

Topics:

- Attention and Transformers

CS 4644-DL / 7643-A

ZSOLT KIRA

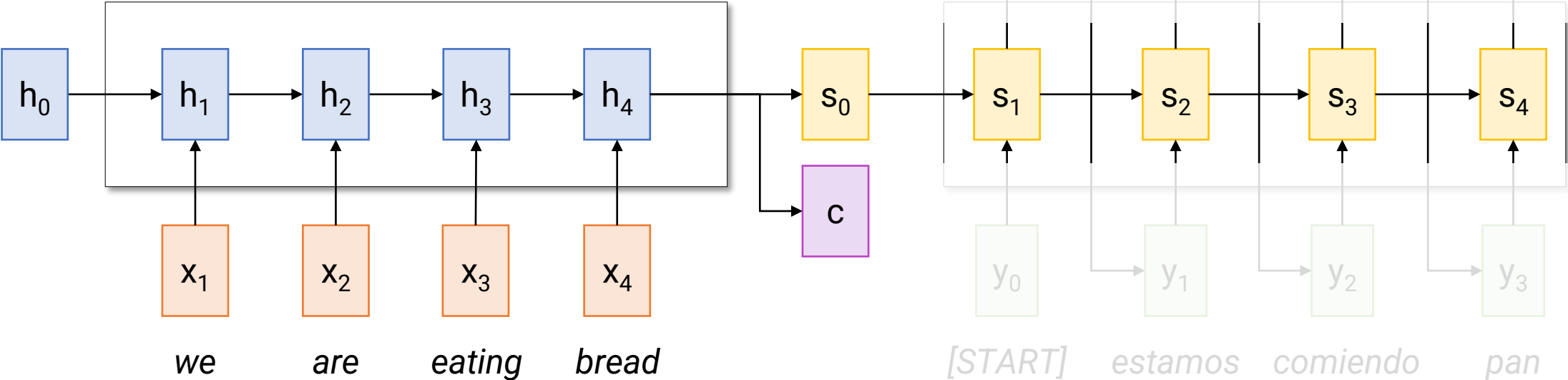
- **Assignment 3**
 - Due **March 9th 11:59pm EST**
 - **Oops.** Diffusion models accidentally included. No need to do it by Mar 9th! @258
- **Projects**
 - Project proposal due **March 15th**
 - Proposal description out on canvas @256
- Meta office hours Friday 3pm ET on language models

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

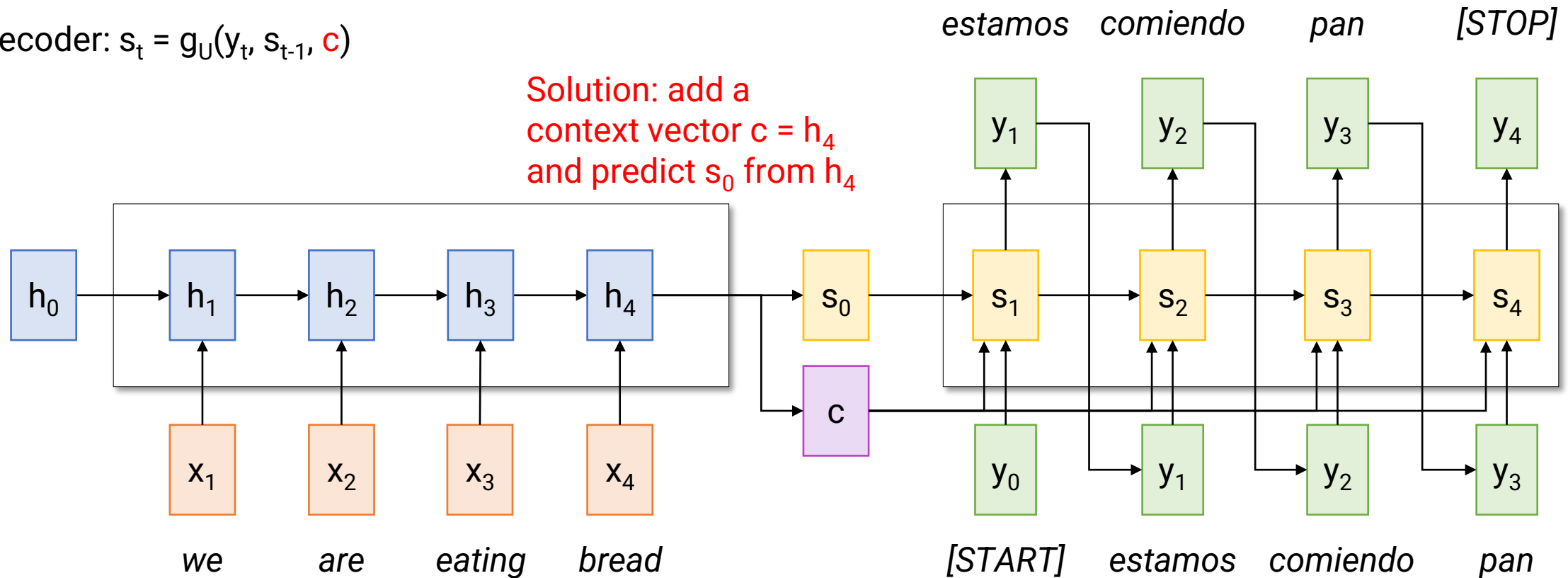


Machine Translation with RNNs

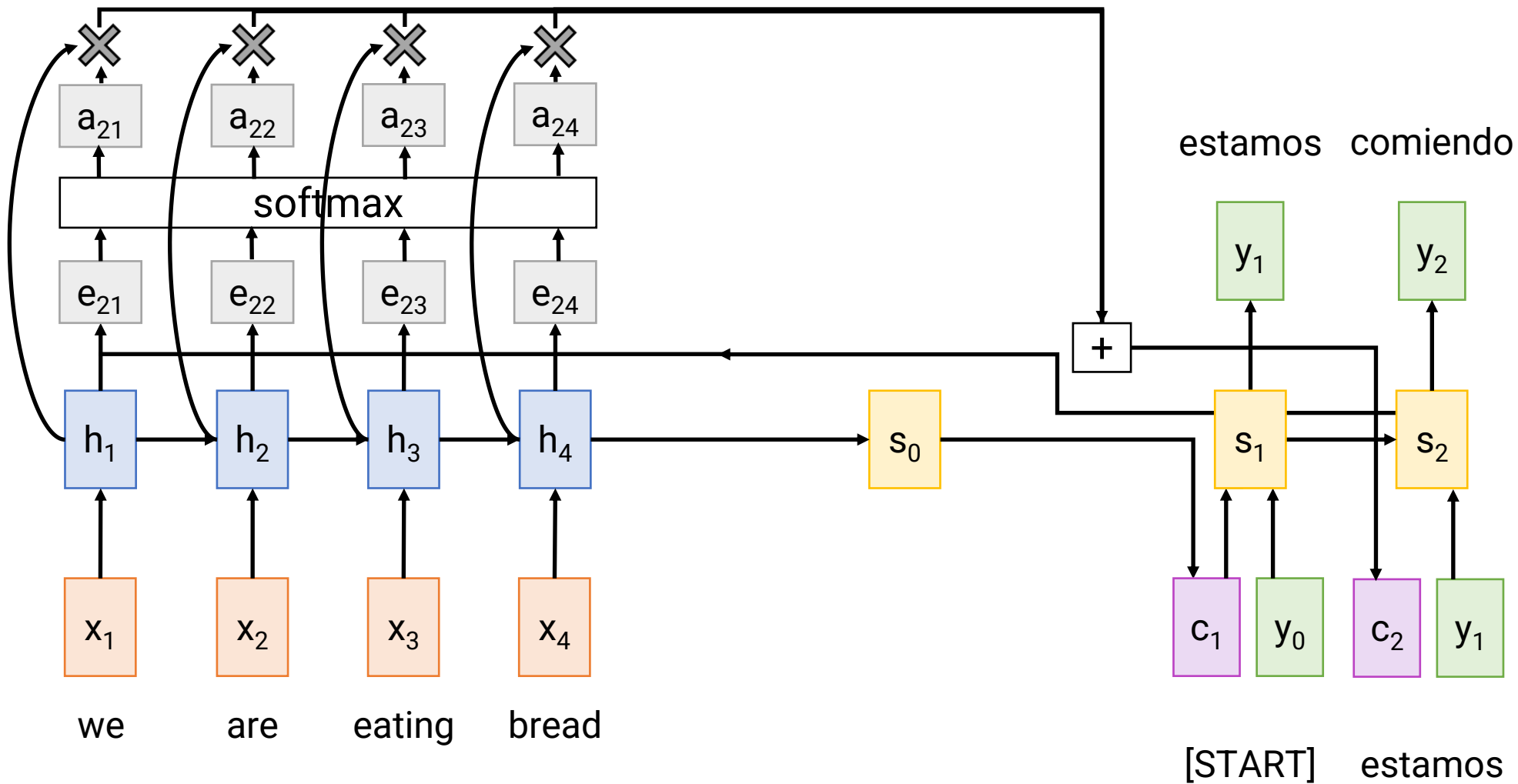
Encoder: $h_t = f_W(x_t, h_{t-1})$

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

Solution: add a context vector $\mathbf{c} = h_4$ and predict s_0 from h_4



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

Machine Translation with RNNs **and Attention**

Example: English to French translation

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

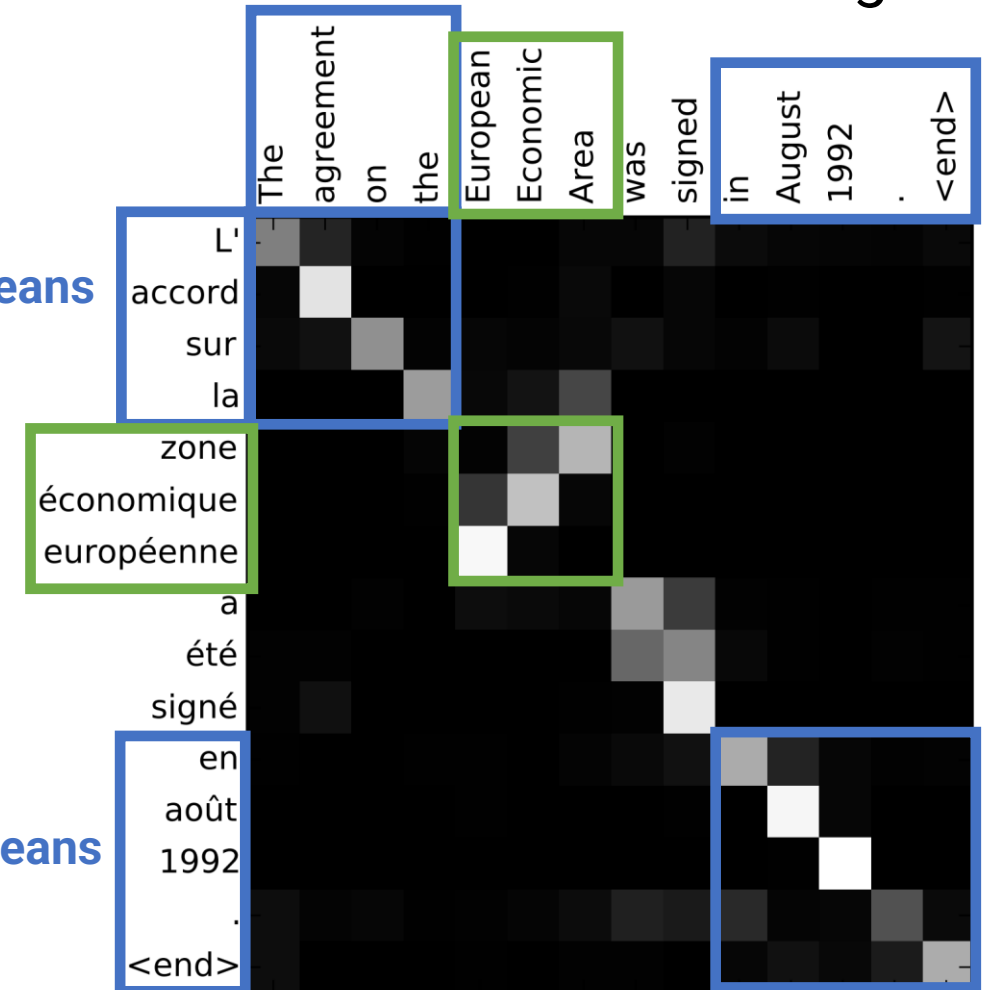
Output: “**L'accord sur la zone économique européenne** a été signé **en août 1992.**”

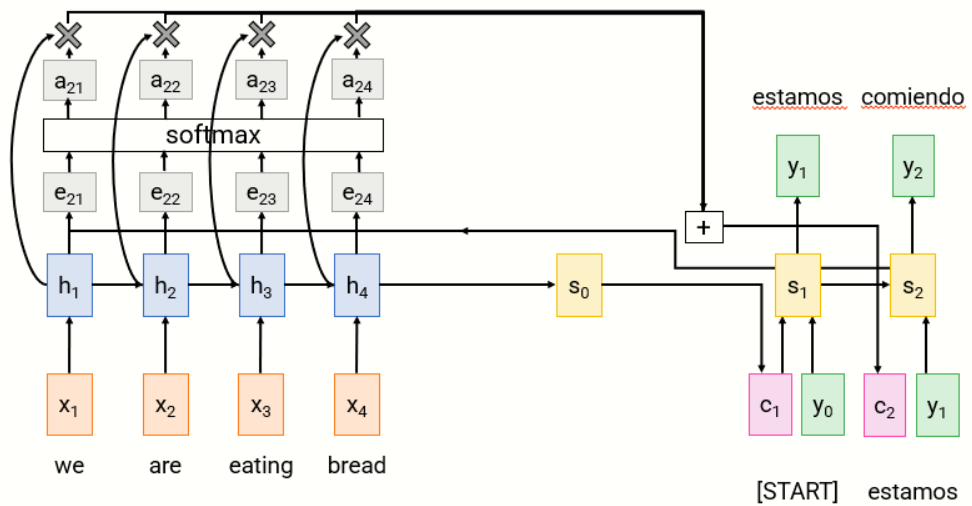
Diagonal attention means words correspond in order

Attention figures out different word orders

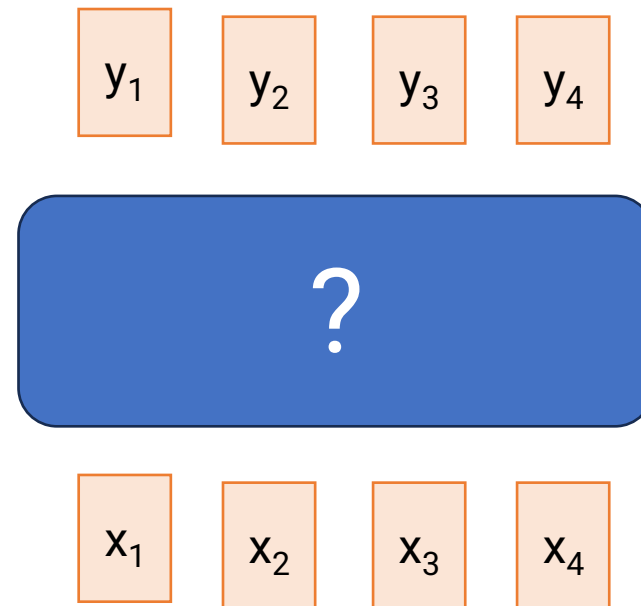
Diagonal attention means words correspond in order

Visualize attention weights $a_{t,i}$





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: $N_X \times D_H$)

