Topics:

- Transformers

CS 8803-VLM
ZSOLT KIRA

Many slides by Justin Johnson

- Read over the website!
- Read up on Deep Learning, Transformers
- **After announcement, sign up for presenting a paper**
  - See the schedule for dates of project proposal, mid-project update, and final presentations.
  - Reminder: Please sign up for onloy one session.
  - Sessions are topic-focused. If there are other papers you recommend or want to present in addition to or instead of, let us know! We will take a look at the quality/relevance and approve.
  - The first one is next Tuesday 09/02 so it would be great to have someone sign up for that one ASAP!

Deep Learning Fundamentals

Linear classification
Loss functions
Optimization
Optimizers
Backpropagation
Computation Graph
Multi-layer Perceptrons

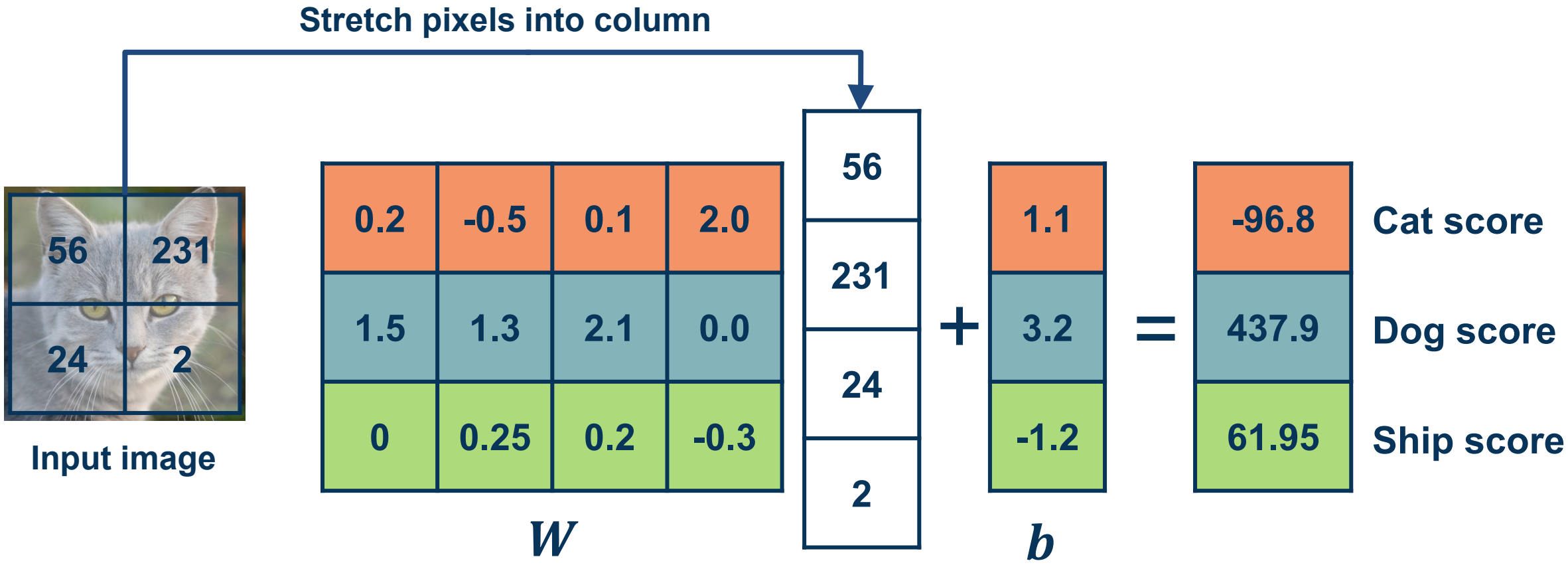
Neural Network Components and Architectures

Hardware & software
Convolutions
Convolution Neural Networks
Pooling
Activation functions
Batch normalization
Transfer learning
Data augmentation
Architecture design
RNN/LSTMs
Attention & Transformers

Applications & Learning Algorithms

Semantic & instance Segmentation
Reinforcement Learning
Large-language Models
Variational Autoencoders
Diffusion Models
Generative Adversarial Nets
Self-supervised Learning
Vision-Language Models
VLM for Robotics

Example with an image with **4 pixels**, and **3 classes (cat/dog/ship)**



Adapted from slides by Fei-Fei Li, Justin Johnson, Serena Yeung, from CS 231n

- We can find the steepest descent direction by computing the **derivative (gradient):**

$$f'(a) = \lim_{h \to 0} \frac{f(a+h) - f(a)}{h}$$

- Steepest descent direction is the **negative gradient**
- **Intuitively:** Measures how the function changes as the argument a changes by a small step size
  - As step size goes to zero
- **In Machine Learning:** Want to know how the **loss function** changes **as weights** are varied
  - Can consider each parameter separately by taking **partial derivative** of loss function with respect to that parameter

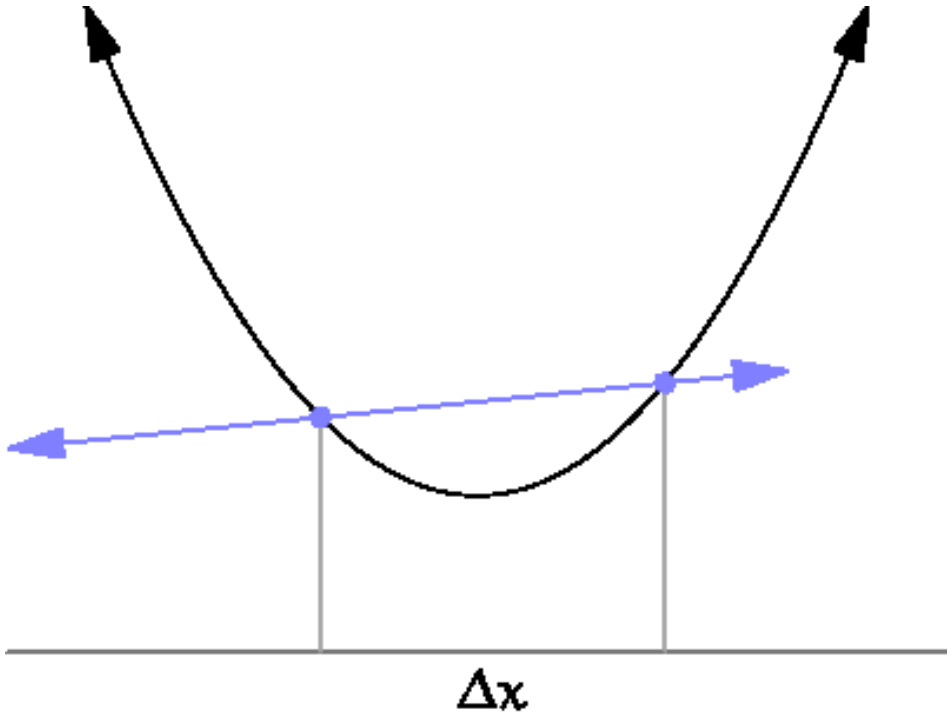
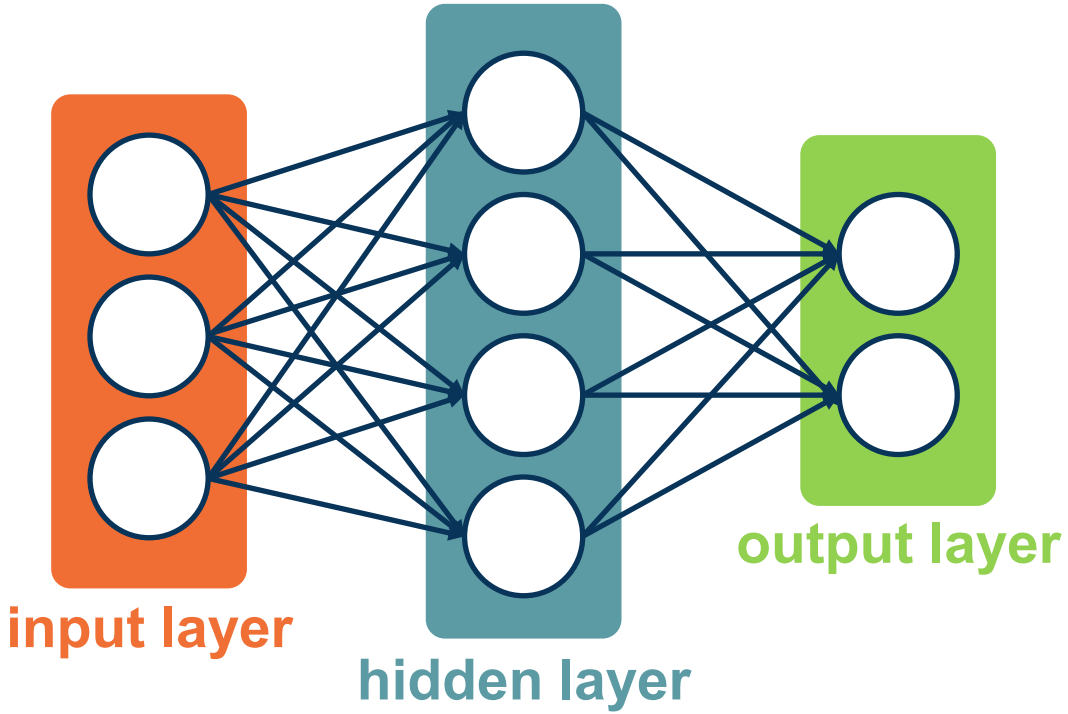


Image and equation from: https://en.wikipedia.org/wiki/Derivative#/media/File:Tangent_animation.gif

The same two-layered neural network **corresponds to adding another weight matrix**

- We will prefer the linear algebra view, but use some terminology from neural networks (& biology)



$$x \quad W_1 \quad W_2$$

$$=$$

$$f(x, W_1, W_2) = \sigma(W_2\sigma(W_1 x))$$

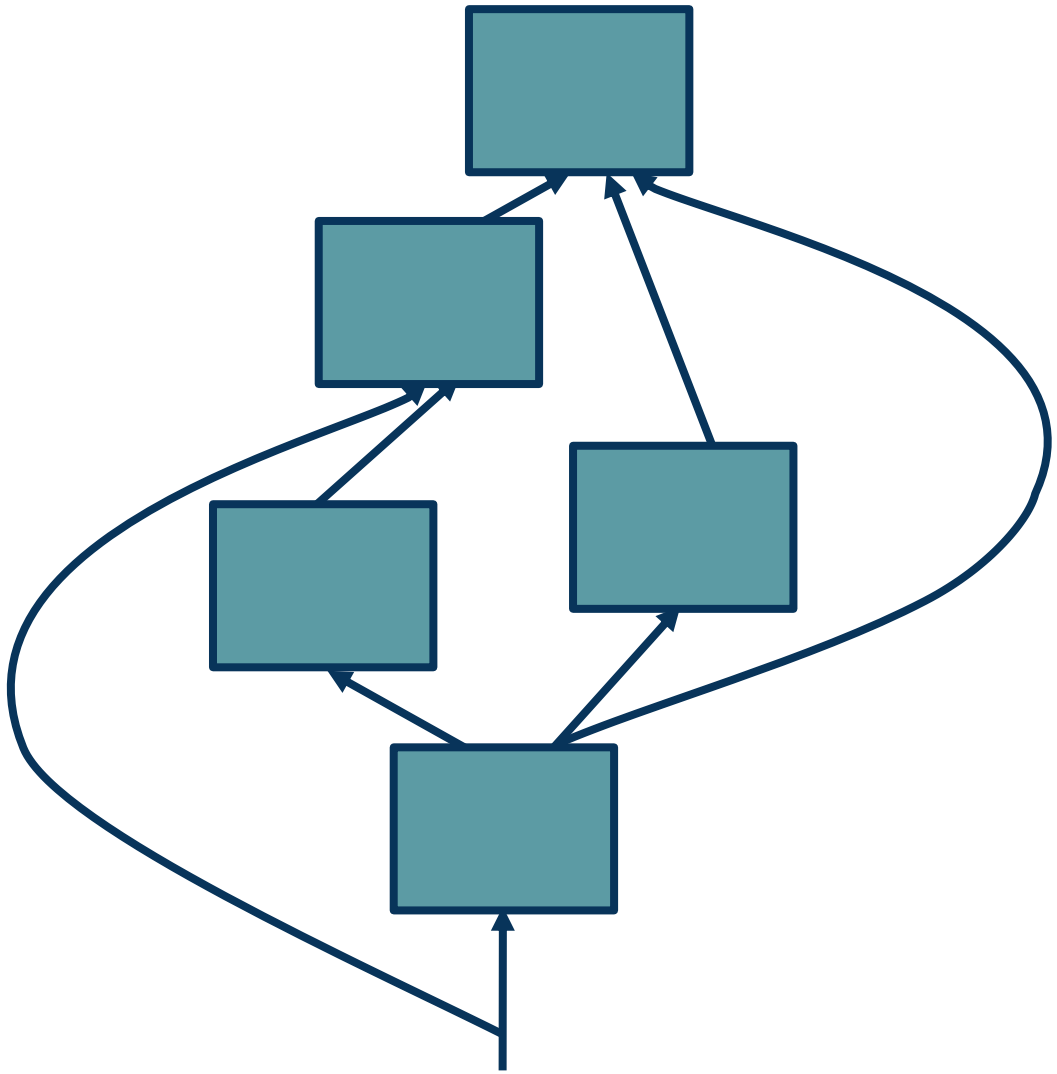
Figure adapted from slides by Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n

To develop a general algorithm for this, we will view the function as a **computation graph**

Graph can be any **directed acyclic graph (DAG)**

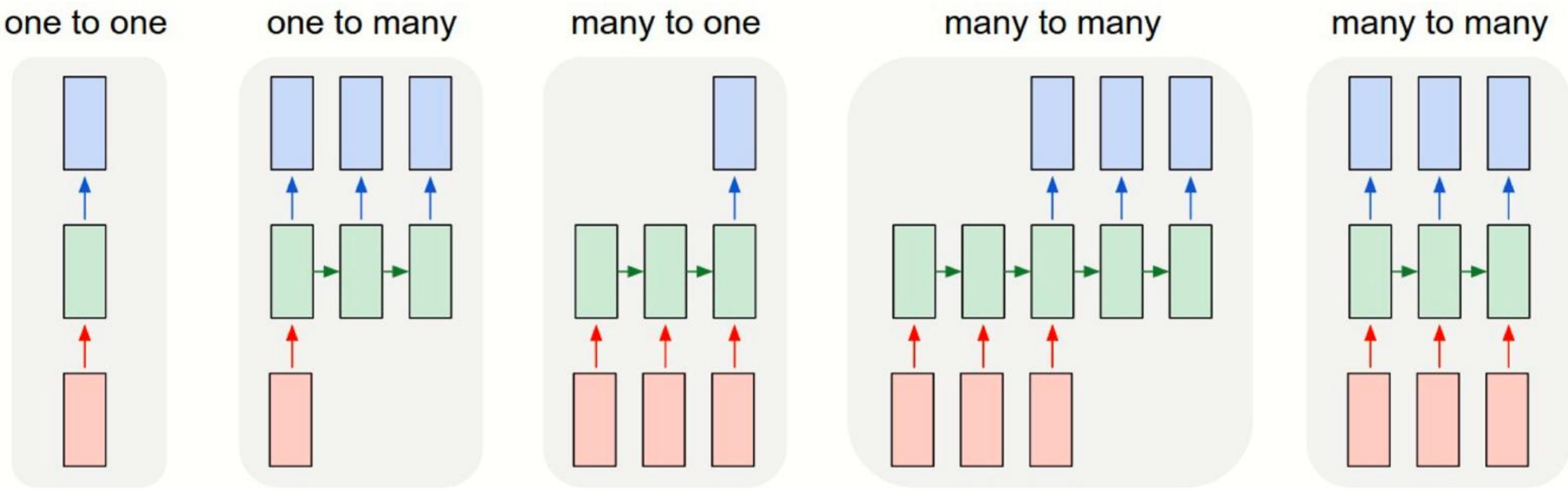
- Modules must be differentiable to support gradient computations for gradient descent

A **training algorithm** will then process this graph, **one module at a time**

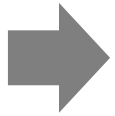


Adapted from figure by Marc'Aurelio Ranzato, Yann LeCun

Task: Sequence to Sequence Modeling

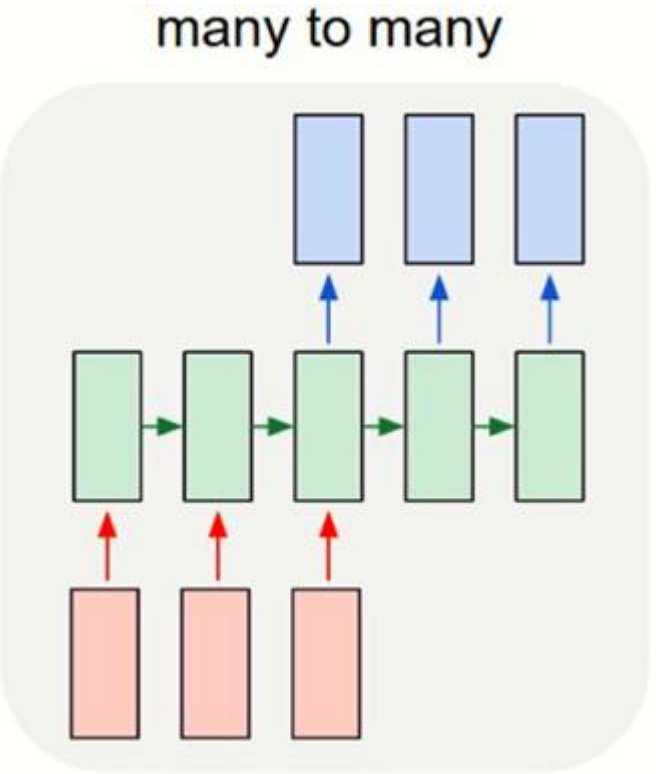


Machine Translation

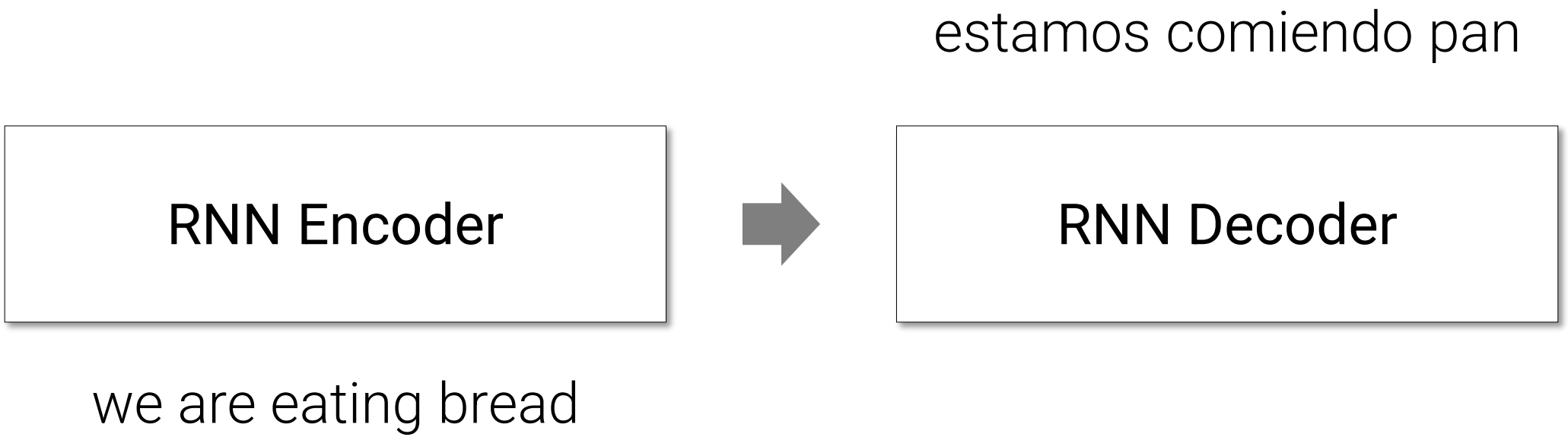
we are eating bread  estamos comiendo pan

Some Important Concepts

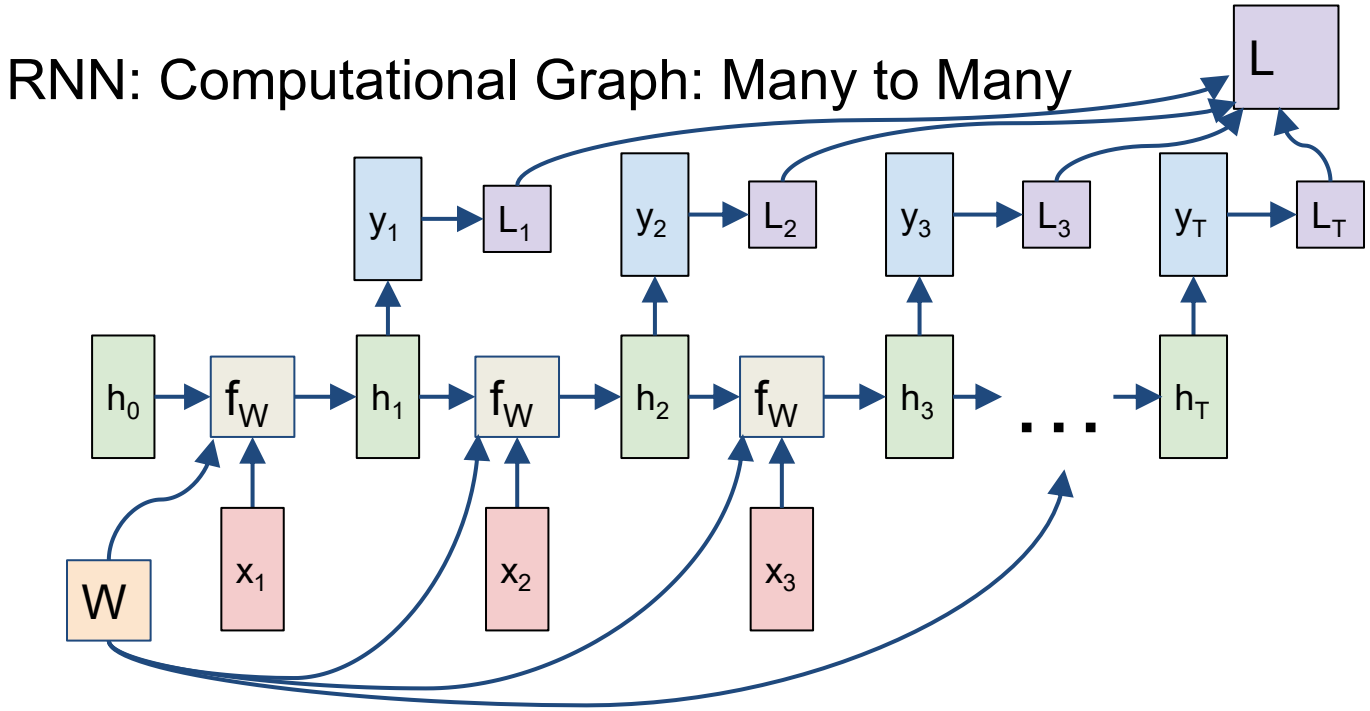
- Propagation of information (forward)
  - Mixing!
  - Two entangled things: Encoded input, state of decoding
- Propagation of gradients backwards



