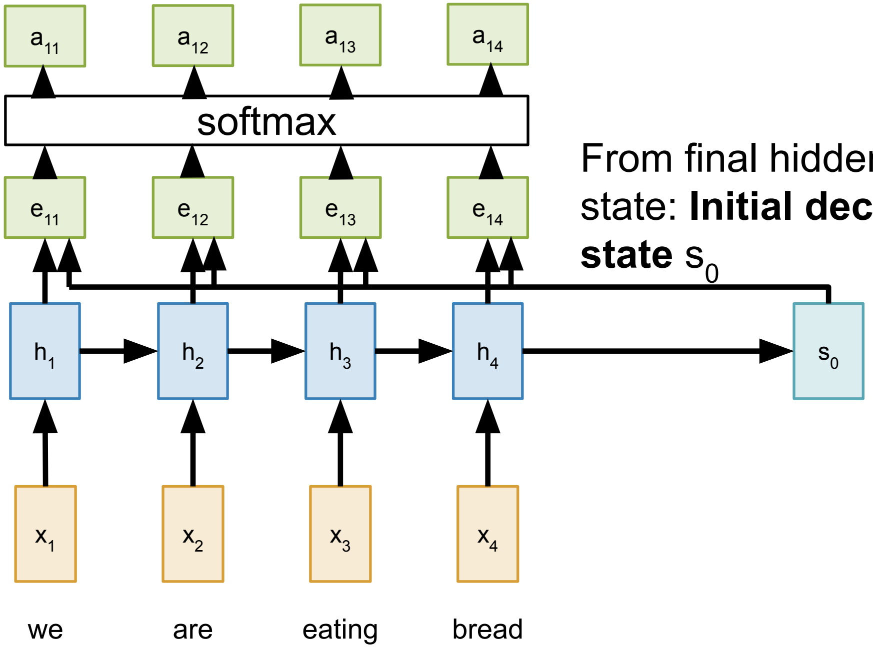
Sequence to Sequence with RNNs and Attention



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

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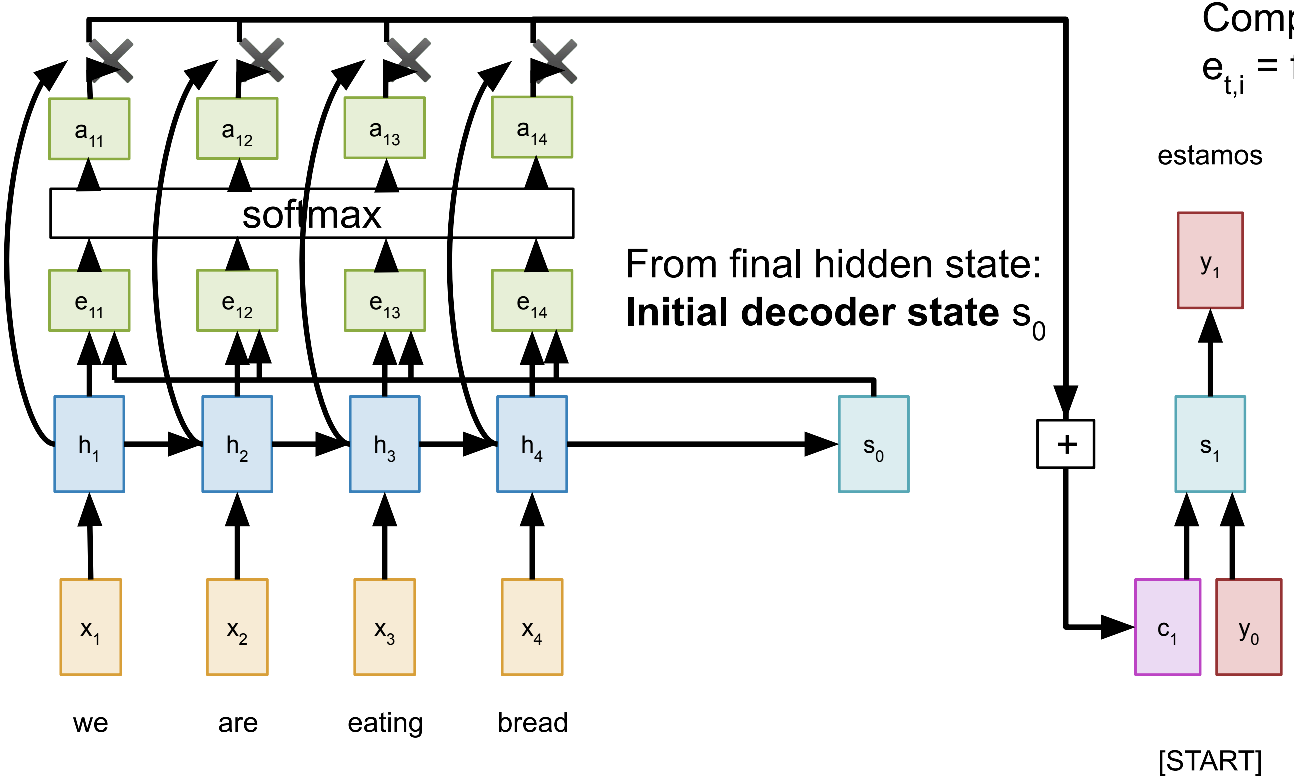
Sequence to Sequence with RNNs and Attention



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

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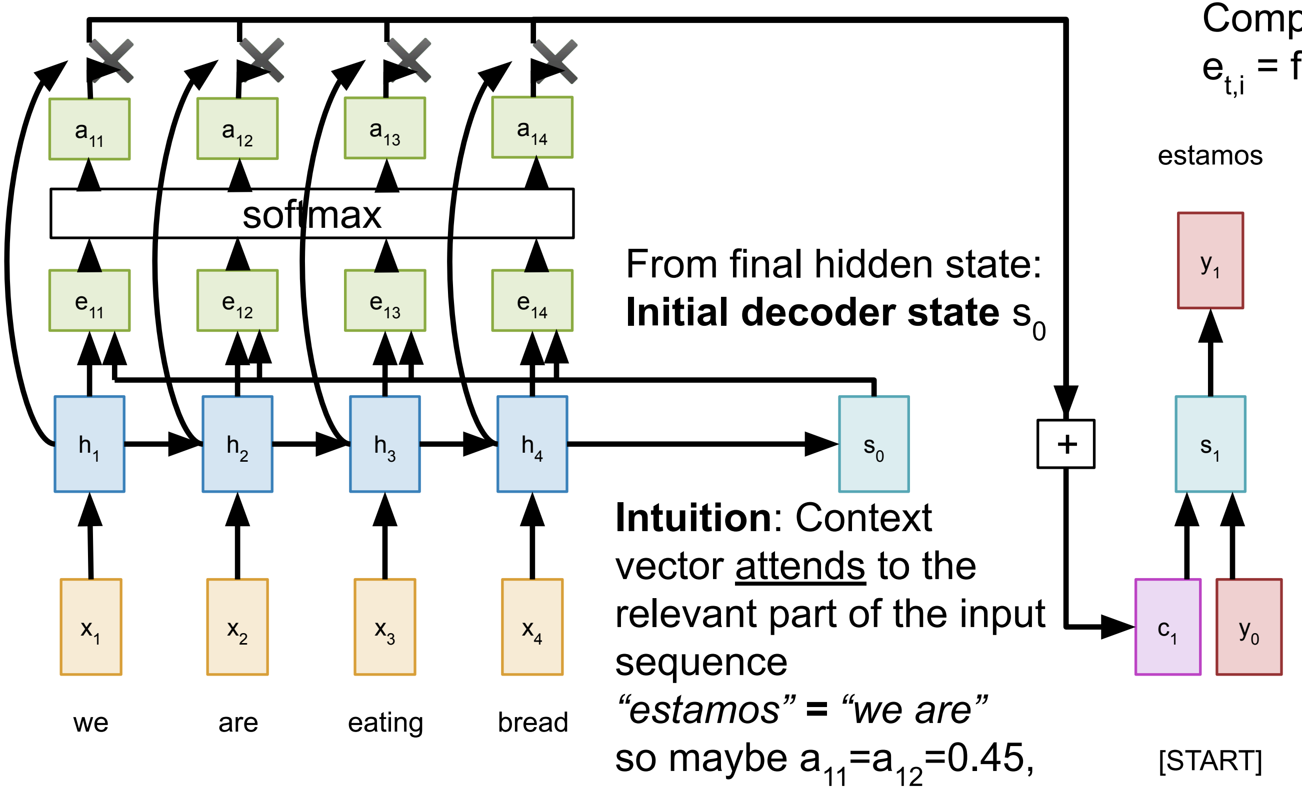
Sequence to Sequence with RNNs and Attention



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

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

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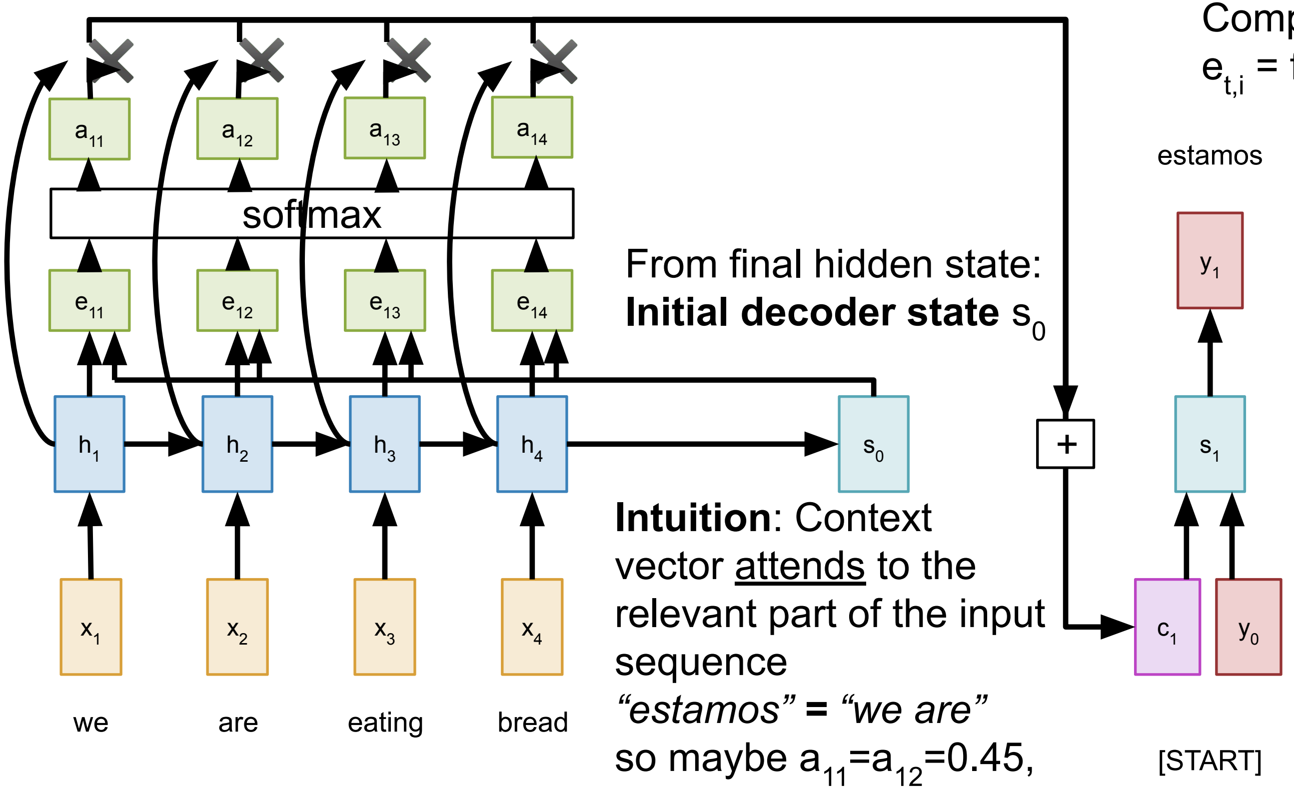
Sequence to Sequence with RNNs and Attention



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

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

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

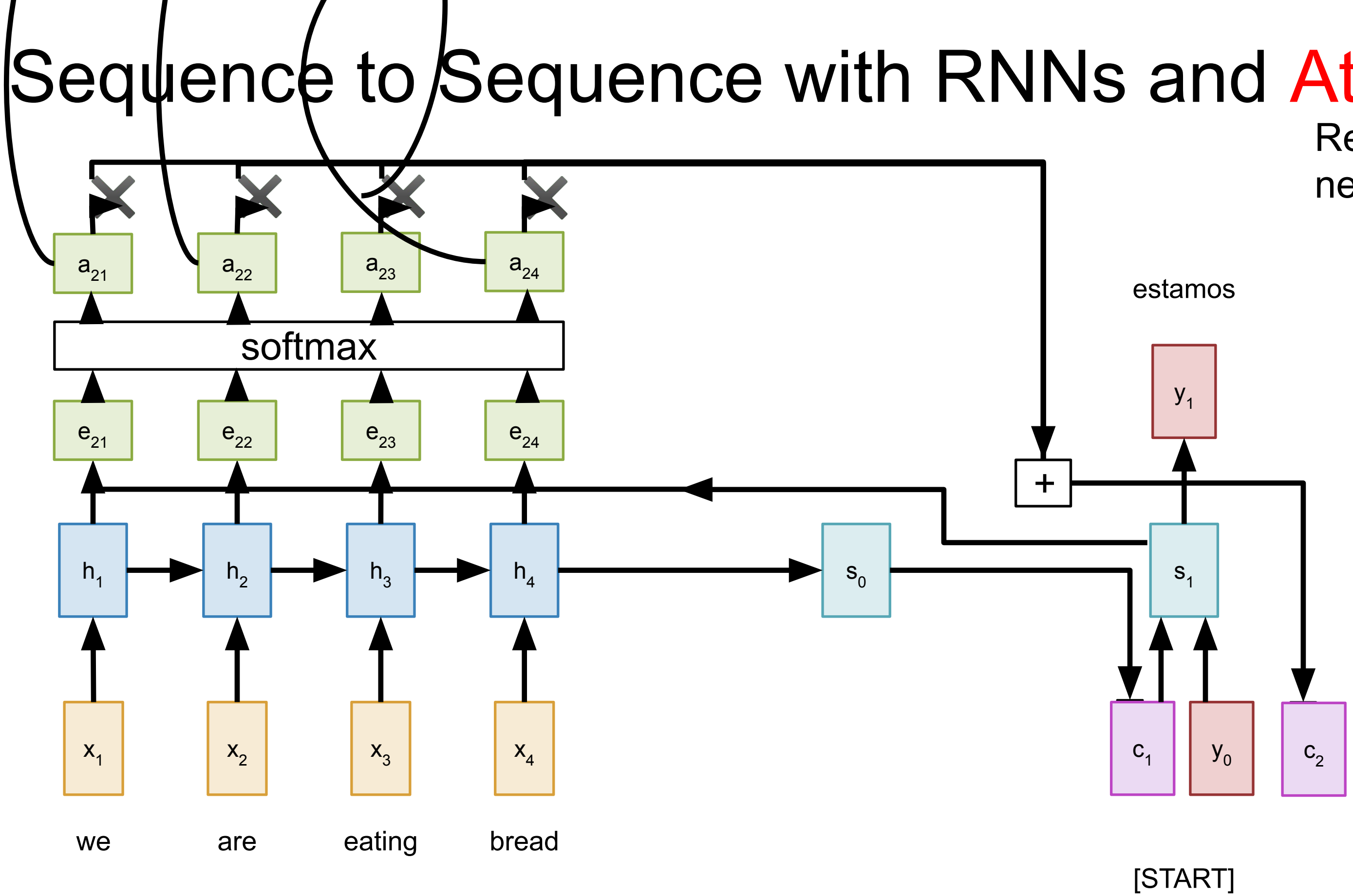
Intuition: Context vector <u>attends</u> to the relevant part of the input sequence
"estamos" = *"we are"*
so maybe $a_{11}=a_{12}=0.45$, $a_{13}=a_{14}=0.05$

This is all differentiable! No supervision on 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 and Attention

