Topics:

- Attention and Transformers

CS 4644-DL / 7643-A

ZSOLT KIRA

- **Assignment 3 out**
    - Due **March 8th 11:59pm EST**

- Meta office hours Friday 3pm ET on Attention/Language Models

Lecture Outline

- Machine Translation with RNNs
- RNNs with Attention
- From Attention to Transformers
- What can Transformers do?

Slides from Justin Johnson, modified by Arjun Madjumdar

Sequence Modeling with RNNs

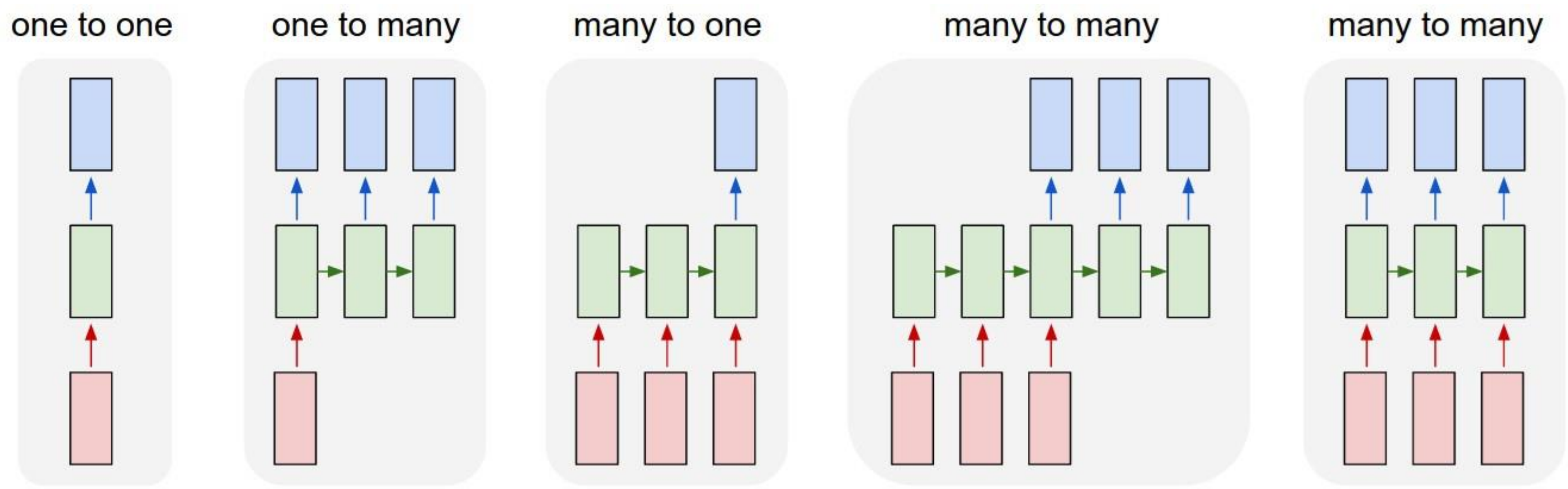
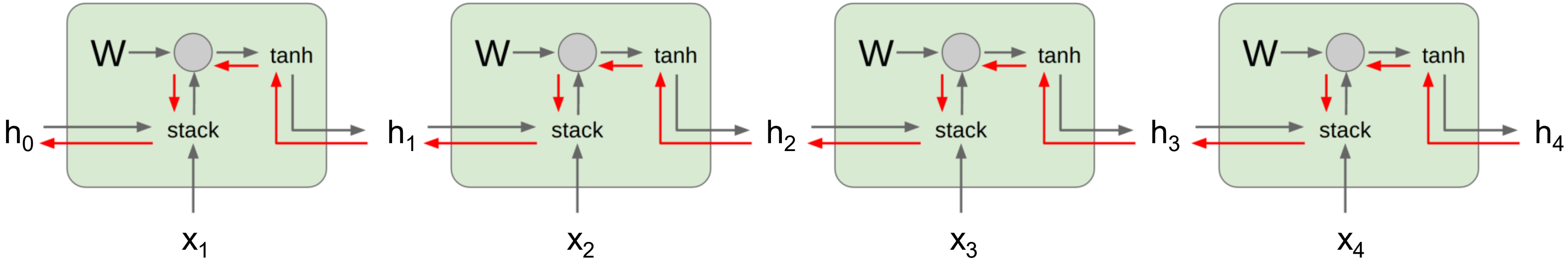


Image Credit: Andrej Karpathy

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



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

How can we train this on language?

- Supervised Learning:
  - Sentiment analysis (sentence -> negative/neutral/positive) labeled by humans
  - Translation -> English and equivalent other language

- Self-supervised: Predict the next letter or word!
  - This is **extremely powerful!!**
  - In order to predict what's next, it needs to really understand not just language statistics but world knowledge!
    - Of course, we need scale for this level of loss reduction / understanding

- **Training:** A large corpus of text from the web
  - Note: No annotation required! It's just "the text"

- **Inference:** Just generate me new text
  - Can condition on some initial input (**prompt**)

```c
#include <asm/io.h>
#include <asm/prom.h>
#include <asm/e820.h>
#include <asm/system_info.h>
#include <asm/setew.h>
#include <asm/pgproto.h>

#define REG_PG    vesa_slot_addr_pack
#define PFM_NOCOMP  AFSR(0, load)
#define STACK_DDR(type)     (func)

#define SWAP_ALLOCATE(nr)     (e)
#define emulate_sigs()  arch_get_unaligned_child()
#define access_rw(TST)  asm volatile("movd %%esp, %0, %3" : : "r" (0));   \
  if (__type & DO_READ)

static void stat_PC_SEC __read_mostly offsetof(struct seq_argsqueue, \
          pC>[1]);

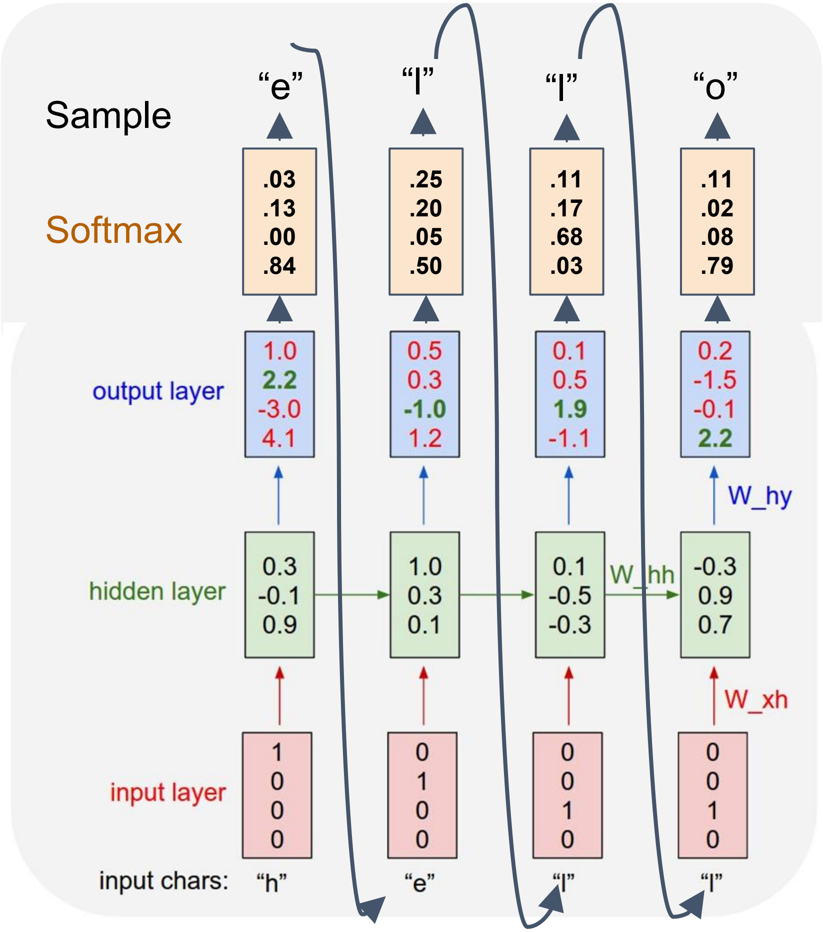
static void
os_prefix(unsigned long sys)
{
#ifdef CONFIG_PREEMPT
  PUT_PARAM_RAID(2, sel) = get_state_state();
  set_pid_sum((unsigned long)state, current_state_str(),
           (unsigned long)-1->lr_full; low;
}
```

Test Time: Sample / Argmax / Beam Search

Example: Character-level Language Model Sampling

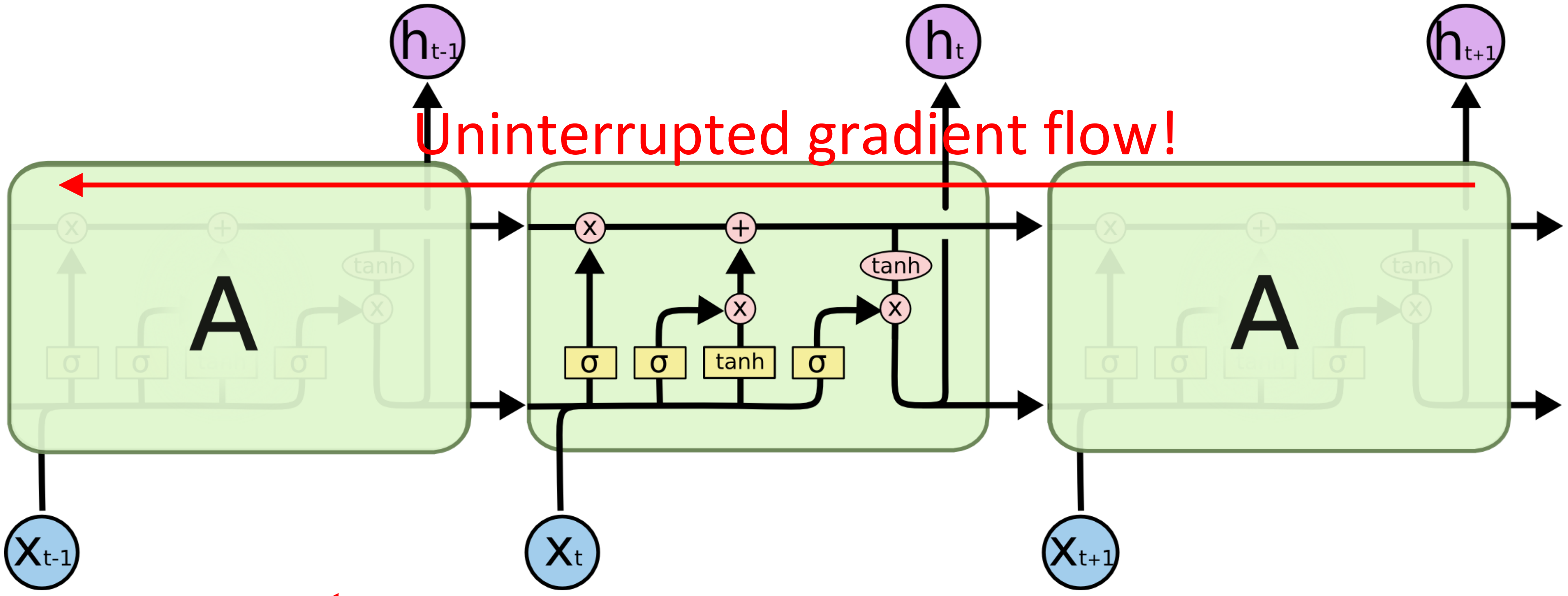
Vocabulary: [h,e,l,o]

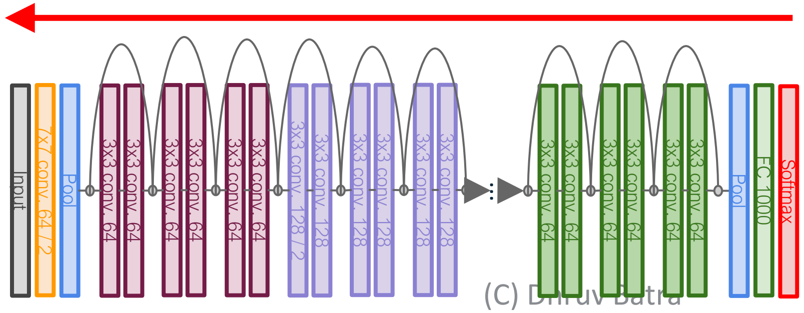
At test-time sample characters one at a time, feed back to model



Can also feed in predictions during training (student forcing)

LSTMs Intuition: Additive Updates





Similar to ResNet!

Image Credit: Christopher Olah (http://colah.github.io/posts/2015-08-Understanding-LSTMs/)

