Transformers / Vision Transformers

EE/CS/CNS148 2022

Neehar Kondapaneni

Transformers (2017)

Attention Is All You Need

Ashish Vaswani* Google Brain avaswani@google.com

Noam Shazeer* Google Brain noam@google.com

Niki Parmar* Google Research nikip@google.com

Jakob Uszkoreit* Google Research usz@google.com

Llion Jones* Google Research llion@google.com

Aidan N. Gomez* † University of Toronto aidan@cs.toronto.edu

Łukasz Kaiser* Google Brain lukaszkaiser@google.com

Illia Polosukhin* ‡ illia.polosukhin@gmail.com

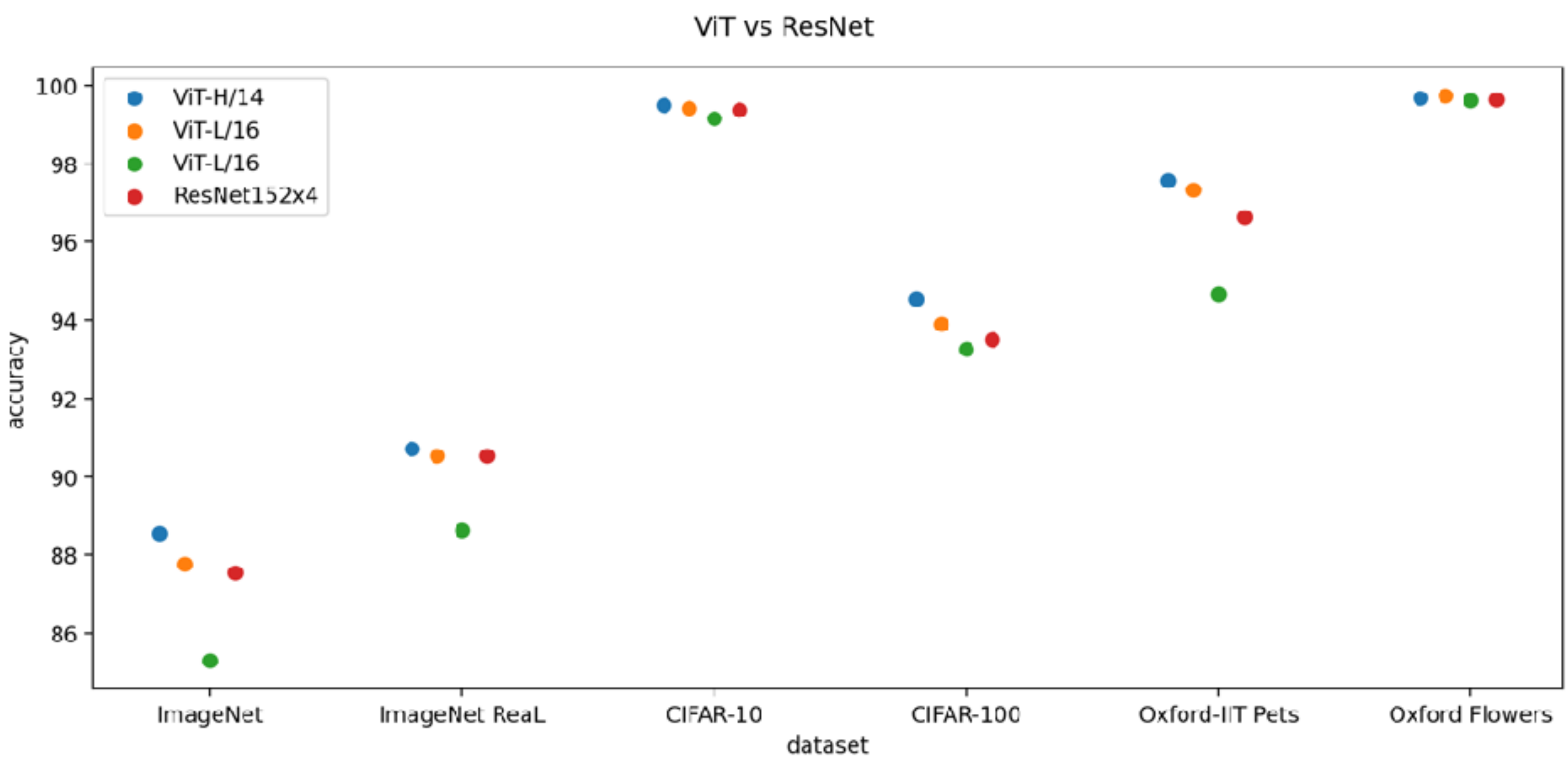
The quality of the text generated by GPT-3 is so high that it can be difficult to determine whether or not it was written by a human, which has both benefits and risks.[4]

Transformers were originally designed for natural language processing… here's a link to an interactive example.

Vision Transformers (ViT) (2021)

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



****Ongoing research on whether ResNets or Transformers are better…**

Lecture Roadmap

1. **Motivation**
2. Word Embeddings
3. Attention
   - What is it, intuitively?
   - What is it, mathematically?
4. Scalar Dot-Product Attention
   - Why?
   - Queries, Keys, Values
   - Computing Attention
5. Multi-Headed Attention
   - MHA Intuition
6. Transformer Architecture
7. Vision Transformers
   - Moving from text to images
   - Comparing transformers and CNNs

Motivation

Suppose we want to do language translation…

Italian: Io la sto mangiando.

Direct Translation: I it am eating.

English: I am eating it.

Motivation

Suppose we want to do language translation…

Italian: Io la sto mangiando.

Direct Translation: I it am eating.

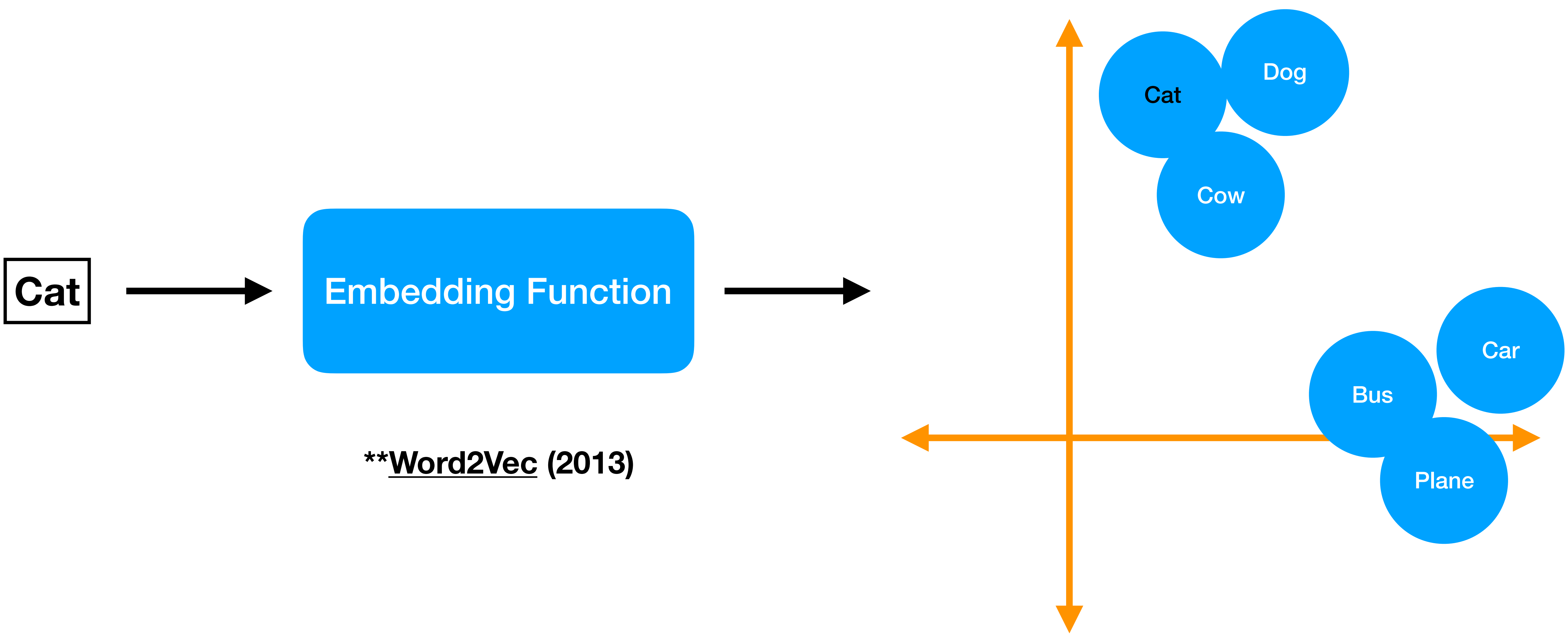
English: I am eating it.

A translator would need to determine what parts of the **Italian** sentence to pay **attention** to, in order to translate it correctly.

Lecture Roadmap

1. Motivation
2. **Word Embeddings**
3. Attention
    - What is it, intuitively?
    - What is it, mathematically?
4. Scalar Dot-Product Attention
    - Why?
    - Queries, Keys, Values
    - Computing Attention
5. Multi-Headed Attention
    - MHA Intuition
6. Transformer Architecture
7. Vision Transformers
    - Moving from text to images
    - Comparing transformers and CNNs

Word Embeddings



****<u>Word2Vec</u> (2013)**

Lecture Roadmap

1. Motivation
2. Word Embeddings
3. **Attention**
    - What is it, intuitively?
    - What is it, mathematically?
4. Scalar Dot-Product Attention
    - Why?
    - Queries, Keys, Values
    - Computing Attention
5. Multi-Headed Attention
    - MHA Intuition
6. Transformer Architecture
7. Vision Transformers
    - Moving from text to images
    - Comparing transformers and CNNs

Attention

Italian: Io la sto mangiando.

When reading a word in this sentence, what do I need to pay **attention** to.

Attention

Italian: Io la sto mangiando.

When reading a word in this sentence, what do I need to pay **attention** to.

English is a **subject - verb - object** language

English: I am eating it.

Attention

Italian: Io la sto mangiando.

When reading a word in this sentence, what do I need to pay **attention** to.

English is a **subject - verb - object** language

English: I am eating it.

What is the subject doing?

Io la sto mangiando.

Attention

Italian: Io la sto mangiando.

When reading a word in this sentence, what do I need to pay **attention** to.

English is a **subject - verb - object** language

English: I am eating it.

What is the subject doing?

Io la sto mangiando.

What is the verb operating on?

Io la sto **mangiando**.

Attention

How might we encode this mathematically using our word embeddings?

Word embedding

$$e_i$$

Attention

How might we encode this mathematically using our word embeddings?

t

Io la sto mangiando.

Word embedding

e_i

Attention

How might we encode this mathematically using our word embeddings?

$$\alpha_{ti} = \begin{array}{cccc} t & & & \\ \left[\; 0.33 \right. & 0.00 & 0.33 & \left. 0.33 \;\right] \\ \textbf{lo} & \text{la} & \text{sto} & \text{mangiando.} \end{array}$$

Attention weights

Word embedding

$$\alpha_{ti} \quad e_i$$

Attention

How might we encode this mathematically using our word embeddings?

$$
\begin{array}{cccccc}
 & t & & & & \\
\alpha_{ti} = [& 0.00 & 0.00 & 0.33 & 0.33 &] \\
 & \textbf{lo} & \text{la} & \text{sto} & \text{mangiando.} &
\end{array}
$$

Attention weights

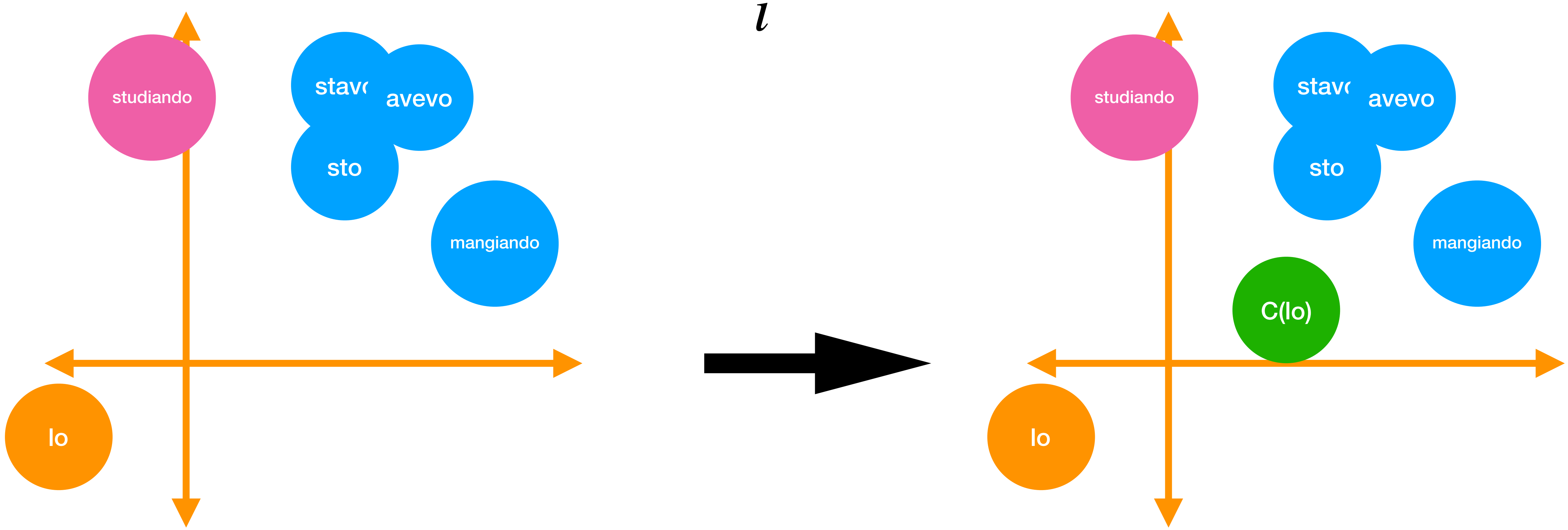
Context vector

Word embedding

$$c_t = \sum_{i}^{T} \alpha_{ti} \cdot e_i$$

Attention

$$c_t = \sum_{i}^{T} \alpha_{ti} \cdot e_i$$



Italian: Io la sto mangiando.

