Attention and Transformers

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Georgia Tech

Slide Credits: Andrej Karpathy, Justin Johnson, Dhruv Batra

Lecture Outline

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

Sequence Modeling with RNNs

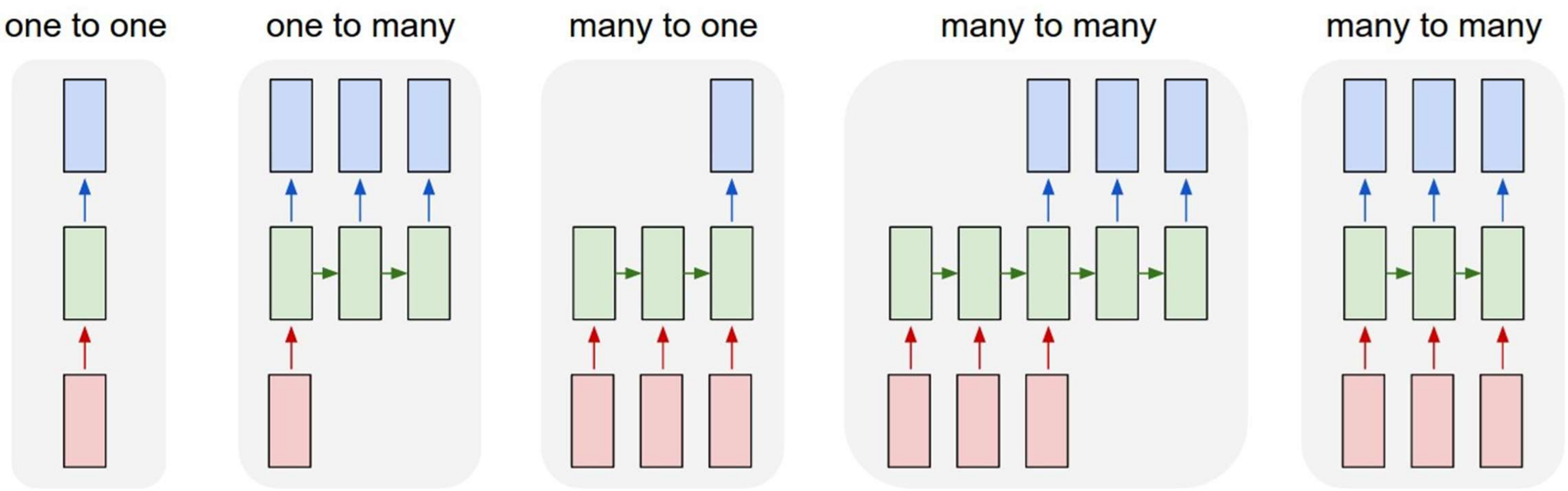
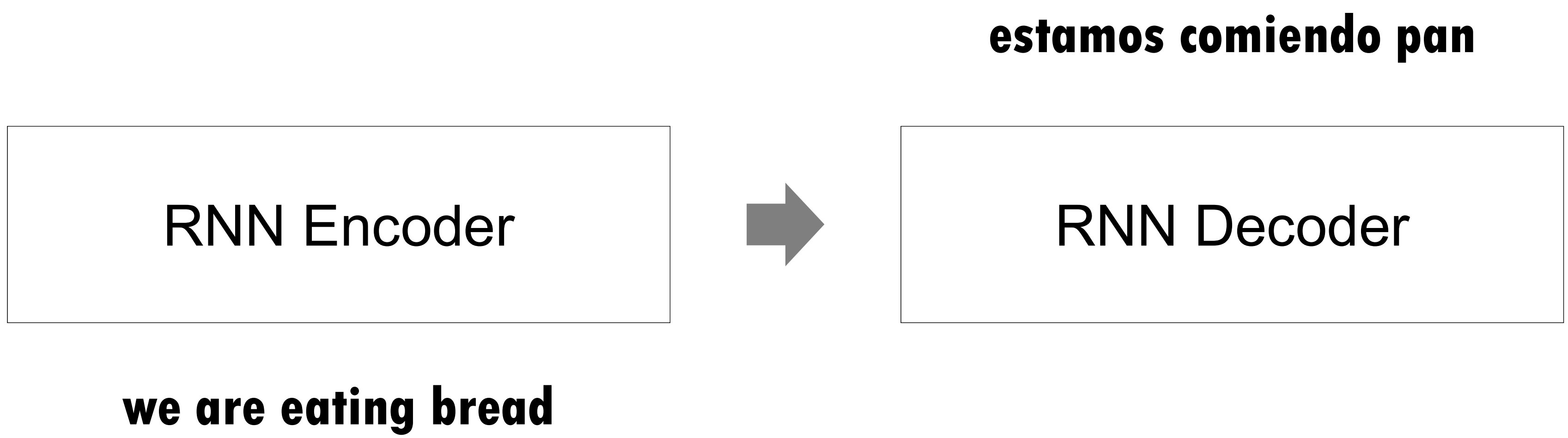


Image Credit: Andrej Karpathy

Machine Translation

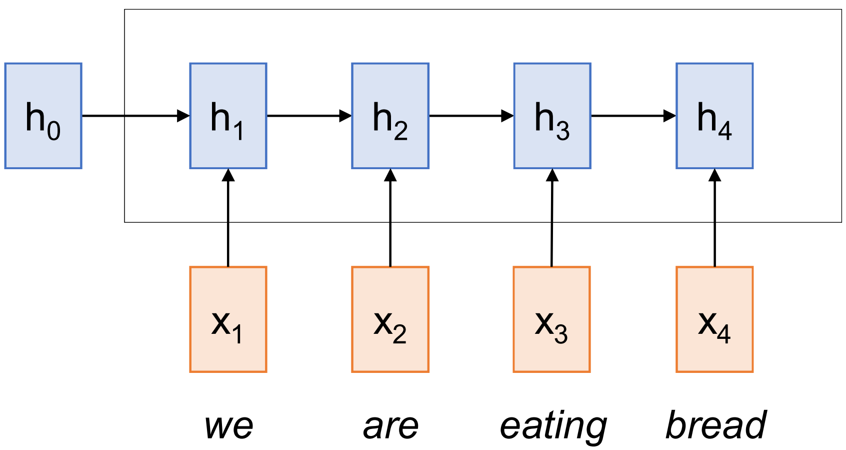
we are eating bread ➡ estamos comiendo pan

Machine Translation



Machine Translation with RNNs

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



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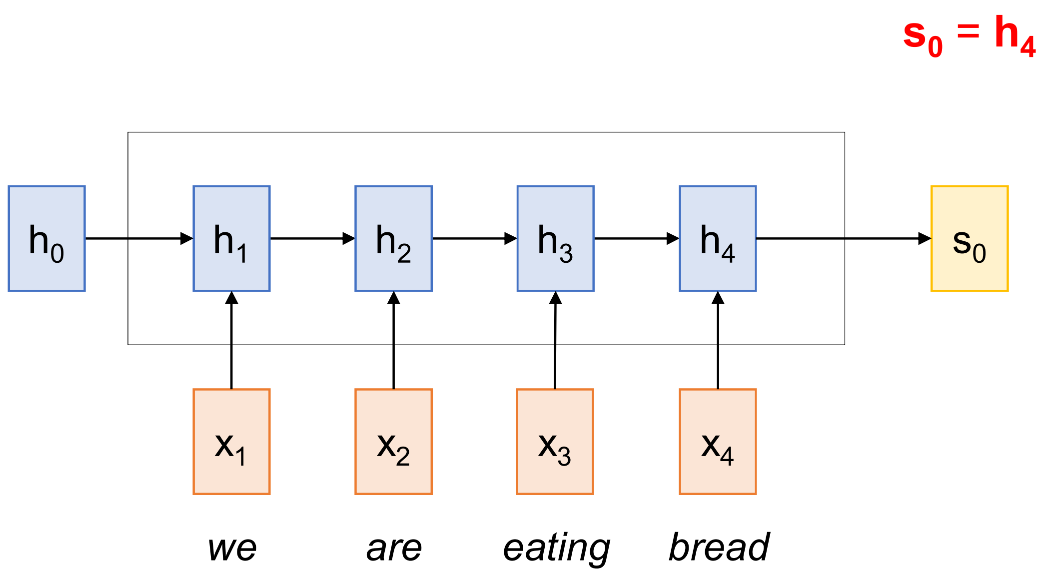
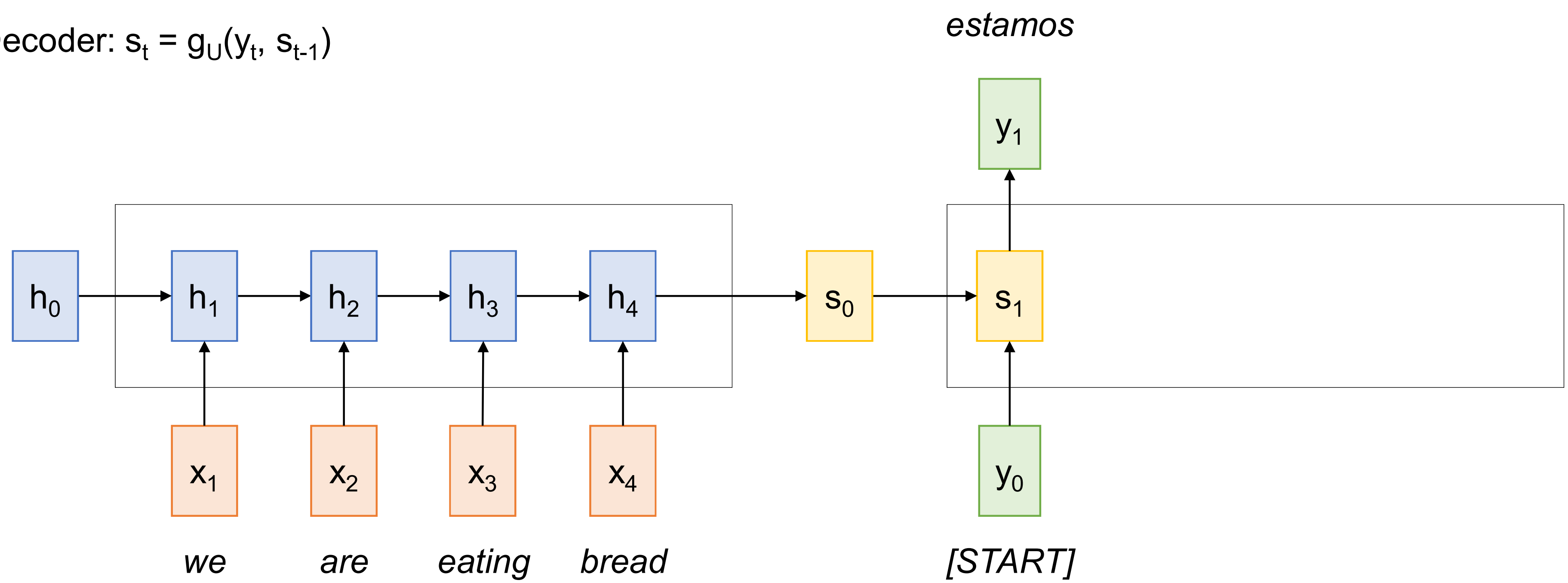


Slide credit: Justin Johnson

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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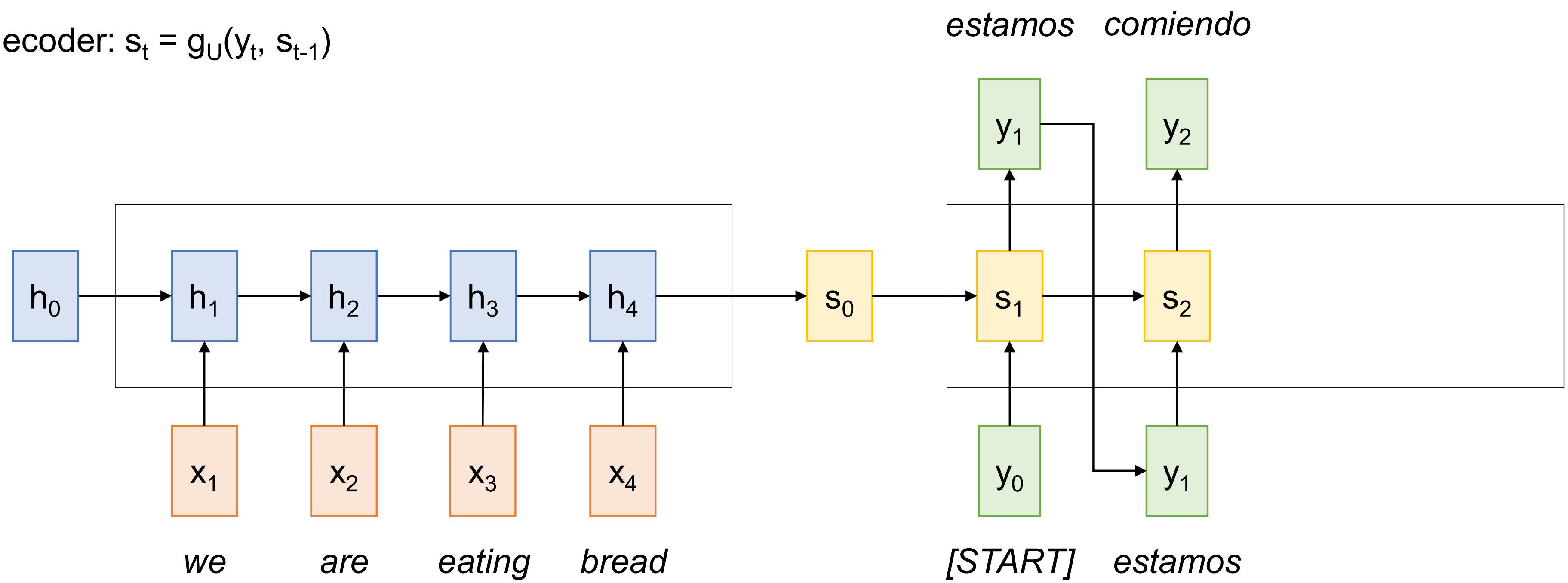

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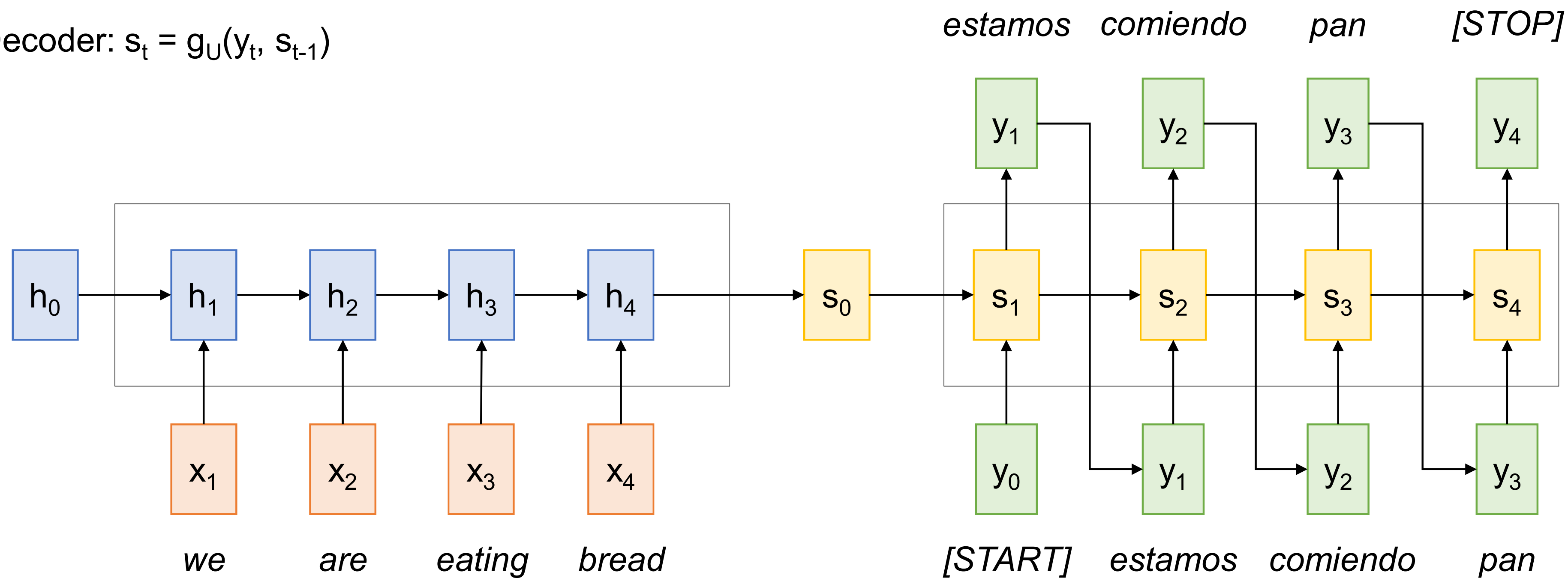