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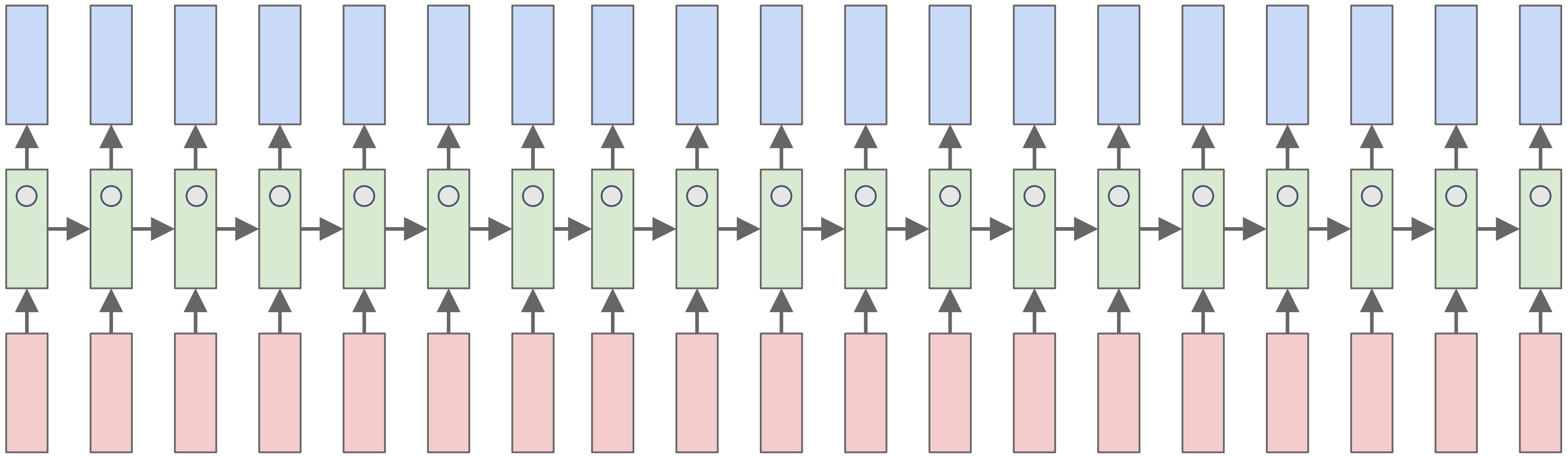
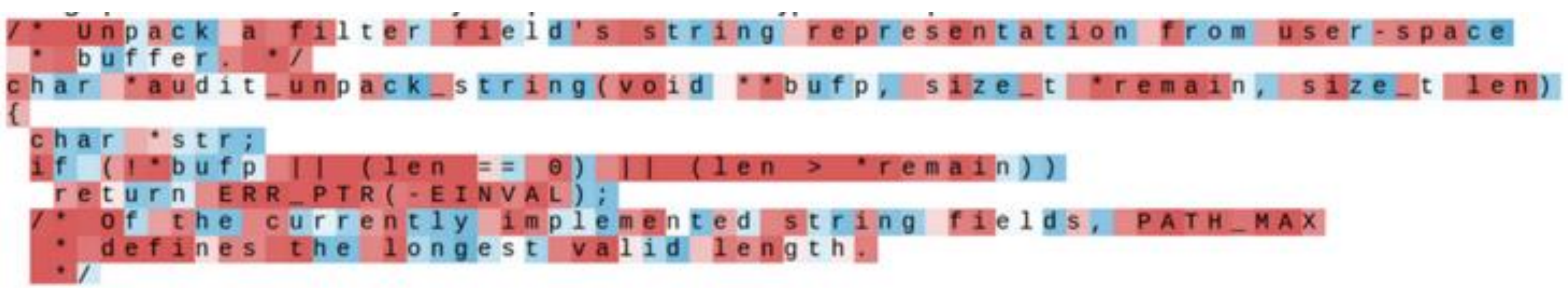
```

Searching for interpretable cells



Karpathy, Johnson, and Fei-Fei: Visualizing and Understanding Recurrent Networks, ICLR Workshop 2016

Searching for interpretable cells



Karpathy, Johnson, and Fei-Fei: Visualizing and Understanding Recurrent Networks, ICLR Workshop 2016

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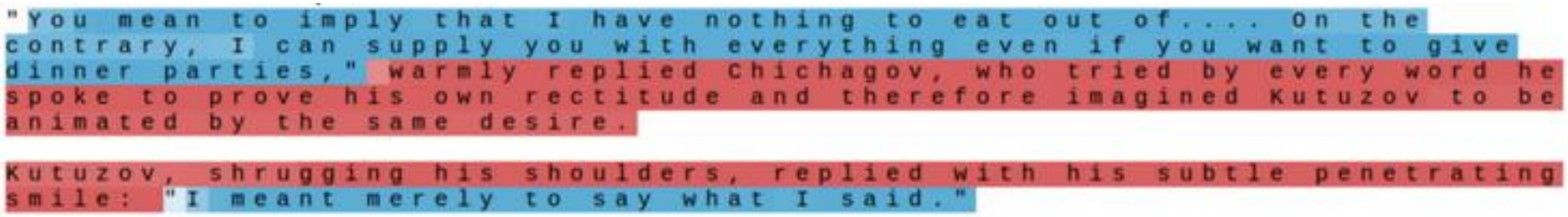
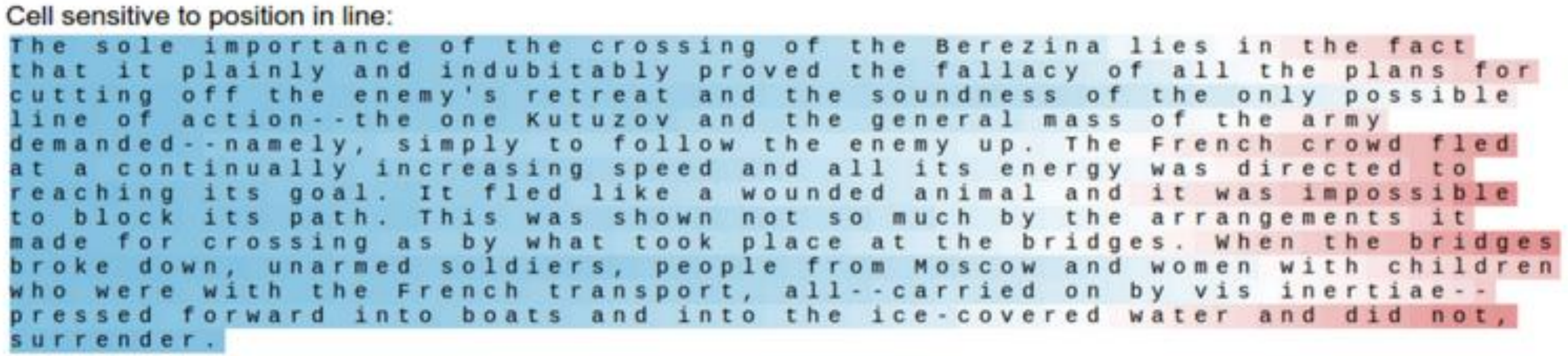


quote detection cell

Karpathy, Johnson, and Fei-Fei: Visualizing and Understanding Recurrent Networks, ICLR Workshop 2016

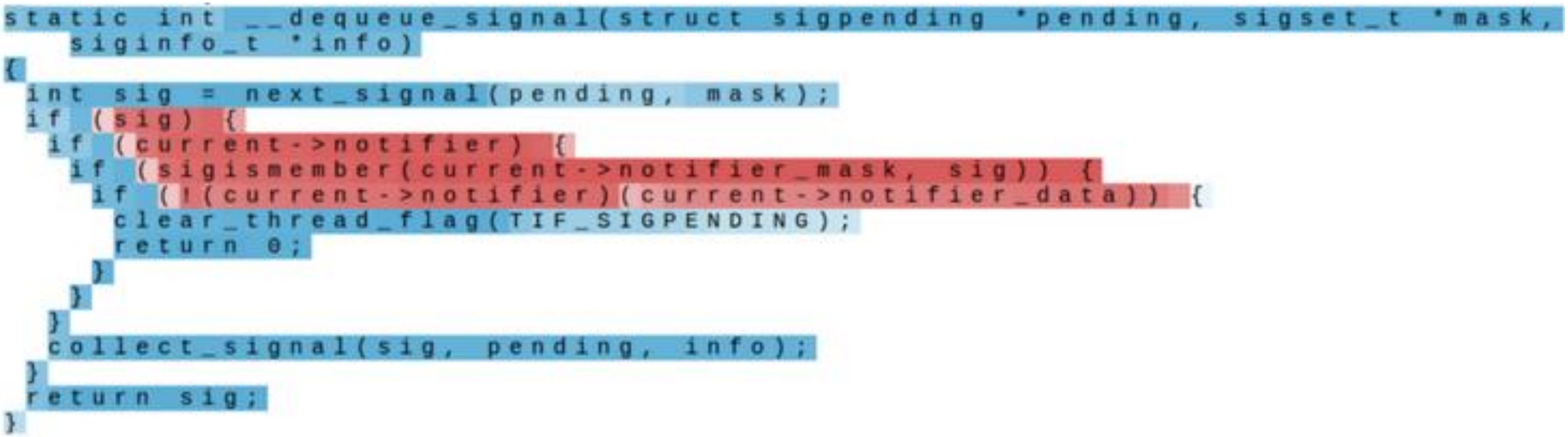
Searching for interpretable cells



line length tracking cell

Karpathy, Johnson, and Fei-Fei: Visualizing and Understanding Recurrent Networks, ICLR Workshop 2016

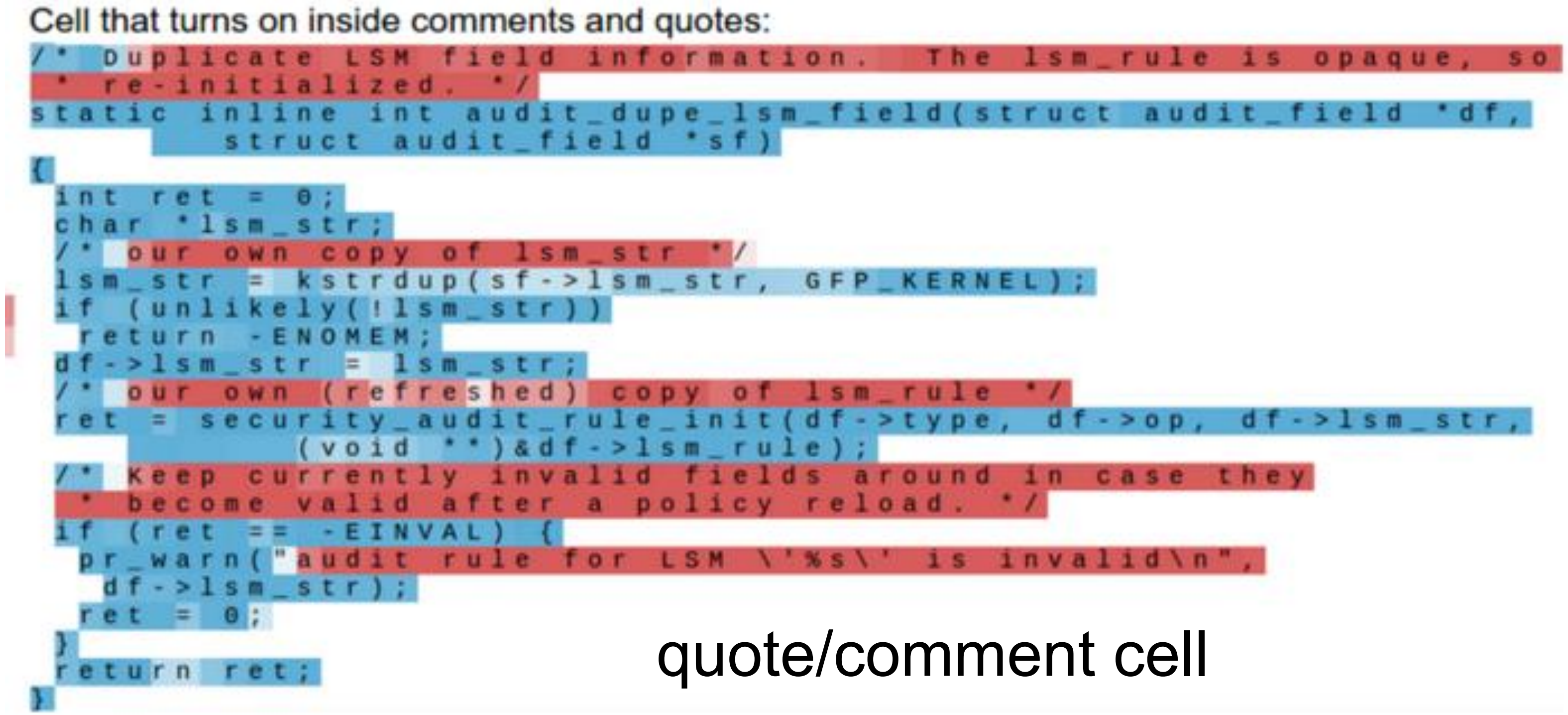
Searching for interpretable cells



if statement cell

Karpathy, Johnson, and Fei-Fei: Visualizing and Understanding Recurrent Networks, ICLR Workshop 2016

Searching for interpretable cells



Karpathy, Johnson, and Fei-Fei: Visualizing and Understanding Recurrent Networks, ICLR Workshop 2016

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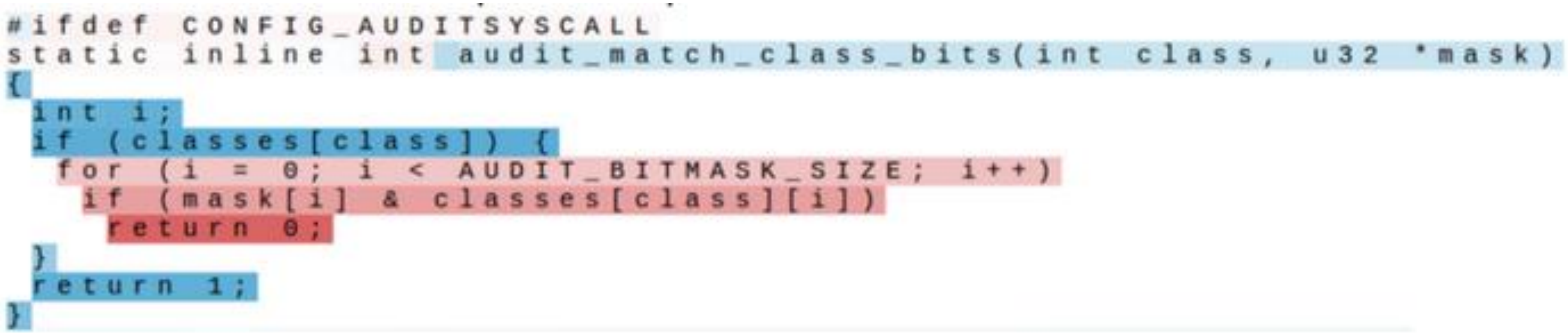
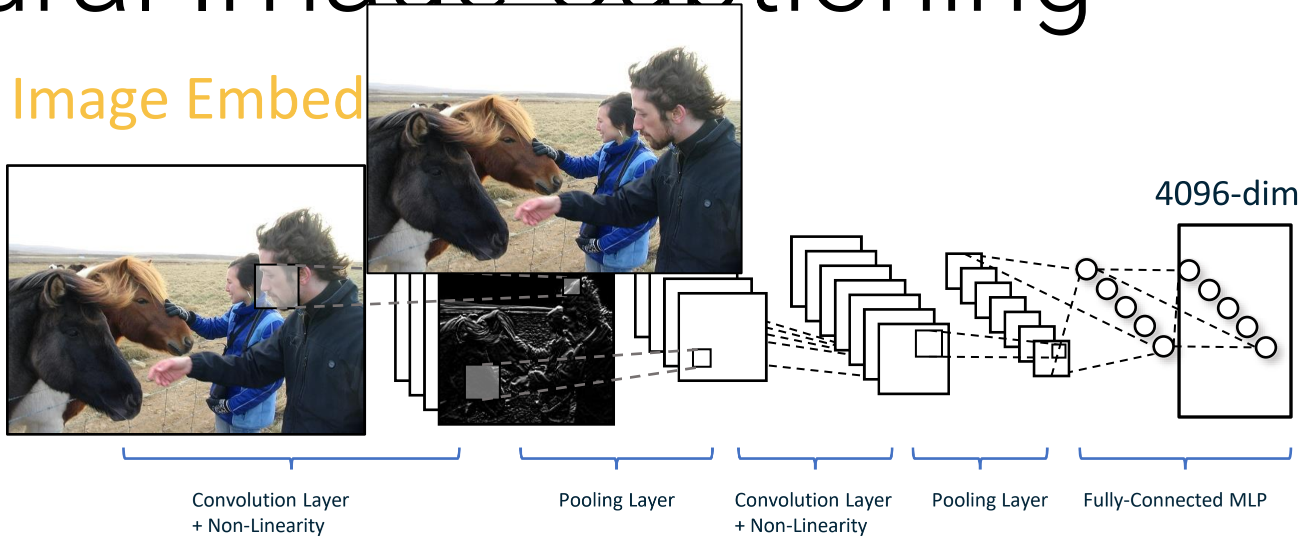


code depth cell

Karpathy, Johnson, and Fei-Fei: Visualizing and Understanding Recurrent Networks, ICLR Workshop 2016

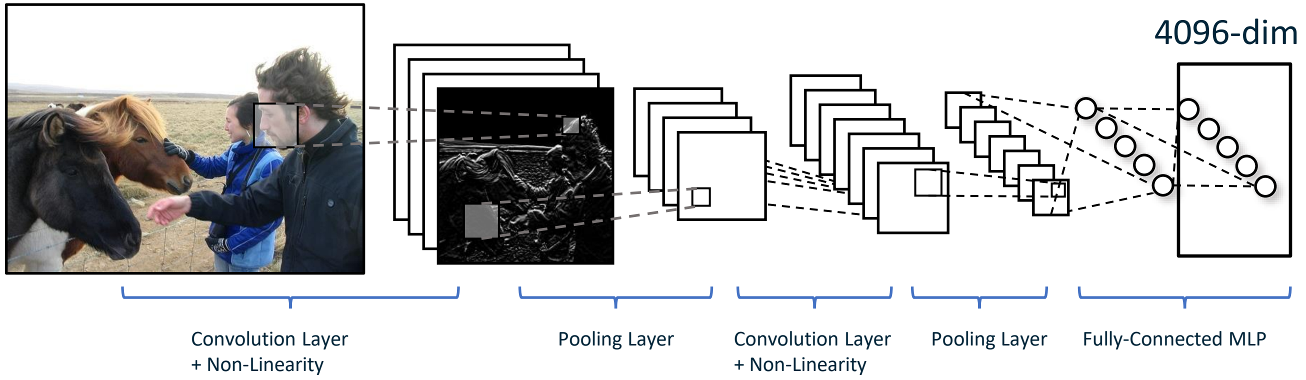
Neural Image Captioning

Image Embedding

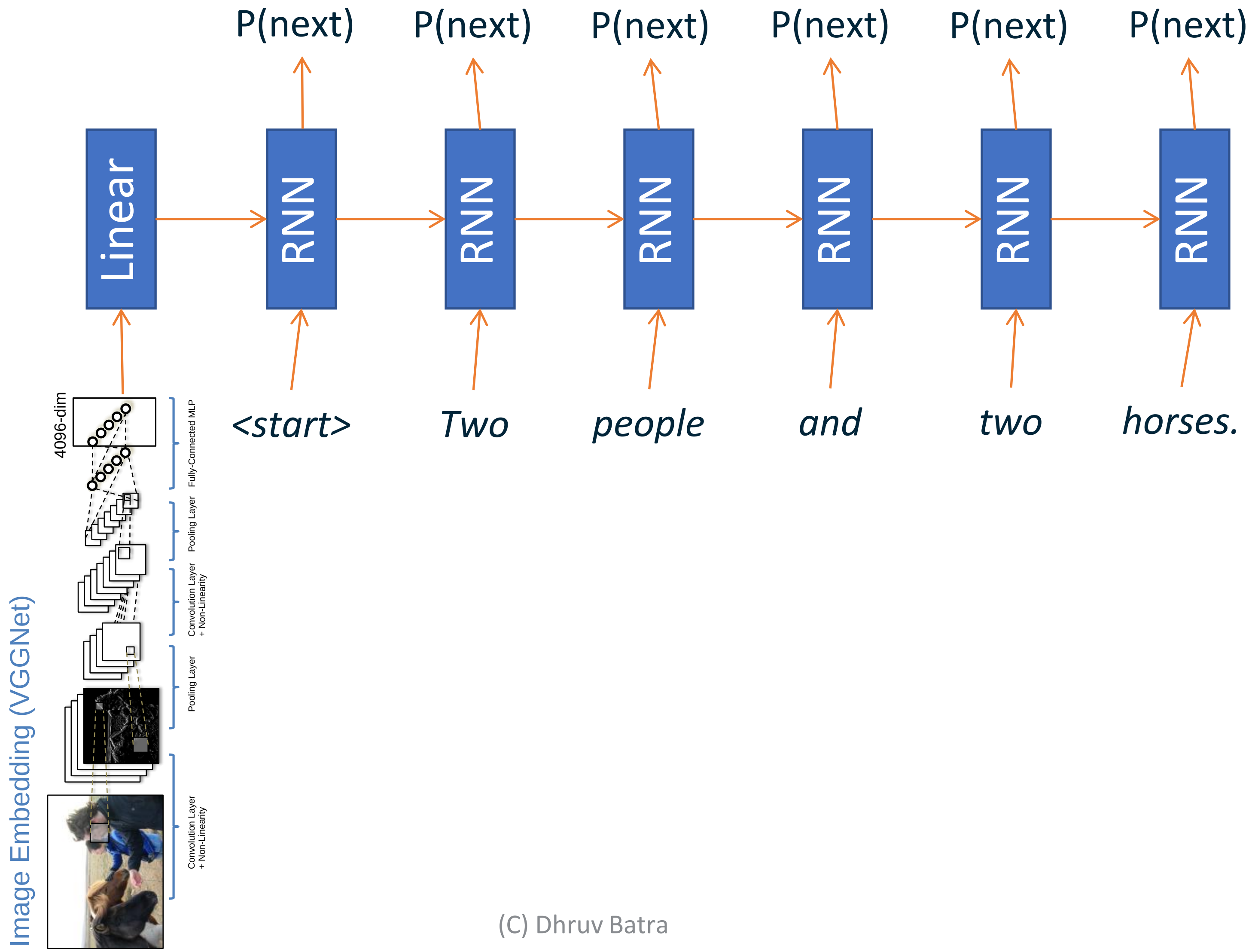


Neural Image Captioning

Image Embedding (VGGNet)



Neural Image Captioning



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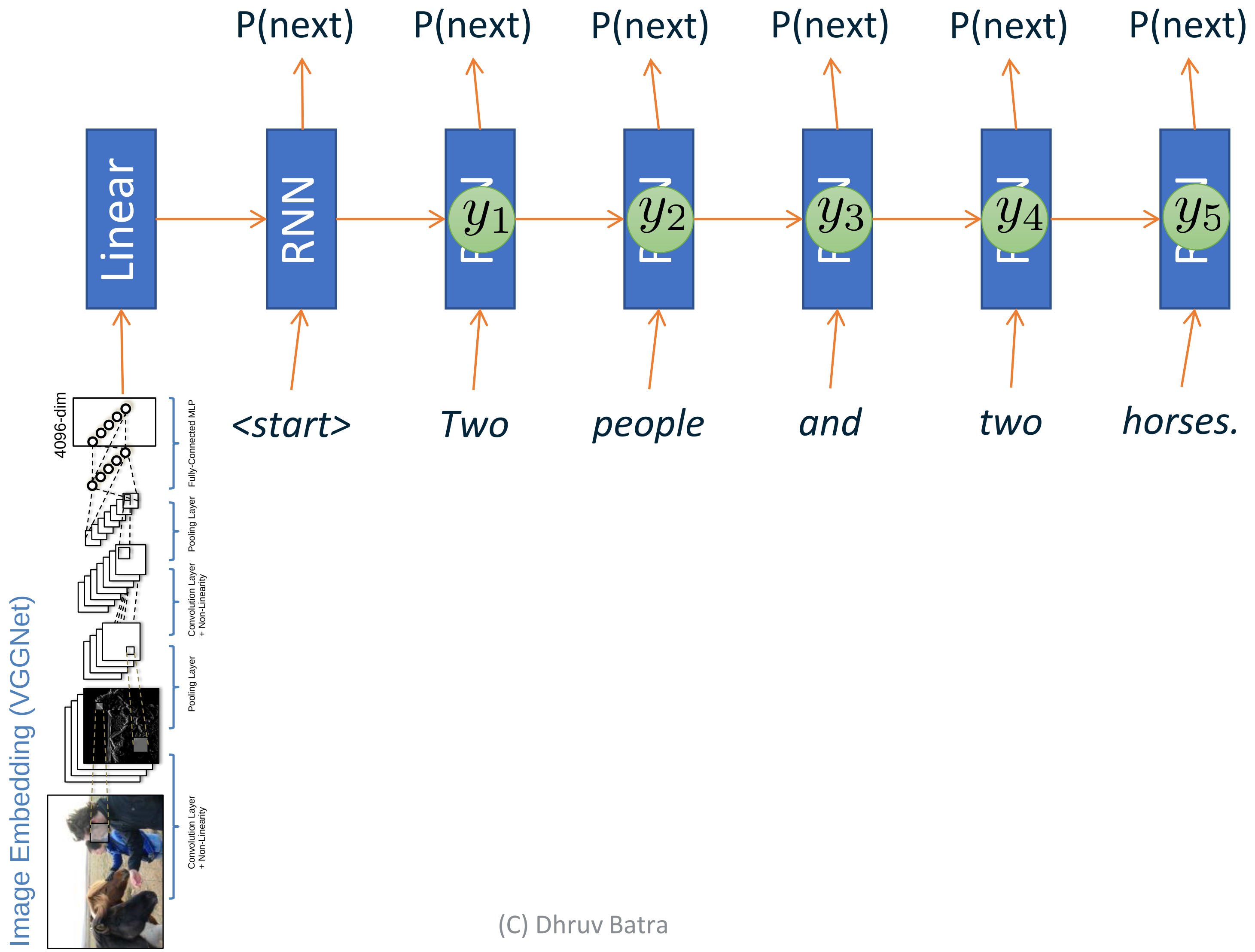
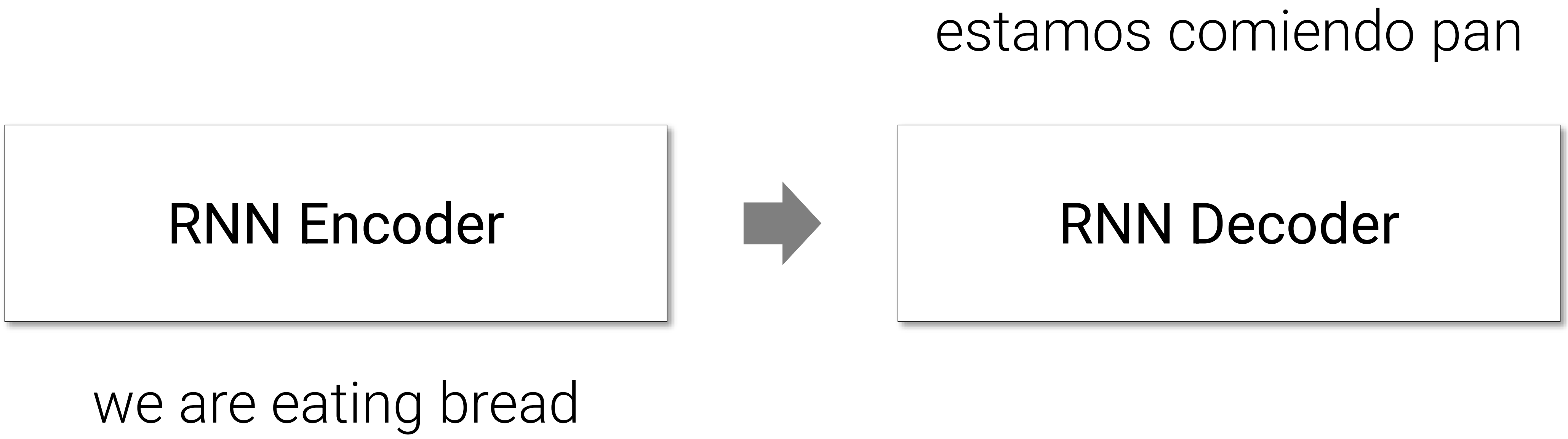


Machine Translation

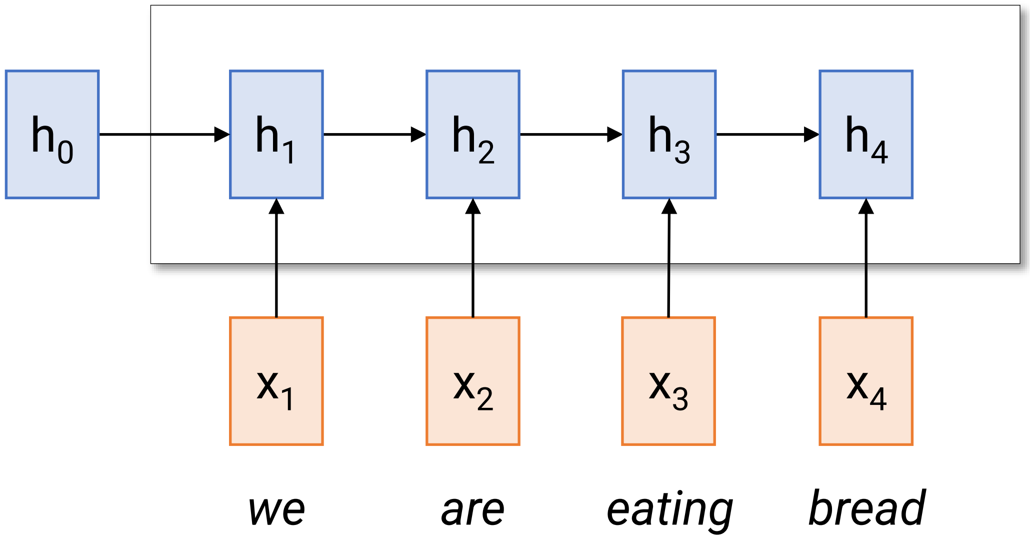
we are eating bread → estamos comiendo pan

Machine Translation



Machine Translation with RNNs

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



Slide credit: Justin Johnson

Machine Translation with RNNs

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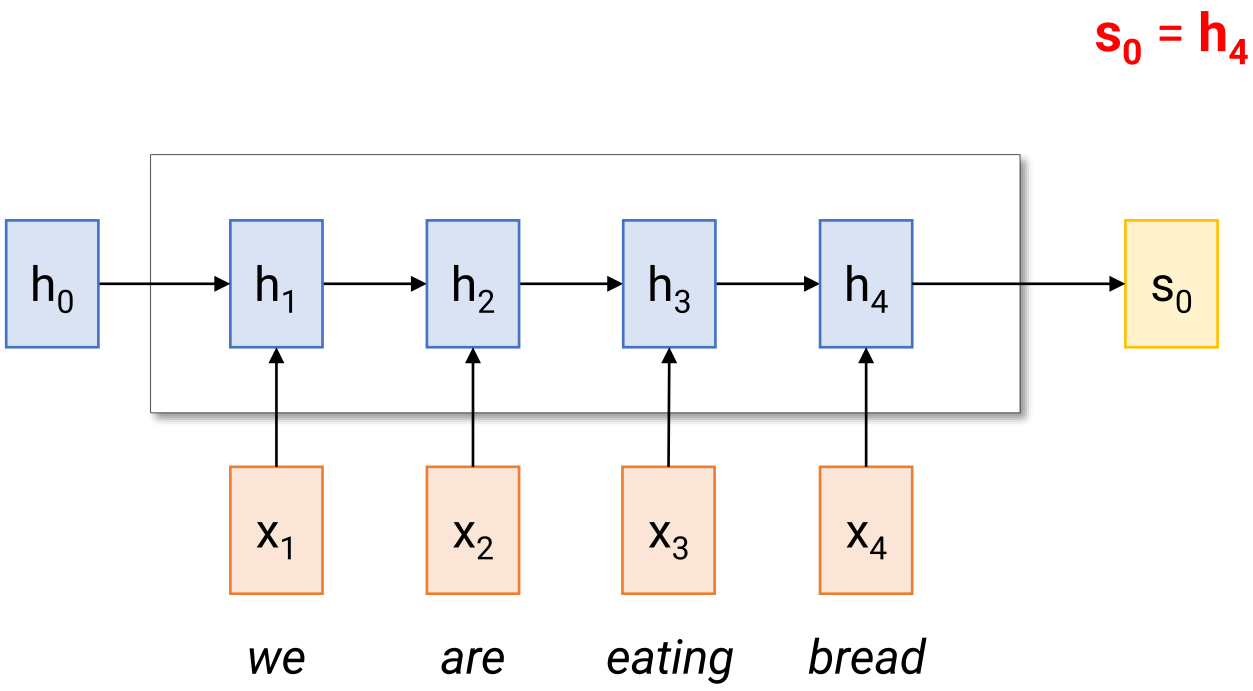
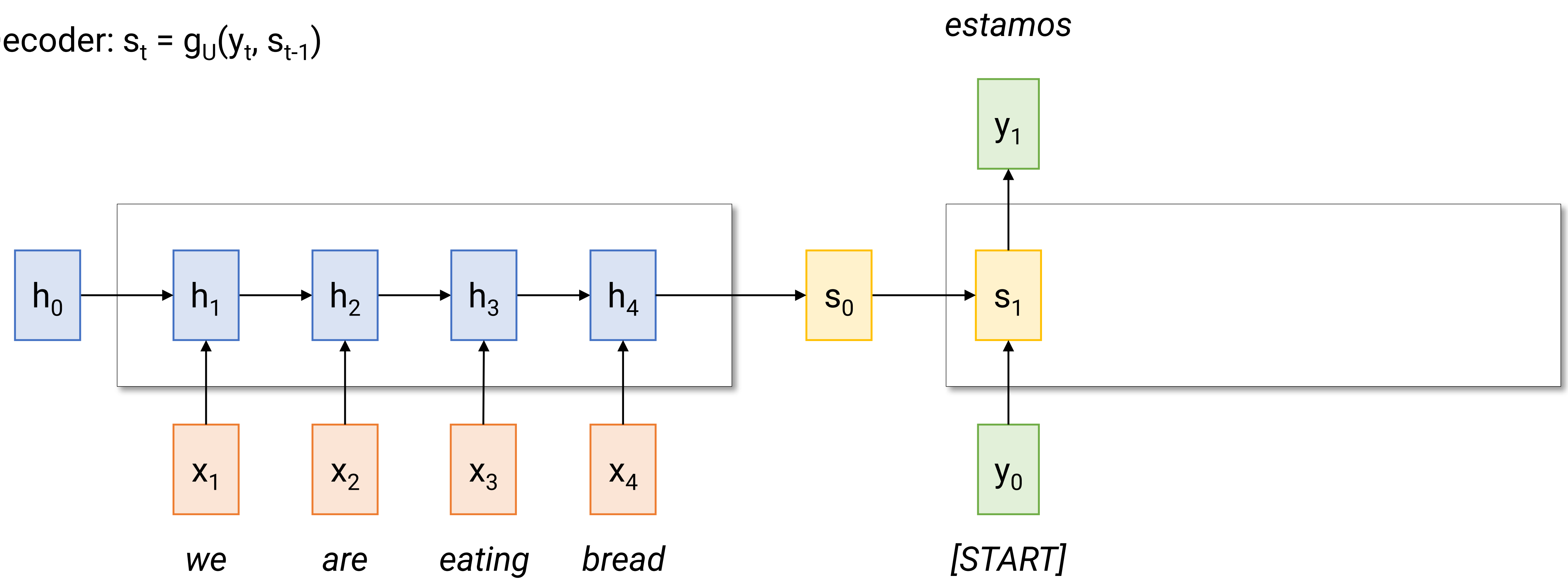


Slide credit: Justin Johnson

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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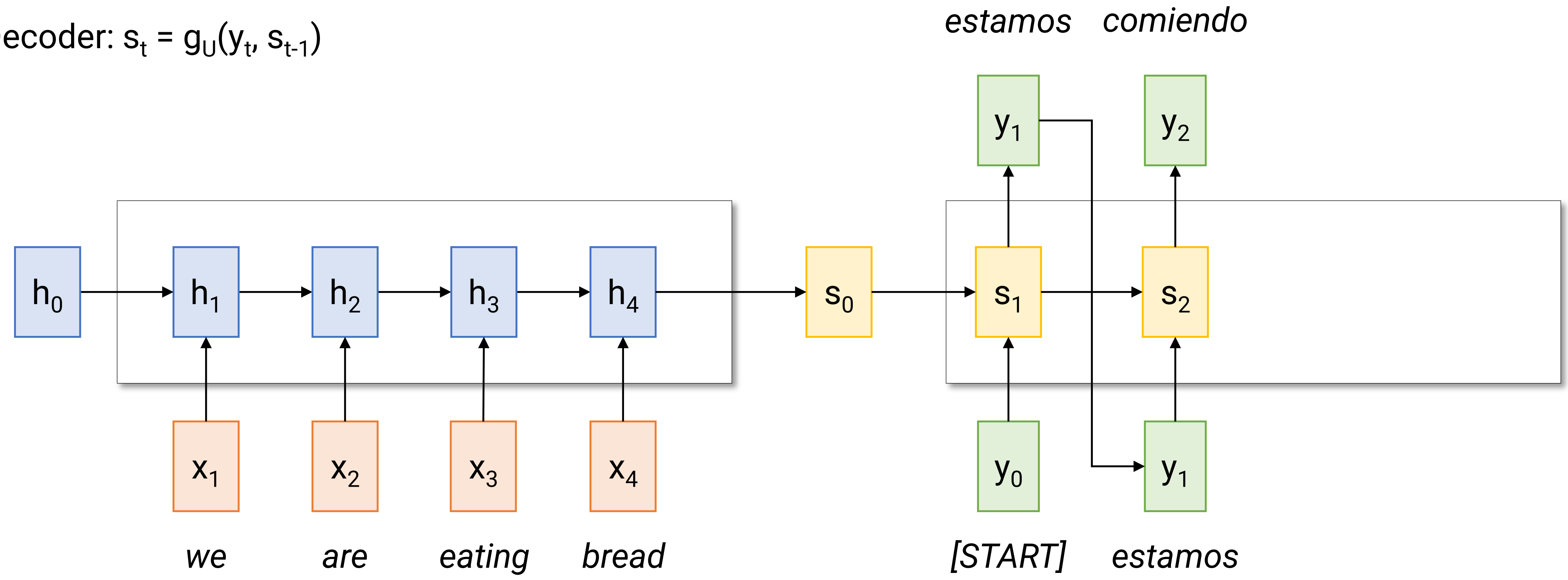


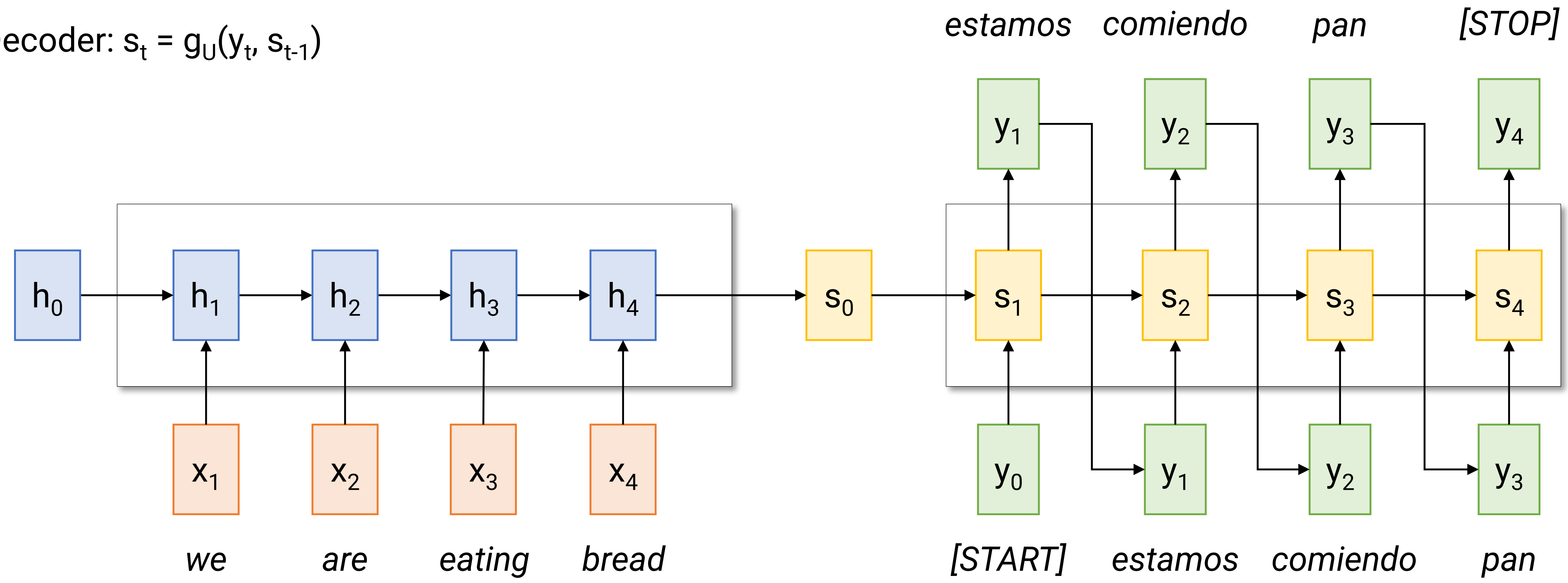
Slide credit: Justin Johnson

Machine Translation with RNNs

