Lecture 12:
Attention and Transformers

Administrative: A4

Pytorch! Visualizations! RNNs!

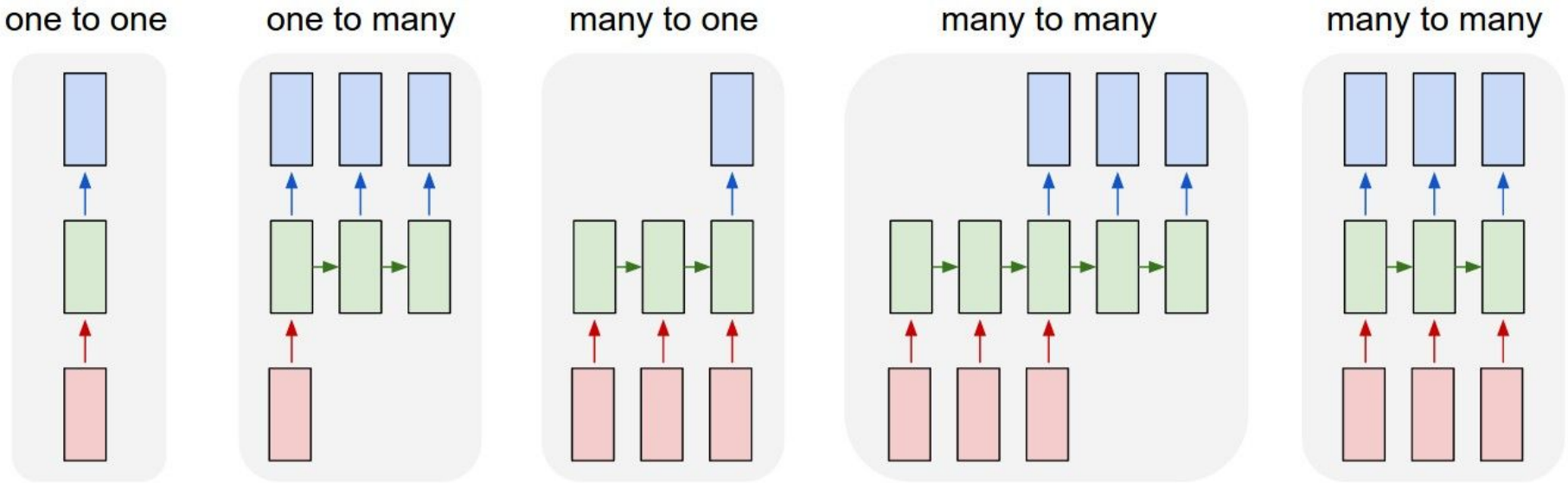
Due Feb 27

Milestone

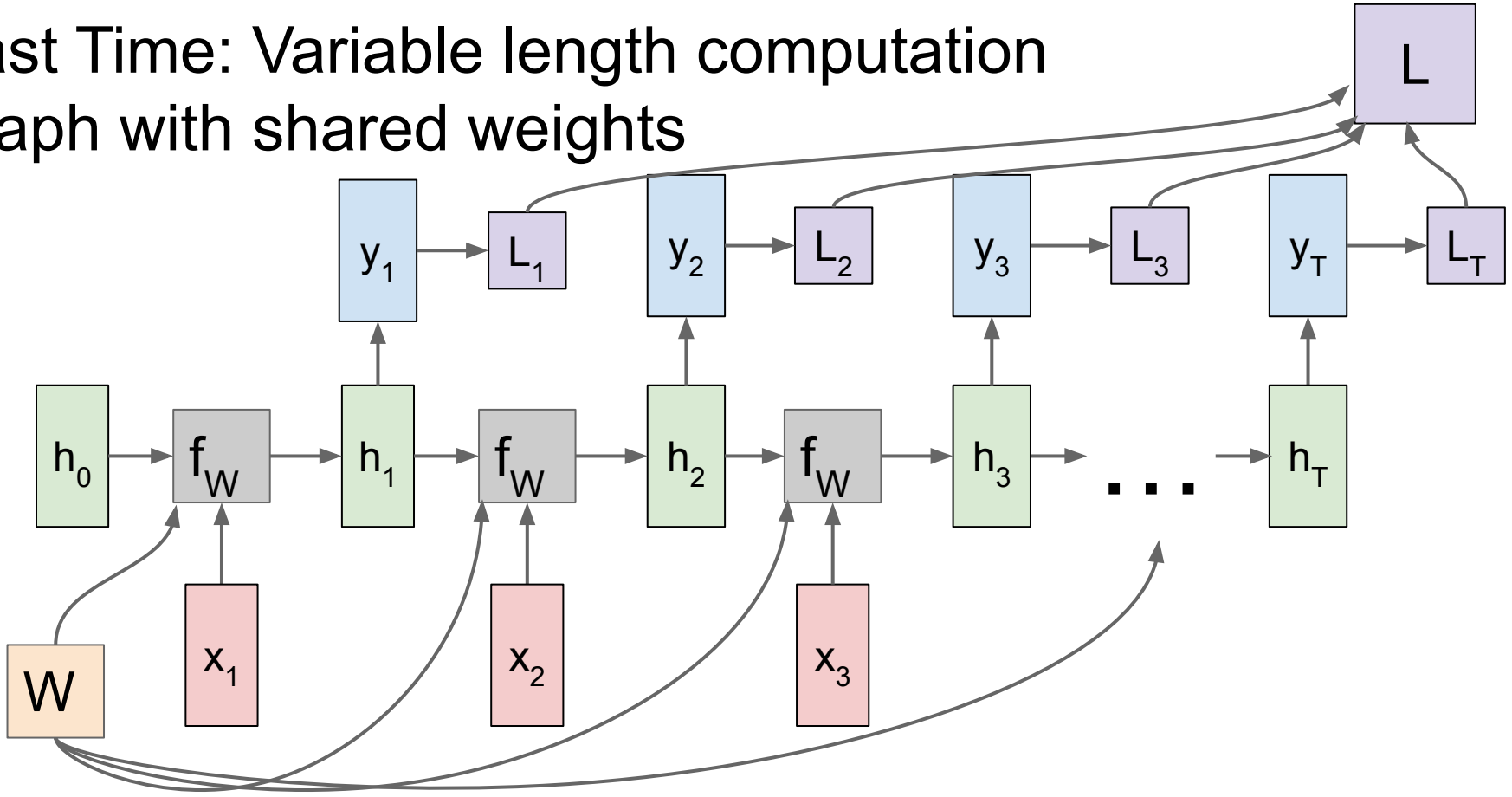
Due in 1 week

Start on your poster

Last Time: Recurrent Neural Networks

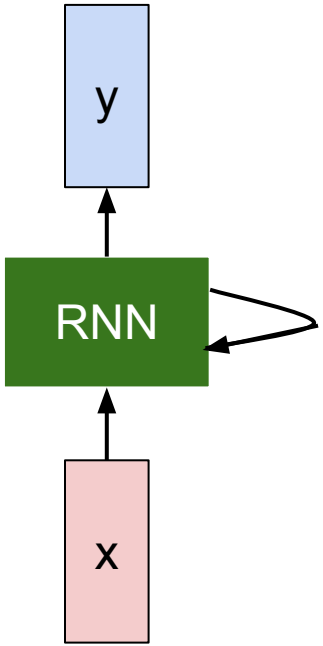


Last Time: Variable length computation graph with shared weights



(Simple) Recurrent Neural Network

The state consists of a single *"hidden"* vector **h**:



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

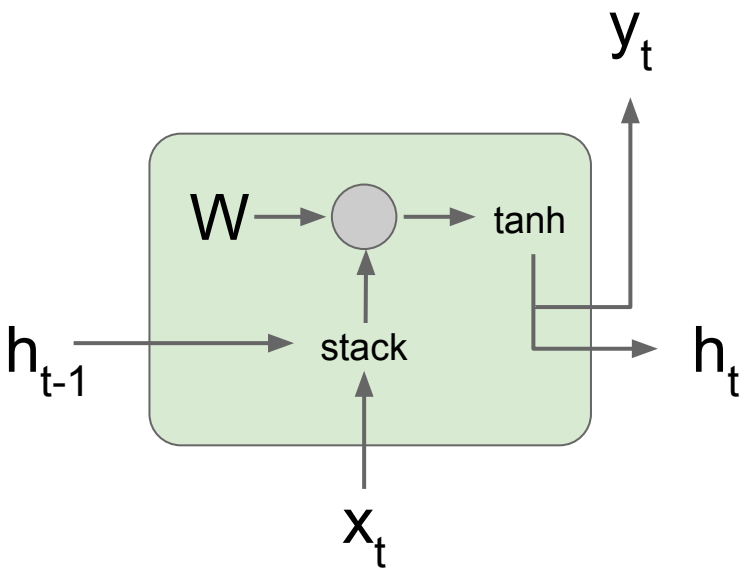
$$h_t = \tanh(W_{hh}h_{t-1} + W_{xh}x_t)$$

$$y_t = W_{hy}h_t$$

Sometimes called a "Vanilla RNN" or an "Elman RNN" after Prof. Jeffrey Elman

Vanilla RNN Gradient Flow

Bengio et al, “Learning long-term dependencies with gradient descent is difficult”, IEEE Transactions on Neural Networks, 1994
Pascanu et al, “On the difficulty of training recurrent neural networks”, ICML 2013



$$
\begin{aligned}
h_t &= \tanh(W_{hh}h_{t-1} + W_{xh}x_t) \\
&= \tanh\left(\begin{pmatrix} W_{hh} & W_{hx} \end{pmatrix} \begin{pmatrix} h_{t-1} \\ x_t \end{pmatrix} \right) \\
&= \tanh\left(W \begin{pmatrix} h_{t-1} \\ x_t \end{pmatrix} \right)
\end{aligned}
$$

Vanilla RNN Gradient Flow

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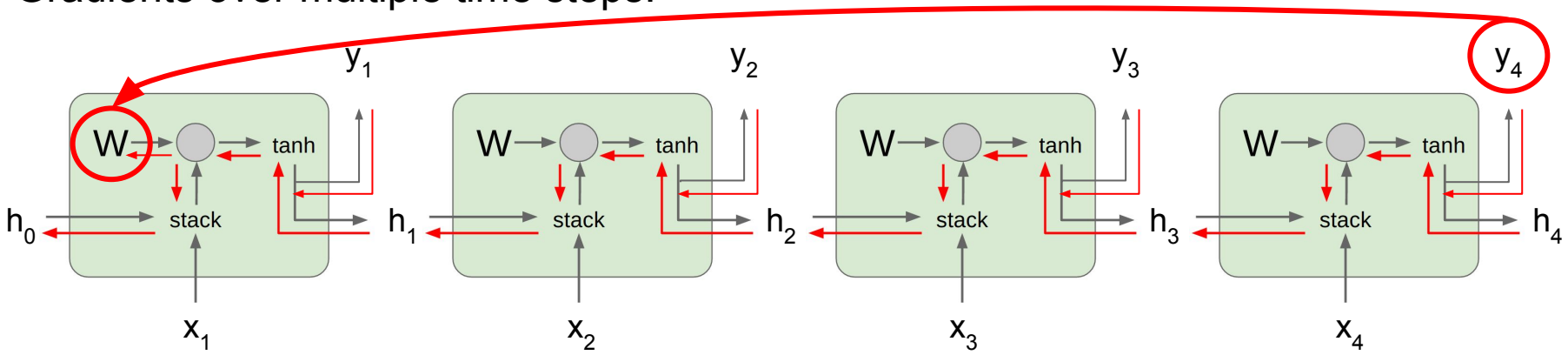
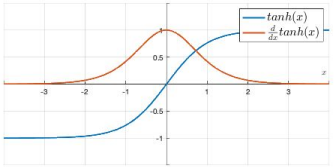
Gradients over multiple time steps:



$$\frac{\partial L}{\partial W} = \sum_{t=1}^{T} \frac{\partial L_t}{\partial W}$$

Almost always < 1
Vanishing gradients



$$\frac{\partial L_T}{\partial W} = \frac{\partial L_T}{\partial h_T}\left(\prod_{t=2}^{T} tanh'\left(W_{hh}h_{t-1} + W_{xh}x_t\right)\right) W_{hh}^{T-1}\frac{\partial h_1}{\partial W}$$

Long Short Term Memory (LSTM)

Vanilla RNN

$$h_t = \tanh\left(W \begin{pmatrix} h_{t-1} \\ x_t \end{pmatrix}\right)$$

LSTM

$$\begin{pmatrix} i \\ f \\ o \\ g \end{pmatrix} = \begin{pmatrix} \sigma \\ \sigma \\ \sigma \\ \tanh \end{pmatrix} W \begin{pmatrix} h_{t-1} \\ x_t \end{pmatrix}$$

$$c_t = f \odot c_{t-1} + i \odot g$$

$$h_t = o \odot \tanh(c_t)$$

Hochreiter and Schmidhuber, “Long Short Term Memory”, Neural Computation 1997

RNNs have a single hidden state (h_t)
LSTMs have two: cell memory c_t and hidden state h_t

Vanilla RNN

$$h_t = \tanh\left(W \begin{pmatrix} h_{t-1} \\ x_t \end{pmatrix}\right)$$

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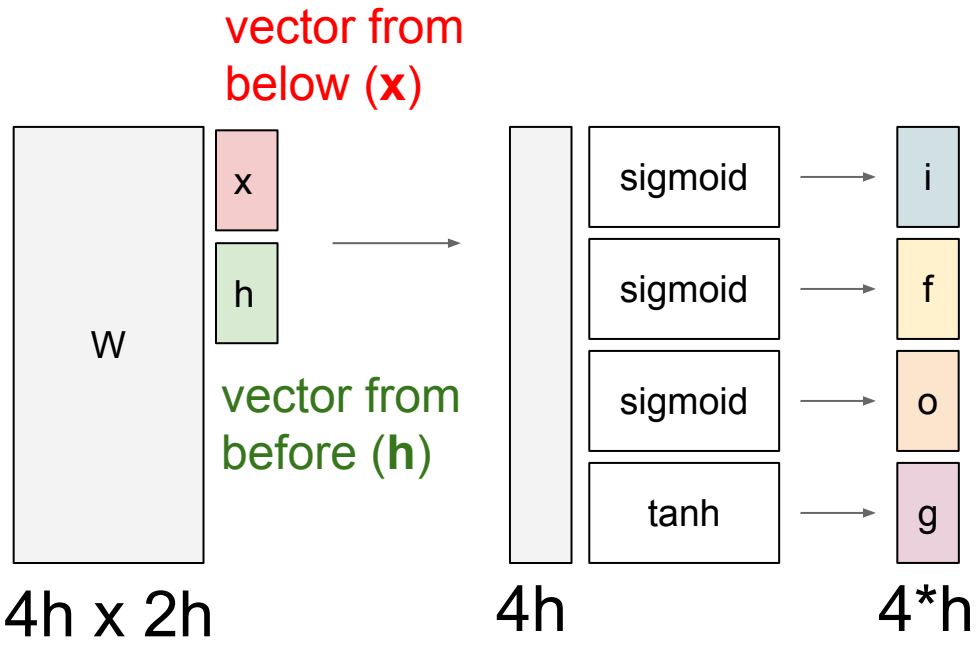
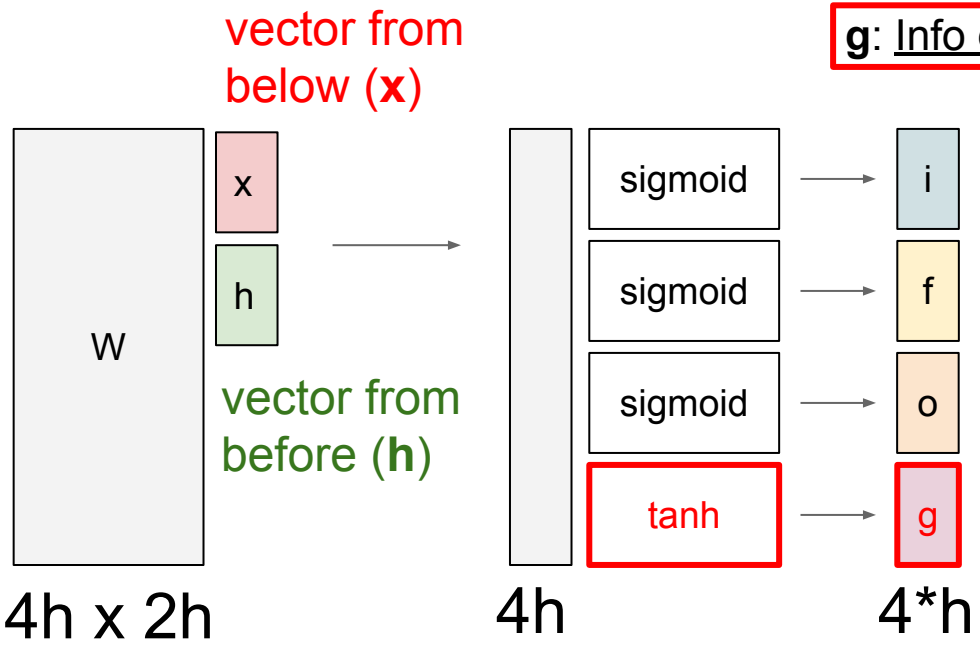
Long Short Term Memory (LSTM)

[Hochreiter et al., 1997]



Long Short Term Memory (LSTM)

[Hochreiter et al., 1997]



g: Info gate, How much to write to cell

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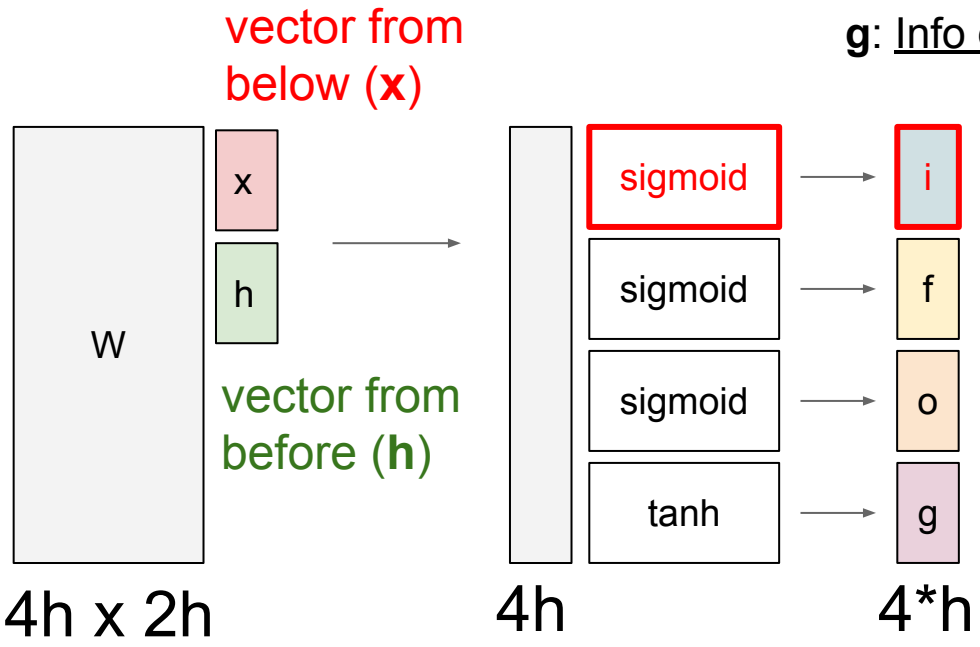
[Hochreiter et al., 1997]

i: Input gate, whether to write to cell

g: Info gate, How much to write to cell



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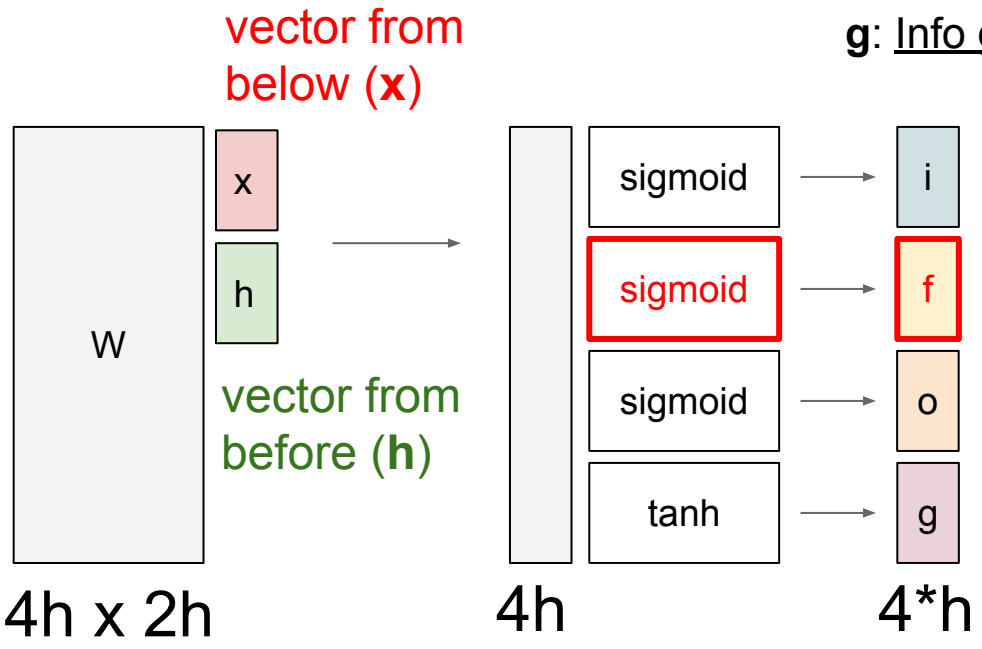
Long Short Term Memory (LSTM)

[Hochreiter et al., 1997]

i: Input gate, whether to write to cell

f: Forget gate, Whether to erase cell

g: Info gate, How much to write to cell



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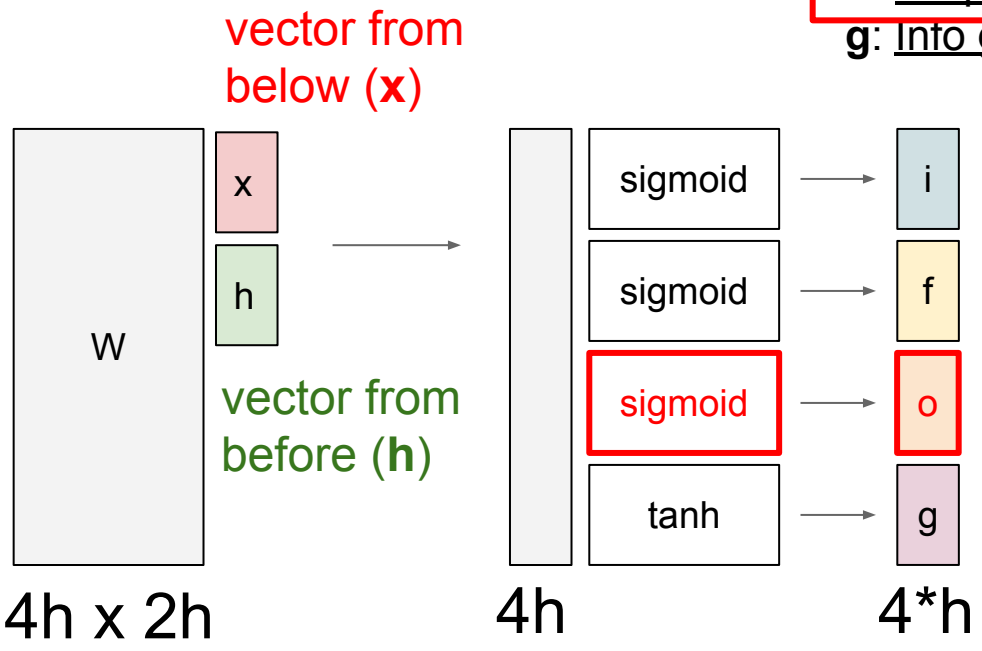
Long Short Term Memory (LSTM)

[Hochreiter et al., 1997]

i: Input gate, whether to write to cell
f: Forget gate, Whether to erase cell
o: Output gate, How much to reveal cell
g: Info gate, How much to write to cell



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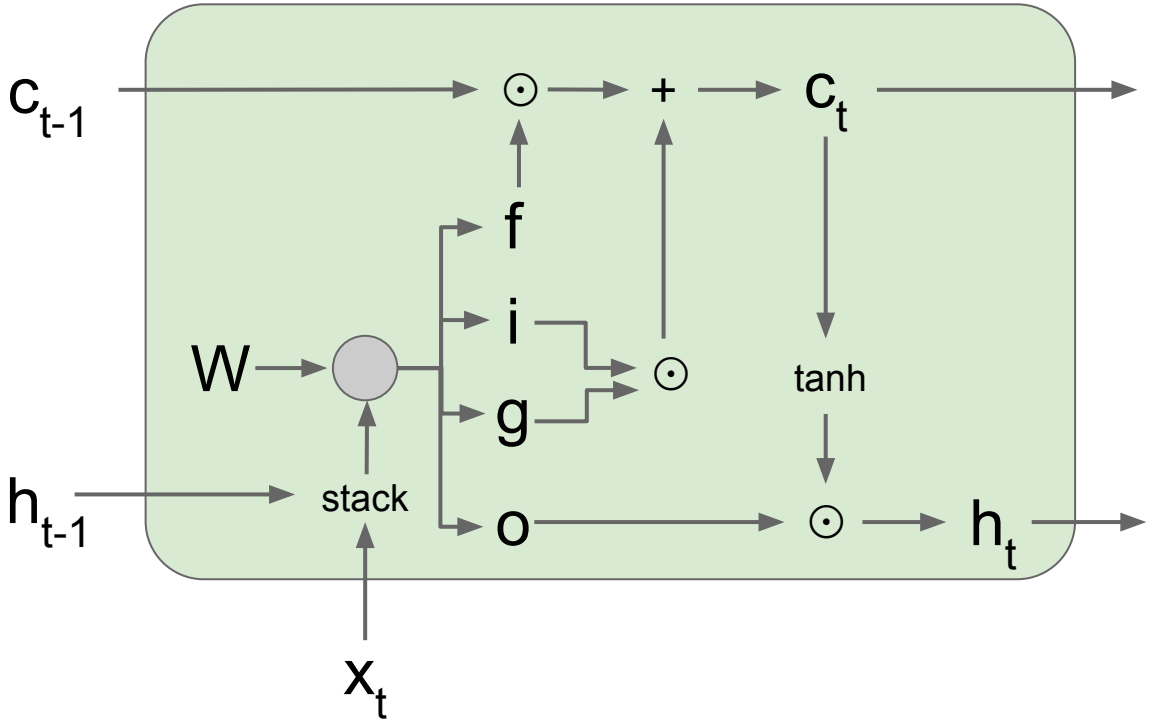

