Topics:

- Transformers continued
- Vision Transformers

CS 4644-DL / 7643-A

ZSOLT KIRA

- **Assignment 2**
  - Due **June 25th (Today!) 11:59pm EST (grace period 27th)**

- **Project Check-In released**
  - Extended to July 3rd (grace July 5th)

- Meta office hours Friday 3pm ET on attention models

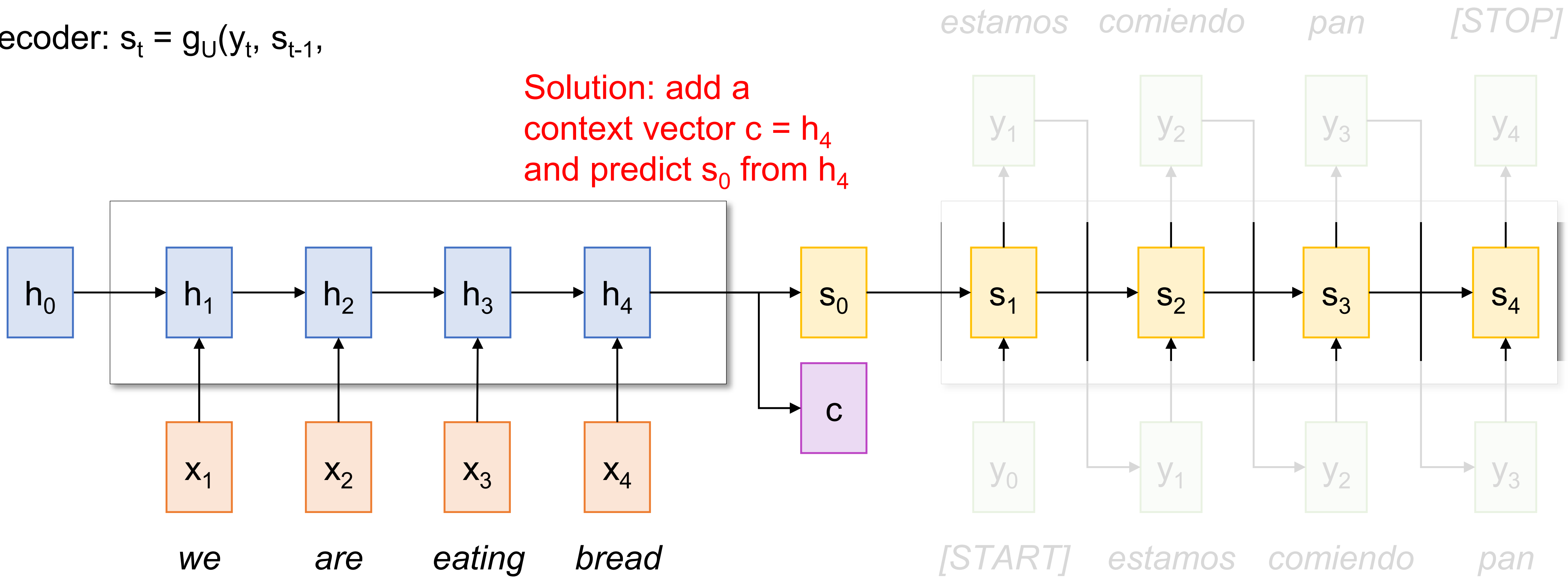
- Monday will be a remote session

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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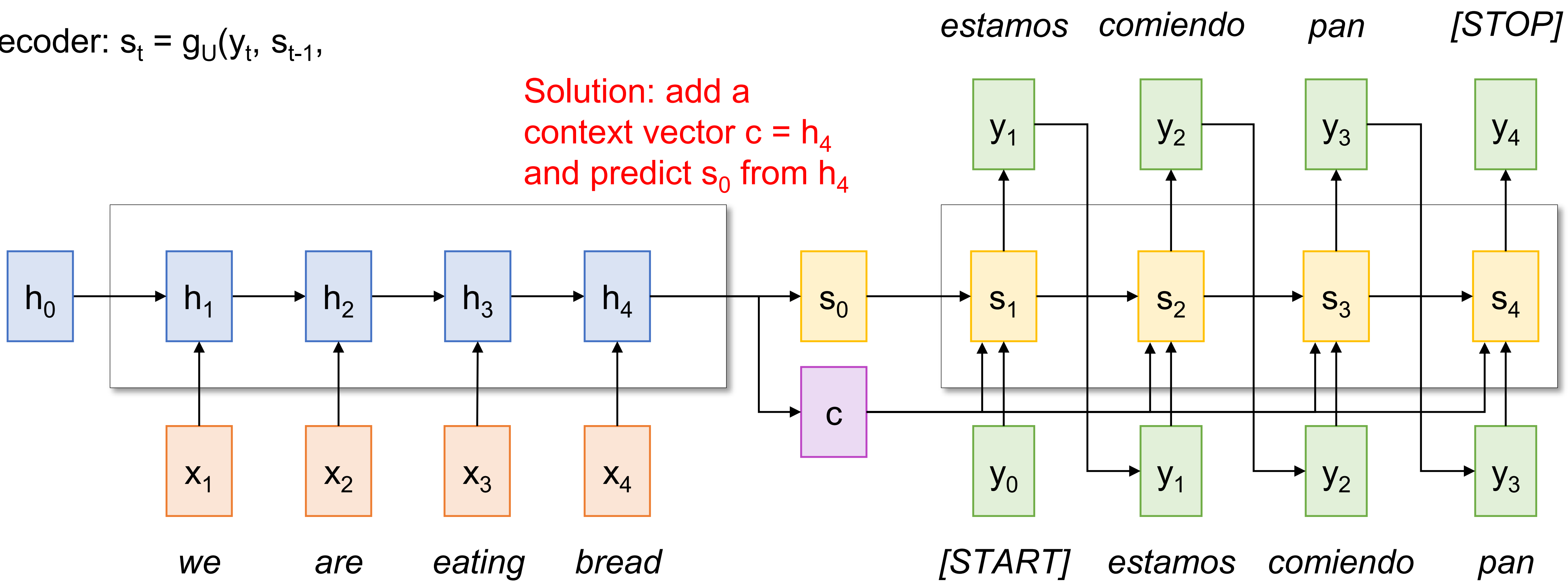

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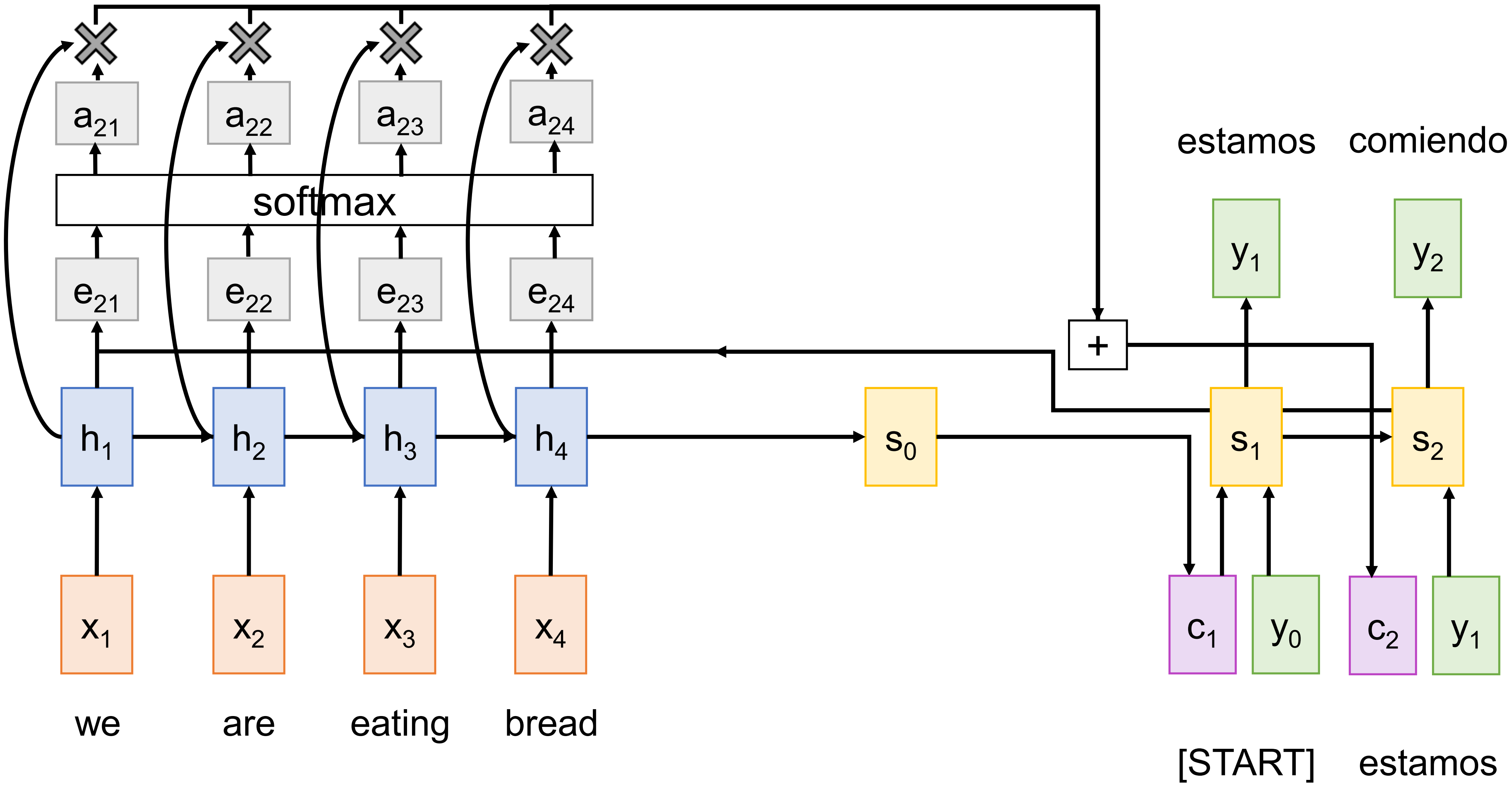
Machine Translation with RNNs **and Attention**



Repeat: Use s_1 to compute new context vector c_2

Use c_2 to compute s_2, y_2

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

Slide credit: Justin Johnson

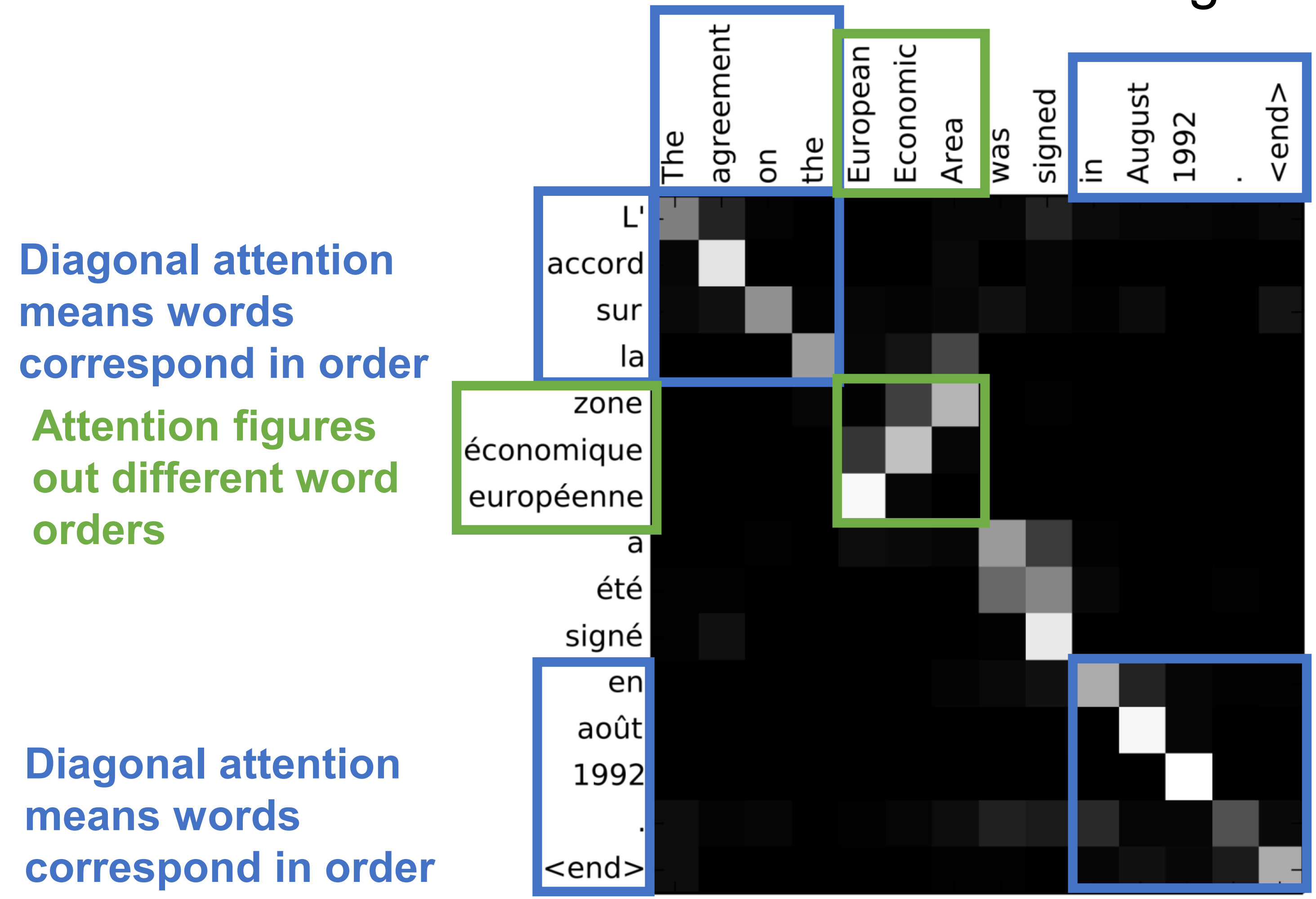
Machine Translation with RNNs **and Attention**

Example: English to French translation

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

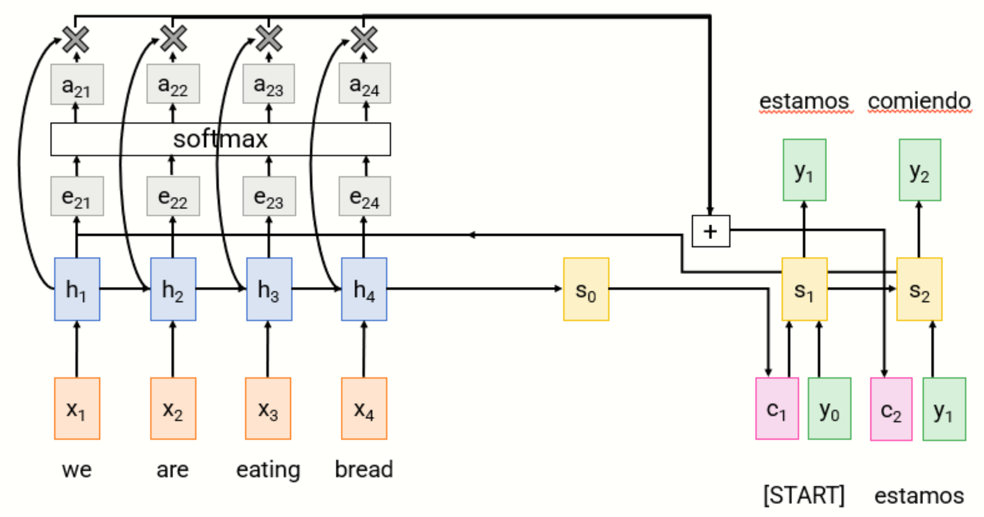
Output: "L'accord sur la zone économique européenne a été signé en août 1992."

Visualize attention weights $a_{t,i}$

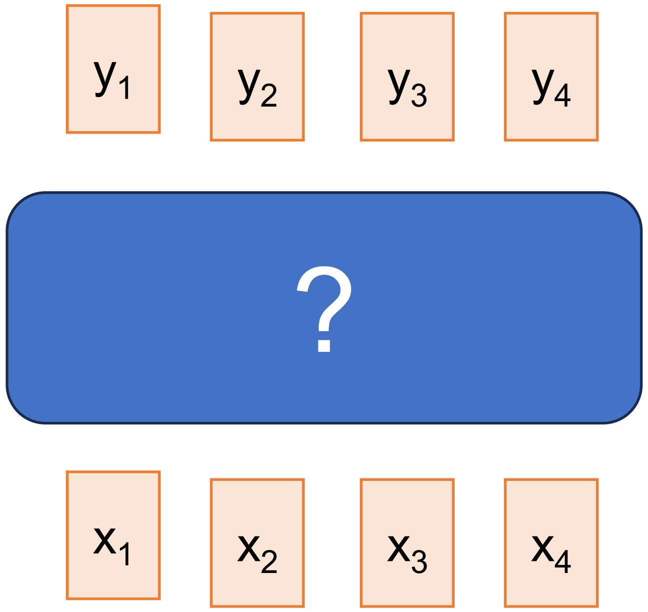


Bahdanau et al, "Neural machine translation by jointly learning to align and translate", ICLR 2015

Slide credit: Justin Johnson

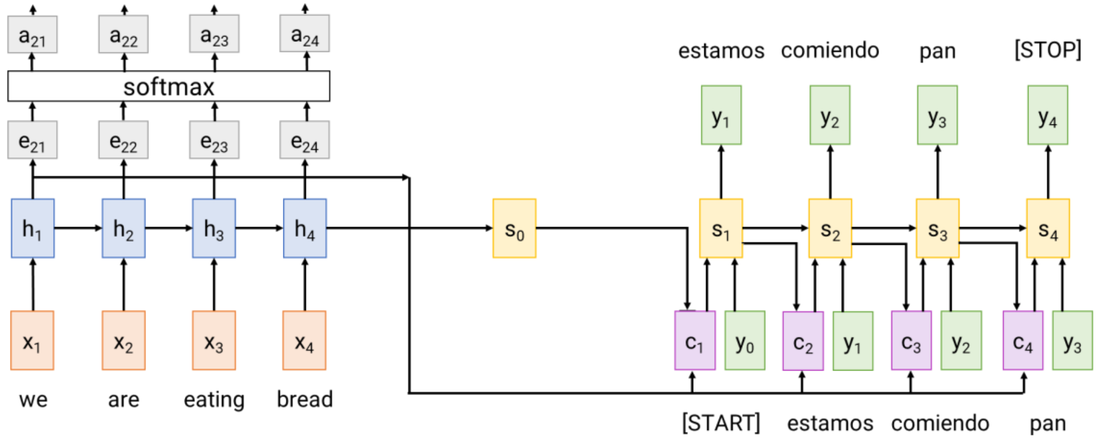


Idea: Can we use **attention** as a fundamental building block for a generic sequence (input) to sequence (output) layer?



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}

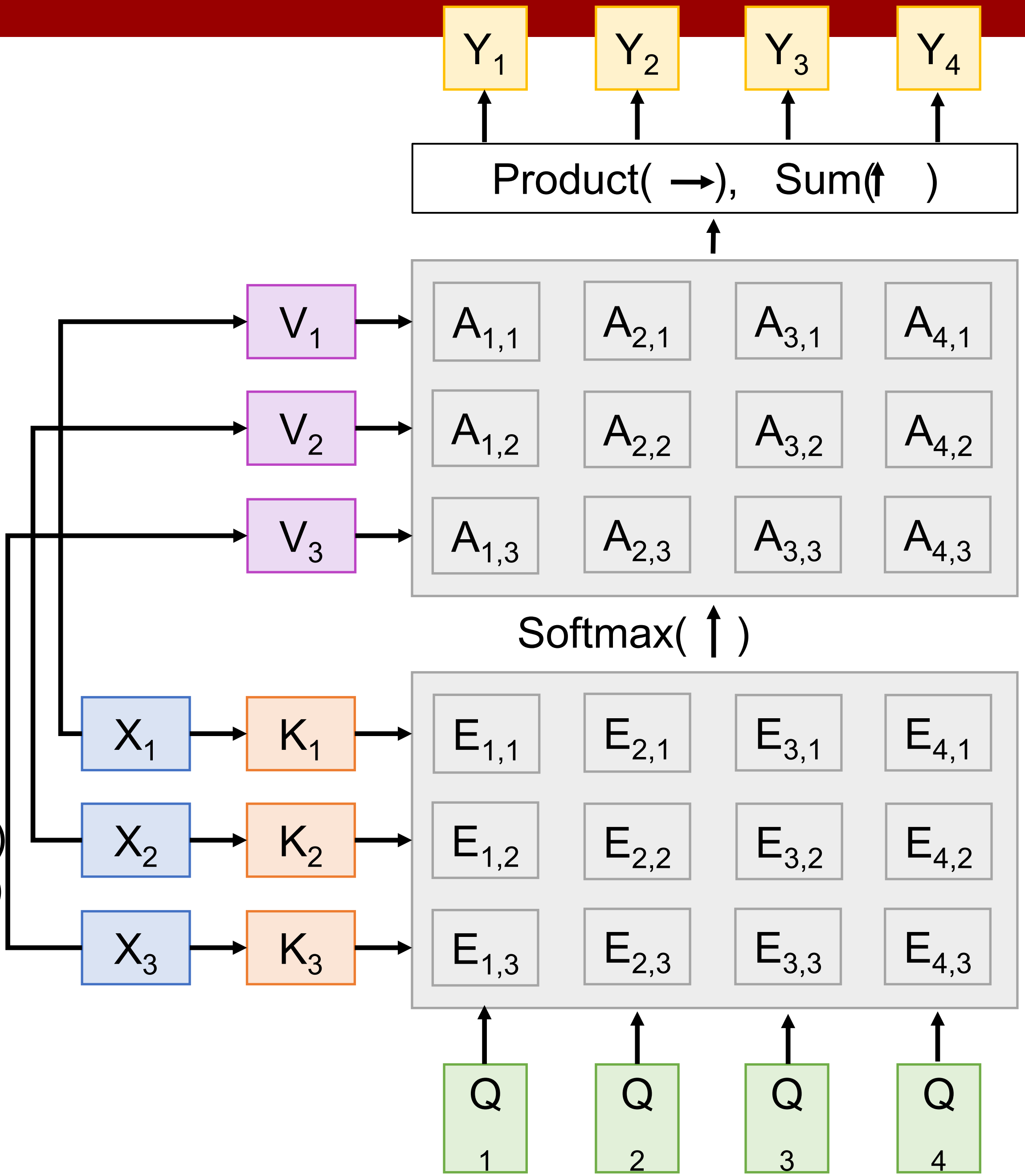


Computation:
Similarities: e (Shape: N_X) $e_i = f_{att}(\mathbf{s_{t-1}}, \mathbf{h_i})$
Attention weights: $a = \text{softmax}(e)$ (Shape: N_X)
Output vector: $y = \sum_i a_i \mathbf{h_i}$ (Shape: D_X)

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



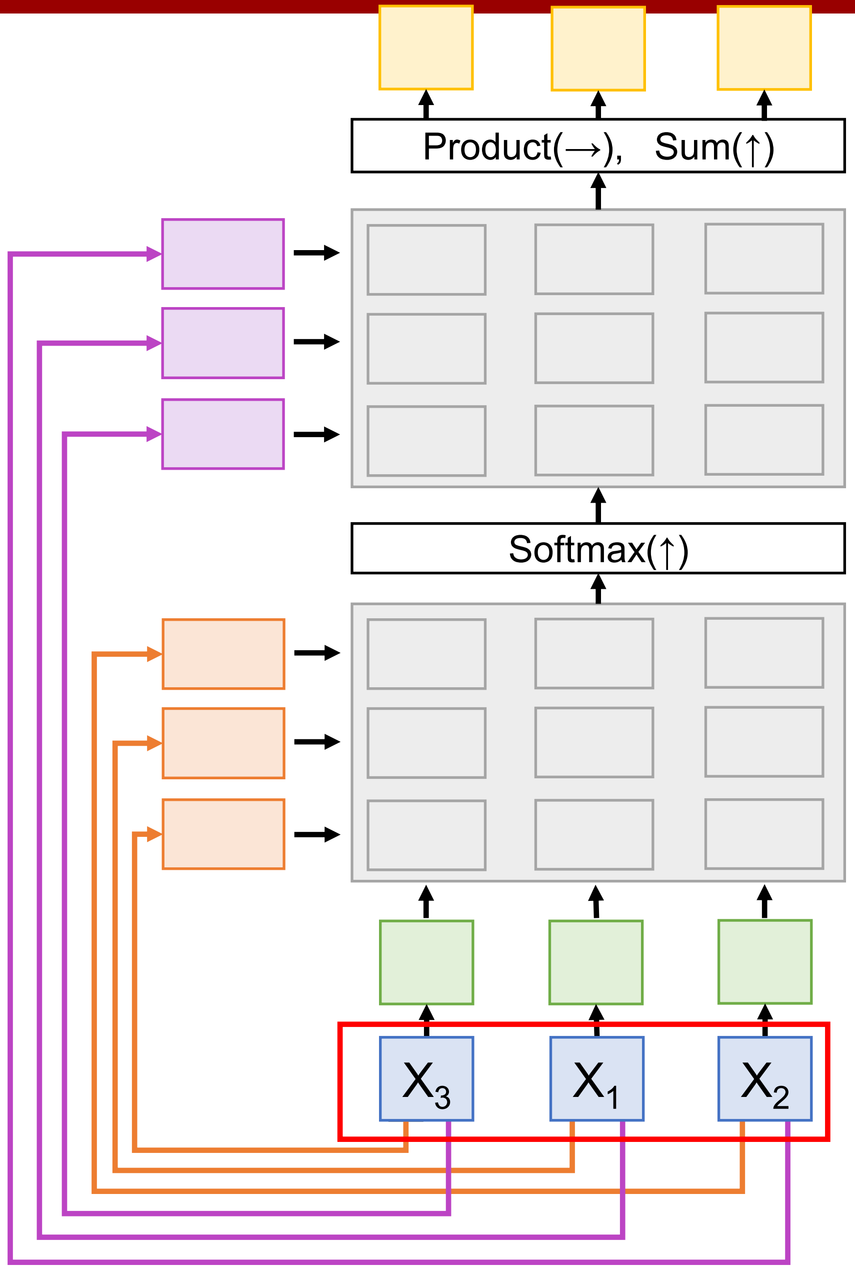
Slide credit: Justin Johnson

Self-Attention Layer

Consider **permuting** the input vectors:

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

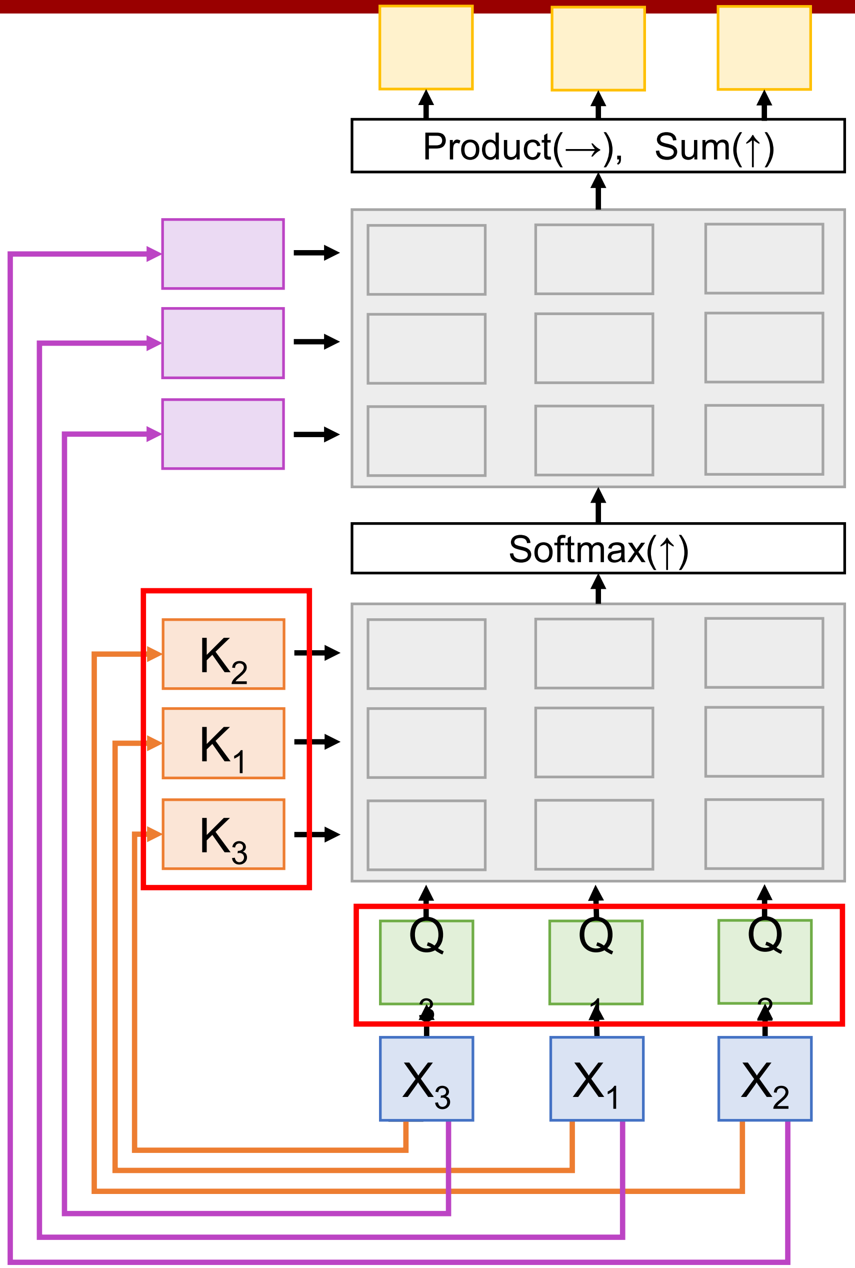
Self-Attention Layer

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)

Consider **permuting** the input vectors:

Queries and Keys 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: $A = \text{softmax}(E, \text{dim}=1)$ (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

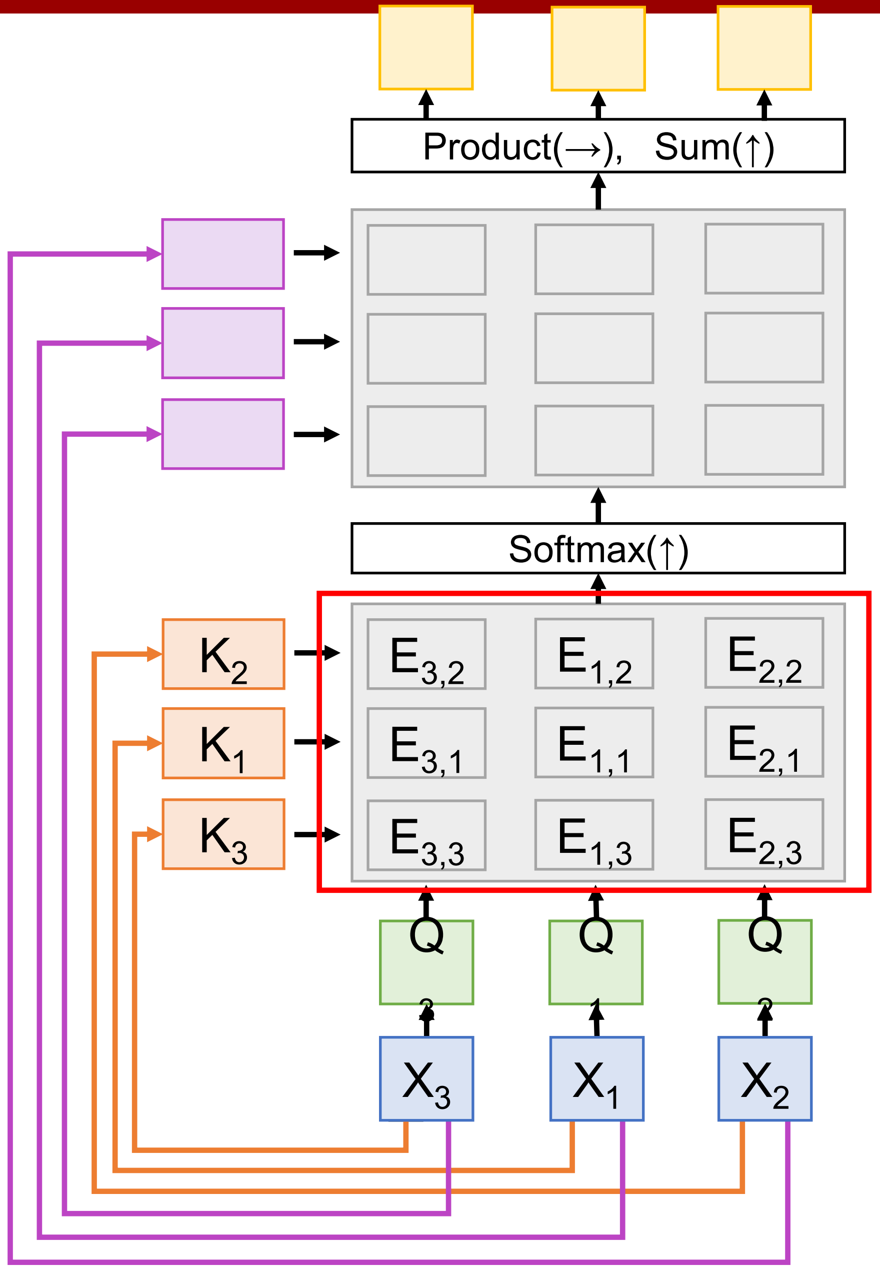
Self-Attention Layer

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** · **K_j** / 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: **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:

Attention weights 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)
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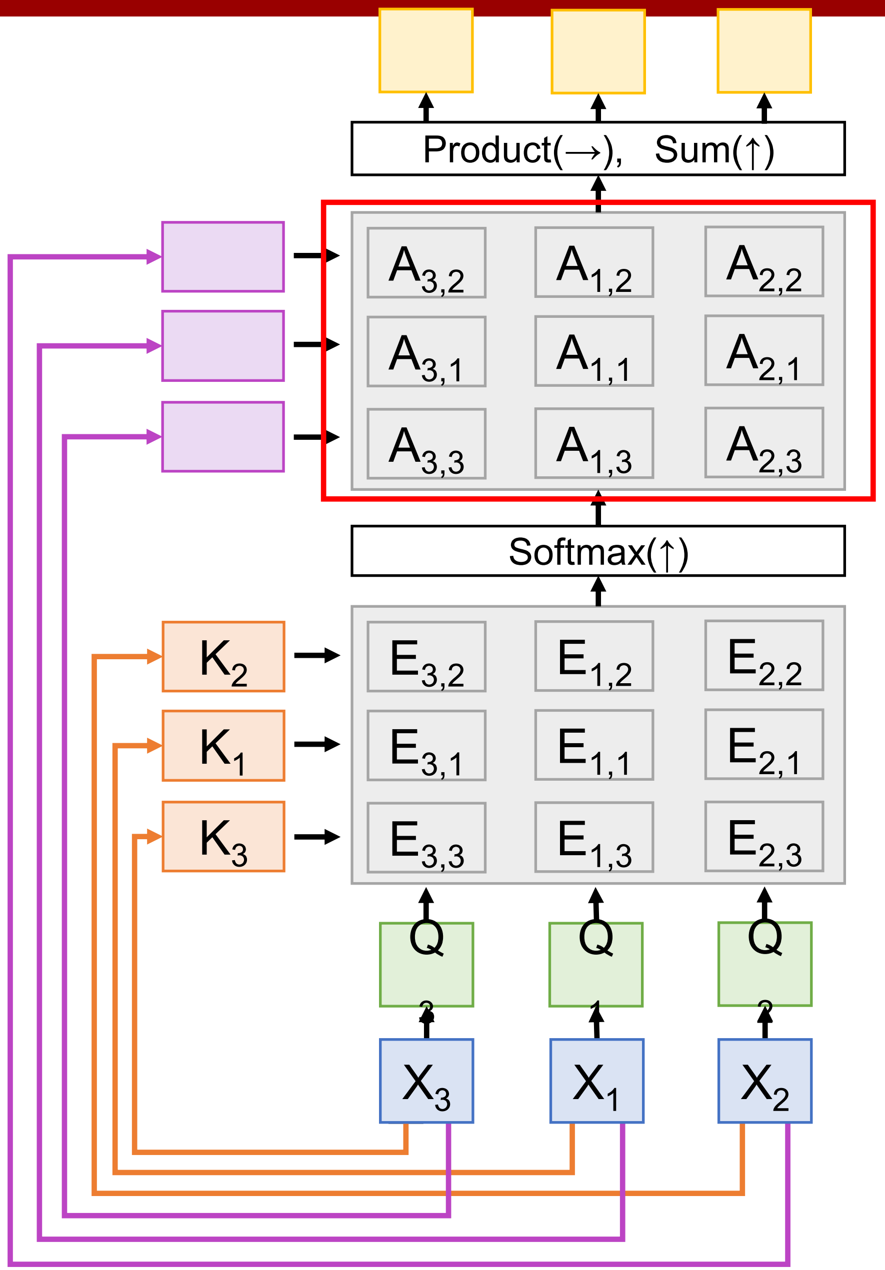


Slide credit: Justin Johnson

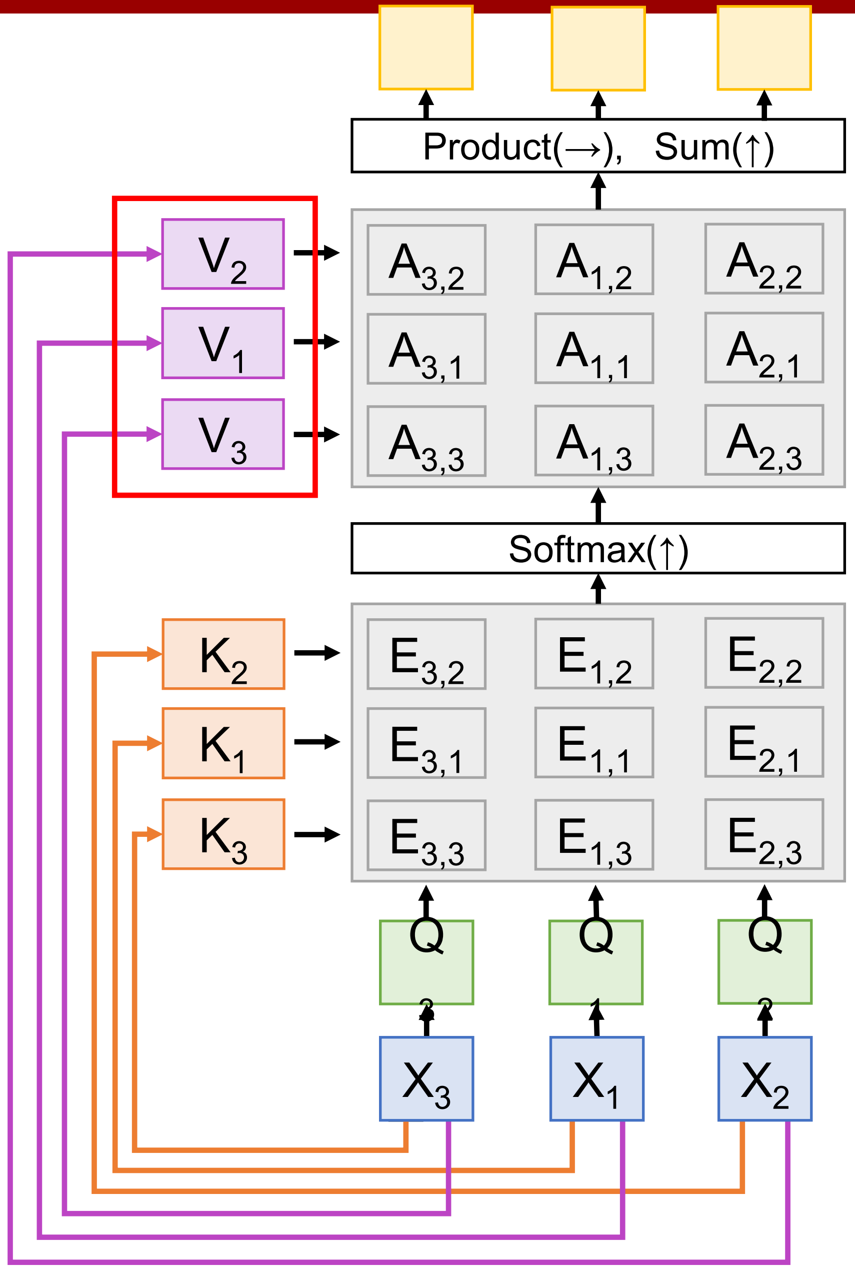
Self-Attention Layer

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: $D_X \times D_Q$)

Consider **permuting** the input vectors:

Values will be the same, but permuted

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

Consider **permuting** the input vectors:

Outputs will be the same, but permuted

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)
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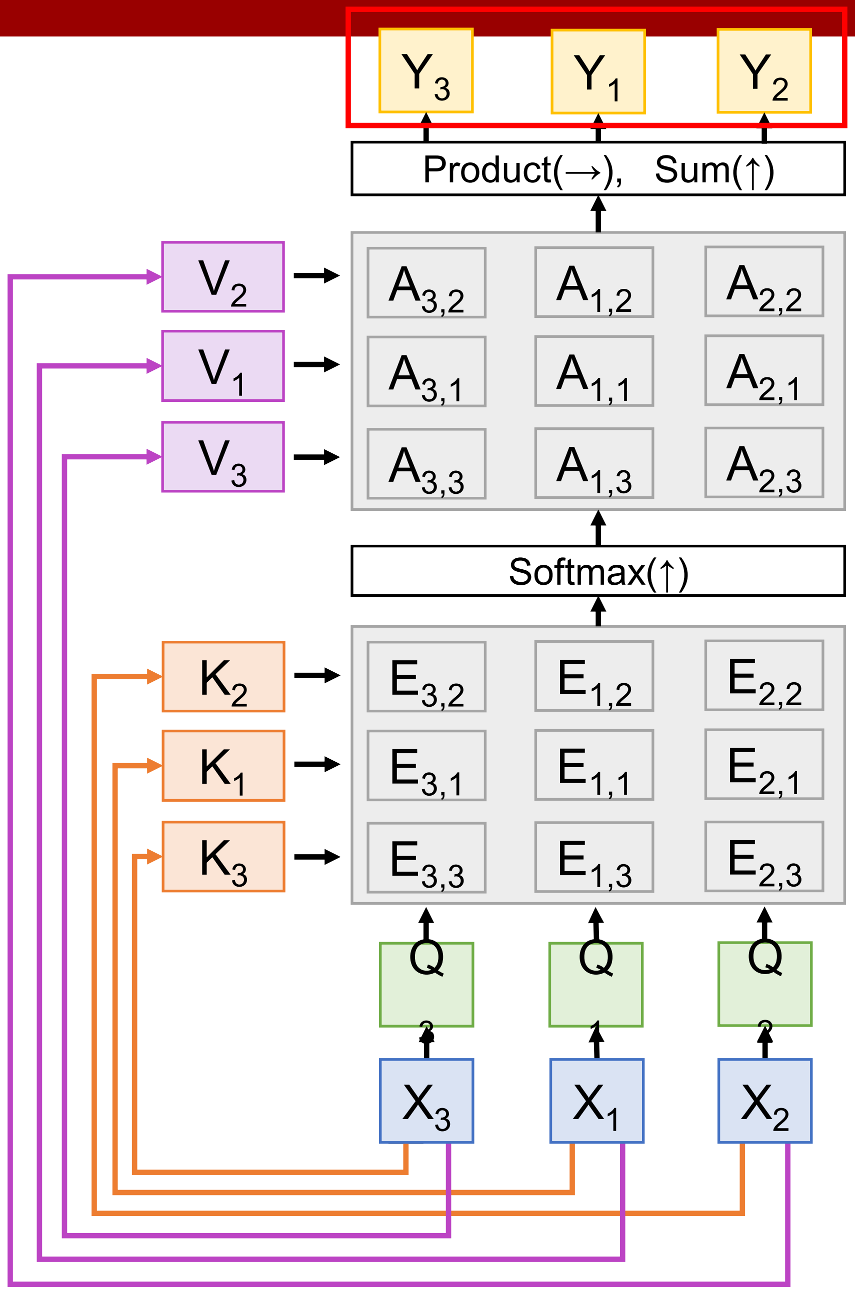

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Inputs:
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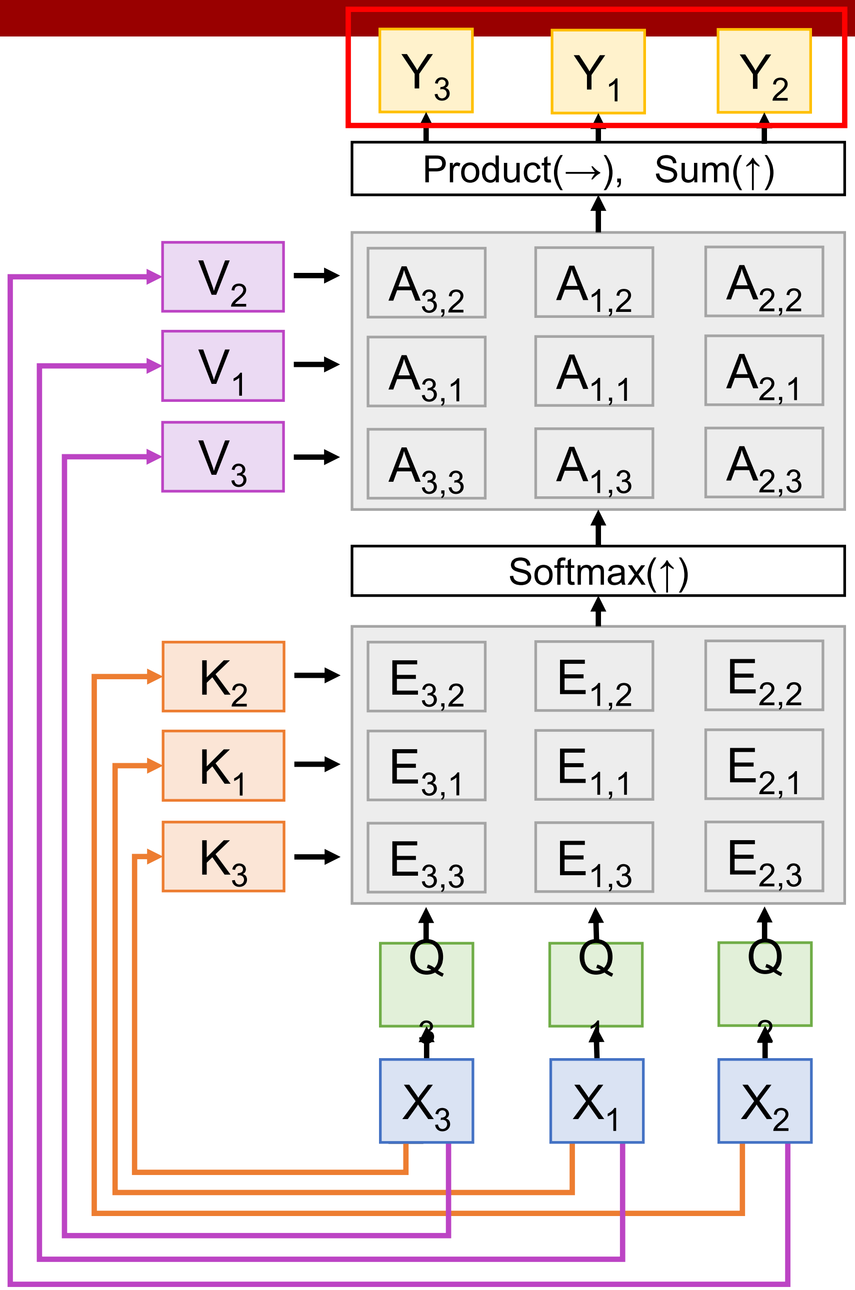
Consider **permuting** the input vectors:

Outputs will be the same, but permuted

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



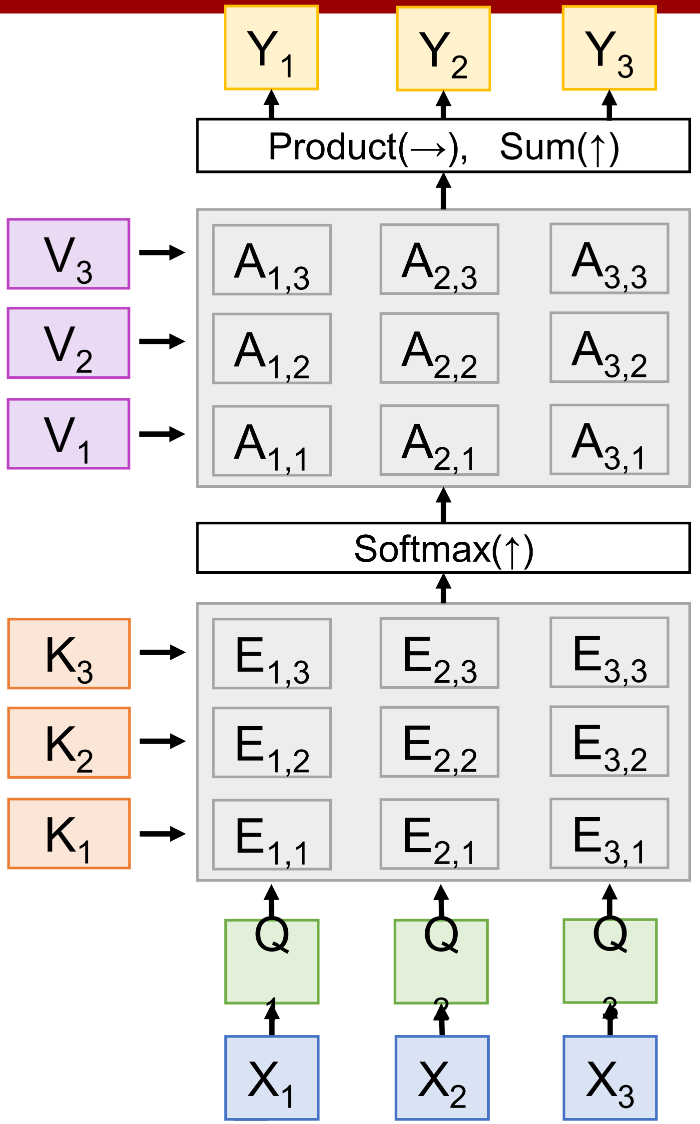
Slide credit: Justin Johnson

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)

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

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

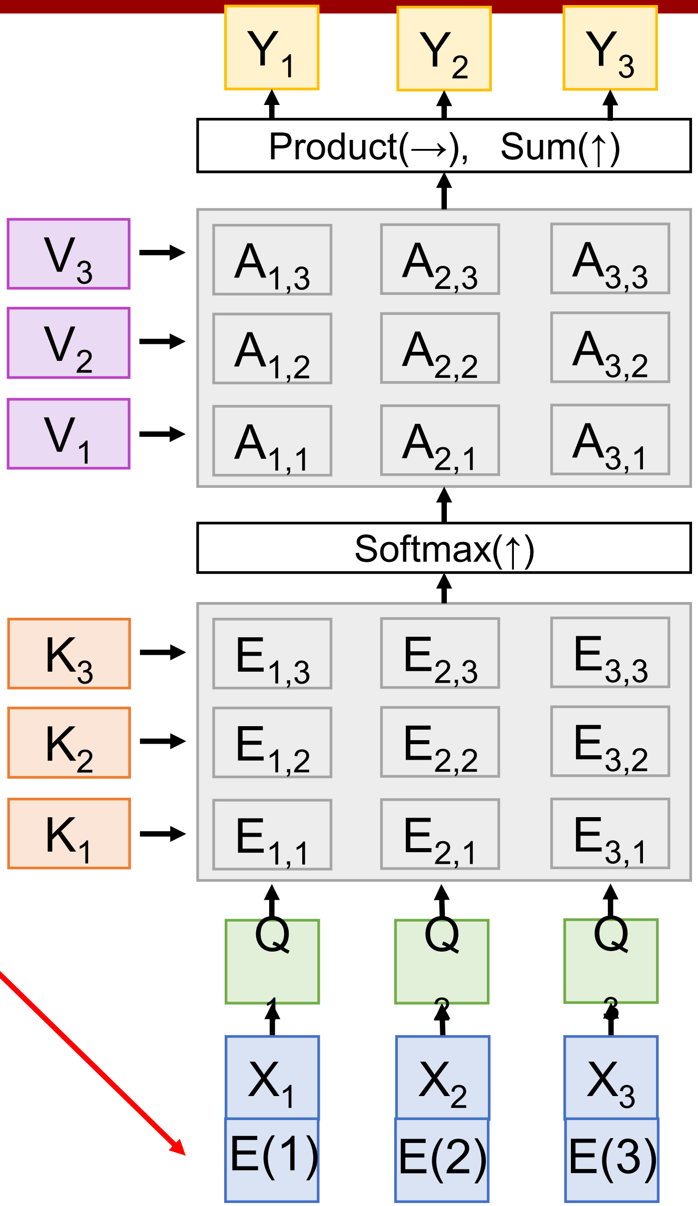
<u>Inputs</u>:
Input vectors: X (Shape: $N_X \times D_X$)
Key matrix: W_K (Shape: $D_X \times D_Q$)
Value matrix: W_V (Shape: $D_X \times D_V$)
Query matrix: W_Q (Shape: $D_X \times D_Q$)