Note [START]/[STOP] words. This can be treated as representation for entire sentence

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

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



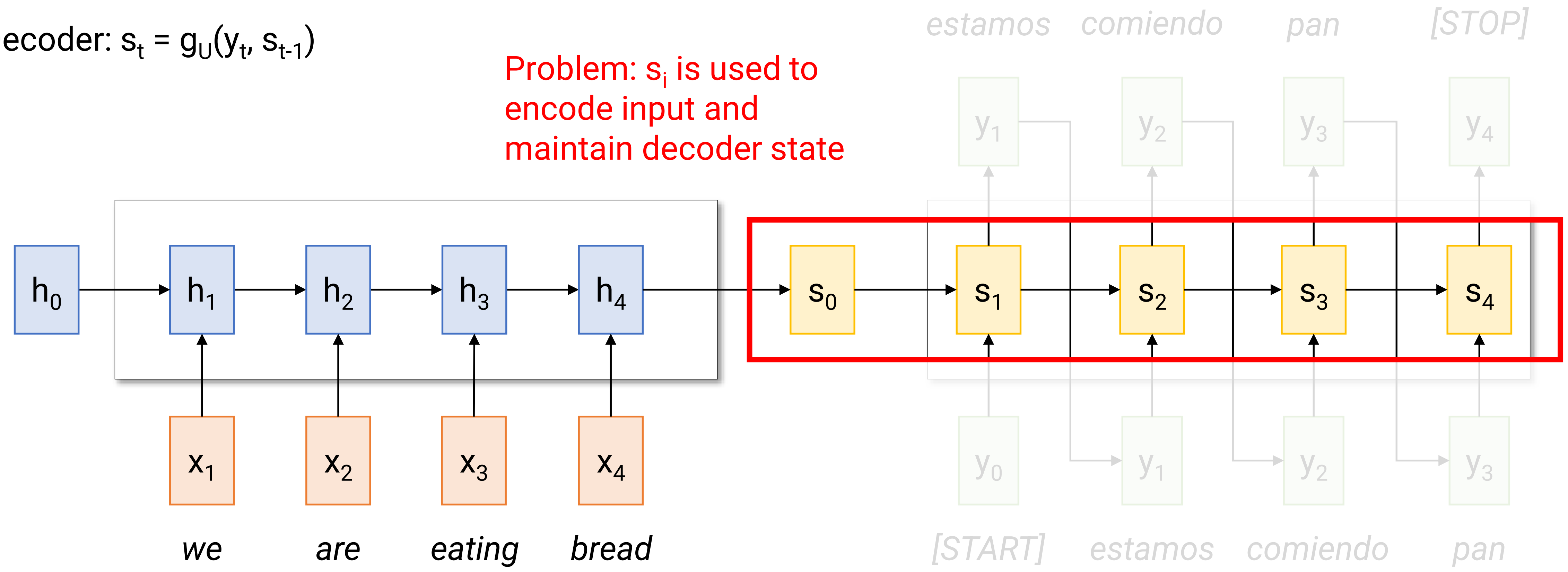
Slide credit: Justin Johnson

Machine Translation with RNNs

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

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

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



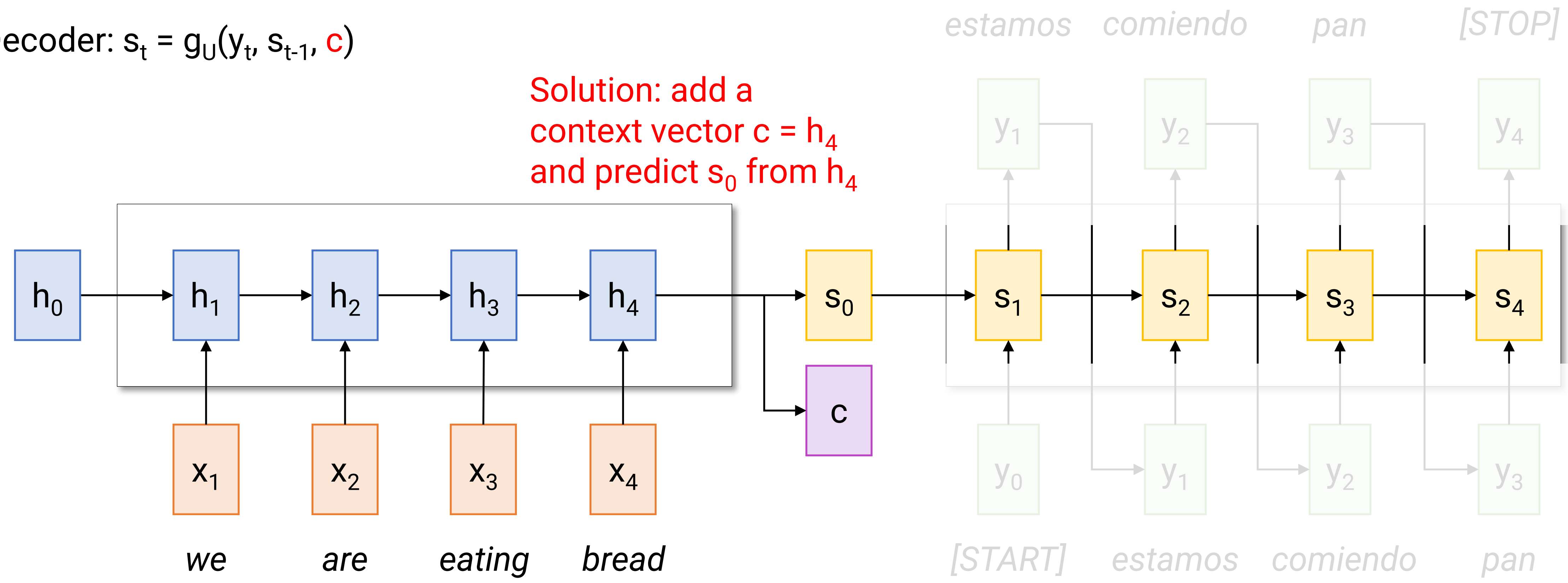
Slide credit: Justin Johnson

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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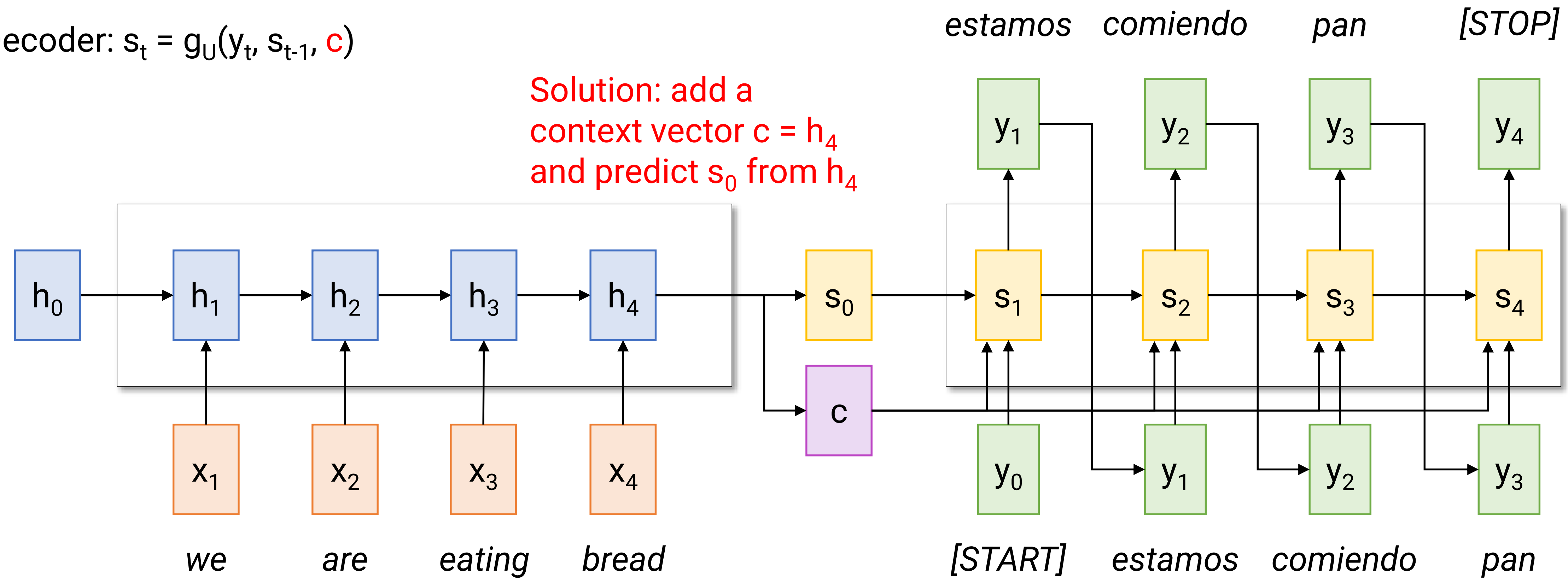

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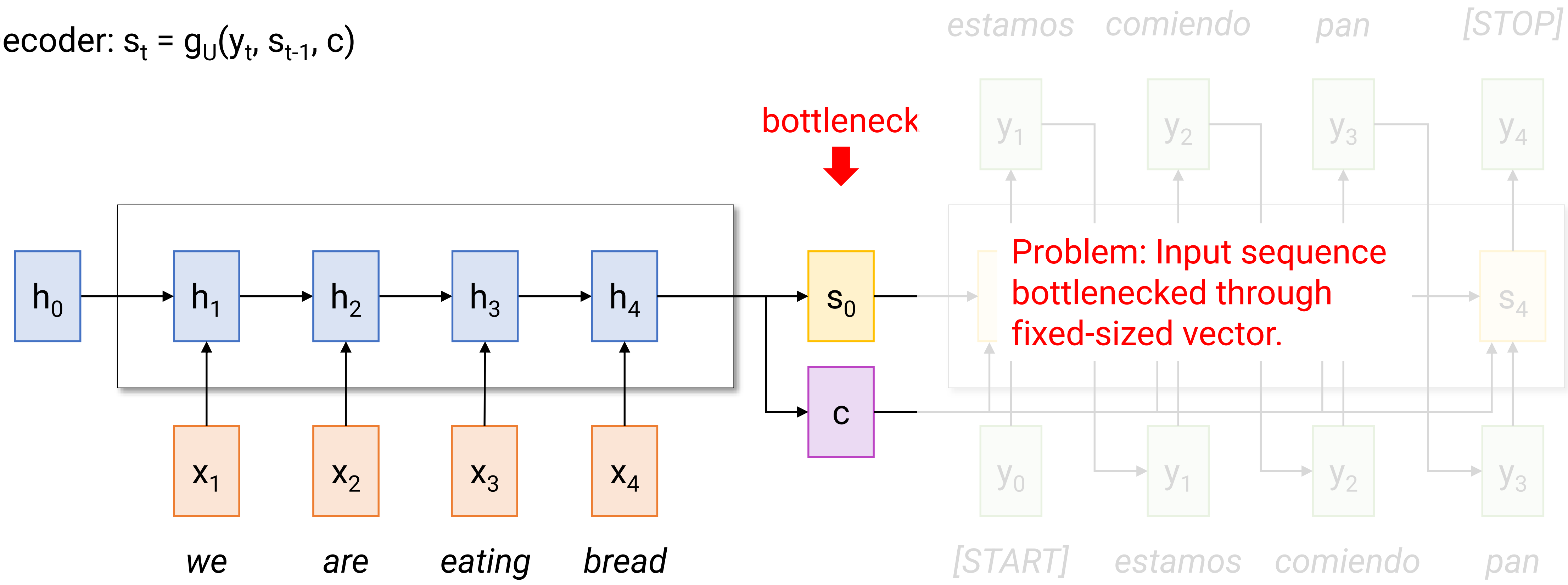

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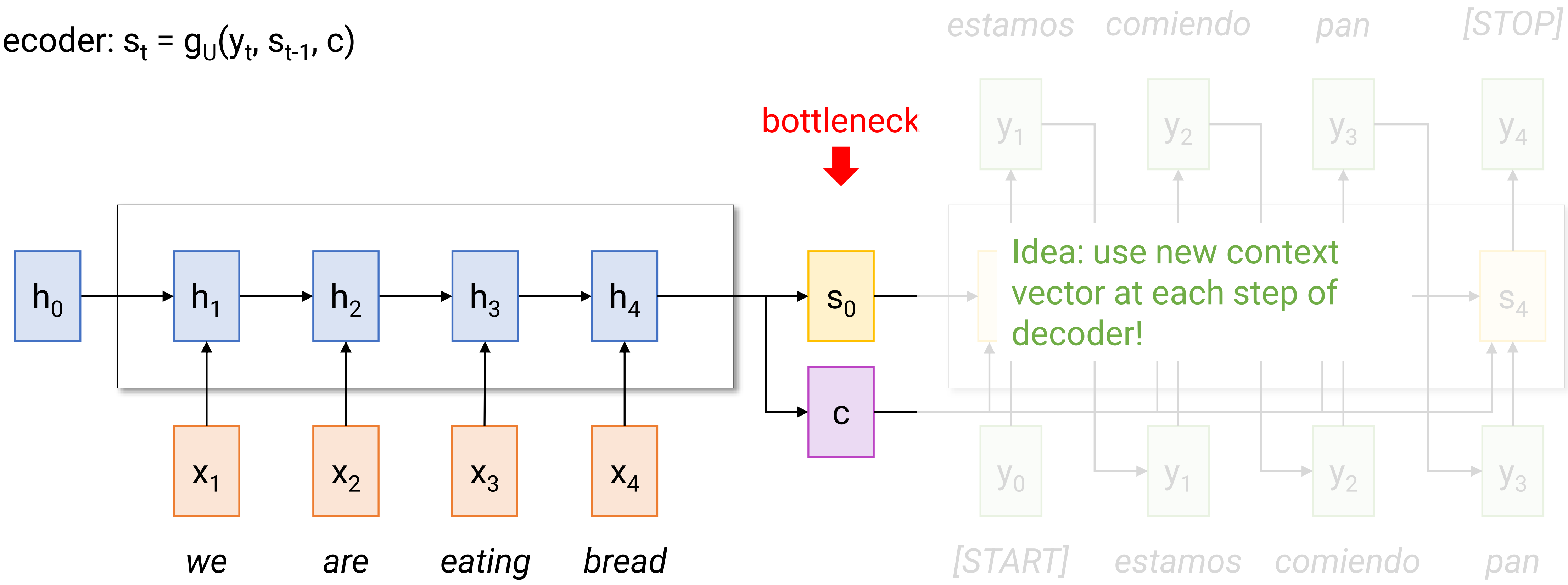
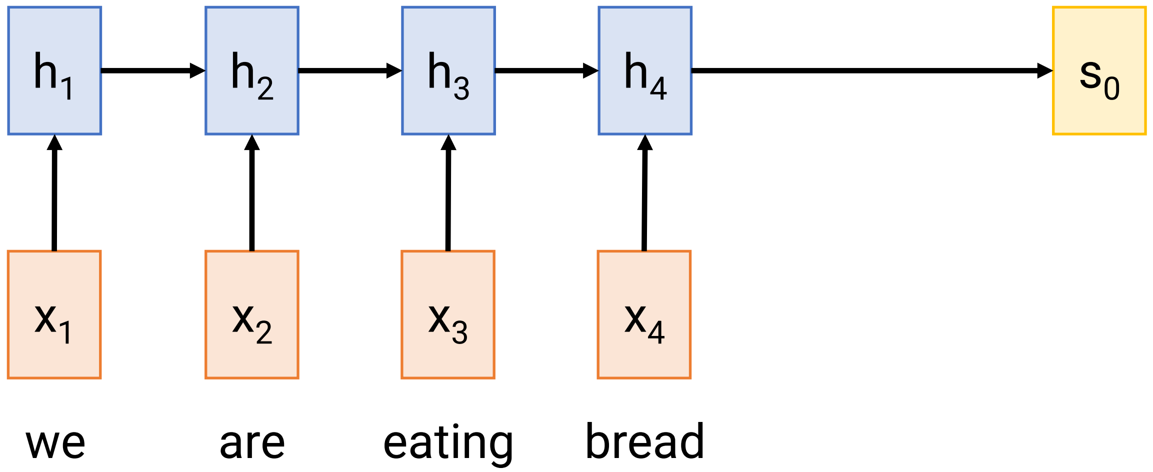


Slide credit: Justin Johnson

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

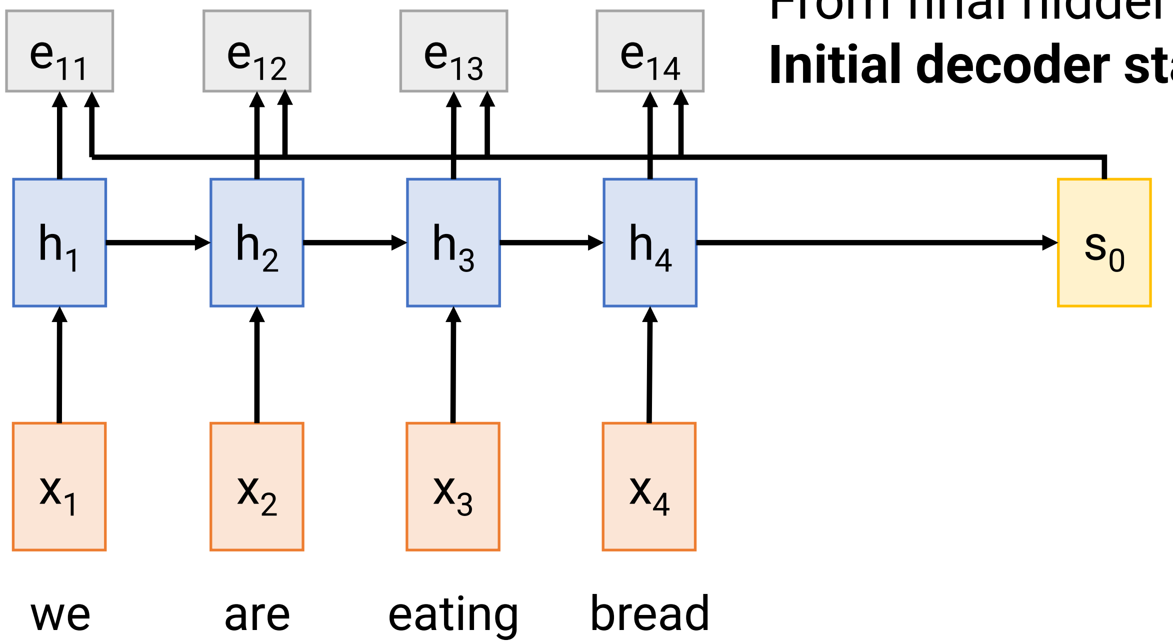
Slide credit: Justin Johnson

Machine Translation with RNNs **and Attention**

Compute **alignment scores**

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

From final hidden state:
Initial decoder state s_0



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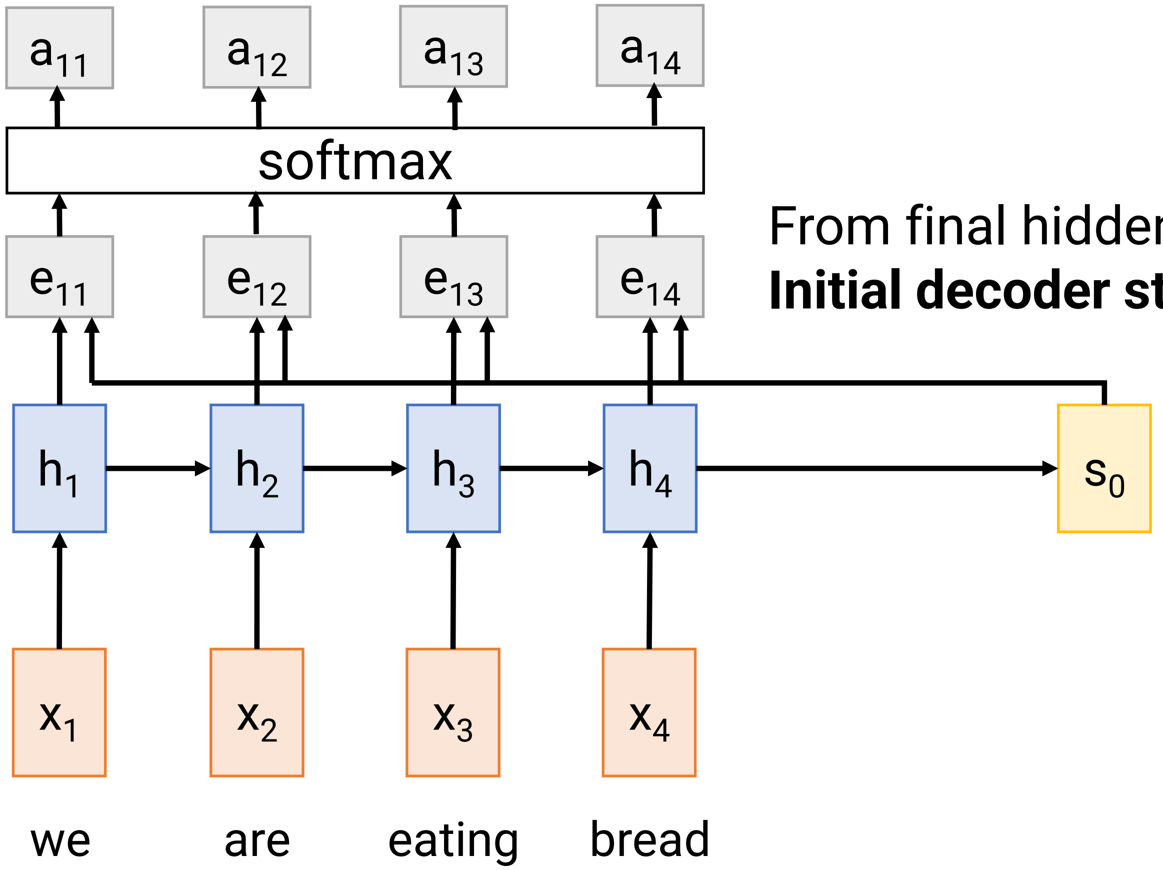

From final hidden state:
Initial decoder state s_0

Compute **alignment scores**

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

Normalize to get
attention weights

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

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

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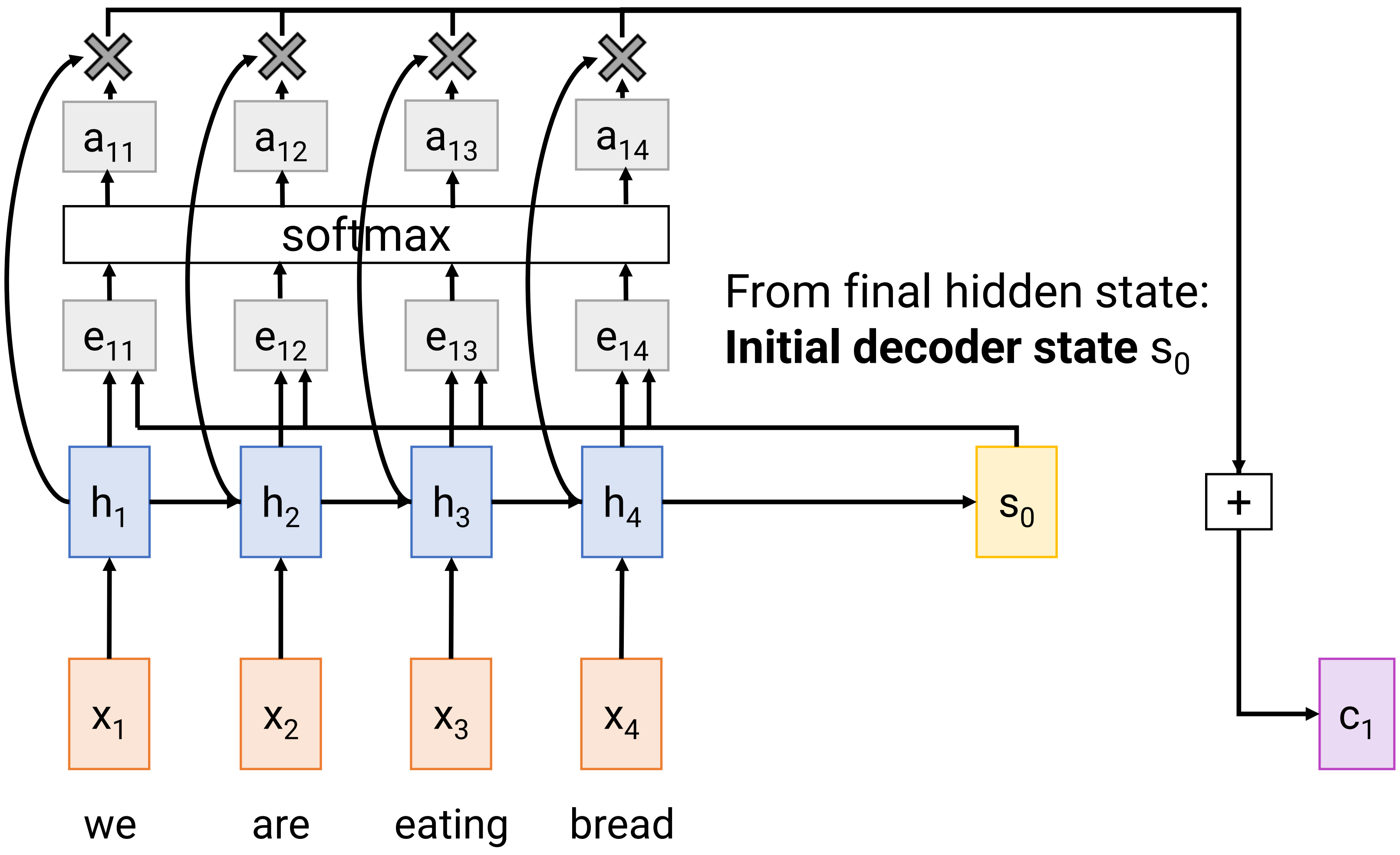
Machine Translation with RNNs **and Attention**



From final hidden state:
Initial decoder state s_0

Compute **alignment scores**

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

Normalize to get **attention weights**

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

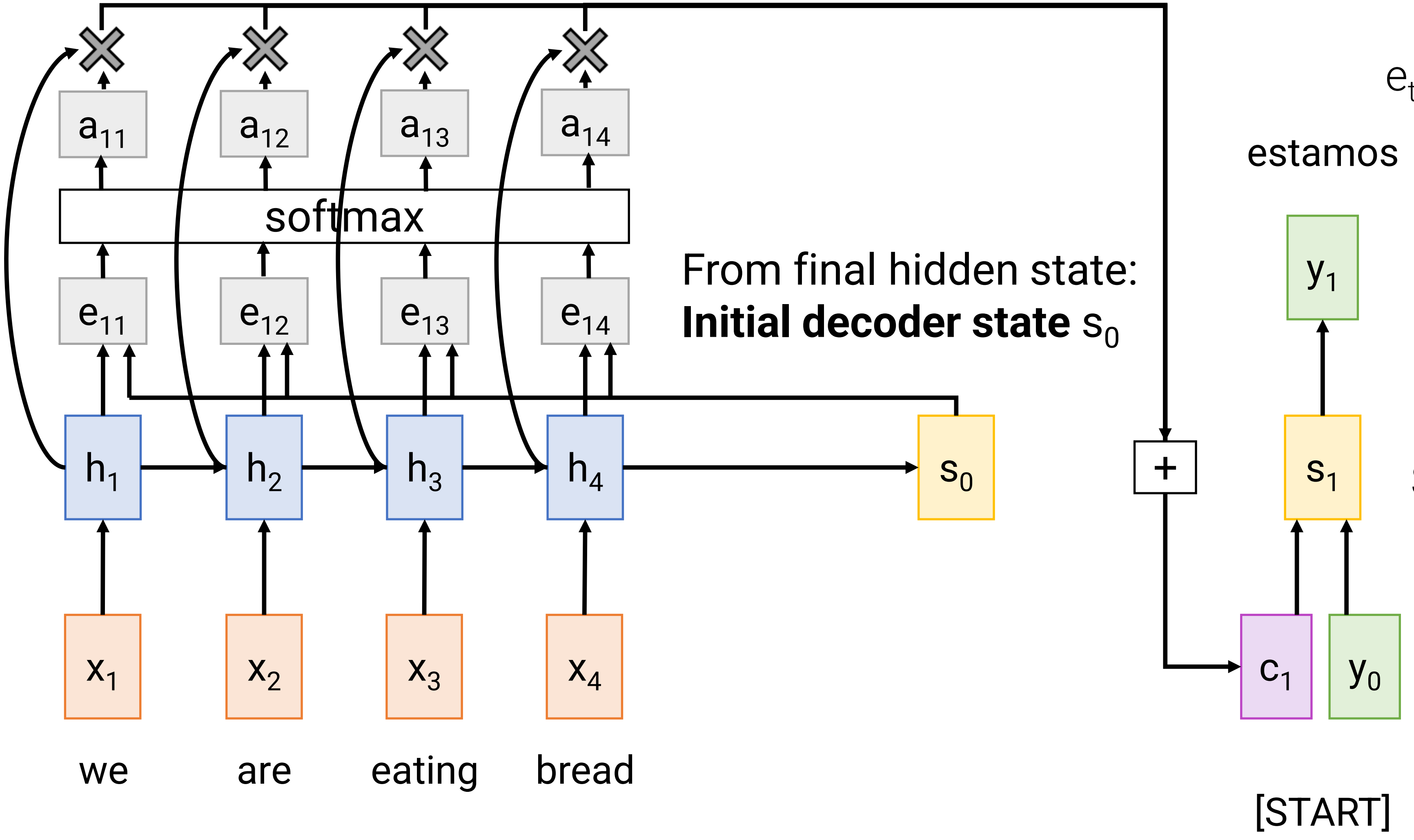
Set context vector **c** to a linear combination of hidden states

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

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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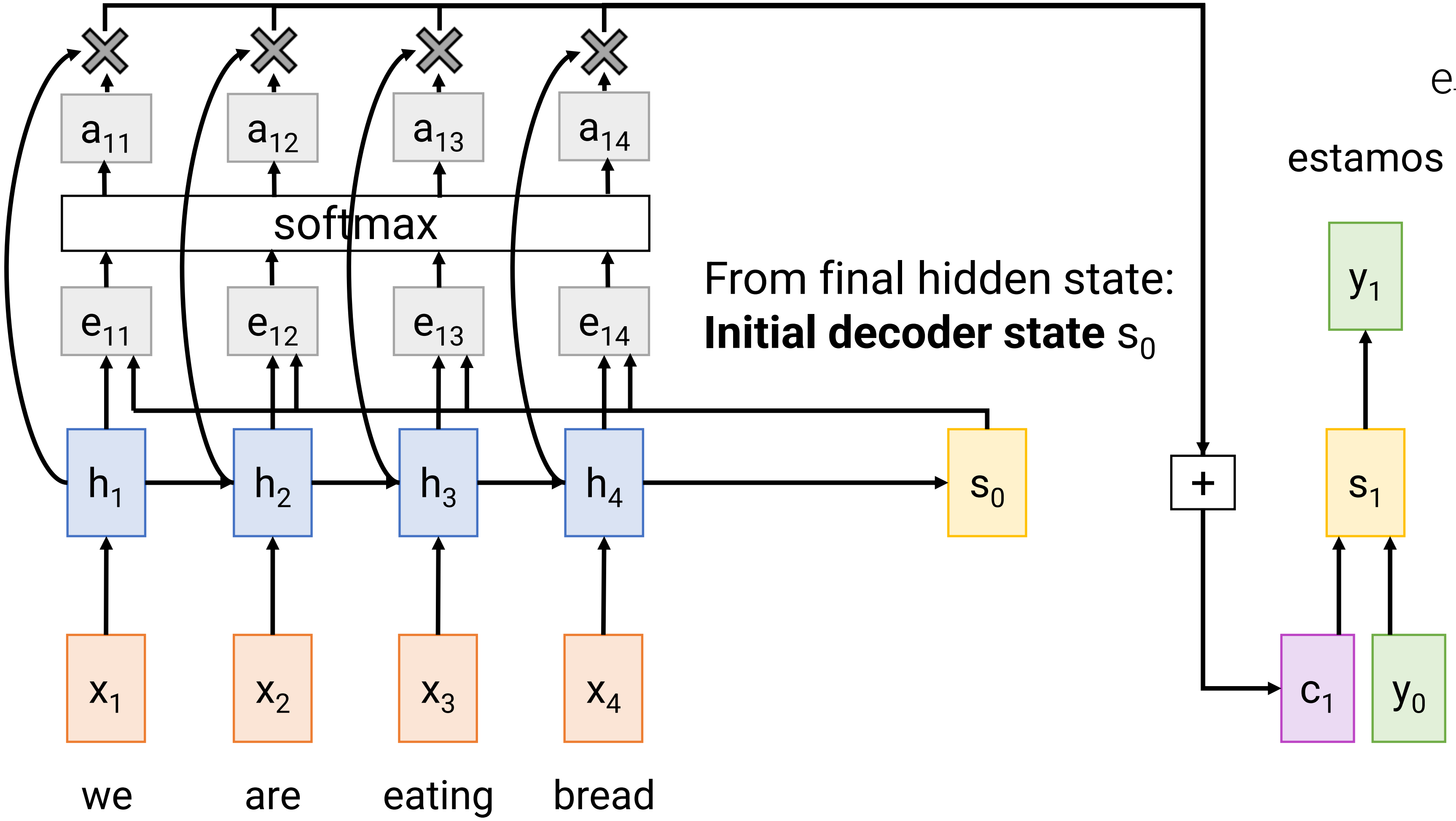
Machine Translation with RNNs **and Attention**



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

Compute **alignment scores**