Machine Translation

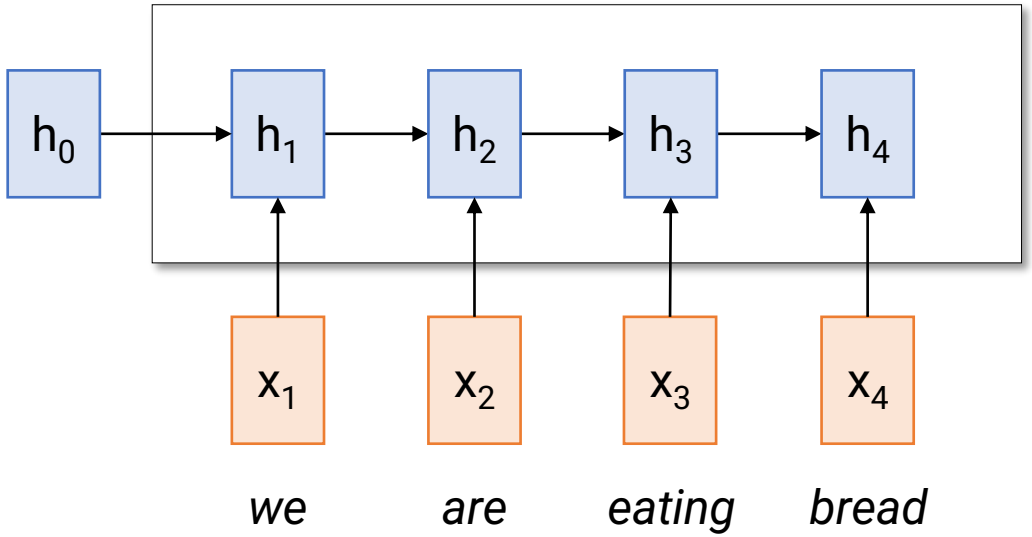


Model: Recurrent Neural Network



Machine Translation with RNNs

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

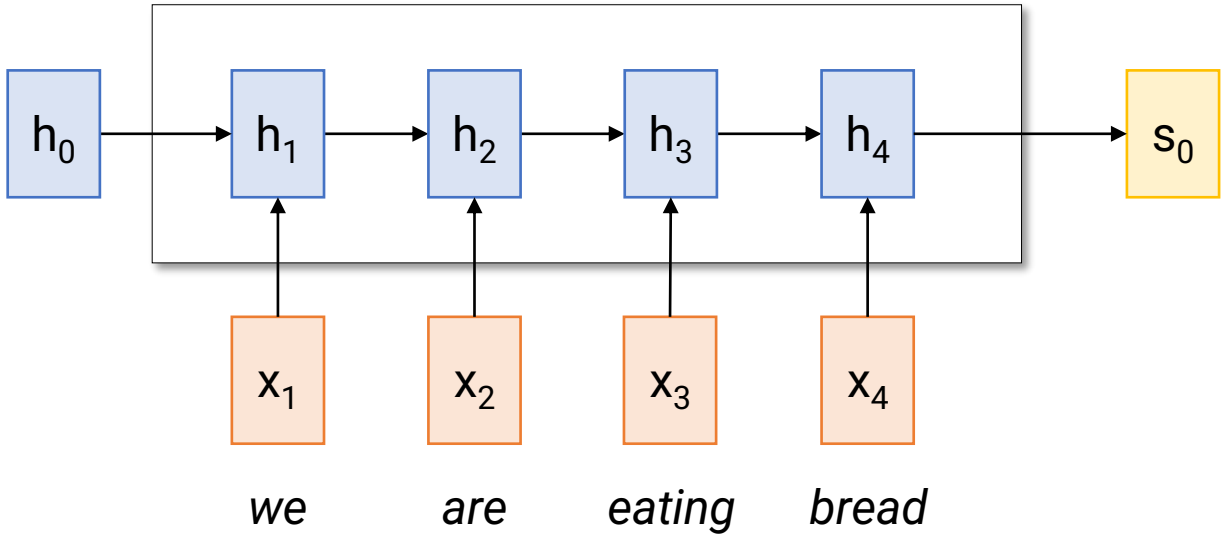


Slide credit: Justin Johnson

Machine Translation with RNNs

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

$s_0 = h_4$

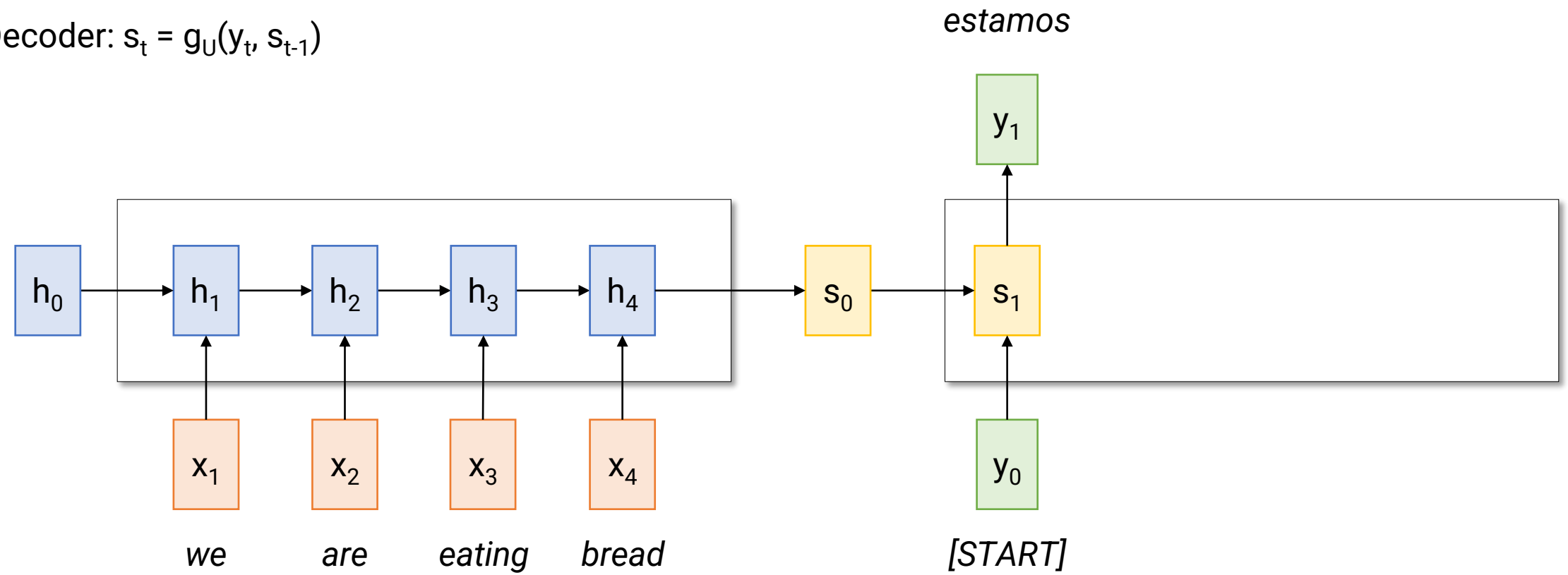


Slide credit: Justin Johnson

Machine Translation with RNNs

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

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



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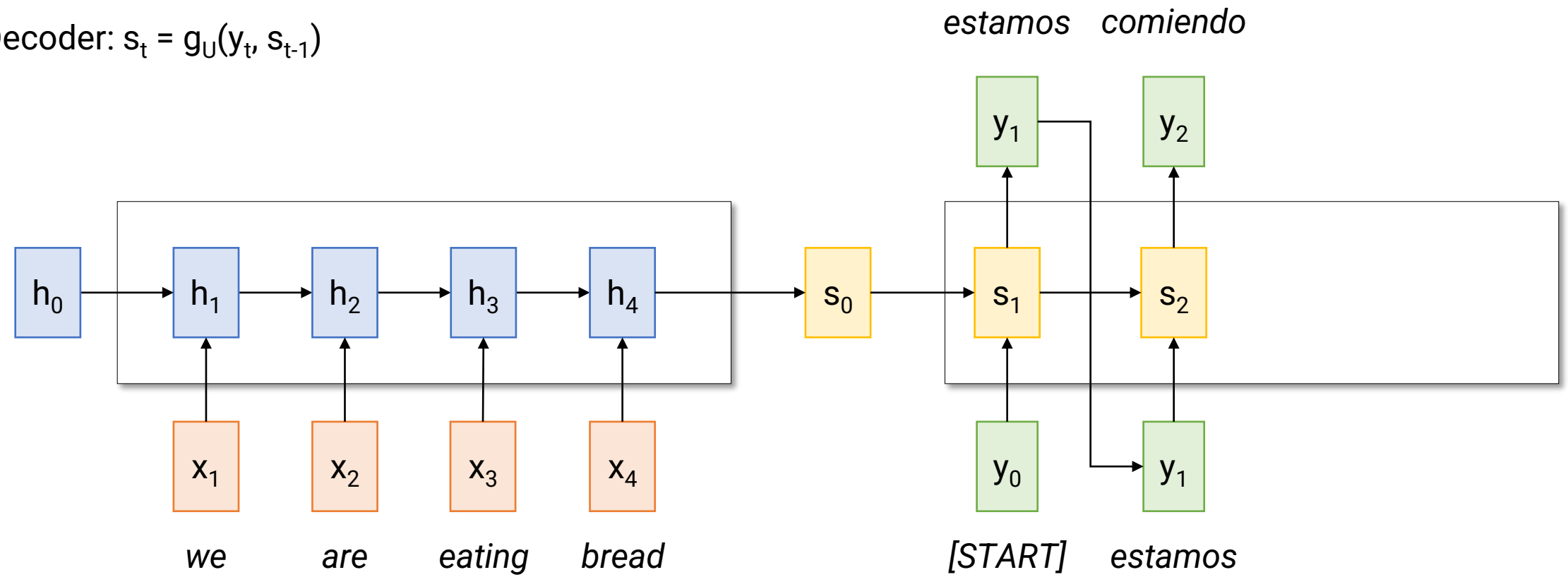

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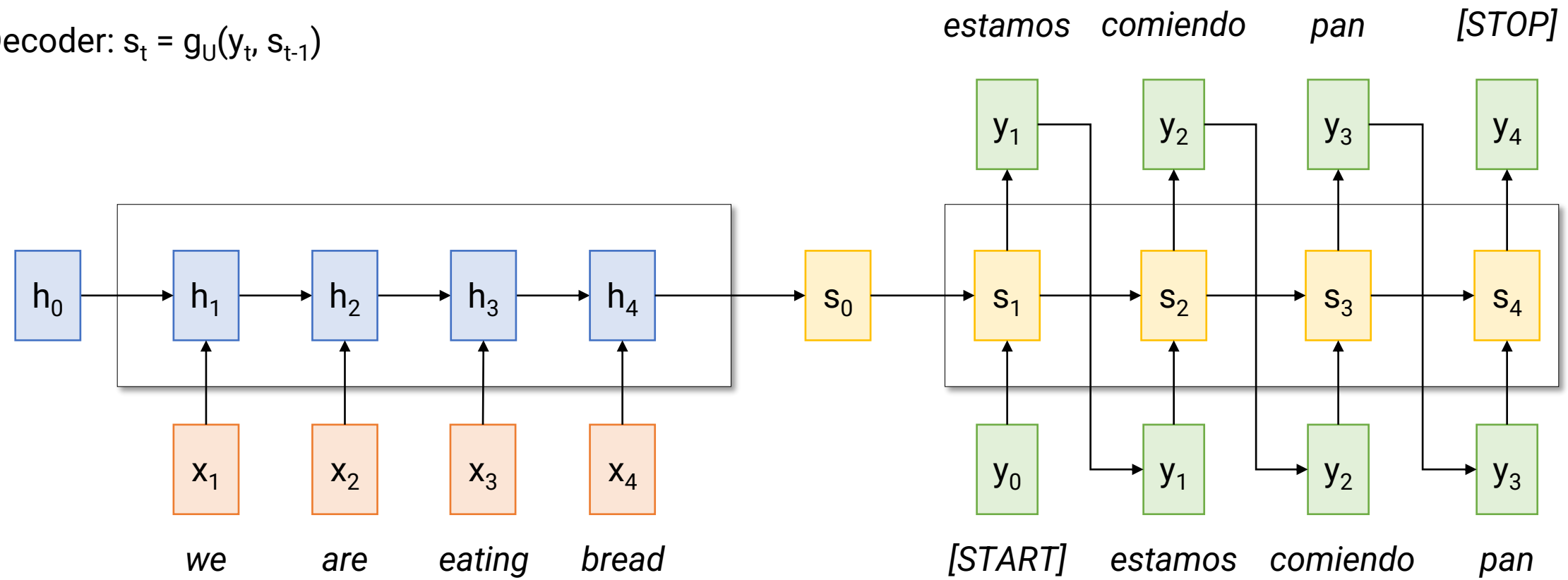

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Machine Translation with RNNs

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

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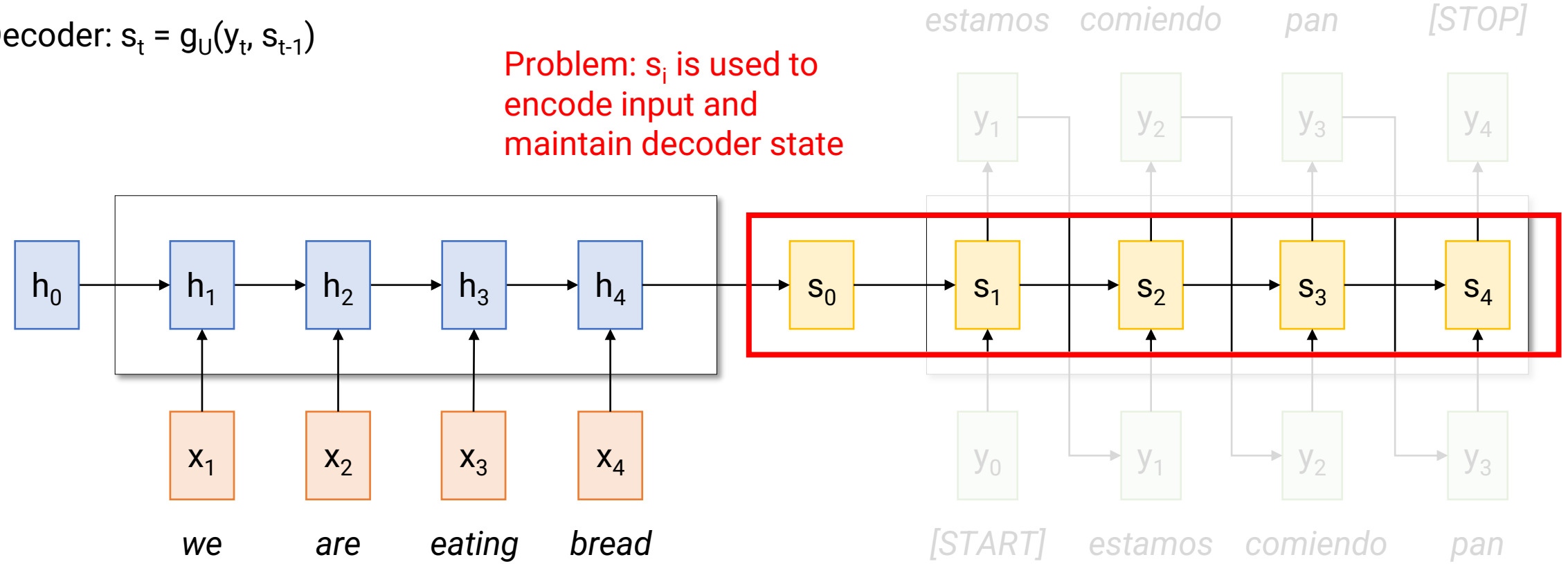
Problem: s_i is used to encode input and maintain decoder state



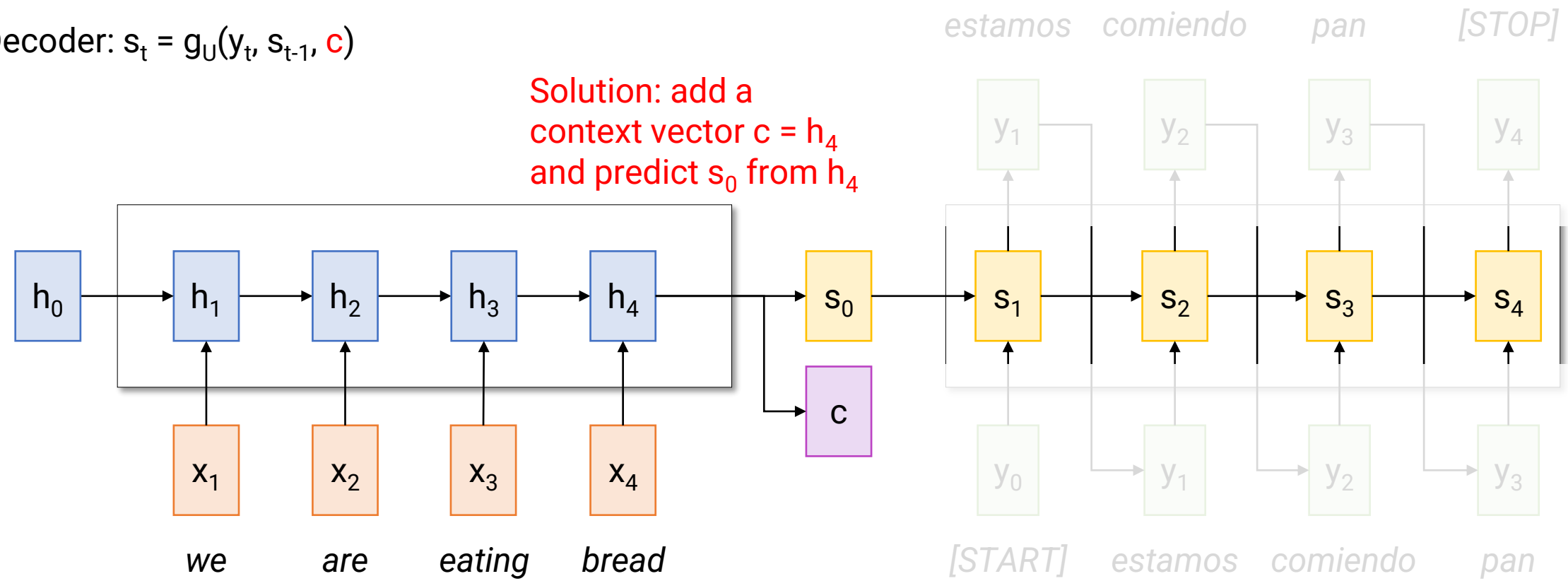
Slide credit: Justin Johnson

Machine Translation with RNNs

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

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

Solution: add a context vector $c = h_4$ and predict s_0 from h_4



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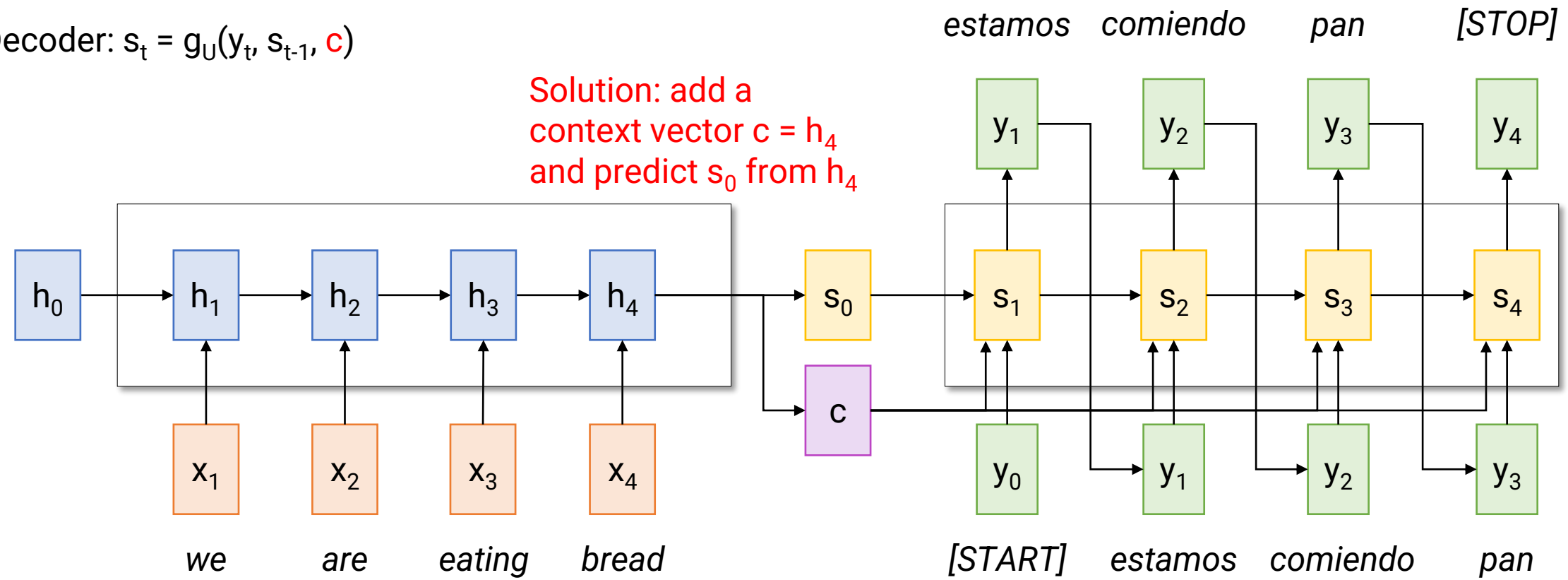

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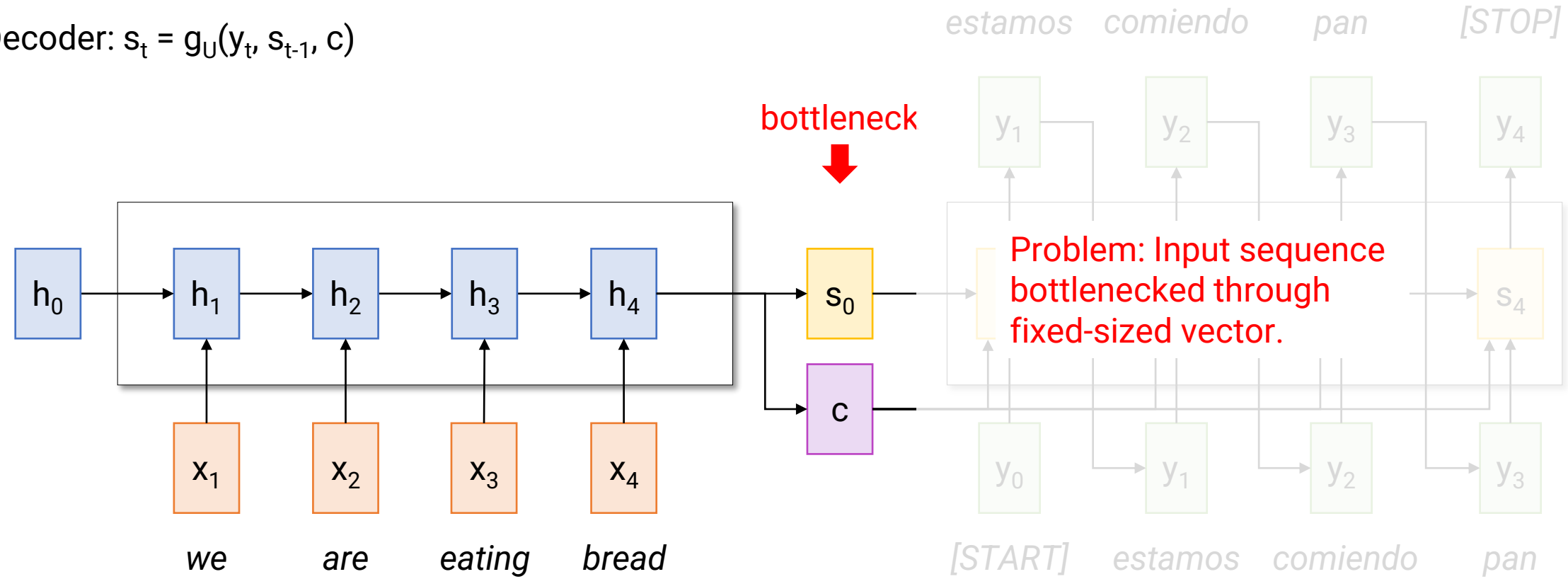

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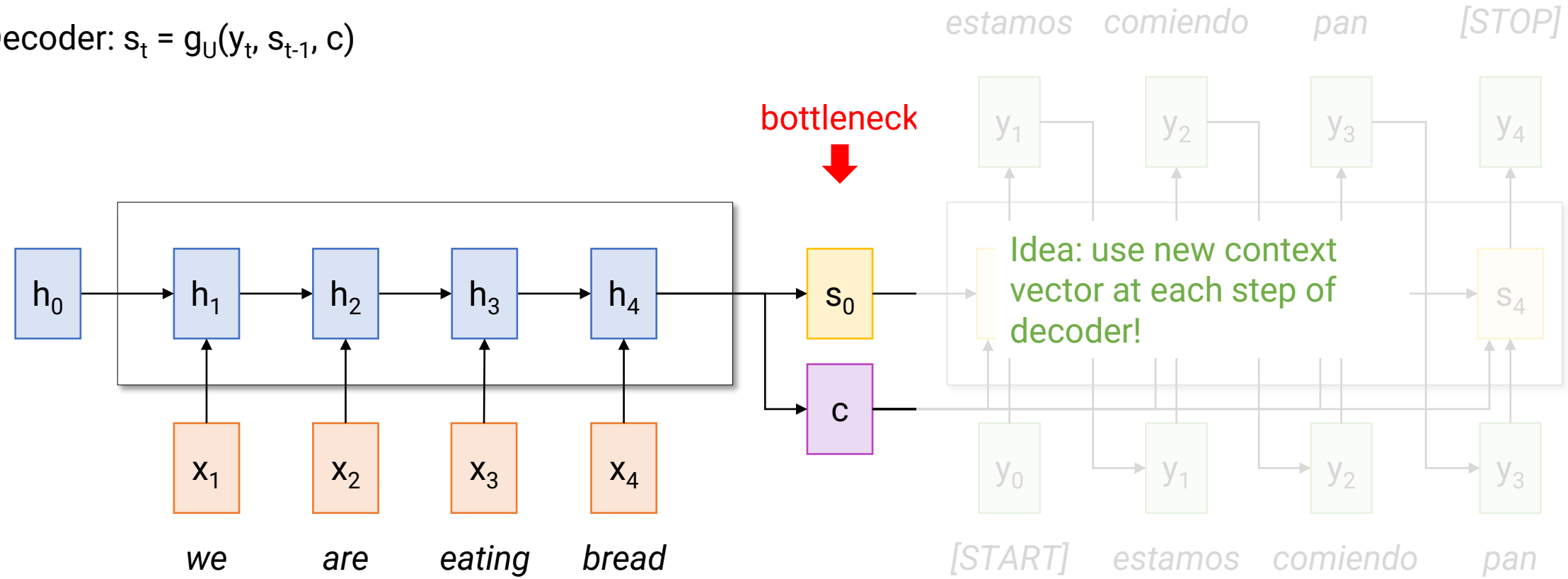
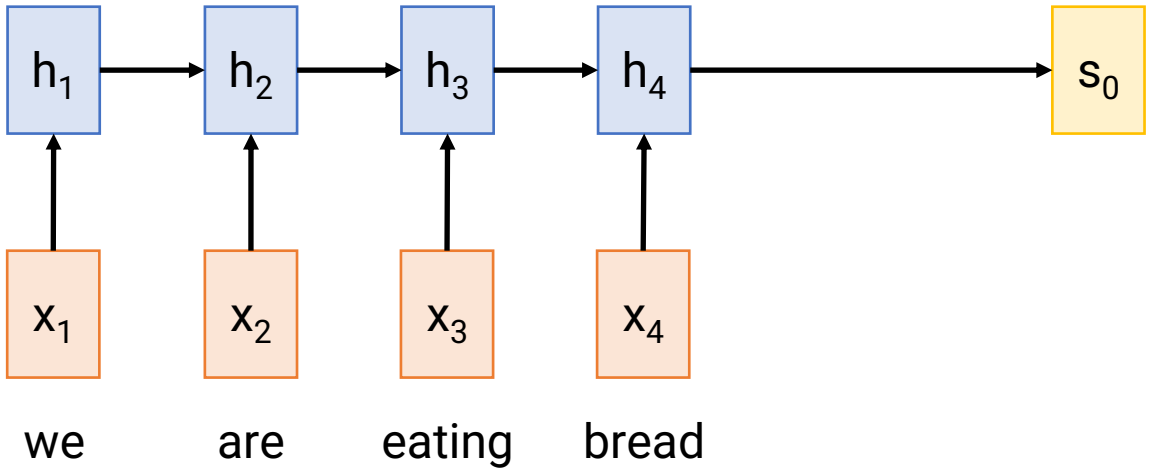


Slide credit: Justin Johnson

Machine Translation with RNNs **and Attention**

From final hidden state:
Initial decoder state s_0



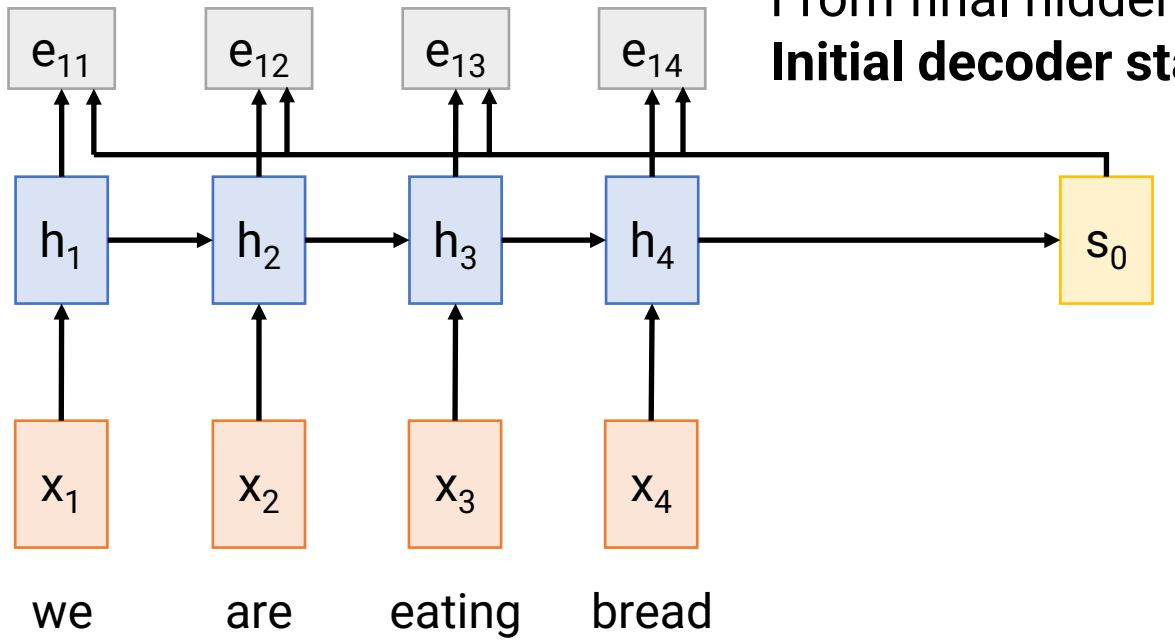
Bahdanau et al, “Neural machine translation by jointly learning to align and translate”, ICLR 2015

