Transformers

Machine Learning Course - CS-433
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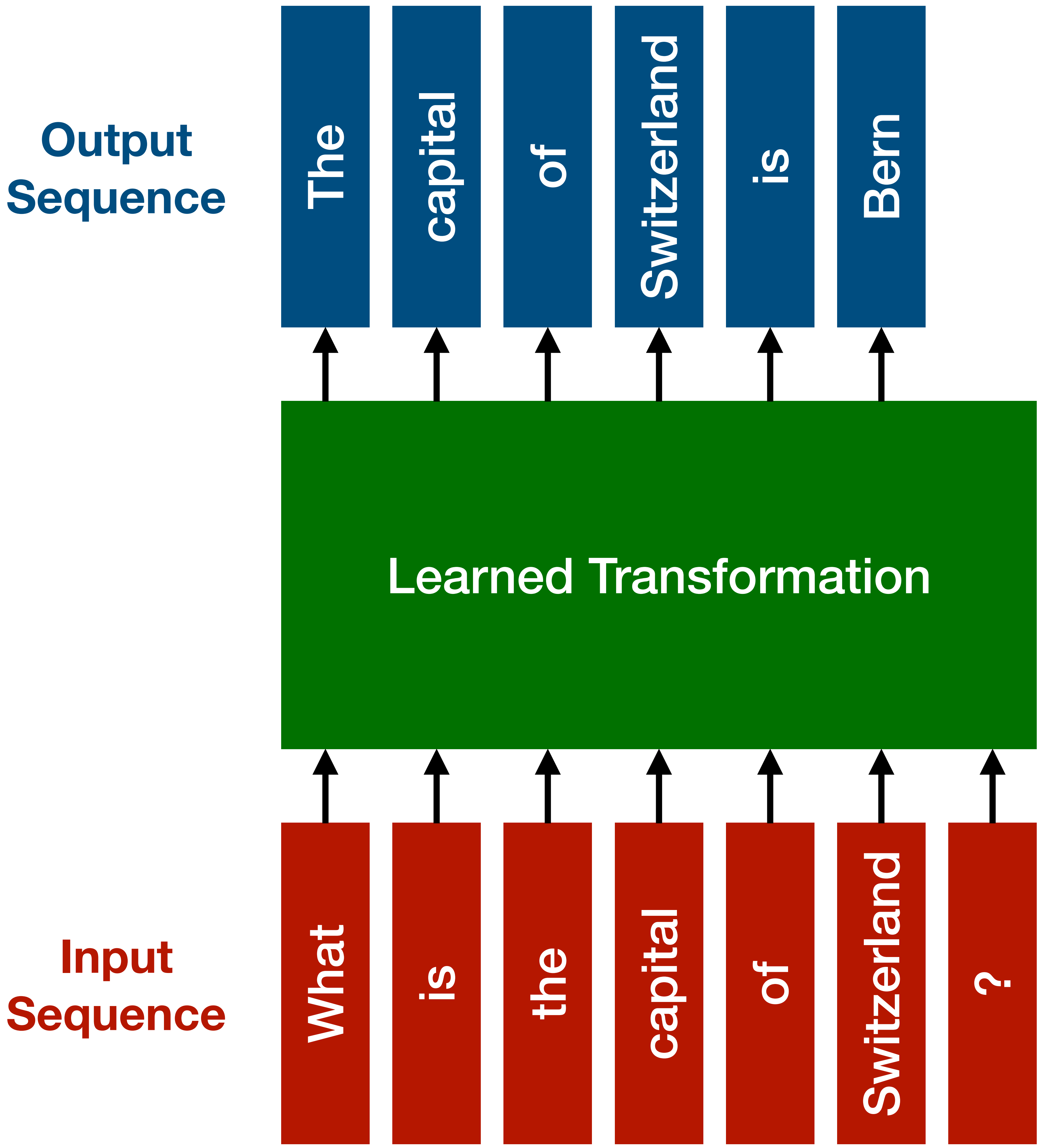
EPFL

Sequence-to-Sequence Transformations

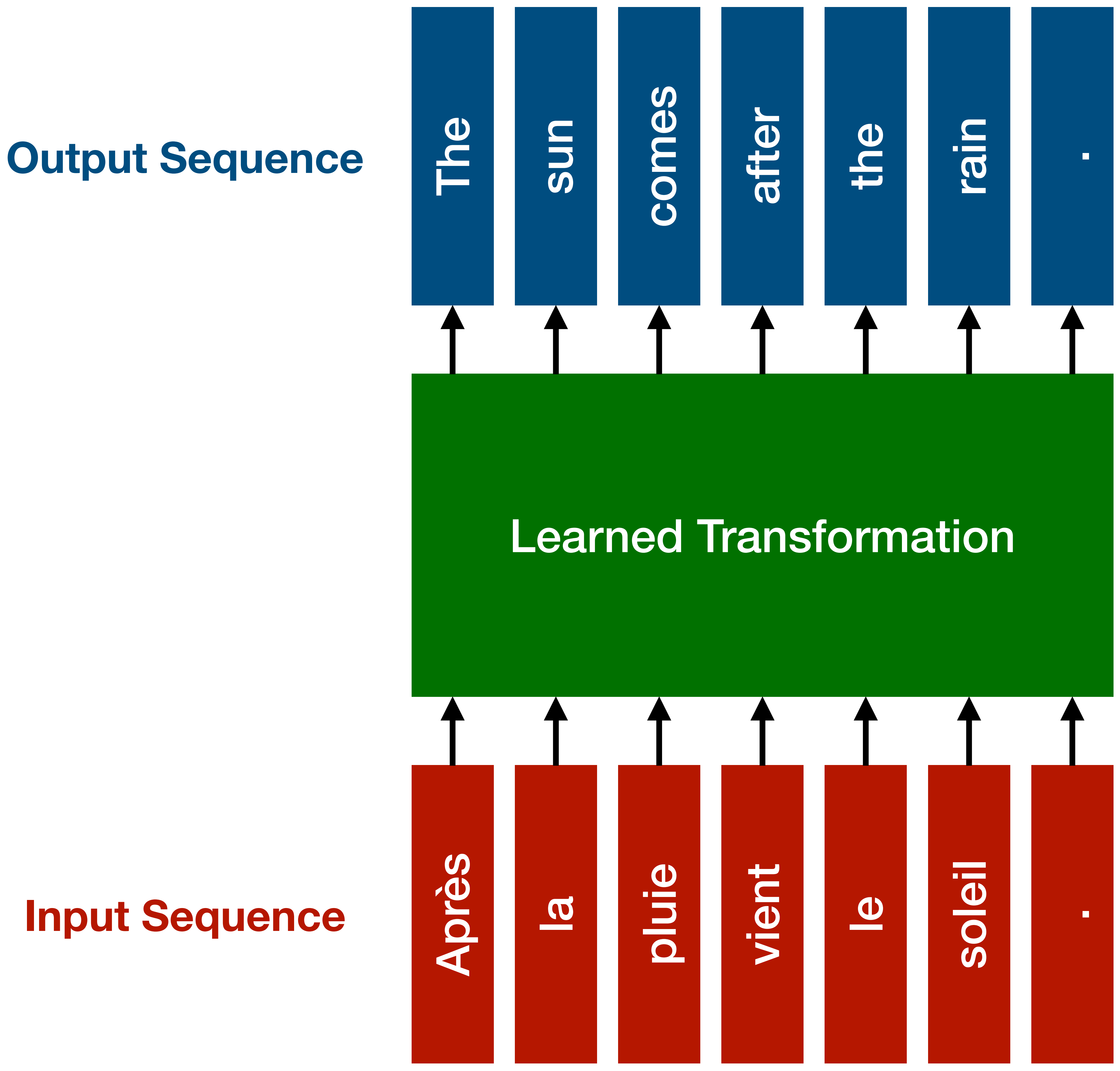
Sequence-to-Sequence Transformations

- Many interesting problems in ML can be expressed as **mapping one sequence to another**
- **Example**: chatbots like ChatGPT
    - Input: question (word sequence)
    - Output: answer (word sequence)
- Input and output sequences can represent various types of data: words, images, etc.