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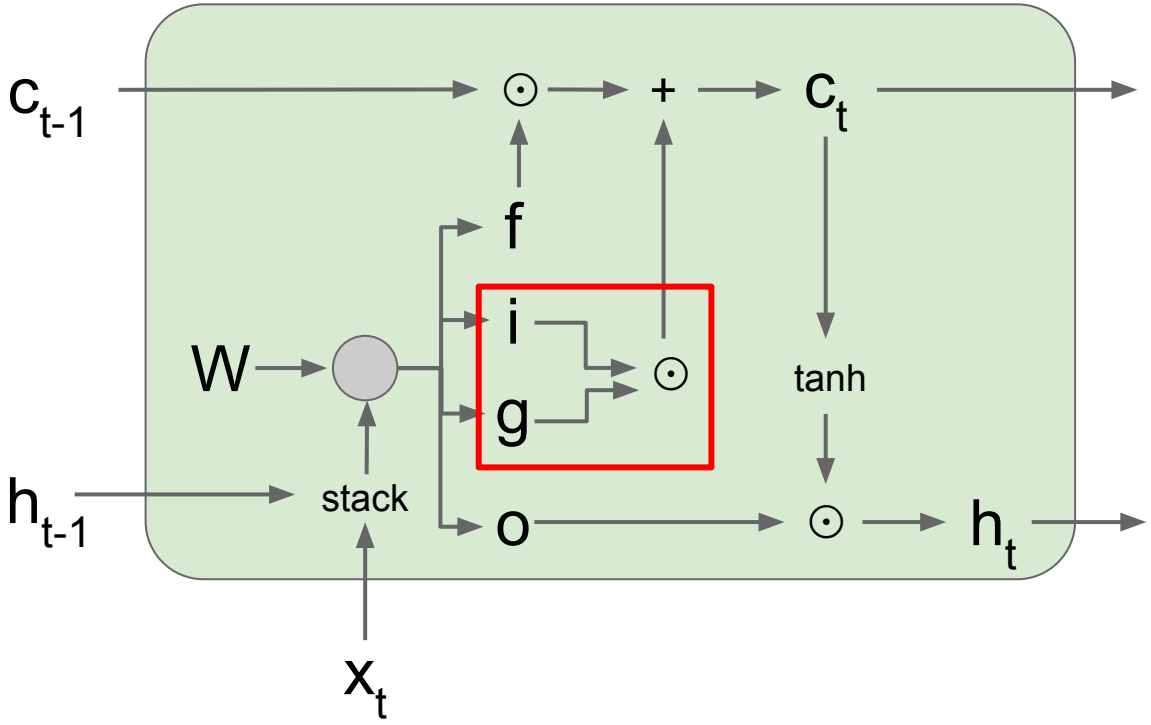

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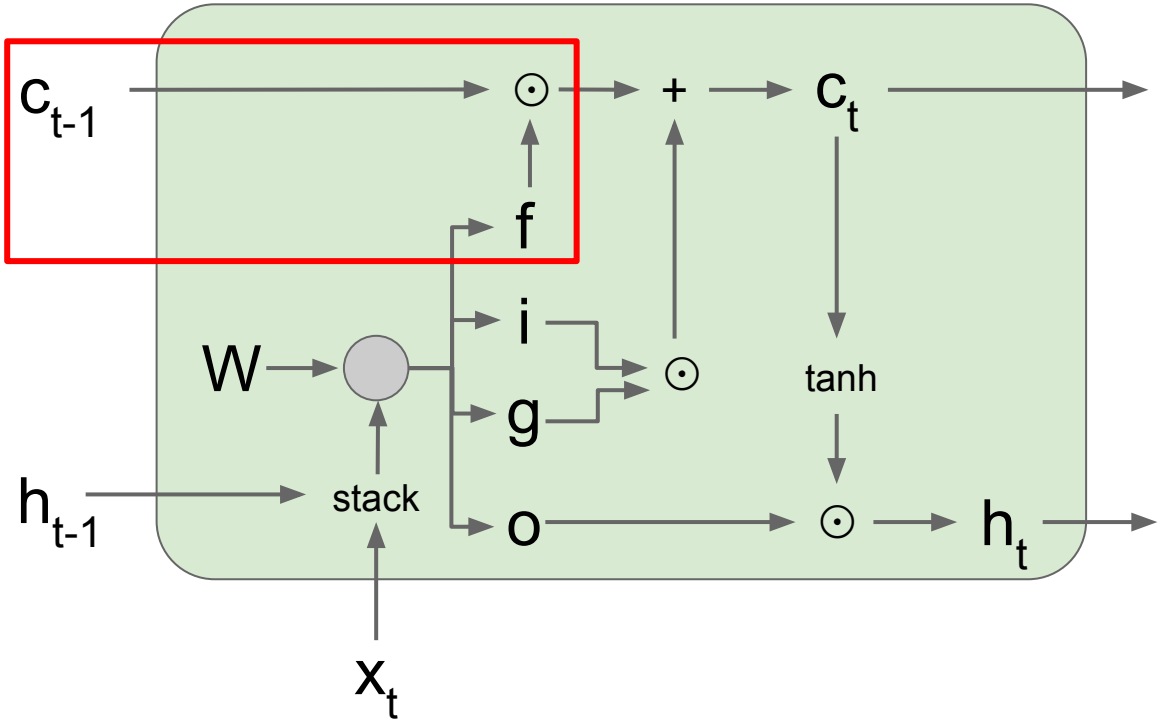

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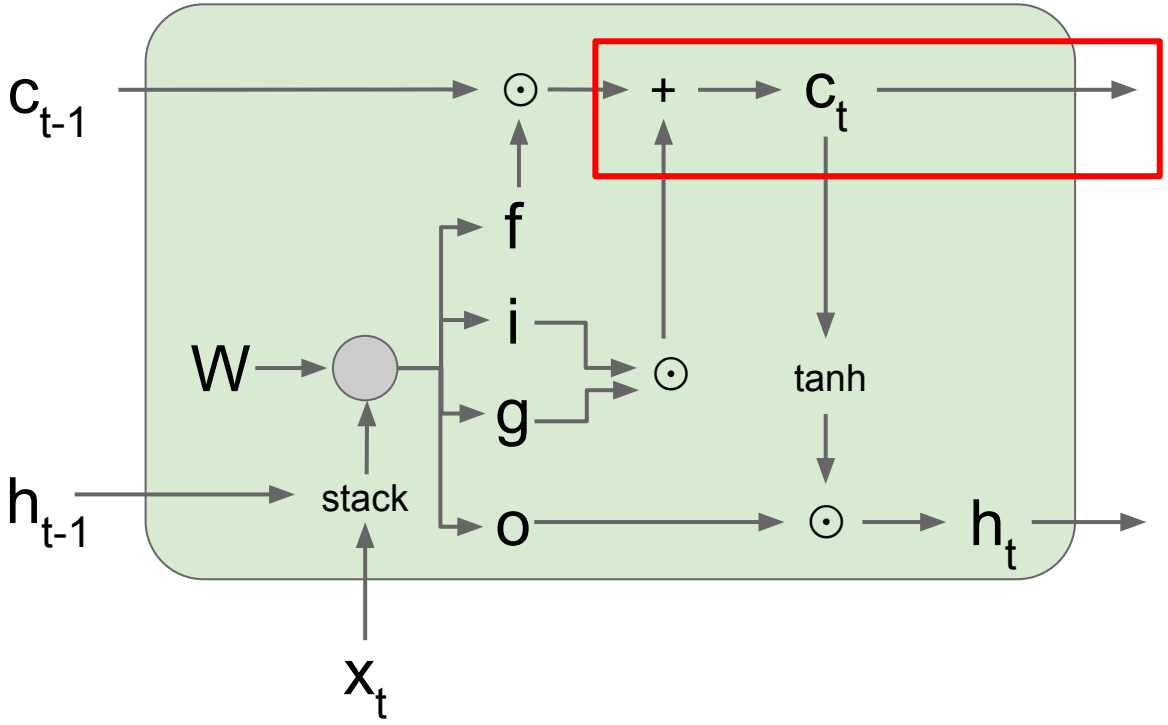

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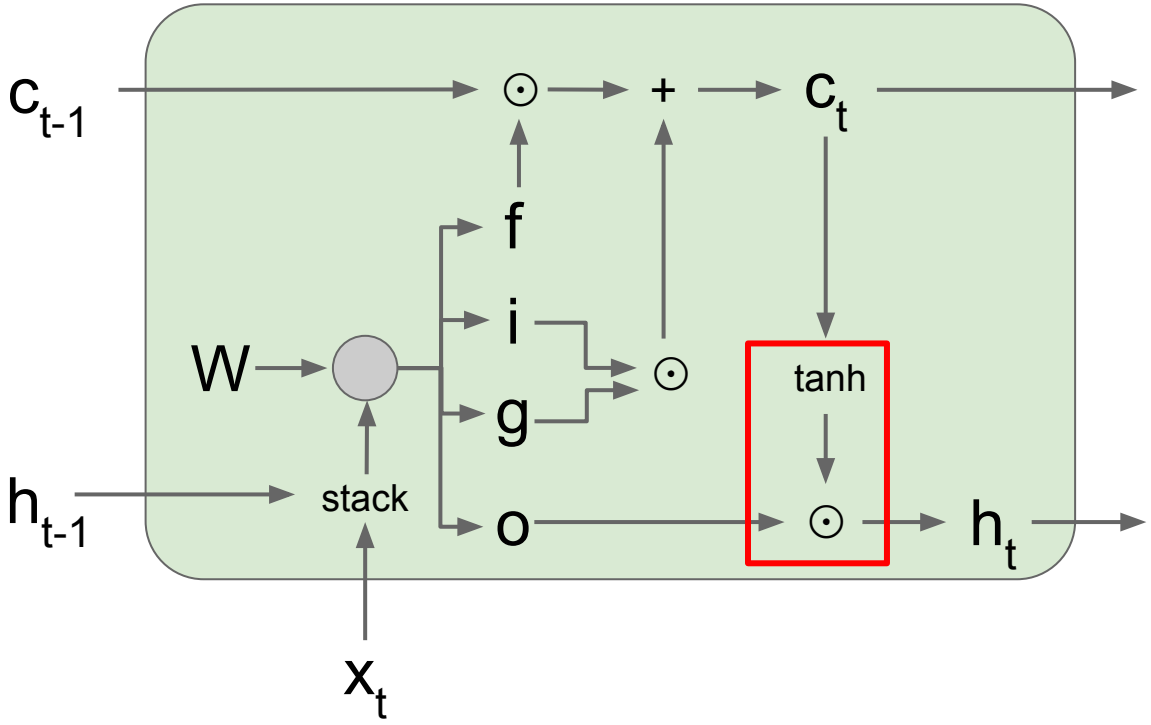

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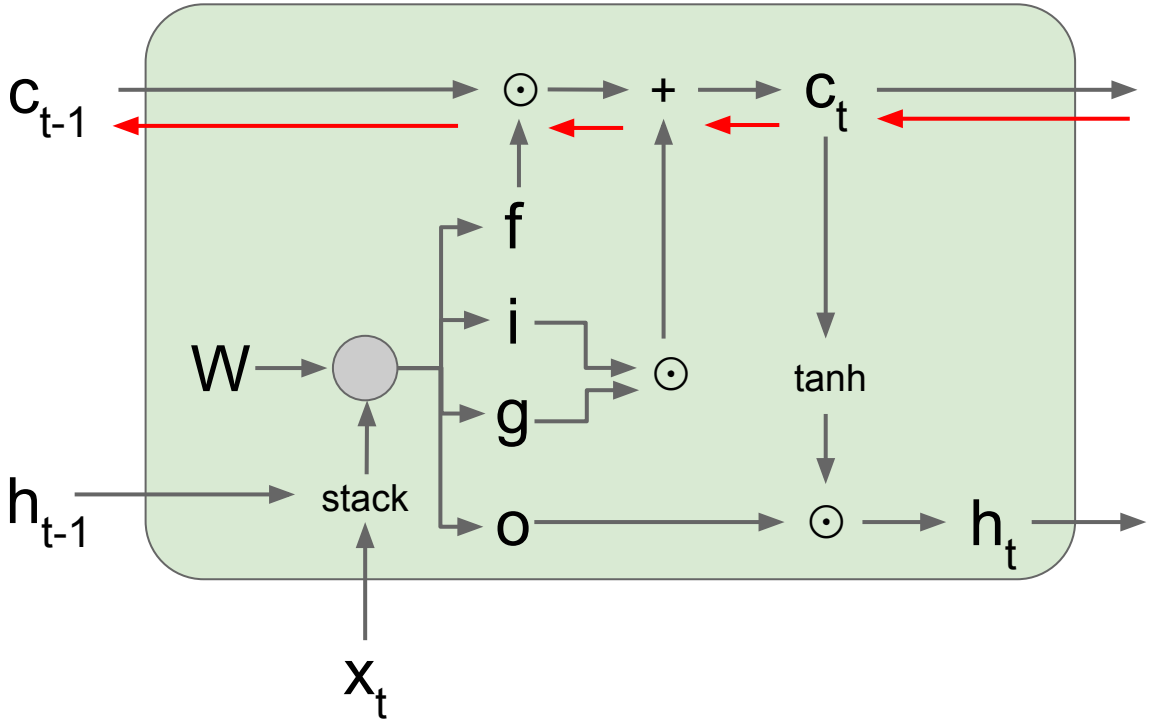
Long Short Term Memory (LSTM): Gradient Flow

[Hochreiter et al., 1997]



Backpropagation from c_t to c_{t-1} only elementwise multiplication by f, no matrix multiply by W

$$\begin{pmatrix} i \\ f \\ o \\ g \end{pmatrix} = \begin{pmatrix} \sigma \\ \sigma \\ \sigma \\ \tanh \end{pmatrix} W \begin{pmatrix} h_{t-1} \\ x_t \end{pmatrix}$$

$$c_t = f \odot c_{t-1} + i \odot g$$

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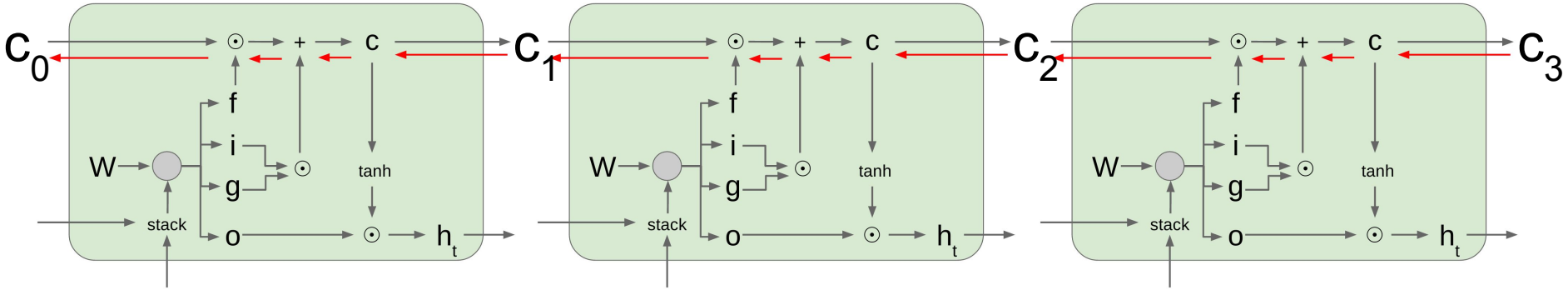
Long Short Term Memory (LSTM): Gradient Flow

[Hochreiter et al., 1997]

Uninterrupted gradient flow!



Notice that the gradient contains the **f** gate's vector of activations

- allows better control of gradients values, using suitable parameter updates of the forget gate.

Also notice that are added through the **f, i, g,** and **o** gates

- better balancing of gradient values

Do LSTMs solve the vanishing gradient problem?

The LSTM architecture makes it easier for the RNN to preserve information over many timesteps

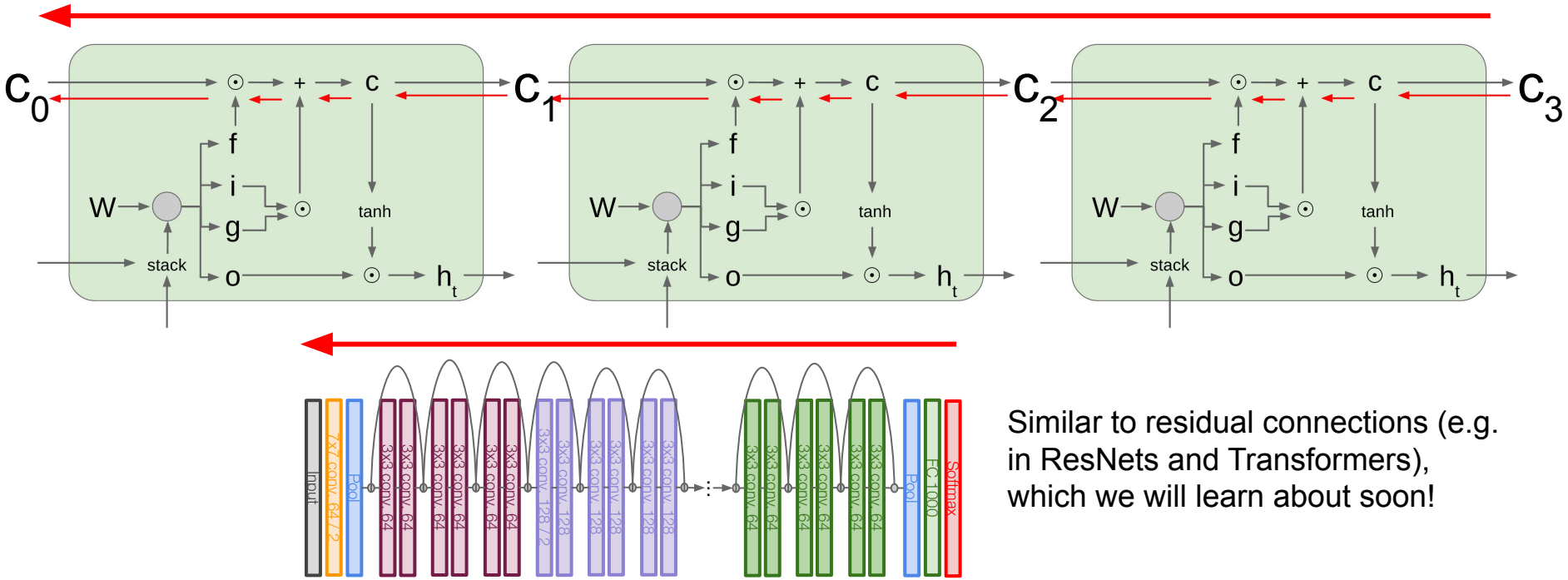
- e.g. **if the f = 1 and the i = 0**, then the information of that cell is preserved indefinitely.
- By contrast, it's harder for vanilla RNN to learn a recurrent weight matrix Wh that preserves info in hidden state

LSTM **doesn't guarantee** that there is no vanishing/exploding gradient, but it does provide an easier way for the model to learn long-distance dependencies

Long Short Term Memory (LSTM): Gradient Flow

[Hochreiter et al., 1997]

Uninterrupted gradient flow!



Similar to residual connections (e.g. in ResNets and Transformers), which we will learn about soon!

Other RNN Variants

GRU [*Learning phrase representations using rnn encoder-decoder for statistical machine translation*, Cho et al. 2014]

$$r_t = \sigma(W_{xr}x_t + W_{hr}h_{t-1} + b_r)$$
$$z_t = \sigma(W_{xz}x_t + W_{hz}h_{t-1} + b_z)$$
$$\tilde{h}_t = \tanh(W_{xh}x_t + W_{hh}(r_t \odot h_{t-1}) + b_h)$$
$$h_t = z_t \odot h_{t-1} + (1 - z_t) \odot \tilde{h}_t$$

[*LSTM: A Search Space Odyssey*, Greff et al., 2015]

[*An Empirical Exploration of Recurrent Network Architectures*, Jozefowicz et al., 2015]

MUT1:

$$\begin{aligned} z &= \text{sigm}(W_{\text{xz}}x_t + b_{\text{z}}) \\ r &= \text{sigm}(W_{\text{xr}}x_t + W_{\text{hr}}h_t + b_{\text{r}}) \\ h_{t+1} &= \tanh(W_{\text{hh}}(r \odot h_t) + \tanh(x_t) + b_{\text{h}}) \odot z \\ &+ h_t \odot (1 - z) \end{aligned}$$

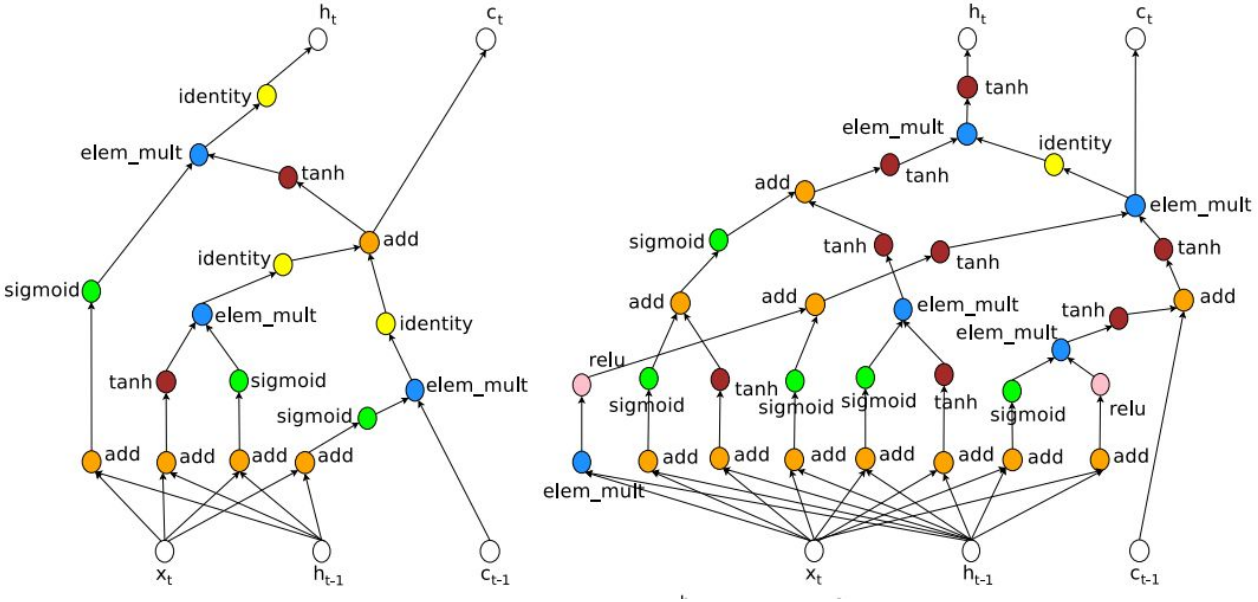
MUT2:

$$\begin{aligned} z &= \text{sigm}(W_{\text{xz}}x_t + W_{\text{hz}}h_t + b_{\text{z}}) \\ r &= \text{sigm}(x_t + W_{\text{hr}}h_t + b_{\text{r}}) \\ h_{t+1} &= \tanh(W_{\text{hh}}(r \odot h_t) + W_{xh}x_t + b_{\text{h}}) \odot z \\ &+ h_t \odot (1 - z) \end{aligned}$$

MUT3:

$$\begin{aligned} z &= \text{sigm}(W_{\text{xz}}x_t + W_{\text{hz}}\tanh(h_t) + b_{\text{z}}) \\ r &= \text{sigm}(W_{\text{xr}}x_t + W_{\text{hr}}h_t + b_{\text{r}}) \\ h_{t+1} &= \tanh(W_{\text{hh}}(r \odot h_t) + W_{xh}x_t + b_{\text{h}}) \odot z \\ &+ h_t \odot (1 - z) \end{aligned}$$

Neural Architecture Search for RNN architectures



LSTM cell

Cell they found

Zoph et Le, “Neural Architecture Search with Reinforcement Learning”, ICLR 2017

Recurrence for Vision

- LSTM were a good default choice until a few years ago
- Use variants like GRU if you want faster compute and less parameters
- Use transformers (next lecture) as they are dominating NLP and also vision models

Su et al. "Vl-bert: Pre-training of generic visual-linguistic representations." ICLR 2020
Lu et al. "Vilbert: Pretraining task-agnostic visiolinguistic representations for vision-and-language tasks." NeurIPS 2019
Li et al. "Visualbert: A simple and performant baseline for vision and language." *arXiv* 2019

Today's Agenda:

- **Attention with RNNs**
  - In Computer Vision
  - In NLP
- **General Attention Layer**
  - Self-attention
  - Positional encoding
  - Masked attention
  - Multi-head attention
- **Transformers**

Today's Agenda:

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  - In Computer Vision
  - In NLP
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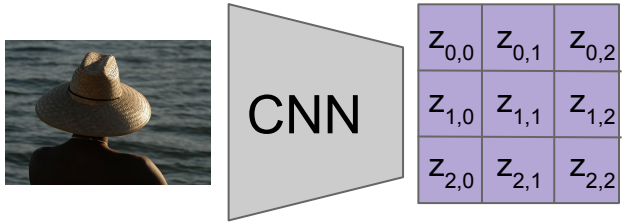
Image Captioning using spatial features

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



Extract spatial features from a pretrained CNN

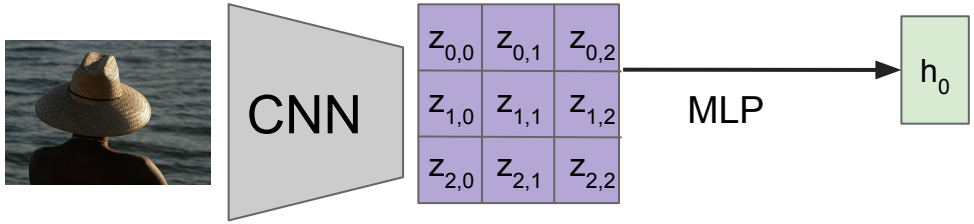
Features: H x W x D

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

Image Captioning using spatial features

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

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



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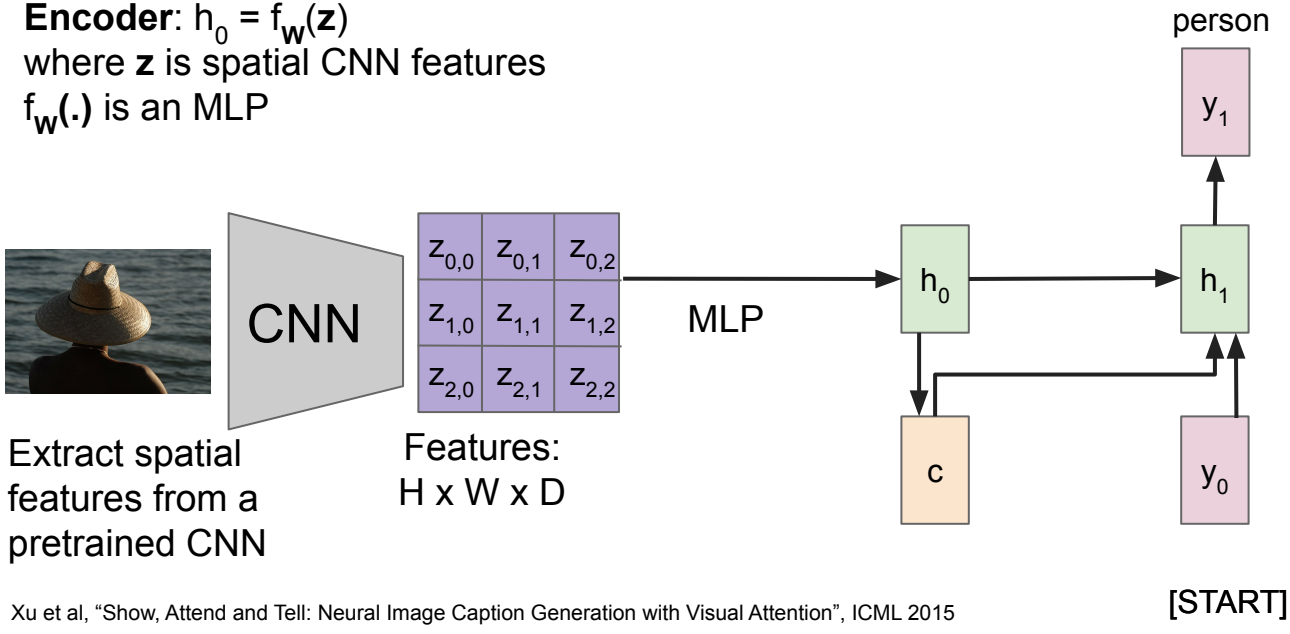

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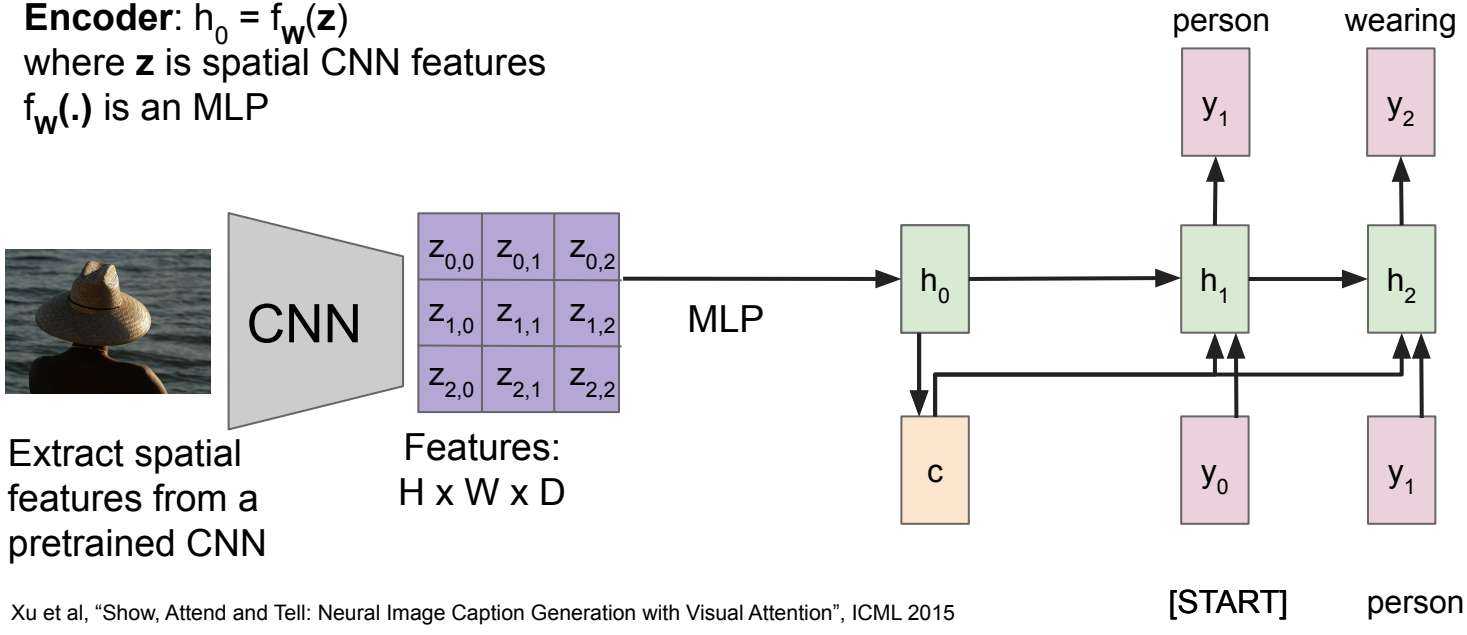

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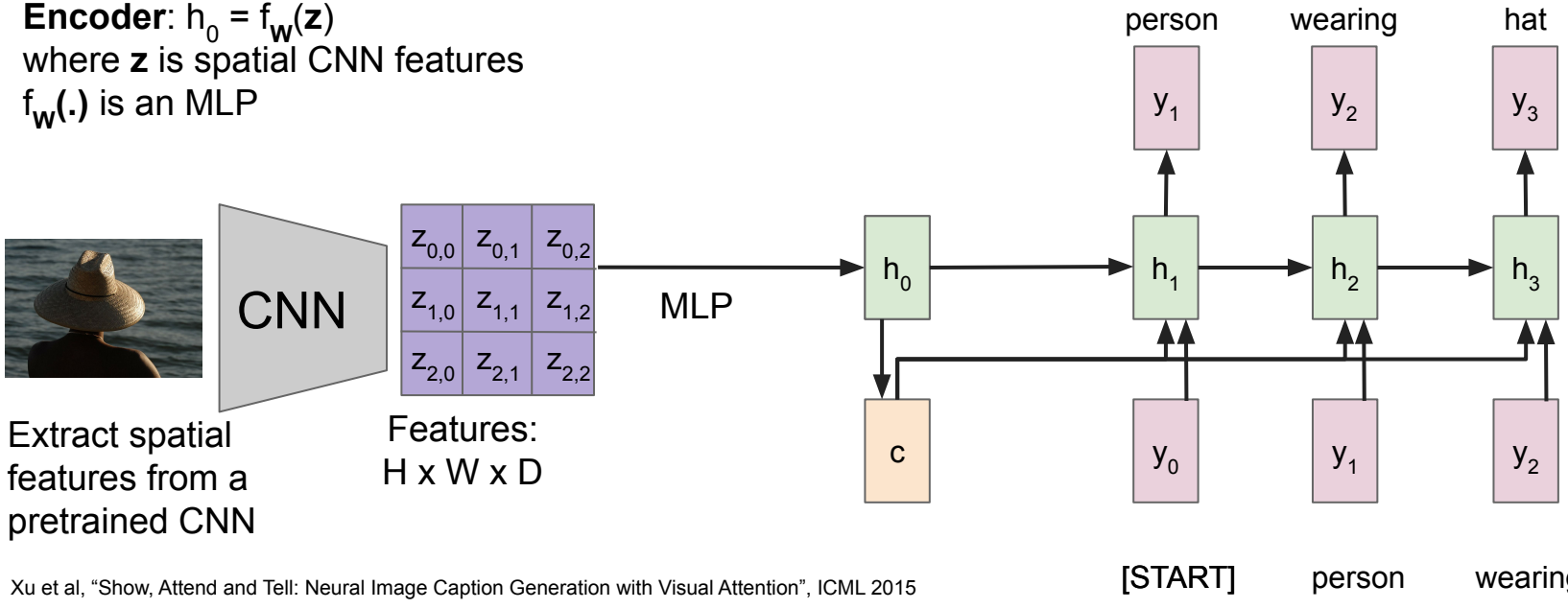

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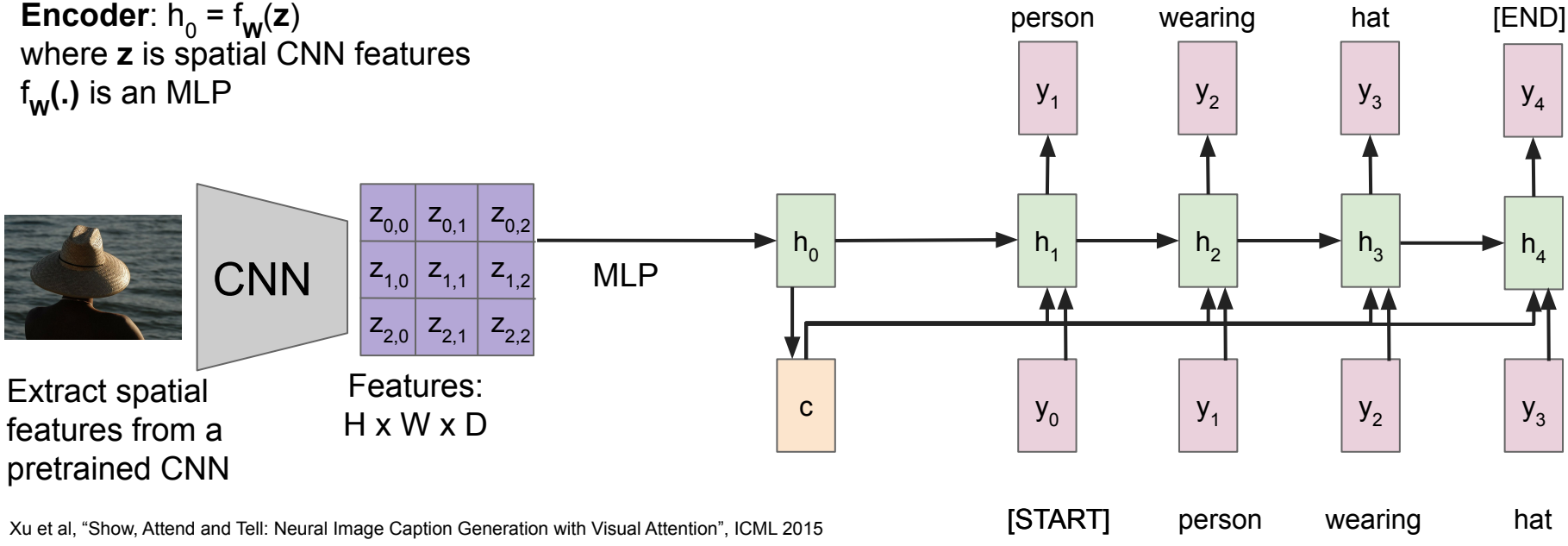

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Image Captioning using spatial features

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

CNN

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

Extract spatial features from a pretrained CNN

Features: H x W x D

MLP

h_0 h_1 h_2 h_3 h_4

c

y_0 y_1 y_2 y_3

[START] person wearing hat

y_1 y_2 y_3 y_4

person wearing hat [END]

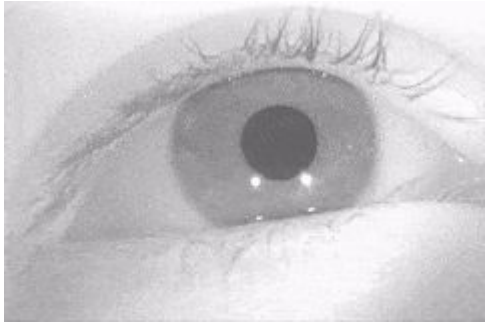
Xu et al, "Show, Attend and Tell: Neural Image Caption Generation with Visual Attention", ICML 2015

Image Captioning with RNNs & Attention

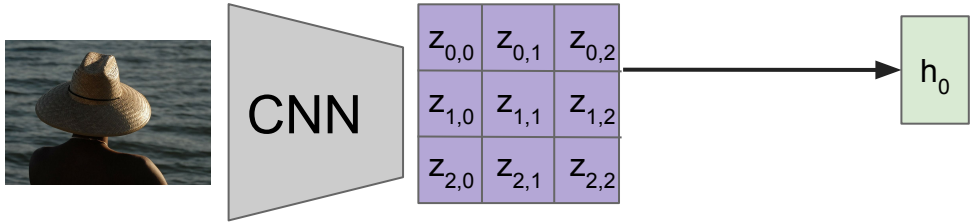
Attention idea: New context vector at every time step.

Each context vector will attend to different image regions

gif source



Attention Saccades in humans

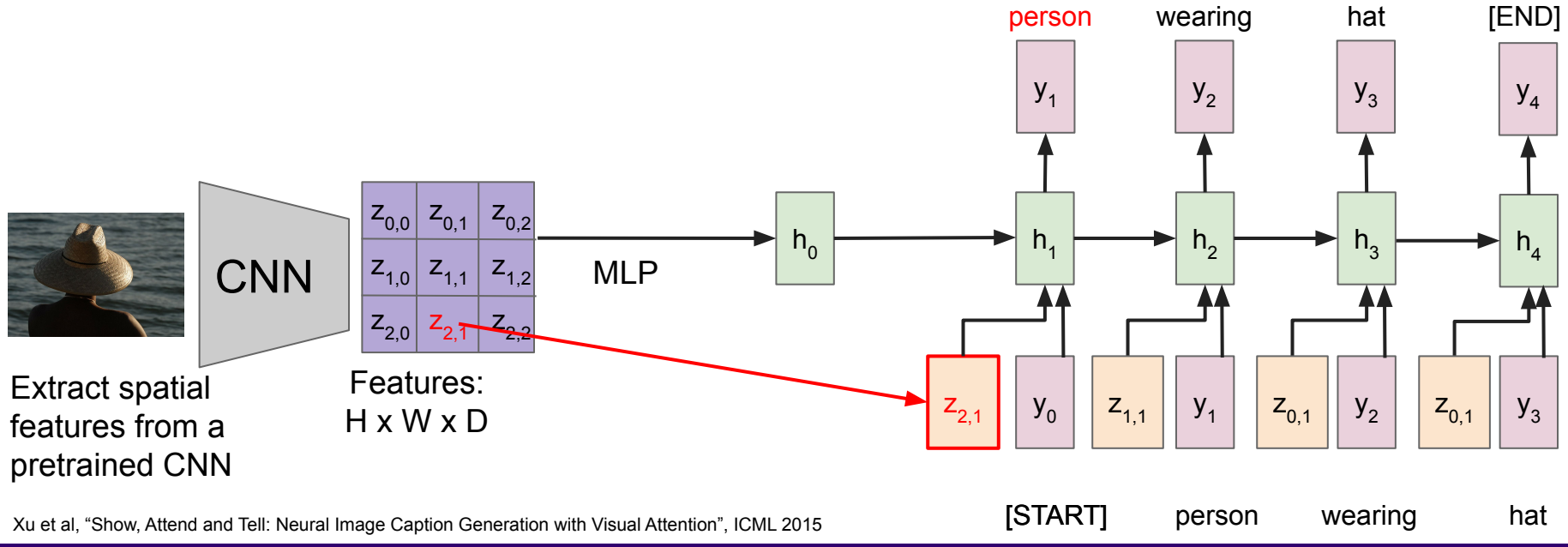


Extract spatial features from a pretrained CNN

Features: H x W x D

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

Ideally what we want is for the model to look at different regions when generating each word



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

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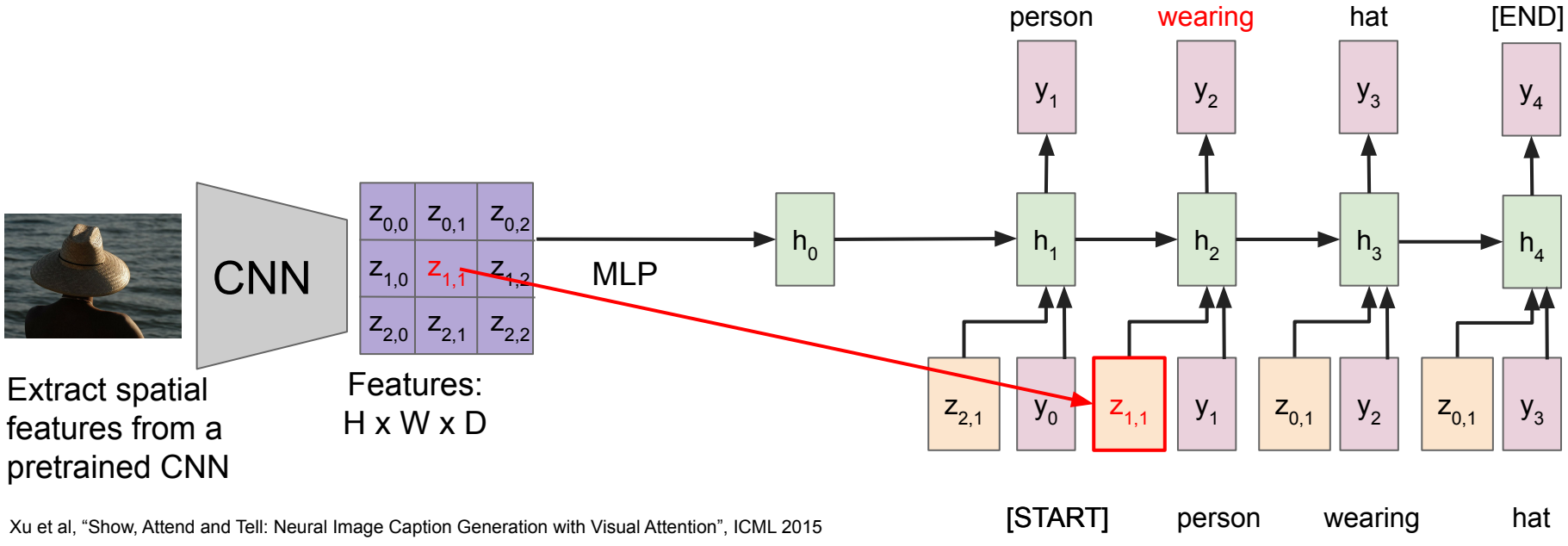
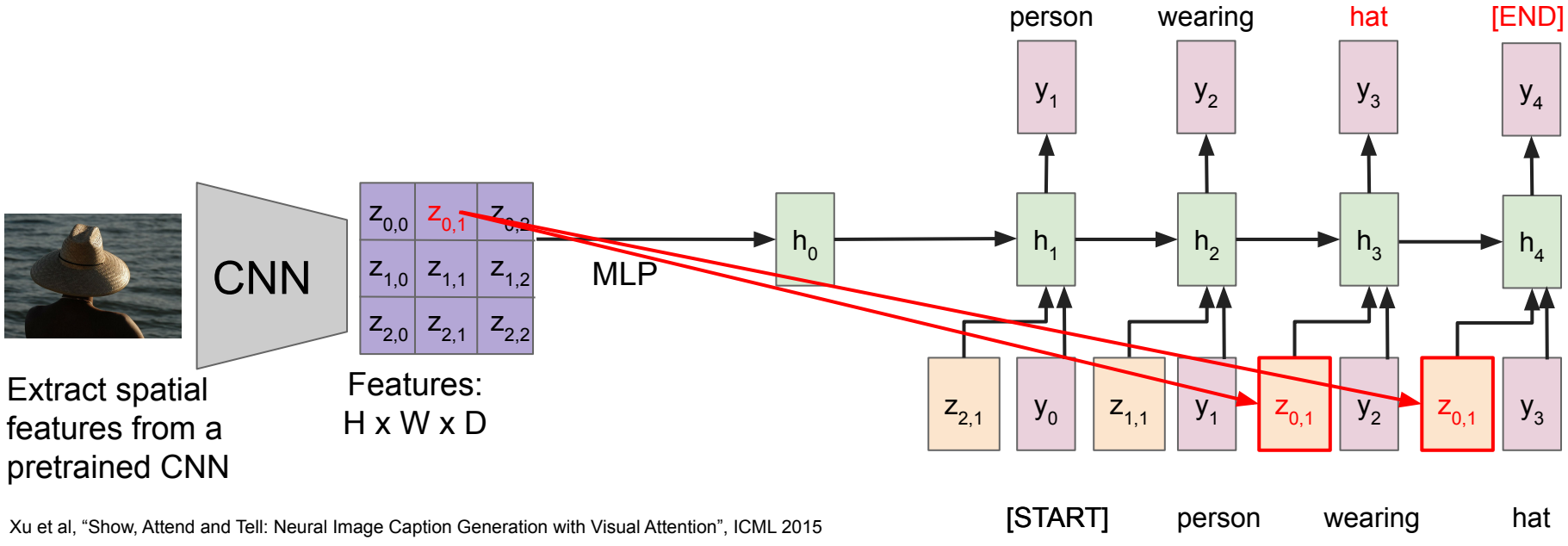


Xu et al, "Show, Attend and Tell: Neural Image Caption Generation with Visual Attention", ICML 2015

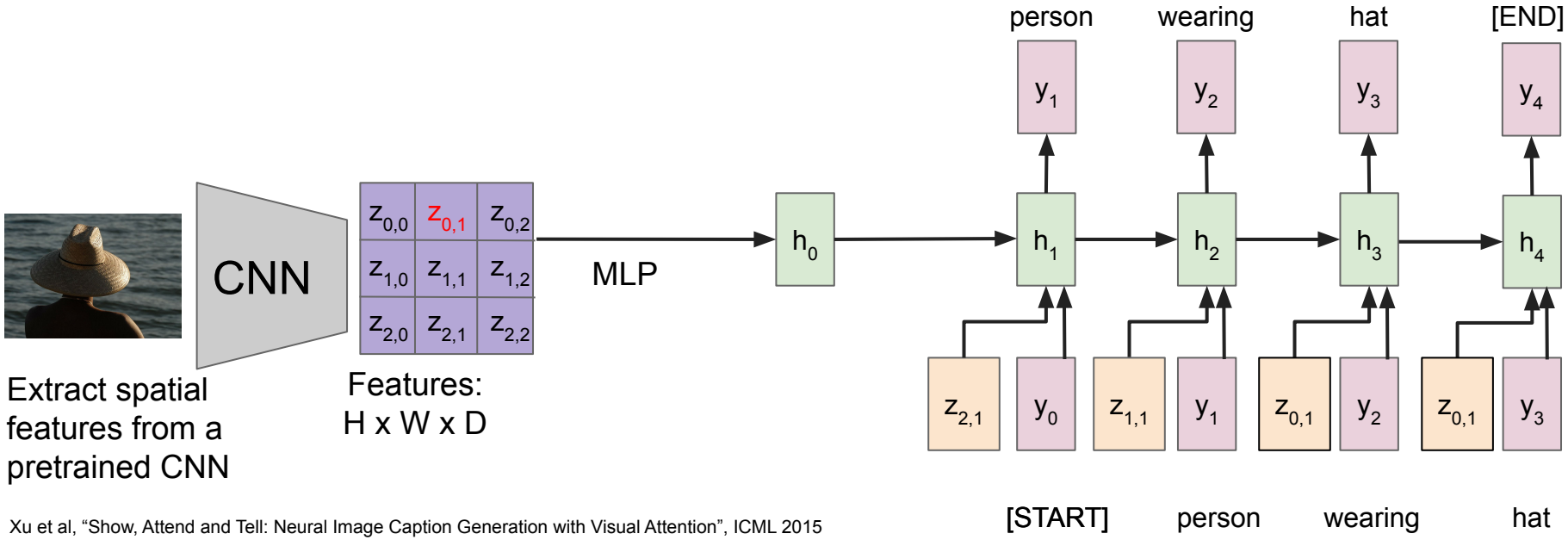
Ideally what we want is for the model to look at different regions when generating each word



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

How do we design a differentiable process that "attends" to different input regions?

Why differentiable? So that we can use backprop!