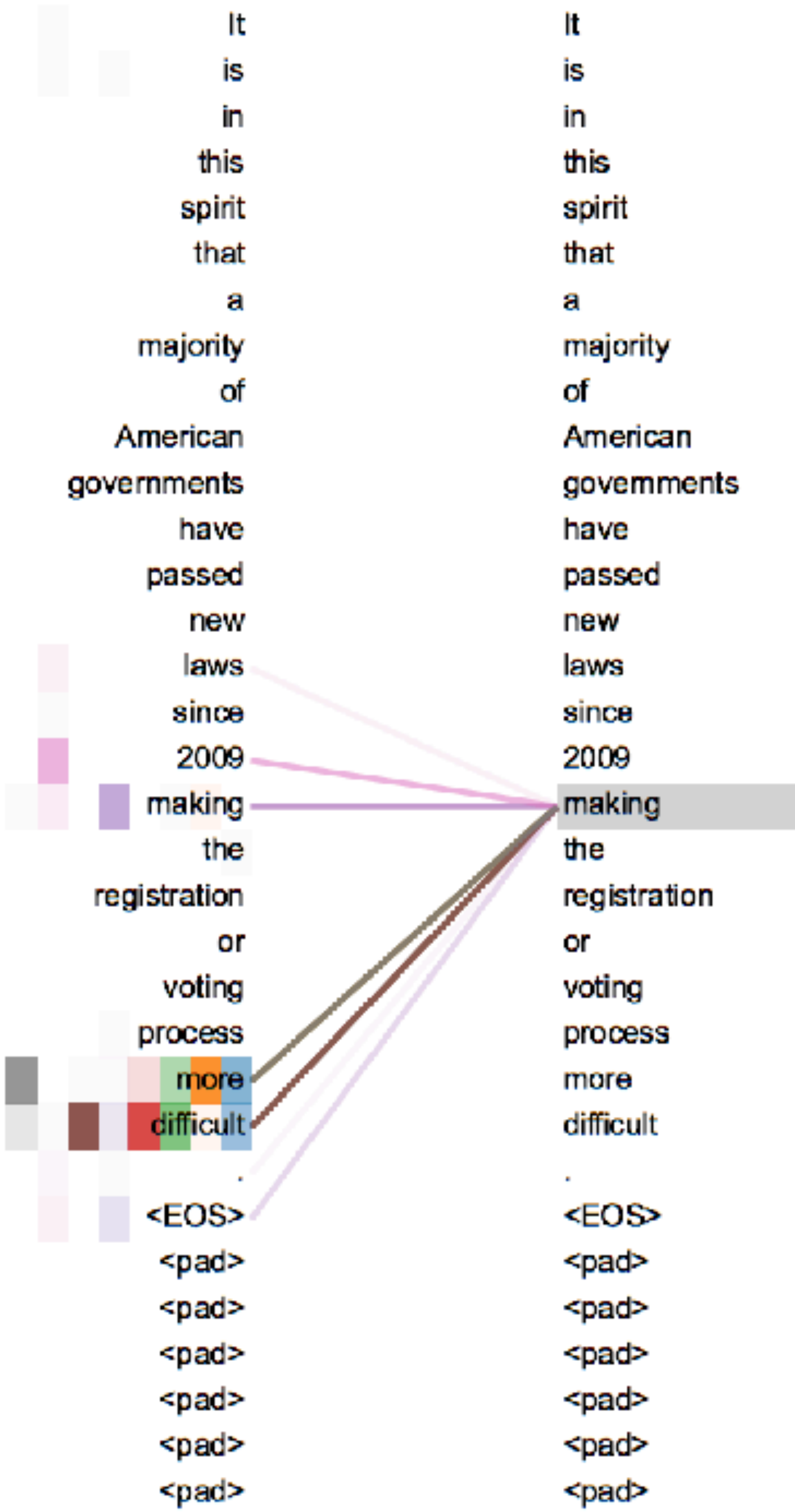
Lecture Roadmap

1. Motivation
2. Word Embeddings
3. Attention
    - What is it, intuitively?
    - What is it, mathematically?
4. **Scalar Dot-Product Attention**
    - Why?
    - Queries, Keys, Values
    - Computing Attention
5. Multi-Headed Attention
    - MHA Intuition
6. Transformer Architecture
7. Vision Transformers
    - Moving from text to images
    - Comparing transformers and CNNs

Why Scalar Dot-Product Attention?

Let's look at a couple of motivating examples…

From here on out, **'query'** will represent the word that we are encoding the context for.

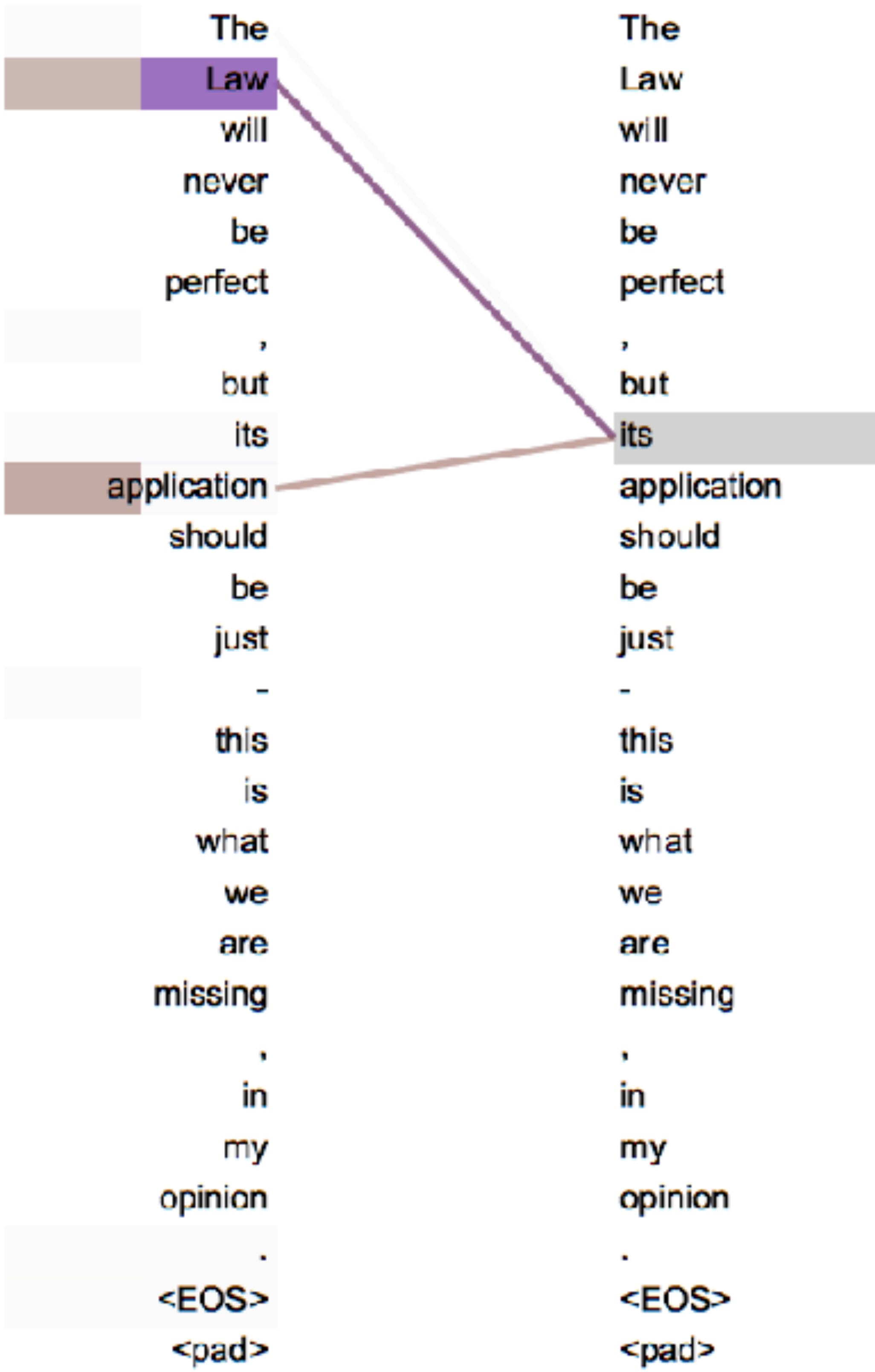


Context for verbs

Here the **query** is *making*.

It puts most **attention** on itself and on the words *more difficult*, creating a **context** for the phrase *making [something] more difficult*.

Anaphora Resolution



Anaphora Example:
Susan dropped the plate. **It** shattered loudly.

This layer resolves what words like “it” refer back to.

Scalar Dot-Product Attention

Each word in the sentence will have three representations.

Query, Key, Value.

Query, Key, Value Intuition

Q, K, V are originally from retrieval systems (search).

In retrieval systems… like youtube search

Queries - The sentences we type in to youtube to look for a video
Keys - The representations of the videos
Values - The videos of interest

Query, Key, Value Intuition

In sentences…

Queries - Representations of the word of interest
Keys - Representations for all the words in the sentence
Values - The abstract, contextual representation of the words

Query, Key, Value Intuition

In sentences…

Queries - Representations of the word of interest
Keys - Representations for all the words in the sentence
Values - The abstract semantic representation of the words

We want to determine how each **query**, relates to each **key** to compute an attention over the **values**.

Query, Key, Value Intuition

In sentences…

Queries - Representations of the word of interest
Keys - Representations for all the words in the sentence
Values - The abstract semantic representation of the words

We want to determine how each **query**, relates to each **key** to compute an attention over the **values**.

First, how do we compute these representations?

Query, Key, Value

Start with the original word embedding.

$$word_i \longrightarrow \boxed{\text{Embedding Function}} \longrightarrow z_i \in R^{d_z}$$

Query, Key, Value

Start with the original word embedding.

$$word_i \longrightarrow \boxed{\text{Embedding Function}} \longrightarrow z_i \in R^{d_z}$$

Linear projections of the original word embedding.

$$z_i \cdot W^Q = q_i \qquad z_i \cdot W^K = k_i \qquad z_i \cdot W^V = v_i$$

Learned

Query, Key, Value

$$W^Q \in R^{d_z \times d} \qquad W^K \in R^{d_z \times d} \qquad W^V \in R^{d_z \times d}$$

W usually **reduces** the dimensionality from the original embedding.
(Tall and skinny matrix)

Query, Key, Value

Collect all the linear projections into matrices.

$$R^{N \times d}$$

$$Q = [q_1, q_2, \ldots, q_N]^T$$

$$K = [k_1, k_2, \ldots, k_N]^T$$

$$V = [v_1, v_2, \ldots, v_N]^T$$

Scalar Dot Product Attention

Let's convert our intuitive ideas about queries, keys and values into an equation.

$$c_t = \sum_{i}^{T} \alpha_{ti} \cdot e_i$$

The original attention equation.

Scalar Dot Product Attention

Let’s convert our intuitive ideas about queries, keys and values into an equation.

$$\boxed{V}$$

$$c_t = \sum_{i}^{T} \alpha_{ti} \cdot e_i$$

Scalar Dot Product Attention

Let's convert our intuitive ideas about queries, keys and values into an equation.

$$\boxed{softmax(\frac{qK^T}{\sqrt{d}})}\boxed{V}$$

$$c_t = \sum_{i}^{T} \alpha_{ti} \cdot e_i$$

Scalar Dot Product Attention

Let’s convert our intuitive ideas about queries, keys and values into an equation.

Note that K, V are not the same as W^K, W^V

$$Attention(q, K, V) = \boxed{softmax(\frac{qK^T}{\sqrt{d}})}\boxed{V}$$

$$c_t = \sum_{i}^{T} \alpha_{ti} \cdot e_i$$

Scalar Dot Product Attention

$$Attention(q, K, V) = softmax(\frac{qK^T}{\sqrt{d}})V$$

Breaking it down…

Scalar Dot Product Attention

$$Attention(q, K, V) = softmax(\frac{qK^T}{\sqrt{d}})V$$

Breaking it down…

$$qK^T$$

Dot product - large when vectors are "similar".
Encodes relevance of keys (other words) to a specific query (word).

so that $(1 \times d) \cdot (d \times N) = (1 \times N)$

Scalar Dot Product Attention

$$Attention(q, K, V) = softmax(\frac{qK^T}{\sqrt{d}})V$$

$$qK^T$$

Dot product - large when vectors are “similar”.
Encodes relevance of keys (other words) to a specific query (word).

$$\frac{qK^T}{\sqrt{d}}$$

Scale the dot products down (to avoid vanishing gradient issues)

Scalar Dot Product Attention

$$Attention(q, K, V) = softmax(\frac{qK^T}{\sqrt{d}})V$$

$$\frac{qK^T}{\sqrt{d}}$$

Scale the dot products down (to avoid vanishing gradient issues)

$$softmax(\frac{qK^T}{\sqrt{d}})$$

Transform the dot products into weights that sum to 1 (in each row of the output matrix)

Scalar Dot Product Attention

$$Attention(q, K, V) = softmax(\frac{qK^T}{\sqrt{d}})V$$

$$softmax(\frac{qK^T}{\sqrt{d}})$$

Transform the dot products into weights that sum to 1 (in each row of the output matrix)

At this point, we have weights that we can apply to our Values representations. These weights dictate what Values we pay *attention* to.

Scalar Dot Product Attention

$$Attention(q, K, V) = softmax(\frac{qK^T}{\sqrt{d}})V$$

$$softmax(\frac{qK^T}{\sqrt{d}})$$

Transform the dot products into weights that sum to 1 (in each row of the output matrix)

$$softmax(\frac{qK^T}{\sqrt{d}})V$$

We now have a representation that abstractly represents the ***context*** with which we read **each** query word.

$$(1 \times N) \times (N \times d) = (1 \times d)$$

Scalar Dot Product Attention

We can compute a batch all at once by using a matrix of queries.

$$Attention(Q, K, V) = softmax(\frac{QK^T}{\sqrt{d}})V$$

$$(N \times N) \times (N \times d) = (N \times d)$$

Why three different representations?

Main answer: It worked better, other types of attentions have been explored, this worked the best.

Why three different representations?

Why can't we fold queries and keys into one representation?

****These are opinions. StackOverflow has some discussion about this.**

Why three different representations?

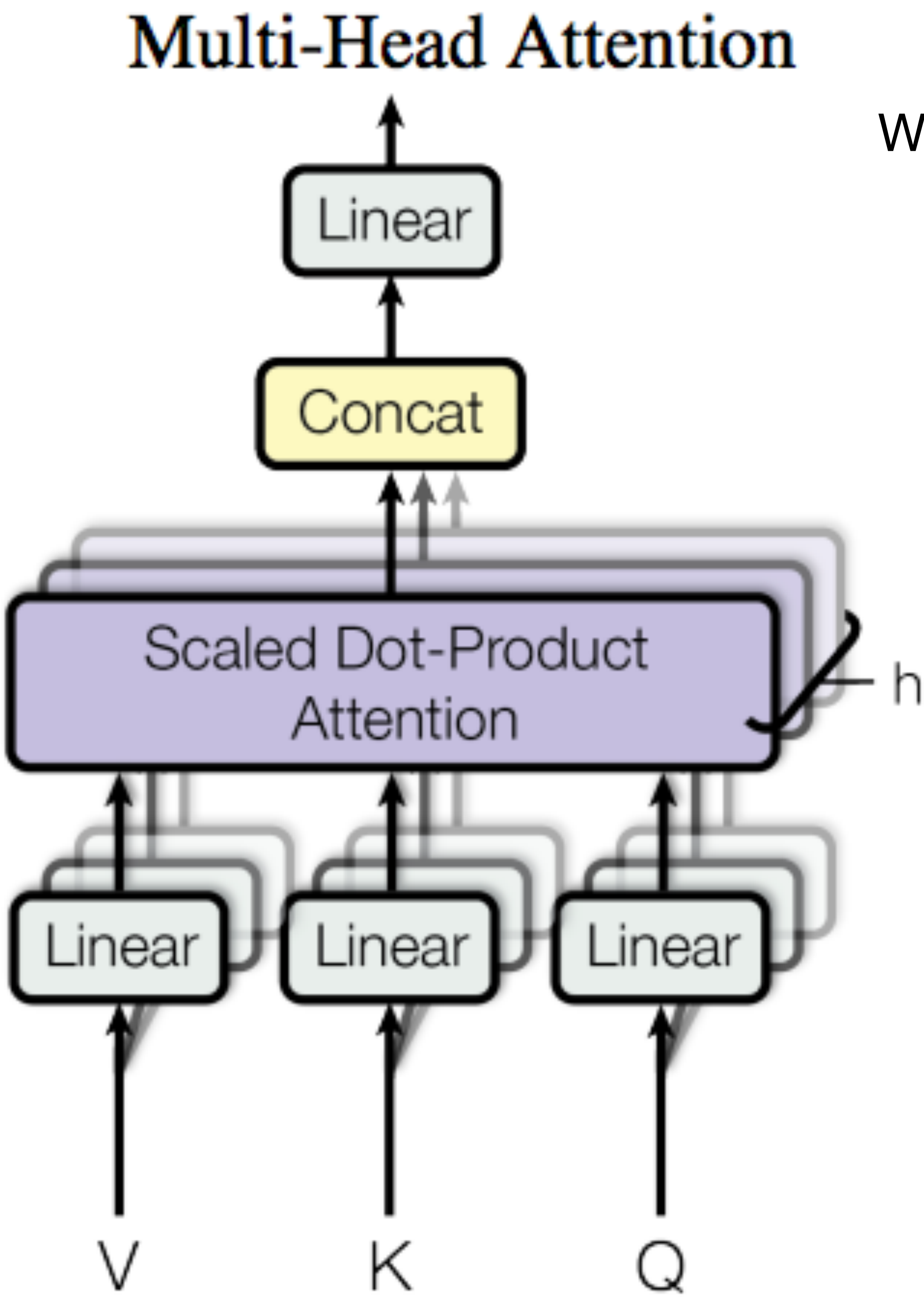
Why can't we fold keys and values into one representation?