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

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

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

E can be learned lookup table, or fixed function



Slide credit: Justin Johnson

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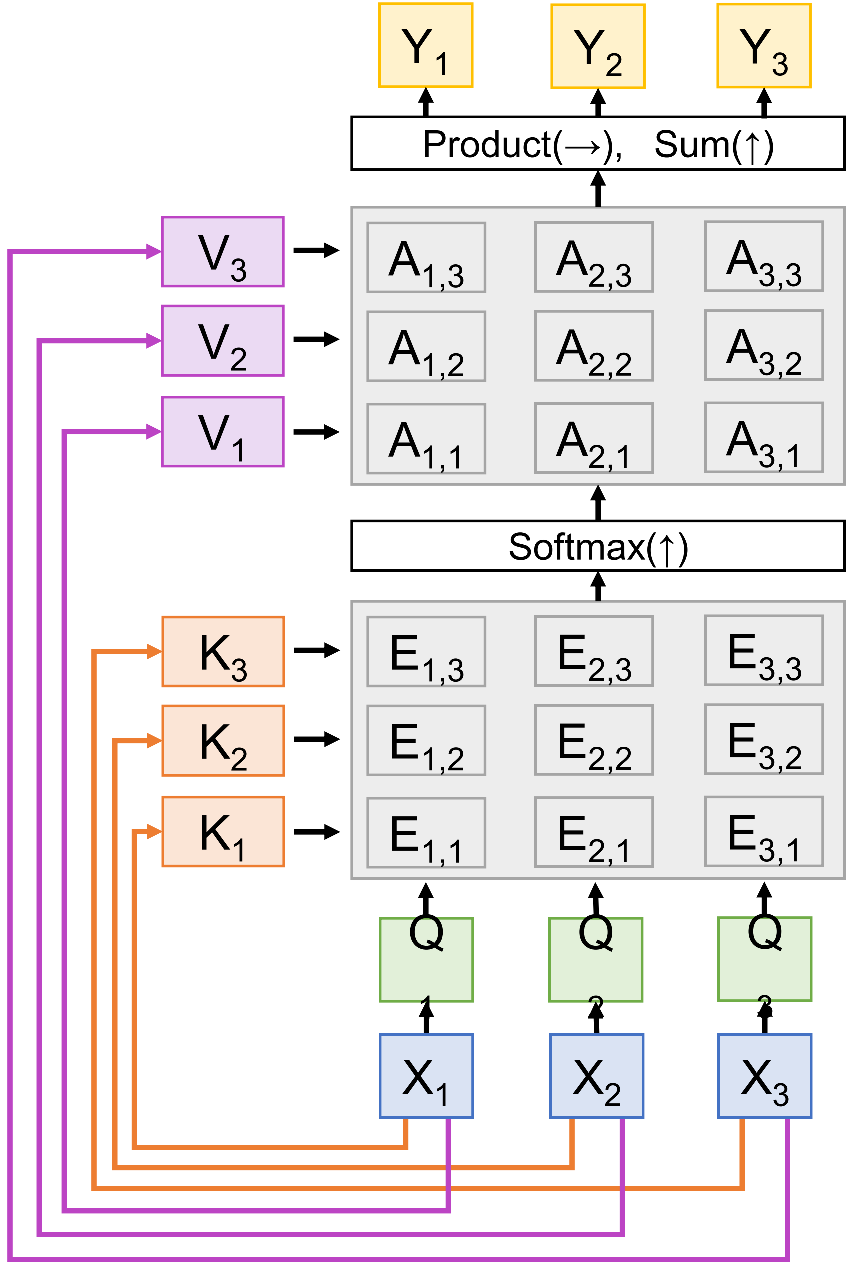
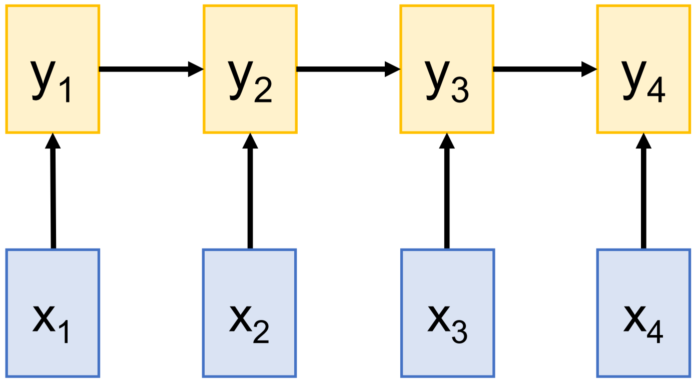


Slide credit: Justin Johnson

Three Ways of Processing Sequences

Recurrent Neural Network

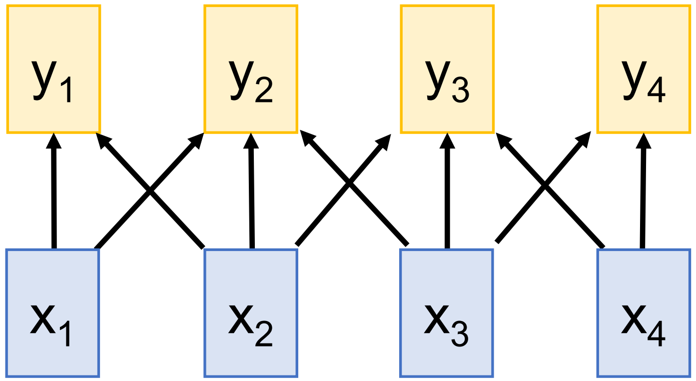


Works on **Ordered Sequences**

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

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

1D Convolution

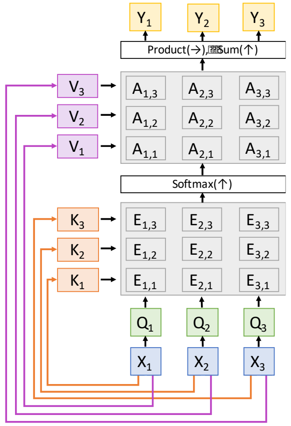


Works on **Multidimensional Grids**

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

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

Self-Attention



Works on **Sets of Vectors**

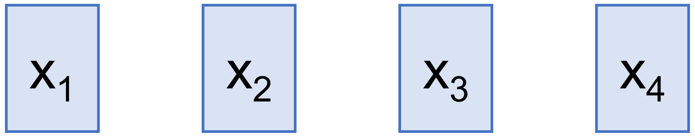
(+) Good at long sequences: after one self-attention layer, each output "sees" all inputs!

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

(-) Very memory intensive

Slide credit: Justin Johnson

The Transformer

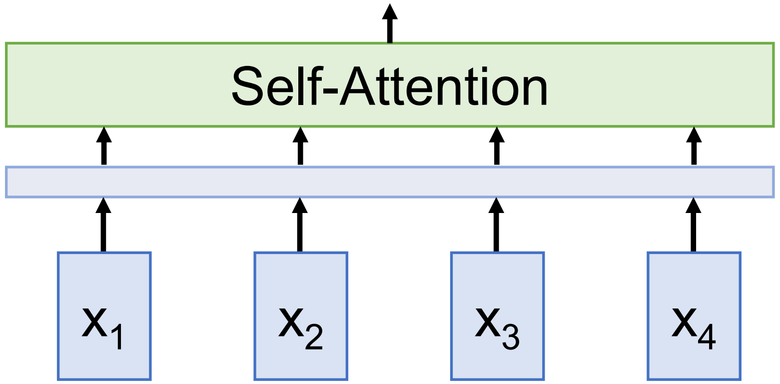


Vaswani et al, “Attention is all you need”, NeurIPS 2017

Slide credit: Justin Johnson

The Transformer

All vectors interact
with each other



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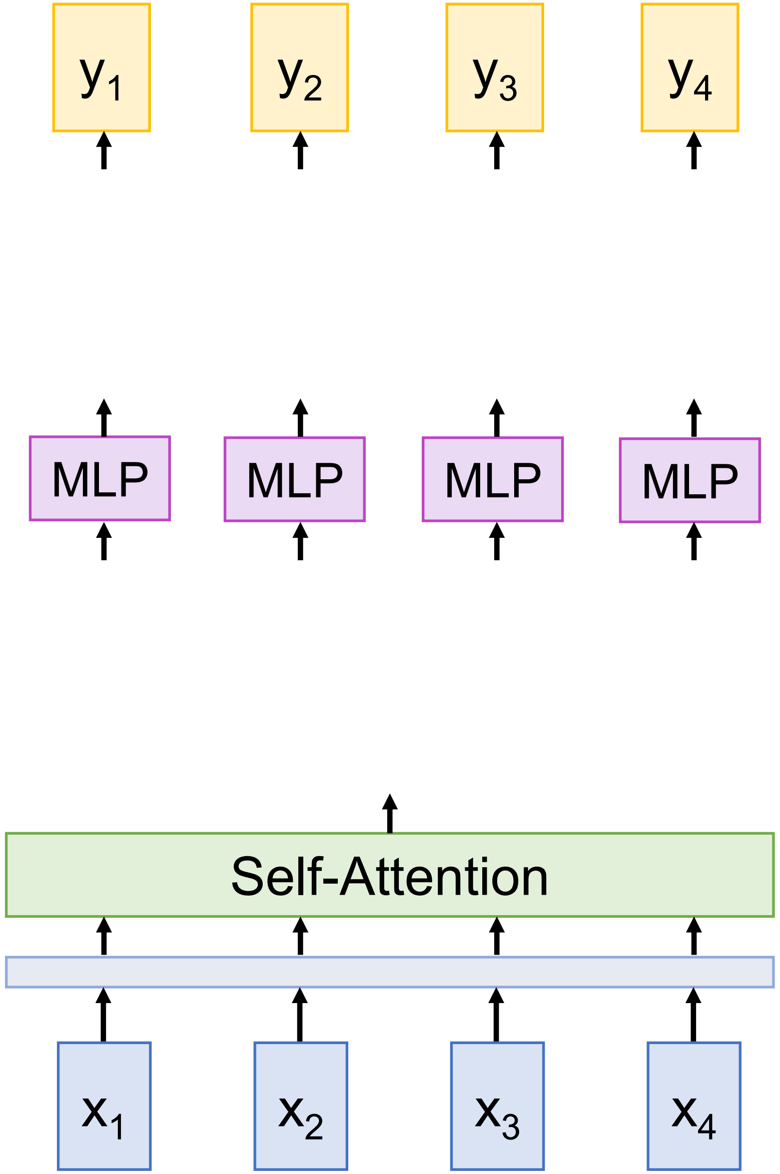
The Transformer



MLP independently
on each vector
(weight shared!)

All vectors interact
with each other

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

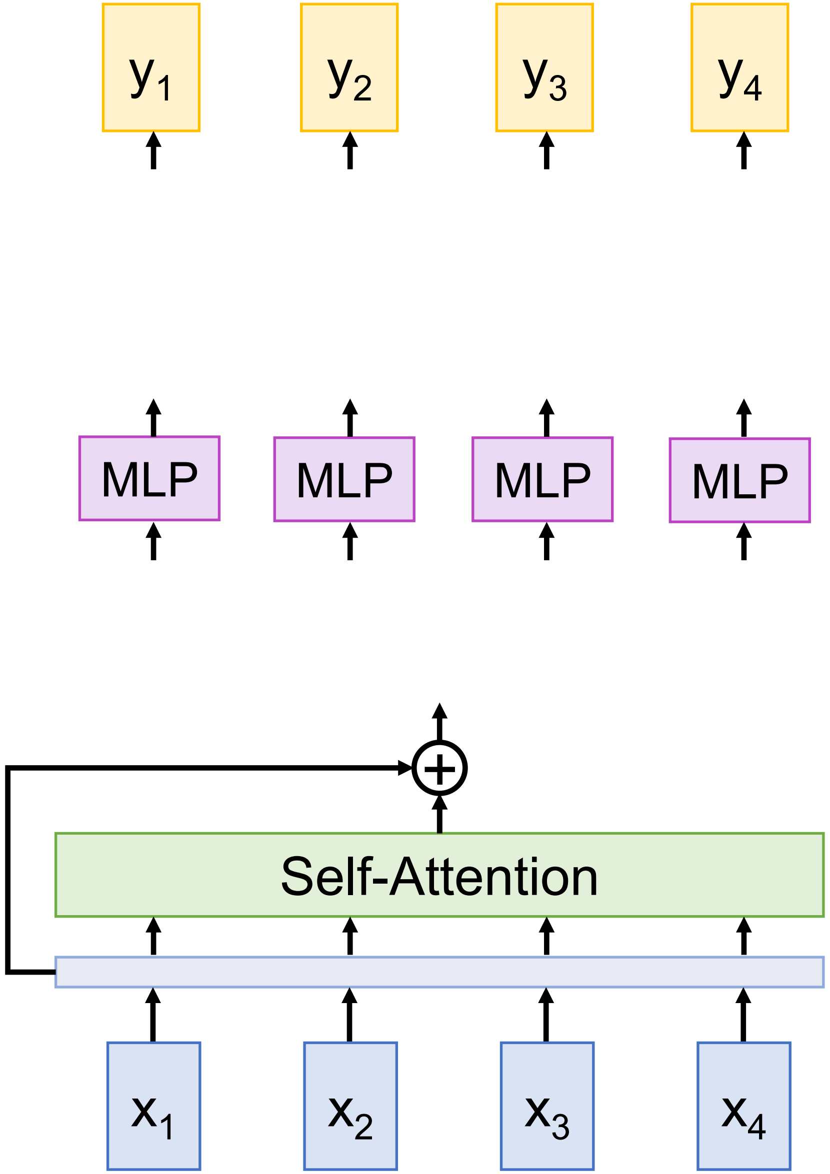
Slide credit: Justin Johnson

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

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)

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

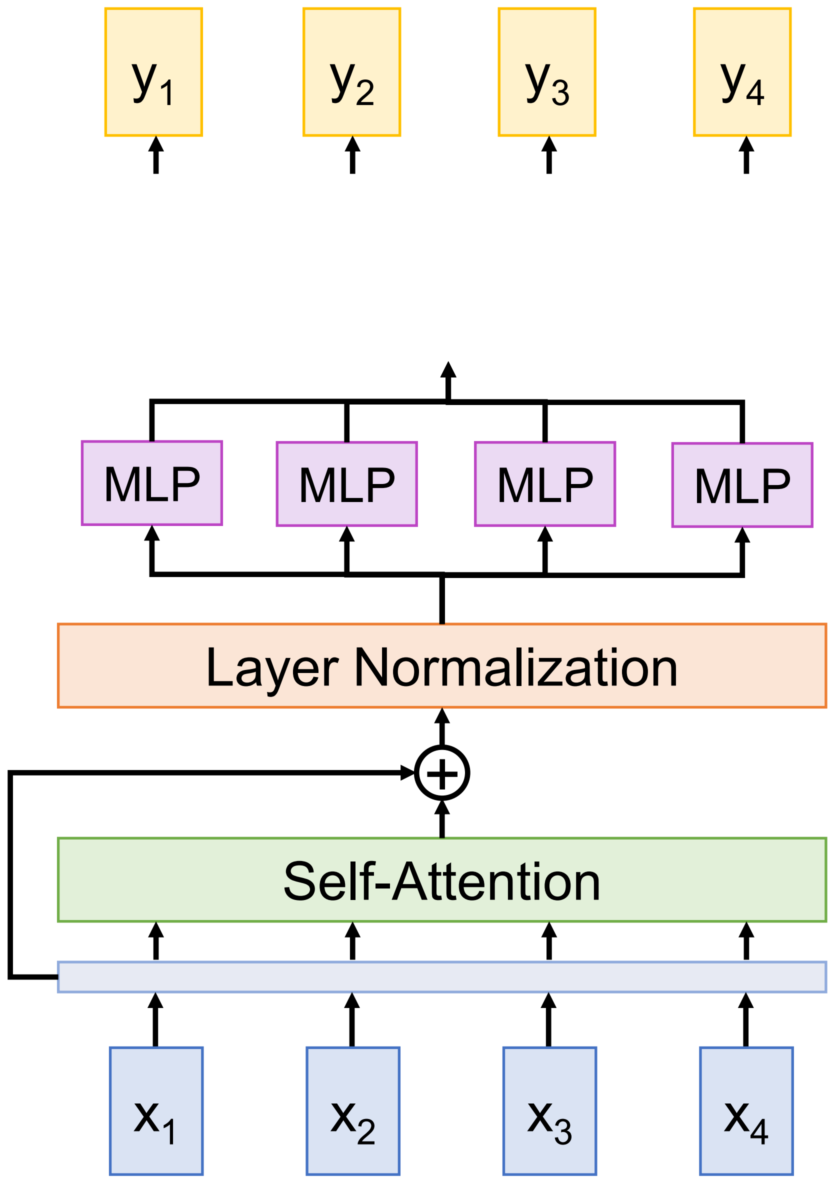
$y_i = \gamma * z_i + \beta$

Ba et al, 2016

MLP independently on each vector

Residual connection

All vectors interact with each other



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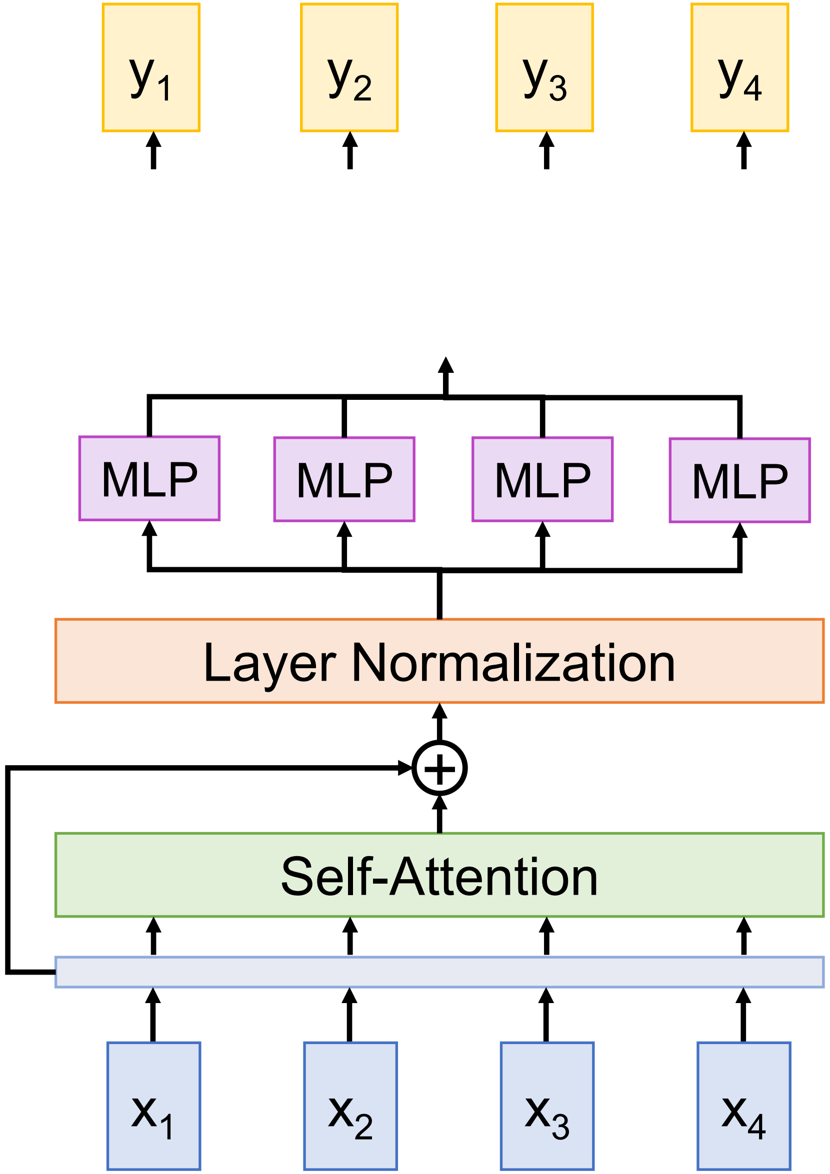
The Transformer

MLP independently on each vector

Residual connection

All vectors interact with each other



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

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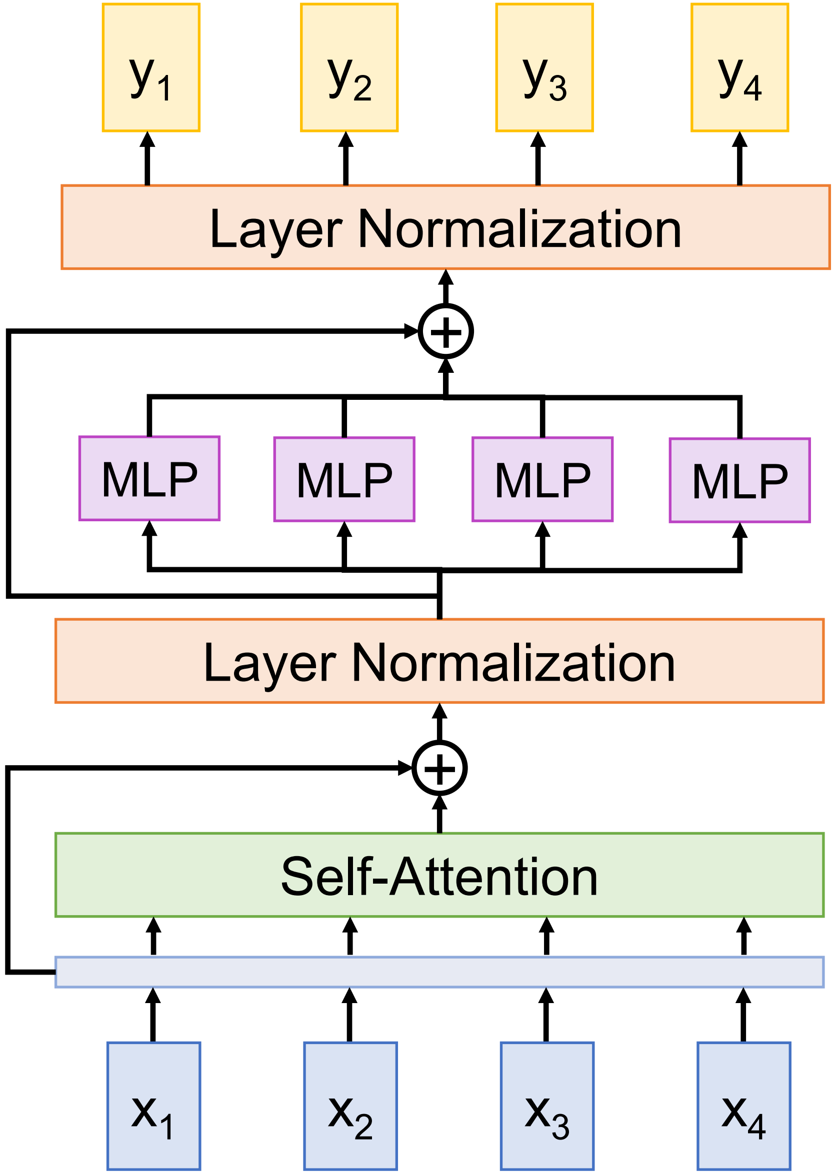
The Transformer

Residual connection

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

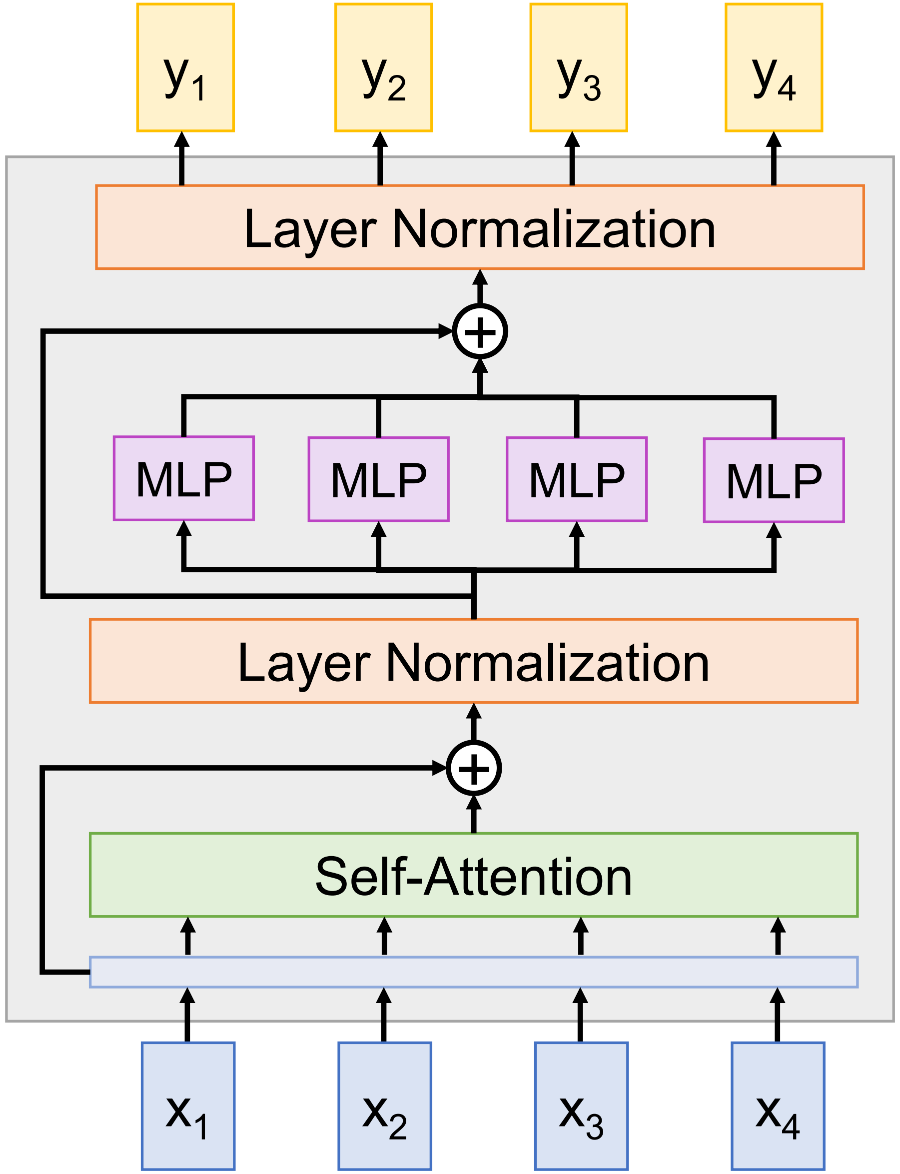
The Transformer

<u>**Transformer Block**</u>:
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

Slide credit: Justin Johnson

The Transformer

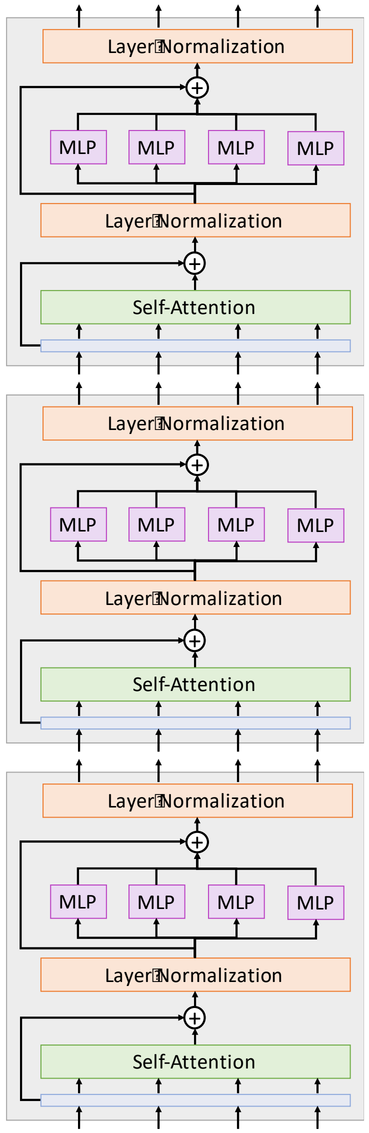
<u>**Transformer Block**</u>**:**
Input: Set of vectors x
Output: Set of vectors y

Self-attention is the only interaction between vectors!