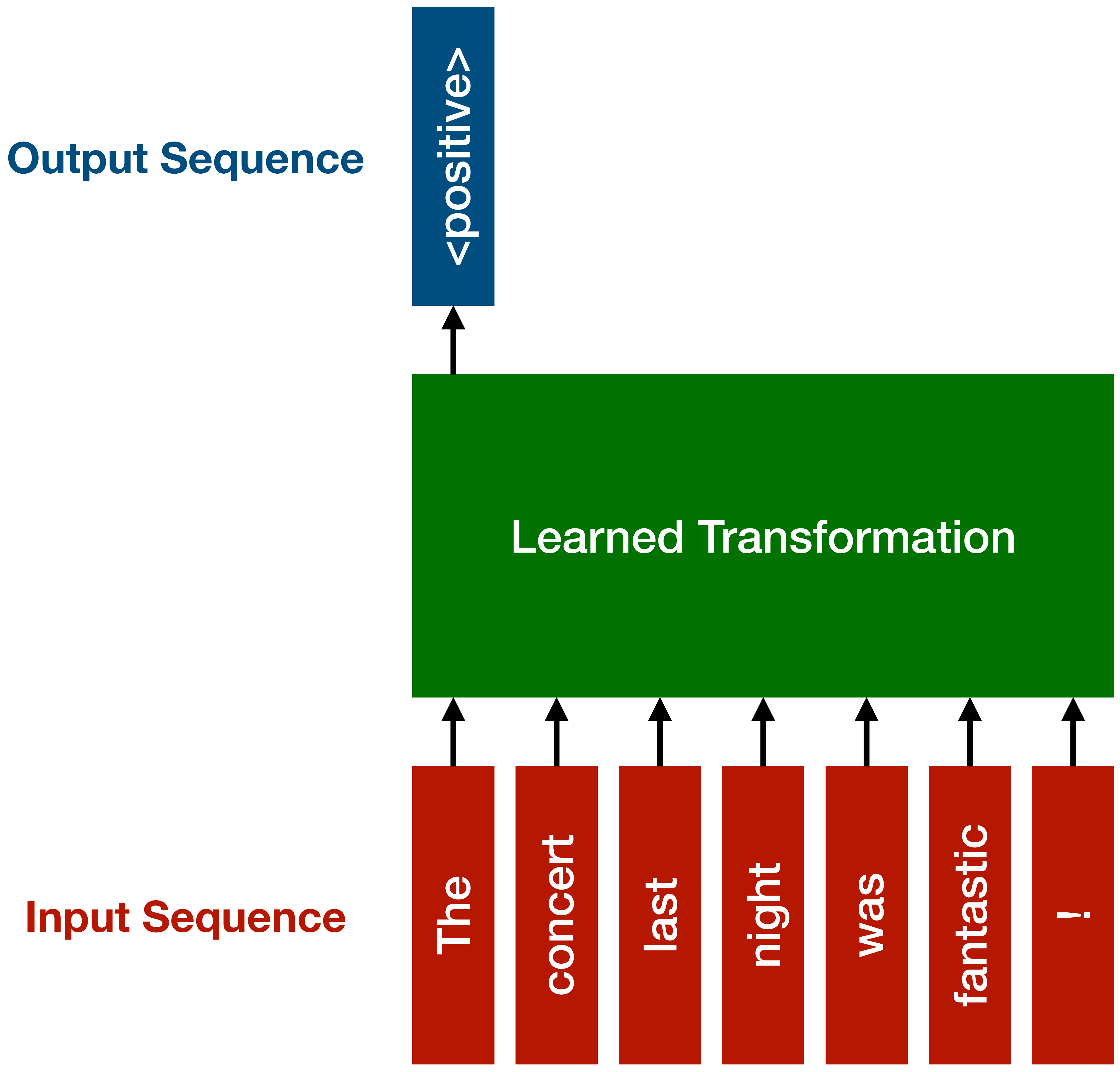


The sequence-to-sequence framework is very general

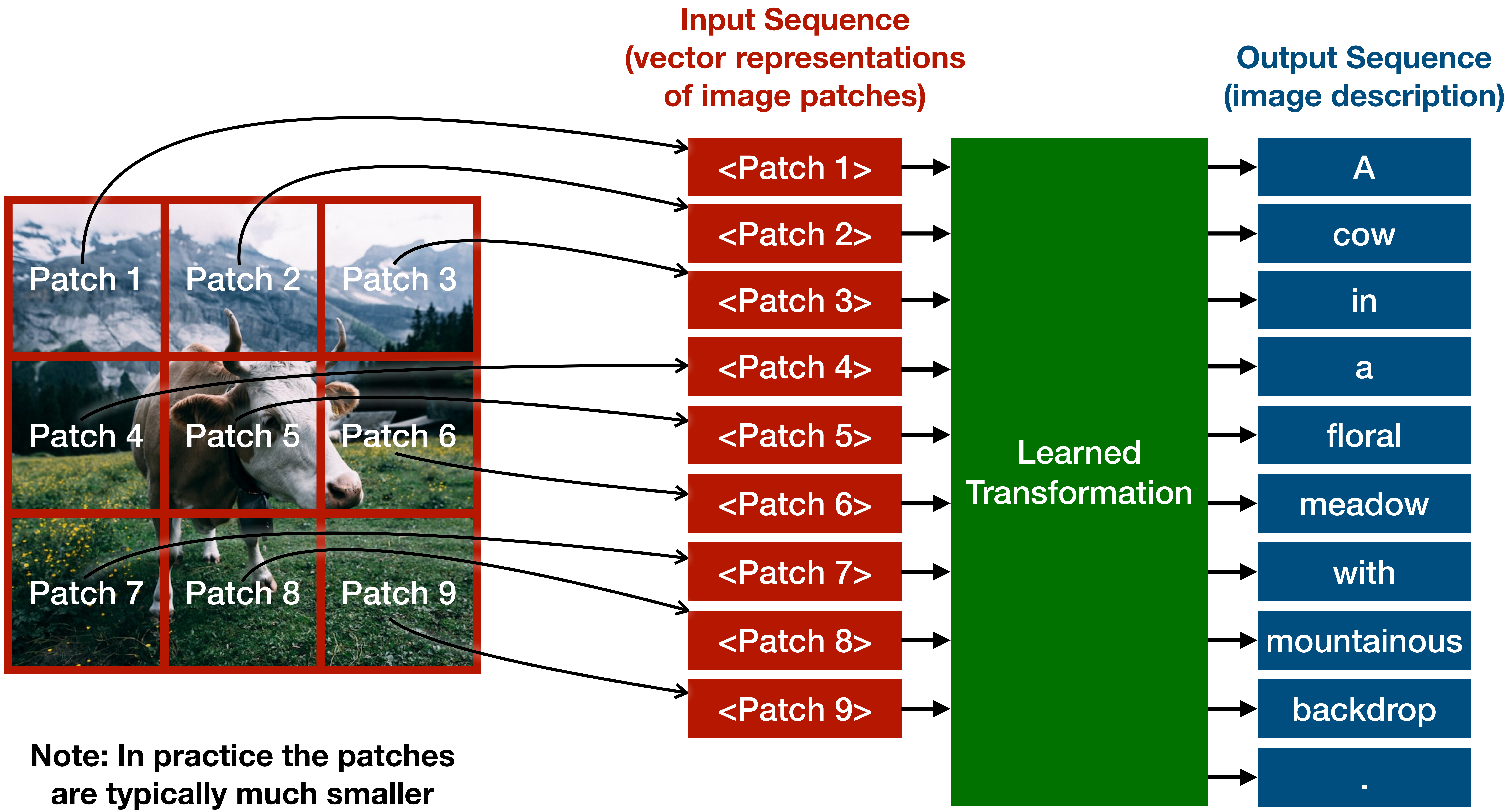
Translation



Sentiment classification
(output is a sequence of length 1)

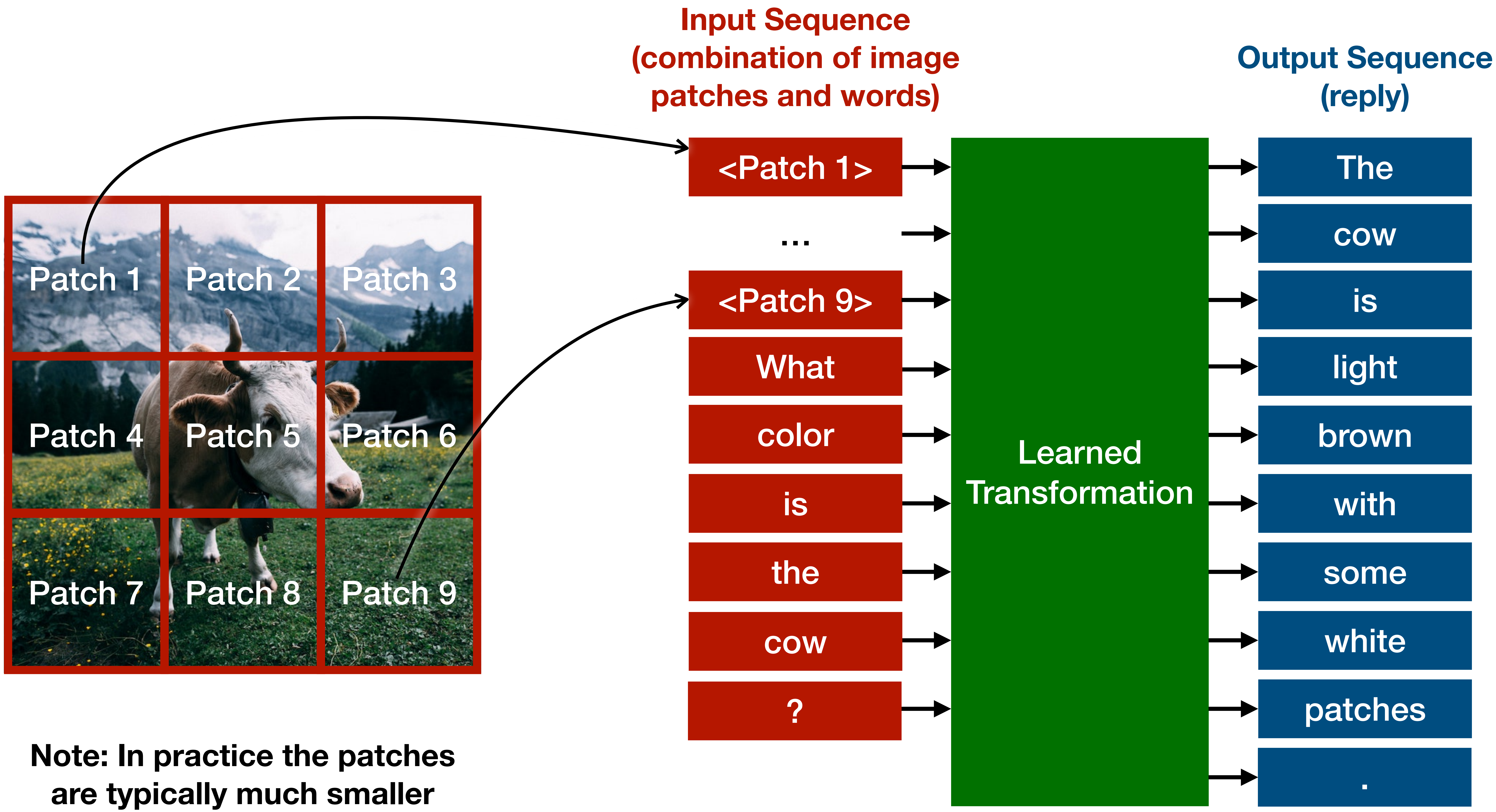


Images can also be represented as sequences



Note: In practice the patches are typically much smaller

Sequences can be multimodal (image + text)