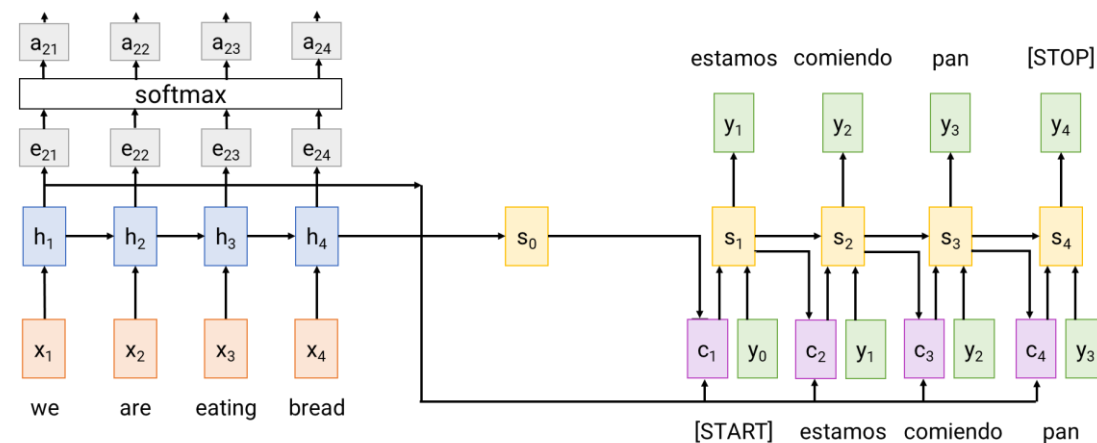
Similarity function: f_{att}

Computation:

Similarities: \mathbf{e} (Shape: N_X) $e_i = f_{\text{att}}(\mathbf{s}_{t-1}, \mathbf{h}_i)$

Attention weights: $\mathbf{a} = \text{softmax}(\mathbf{e})$ (Shape: N_X)

Output vector: $\mathbf{y} = \sum_i a_i \mathbf{h}_i$ (Shape: D_X)



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:

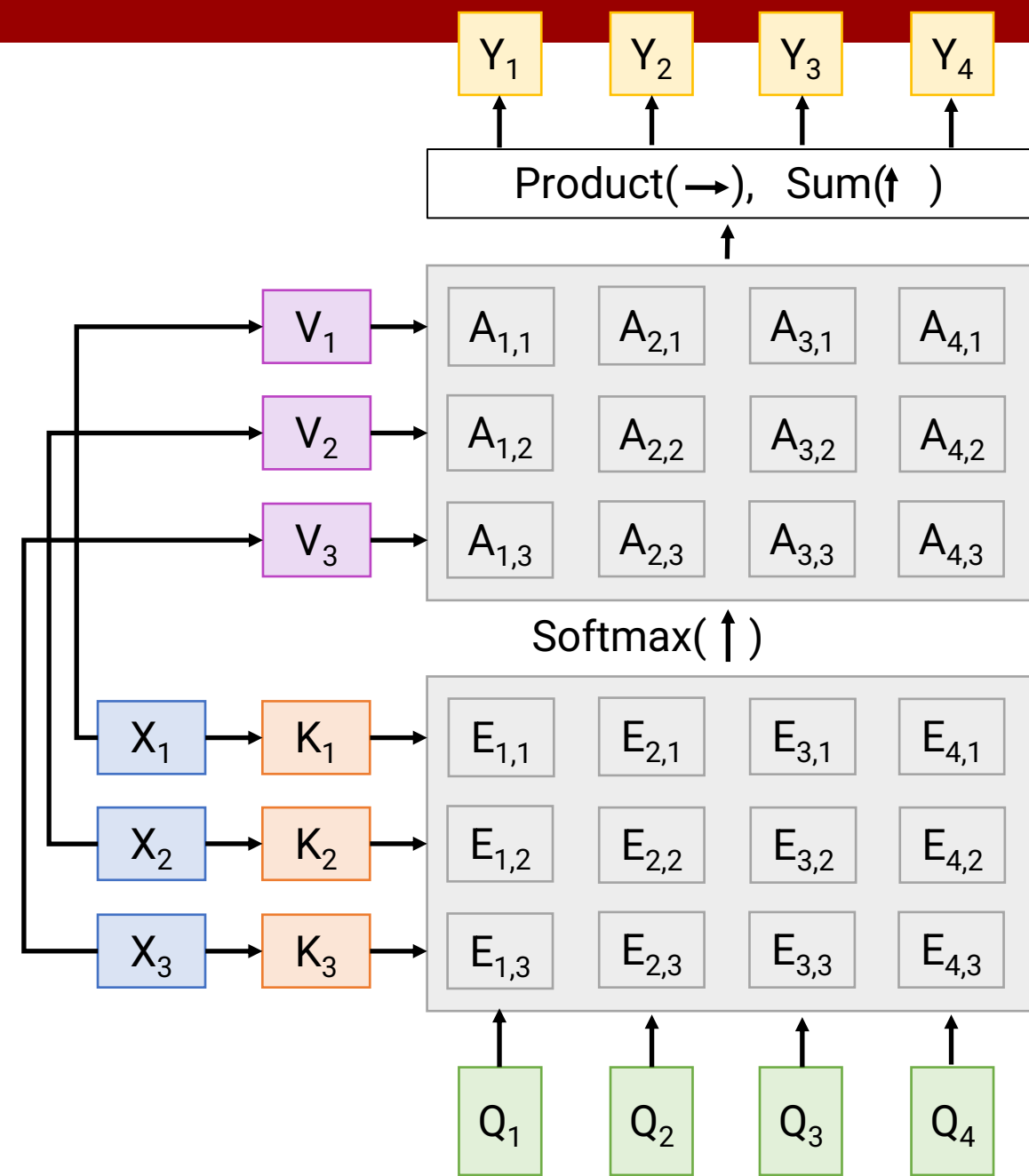
Key vectors: $\mathbf{K} = \mathbf{XW}_K$ (Shape: $N_X \times D_Q$)

Value vectors: $\mathbf{V} = \mathbf{XW}_V$ (Shape: $N_X \times D_V$)

Similarities: $\mathbf{E} = \mathbf{QK}^T$ (Shape: $N_Q \times N_X$) $E_{i,j} = \mathbf{Q}_i \cdot \mathbf{K}_j / \text{sqrt}(D_Q)$

Attention weights: $\mathbf{A} = \text{softmax}(\mathbf{E}, \text{dim}=1)$ (Shape: $N_Q \times N_X$)

Output vectors: $\mathbf{Y} = \mathbf{AV}$ (Shape: $N_Q \times D_V$) $Y_i = \sum_j A_{i,j} \mathbf{V}_j$



Self-Attention Layer

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

Inputs:

Input vectors: \mathbf{X} (Shape: $N_X \times D_X$)

Key matrix: \mathbf{W}_K (Shape: $D_X \times D_Q$)

Value matrix: \mathbf{W}_V (Shape: $D_X \times D_V$)

Query matrix: \mathbf{W}_Q (Shape: $D_X \times D_Q$)

Computation:

Query vectors: $\mathbf{Q} = \mathbf{XW}_Q$

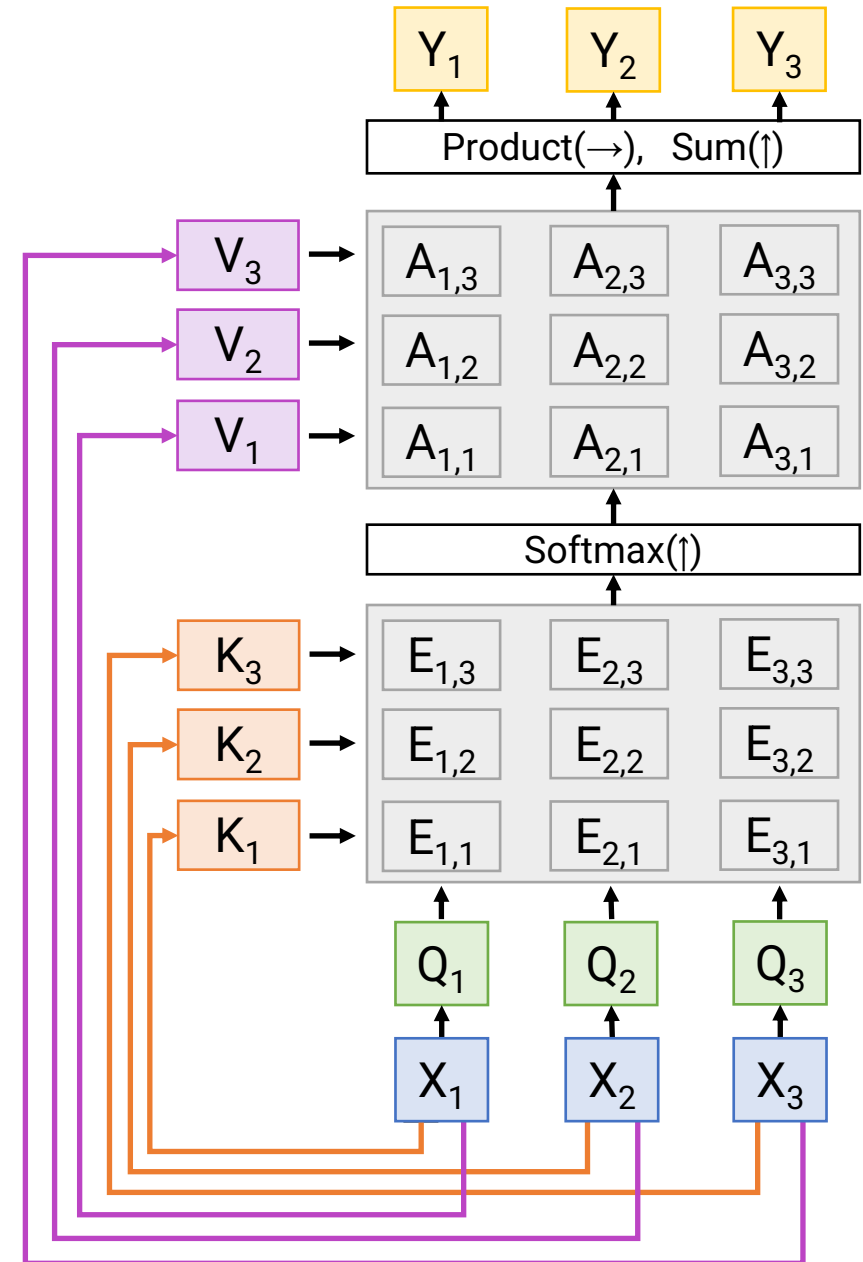
Key vectors: $\mathbf{K} = \mathbf{XW}_K$ (Shape: $N_X \times D_Q$)

Value vectors: $\mathbf{V} = \mathbf{XW}_V$ (Shape: $N_X \times D_V$)

Similarities: $\mathbf{E} = \mathbf{QK}^T$ (Shape: $N_X \times N_X$) $E_{i,j} = \mathbf{Q}_i \cdot \mathbf{K}_j / \text{sqrt}(D_Q)$

Attention weights: $\mathbf{A} = \text{softmax}(\mathbf{E}, \text{dim}=1)$ (Shape: $N_X \times N_X$)

Output vectors: $\mathbf{Y} = \mathbf{AV}$ (Shape: $N_X \times D_V$) $Y_i = \sum_j A_{i,j} \mathbf{V}_j$



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: $D_x \times D_Q$)

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: $\mathbf{E} = \mathbf{QK}^T$ (Shape: $N_x \times N_x$) $E_{i,j} = \mathbf{Q}_i \cdot \mathbf{K}_j / \text{sqrt}(D_Q)$

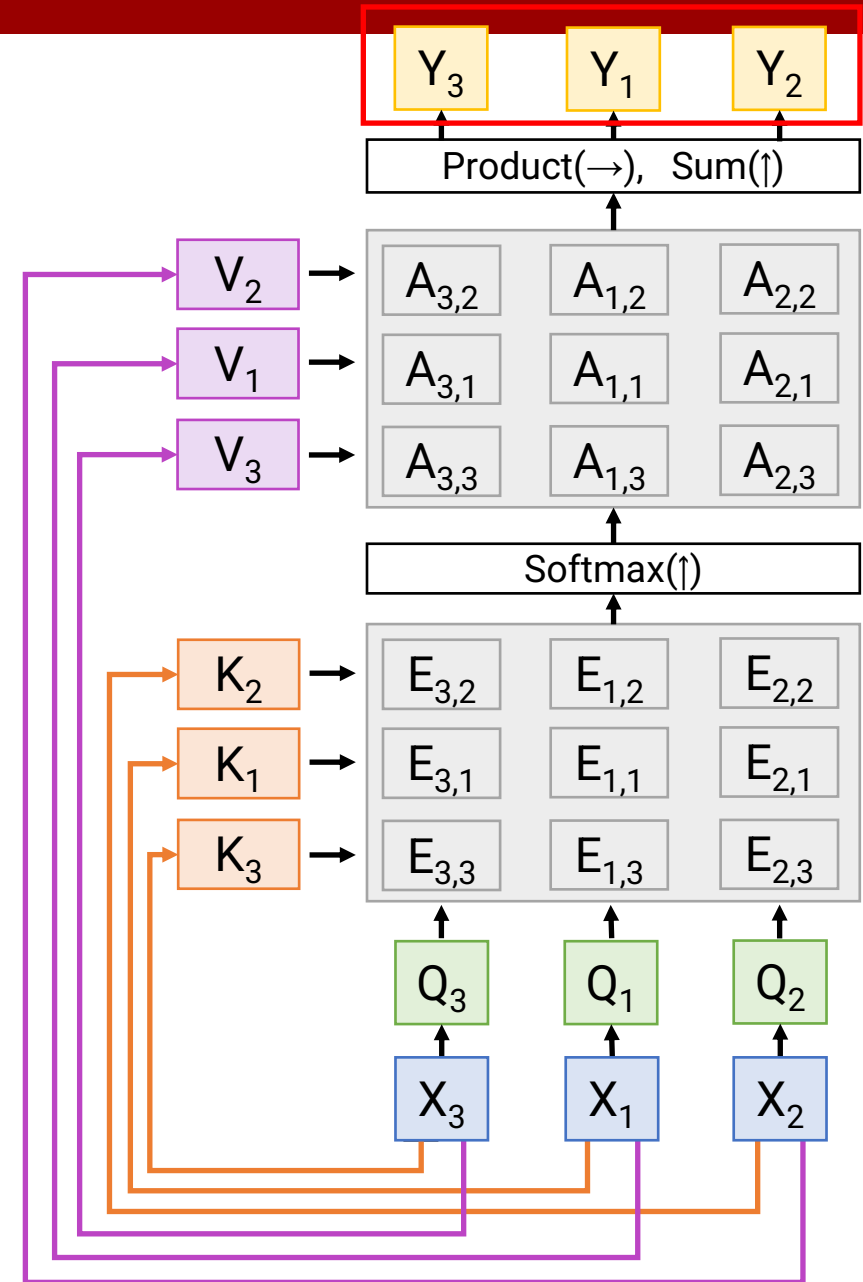
Attention weights: $\mathbf{A} = \text{softmax}(\mathbf{E}, \text{dim}=1)$ (Shape: $N_x \times N_x$)

Output vectors: $\mathbf{Y} = \mathbf{AV}$ (Shape: $N_x \times D_V$) $Y_i = \sum_j A_{i,j} \mathbf{V}_j$

Consider **permuting**
the input vectors:

Outputs will be the
same, but permuted

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



Self-Attention Layer

Inputs:

Input vectors: X (Shape: $N_x \times D_x$)

Key matrix: W_k (Shape: $D_x \times D_Q$)

Value matrix: W_v (Shape: $D_x \times D_V$)

Query matrix: W_Q (Shape: $D_x \times D_Q$)

Computation:

Query vectors: $Q = XW_Q$

Key vectors: $K = XW_k$ (Shape: $N_x \times D_Q$)

Value vectors: $V = XW_v$ (Shape: $N_x \times D_V$)

Similarities: $E = QK^T$ (Shape: $N_x \times N_x$) $E_{i,j} = Q_i \cdot K_j / \text{sqrt}(D_Q)$