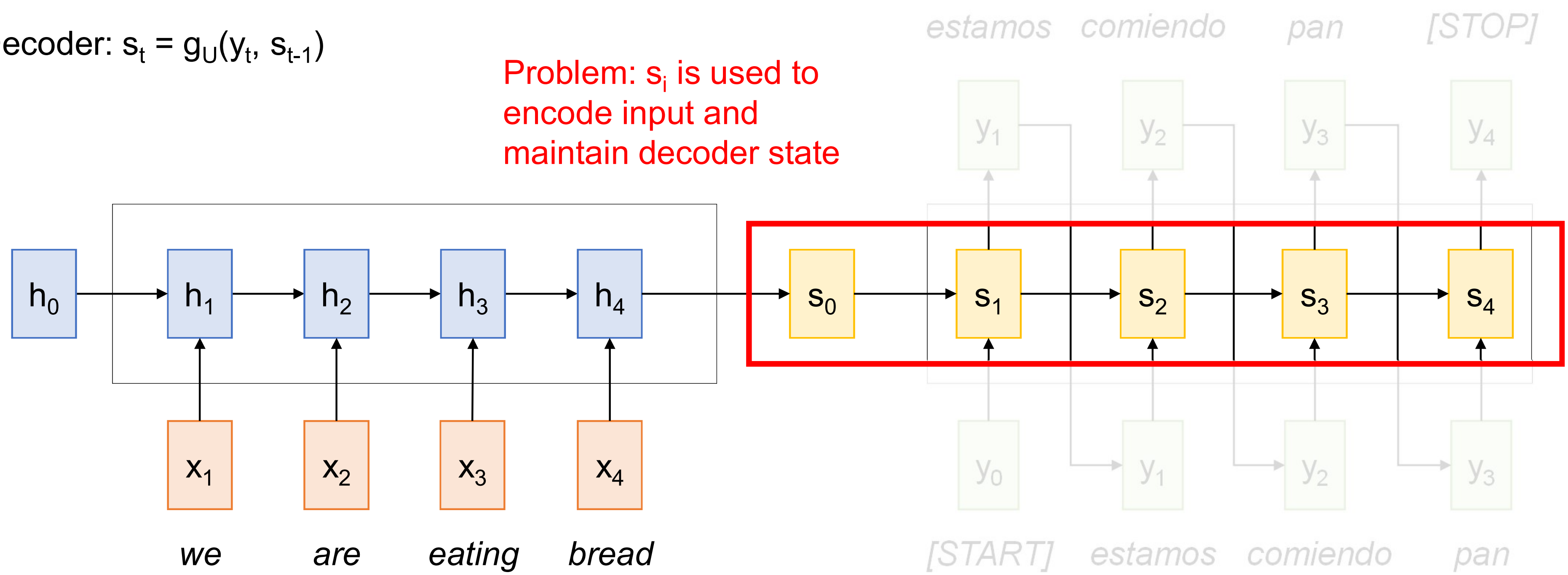
Slide credit: Justin Johnson

Machine Translation with RNNs

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

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

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



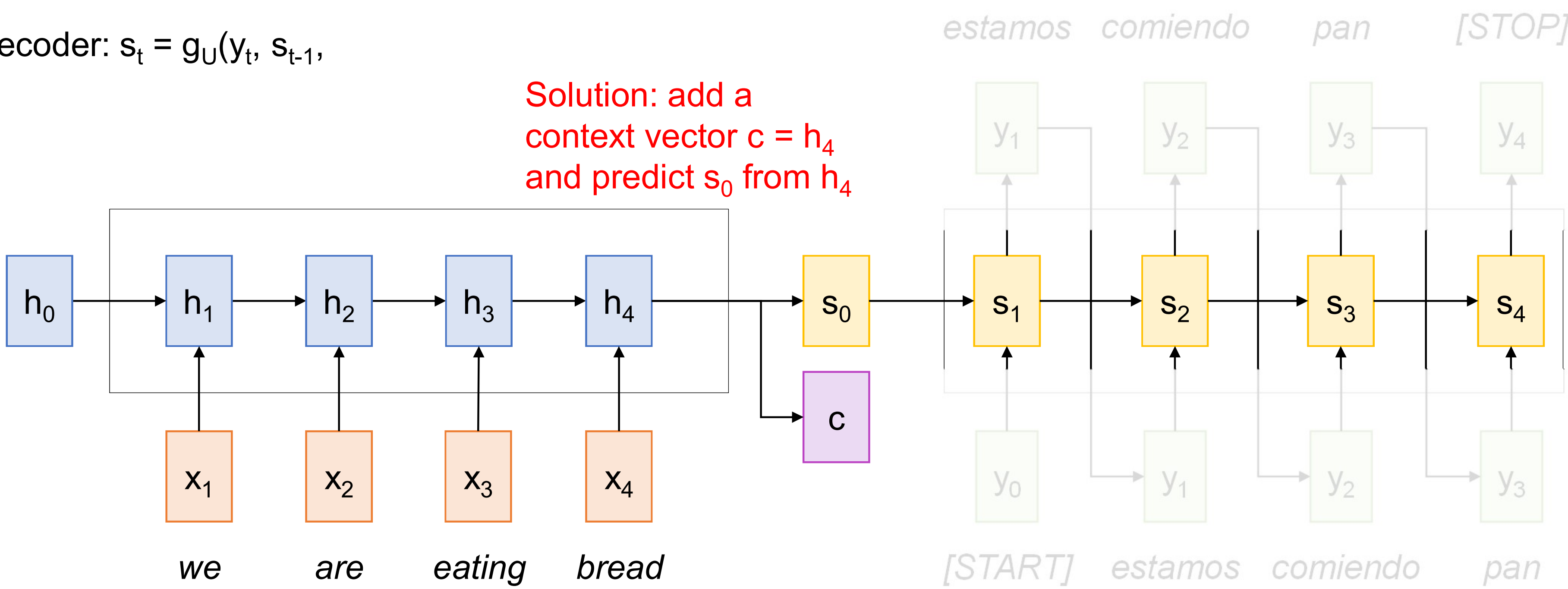
Slide credit: Justin Johnson

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



Slide credit: Justin Johnson

Machine Translation with RNNs

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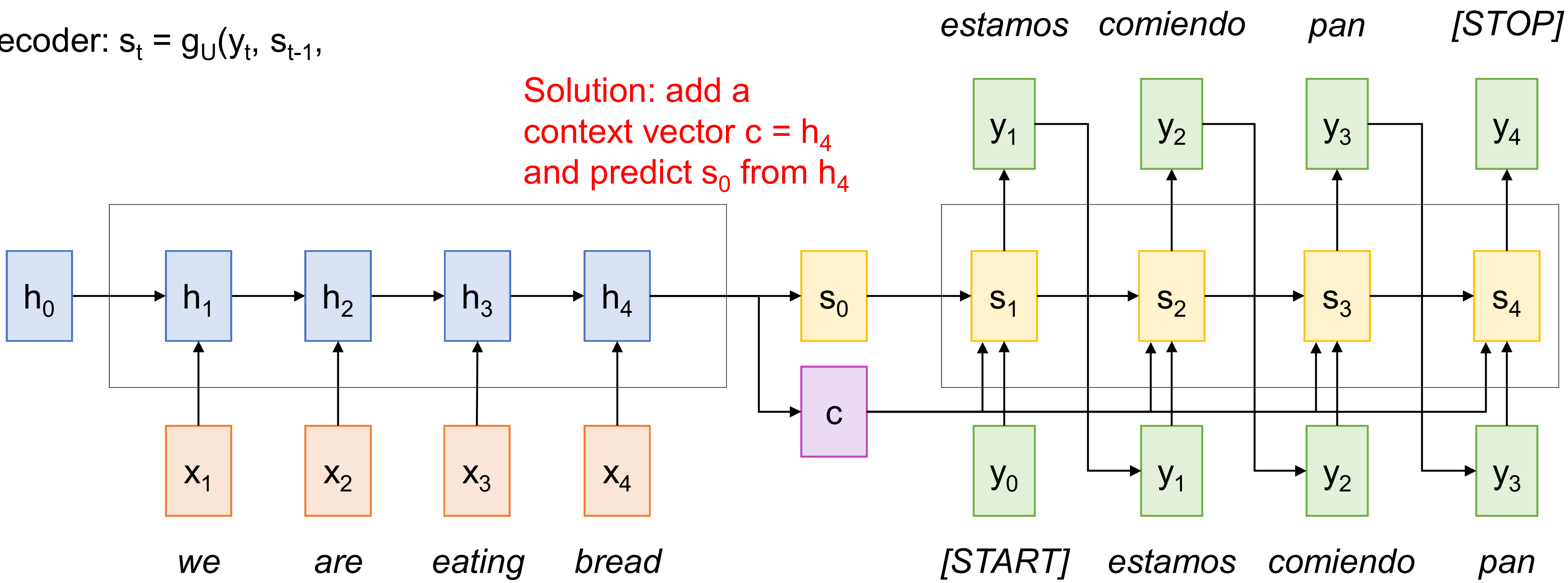

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Machine Translation with RNNs

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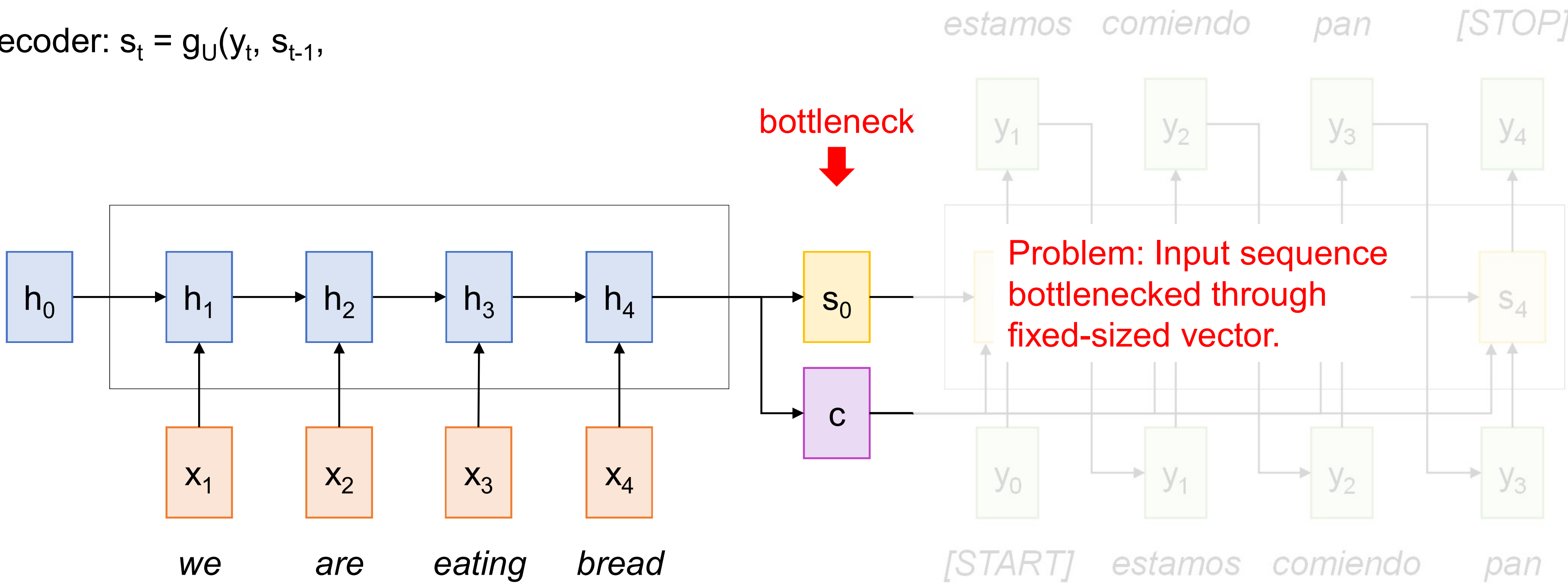

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Machine Translation with RNNs

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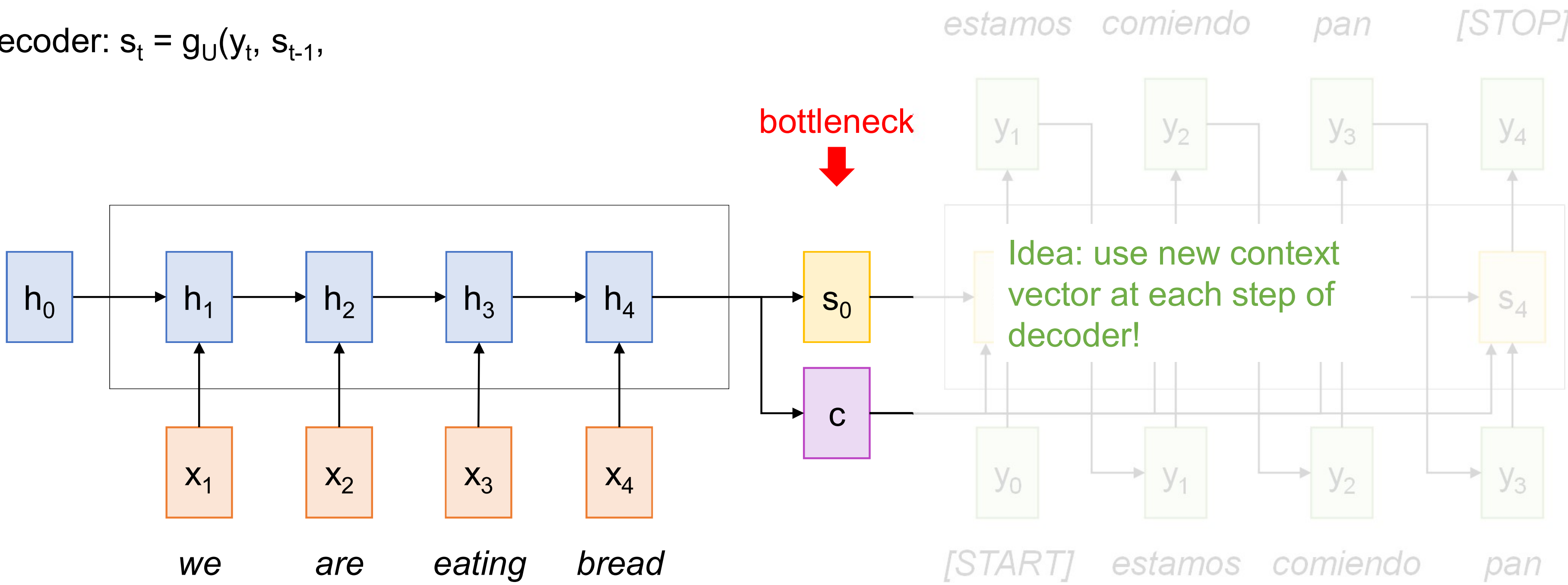

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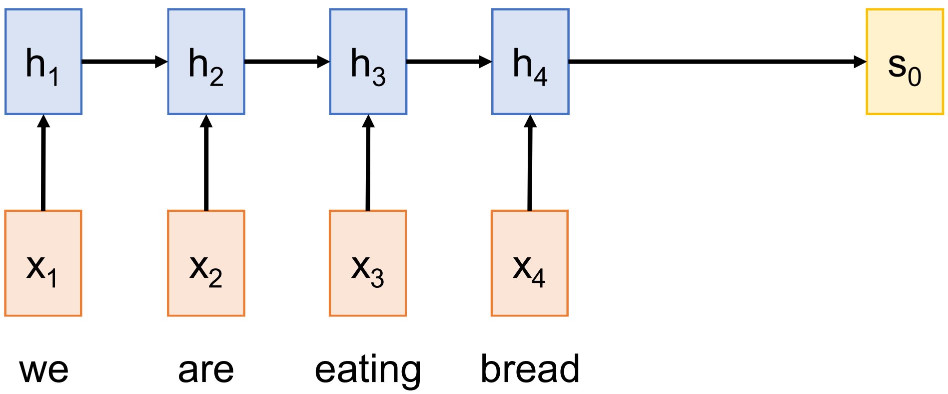
Machine Translation with RNNs and Attention

From final hidden state:
Initial decoder state s_0



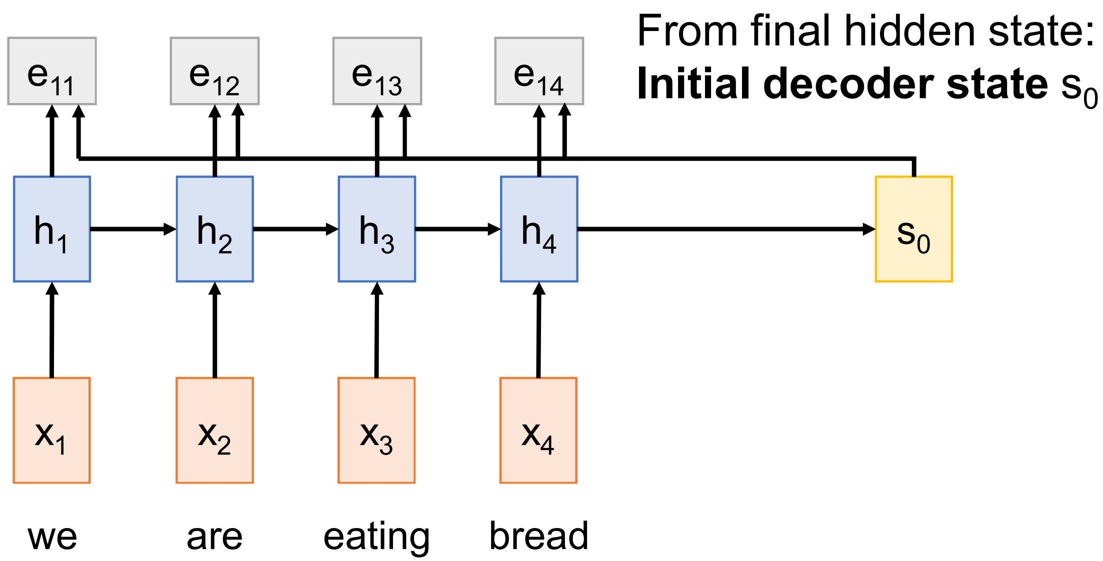
Bahdanau et al, "Neural machine translation by jointly learning to align and translate", ICLR 2015

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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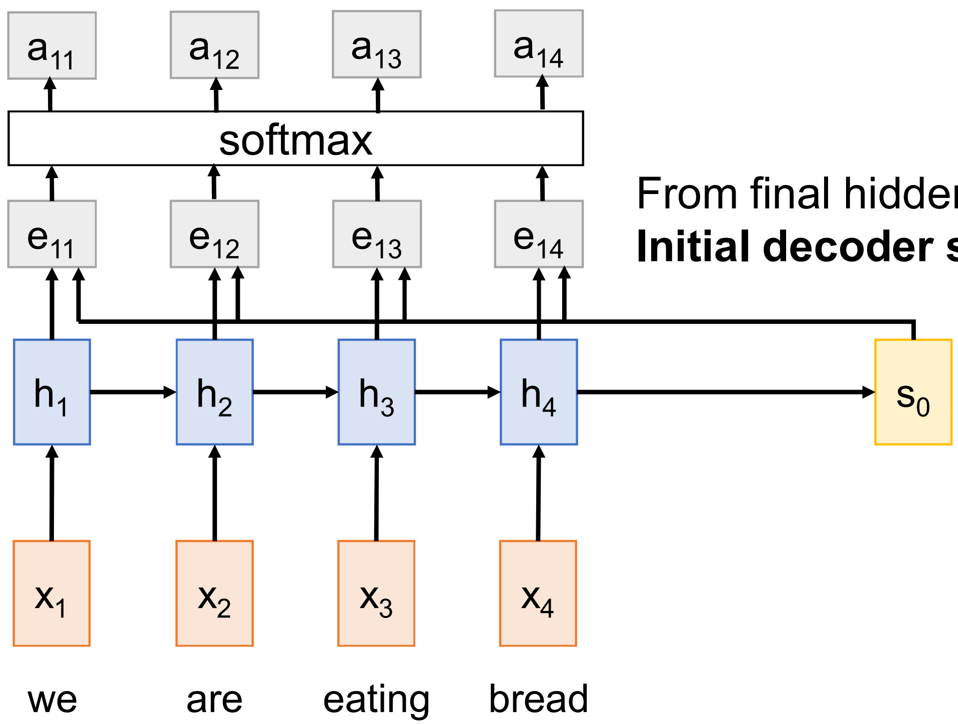
Machine Translation with RNNs and Attention



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

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

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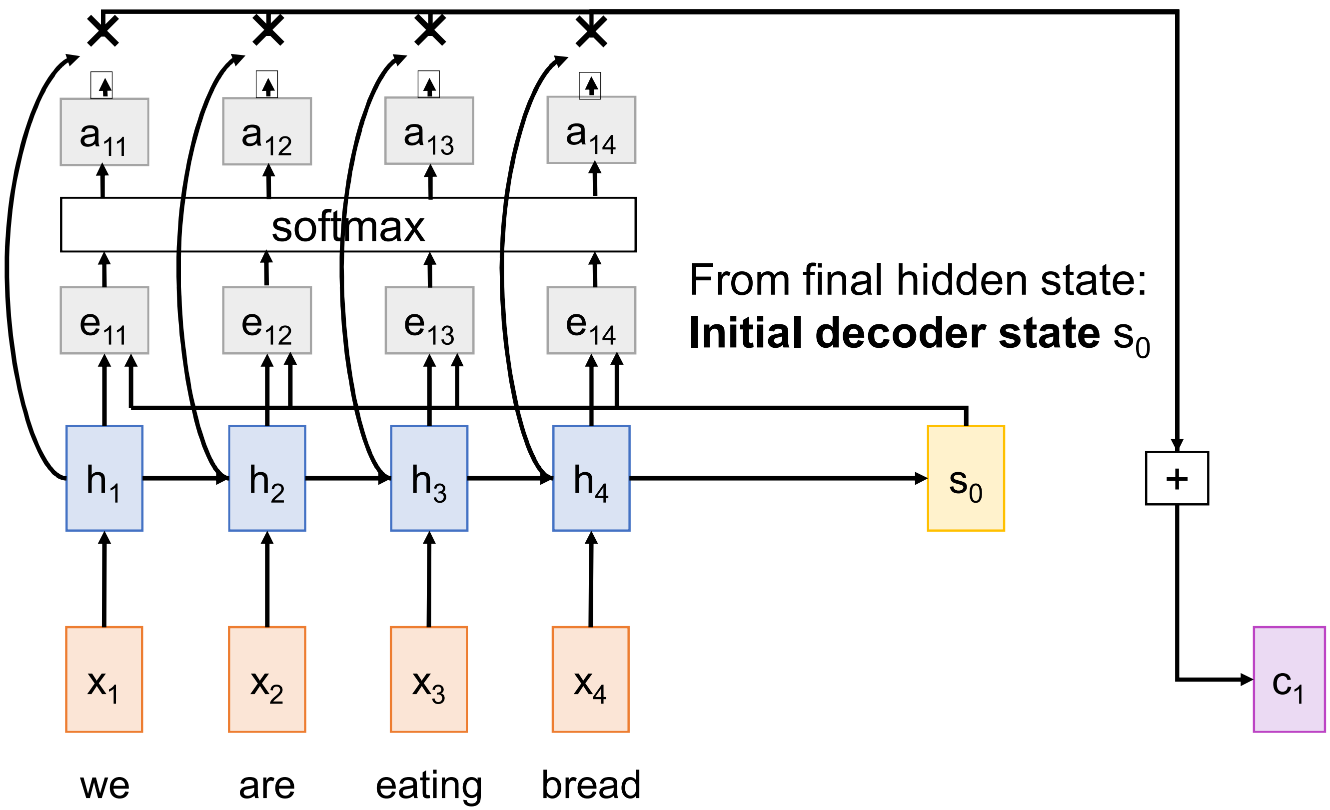
Machine Translation with RNNs and Attention



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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

