Lectures on AI-driven Drug Discovery

Attention: Part I

Sung-eui Yoon (윤성의)

https://sgvr.kaist.ac.kr/~sungeui/

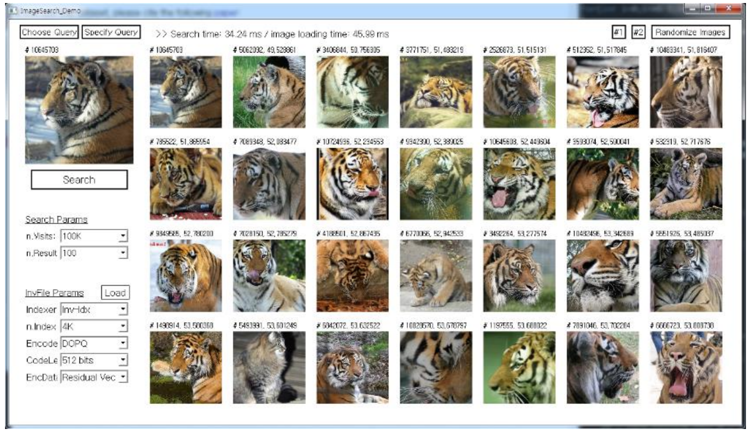
School of Computing & Graduate School of Artificial Intelli

KAIST

Present: Intelligent Ray Tracing, Image Search, Motion Planning

- **Designing *scalable and intelligent graphics, vision and robotics algorithms* to efficiently handle massive models on commodity hardware**

Graphics, photo-realistic rendering



Vision, image search

Robotics, motion planning

My Recent Work

- Workshop at ICRA 19 about:
  - Sound Source Localization and its Applications for Robots
  - Main organizer: Sung-eui Yoon

- Tutorial at CVPR 16 about:
  - Recent Image Search Techniques
  - Organizers: Sung-eui Yoon and Zhe Lin

KAIST

Recognitions and Collaborations

- **Test-of-Time Award 2006 at 2015, High Performance Graphics**
  - **차세대 과학자상 (IT 부문), 2019**
  - **국내외 학회 여러 논문 우수상**

- **Produced a few professors at GIST, SKKU, KOREATECH**
- **Worked on research collaborations with many domestic and international companies, and funding agencies**

Topics

Part I

Preliminary topics:

- Recurrent neural network

Sequence-to-Sequence with RNNs and Attention

- Image Captioning with RNNs and Attention

Part II

Self-Attention Layer

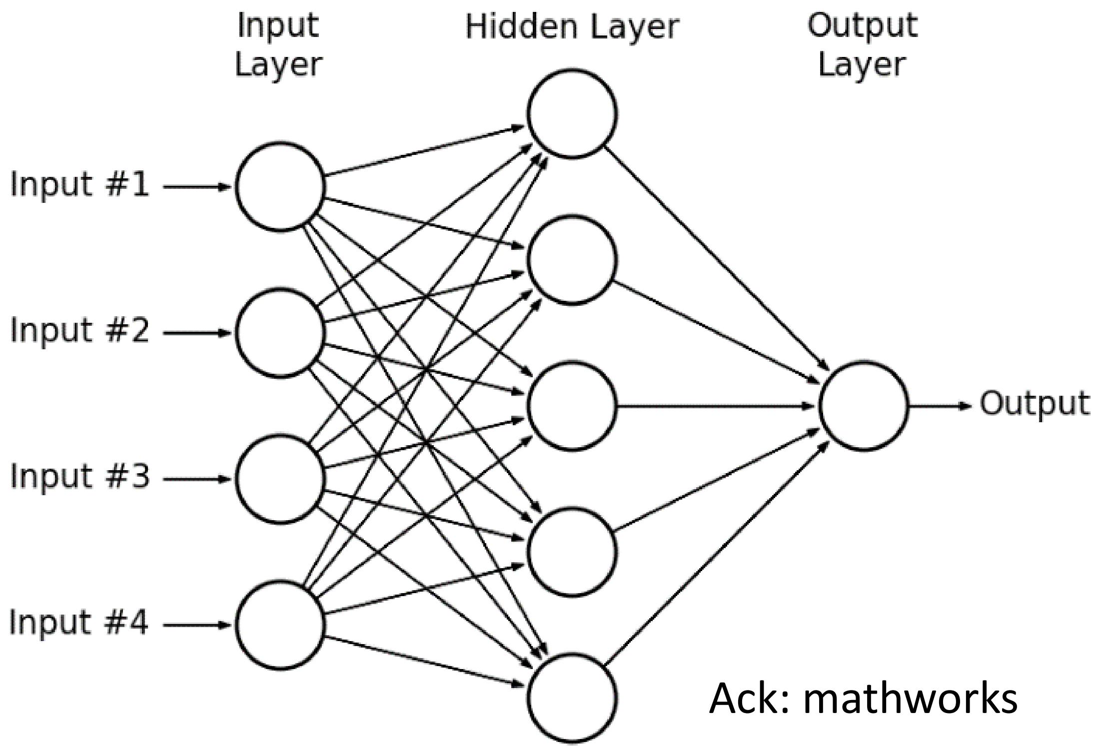
The Transformer

Ack.: Slides of Justin Johnson

Preliminary: Neural Network

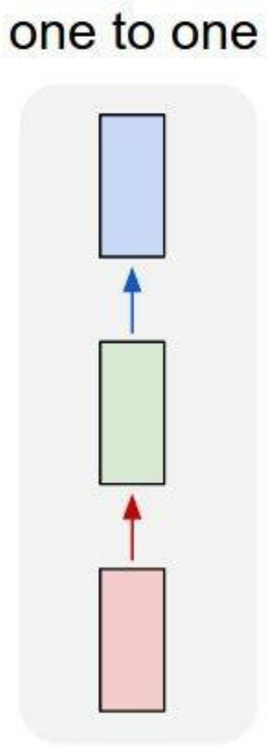
"Neural Network" is a very broad term

More accurately called "fully-connected networks" or sometimes "multi-layer perceptrons" (MLP)



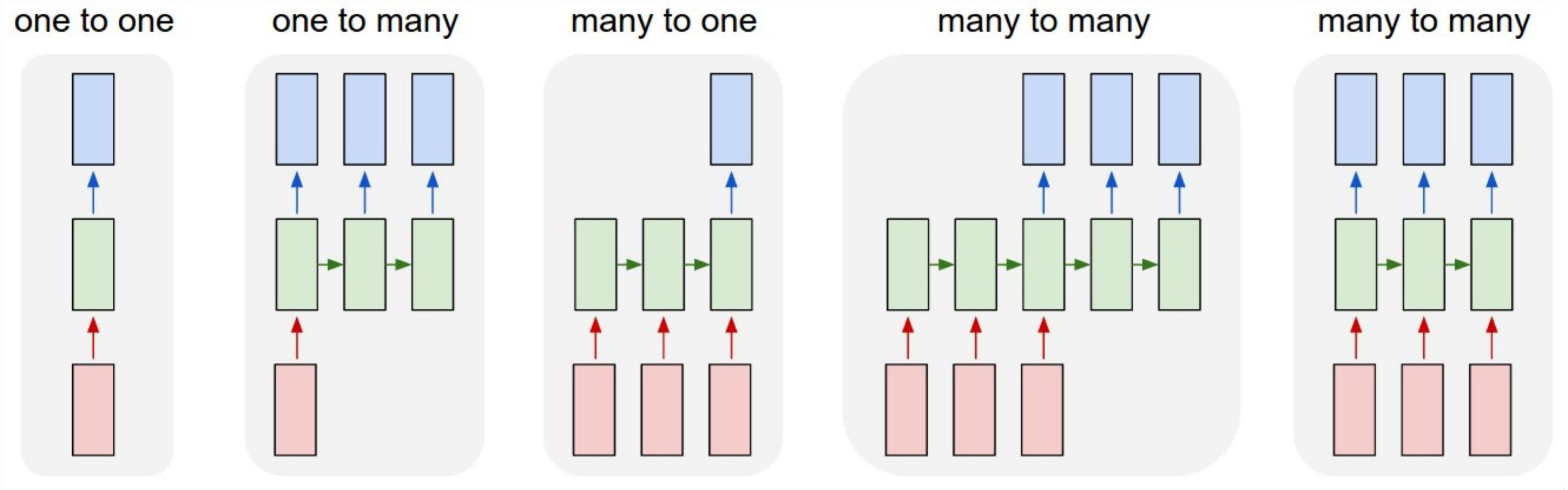
Ack: mathworks

Preliminary: "Vanilla" Neural Network



Vanilla Neural Networks

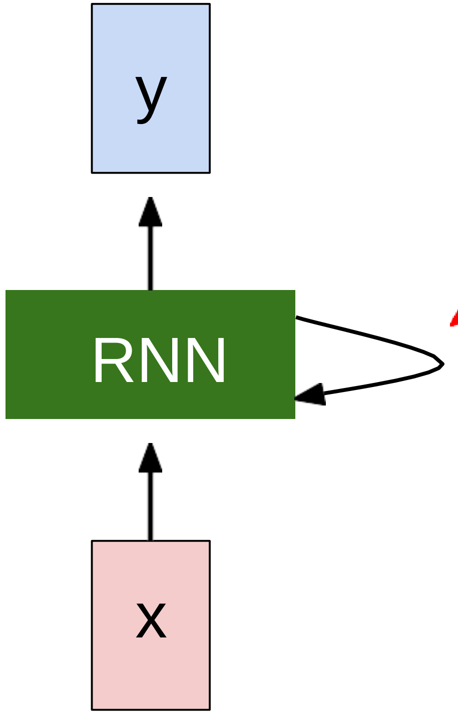
Preliminary: Recurrent Neural Networks



e.g. **Image Captioning**
image -> sequence of words

e.g. **Machine Translation**
seq of words -> seq of words

Recurrent Neural Network



Key idea: RNNs have an "internal state" that is updated as a sequence is processed

Recurrent Neural Network

We can process a sequence of vectors **x** by applying a **recurrence formula** at every time step:

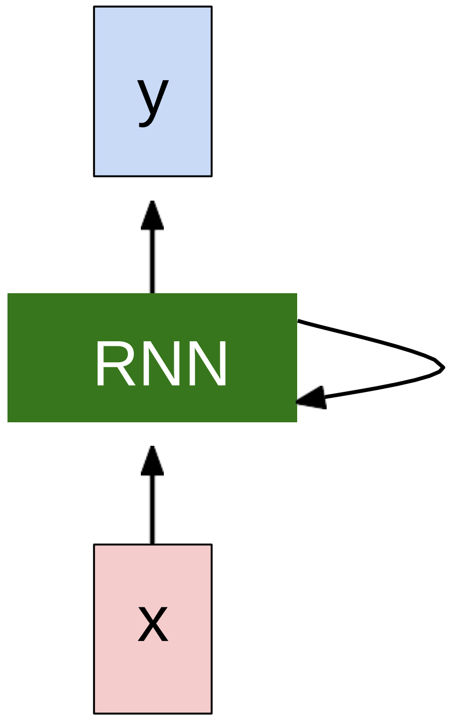
$$\boxed{h_t} = \boxed{f_W}(\boxed{h_{t-1}}, \boxed{x_t})$$

new state

old state

input vector at some time step

some function with parameters W



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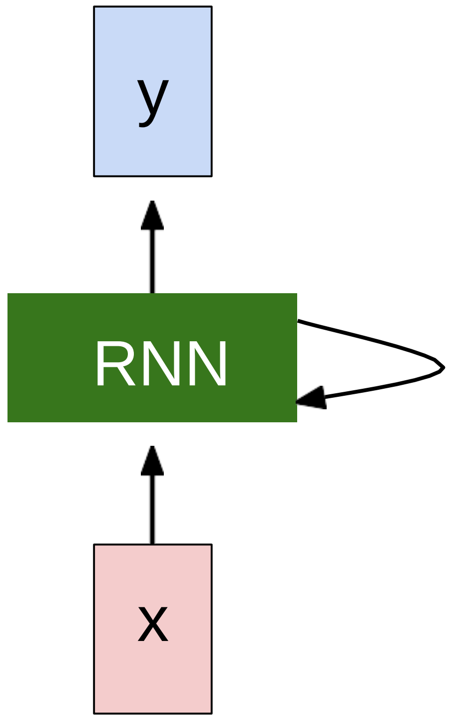
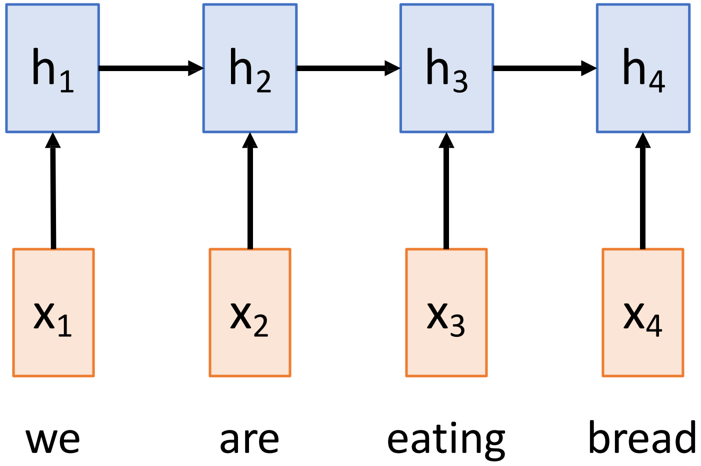


Notice: the same function and the same set of parameters are used at every time step.