Slide credit: Justin Johnson

Machine Translation with RNNs **and Attention**

Compute **alignment scores**

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



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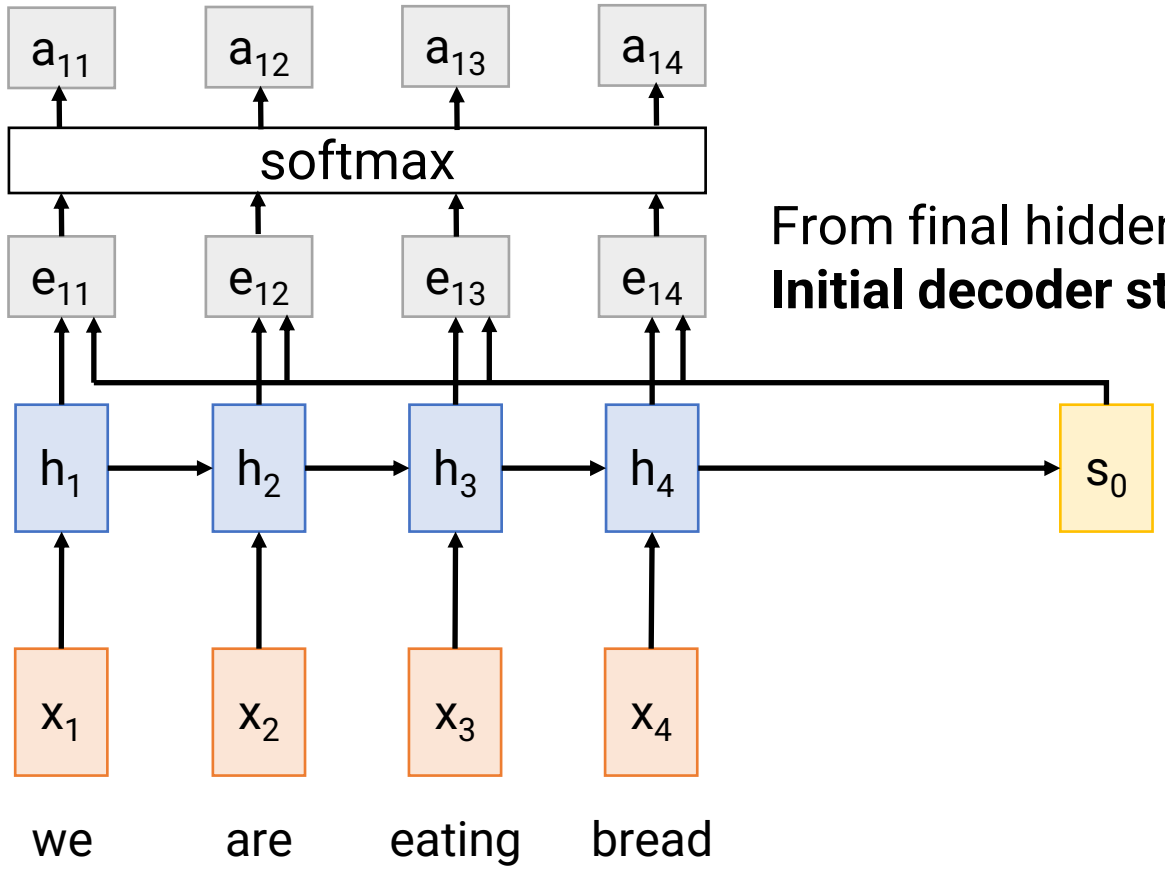

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Normalize to get
attention weights

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

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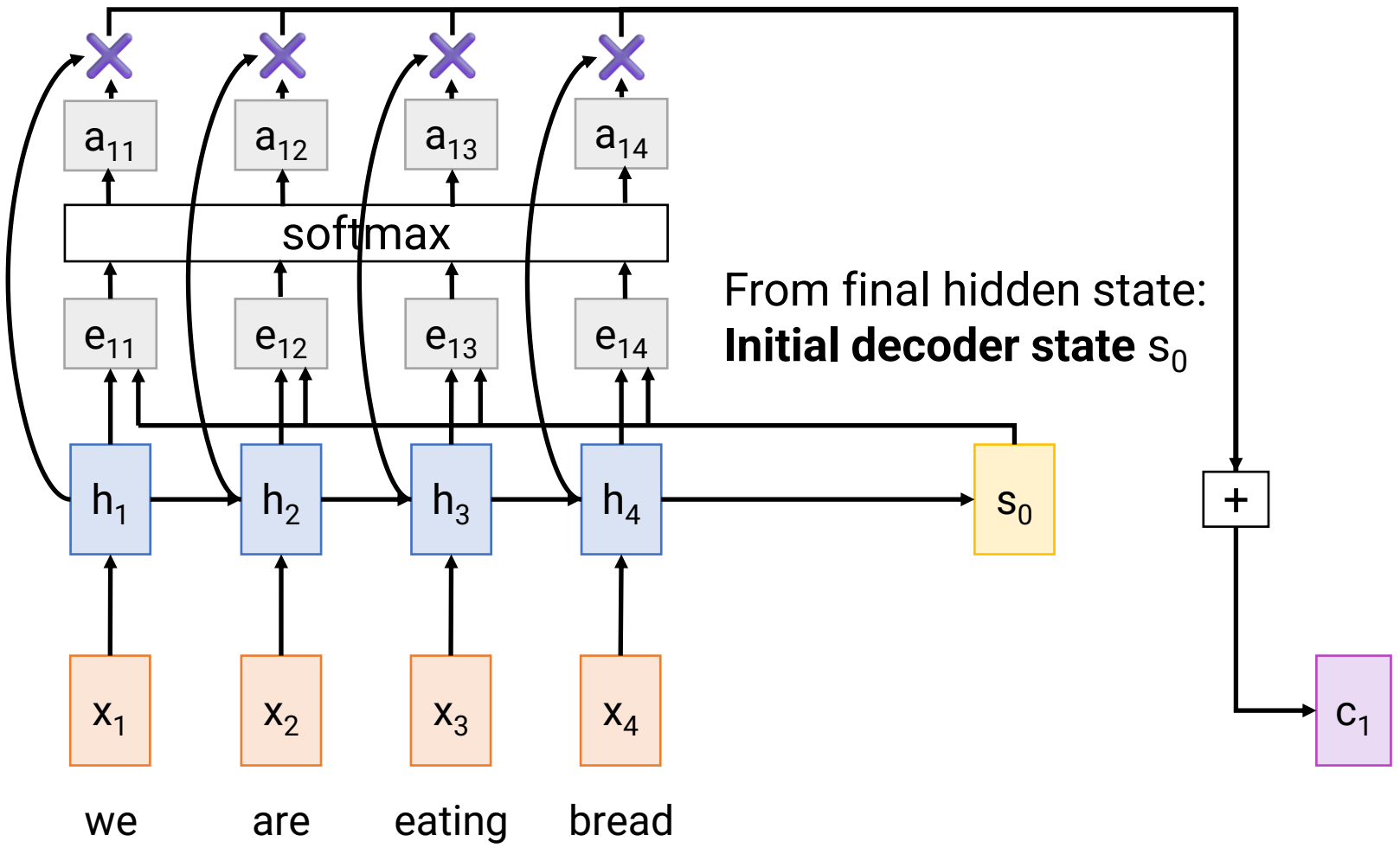
Machine Translation with RNNs **and Attention**



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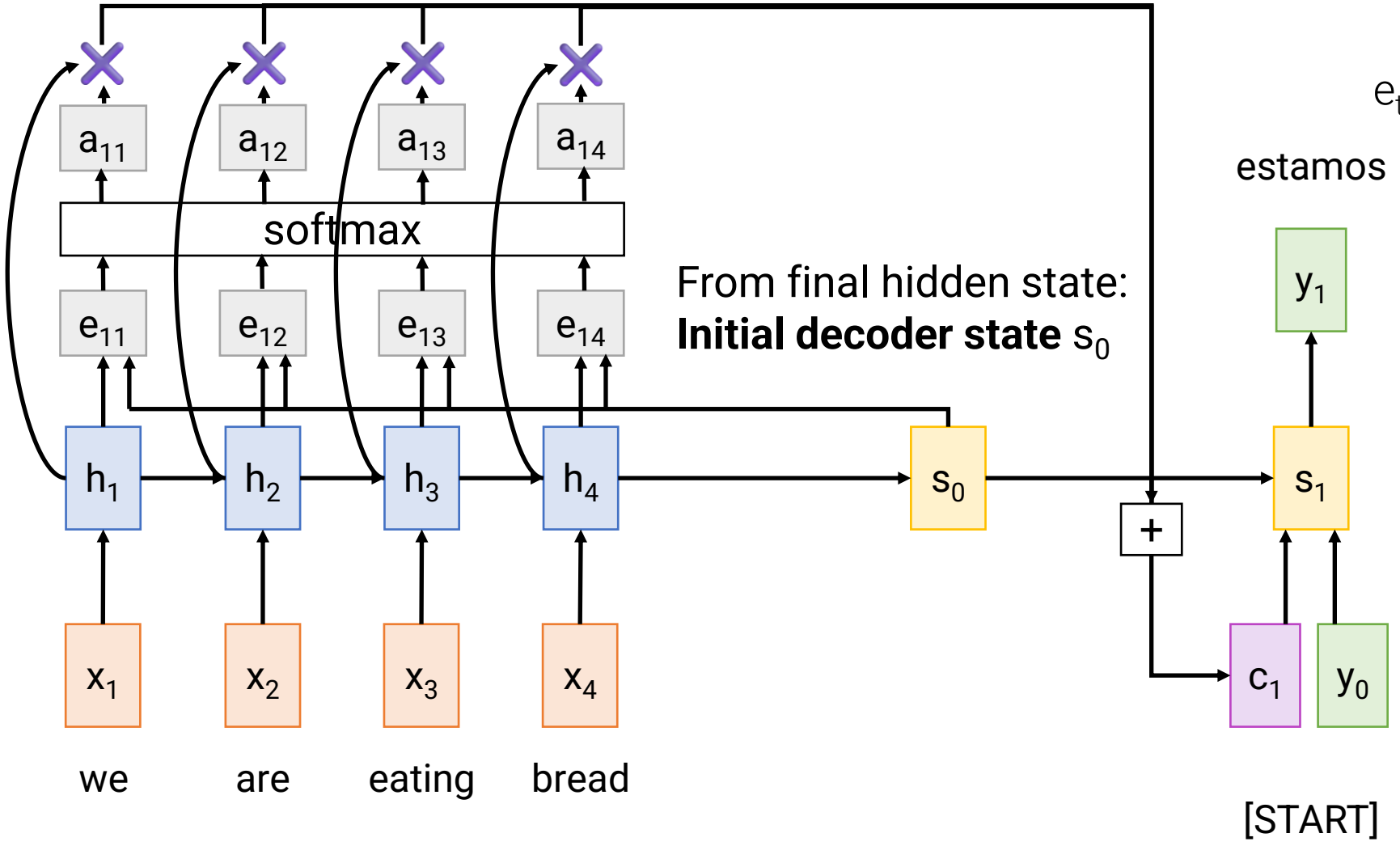
Set context vector **c** to a linear combination of hidden states

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

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

Slide credit: Justin Johnson

Machine Translation with RNNs **and Attention**



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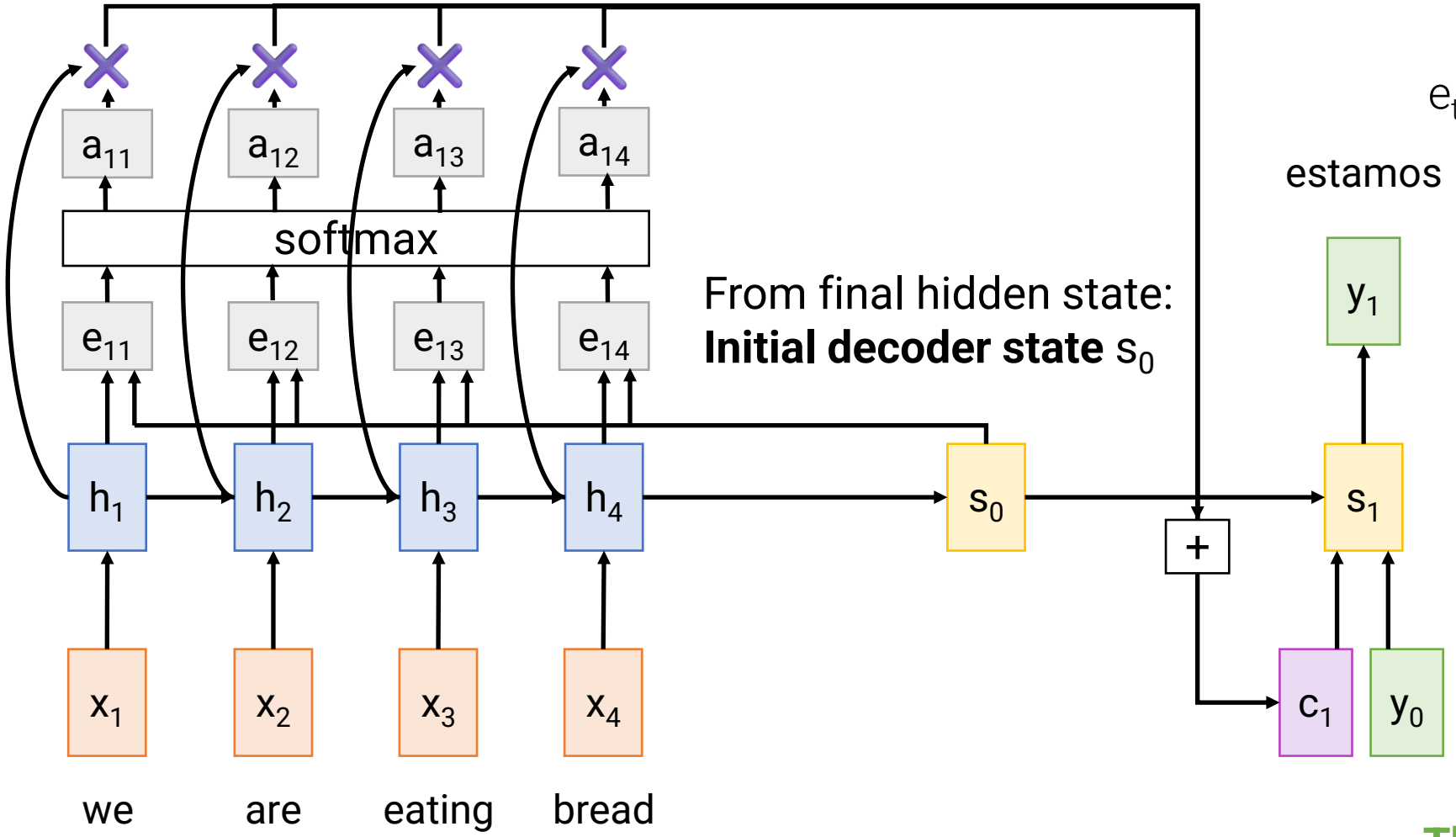

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This is all differentiable! Do not supervise attention weights – backprop through everything

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

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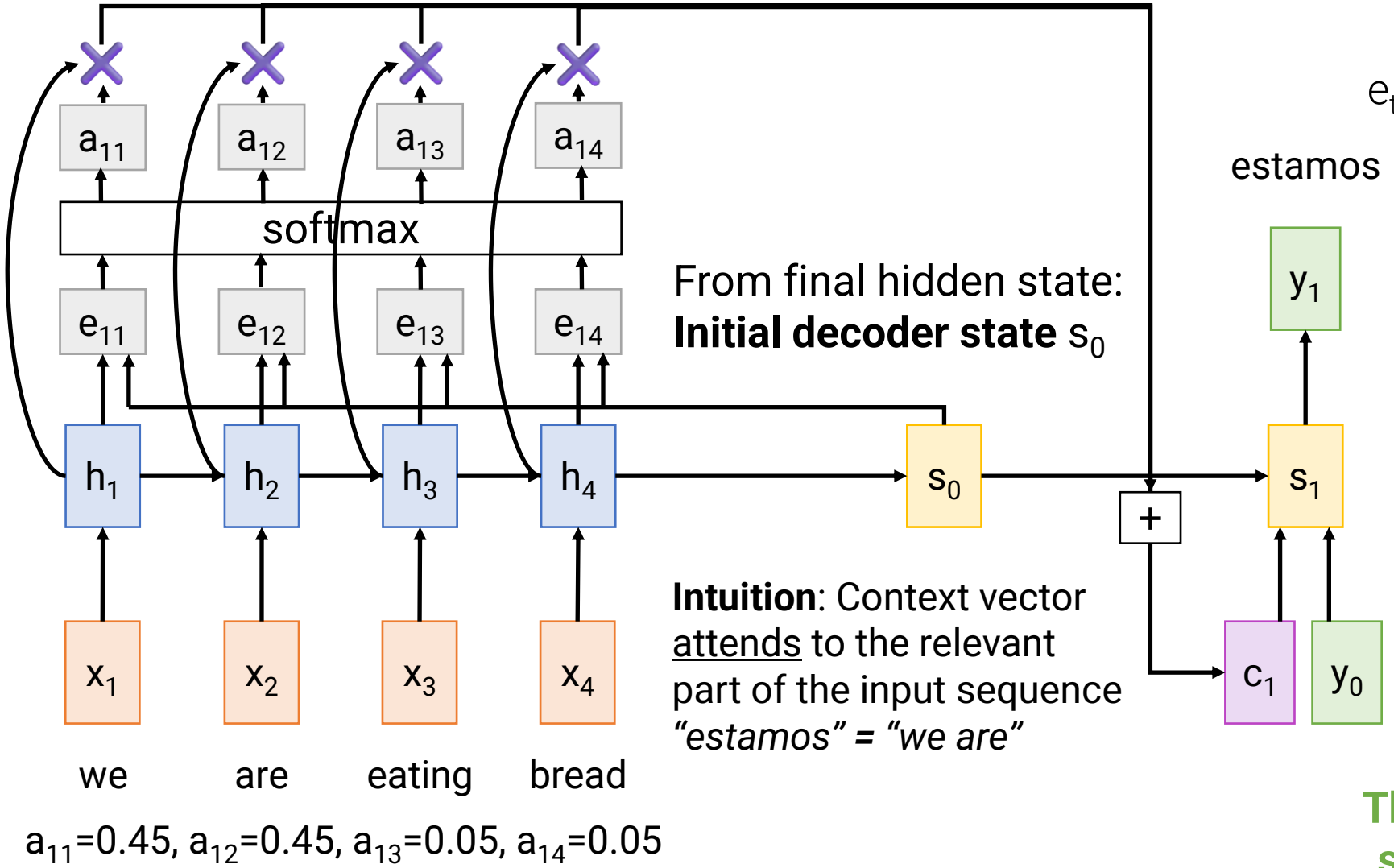
Machine Translation with RNNs **and Attention**



From final hidden state:
Initial decoder state s_0

Intuition: Context vector attends to the relevant part of the input sequence
"estamos" = "we are"

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

Compute **alignment scores**

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

Normalize to get **attention weights**

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

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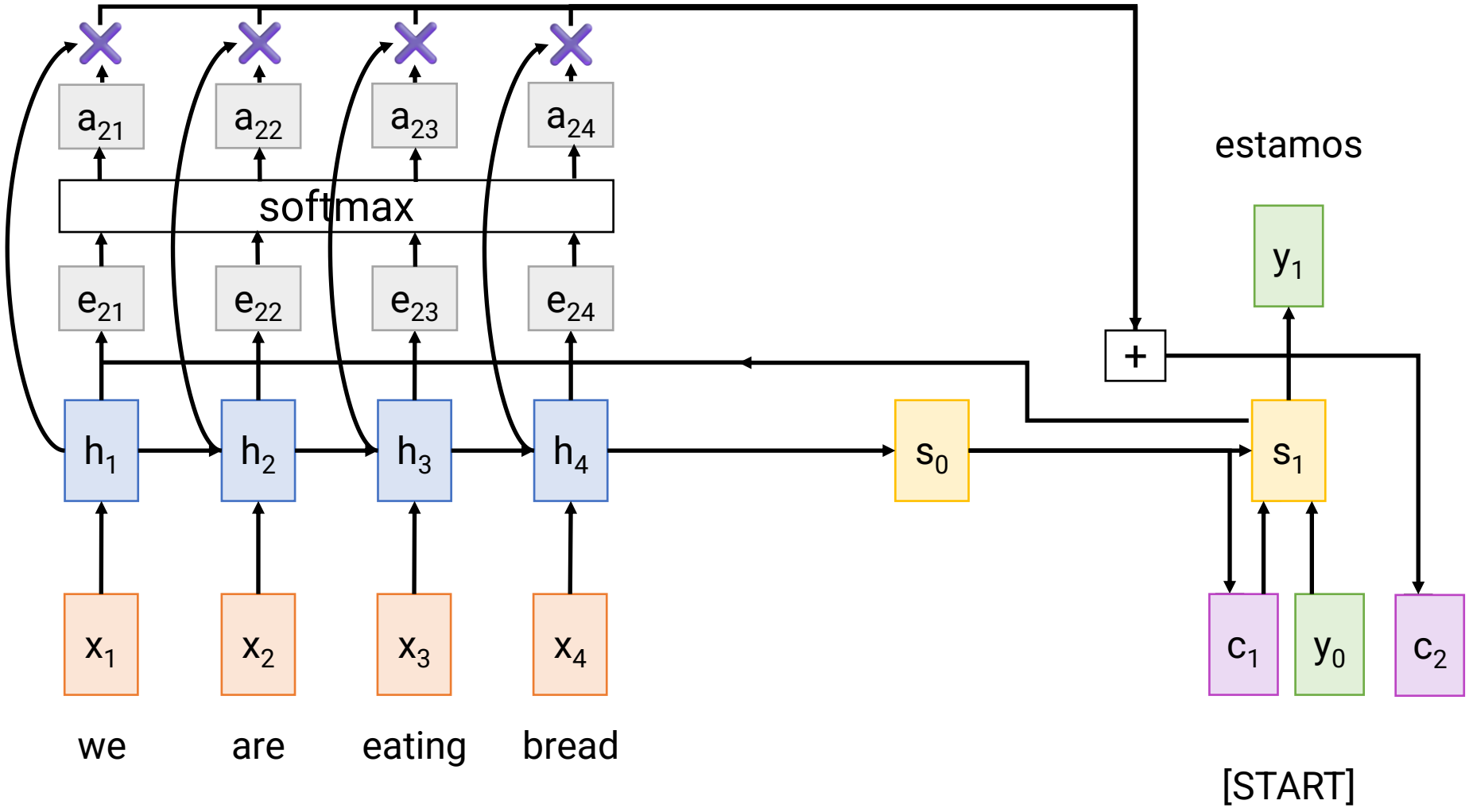
Machine Translation with RNNs **and Attention**

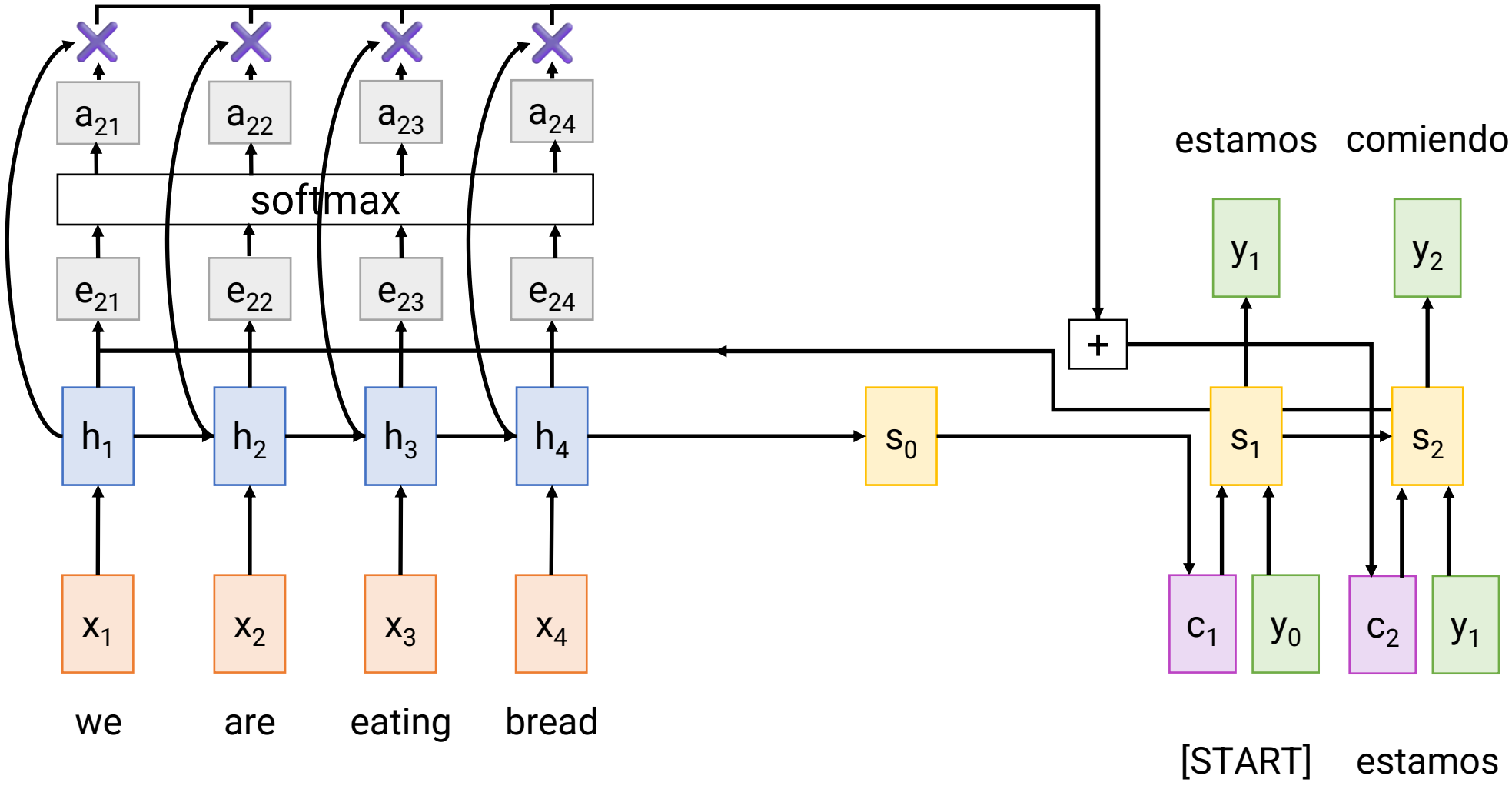


Repeat: Use s_1 to compute new context vector c_2

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

Slide credit: Justin Johnson

Machine Translation with RNNs **and Attention**



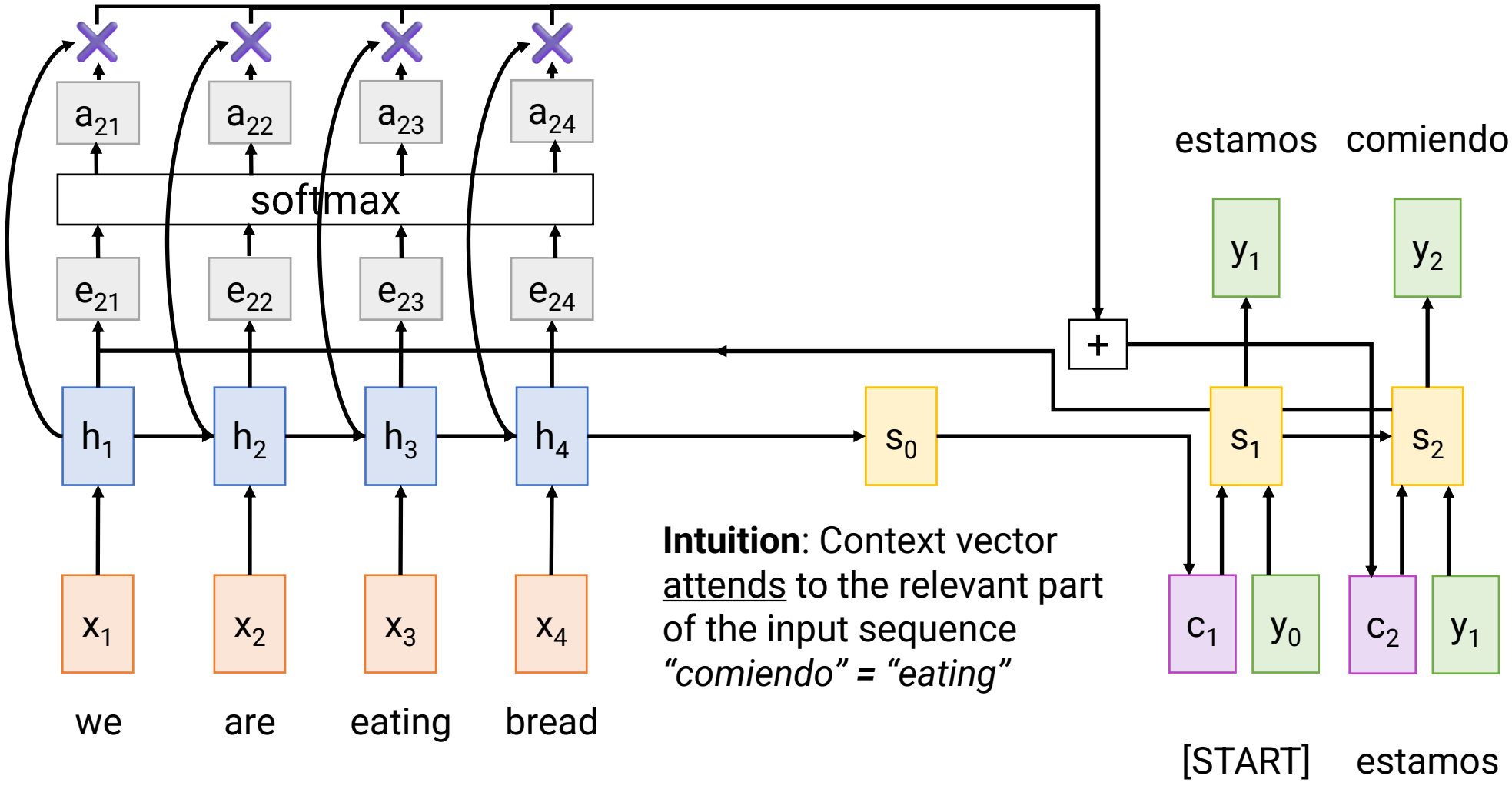
Repeat: Use s_1 to compute new context vector c_2