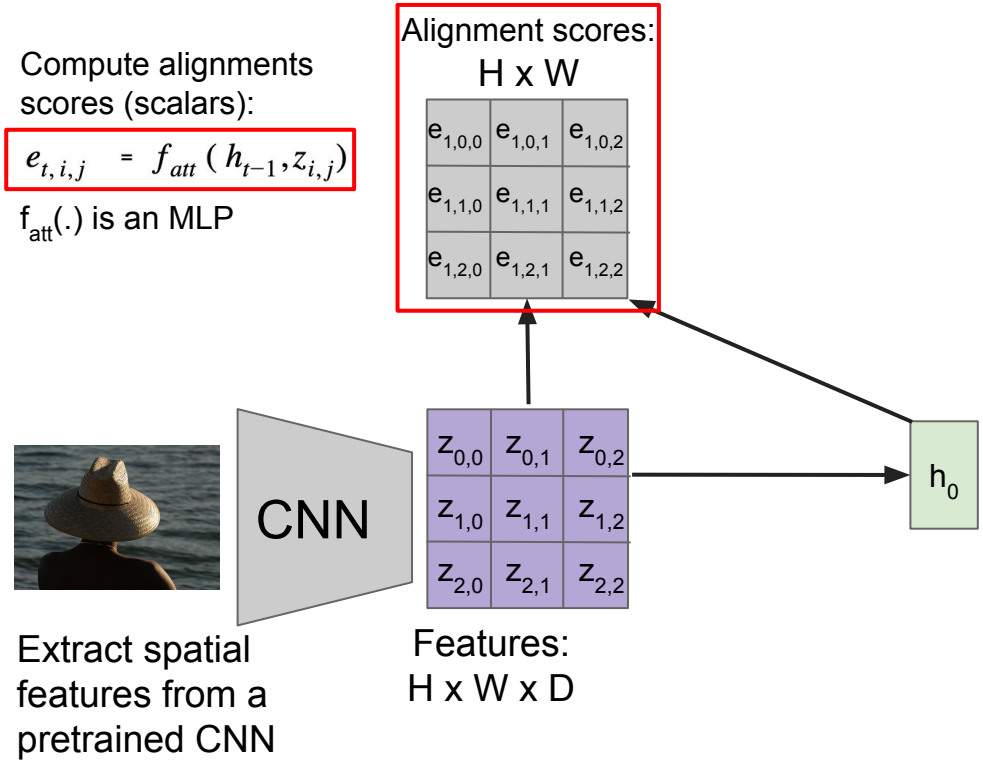
Xu et al, "Show, Attend and Tell: Neural Image Caption Generation with Visual Attention", ICML 2015

Image Captioning with RNNs & Attention

Compute alignments scores (scalars):

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

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



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

Image Captioning with RNNs & Attention

Compute alignments scores (scalars):

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$f_{att}(.)$ 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:

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

$0 < a_{t,i,j} < 1$, 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

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

Image Captioning with RNNs & 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

CNN

Extract spatial features from a pretrained CNN

Features: H x W x D

h_0

c_1

Normalize to get attention weights:

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

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

Compute context vector:

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

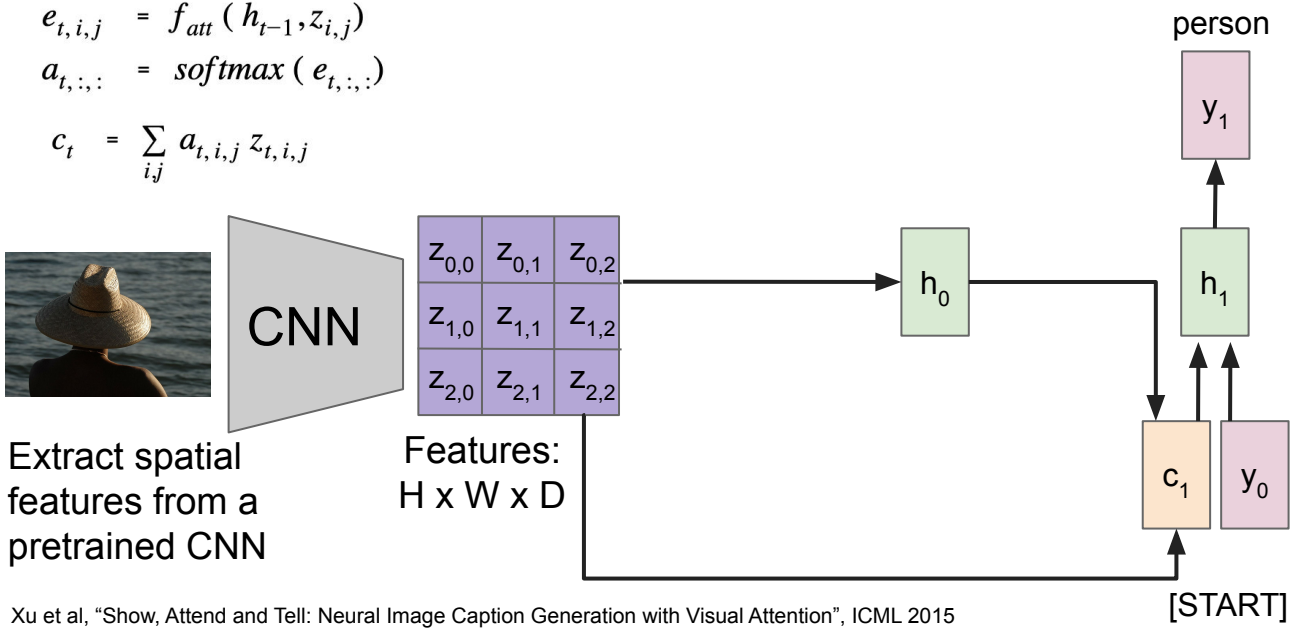
Xu et al, "Show, Attend and Tell: Neural Image Caption Generation with Visual Attention", ICML 2015

Image Captioning with RNNs & 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

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



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

Image Captioning with RNNs & Attention

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

Alignment scores: H x W

Attention: H x W

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

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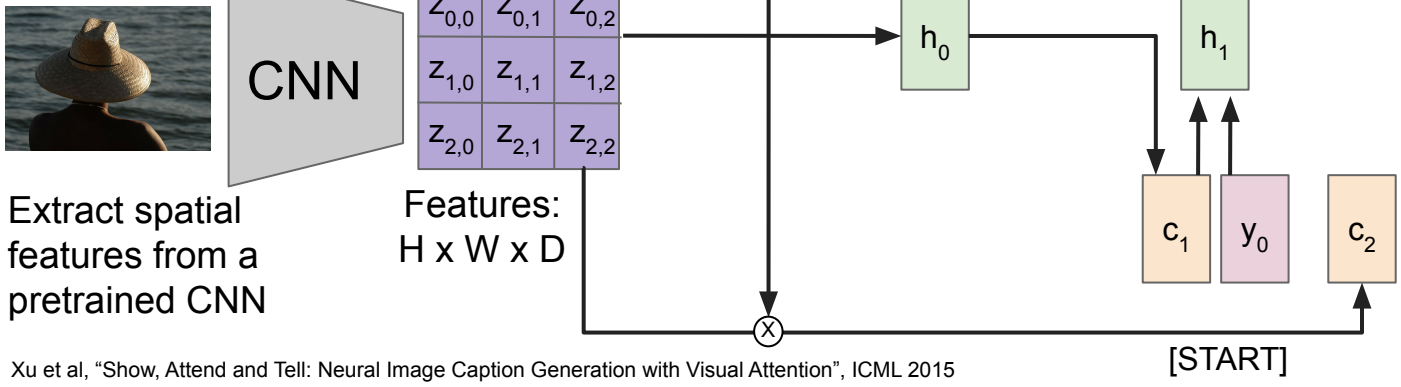
$$c_t = \sum_{i,j} a_{t,i,j} z_{t,i,j}$$



Extract spatial features from a pretrained CNN

Features: H x W x D

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

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

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

y_1 y_2

person wearing

c_1 y_0 c_2 y_1

[START] person

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

Image Captioning with RNNs & 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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$$c_t = \sum_{i,j} a_{t,i,j} z_{t,i,j}$$

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

y_1 y_2 y_3

person wearing hat

c_1 y_0 c_2 y_1 c_3 y_2

[START] person wearing

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

Image Captioning with RNNs & Attention

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

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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

y_1 y_2 y_3 y_4

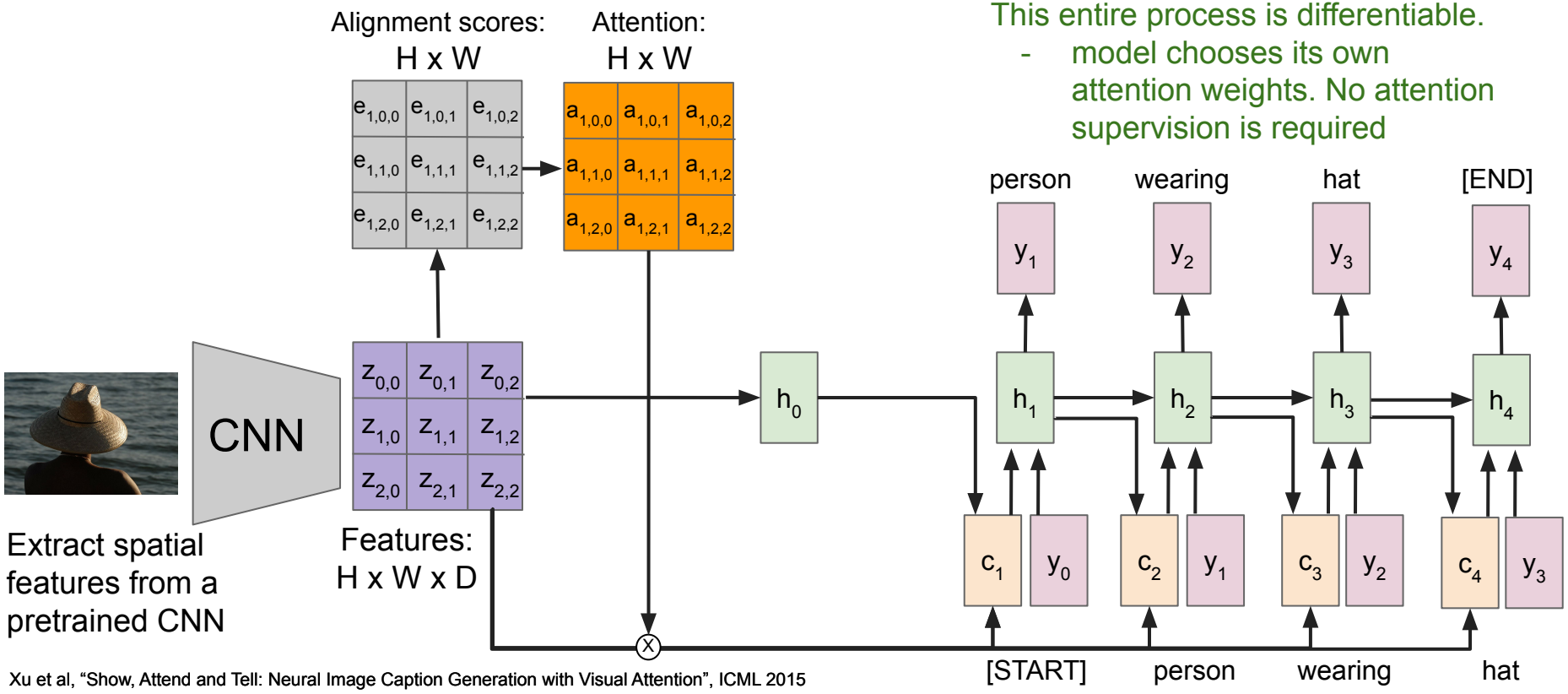
person wearing hat [END]

c_1 y_0 c_2 y_1 c_3 y_2 c_4 y_3

[START] person wearing hat

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

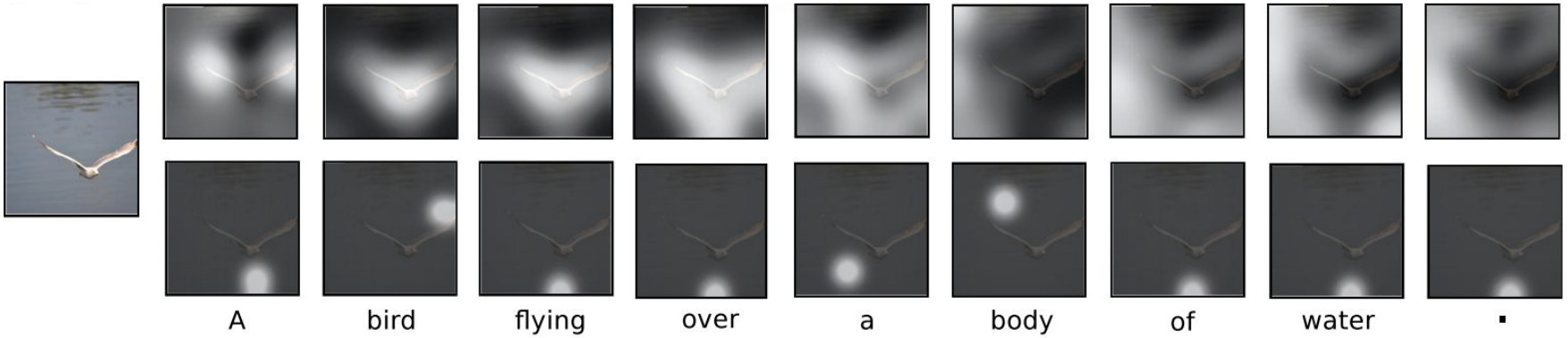
Image Captioning with RNNs & Attention



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

Image Captioning with Attention

Top row: Attention



Bottom row: visualizing the patch with highest attention

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

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.

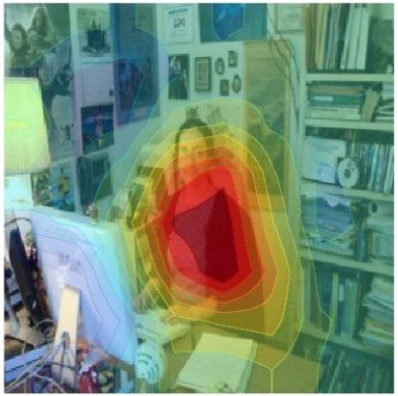
Xu et al, "Show, Attend, and Tell: Neural Image Caption Generation with Visual Attention", ICML 2015

Attention can detect Gender Bias

Wrong

Baseline:
*A **man** sitting at a desk with a laptop computer.*

Right for the Right Reasons

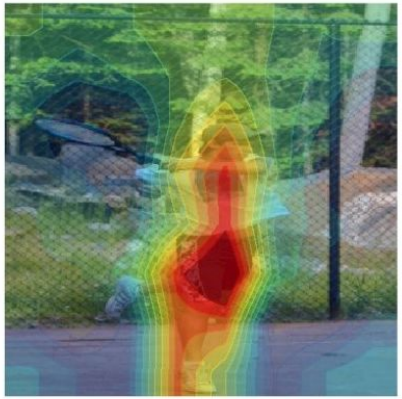


Our Model:
*A **woman** sitting in front of a laptop computer.*

Right for the Wrong Reasons

Baseline:
*A **man** holding a tennis racquet on a tennis court.*

Right for the Right Reasons

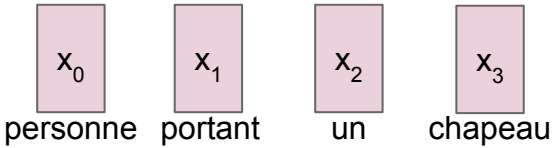


Our Model:
*A **man** holding a tennis racquet on a tennis court.*

Burns et al. "Women also Snowboard: Overcoming Bias in Captioning Models" ECCV 2018

Similar tasks in NLP - Language translation example

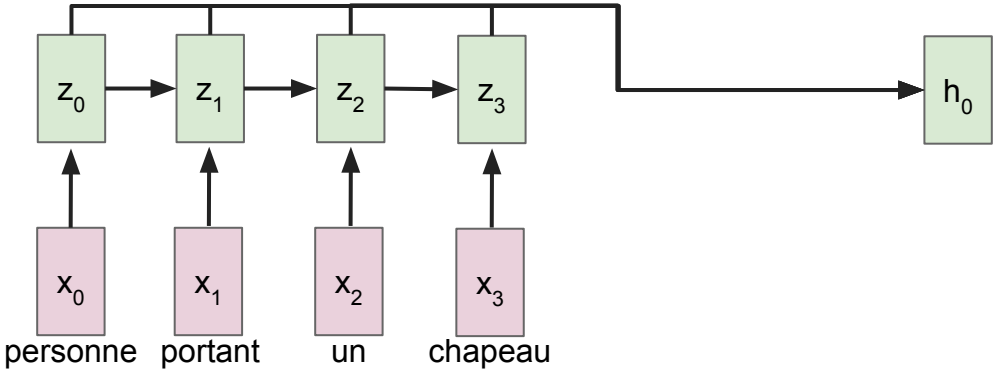
Input: Sequence **x** = $x_1, x_2, \ldots, x_T$
Output: Sequence **y** = $y_1, y_2, \ldots, y_T$



Similar tasks in NLP - Language translation example

Input: Sequence **x** = $x_1, x_2, \ldots, x_T$
Output: Sequence **y** = $y_1, y_2, \ldots, y_T$

Encoder: $h_0 = f_{\mathbf{W}}(\mathbf{z})$
where $z_t = \text{RNN}(x_t, u_{t-1})$
$f_{\mathbf{W}}(.)$ is MLP
u is the hidden RNN state



Similar tasks in NLP - Language translation example

Input: Sequence $\mathbf{x} = x_1, x_2, ..., x_T$
Output: Sequence $\mathbf{y} = y_1, y_2, ..., y_T$

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

Encoder: $h_0 = f_{\mathbf{W}}(\mathbf{z})$
where $z_t = RNN(x_t, u_{t-1})$
$f_{\mathbf{W}}(.)$ is MLP
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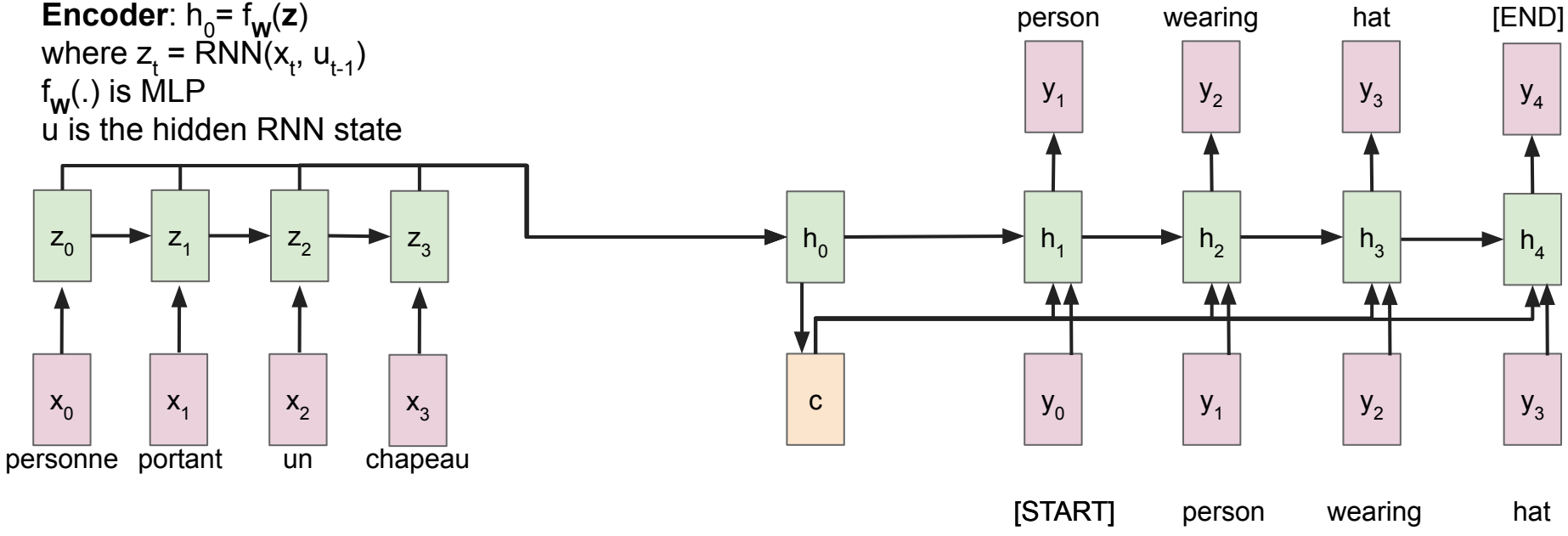
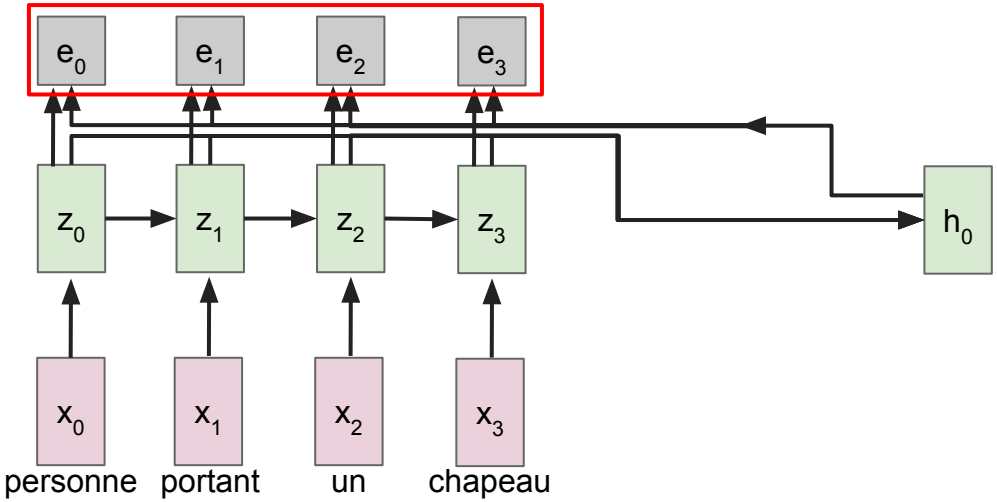


Attention in NLP - Language translation example

Compute alignments scores (scalars):

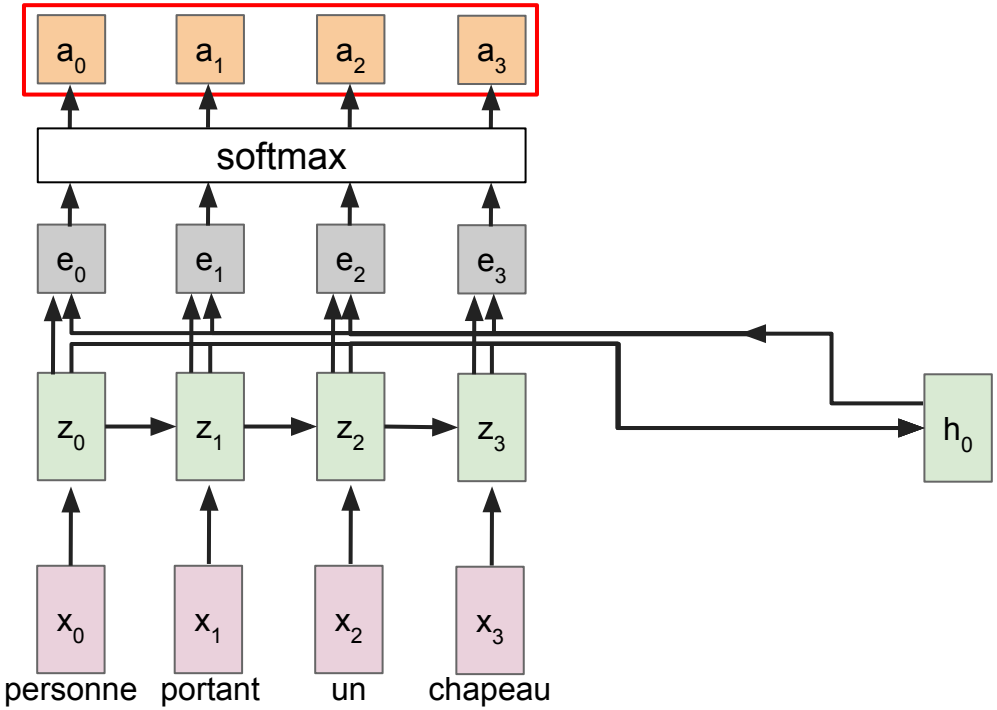
$$e_{t,i} = f_{att}(h_{t-1}, z_i)$$

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



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

Attention in NLP - Language translation example



Compute alignments scores (scalars):