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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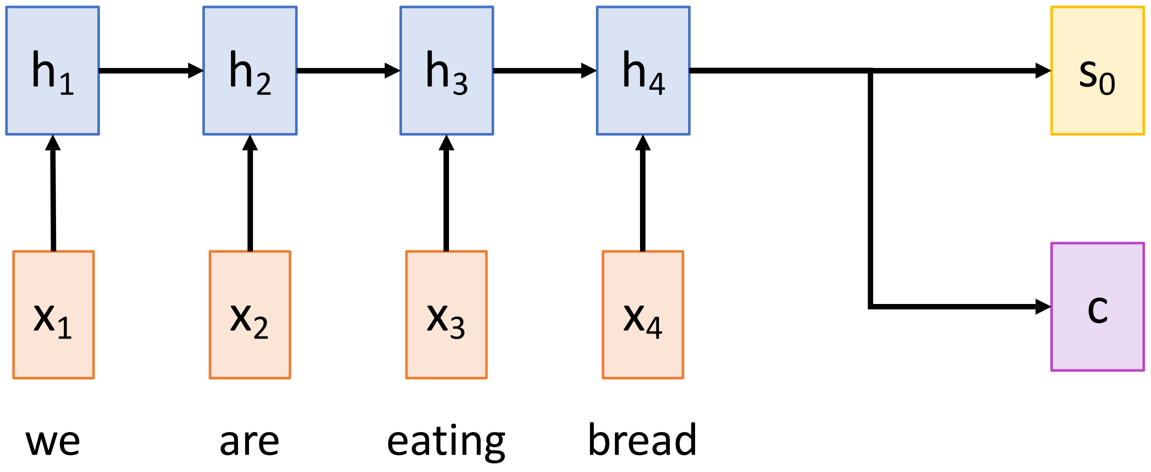
From final hidden state predict:

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

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From final hidden state predict:

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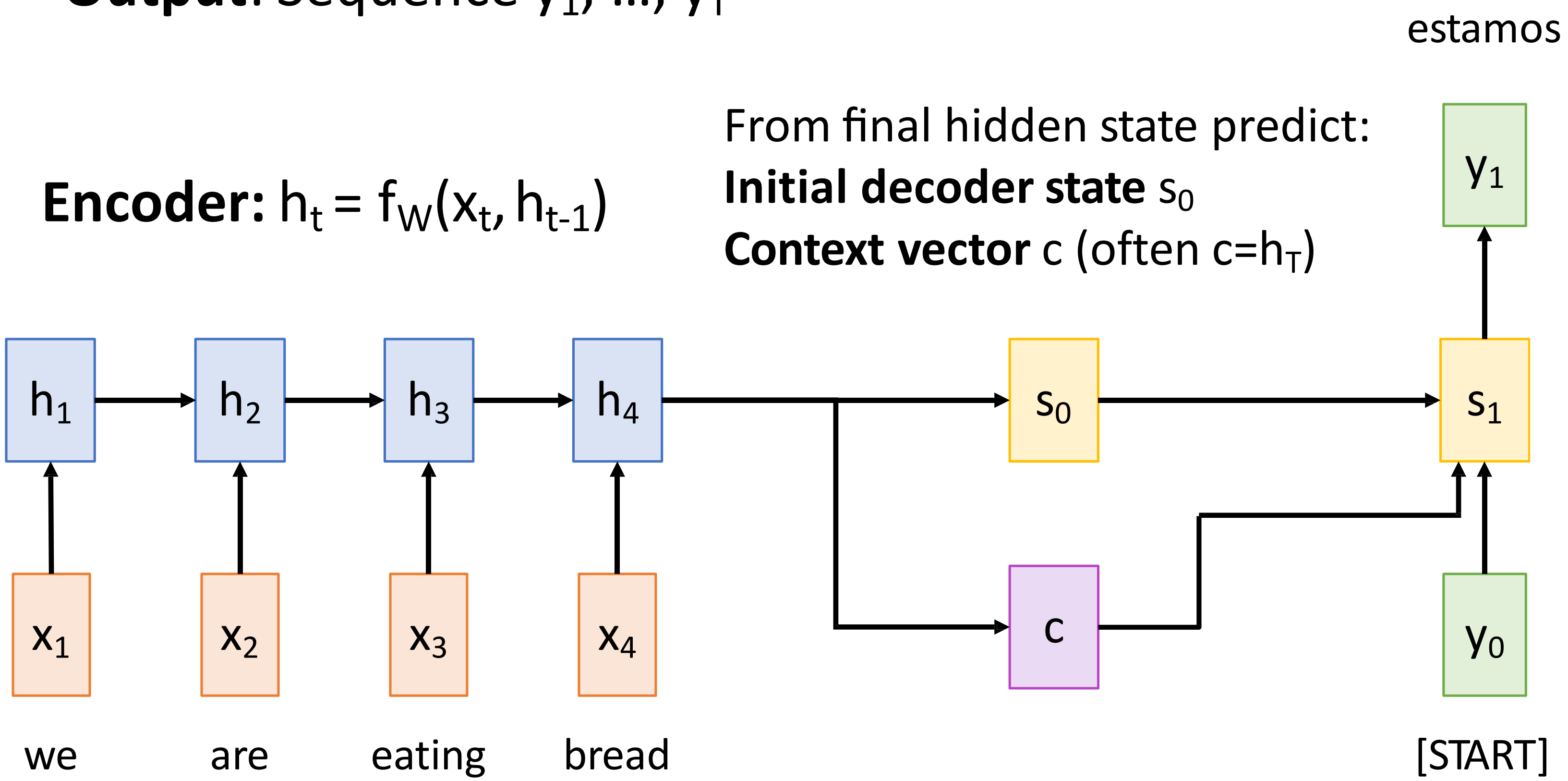

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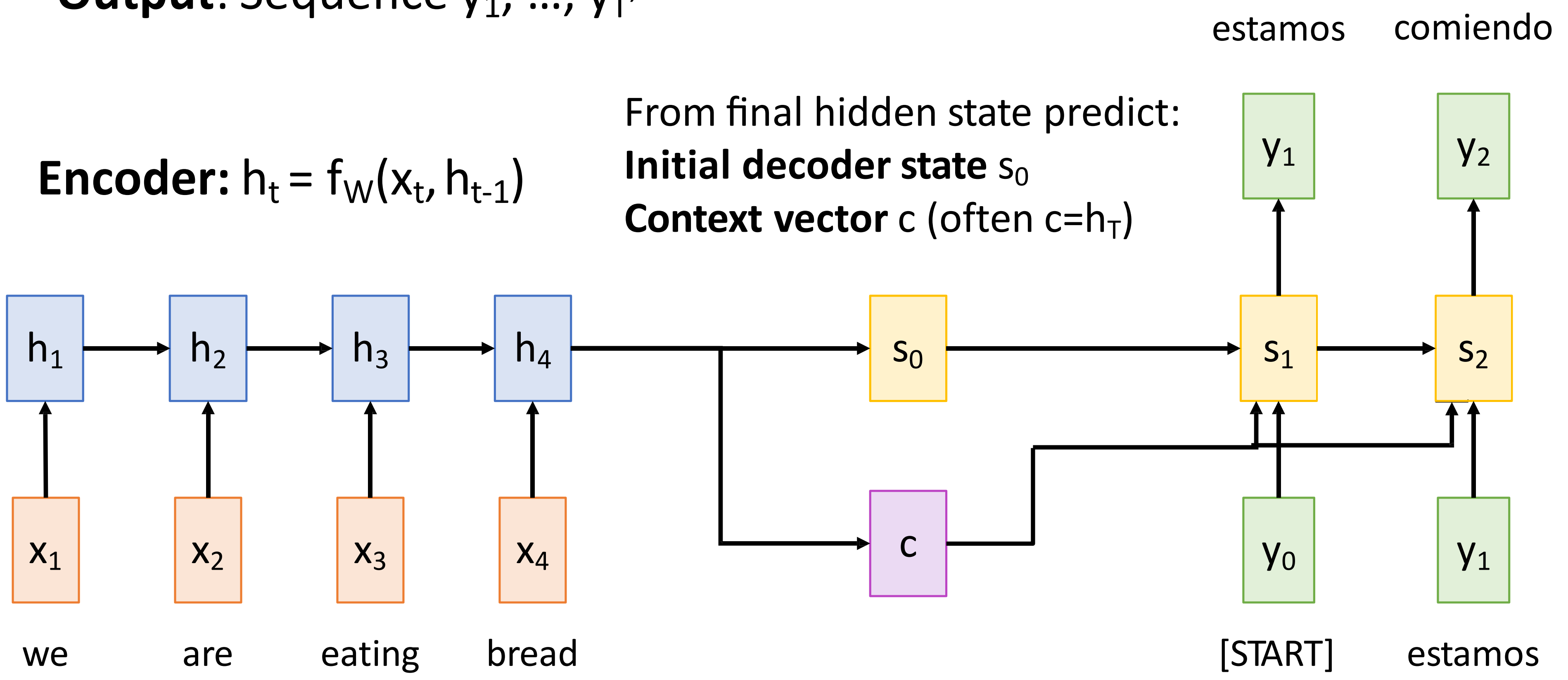

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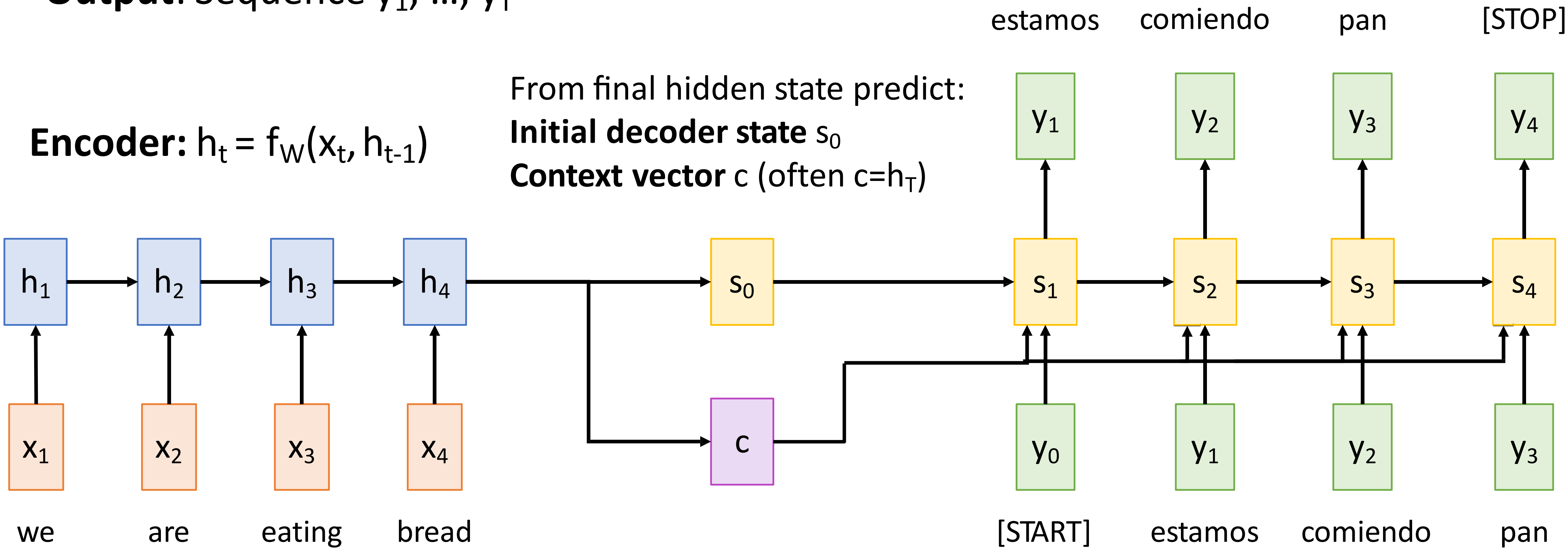

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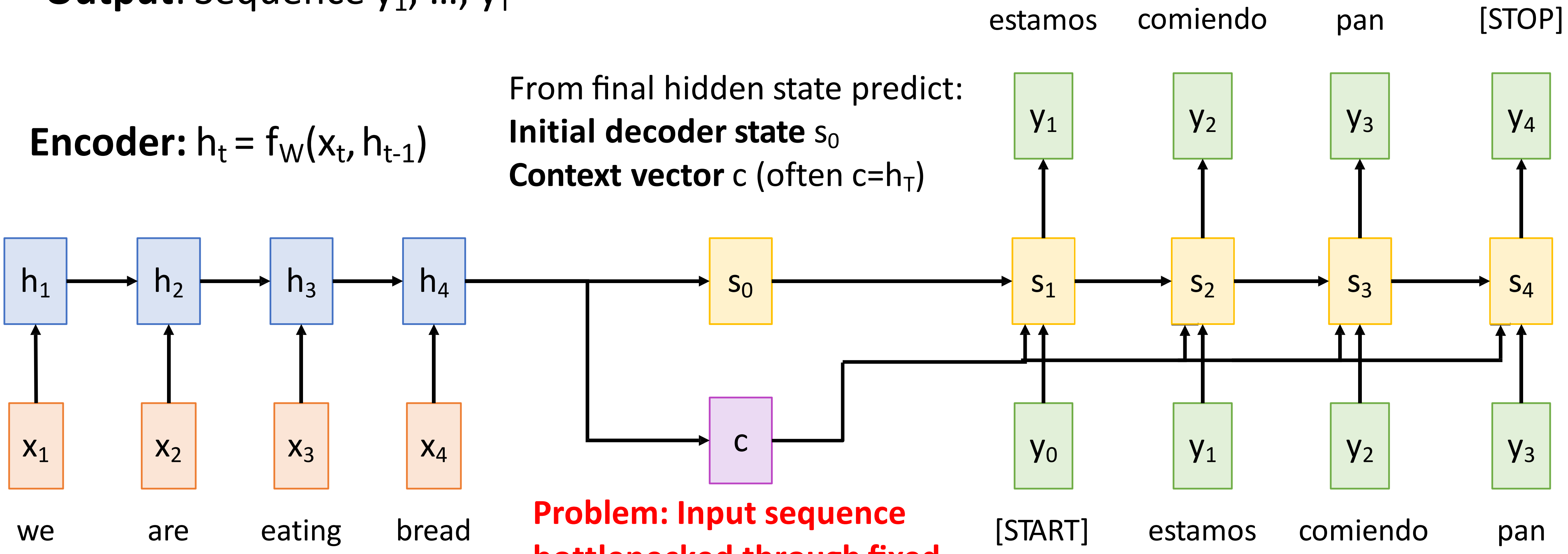

Problem: Input sequence bottlenecked through fixed-sized vector. What if T=1000?

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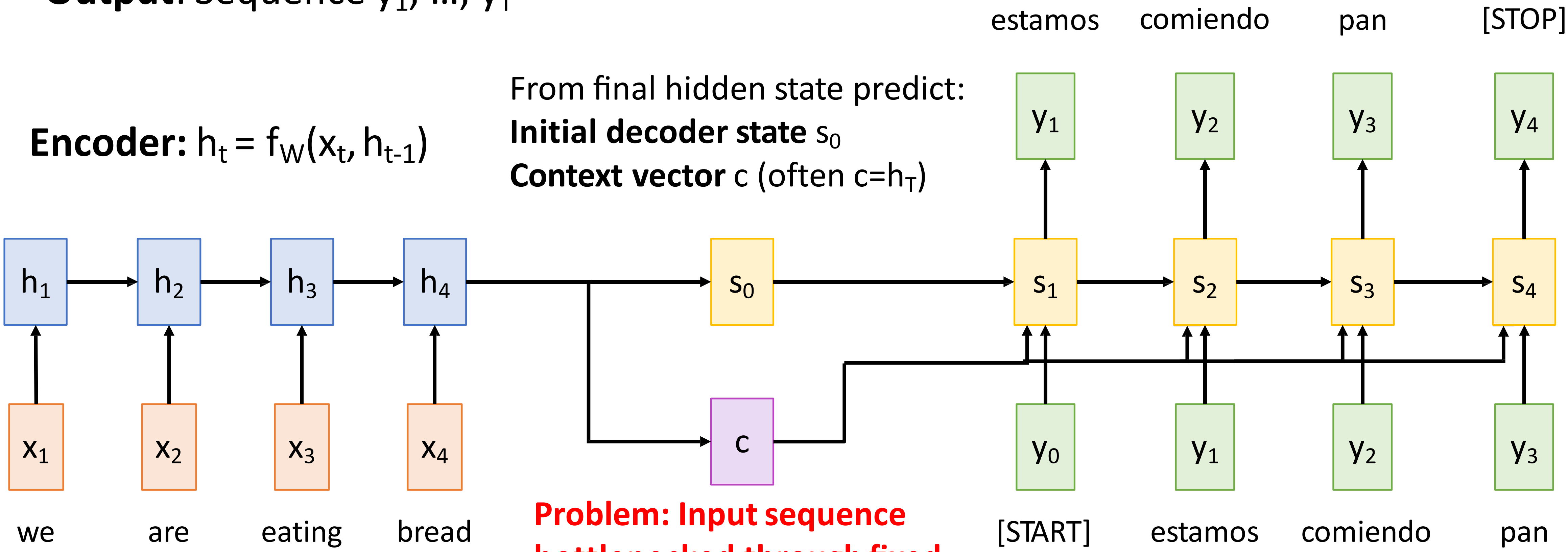

Problem: Input sequence bottlenecked through fixed sized vector. What if T=1000?