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

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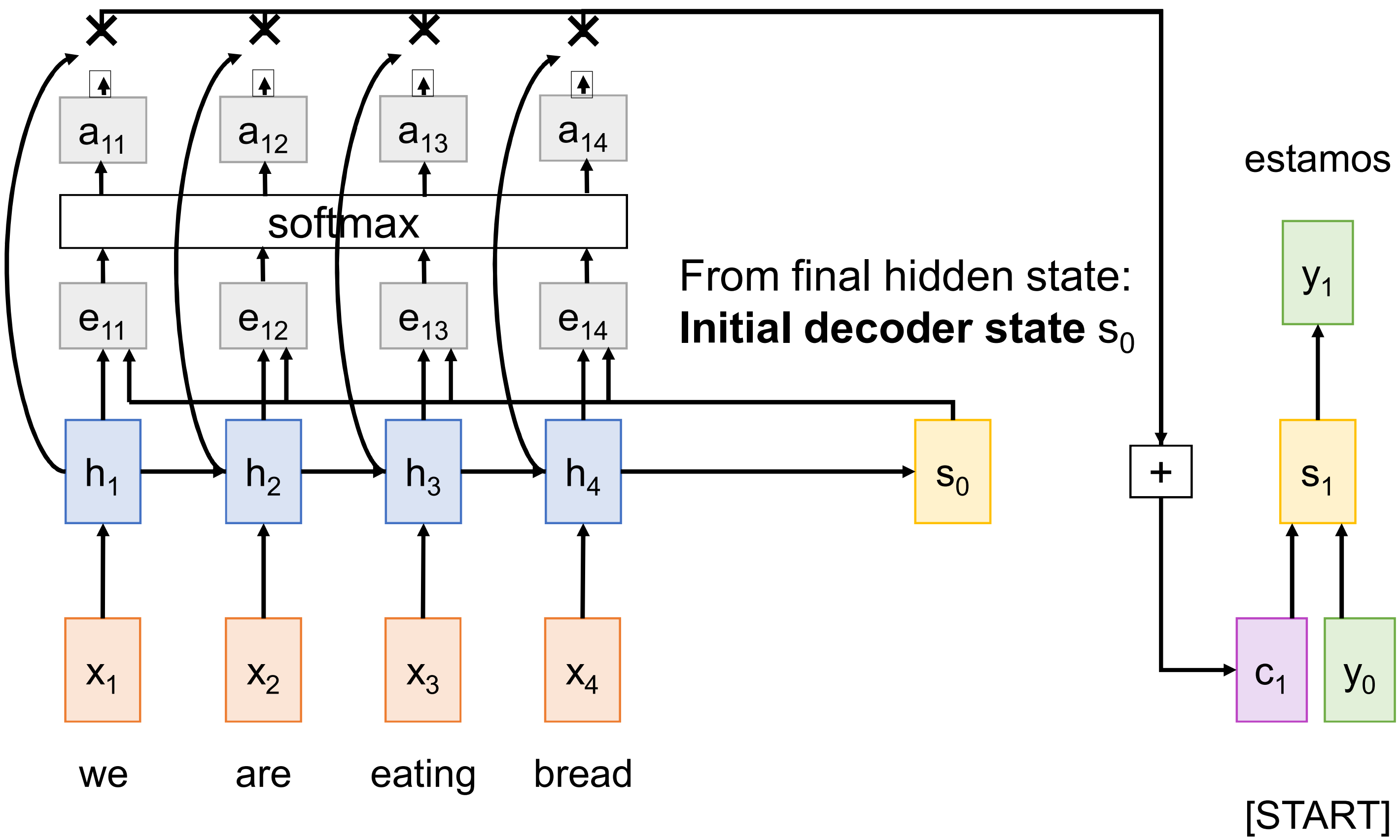
Machine Translation with RNNs and Attention



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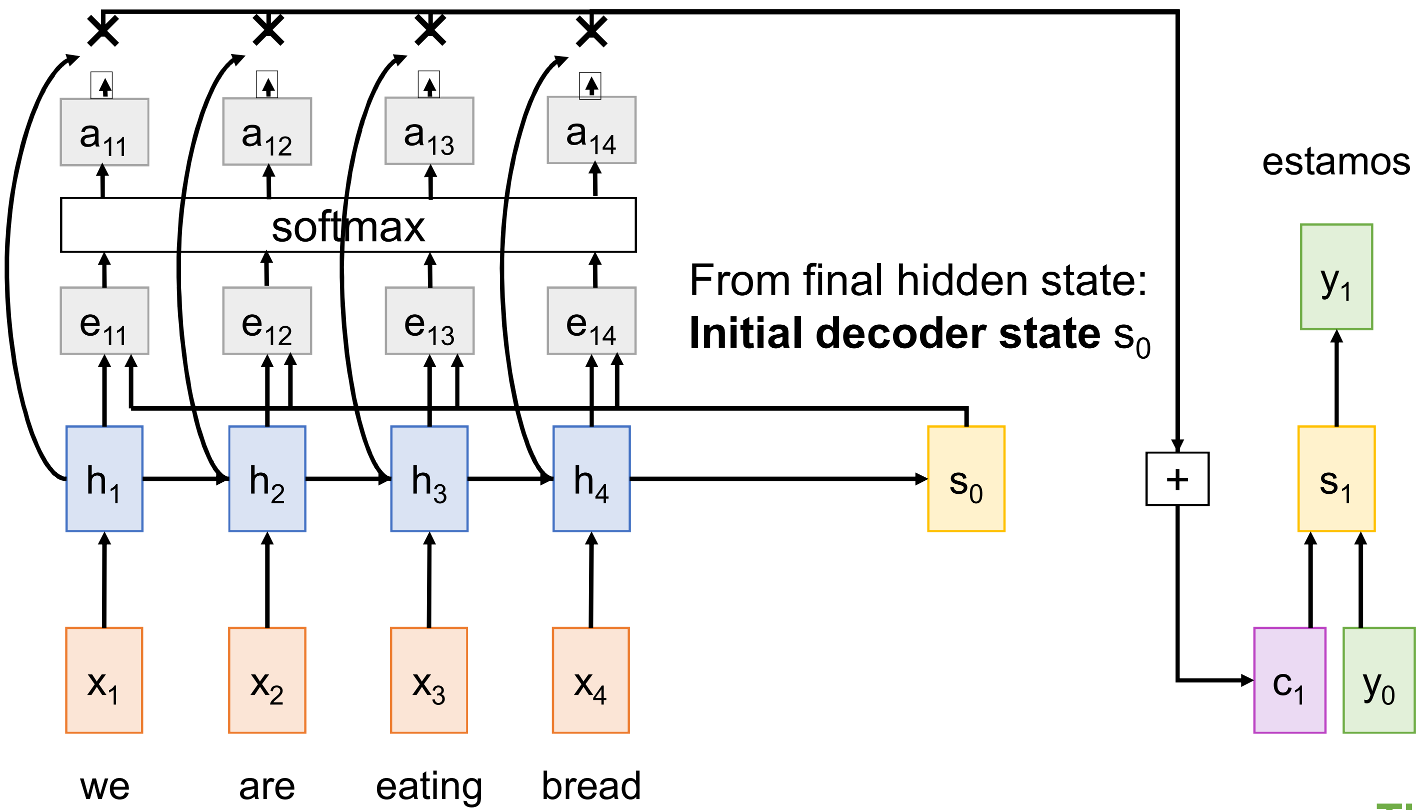
Machine Translation with RNNs and Attention



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Set context vector c to a linear combination of hidden states

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

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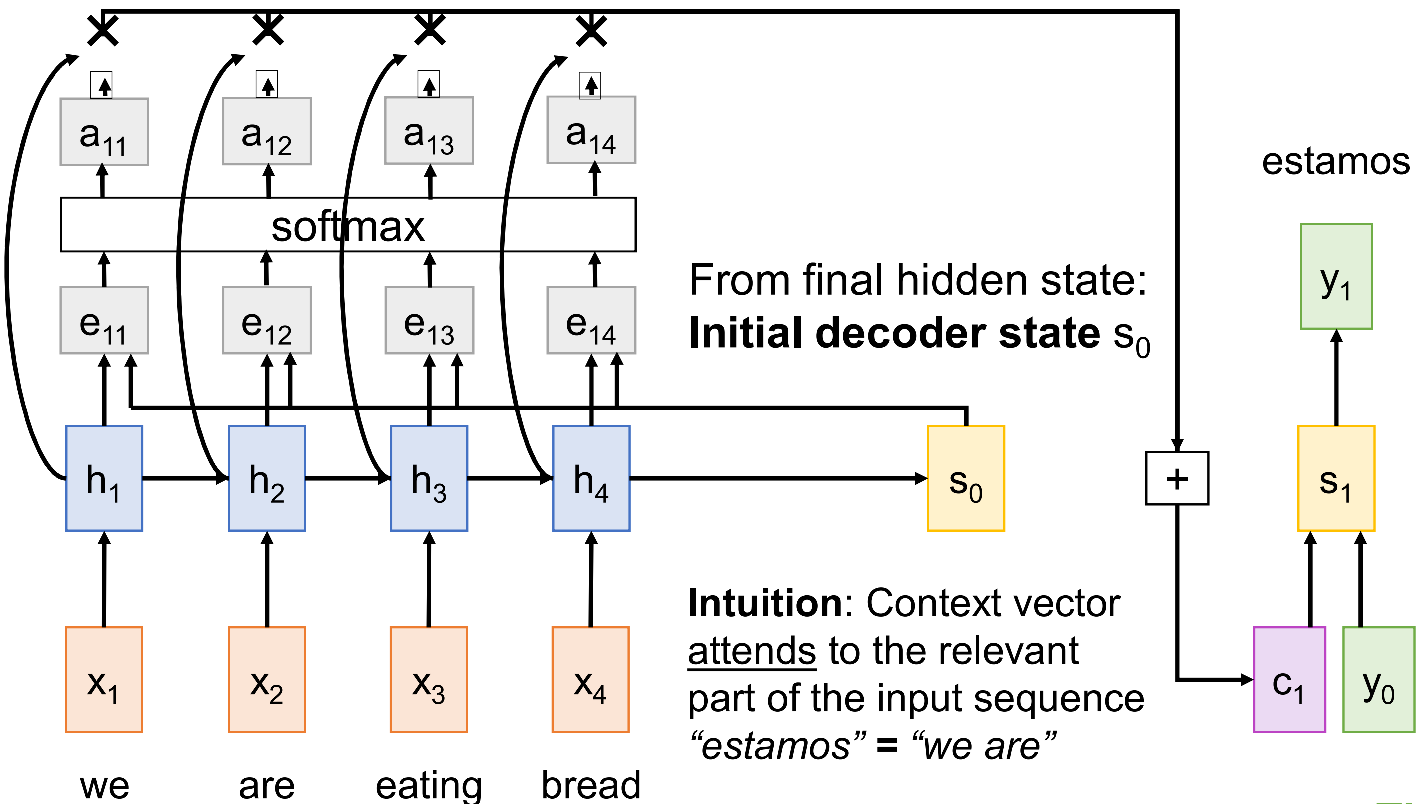
Machine Translation with RNNs and Attention



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

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

Set context vector c to a linear combination of hidden states

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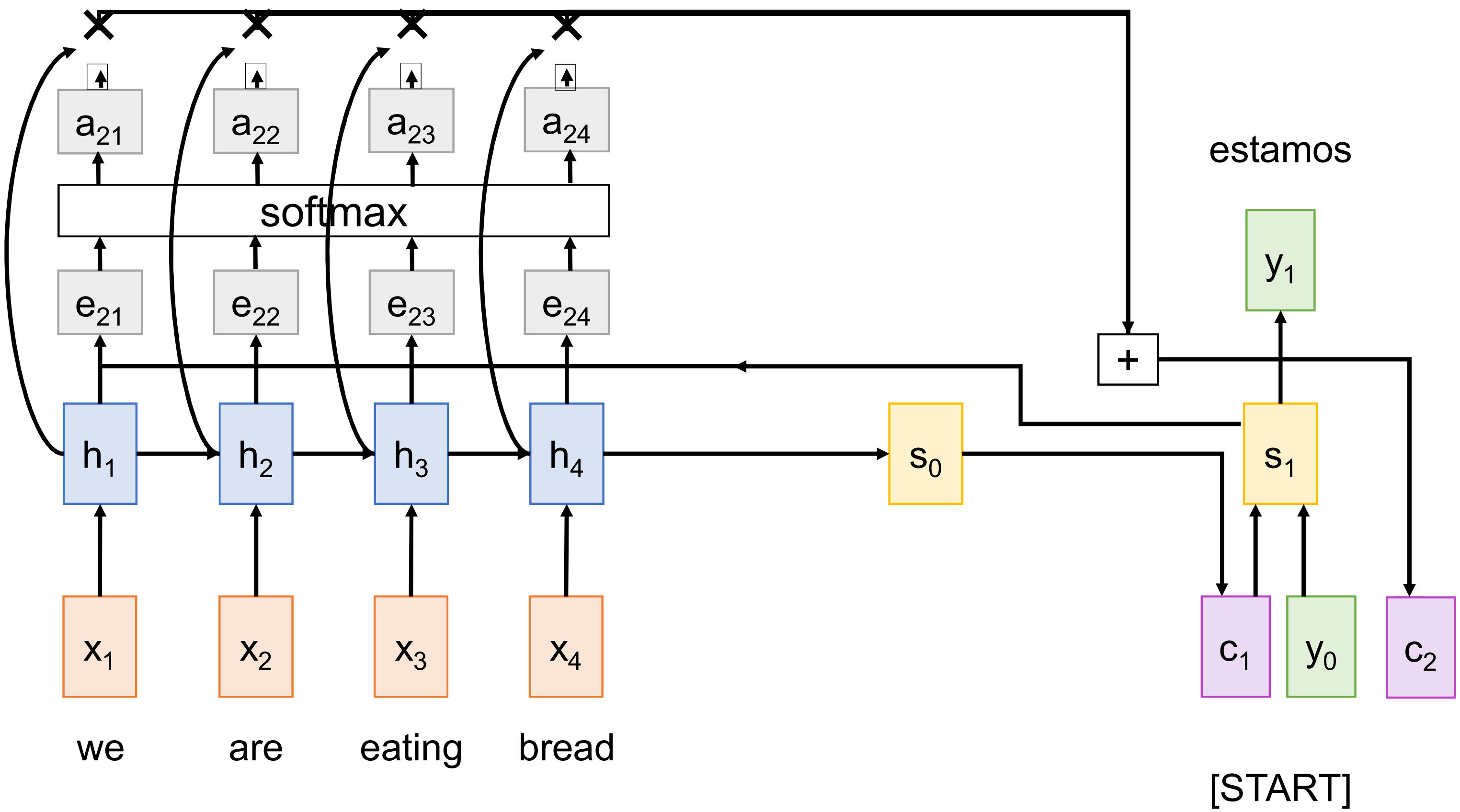
Machine Translation with RNNs and Attention



Repeat: Use s_1 to compute new context vector c_2

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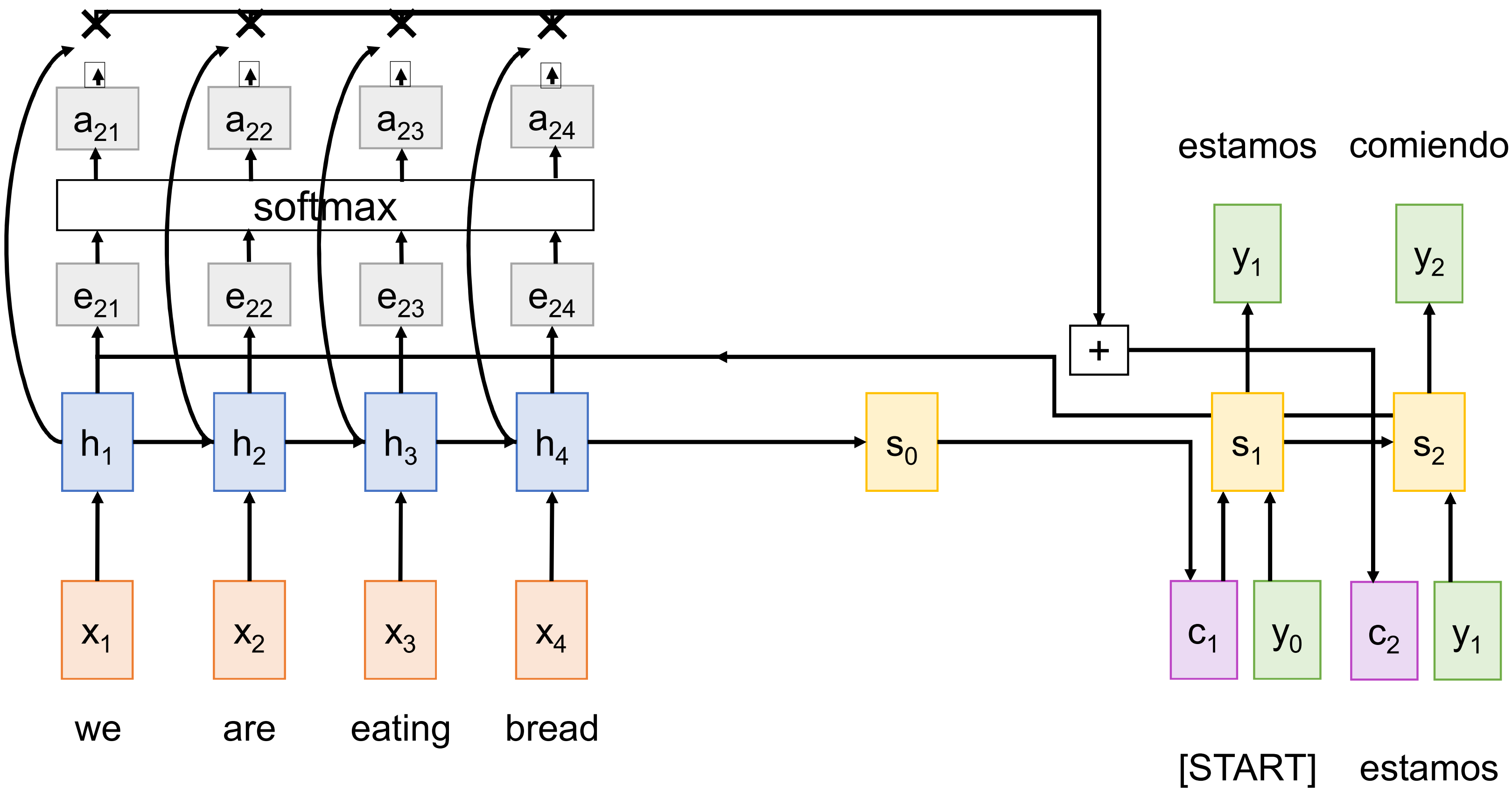
Machine Translation with RNNs and Attention



Repeat: Use s_1 to compute new context vector c_2

Use c_2 to compute s_2, y_2

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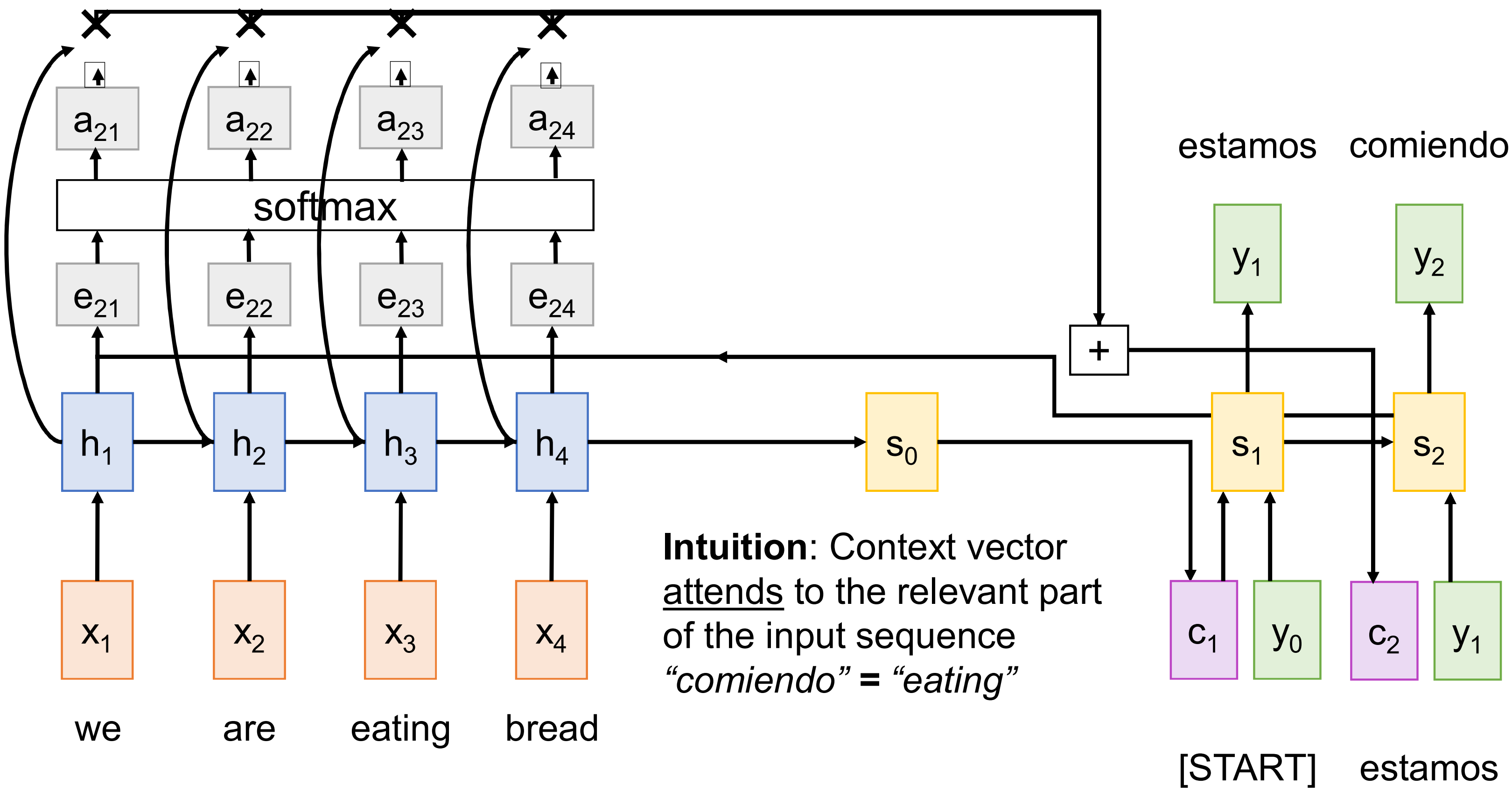
Machine Translation with RNNs and Attention