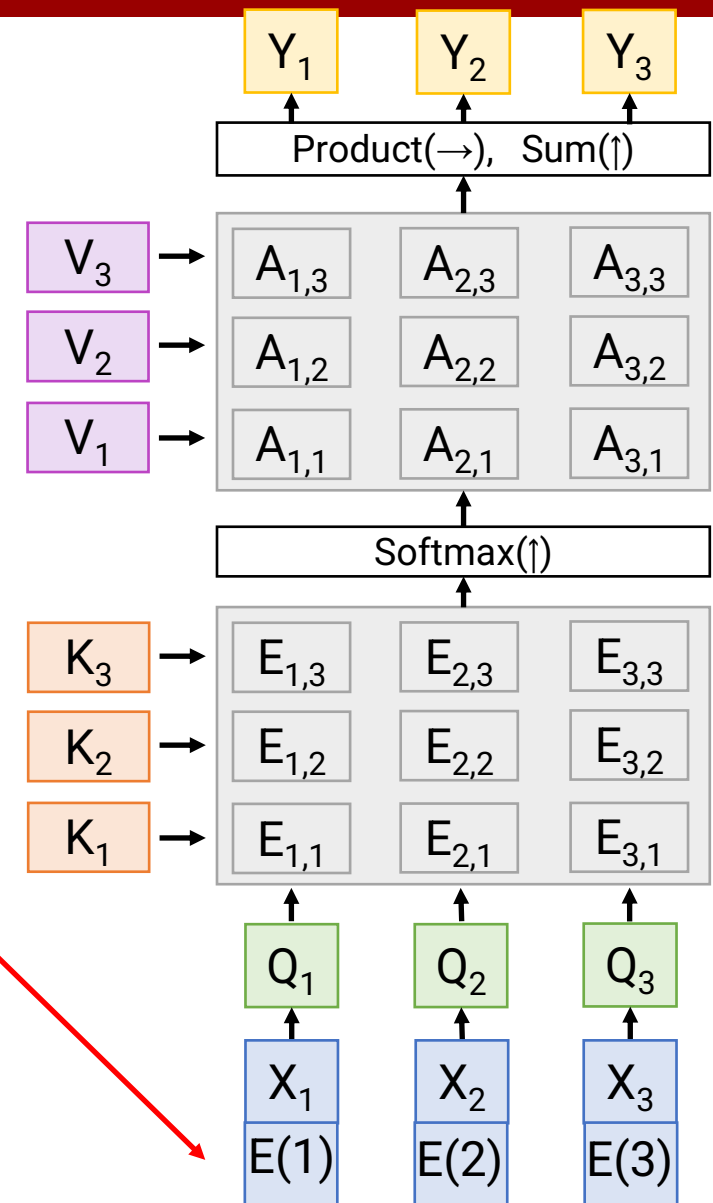
Attention weights: $A = \text{softmax}(E, \text{dim}=1)$ (Shape: $N_x \times N_x$)

Output vectors: $Y = AV$ (Shape: $N_x \times D_V$) $Y_i = \sum_j A_{i,j} V_j$

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

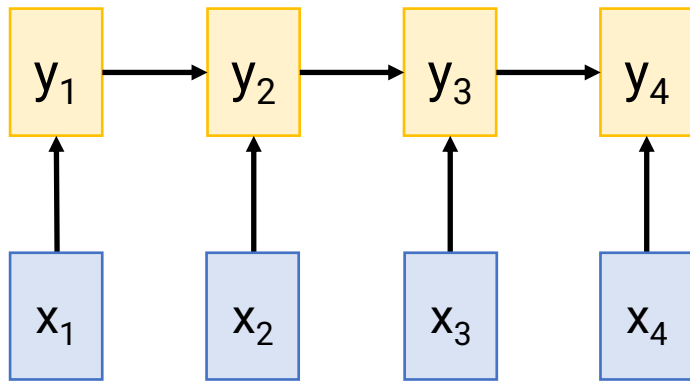
In order to make processing position-aware, concatenate input with **positional encoding**

E can be learned lookup table, or fixed function



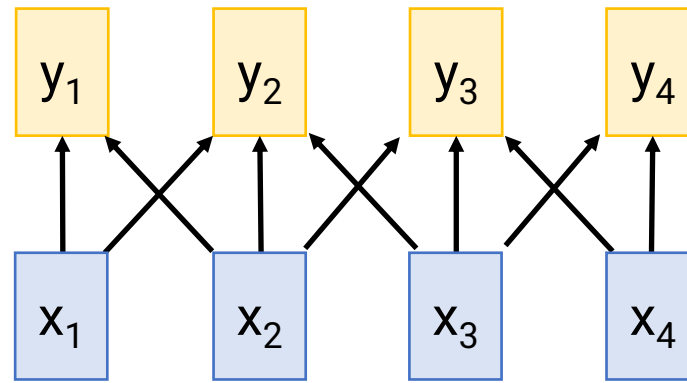
Three Ways of Processing Sequences

Recurrent Neural Network



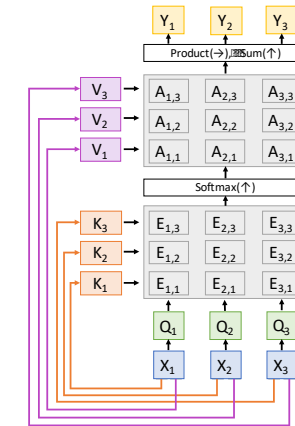
- Works on **Ordered Sequences**
- (+) **Good at long sequences:** After one RNN layer, h_T "sees" the whole sequence
- (-) **Not parallelizable:** need to compute hidden states sequentially

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



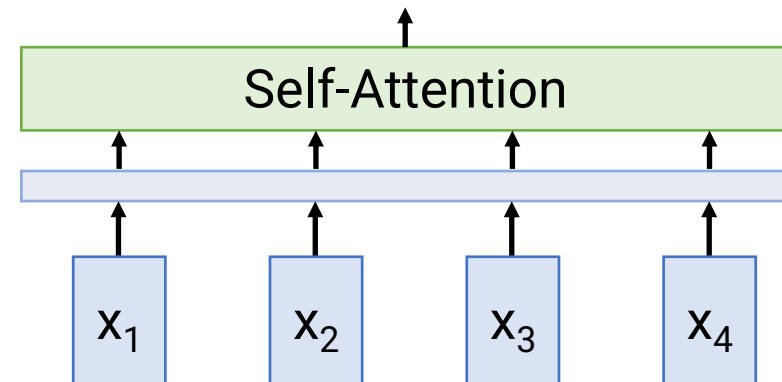
- Works on **Sets of Vectors**
- (+) **Good at long sequences:** after one self-attention layer, each output "sees" all inputs!
- (+) **Highly parallel:** Each output can be computed in parallel
- (-) **Very memory intensive**

The Transformer



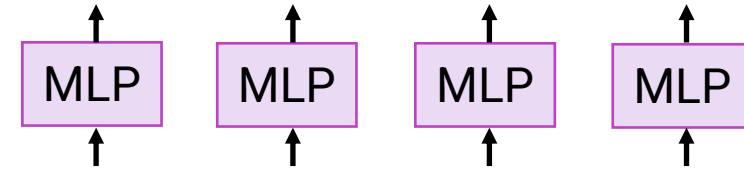
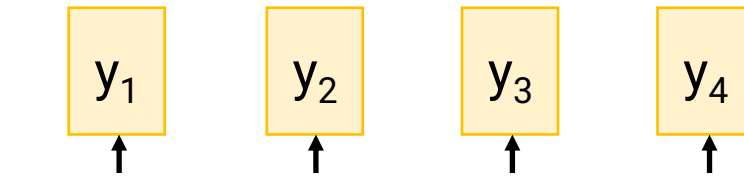
The Transformer

All vectors interact
with each other

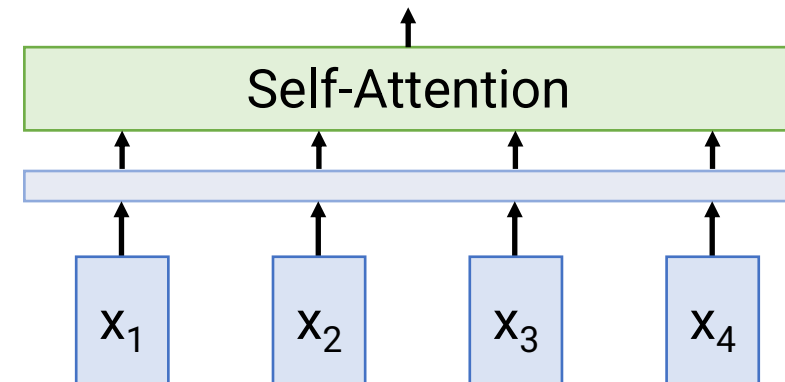


The Transformer

MLP independently
on each vector
(**weight shared!**)

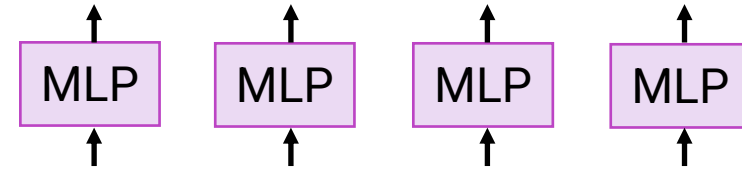
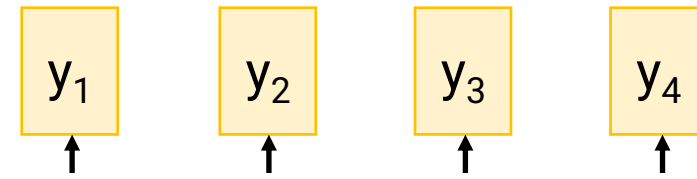


All vectors interact
with each other



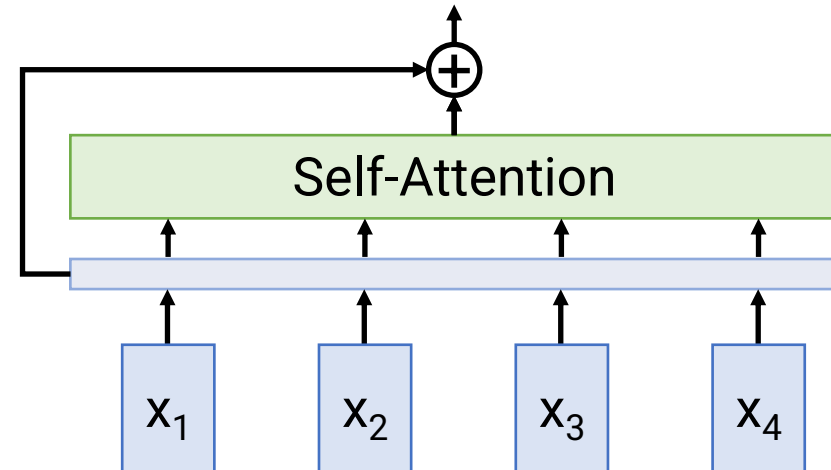
The Transformer

MLP independently
on each vector



Residual connection

All vectors interact
with each other



The Transformer

Recall **Layer Normalization**:

Given h_1, \dots, 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)