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

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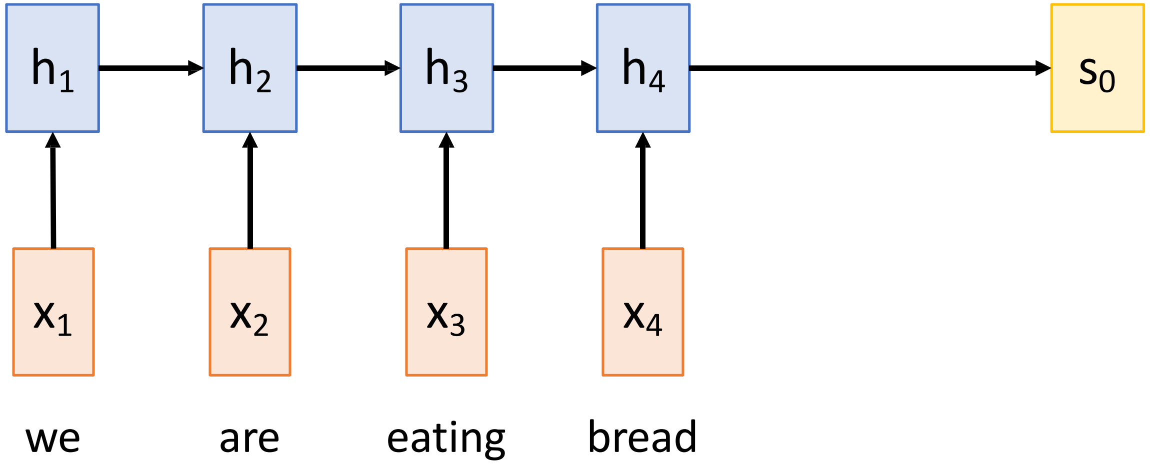
Sequence-to-Sequence with RNNs and Attention

Input: Sequence $x_1, \ldots x_T$
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



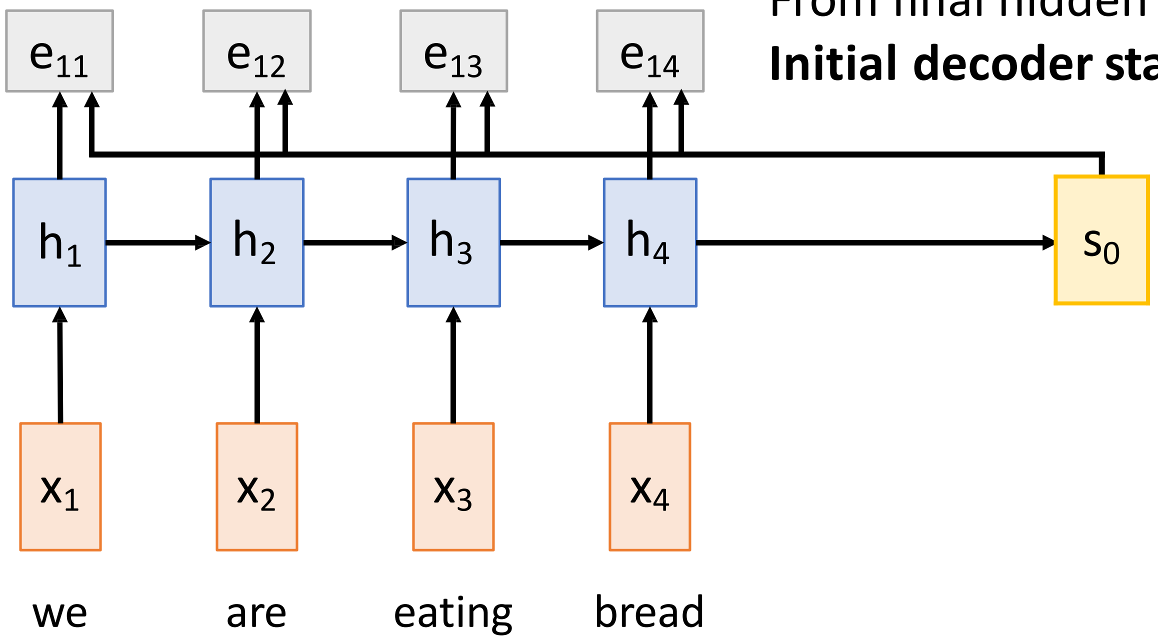
Bahdanau et al, "Neural machine translation by jointly learning to align and translate", ICLR 2015

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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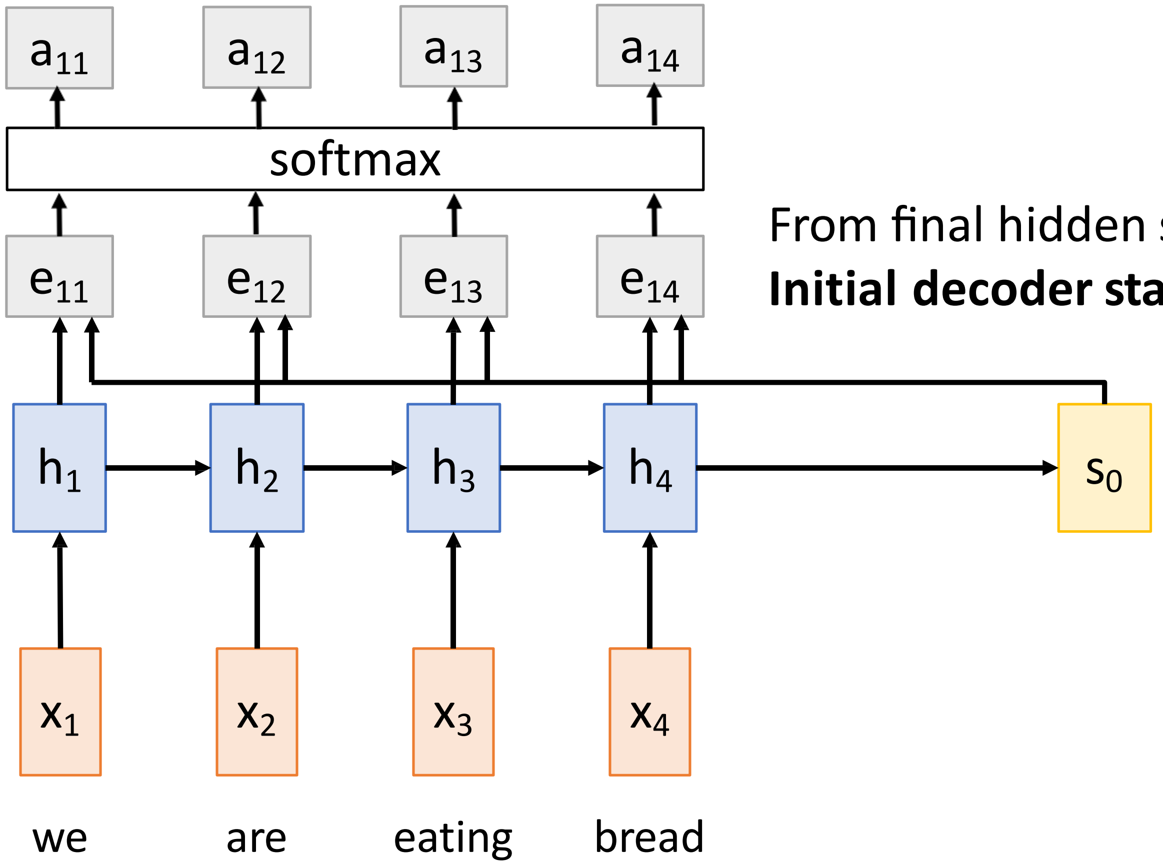

From final hidden state:
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Compute (scalar) **alignment scores**
$e_{t,i} = f_{att}(s_{t-1}, h_i)$ (f_{att} is an MLP)

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

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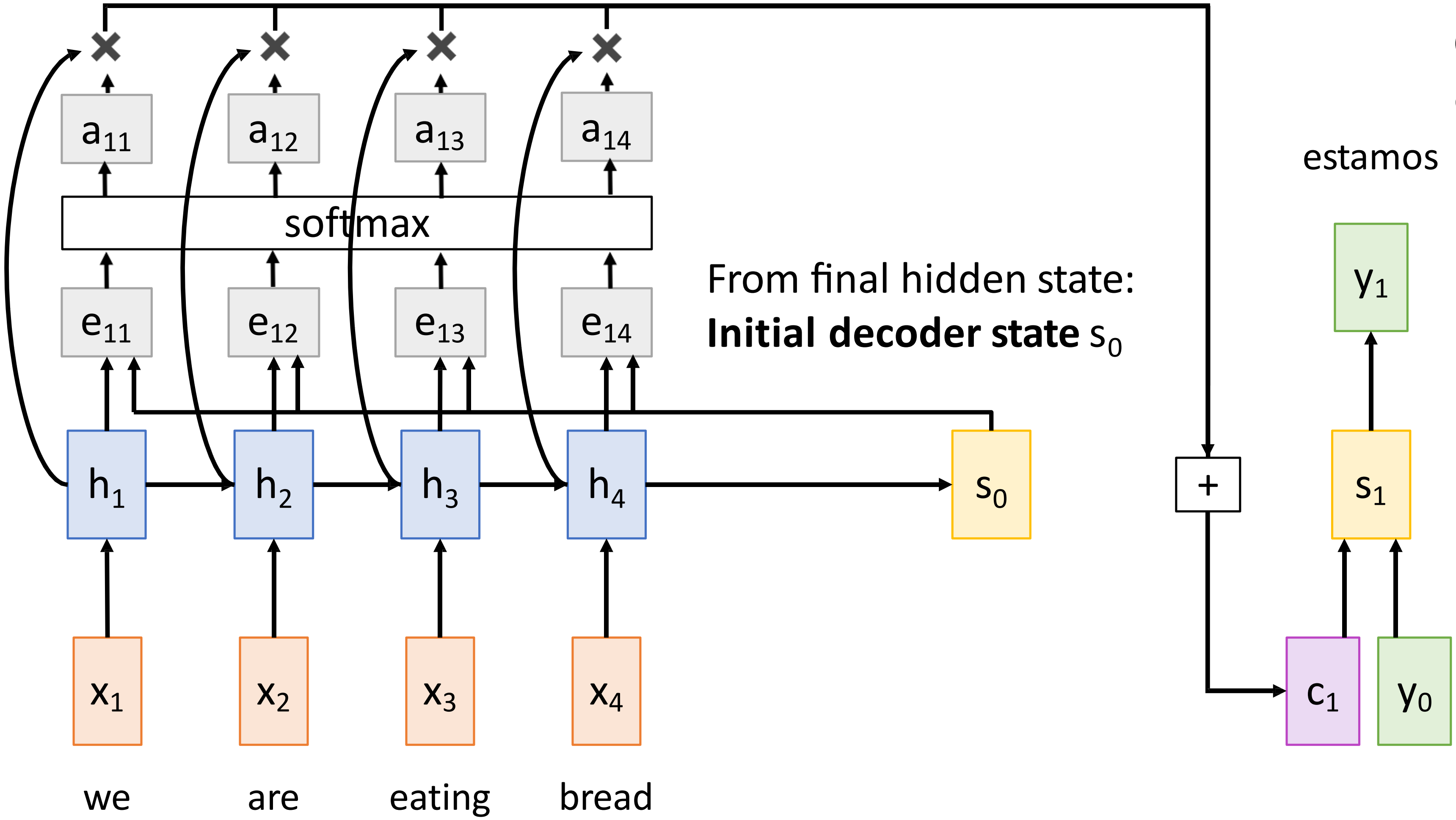
Sequence-to-Sequence with RNNs and Attention



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

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

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

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

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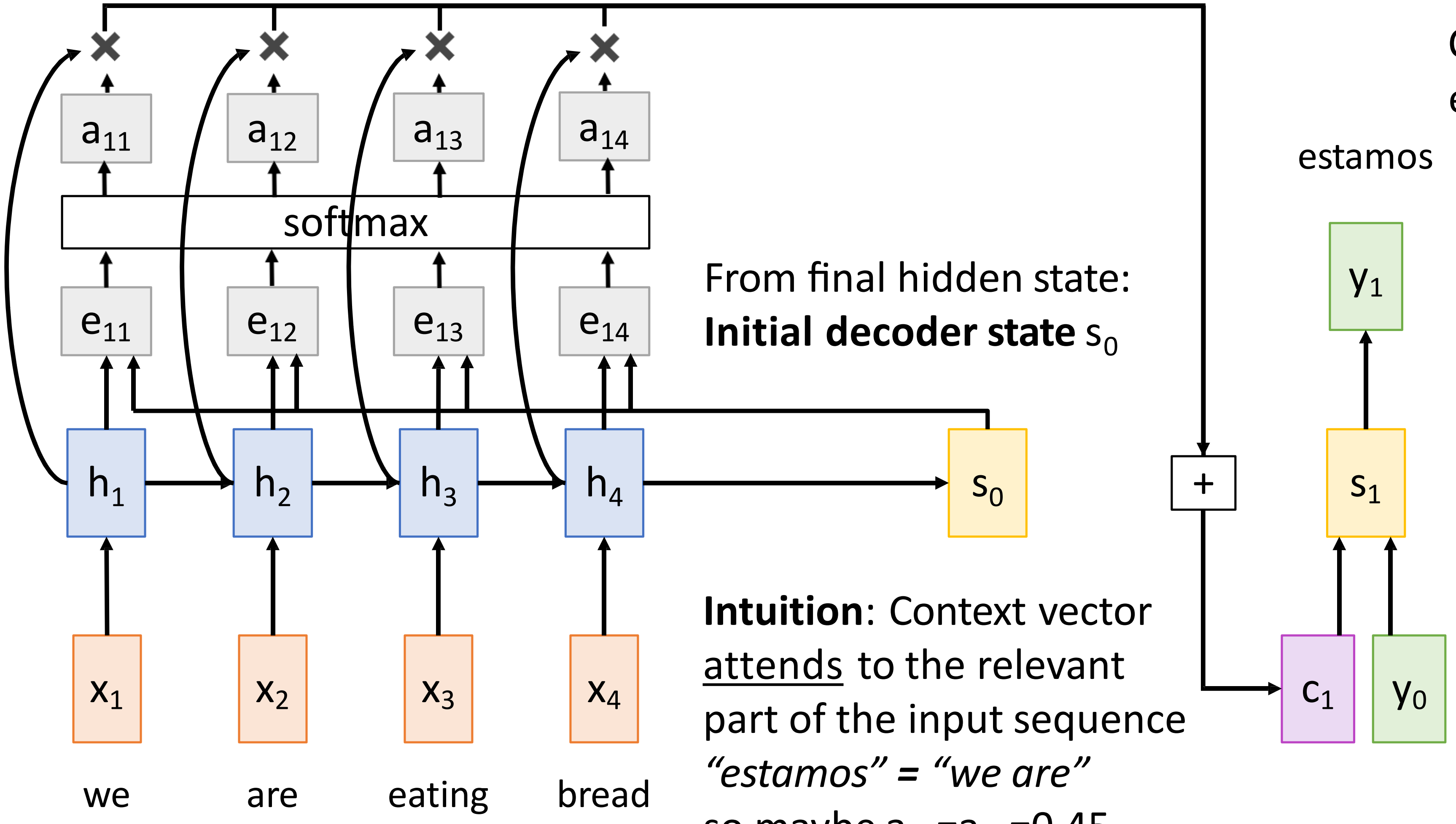
Sequence-to-Sequence with RNNs and Attention