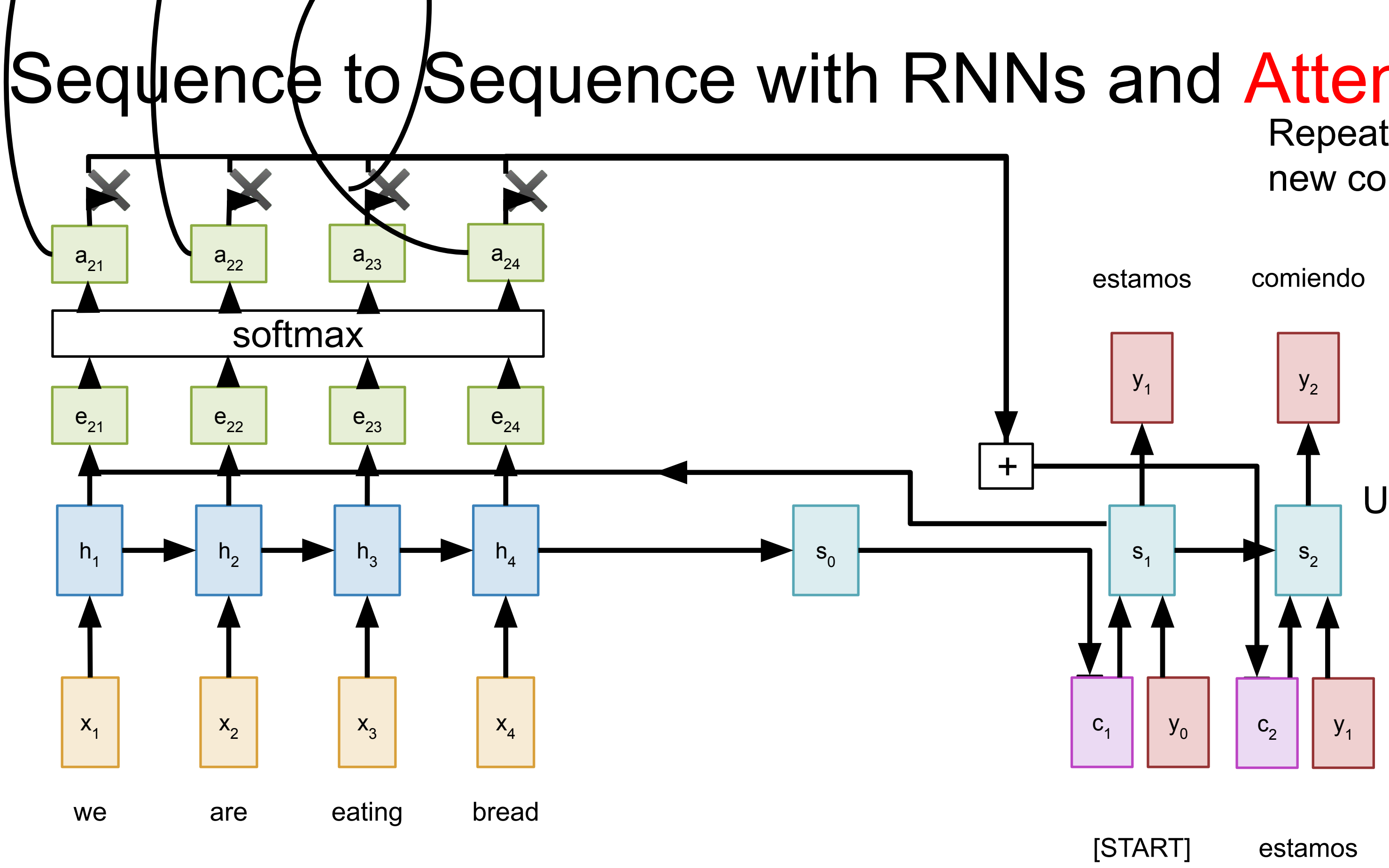
Repeat: Use s_1 to compute new context vector c_2



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

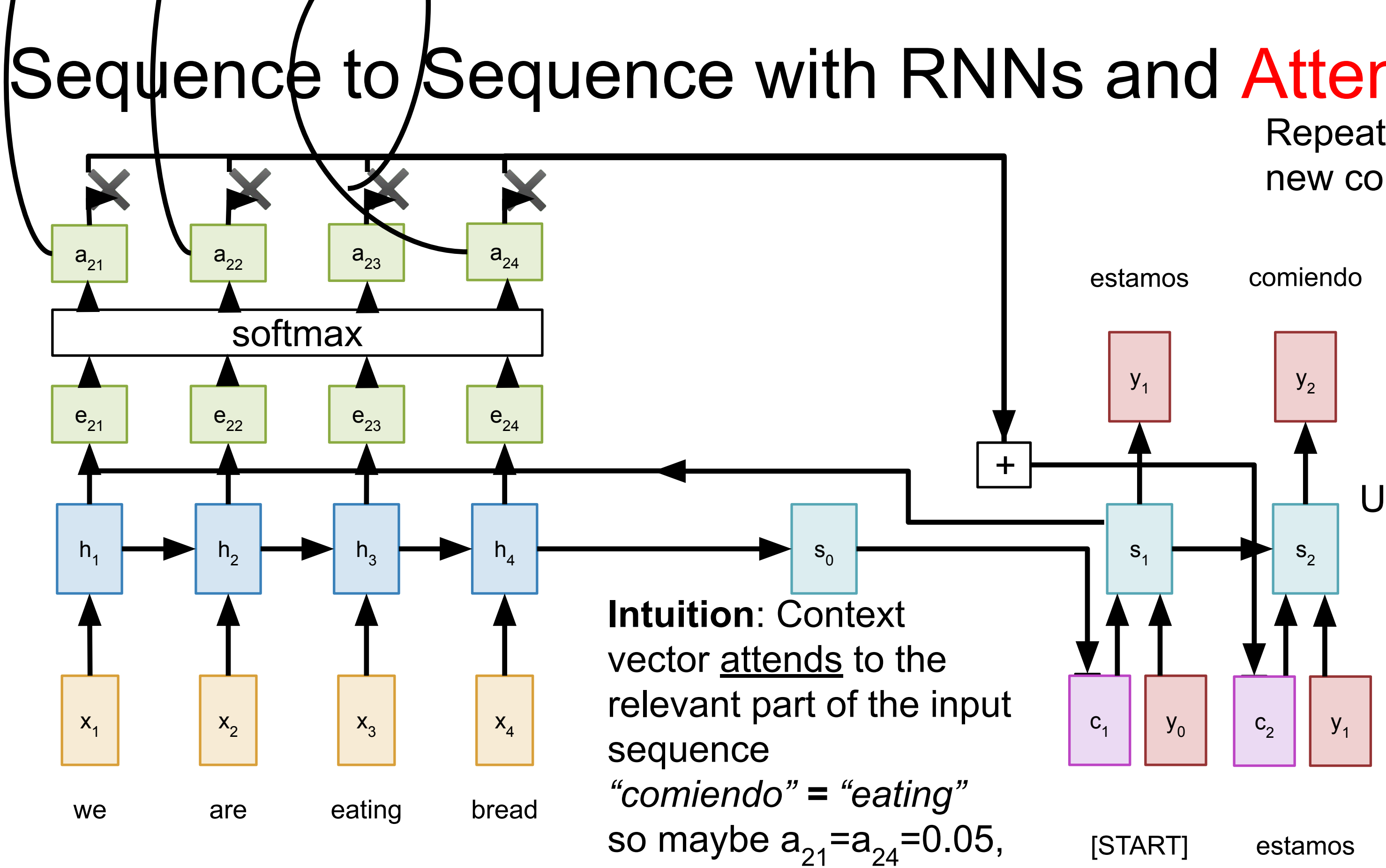


Use c_2 to compute s_2, y_2

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

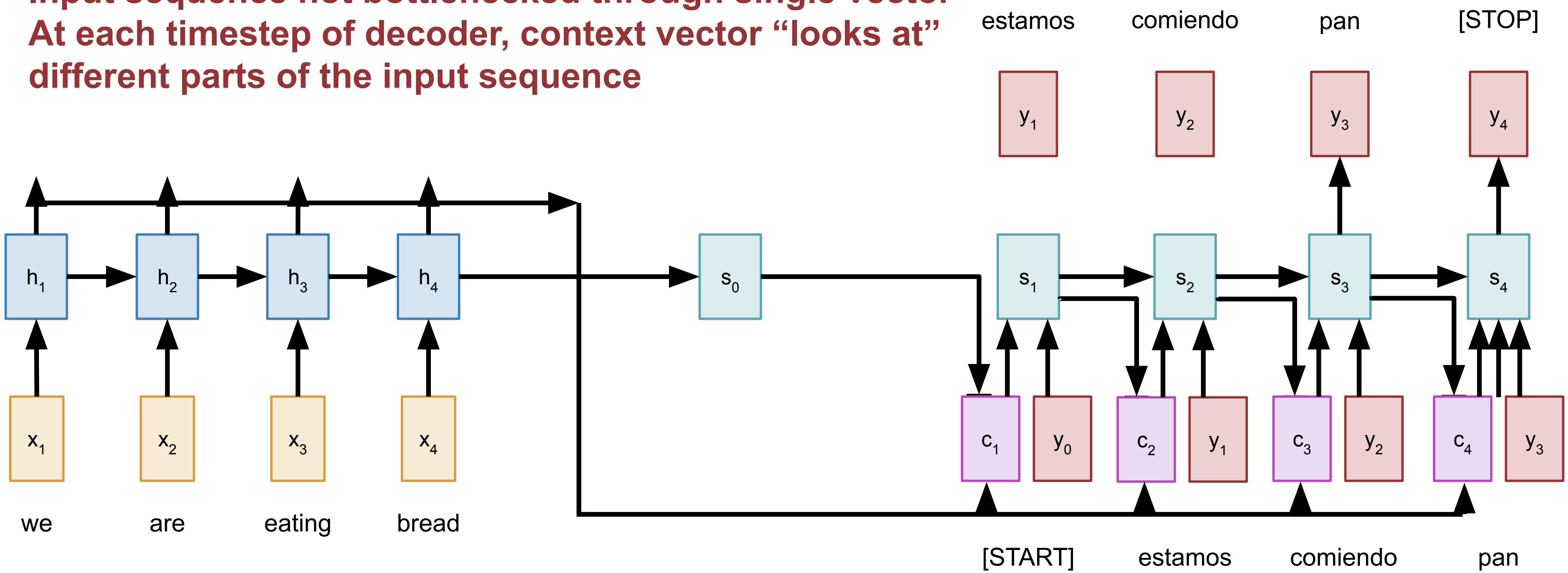
Intuition: Context vector attends to the relevant part of the input sequence
"comiendo" **=** *"eating"*
so maybe $a_{21}=a_{24}=0.05$, $a_{22}=0.1$, $a_{23}=0.8$

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

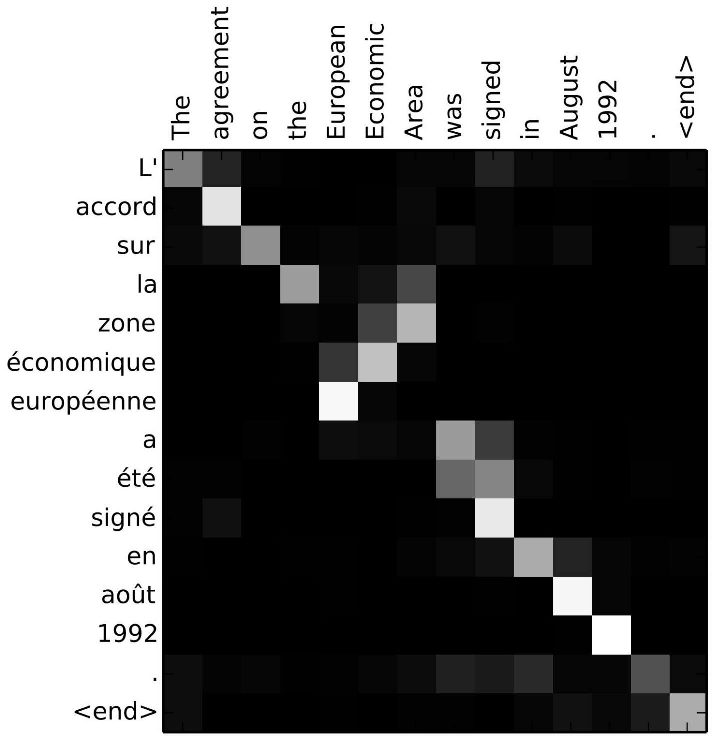
Sequence to Sequence with RNNs and Attention

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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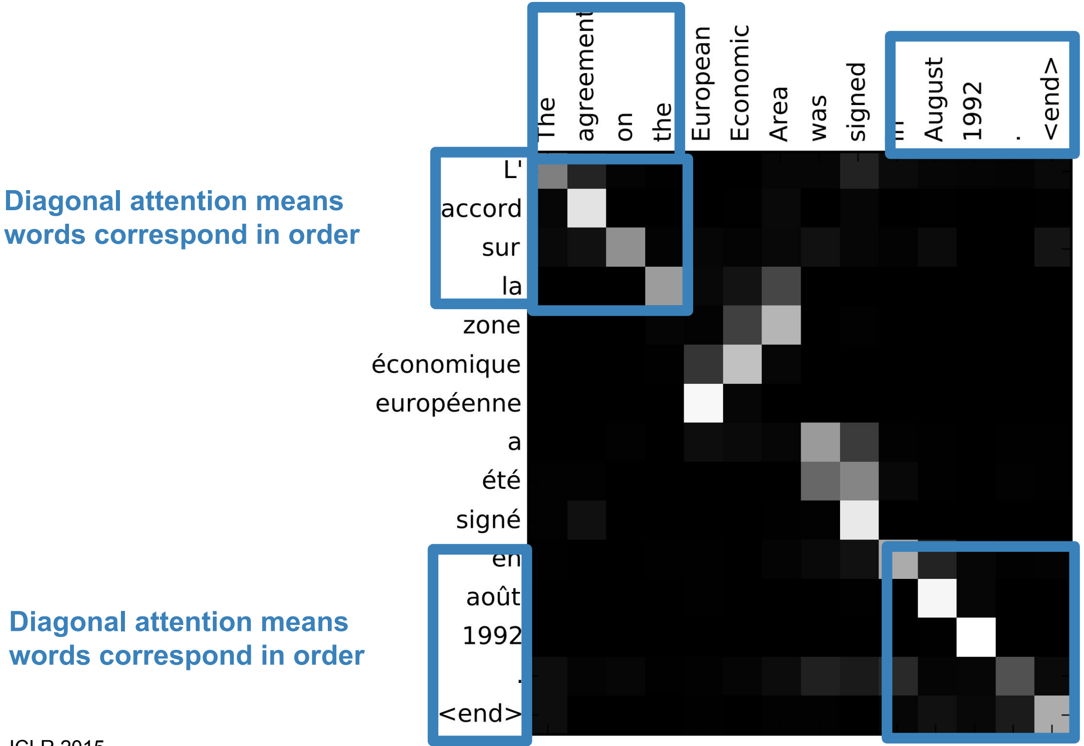

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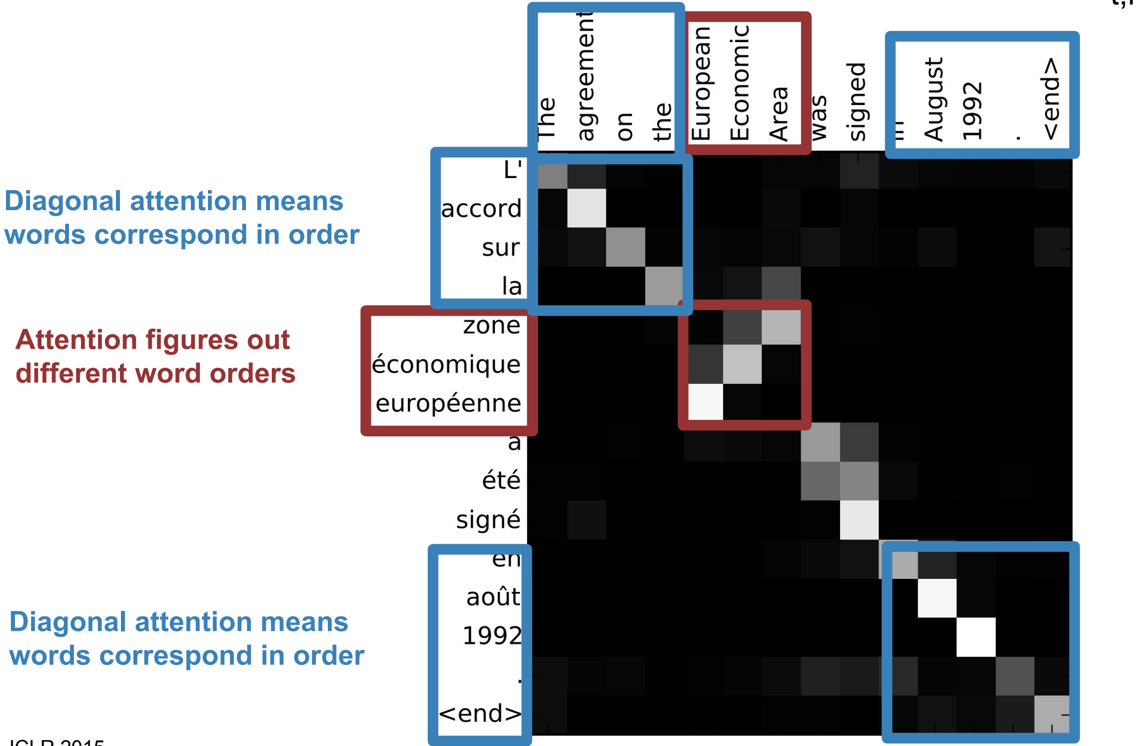

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Sequence to Sequence with RNNs and Attention

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 $\{h_i\}$!