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

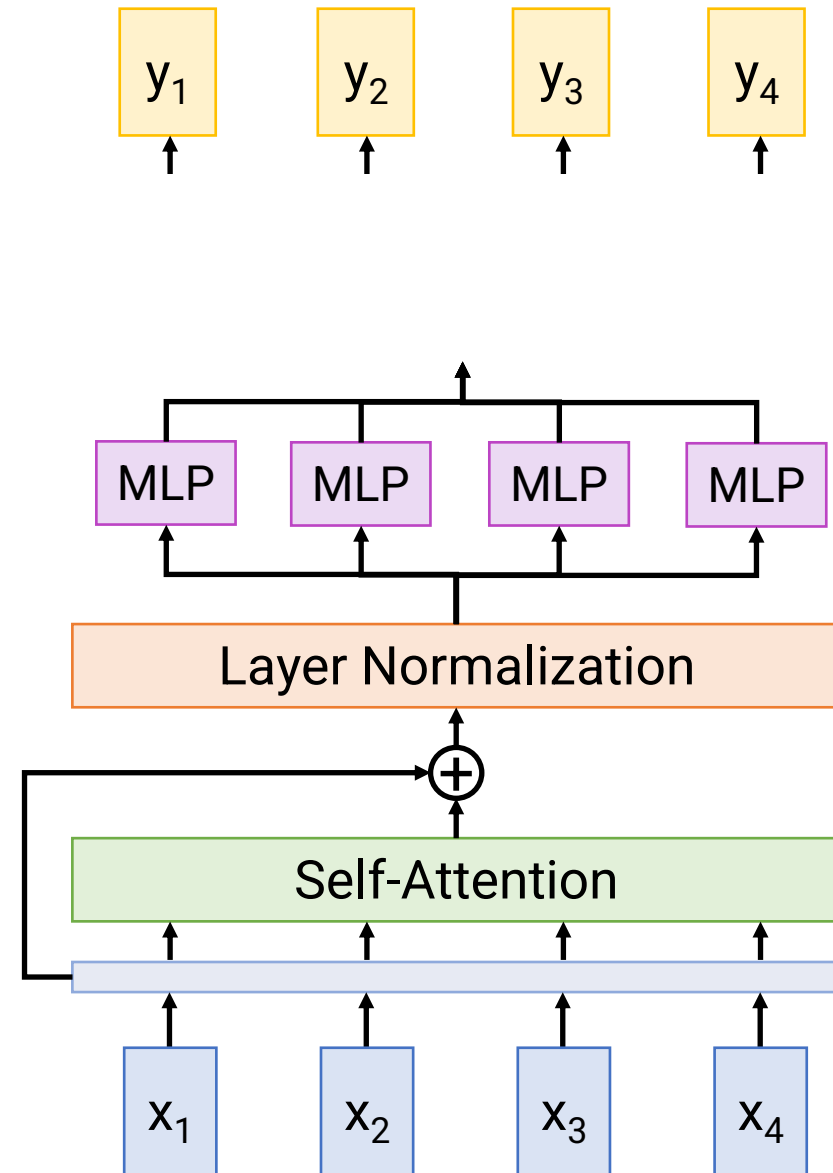
$y_i = \gamma * z_i + \beta$

Ba et al, 2016

MLP independently
on each vector

Residual connection

All vectors interact
with each other

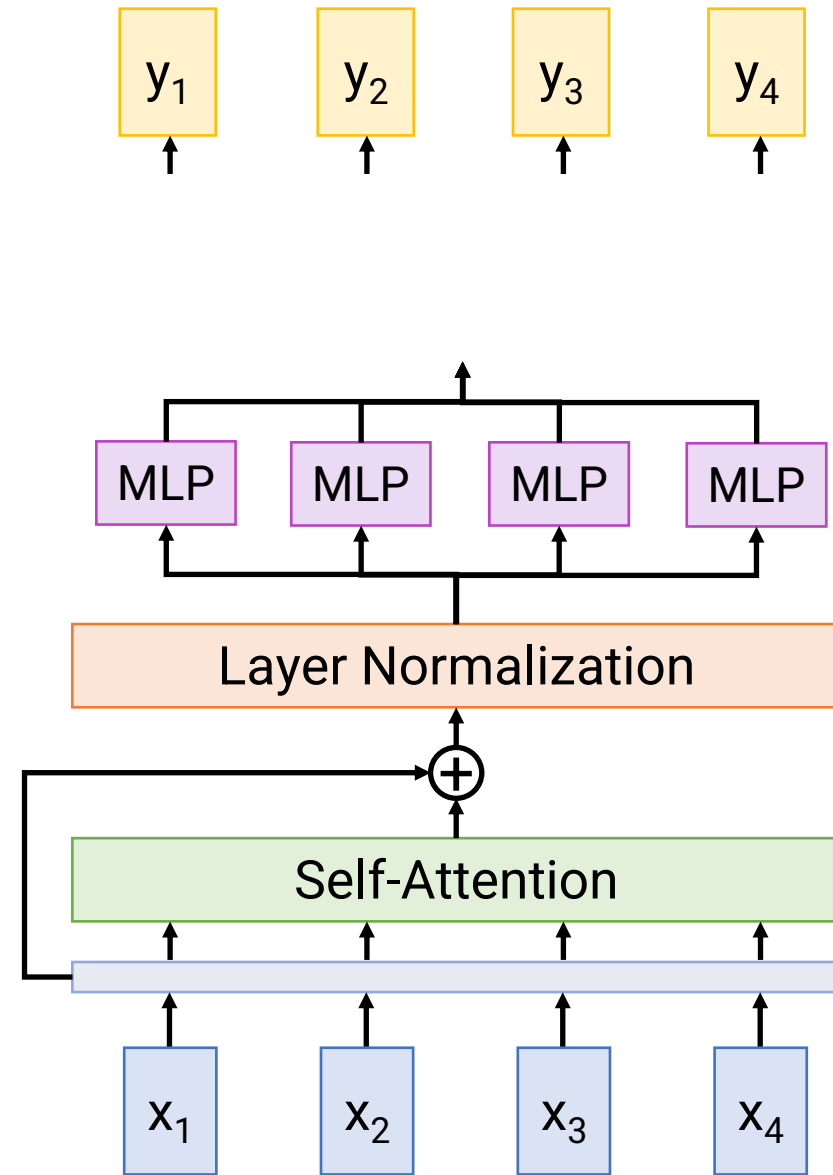


The Transformer

MLP independently
on each vector

Residual connection

All vectors interact
with each other



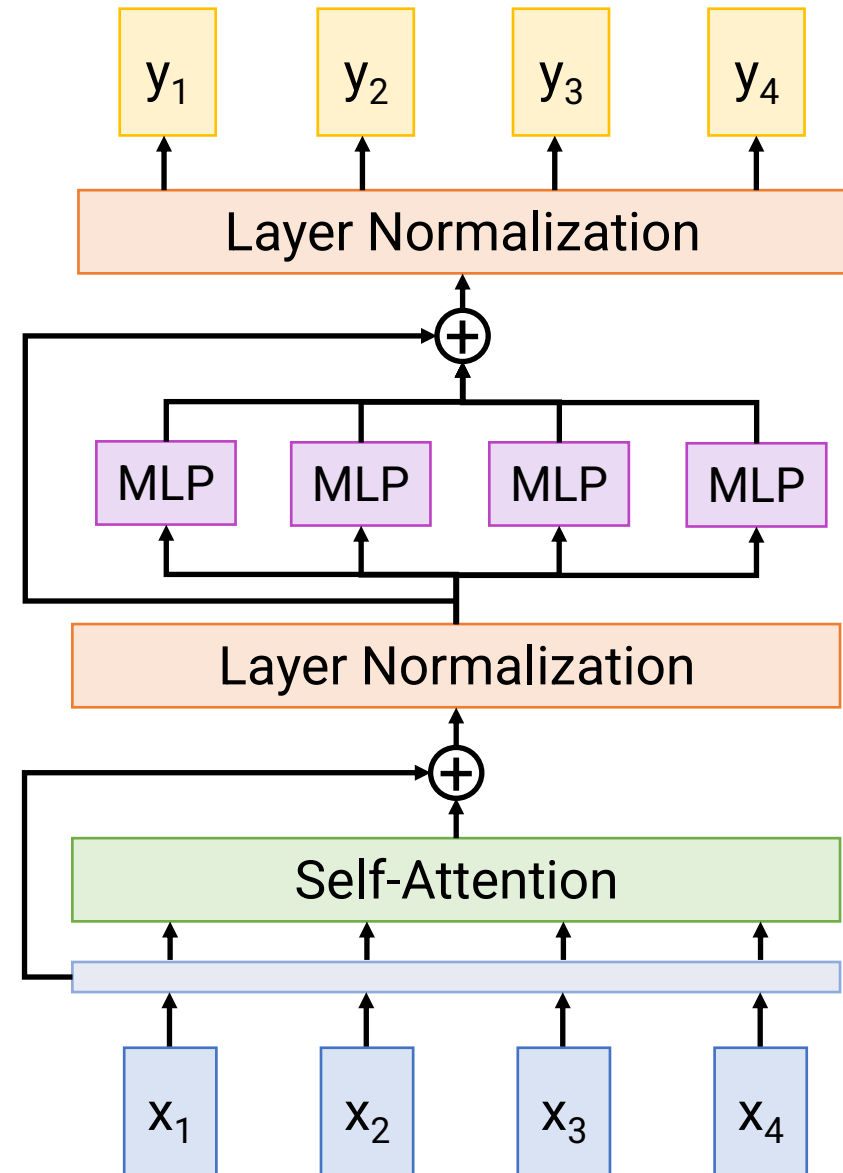
The Transformer

Residual connection

MLP independently
on each vector

Residual connection

All vectors interact
with each other



The Transformer

Transformer Block:

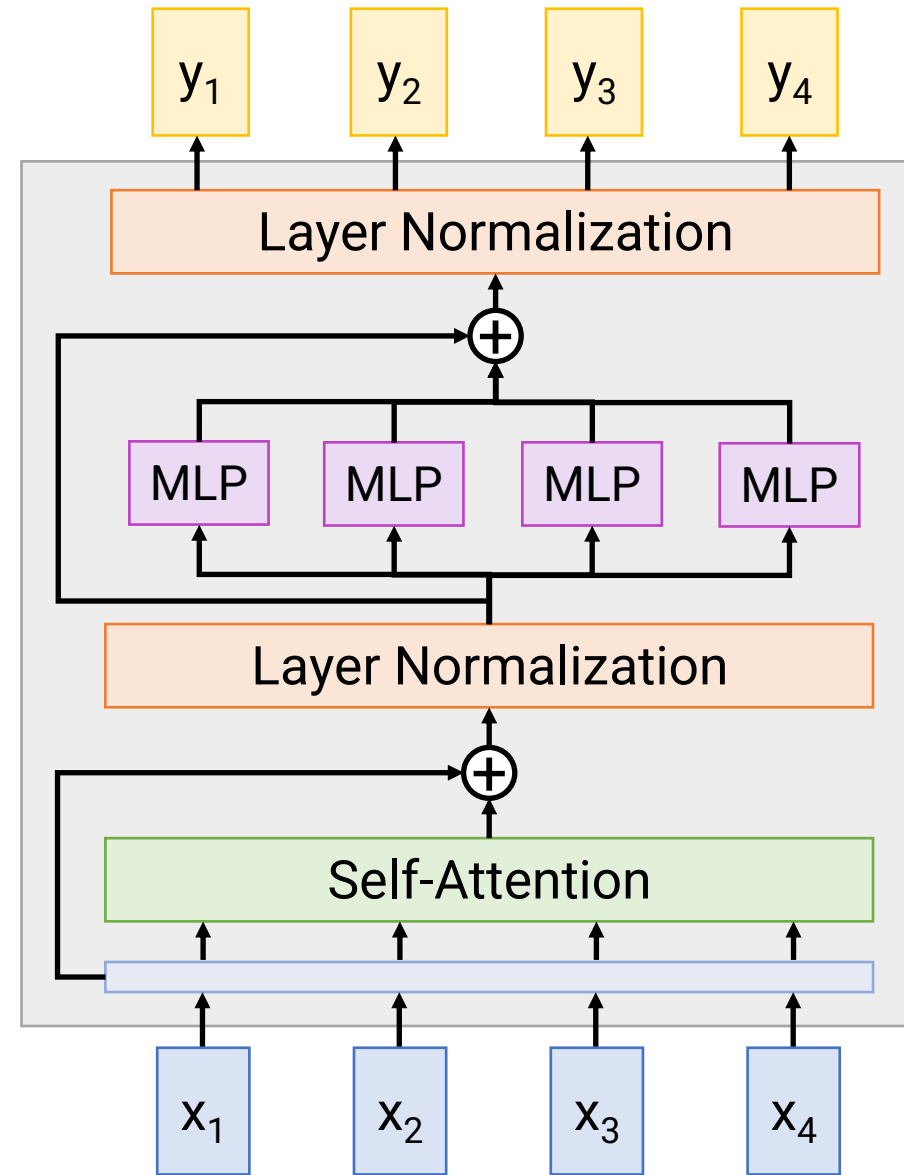
Input: Set of vectors x

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



The Transformer

Transformer Block:

Input: Set of vectors x

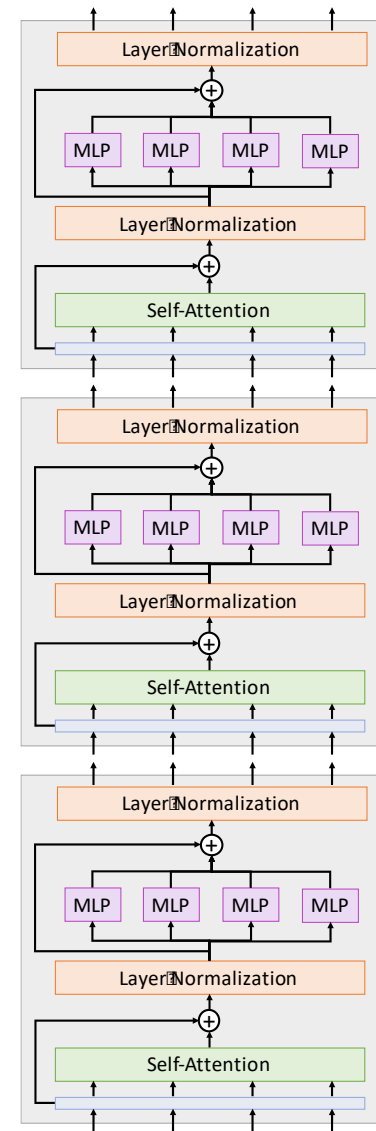
Output: Set of vectors y

Self-attention is the only interaction between vectors!

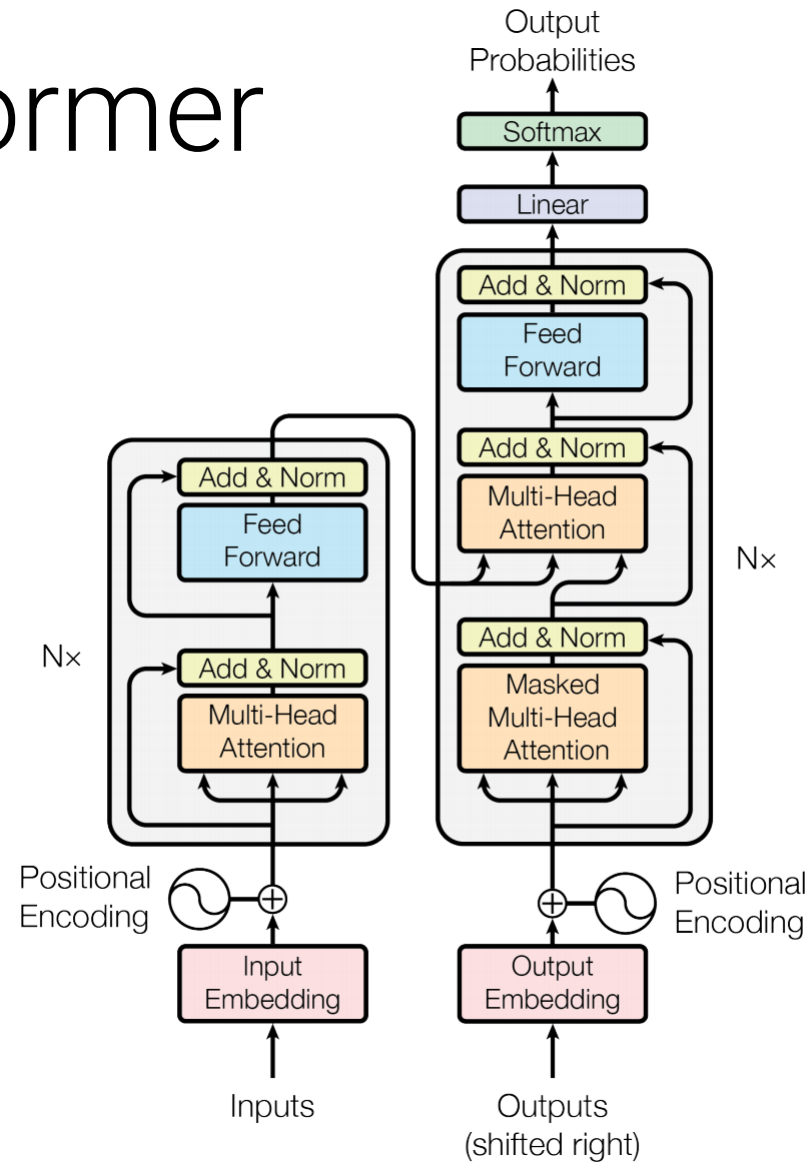
Layer norm and MLP work independently per vector

Highly scalable, highly parallelizable

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



The Transformer



Encoder-Decoder

Details:

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

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

GLUE Benchmark

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	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

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.



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_yvlzX0nPa?dl=0

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

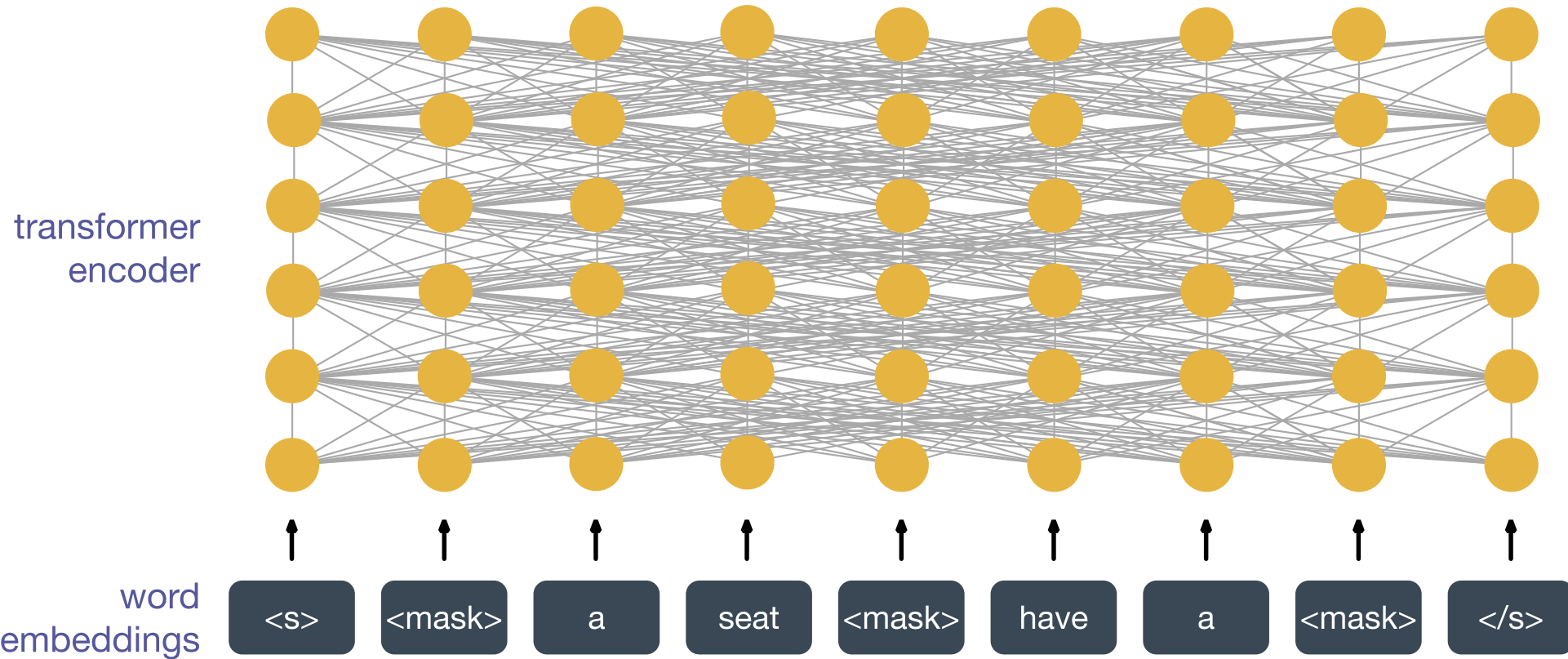
$$p(\mathbf{s}) = p(w_1, w_2, \dots, w_n)$$

- ◆ **Another 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.
- ◆ 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.