Layer norm and MLP work independently per vector

Highly scalable, highly parallelizable

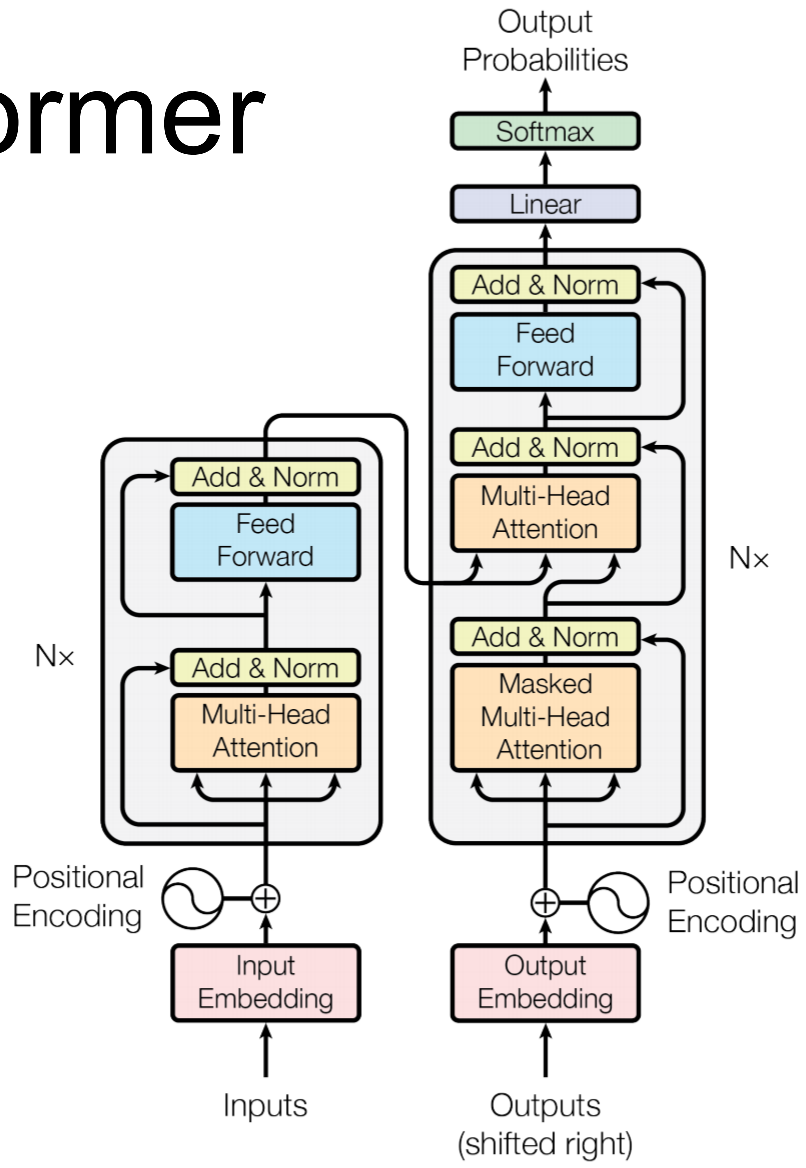
A **Transformer** is a sequence of transformer blocks



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

Slide credit: Justin Johnson

The Transformer



Encoder-Decoder

Details:

- Tokenization is messy! Trained chunking mechanism
- Position encoding
  - sin/cos: Normalized, nearby tokens have similar values, etc.
  - Added to input embedding
- When to use decoder-only versus encoder-decoder model is open problem
  - GPT is decoder only!

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

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
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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
+ 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

Task: Train for next-token prediction on massive web-scale corpus

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/

Jean Maillard

Jean Maillard is a Research Scientist on the Language And Translation Technologies Team (LATTE) at Facebook AI. His research interests within NLP include word- and sentence-level semantics, structured prediction, and low-resource languages. Prior to joining Facebook in 2019, he

Module 3 Lesson 12 (M3L12) on Dropbox

https://www.dropbox.com/sh/iviro188gq0b4vs/AADdHxX_Uy1TkpF_yvIzX0nPa?dl=0

- **Recall:** language models estimate the probability of sequences of words:

$$p(\boldsymbol{s}) = p(w_1, w_2, \ldots, w_n)$$

- ***More general task: Masked language modeling*** is a related ***pre-training task*** – an auxiliary task, different from the final task we're really interested in, but which can help us achieve better performance by finding good initial parameters for the model.
- **Key idea:** Mask out (ignore) some parts of the input and then have model predict it
- By pre-training on masked language modeling before training on our final task, it is usually possible to obtain higher performance than by simply training on the final task.

Masked Self-Attention Layer

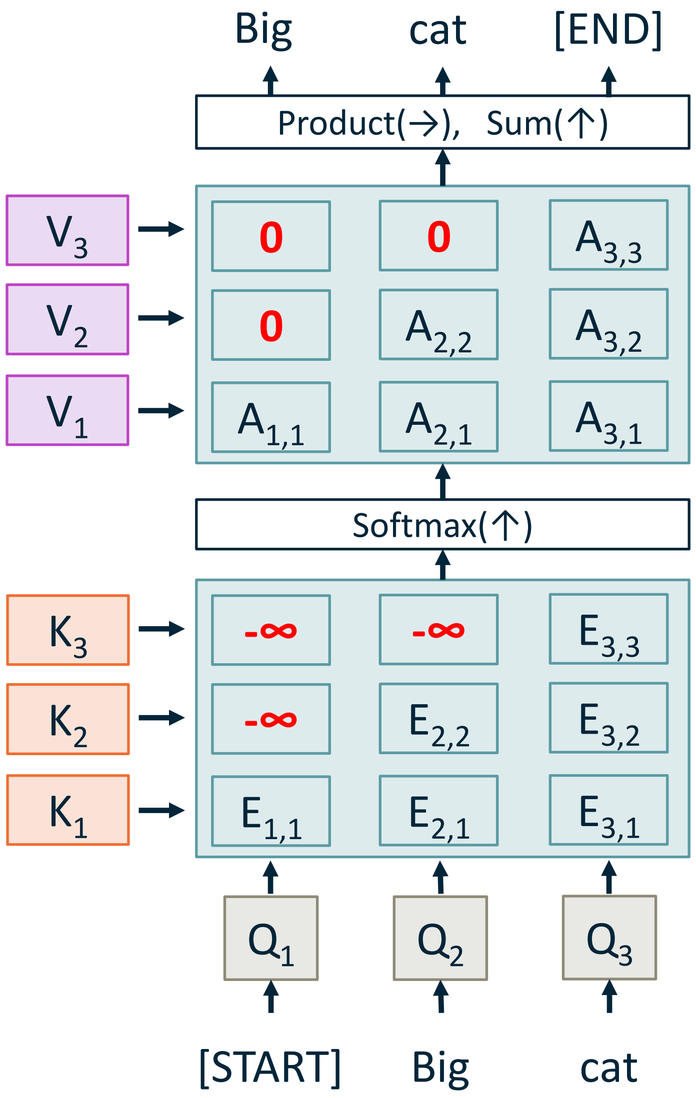
- **We can implement prediction of next word as causal masked language modeling**

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

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

Used for language modeling (predict next word)



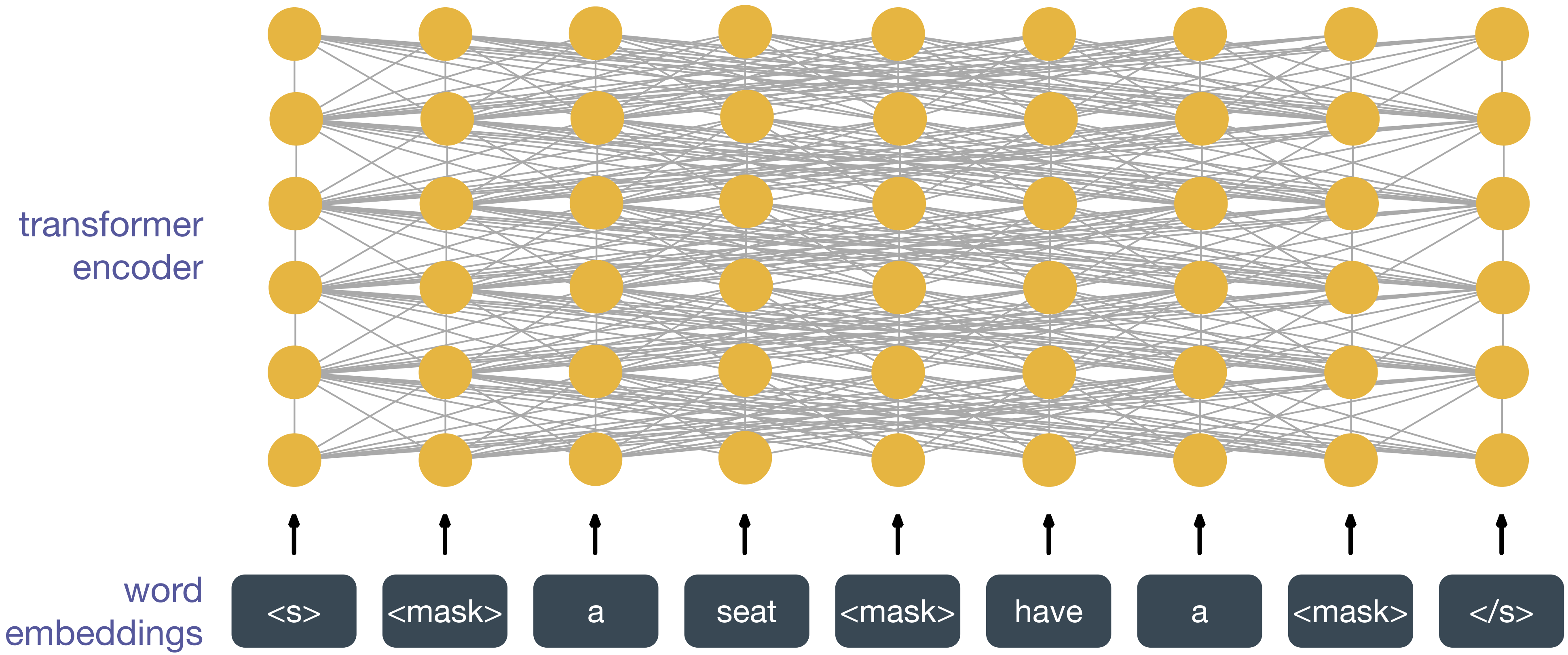
But the idea is more general!