Note: In practice the patches are typically much smaller

Transformers

What Is a Transformer?

$$\boxed{f : sequence \underset{\text{(using \textbf{self-attention})}}{\rightarrow} sequence}$$

Transformer is a neural network f that iteratively transforms a sequence to another sequence and mixes the information between the sequence elements via **self-attention**

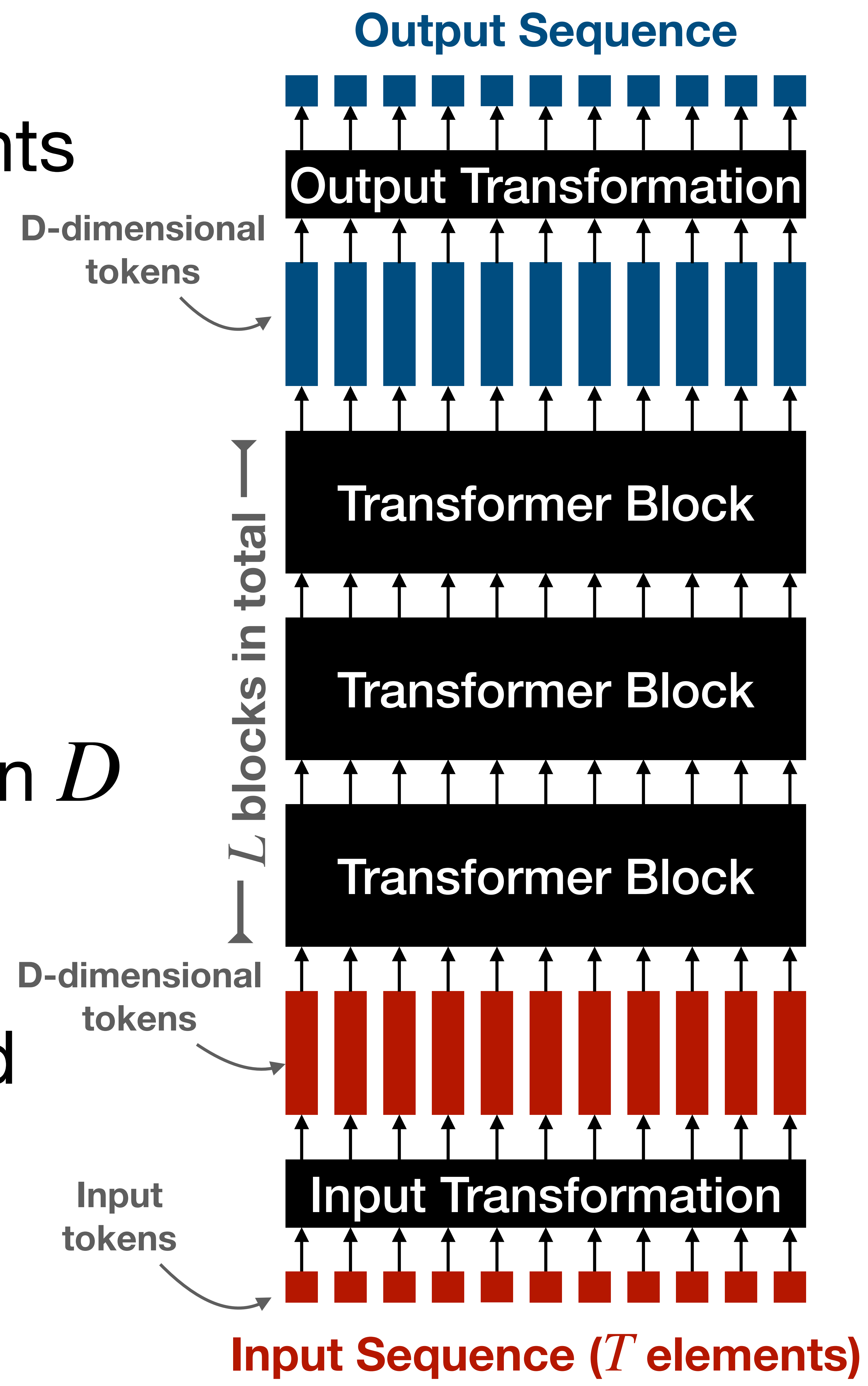
Basic Transformer Architecture

Input transformation: converts the input sequence elements into real-valued vector representations (aka **tokens**):

- maps a one-hot word vector to a real-valued vector
- extracts an image patch and flattens it into a vector

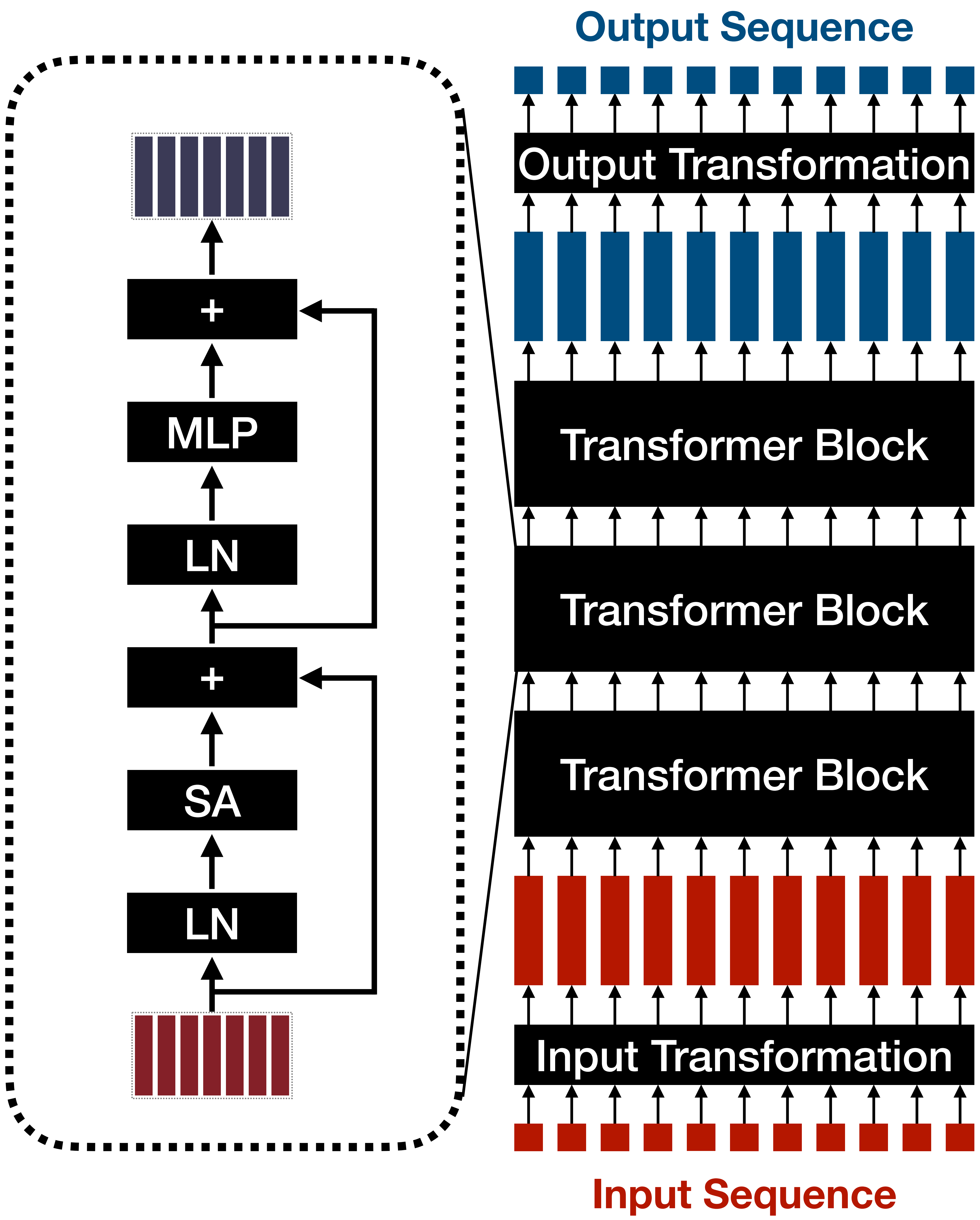
Transformer block: transforms a sequence of T vectors of dimension D into a new sequence of T vectors of dimension D using **self-attention** and **MLP sub-blocks**

Output transformation: converts the vectors to the desired output format (e.g., single-element sequence for classification, multiple-element sequence of words)