****StackOverflow has some discussion about this.**

Lecture Roadmap

1. Motivation
2. Word Embeddings
3. Attention
    - What is it, intuitively?
    - What is it, mathematically?
4. Scalar Dot-Product Attention
    - Why?
    - Queries, Keys, Values
    - Computing Attention
5. **Multi-Headed Attention**
    - MHA Intuition
6. Transformer Architecture
7. Vision Transformers
    - Moving from text to images
    - Comparing transformers and CNNs

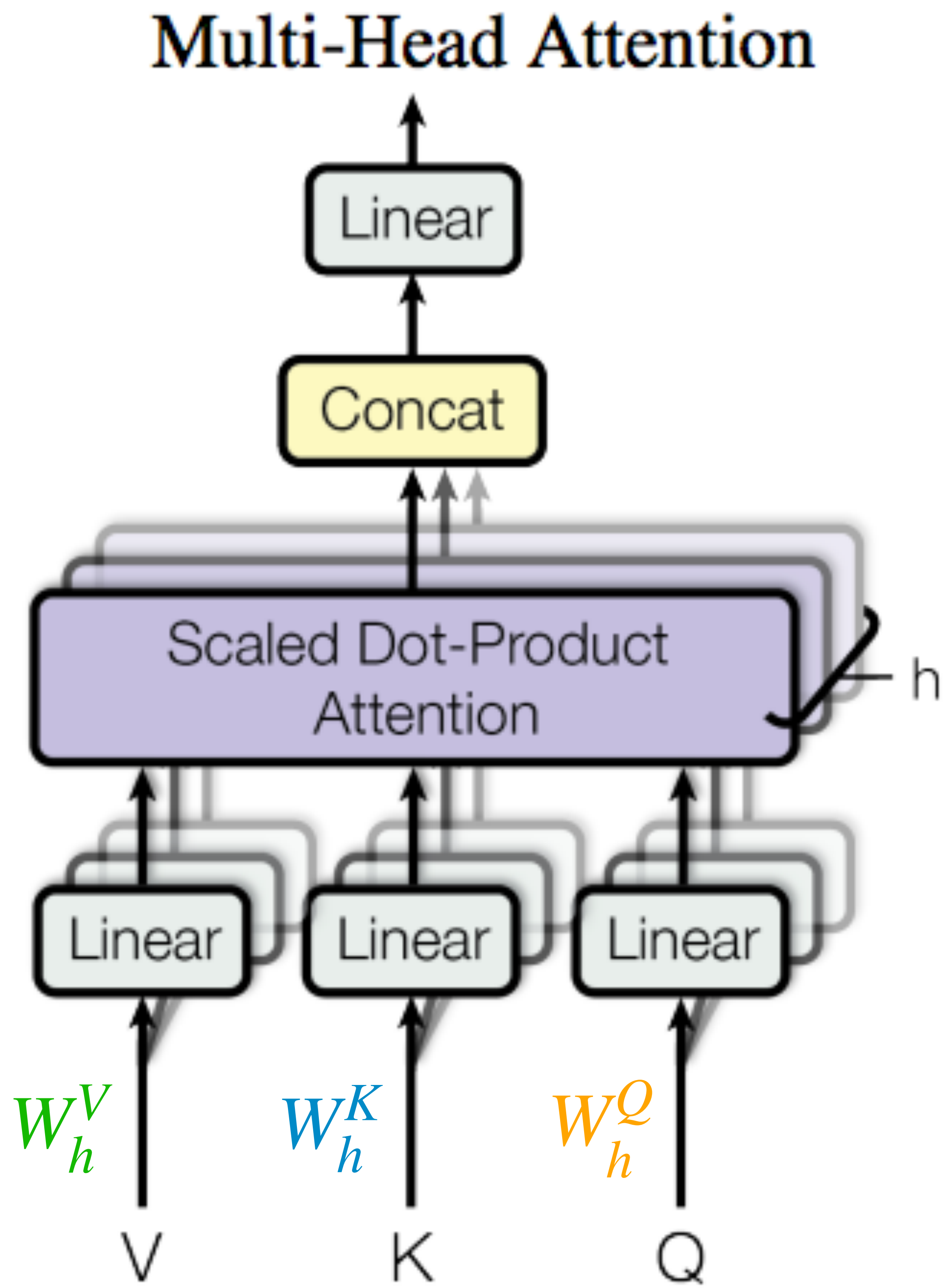
Multi-Head Attention



We are learning a different transformation per head.

W_h^V W_h^K W_h^Q

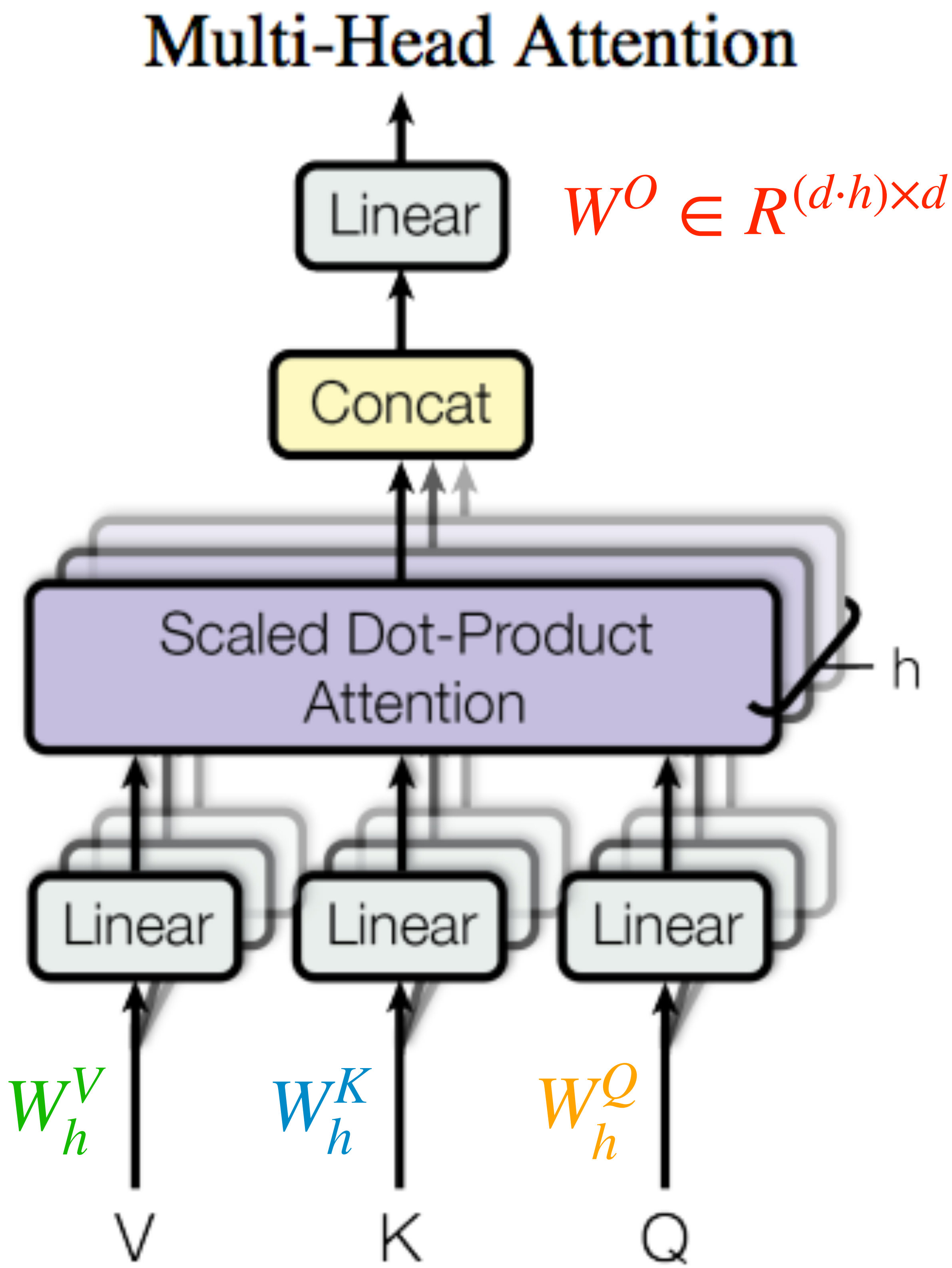
Multi-Head Attention



$(N \times dh)$

Concatenate output of SDPA layers

Multi-Head Attention



$$(N \times d) = (N \times dh) \cdot (dh \times d)$$

$$MHA = ConcatVec \cdot W^O$$

$$(N \times dh)$$

Concatenate output of SDPA layers

MHA Intuition

Why multiple heads?

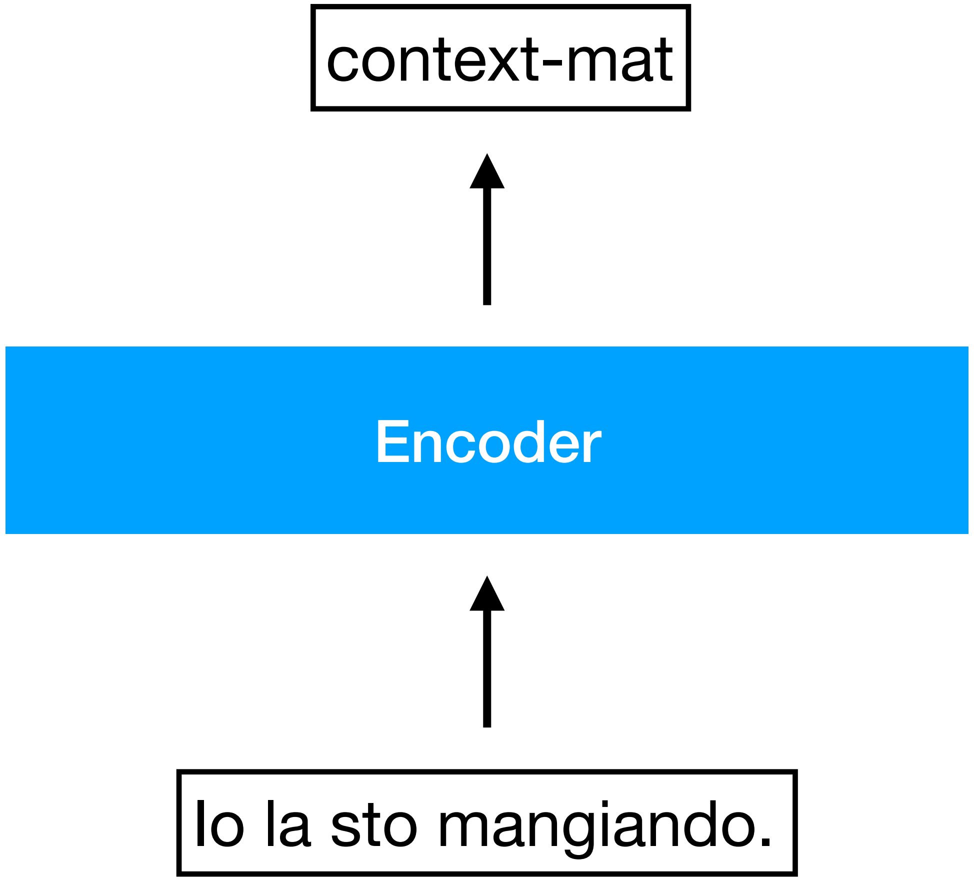
It worked better in their paper.

The real answer is more nuanced and has to do with training stability.
https://arxiv.org/pdf/2106.09650.pdf

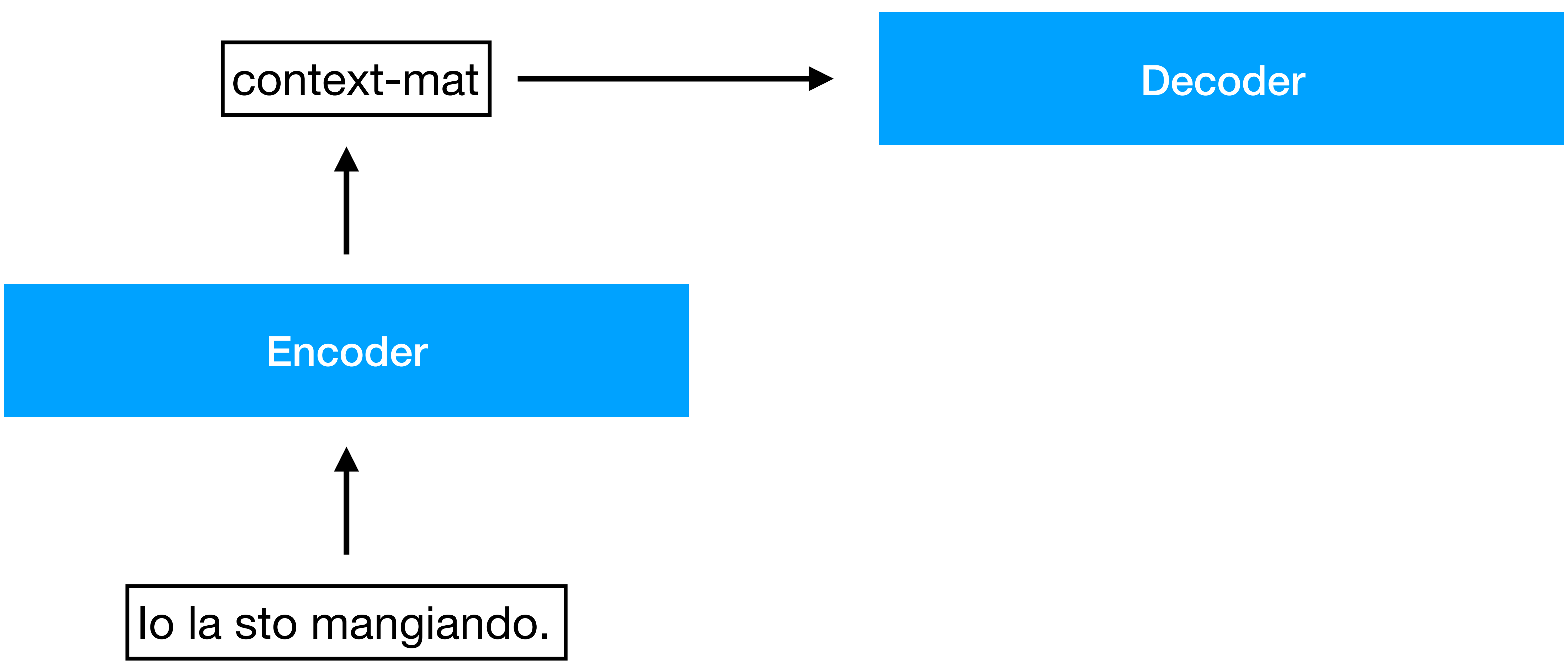
Lecture Roadmap

1. Motivation
2. Word Embeddings
3. Attention
    - What is it, intuitively?
    - What is it, mathematically?
4. Scalar Dot-Product Attention
    - Why?
    - Queries, Keys, Values
    - Computing Attention
5. Multi-Headed Attention
    - MHA Intuition
6. **Transformer Architecture**
7. Vision Transformers
    - Moving from text to images
    - Comparing transformers and CNNs