take | a | seat | , | have | a | drink

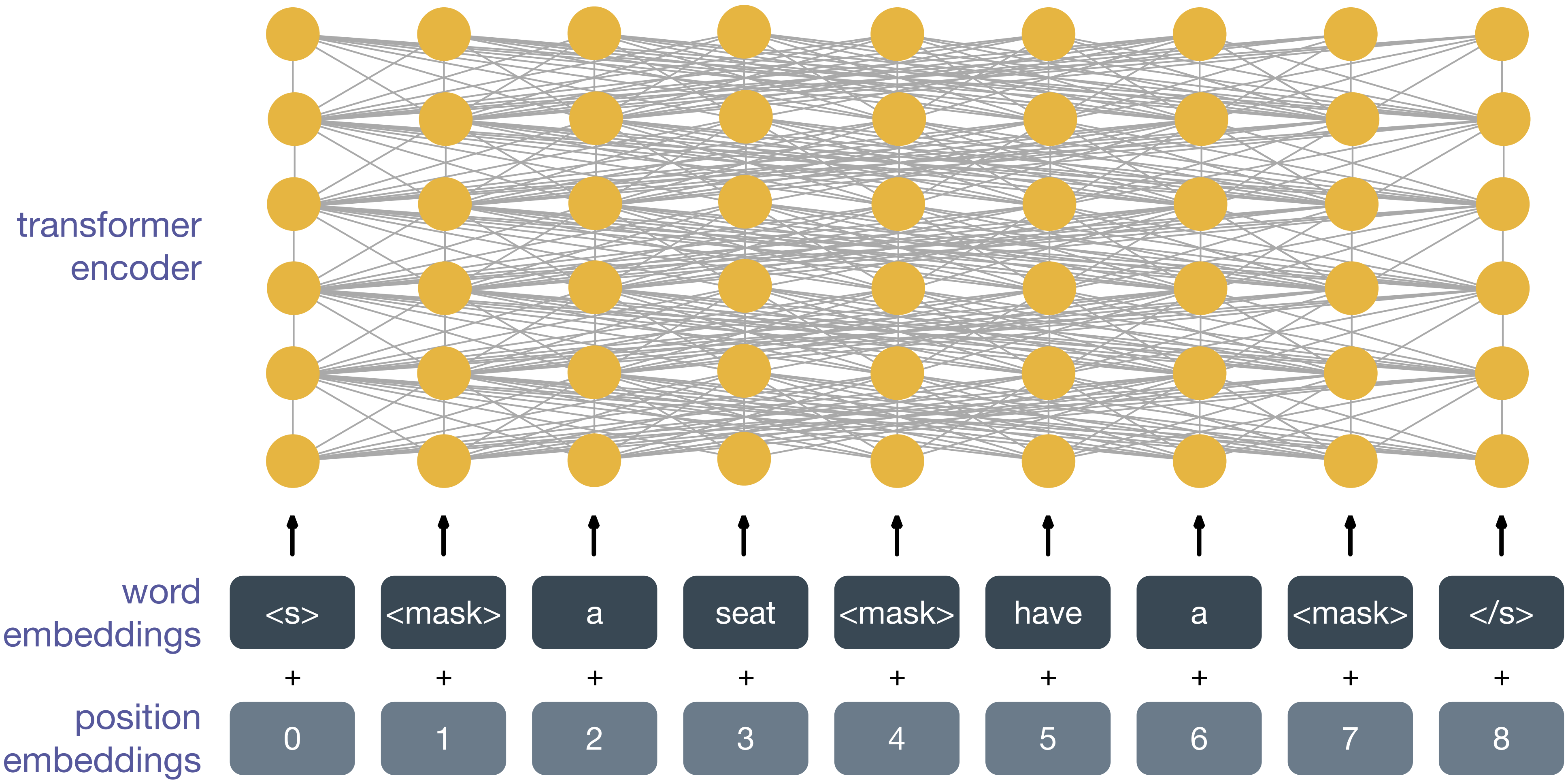
Masked Language Models

<s> <mask> a seat <mask> have a <mask> </s>

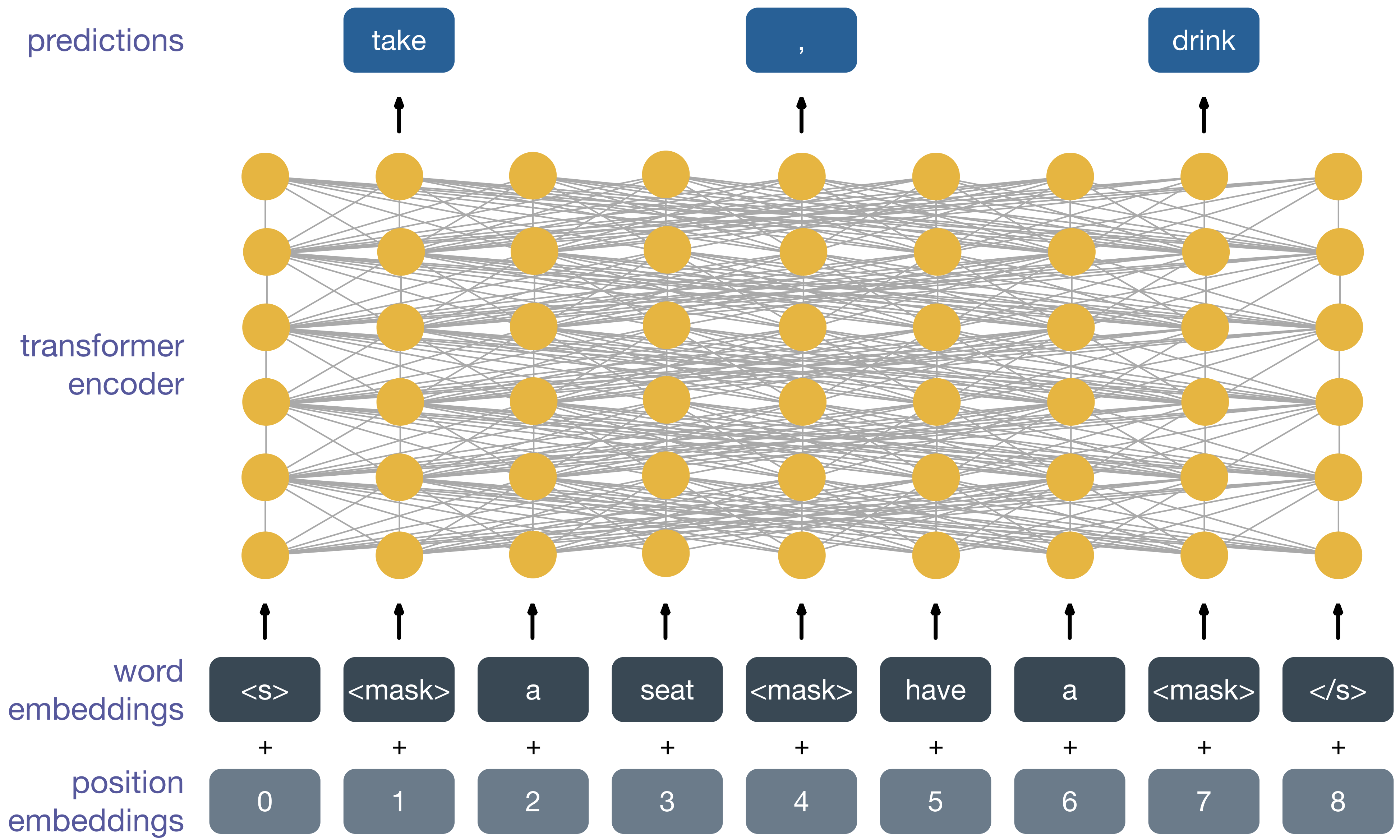
Masked Language Models



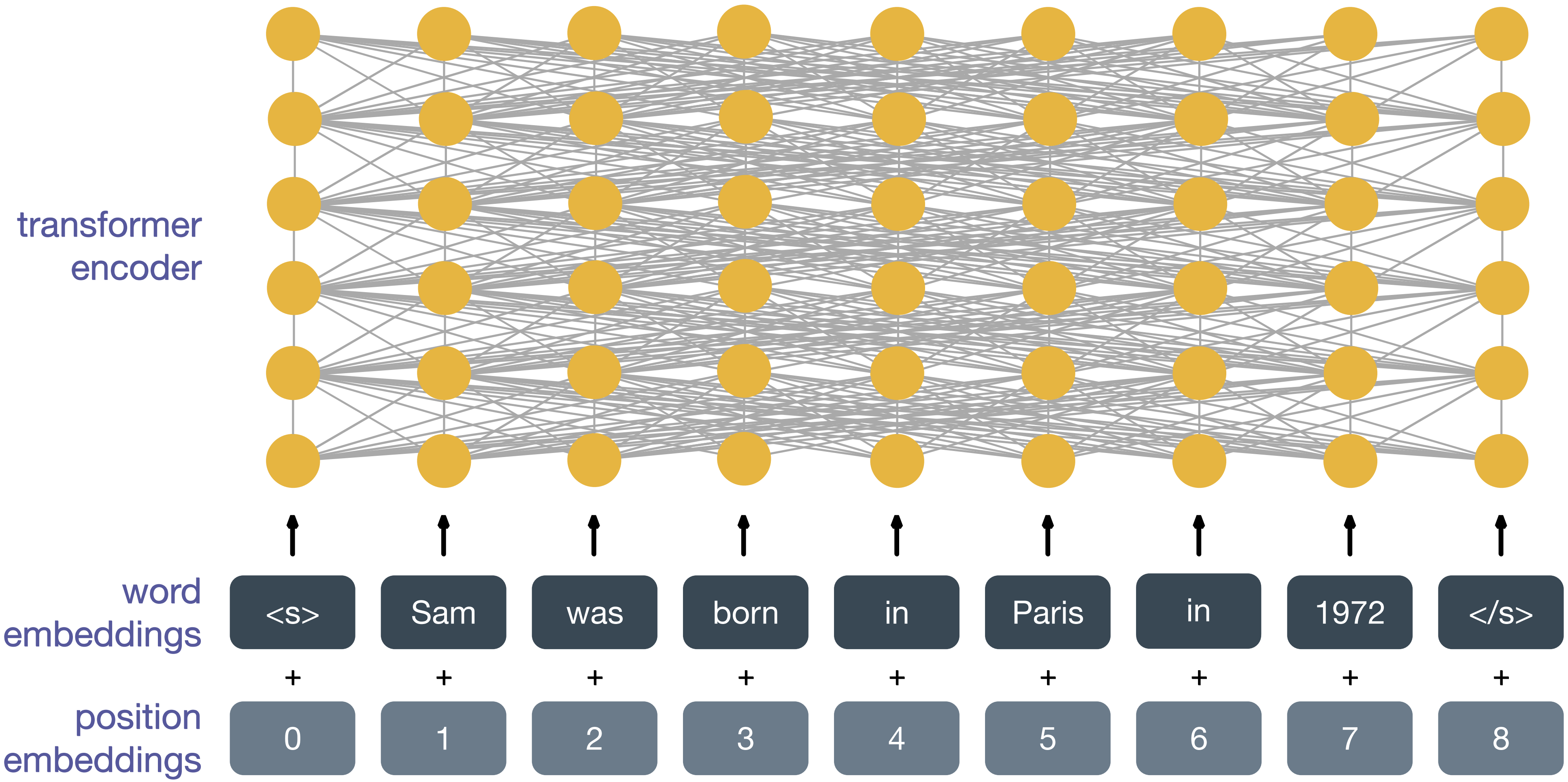
Masked Language Models



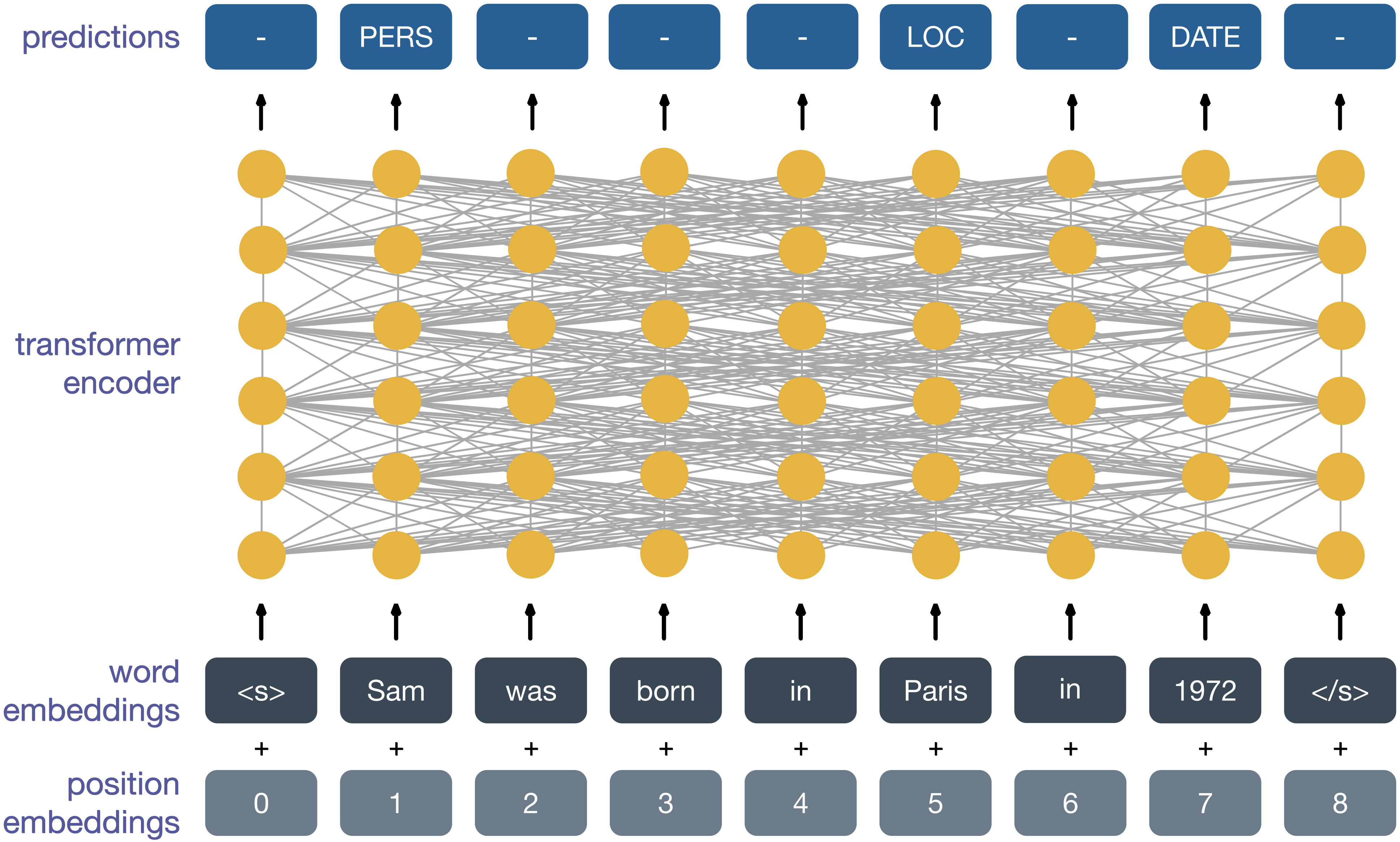
Masked Language Models



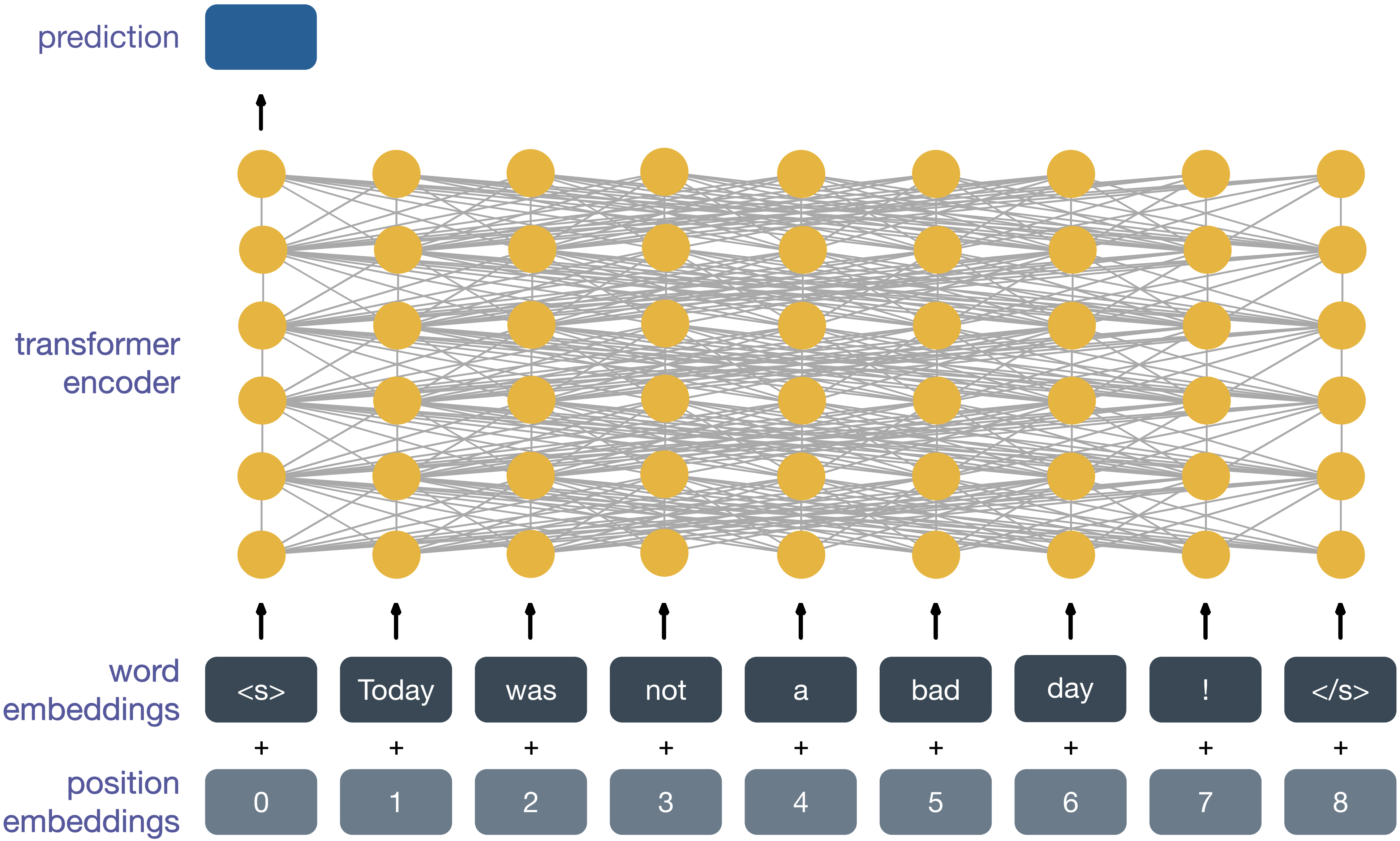
Self-Supervised: Masked Language Models



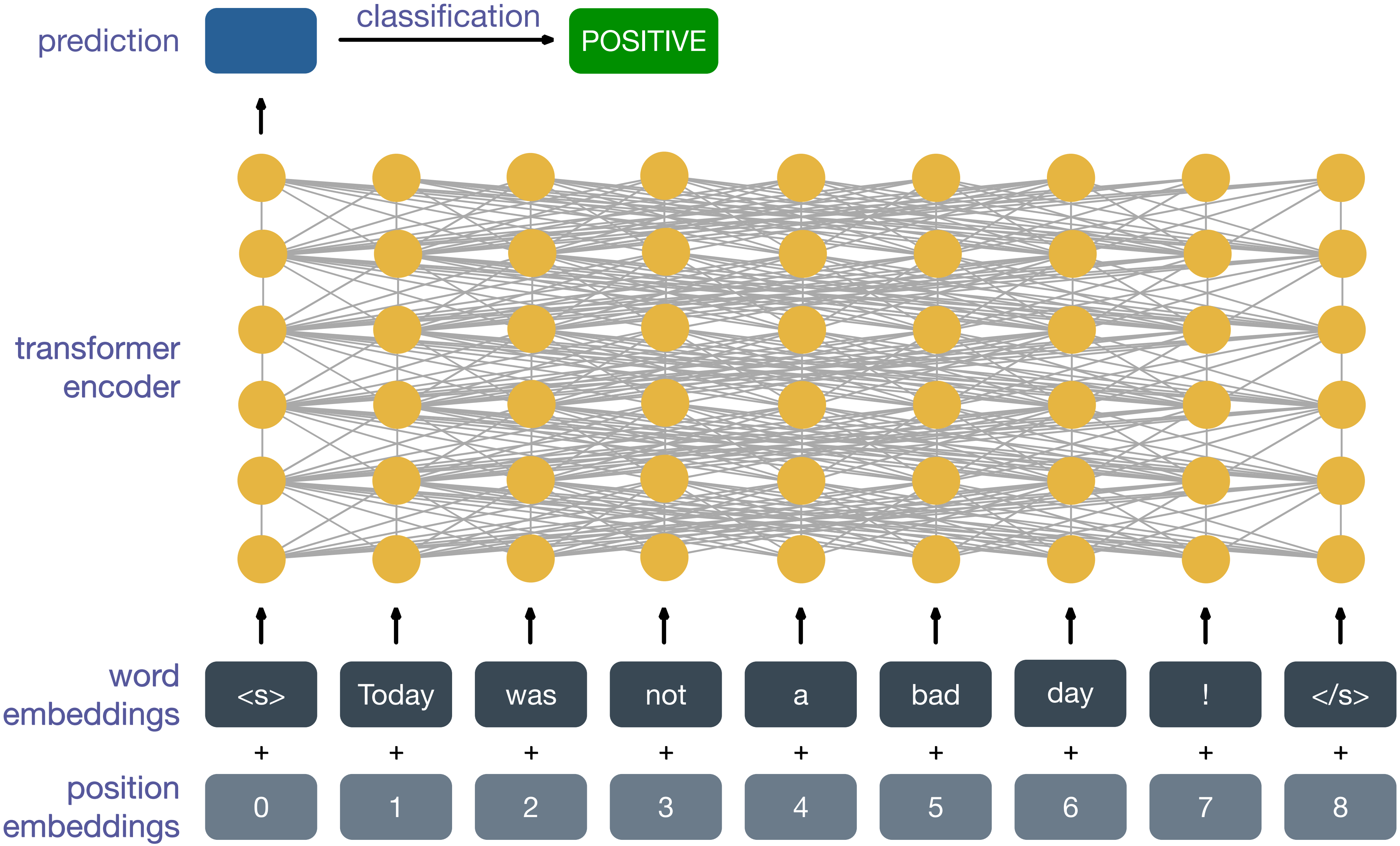
Supervised: Token-level Tasks



Supervised: Token-level Tasks



Supervised: Sentence-level Tasks



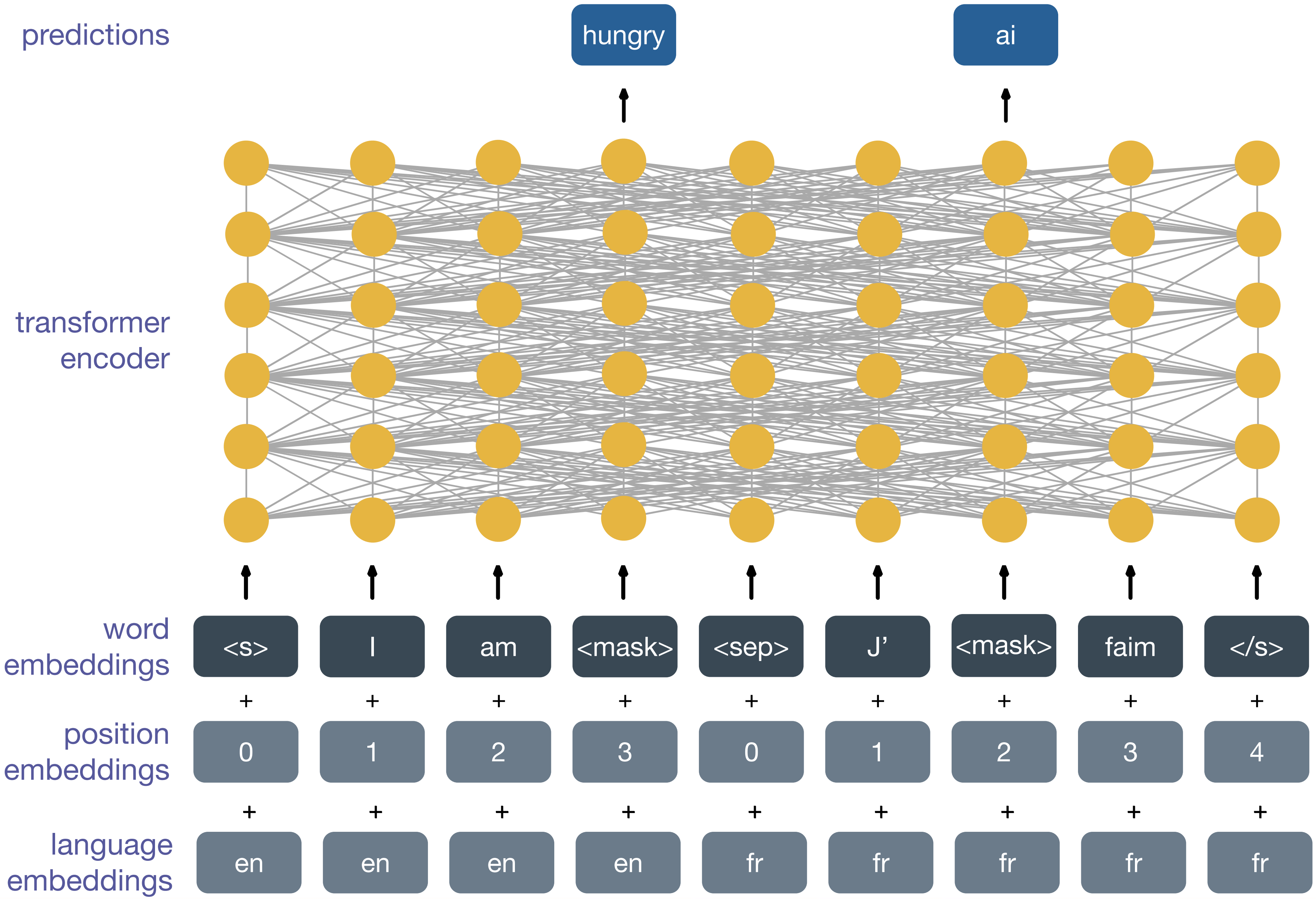
Supervised: Sentence-level Tasks

I am hungry J’ ai faim

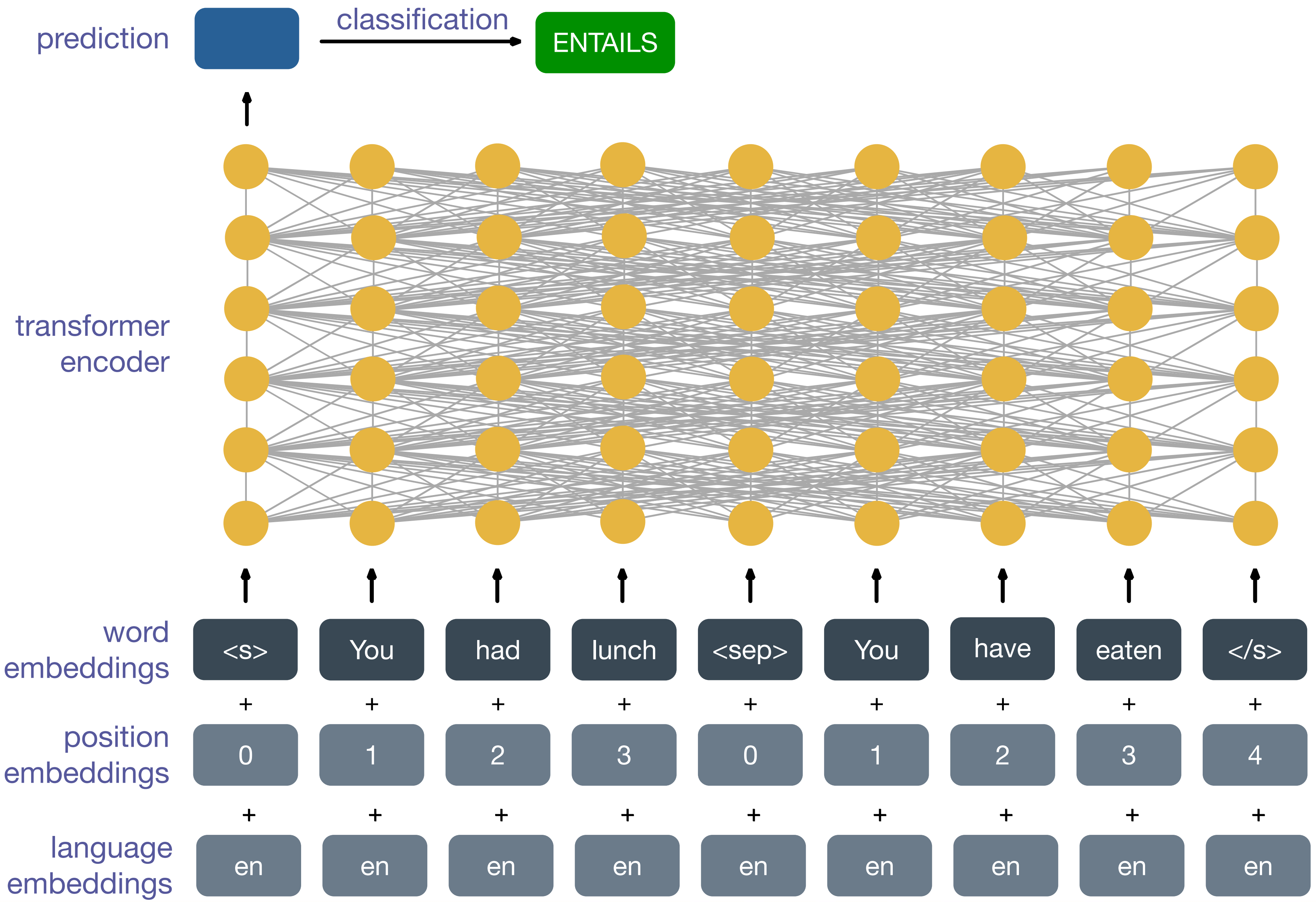
Cross-lingual Masked Language Modeling

<s> I am <mask> <sep> J’ <mask> faim </s>

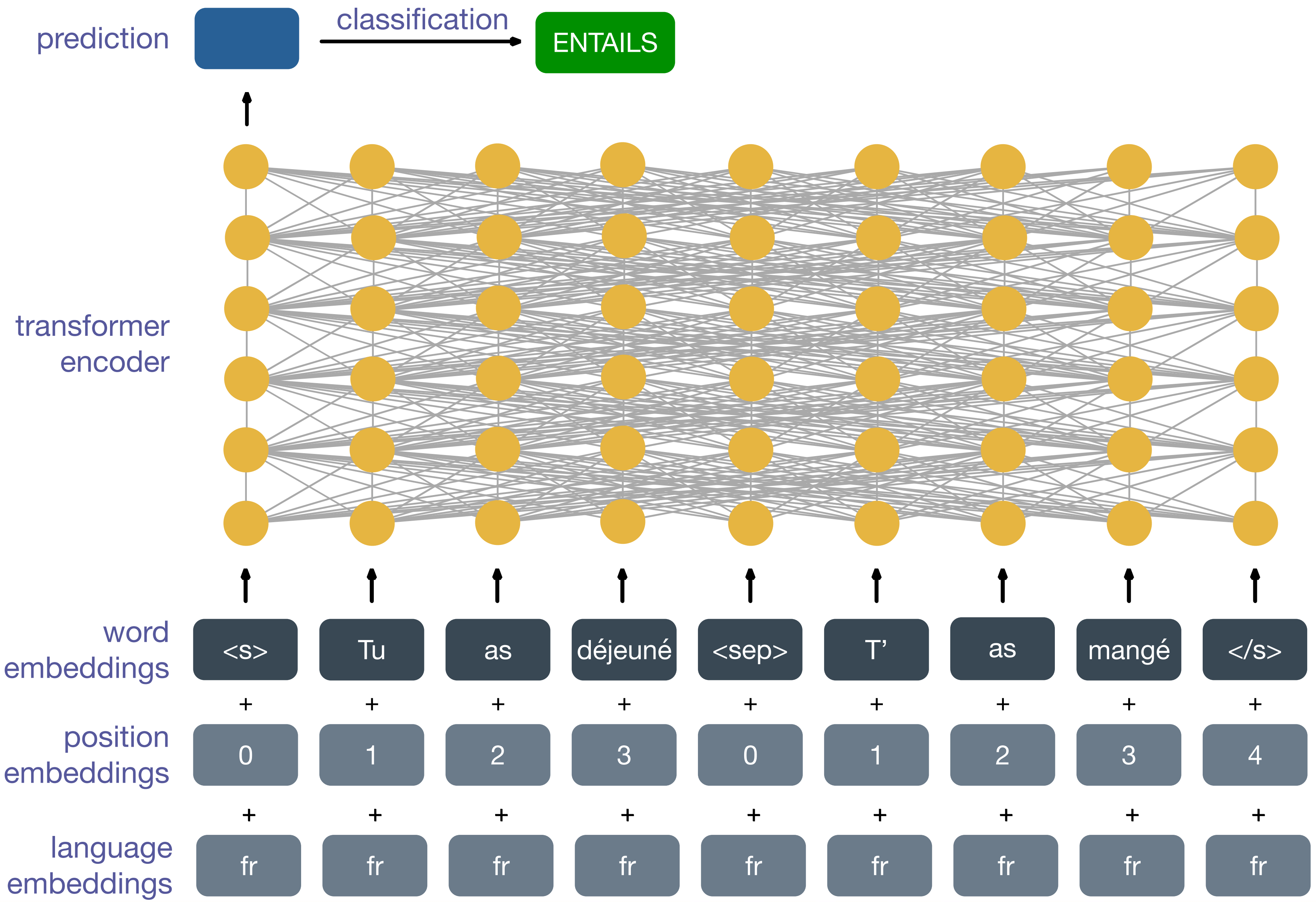
Cross-lingual Masked Language Modeling



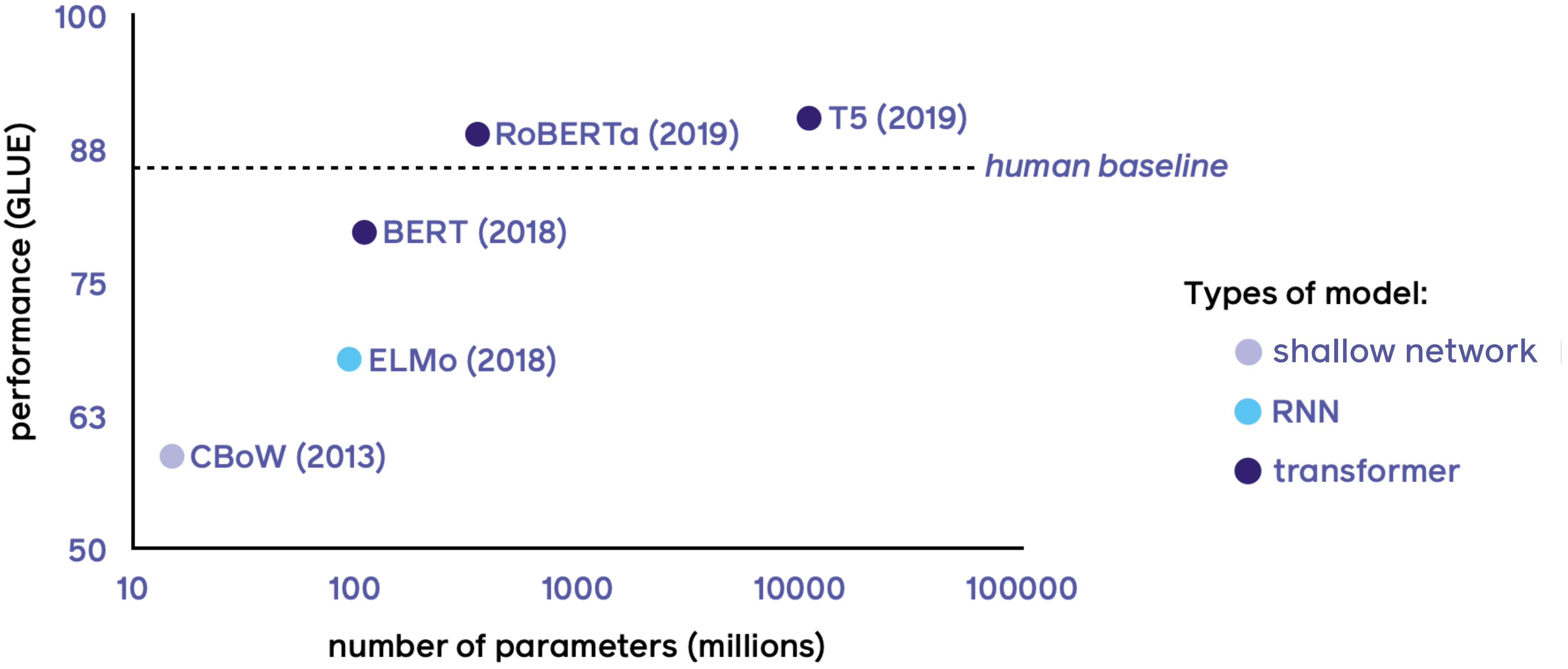
Cross-lingual Masked Language Modeling



Cross-lingual Task: Natural Language Inference



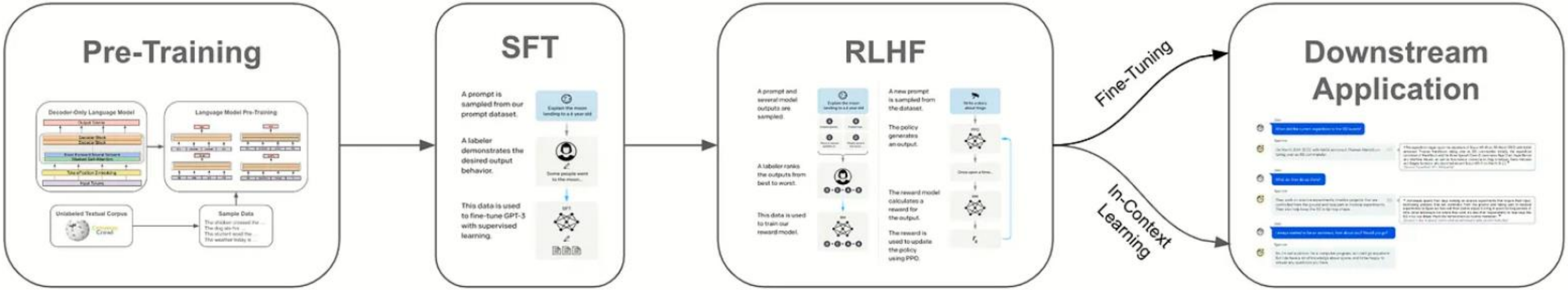
Cross-lingual Task: Natural Language Inference



Current rough guidelines:

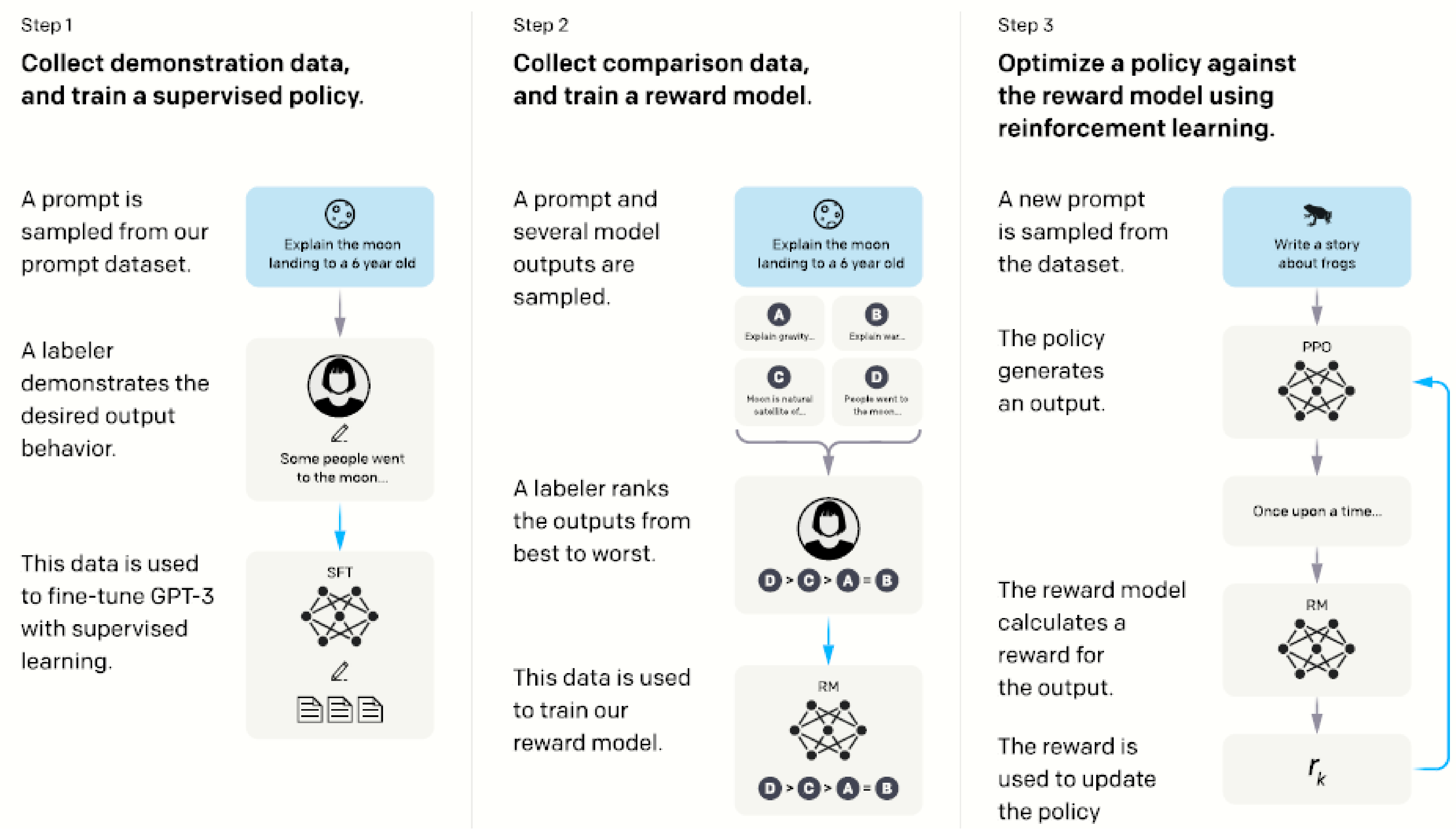
- For **self-supervised pre-training** of LLMs, use **causal mask** (predict next word) with **decoder-only model**
- Note: Large language models (ChatGPT) have several stages of training after pre-training (incl. reinforcement learning)
- For **classification/supervised tasks**, use **encoder-decoder models** often trained with **non-causal masked training**

Model Size in Perspective



Ouyang et al., Training language models to follow instructions with human feedback

Post-Training



Ouyang et al., Training language models to follow instructions with human feedback

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

ViLBERT: A Visolinguistic Transformer

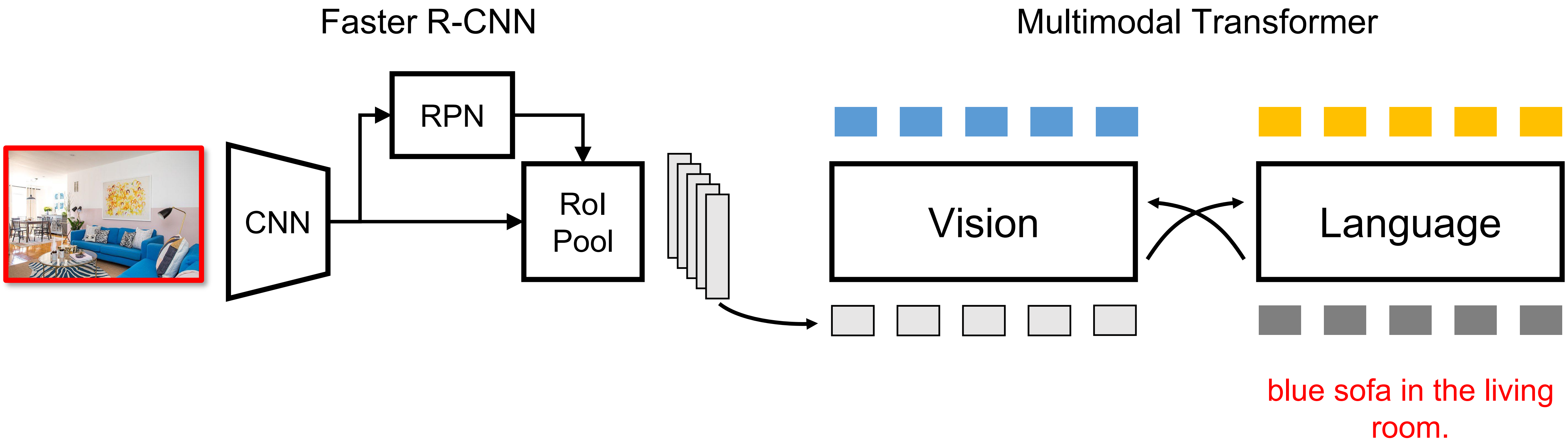
pop artist performs at the festival in a city.