Use c_2 to compute s_2, y_2

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

Slide credit: Justin Johnson

Machine Translation with RNNs **and Attention**



Intuition: Context vector attends to the relevant part of the input sequence
"comiendo" = "eating"

Repeat: Use s_1 to compute new context vector c_2

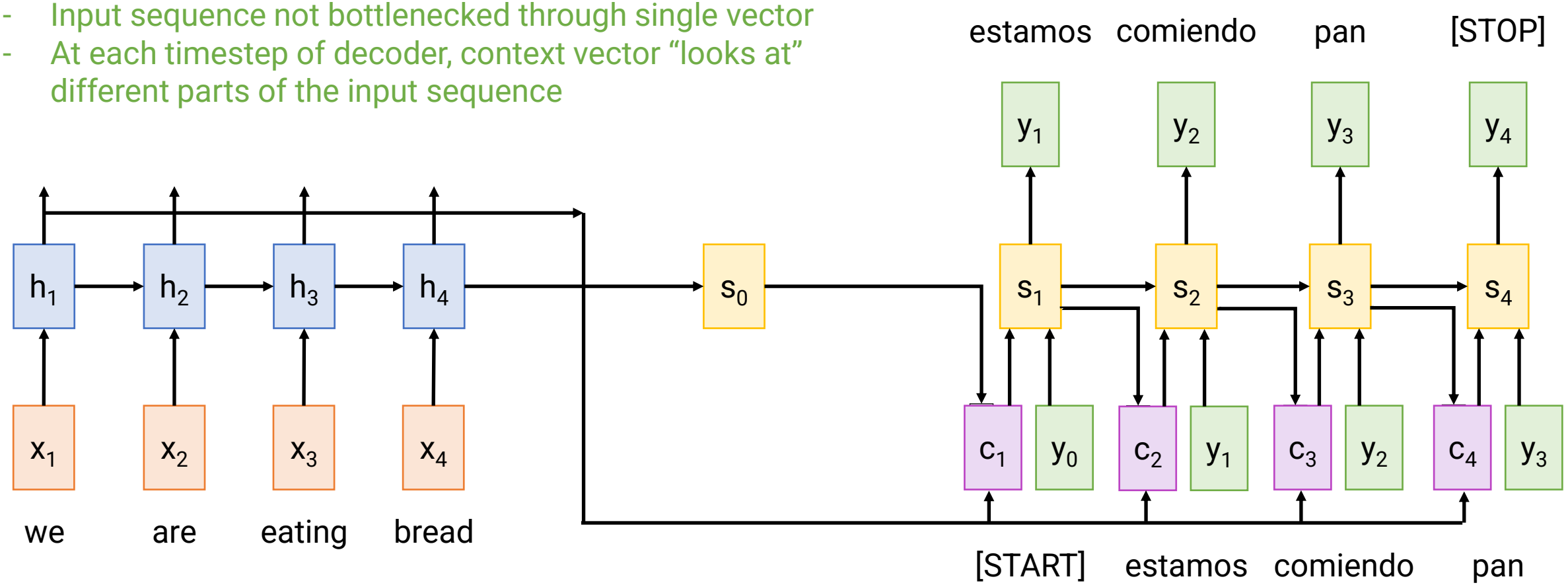
Use c_2 to compute s_2, y_2

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

Slide credit: Justin Johnson

Machine Translation 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

Slide credit: Justin Johnson

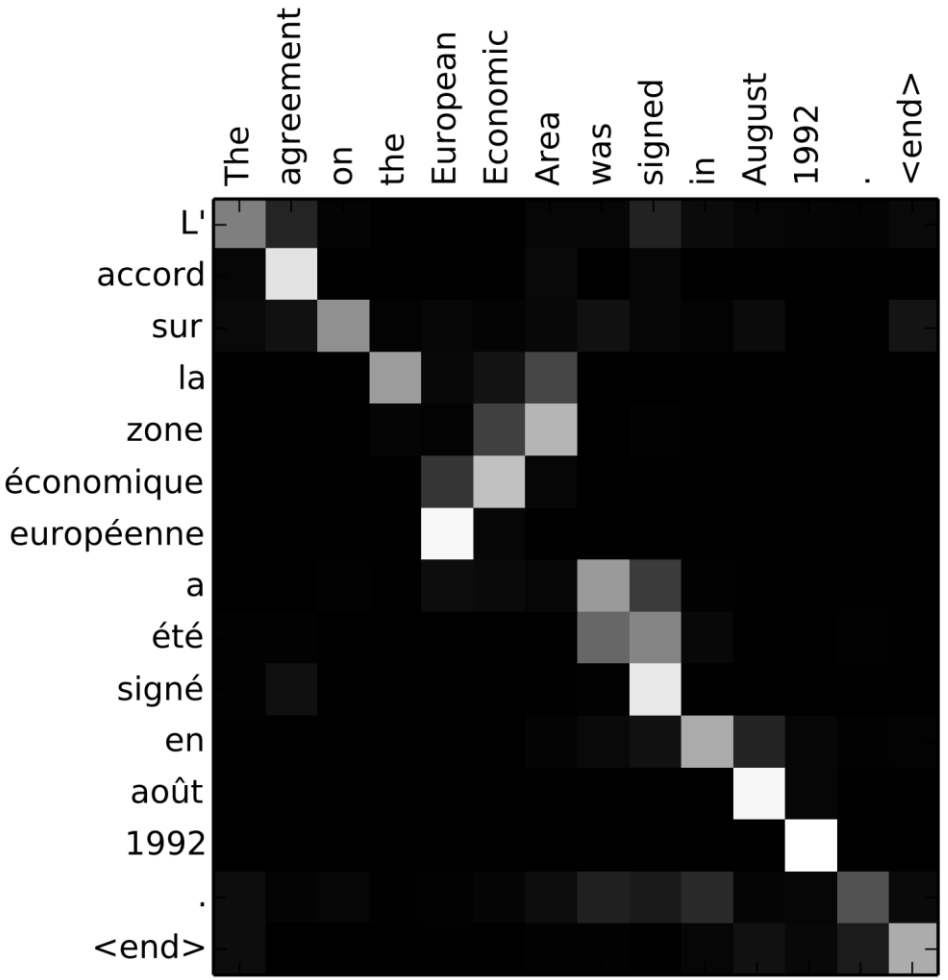
Machine Translation with RNNs **and Attention**

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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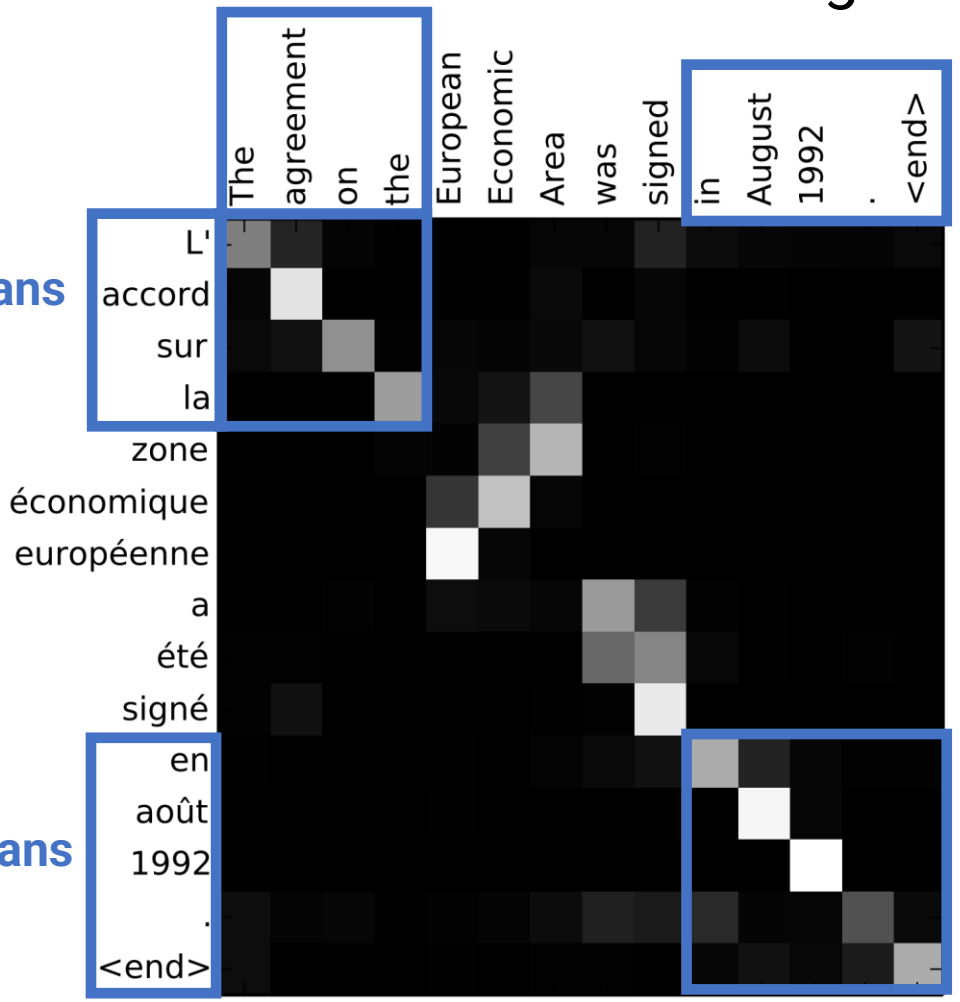

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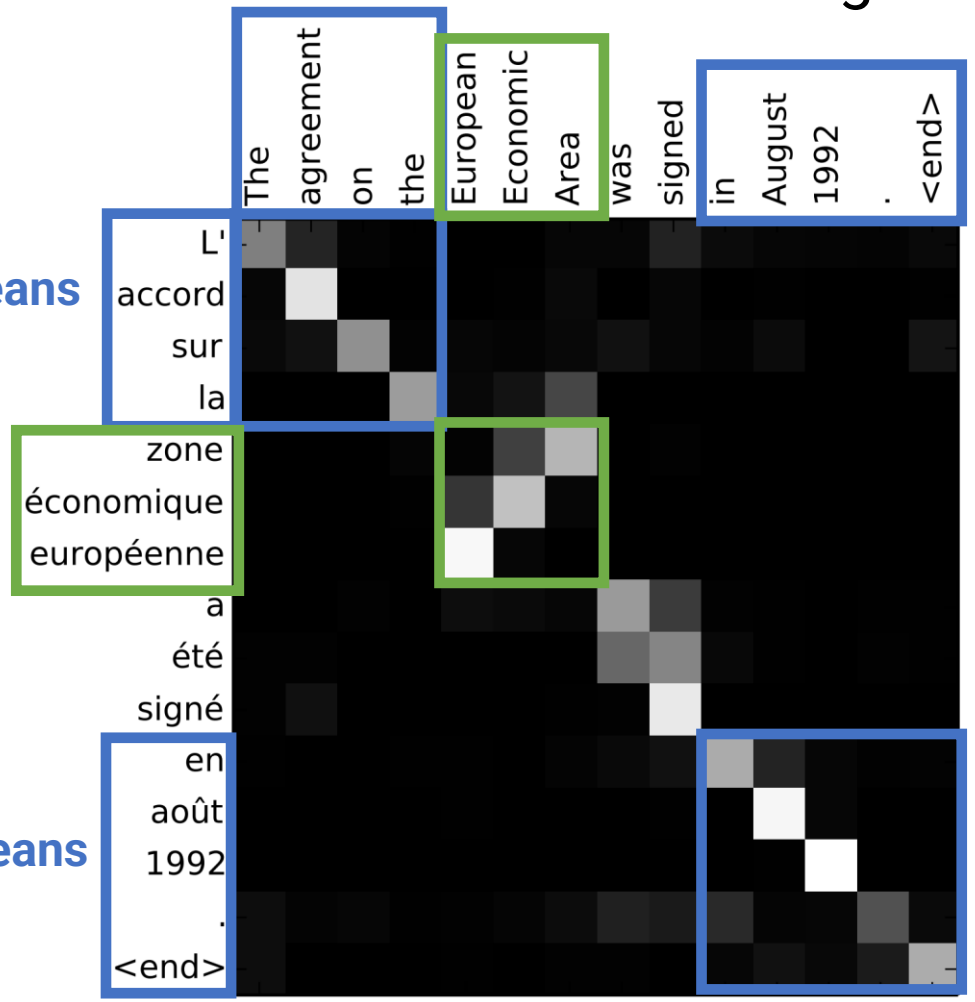


Diagonal attention means words correspond in order

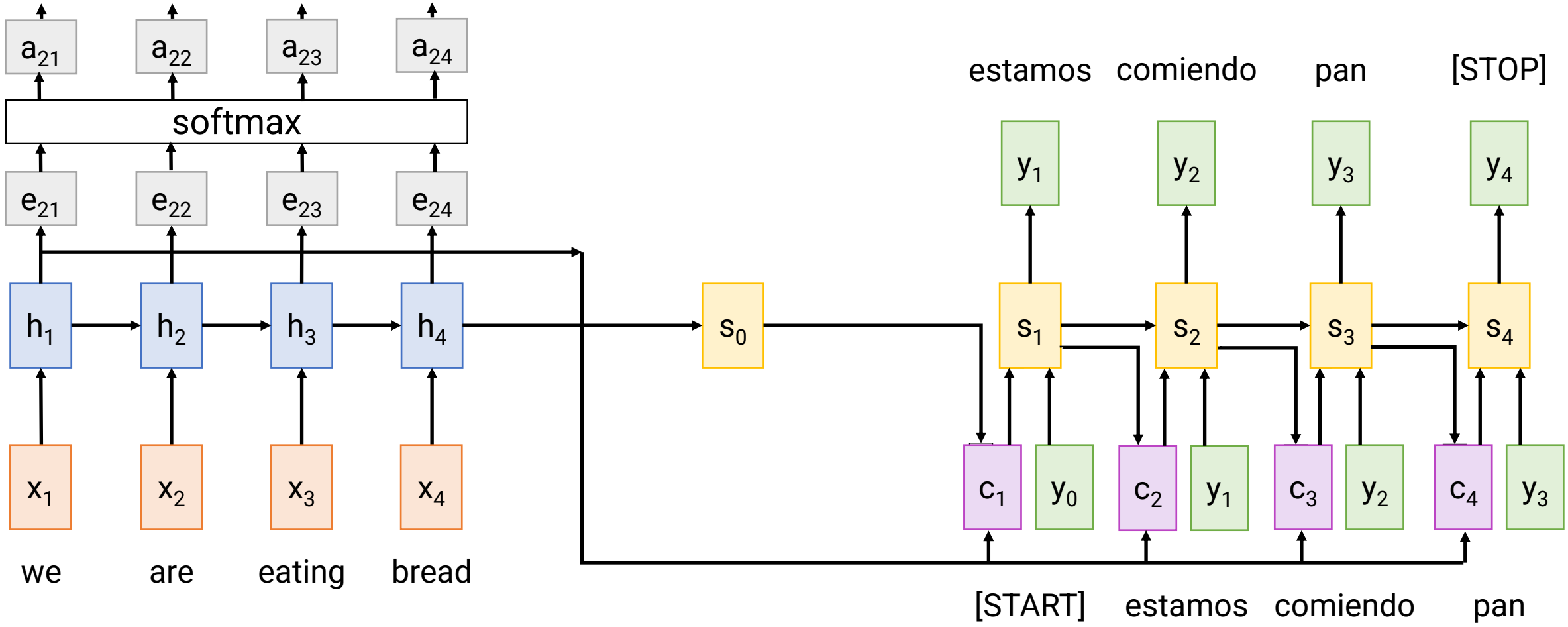
Attention figures out different word orders

Diagonal attention means words correspond in order

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

Slide credit: Justin Johnson

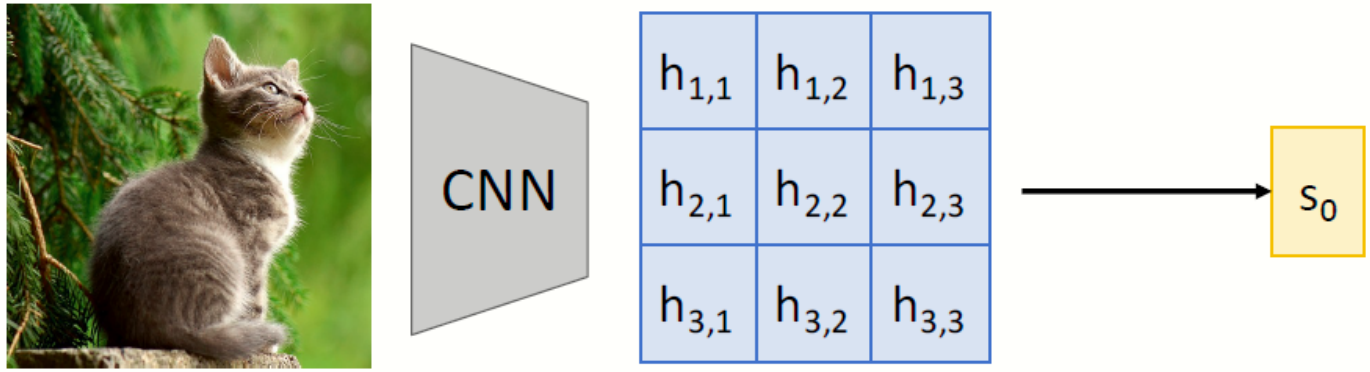
Machine Translation with RNNs **and Attention**



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

Slide credit: Justin Johnson

Image Captioning with RNNs and Attention



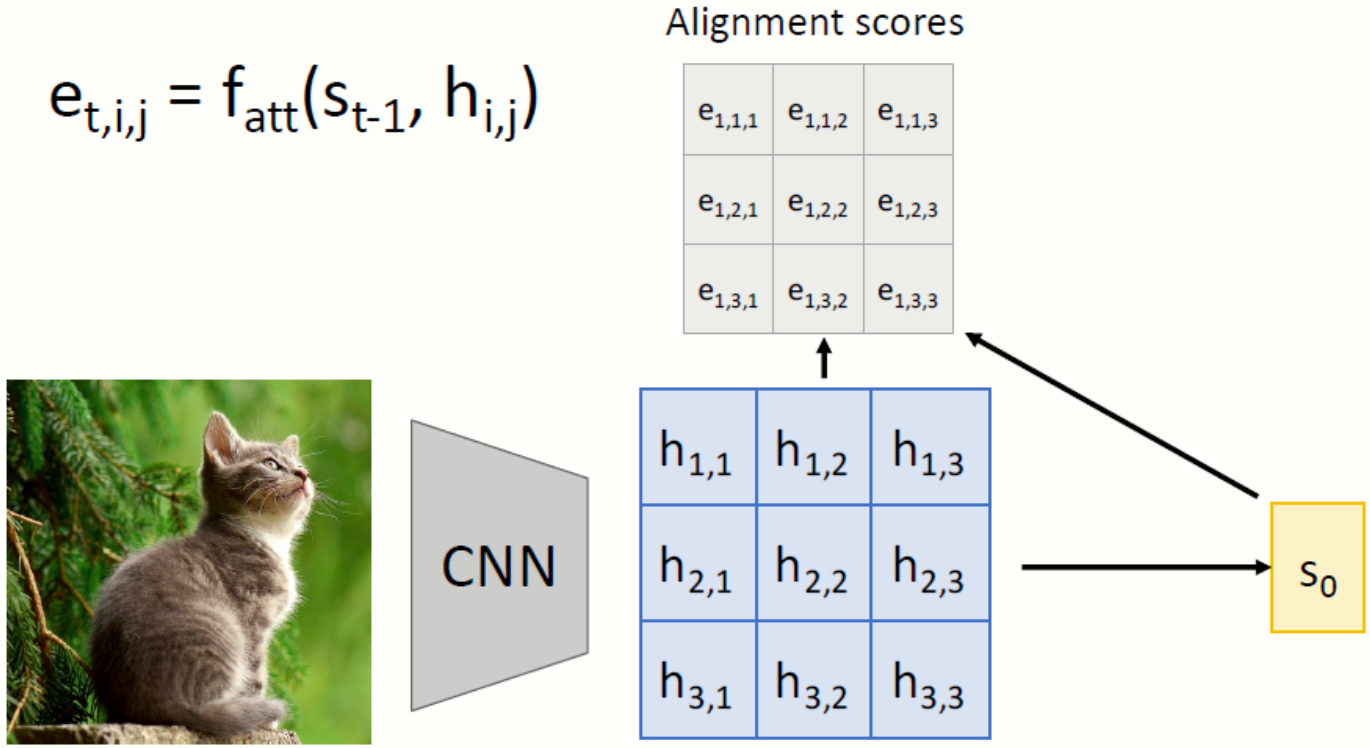
Use a CNN to compute a grid of features for an image

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

Slide credit: Justin Johnson

Image Captioning with RNNs and Attention

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



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

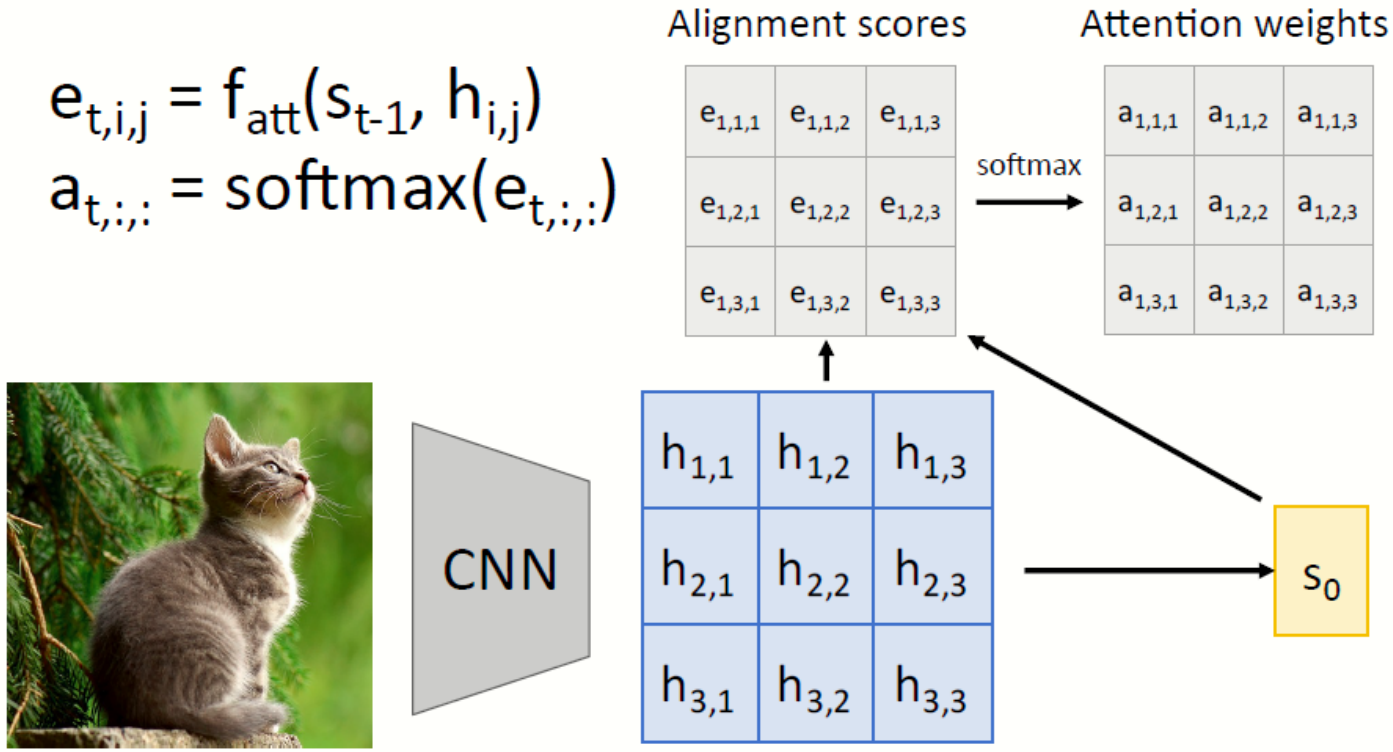
Xu et al, "Show, Attend, and Tell: Neural Image Caption Generation with Visual Attention", ICML 2015