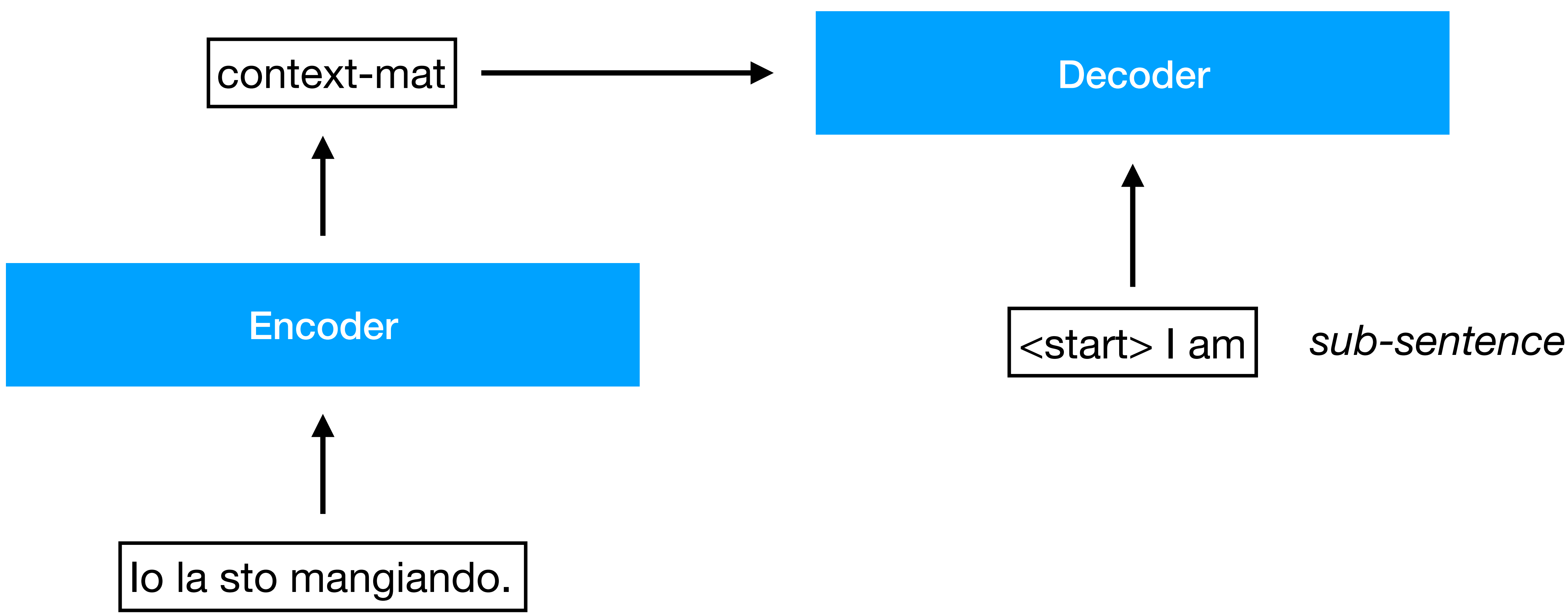
Transformer Architecture



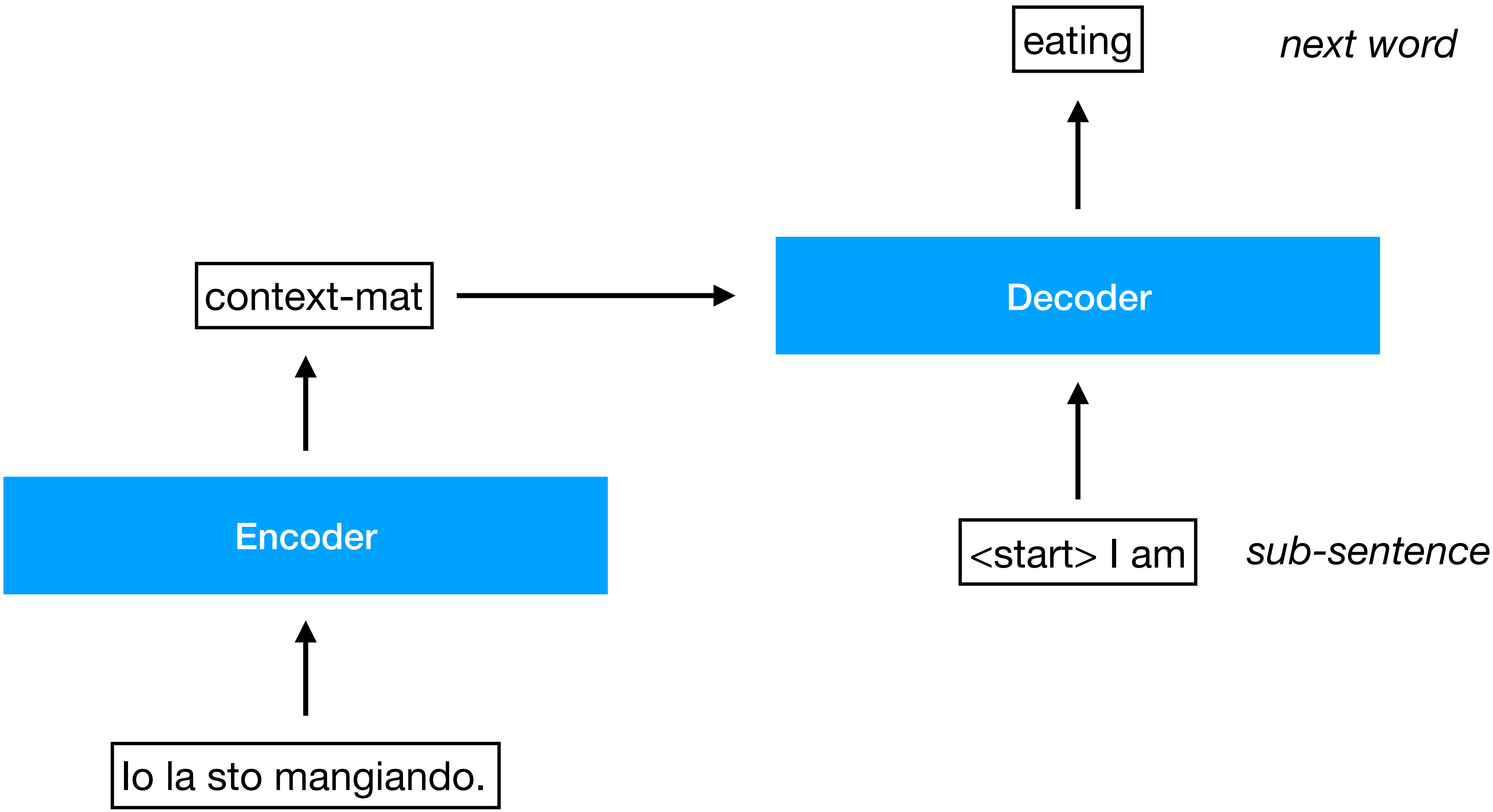
Transformer Architecture



Transformer Architecture

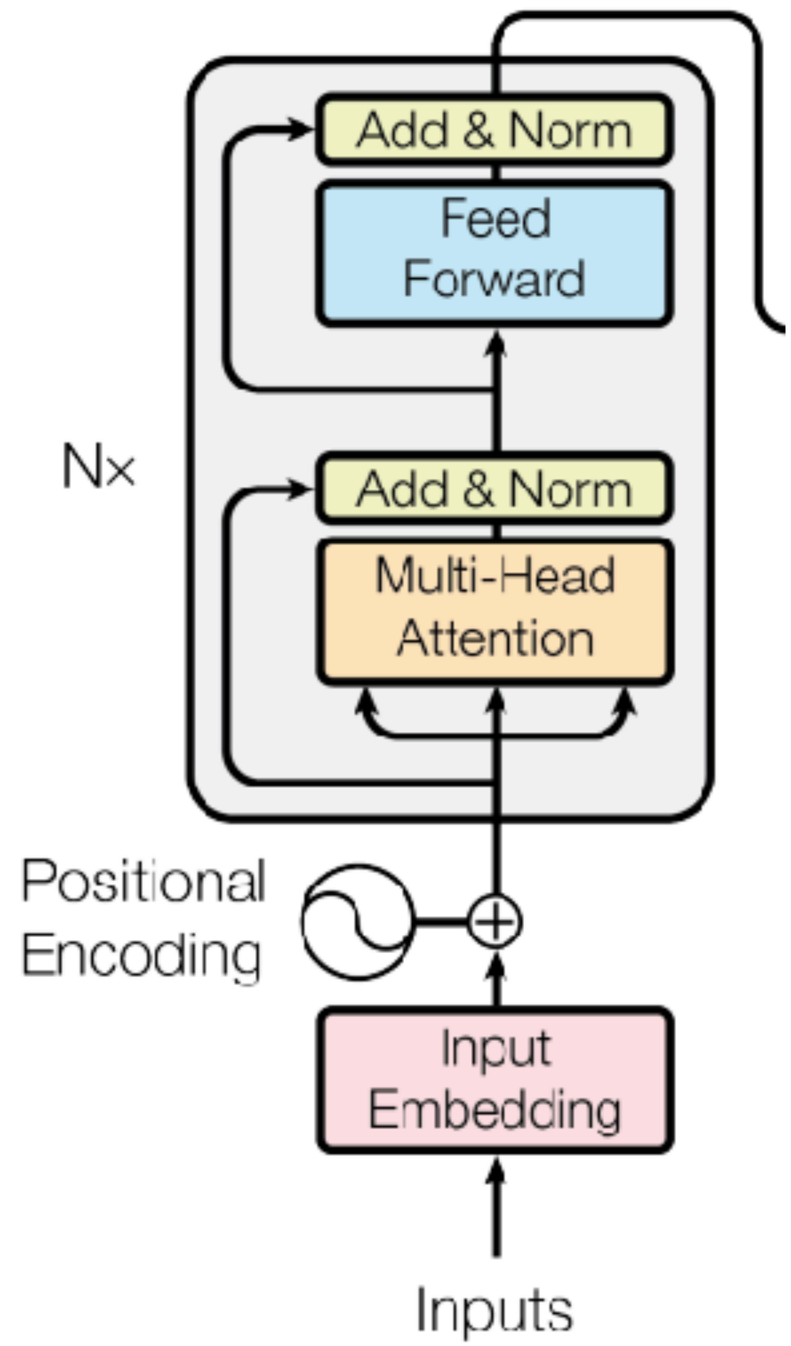


Transformer Architecture



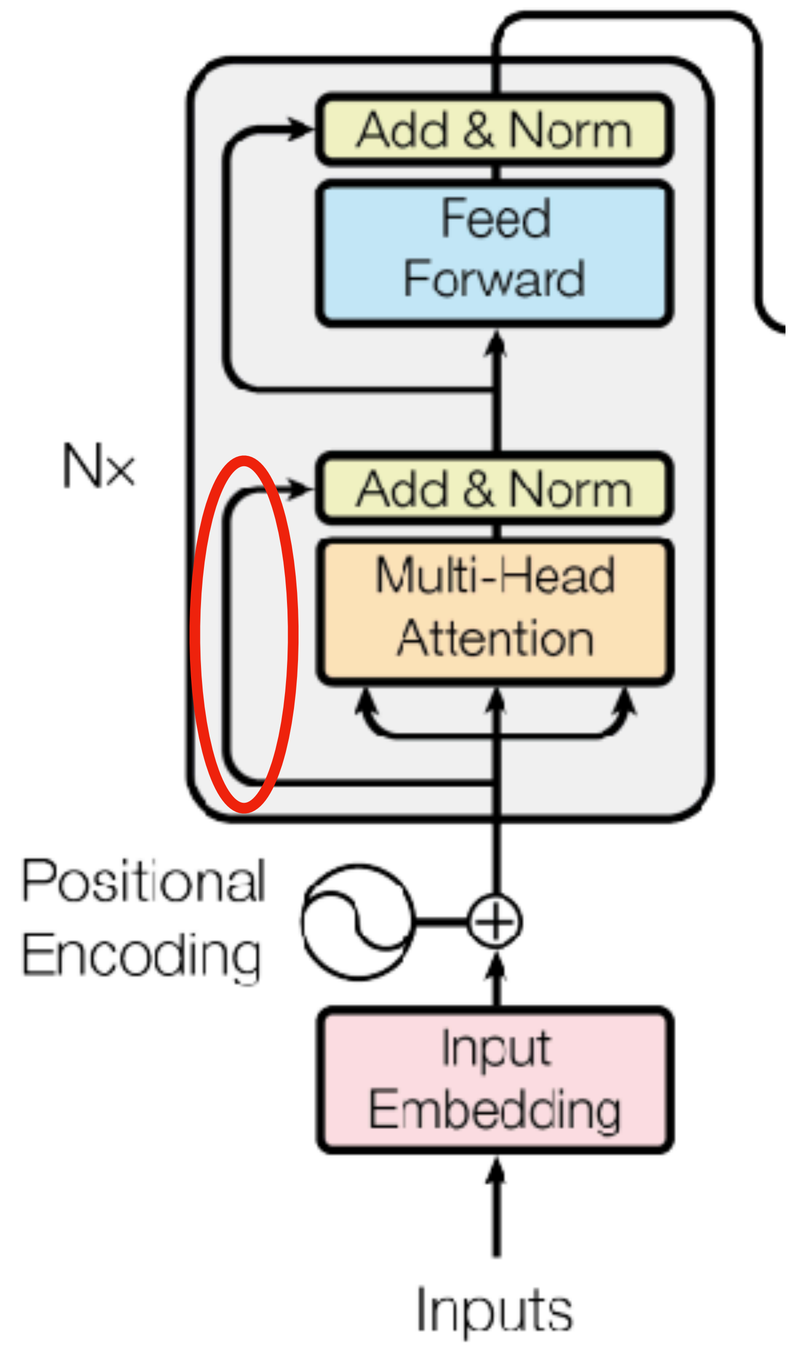
Transformer Encoder

Encoder



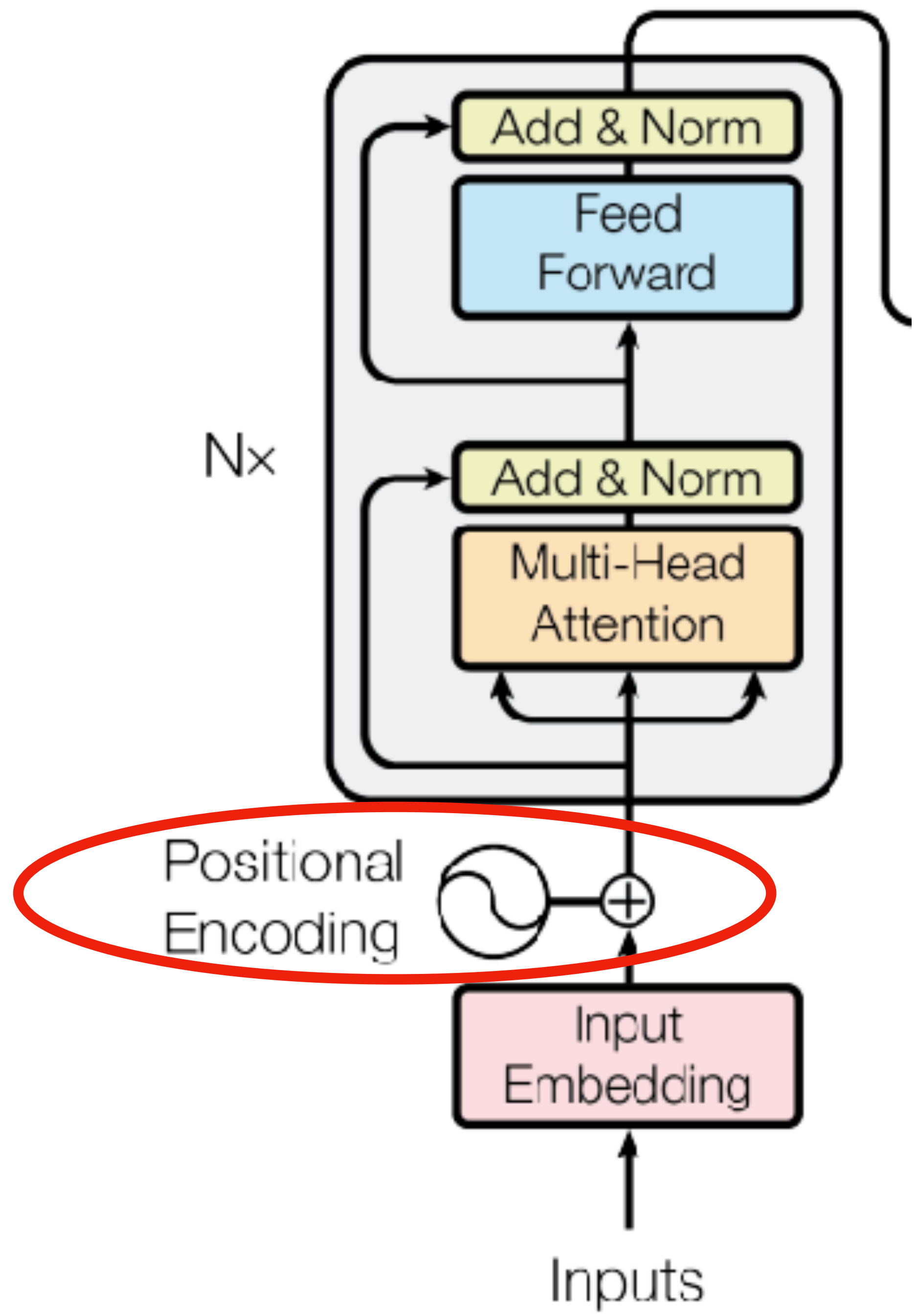
Transformer Encoder

Encoder



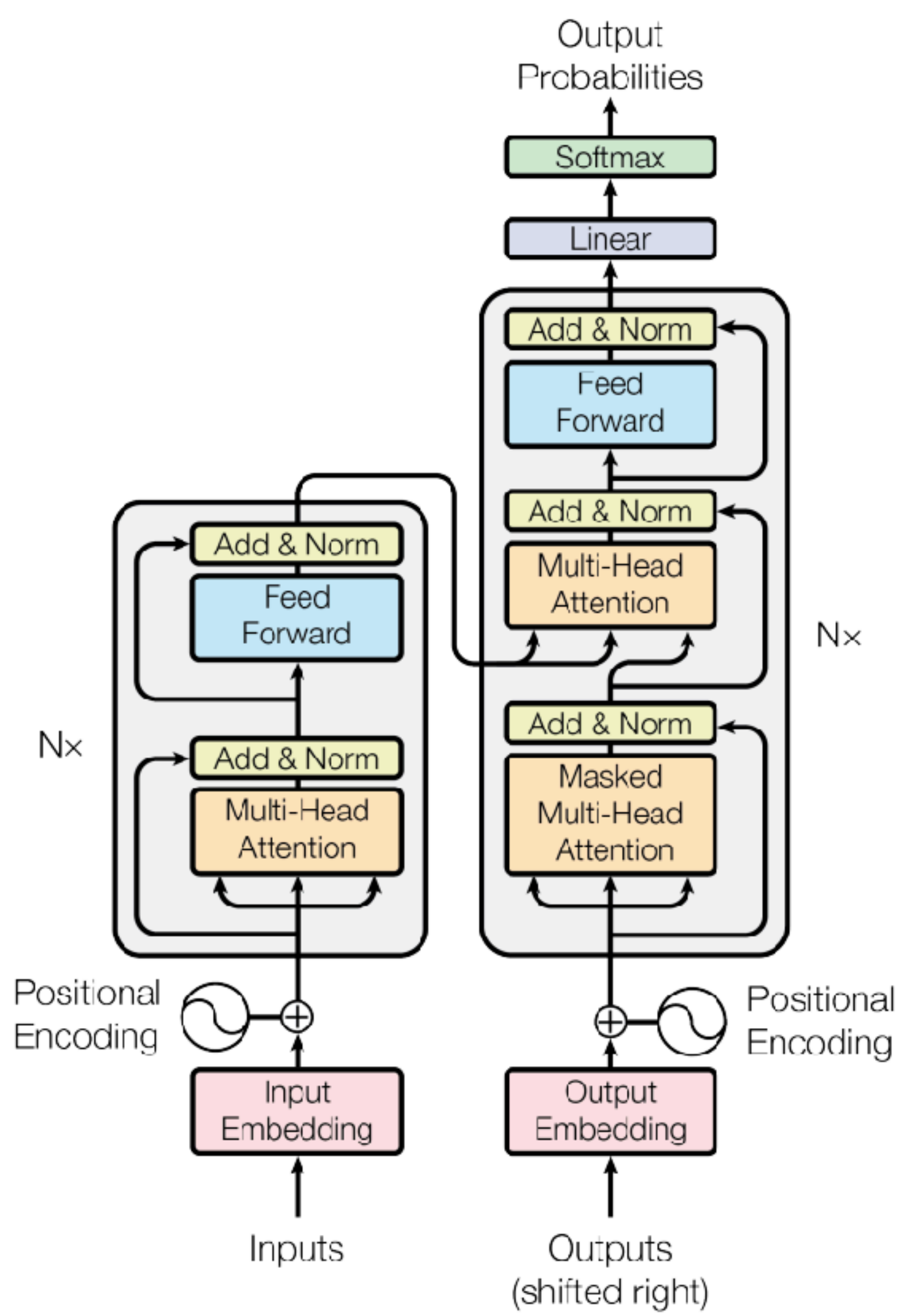
Transformer Encoder

Encoder



Transformer Architecture

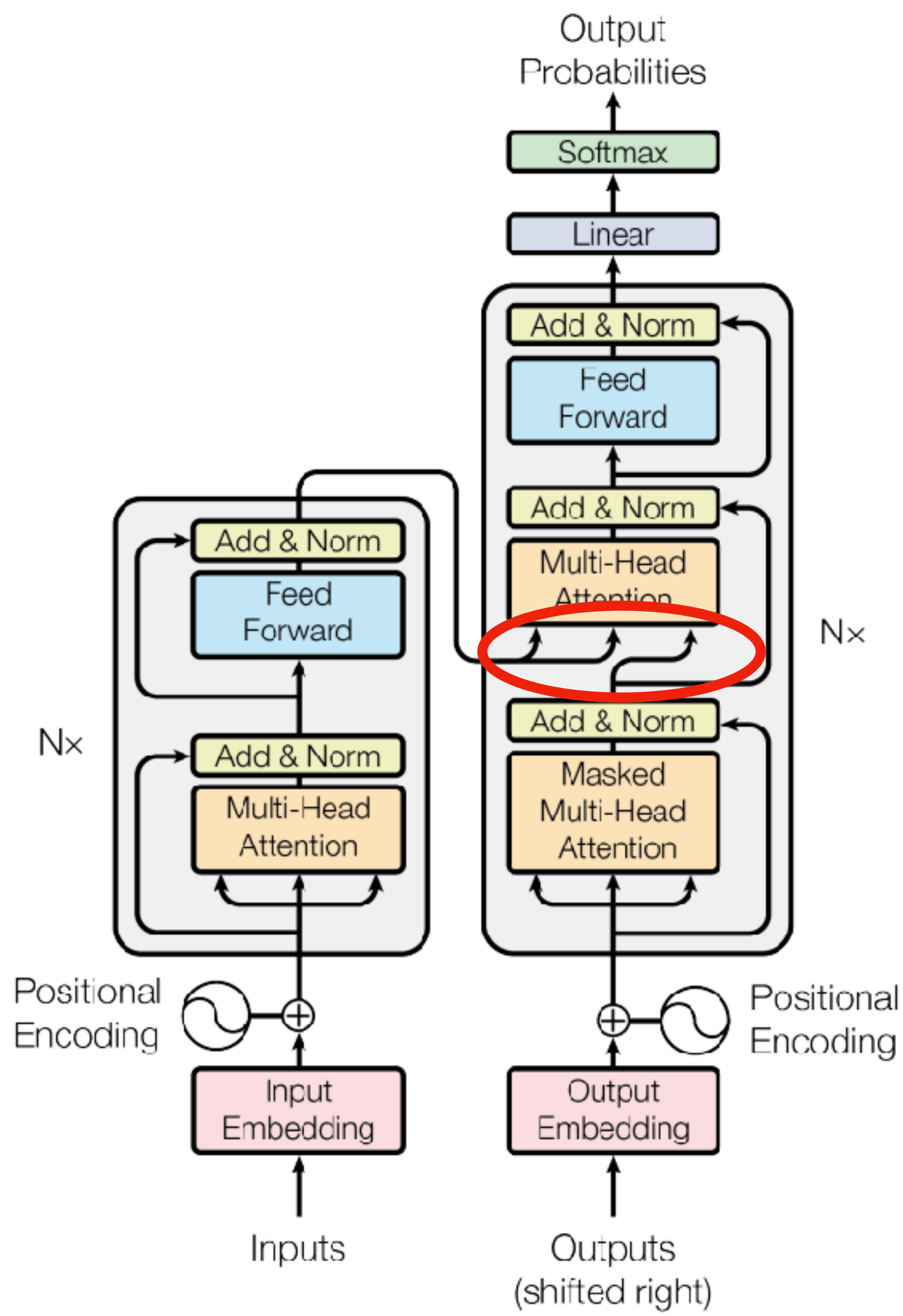
Encoder



Decoder

Transformer Architecture

Encoder



Decoder

Questions?

1. Motivation
2. Word Embeddings
3. Attention
    - What is it, intuitively?
    - What is it, mathematically?
4. Scalar Dot-Product Attention
    - Why?
    - Queries, Keys, Values
    - Computing Attention
5. Multi-Headed Attention