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

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

"estamos" = "we are"

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

Compute (scalar) **alignment scores**

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Normalize alignment scores to get **attention weights**

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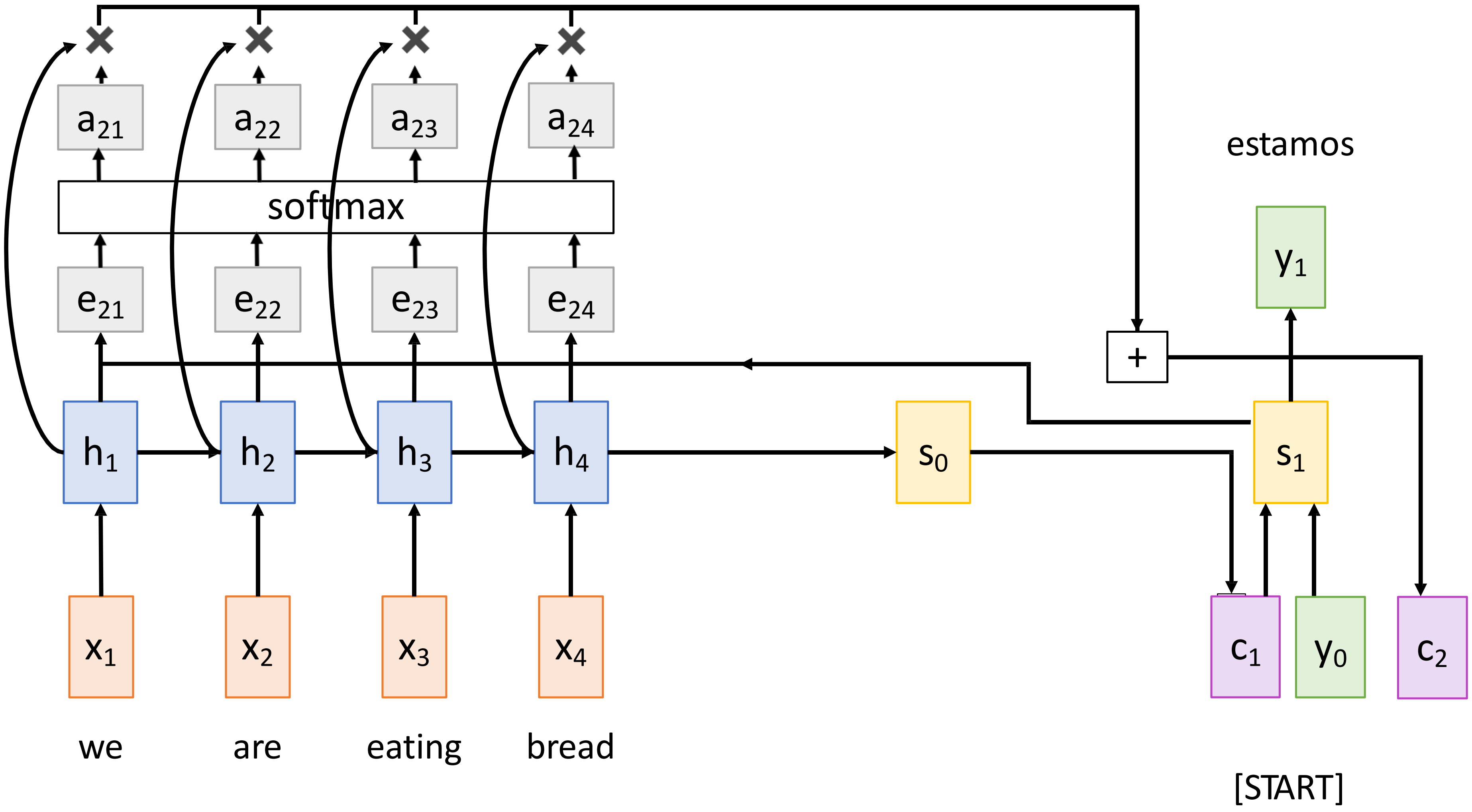
Sequence-to-Sequence with RNNs

Repeat: Use s_1 to compute new context vector c_2



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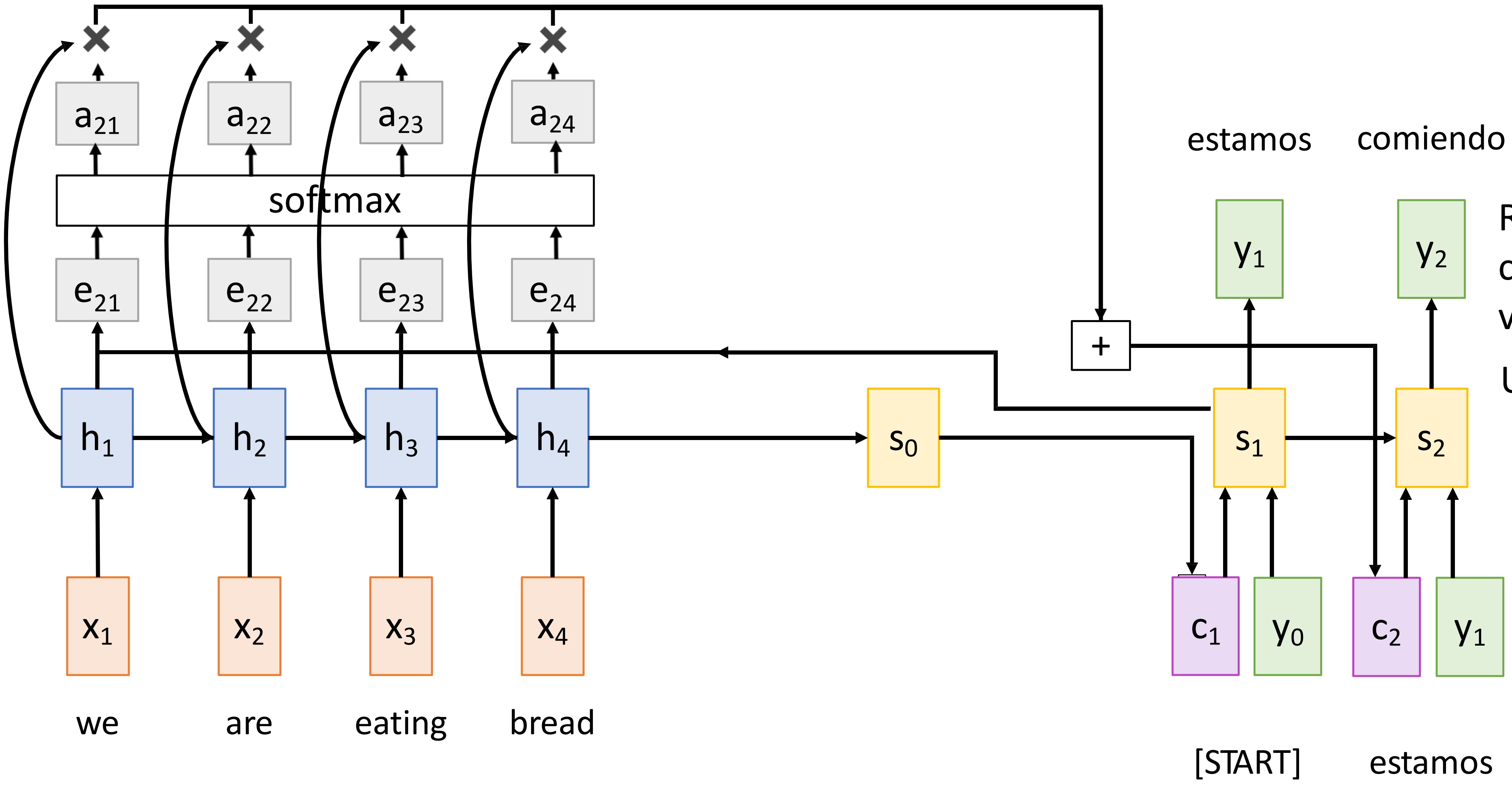
Sequence-to-Sequence with RNNs and Attention



Repeat: Use s_1 to compute new context vector c_2

Use c_2 to compute s_2, y_2

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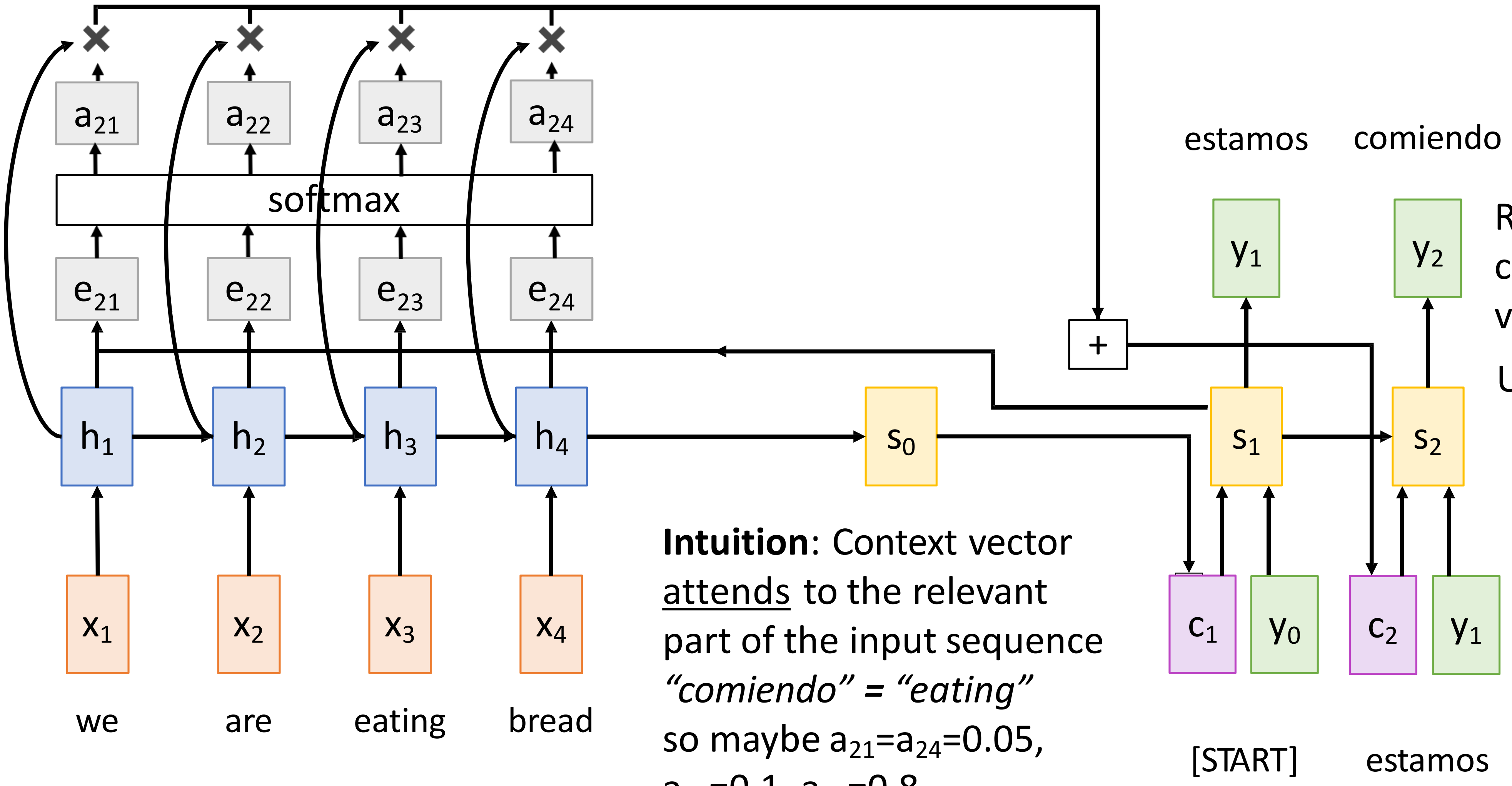
Sequence-to-Sequence with RNNs and Attention