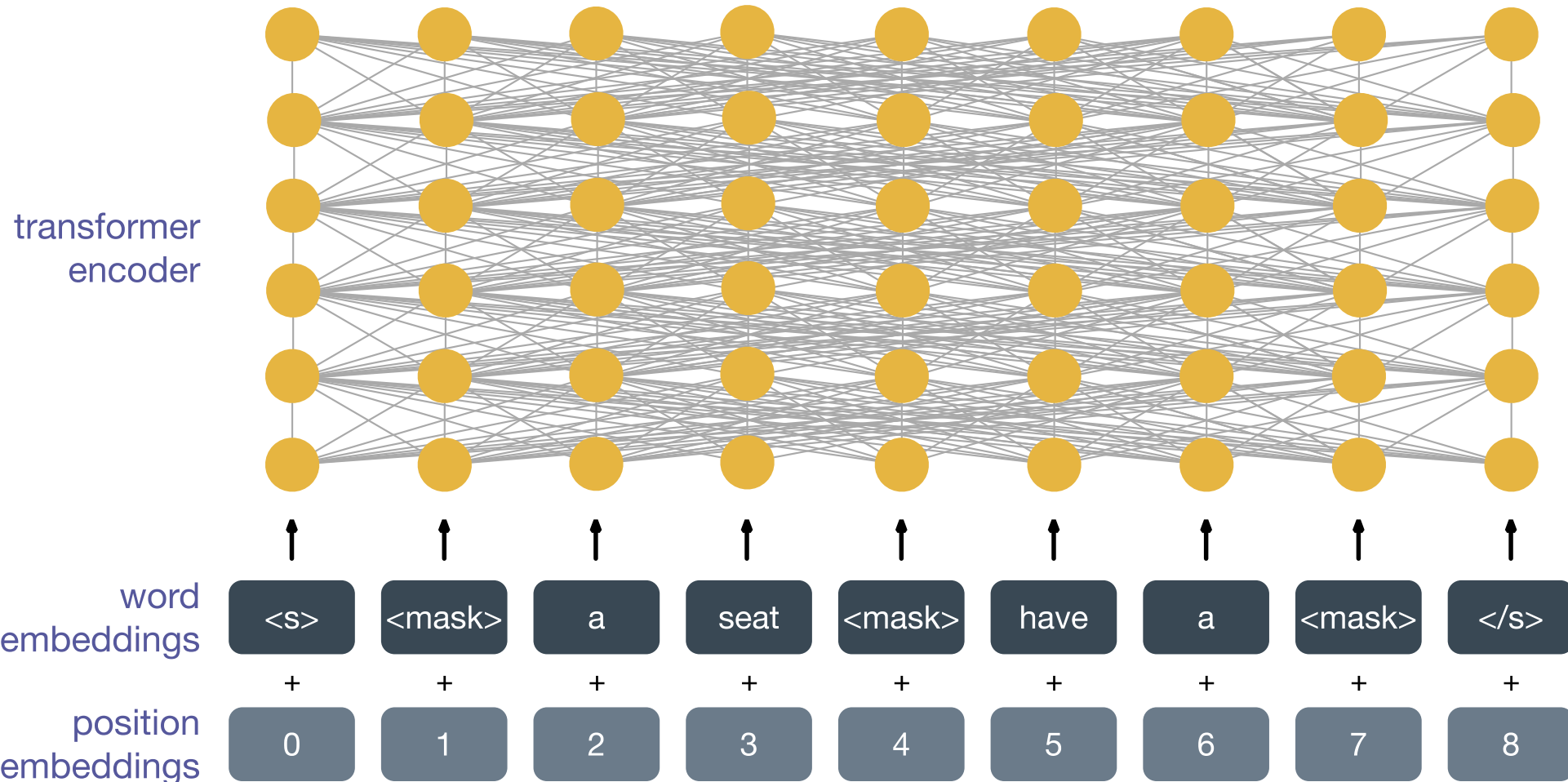
take a seat , have a drink

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

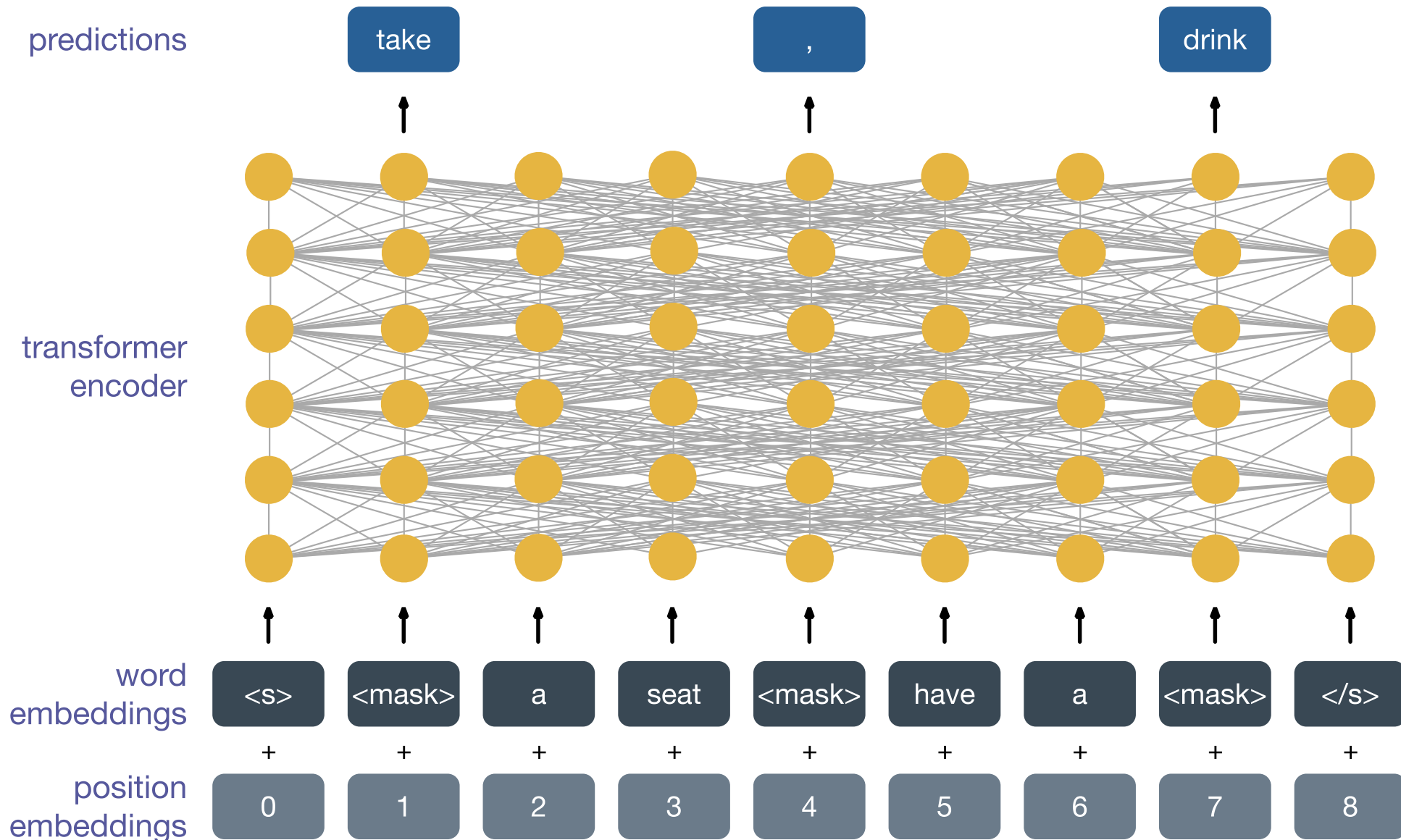
Masked Language Models



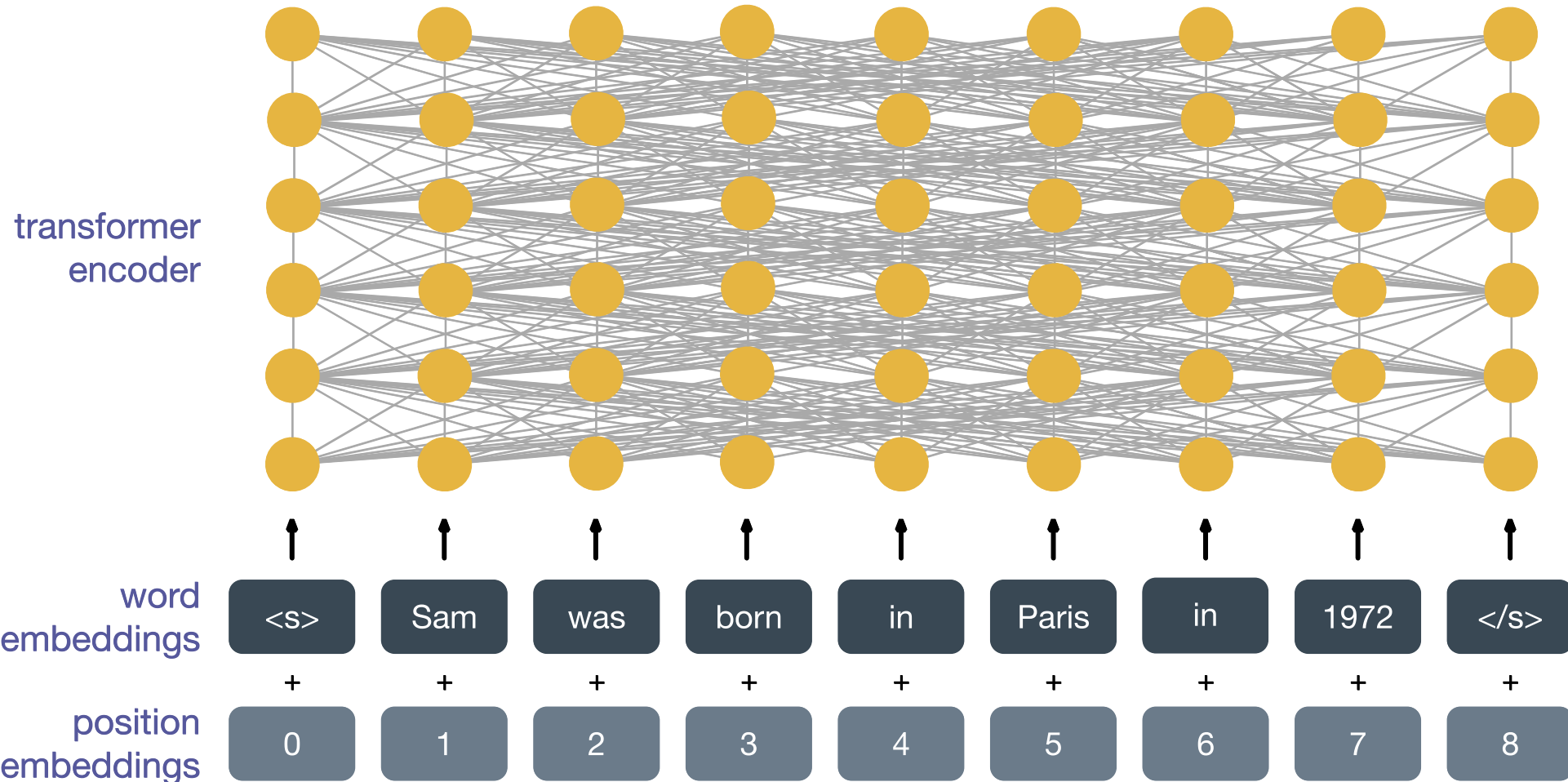
Masked Language Models



Masked Language Models



Masked Language Models

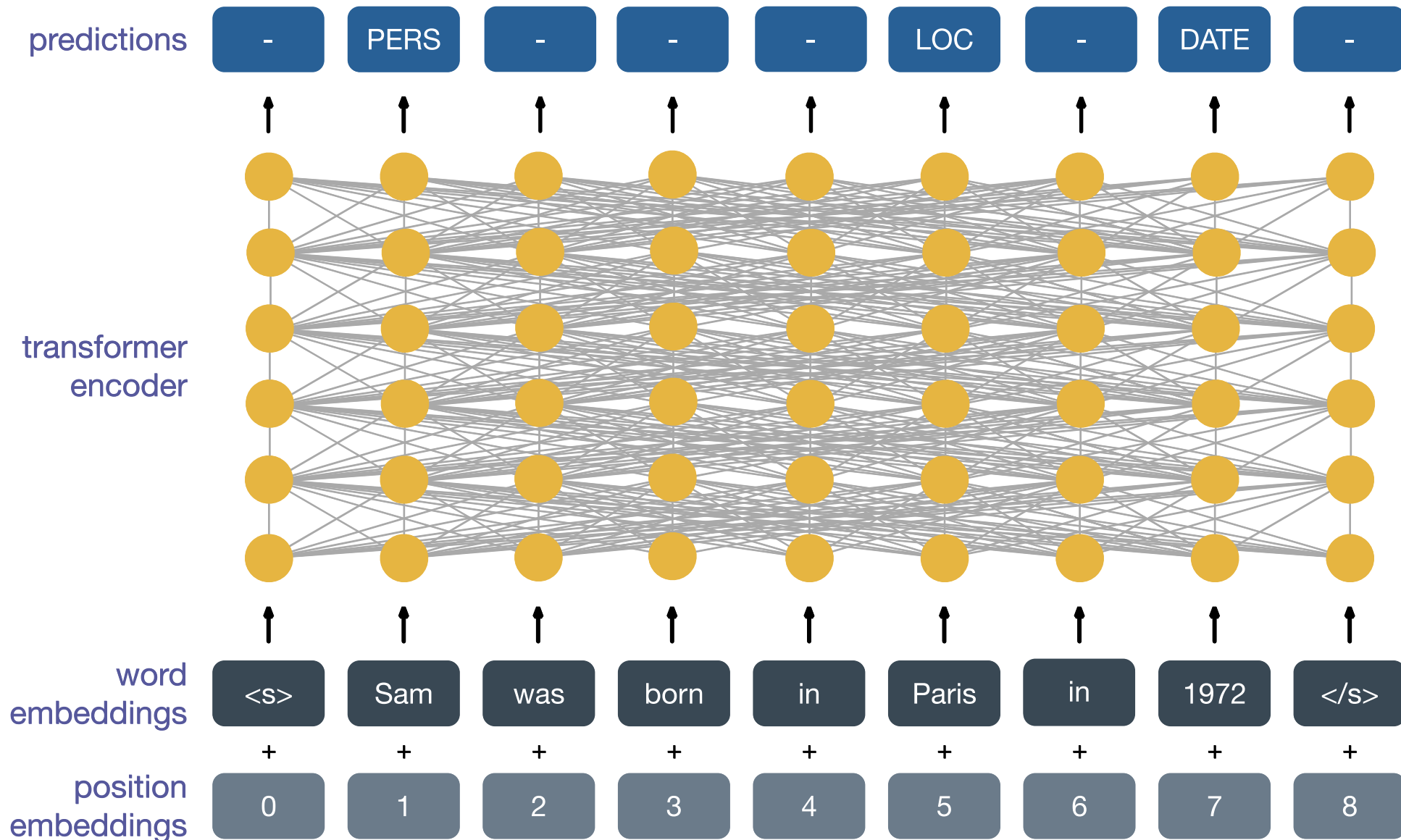


transformer