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.

What about for just image inputs? Without Convolution?

Preprint. Under review.

[cs.CV] 22 Oct 2020

An Image is Worth 16x16 Words: Transformers for Image Recognition at Scale

Alexey Dosovitskiy*,†, Lucas Beyer*, Alexander Kolesnikov*, Dirk Weissenborn*, Xiaohua Zhai*, Thomas Unterthiner, Mostafa Dehghani, Matthias Minderer, Georg Heigold, Sylvain Gelly, Jakob Uszkoreit, Neil Houlsby*,†

*equal technical contribution, †equal advising

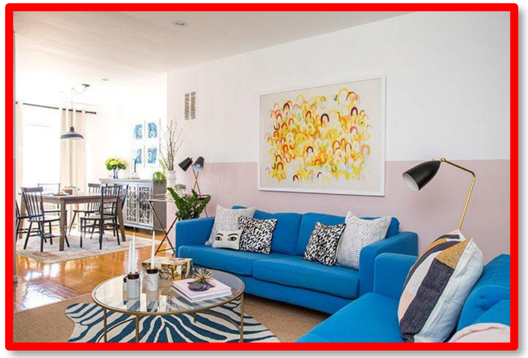
Google Research, Brain Team

{adosovitskiy, neilhoulsby}@google.com

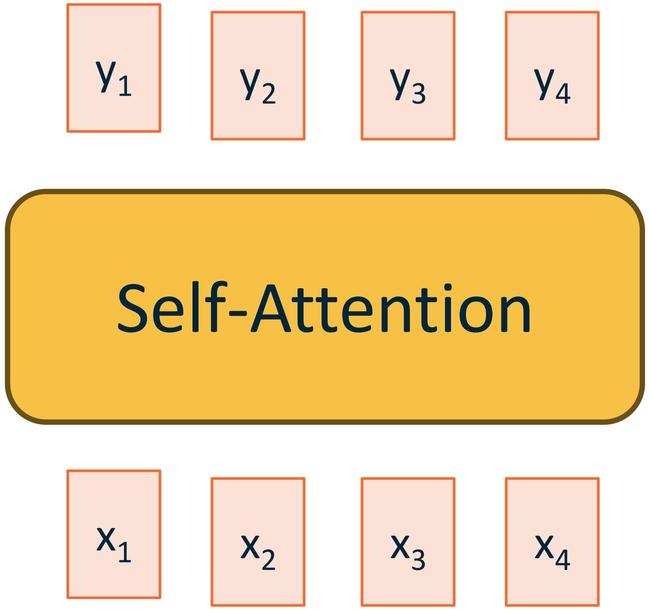
Abstract

While the Transformer architecture has become the de-facto standard for natural language processing tasks, its applications to computer vision remain limited. In vision, attention is either applied in conjunction with convolutional networks, or used to replace certain components of convolutional networks while keeping their overall structure in place. We show that this reliance on CNNs is not necessary and a pure transformer applied directly to sequences of image patches can perform very well on image classification tasks. When pre-trained on large amounts of data and transferred to multiple mid-sized or small image recognition benchmarks (ImageNet, CIFAR-100, VTAB, etc.), Vision Transformer (ViT) attains excellent results compared to state-of-the-art convolutional networks while requiring substantially fewer computational resources to train.[1]

Slide progression inspired by Soheil Feizi

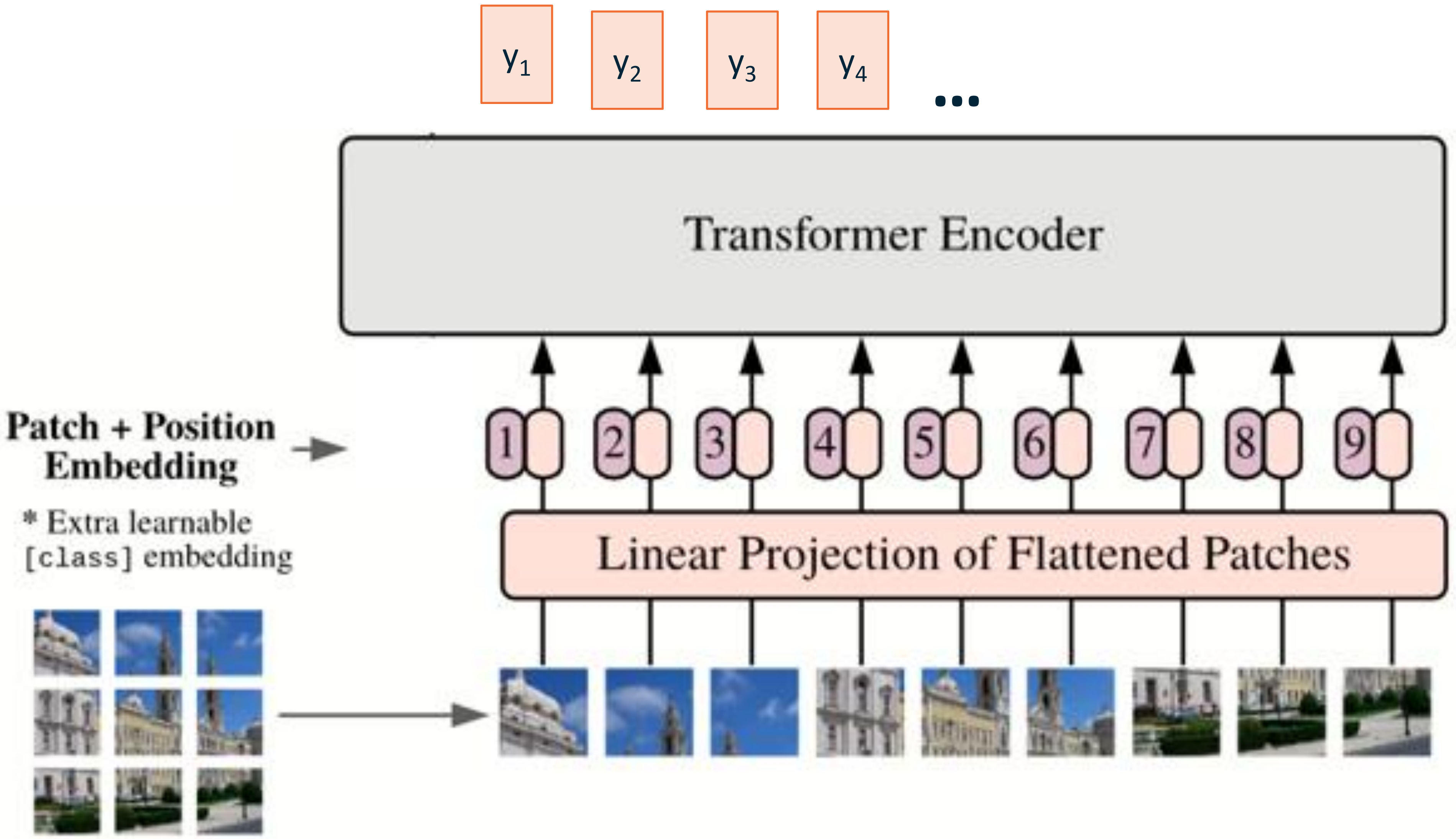


How should we "tokenize" images?



- Pixels? Too computationally intensive $O(n^2)$!
- Patches!

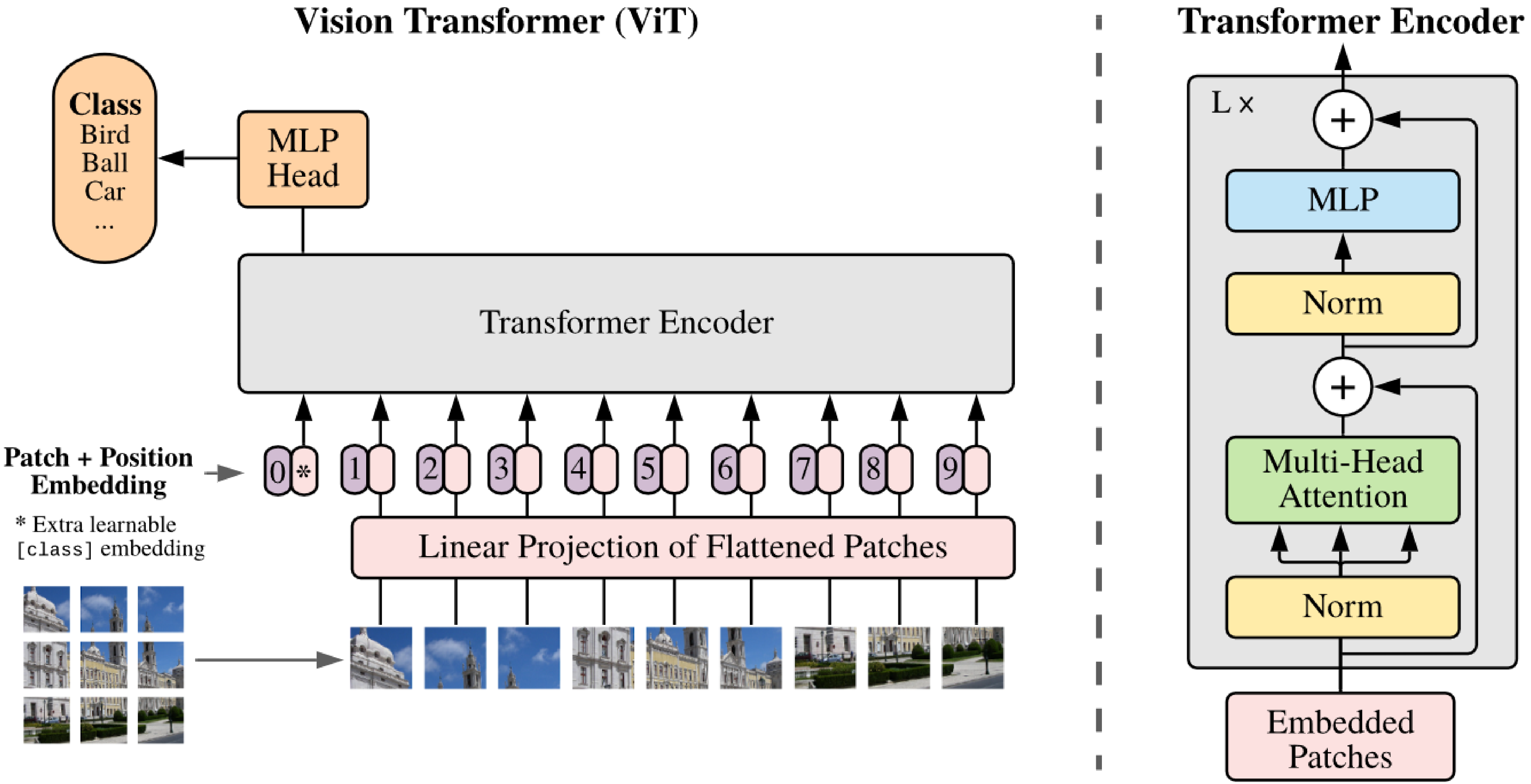
What to do with images?



- How do we do classification?

Patches as input to Self-Attention

Vision Transformer (ViT)



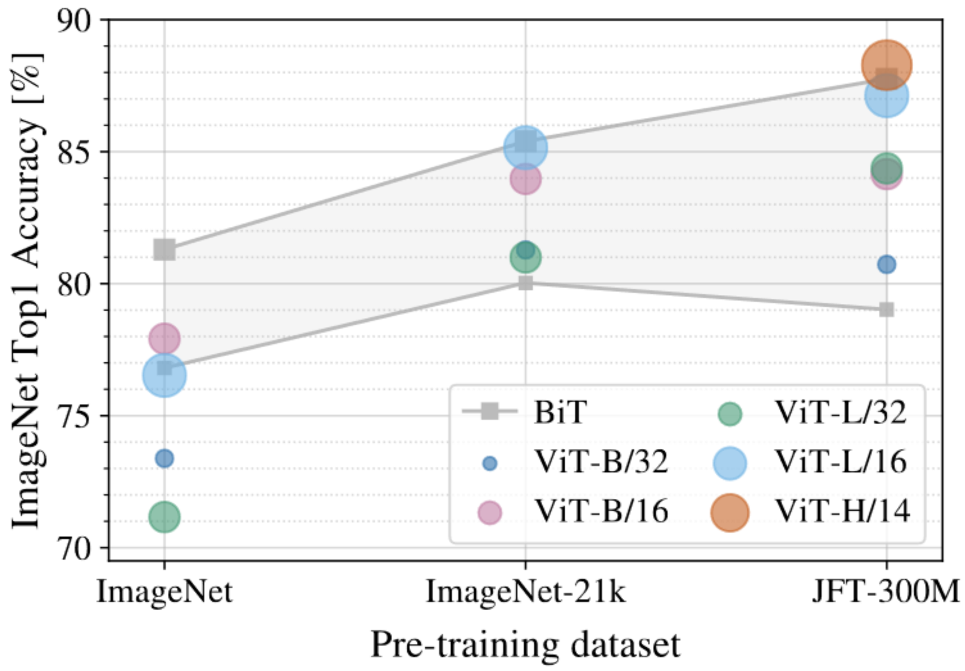


Figure 3: Transfer to ImageNet. While large ViT models perform worse than BiT ResNets (shaded area) when pre-trained on small datasets, they shine when pre-trained on larger datasets. Similarly, larger ViT variants overtake smaller ones as the dataset grows.

When trained on mid-sized datasets such as ImageNet, such models yield modest accuracies of a few percentage points below ResNets of comparable size.

Why?

Lacks some of the inductive biases:

- Spatial locality
- Translation equivariance

How can we overcome this?

https://paperswithcode.com/sota/image-classification-on-imagenet

However, the picture changes if the models are trained on larger datasets (14M-300M images). We find that large scale training trumps inductive bias.

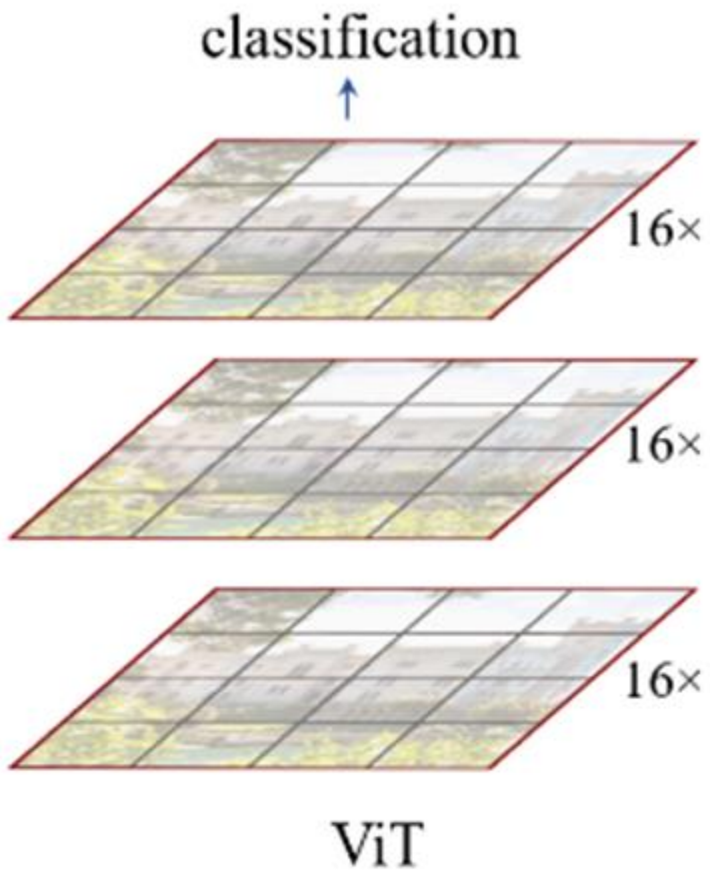
Model	Layers	Hidden size D	MLP size	Heads	Params
ViT-Base	12	768	3072	12	86M
ViT-Large	24	1024	4096	16	307M
ViT-Huge	32	1280	5120	16	632M

Table 1: Details of Vision Transformer model variants.

	Ours-JFT (ViT-H/14)	Ours-JFT (ViT-L/16)	Ours-I21K (ViT-L/16)	BiT-L (ResNet152x4)	Noisy Student (EfficientNet-L2)
ImageNet	**88.55** $\pm$ 0.04	87.76 $\pm$ 0.03	85.30 $\pm$ 0.02	87.54 $\pm$ 0.02	88.4/88.5*
ImageNet ReaL	**90.72** $\pm$ 0.05	90.54 $\pm$ 0.03	88.62 $\pm$ 0.05	90.54	90.55
CIFAR-10	**99.50** $\pm$ 0.06	99.42 $\pm$ 0.03	99.15 $\pm$ 0.03	99.37 $\pm$ 0.06	–
CIFAR-100	**94.55** $\pm$ 0.04	93.90 $\pm$ 0.05	93.25 $\pm$ 0.05	93.51 $\pm$ 0.08	–
Oxford-IIIT Pets	**97.56** $\pm$ 0.03	97.32 $\pm$ 0.11	94.67 $\pm$ 0.15	96.62 $\pm$ 0.23	–
Oxford Flowers-102	99.68 $\pm$ 0.02	**99.74** $\pm$ 0.00	99.61 $\pm$ 0.02	99.63 $\pm$ 0.03	–
VTAB (19 tasks)	**77.63** $\pm$ 0.23	76.28 $\pm$ 0.46	72.72 $\pm$ 0.21	76.29 $\pm$ 1.70	–
TPUv3-core-days	2.5k	0.68k	0.23k	9.9k	12.3k

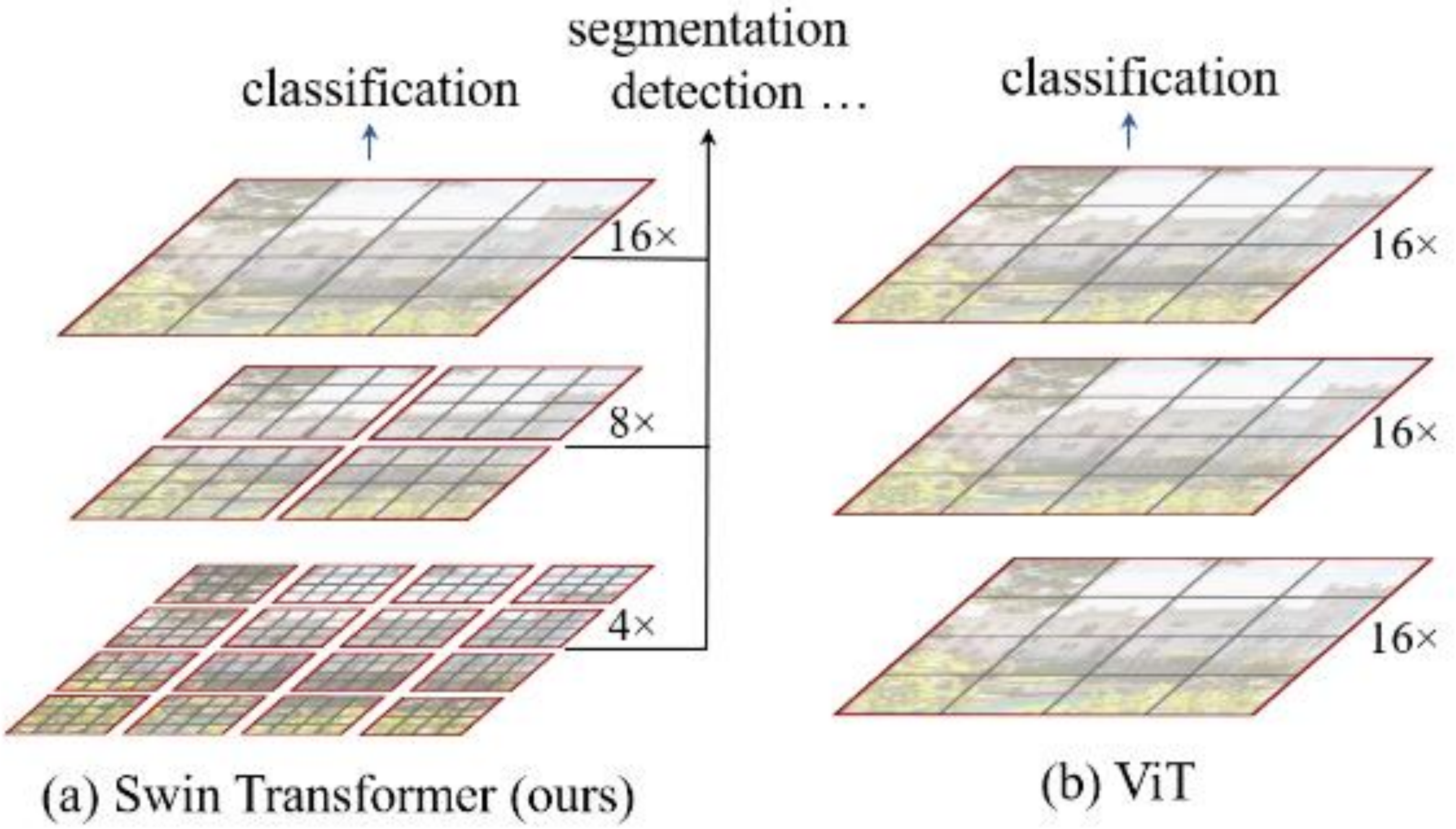
Can we add some inductive biases?

ViT Results



What is wrong with this?