Transformer Block

- **Self-Attention (SA):** mixes information **between** tokens
- **Multi-Layer Perceptron (MLP):** mixes information **within** each token
- Other standard components:
  - Skip connections are widely used
  - Layer normalization (LN) is usually placed at the start of a residual branch



Input Transformations

Text Token Embeddings

Tokenization: split the input text into a sequence of *input tokens* (typically word fragments + some special symbols) according to some predefined *tokenizer procedure*:

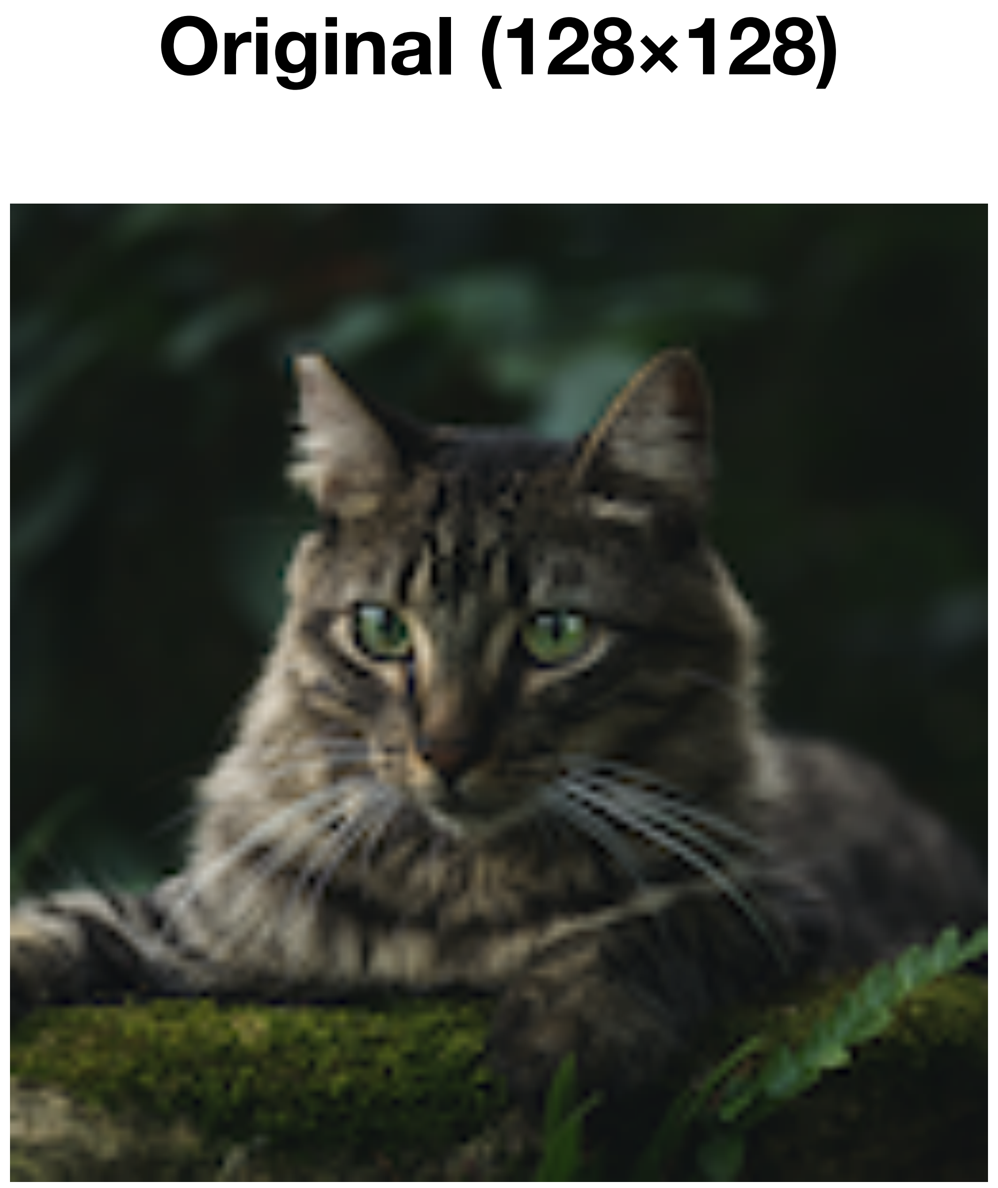
- `Text: "<User:>Transformers are awesome!"`
- `Tokens: [<User token>, "trans", "form", "ers_", "are_", "awe", "some", "!"]`
- `Token IDs: [0, 5124, 1029, 645, 3001, 6931, 7330, 10] (each token corresponds to some number` $i \in \{1, \ldots, N_{vocab}\}$`)`

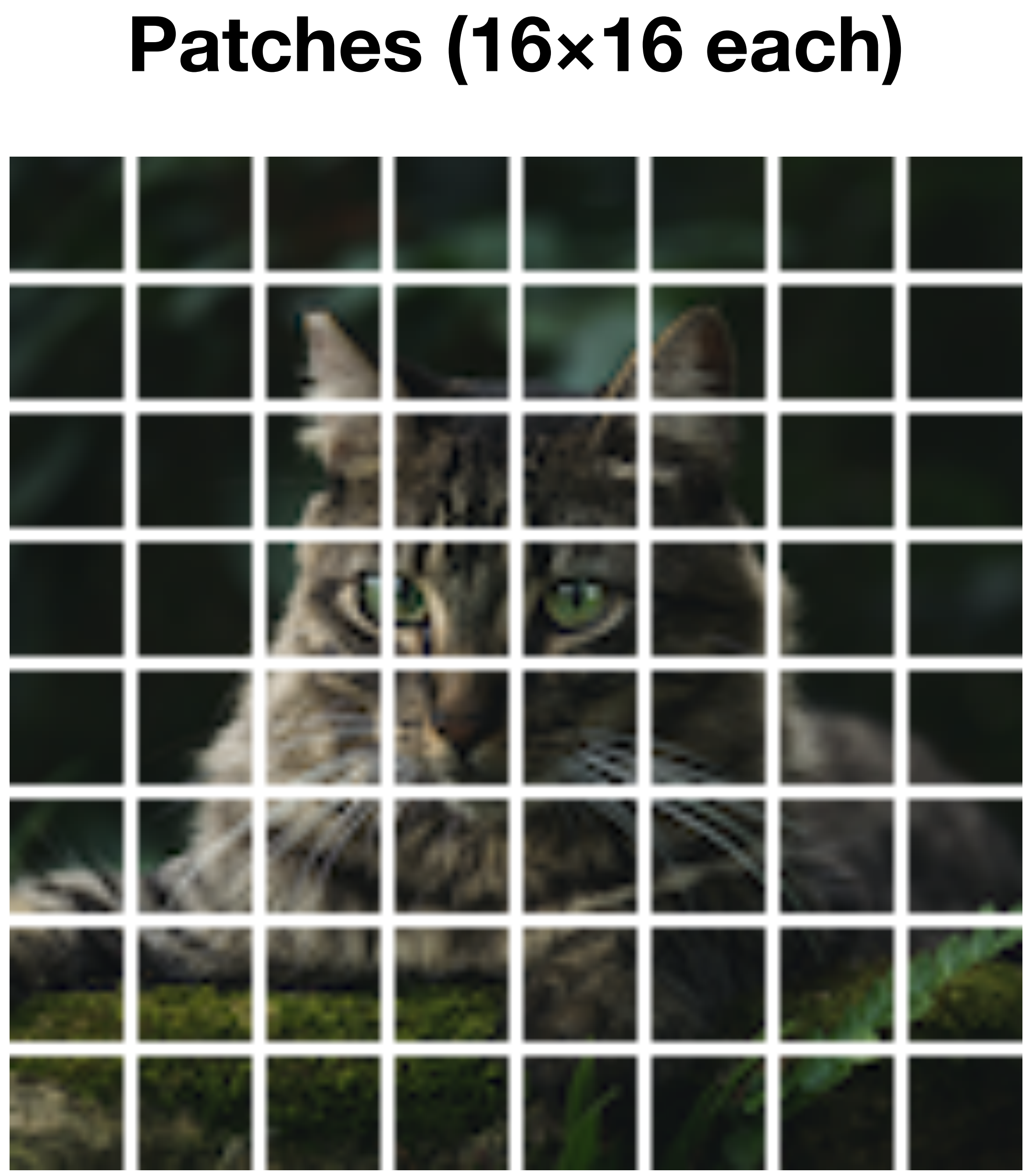
Token embedding: convert token IDs to real-valued token vectors