Slide credit: Justin Johnson

Image Captioning with RNNs and Attention

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

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



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

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

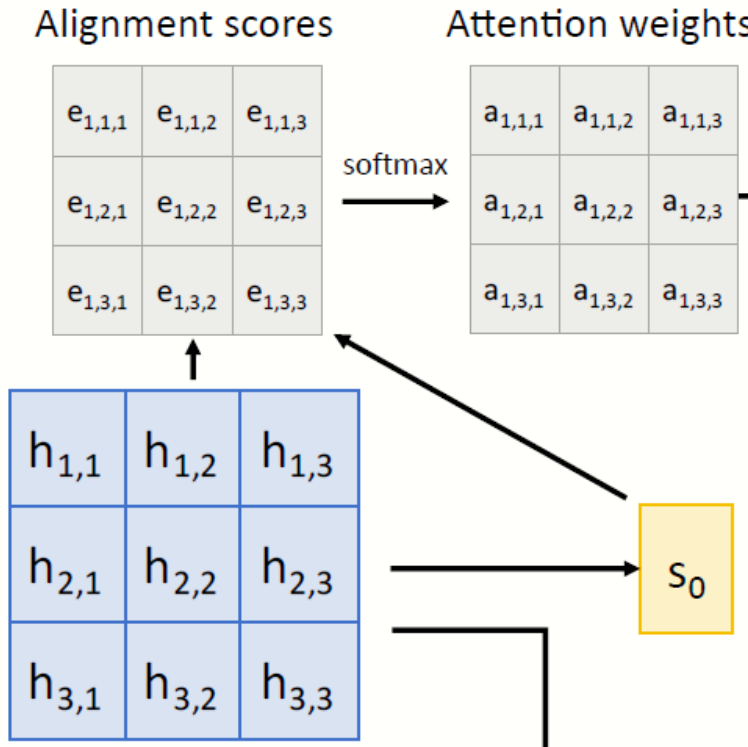
Slide credit: Justin Johnson

Image Captioning with RNNs and Attention

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

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

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



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

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

Slide credit: Justin Johnson

Image Captioning with RNNs and Attention

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

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

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

CNN

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

Alignment scores

$e_{1,1,1}$ $e_{1,1,2}$ $e_{1,1,3}$
$e_{1,2,1}$ $e_{1,2,2}$ $e_{1,2,3}$
$e_{1,3,1}$ $e_{1,3,2}$ $e_{1,3,3}$

softmax

Attention weights

$a_{1,1,1}$ $a_{1,1,2}$ $a_{1,1,3}$
$a_{1,2,1}$ $a_{1,2,2}$ $a_{1,2,3}$
$a_{1,3,1}$ $a_{1,3,2}$ $a_{1,3,3}$

$h_{1,1}$ $h_{1,2}$ $h_{1,3}$
$h_{2,1}$ $h_{2,2}$ $h_{2,3}$
$h_{3,1}$ $h_{3,2}$ $h_{3,3}$

s_0 s_1

y_1 cat

c_1 y_0

[START]

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

Slide credit: Justin Johnson

Image Captioning with RNNs and Attention

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

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

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

CNN

$h_{1,1}$ $h_{1,2}$ $h_{1,3}$

$h_{2,1}$ $h_{2,2}$ $h_{2,3}$

$h_{3,1}$ $h_{3,2}$ $h_{3,3}$

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

cat

y_1

s_0 s_1

c_1 y_0

[START]

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

Slide credit: Justin Johnson

Image Captioning with RNNs and Attention

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

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

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

Alignment scores

CNN

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

cat

[START]

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

Slide credit: Justin Johnson

Image Captioning with RNNs and Attention

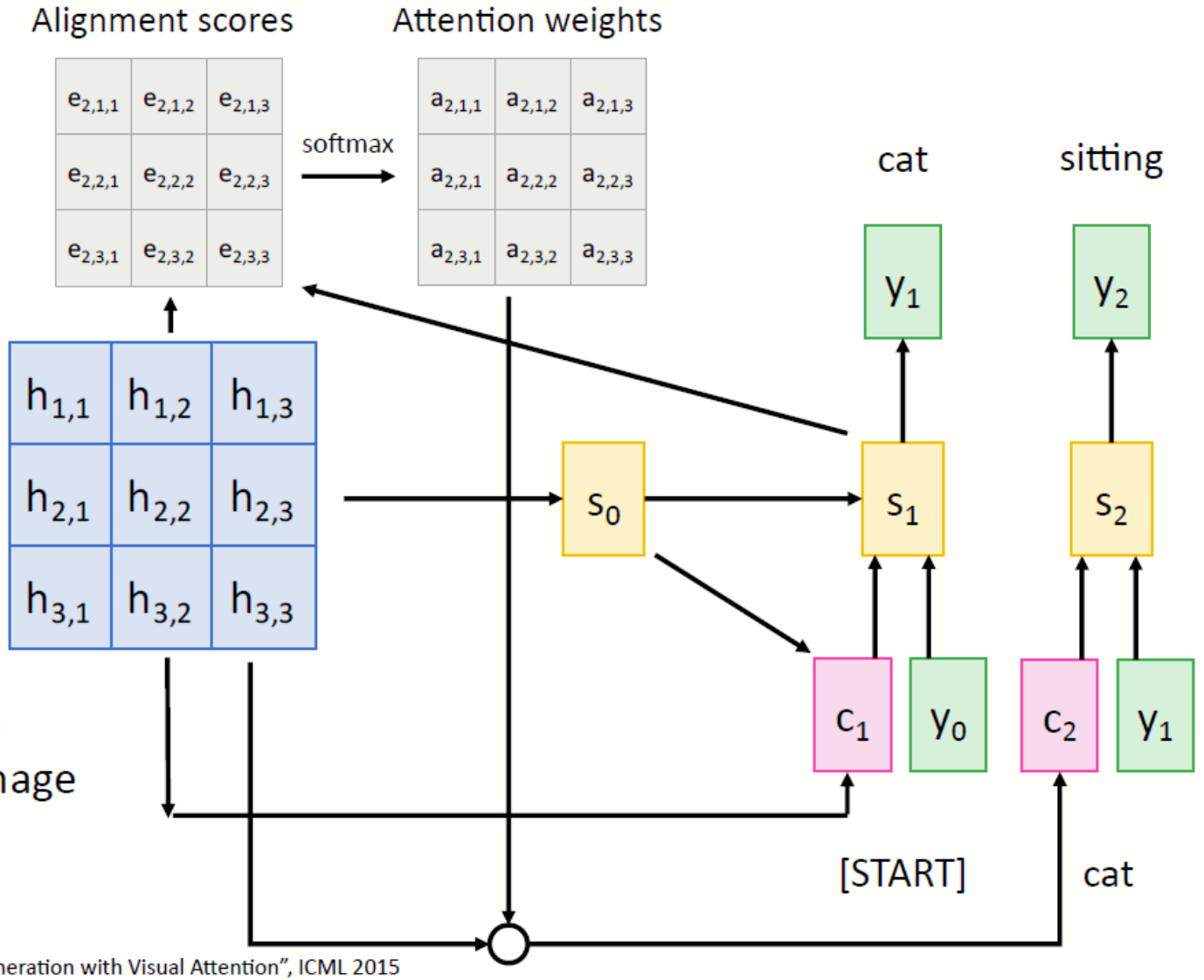
$e_{t,i,j} = f_{att}(s_{t-1}, h_{i,j})$

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

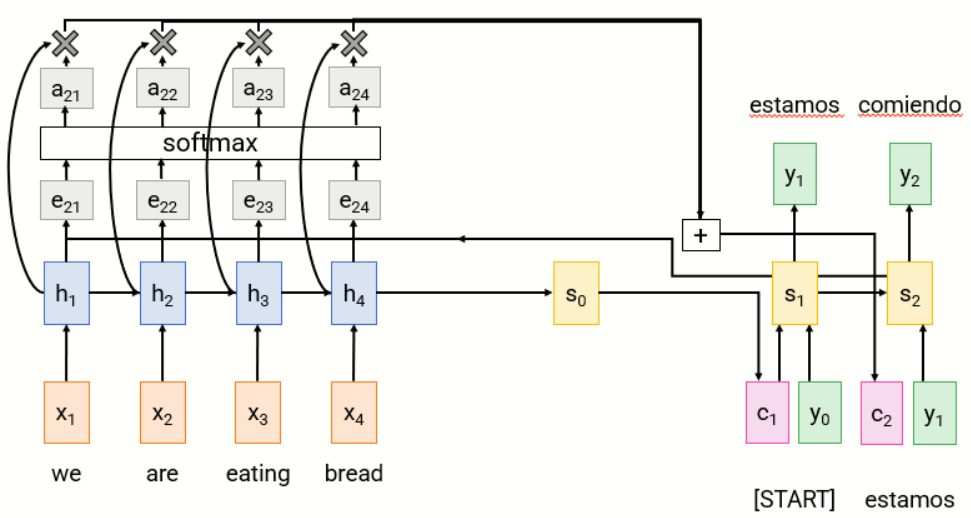
$c_t = \sum_{i,j} a_{t,i,j} h_{i,j}$

CNN

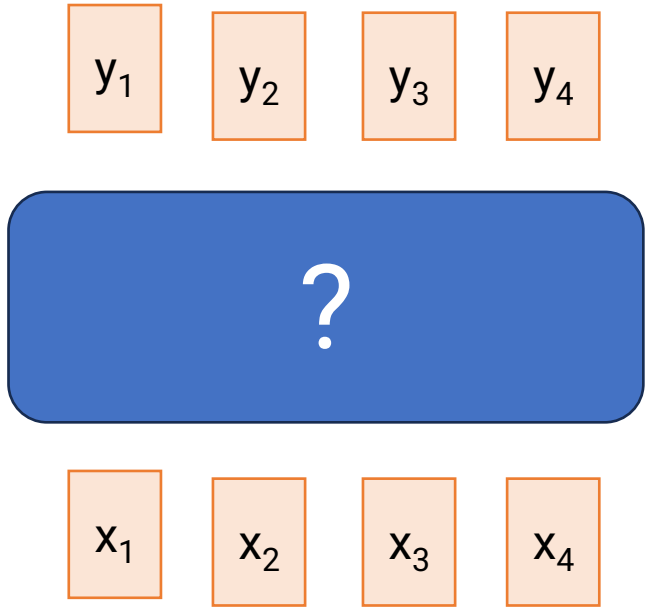
Use a CNN to compute a grid of features for an image



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

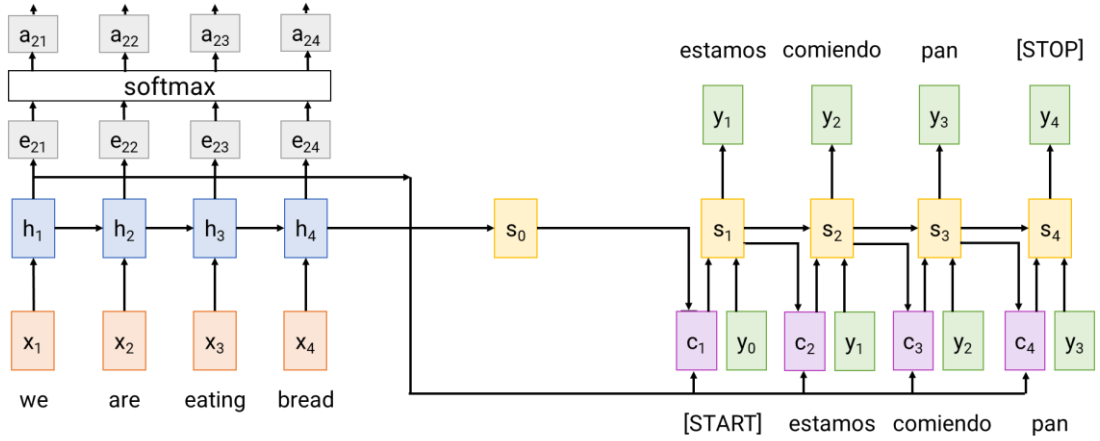


Idea: Can we use **attention** as a fundamental building block for a generic sequence (input) to sequence (output) layer?



Attention Layer

Inputs:
State vector: s_i (Shape: D_Q)
Hidden vectors: h_i (Shape: N_X x D_H)
Similarity function: f_{att}

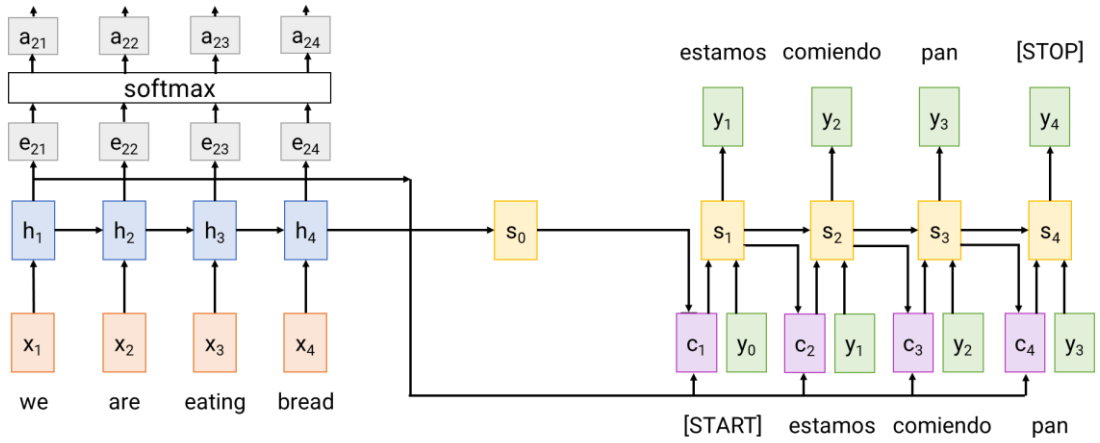


Computation:
Similarities: e (Shape: N_X) $e_i = f_{att}(s_{t-1}, h_i)$
Attention weights: a = softmax(e) (Shape: N_X)
Output vector: $y = \sum_i a_i h_i$ (Shape: D_X)

Slide credit: Justin Johnson

Attention Layer

Inputs:
Query vector: **q** (Shape: D_Q)
Input vectors: **X** (Shape: N_X x D_X)
Similarity function: f_{att}

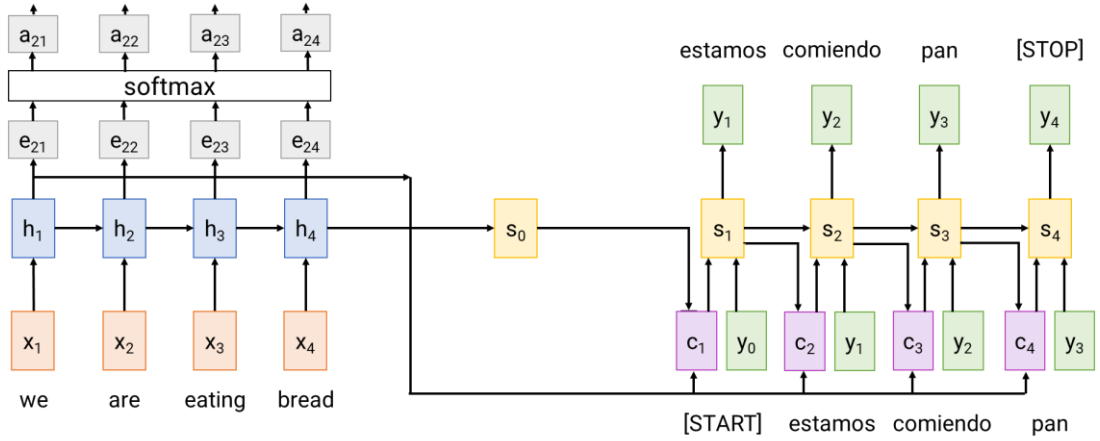


Computation:
Similarities: e (Shape: N_X) $e_i = f_{att}(\mathbf{q}, \mathbf{X}_i)$
Attention weights: a = softmax(e) (Shape: N_X)
Output vector: $y = \sum_i a_i \mathbf{X}_i$ (Shape: D_X)

Slide credit: Justin Johnson

Attention Layer

Inputs:
Query vector: **q** (Shape: D_Q)
Input vectors: **X** (Shape: N_X x D_Q)
Similarity function: dot product



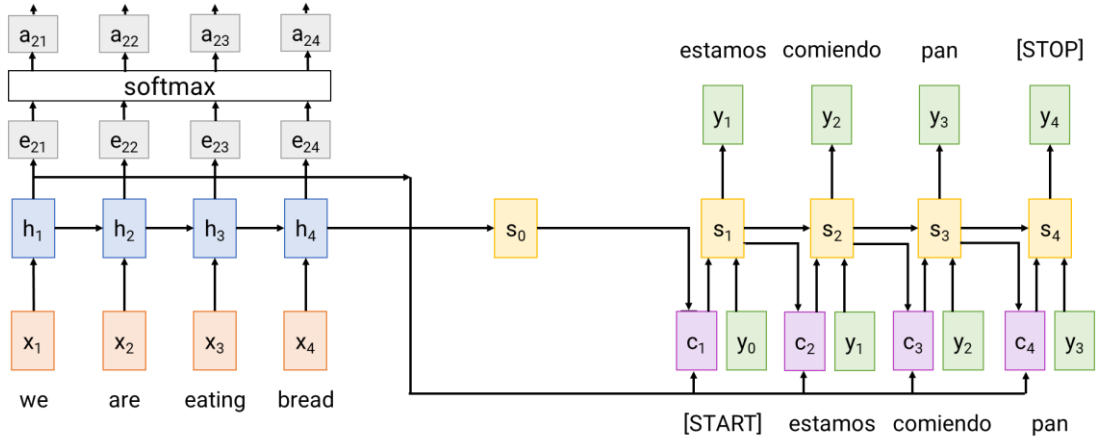
Computation:
Similarities: e (Shape: N_X) $e_i = \mathbf{q} \cdot \mathbf{X}_i$
Attention weights: a = softmax(e) (Shape: N_X)
Output vector: $y = \sum_i a_i \mathbf{X}_i$ (Shape: D_X)

Changes:
- Use dot product for similarity

Slide credit: Justin Johnson

Attention Layer

Inputs:
Query vector: **q** (Shape: D_Q)
Input vectors: **X** (Shape: N_X x D_Q)
Similarity function: scaled dot product



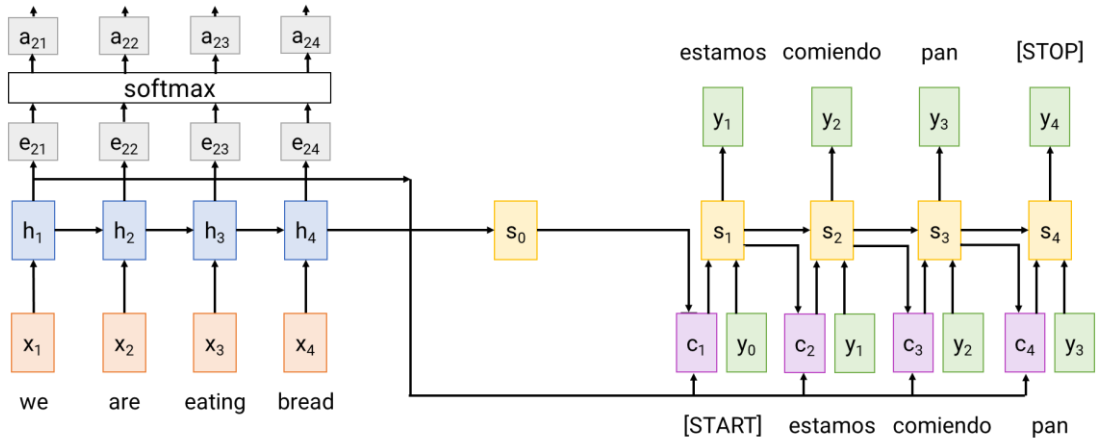
Computation:
Similarities: e (Shape: N_X) $e_i = \mathbf{q} \cdot \mathbf{X}_i / \text{sqrt}(D_Q)$
Attention weights: a = softmax(e) (Shape: N_X)
Output vector: $y = \sum_i a_i \mathbf{X}_i$ (Shape: D_X)

Changes:
- Use **scaled** dot product for similarity

Slide credit: Justin Johnson

Attention Layer

Inputs:
Query vectors: Q (Shape: N_Q x D_Q)
Input vectors: X (Shape: N_X x D_Q)



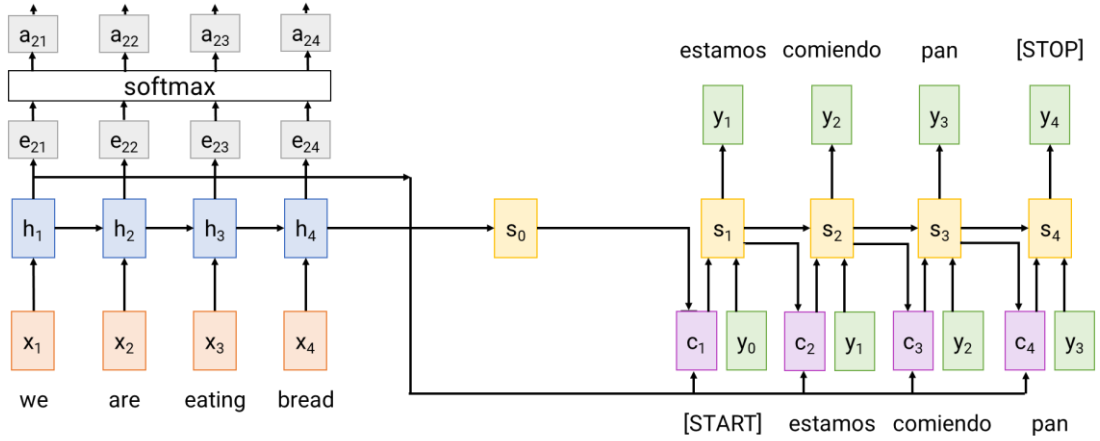
Computation:
Similarities: $E = QX^T$ (Shape: N_Q x N_X) $E_{i,j} = Q_i \cdot X_j / \sqrt{D_Q}$
Attention weights: $A = \text{softmax}(E, \text{dim}=1)$ (Shape: N_Q x N_X)
Output vectors: $Y = AX$ (Shape: N_Q x D_X) $Y_i = \sum_j A_{i,j} X_j$

Changes:
- Use dot product for similarity
- Multiple **query** vectors

Slide credit: Justin Johnson

Attention Layer

Inputs:
Query vectors: Q (Shape: N_Q x D_Q)
Input vectors: X (Shape: N_X x D_X)
Key matrix: W_K (Shape: D_X x D_Q)
Value matrix: W_V (Shape: D_X x D_V)



Computation:
Key vectors: $K = XW_K$ (Shape: N_X x D_Q)
Value vectors: $V = XW_V$ (Shape: N_X x D_V)
Similarities: $E = QK^T$ (Shape: N_Q x N_X) $E_{i,j} = Q_i \cdot K_j / \sqrt{D_Q}$
Attention weights: A = softmax(E, dim=1) (Shape: N_Q x N_X)
Output vectors: $Y = AV$ (Shape: N_Q x D_V) $Y_i = \sum_j A_{i,j} V_j$

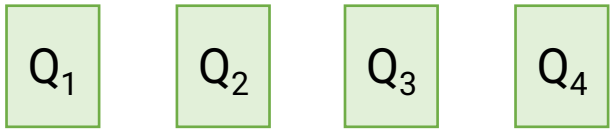
Changes:
- Use dot product for similarity
- Multiple **query** vectors
- Separate **key** and **value**

Slide credit: Justin Johnson

Attention Layer

Inputs:
Query vectors: Q (Shape: N_Q x D_Q)
Input vectors: X (Shape: N_X x D_X)
Key matrix: W_K (Shape: D_X x D_Q)
Value matrix: W_V (Shape: D_X x D_V)

Computation:
Key vectors: $K = XW_K$ (Shape: N_X x D_Q)
Value vectors: $V = XW_V$ (Shape: N_X x D_V)
Similarities: $E = QK^T$ (Shape: N_Q x N_X) $E_{i,j} = Q_i \cdot K_j / \text{sqrt}(D_Q)$
Attention weights: A = softmax(E, dim=1) (Shape: N_Q x N_X)
Output vectors: $Y = AV$ (Shape: N_Q x D_V) $Y_i = \sum_j A_{i,j} V_j$

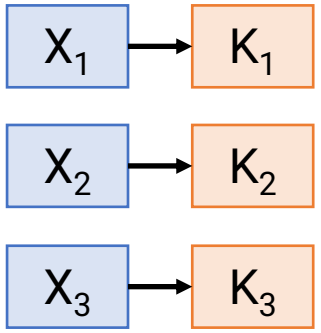


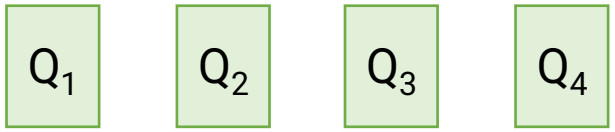
Slide credit: Justin Johnson

Attention Layer

Inputs:
Query vectors: Q (Shape: N_Q x D_Q)
Input vectors: X (Shape: N_X x D_X)
Key matrix: W_K (Shape: D_X x D_Q)
Value matrix: W_V (Shape: D_X x D_V)

Computation:
Key vectors: $K = XW_K$ (Shape: N_X x D_Q)
Value vectors: $V = XW_V$ (Shape: N_X x D_V)
Similarities: $E = QK^T$ (Shape: N_Q x N_X) $E_{i,j} = Q_i \cdot K_j / \text{sqrt}(D_Q)$
Attention weights: A = softmax(E, dim=1) (Shape: N_Q x N_X)
Output vectors: $Y = AV$ (Shape: N_Q x D_V) $Y_i = \sum_j A_{i,j} V_j$