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Normalize to get **attention weights**

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

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

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

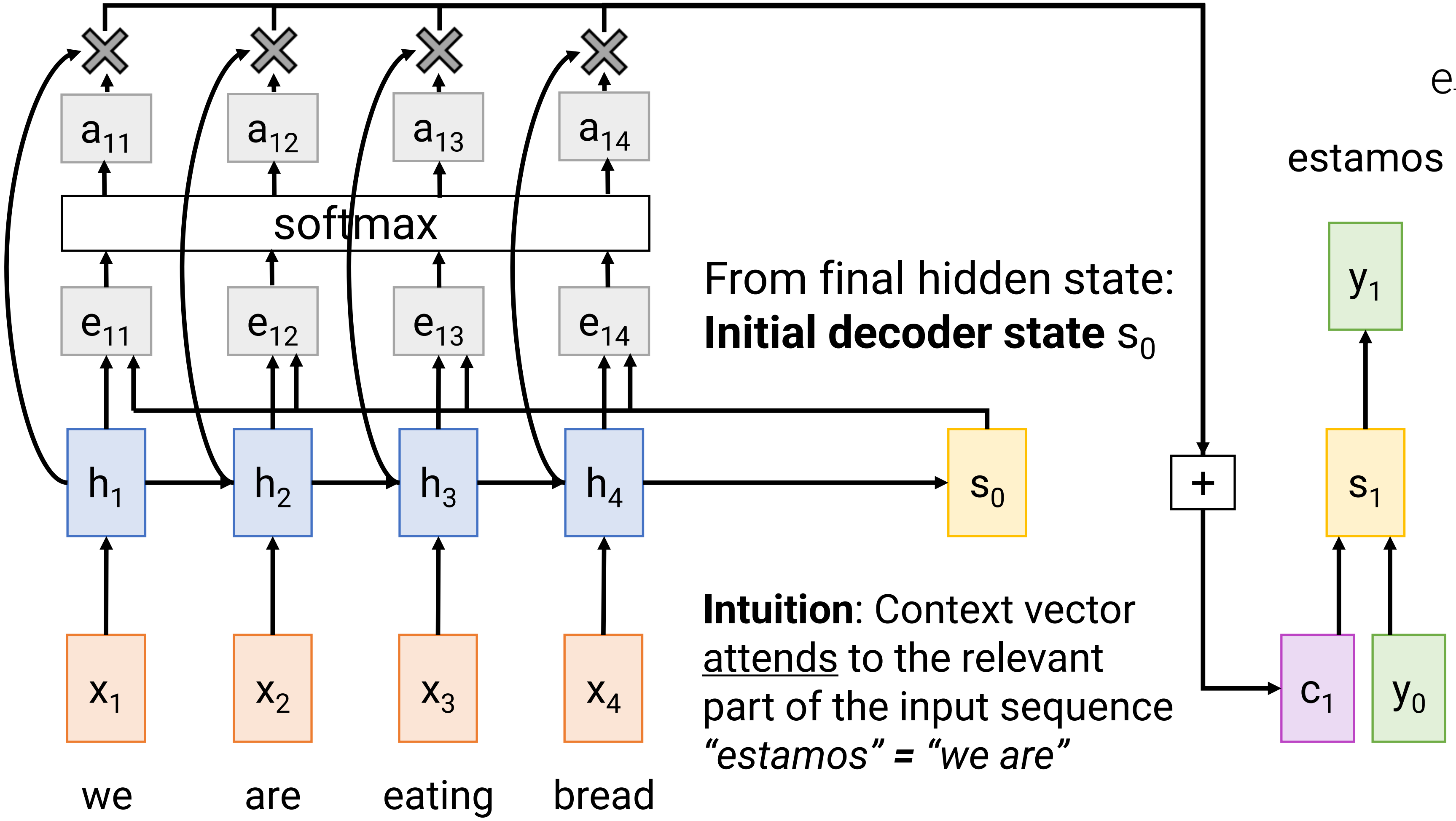
This is all differentiable! Do not supervise attention weights – backprop through everything

Can be seen as a input-dependent weighting (rather than MLP)

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**



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

Intuition: Context vector <u>attends</u> to the relevant part of the input sequence *"estamos" = "we are"*

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**

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

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

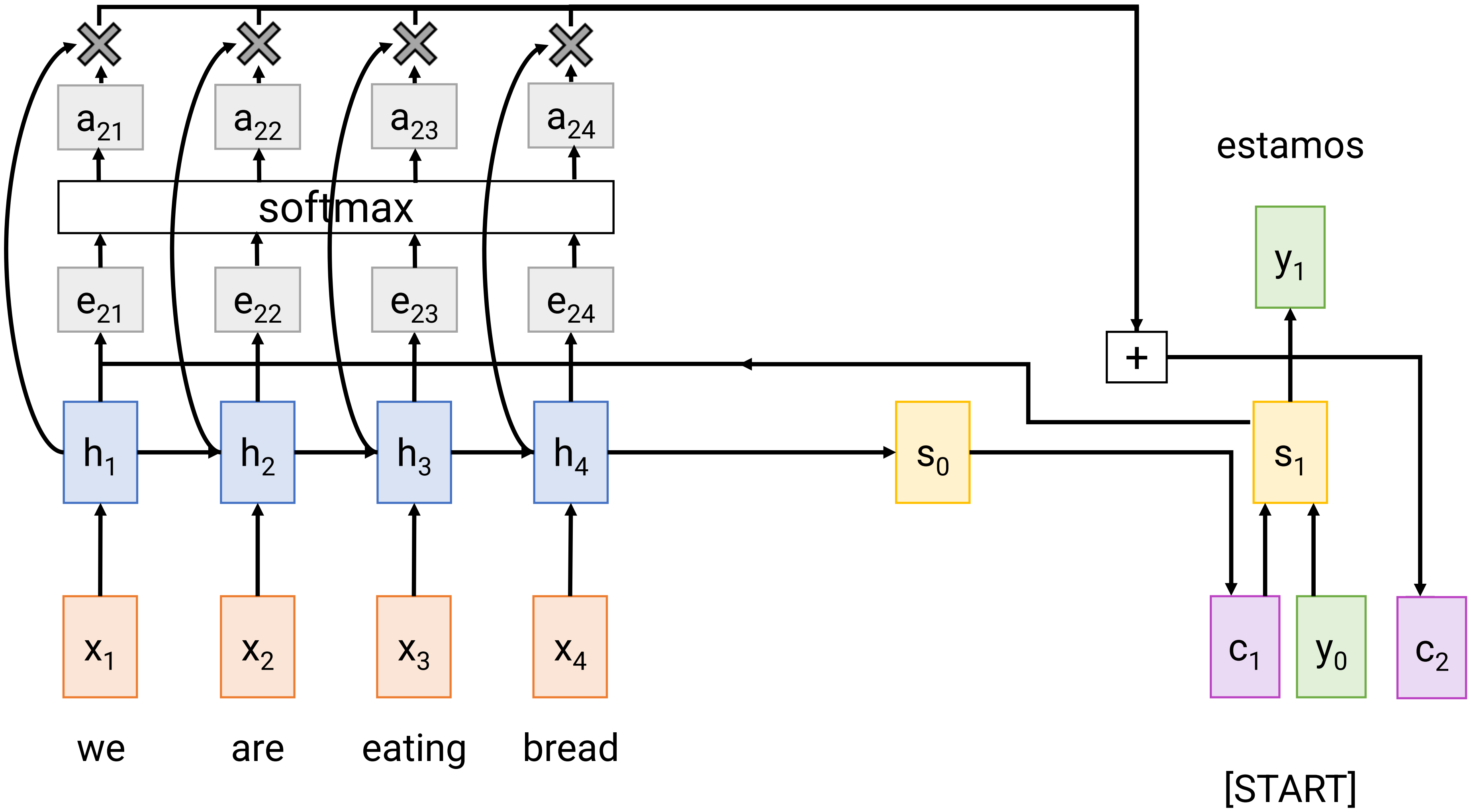
$c_t = \sum_i a_{t,i} h_i$

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

This is an inductive bias we think is reasonable for this task. Need to verify empirically though!

Slide credit: Justin Johnson

Machine Translation with RNNs **and Attention**

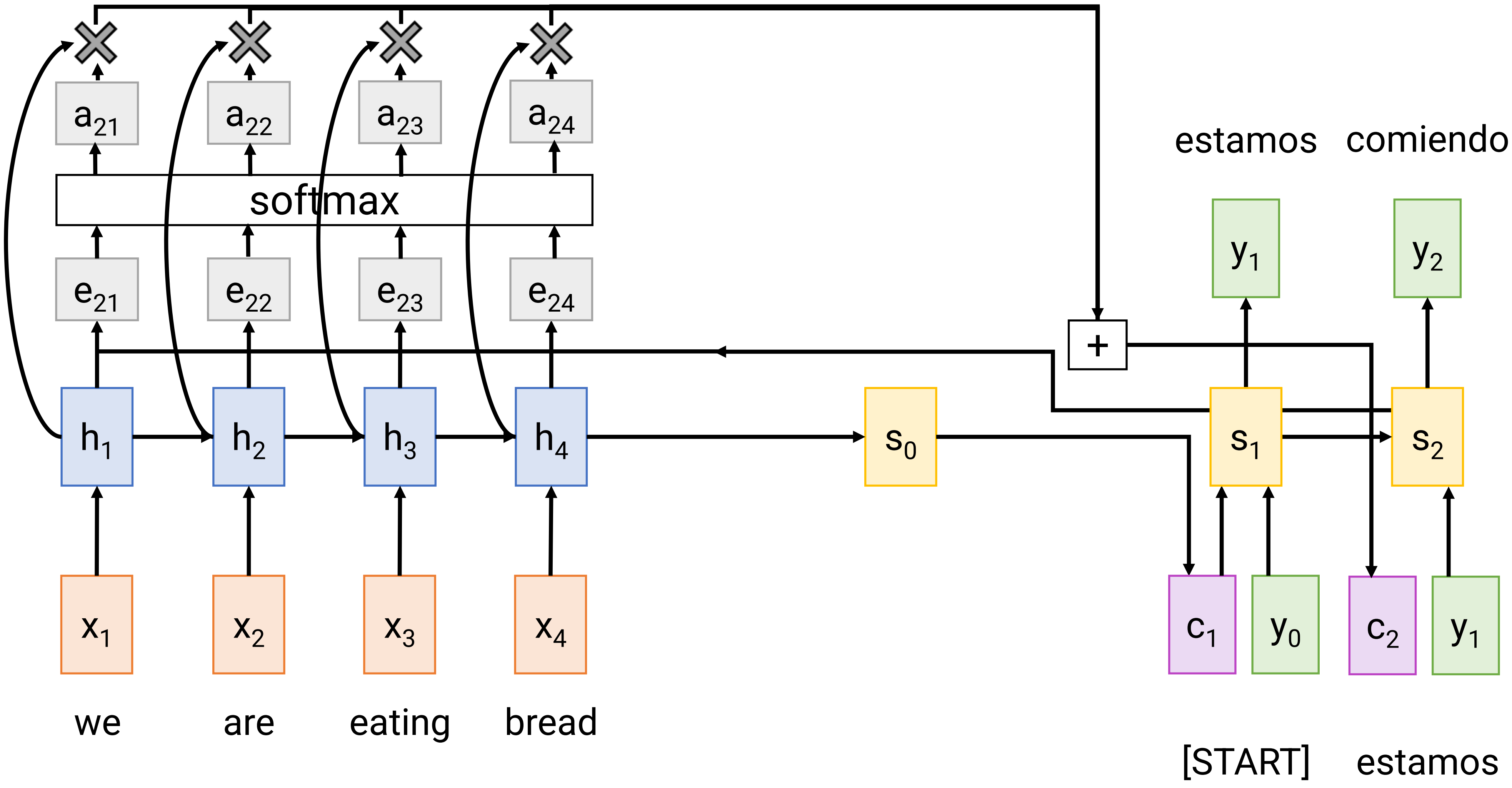


Repeat: Use s_1 to compute new context vector c_2

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**

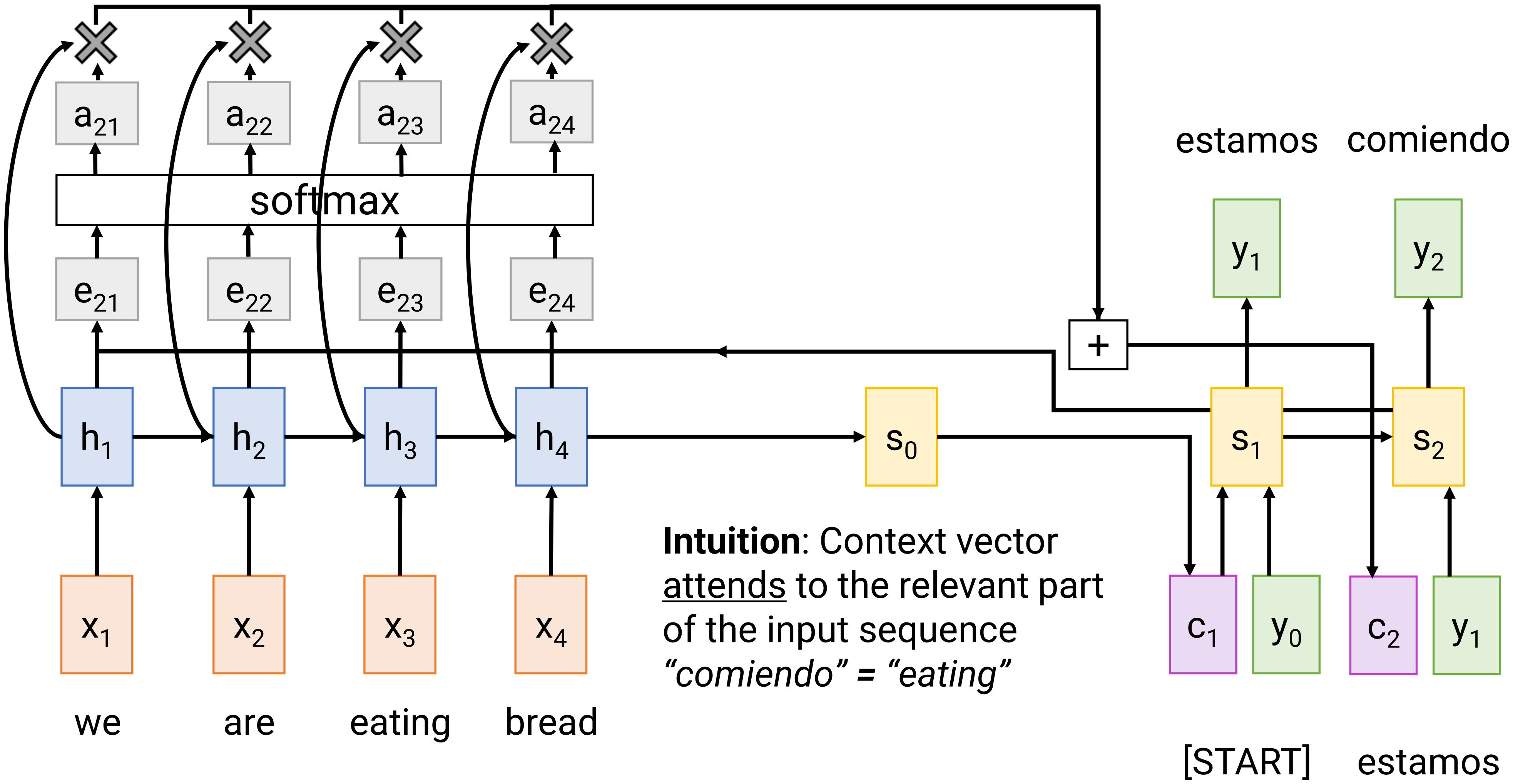


Repeat: Use s_1 to compute new context vector c_2

Use c_2 to compute s_2, y_2

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

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

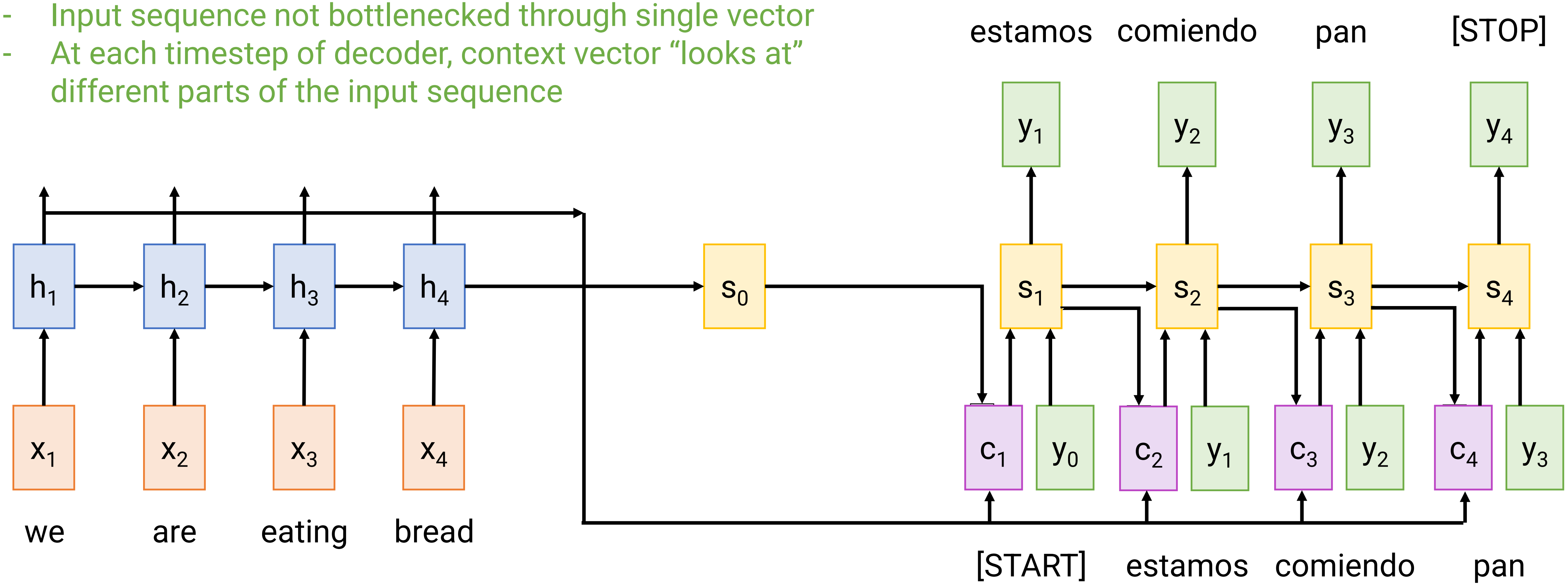
Intuition: Context vector attends to the relevant part of the input sequence
“comiendo” = “eating”

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

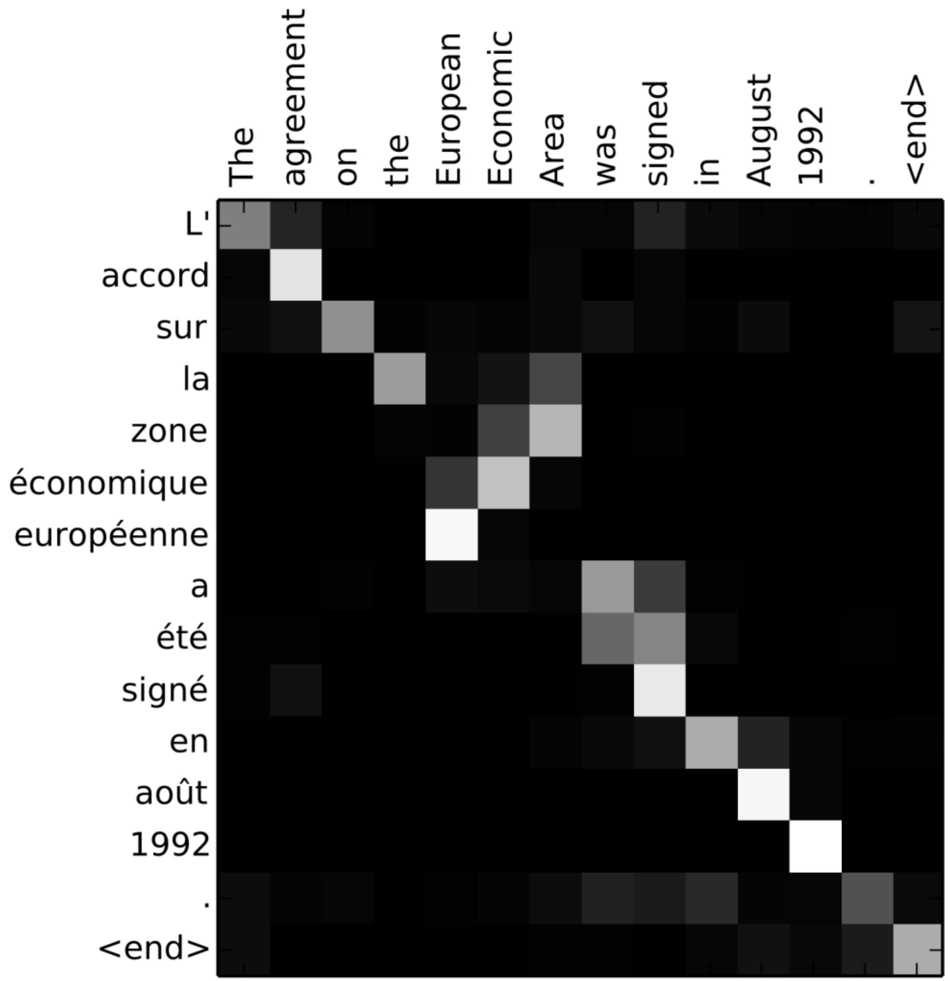
Machine Translation with RNNs **and Attention**

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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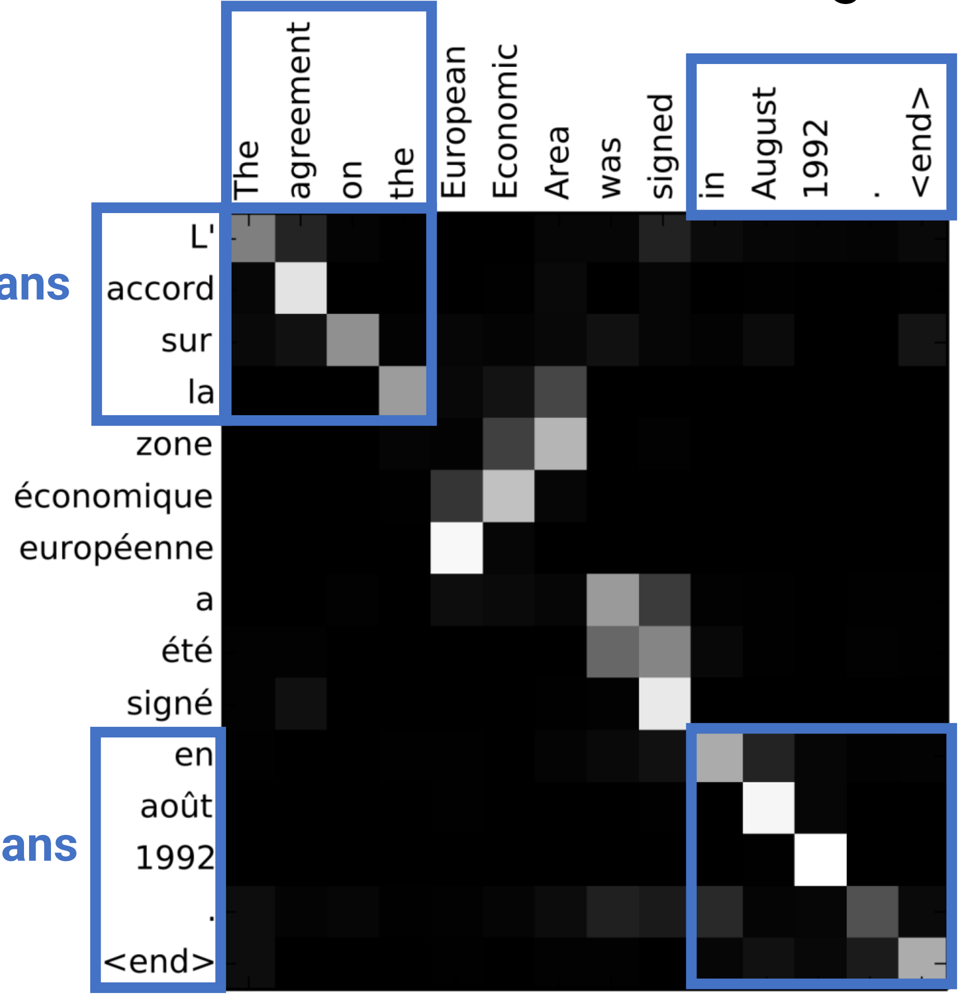
Example: English to French translation

Input: "**The agreement on the** European Economic Area was signed **in August 1992**."

Output: "**L'accord sur la** zone économique européenne a été signé **en août 1992**."

Visualize attention weights $a_{t,i}$

Diagonal attention means words correspond in order



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Example: English to French translation

Input: "**The agreement on the European Economic Area** was signed **in August 1992**."

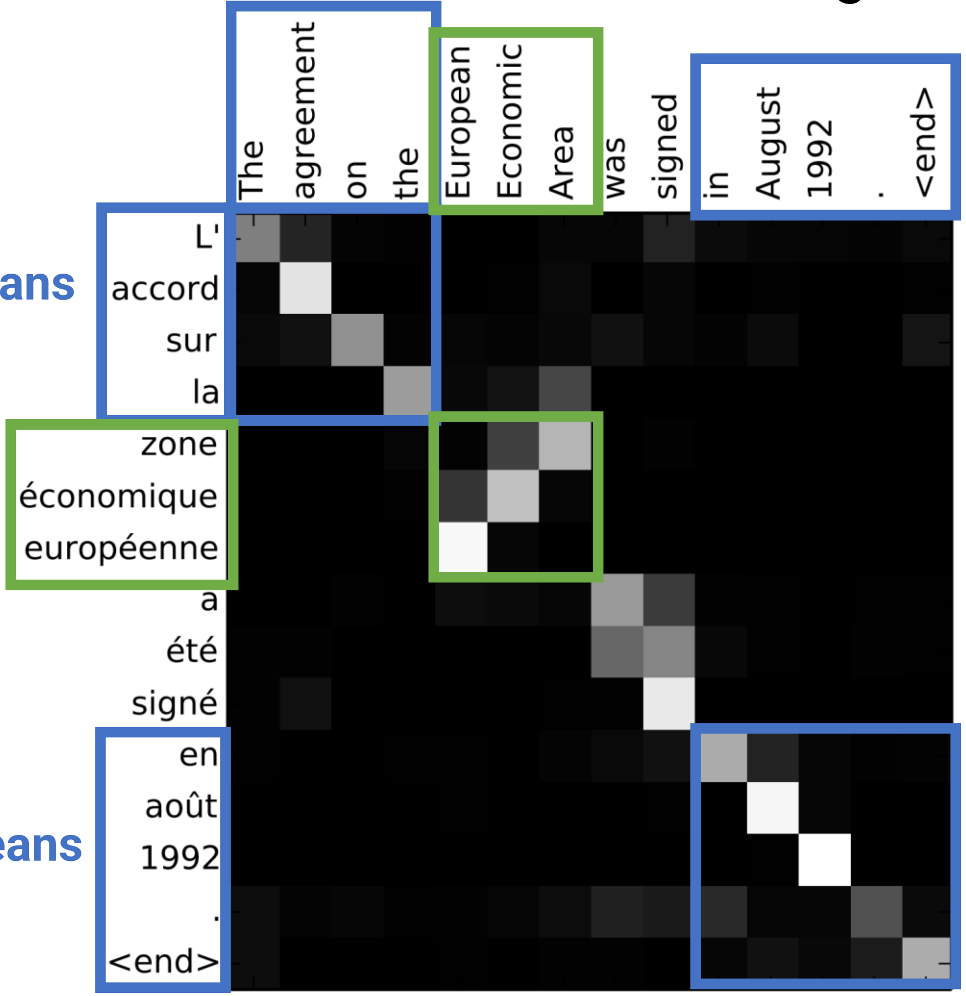
Output: "**L'accord sur la zone économique européenne** a été signé **en août 1992**."