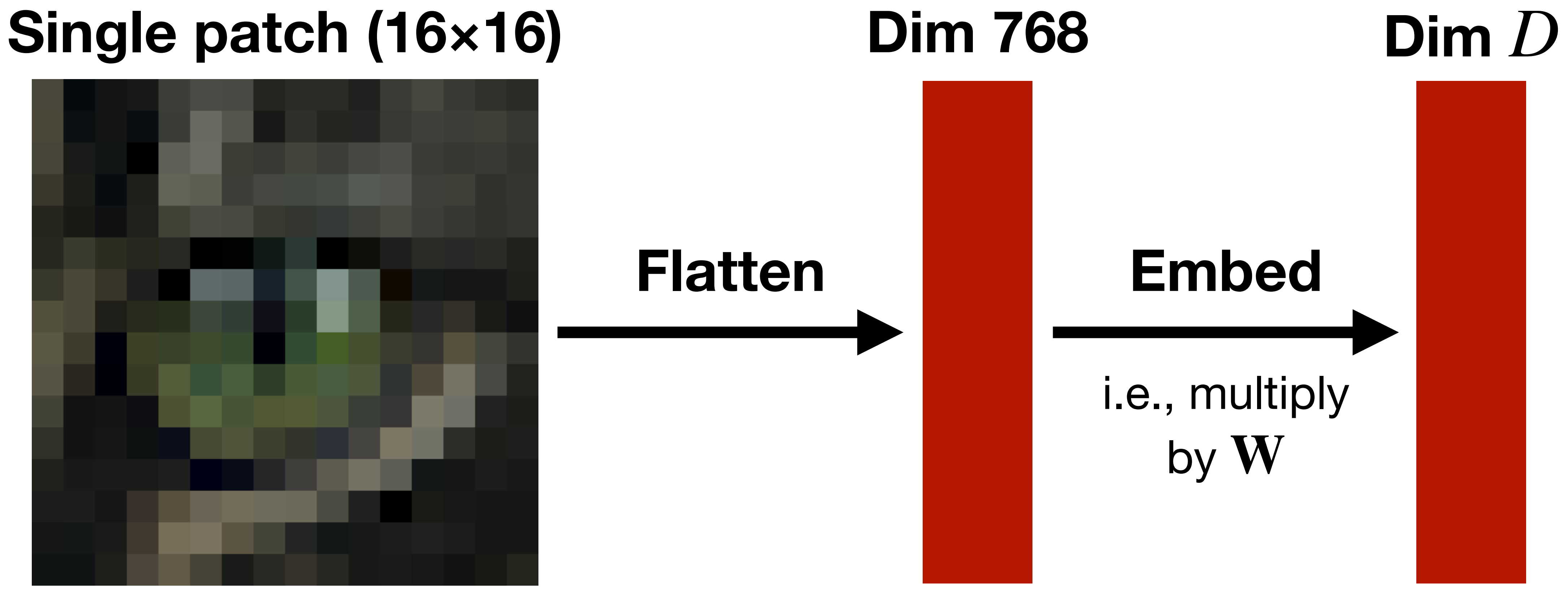
- Convert each token ID $i \in \{1, \ldots, N_{vocab}\}$ into a real-valued vector $\mathbf{w}_i \in \mathbb{R}^D$
- This can be seen as a matrix multiplication $\mathbf{W} \cdot \mathbf{e}_i = \mathbf{W}_{:,i} = \mathbf{w}_i$ (with $\mathbf{W} \in \mathbb{R}^{D \times N_{vocab}}$)
- $\mathbf{W}$ is learned via backpropagation, along with all other transformer parameters (however, the tokenizer procedure is typically fixed in advance and not learned)
- The whole input sequence of T tokens leads to an input matrix $X \in \mathbb{R}^{T \times D}$

Image Patch Embeddings

- Divide image into patches of a given size (typical choice: 16×16 pixels each)
- Flatten each patch into a vector of size $16 \cdot 16 \cdot 3 = 768$ (height*width*color channels)
- Multiply each resulting vector by an embedding matrix $\mathbf{W} \in \mathbb{R}^{768 \times D}$ which is shared for all inputs
- Learn $\mathbf{W}$ through backpropagation, along with all other transformer parameters
- The whole input sequence of T embedded patches leads to an input matrix $X \in \mathbb{R}^{T \times D}$







Attention

What Is Attention?

$$A : tokens \rightarrow tokens$$

(using a **weighted average**)

Reminder: a token is simply a real-valued vector

Attention is a function that transforms a sequence of tokens to a new sequence of tokens using a **learned input-dependent weighted average**

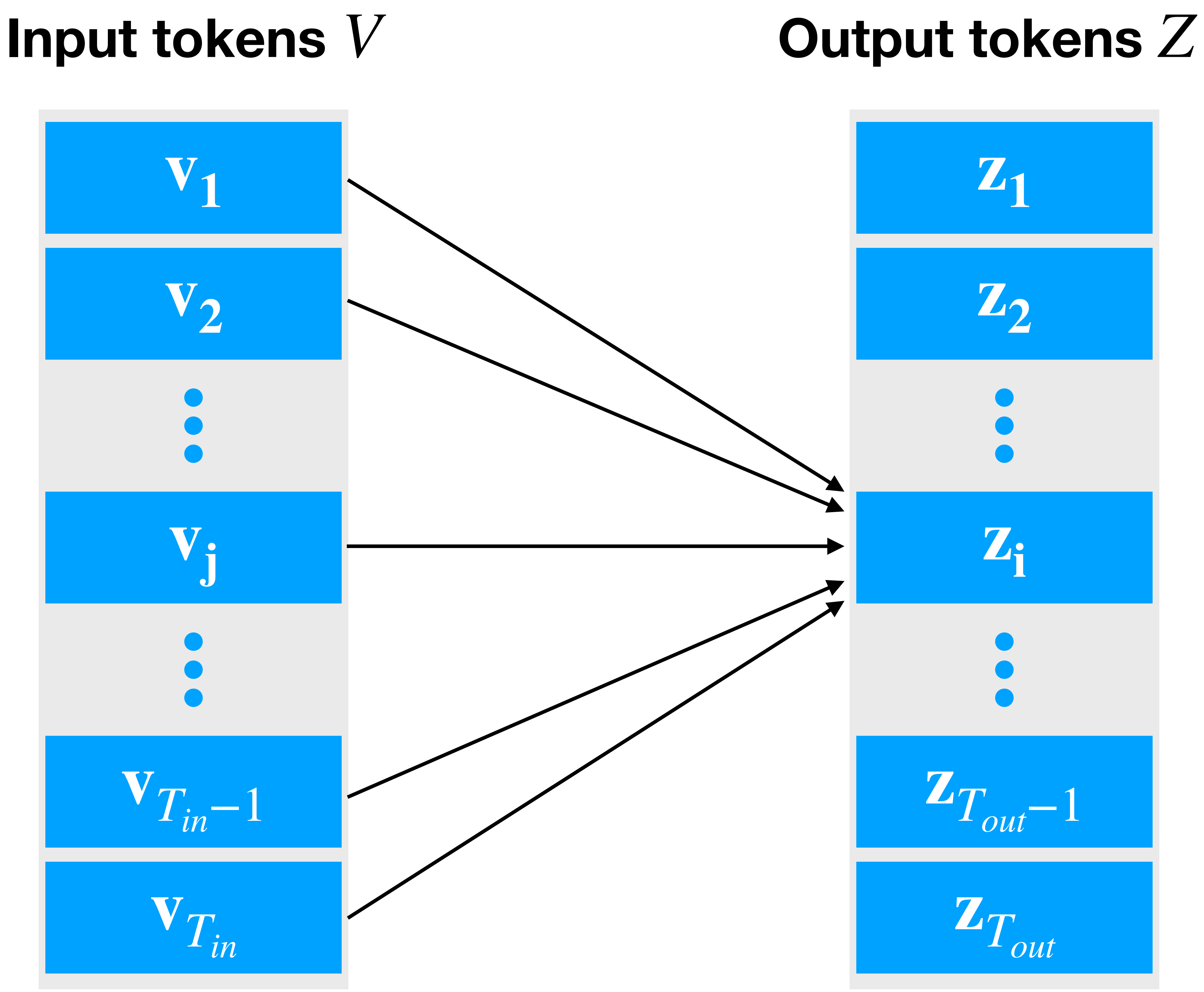
Attention as a Weighted Average

- T_{in} **input tokens**: $V \in \mathbb{R}^{T_{in} \times D_V}$
- T_{out} **output tokens**: $Z \in \mathbb{R}^{T_{out} \times D_V}$
- Output tokens are simply a **weighted average** of the input tokens:

$$\mathbf{z_i} = \sum_{j=1}^{T_{in}} p_{i,j} \mathbf{v_j} \quad \text{or in matrix form} \quad Z = PV$$

- Weighting coefficients $P \in [0,1]^{T_{out} \times T_{in}}$ form valid probability distributions over the input tokens $\sum_{j=1}^{T_{in}} p_{i,j} = 1$ (i.e., each row sums to one)

Notation: throughout this lecture, the j-th **rows** of V and Z are denoted by $\mathbf{v}_j$ and $\mathbf{z}_j$