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

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

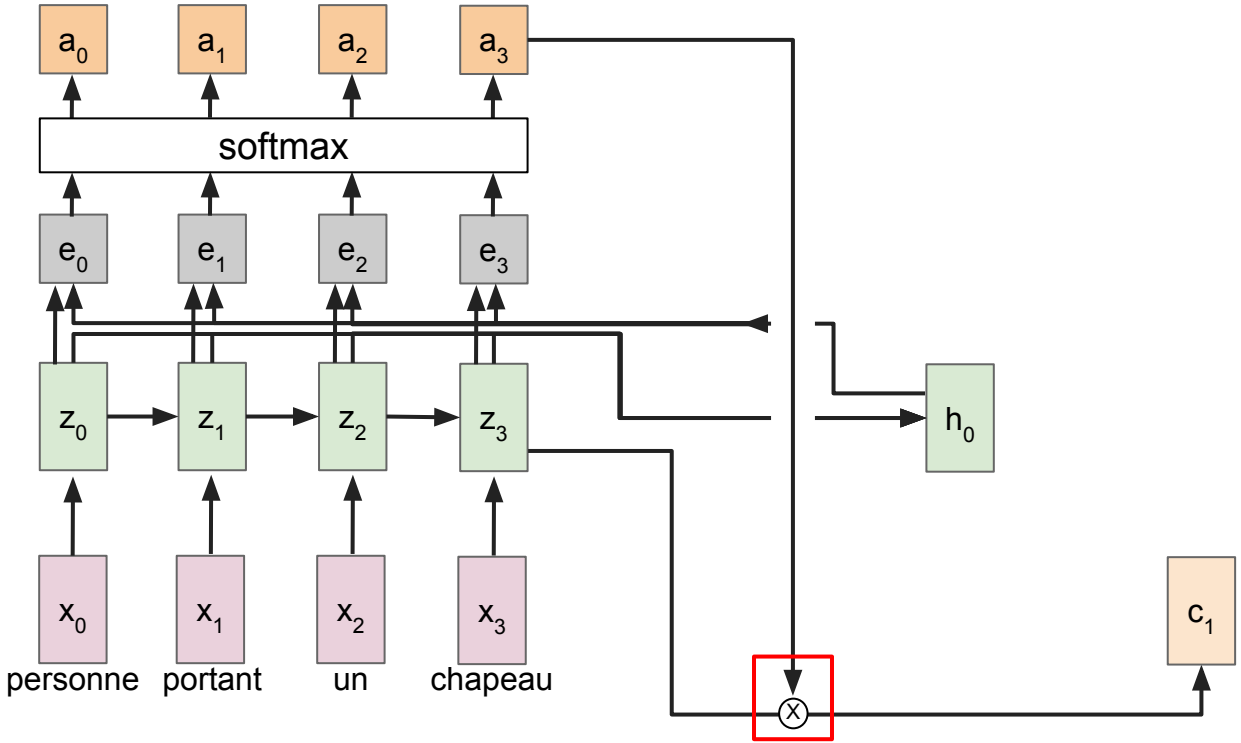
Normalize to get attention weights:

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

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

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

Attention in NLP - Language translation example



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attention values sum to 1

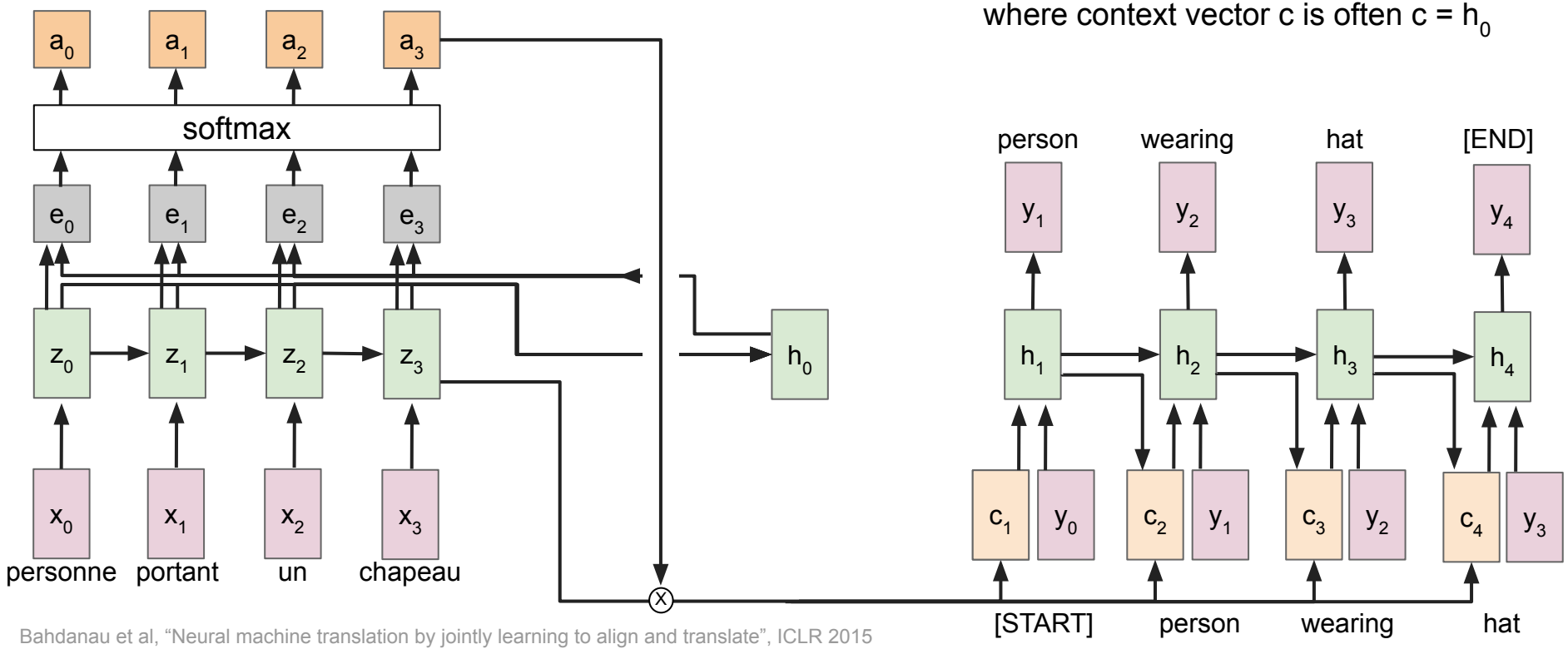
Compute context vector:

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

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

Attention in NLP - Language translation example

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



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

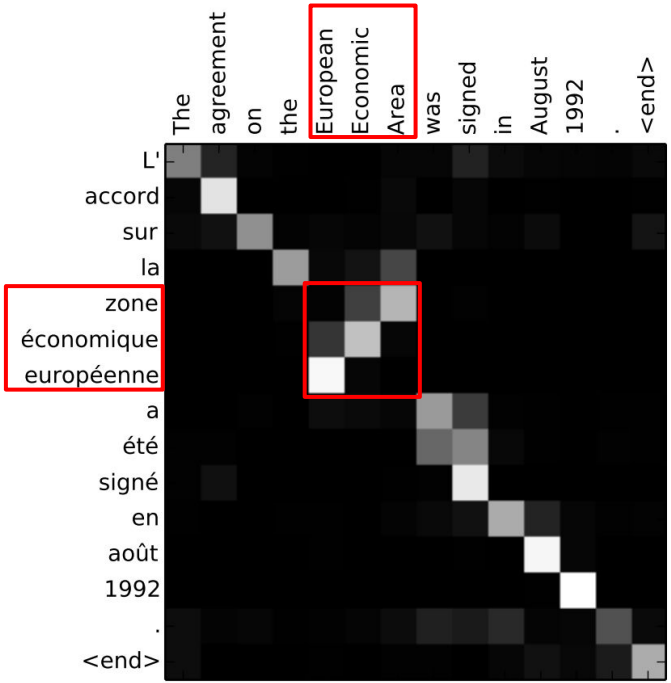
Similar visualization of attention weights

English to French translation example:

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."

Without any attention supervision, model learns different word orderings for different languages

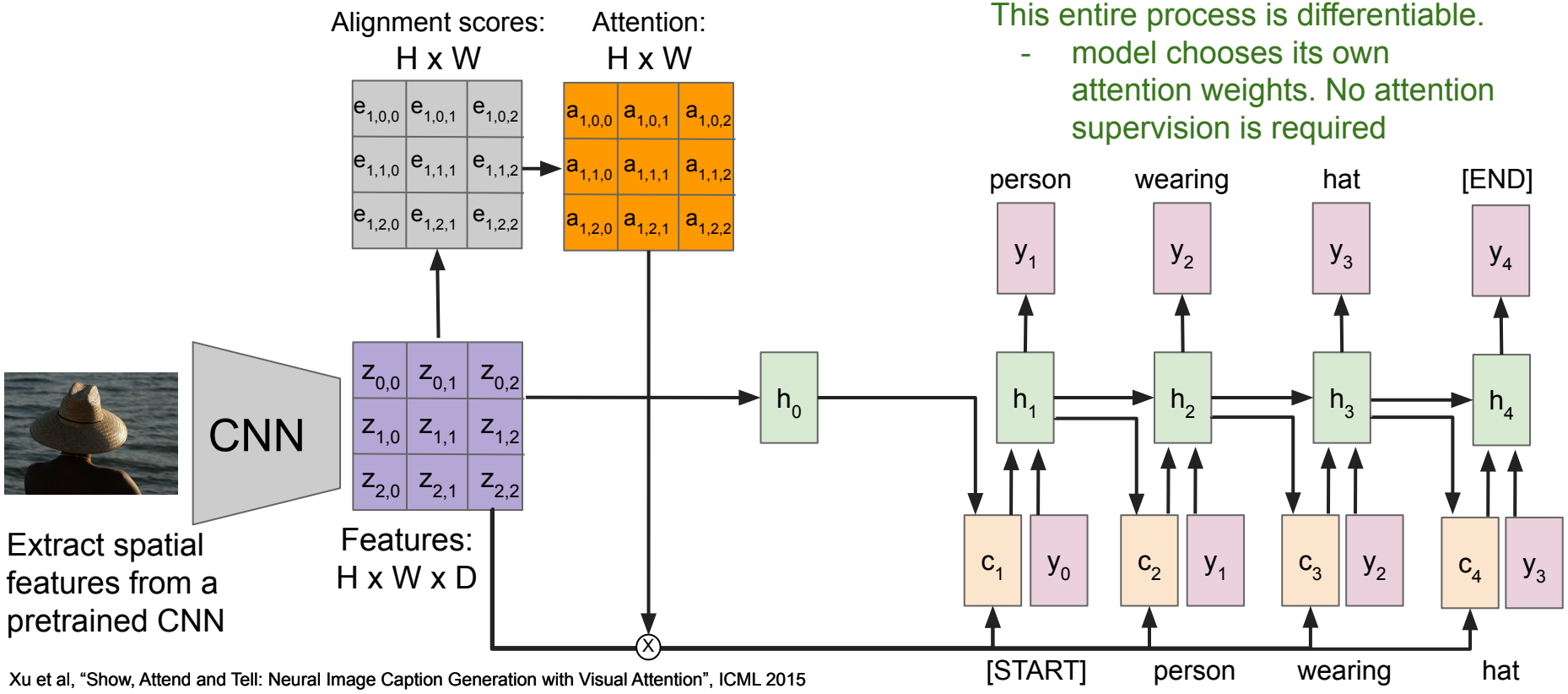


Bahdanau et al, "Neural machine translation by jointly learning to align and translate", ICLR 2015

Today's Agenda:

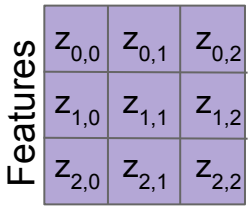
- **Attention with RNNs**
  - In Computer Vision
  - In NLP
- **General Attention Layer**
  - Self-attention
  - Positional encoding
  - Masked attention
  - Multi-head attention
- **Transformers**

Image Captioning with RNNs & Attention



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

Attention we just saw in image captioning

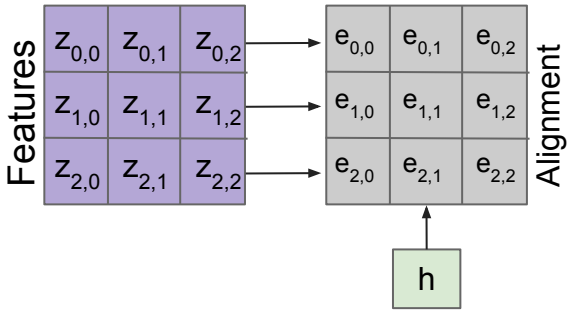


h

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

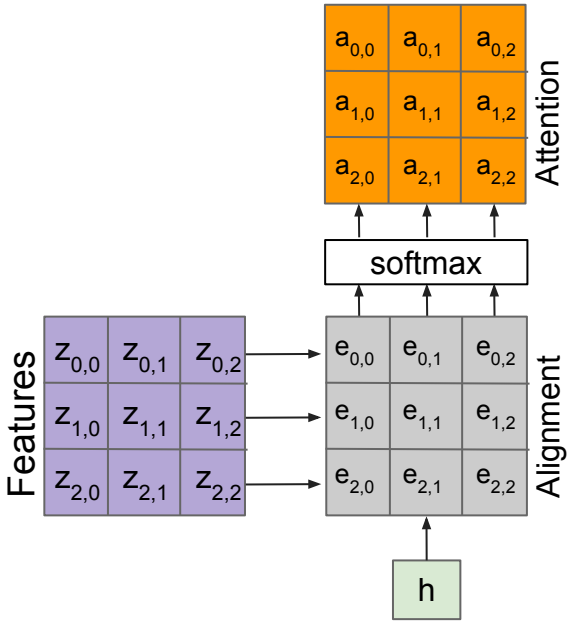
Attention we just saw in image captioning

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



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

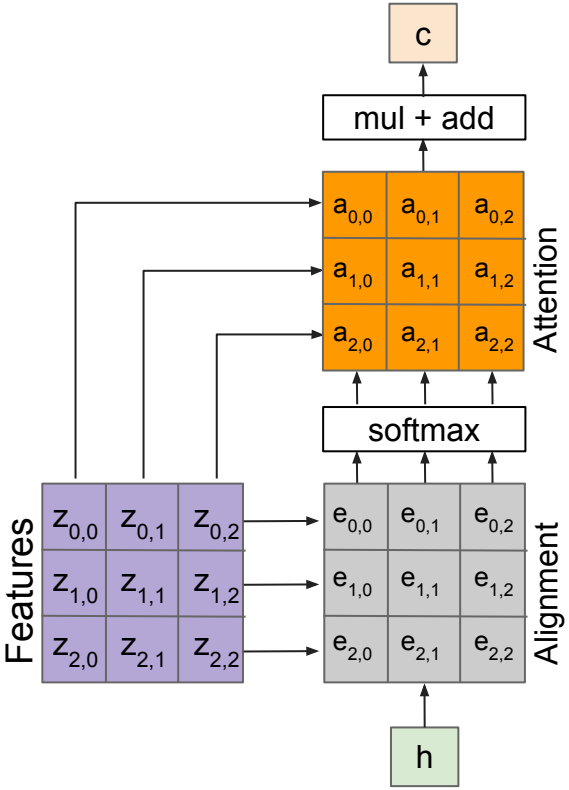
Attention we just saw in image captioning



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

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

Attention we just saw in image captioning

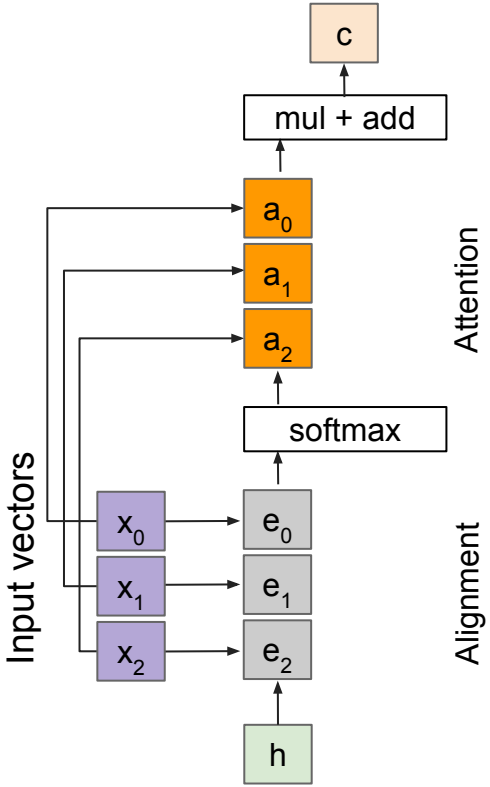


Outputs:
context vector: **c** (shape: D)

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

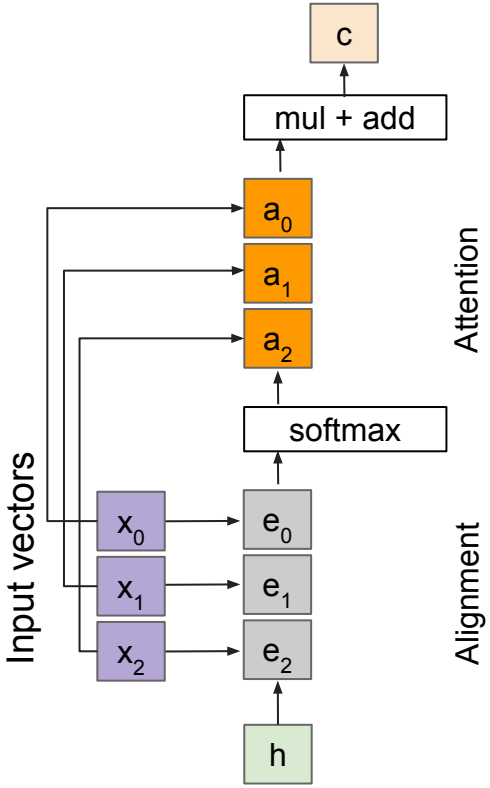
Operations:
Alignment: $e_i = f_{att}(h, x_i)$
Attention: **a** = softmax(**e**)
Output: $\mathbf{c} = \sum_i a_i x_i$

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)

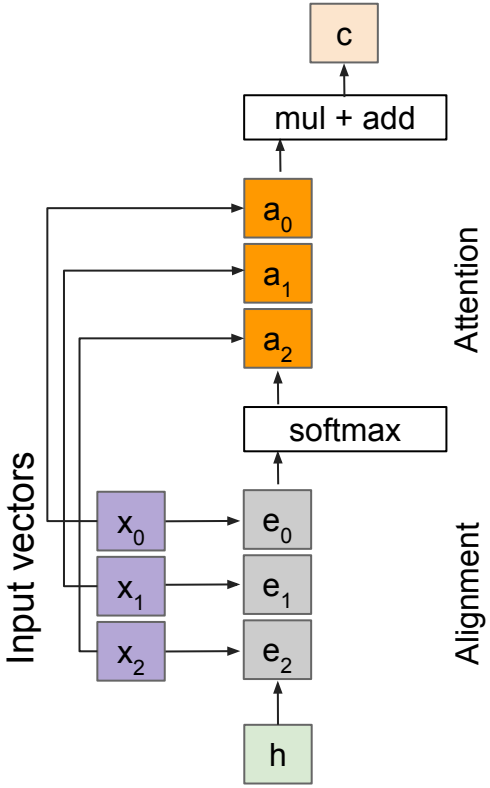
Operations:
Alignment: $e_i = h \cdot x_i$
Attention: **a** = softmax(**e**)
Output: **c** = $\sum_i a_i x_i$

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)

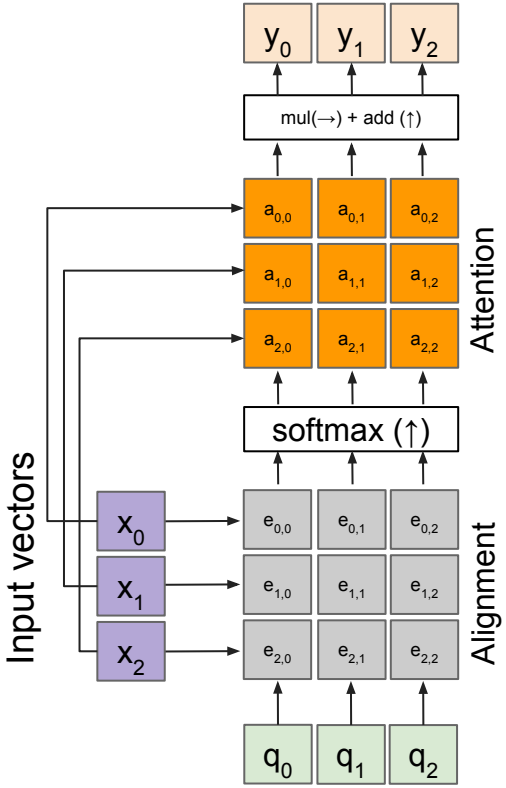
Operations:
Alignment: $e_i = h \cdot x_i / \sqrt{D}$
Attention: **a** = softmax(**e**)
Output: $\mathbf{c} = \sum_i a_i x_i$

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

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

- High dimensionality means more terms in the dot product sum.
- Large magnitude vectors will cause softmax to peak and assign very little weight to all others
- Dividing by $\sqrt{D}$ will reduce effect of large magnitude vectors

General attention layer



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

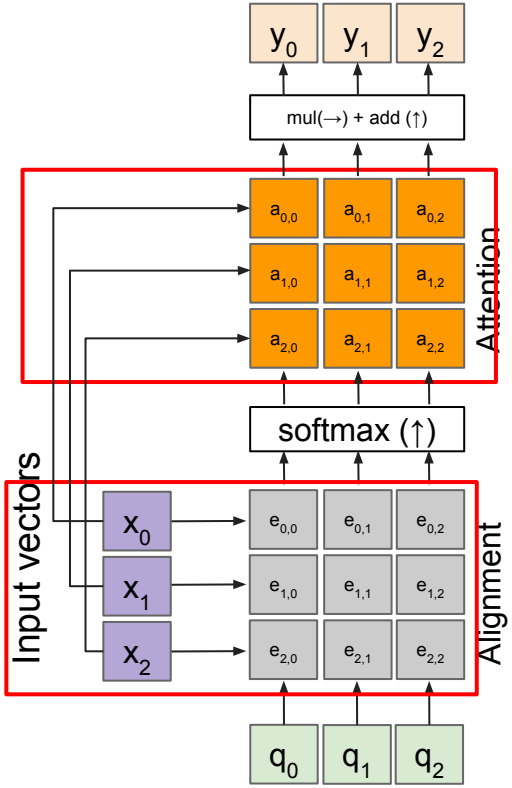
Multiple query vectors
- each query creates a new output context vector

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: M x D)

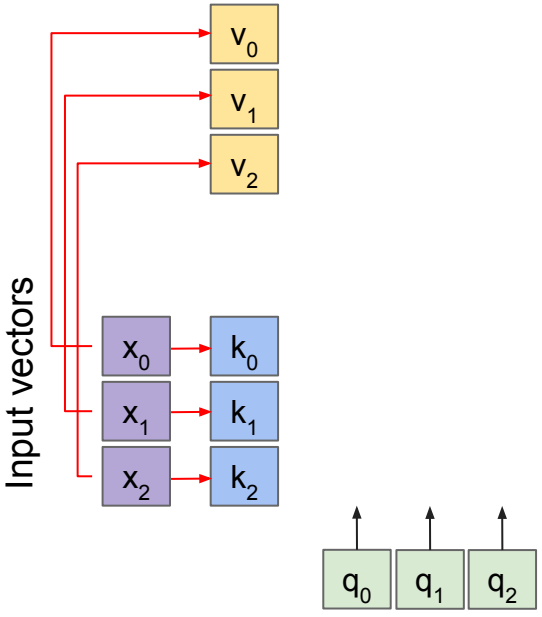
Operations:
Alignment: $e_{i,j} = q_j \cdot x_i / \sqrt{D}$
Attention: **a** = softmax(**e**)
Output: $y_j = \sum_i a_{i,j} x_i$

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

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



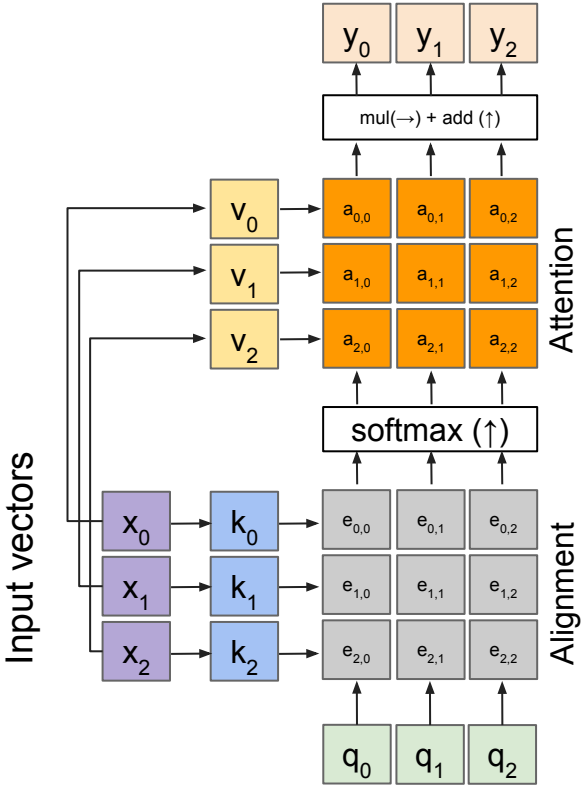
Operations:
Key vectors: $k = xW_k$
Value vectors: $v = xW_v$

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

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: M x 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)

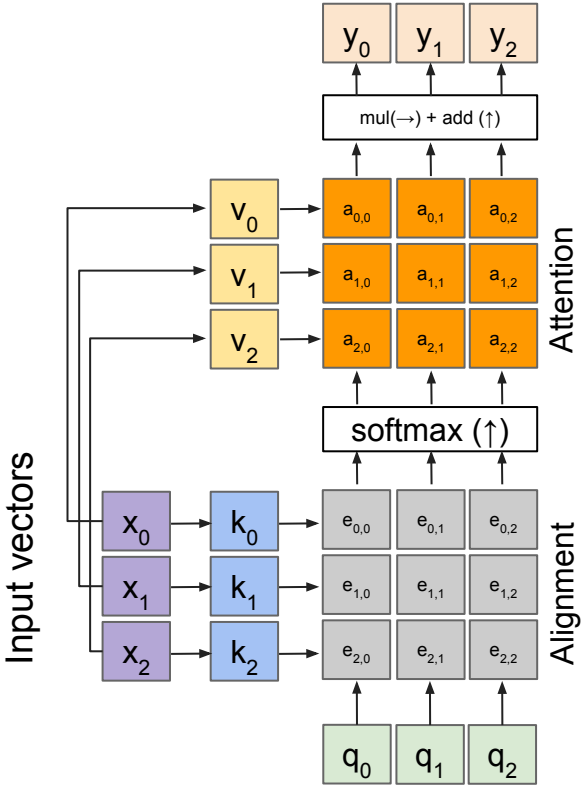
The input and output dimensions can now change depending on the key and value FC layers

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.