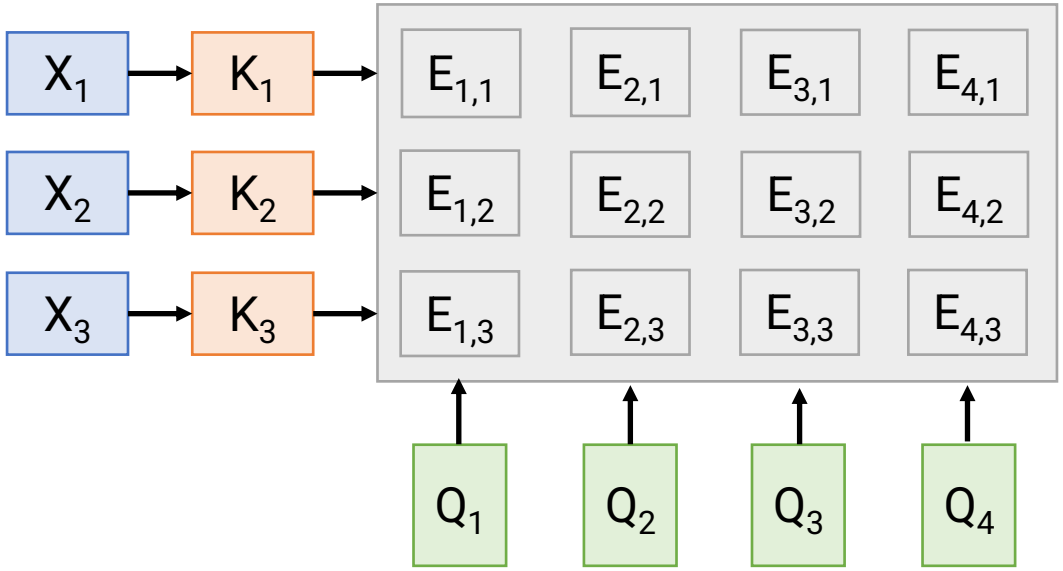


Slide credit: Justin Johnson

Attention Layer

Inputs:
Query vectors: Q (Shape: N_Q x D_Q)
Input vectors: X (Shape: N_X x D_X)
Key matrix: W_K (Shape: D_X x D_Q)
Value matrix: W_V (Shape: D_X x D_V)

Computation:
Key vectors: $K = XW_K$ (Shape: N_X x D_Q)
Value vectors: $V = XW_V$ (Shape: N_X x D_V)
Similarities: $E = QK^T$ (Shape: N_Q x N_X) $E_{i,j} = Q_i \cdot K_j / \text{sqrt}(D_Q)$
Attention weights: A = softmax(E, dim=1) (Shape: N_Q x N_X)
Output vectors: $Y = AV$ (Shape: N_Q x D_V) $Y_i = \sum_j A_{i,j} V_j$

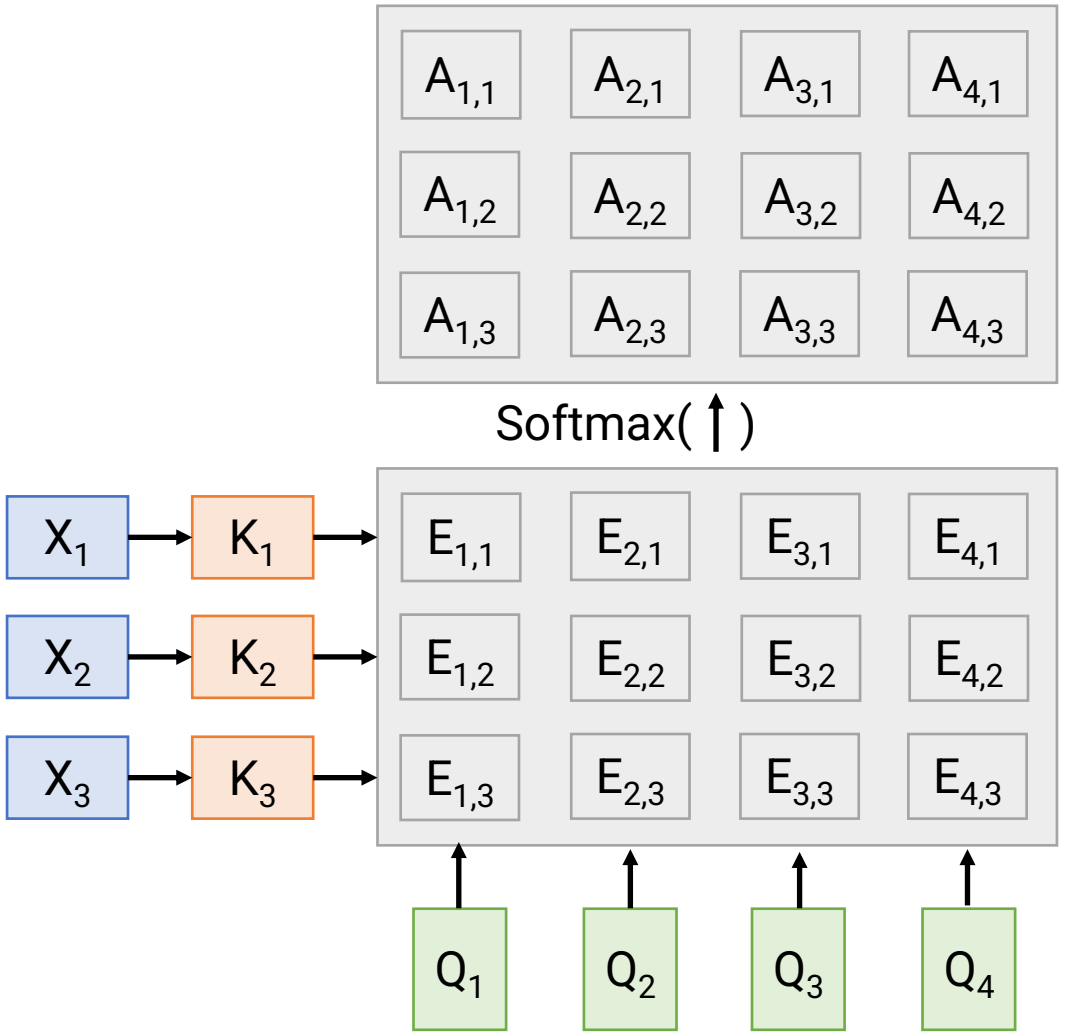


Slide credit: Justin Johnson

Attention Layer

Inputs:
Query vectors: Q (Shape: N_Q x D_Q)
Input vectors: X (Shape: N_X x D_X)
Key matrix: W_K (Shape: D_X x D_Q)
Value matrix: W_V (Shape: D_X x D_V)

Computation:
Key vectors: $K = XW_K$ (Shape: N_X x D_Q)
Value vectors: $V = XW_V$ (Shape: N_X x D_V)
Similarities: $E = QK^T$ (Shape: N_Q x N_X) $E_{i,j} = Q_i \cdot K_j / \text{sqrt}(D_Q)$
Attention weights: A = softmax(E, dim=1) (Shape: N_Q x N_X)
Output vectors: $Y = AV$ (Shape: N_Q x D_V) $Y_i = \sum_j A_{i,j} V_j$

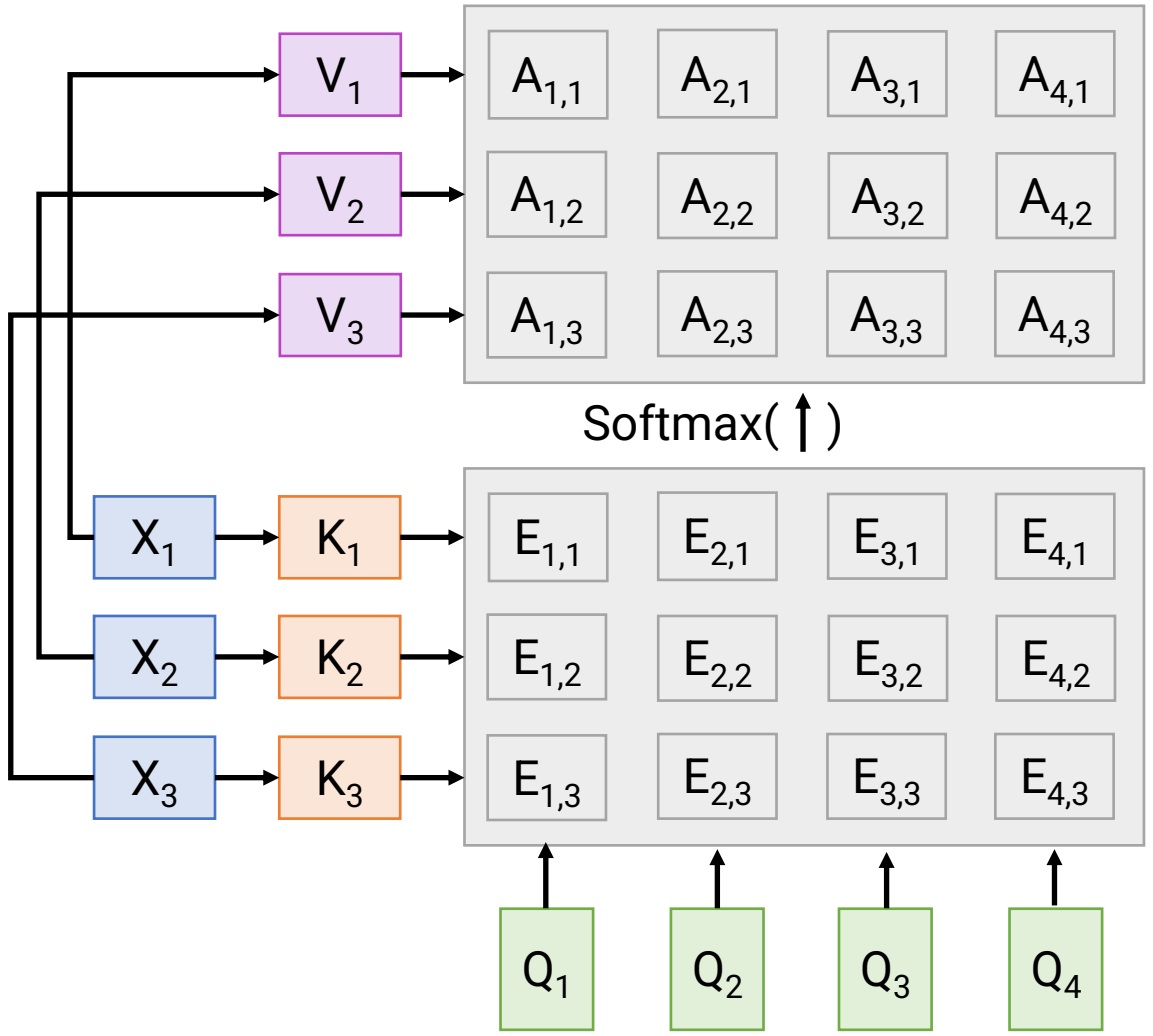


Slide credit: Justin Johnson

Attention Layer

Inputs:
Query vectors: Q (Shape: N_Q x D_Q)
Input vectors: X (Shape: N_X x D_X)
Key matrix: W_K (Shape: D_X x D_Q)
Value matrix: W_V (Shape: D_X x D_V)

Computation:
Key vectors: $K = XW_K$ (Shape: N_X x D_Q)
Value vectors: $V = XW_V$ (Shape: N_X x D_V)
Similarities: $E = QK^T$ (Shape: N_Q x N_X) $E_{i,j} = Q_i \cdot K_j / \sqrt{D_Q}$
Attention weights: A = softmax(E, dim=1) (Shape: N_Q x N_X)
Output vectors: $Y = AV$ (Shape: N_Q x D_V) $Y_i = \sum_j A_{i,j} V_j$

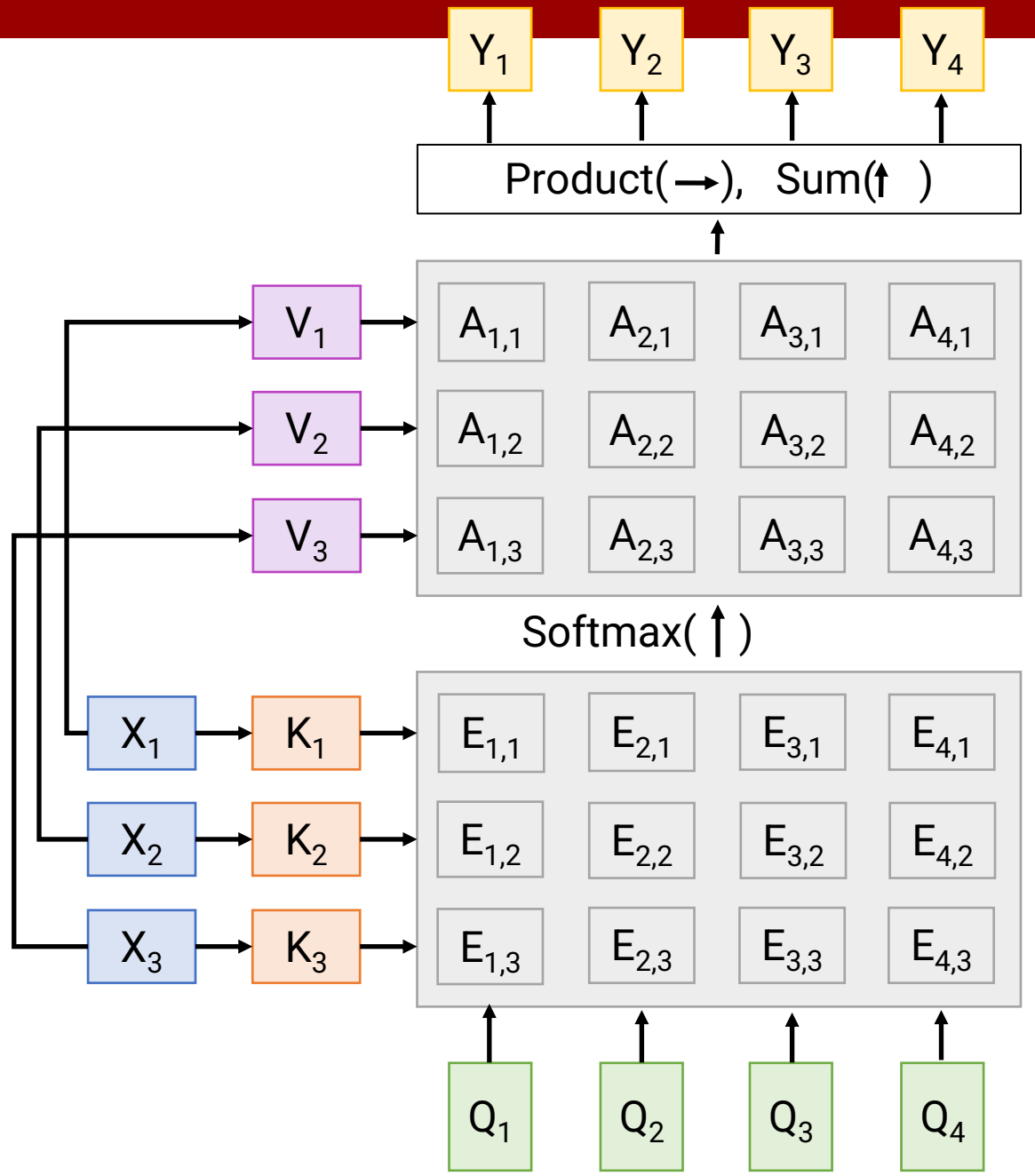


Slide credit: Justin Johnson

Attention Layer

Inputs:
Query vectors: Q (Shape: N_Q x D_Q)
Input vectors: X (Shape: N_X x D_X)
Key matrix: W_K (Shape: D_X x D_Q)
Value matrix: W_V (Shape: D_X x D_V)

Computation:
Key vectors: $K = XW_K$ (Shape: N_X x D_Q)
Value vectors: $V = XW_V$ (Shape: N_X x D_V)
Similarities: $E = QK^T$ (Shape: N_Q x N_X) $E_{i,j} = Q_i \cdot K_j / \text{sqrt}(D_Q)$
Attention weights: A = softmax(E, dim=1) (Shape: N_Q x N_X)
Output vectors: $Y = AV$ (Shape: N_Q x D_V) $Y_i = \sum_j A_{i,j} V_j$



Slide credit: Justin Johnson

Self-Attention Layer

One **query** per **input vector**

Inputs:
Input vectors: **X** (Shape: N_X x D_X)
Key matrix: W_K (Shape: D_X x D_Q)
Value matrix: W_V (Shape: D_X x D_V)
Query matrix: W_Q (Shape: D_X x D_Q)

Computation:
Query vectors: $Q = XW_Q$
Key vectors: $K = XW_K$ (Shape: N_X x D_Q)
Value vectors: $V = XW_V$ (Shape: N_X x D_V)
Similarities: $E = QK^T$ (Shape: N_X x N_X) $E_{i,j} = Q_i \cdot K_j / \sqrt{D_Q}$
Attention weights: $A = \text{softmax}(E, \text{dim}=1)$ (Shape: N_X x N_X)
Output vectors: $Y = AV$ (Shape: N_X x D_V) $Y_i = \sum_j A_{i,j} V_j$

X_1 X_2 X_3

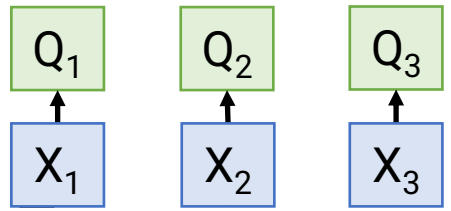
Slide credit: Justin Johnson

Self-Attention Layer

One **query** per **input vector**

Inputs:
Input vectors: **X** (Shape: N_X x D_X)
Key matrix: W_K (Shape: D_X x D_Q)
Value matrix: W_V (Shape: D_X x D_V)
Query matrix: W_Q (Shape: D_X x D_Q)

Computation:
Query vectors: $Q = XW_Q$
Key vectors: $K = XW_K$ (Shape: N_X x D_Q)
Value vectors: $V = XW_V$ (Shape: N_X x D_V)
Similarities: $E = QK^T$ (Shape: N_X x N_X) $E_{i,j} = Q_i \cdot K_j / \text{sqrt}(D_Q)$
Attention weights: A = softmax(E, dim=1) (Shape: N_X x N_X)
Output vectors: $Y = AV$ (Shape: N_X x D_V) $Y_i = \sum_j A_{i,j} V_j$



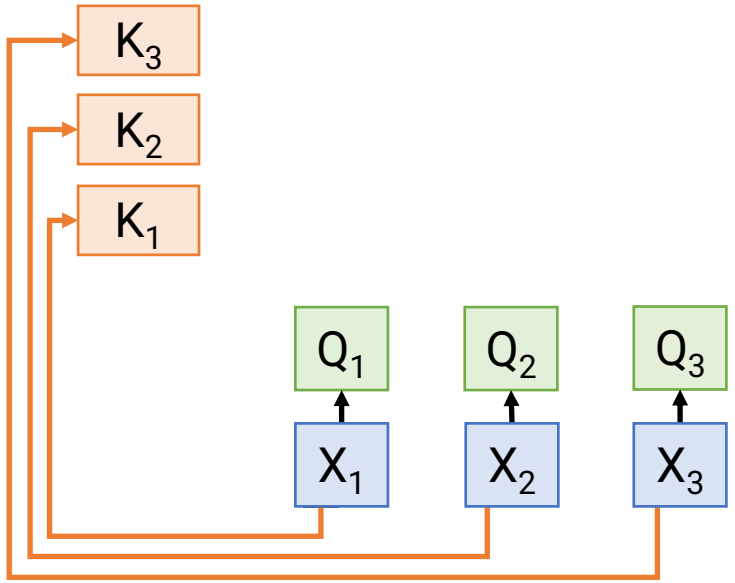
Slide credit: Justin Johnson

Self-Attention Layer

One **query** per **input vector**

Inputs:
Input vectors: X (Shape: $N_X \times D_X$)
Key matrix: W_K (Shape: $D_X \times D_Q$)
Value matrix: W_V (Shape: $D_X \times D_V$)
Query matrix: W_Q (Shape: $D_X \times D_Q$)

Computation:
Query vectors: $Q = XW_Q$
Key vectors: $K = XW_K$ (Shape: $N_X \times D_Q$)
Value vectors: $V = XW_V$ (Shape: $N_X \times D_V$)
Similarities: $E = QK^T$ (Shape: $N_X \times N_X$) $E_{i,j} = Q_i \cdot K_j / \sqrt{D_Q}$
Attention weights: $A = \text{softmax}(E, \text{dim}=1)$ (Shape: $N_X \times N_X$)
Output vectors: $Y = AV$ (Shape: $N_X \times D_V$) $Y_i = \sum_j A_{i,j} V_j$



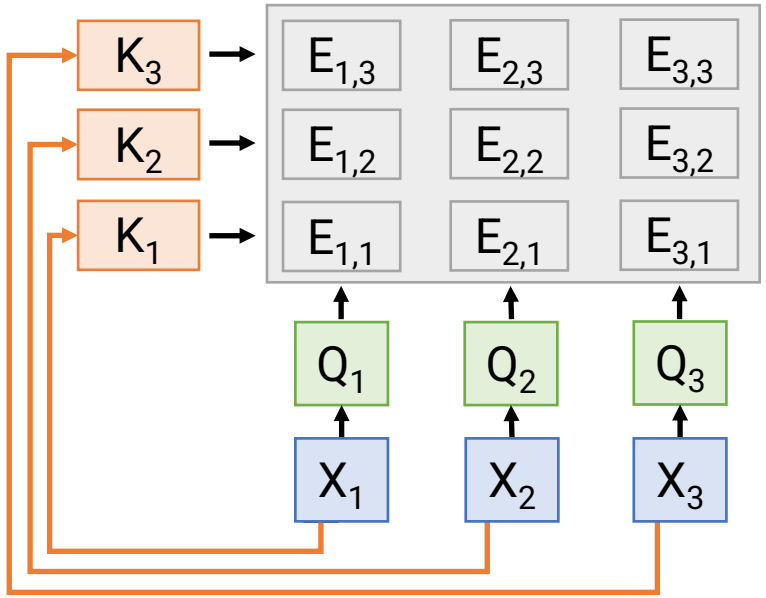
Slide credit: Justin Johnson

Self-Attention Layer

One **query** per **input vector**

Inputs:
Input vectors: X (Shape: $N_X \times D_X$)
Key matrix: W_K (Shape: $D_X \times D_Q$)
Value matrix: W_V (Shape: $D_X \times D_V$)
Query matrix: W_Q (Shape: $D_X \times D_Q$)

Computation:
Query vectors: $Q = XW_Q$
Key vectors: $K = XW_K$ (Shape: $N_X \times D_Q$)
Value vectors: $V = XW_V$ (Shape: $N_X \times D_V$)
Similarities: $E = QK^T$ (Shape: $N_X \times N_X$) $E_{i,j} = Q_i \cdot K_j / \sqrt{D_Q}$
Attention weights: $A = \text{softmax}(E, \text{dim}=1)$ (Shape: $N_X \times N_X$)
Output vectors: $Y = AV$ (Shape: $N_X \times D_V$) $Y_i = \sum_j A_{i,j} V_j$



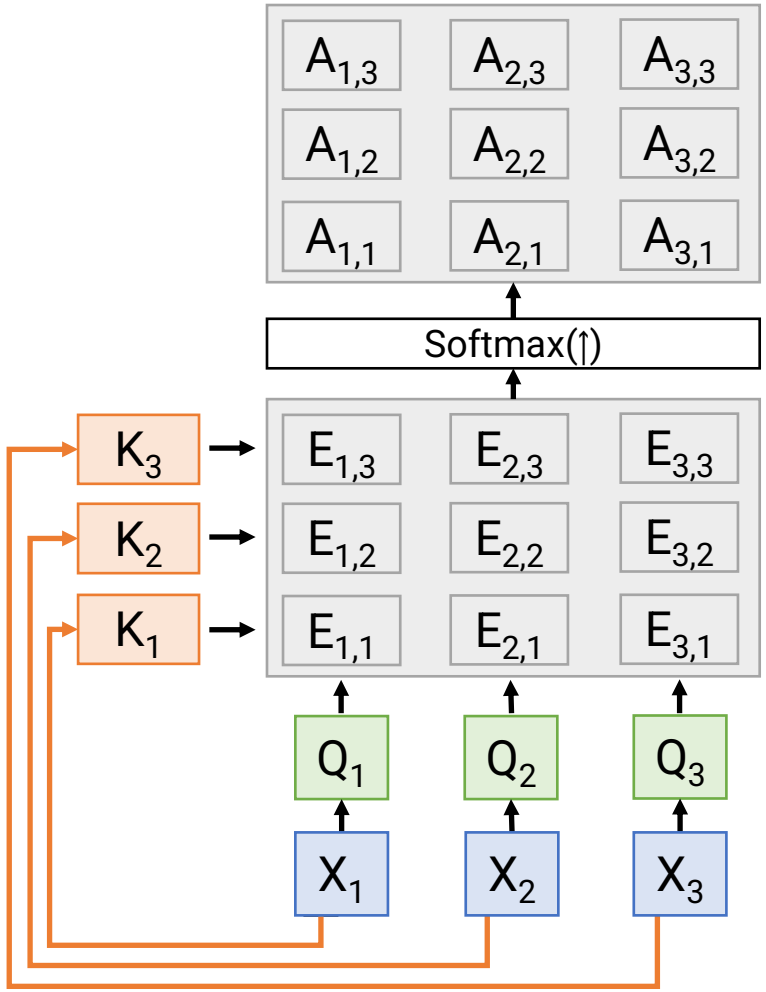
Slide credit: Justin Johnson

Self-Attention Layer

One **query** per **input vector**

Inputs:
Input vectors: **X** (Shape: N_X x D_X)
Key matrix: W_K (Shape: D_X x D_Q)
Value matrix: W_V (Shape: D_X x D_V)
Query matrix: W_Q (Shape: D_X x D_Q)

Computation:
Query vectors: $Q = XW_Q$
Key vectors: $K = XW_K$ (Shape: N_X x D_Q)
Value vectors: $V = XW_V$ (Shape: N_X x D_V)
Similarities: $E = QK^T$ (Shape: N_X x N_X) $E_{i,j} = Q_i \cdot K_j / \sqrt{D_Q}$
Attention weights: A = softmax(E, dim=1) (Shape: N_X x N_X)
Output vectors: $Y = AV$ (Shape: N_X x D_V) $Y_i = \sum_j A_{i,j} V_j$



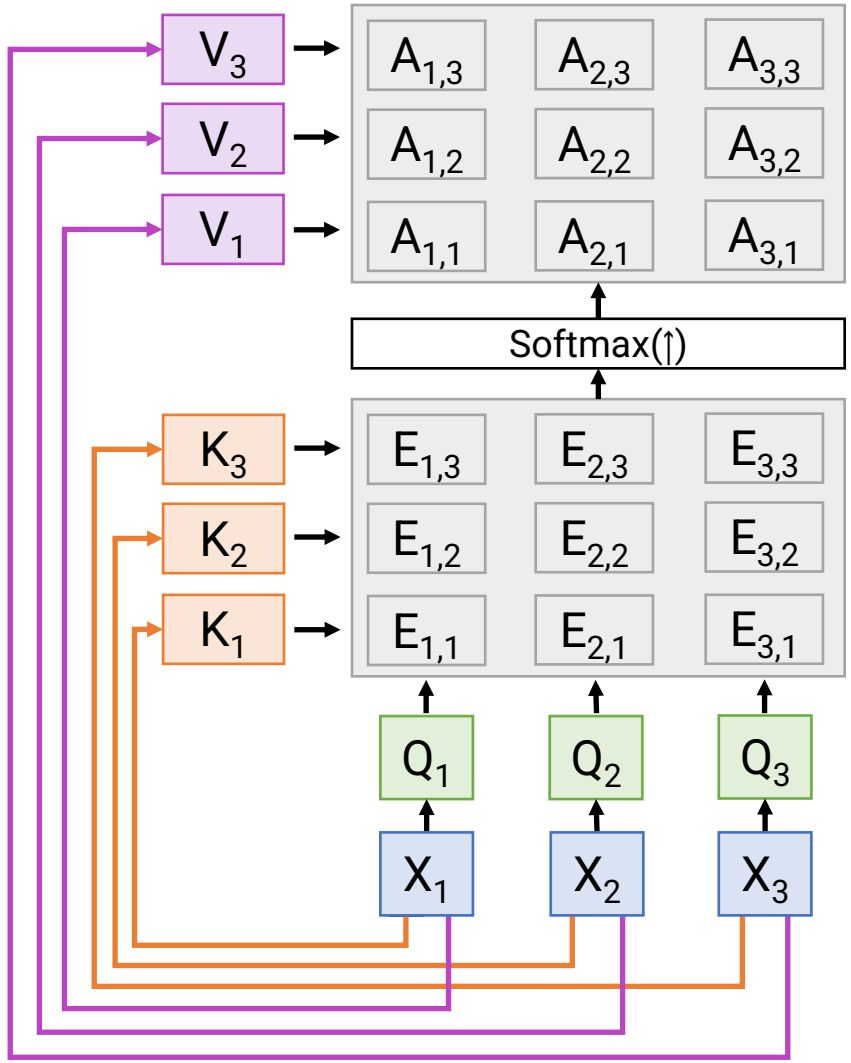
Slide credit: Justin Johnson

Self-Attention Layer

One **query** per **input vector**

Inputs:
Input vectors: X (Shape: $N_X \times D_X$)
Key matrix: W_K (Shape: $D_X \times D_Q$)
Value matrix: W_V (Shape: $D_X \times D_V$)
Query matrix: W_Q (Shape: $D_X \times D_Q$)