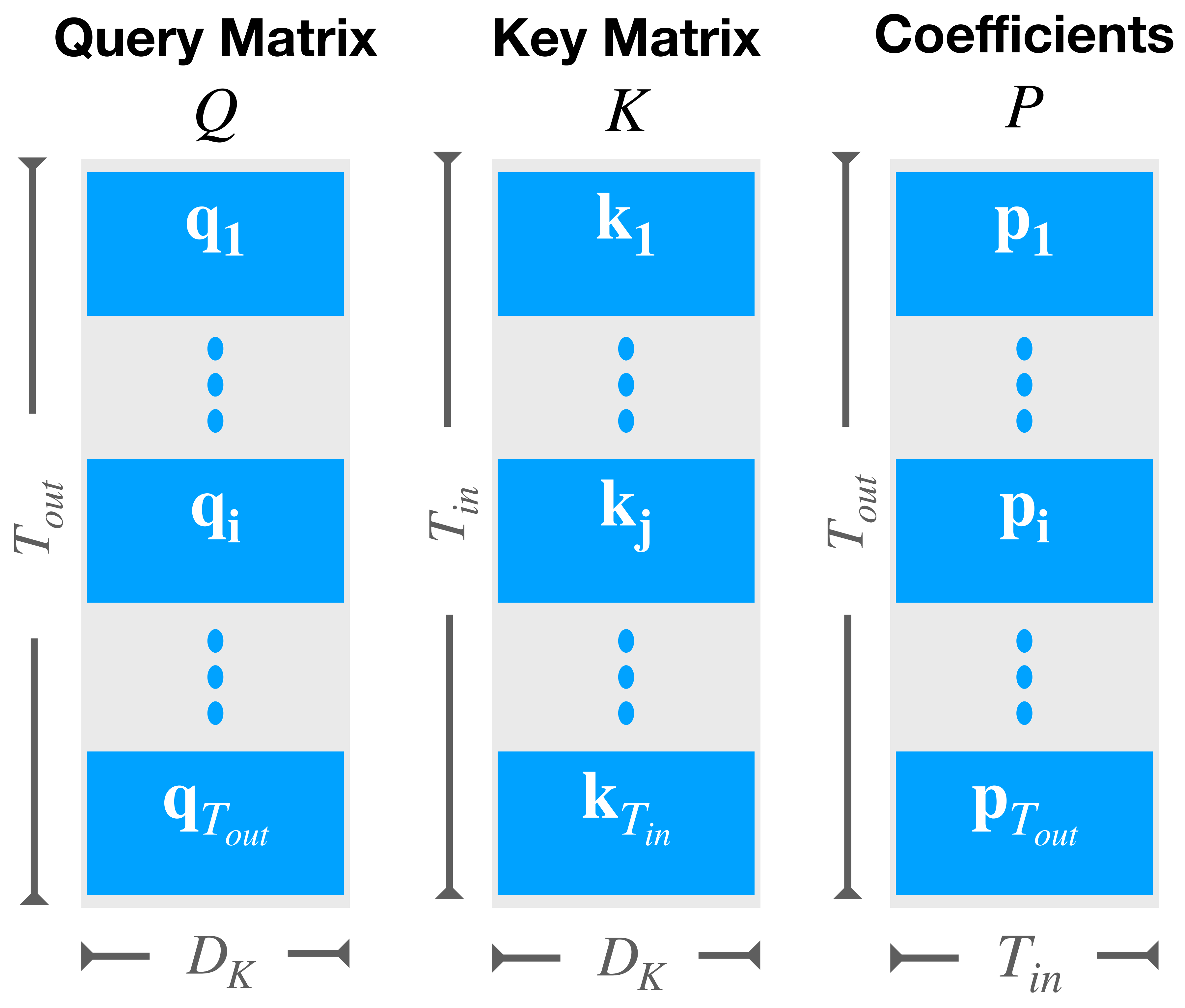
The Weighting Coefficients P

- **Query tokens** $Q \in \mathbb{R}^{T_{out} \times D_K}$ (one query per output token)
- **Key tokens** $K \in \mathbb{R}^{T_{in} \times D_K}$ (one key per input token)
- Determine weight $p_{i,j}$ based on **how similar $\mathbf{q}_i$ and $\mathbf{k}_j$** are
  - Use inner product to obtain raw similarity scores
  - Normalize with softmax (scaled by temperature by $\sqrt{D_K}$) to obtain a probability distribution
- This can be expressed as:

Element-wise: $$p_{i,j} = \frac{\exp\left(\mathbf{q}_i \mathbf{k}_j^\top / \sqrt{D_K}\right)}{\sum_{t=1}^{T_{in}} \exp\left(\mathbf{q}_i \mathbf{k}_t^\top / \sqrt{D_K}\right)}$$

Matrix form: $$P = \text{softmax}\left(\frac{QK^\top}{\sqrt{D_K}}\right)$$

The softmax
is applied on each
row *independently*



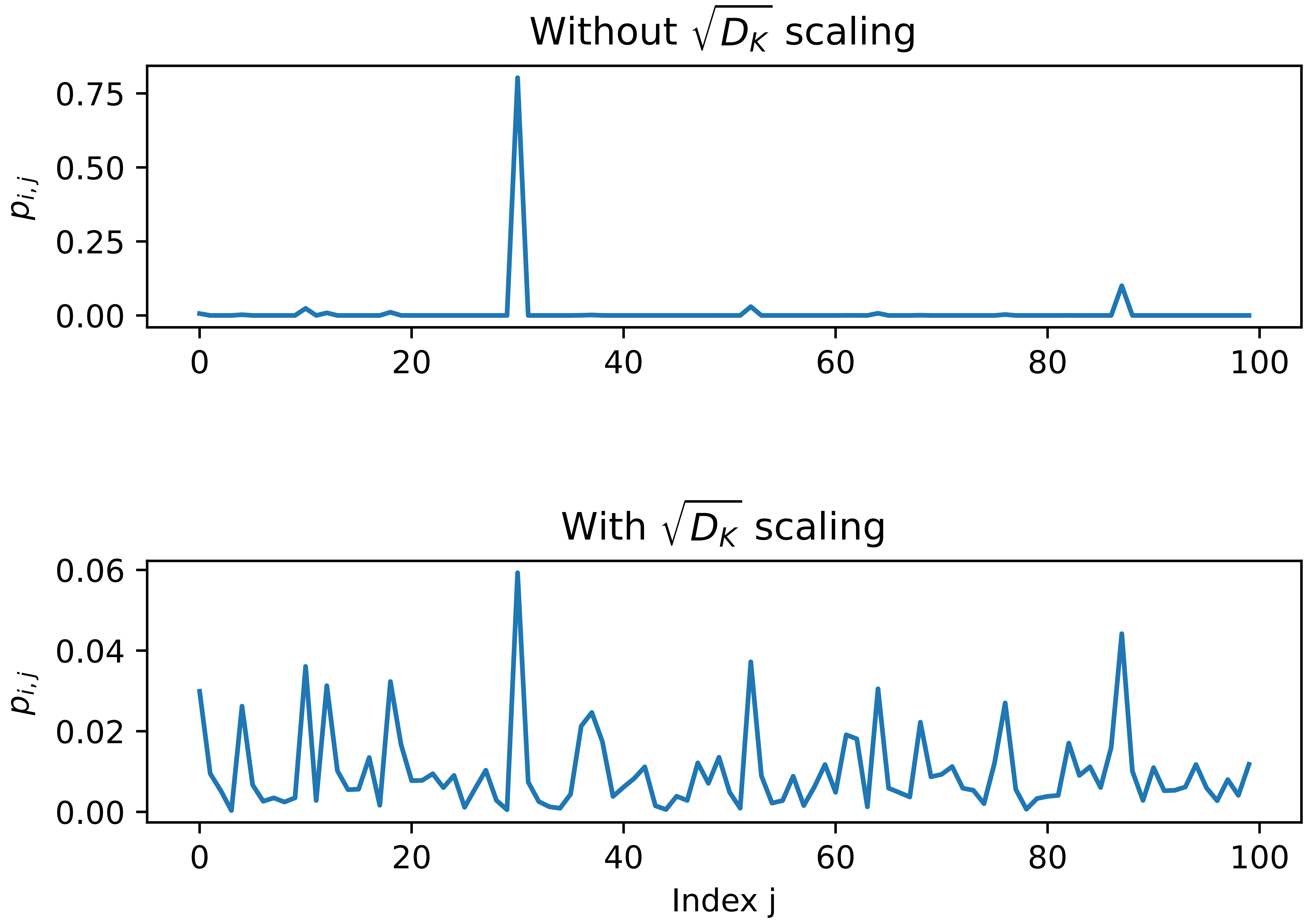
Why Use the $1/\sqrt{D_k}$ Scaling?

$$P = \text{softmax}\left(\frac{QK^\top}{\sqrt{D_K}}\right)$$

- **Without scaling**: sharp distribution of the attention weights $p_{i,j}$ at random initialization

- The model takes much more time to adjust from the initial peak due to vanishing gradients

- The $1/\sqrt{D_k}$ scaling ensures uniformity at initialization and faster convergence



Self-Attention

V, K, Q are all derived from the **same** input token sequence $X \in \mathbb{R}^{T \times D}$ (note that $T := T_{in} = T_{out}$)