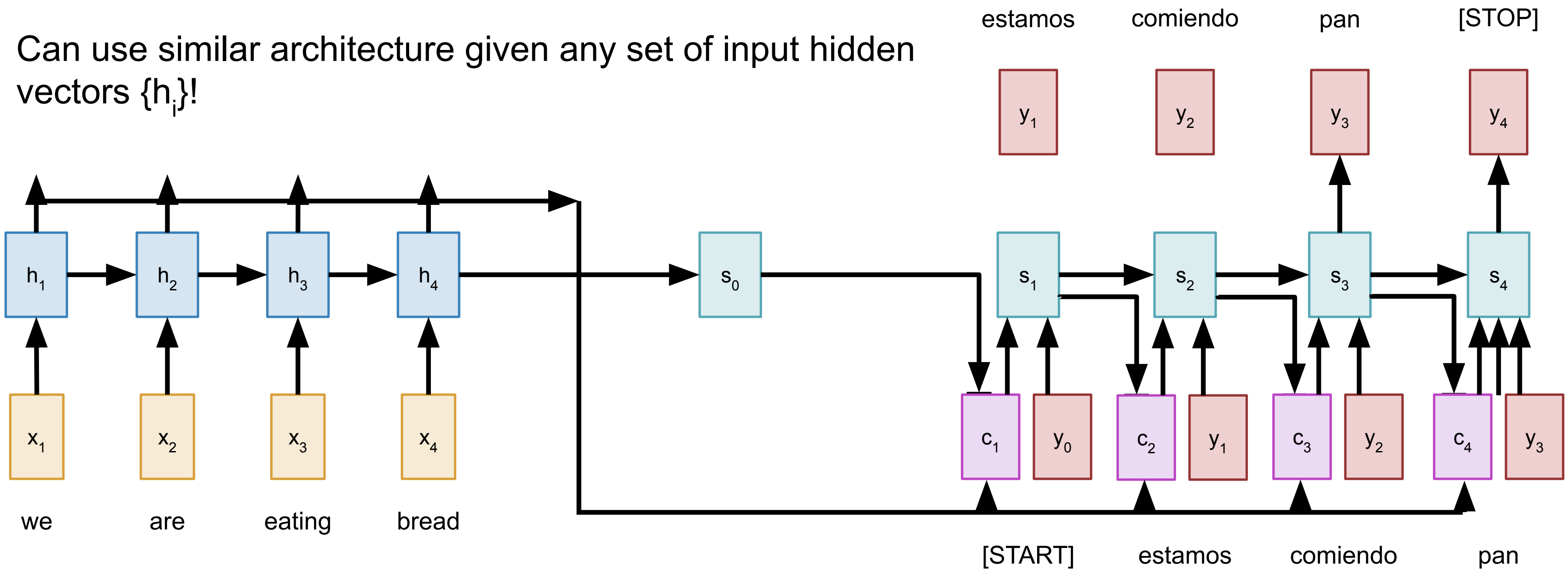

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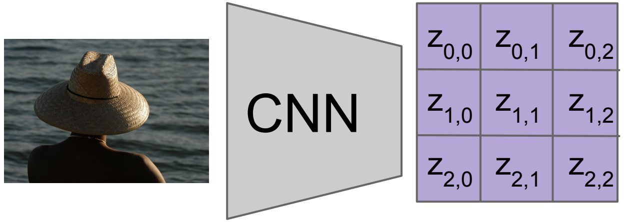
Image Captioning using spatial features

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

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

Image Captioning using spatial features

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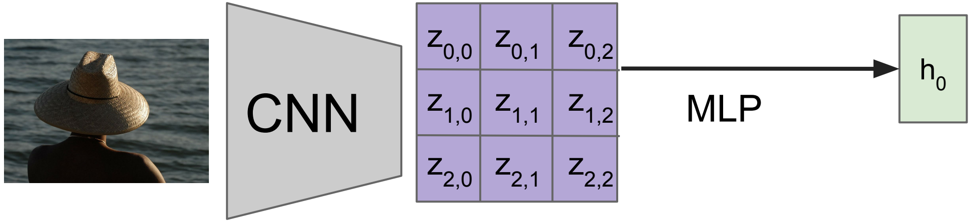
Encoder: $h_0 = f_{\mathbf{W}}(\mathbf{z})$
where **z** is spatial CNN features
$f_{\mathbf{W}}(.)$ is an MLP



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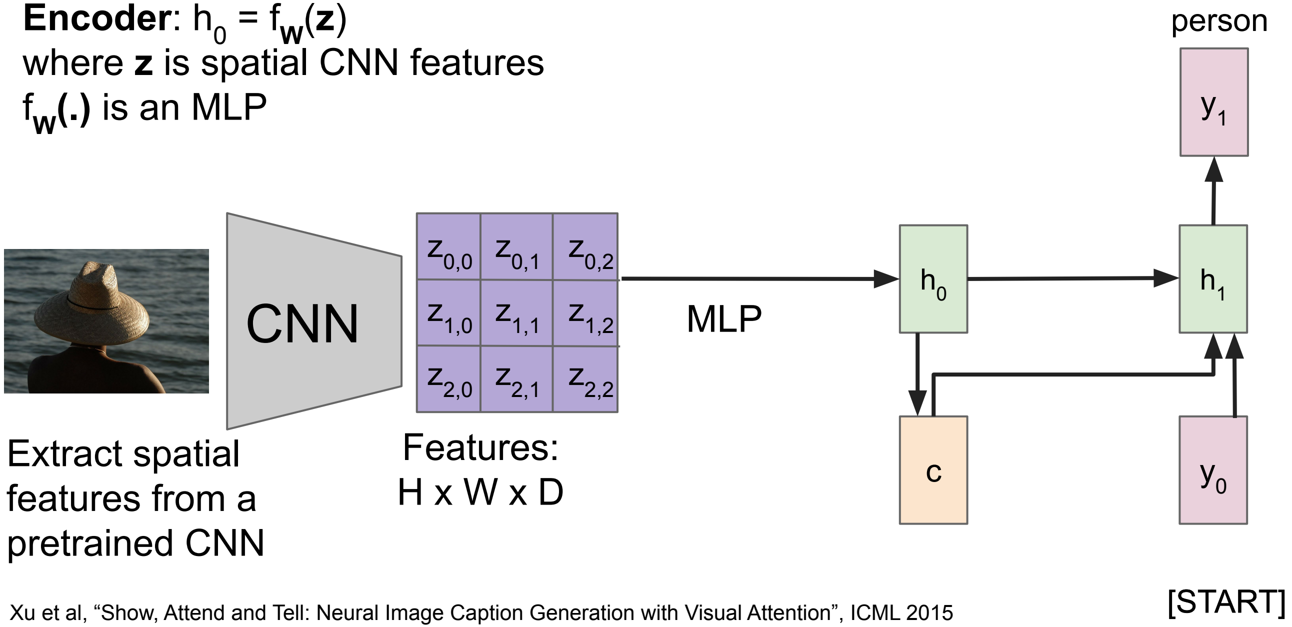

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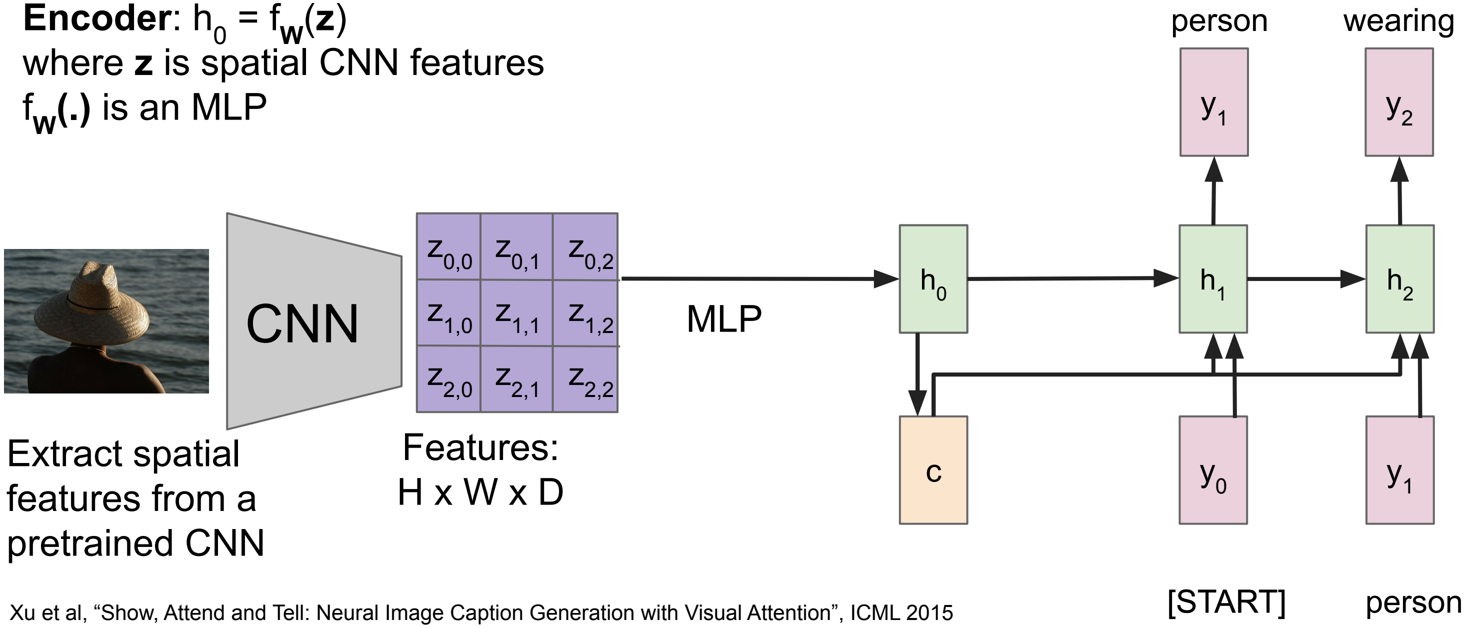

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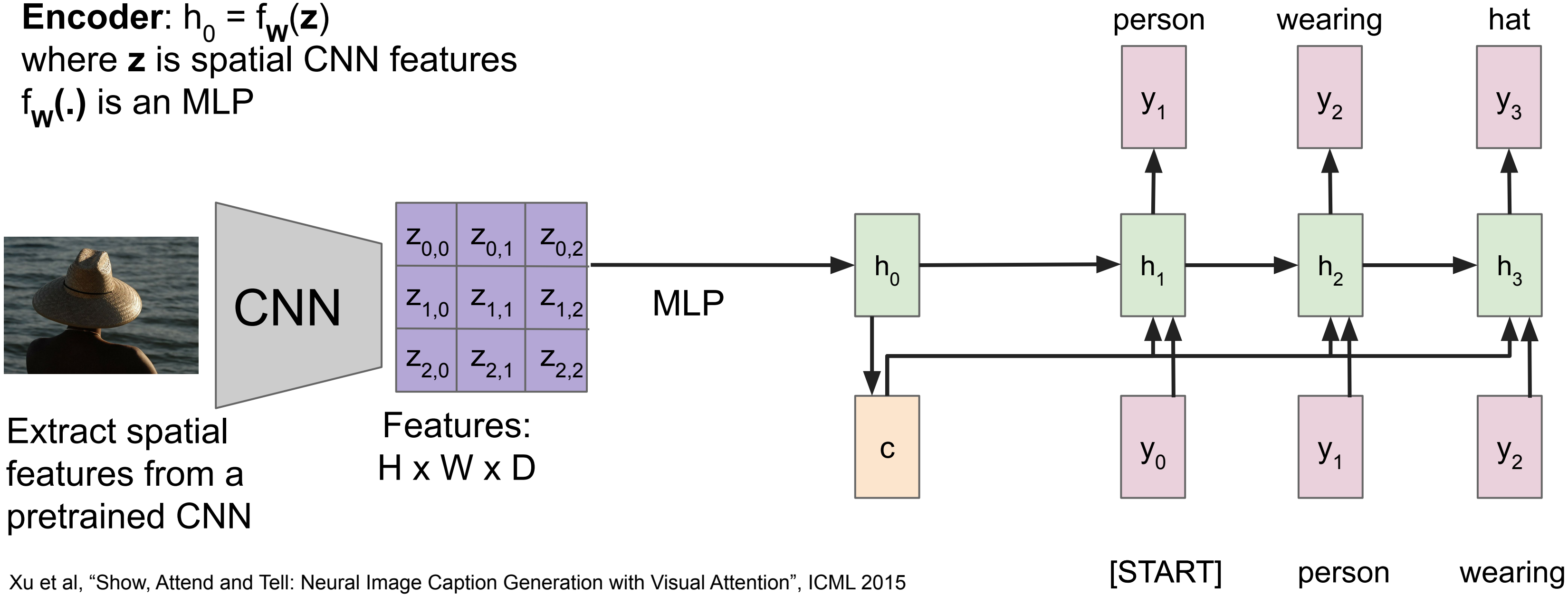

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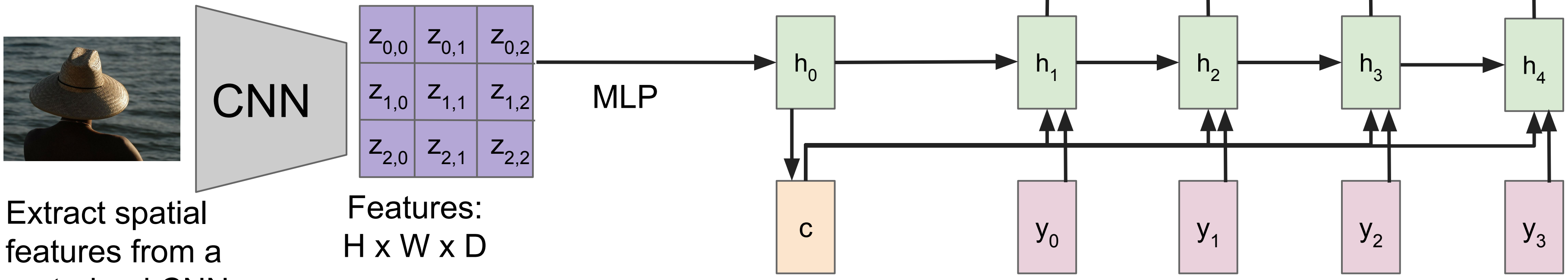

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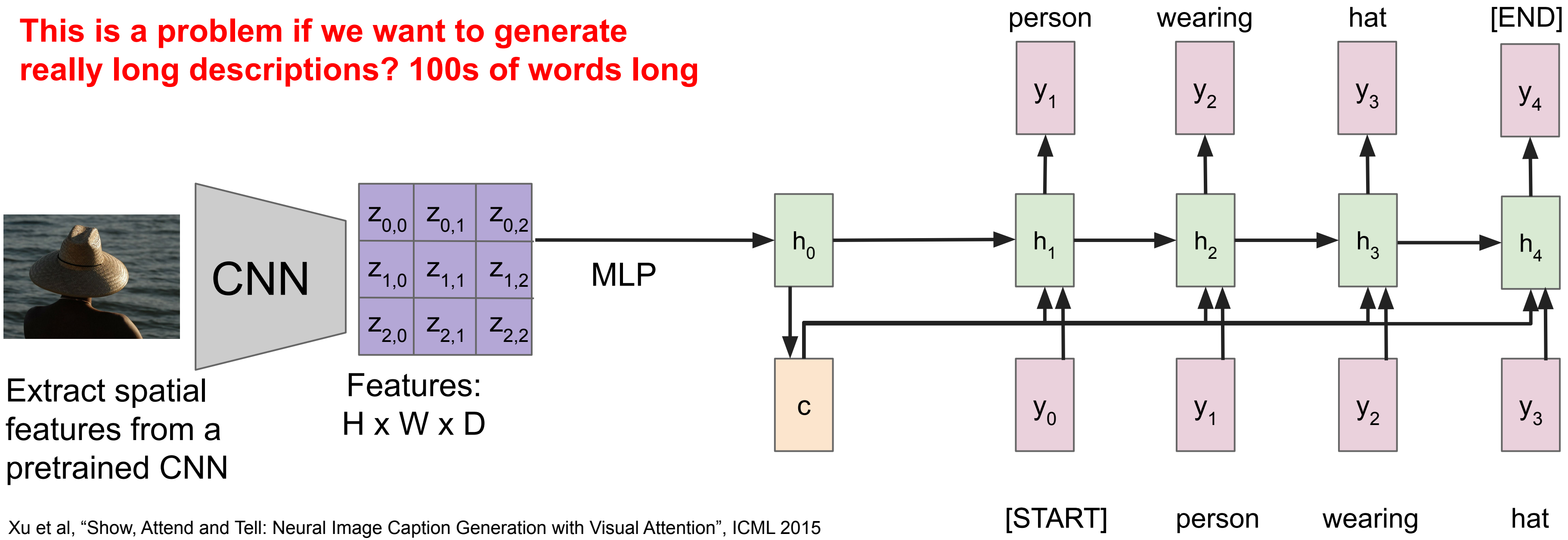
Image Captioning using spatial features