Deriving self-attention from this general attention layer

General attention layer



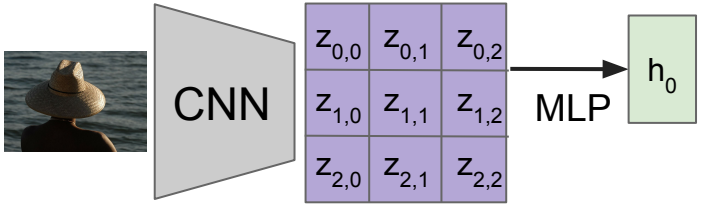
Outputs:
context vectors: **y** (shape: D_v)

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

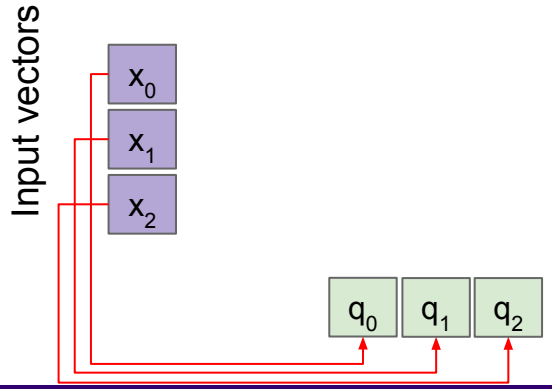
Inputs:
Input vectors: **x** (shape: N x D)
Queries: **q** (shape: M x D_k)

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: $\mathbf{k} = \mathbf{x}W_k$
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: $y_j = \sum_i a_{i,j} v_i$

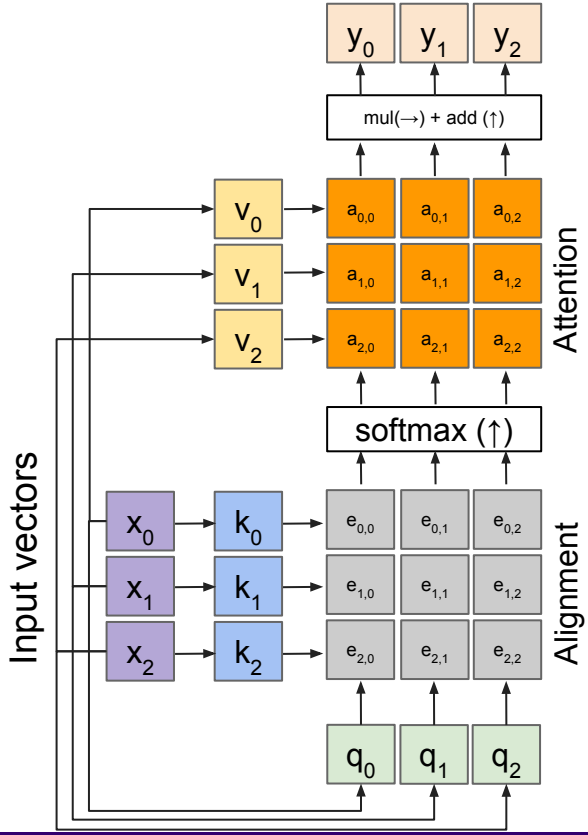
We can calculate the query vectors from the input vectors, therefore, defining a "self-attention" layer.

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

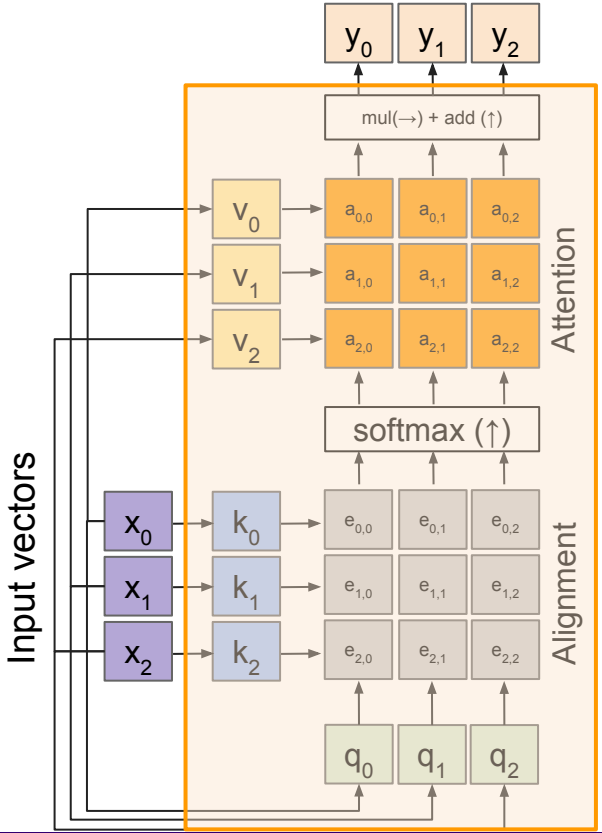


Outputs:
context vectors: **y** (shape: D_v)

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)

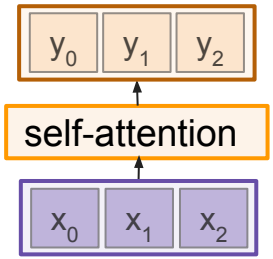
Self attention layer - attends over sets of inputs



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

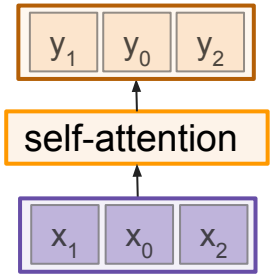
Inputs:
Input vectors: **x** (shape: N x D)

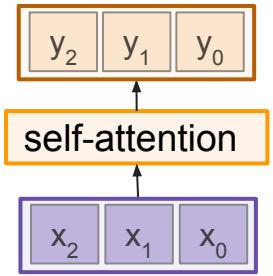


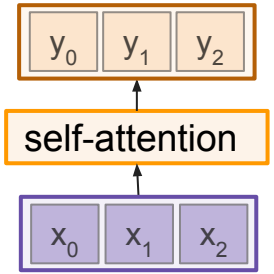
Self attention layer - attends over sets of inputs

Permutation invariant

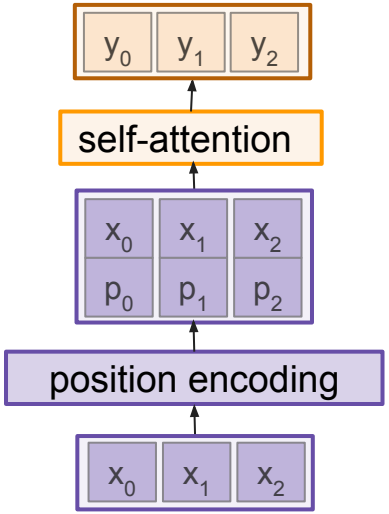
Problem: how can we encode ordered sequences like language or spatially ordered image features?







Positional encoding



Concatenate special positional encoding p_j to each input vector x_j

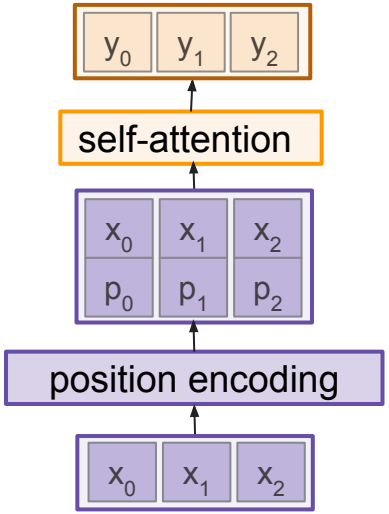
We use a function *pos*: $N \rightarrow R^d$
to process the position j of the vector into a d-dimensional vector

So, $p_j = pos(j)$

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_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.

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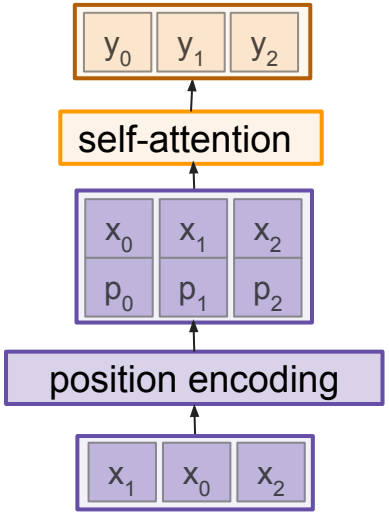
Vaswani et al, "Attention is all you need", NeurIPS 2017

Positional encoding



Concatenate special positional encoding p_j to each input vector x_j

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Options for *pos*(.)

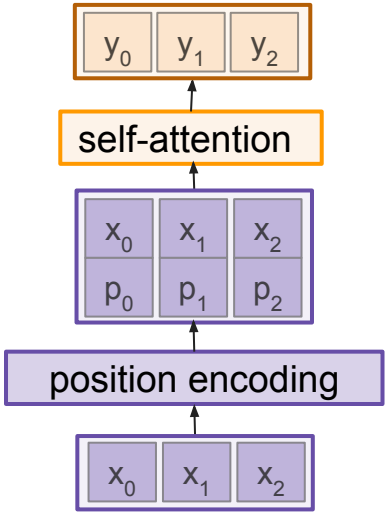
1. Learn a lookup table:
   - Learn parameters to use for *pos*(t) for t ε [0, T)
   - Lookup table contains T x d parameters.

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

We use a function *pos*: N $\rightarrow R^d$
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Intuition:

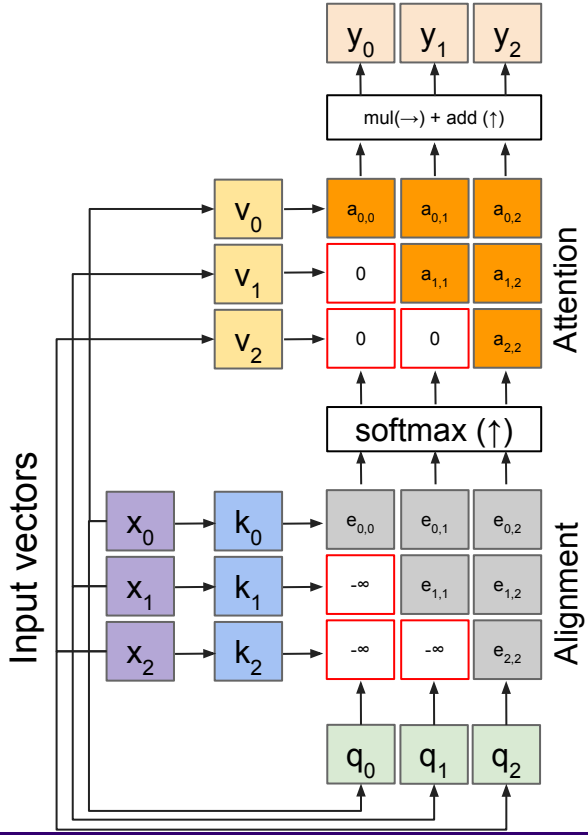
0 :	0	0	0	0	8 :	1	0	0	0
1 :	0	0	0	1	9 :	1	0	0	1
2 :	0	0	1	0	10 :	1	0	1	0
3 :	0	0	1	1	11 :	1	0	1	1
4 :	0	1	0	0	12 :	1	1	0	0
5 :	0	1	0	1	13 :	1	1	0	1
6 :	0	1	1	0	14 :	1	1	1	0
7 :	0	1	1	1	15 :	1	1	1	1

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

image source

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

Causal attention layer



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

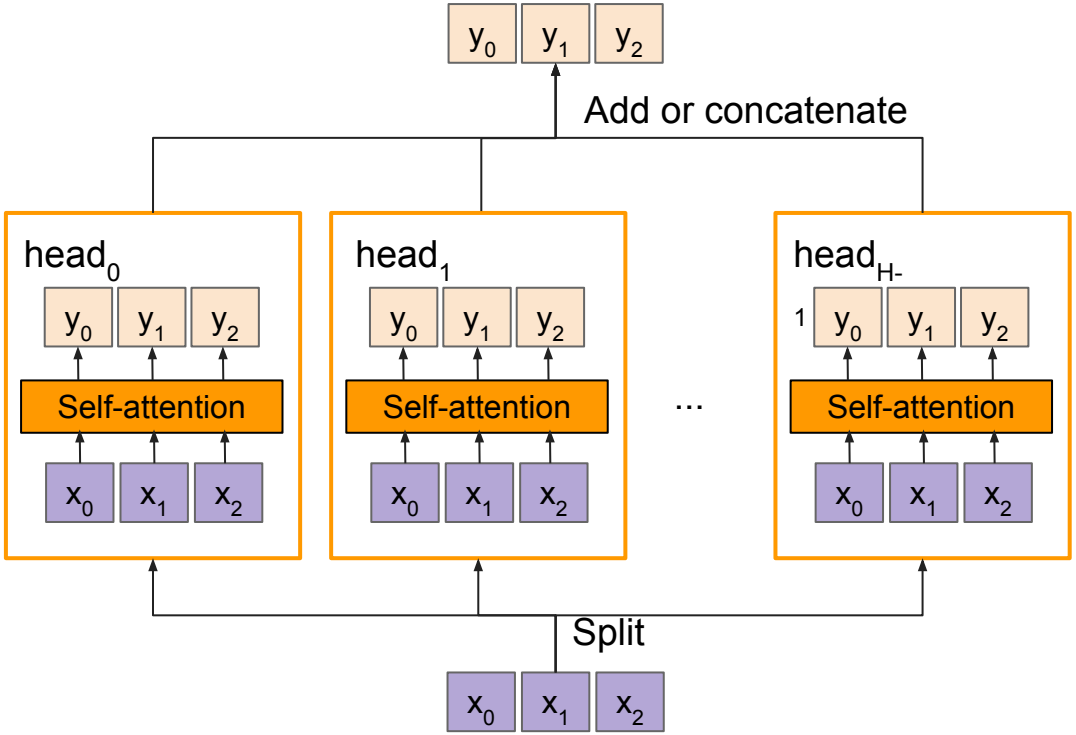
Operations:
Key vectors: $\mathbf{k} = \mathbf{x}W_k$
Value vectors: $\mathbf{v} = \mathbf{x}W_v$
Query vectors: $\mathbf{q} = \mathbf{x}W_q$
Alignment: $e_{i,j} = q_j \cdot k_i / \sqrt{D}$
Attention: $\mathbf{a} = \text{softmax}(\mathbf{e})$
Output: $y_j = \sum_i a_{i,j} v_i$

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

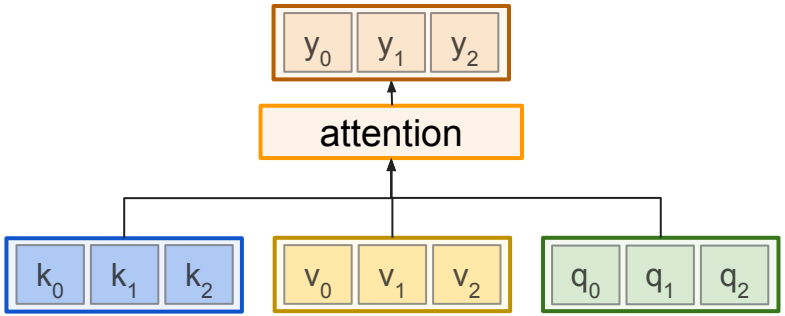
- Prevent vectors from looking at future vectors.
- Manually set alignment scores to -infinity

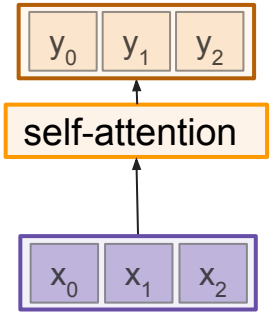
Multi-head self-attention layer

- Multiple self-attention heads in parallel

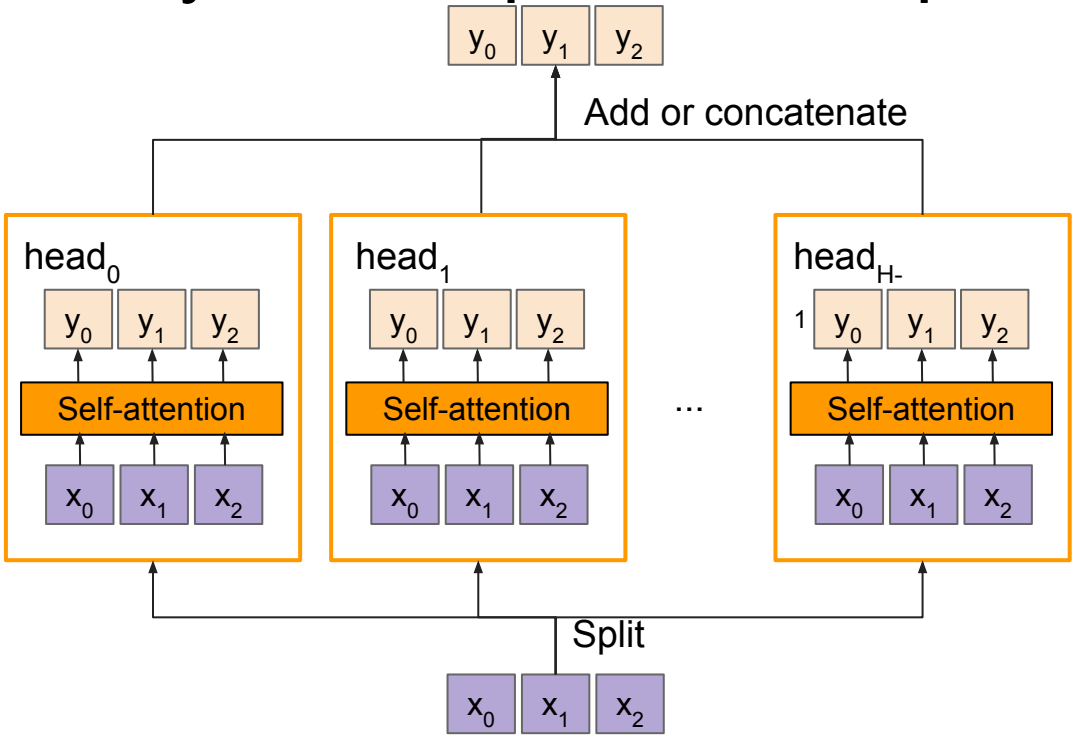


General attention versus self-attention





Attention layers can process sequential inputs



Self-attention layers are masked

Comparing RNNs to masked multi-headed attention

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.

Masked multi-headed attention:

(+) 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.

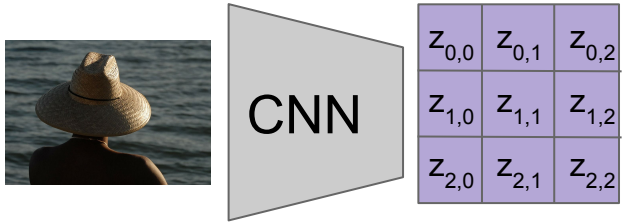
(-) Requires a lot of memory: N x M alignment and attention scalers need to be calculated and stored for a single self-attention head. (but GPUs are getting bigger and better)

Today's Agenda:

- **Attention with RNNs**
  - In Computer Vision
  - In NLP
- **General Attention Layer**
  - Self-attention
  - Positional encoding
  - Masked attention
  - Multi-head attention
- **Transformers**

Image Captioning using transformers

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



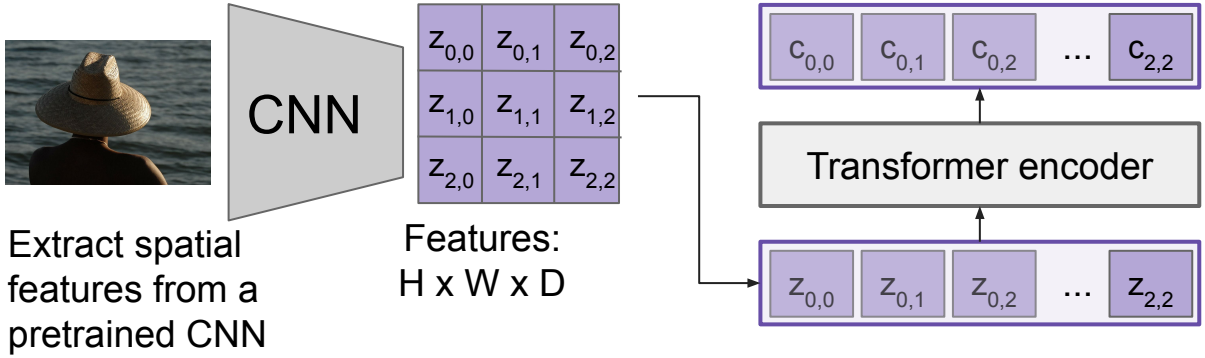
Extract spatial features from a pretrained CNN

Features: H x W x D

Image Captioning using transformers

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

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



Extract spatial features from a pretrained CNN

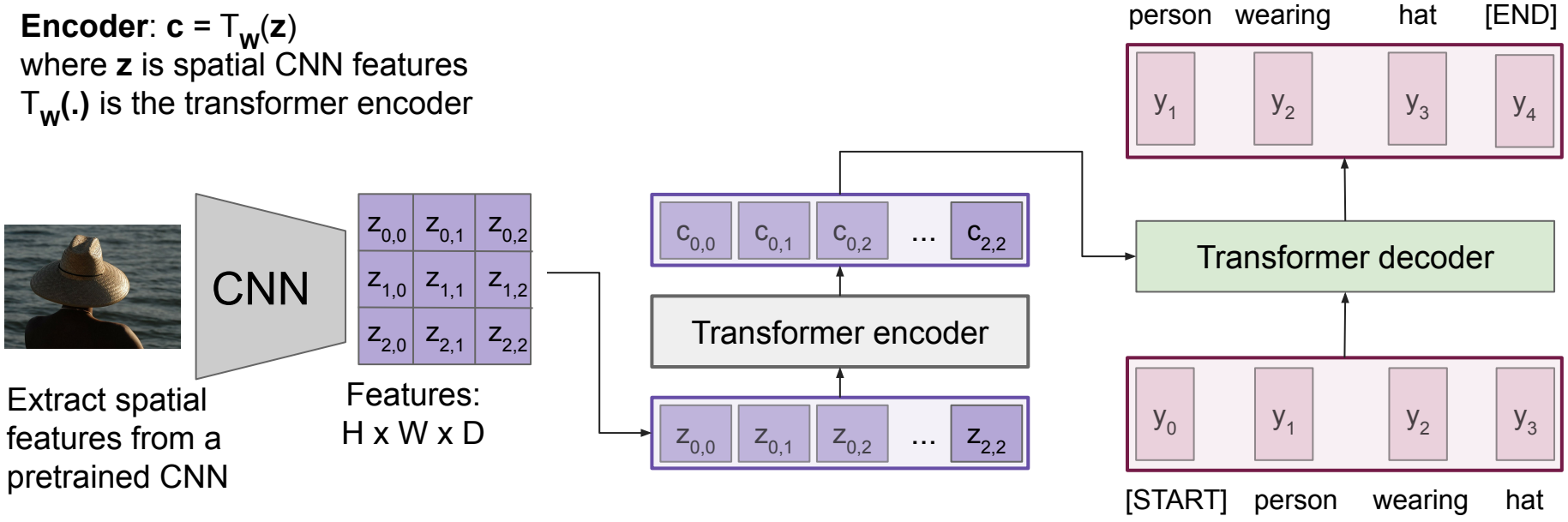
Features: H x W x D

Image Captioning using transformers

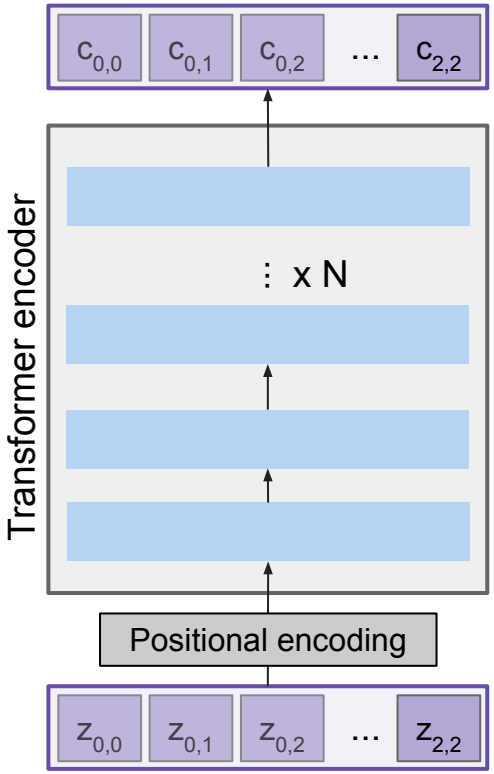
Input: Image **I**
Output: Sequence **y** = $y_1, y_2, ..., y_T$

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

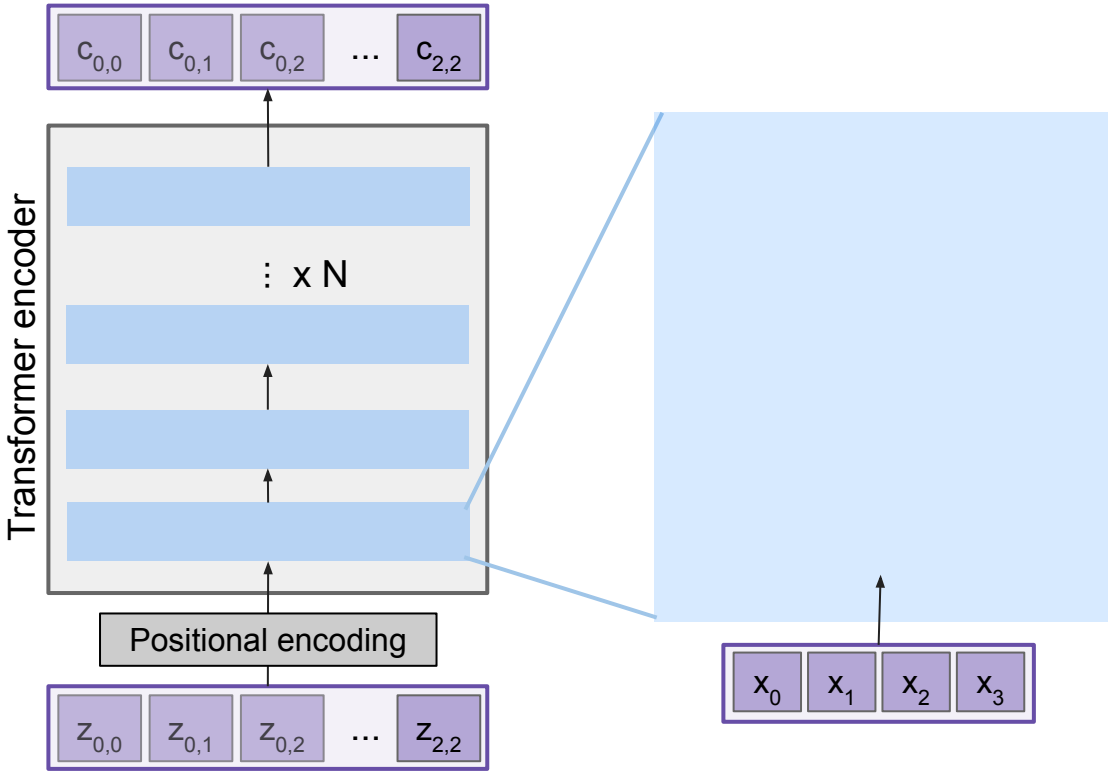


Made up of N encoder blocks.