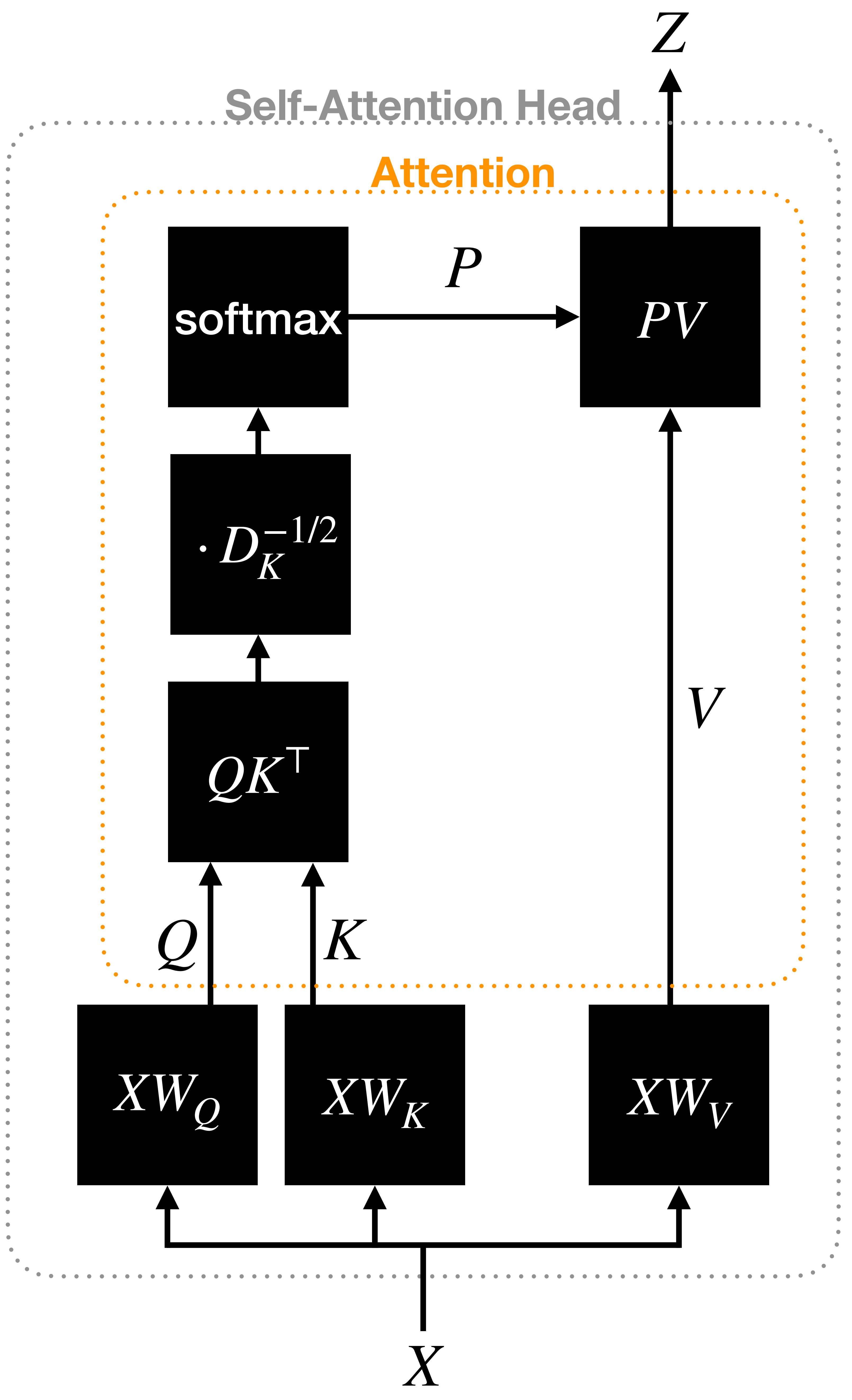
$\Rightarrow$ This forms the basis for **self-attention**:

- **Values:** $V = XW_V \in \mathbb{R}^{T \times D}$, $W_V \in \mathbb{R}^{D \times D}$
- **Keys**: $K = XW_K \in \mathbb{R}^{T \times D_K}$, $W_K \in \mathbb{R}^{D \times D_K}$
- **Queries**: $Q = XW_Q \in \mathbb{R}^{T \times D_K}$, $W_Q \in \mathbb{R}^{D \times D_K}$

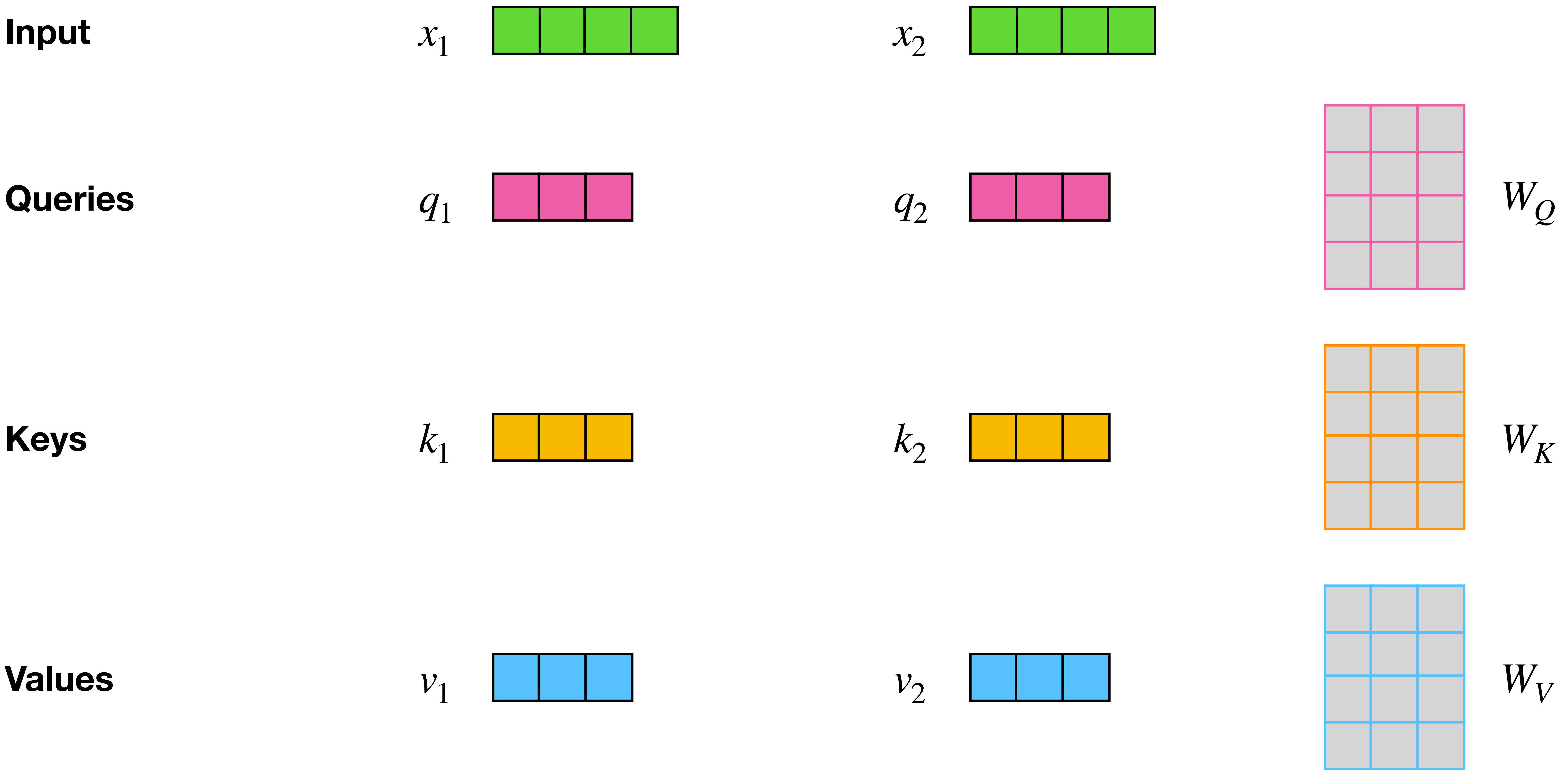
➡ W_Q, W_V, W_K are learned parameters

The output is given by:

$$Z = \mathrm{softmax}\left(\frac{XW_Q W_K^\top X^\top}{\sqrt{D_K}}\right) XW_V$$



Self-Attention: Step-by-Step

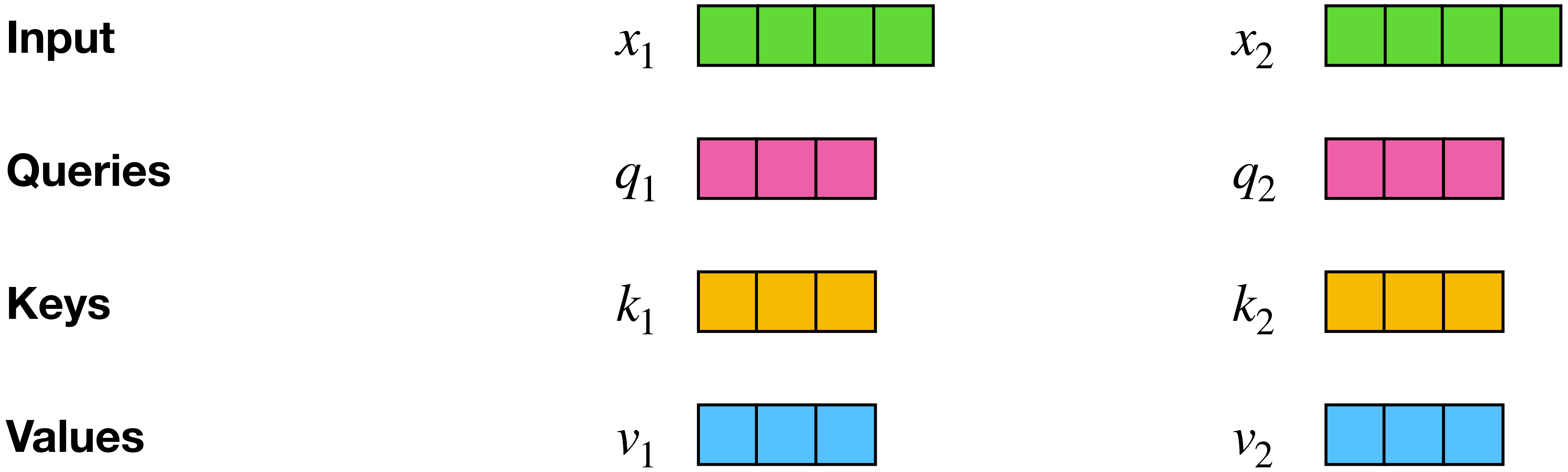


$$\boxed{\begin{aligned} Q &= XW_Q \\ K &= XW_K \\ V &= XW_V \end{aligned}}$$

Multiplying the input by the Q/K/V weight matrices, we create a query, a key and a value projection of each input of the input sequence