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



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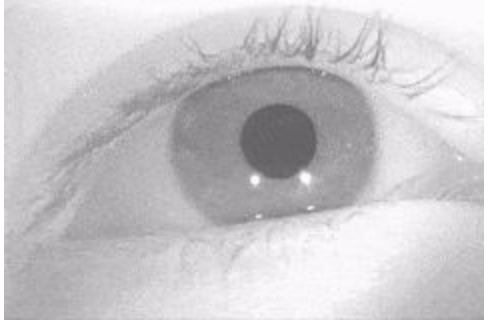
Xu et al, “Show, Attend and Tell: Neural Image Caption Generation with Visual Attention”, ICML 2015

Image Captioning with RNNs and Attention

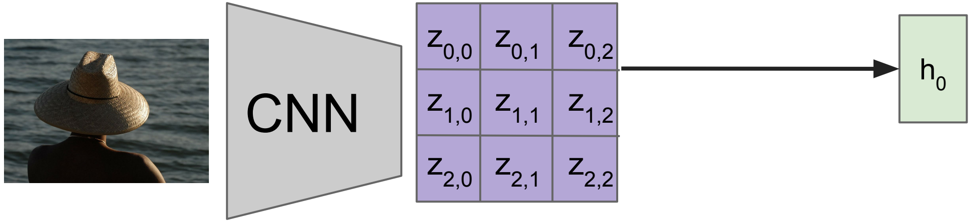
gif source

Attention idea: New context vector at every time step.

Each context vector will attend to different image regions



Attention Saccades in humans



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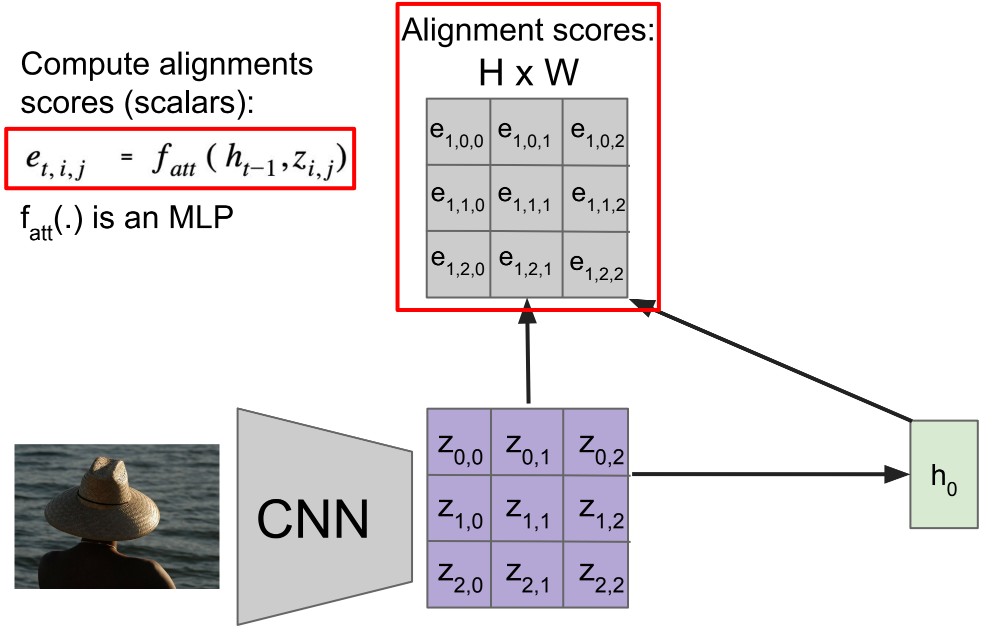
Xu et al, "Show, Attend and Tell: Neural Image Caption Generation with Visual Attention", ICML 2015

Image Captioning with RNNs and Attention

Compute alignments scores (scalars):

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

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



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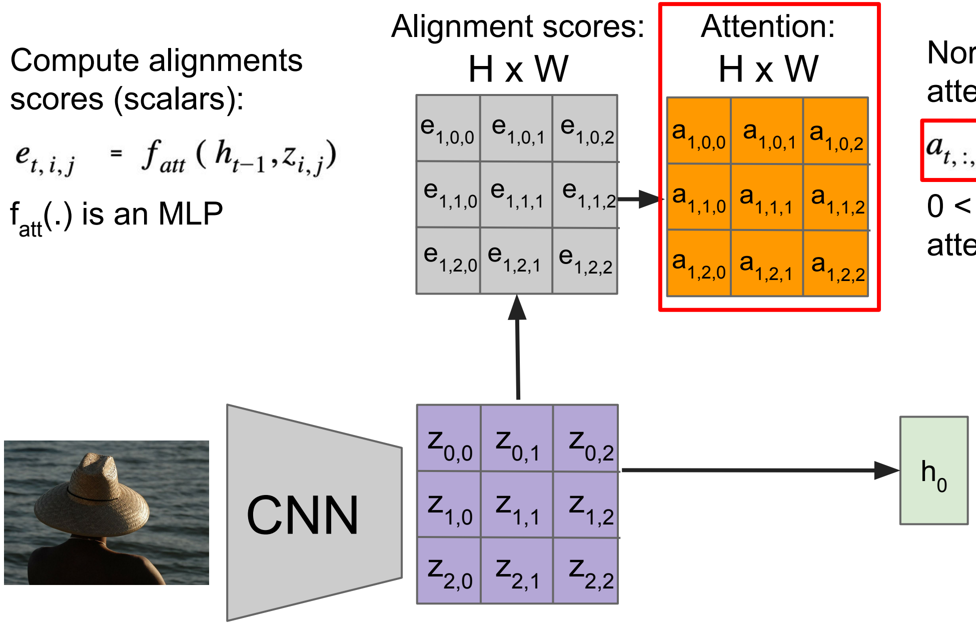
Normalize to get attention weights:

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

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



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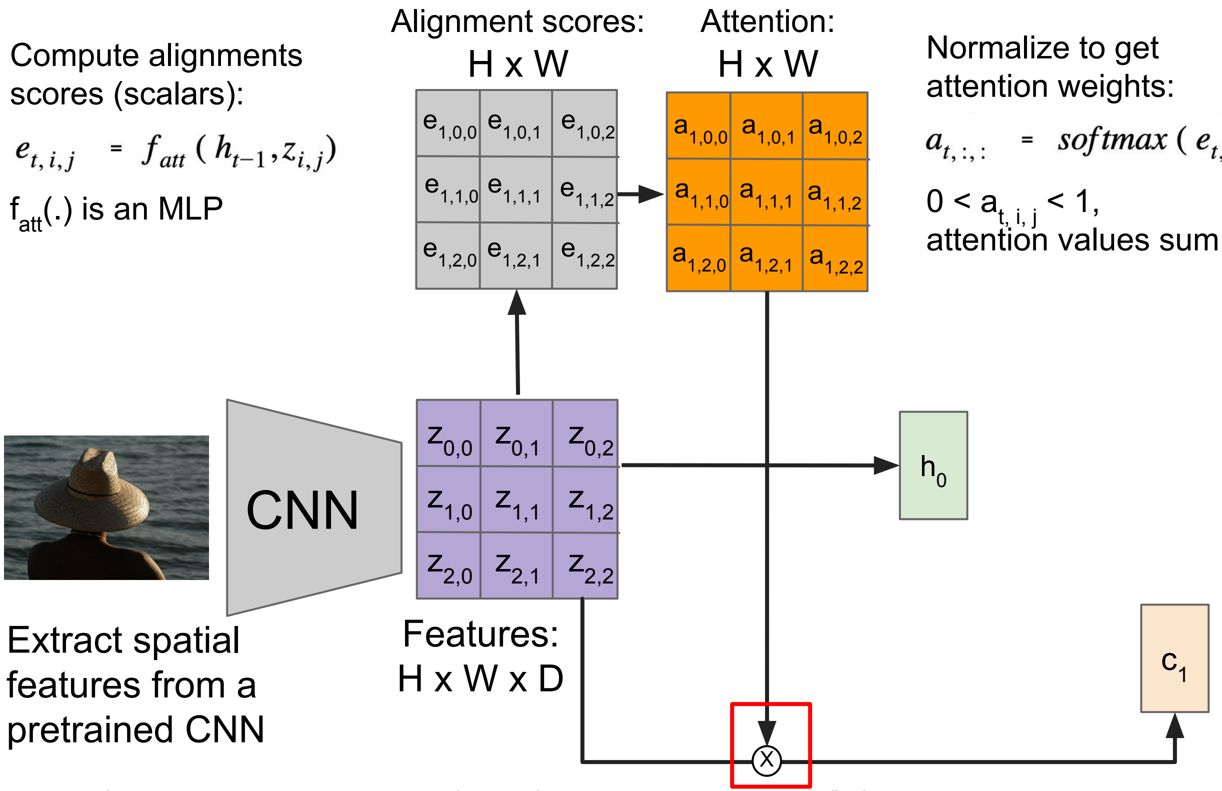

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attention values sum to 1

Compute context vector:

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

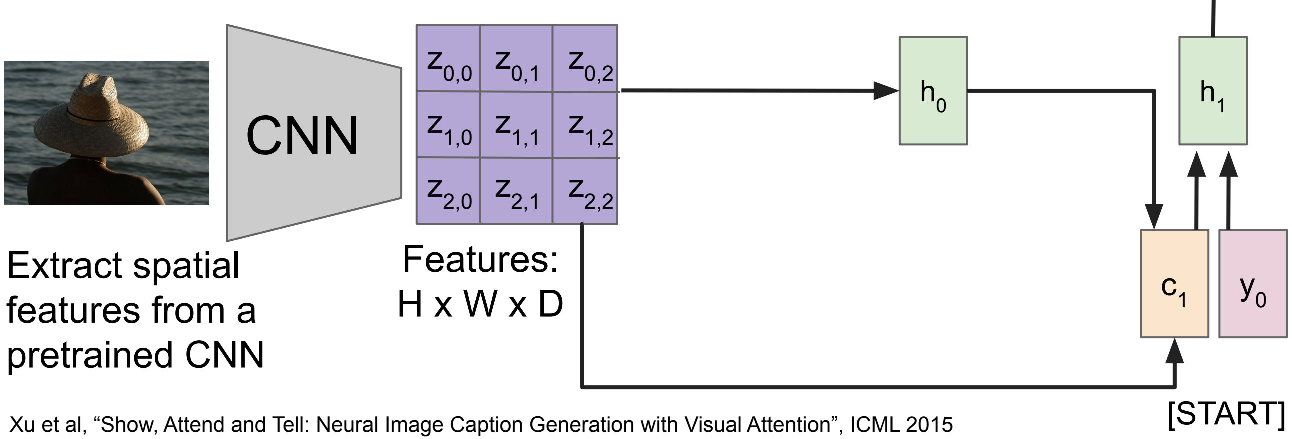
Xu et al, “Show, Attend and Tell: Neural Image Caption Generation with Visual Attention”, ICML 2015

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

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



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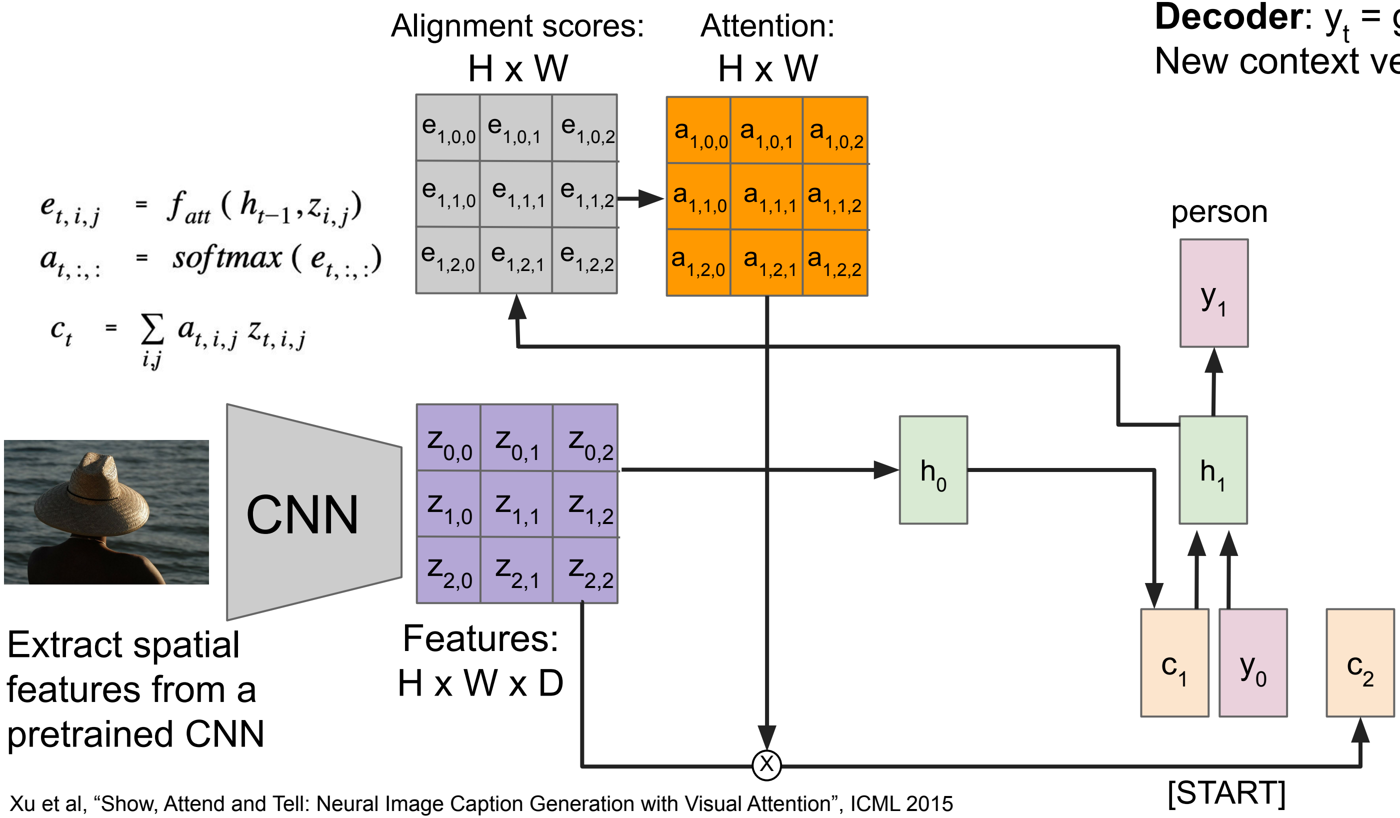
New context vector at every time step