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

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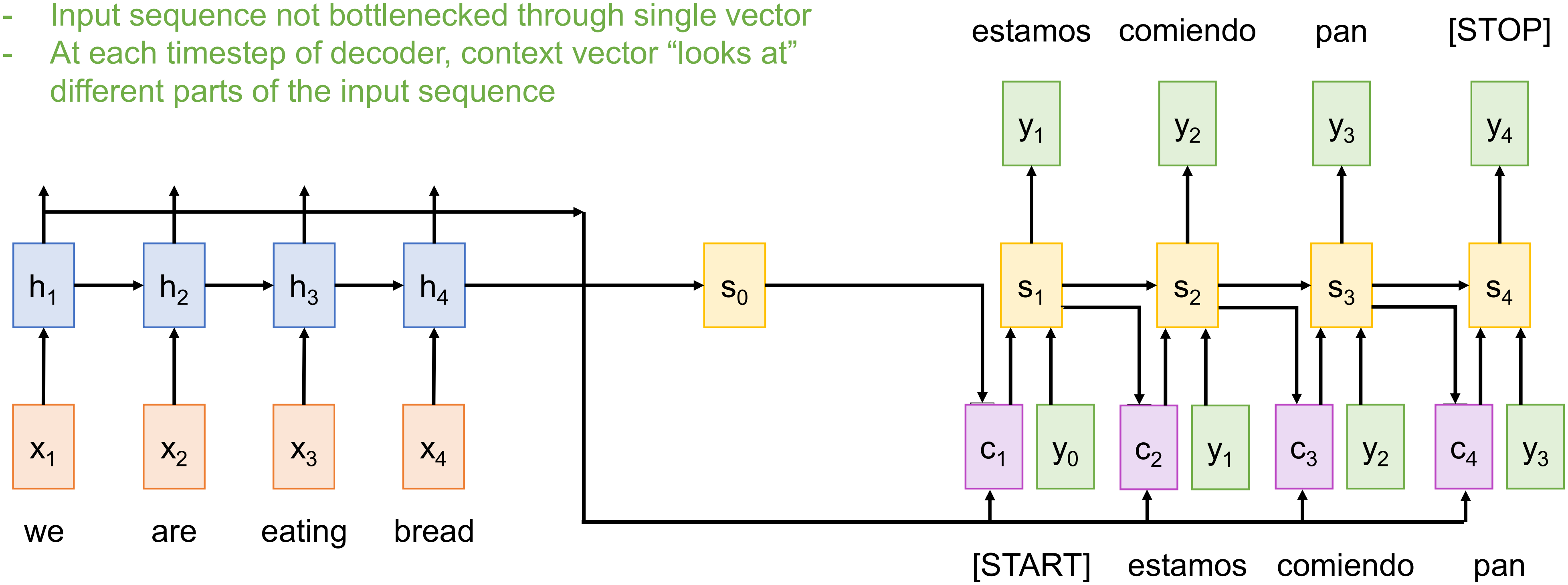
Machine Translation with RNNs and Attention

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



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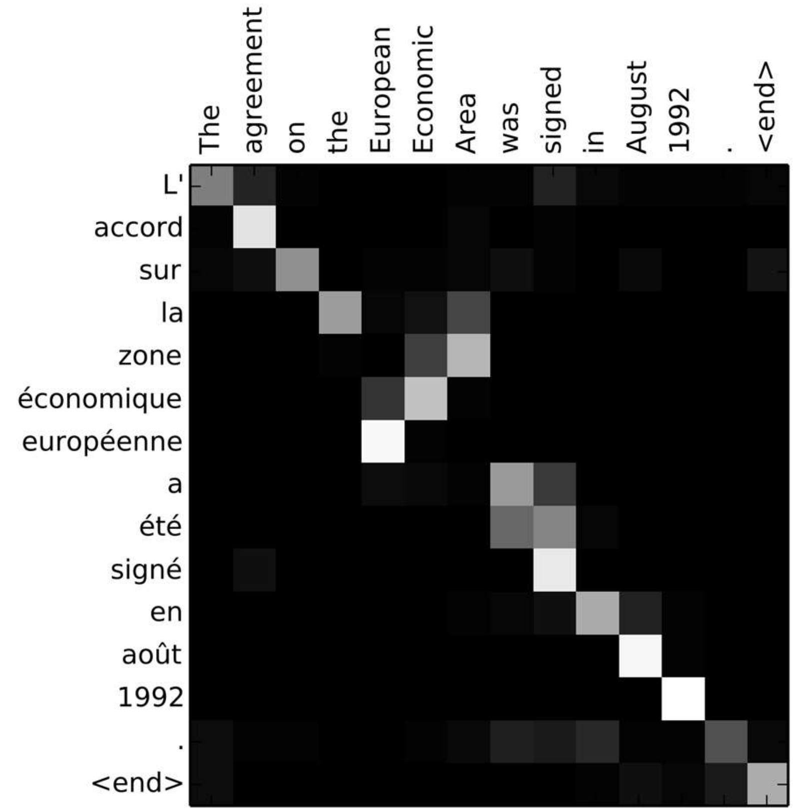
Machine Translation with RNNs and Attention

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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Machine Translation with RNNs and Attention

Example: English to French translation

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Diagonal attention means words correspond in order

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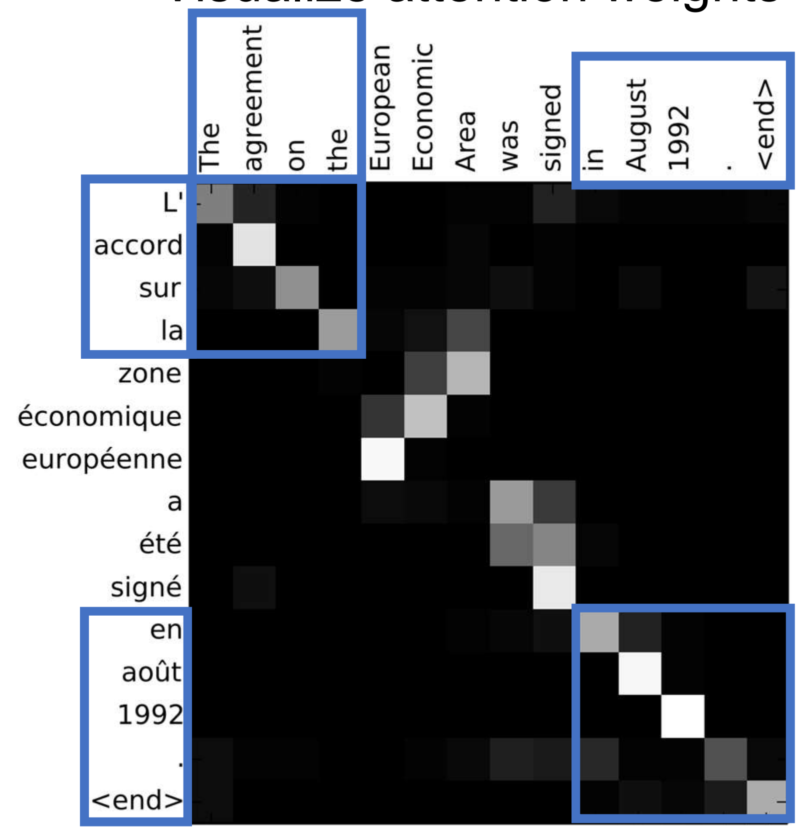

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Machine Translation with RNNs and Attention

Example: English to French translation

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

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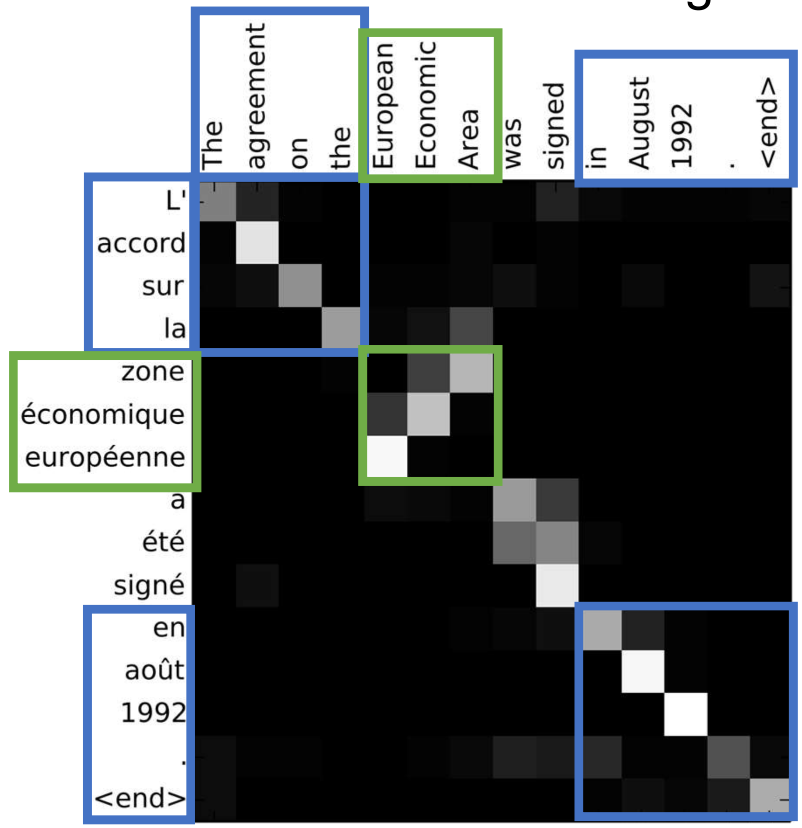
Diagonal attention means words correspond in order

Attention figures out different word orders

Diagonal attention means words correspond in order

Visualize attention weights $a_{t,i}$



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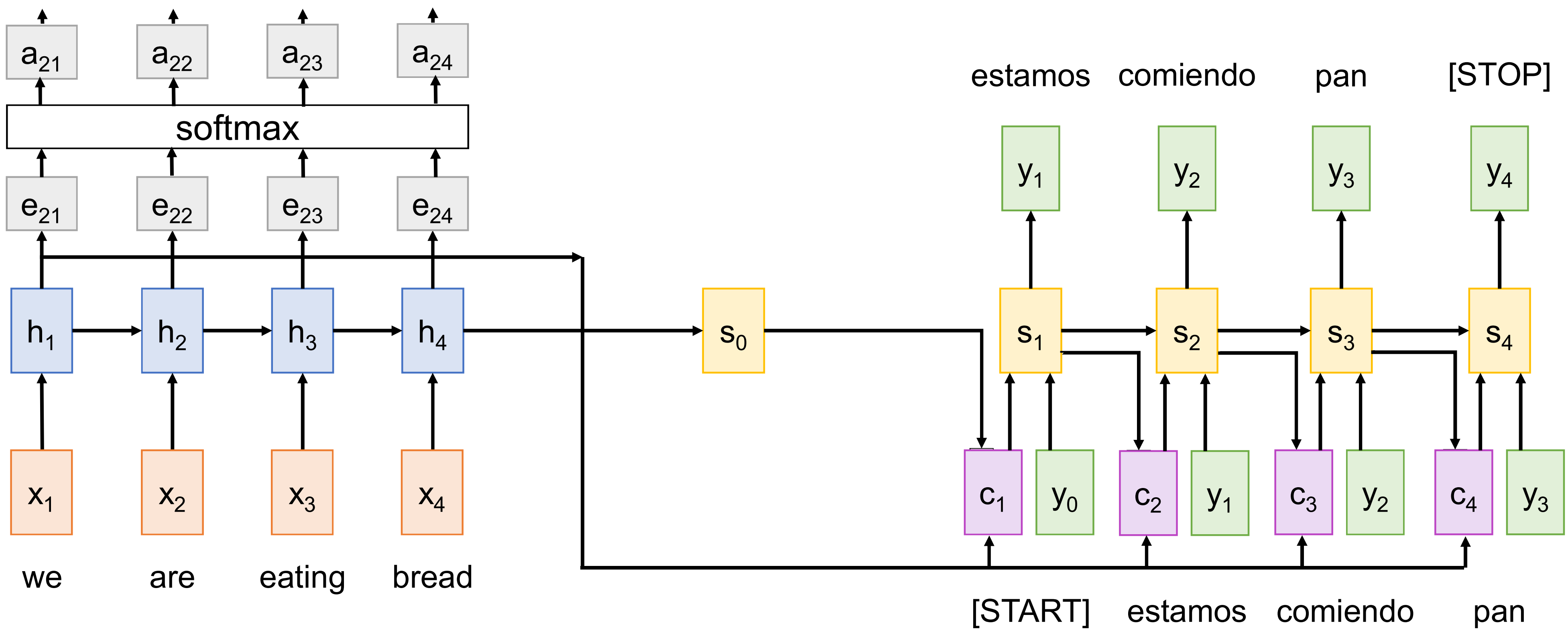
Machine Translation with RNNs and Attention



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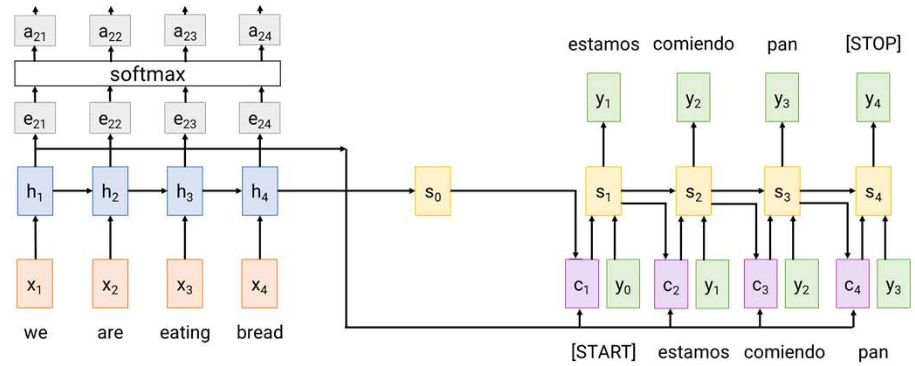
Attention Layer

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

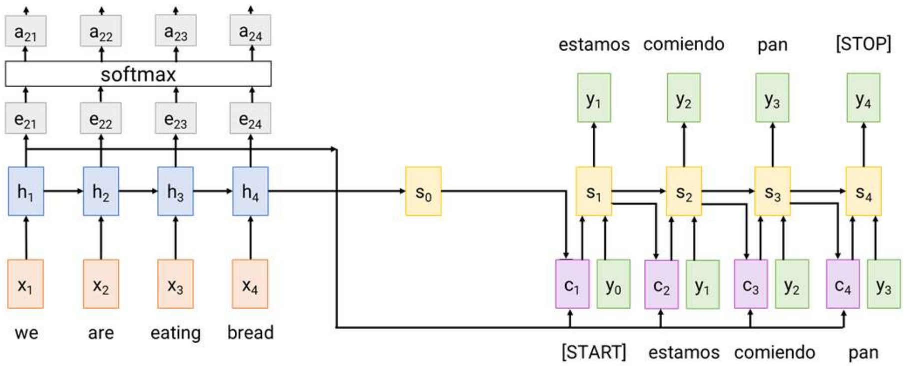


Computation:
Similarities: e (Shape: N_X) $e_i = f_{att}(\mathbf{s_{t-1}}, \mathbf{h_i})$
Attention weights: a = softmax(e) (Shape: N_X)
Output vector: $y = \sum_i a_i \mathbf{h_i}$ (Shape: D_X)

Slide credit: Justin Johnson

Attention Layer

Inputs:
Query vector: $\mathbf{q}$ (Shape: D_Q)
Input vectors: $\mathbf{X}$ (Shape: $N_X \times D_X$)
Similarity function: f_{att}

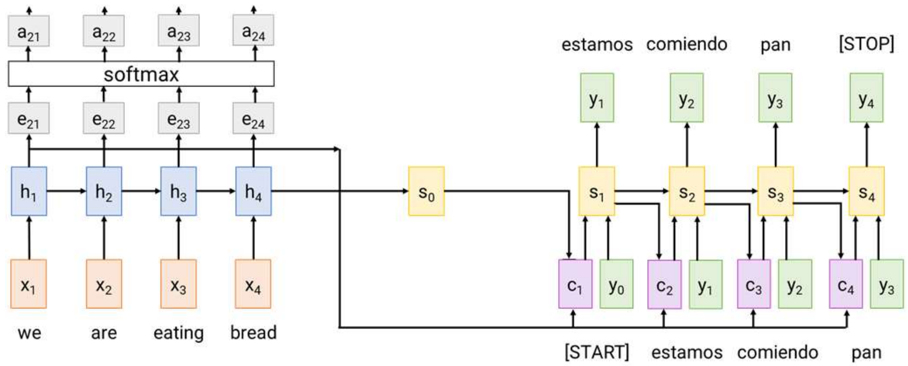


Computation:
Similarities: e (Shape: N_X) $e_i = f_{att}(\mathbf{q}, \mathbf{X_i})$
Attention weights: a = softmax(e) (Shape: N_X)
Output vector: $y = \sum_i a_i \mathbf{X_i}$ (Shape: D_X)

Slide credit: Justin Johnson

Attention Layer

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



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

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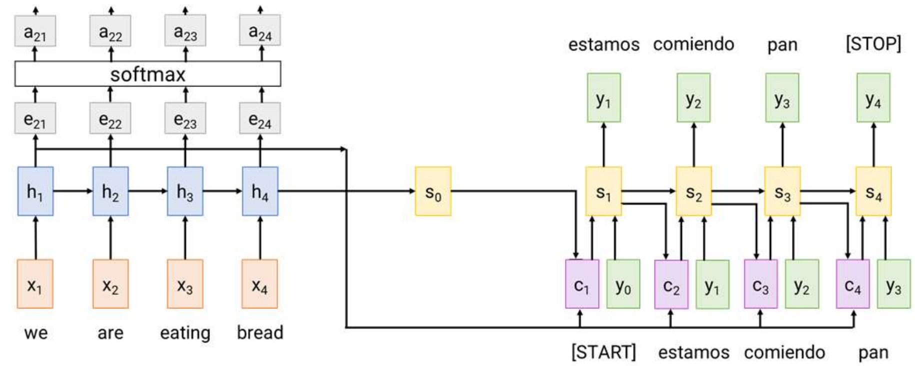
Attention Layer

Inputs:
Query vector: $\mathbf{q}$ (Shape: D_Q)
Input vectors: $\mathbf{X}$ (Shape: $N_X \times D_Q$)
Similarity function: scaled dot product



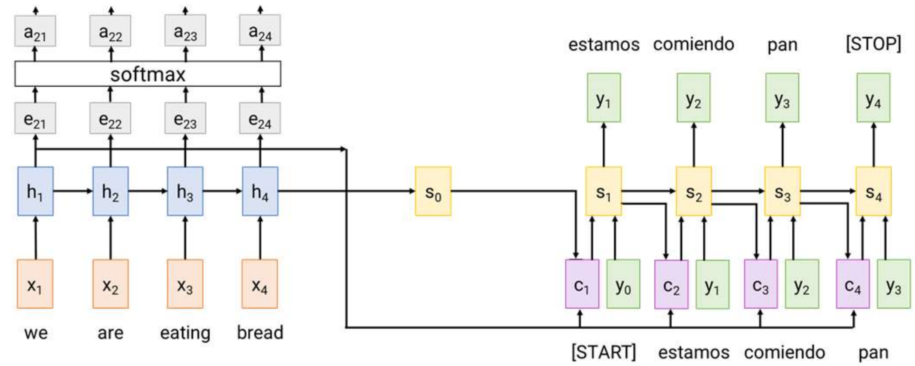
Computation:
Similarities: e (Shape: N_X) $e_i = \mathbf{q} \cdot \mathbf{X_i} / \text{sqrt}(D_Q)$
Attention weights: $a = \text{softmax}(e)$ (Shape: N_X)
Output vector: $y = \sum_i a_i \mathbf{X_i}$ (Shape: D_X)

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)



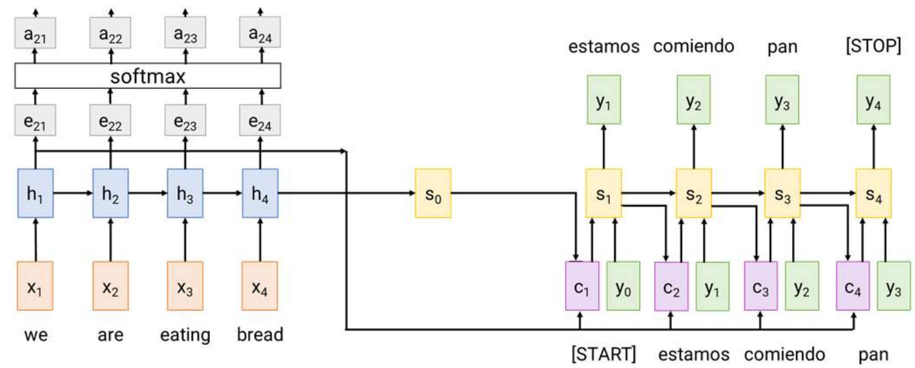
Computation:
Similarities: $E = QX^T$ (Shape: N_Q x N_X) $E_{i,j} = Q_i \cdot X_j / \text{sqrt}(D_Q)$
Attention weights: A = softmax(E, dim=1) (Shape: N_Q x N_X)
Output vectors: $Y = AX$ (Shape: N_Q x D_X) $Y_i = \sum_j A_{i,j} X_j$