encoder

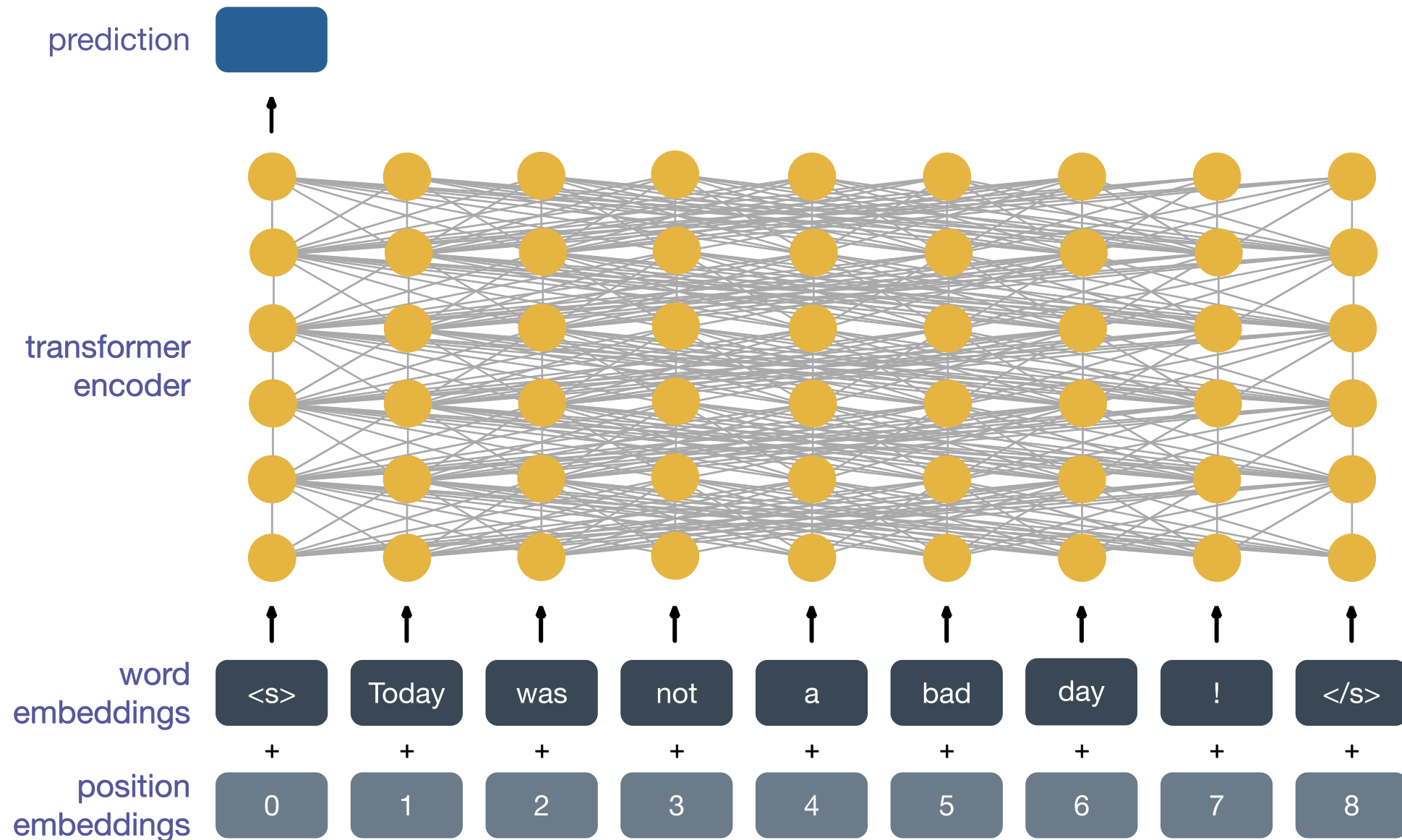
word
embeddings

position
embeddings

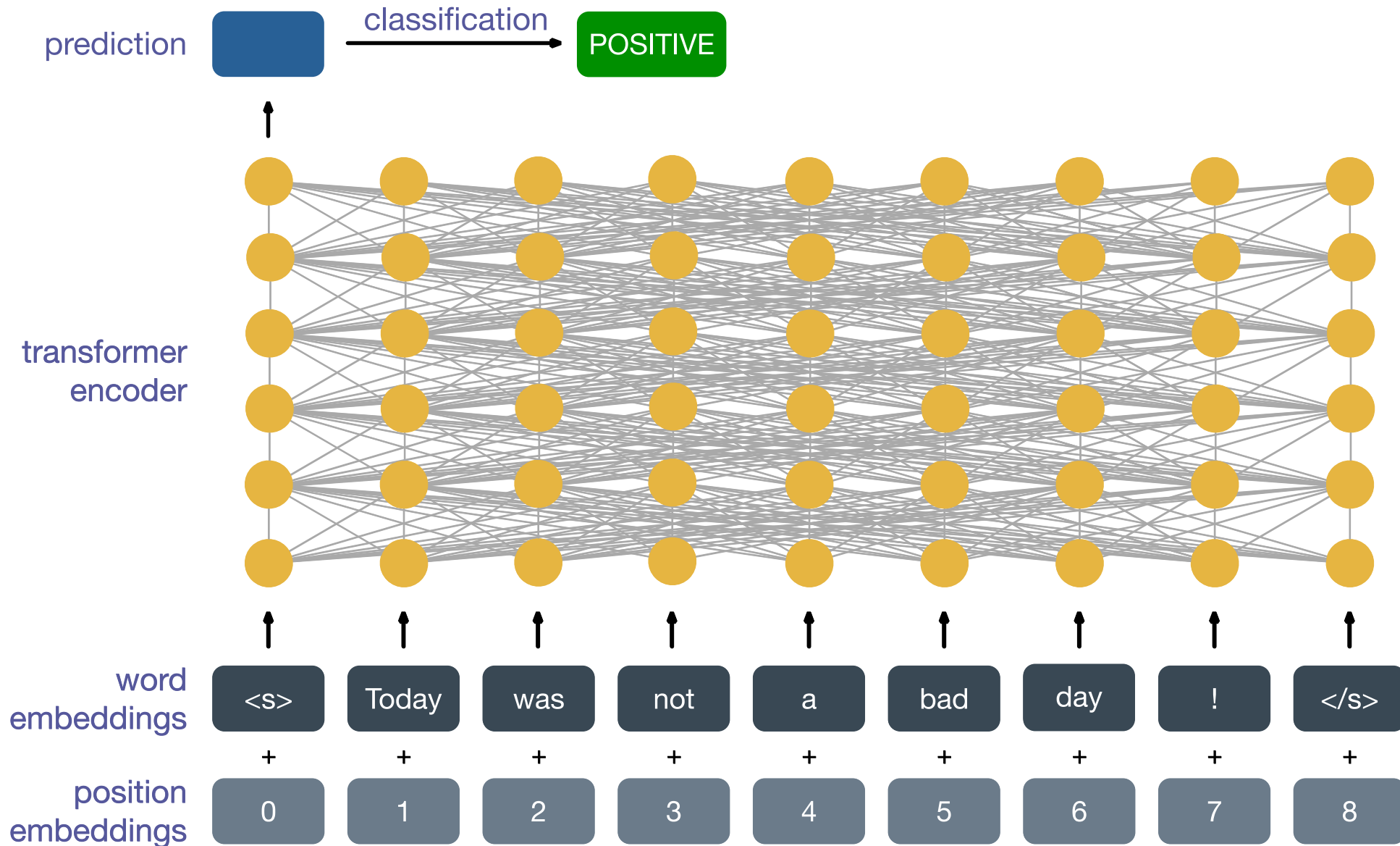
Token-level Tasks



Token-level Tasks



Sentence-level Tasks

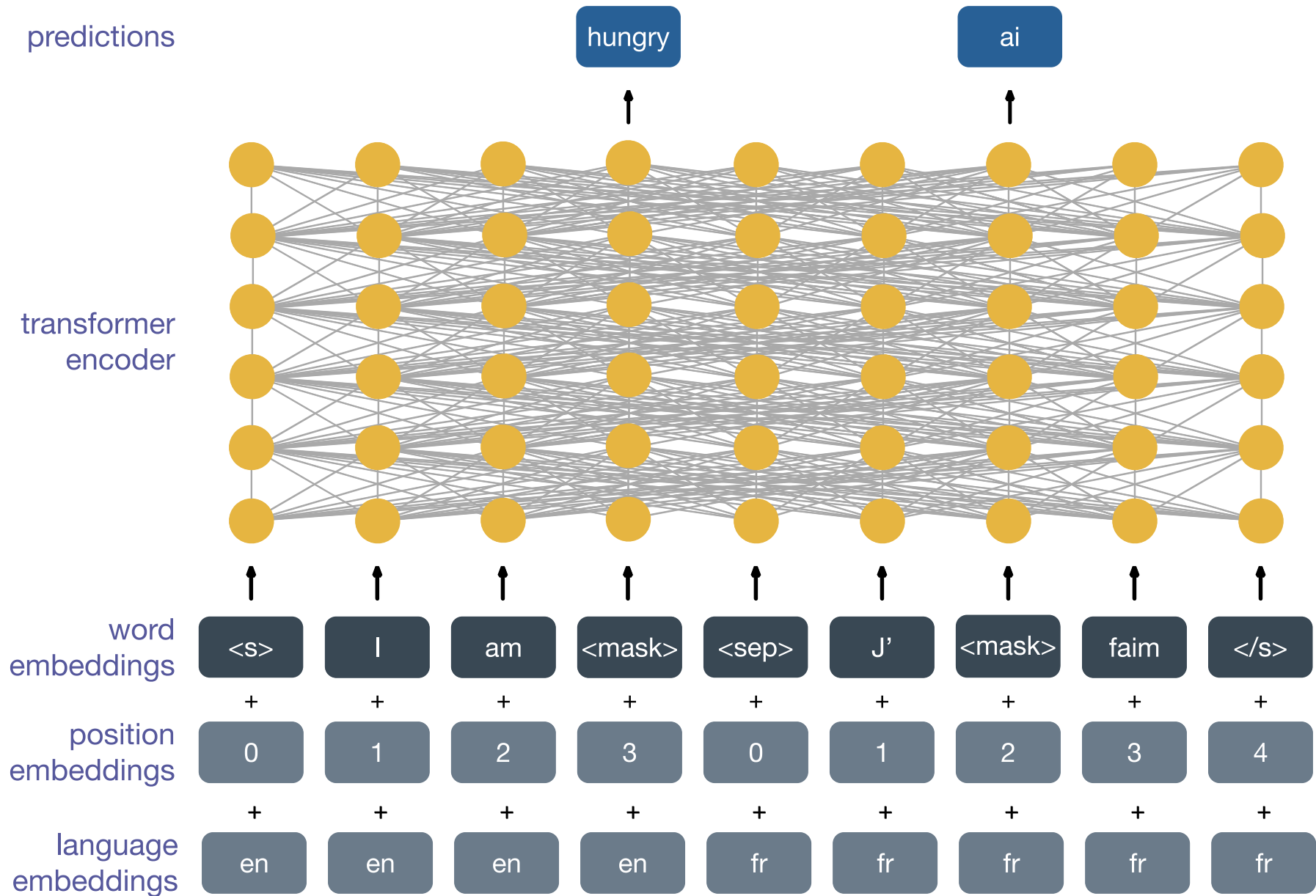


Sentence-level Tasks

I am hungry

J' ai faim

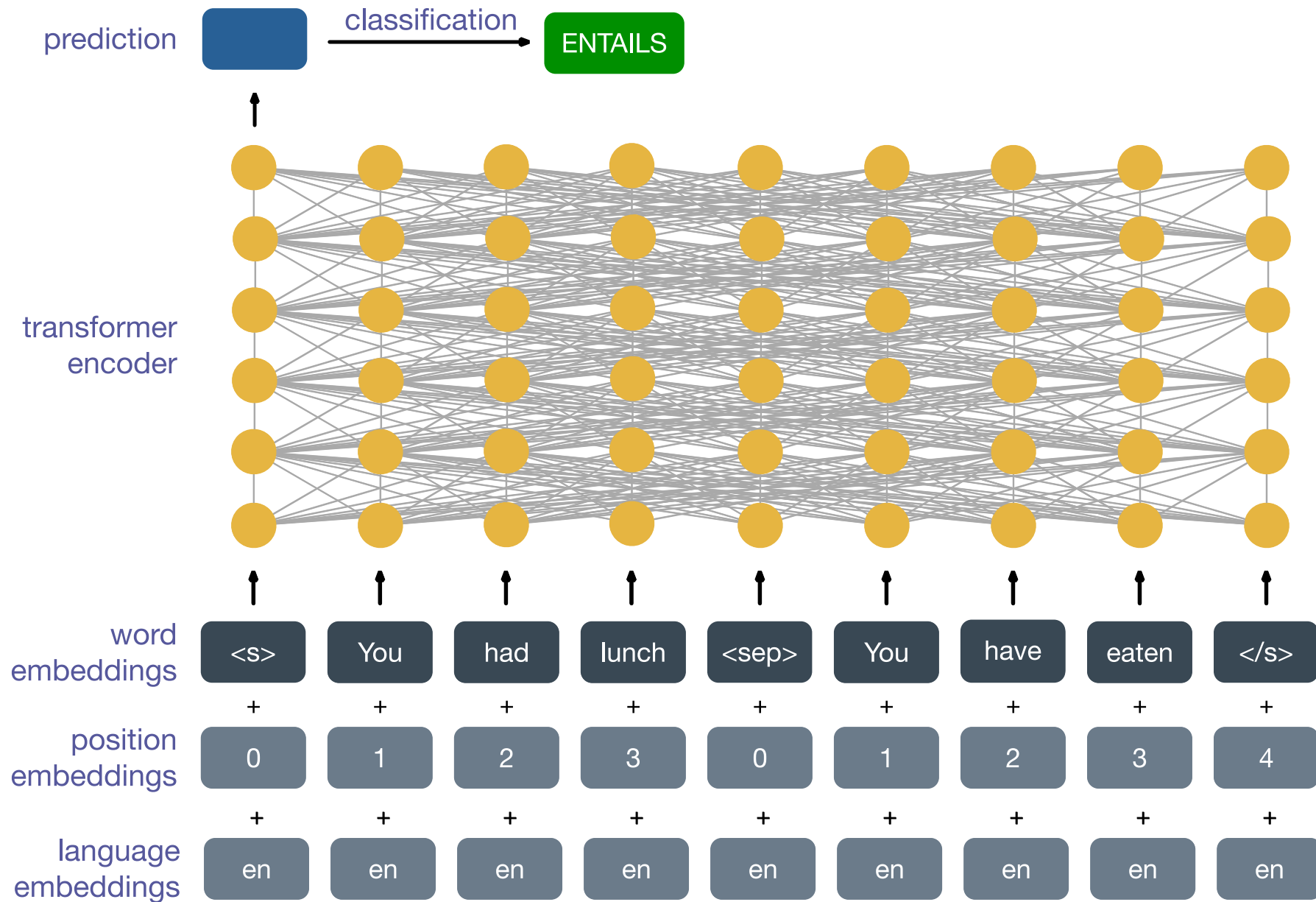
<s> I am <mask> <sep> J' <mask> faim </s>