Repeat: Use s_1 to compute new context vector c_2

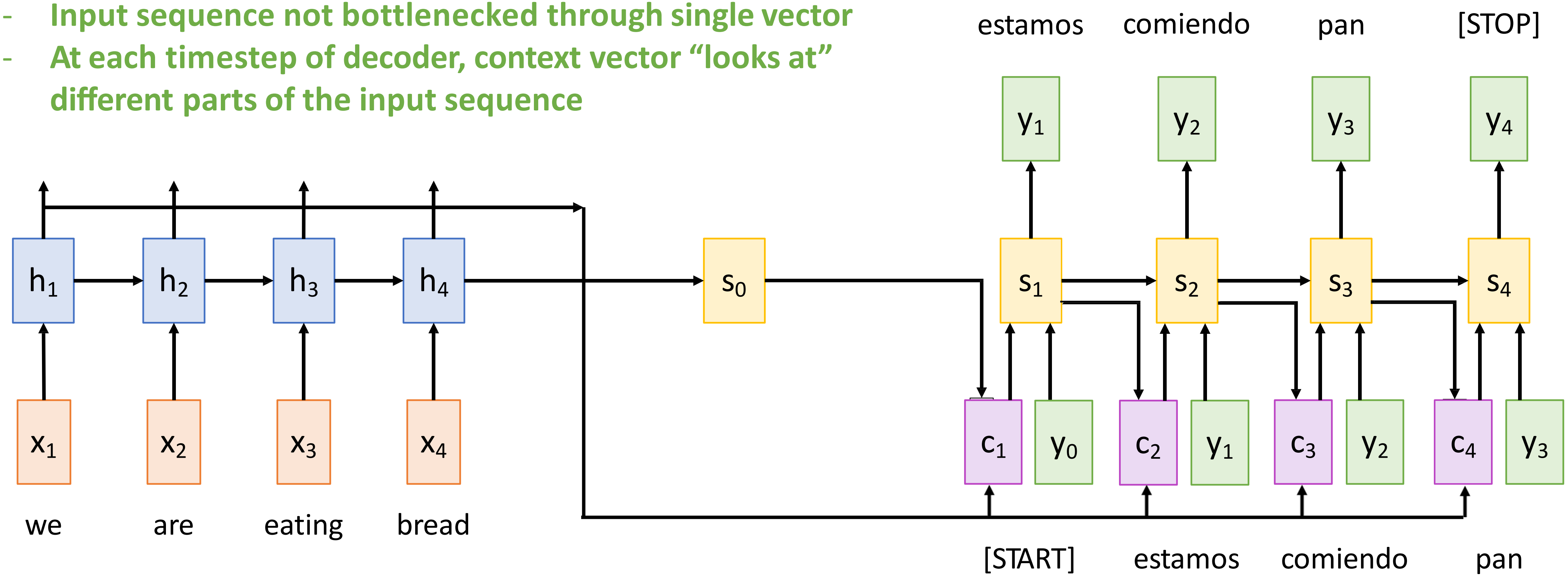
Use c_2 to compute s_2, y_2

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**



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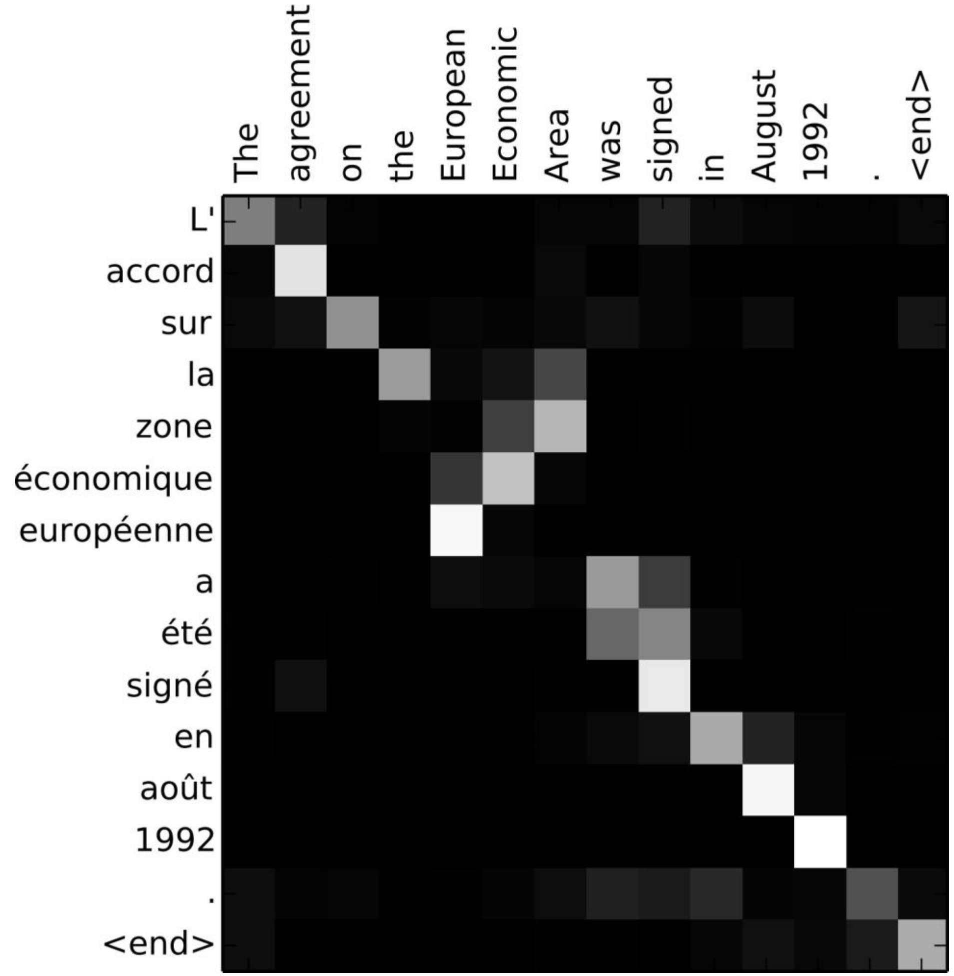
Sequence-to-Sequence with RNNs and Attention

Visualize attention weights $a_{t,i}$

Example: English to French translation

Input: “The agreement on the European Economic Area was signed in August 1992.”

Output: “L’accord sur la zone économique européenne a été signé en août 1992.”



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Sequence-to-Sequence with RNNs and Attention

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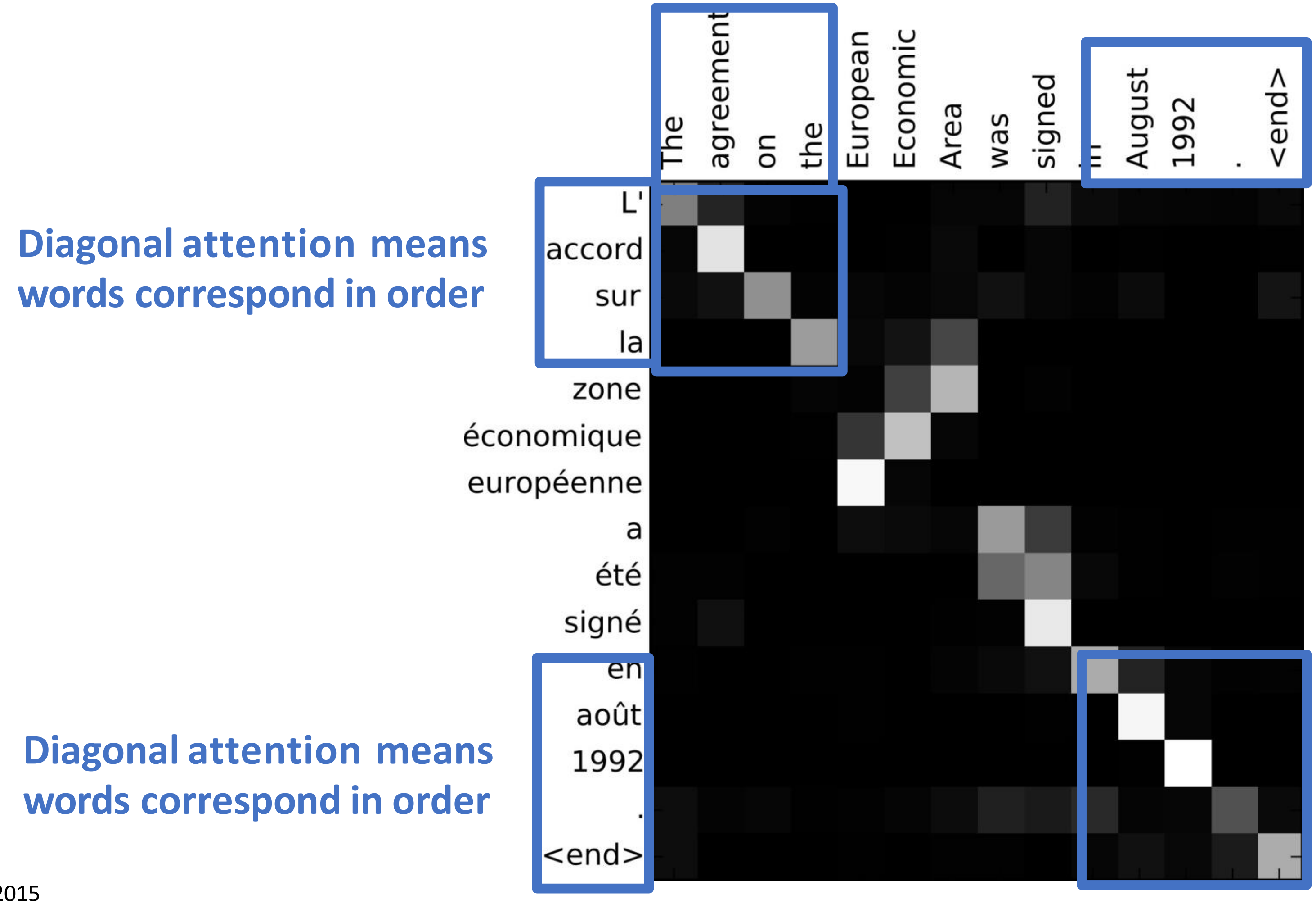

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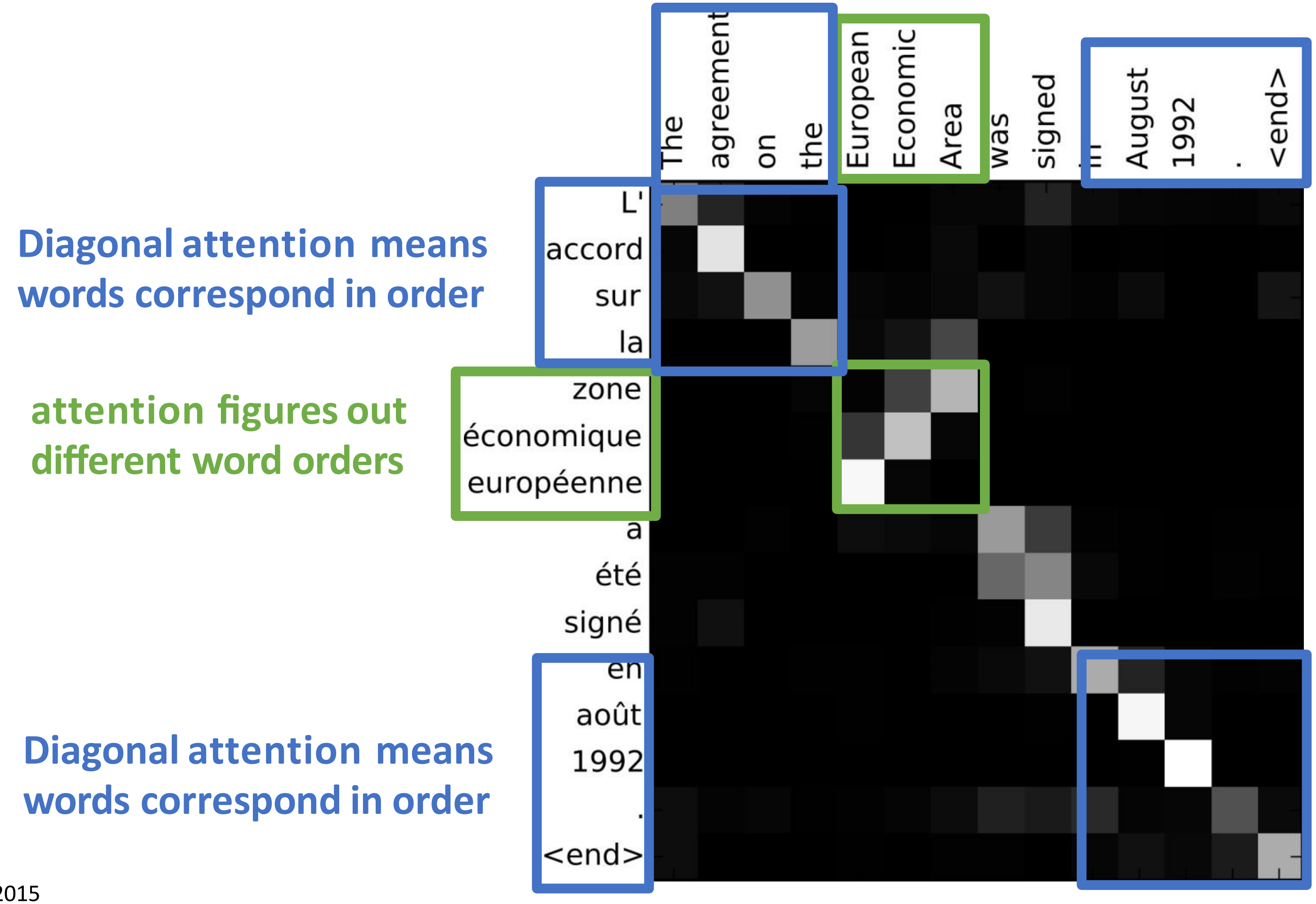

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Sequence-to-Sequence with RNNs and Attention

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 $\{h_i\}$!

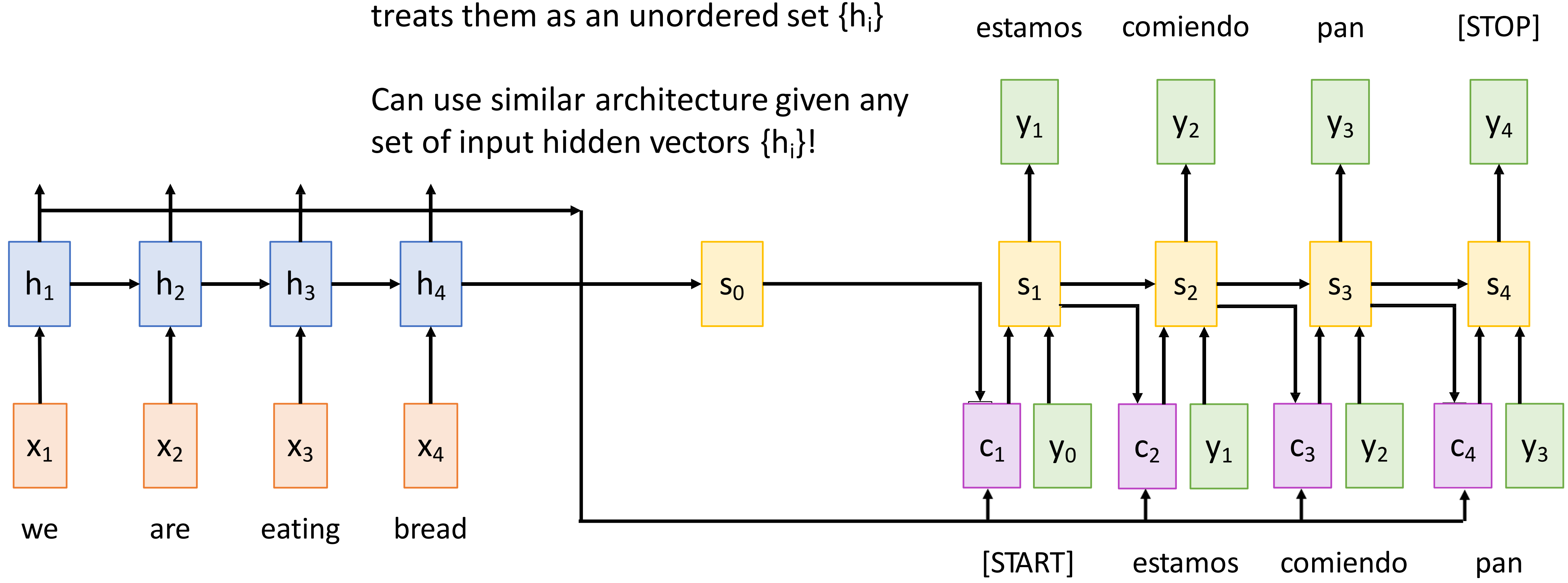

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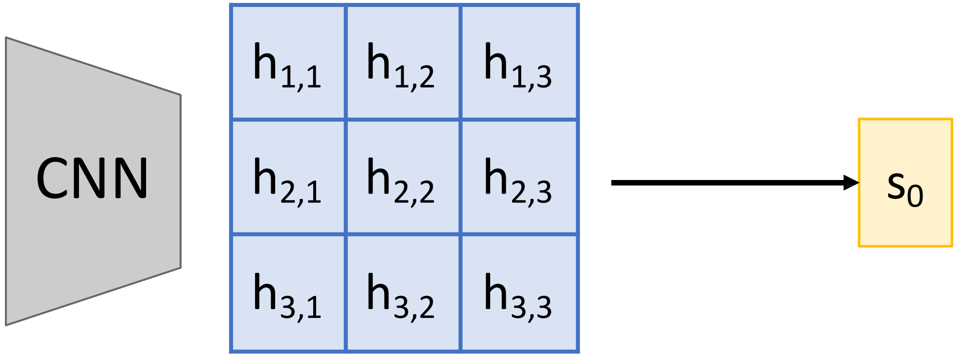
Image Captioning with RNNs and Attention