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: $\mathbf{W_K}$ (Shape: D_X x D_Q)
Value matrix: $\mathbf{W_V}$ (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 = $\mathbf{QK}^T$ (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) $Y_i = \sum_j A_{i,j} \mathbf{V_j}$

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

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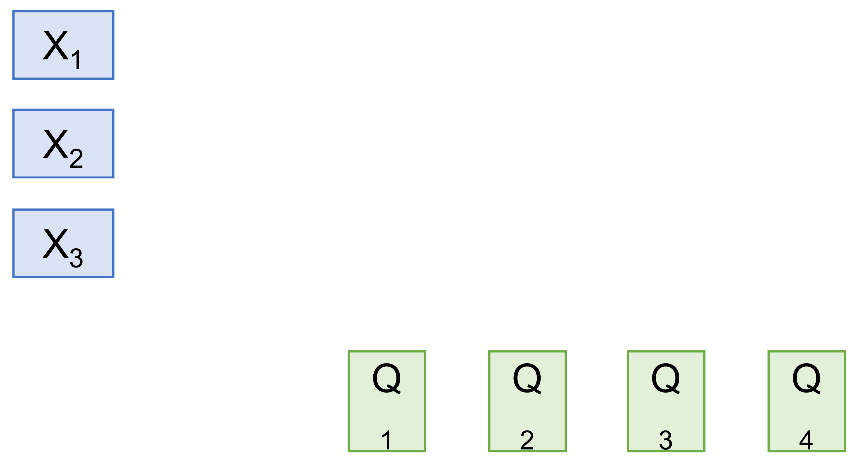
Attention Layer

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

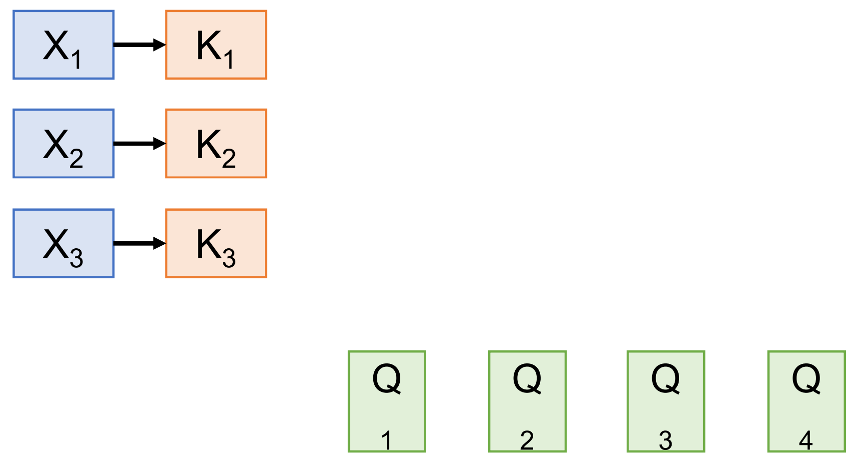


Slide credit: Justin Johnson

Attention Layer

Inputs:
Query vectors: $\mathbf{Q}$ (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: $N_Q \times D_V$) $Y_i = \sum_j A_{i,j}\mathbf{V_j}$

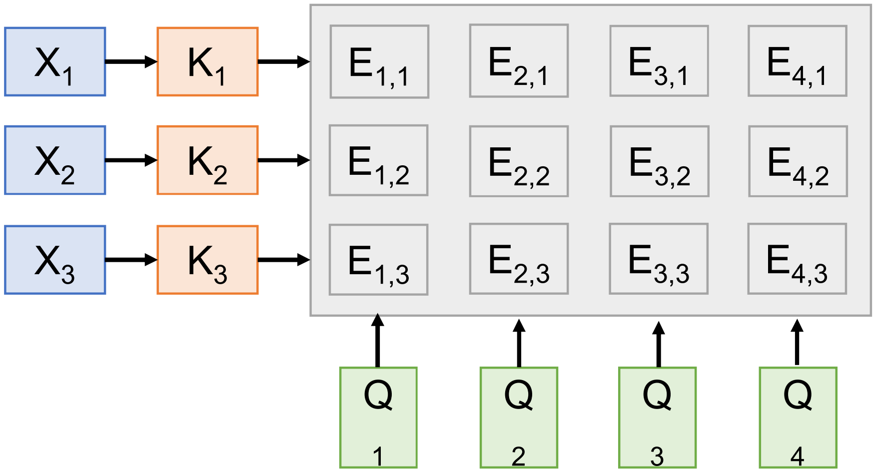


Slide credit: Justin Johnson

Attention Layer

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

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

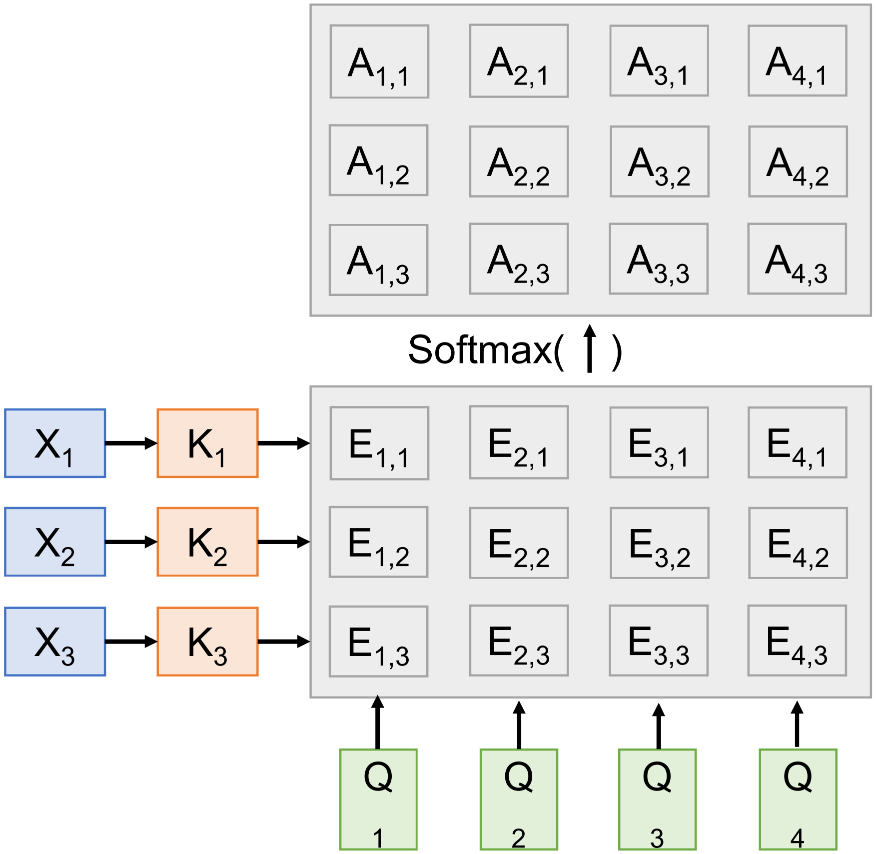


Slide credit: Justin Johnson

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

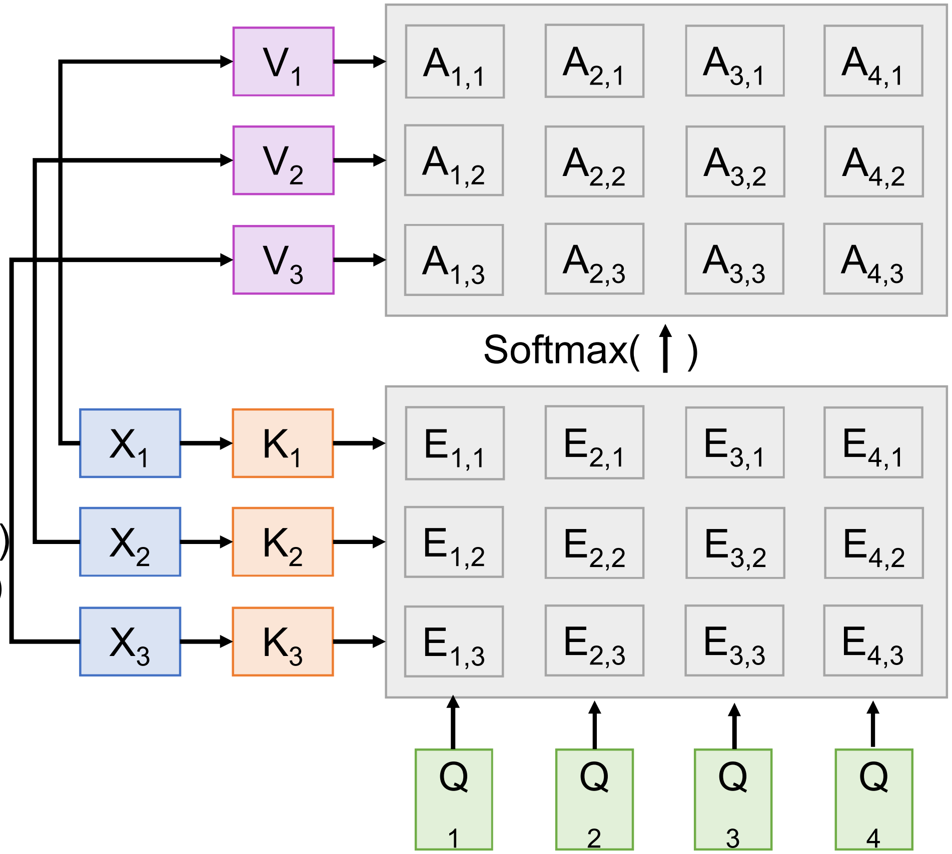


Slide credit: Justin Johnson

Attention Layer

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

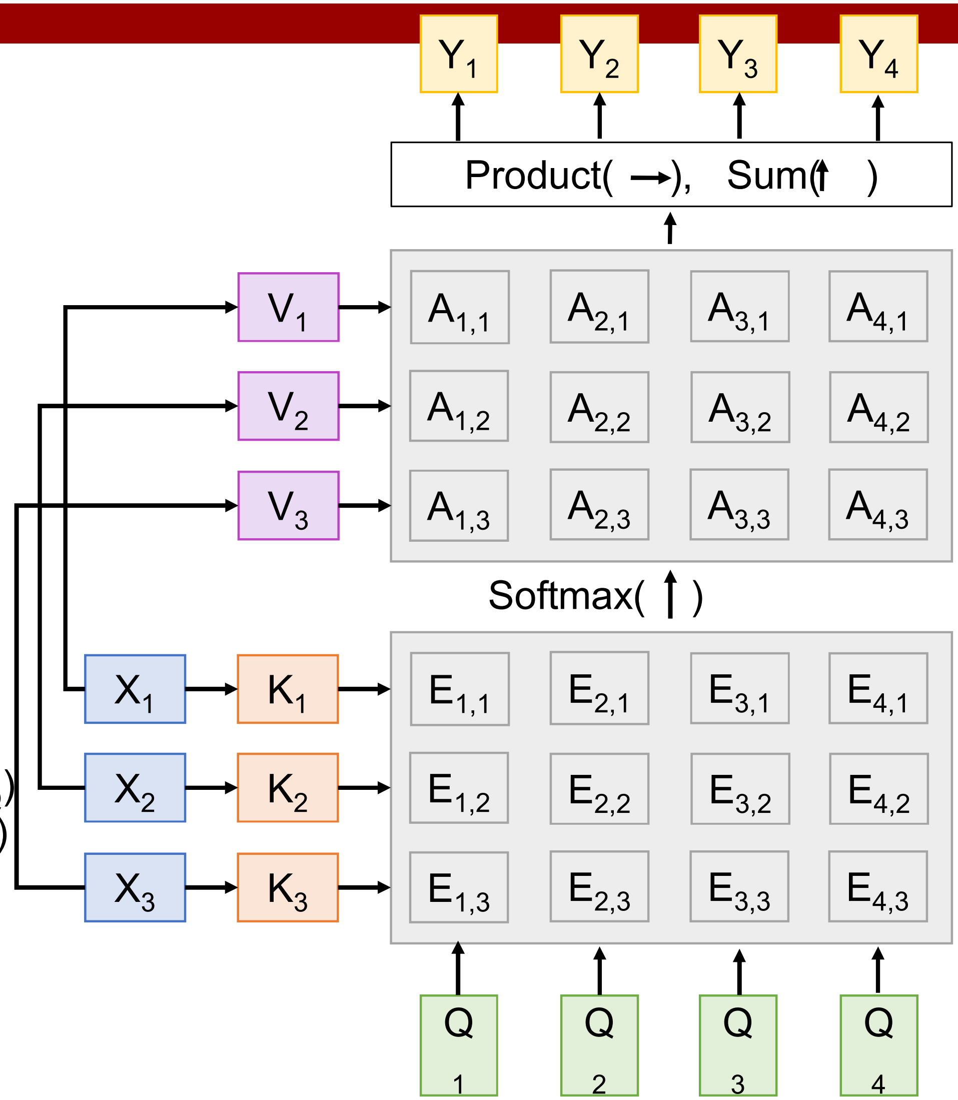


Slide credit: Justin Johnson

Attention Layer

Inputs:
Query vectors: $\mathbf{Q}$ (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: $A = \mathrm{softmax}(E, \mathrm{dim}=1)$ (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

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

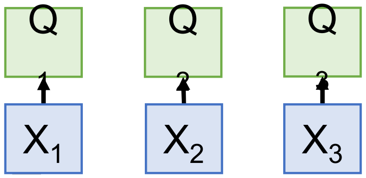
Slide credit: Justin Johnson

Self-Attention Layer

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

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

<u>**Computation**</u>:
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) $Y_i = \sum_j A_{i,j} \mathbf{V_j}$



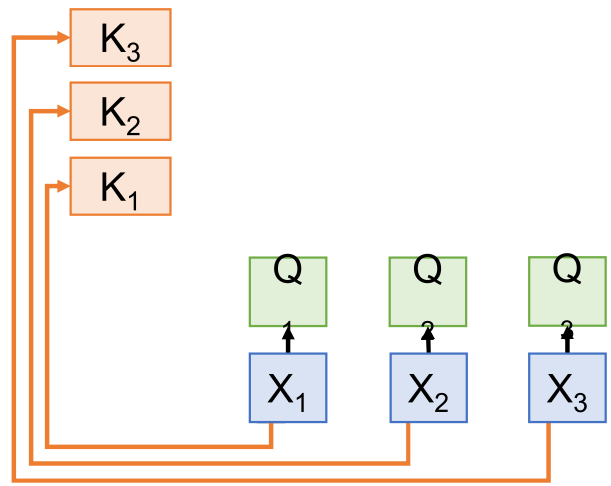
Slide credit: Justin Johnson

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



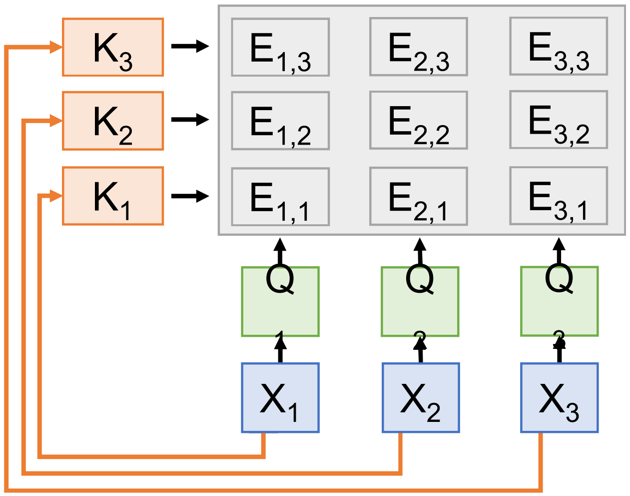
Slide credit: Justin Johnson

Self-Attention Layer

One query per input vector

Inputs:
Input vectors: X (Shape: $N_X \times D_X$)
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: $N_X \times D_V$) $Y_i = \sum_j A_{i,j} V_j$



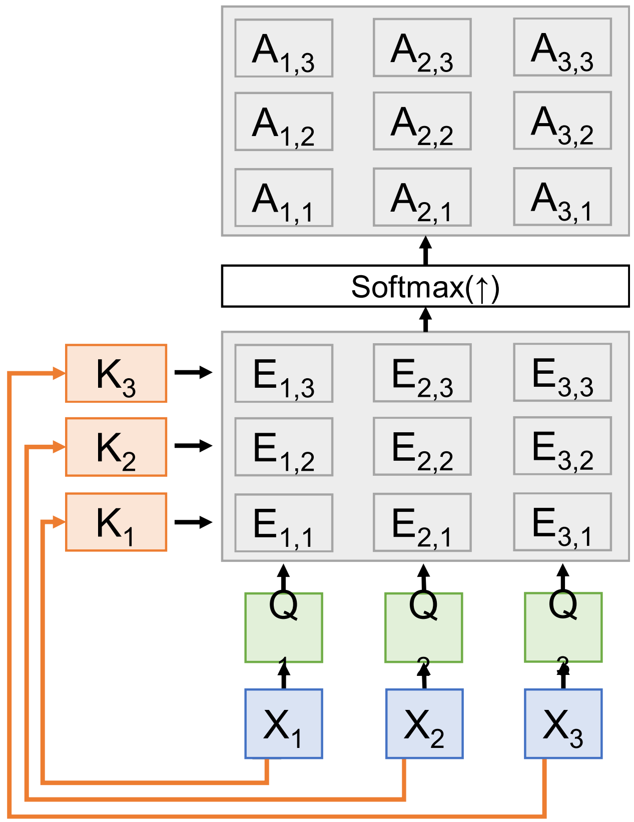
Slide credit: Justin Johnson

Self-Attention Layer

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



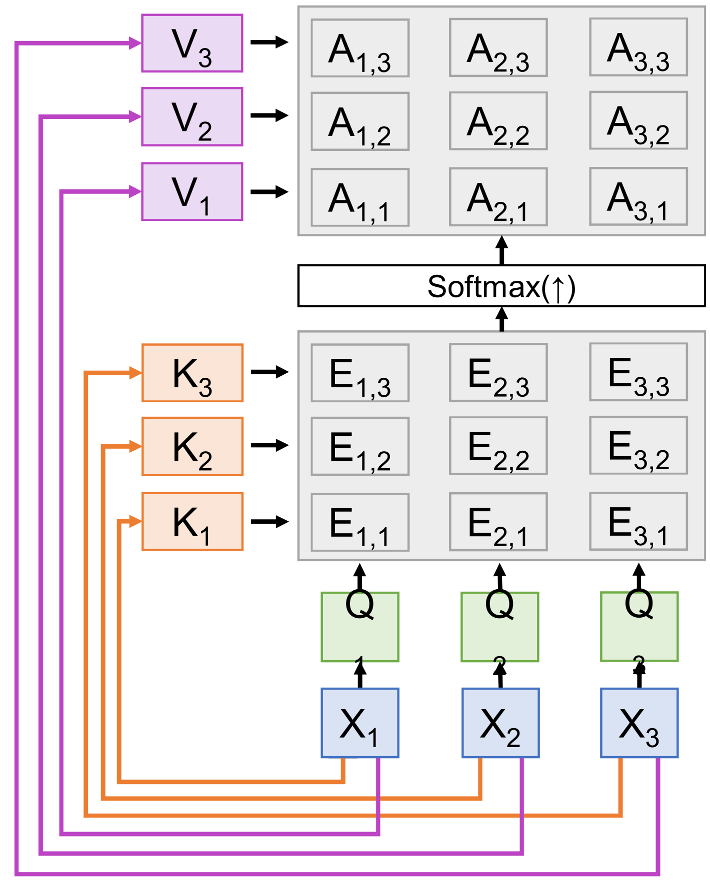
Slide credit: Justin Johnson

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



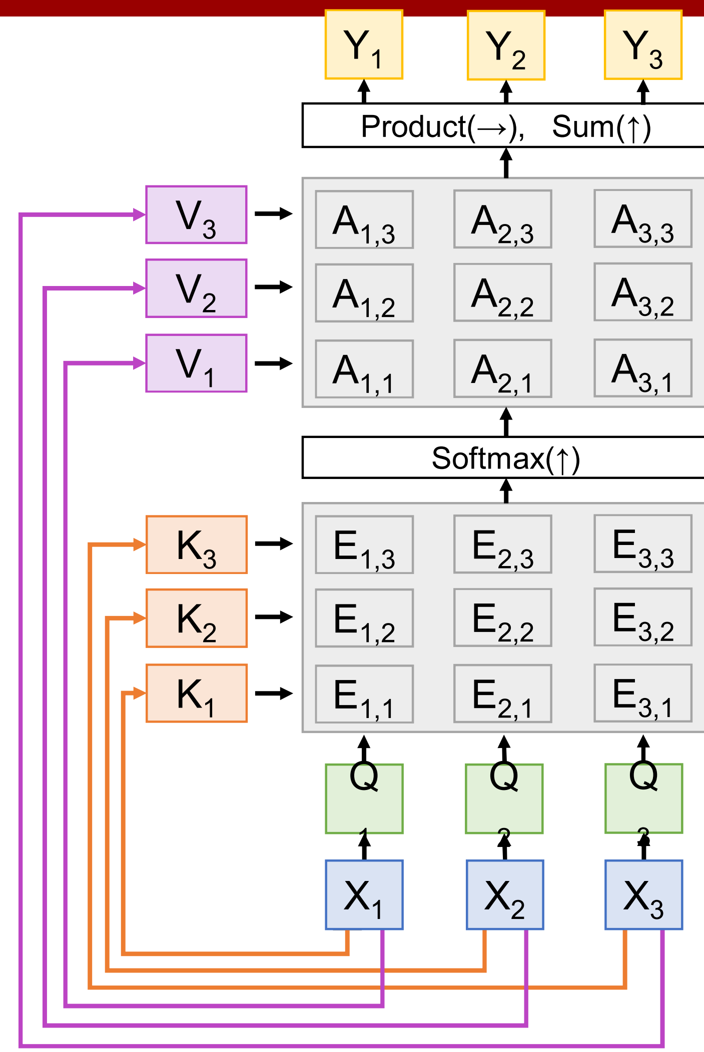
Slide credit: Justin Johnson

Self-Attention Layer

One query per input vector

Inputs:
Input vectors: X (Shape: $N_X \times D_X$)
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: $N_X \times D_V$) $Y_i = \sum_j A_{i,j} V_j$