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



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

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

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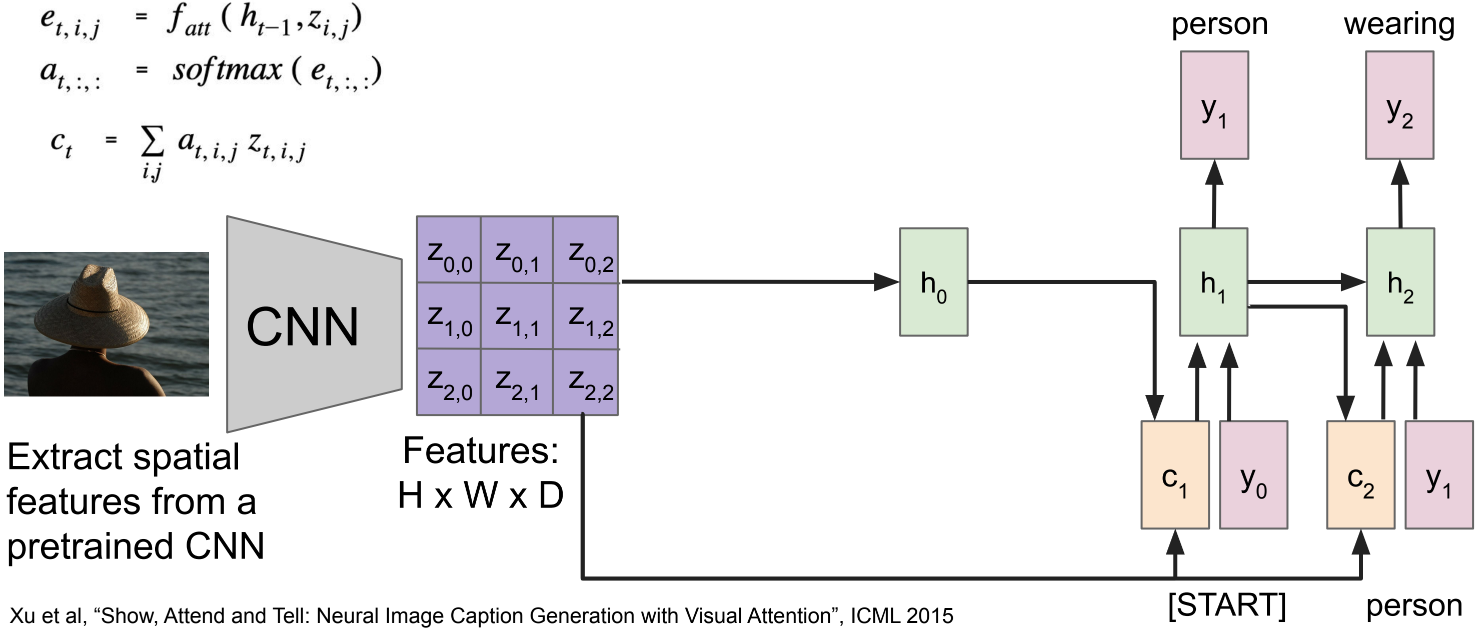

Extract spatial features from a pretrained CNN

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

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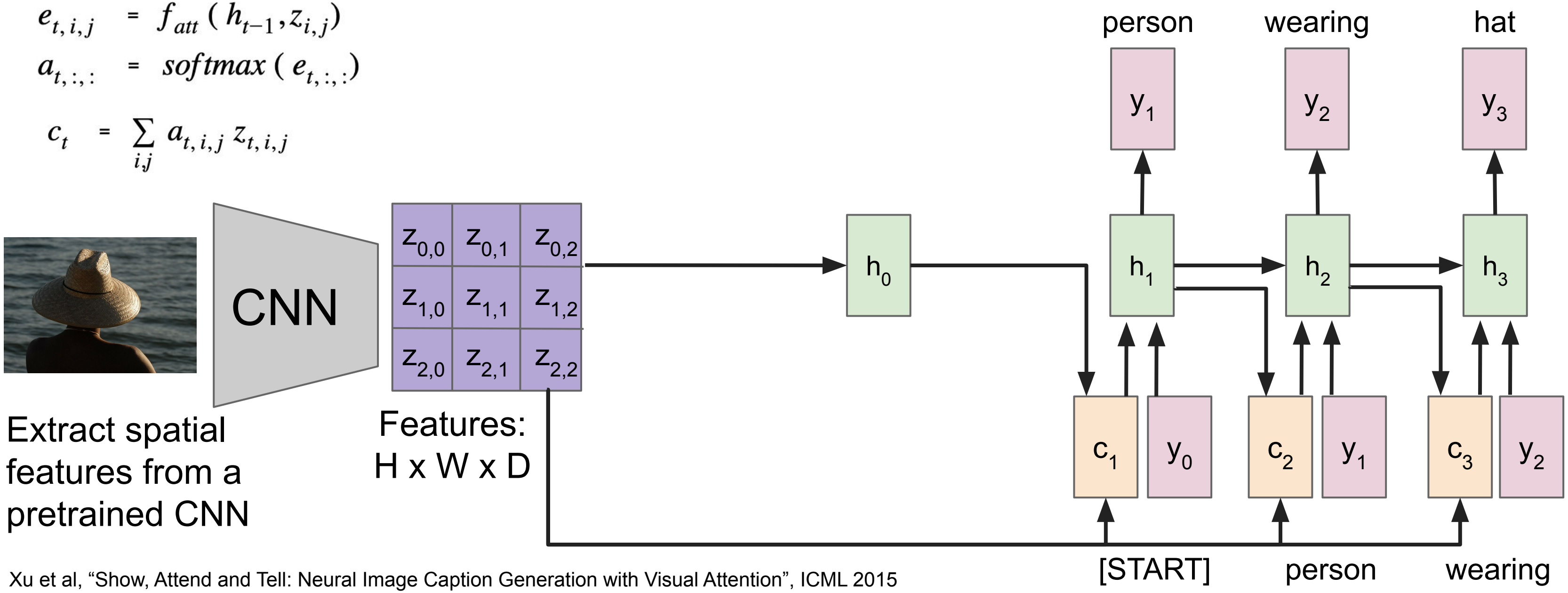

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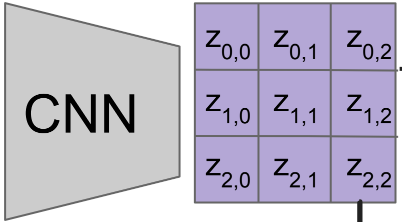

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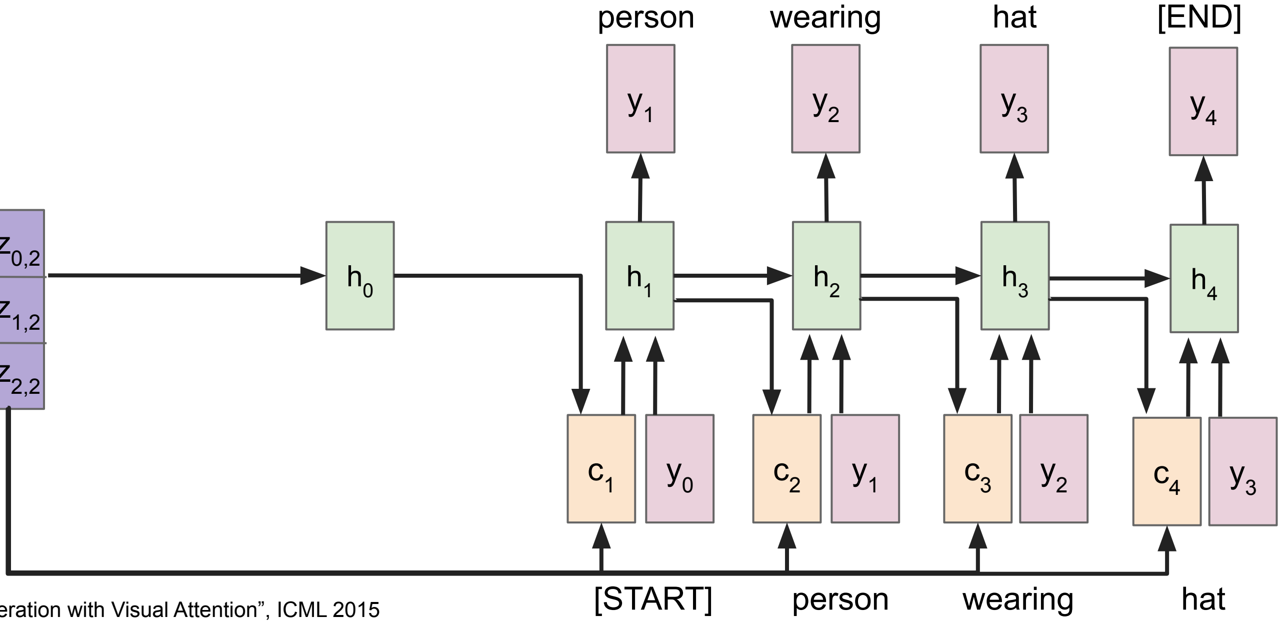
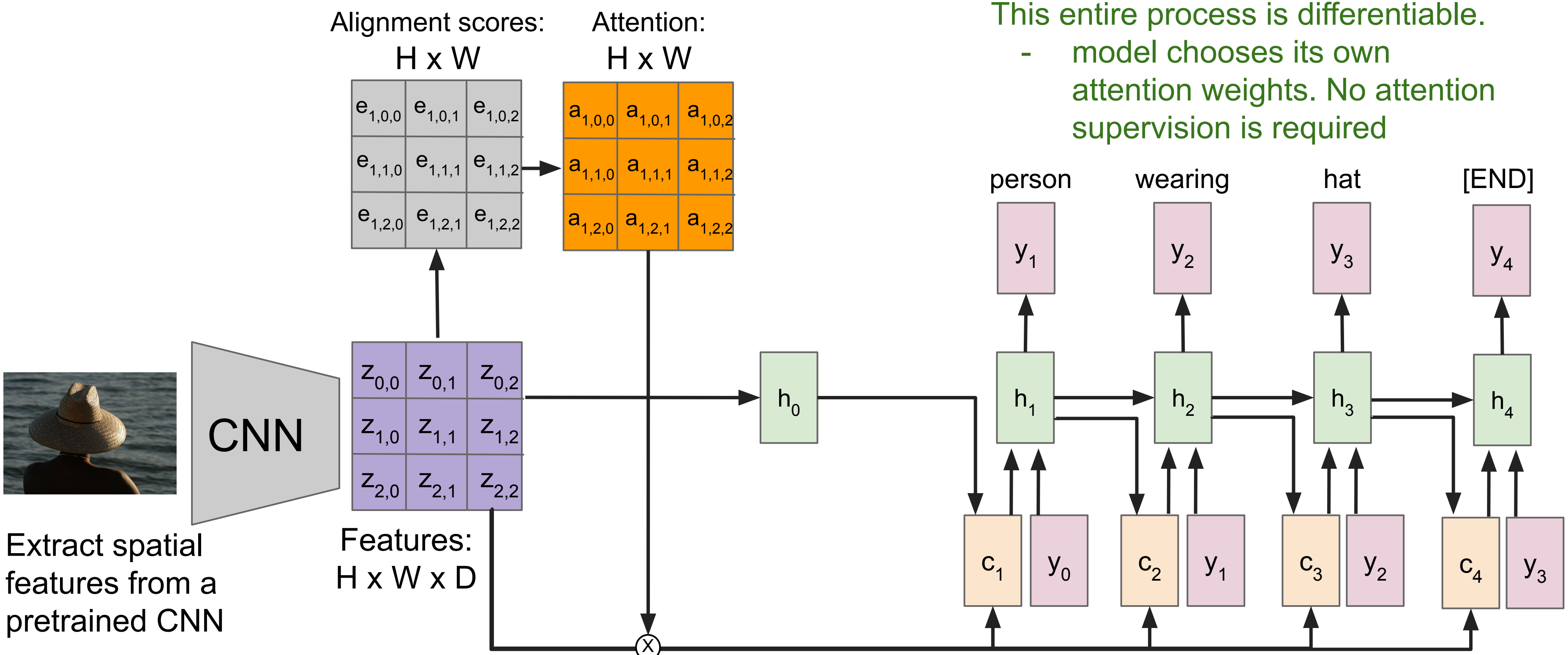


Xu et al, “Show, Attend and Tell: Neural Image Caption Generation with Visual Attention”, ICML 2015

Image Captioning with RNNs and Attention



This entire process is differentiable.

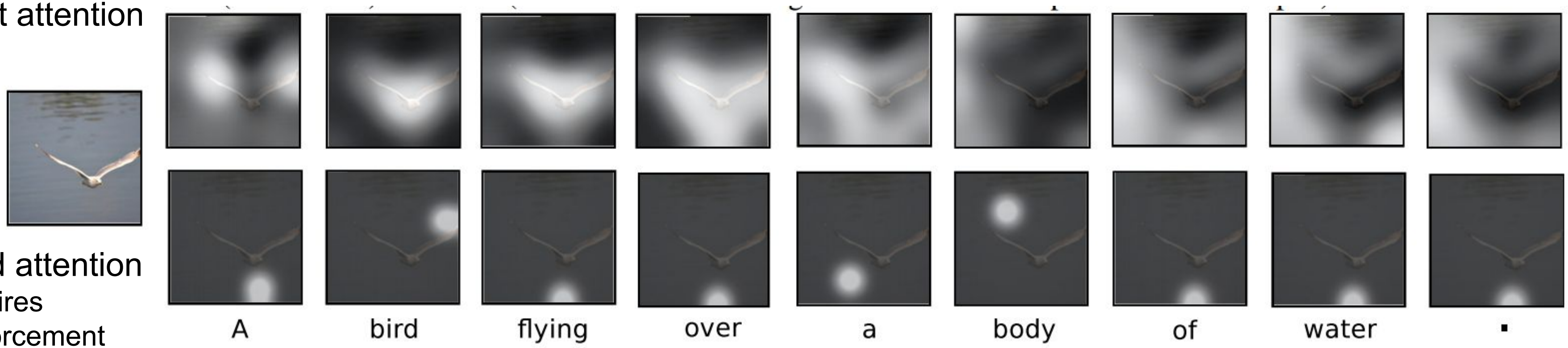
- model chooses its own attention weights. No attention supervision is required

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

Image Captioning with Attention

Soft attention

Hard attention
(requires
reinforcement
learning)



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

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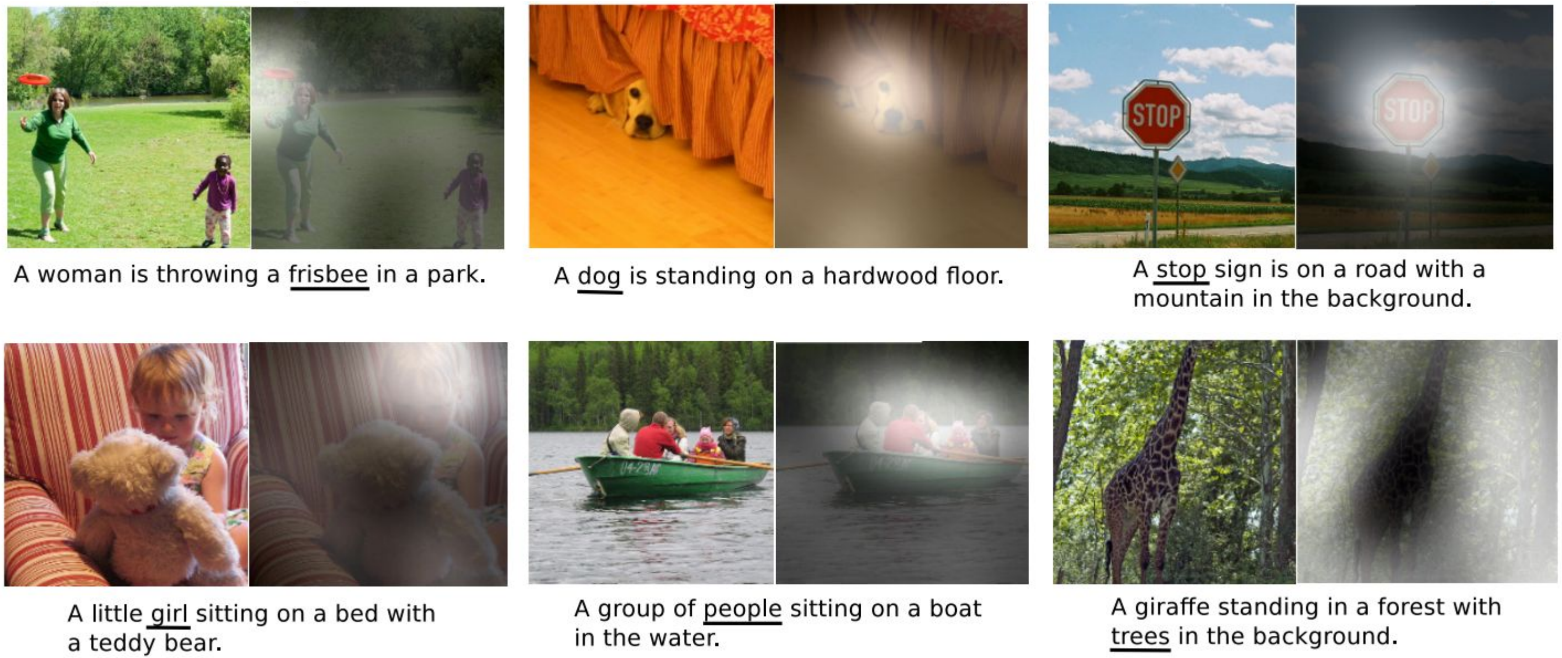
Image Captioning with Attention