Diagonal attention means words correspond in order

Attention figures out different word orders

Diagonal attention means words correspond in order

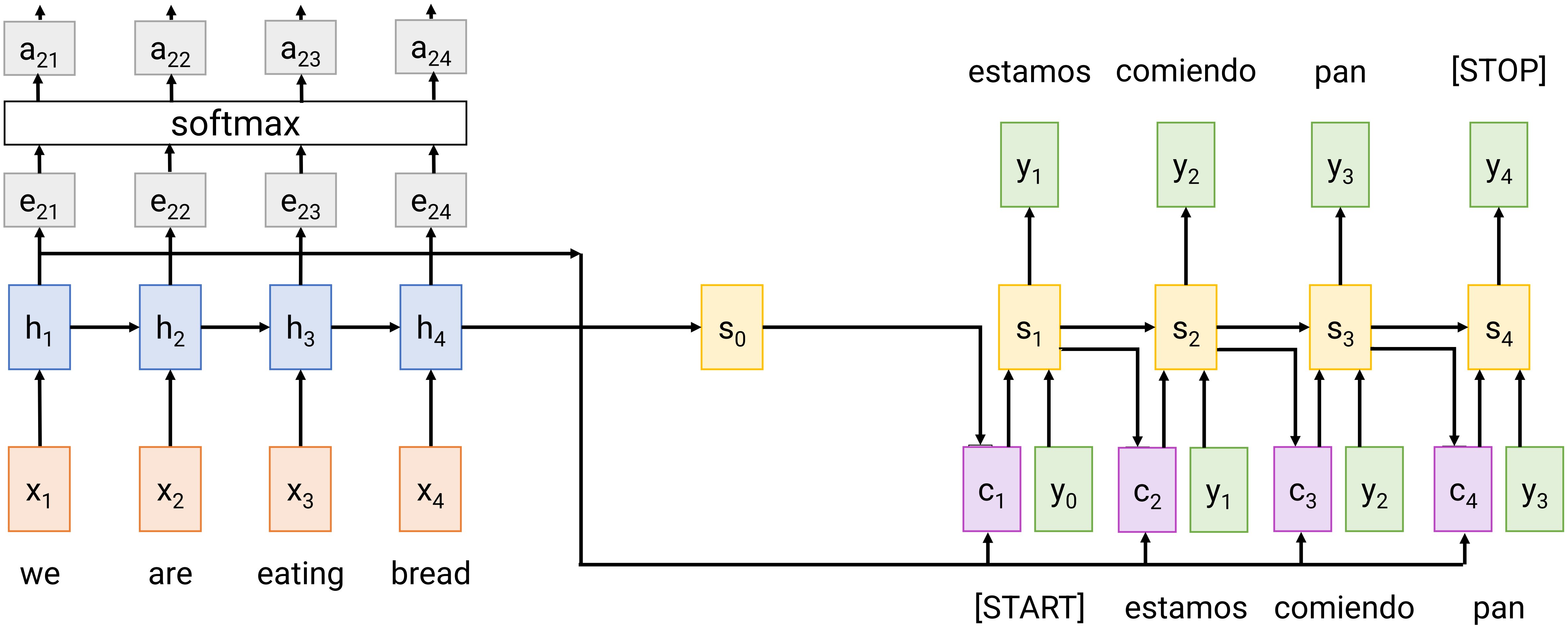
Visualize attention weights $a_{t,i}$



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**



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

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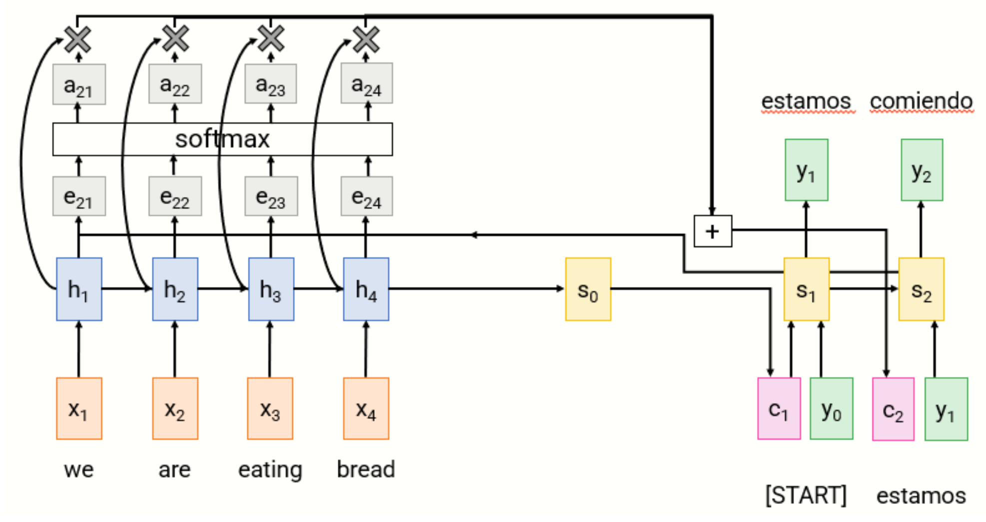
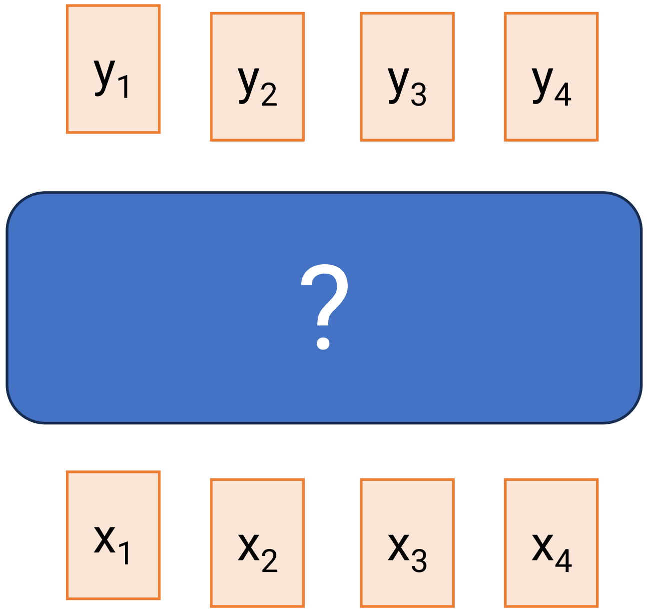


Idea: Can we use **attention** as a fundamental building block for a generic sequence (input) to sequence (output) layer?



Note: We just want a generic sequence-in, sequence-out model that will represent each input *contextualized* with rest of inputs, and encode meaning of entire sequence

We will progressively develop a generic mechanism using idea of attention.
Don't try to map to RNN translation example!

Attention Layer

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

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

Make the module generic:
Input (X), Query (q)
Output (Weighted sum of inputs)

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: $\mathbf{q}$ (Shape: D_Q)
Input vectors: $\mathbf{X}$ (Shape: N_X x D_Q)
Similarity function: $\boxed{\text{dot product}}$

Computation:
Similarities: e (Shape: N_X) $\boxed{e_i = \mathbf{q} \cdot \mathbf{X}_i}$
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) $e_i = \mathbf{q} \cdot \mathbf{X}_i / \mathrm{sqrt}(D_Q)$
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: $\boxed{\mathbf{Q} \text{ (Shape: } N_Q \times D_Q)}$
Input vectors: $\mathbf{X}$ (Shape: $N_X \times D_Q$)

Make the module generic:
Sequence Input (X), Sequence Query (Q)
Output: Sequence (Weighted sum/mixture of inputs)

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

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

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)

Separate concerns:
1) *Matching* (similarity) -> Key,
2) Output given weighting -> Value

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 = A**V** (Shape: N_Q x D_V) $Y_i = \sum_j A_{i,j} V_j$

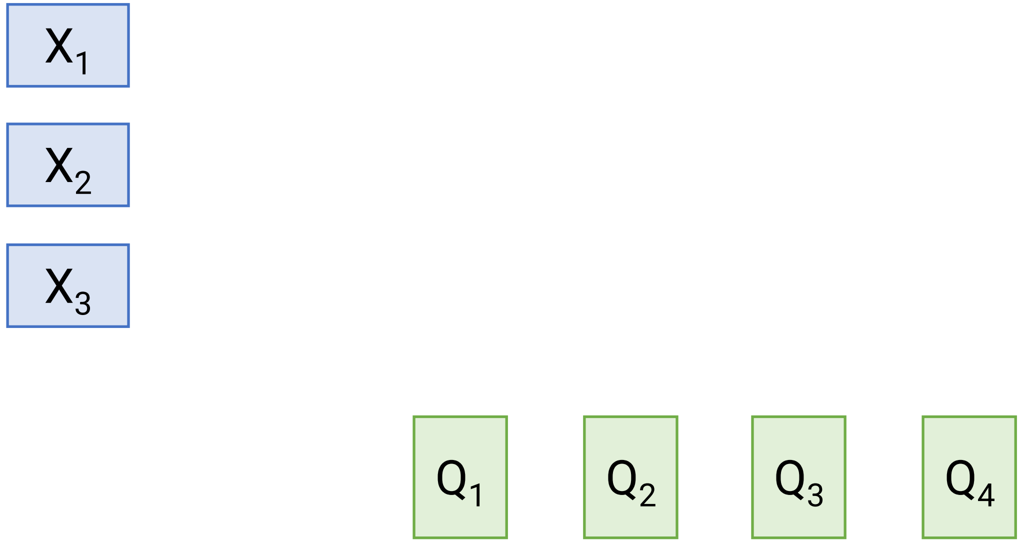
Changes:
- Use dot product for similarity
- Multiple **query** vectors
- Separate **key** and **value**

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) $Y_i = \sum_j A_{i,j} V_j$

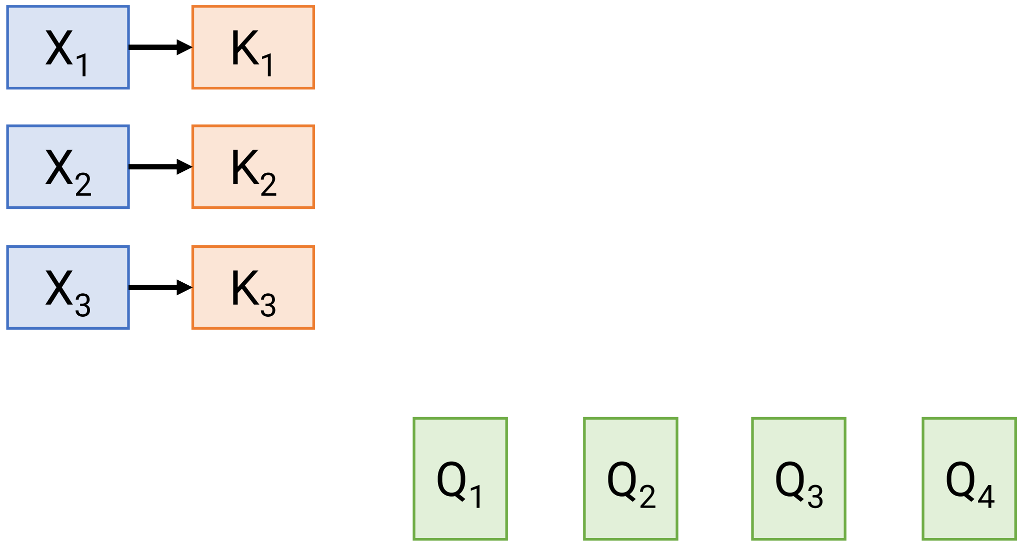


Slide credit: Justin Johnson

Attention Layer

Inputs:
Query vectors: **Q** (Shape: N_Q x D_Q)