    - MHA Intuition
6. Transformer Architecture

Lecture Roadmap

1. Motivation
2. Word Embeddings
3. Attention
    - What is it, intuitively?
    - What is it, mathematically?
4. Scalar Dot-Product Attention
    - Why?
    - Queries, Keys, Values
    - Computing Attention
5. Multi-Headed Attention
    - MHA Intuition
6. Transformer Architecture
7. **Vision Transformers**
    - Moving from text to images
    - Comparing transformers and CNNs

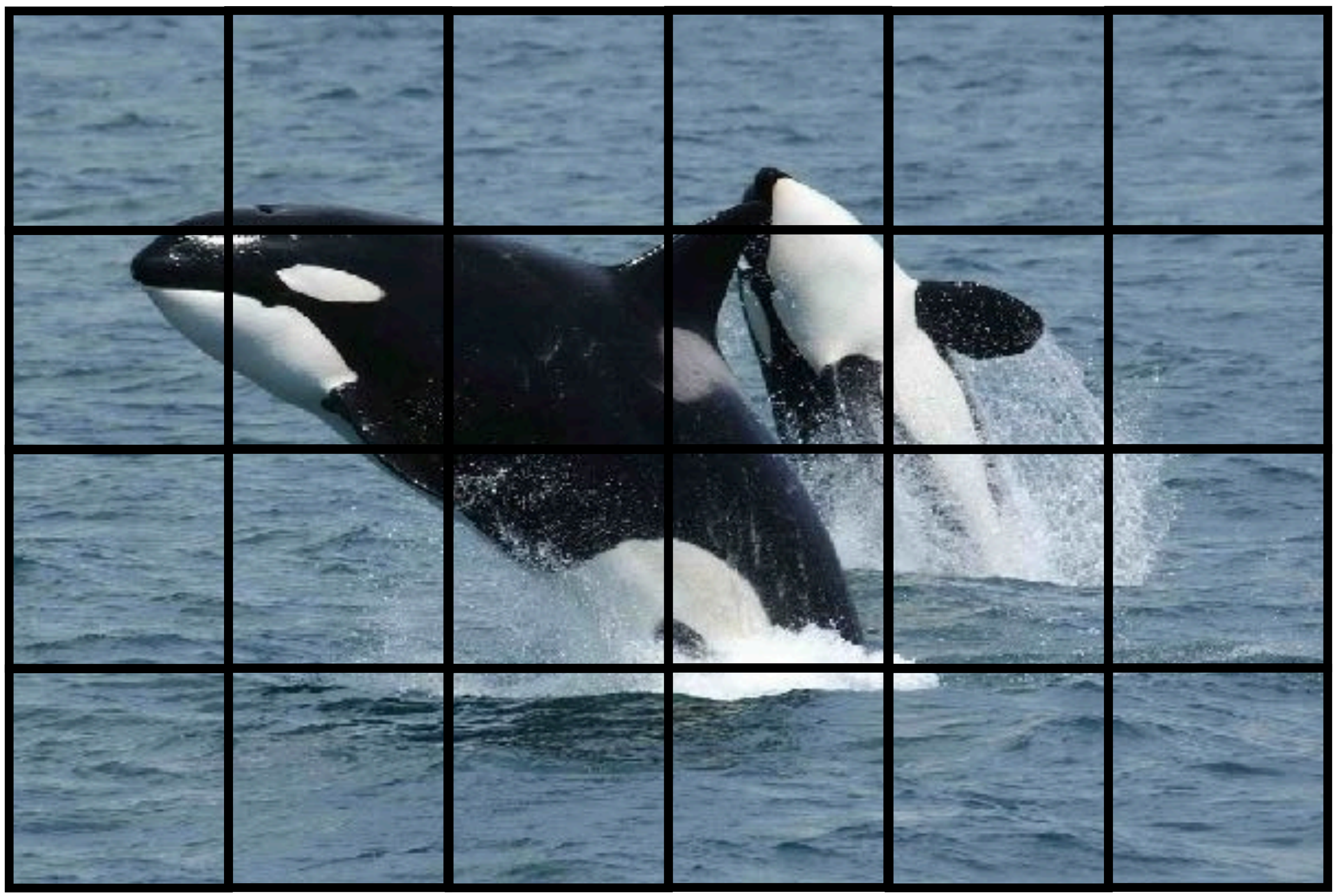
What is the most naive way to generalize the transformer encoder for images?

What is a “word” in an image?

What is a more realistic, efficient way to generalize the transformer encoder for images?

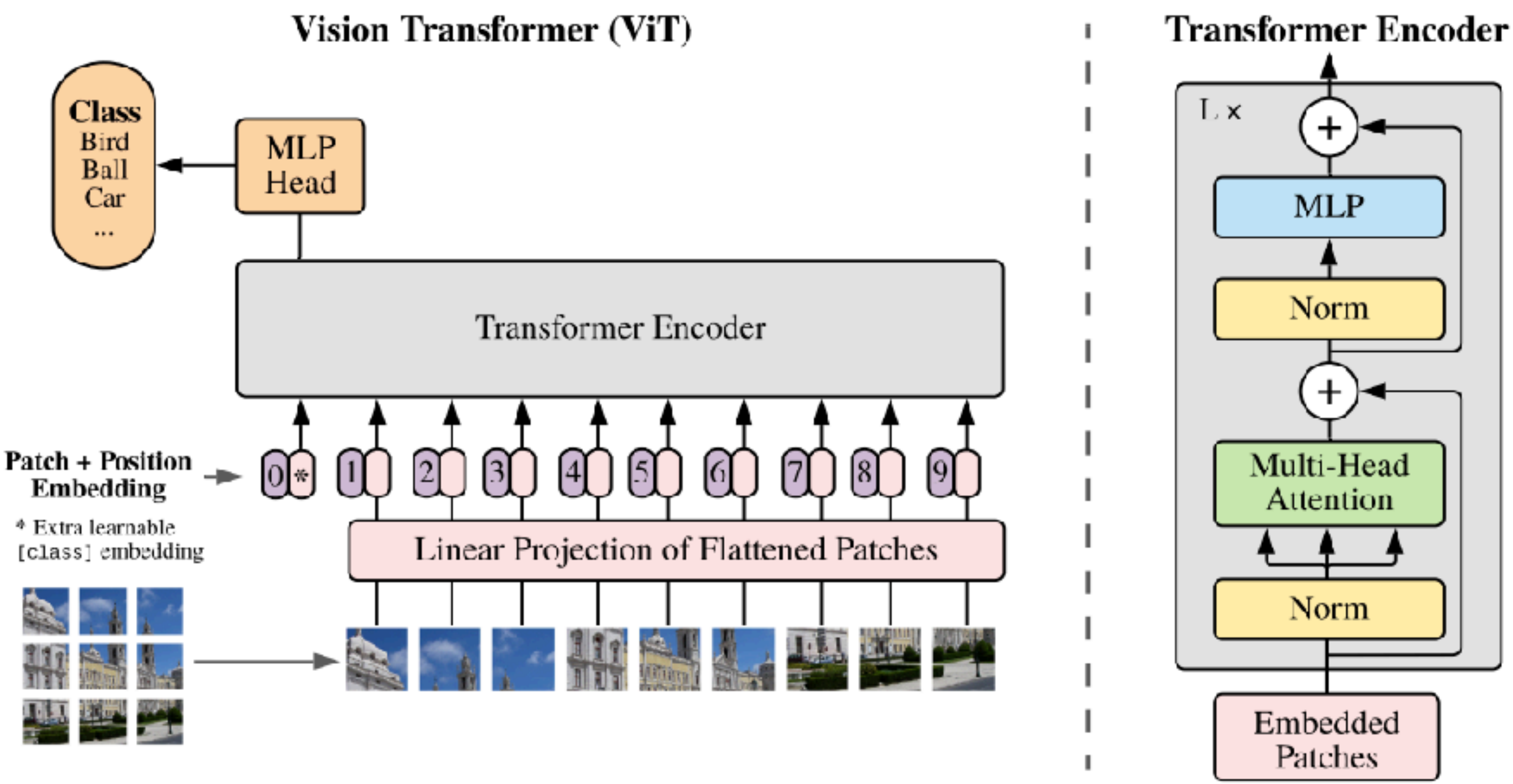
What is a more realistic, efficient way to generalize the transformer encoder for images?