Cross-lingual Masked Language Modeling

FACEBOOK AI

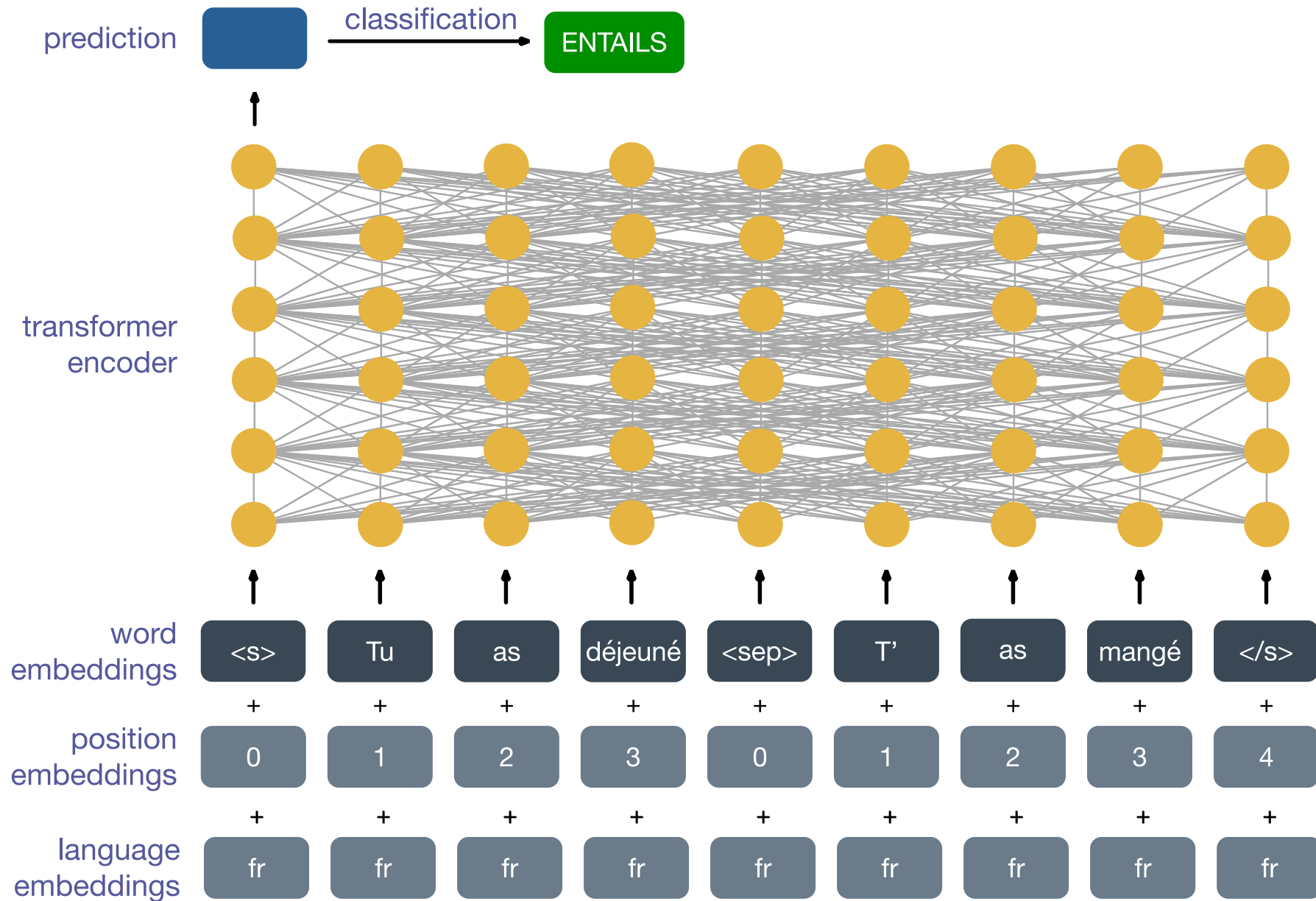




Cross-lingual Task: Natural Language Inference

FACEBOOK AI

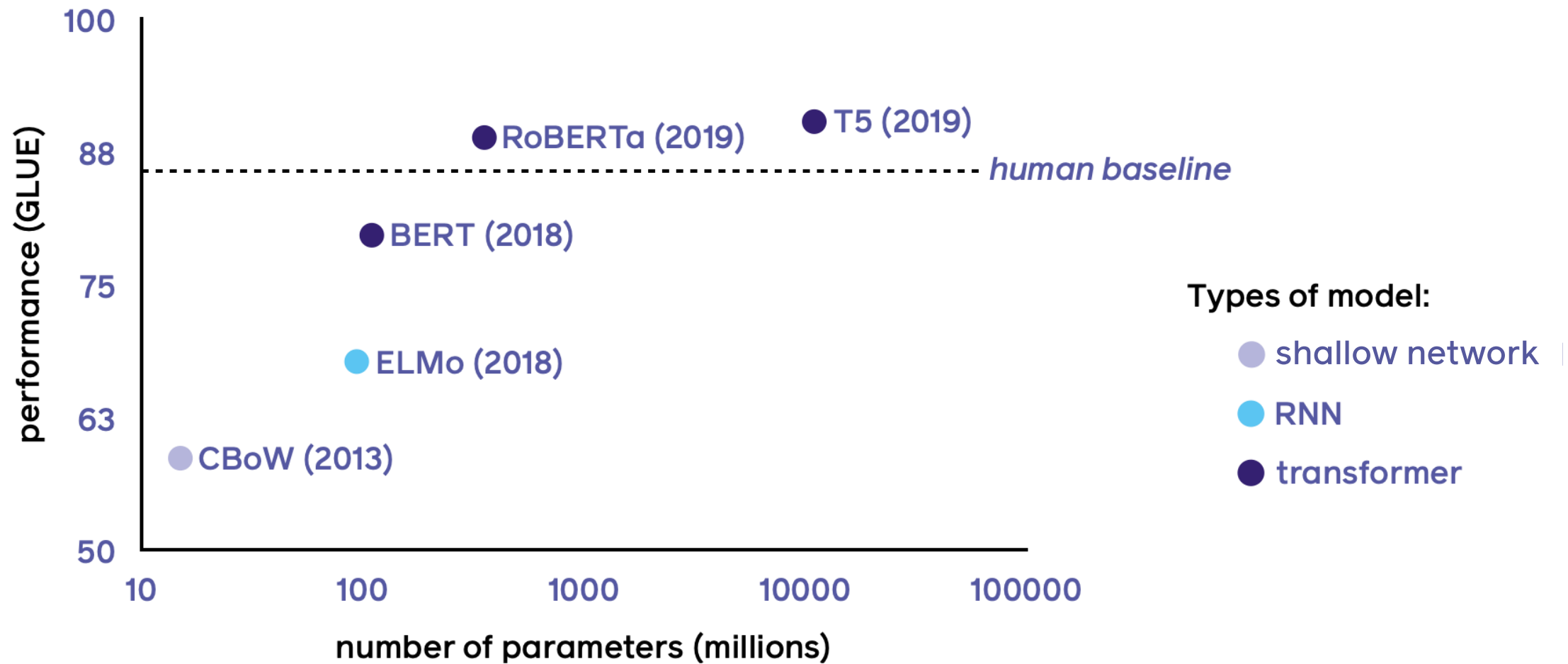




Cross-lingual Task: Natural Language Inference

FACEBOOK AI





Model Size in Perspective

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

ViLBERT: A Visolinguistic Transformer



pop artist performs at the festival in a city.

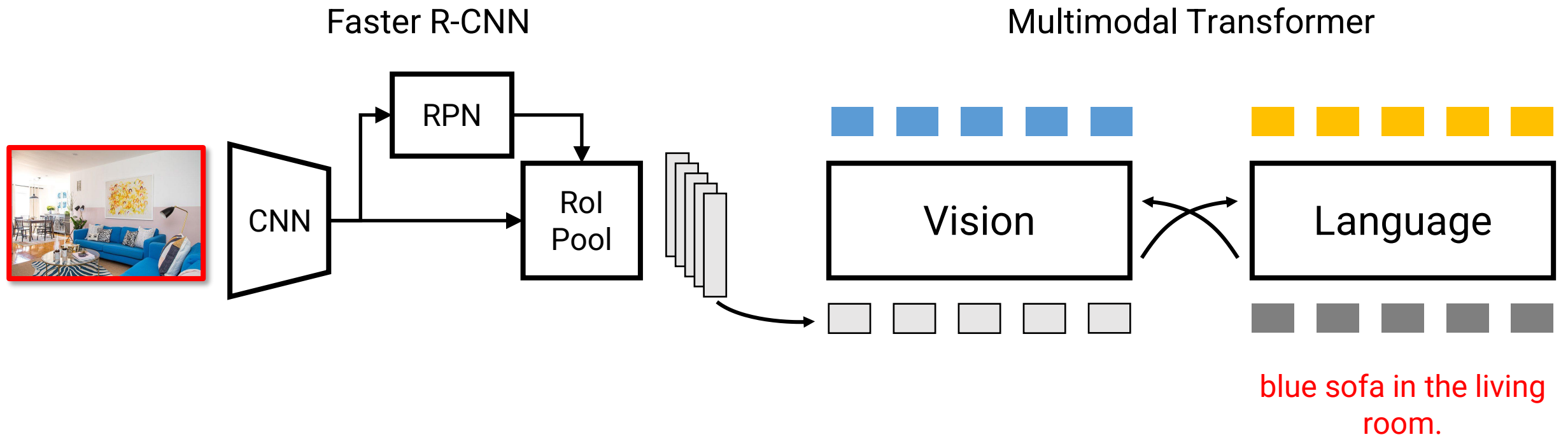


a worker helps to clear the debris.



blue sofa in the living room.

ViLBERT: A Visolinguistic Transformer



What about for just image inputs? Without Convolution?

Preprint. Under review.

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, neilhoulby}@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. 

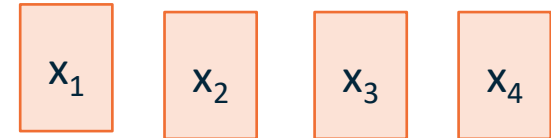
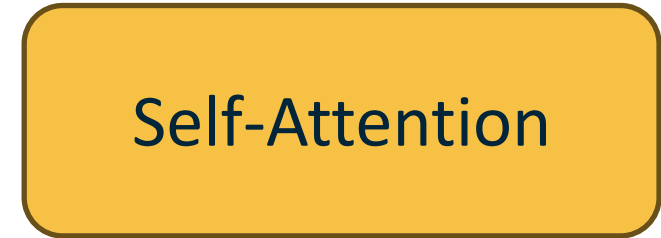
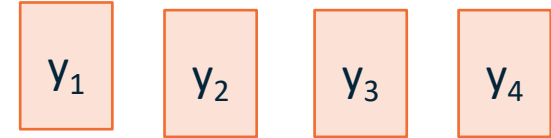
[cs.CV] 22 Oct 2020

Slide progression inspired by Soheil Feizi

What About Vision with just Self-Attention?



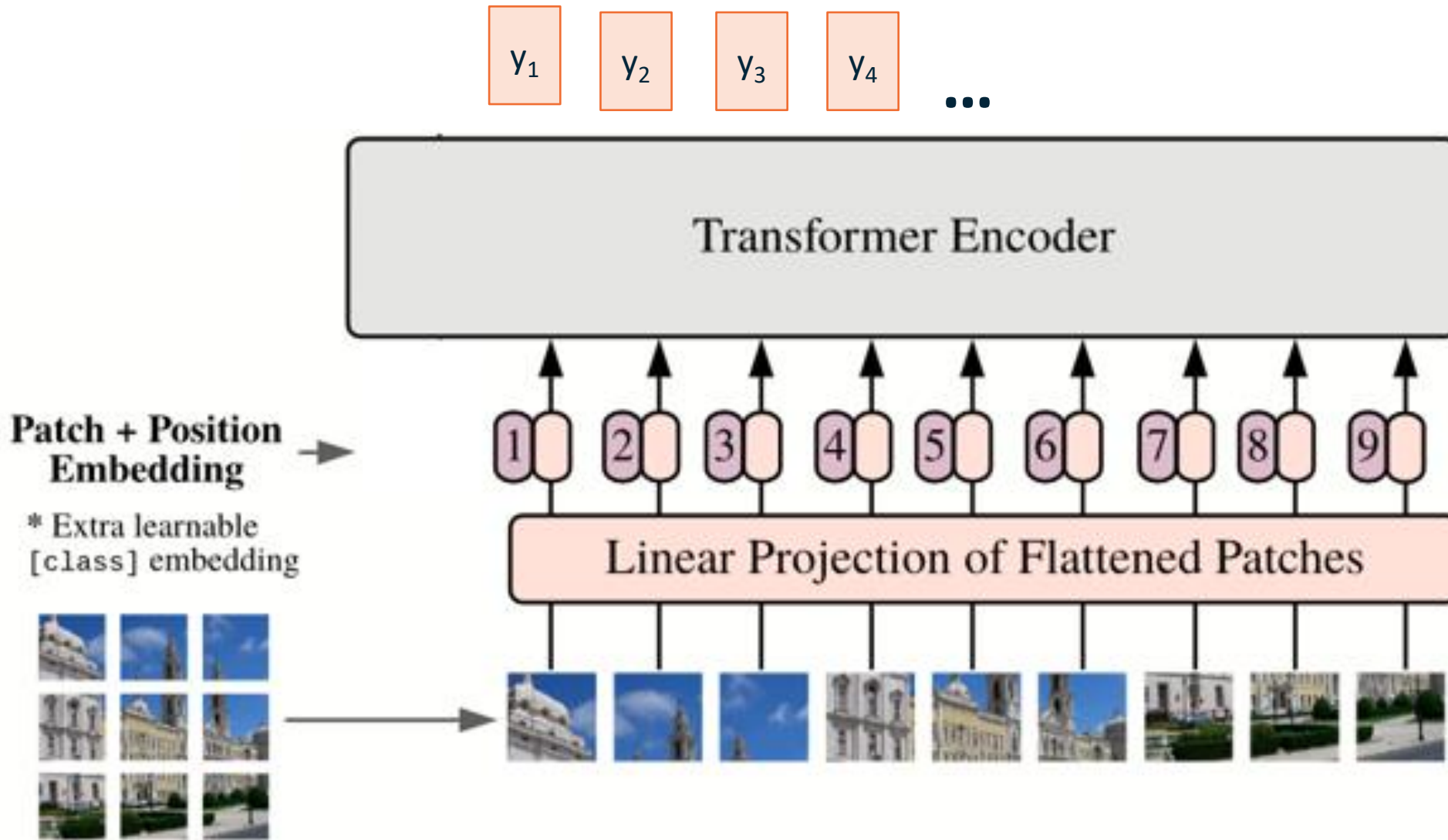
How should we
“tokenize” images?



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

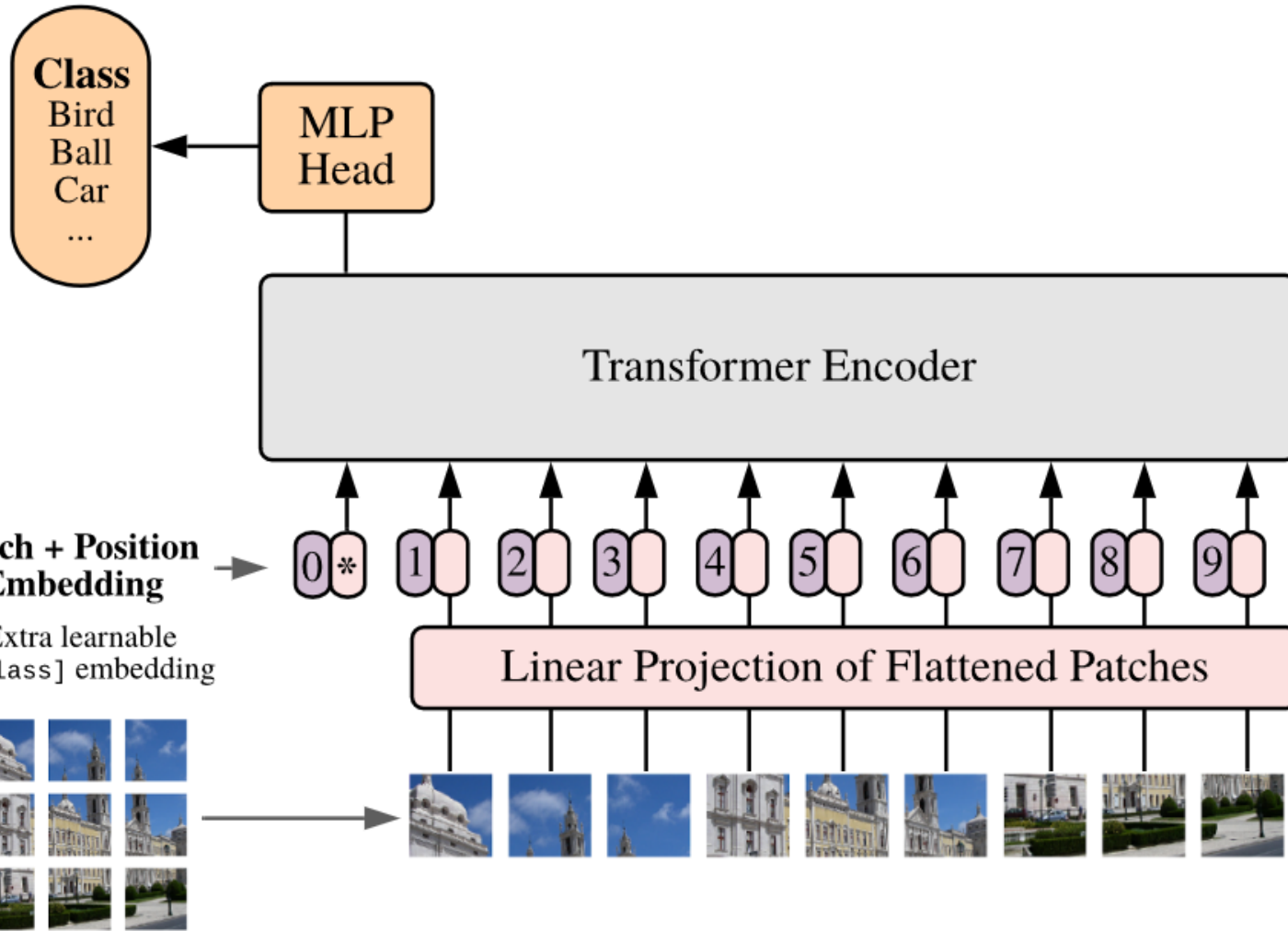
What to do with images?

- How do we do classification?