Input vectors: **X** (Shape: N_X x D_X)
Key matrix: $\mathbf{W_K}$ (Shape: D_X x D_Q)
Value matrix: $\mathbf{W_V}$ (Shape: D_X x D_V)

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

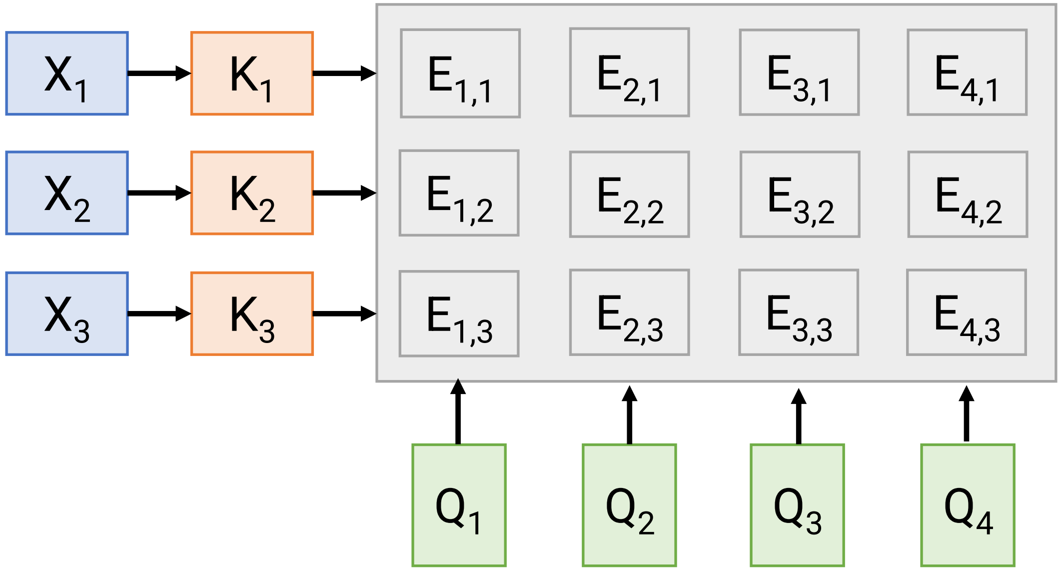


Slide credit: Justin Johnson

Attention Layer

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

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

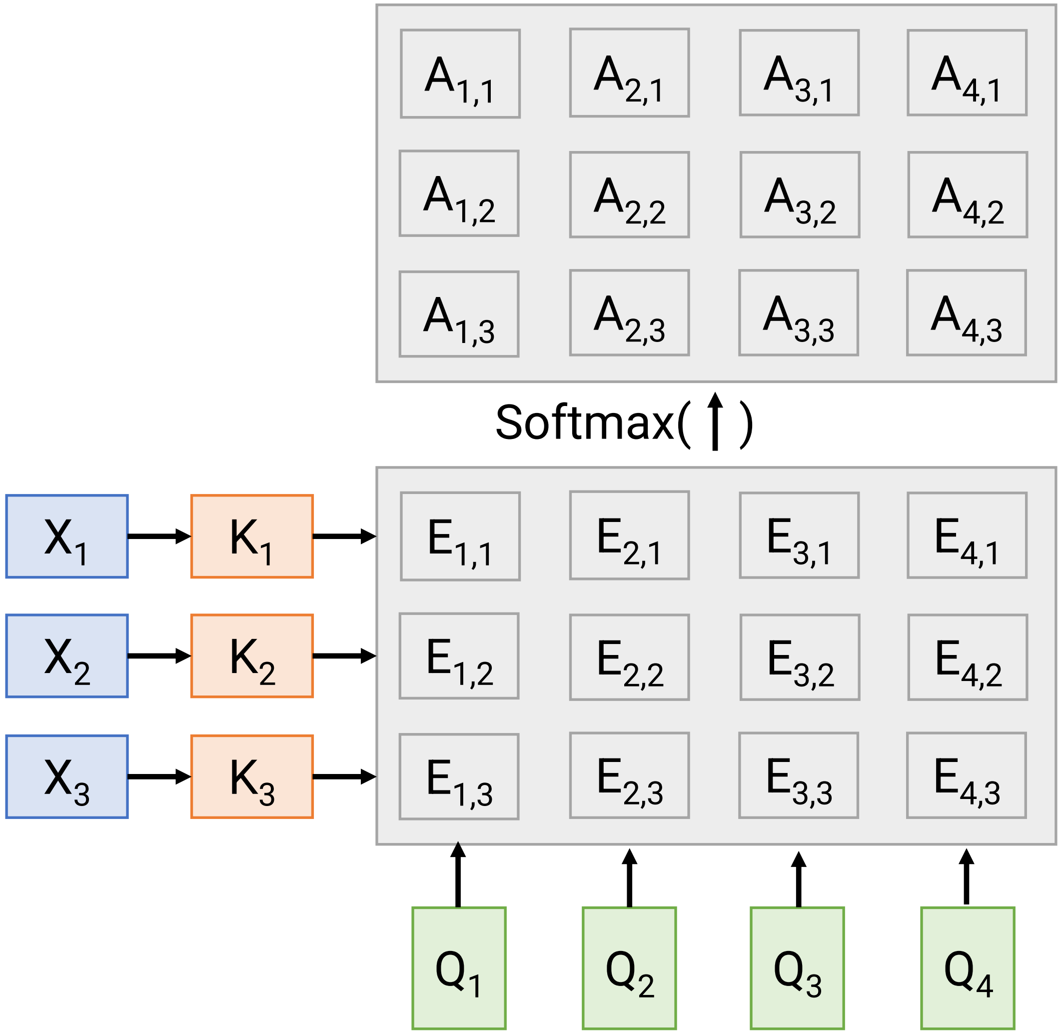


Slide credit: Justin Johnson

Attention Layer

Inputs:
Query vectors: **Q** (Shape: N_Q x D_Q)
Input vectors: **X** (Shape: N_X x D_X)
Key matrix: $\mathbf{W_K}$ (Shape: D_X x D_Q)
Value matrix: $\mathbf{W_V}$ (Shape: D_X x D_V)

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

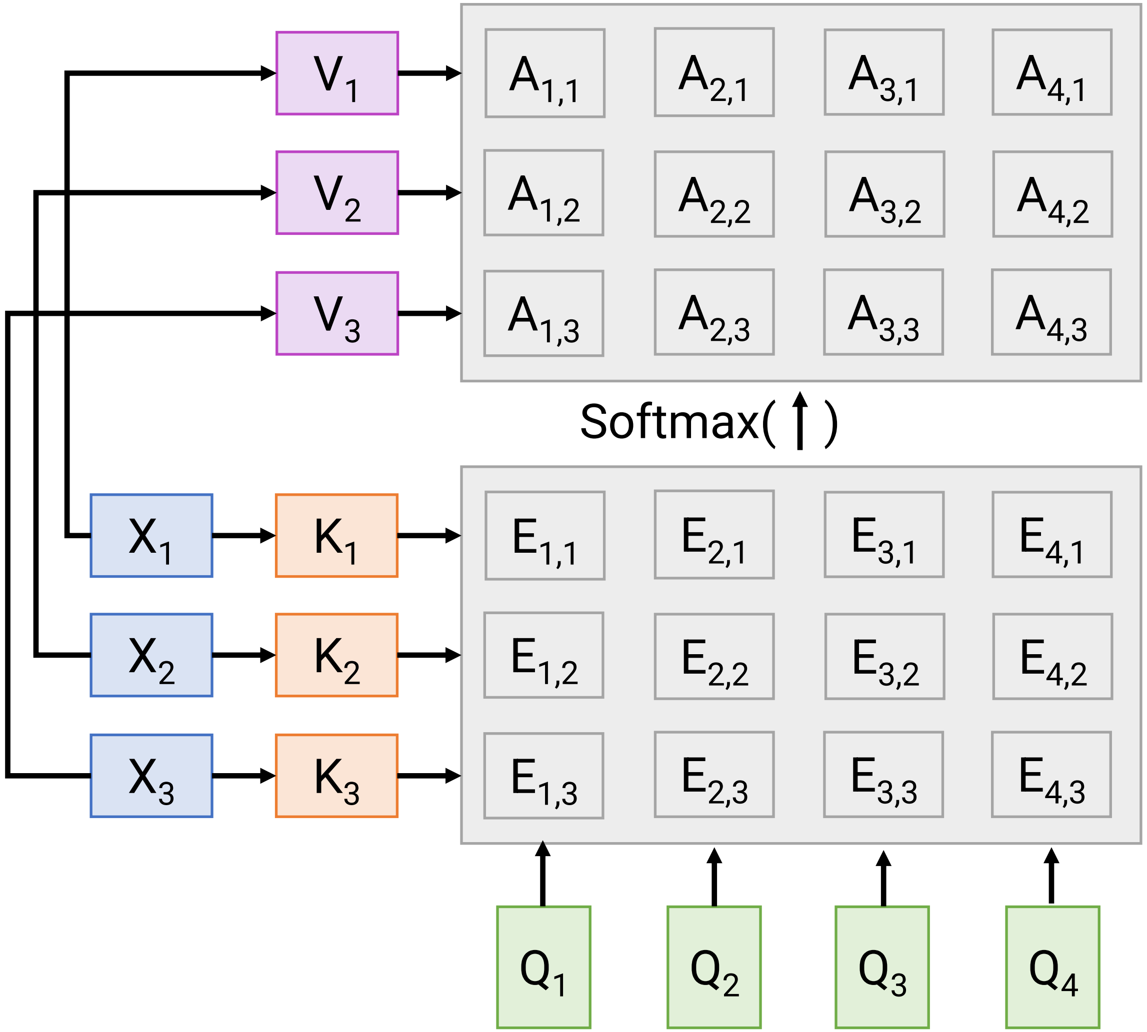


Slide credit: Justin Johnson

Attention Layer

Inputs:
Query vectors: $\mathbf{Q}$ (Shape: $N_Q \times D_Q$)
Input vectors: $\mathbf{X}$ (Shape: $N_X \times D_X$)
Key matrix: $\mathbf{W_K}$ (Shape: $D_X \times D_Q$)
Value matrix: $\mathbf{W_V}$ (Shape: $D_X \times D_V$)

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

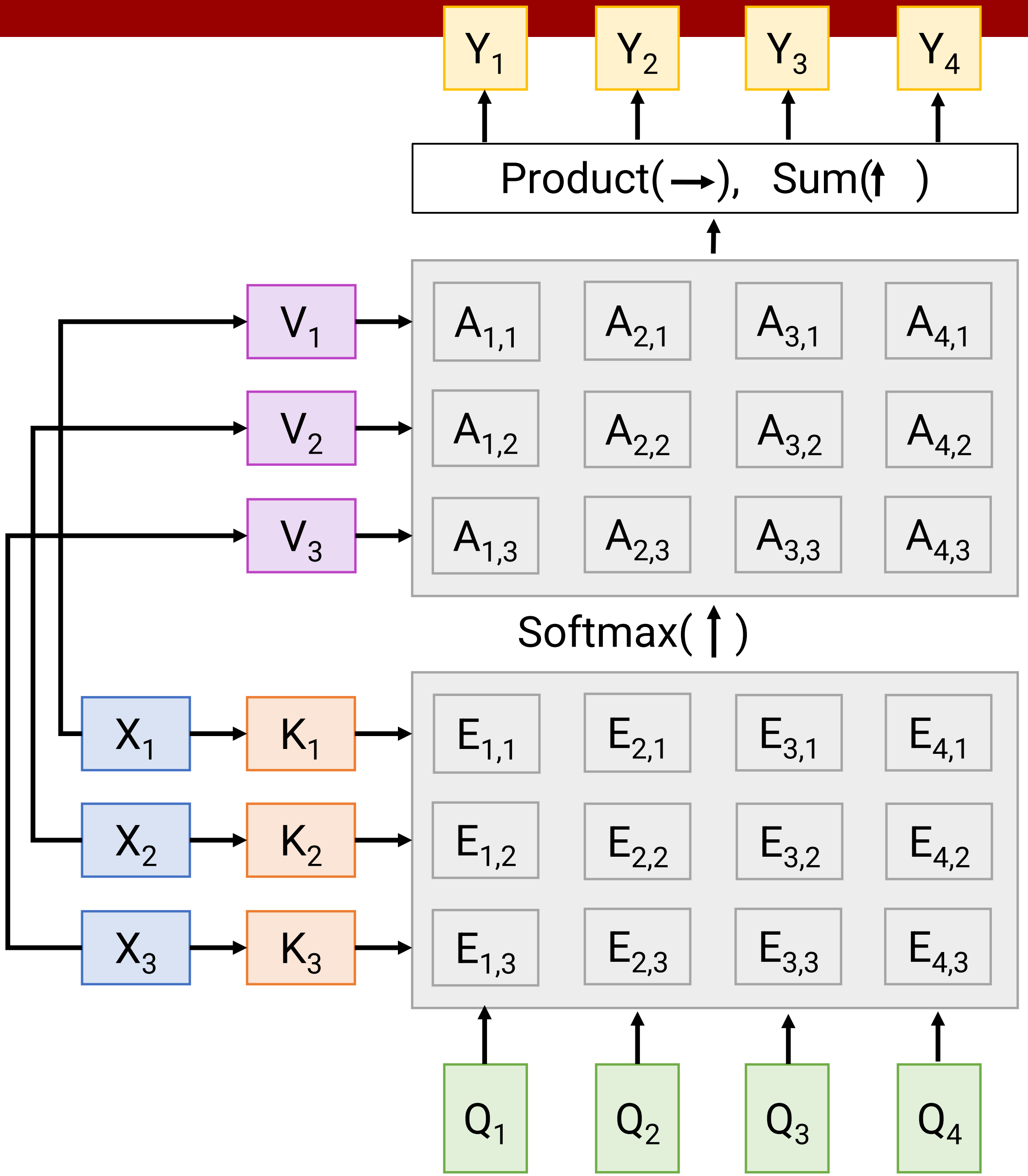


Slide credit: Justin Johnson

Attention Layer

Inputs:
Query vectors: **Q** (Shape: N_Q x D_Q)
Input vectors: **X** (Shape: N_X x D_X)
Key matrix: $\mathbf{W_K}$ (Shape: D_X x D_Q)
Value matrix: $\mathbf{W_V}$ (Shape: D_X x D_V)

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



Slide credit: Justin Johnson

Self-Attention Layer

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

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

Make the module generic:
Input: Sequence (X)
Output: Sequence (Weighted sum/mixture of inputs)

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

X_1 X_2 X_3

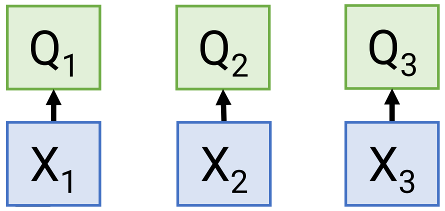
Slide credit: Justin Johnson

Self-Attention Layer

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

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

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



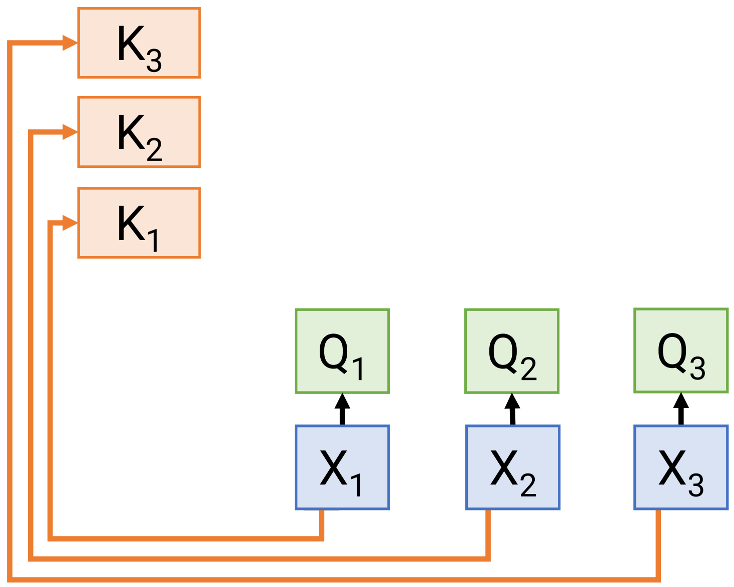
Slide credit: Justin Johnson

Self-Attention Layer

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

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

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



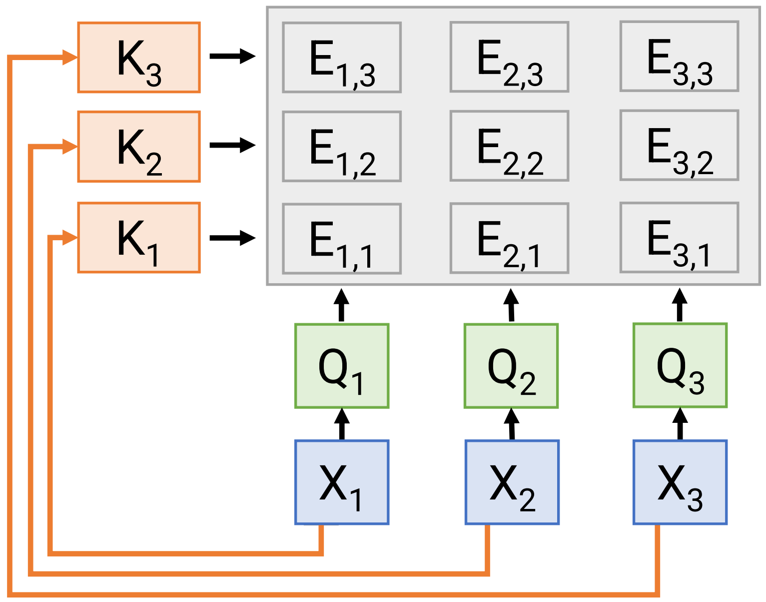
Slide credit: Justin Johnson

Self-Attention Layer

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

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

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