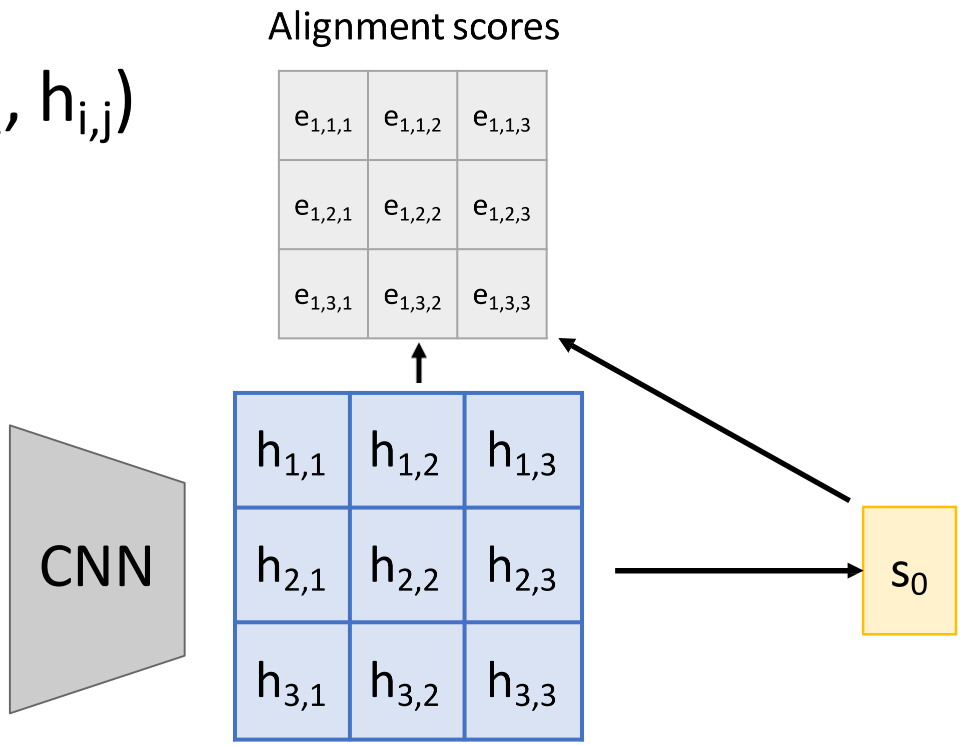


Use a CNN to compute a
grid of features for an image

Xu et al, "Show, attend, and Tell: Neural Image Cap$on Genera$on with Visual attention", ICML 2015

Image Captioning with RNNs and Attention

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



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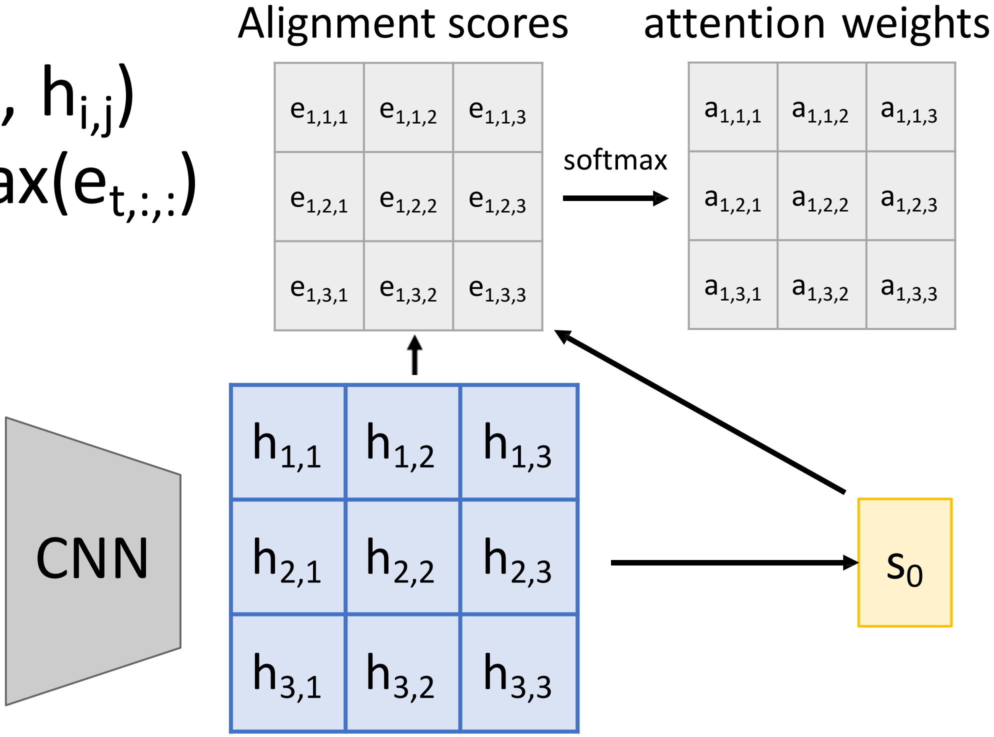
$e_{t,i,j} = f_{att}(s_{t-1}, h_{i,j})$

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



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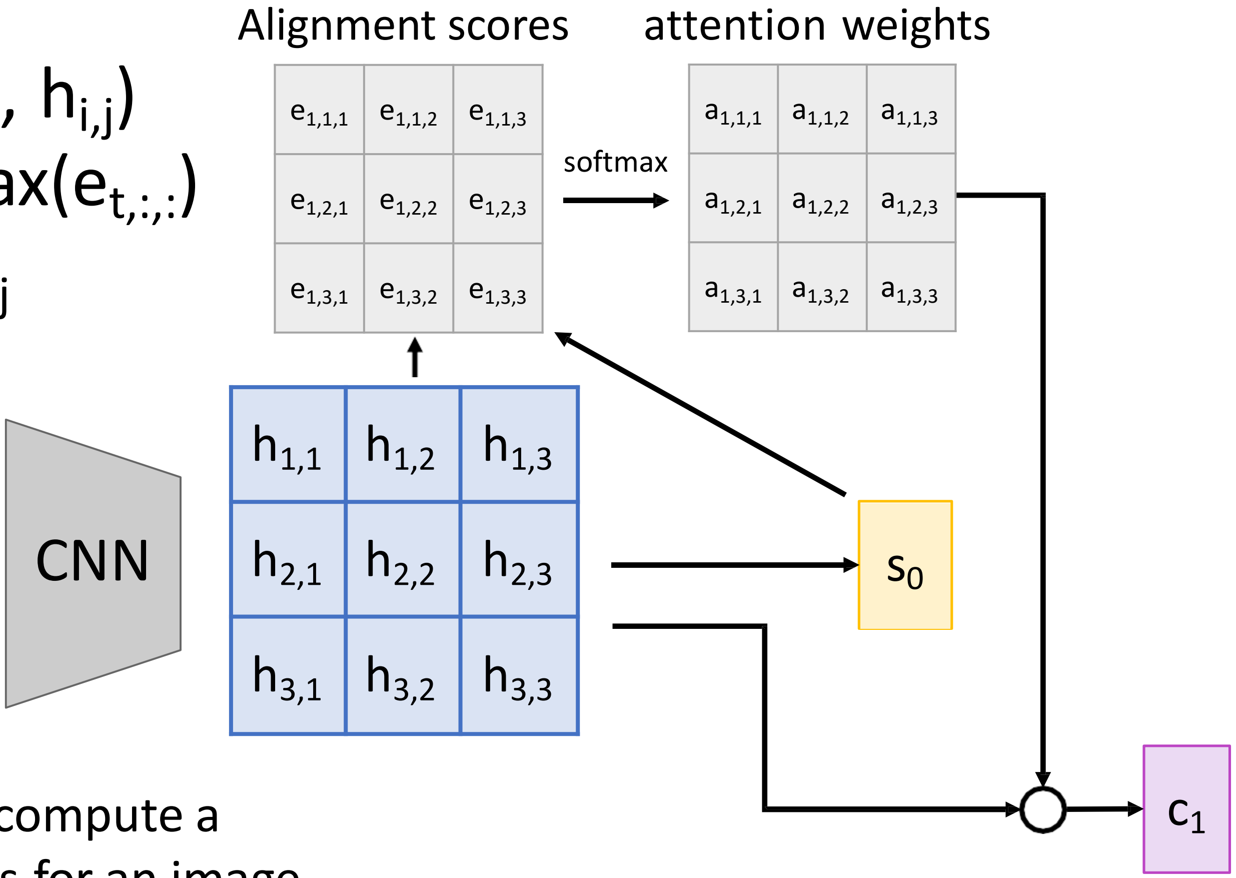

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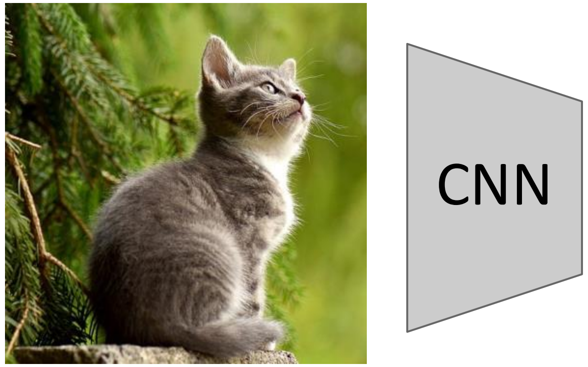