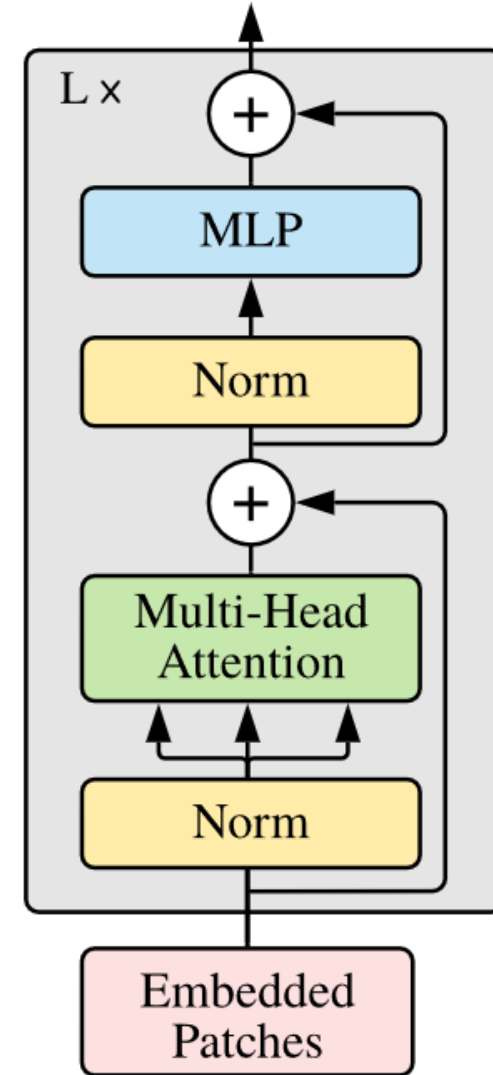


Patches as input to Self-Attention

Vision Transformer (ViT)



Transformer Encoder



Vision Transformer (ViT)

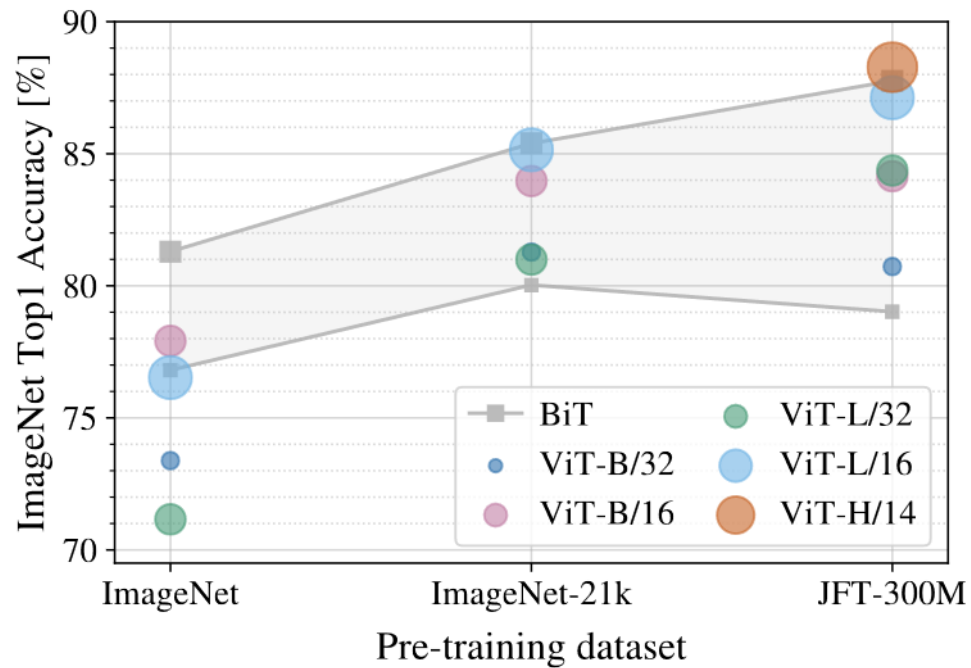


Figure 3: Transfer to ImageNet. While large ViT models perform worse than BiT ResNets (shaded area) when pre-trained on small datasets, they shine when pre-trained on larger datasets. Similarly, larger ViT variants overtake smaller ones as the dataset grows.

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?

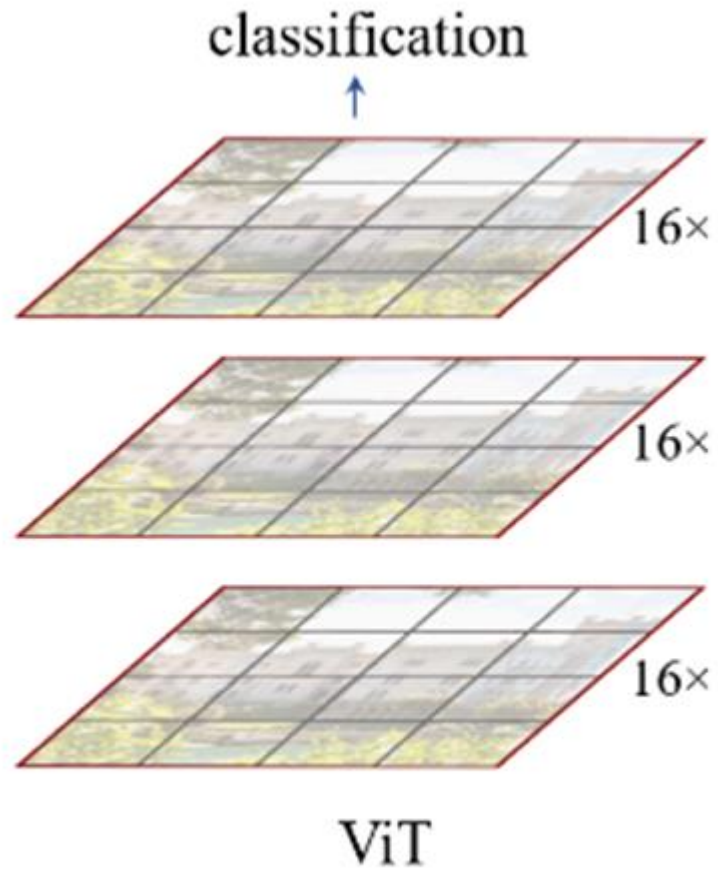
However, the picture changes if the models are trained on larger datasets (14M-300M images). We find that large scale training trumps inductive bias.

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

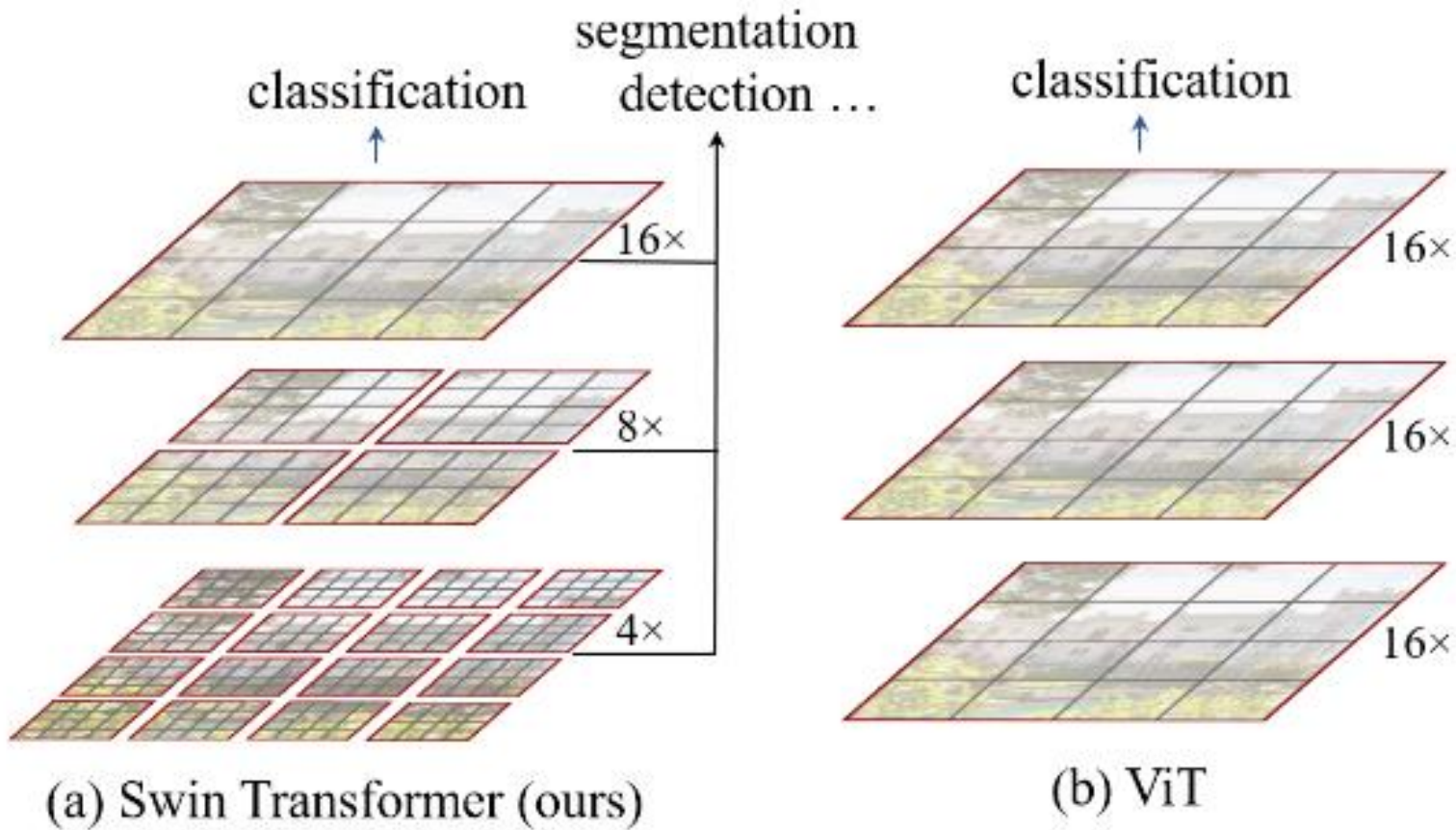
Table 1: Details of Vision Transformer model variants.

	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 ± 0.04	87.76 ± 0.03	85.30 ± 0.02	87.54 ± 0.02	88.4/88.5*
ImageNet ReaL	90.72 ± 0.05	90.54 ± 0.03	88.62 ± 0.05	90.54	90.55
CIFAR-10	99.50 ± 0.06	99.42 ± 0.03	99.15 ± 0.03	99.37 ± 0.06	—
CIFAR-100	94.55 ± 0.04	93.90 ± 0.05	93.25 ± 0.05	93.51 ± 0.08	—
Oxford-IIIT Pets	97.56 ± 0.03	97.32 ± 0.11	94.67 ± 0.15	96.62 ± 0.23	—
Oxford Flowers-102	99.68 ± 0.02	99.74 ± 0.00	99.61 ± 0.02	99.63 ± 0.03	—
VTAB (19 tasks)	77.63 ± 0.23	76.28 ± 0.46	72.72 ± 0.21	76.29 ± 1.70	—
TPUv3-core-days	2.5k	0.68k	0.23k	9.9k	12.3k

Can we add some inductive biases?



What is wrong with this?



Ideas:

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

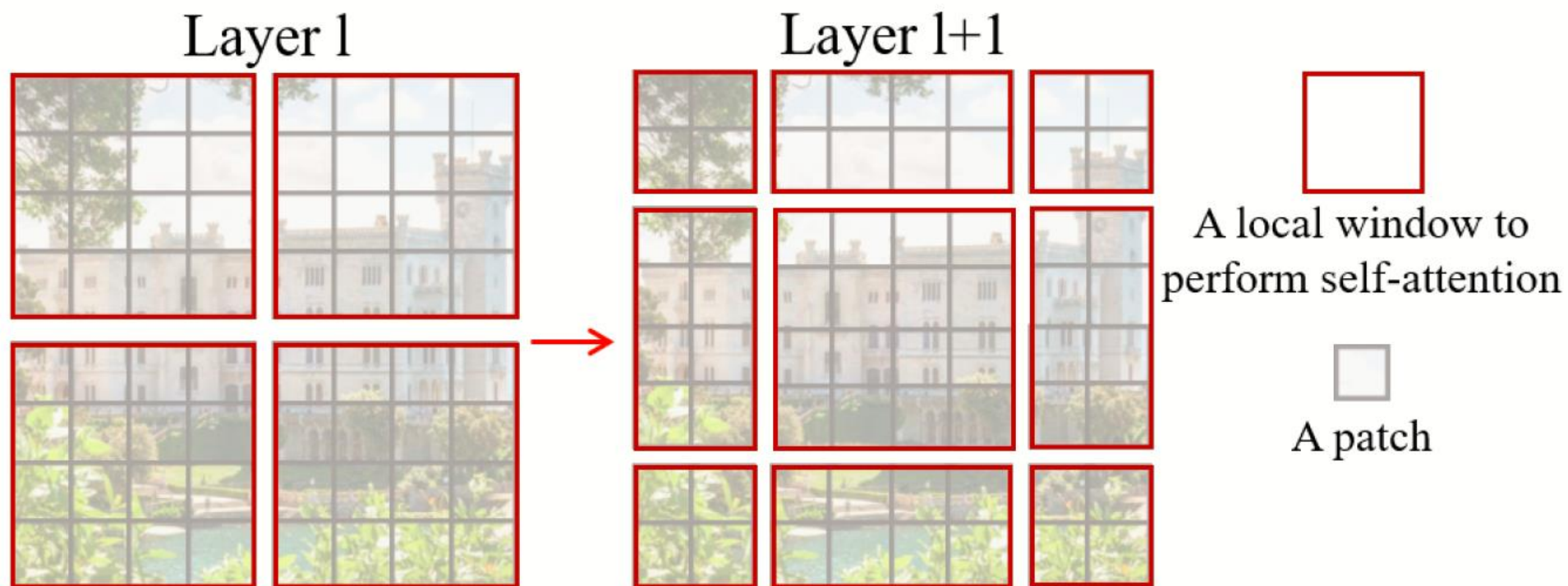
Swin Transformer: Hierarchical Vision Transformer using Shifted Windows

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-duco>





Swin Transformer: Hierarchical Vision Transformer using Shifted Windows

Ze Liu, Yutong Lin, Yue Cao, Han Hu, Yixuan Wei, Zheng Zhang, Stephen Lin, Baining Guo

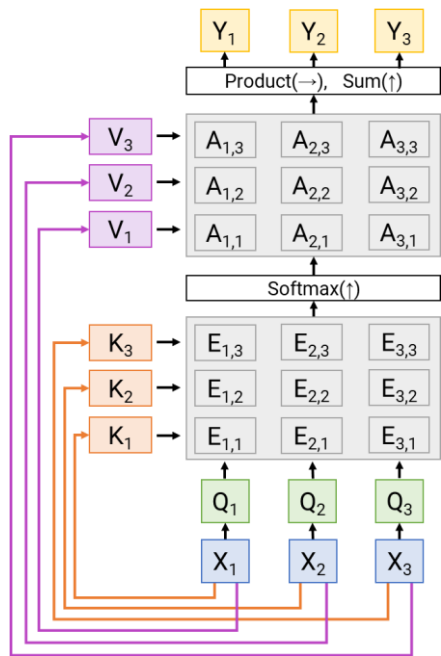
Shifted Window Attention

Summary

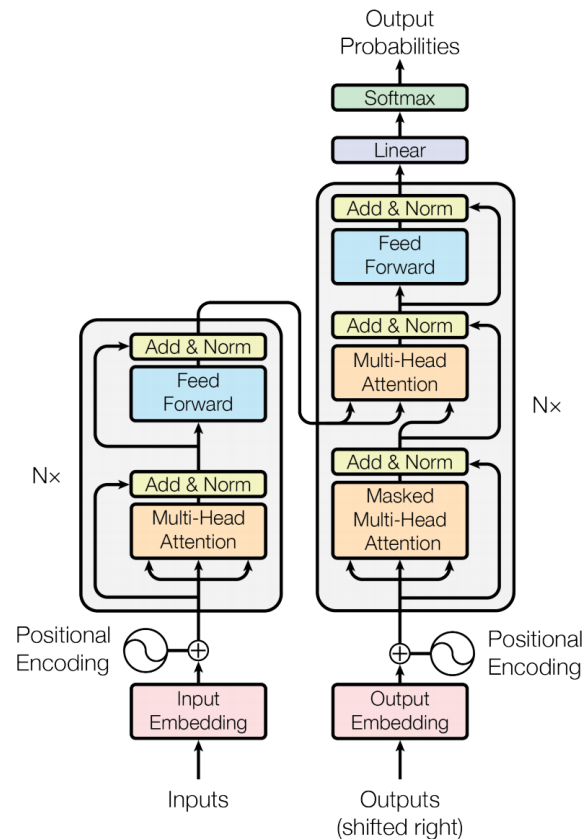
- “Attention” models outperform recurrent models and convolutional models for sequence processing. They allow long range interactions.
- These models do best with LOTS of training data
- Surprisingly, they seem to outperform convolutional networks for image processing tasks.
 - Long(er) range interactions might be more important than we realized.
- Naïve attention mechanisms have quadratic complexity with the number of input tokens, but there are often workarounds for this.

Summary

Self-Attention



Transformer Model



ViLBERT