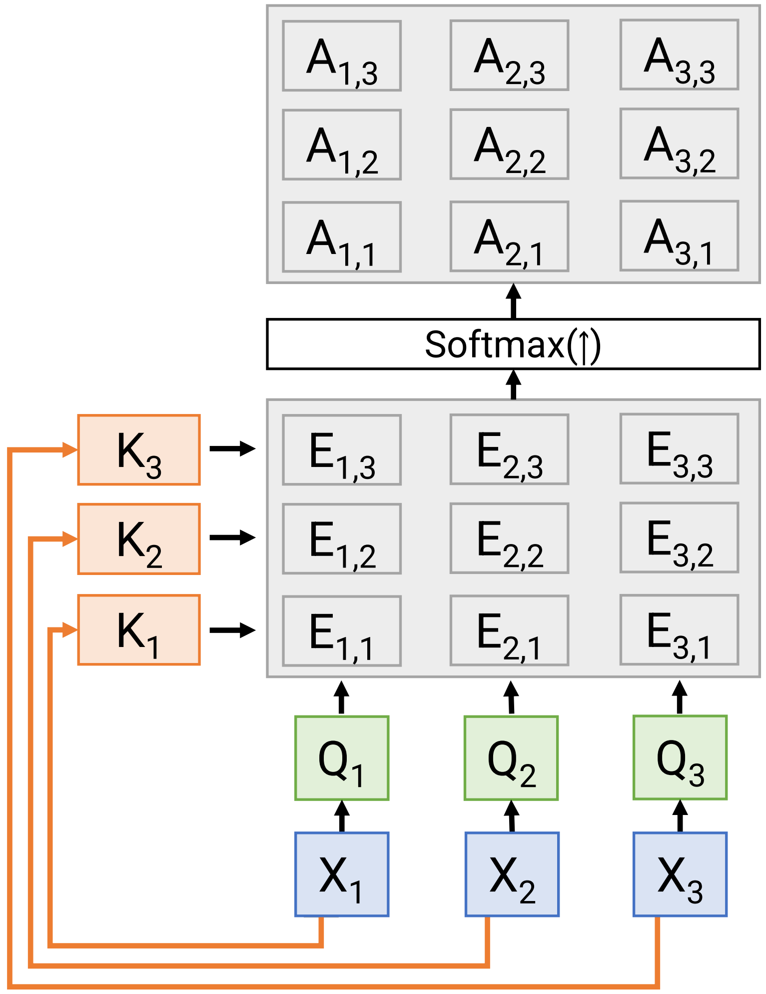
Slide credit: Justin Johnson

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) $E_{i,j} = Q_i \cdot K_j / \text{sqrt}(D_Q)$
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) $Y_i = \sum_j A_{i,j} V_j$

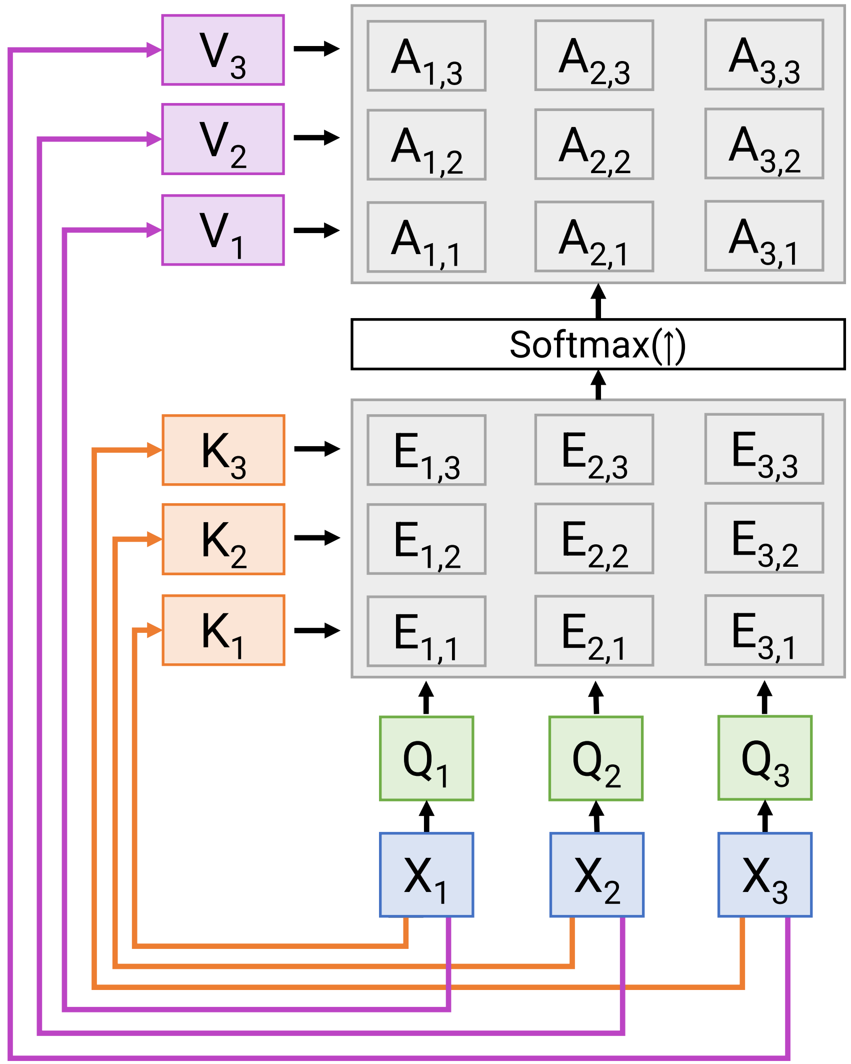


Self-Attention Layer

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

<u>Inputs</u>:
Input vectors: $\mathbf{X}$ (Shape: $N_X \times D_X$)
Key matrix: $\mathbf{W_K}$ (Shape: $D_X \times D_Q$)
Value matrix: $\mathbf{W_V}$ (Shape: $D_X \times D_V$)
Query matrix: $\mathbf{W_Q}$ (Shape: $D_X \times D_Q$)

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



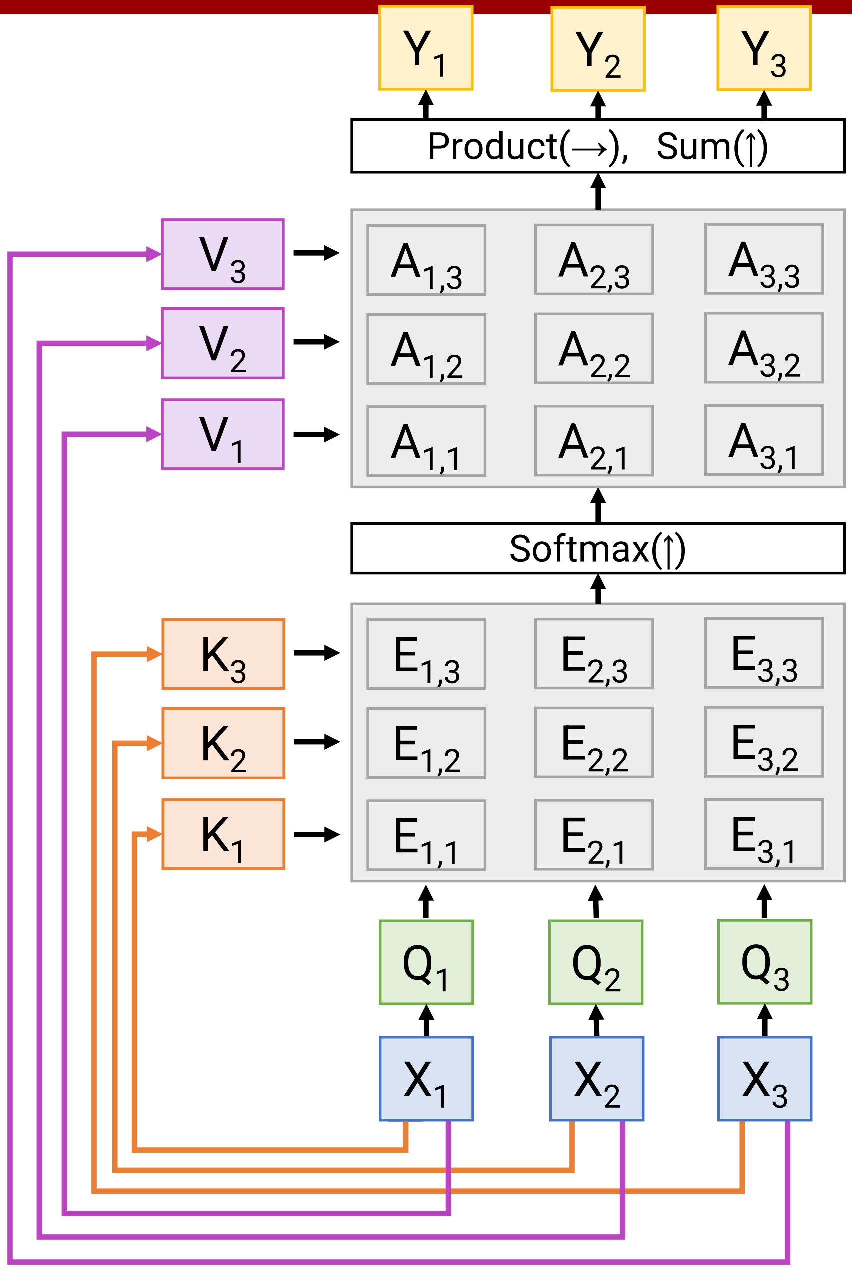
Slide credit: Justin Johnson

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: $N_X \times N_X$) $E_{i,j} = Q_i \cdot K_j / \mathrm{sqrt}(D_Q)$
Attention weights: $A = \mathrm{softmax}(E, \mathrm{dim}=1)$ (Shape: $N_X \times N_X$)
Output vectors: $Y = AV$ (Shape: $N_X \times D_V$) $Y_i = \sum_j A_{i,j} V_j$



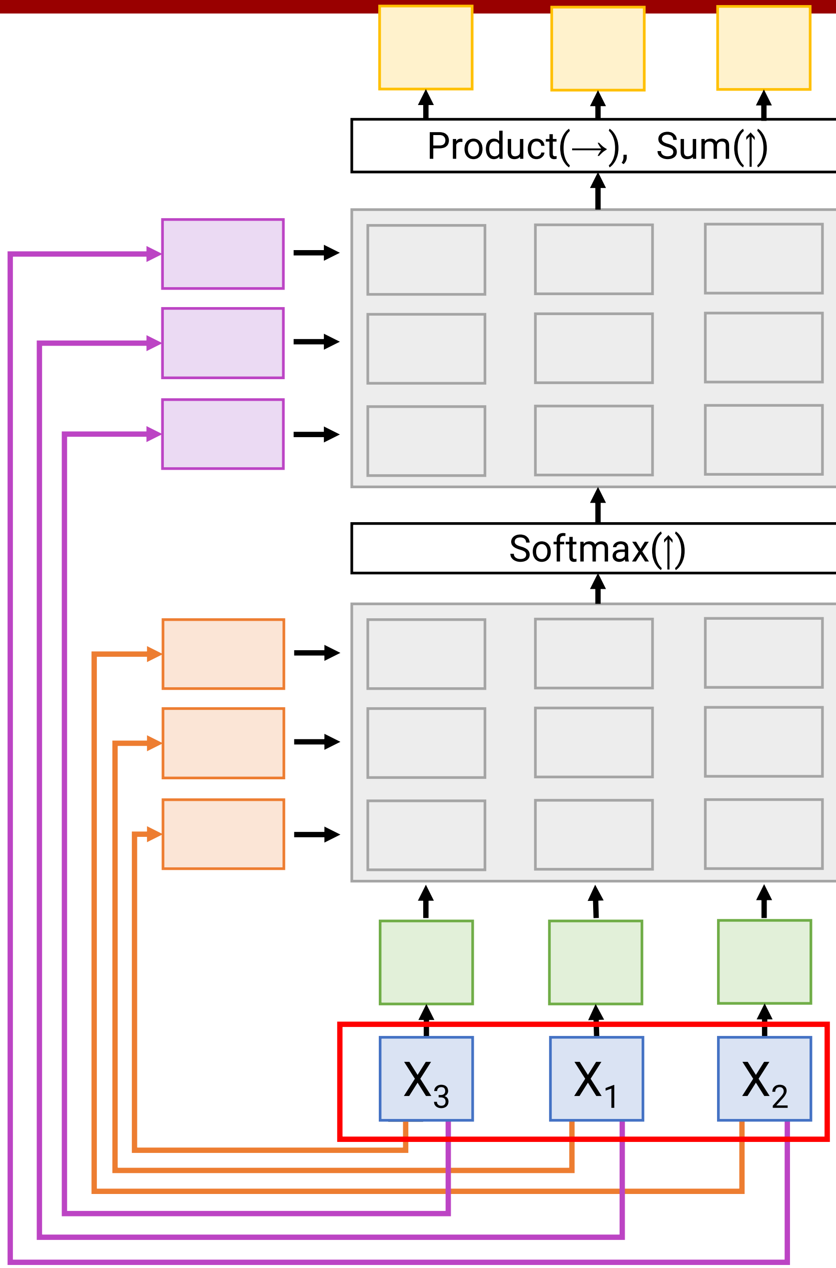
Slide credit: Justin Johnson

Self-Attention Layer

Consider **permuting** the input vectors:

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) $E_{i,j} = Q_i \cdot K_j / \mathrm{sqrt}(D_Q)$
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

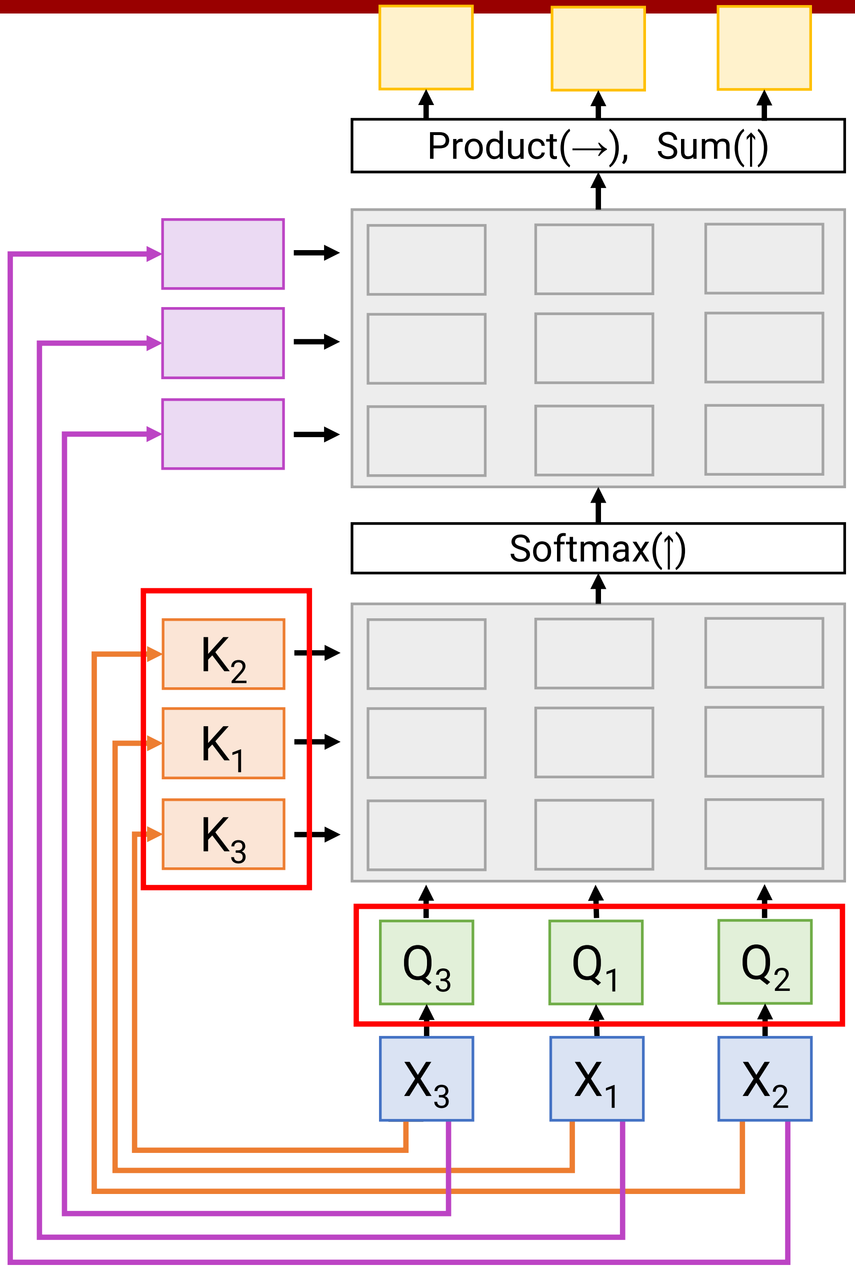
Self-Attention Layer

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

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

Consider **permuting** the input vectors:

Queries and Keys will be the same, but permuted



Slide credit: Justin Johnson

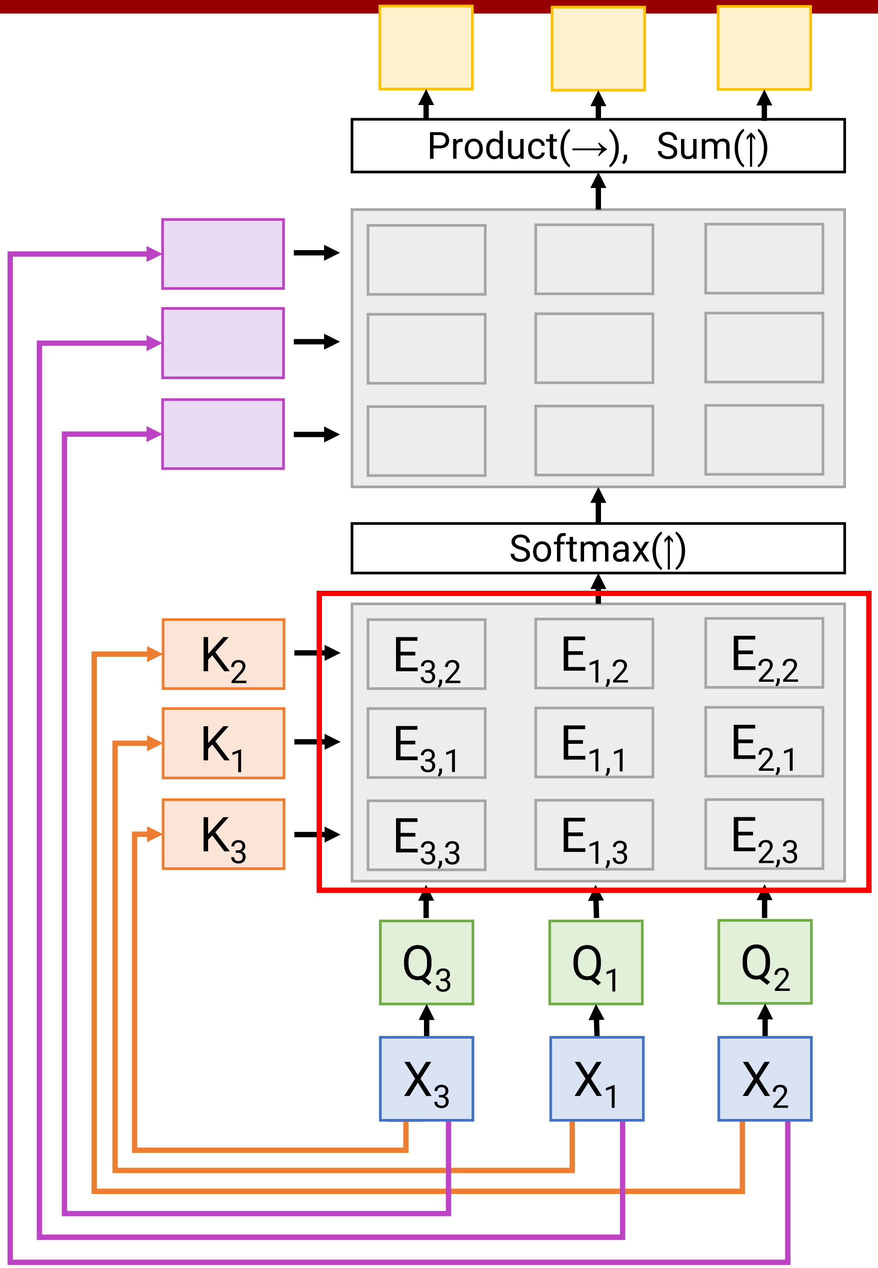
Self-Attention Layer

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:

Similarities 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 = A**V** (Shape: N_X x D_V) $Y_i = \sum_j A_{i,j} V_j$



Slide credit: Justin Johnson

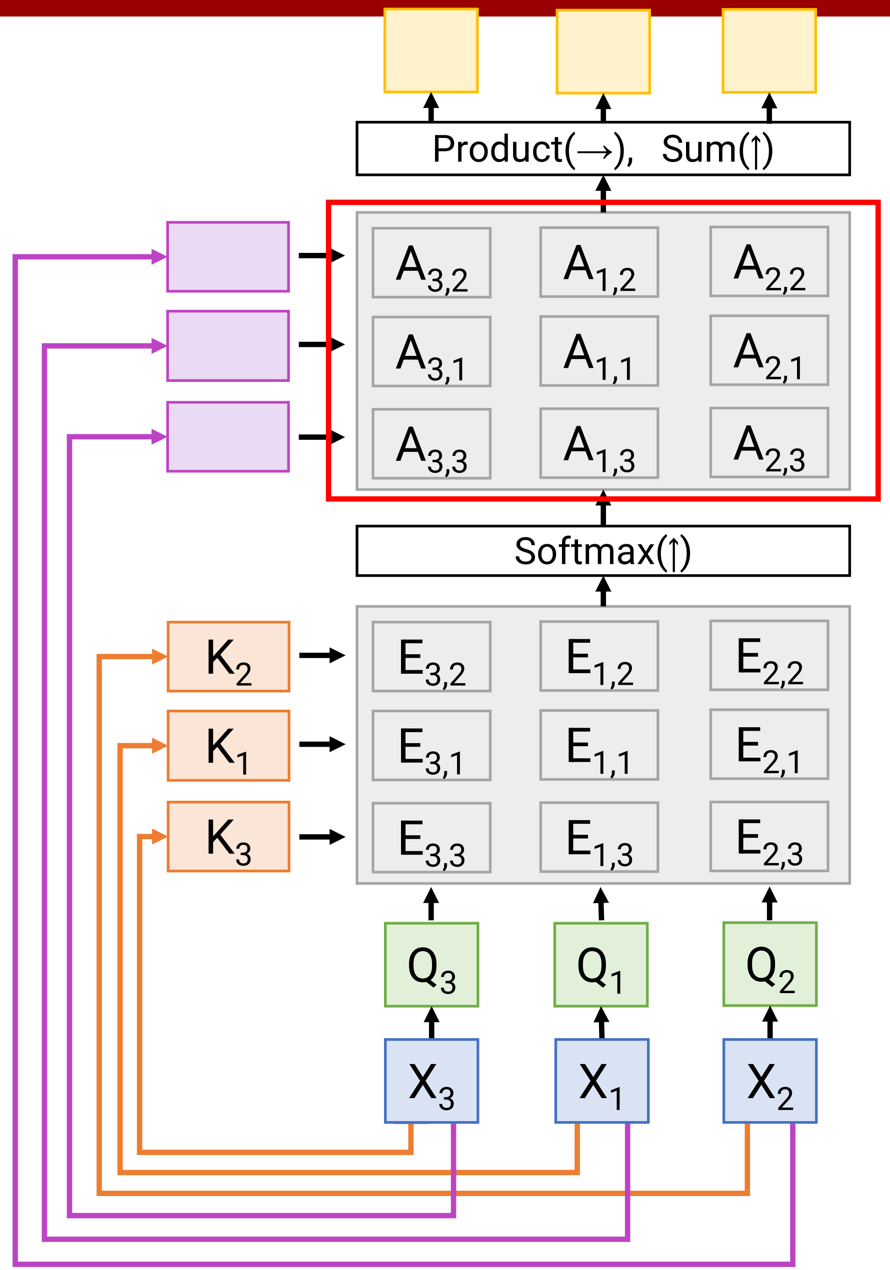
Self-Attention Layer

<u>Inputs</u>:
Input vectors: $\mathbf{X}$ (Shape: $N_X \times D_X$)
Key matrix: $\mathbf{W_K}$ (Shape: $D_X \times D_Q$)
Value matrix: $\mathbf{W_V}$ (Shape: $D_X \times D_V$)
Query matrix: $\mathbf{W_Q}$ (Shape: $D_X \times D_Q$)

Consider **permuting** the input vectors:

Attention weights will be the same, but permuted

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



Slide credit: Justin Johnson

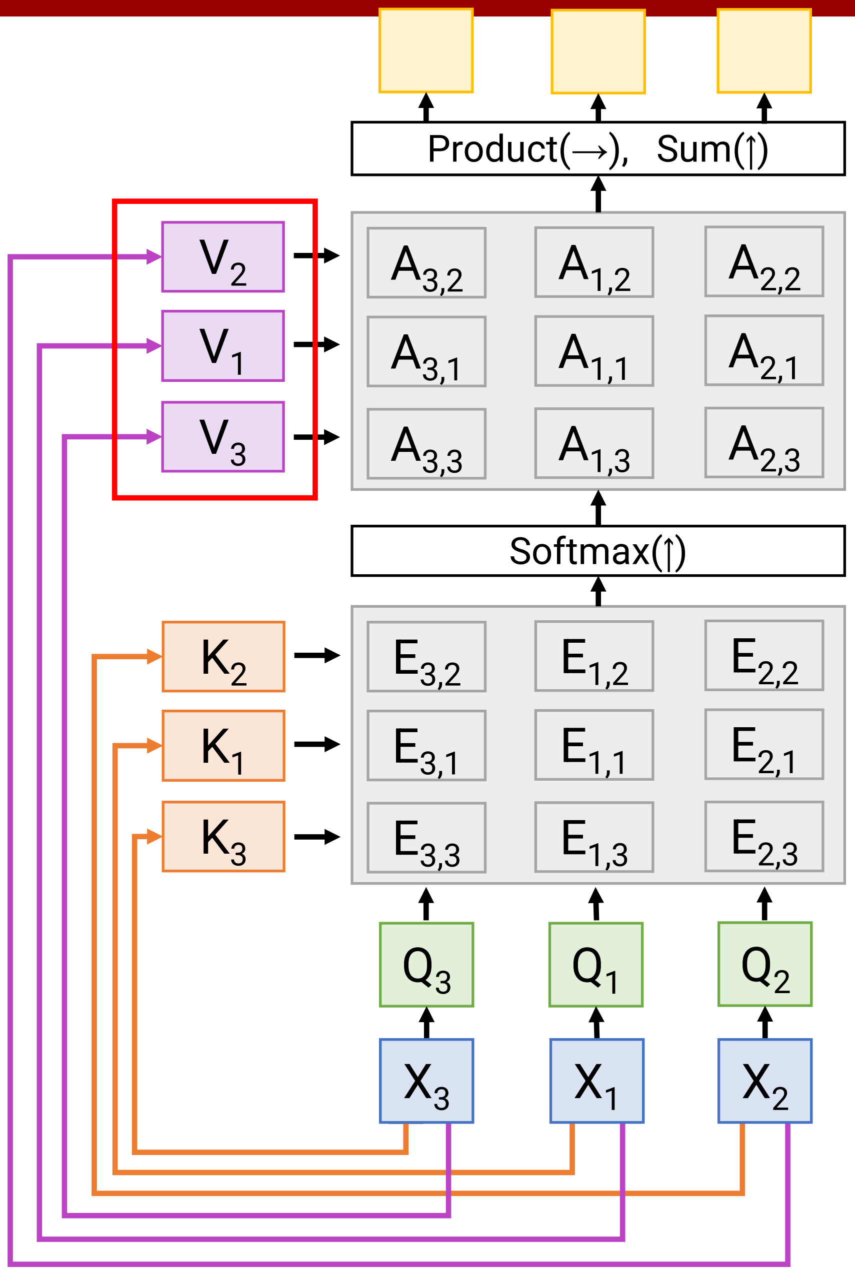
Self-Attention Layer

Consider **permuting** the input vectors:

Values will be the same, but permuted