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

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

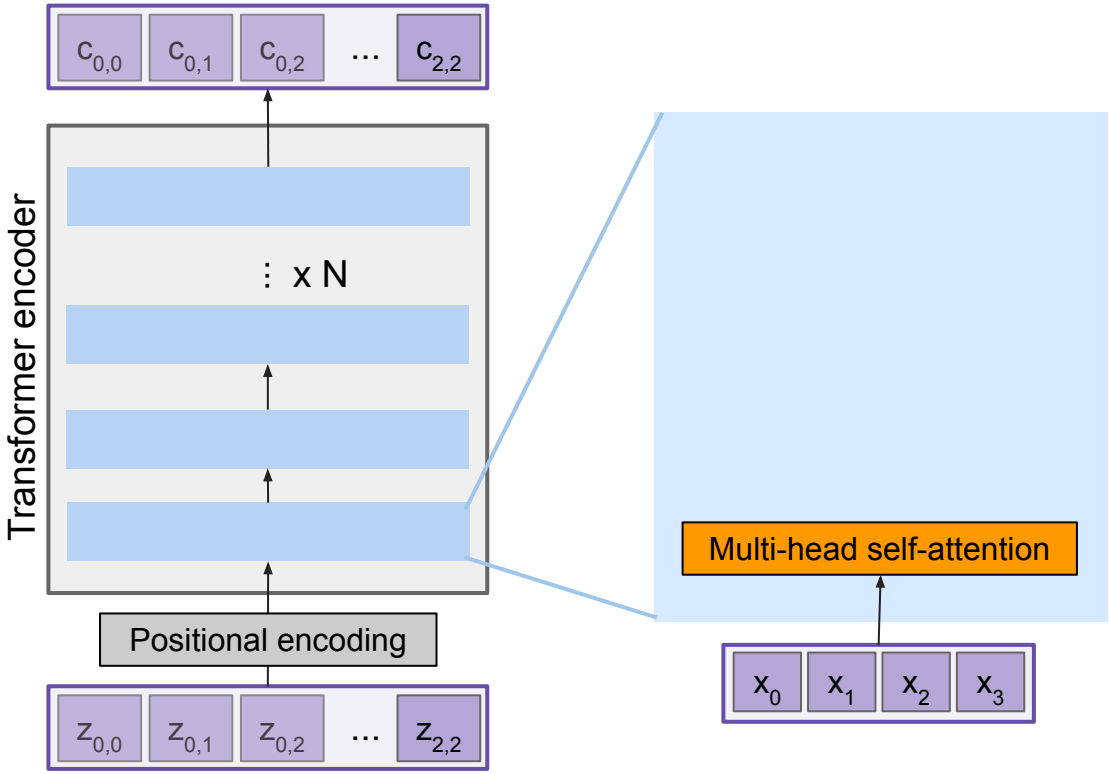
The Transformer encoder block



Let's dive into one encoder block

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

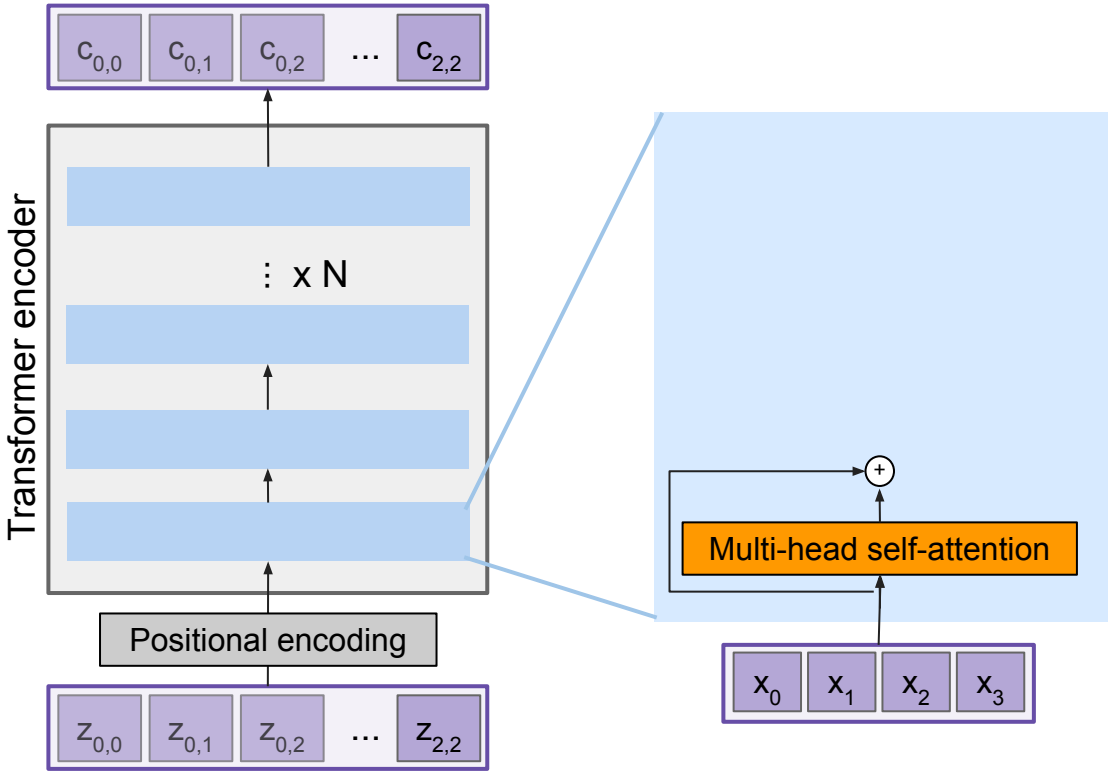
The Transformer encoder block



Attention attends over all the vectors

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

The Transformer encoder block

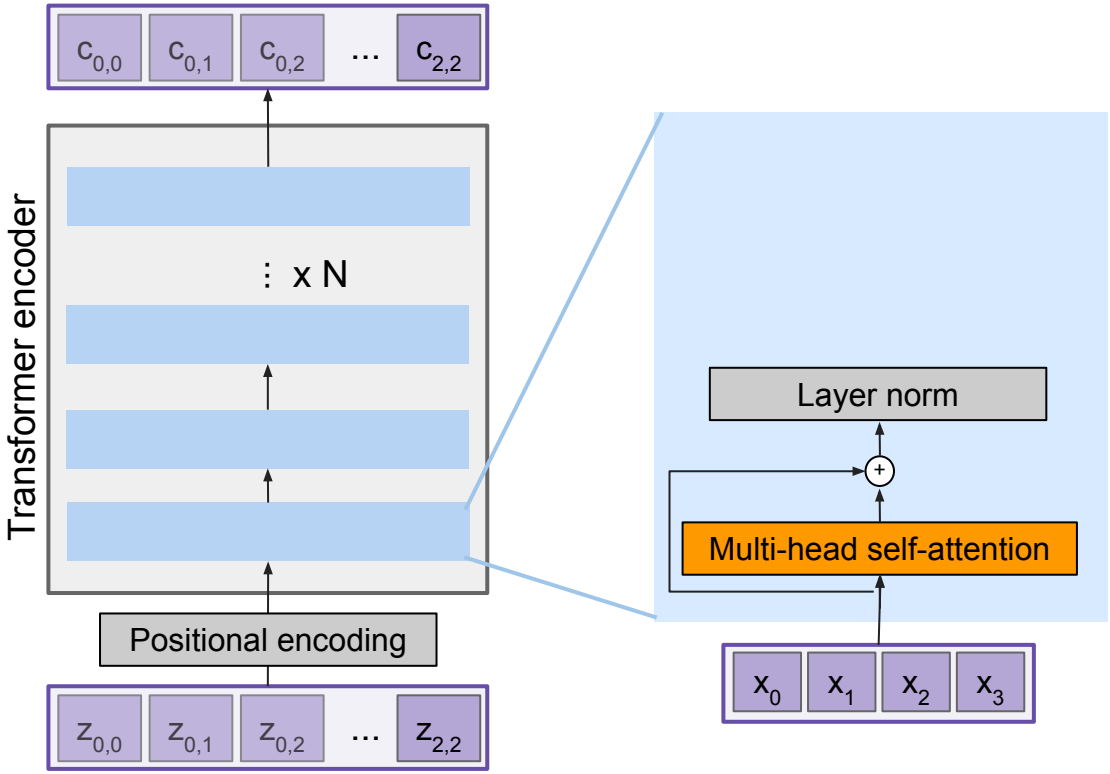


Residual connection

Attention attends over all the vectors

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

The Transformer encoder block



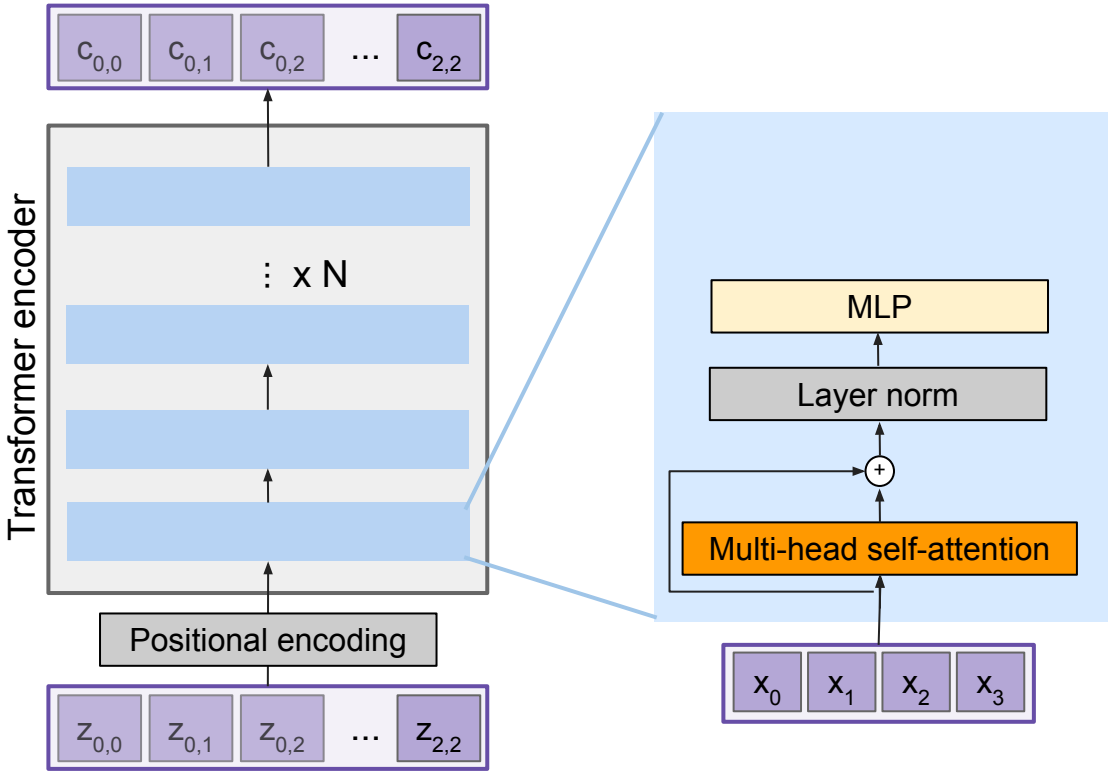
LayerNorm over each vector individually

Residual connection

Attention attends over all the vectors

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

The Transformer encoder block



MLP (2 layers with GeLU) over each vector individually

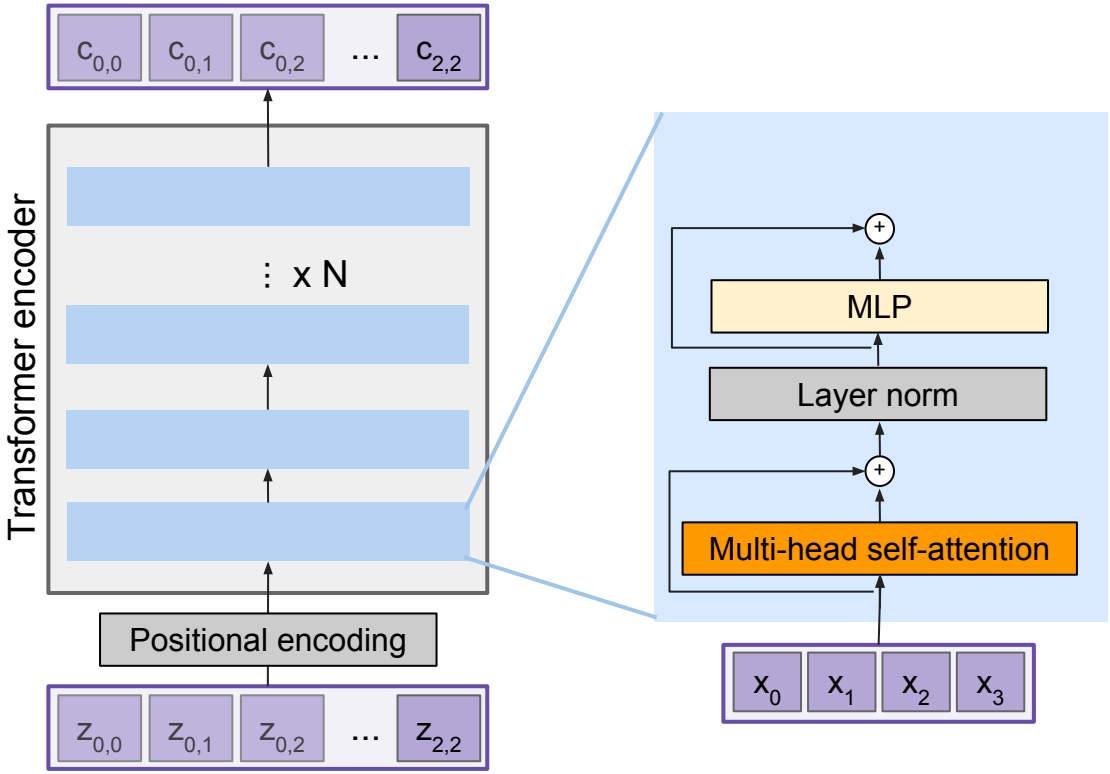
LayerNorm over each vector individually

Residual connection

Attention attends over all the vectors

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

The Transformer encoder block



Residual connection

MLP (2 layers with GeLU) over each vector individually

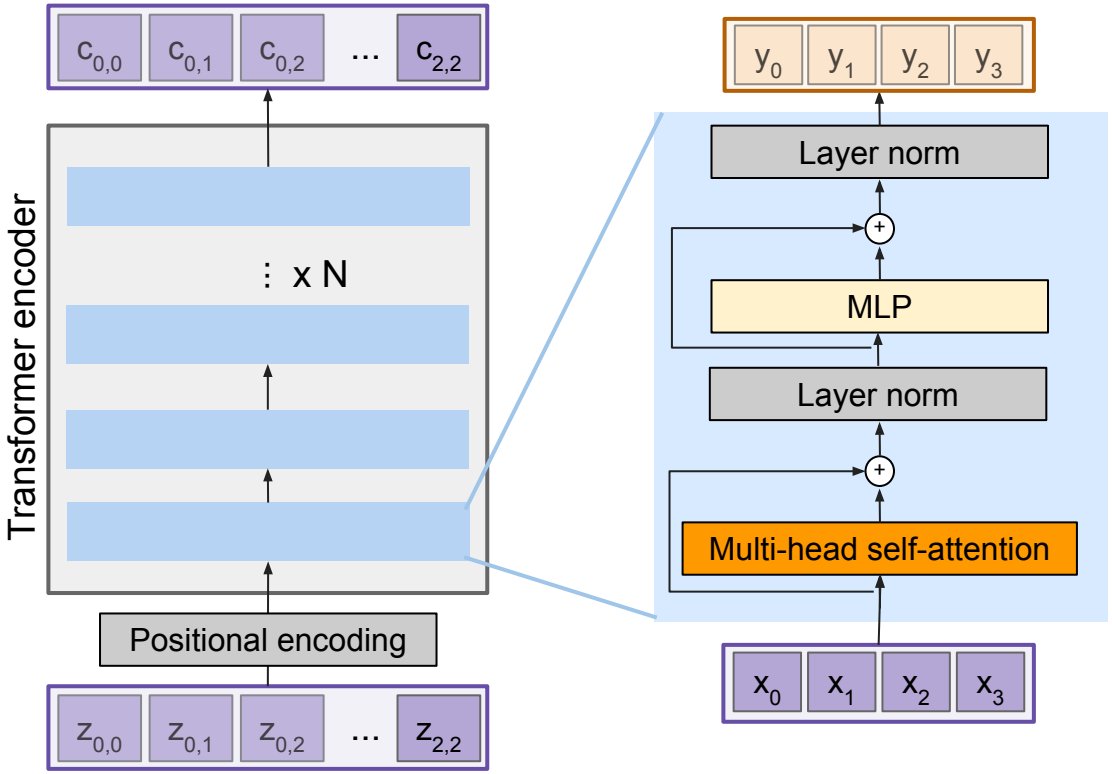
LayerNorm over each vector individually

Residual connection

Attention attends over all the vectors

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

The Transformer encoder block



Transformer Encoder Block:

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

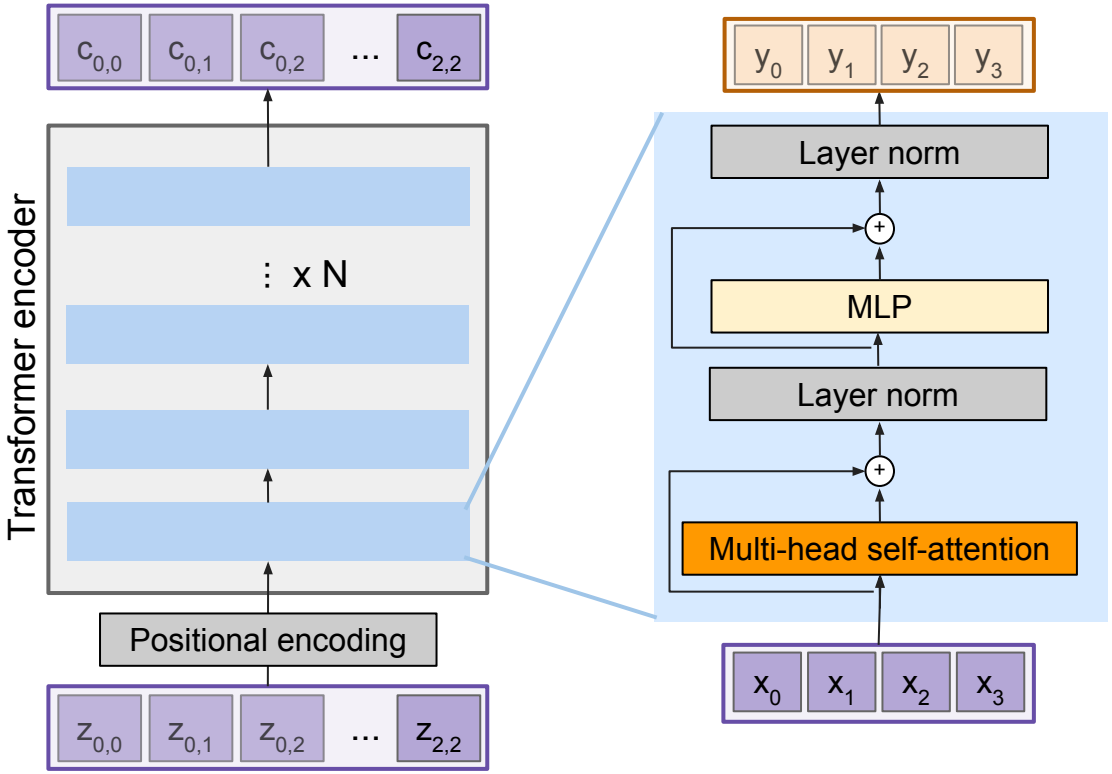
Self-attention is the only interaction between vectors.

Layer norm and MLP operate independently per vector.

Highly scalable, highly parallelizable, but high memory usage.

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

The Transformer encoder block



Now very common for LN to come before operations instead of after

Transformer Encoder Block:

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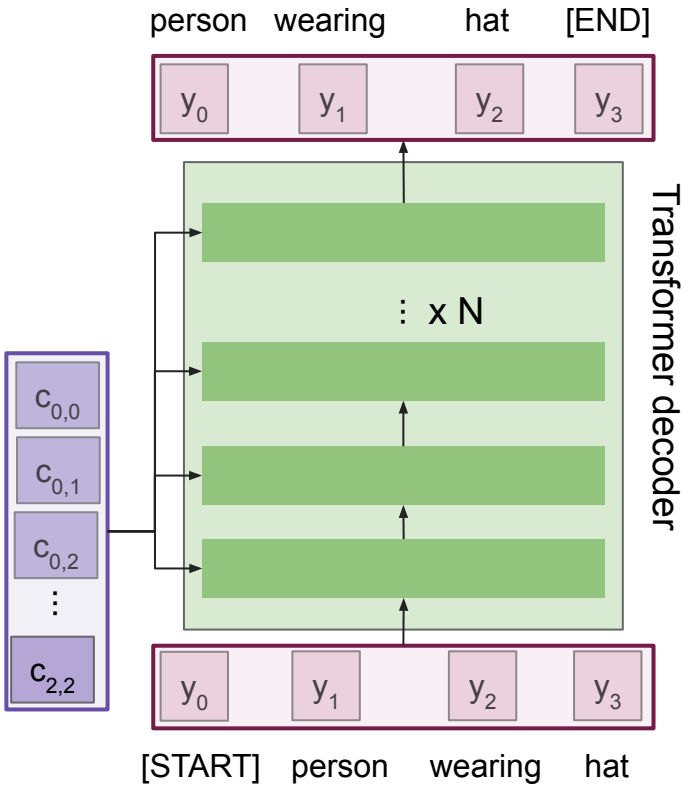
Vaswani et al, "Attention is all you need", NeurIPS 2017

The Transformer Decoder block

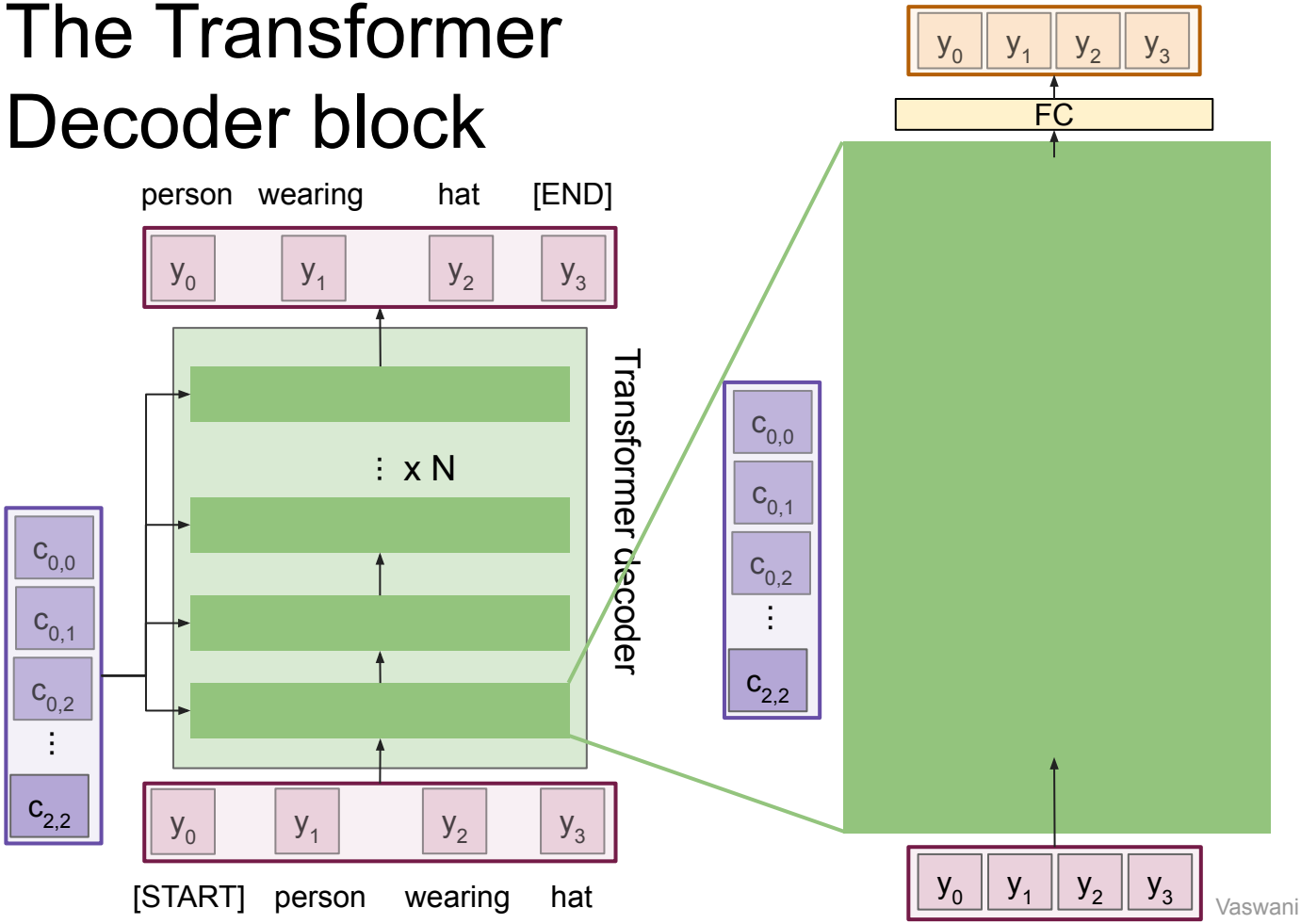


Made up of N decoder blocks.