Patches

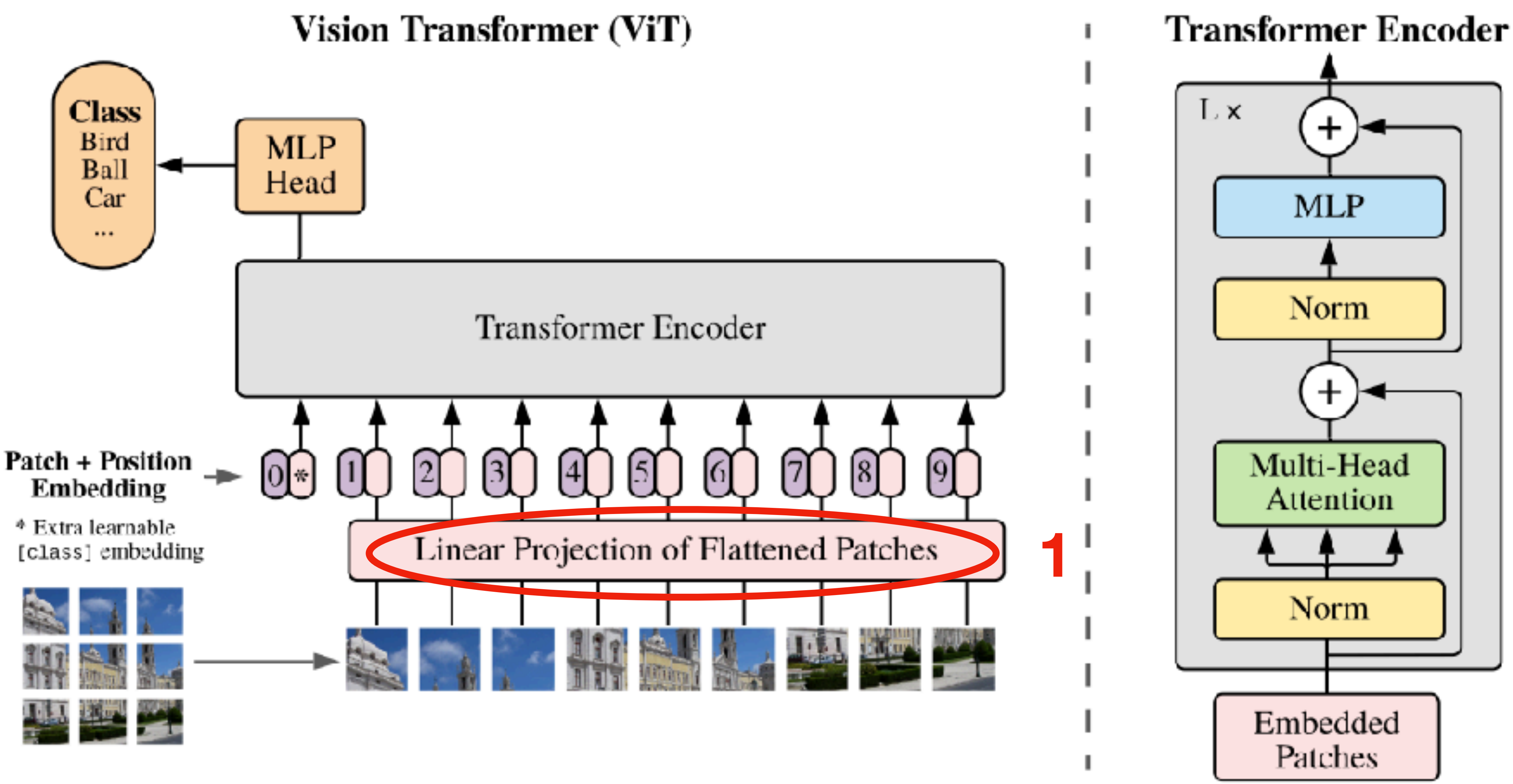


Vision Transformers (ViT)

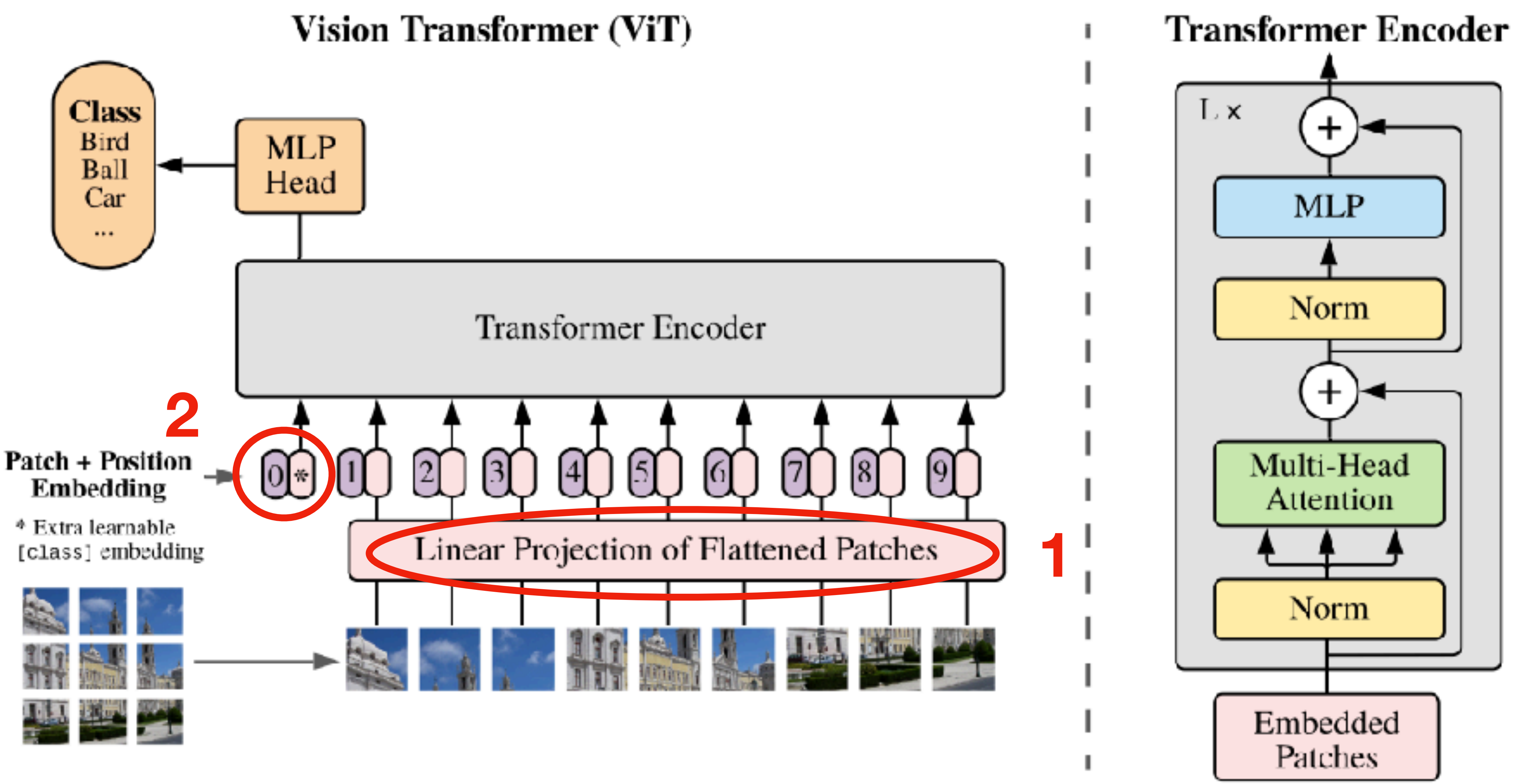
What's new?



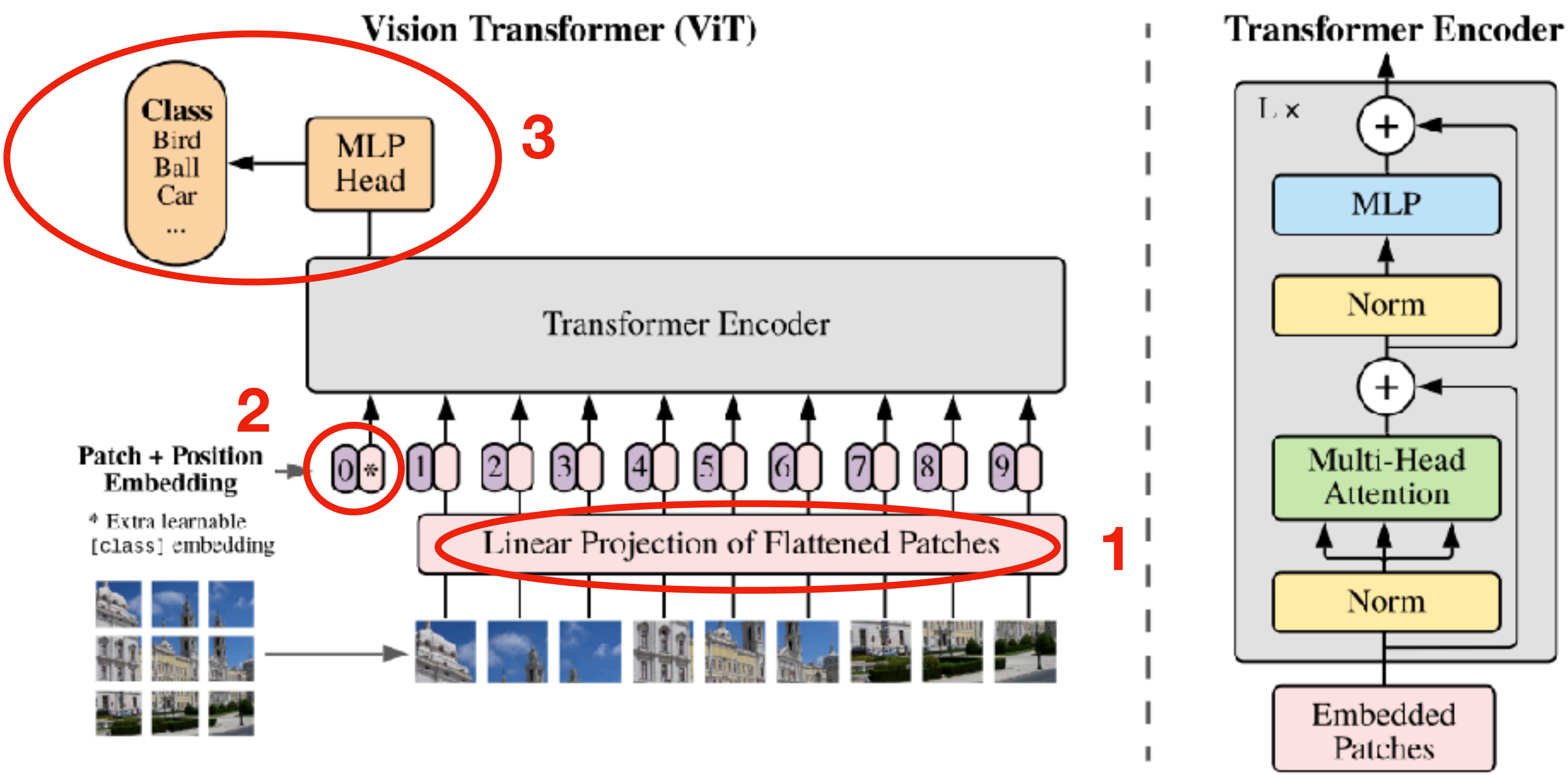
Vision Transformers (ViT)



Vision Transformers (ViT)



Vision Transformers (ViT)