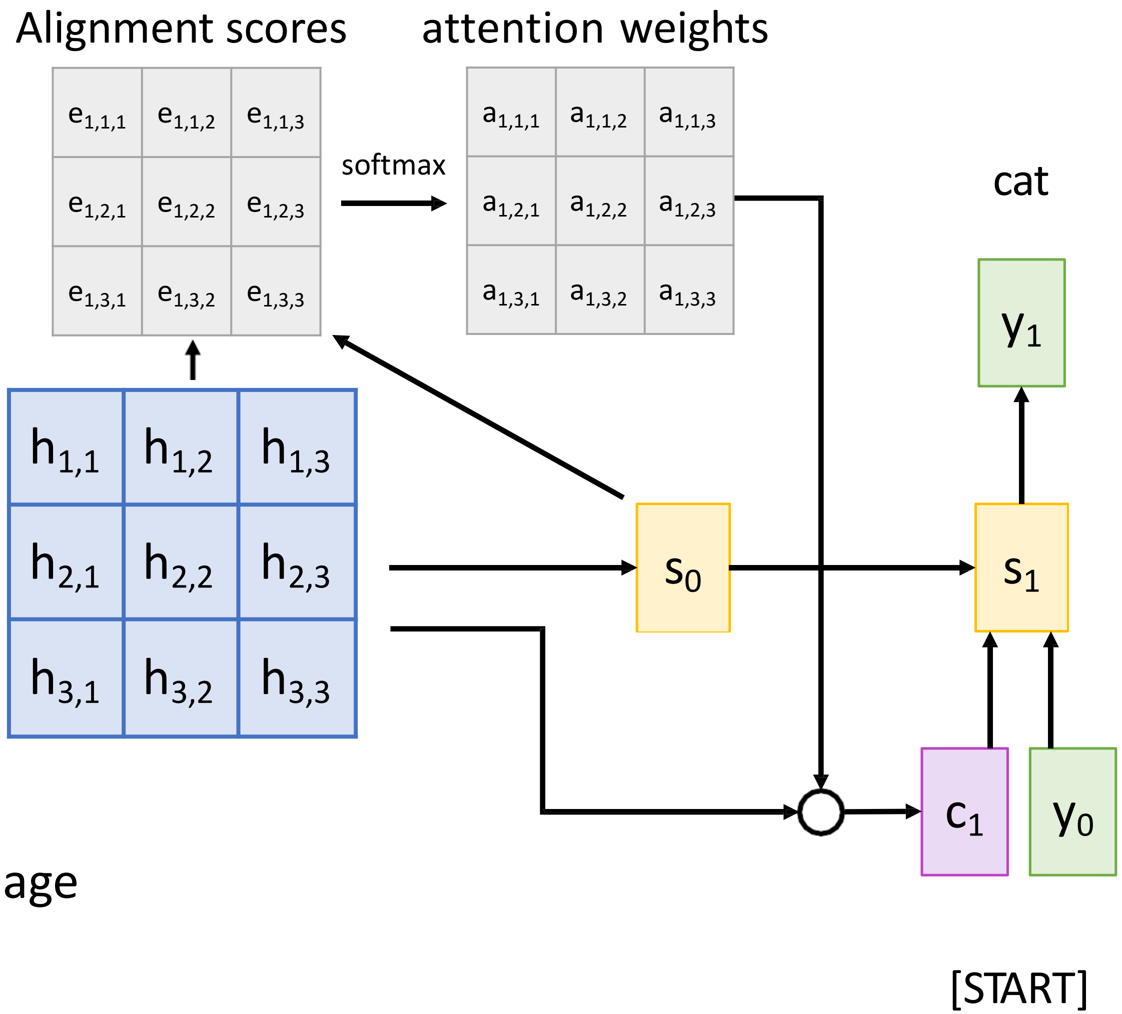

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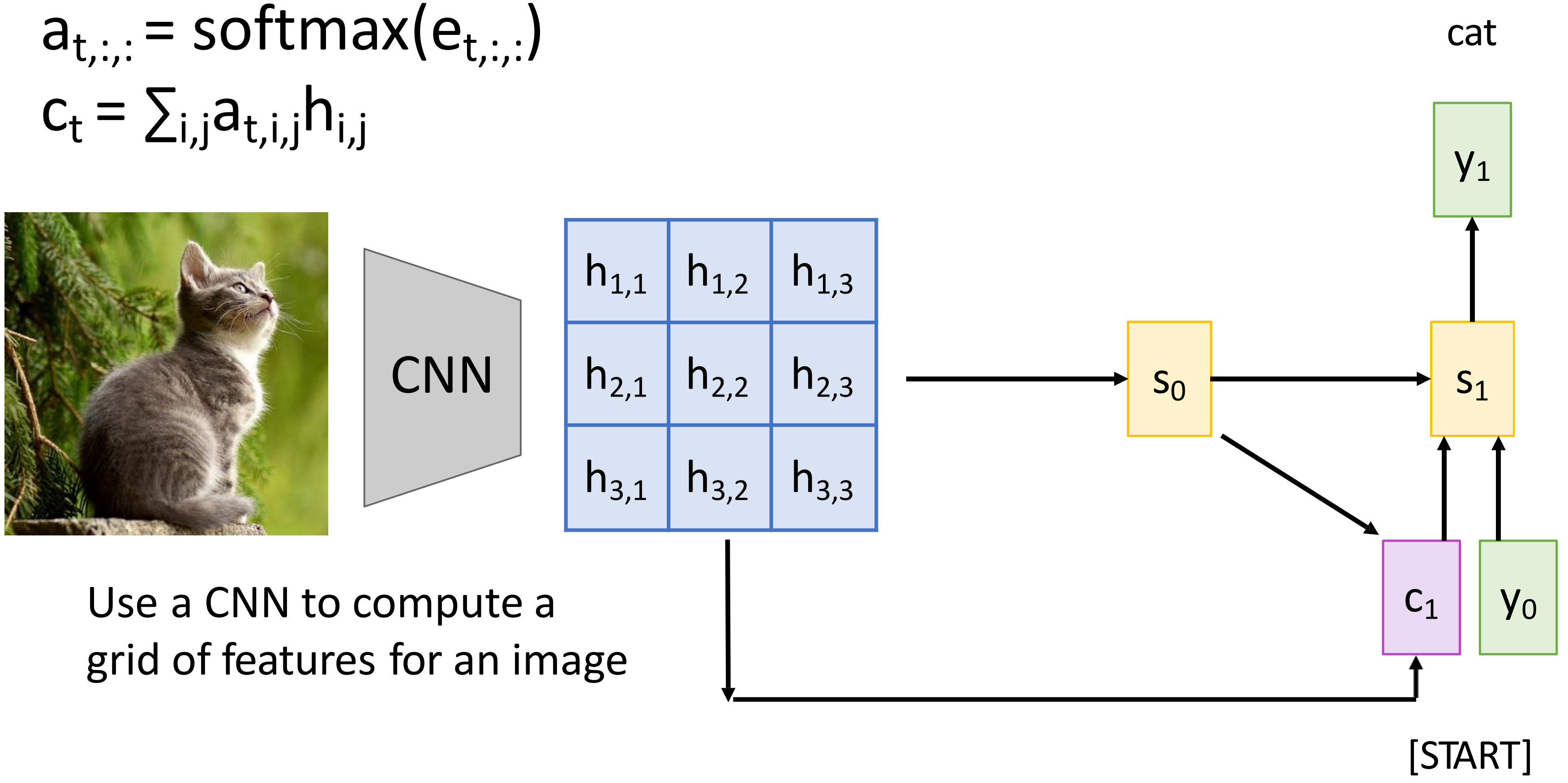

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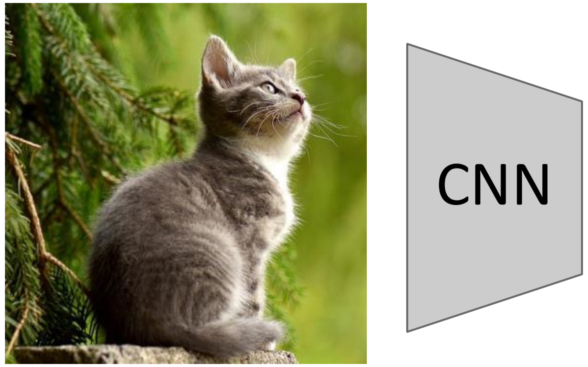

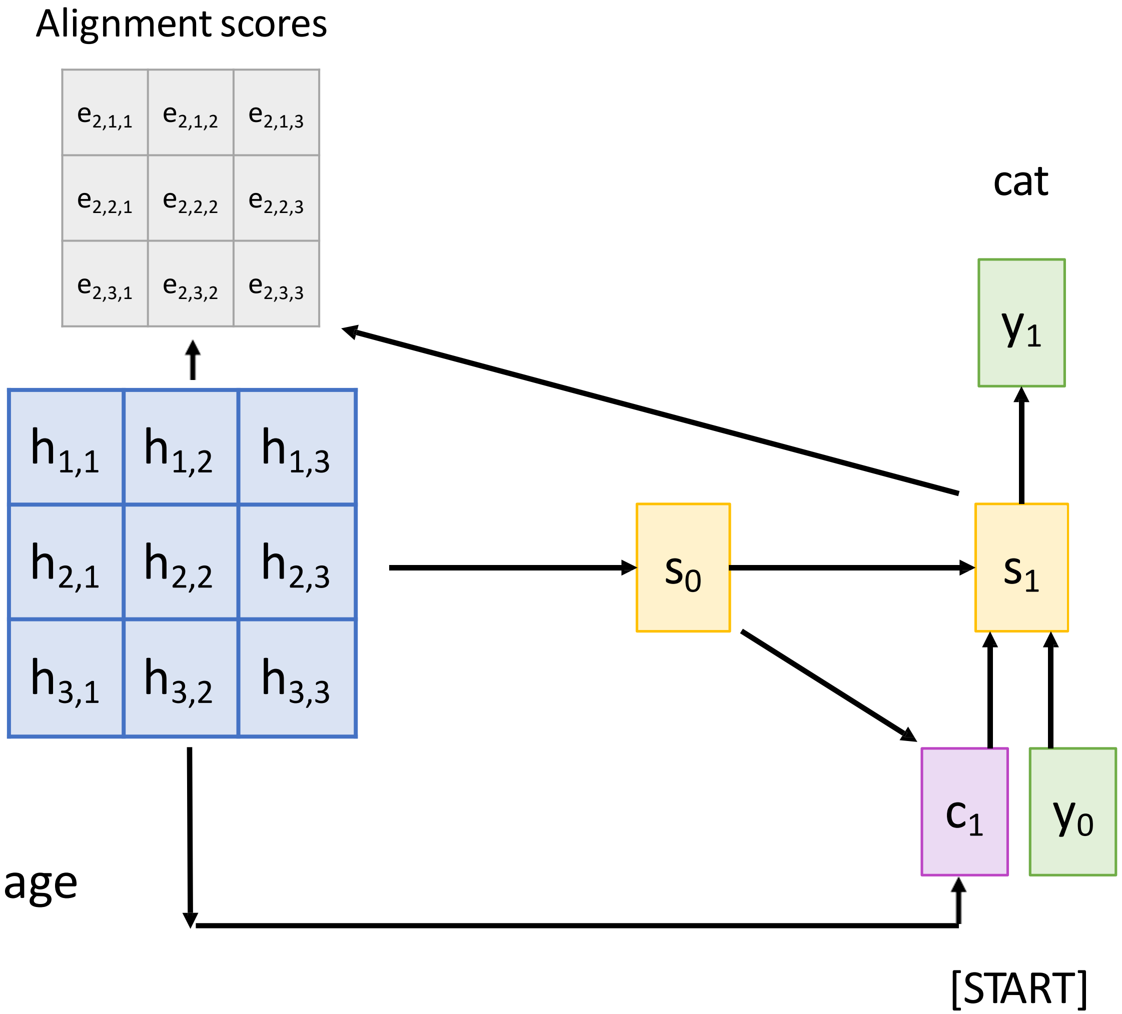

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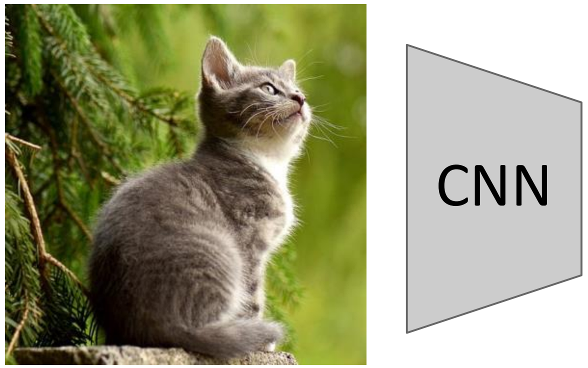
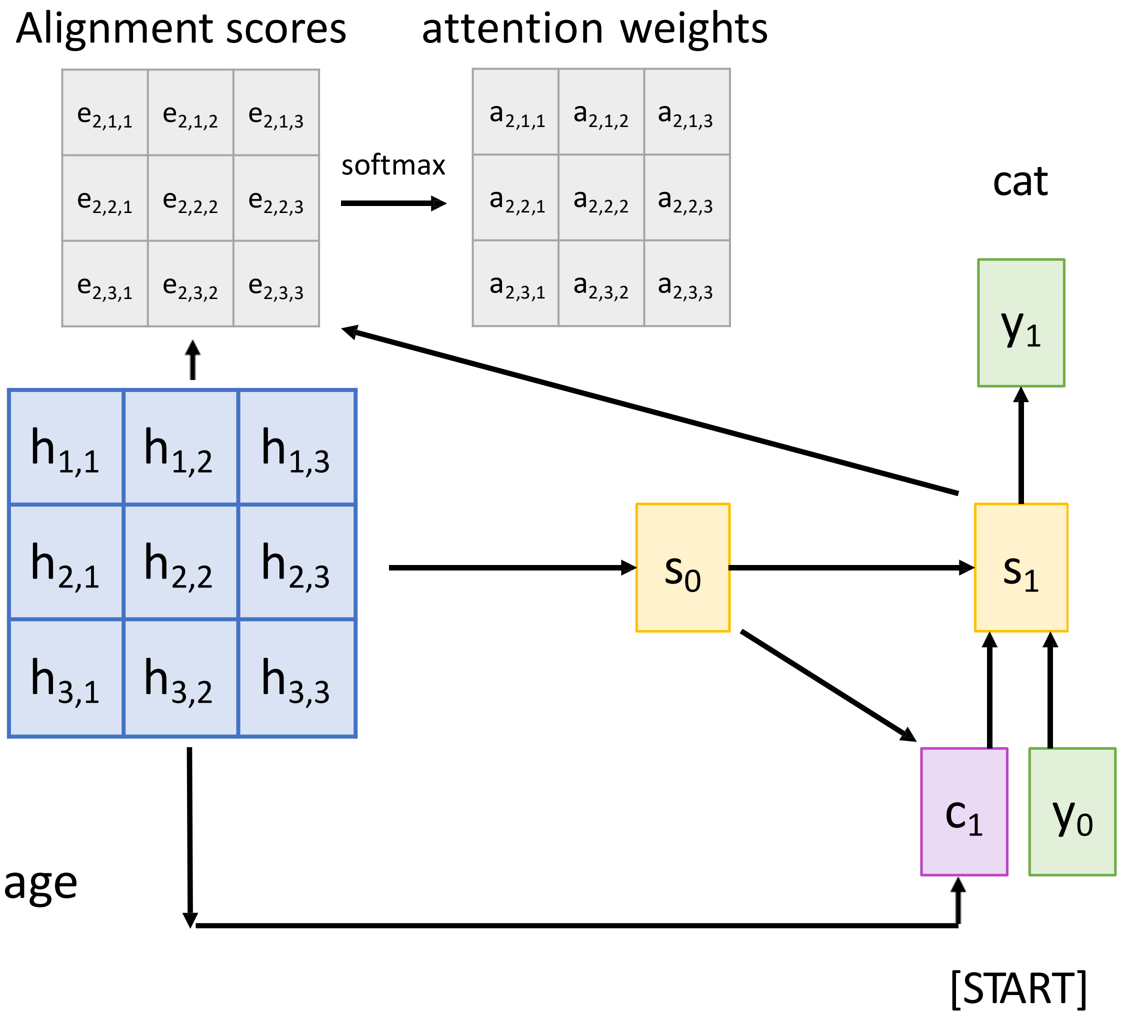


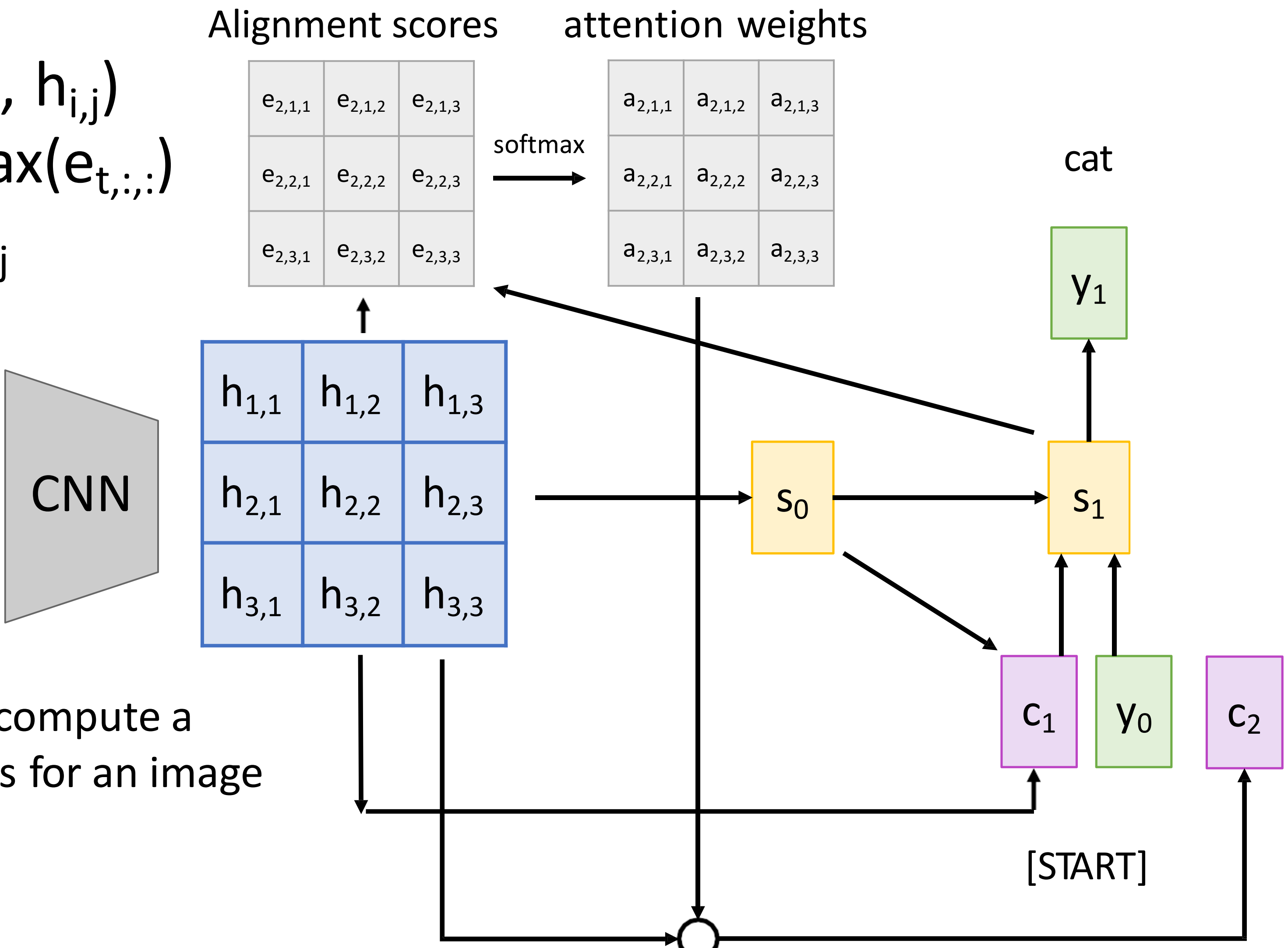


Use a CNN to compute a grid of features for an image

Xu et al, "Show, attend, and Tell: Neural Image Cap$on Genera$on with Visual attention", ICML 2015