Current deep ViT



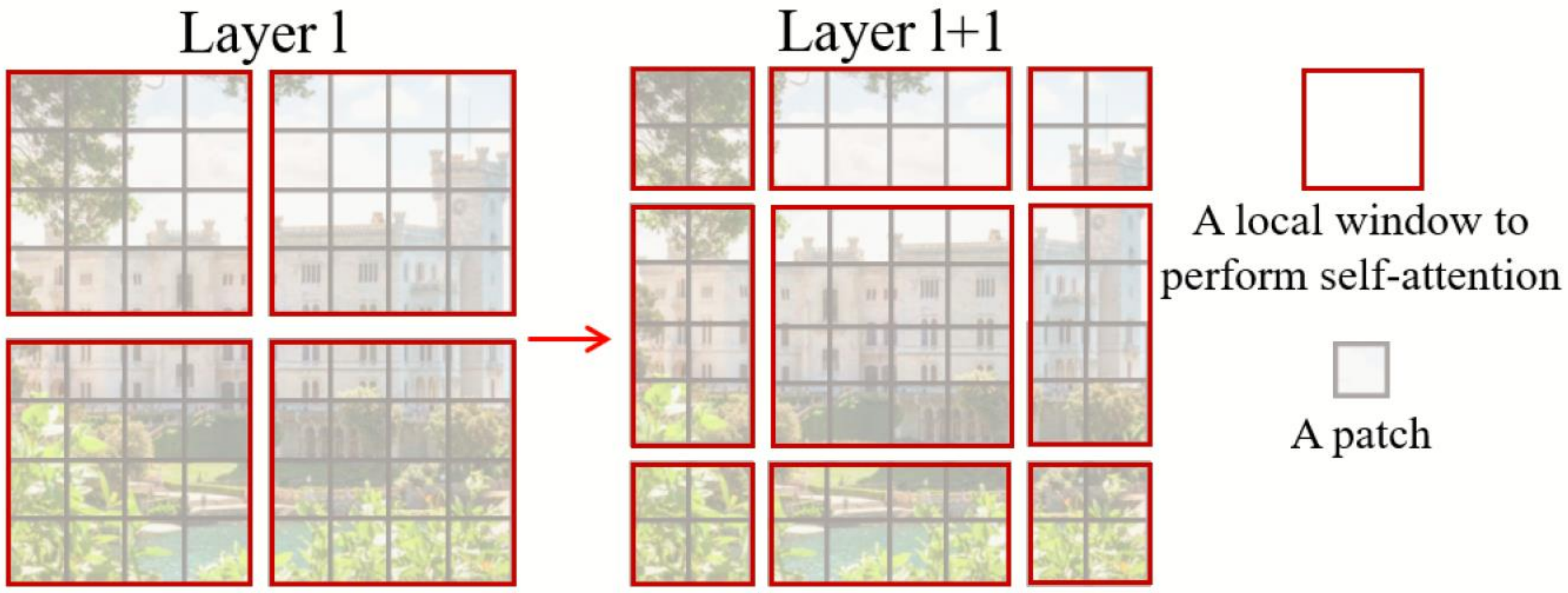
Ideas:

- Use smaller patches (4x4x3)
- Project them to lower dimension (4)
- Merge tokens at deeper levels
- Full attention => Window attention
    - => Shifted window attention

Swin Transformer: Hierarchical Vision Transformer using Shifted Windows
Ze Liu, Yutong Lin, Yue Cao, Han Hu, Yixuan Wei, Zheng Zhang, Stephen Lin, Baining Guo

Swin Transformers

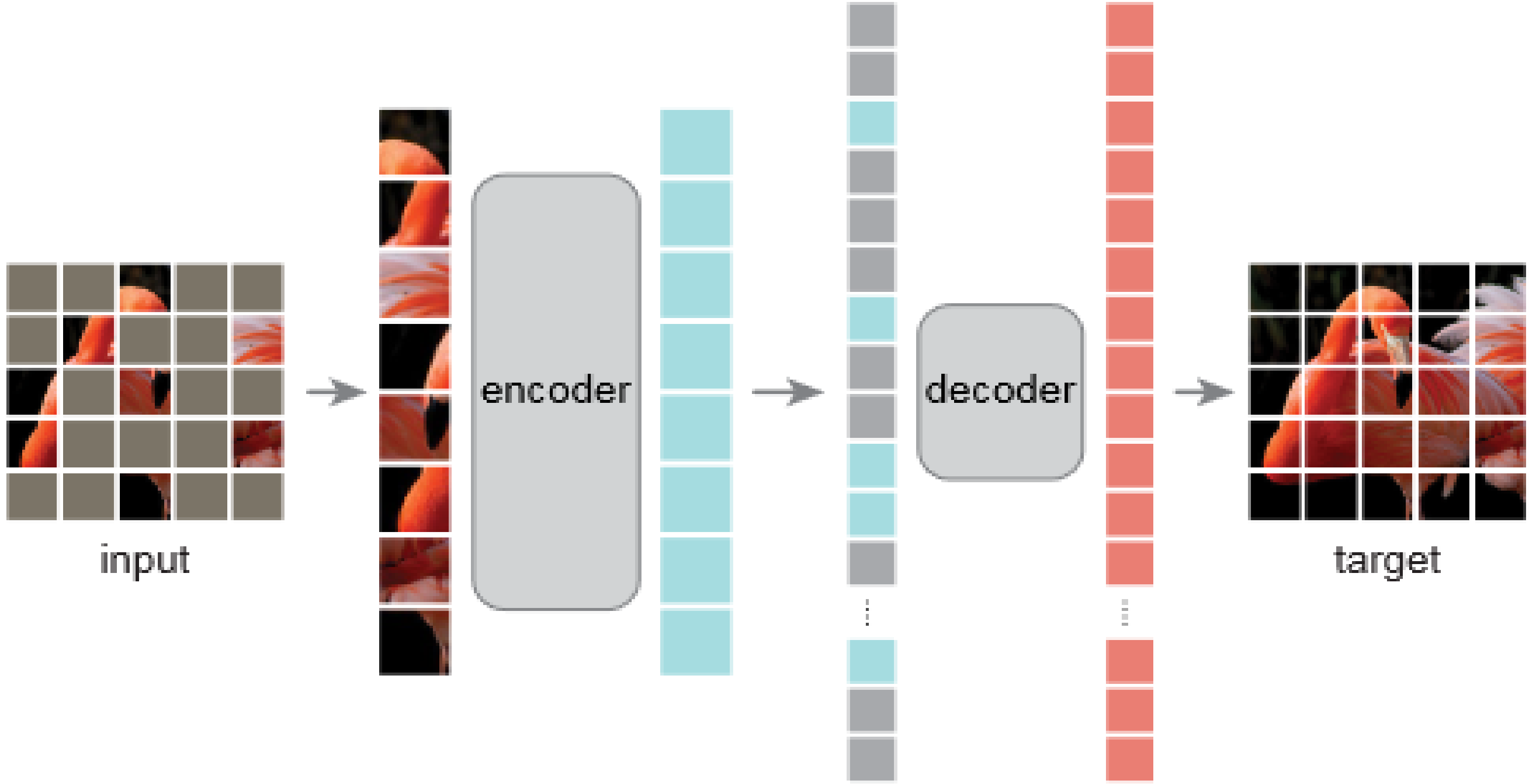
https://paperswithcode.com/sota/instance-segmentation-on-coco



Swin Transformer: Hierarchical Vision Transformer using Shifted Windows
Ze Liu, Yutong Lin, Yue Cao, Han Hu, Yixuan Wei, Zheng Zhang, Stephen Lin, Baining Guo

Shifted Window Attention

https://paperswithcode.com/sota/instance-segmentation-on-coco



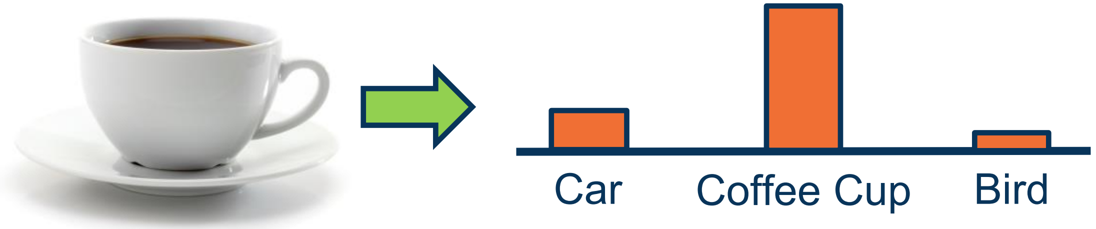
How can we learn unsupervised representations?

He et al., Masked Autoencoders Are Scalable Vision Learners

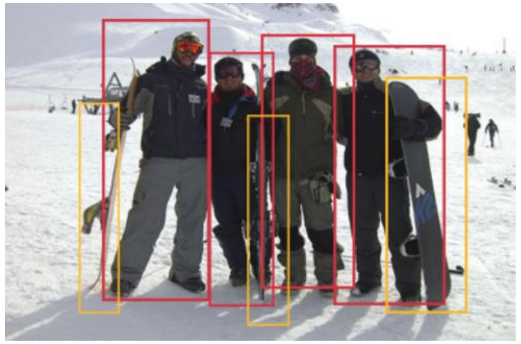
Masked Autoencoders

https://paperswithcode.com/sota/instance-segmentation-on-coco

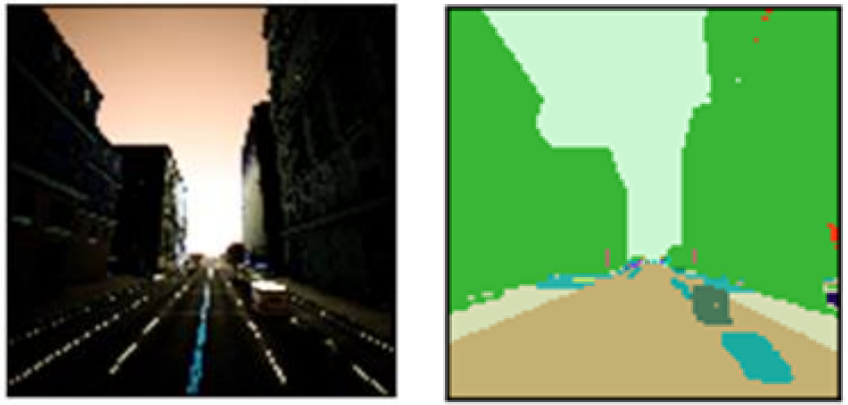
Image to Image CNNs



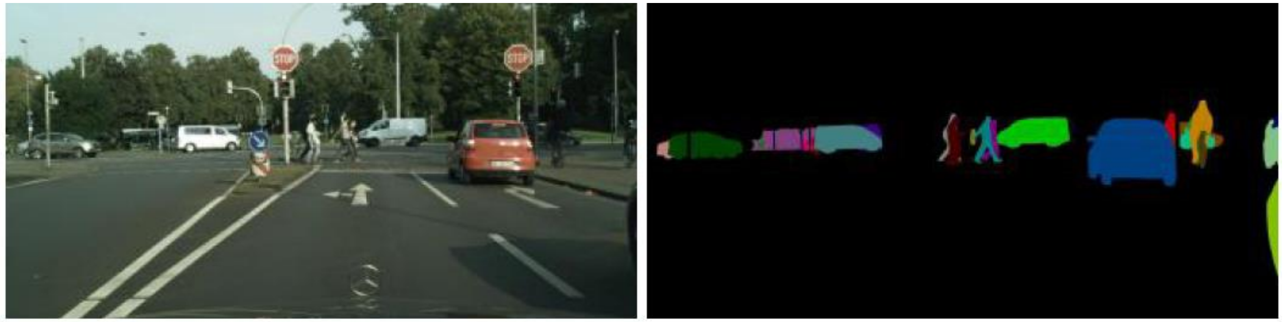
Classification
(Class distribution per image)



Object Detection
(List of bounding boxes with class distribution per box)



Semantic Segmentation
(Class distribution per pixel)



Instance Segmentation
(Class distribution per pixel with unique ID)

Computer Vision Tasks

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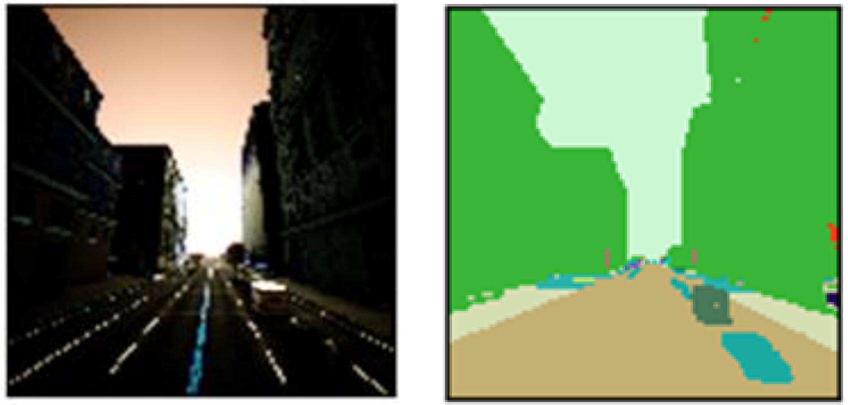
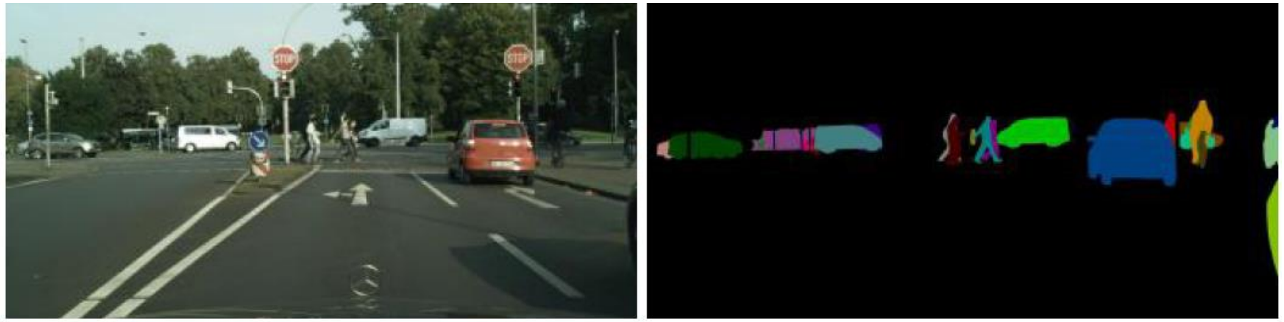
Given an image, output another image

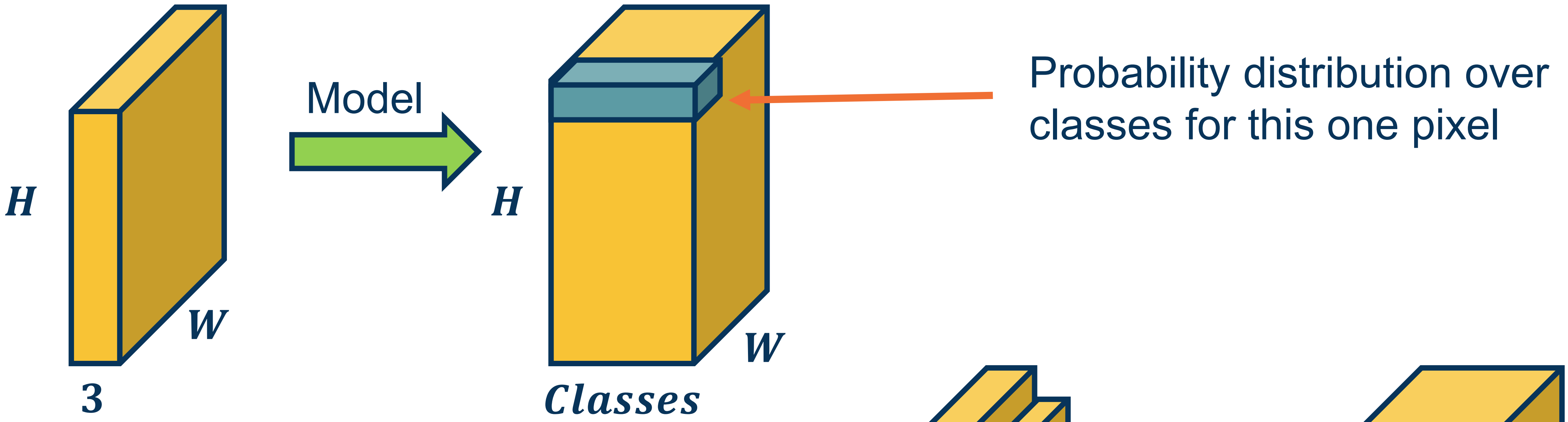
- Each output contains class distribution per pixel
- More generally an image-to-image problem

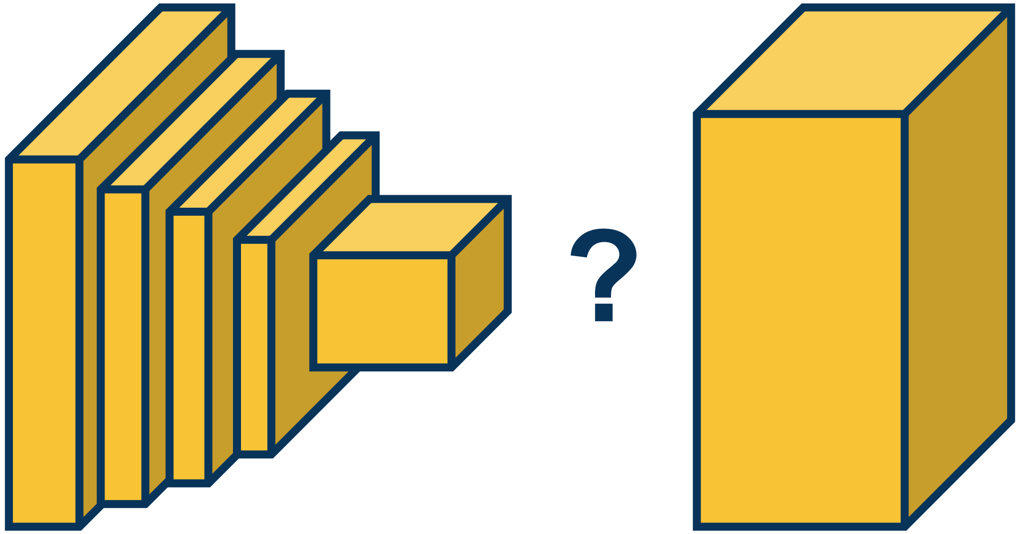


Semantic Segmentation
(Class distribution per pixel)

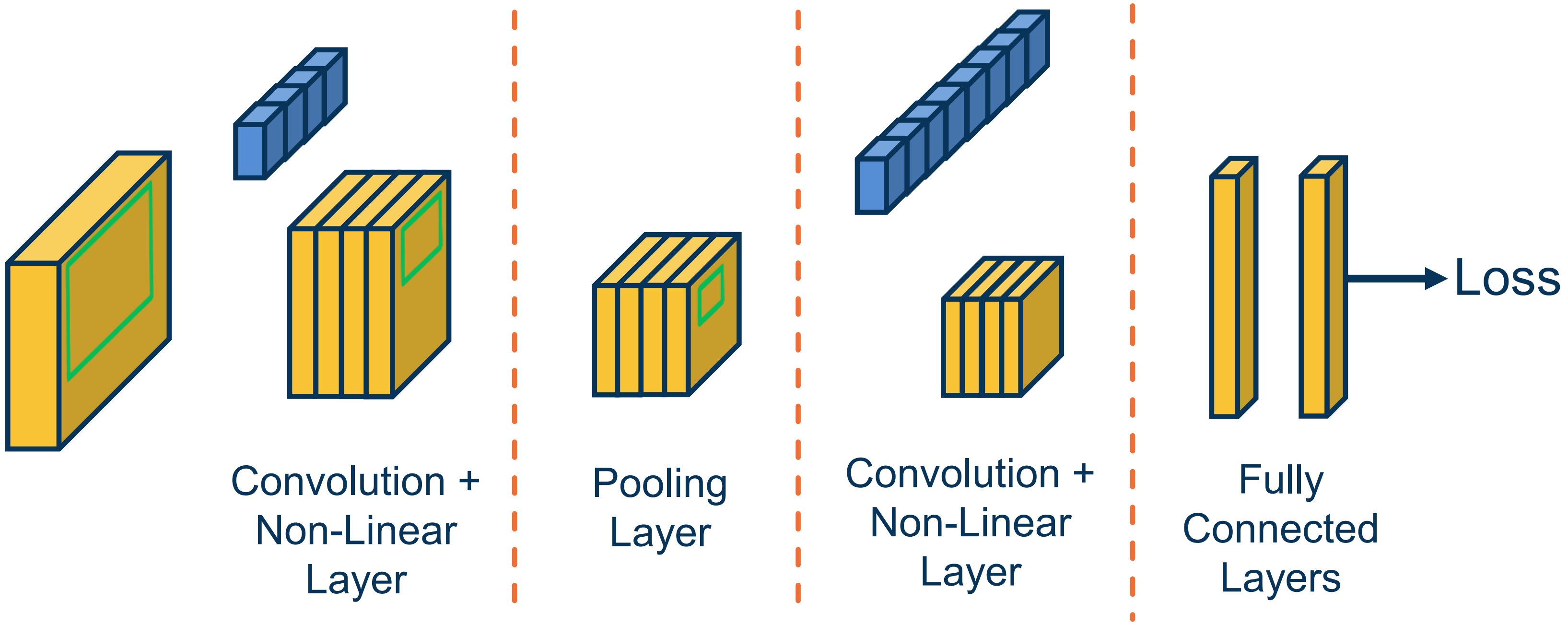


Instance Segmentation
(Class distribution per pixel with unique ID)





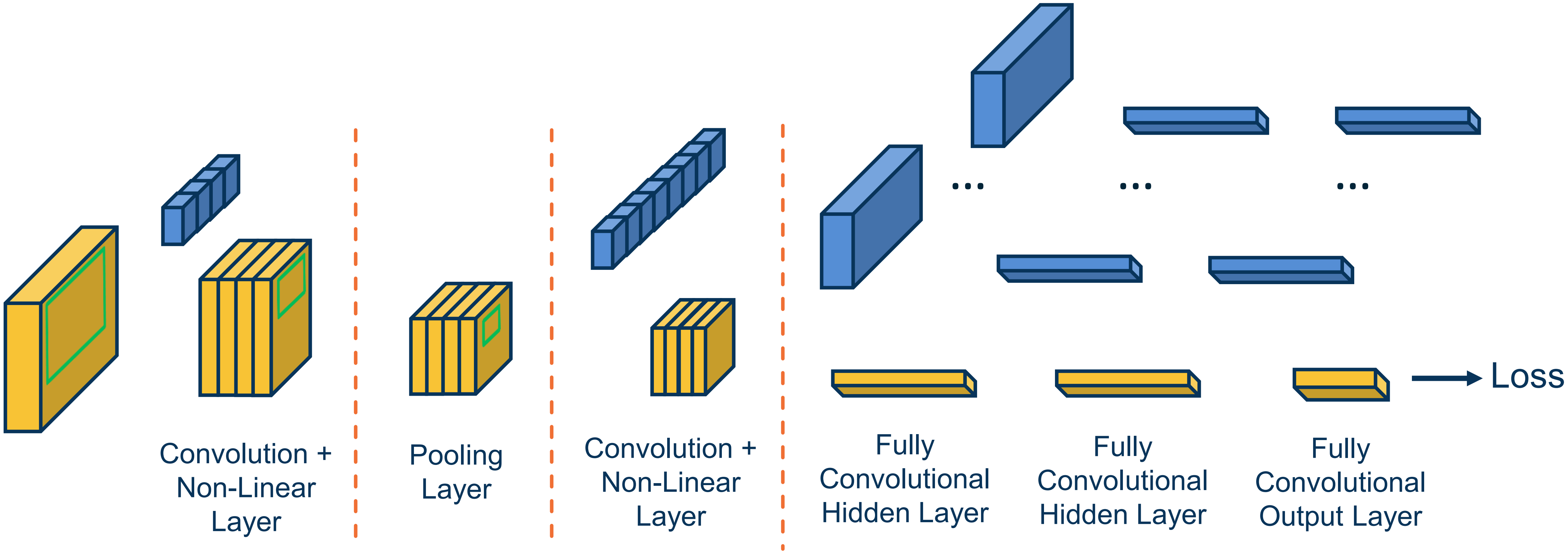
Input & Output



Fully connected layers no longer explicitly retain spatial information (though the network can still learn to do so)

Idea: Convert fully connected layer to convolution!

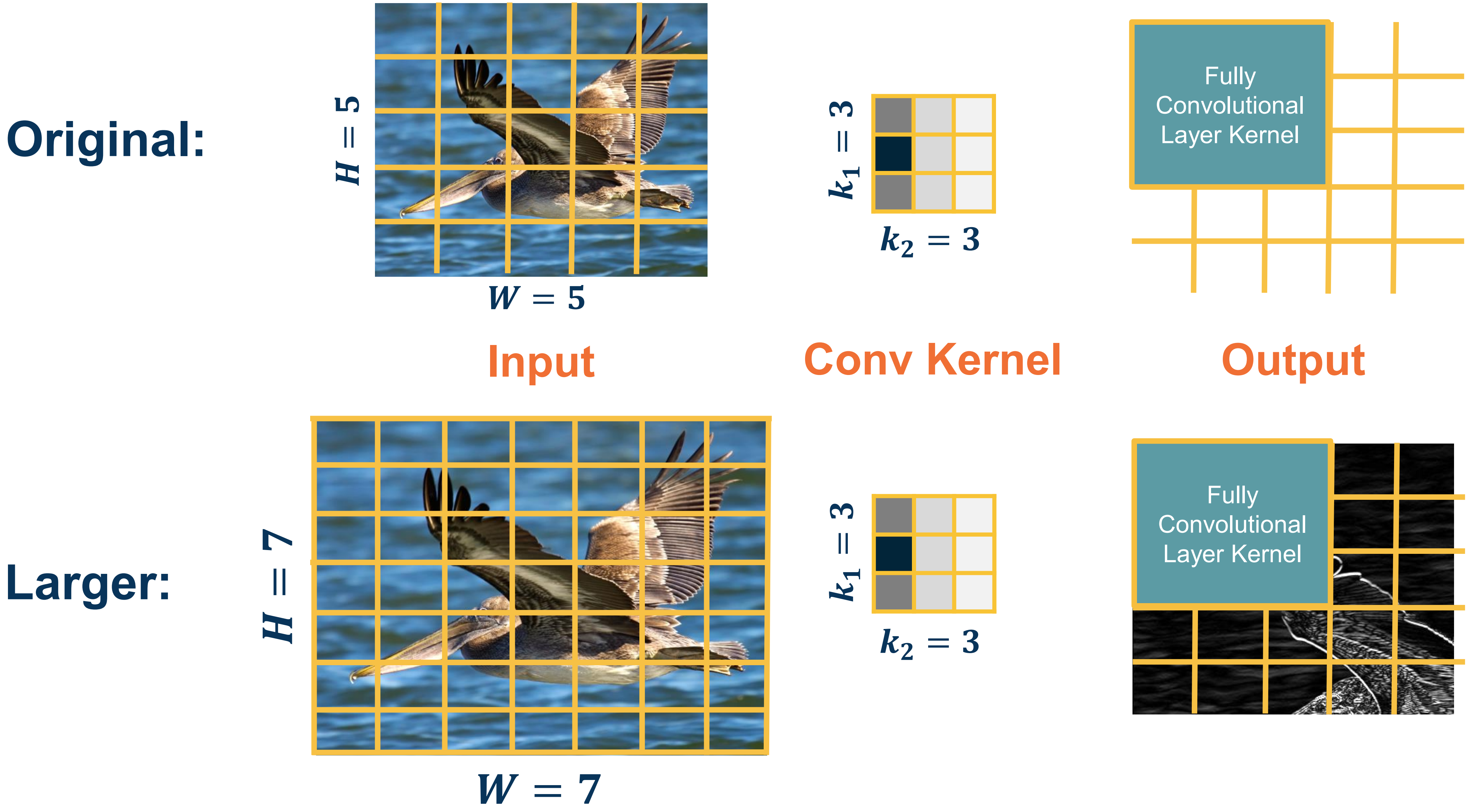
Idea 1: Fully-Convolutional Network



Each kernel has the size of entire input! (output is 1 scalar)

- This is equivalent to Wx+b!
- We have one kernel per output node

Converting FC Layers to Conv Layers



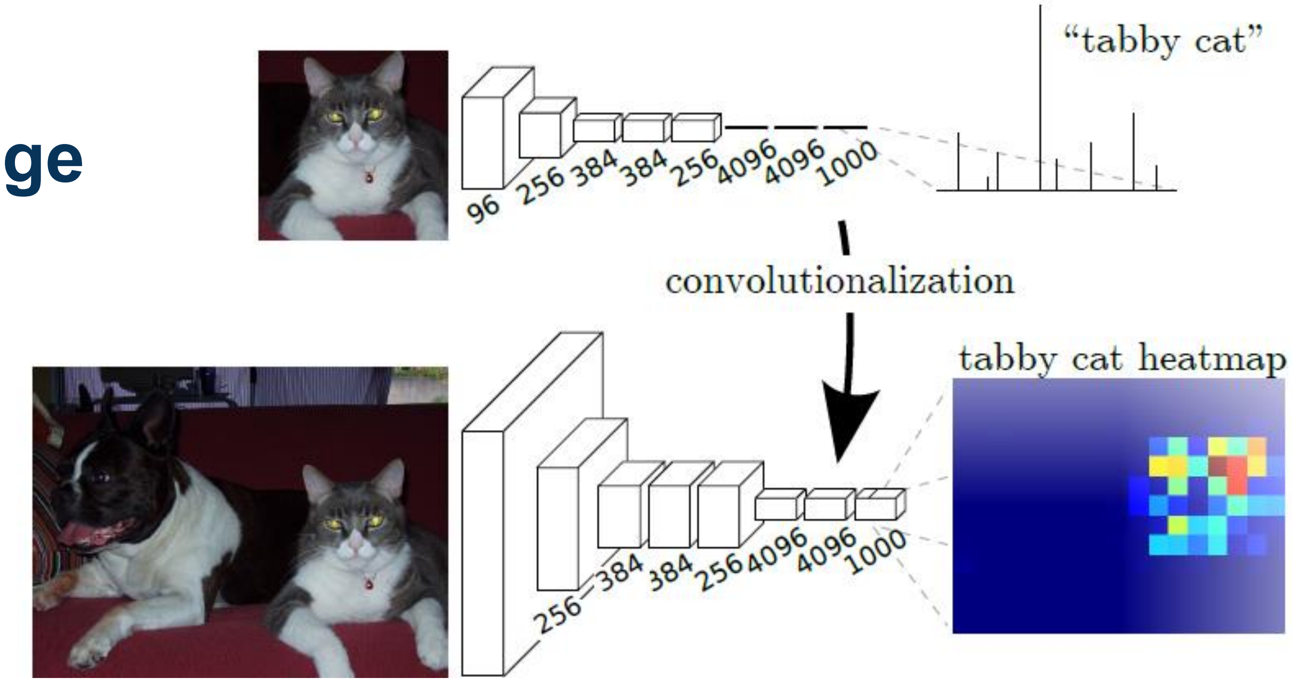
Same Kernel, Larger Input

Why does this matter?