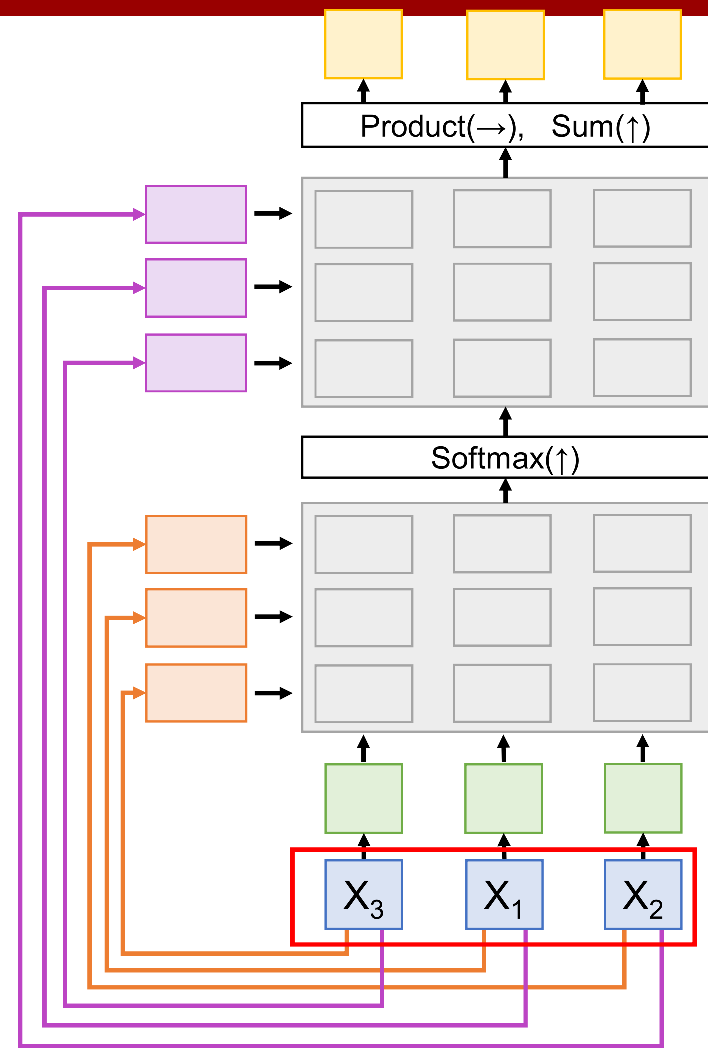
Slide credit: Justin Johnson

Self-Attention Layer

Inputs:
Input vectors: **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:

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

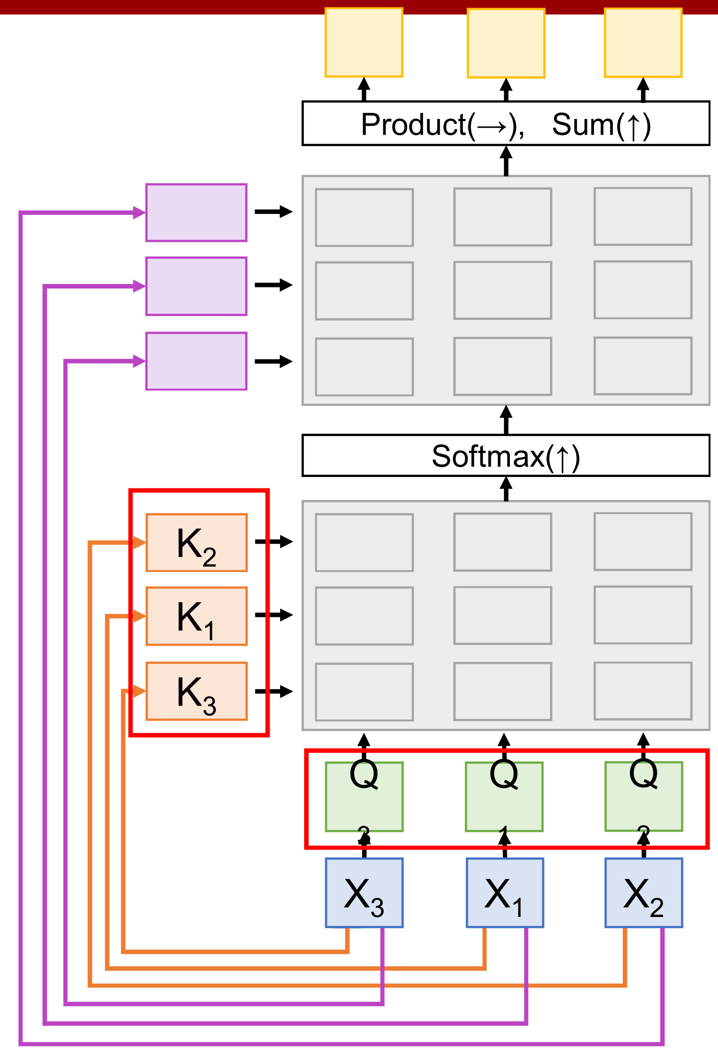
Self-Attention Layer

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



Slide credit: Justin Johnson

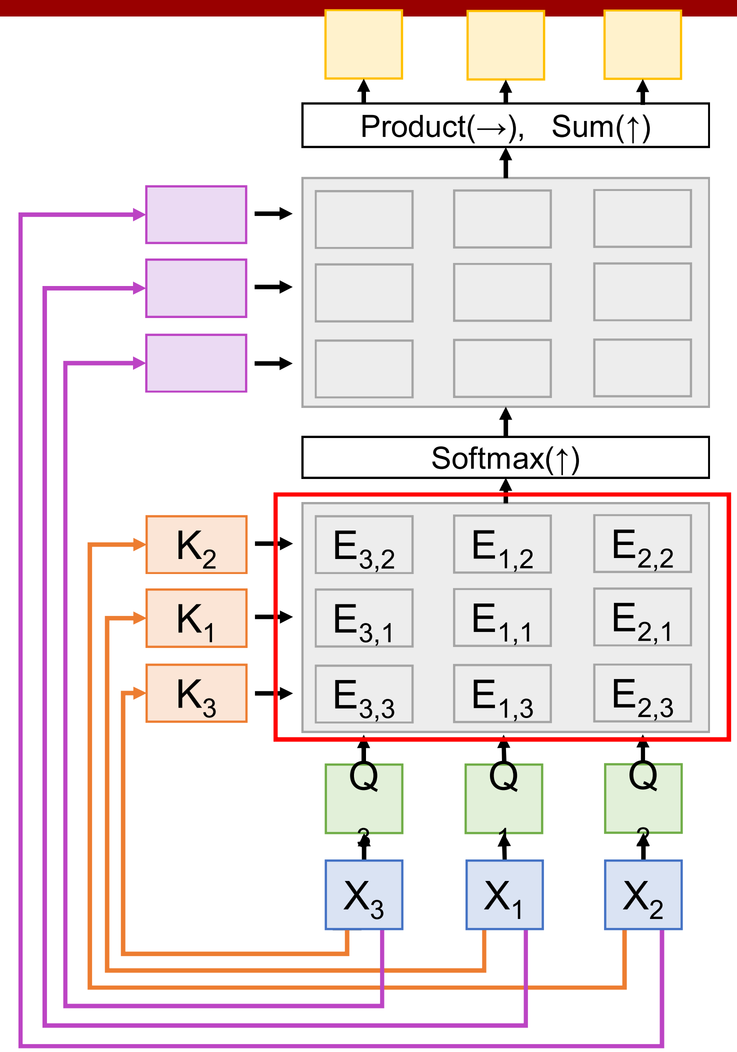
Self-Attention Layer

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)

Consider **permuting** the input vectors:

Similarities will be the same, but permuted

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



Slide credit: Justin Johnson

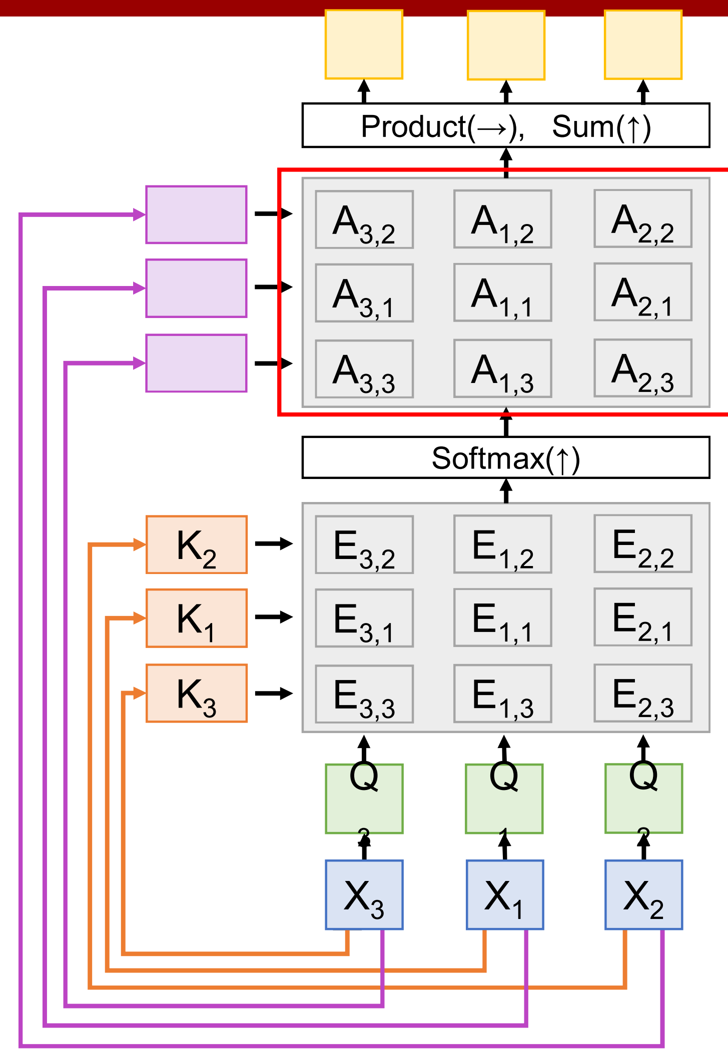
Self-Attention Layer

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:

Attention weights will be the same, but permuted



Slide credit: Justin Johnson

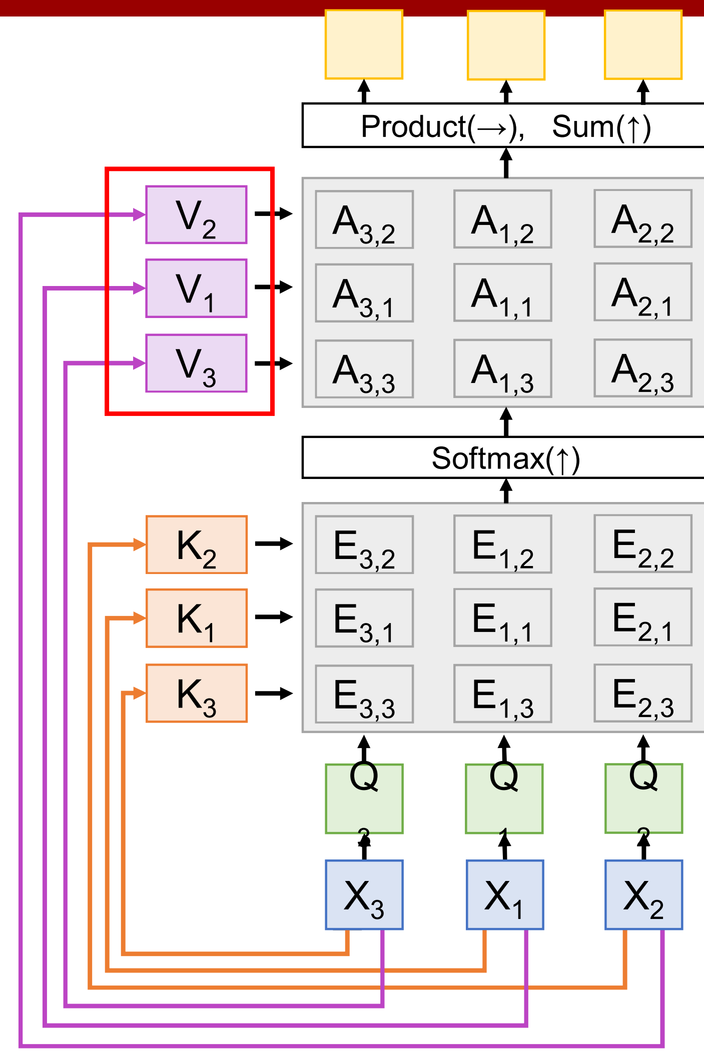
Self-Attention Layer

Inputs:
Input vectors: **X** (Shape: N_X x D_X)
Key matrix: $\mathbf{W_K}$ (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:

Values will be the same, but permuted



Slide credit: Justin Johnson

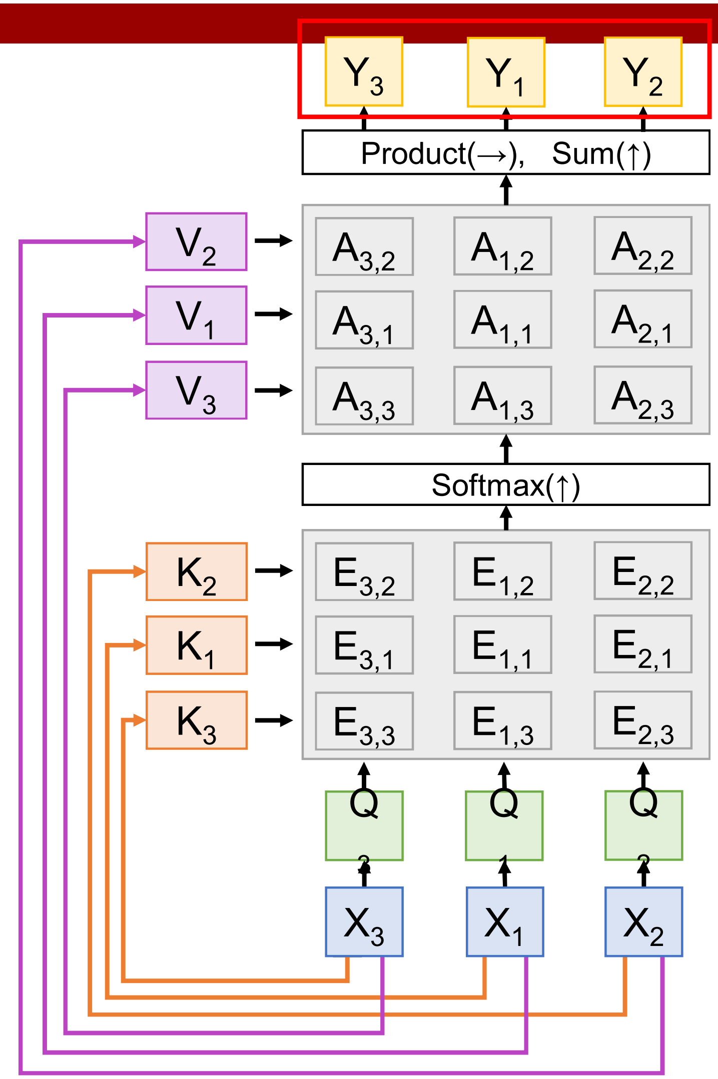
Self-Attention Layer

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:

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

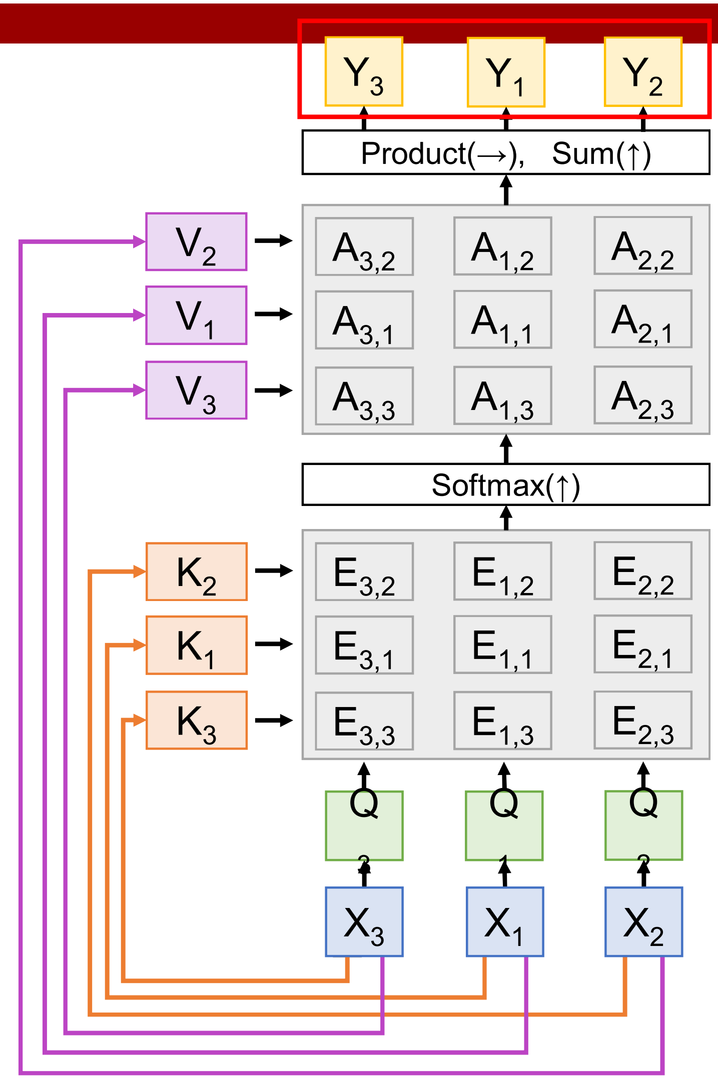
Inputs:
Input vectors: $\mathbf{X}$ (Shape: N_X x D_X)
Key matrix: $\mathbf{W_K}$ (Shape: D_X x D_Q)
Value matrix: $\mathbf{W_V}$ (Shape: D_X x D_V)
Query matrix: $\mathbf{W_Q}$ (Shape: D_X x D_Q)

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

Consider **permuting** the input vectors:

Outputs will be the same, but permuted

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



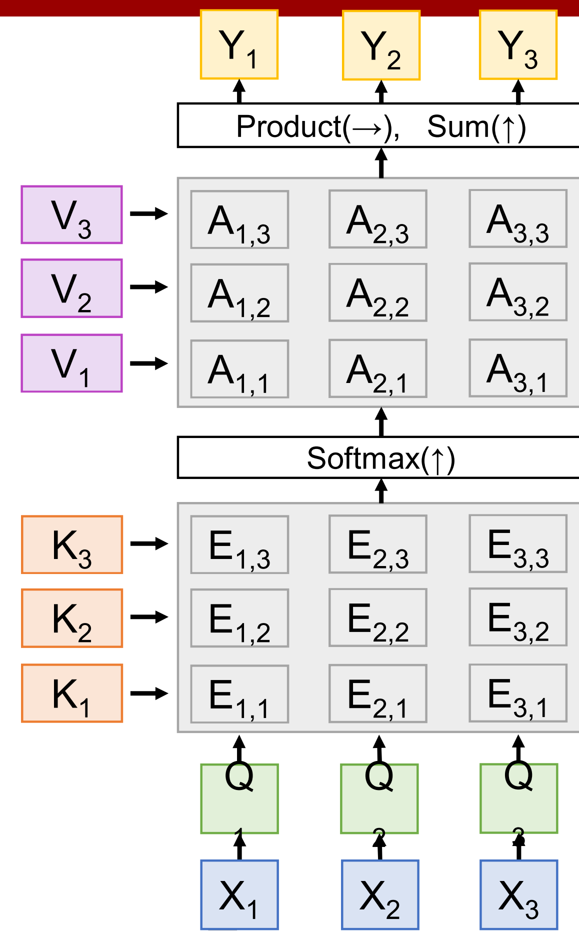
Slide credit: Justin Johnson

Self-Attention Layer

<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)