Image Captioning with RNNs and Attention

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



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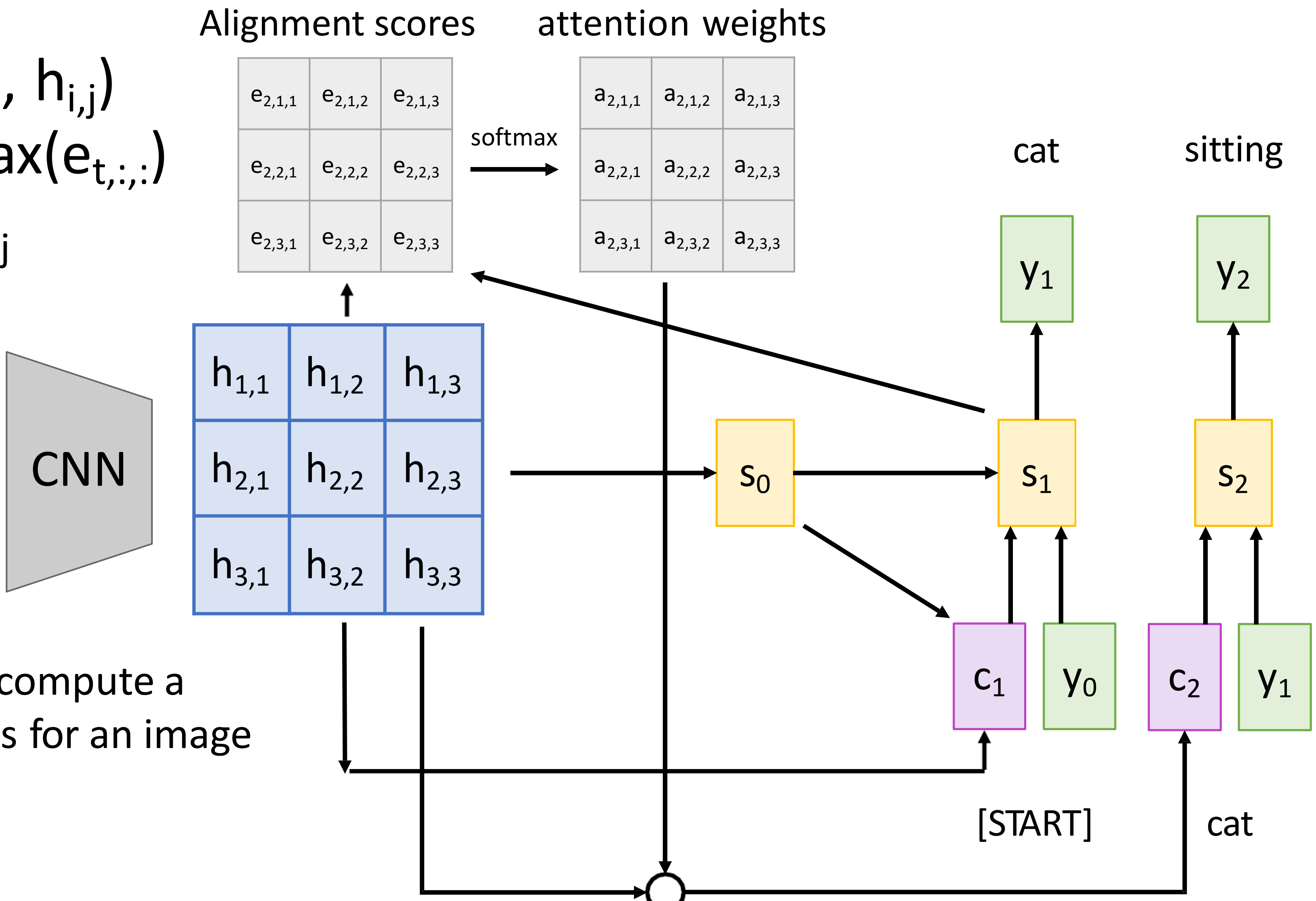

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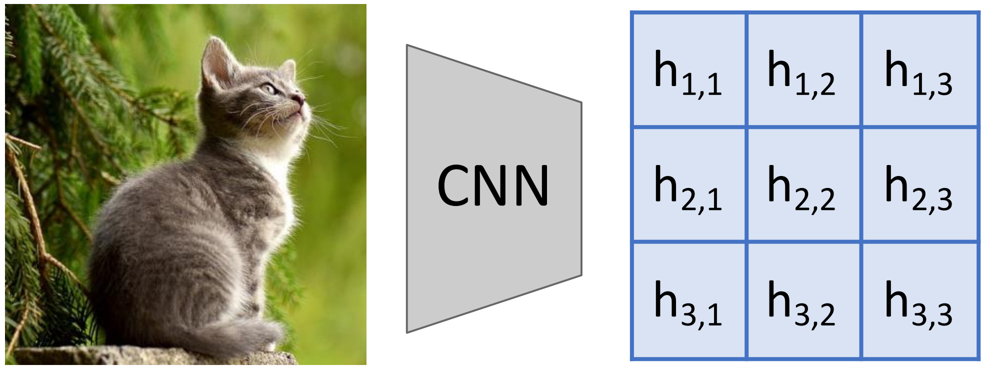
Each timestep of decoder uses a different context vector that looks at different parts of the input image



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

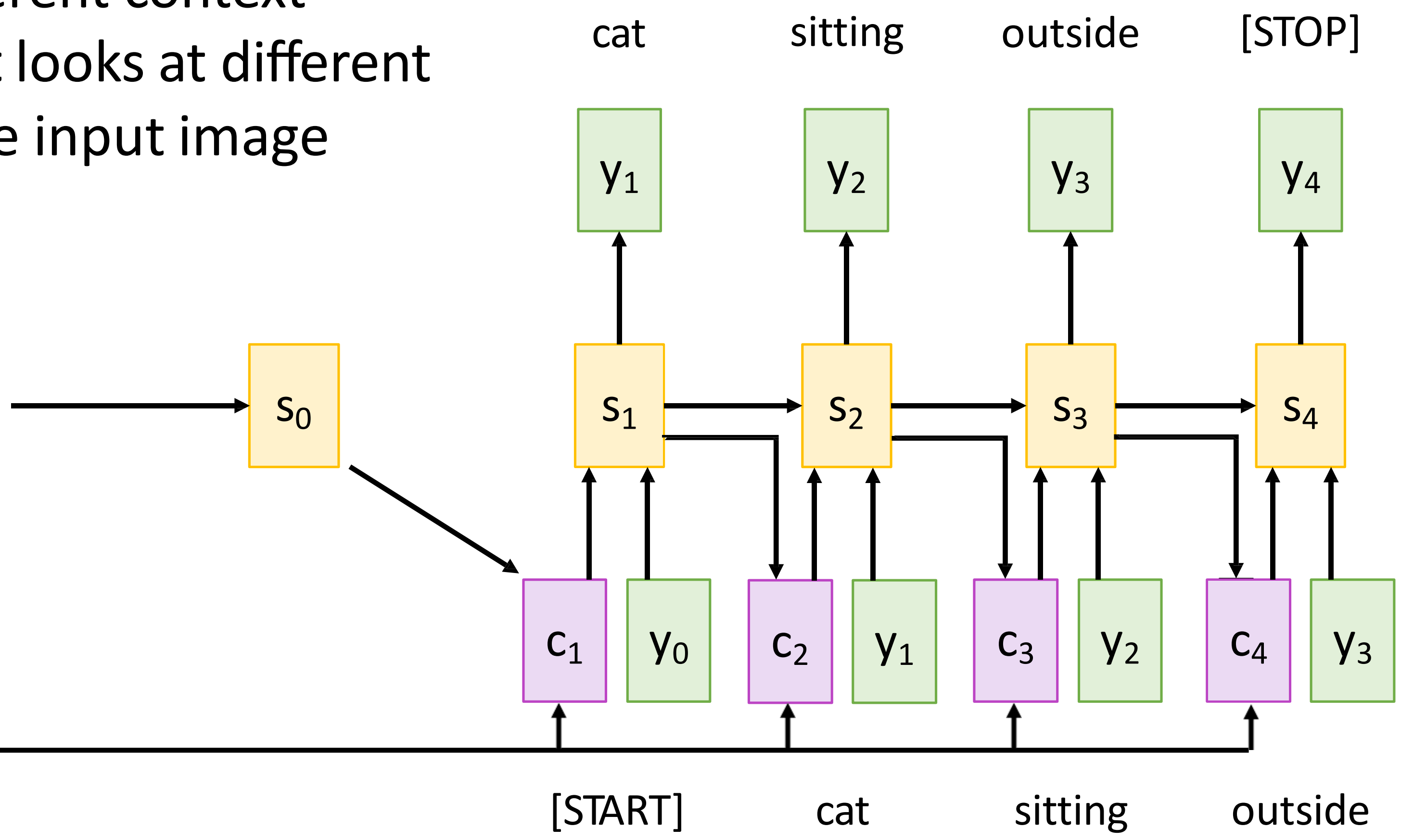


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Image Captioning with RNNs and Attention

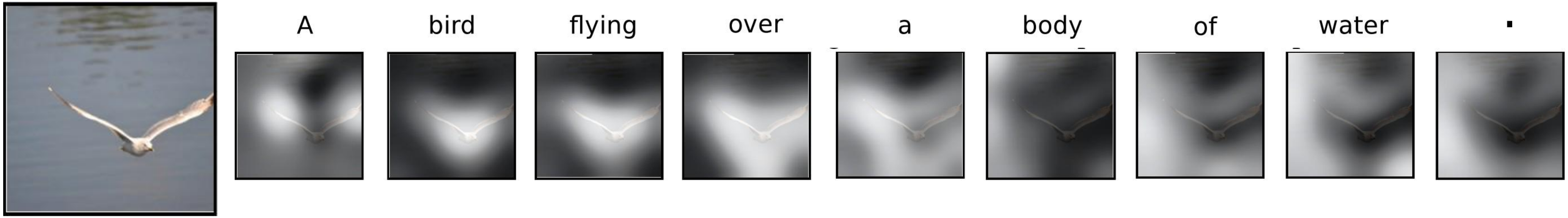

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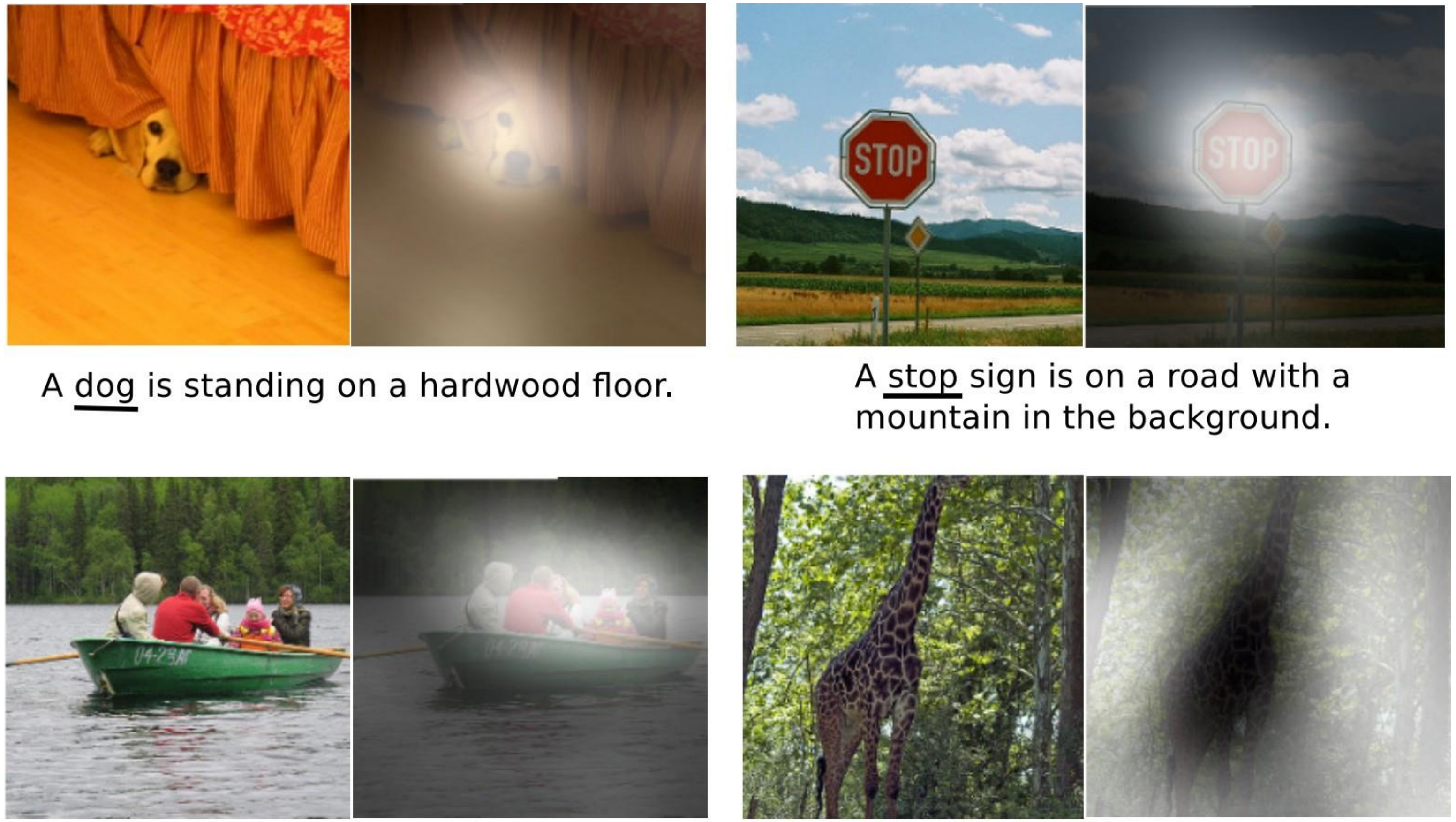
Image Captioning with RNNs and Attention



A dog is standing on a hardwood floor.

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

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

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

Xu et al, “Show, attend, and Tell: Neural Image Cap$on Genera$on with Visual attention”, ICML 2015

X, Attend, and Y

“**Show, attend, and tell**” *(Xu et al, ICML 2015)*
Look at image, attend to image regions, produce question

“**Ask, attend, and answer**” *(Xu and Sattnko, ECCV 2016)*
“**Show, ask, attend, and answer”** *(Kazemi and Elqursh, 2017)*
Read text of question, attend to image regions, produce answer

“**Listen, attend, and spell**” *(Chan et al, ICASSP 2016)*
Process raw audio, attend to audio regions while producing text

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

“**Show, attend, and interact**” *(Qureshi et al, ICRA 2017)*
Process image, attend to image regions, output robot control commands

“**Show, attend, and read**” *(Li et al, AAAI 2019)*
Process image, attend to image regions, output text

Summary

Part I

Preliminary topics:

- Recurrent neural network

Sequence-to-Sequence with RNNs and Attention

- Image Captioning with RNNs and Attention

Part II

Self-Attention Layer

The Transformer