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

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

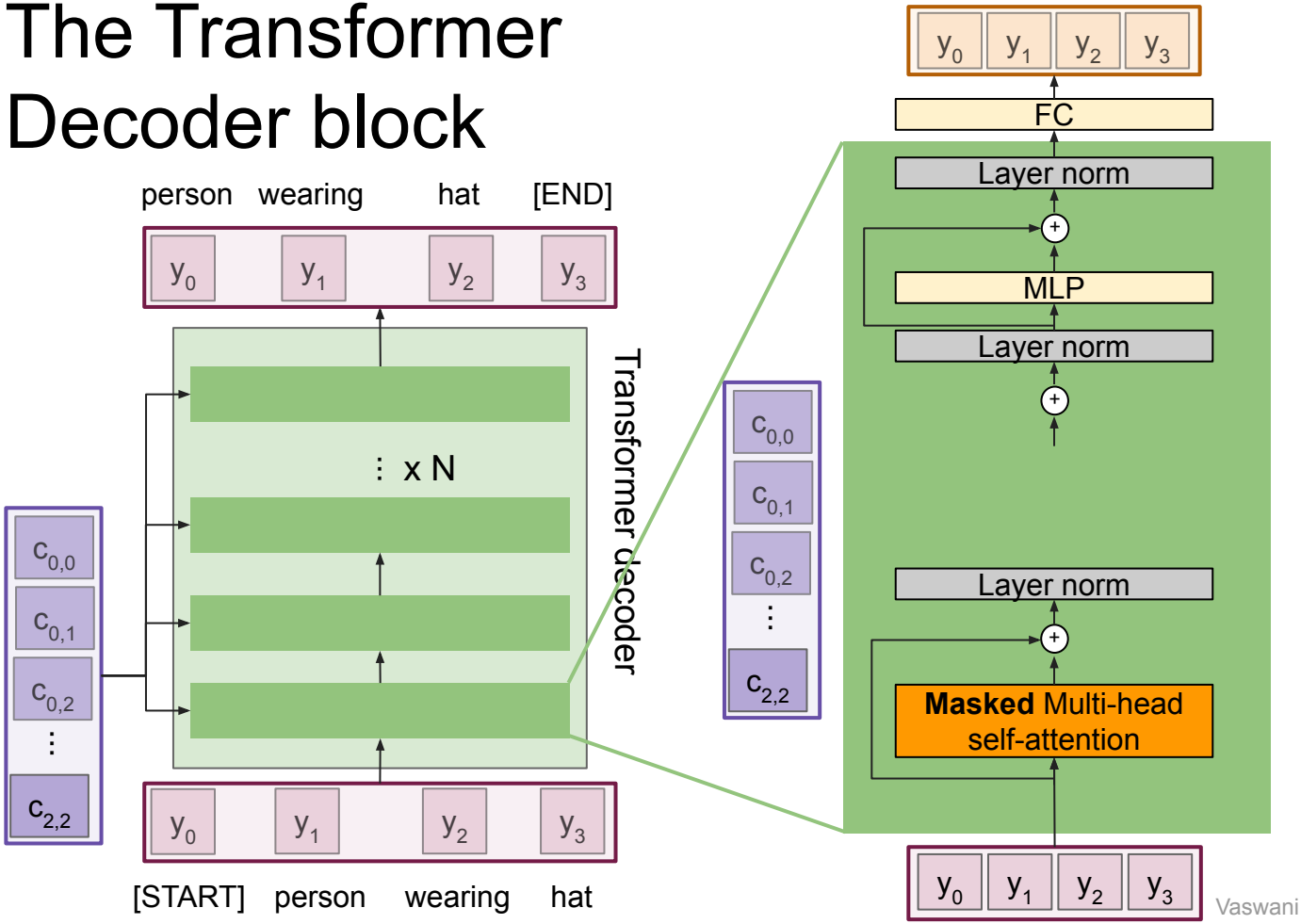
The Transformer Decoder block



Let's dive into the transformer decoder block

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

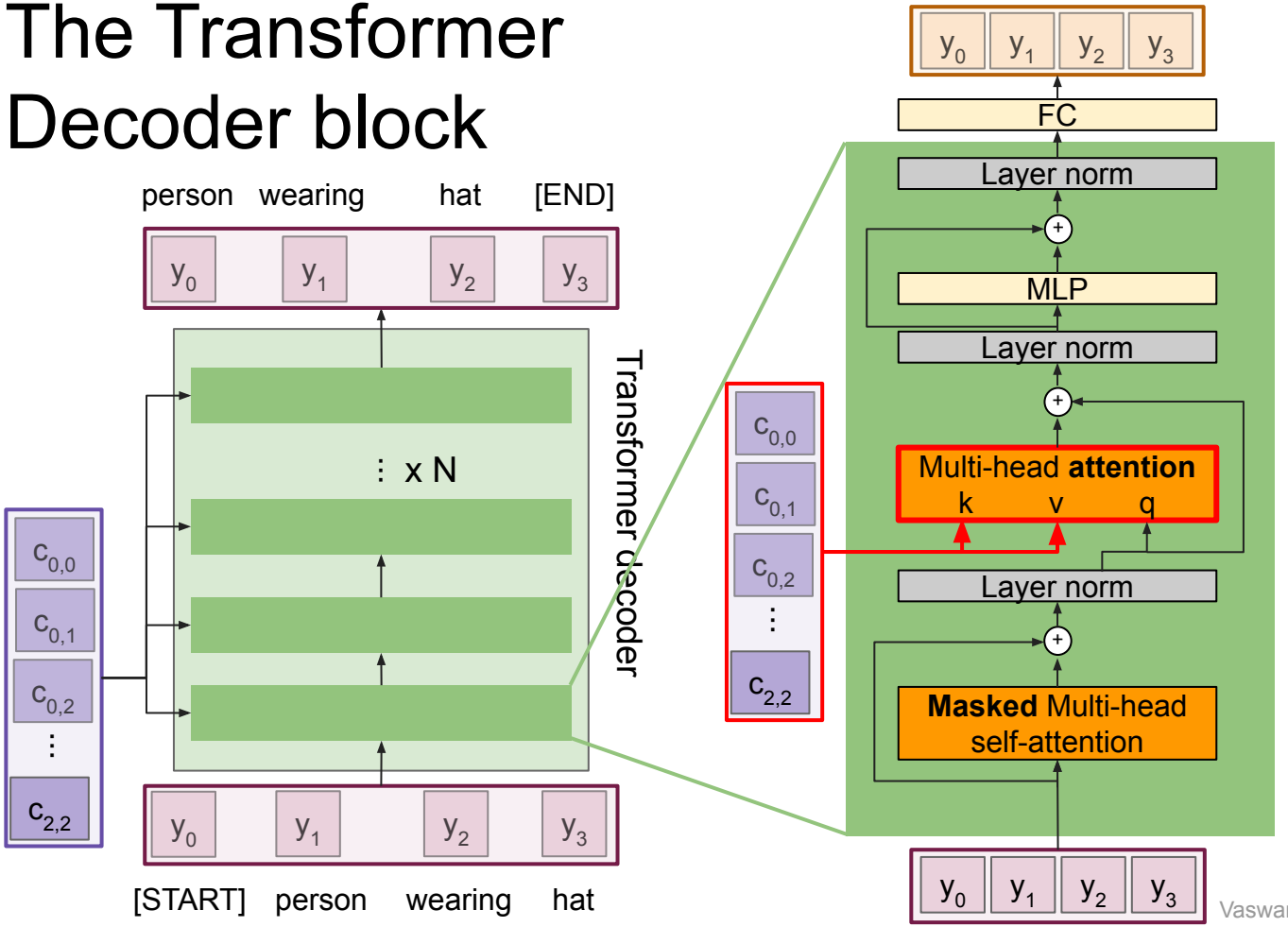
The Transformer Decoder block



Most of the network is the same the transformer encoder.

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

The Transformer Decoder block

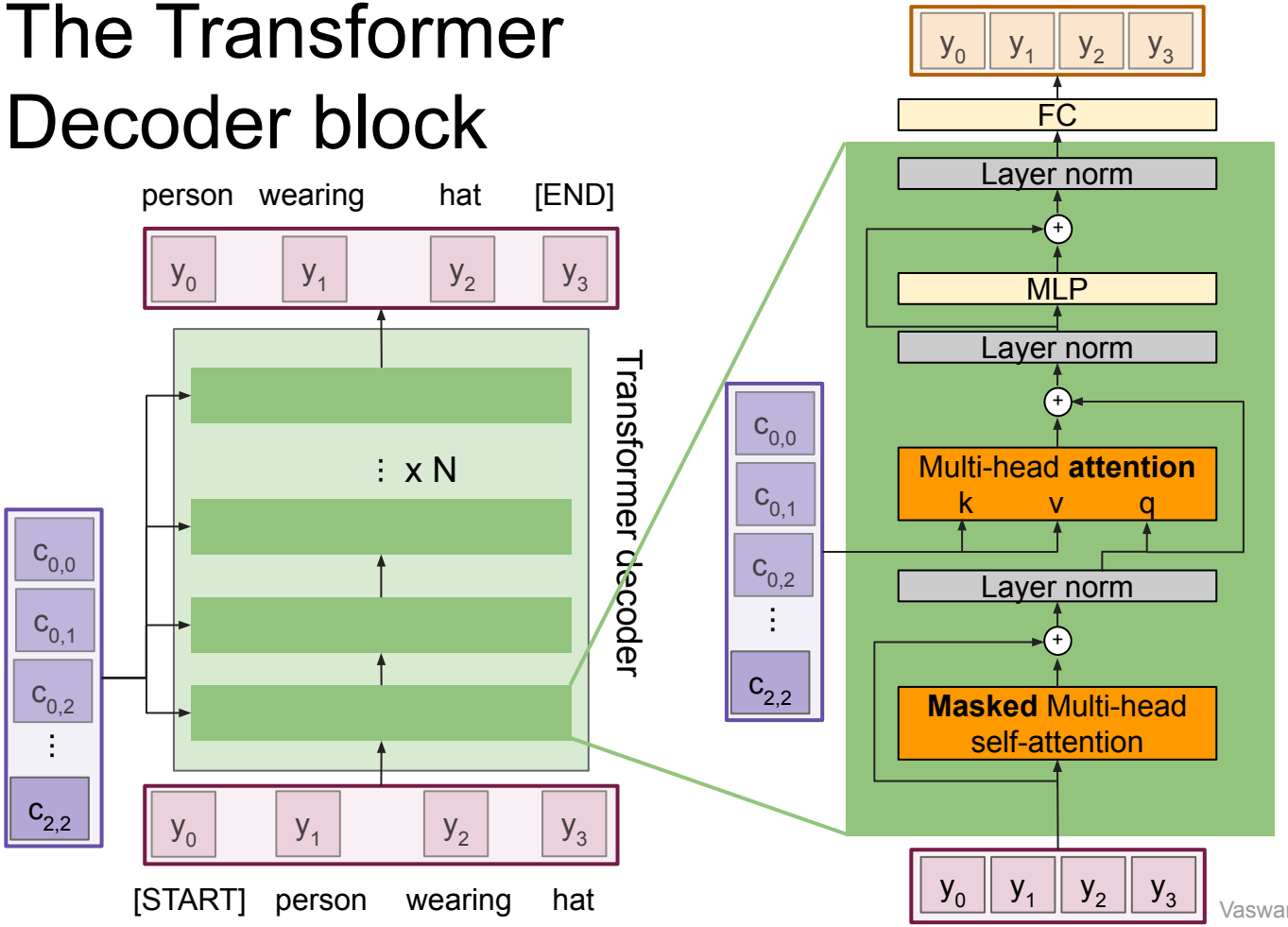


Multi-head attention block attends over the transformer encoder outputs.

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

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

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

- **No recurrence at all**

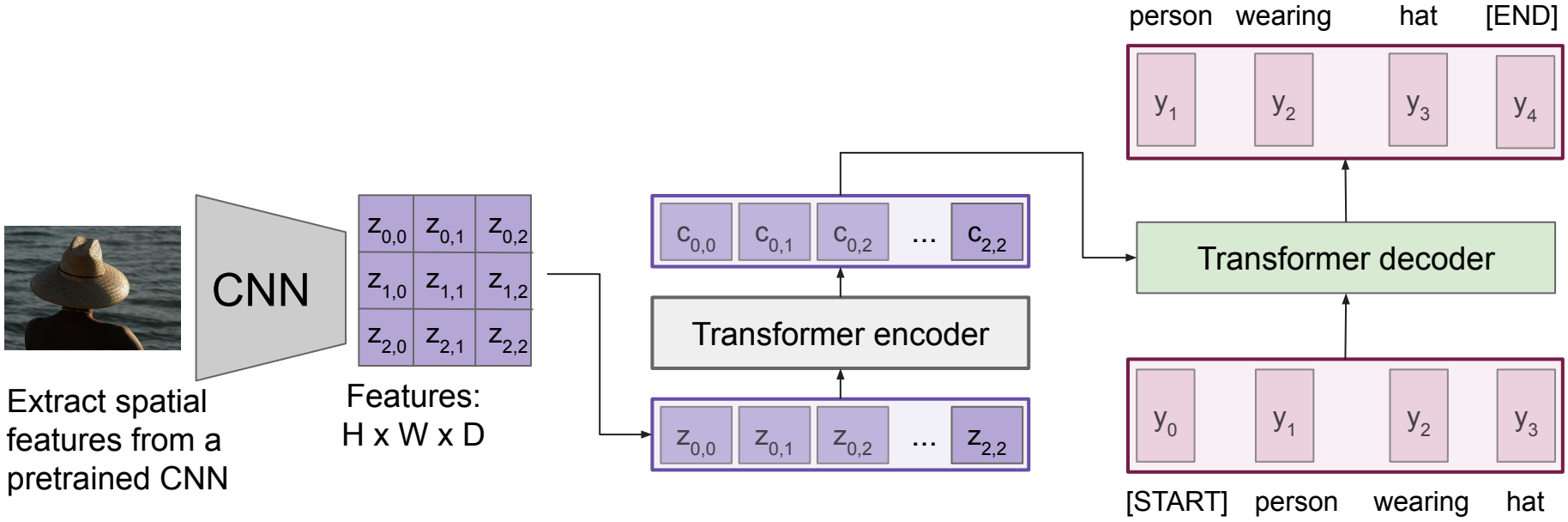


Image Captioning using transformers

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

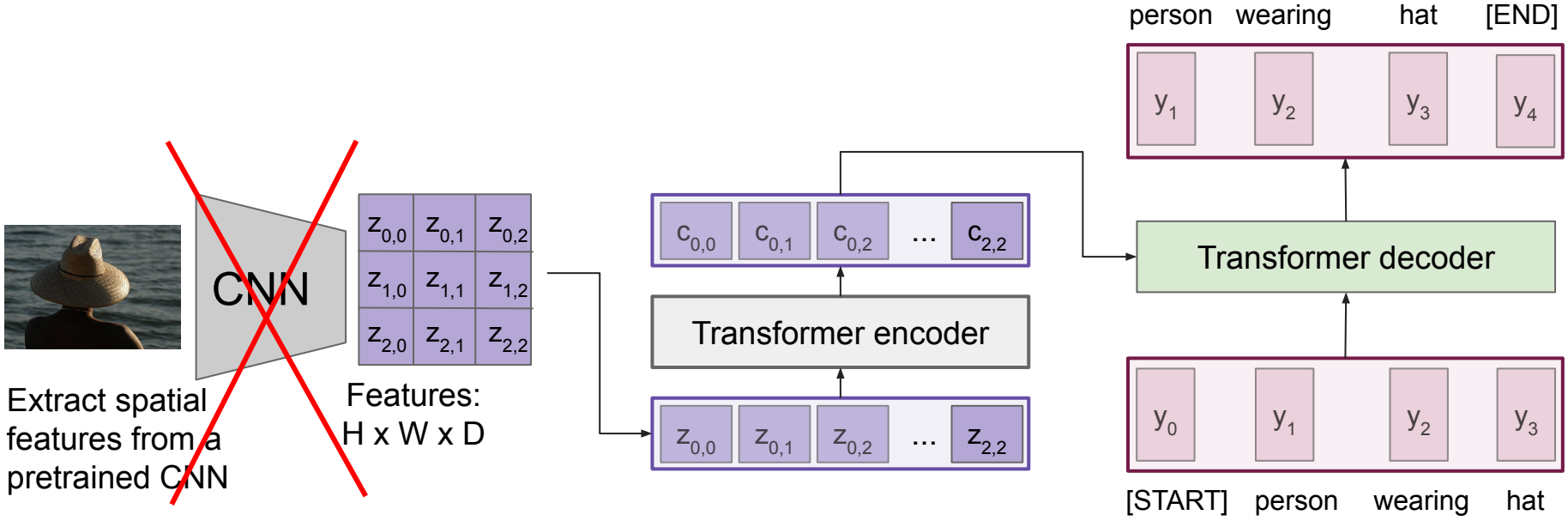
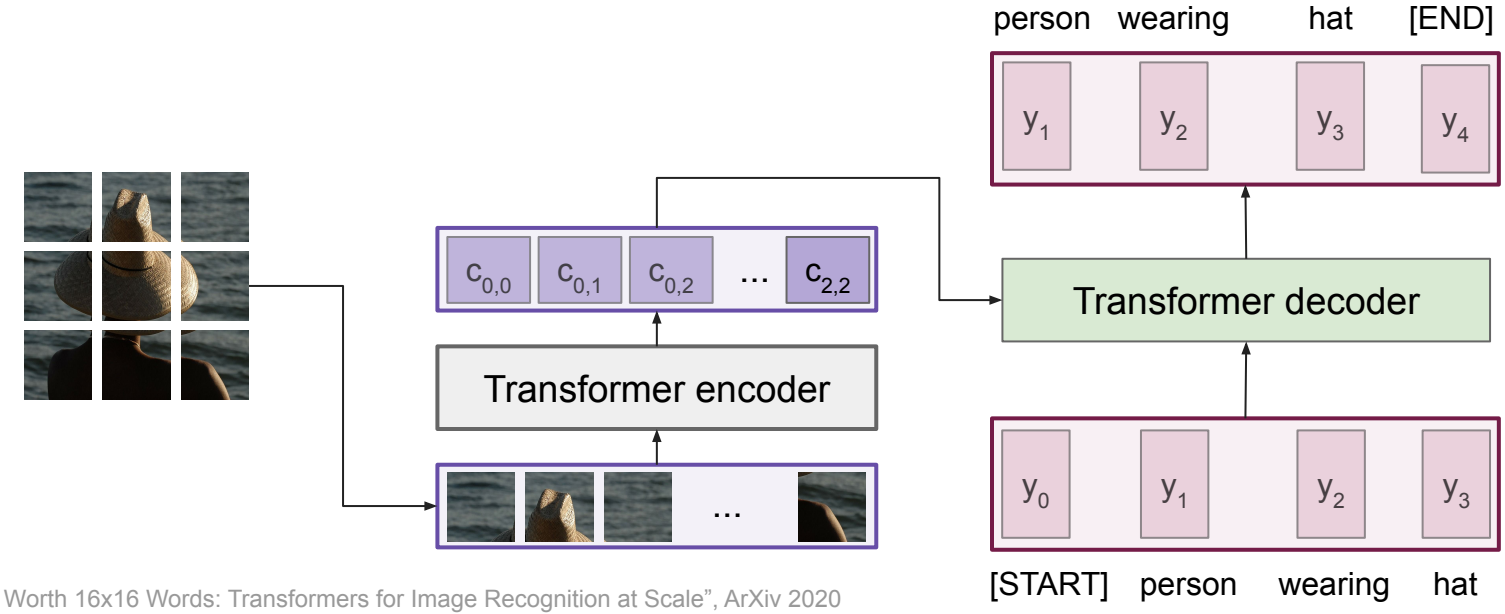


Image Captioning using ONLY transformers

- **Transformers from pixels to language**



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

Image Captioning using ONLY transformers

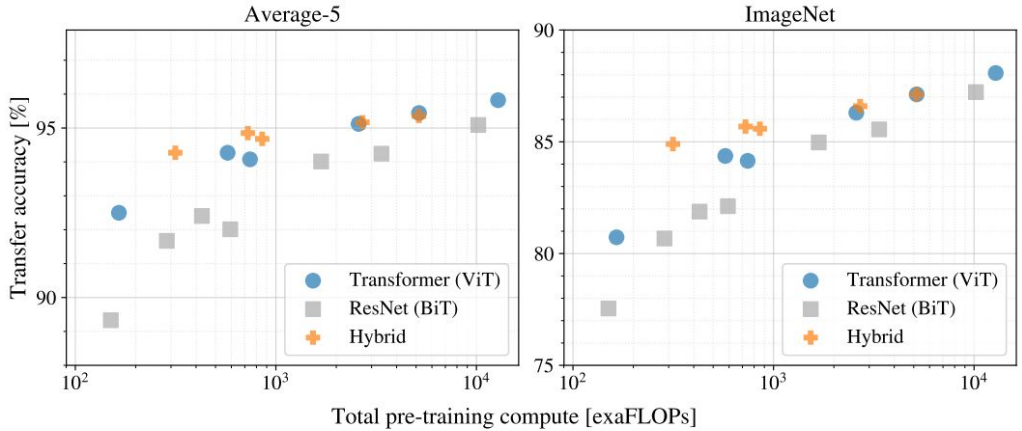


Figure 5: Performance versus cost for different architectures: Vision Transformers, ResNets, and hybrids. Vision Transformers generally outperform ResNets with the same computational budget. Hybrids improve upon pure Transformers for smaller model sizes, but the gap vanishes for larger models.

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

New large-scale transformer models

TEXT PROMPT

an illustration of a baby daikon radish in a tutu walking a dog

AI-GENERATED IMAGES

Edit prompt or view more images↓

TEXT PROMPT

an armchair in the shape of an avocado [...]

AI-GENERATED IMAGES

Edit prompt or view more images↓

link to more examples

Transformers today

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

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

Transformers today

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Transformer-Large	12	1024	16	213M	?	8x P100 (3.5 days)
BERT-Base	12	768	12	119M	13GB	?
BERT-Large	24	1024	16	340M	13GB	?

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

Transformers today

Model	Layers	Width	Heads	Params	Data	Training
Transformer-Base	12	512	8	65M	?	8x P100 (12 hours)
Transformer-Large	12	1024	16	213M	?	8x P100 (3.5 days)
BERT-Base	12	768	12	119M	13GB	?
BERT-Large	24	1024	16	340M	13GB	?
XLNet-Large	24	1024	16	~340M	126GB	512x TPU-v3 (2.5 days)
RoBERTa	24	1024	16	355M	160GB	1024x V100 GPUs (1 day)

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

Transformers today

Model	Layers	Width	Heads	Params	Data	Training
Transformer-Base	12	512	8	65M	?	8x P100 (12 hours)
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RoBERTa	24	1024	16	355M	160GB	1024x V100 GPUs (1 day)
GPT-2	48	1600	25	1.5B	40GB	?

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

Transformers today

Model	Layers	Width	Heads	Params	Data	Training
Transformer-Base	12	512	8	65M	?	8x P100 (12 hours)
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GPT-2	48	1600	25	1.5B	40GB	?
Megatron-LM	72	3072	32	8.3B	174GB	512x V100 GPU (9 days)

Shoeybi et al. "Megatron-lm: Training multi-billion parameter language models using model parallelism." 2019. (Google)

Transformers today

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Megatron-LM	72	3072	32	8.3B	174GB	512x V100 GPU (9 days)
Turing-NLG	78	4256	28	17B	?	256x V100 GPUs

Microsoft, "Turing-NLG: A 17-billion parameter language model by Microsoft", 2020

Transformers today

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Turing-NLG	78	4256	28	17B	?	256x V100 GPUs
GPT-3	96	12288	96	175B	694GB	?

Brown et al, "Language Models are Few-Shot Learners", NeurIPS 2020

Transformers today

Rae et al, “Scaling Language Models: Methods, Analysis, & Insights from Training Gopher”, arXiv 2021 (Google)

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Turing-NLG	78	4256	28	17B	?	256x V100 GPUs
GPT-3	96	12288	96	175B	694GB	?
Gopher	80	16384	128	280B	10.55TB	4096x TPU-v3 (38 days)

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GPT-3	96	12288	96	175B	694GB	?
Gopher	80	16384	128	280B	10.55TB	4096x TPU-v3 (38 days)
GPT-4	?	?	?	1.8T	?	?

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.

Next time: Modern architectures