<u>**Inputs**</u>:
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)

<u>**Computation**</u>:
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) $E_{i,j} = Q_i \cdot K_j / \mathrm{sqrt}(D_Q)$
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

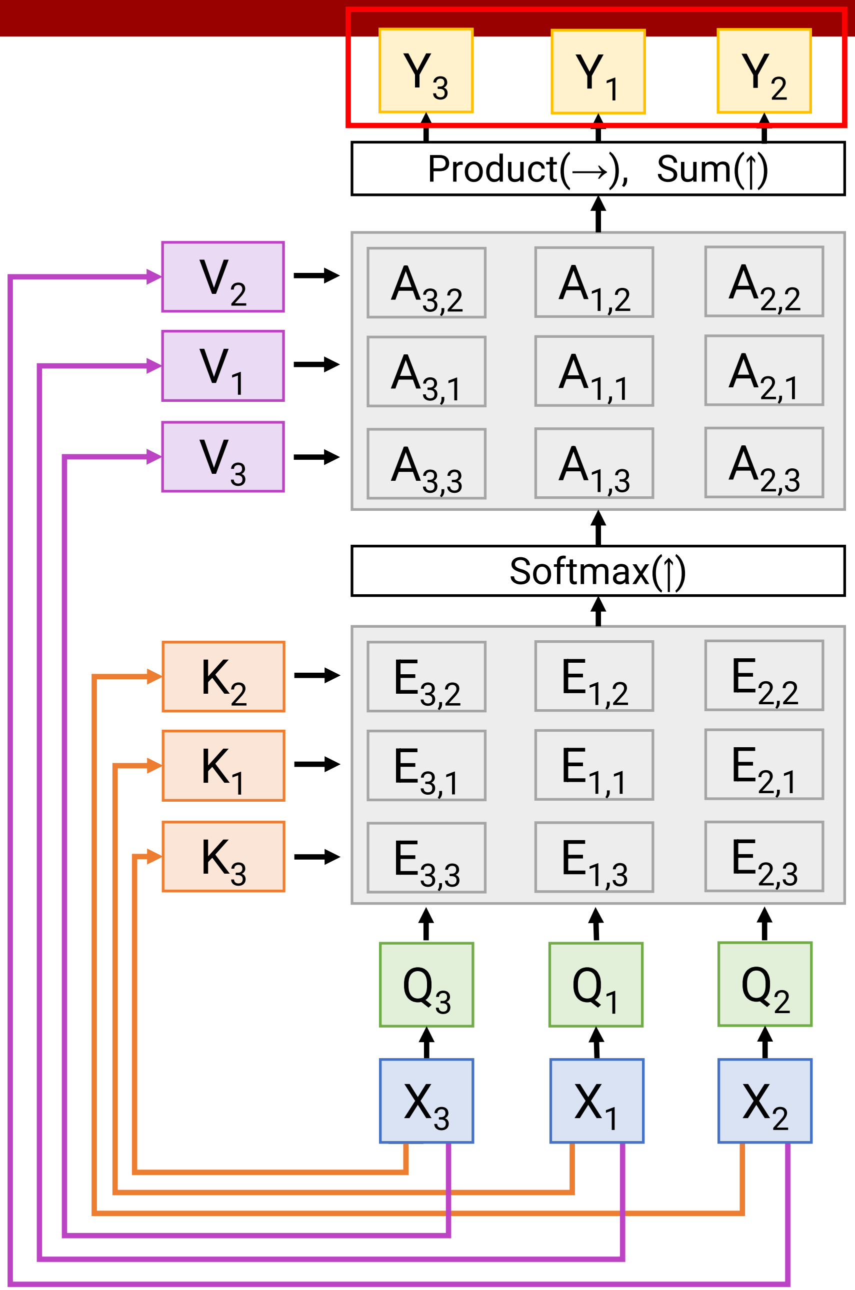
Self-Attention Layer

Consider **permuting** the input vectors:

Outputs will be the same, but permuted

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

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



Slide credit: Justin Johnson

Self-Attention Layer

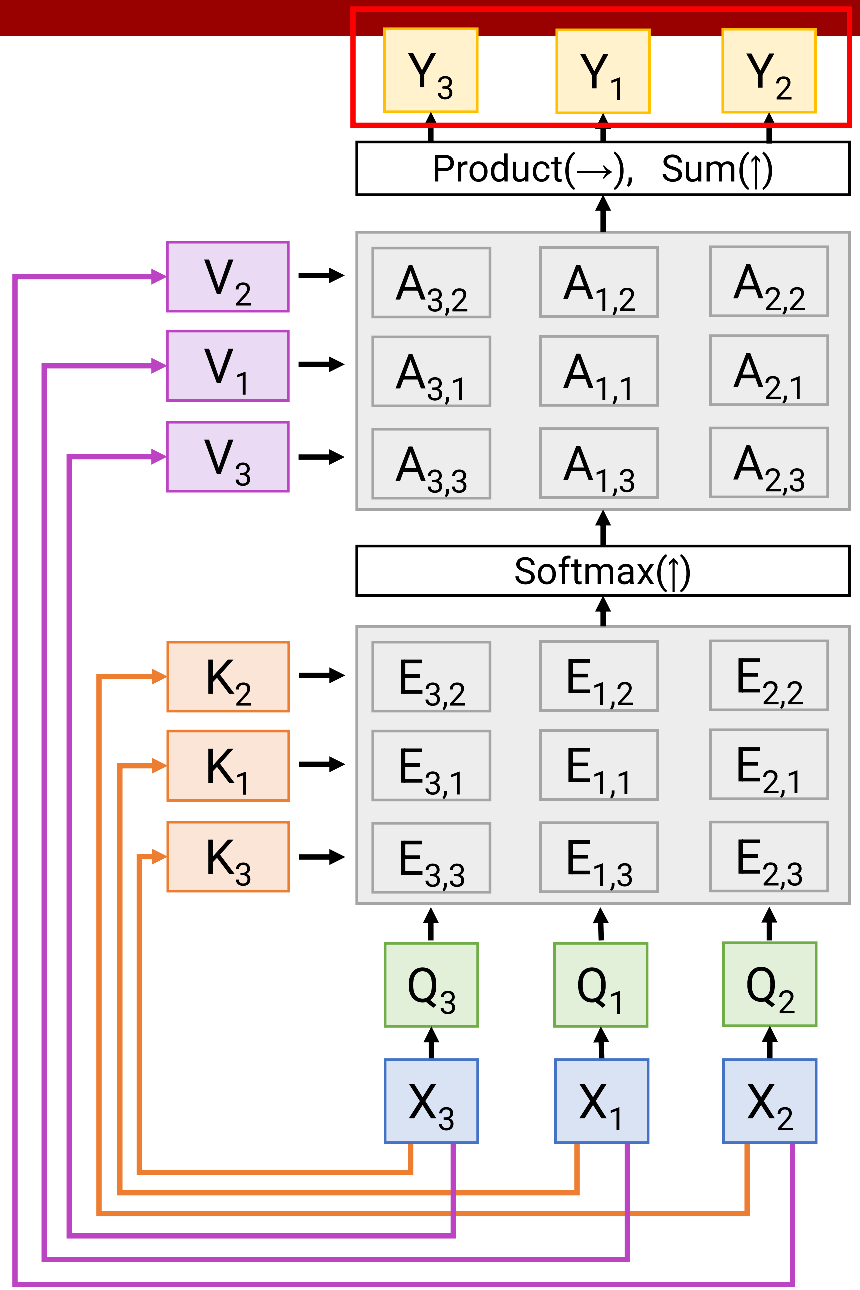
Inputs:
Input vectors: X (Shape: $N_X \times D_X$)
Key matrix: W_K (Shape: $D_X \times D_Q$)
Value matrix: W_V (Shape: $D_X \times D_V$)
Query matrix: W_Q (Shape: $D_X \times D_Q$)

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: $N_X \times N_X$) $E_{i,j} = Q_i \cdot K_j / \mathrm{sqrt}(D_Q)$
Attention weights: $A = \mathrm{softmax}(E, \mathrm{dim}=1)$ (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**
$f(s(x)) = s(f(x))$



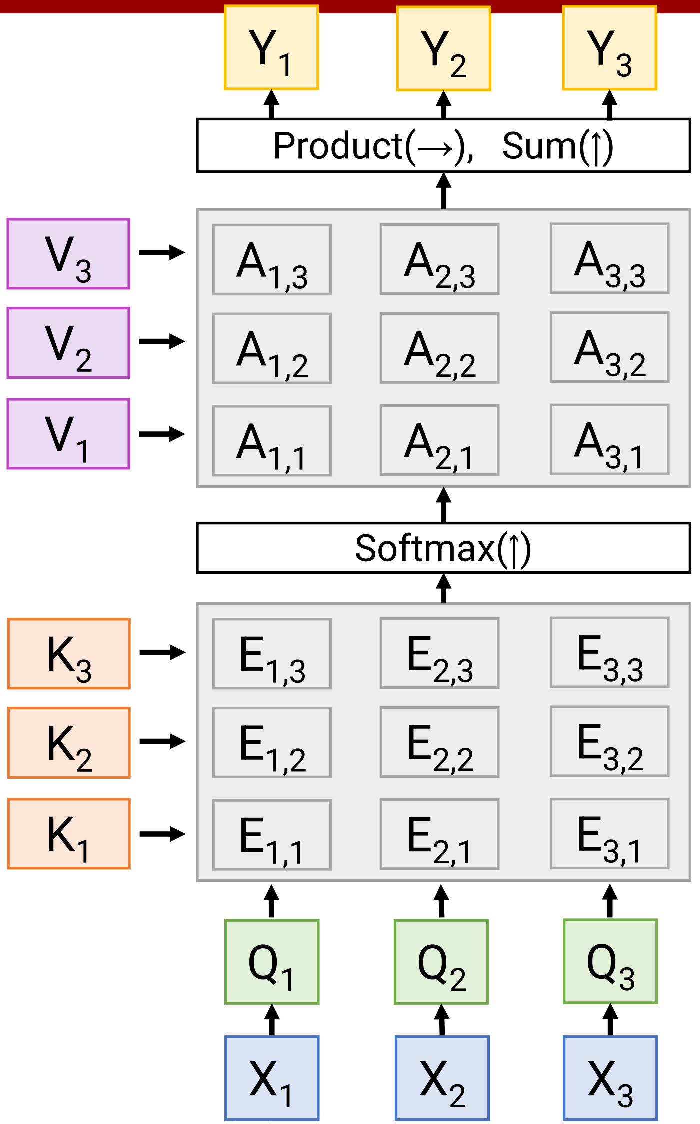
Slide credit: Justin Johnson

Self-Attention Layer

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

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

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



Slide credit: Justin Johnson

Self-Attention Layer

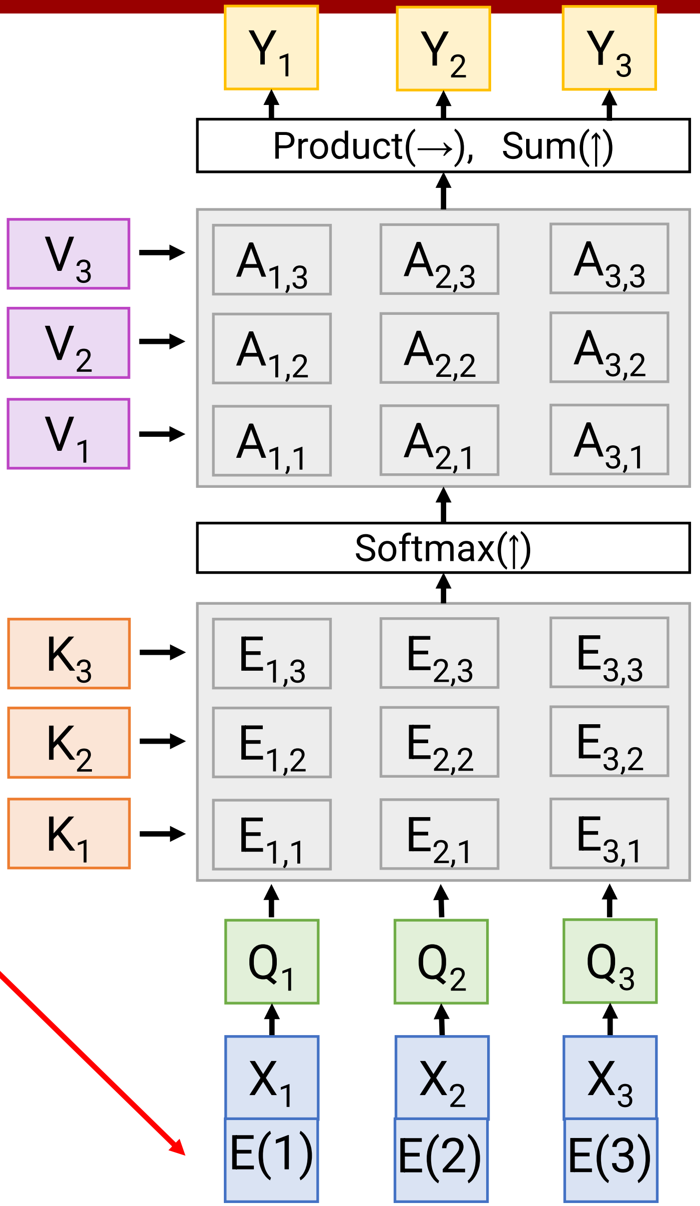
Inputs:
Input vectors: **X** (Shape: N_X x D_X)
Key matrix: **W_K** (Shape: D_X x D_Q)
Value matrix: **W_V** (Shape: D_X x D_V)
Query matrix: **W_Q** (Shape: D_X x D_Q)

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) $E_{i,j} = Q_i \cdot K_j / \mathrm{sqrt}(D_Q)$
Attention weights: A = softmax(E, dim=1) (Shape: N_X x N_X)
Output vectors: Y = A**V** (Shape: N_X x 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

Summary

- We have made a generic sequence-in to sequence-out layer
  - This is what we want for language processing!
  - Each output is a contextualized representation of the corresponding input word
  - Vector for stop word can be treated as representation of entire sentence (e.g. project its output to classifier and add loss)

- Unlike RNNs/LSTMs, it processes all inputs (e.g. entire sentence) **at once**
  - **Highly parallelizable**
  - **-> SCALE! -> Reduction of loss -> Magic**

- Next time: Entire transformer architecture that combines this new layer with other layers/concepts we know about (fully-connected, normalization, residual/skip connections)