Computation:
Query vectors: $Q = XW_Q$
Key vectors: $K = XW_K$ (Shape: $N_X \times D_Q$)
Value vectors: $V = XW_V$ (Shape: $N_X \times D_V$)
Similarities: $E = QK^T$ (Shape: $N_X \times N_X$) $E_{i,j} = Q_i \cdot K_j / \sqrt{D_Q}$
Attention weights: $A = \text{softmax}(E, \text{dim}=1)$ (Shape: $N_X \times N_X$)
Output vectors: $Y = AV$ (Shape: $N_X \times D_V$) $Y_i = \sum_j A_{i,j} V_j$



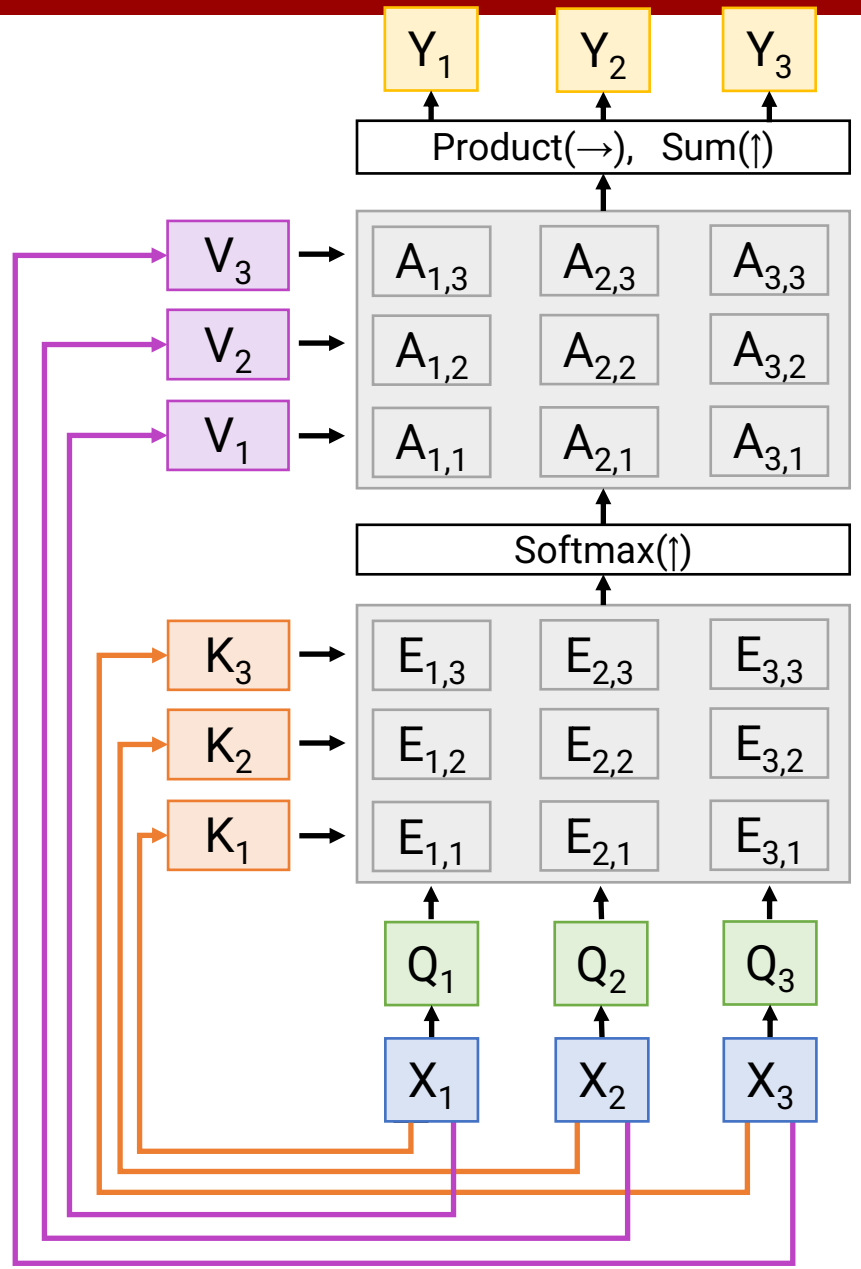
Slide credit: Justin Johnson

Self-Attention Layer

One **query** per **input vector**

Inputs:
Input vectors: X (Shape: $N_X \times D_X$)
Key matrix: W_K (Shape: $D_X \times D_Q$)
Value matrix: W_V (Shape: $D_X \times D_V$)
Query matrix: W_Q (Shape: $D_X \times D_Q$)

Computation:
Query vectors: $Q = XW_Q$
Key vectors: $K = XW_K$ (Shape: $N_X \times D_Q$)
Value vectors: $V = XW_V$ (Shape: $N_X \times D_V$)
Similarities: $E = QK^T$ (Shape: $N_X \times N_X$) $E_{i,j} = Q_i \cdot K_j / \sqrt{D_Q}$
Attention weights: $A = \text{softmax}(E, \text{dim}=1)$ (Shape: $N_X \times N_X$)
Output vectors: $Y = AV$ (Shape: $N_X \times D_V$) $Y_i = \sum_j A_{i,j} V_j$



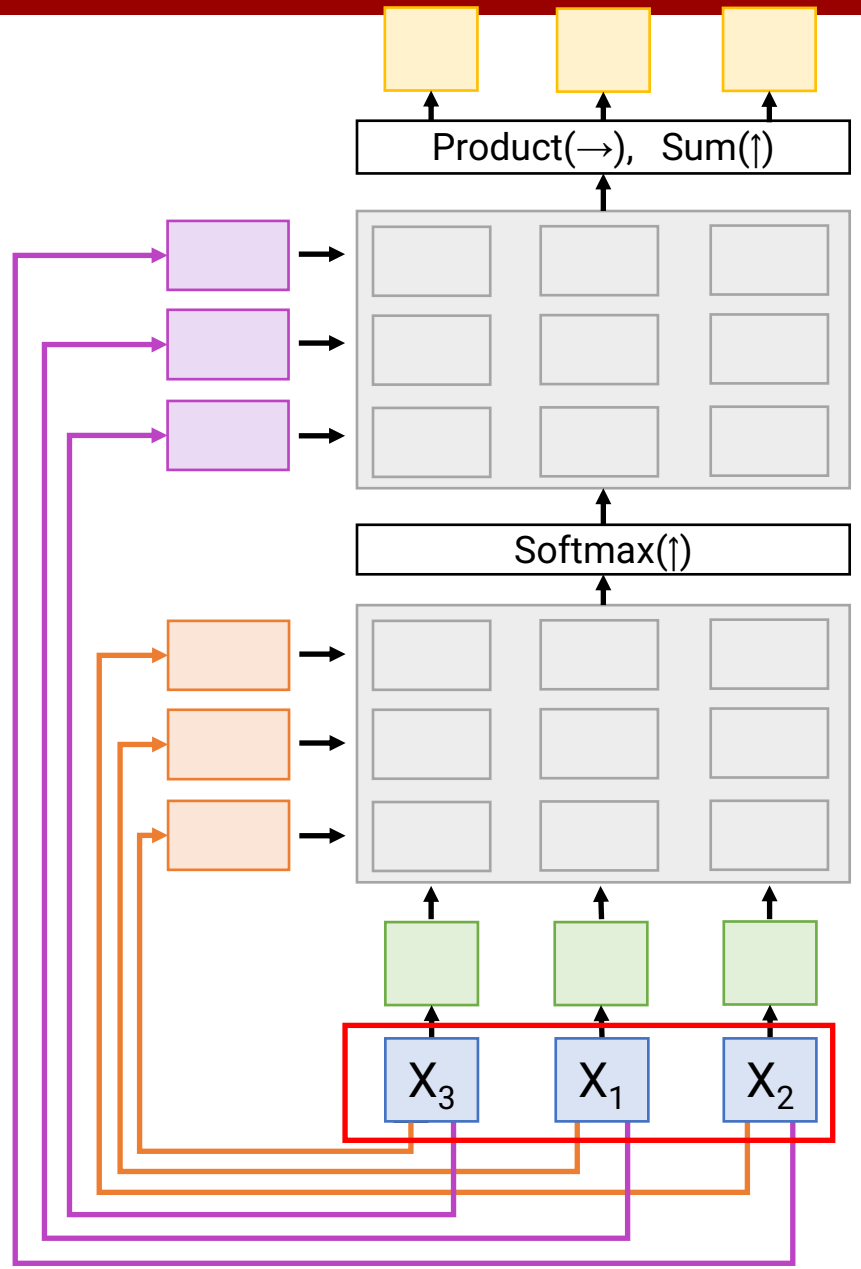
Slide credit: Justin Johnson

Self-Attention Layer

Inputs:
Input vectors: X (Shape: N_X x D_X)
Key matrix: W_K (Shape: D_X x D_Q)
Value matrix: W_V (Shape: D_X x D_V)
Query matrix: W_Q (Shape: D_X x D_Q)

Consider **permuting** the input vectors:

Computation:
Query vectors: $Q = XW_Q$
Key vectors: $K = XW_K$ (Shape: N_X x D_Q)
Value vectors: $V = XW_V$ (Shape: N_X x D_V)
Similarities: $E = QK^T$ (Shape: N_X x N_X) $E_{i,j} = Q_i \cdot K_j / \text{sqrt}(D_Q)$
Attention weights: $A = \text{softmax}(E, \text{dim}=1)$ (Shape: N_X x N_X)
Output vectors: $Y = AV$ (Shape: N_X x D_V) $Y_i = \sum_j A_{i,j} V_j$



Slide credit: Justin Johnson

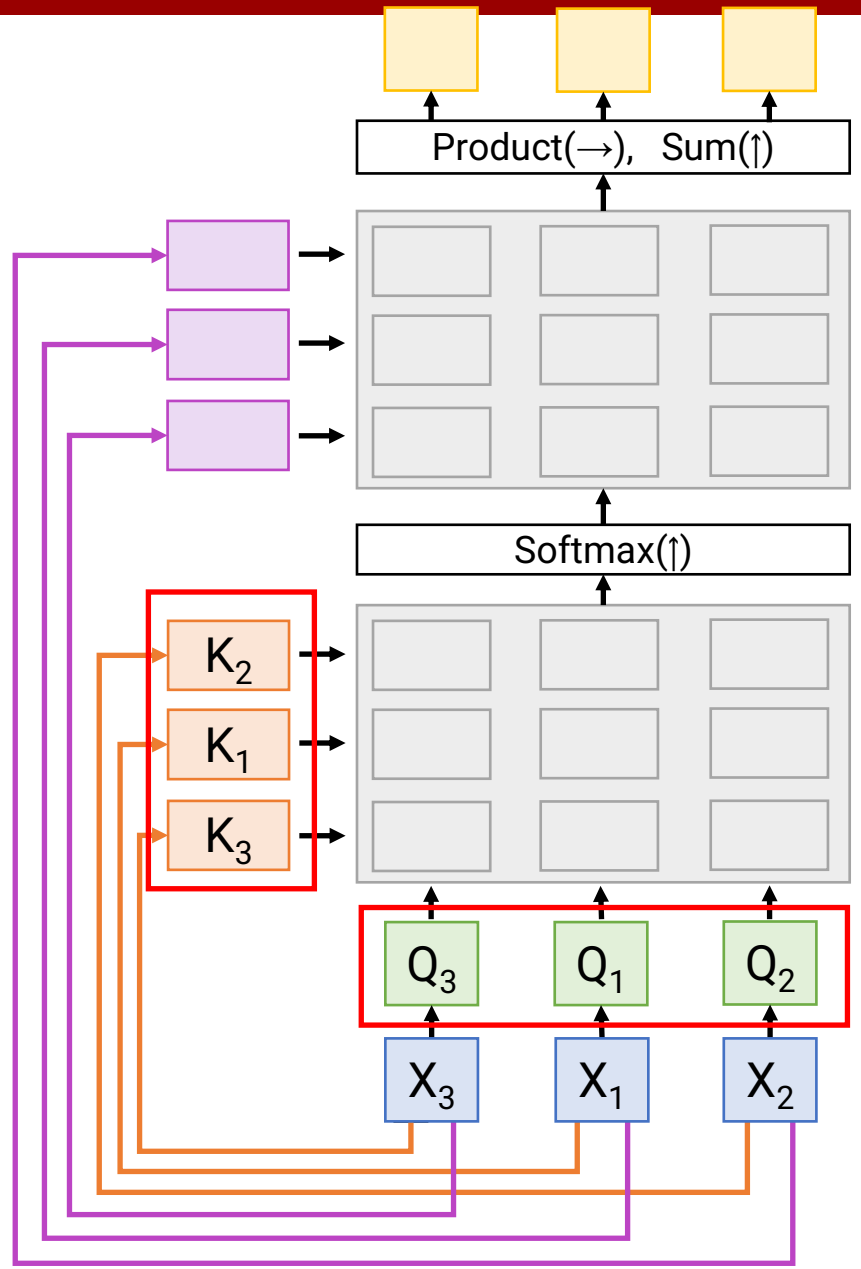
Self-Attention Layer

Inputs:
Input vectors: X (Shape: N_X x D_X)
Key matrix: W_K (Shape: D_X x D_Q)
Value matrix: W_V (Shape: D_X x D_V)
Query matrix: W_Q (Shape: D_X x D_Q)

Consider **permuting** the input vectors:

Queries and Keys will be the same, but permuted

Computation:
Query vectors: $Q = XW_Q$
Key vectors: $K = XW_K$ (Shape: N_X x D_Q)
Value Vectors: $V = XW_V$ (Shape: N_X x D_V)
Similarities: $E = QK^T$ (Shape: N_X x N_X) $E_{i,j} = Q_i \cdot K_j / \sqrt{D_Q}$
Attention weights: A = softmax(E, dim=1) (Shape: N_X x N_X)
Output vectors: $Y = AV$ (Shape: N_X x D_V) $Y_i = \sum_j A_{i,j} V_j$



Slide credit: Justin Johnson

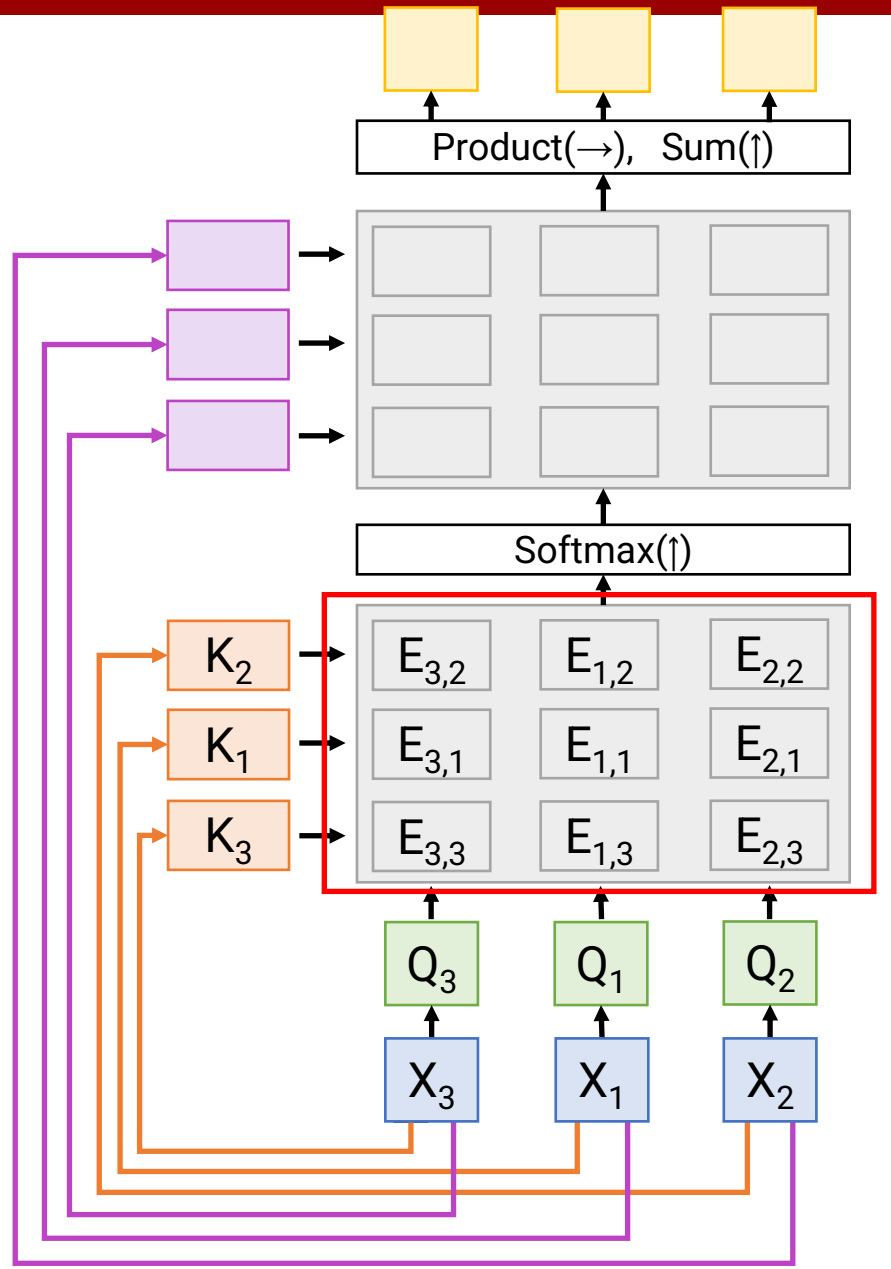
Self-Attention Layer

Inputs:
Input vectors: X (Shape: $N_X \times D_X$)
Key matrix: W_K (Shape: $D_X \times D_Q$)
Value matrix: W_V (Shape: $D_X \times D_V$)
Query matrix: W_Q (Shape: $D_X \times D_Q$)

Consider **permuting** the input vectors:

Similarities will be the same, but permuted

Computation:
Query vectors: $Q = XW_Q$
Key vectors: $K = XW_K$ (Shape: $N_X \times D_Q$)
Value vectors: $V = XW_V$ (Shape: $N_X \times D_V$)
Similarities: $E = QK^T$ (Shape: $N_X \times N_X$) $E_{i,j} = Q_i \cdot K_j / \sqrt{D_Q}$
Attention weights: $A = \text{softmax}(E, \text{dim}=1)$ (Shape: $N_X \times N_X$)
Output vectors: $Y = AV$ (Shape: $N_X \times D_V$) $Y_i = \sum_j A_{i,j} V_j$



Slide credit: Justin Johnson

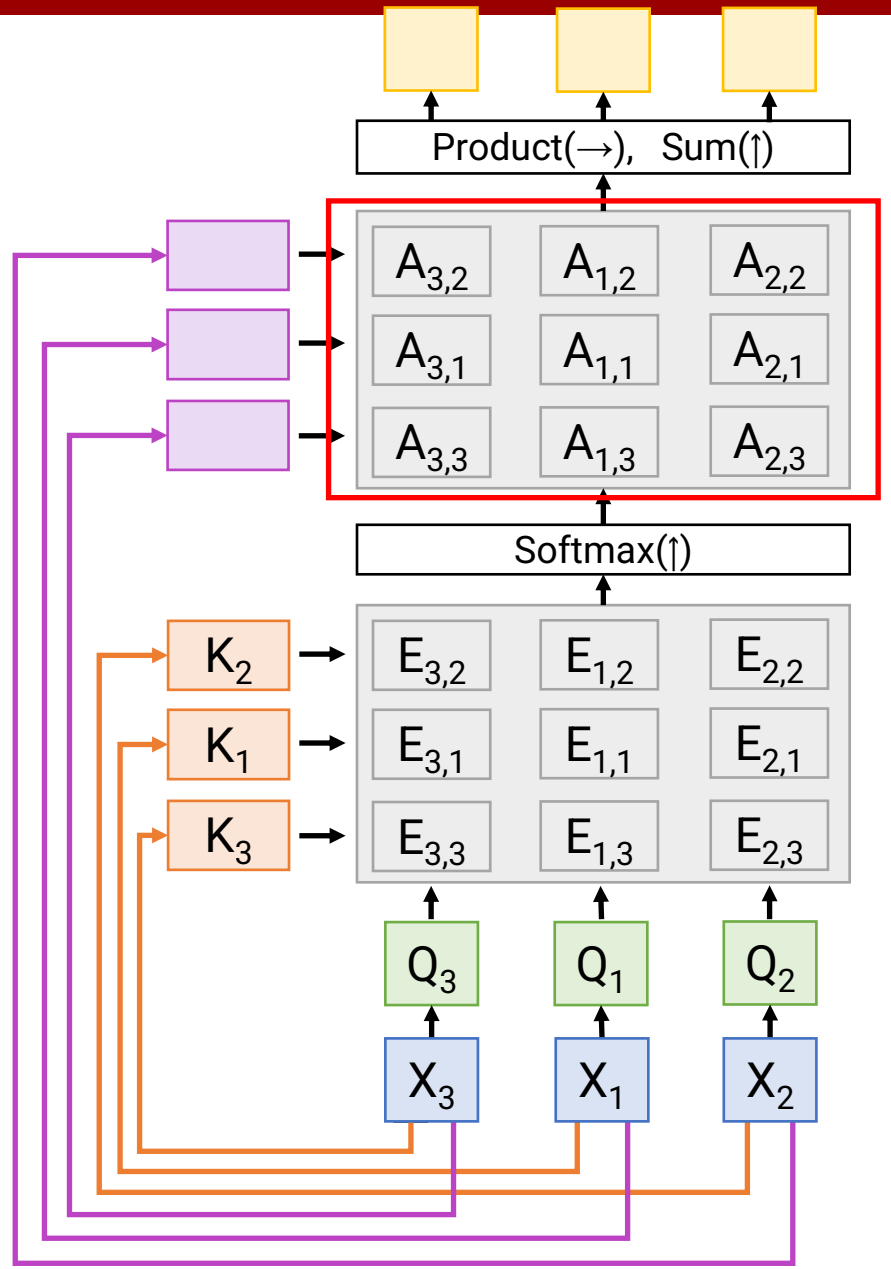
Self-Attention Layer

Inputs:
Input vectors: X (Shape: N_X x D_X)
Key matrix: W_K (Shape: D_X x D_Q)
Value matrix: W_V (Shape: D_X x D_V)
Query matrix: W_Q (Shape: D_X x D_Q)

Consider **permuting** the input vectors:

Attention weights will be the same, but permuted

Computation:
Query vectors: $Q = XW_Q$
Key vectors: $K = XW_K$ (Shape: N_X x D_Q)
Value vectors: $V = XW_V$ (Shape: N_X x D_V)
Similarities: $E = QK^T$ (Shape: N_X x N_X) $E_{i,j} = Q_i \cdot K_j / \text{sqrt}(D_Q)$
Attention weights: A = softmax(E, dim=1) (Shape: N_X x N_X)
Output vectors: $Y = AV$ (Shape: N_X x D_V) $Y_i = \sum_j A_{i,j} V_j$



Slide credit: Justin Johnson

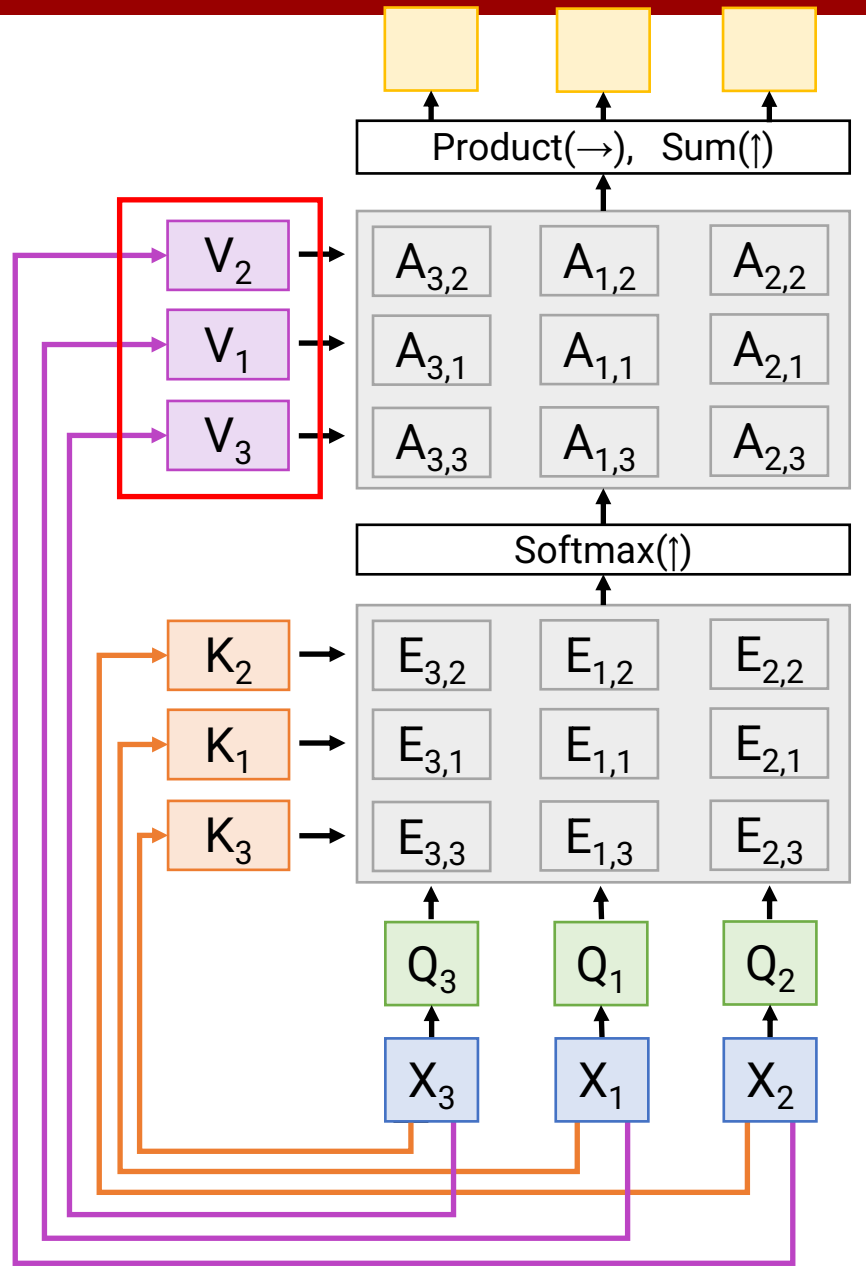
Self-Attention Layer

Inputs:
Input vectors: X (Shape: N_X x D_X)
Key matrix: W_K (Shape: D_X x D_Q)
Value matrix: W_V (Shape: D_X x D_V)
Query matrix: W_Q (Shape: D_X x D_Q)