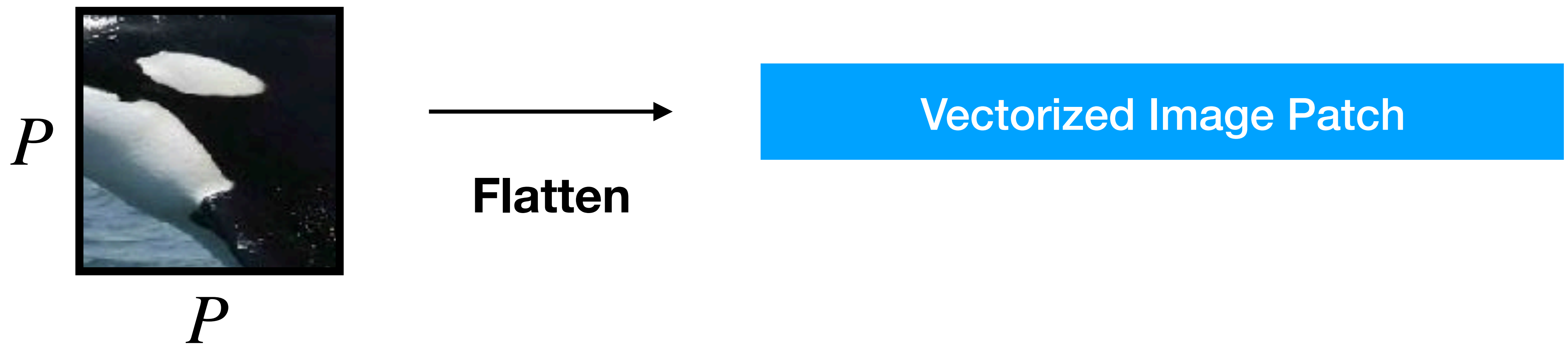


1 Linear Projections of Flattened Patches

P

P

1 Linear Projections of Flattened Patches



1 Linear Projections of Flattened Patches

P

P

Flatten

Vectorized Image Patch

$$x_p \in R^{P^2}$$

1 Linear Projections of Flattened Patches

P

P

Flatten

Vectorized Image Patch

$x_p \in R^{P^2}$

$$x_p \cdot E = \hat{x}_p$$

The matrix E is learned

1 Linear Projections of Flattened Patches

P

P

Flatten

Vectorized Image Patch

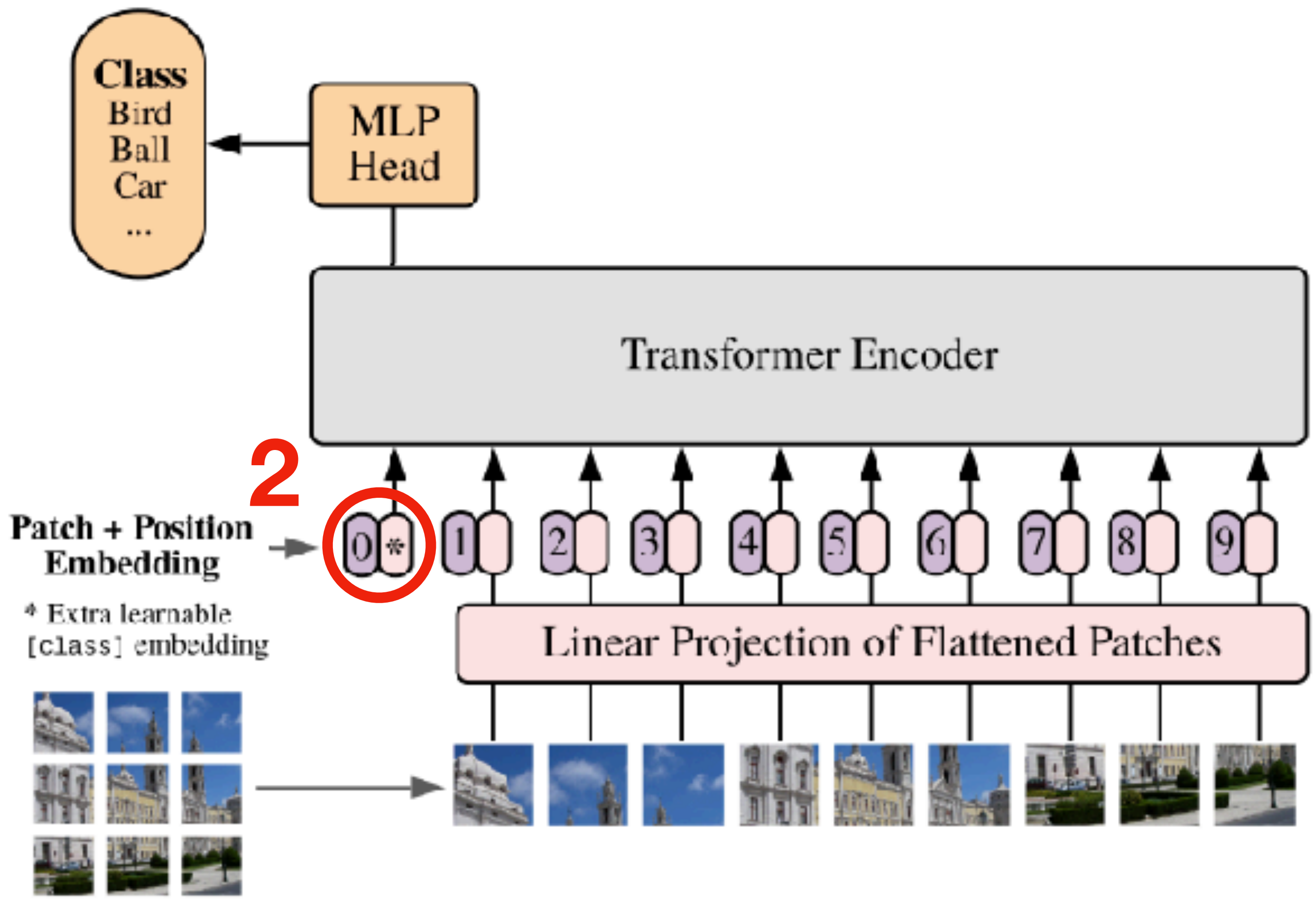
$x_p \in R^{P^2}$

$$x_p \cdot E = \hat{x}_p \qquad E \in R^{P^2 \times D}, \hat{x}_p \in R^D$$

The matrix E is learned

Extra learnable class embedding

Recall from multi-head attention, the output is $(N \times d)$

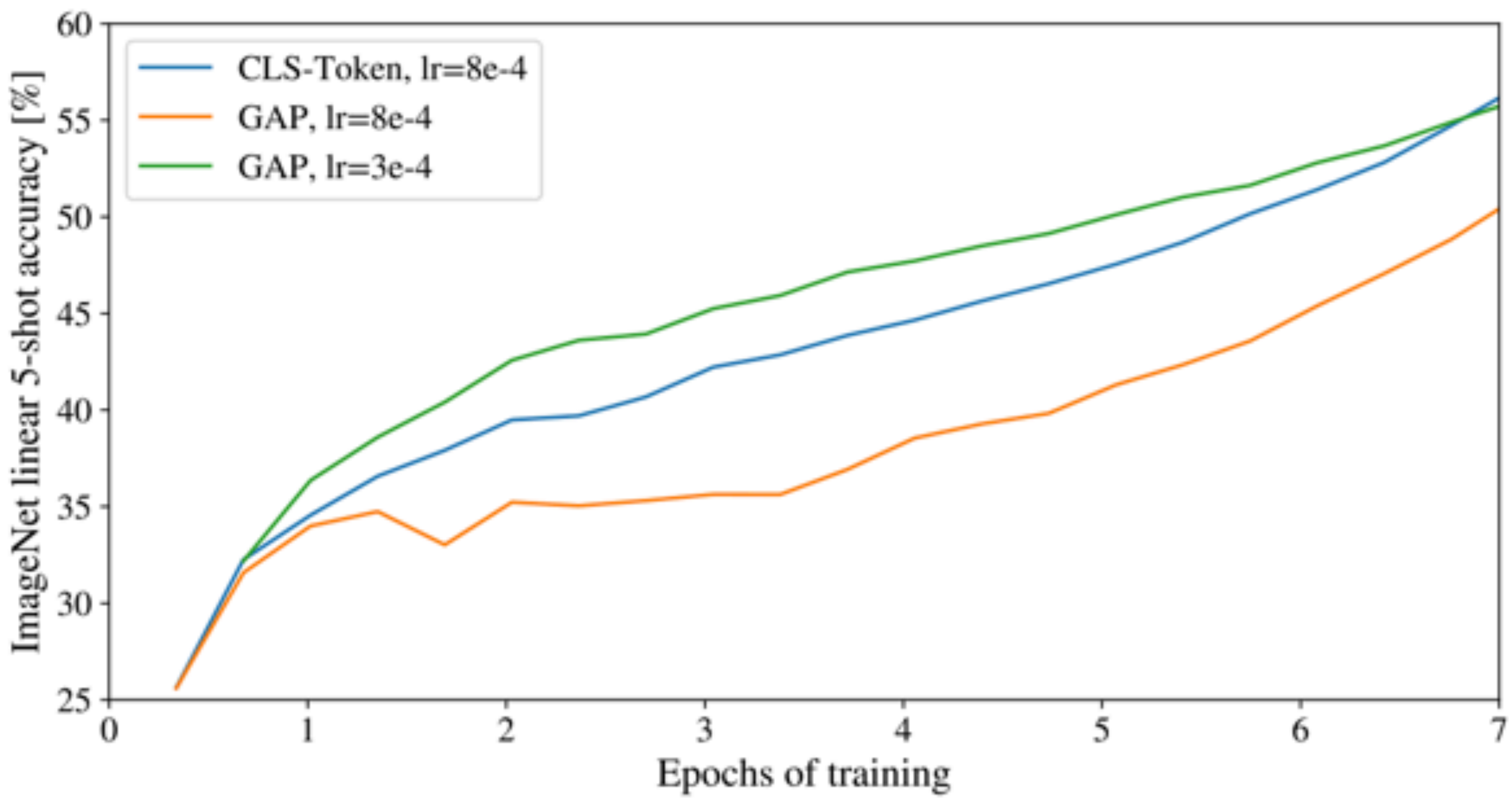


The extra learnable class embedding is the ***query*** that stores the ***context*** representation that is classified by the MLP (3).

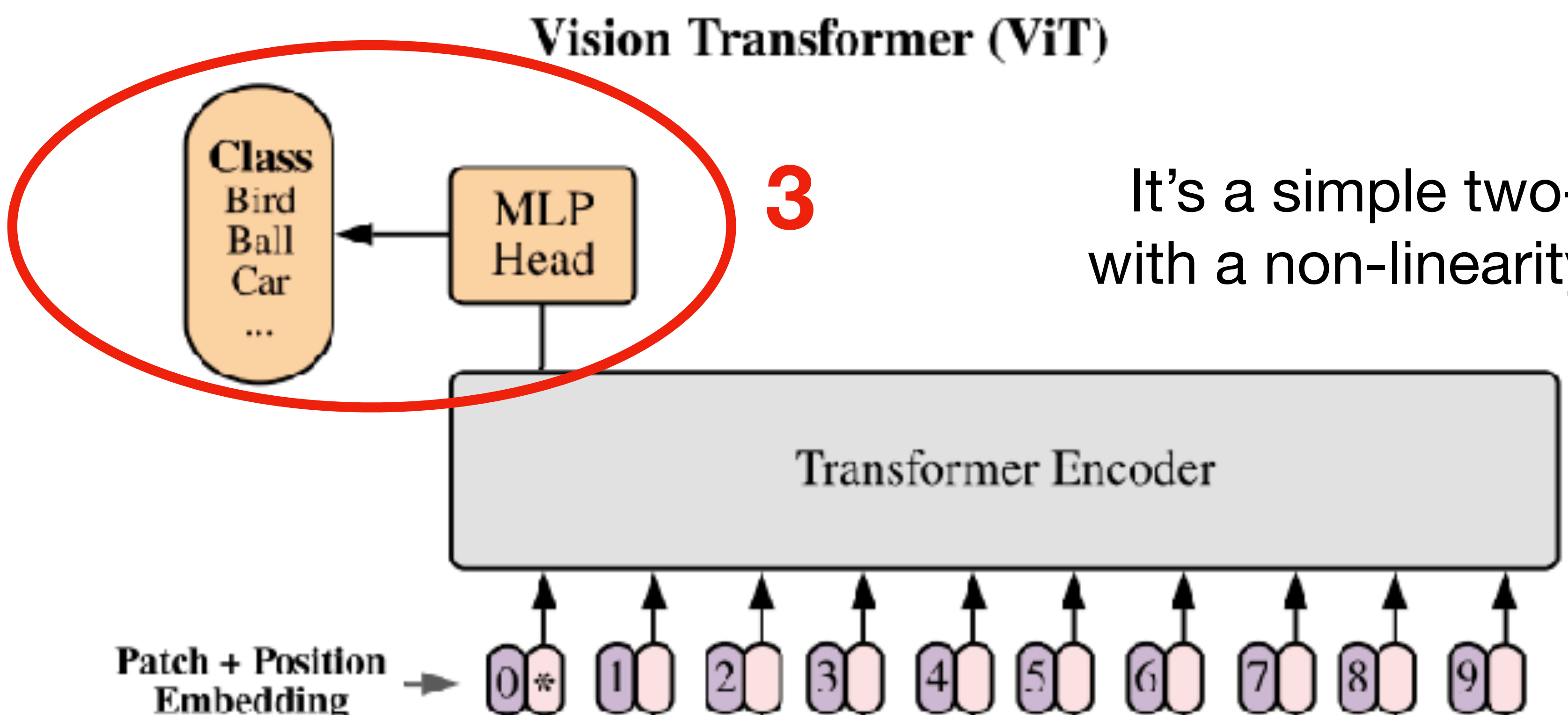
Extra learnable class embedding

Do we need this?

GAP - global average pooling only
CLS-Token - include a class token in input



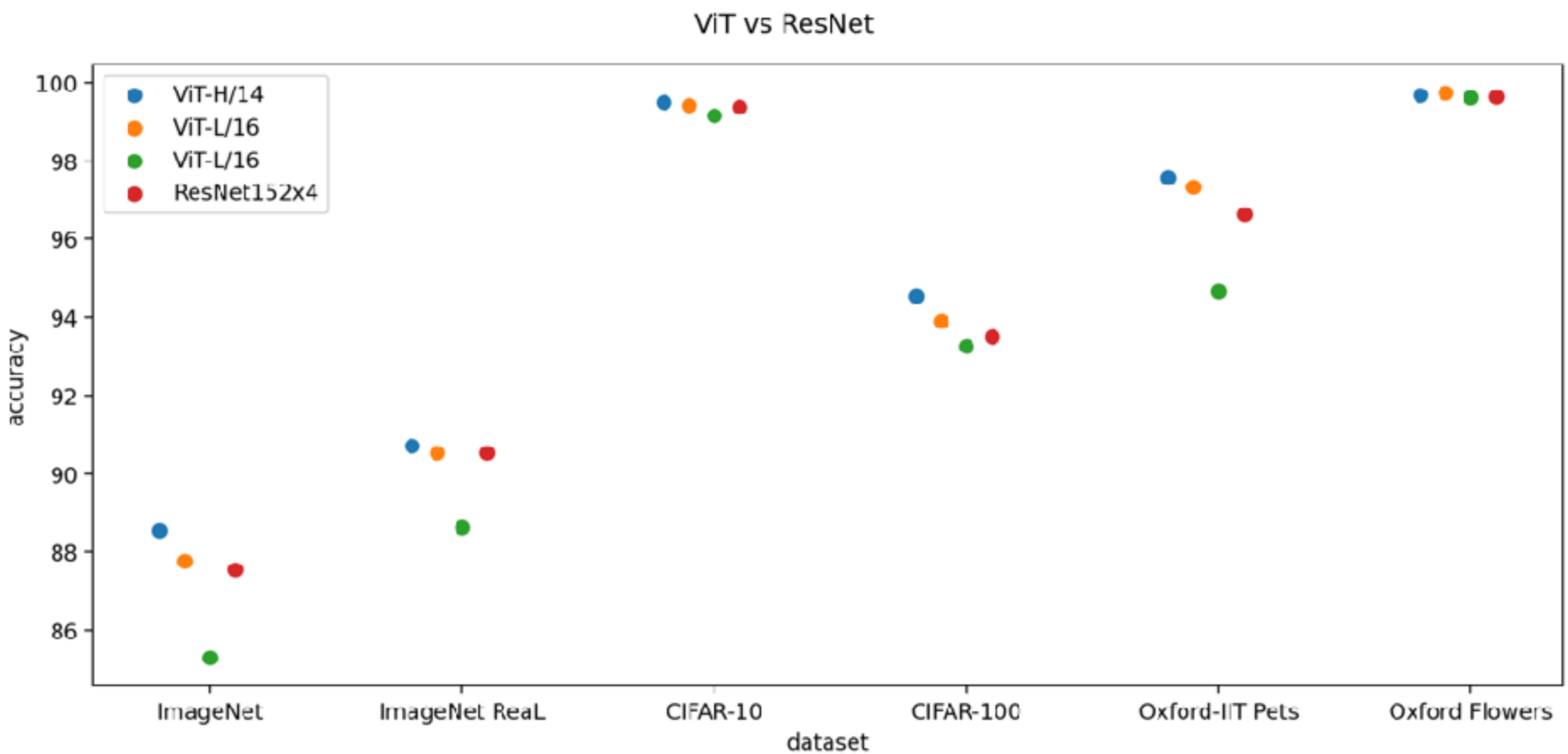
Multi-layer Perceptron (MLP) head



It’s a simple two-layer network with a non-linearity on the output.

Takes output of the encoder at the position of the class-token and predicts a class for the image.

ViT (2021) Performance



Slightly outperforms the ResNet152 based model.

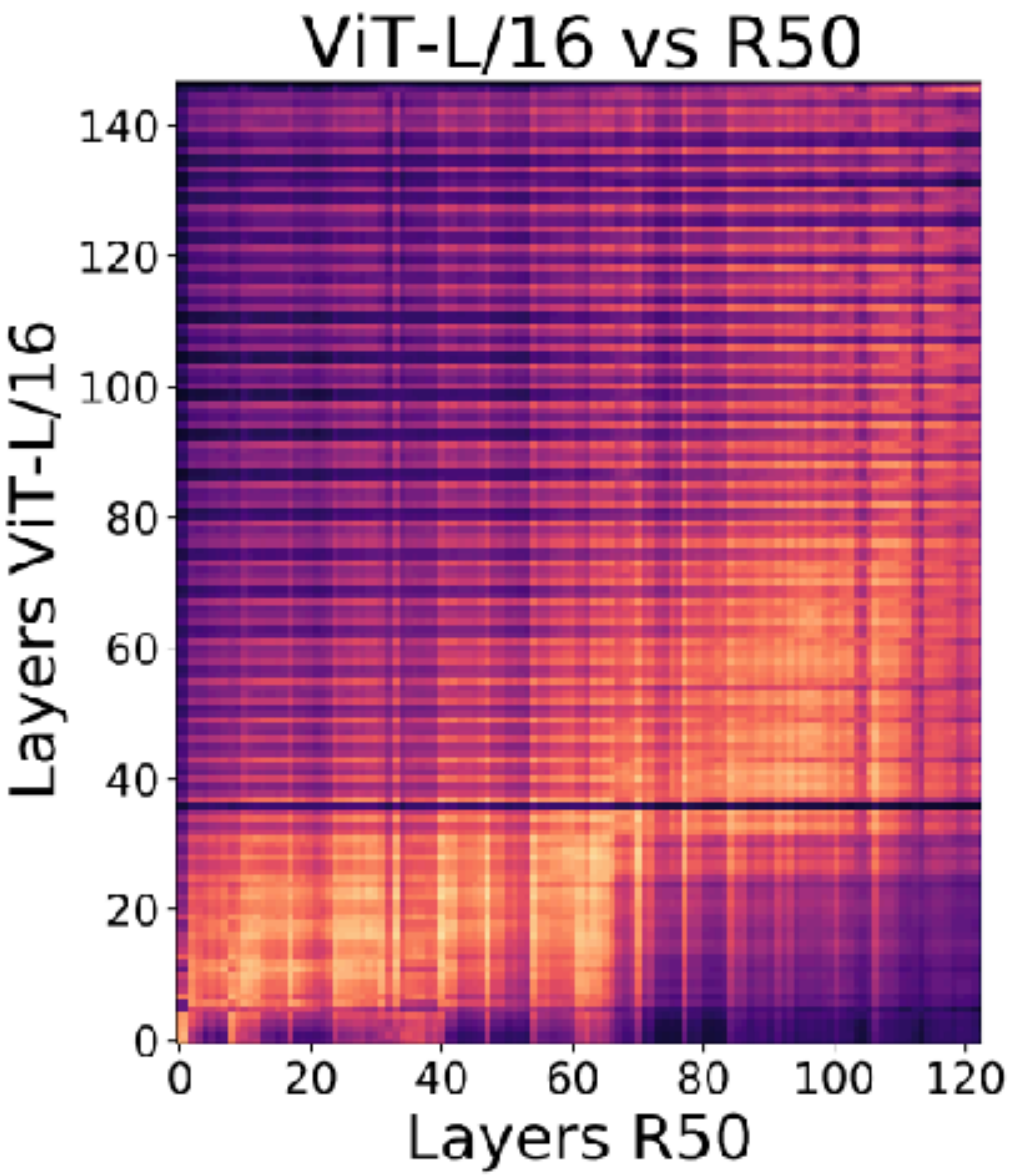
Some interesting questions…

What do the learned attention maps look like?