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

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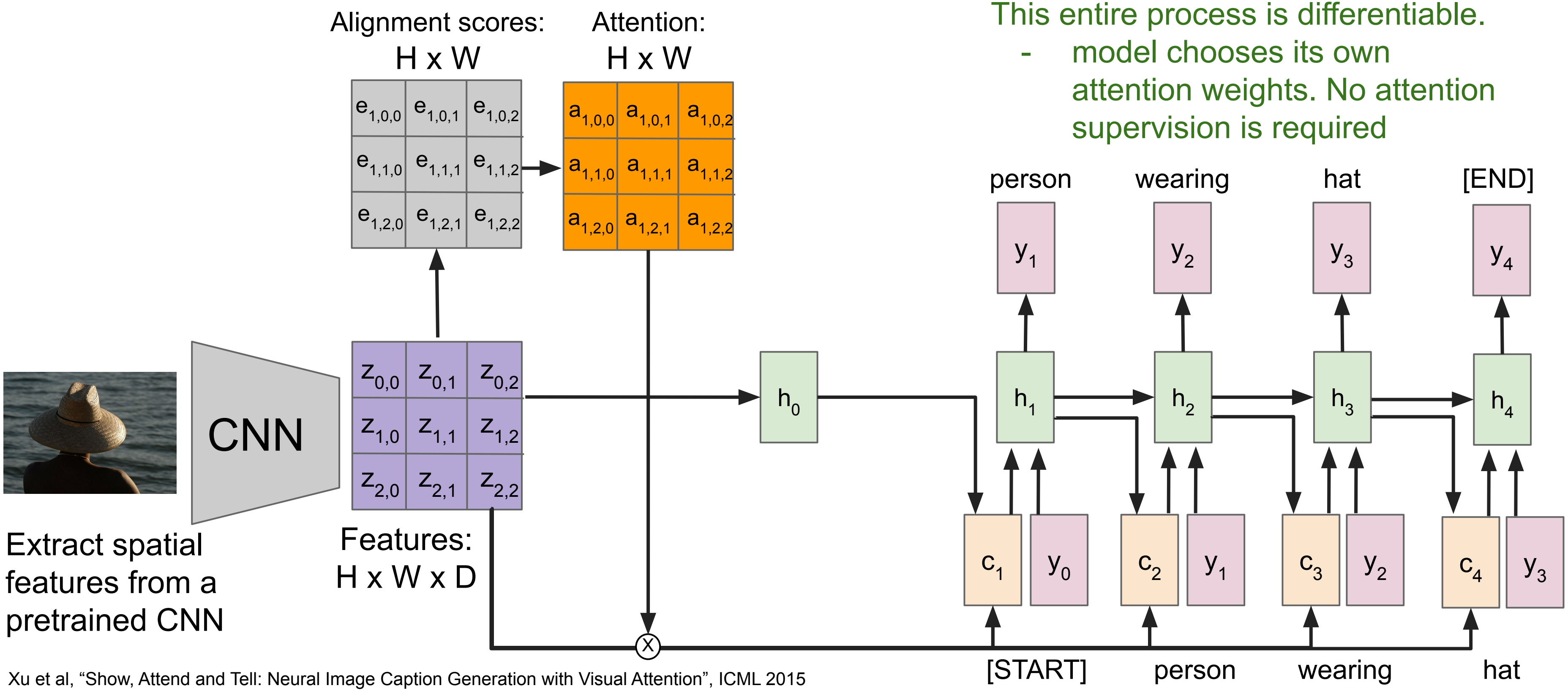
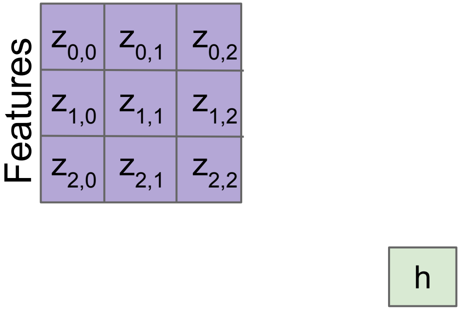
Image Captioning with RNNs and Attention

This entire process is differentiable.
- model chooses its own attention weights. No attention supervision is required



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

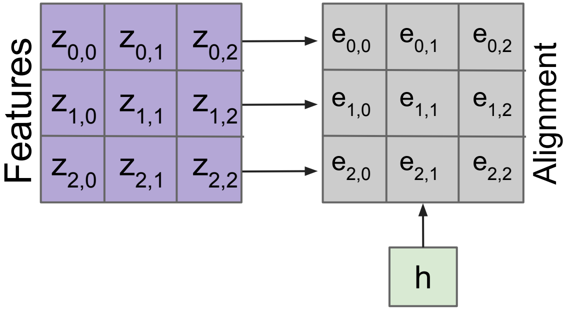
Attention we just saw in image captioning



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

Attention we just saw in image captioning

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



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Query: **h** (shape: D)

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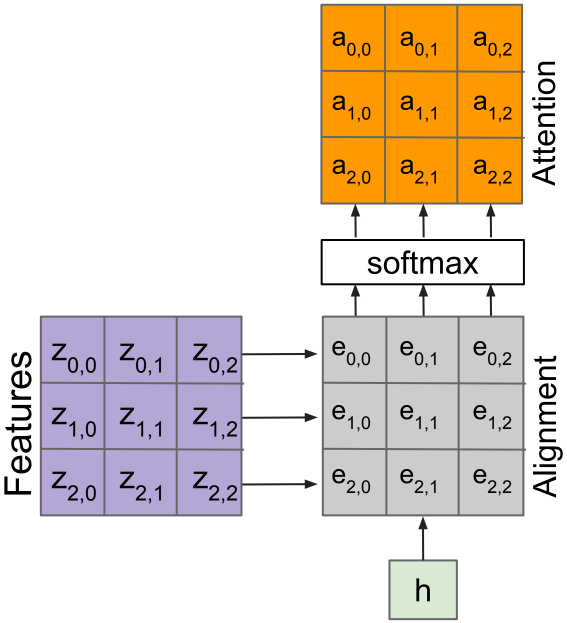
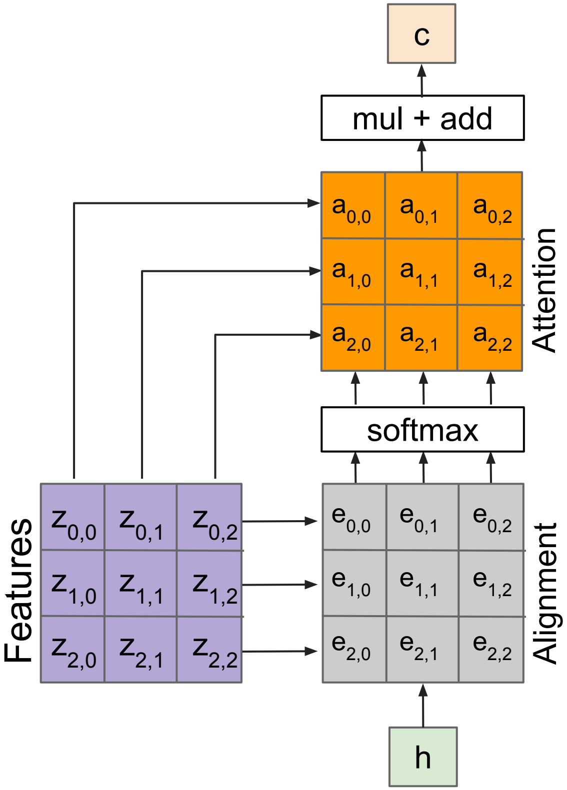


Operations:
Alignment: $e_{i,j} = f_{att}(h, z_{i,j})$
Attention: $\mathbf{a} = \text{softmax}(\mathbf{e})$

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

Attention we just saw in image captioning

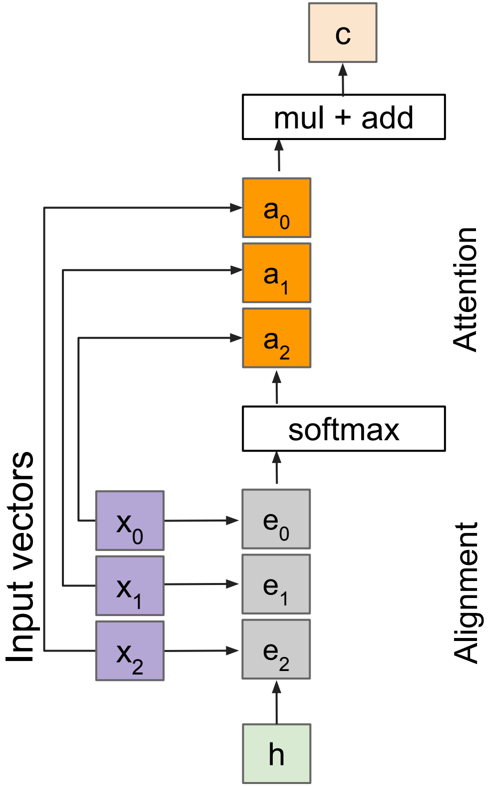


Outputs:
context vector: **c** (shape: D)

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)

General attention layer



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

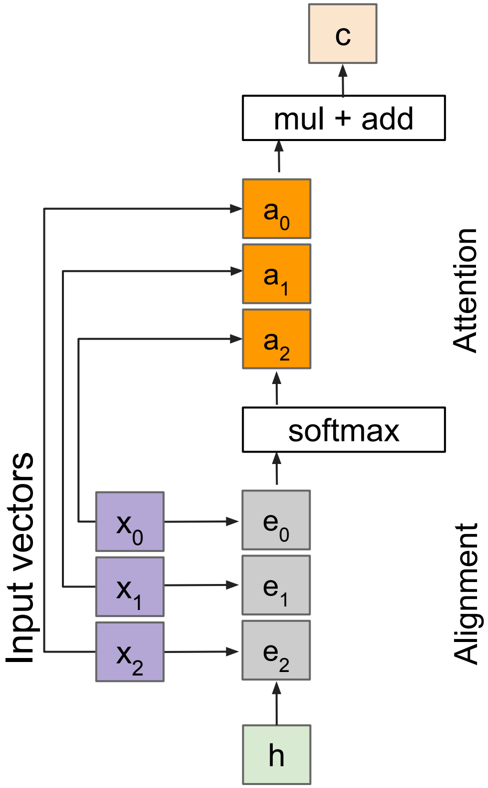
Operations:
Alignment: $e_i = f_{att}(h, x_i)$
Attention: $\mathbf{a} = \text{softmax}(\mathbf{e})$
Output: $\mathbf{c} = \sum_i a_i x_i$

Attention operation is **permutation invariant.**

- Doesn't care about ordering of the features
- Stretch H x W = N into N vectors

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

General attention layer



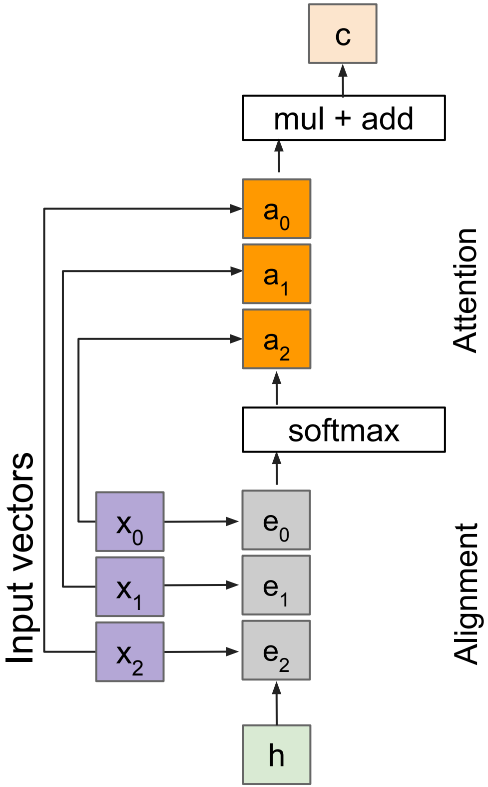
Outputs:
context vector: **c** (shape: D)

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 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)

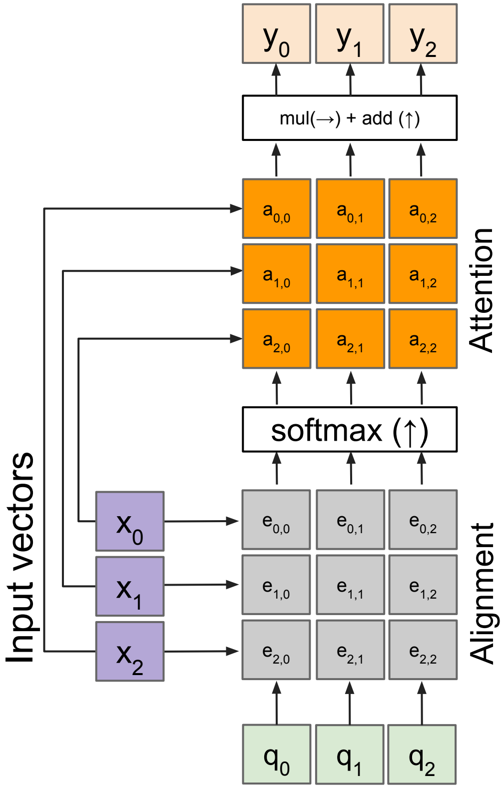
Operations:
$\boxed{\text{Alignment: } e_i = h \cdot x_i / \sqrt{D}}$
Attention: **a** = softmax(**e**)
Output: **c** = $\sum_i a_i x_i$

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)

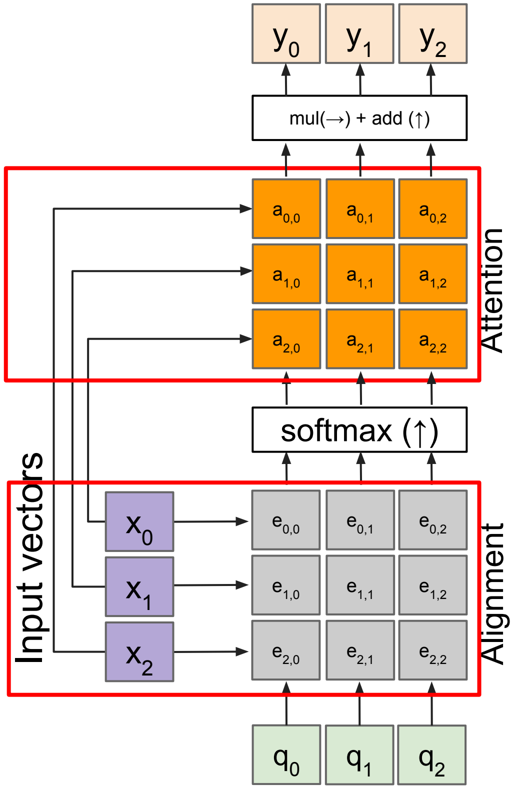
Multiple query vectors
- each query creates a new output context vector

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

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

Multiple query vectors

General attention layer



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

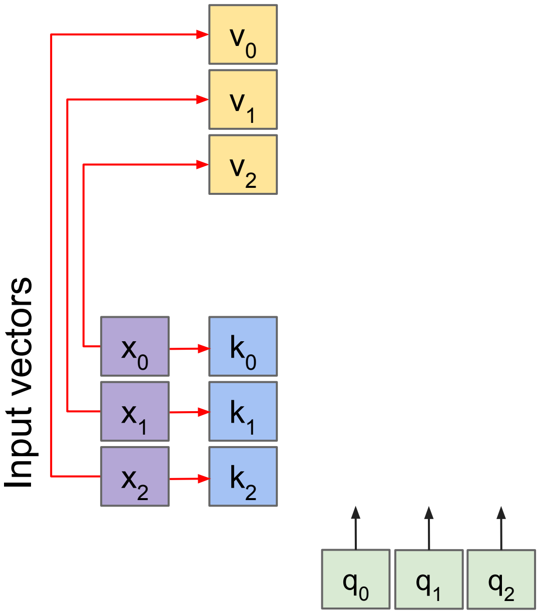
Operations:
Alignment: $e_{i,j} = q_j \cdot x_i / \sqrt{D}$
Attention: $\mathbf{a} = \text{softmax}(\mathbf{e})$
Output: $y_j = \sum_i a_{i,j} x_i$