Consider **permuting** the input vectors:

Values will be the same, but permuted

Computation:
Query vectors: $Q = XW_Q$
Key vectors: $K = XW_K$ (Shape: N_X x D_Q)
Value vectors: $V = XW_V$ (Shape: N_X x D_V)
Similarities: $E = QK^T$ (Shape: N_X x N_X) $E_{i,j} = Q_i \cdot K_j / \sqrt{D_Q}$
Attention weights: $A = \text{softmax}(E, \text{dim}=1)$ (Shape: N_X x N_X)
Output vectors: $Y = AV$ (Shape: N_X x D_V) $Y_i = \sum_j A_{i,j} V_j$



Slide credit: Justin Johnson

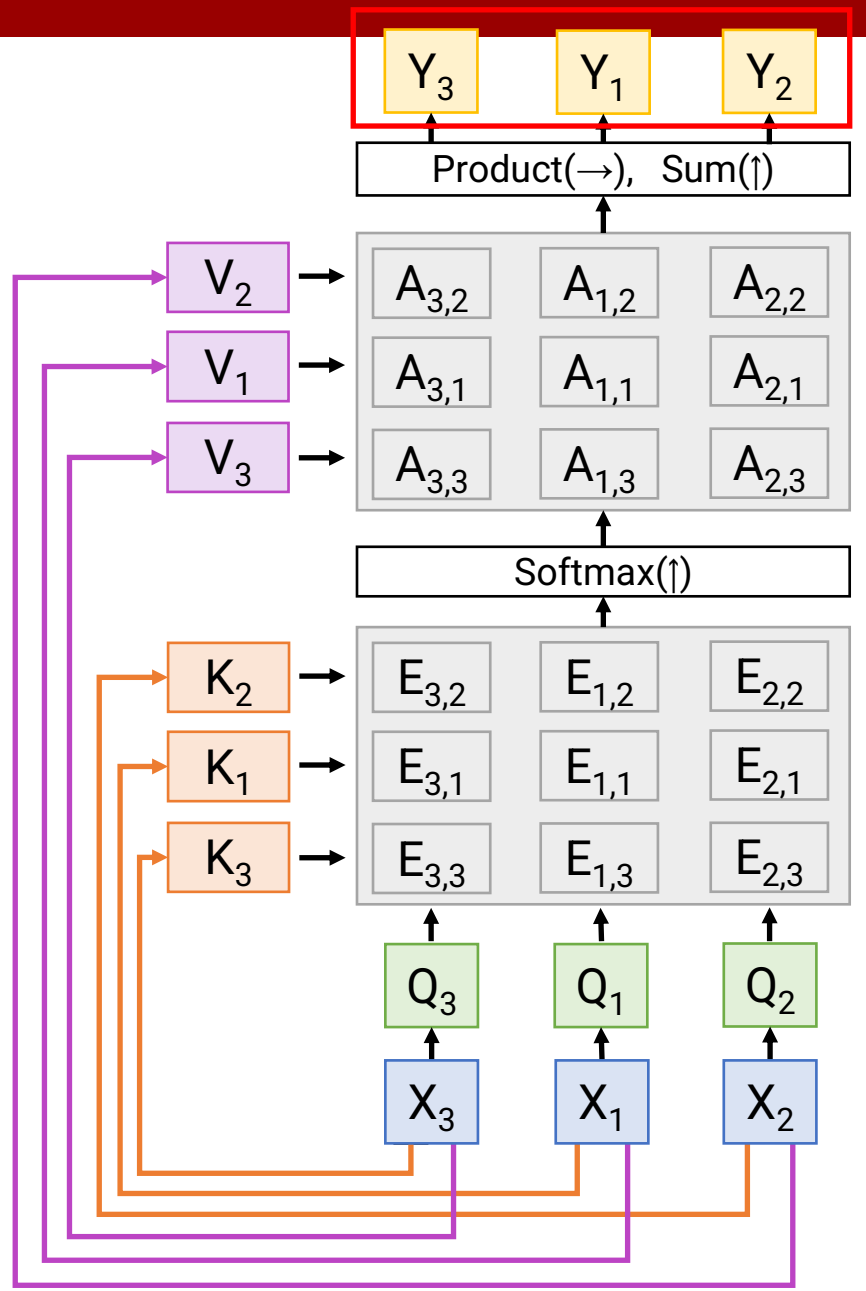
Self-Attention Layer

Inputs:
Input vectors: X (Shape: N_X x D_X)
Key matrix: W_K (Shape: D_X x D_Q)
Value matrix: W_V (Shape: D_X x D_V)
Query matrix: W_Q (Shape: D_X x D_Q)

Consider **permuting** the input vectors:

Outputs will be the same, but permuted

Computation:
Query vectors: $Q = XW_Q$
Key vectors: $K = XW_K$ (Shape: N_X x D_Q)
Value vectors: $V = XW_V$ (Shape: N_X x D_V)
Similarities: $E = QK^T$ (Shape: N_X x N_X) $E_{i,j} = Q_i \cdot K_j / \text{sqrt}(D_Q)$
Attention weights: A = softmax(E, dim=1) (Shape: N_X x N_X)
Output vectors: $Y = AV$ (Shape: N_X x D_V) $Y_i = \sum_j A_{i,j} V_j$



Slide credit: Justin Johnson

Self-Attention Layer

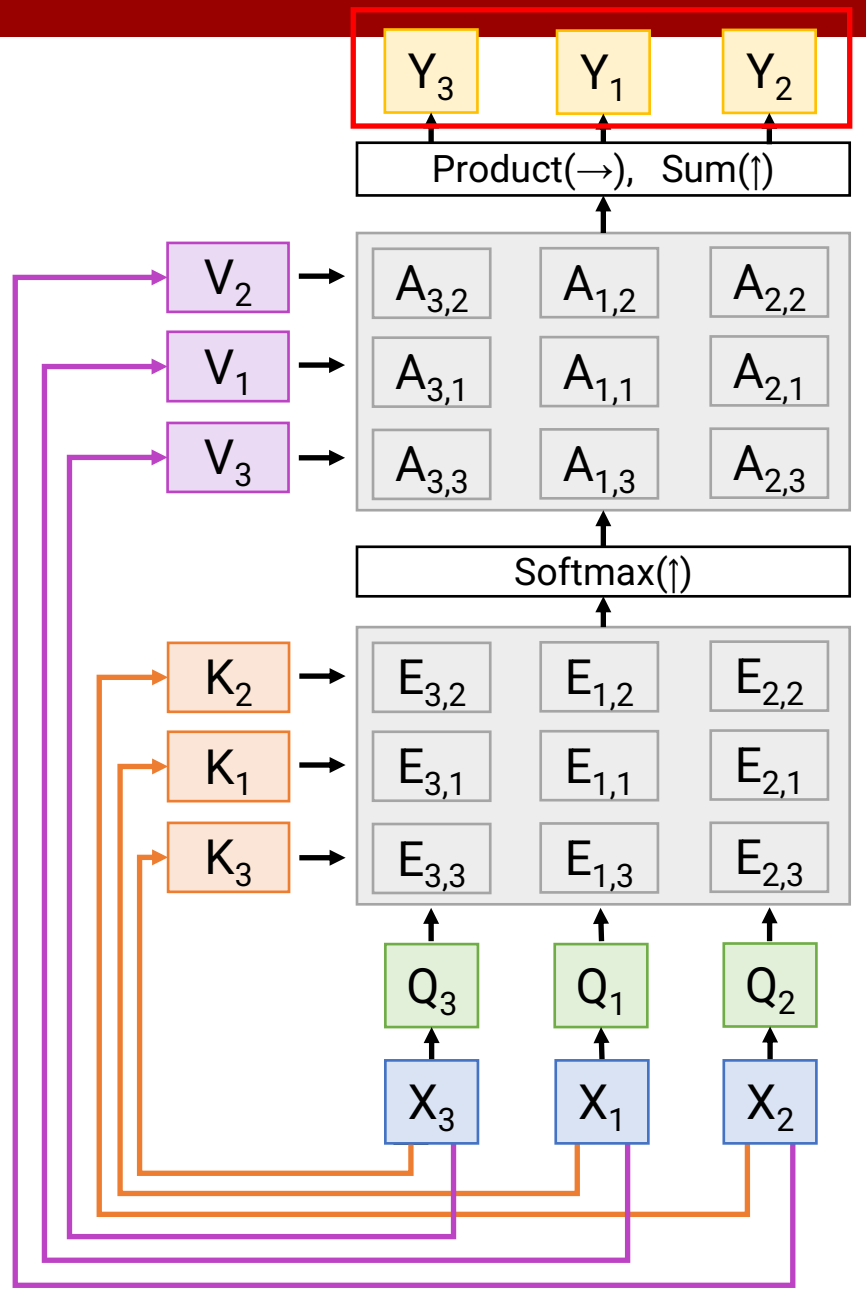
Inputs:
Input vectors: X (Shape: $N_X \times D_X$)
Key matrix: W_K (Shape: $D_X \times D_Q$)
Value matrix: W_V (Shape: $D_X \times D_V$)
Query matrix: W_Q (Shape: $D_X \times D_Q$)

Computation:
Query vectors: $Q = XW_Q$
Key vectors: $K = XW_K$ (Shape: $N_X \times D_Q$)
Value vectors: $V = XW_V$ (Shape: $N_X \times D_V$)
Similarities: $E = QK^T$ (Shape: $N_X \times N_X$) $E_{i,j} = Q_i \cdot K_j / \sqrt{D_Q}$
Attention weights: $A = \text{softmax}(E, \text{dim}=1)$ (Shape: $N_X \times N_X$)
Output vectors: $Y = AV$ (Shape: $N_X \times D_V$) $Y_i = \sum_j A_{i,j} V_j$

Consider **permuting** the input vectors:

Outputs will be the same, but permuted

Self-attention layer is **Permutation Equivariant**
$f(s(x)) = s(f(x))$



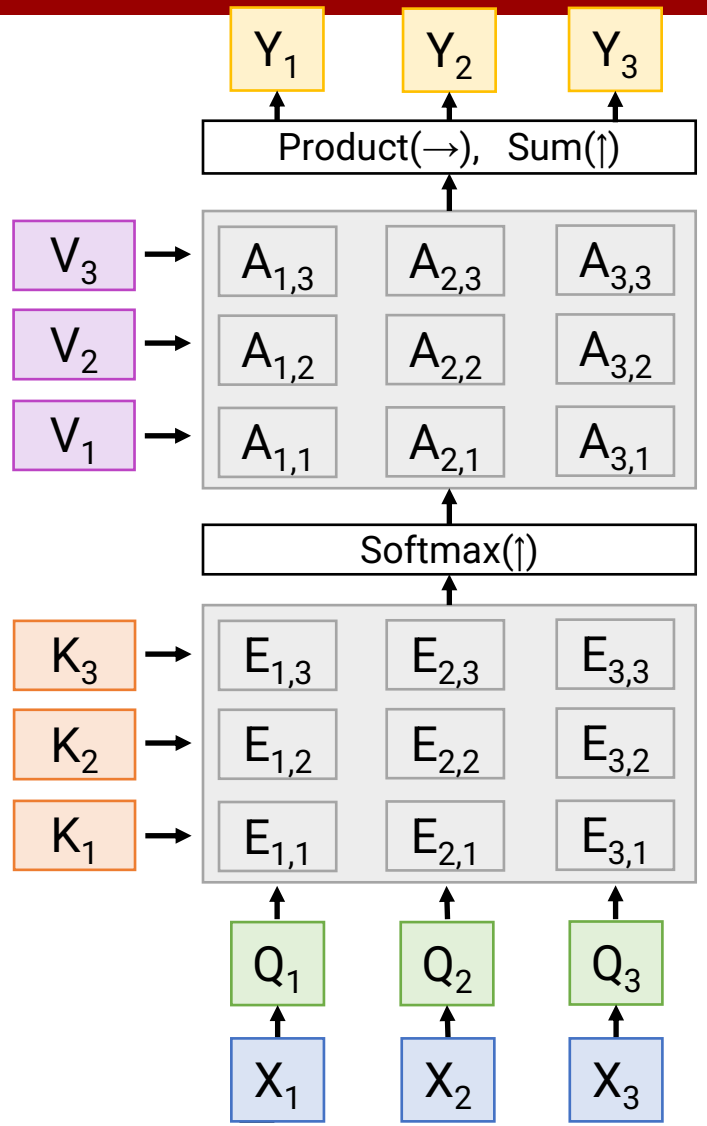
Slide credit: Justin Johnson

Self-Attention Layer

Inputs:
Input vectors: X (Shape: N_X x D_X)
Key matrix: W_K (Shape: D_X x D_Q)
Value matrix: W_V (Shape: D_X x D_V)
Query matrix: W_Q (Shape: D_X x D_Q)

Self attention doesn't "know" the order of the vectors it is processing!

Computation:
Query vectors: $Q = XW_Q$
Key vectors: $K = XW_K$ (Shape: N_X x D_Q)
Value vectors: $V = XW_V$ (Shape: N_X x D_V)
Similarities: $E = QK^T$ (Shape: N_X x N_X) $E_{i,j} = Q_i \cdot K_j / \sqrt{D_Q}$
Attention weights: $A = \text{softmax}(E, \text{dim}=1)$ (Shape: N_X x N_X)
Output vectors: $Y = AV$ (Shape: N_X x D_V) $Y_i = \sum_j A_{i,j} V_j$



Slide credit: Justin Johnson

Self-Attention Layer

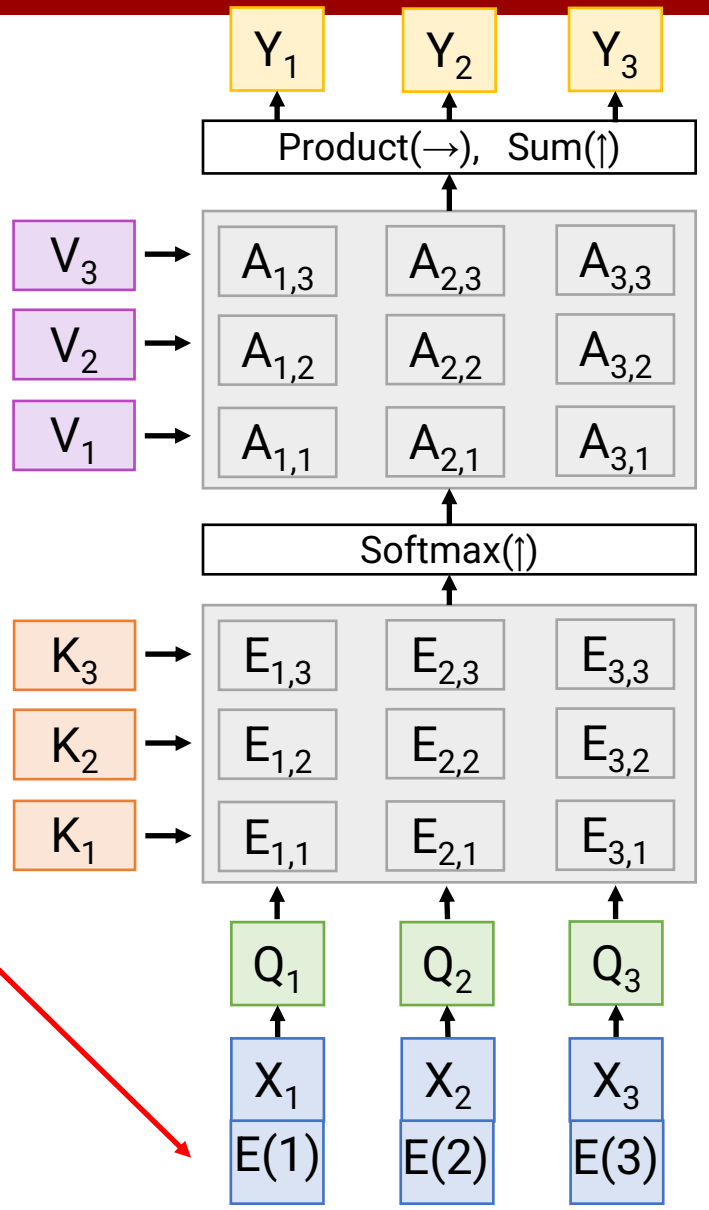
Inputs:
Input vectors: X (Shape: $N_X \times D_X$)
Key matrix: W_K (Shape: $D_X \times D_Q$)
Value matrix: W_V (Shape: $D_X \times D_V$)
Query matrix: W_Q (Shape: $D_X \times D_Q$)

Computation:
Query vectors: $Q = XW_Q$
Key vectors: $K = XW_K$ (Shape: $N_X \times D_Q$)
Value vectors: $V = XW_V$ (Shape: $N_X \times D_V$)
Similarities: $E = QK^T$ (Shape: $N_X \times N_X$) $E_{i,j} = Q_i \cdot K_j / \text{sqrt}(D_Q)$
Attention weights: $A = \text{softmax}(E, \text{dim}=1)$ (Shape: $N_X \times N_X$)
Output vectors: $Y = AV$ (Shape: $N_X \times D_V$) $Y_i = \sum_j A_{i,j} V_j$

Self attention doesn't "know" the order of the vectors it is processing!

In order to make processing position-aware, concatenate input with **positional encoding**

E can be learned lookup table, or fixed function



Slide credit: Justin Johnson

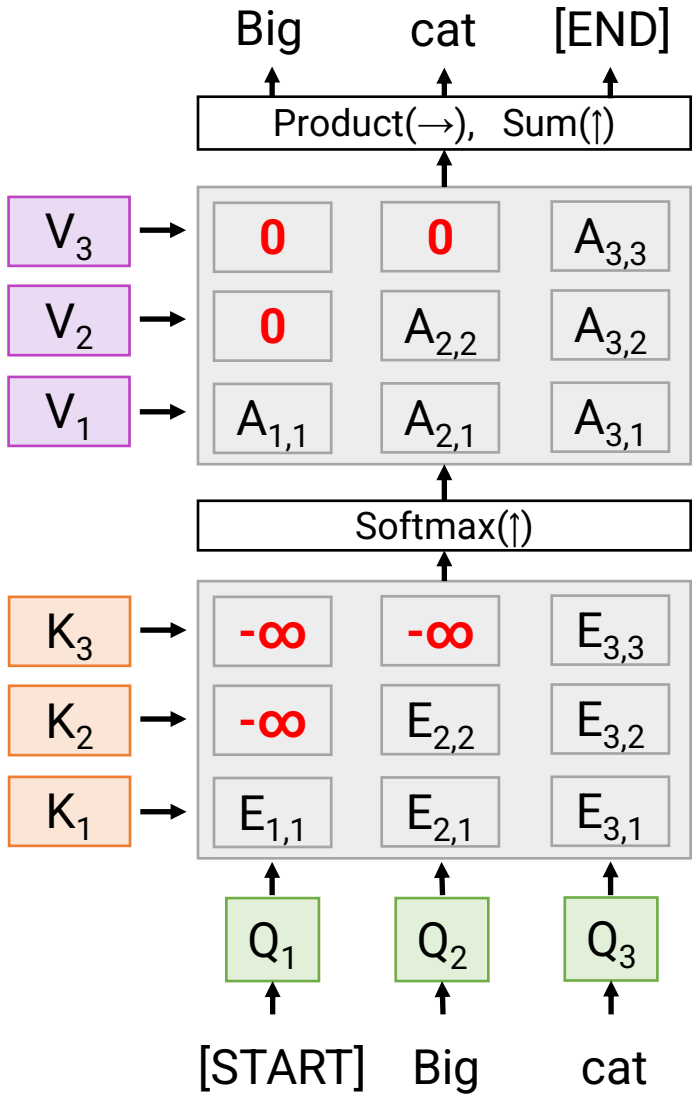
Masked Self-Attention Layer

Inputs:
Input vectors: X (Shape: N_X x D_X)
Key matrix: W_K (Shape: D_X x D_Q)
Value matrix: W_V (Shape: D_X x D_V)
Query matrix: W_Q (Shape: D_X x D_Q)

Don't let vectors "look ahead" in the sequence

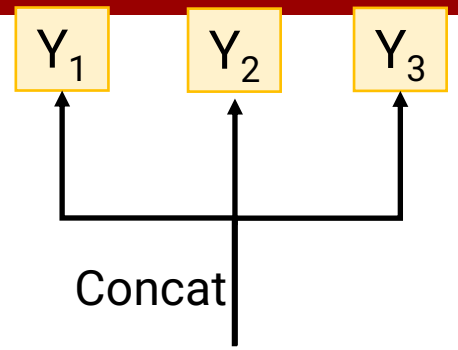
Used for language modeling (predict next word)

Computation:
Query vectors: $Q = XW_Q$
Key vectors: $K = XW_K$ (Shape: N_X x D_Q)
Value vectors: $V = XW_V$ (Shape: N_X x D_V)
Similarities: $E = QK^T$ (Shape: N_X x N_X) $E_{i,j} = Q_i \cdot K_j / \text{sqrt}(D_Q)$
Attention weights: A = softmax(E, dim=1) (Shape: N_X x N_X)
Output vectors: $Y = AV$ (Shape: N_X x D_V) $Y_i = \sum_j A_{i,j} V_j$



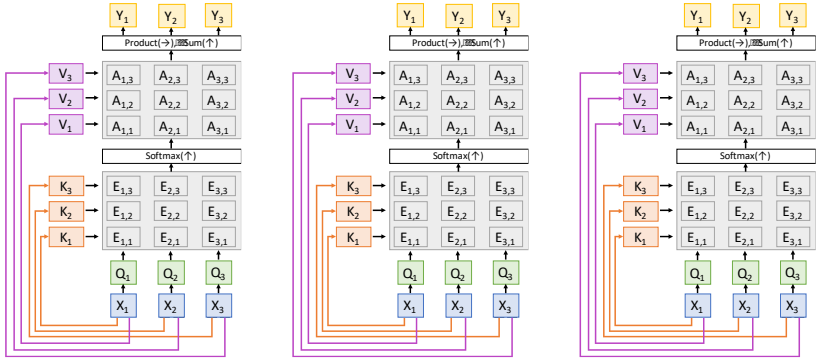
Slide credit: Justin Johnson

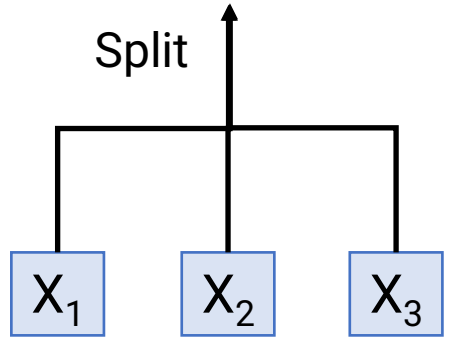
Multihead Self-Attention Layer



Inputs:
Input vectors: X (Shape: N_X x D_X)
Key matrix: W_K (Shape: D_X x D_Q)
Value matrix: W_V (Shape: D_X x D_V)
Query matrix: W_Q (Shape: D_X x D_Q)

Use H independent "Attention Heads" in parallel



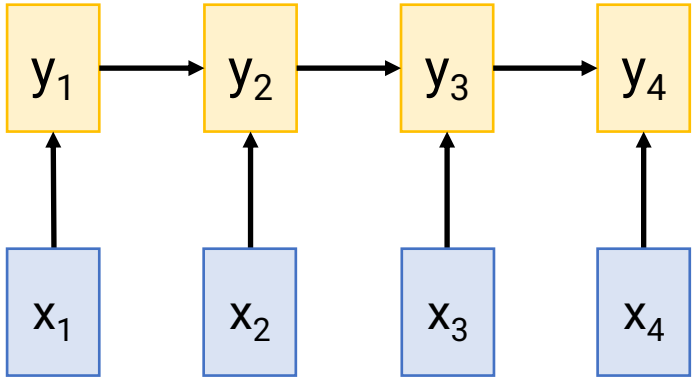


Computation:
Query vectors: $Q = XW_Q$
Key vectors: $K = XW_K$ (Shape: N_X x D_Q)
Value vectors: $V = XW_V$ (Shape: N_X x D_V)
Similarities: $E = QK^T$ (Shape: N_X x N_X) $E_{i,j} = Q_i \cdot K_j / \sqrt{D_Q}$
Attention weights: $A = softmax(E, dim=1)$ (Shape: N_X x N_X)
Output vectors: $Y = AV$ (Shape: N_X x D_V) $Y_i = \sum_j A_{i,j} V_j$

Slide credit: Justin Johnson

Three Ways of Processing Sequences

Recurrent Neural Network

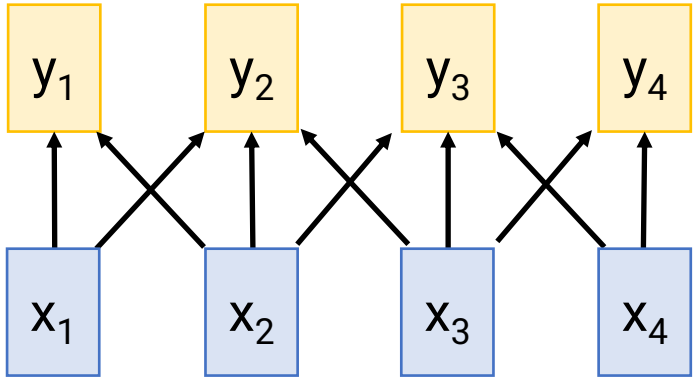


Works on **Ordered Sequences**

(+) Good at long sequences: After one RNN layer, h_T "sees" the whole sequence

(-) Not parallelizable: need to compute hidden states sequentially

1D Convolution

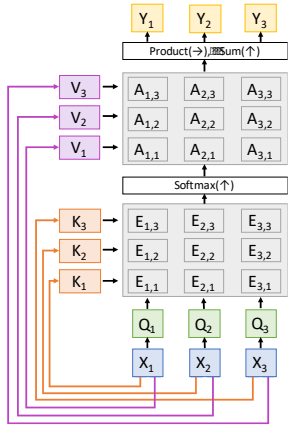


Works on **Multidimensional Grids**

(-) Bad at long sequences: Need to stack many conv layers for outputs to "see" the whole sequence

(+) Highly parallel: Each output can be computed in parallel

Self-Attention



Works on **Sets of Vectors**

(+) Good at long sequences: after one self-attention layer, each output "sees" all inputs!

(+) Highly parallel: Each output can be computed in parallel

(-) Very memory intensive

Slide credit: Justin Johnson