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

<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: $A = \mathrm{softmax}(E, \mathrm{dim}=1)$ (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

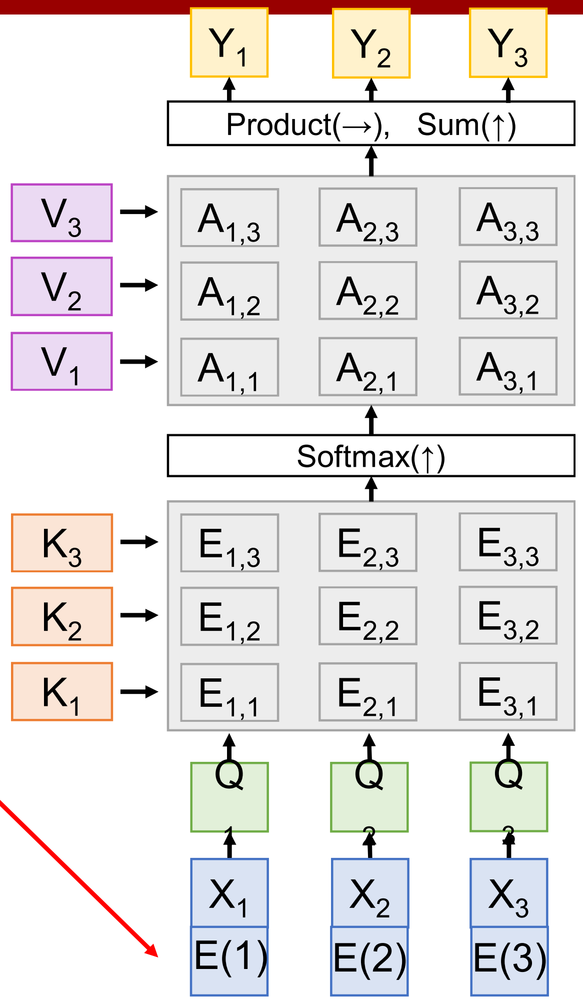
Inputs:
Input vectors: **X** (Shape: $N_X \times D_X$)
Key matrix: $\mathbf{W_K}$ (Shape: $D_X \times D_Q$)
Value matrix: $\mathbf{W_V}$ (Shape: $D_X \times D_V$)
Query matrix: $\mathbf{W_Q}$ (Shape: $D_X \times D_Q$)

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: $N_X \times D_V$) $Y_i = \sum_j A_{i,j}\mathbf{V_j}$

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

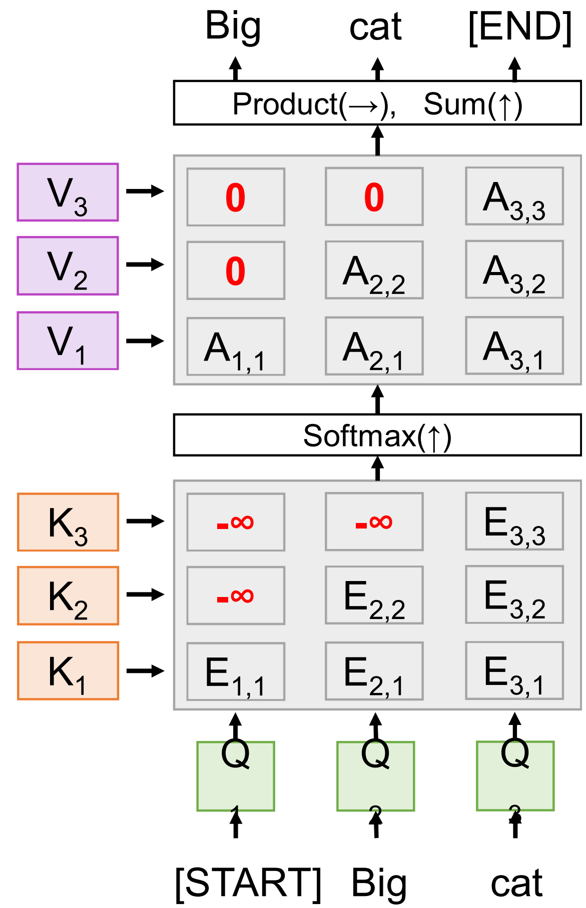
Masked Self-Attention Layer

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)

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: $A = \mathrm{softmax}(E, \mathrm{dim}=1)$ (Shape: N_X x N_X)
Output vectors: $Y = AV$ (Shape: N_X x D_V) $Y_i = \sum_j A_{i,j} V_j$

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

Used for language modeling (predict next word)



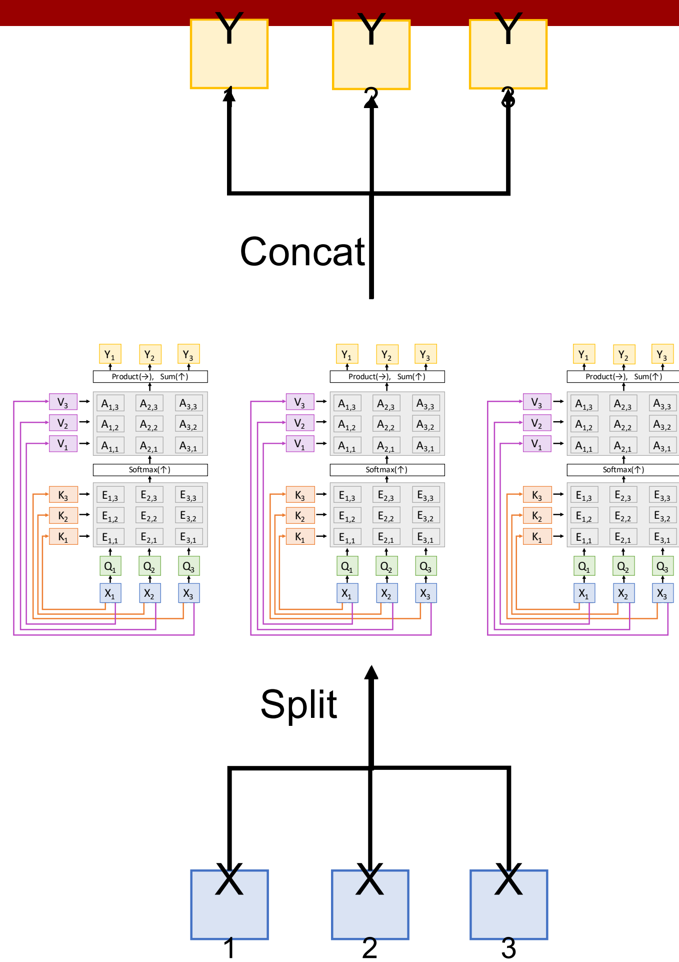
Slide credit: Justin Johnson

Multihead 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: $D_X \times D_Q$)

Use H independent "Attention Heads" in parallel

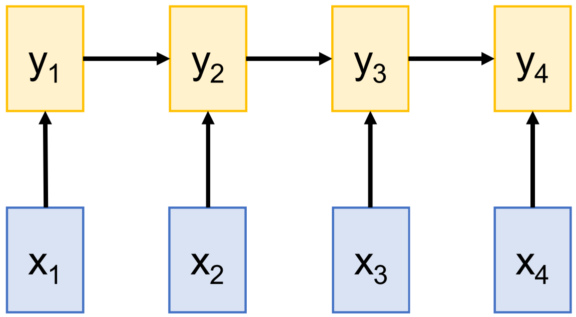
Computation:
Query vectors: $Q = XW_Q$
Key vectors: $K = XW_K$ (Shape: $N_X \times D_Q$)
Value vectors: $V = XW_V$ (Shape: $N_X \times D_V$)
Similarities: $E = QK^T$ (Shape: $N_X \times N_X$) $E_{i,j} = Q_i \cdot K_j / \mathrm{sqrt}(D_Q)$
Attention weights: $A = \mathrm{softmax}(E, \mathrm{dim}=1)$ (Shape: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



Slide credit: Justin Johnson

Three Ways of Processing Sequences

Recurrent Neural Network



Works on **Ordered Sequences**

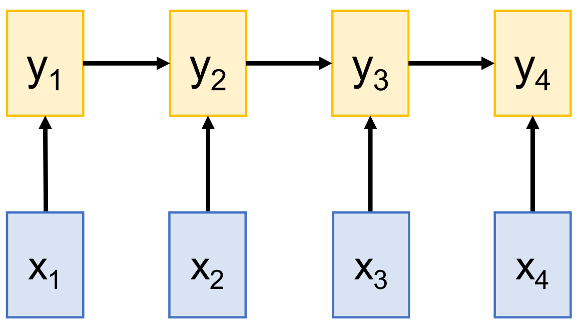
(+) Good at long sequences: After one RNN layer, h_T "sees" the whole sequence

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

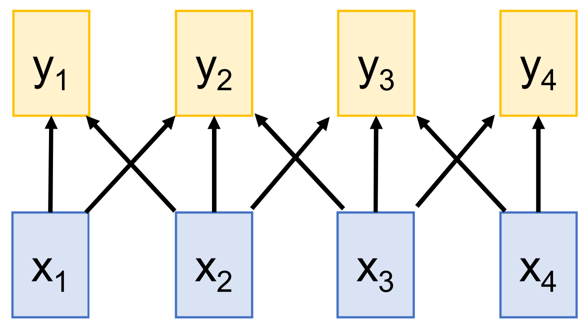
Slide credit: Justin Johnson

Three Ways of Processing Sequences

Recurrent Neural Network



1D Convolution



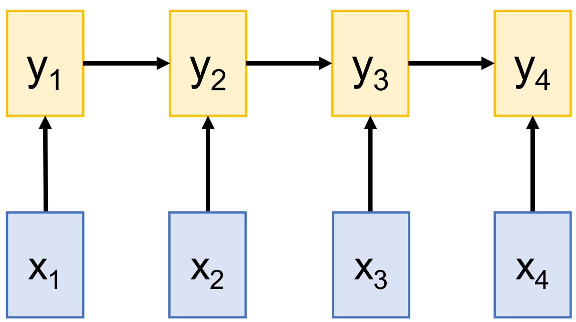
Works on **Ordered Sequences**
(+) Good at long sequences: After one RNN layer, h_T "sees" the whole sequence
(-) Not parallelizable: need to compute hidden states sequentially

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

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

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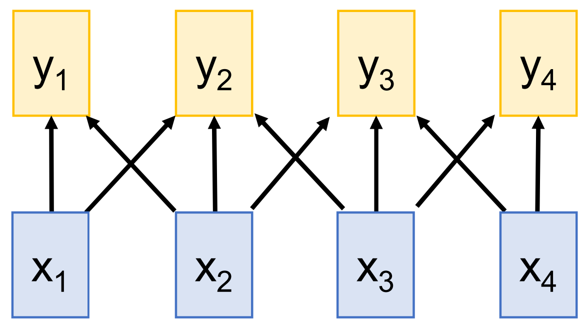
1D Convolution

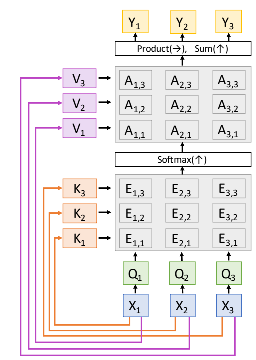


Works on **Multidimensional Grids**

(-) 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

Three Ways of Processing Sequences

Recurrent Neural Network | 1D Convolution | Self-Attention

Attention is all you need

Vaswani et al, NeurIPS 2017

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**

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Self-Attention

Works on **Sets of Vectors**

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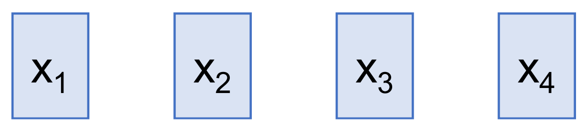
Slide credit: Justin Johnson

The Transformer

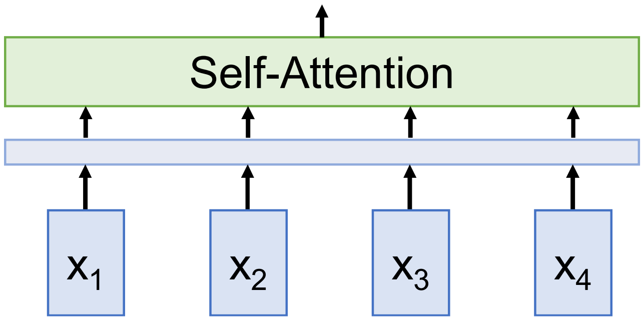


Vaswani et al, “Attention is all you need”, NeurIPS 2017

Slide credit: Justin Johnson

The Transformer

All vectors interact
with each other



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

Slide credit: Justin Johnson

The Transformer

MLP independently
on each vector

All vectors interact
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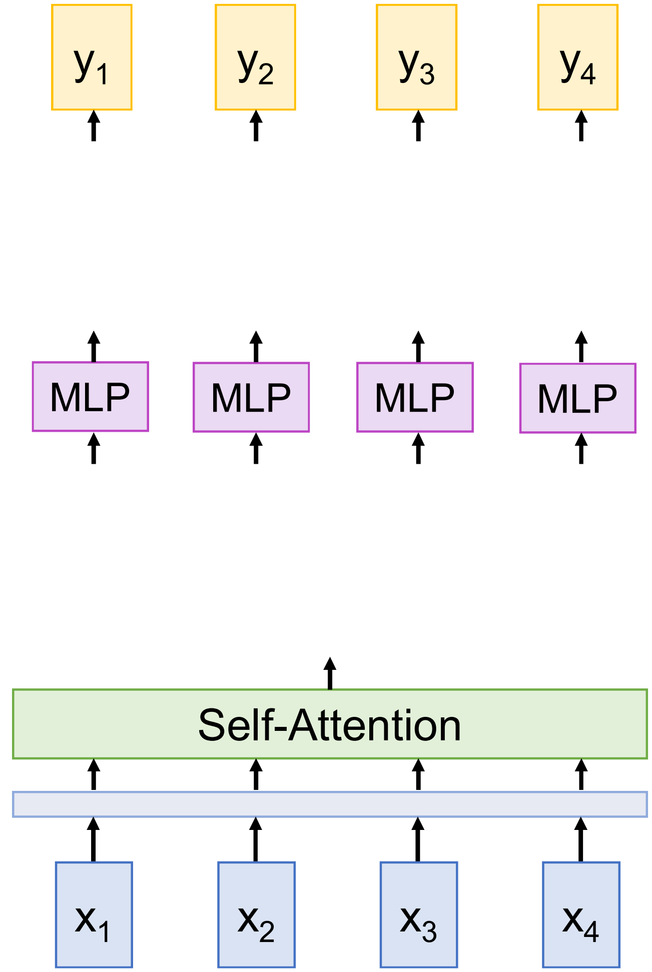
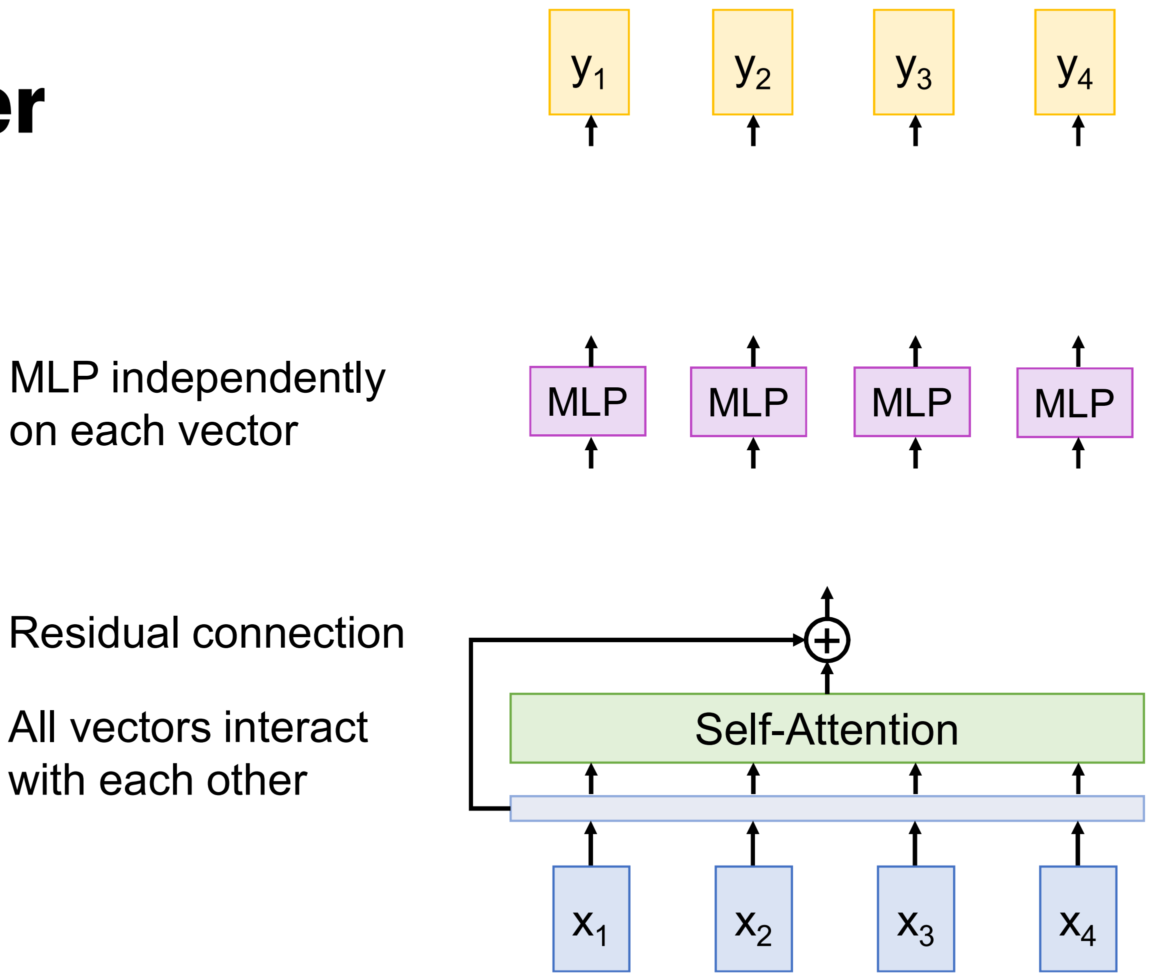


Vaswani et al, "Attention is all you need", NeurIPS 2017

Slide credit: Justin Johnson

The Transformer



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

Slide credit: Justin Johnson

The Transformer

Recall **Layer Normalization**:

Given $h_1, \ldots, h_N$ (Shape: D)

scale: γ (Shape: D)

shift: β (Shape: D)

$\mu_i = (1/D)\sum_j h_{i,j}$ (scalar)

$\sigma_i = (\sum_j (h_{i,j} - \mu_i)^2)^{1/2}$ (scalar)