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



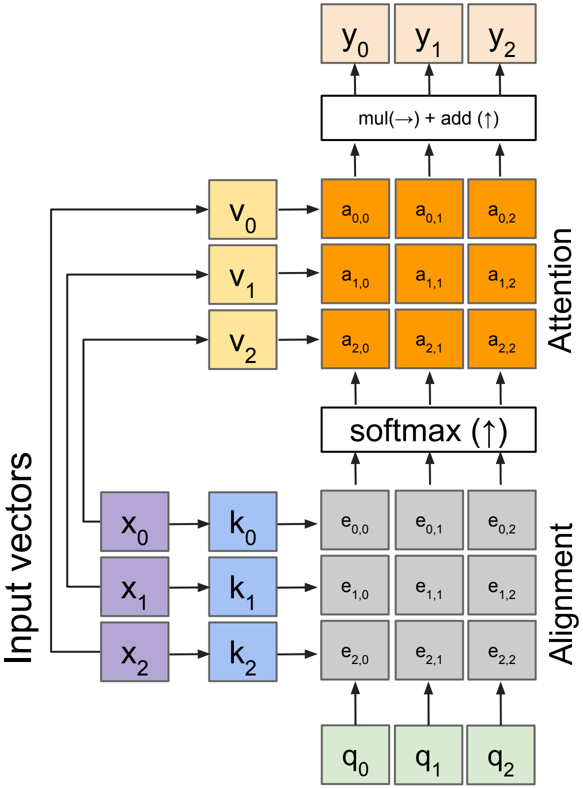
Operations:
Key vectors: $\mathbf{k} = \mathbf{x}\mathbf{W}_k$
Value vectors: $\mathbf{v} = \mathbf{x}\mathbf{W}_v$

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

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: $\boxed{D_v}$)

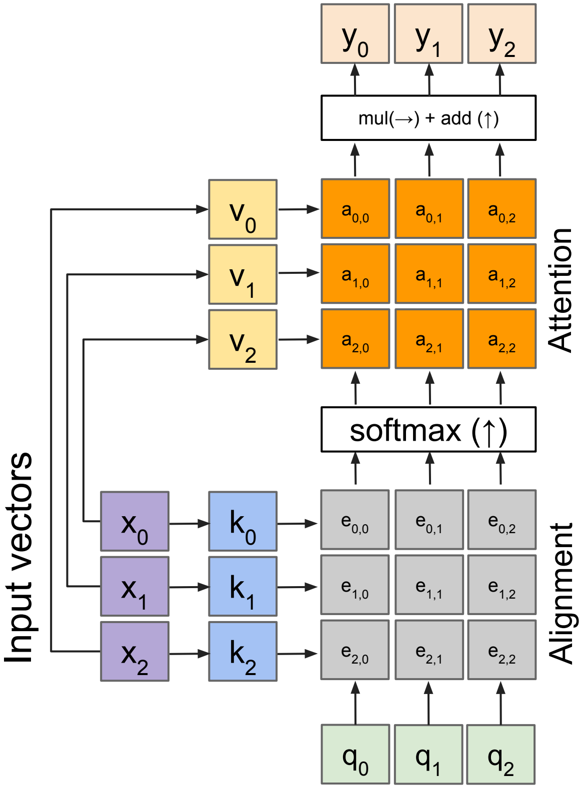
The input and output dimensions can now change depending on the key and value FC layers

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: $y_j = \sum_i a_{i,j} v_i$

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 $\boxed{D_k}$)

General attention layer



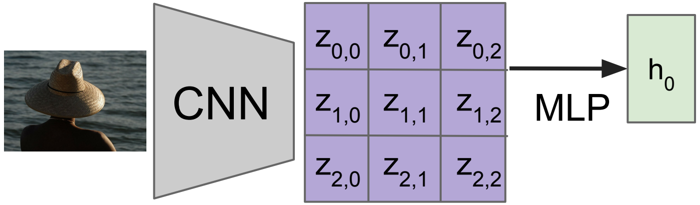
Outputs:
context vectors: **y** (shape: D_v)

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)

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

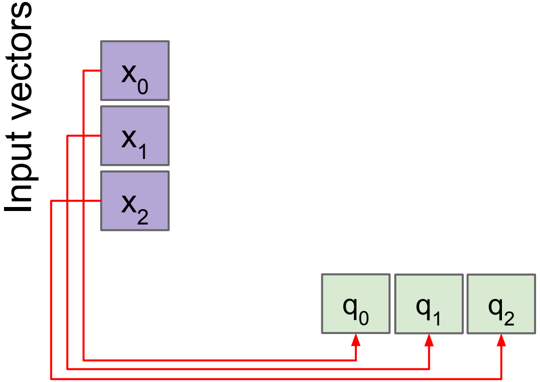


Self attention layer

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: $\mathbf{v} = \mathbf{x}\mathbf{W_v}$
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: $y_j = \sum_i a_{i,j} v_i$

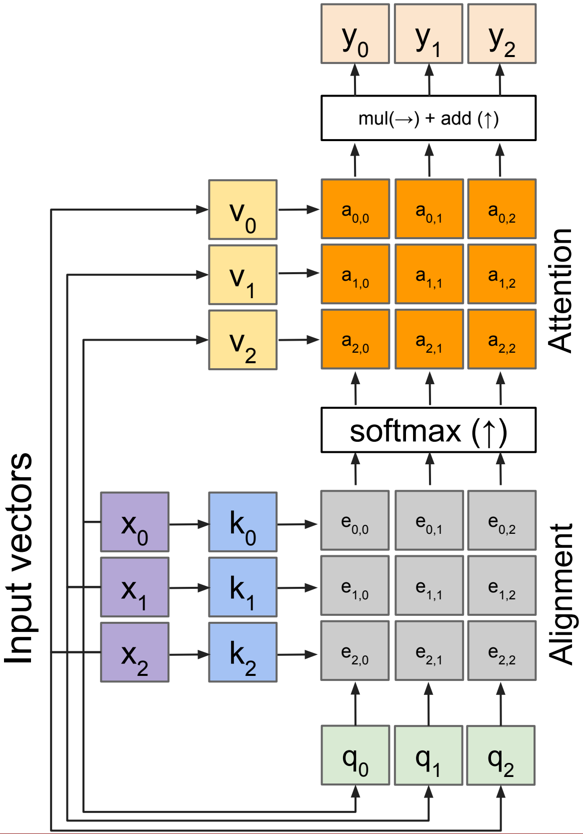
Instead, query vectors are calculated using a FC layer.



No input query vectors anymore

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

Self attention layer

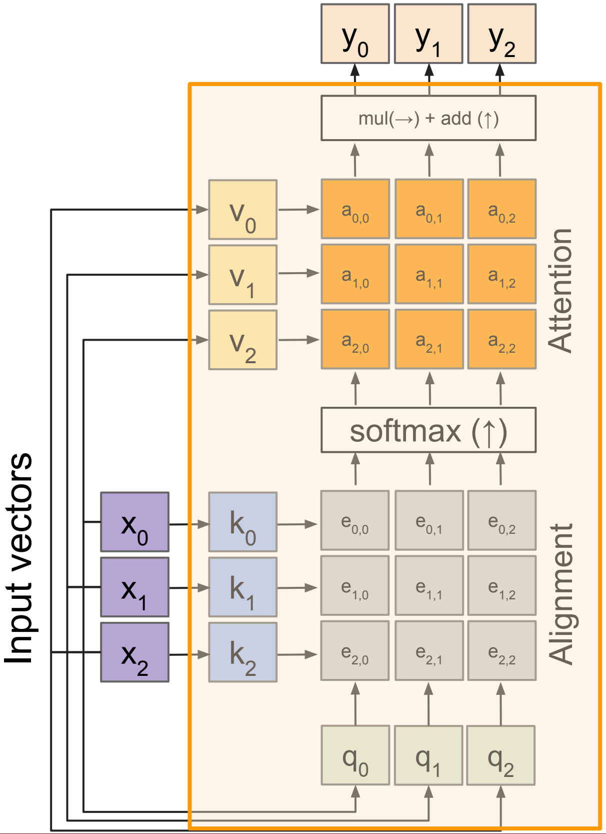


Outputs:
context vectors: **y** (shape: D_v)

Operations:
Key vectors: $\mathbf{k} = \mathbf{x}\mathbf{W}_\mathbf{k}$
Value vectors: $\mathbf{v} = \mathbf{x}\mathbf{W}_\mathbf{v}$
Query vectors: $\mathbf{q} = \mathbf{x}\mathbf{W}_\mathbf{q}$
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: $\mathbf{k} = \mathbf{x}\mathbf{W}_k$
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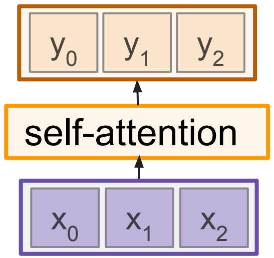
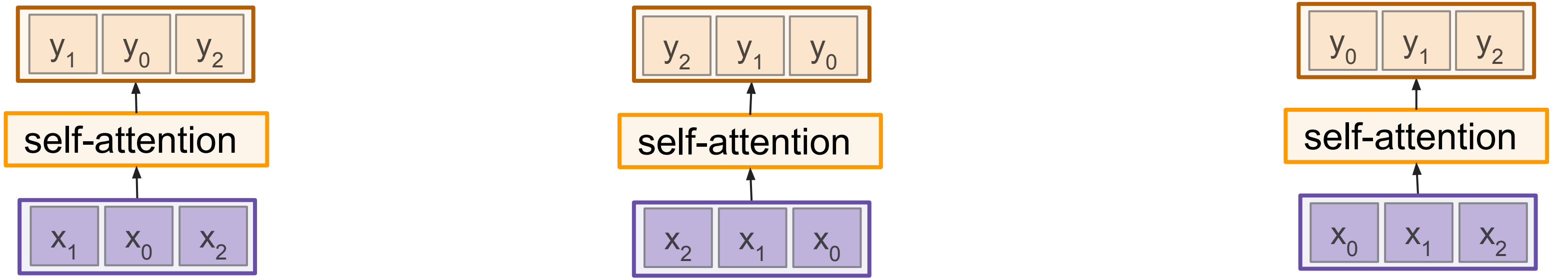
Output: $y_j = \sum_i a_{i,j} v_i$

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



Self attention layer - attends over sets of inputs

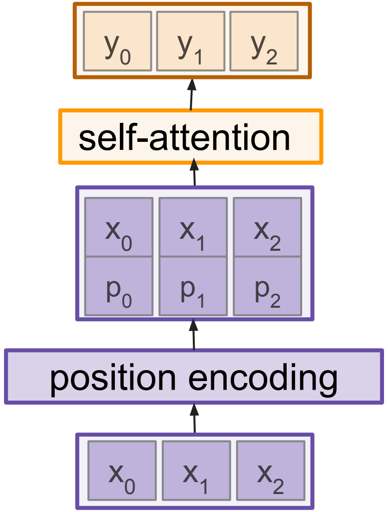


Permutation equivariant

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

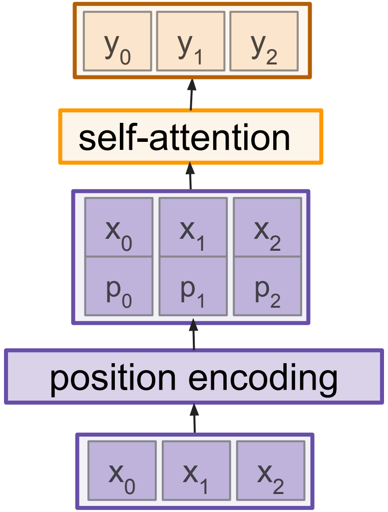
We use a function *pos*: $N \rightarrow R^d$
to process the position j of the vector into a d-dimensional vector

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

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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.

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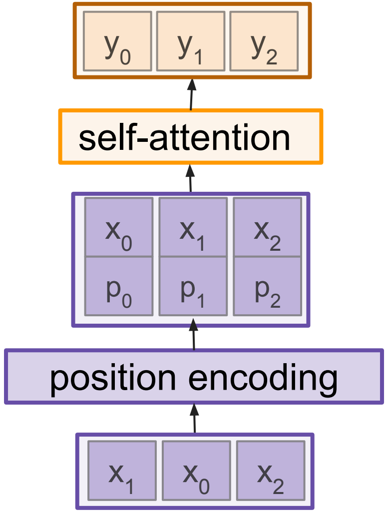
Vaswani et al, "Attention is all you need", NeurIPS 2017

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*(.)

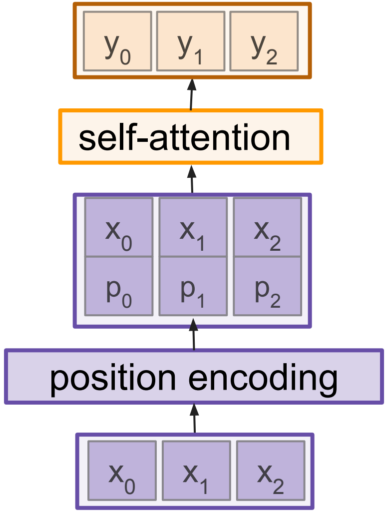
1. Learn a lookup table:
   - Learn parameters to use for *pos*(t) for t ε [0, T)
   - Lookup table contains T x d parameters.

2. Design a fixed function with the desiderata

$$\mathbf{p(t)} = \begin{bmatrix} \sin(\omega_1 . t) \\ \cos(\omega_1 . t) \\ \\ \sin(\omega_2 . t) \\ \cos(\omega_2 . t) \\ \\ \vdots \\ \\ \sin(\omega_{d/2} . t) \\ \cos(\omega_{d/2} . t) \end{bmatrix}_d \quad \text{where } \omega_k = \frac{1}{10000^{2k/d}}$$

Vaswani et al, “Attention is all you need”, NeurIPS 2017

Positional encoding



Concatenate special positional encoding p_j to each input vector x_j

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Options for *pos*(.)

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Intuition:

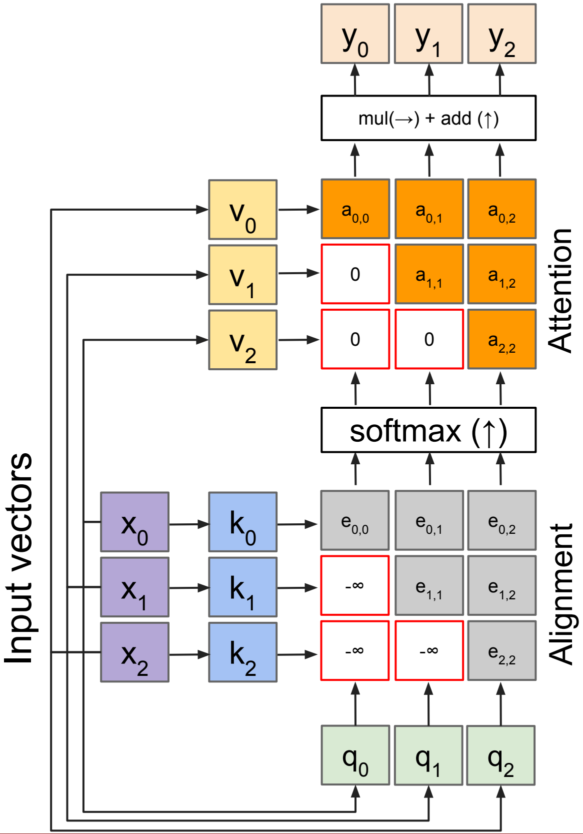
0 :	0	0	0	0	8 :	1	0	0	0
1 :	0	0	0	1	9 :	1	0	0	1
2 :	0	0	1	0	10 :	1	0	1	0
3 :	0	0	1	1	11 :	1	0	1	1
4 :	0	1	0	0	12 :	1	1	0	0
5 :	0	1	0	1	13 :	1	1	0	1
6 :	0	1	1	0	14 :	1	1	1	0
7 :	0	1	1	1	15 :	1	1	1	1

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)