- We can stride the “fully connected” classifier across larger inputs!
- Convolutions work on arbitrary input sizes (because of striding)

Original sized image

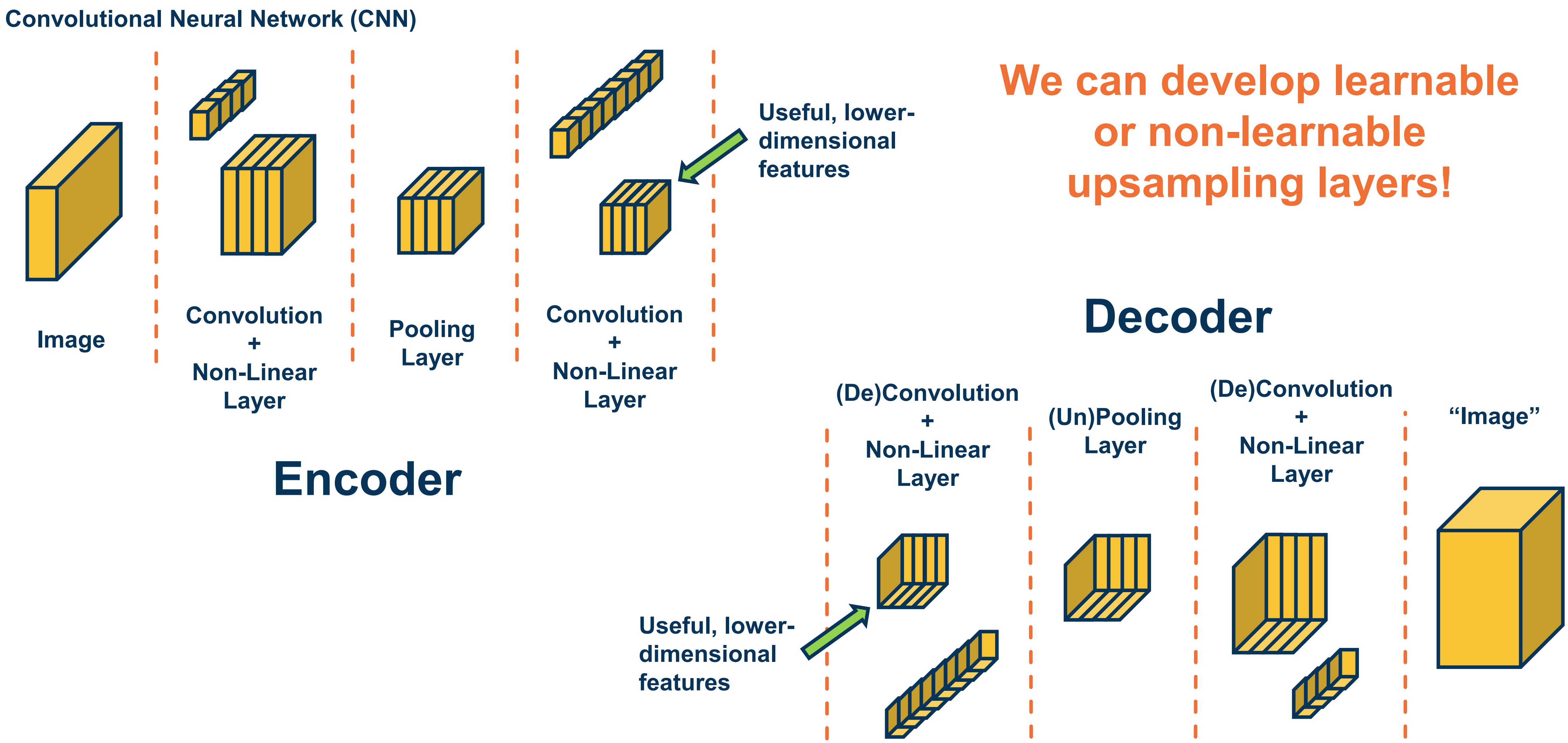
Larger Image



Larger Output Size!

Larger Output Maps

Long, et al., “Fully Convolutional Networks for Semantic Segmentation”, 2015



We can develop learnable or non-learnable upsampling layers!

Idea 2: "De"Convolution and UnPooling

Example : Max pooling

- Stride window across image but perform per-patch **max operation**

$$X(0{:}1, 0{:}1) = \begin{bmatrix} 100 & 150 \\ 100 & 200 \end{bmatrix} \Rightarrow \max(0{:}1,0{:}1) = 200$$

Copy value to position chosen as max in encoder, fill reset of this window with zeros

Idea: Remember max elements in encoder! Copy value from equivalent position, rest are zeros

$$X = \begin{bmatrix} 120 & 150 & 120 \\ 100 & 50 & 110 \\ 25 & 25 & 10 \end{bmatrix} \xrightarrow[\text{2x2 max pool}]{} Y = \begin{bmatrix} 150 & 150 \\ 100 & 110 \end{bmatrix}$$

Encoder

Decoder

$$X = \begin{bmatrix} 300 & 450 \\ 100 & 250 \end{bmatrix} \xrightarrow[]{\text{2x2 max unpool}} Y = \begin{bmatrix} 0 & 300 & - \\ 0 & 0 & - \\ - & - & - \end{bmatrix}$$

Max Unpooling Example (one window)

$$X_{enc} = \begin{bmatrix} 120 & 150 & 120 \\ 100 & 50 & 110 \\ 25 & 25 & 10 \end{bmatrix} \xrightarrow{\text{2x2 max pool}} Y_{enc} = \begin{bmatrix} 150 & 150 \\ 100 & 110 \end{bmatrix}$$

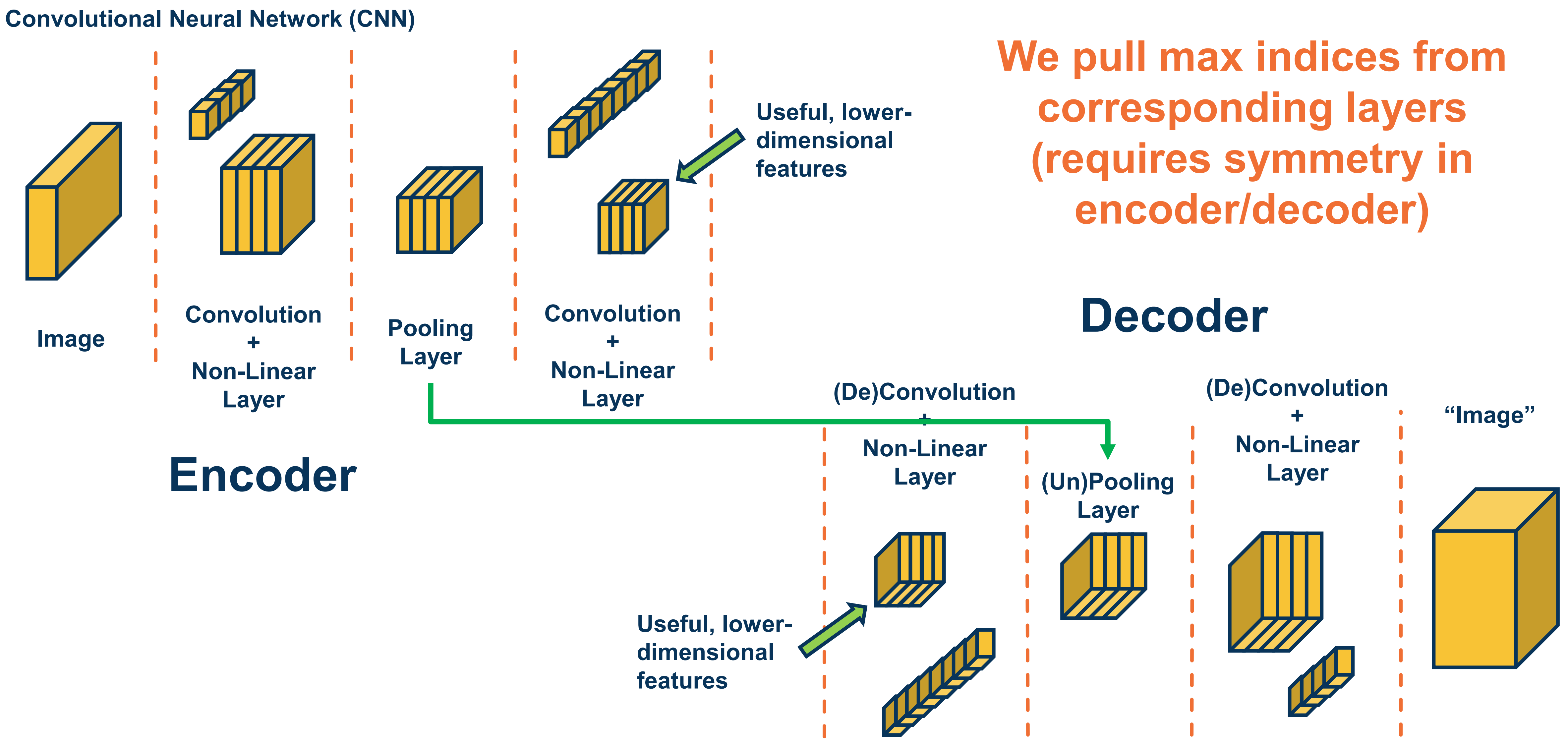
Encoder

Contributions from multiple windows are summed

Decoder

$$X_{dec} = \begin{bmatrix} 300 & 450 \\ 100 & 250 \end{bmatrix} \xrightarrow{\text{2x2 max unpool}} Y_{dec} = \begin{bmatrix} 0 & 300 + 450 & 0 \\ 100 & 0 & 250 \\ 0 & 0 & 0 \end{bmatrix}$$

Max Unpooling Example

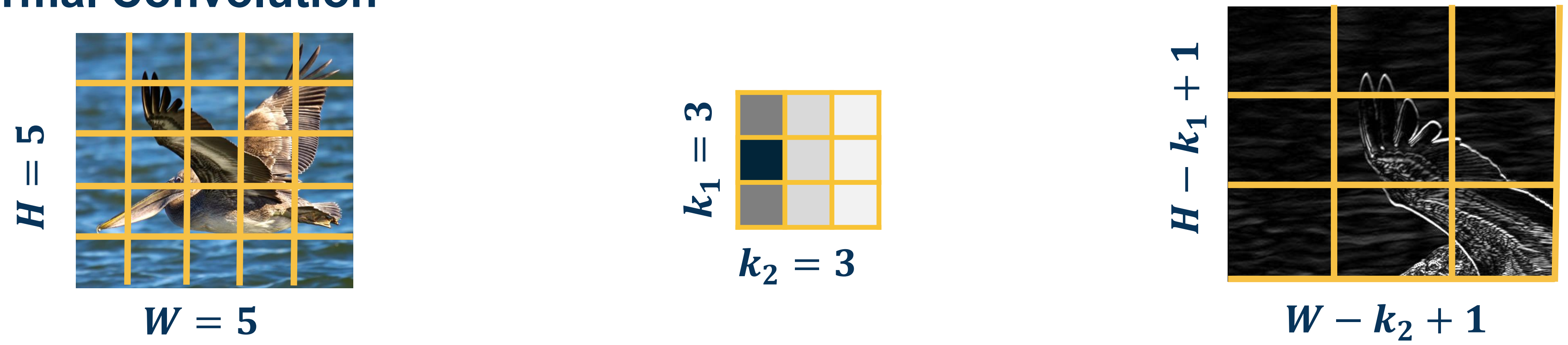


We pull max indices from corresponding layers (requires symmetry in encoder/decoder)

Symmetry in Encoder/Decoder

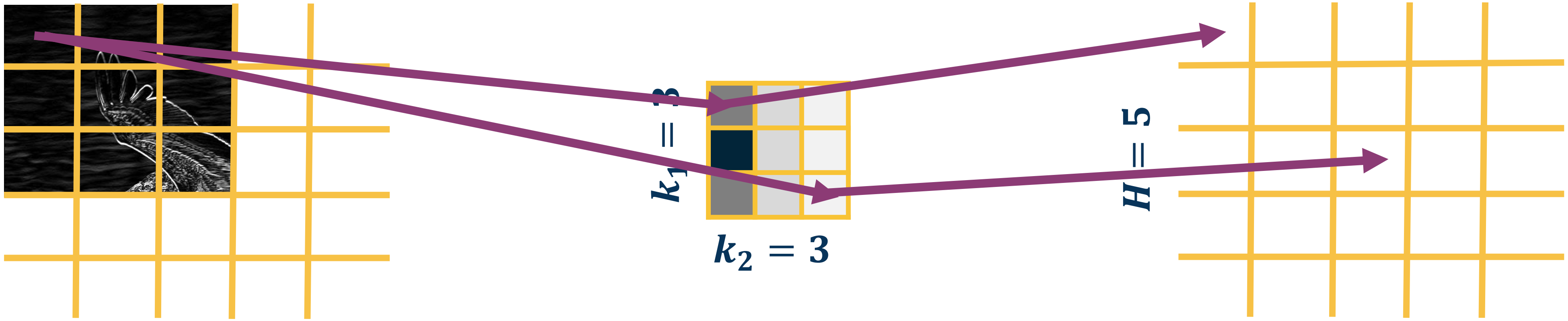
How can we *upsample* using convolutions and learnable kernel?

Normal Convolution



Transposed Convolution (also known as “deconvolution”, fractionally strided conv)

Idea: Take each input pixel, multiply by learnable kernel, “stamp” it on output



“De”Convolution (Transposed Convolution)

$$X = \begin{bmatrix} 120 & 150 & 120 \\ 100 & 50 & 110 \\ 25 & 25 & 10 \end{bmatrix} \qquad K = \begin{bmatrix} 1 & -1 \\ 2 & -2 \end{bmatrix}$$

Contributions from multiple windows are summed

$$\begin{bmatrix} 120 & -120 & 0 & 0 \\ 240 & -240 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

Incorporate
$X(0,0)$

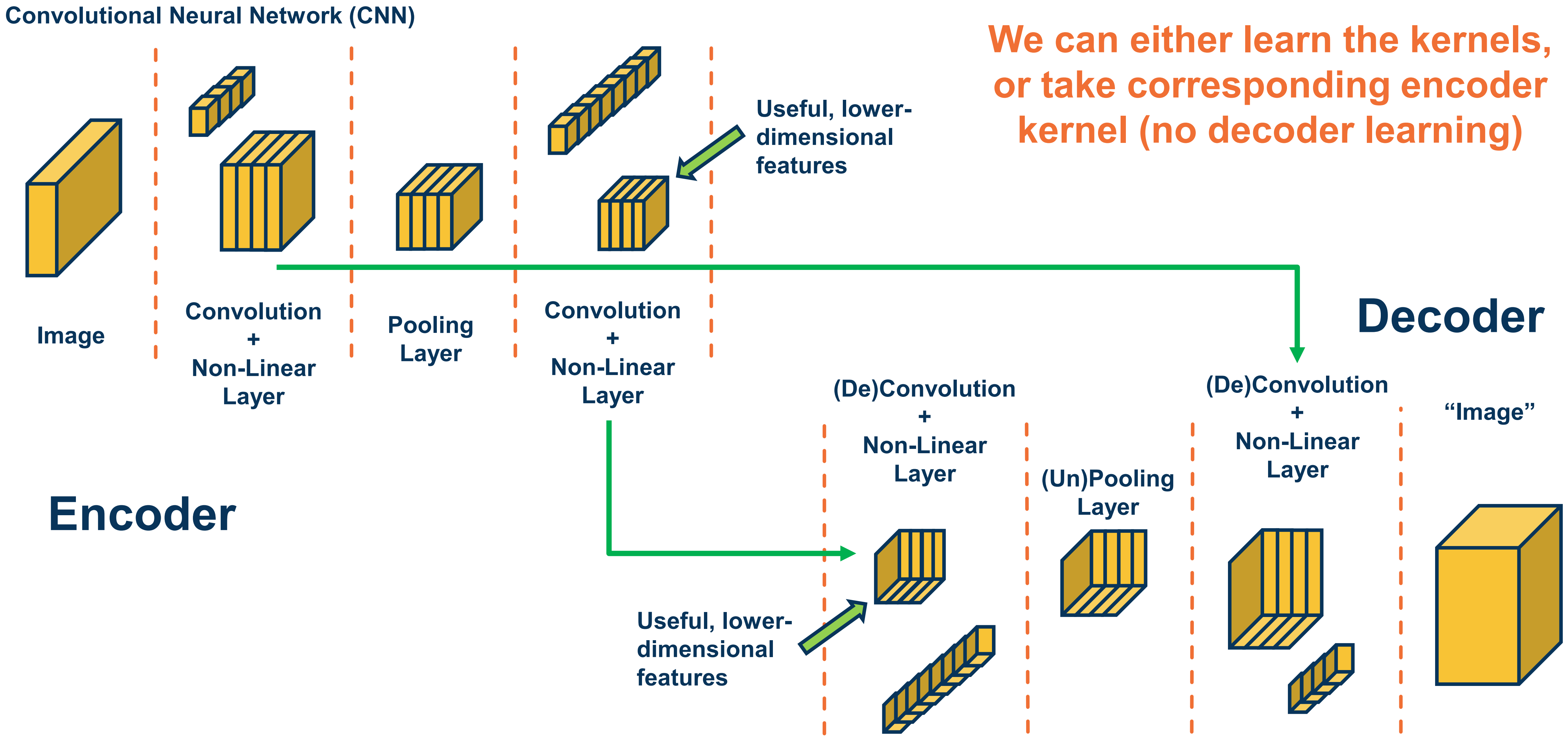
$$\begin{bmatrix} 120 & -120+150 & -150 & 0 \\ 240 & -240+300 & -300 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

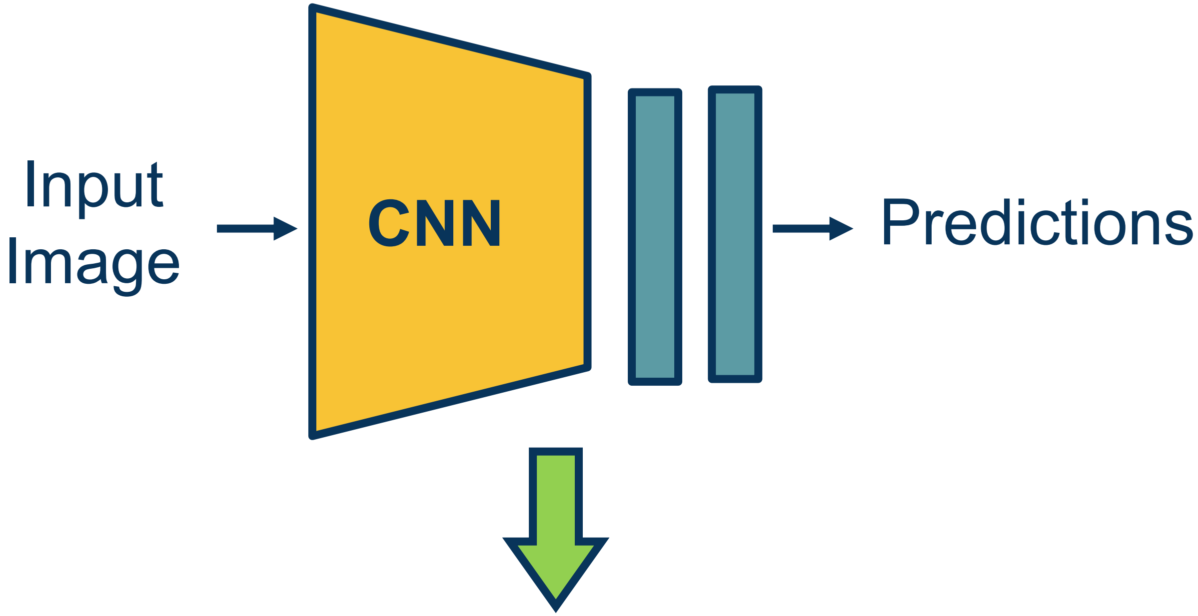
Incorporate
$X(1,0)$

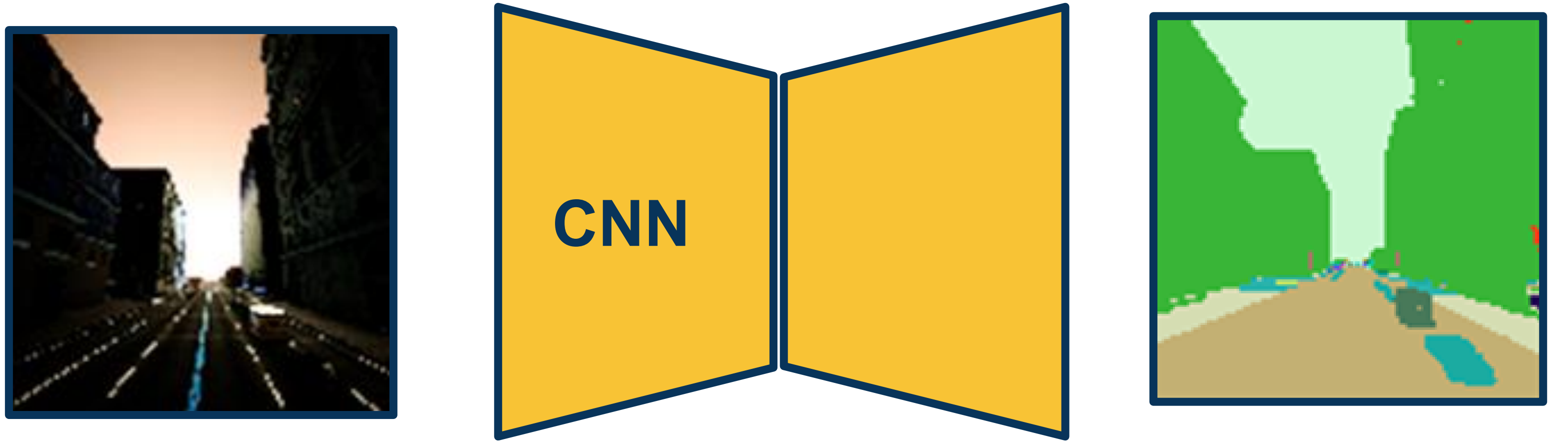
Transposed Convolution Example

Symmetry in Encoder/Decoder

We can either learn the kernels, or take corresponding encoder kernel (no decoder learning)



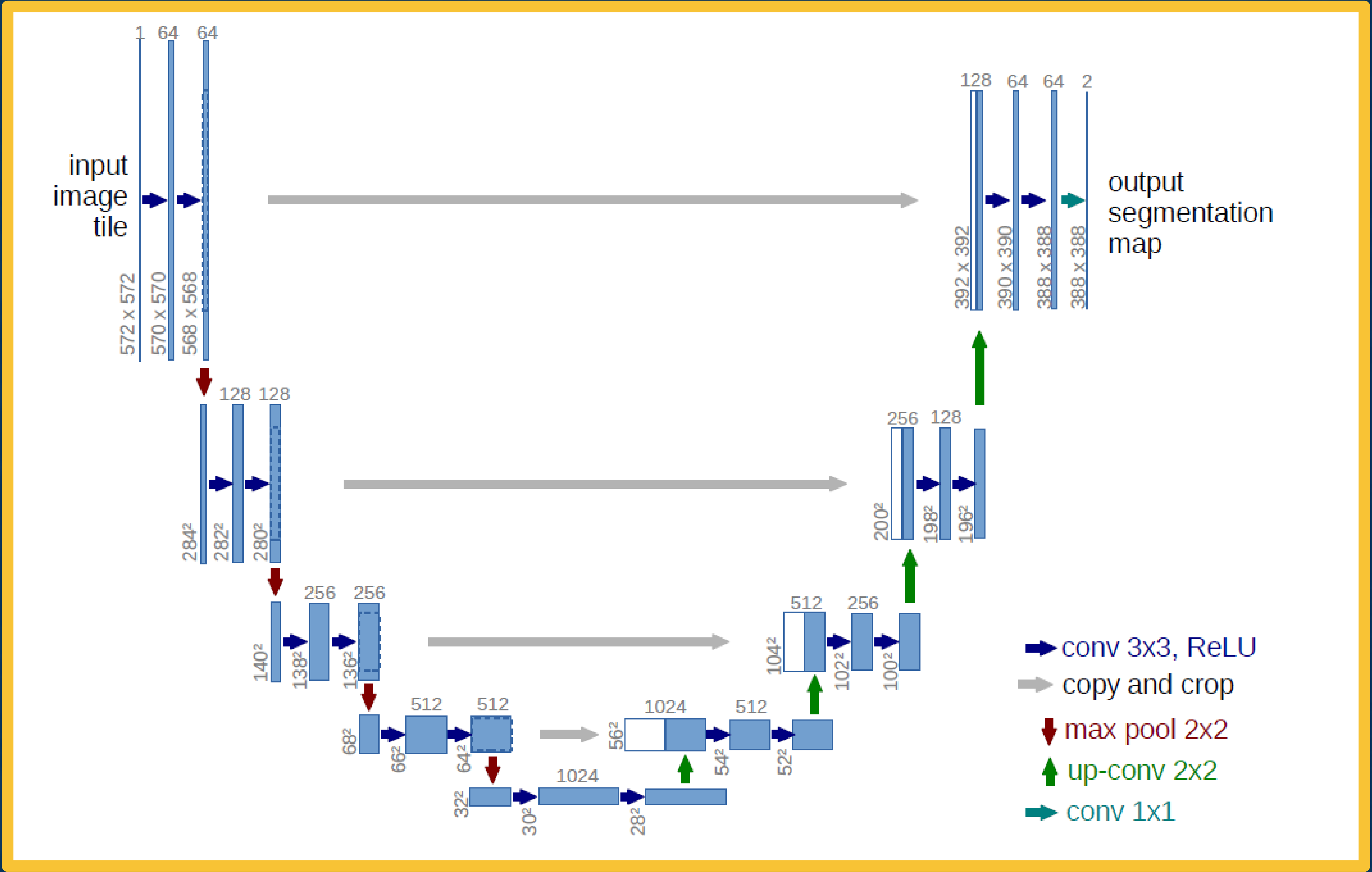




We can start with a pre-trained trunk/backbone (e.g. network pretrained on ImageNet)!

U-Net

You can have skip connections to bypass bottleneck!



Ronneberger, et al., "U-Net: Convolutional Networks for Biomedical Image Segmentation", 2015

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Summary

- Various ways to get **image-like outputs,** for example to predict segmentations of input images
- Fully convolutional layers essentially apply the striding idea to the output classifiers, supporting arbitrary input sizes
  - (without output size depending on what the input size is)
- We can have various upsampling layers that actually increase the size
- Encoder/decoder architectures are popular ways to leverage these to perform general image-to-image tasks