Vaswani et al. (2017)

How does the way vision transformers "see" differ from CNNs?

Representational Similarity



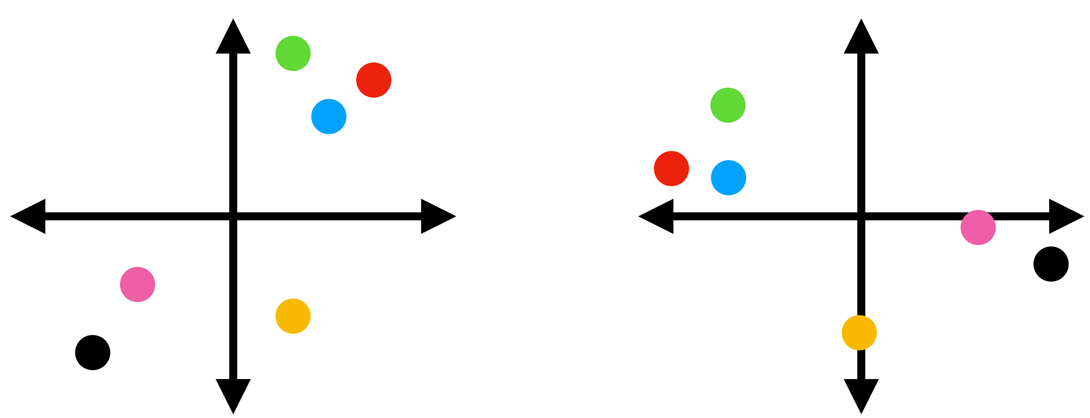
ViT uses a different method to compute low-level representations.

Maithra et al. (2017)

Sub-question: how to compute representational similarity?

Centered Kernel Alignment (CKA)

High level: Compute a **similarity** between the **similarities** in two different layers.



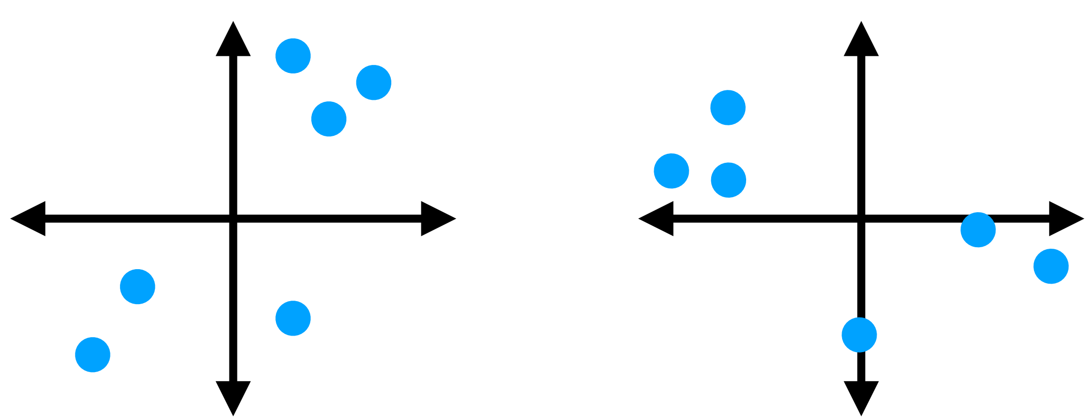
These are effectively the same representation, but directly comparing them won't work.

Sub-question: how to compute representational similarity?

Centered Kernel Alignment (CKA)

High level: Compute a similarity between the similarities in two different layers.

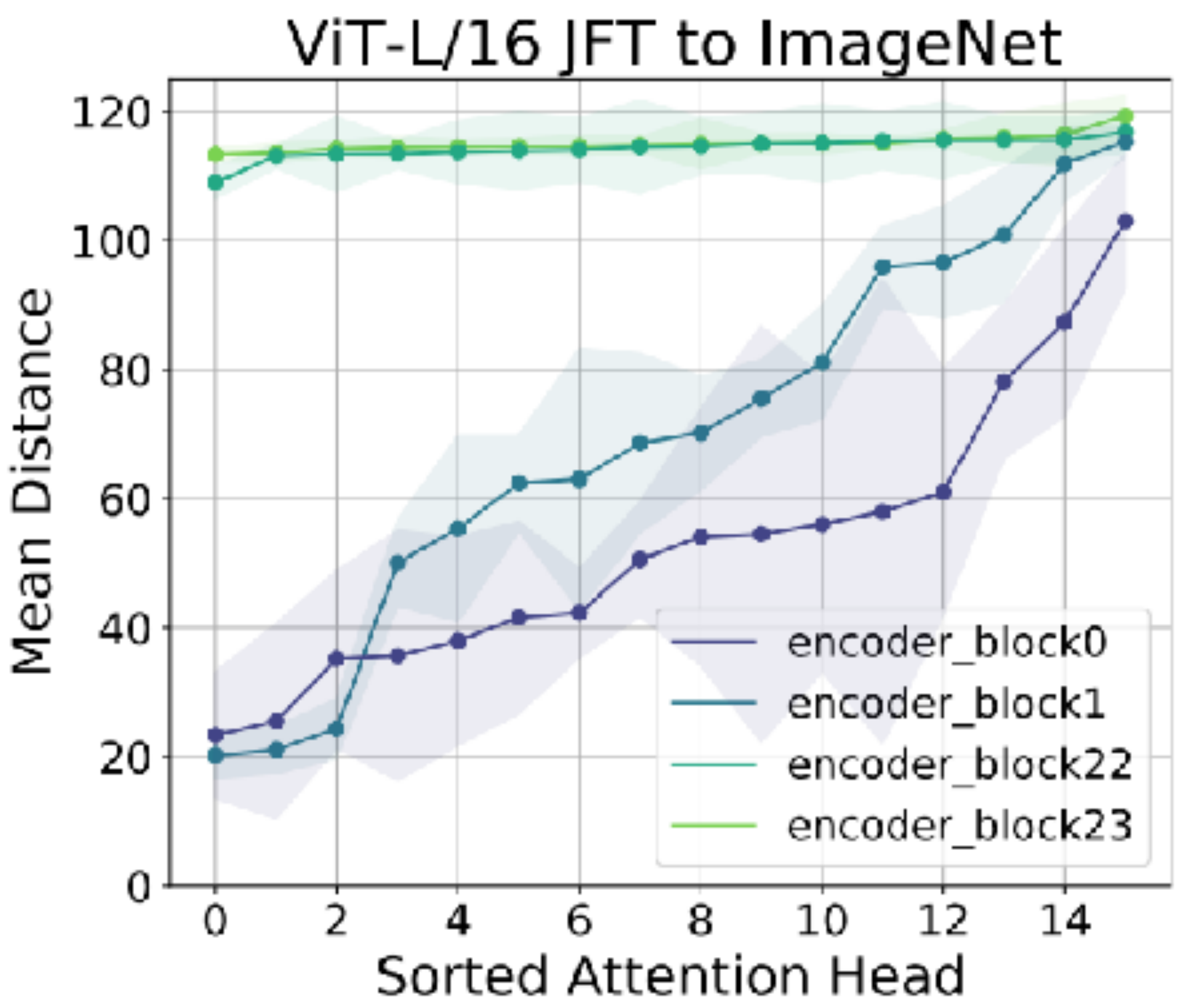
1. Generate the embeddings at two specific layers for the same set of data-points.
2. Compute the Gram matrices (measure the similarity between points in the same representation)
3. Compute a similarity between the Gram matrices



These are effectively the same representation, but directly comparing them won't work.

How does the way vision transformers "see" differ from CNNs?

Local and Global Information



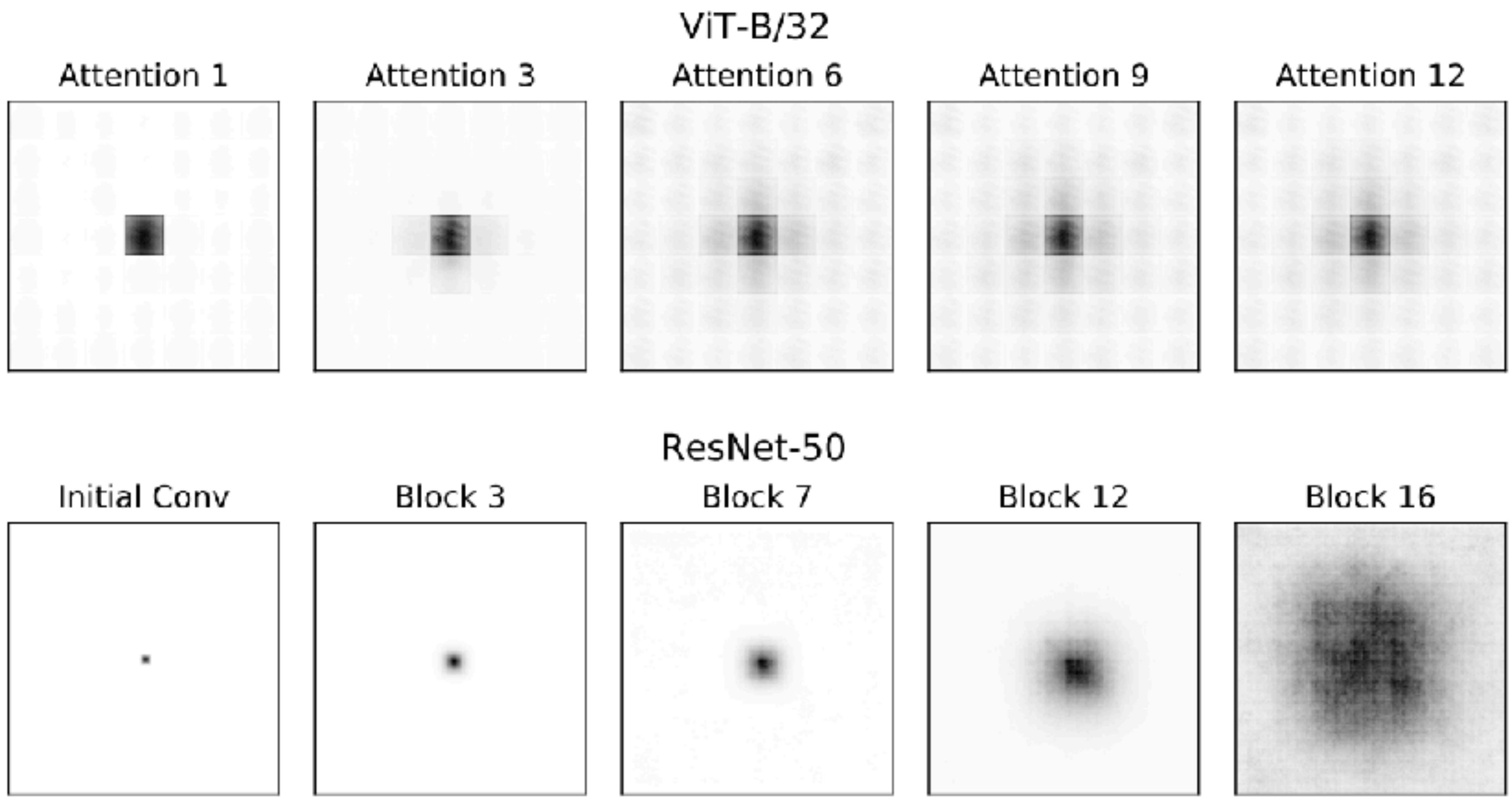
ViT early layers (block0, block1) encode both local and global relationships.

By structure CNNs only encode local information early on.

Maithra et al. (2017)

How does the way vision transformers "see" differ from CNNs?

Receptive Fields



ViT starts incorporating global information much earlier.

Maithra et al. (2017)

Are transformers actually better than CNNs (ResNet)?

These models are still undergoing training procedure improvements.

ResNet strikes back: An improved training procedure in timm

Ross Wightman[°] Hugo Touvron[*,†] Hervé Jégou[*]

[°]Independent researcher [*]Facebook AI [†]Sorbonne University

(Oct 2021) - Propose a new, state-of-the-art training procedure for ResNets that beats the best ViT under some conditions.

DeiT III: Revenge of the ViT

Hugo Touvron[*,†] Matthieu Cord[†] Hervé Jégou[*]

[*]Meta AI [†]Sorbonne University

(Apr 2022) - Propose a new, state-of-the-art supervised training procedure for ViT, which beats ResNet under some conditions.

ResNet strikes back: An improved training procedure in timm
DeiT III: Revenge of the ViT

References

1. Dosovitskiy, Alexey, Lucas Beyer, Alexander Kolesnikov, Dirk Weissenborn, Xiaohua Zhai, Thomas Unterthiner, Mostafa Dehghani, et al. “An Image Is Worth 16x16 Words: Transformers for Image Recognition at Scale.” arXiv, June 3, 2021. http://arxiv.org/abs/2010.11929.

2. Raghu, Maithra, Thomas Unterthiner, Simon Kornblith, Chiyuan Zhang, and Alexey Dosovitskiy. “Do Vision Transformers See Like Convolutional Neural Networks?” arXiv, March 3, 2022. http://arxiv.org/abs/2108.08810.

3. Touvron, Hugo, Matthieu Cord, and Hervé Jégou. “DeiT III: Revenge of the ViT.” arXiv, April 14, 2022. http://arxiv.org/abs/2204.07118.

4. Vaswani, Ashish, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N. Gomez, Lukasz Kaiser, and Illia Polosukhin. “Attention Is All You Need.” arXiv, December 5, 2017. http://arxiv.org/abs/1706.03762.

5. Wightman, Ross, Hugo Touvron, and Hervé Jégou. “ResNet Strikes Back: An Improved Training Procedure in Timm.” arXiv, October 1, 2021. http://arxiv.org/abs/2110.00476.

Useful demos, blogs, stack-overflow posts

1. https://demo.allennlp.org/next-token-lm
2. https://medium.com/deeper-learning/glossary-of-deep-learning-word-embedding-f90c3cec34ca
3. https://jalammar.github.io/illustrated-transformer/
4. https://towardsdatascience.com/illustrated-guide-to-transformers-step-by-step-explanation-f74876522bc0
5. https://stats.stackexchange.com/questions/498955/in-the-attention-mechanism-why-are-there-separate-weight-matrices-for-the-queri
6. https://stats.stackexchange.com/questions/421935/what-exactly-are-keys-queries-and-values-in-attention-mechanisms?rq=1
7. https://stats.stackexchange.com/questions/515477/when-calculating-self-attention-for-transformer-ml-architectures-why-do-we-need
8. https://stats.stackexchange.com/questions/430812/why-k-and-v-are-not-the-same-in-transformer-attention?rq=1