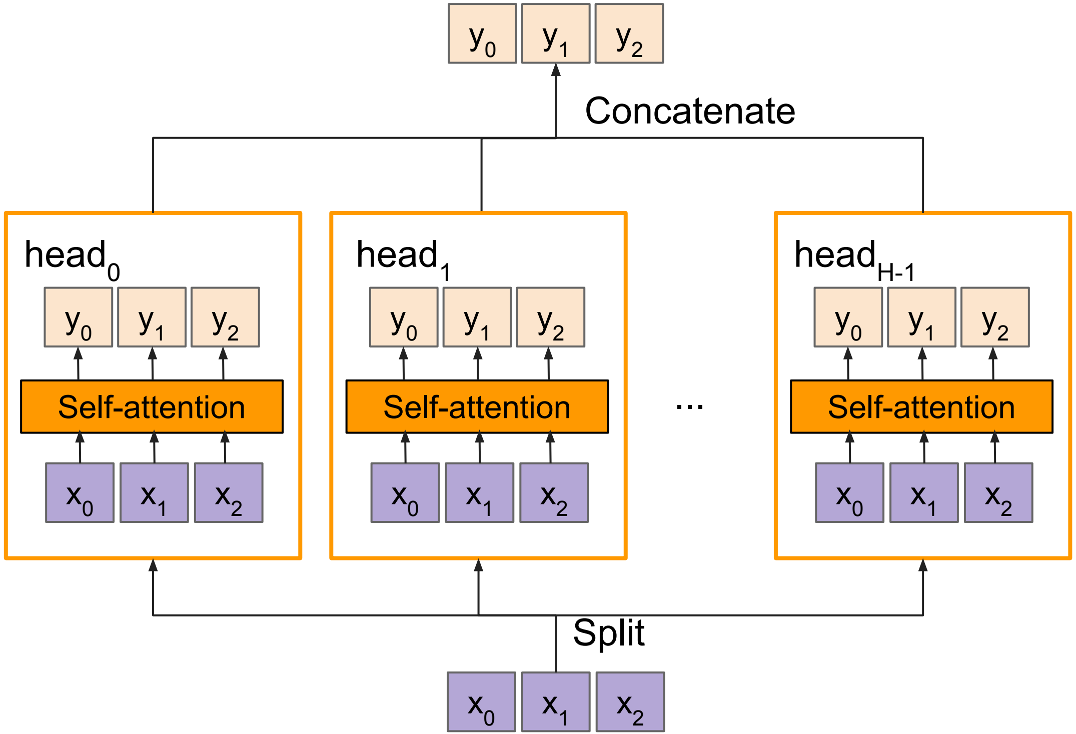
Operations:
Key vectors: $\mathbf{k} = \mathbf{x}\mathbf{W}_k$
Value vectors: $\mathbf{v} = \mathbf{x}\mathbf{W}_v$
Query vectors: $\mathbf{q} = \mathbf{x}\mathbf{W}_q$
Alignment: $e_{i,j} = q_j \cdot k_i / \sqrt{D}$
Attention: $\mathbf{a} = \mathrm{softmax}(\mathbf{e})$
Output: $y_j = \sum_i a_{i,j}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

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

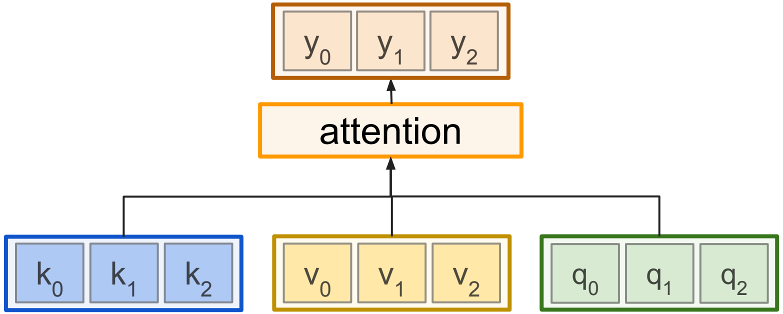
- Prevent vectors from looking at future vectors.
- Manually set alignment scores to -infinity

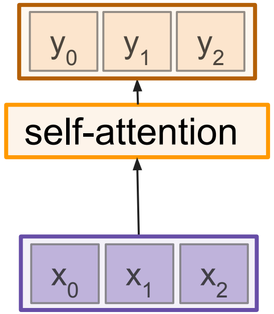
Multi-head self-attention layer

- Multiple self-attention heads in parallel



General attention versus self-attention





Example: CNN with Self-Attention

Input Image

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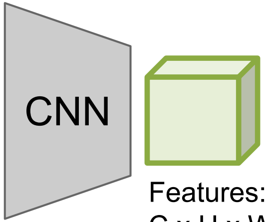
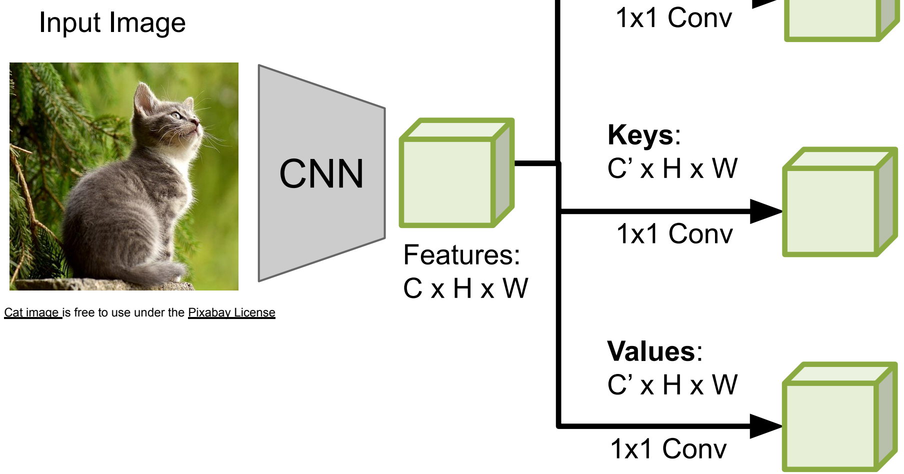


Zhang et al, “Self-Attention Generative Adversarial Networks”, ICML 2018

Slide credit: Justin Johnson

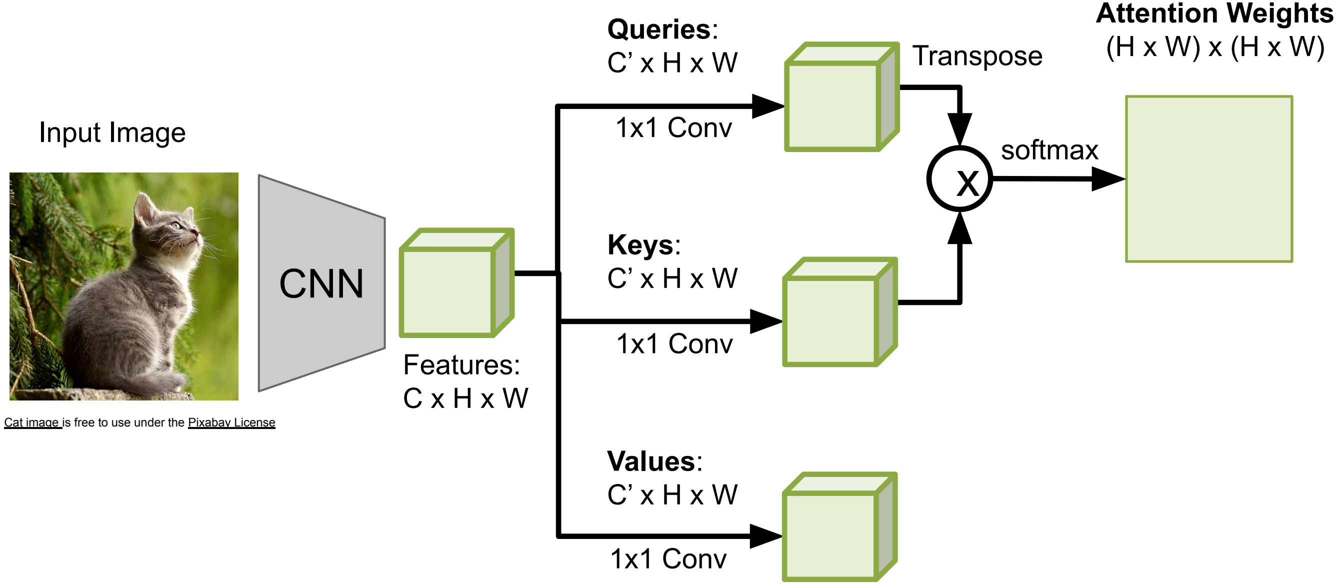
Example: CNN with Self-Attention



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

Slide credit: Justin Johnson

Example: CNN with Self-Attention



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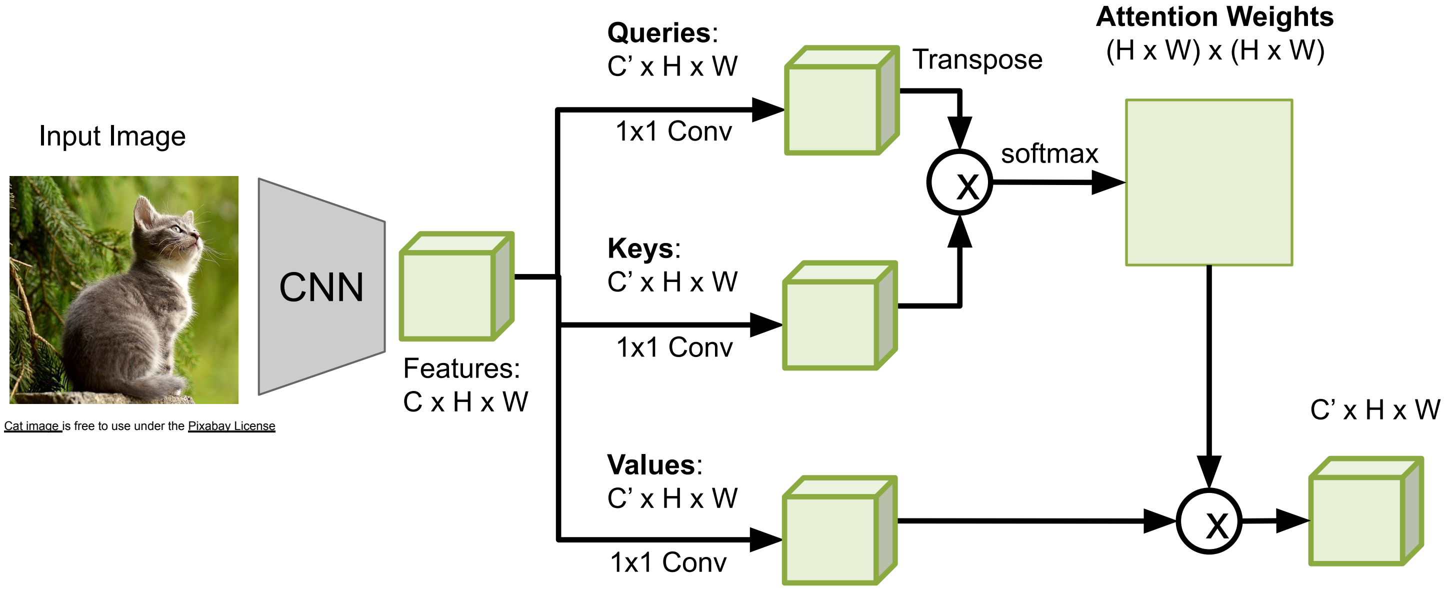
Example: CNN with Self-Attention



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

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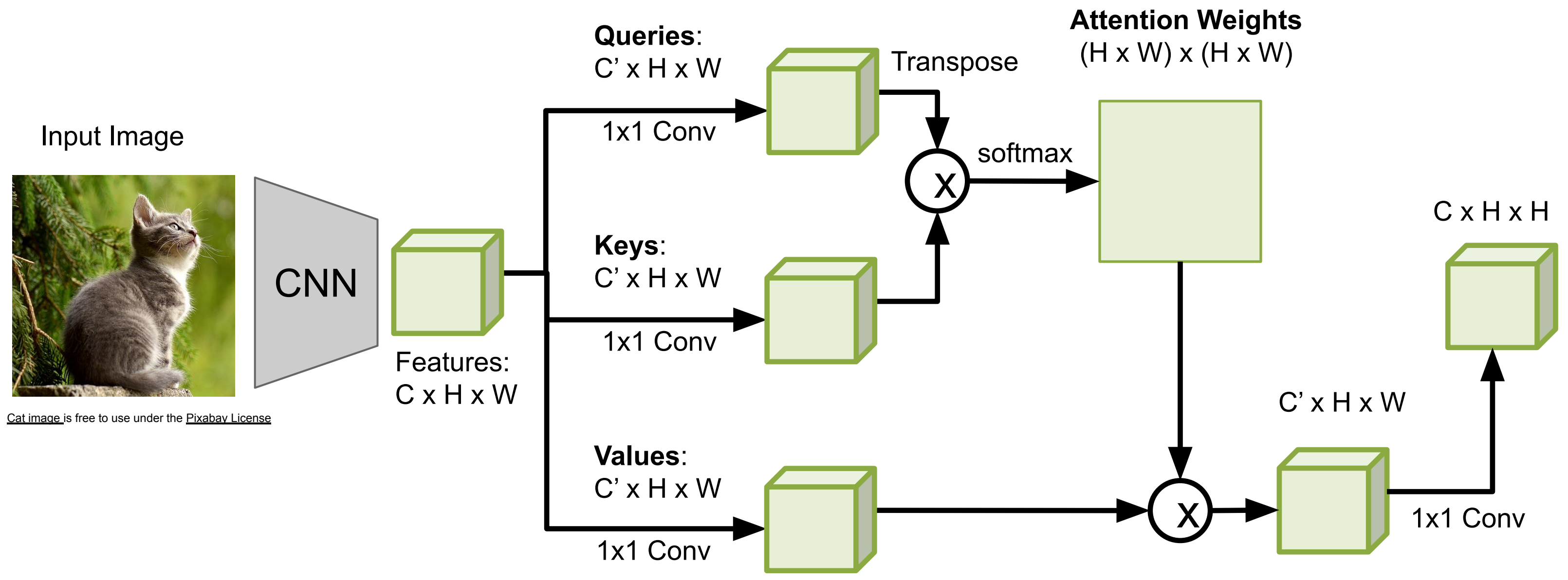
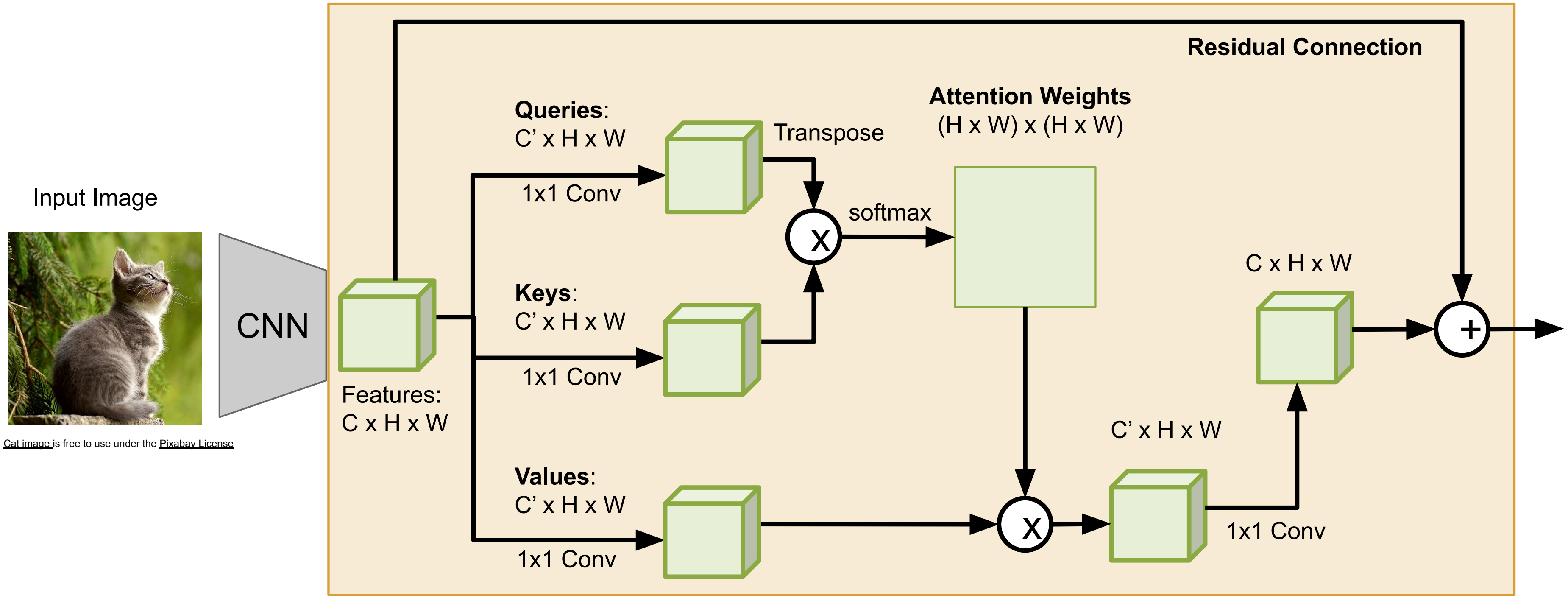
Example: CNN with Self-Attention



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

Slide credit: Justin Johnson

Example: CNN with Self-Attention



Self-Attention Module

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

Slide credit: Justin Johnson

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

On the Opportunities and Risks of Foundation Models

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