$z_i = (h_i - \mu_i) / \sigma_i$

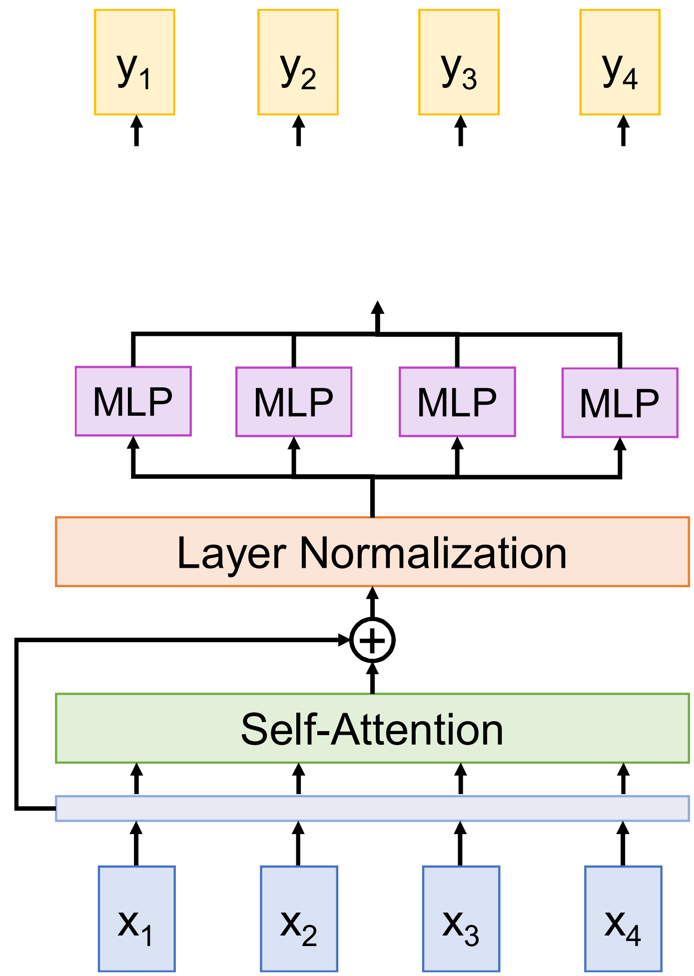
$y_i = \gamma * z_i + \beta$

Ba et al, 2016

MLP independently on each vector

Residual connection

All vectors interact with each other



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

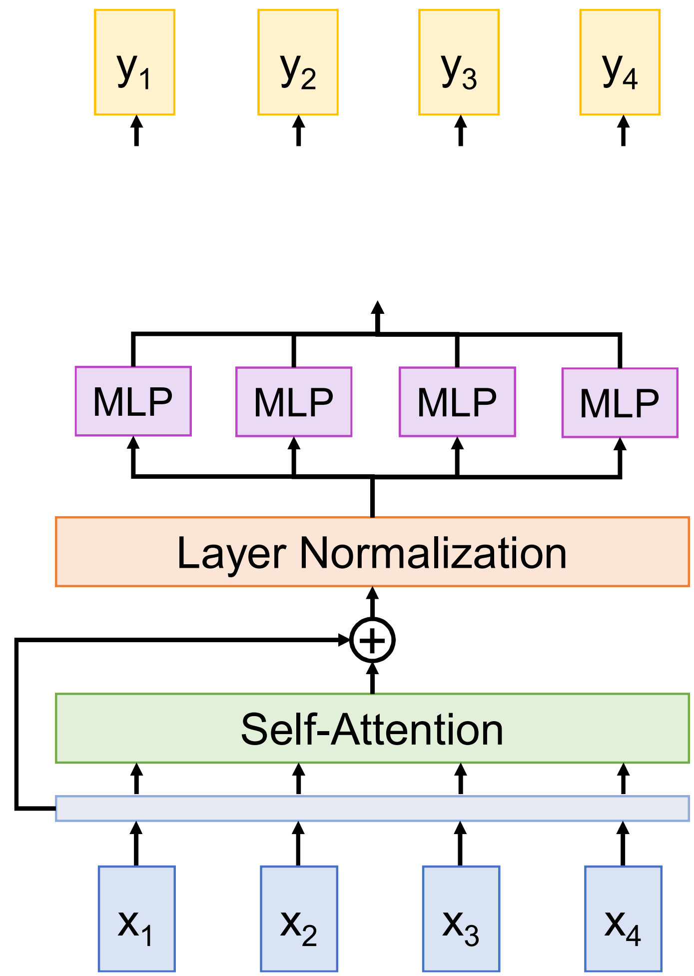
Slide credit: Justin Johnson

The Transformer

MLP independently on each vector

Residual connection

All vectors interact with each other



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

Slide credit: Justin Johnson

The Transformer

Residual connection

MLP independently on each vector

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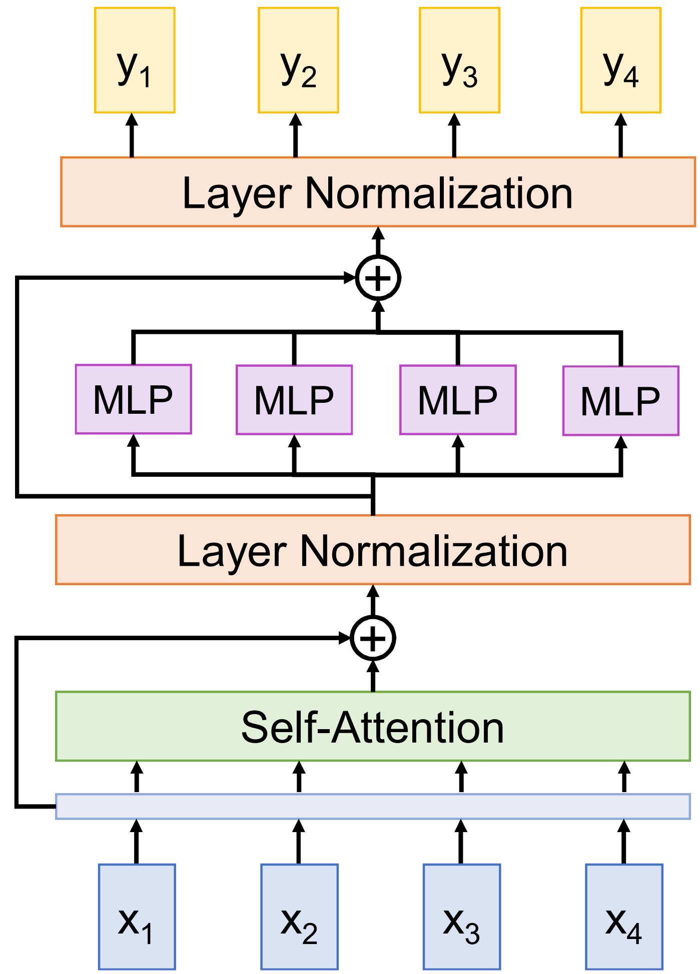


Vaswani et al, “Attention is all you need”, NeurIPS 2017

Slide credit: Justin Johnson

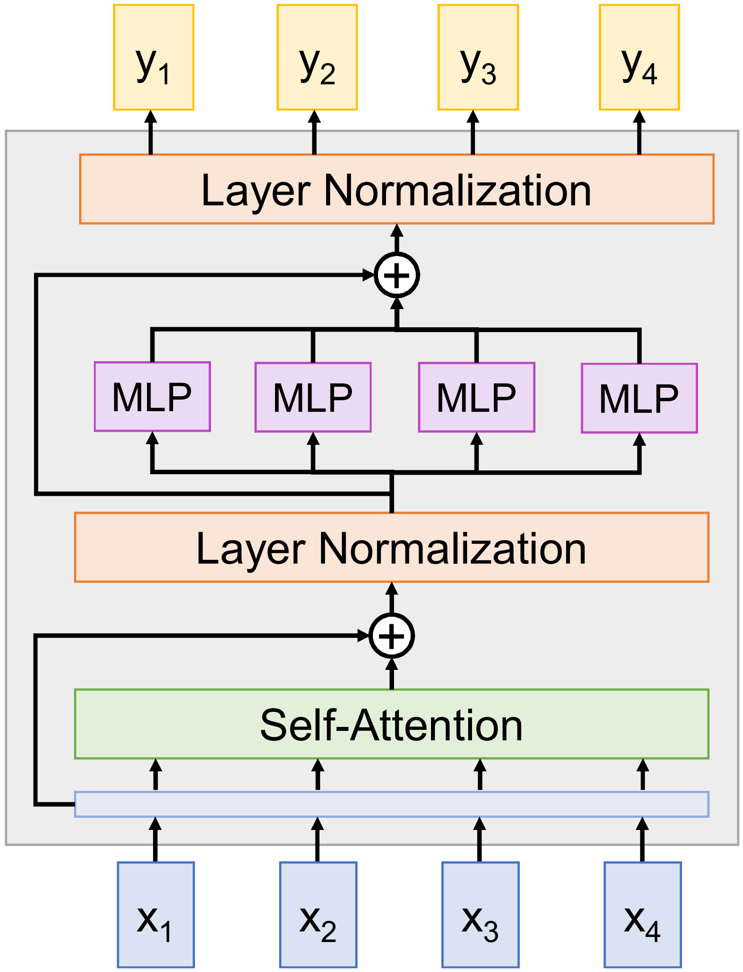
The Transformer

Transformer Block:
Input: Set of vectors x
Output: Set of vectors y

Self-attention is the only interaction between vectors!

Layer norm and MLP work independently per vector

Highly scalable, highly parallelizable



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

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The Transformer

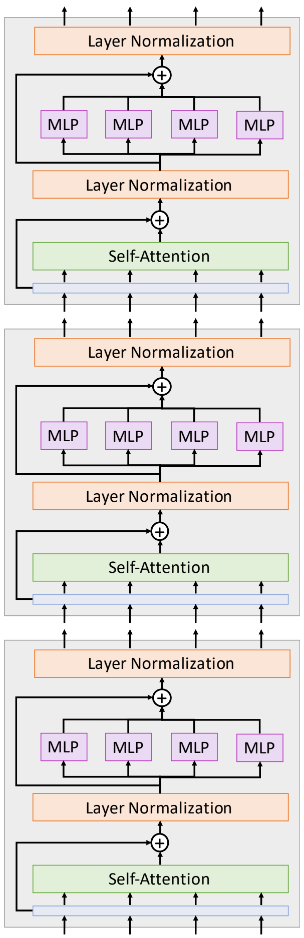
Transformer Block:
Input: Set of vectors x
Output: Set of vectors y

Self-attention is the only interaction between vectors!

Layer norm and MLP work independently per vector

Highly scalable, highly parallelizable

A **Transformer** is a sequence of transformer blocks



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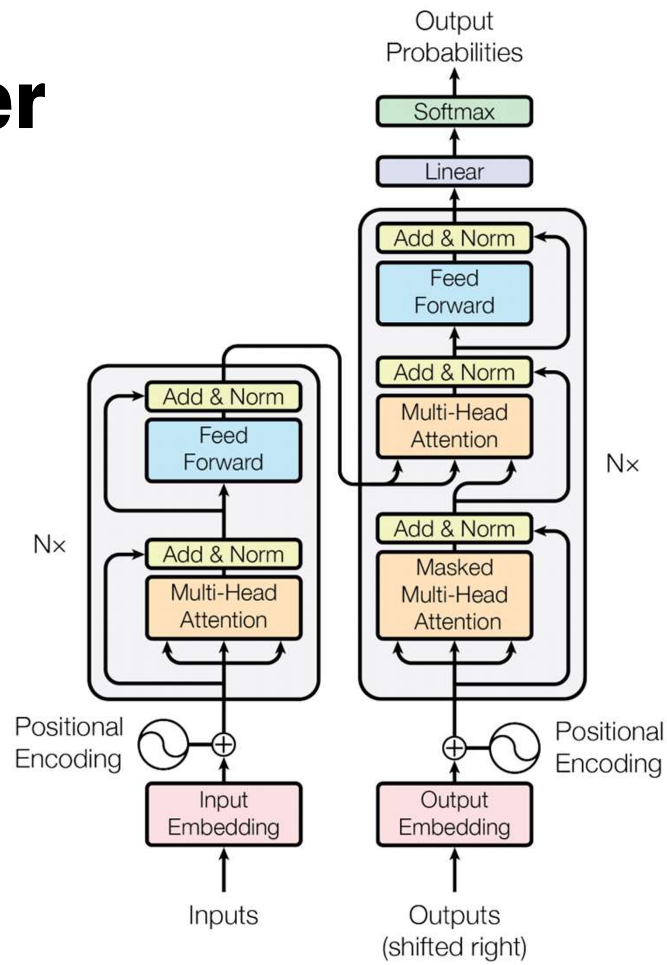
Slide credit: Justin Johnson

The Transformer



Encoder-Decoder

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

GLUE Benchmark

	Rank	Name	Model	URL	Score	CoLA	SST-2	MRPC	STS-B	QQP	MNLI-m	MNLI-mm	QNLI	RTE	WNLI	AX
	1	HFL iFLYTEK	MacALBERT + DKM		90.7	74.8	97.0	94.5/92.6	92.8/92.6	74.7/90.6	91.3	91.1	97.8	92.0	94.5	52.6
+	2	Alibaba DAMO NLP	StructBERT + TAPT		90.6	75.3	97.3	93.9/91.9	93.2/92.7	74.8/91.0	90.9	90.7	97.4	91.2	94.5	49.1
+	3	PING-AN Omni-Sinitic	ALBERT + DAAF + NAS		90.6	73.5	97.2	94.0/92.0	93.0/92.4	76.1/91.0	91.6	91.3	97.5	91.7	94.5	51.2
	4	ERNIE Team - Baidu	ERNIE		90.4	74.4	97.5	93.5/91.4	93.0/92.6	75.2/90.9	91.4	91.0	96.6	90.9	94.5	51.7
	5	T5 Team - Google	T5		90.3	71.6	97.5	92.8/90.4	93.1/92.8	75.1/90.6	92.2	91.9	96.9	92.8	94.5	53.1
	6	Microsoft D365 AI & MSR AI & GATECH	MT-DNN-SMART		89.9	69.5	97.5	93.7/91.6	92.9/92.5	73.9/90.2	91.0	90.8	99.2	89.7	94.5	50.2
+	7	Zihang Dai	Funnel-Transformer (Ensemble B10-10-10H1024)		89.7	70.5	97.5	93.4/91.2	92.6/92.3	75.4/90.7	91.4	91.1	95.8	90.0	94.5	51.6
+	8	ELECTRA Team	ELECTRA-Large + Standard Tricks		89.4	71.7	97.1	93.1/90.7	92.9/92.5	75.6/90.8	91.3	90.8	95.8	89.8	91.8	50.7
+	9	Huawei Noah's Ark Lab	NEZHA-Large		89.1	69.9	97.3	93.3/91.0	92.4/91.9	74.2/90.6	91.0	90.7	95.7	88.7	93.2	47.9
+	10	Microsoft D365 AI & UMD	FreeLB-RoBERTa (ensemble)		88.4	68.0	96.8	93.1/90.8	92.3/92.1	74.8/90.3	91.1	90.7	95.6	88.7	89.0	50.1
	11	Junjie Yang	HIRE-RoBERTa		88.3	68.6	97.1	93.0/90.7	92.4/92.0	74.3/90.2	90.7	90.4	95.5	87.9	89.0	49.3
	12	Facebook AI	RoBERTa		88.1	67.8	96.7	92.3/89.8	92.2/91.9	74.3/90.2	90.8	90.2	95.4	88.2	89.0	48.7
+	13	Microsoft D365 AI & MSR AI	MT-DNN-ensemble		87.6	68.4	96.5	92.7/90.3	91.1/90.7	73.7/89.9	87.9	87.4	96.0	86.3	89.0	42.8
	14	GLUE Human Baselines	GLUE Human Baselines		87.1	66.4	97.8	86.3/80.8	92.7/92.6	59.5/80.4	92.0	92.8	91.2	93.6	95.9	-
	15	Stanford Hazy Research	Snorkel MeTaL		83.2	63.8	96.2	91.5/88.5	90.1/89.7	73.1/89.9	87.6	87.2	93.9	80.9	65.1	39.9

source: https://gluebenchmark.com/leaderboard

GLUE Benchmark

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	6	Microsoft D365 AI & MSR AI & GATECH	MT-DNN-SMART		89.9	69.5	97.5	93.7/91.6	92.9/92.5	73.9/90.2	91.0	90.8	99.2	89.7	94.5	50.2
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+	10	Microsoft D365 AI & UMD	FreeLB-RoBERTa (ensemble)		88.4	68.0	96.8	93.1/90.8	92.3/92.1	74.8/90.3	91.1	90.7	95.6	88.7	89.0	50.1
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source: https://gluebenchmark.com/leaderboard

SYSTEM PROMPT (HUMAN-WRITTEN)
In a shocking finding, scientist discovered a herd of unicorns living in a remote, previously unexplored valley, in the Andes Mountains. Even more surprising to the researchers was the fact that the unicorns spoke perfect English.

MODEL COMPLETION (MACHINE-WRITTEN, 10 TRIES)
The scientist named the population, after their distinctive horn, Ovid's Unicorn. These four-horned, silver-white unicorns were previously unknown to science.

Now, after almost two centuries, the mystery of what sparked this odd phenomenon is finally solved.

Dr. Jorge Pérez, an evolutionary biologist from the University of La Paz, and several companions, were exploring the Andes Mountains when they found a small valley, with no other animals or humans. Pérez noticed that the valley had what appeared to be a natural fountain, surrounded by two peaks of rock and silver snow.

Pérez and the others then ventured further into the valley. "By the time we reached the top of one peak, the water looked blue, with some crystals on top," said Pérez.

Source: OpenAI, "Better Language Models and Their Implications"
https://openai.com/blog/better-language-models/

Can Attention/Transformers be used from more than text processing?

ViLBERT: A Visolinguistic Transformer

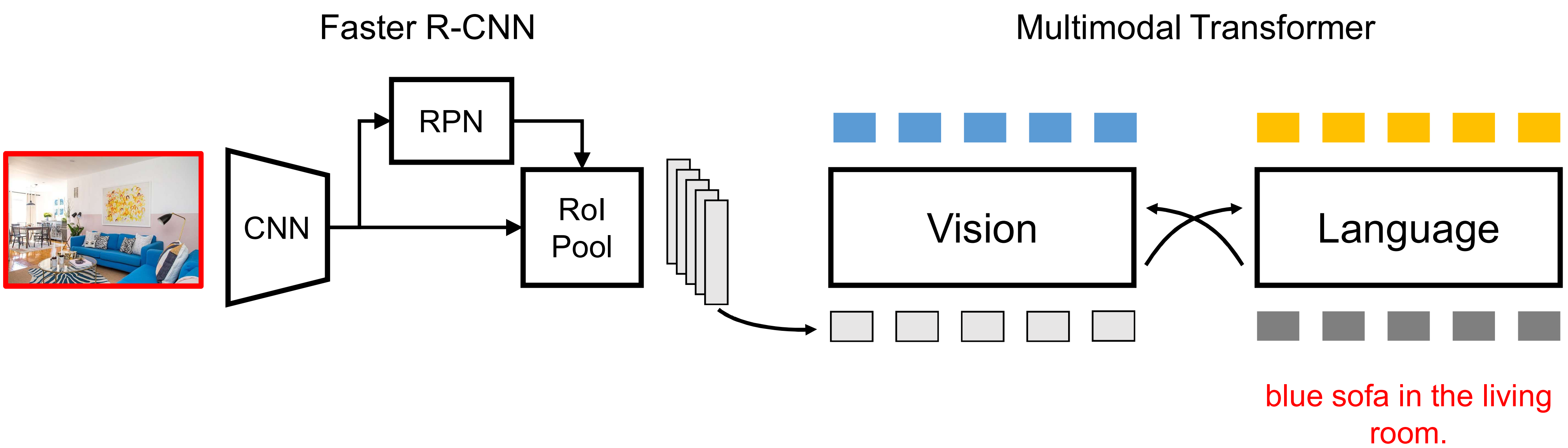
pop artist performs at the festival in a city.

a worker helps to clear the debris.

blue sofa in the living room.

Image and captions from: Sharma, Piyush, et al. "Conceptual captions: A cleaned, hypernymed, image alt-text dataset for automatic image captioning." ACL. 2018.

ViLBERT: A Visolinguistic Transformer



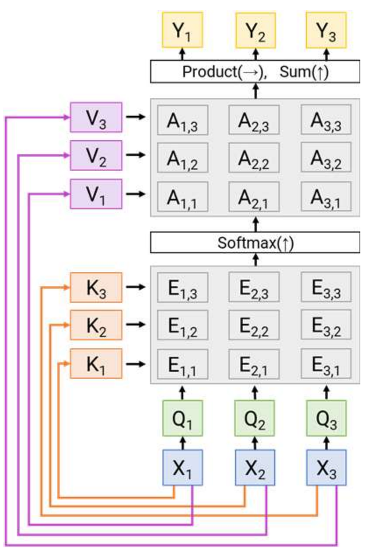
Lu et al "Vilbert: Pretraining task-agnostic visiolinguistic representations for vision-and-language tasks." *NeurIPS*. 2019.
Ren et al. "Faster r-cnn: Towards real-time object detection with region proposal networks." *NeurIPS*. 2015.

ViLBERT Demo:

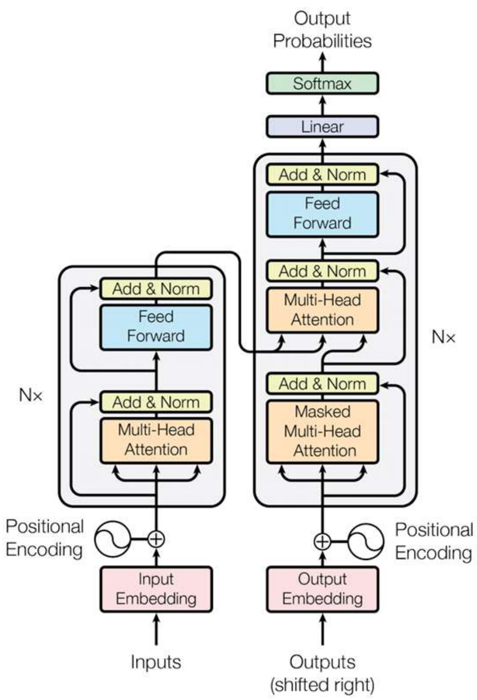
https://demo.allennlp.org/visual-question-answering

Summary

Self-Attention



Transformer Model



ViLBERT