Illustrations borrowed from The Illustrated Transformer

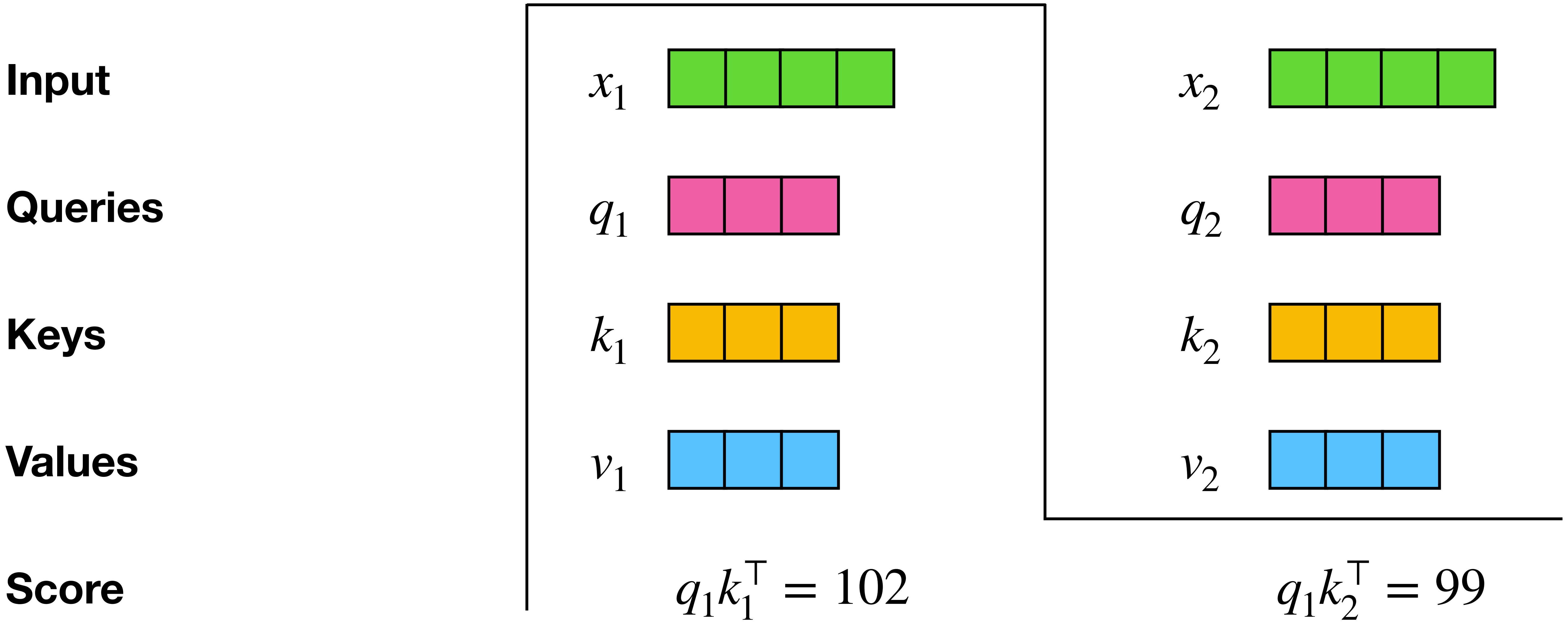
Self-Attention: Step-by-Step



Step 1: create query, key and value vectors for each input token

$$
\boxed{\begin{aligned} Q &= XW_Q \\ K &= XW_K \\ V &= XW_V \end{aligned}}
$$

Self-Attention: Step-by-Step



Step 2: calculate the scores by taking scalar product of the query and key vectors

$$\boxed{QK^\top = XW_Q W_K^\top X^\top}$$

Illustrations borrowed from The Illustrated Transformer

Self-Attention: Step-by-Step

Input	x_1	x_2
Queries	q_1	q_2
Keys	k_1	k_2
Values	v_1	v_2
Score	$q_1k_1^\top = 102$	$q_1k_2^\top = 99$
Divide by $\sqrt{D_K}$	$\frac{q_1k_1^\top}{\sqrt{D_K}} = 58.9$	$\frac{q_1k_2^\top}{\sqrt{D_K}} = 57.2$
Softmax	$p_{1,1} = 0.85$	$p_{1,2} = 0.15$

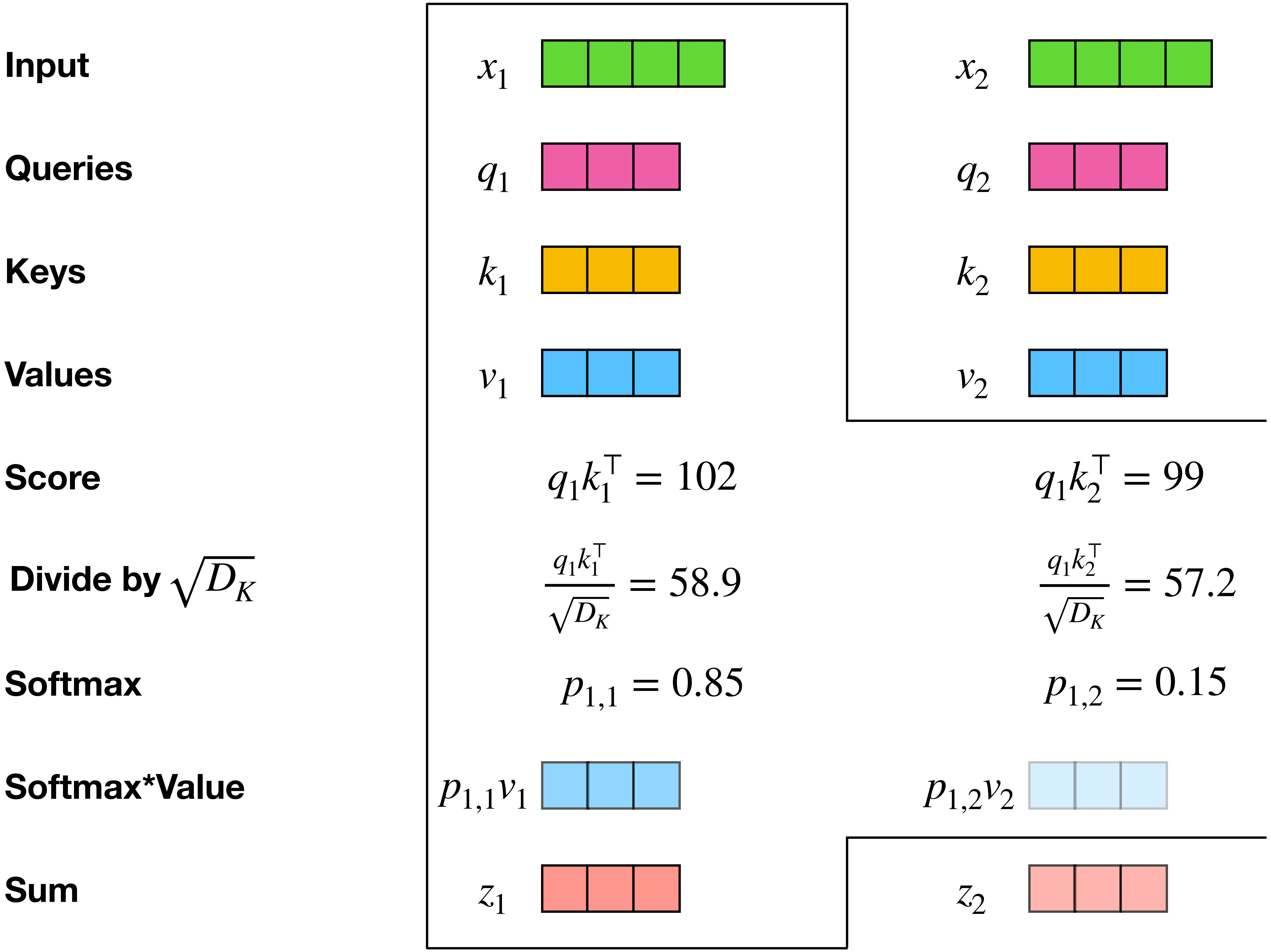
Step 3: divide the scores by $\sqrt{D_K}$

Step 4: Compute the softmax of these values

$$\boxed{P = \mathrm{softmax}\left(\frac{QK^\top}{\sqrt{D_K}}\right)}$$

Illustrations borrowed from The Illustrated Transformer

Self-Attention: Step-by-Step



Step 5: Multiply each value vector by the softmax score

Step 6: Sum up the weighted value vectors

$$\boxed{Z = PV}$$

Illustrations borrowed from The Illustrated Transformer

Self-Attention: Step-by-Step

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Values	v_1	v_2
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Divide by $\sqrt{D_K}$	$\frac{q_1 k_1^\top}{\sqrt{D_K}} = 58.9$	$\frac{q_1 k_2^\top}{\sqrt{D_K}} = 57.2$
Softmax	$p_{1,1} = 0.85$	$p_{1,2} = 0.15$
Softmax*Value	$p_{1,1} v_1$	$p_{1,2} v_2$
Sum	z_1	z_2

$$\boxed{Z = \text{softmax}\left(\frac{X W_Q W_K^\top X^\top}{\sqrt{D_K}}\right) X W_V}$$

Illustrations borrowed from The Illustrated Transformer

Multi-Head Self-Attention

- It is desirable to have multiple attention patterns per layer, similar to having multiple convolutions in a convolutional layer

  => Run H Self-Attention “heads” in parallel

- The output of head h is given by:

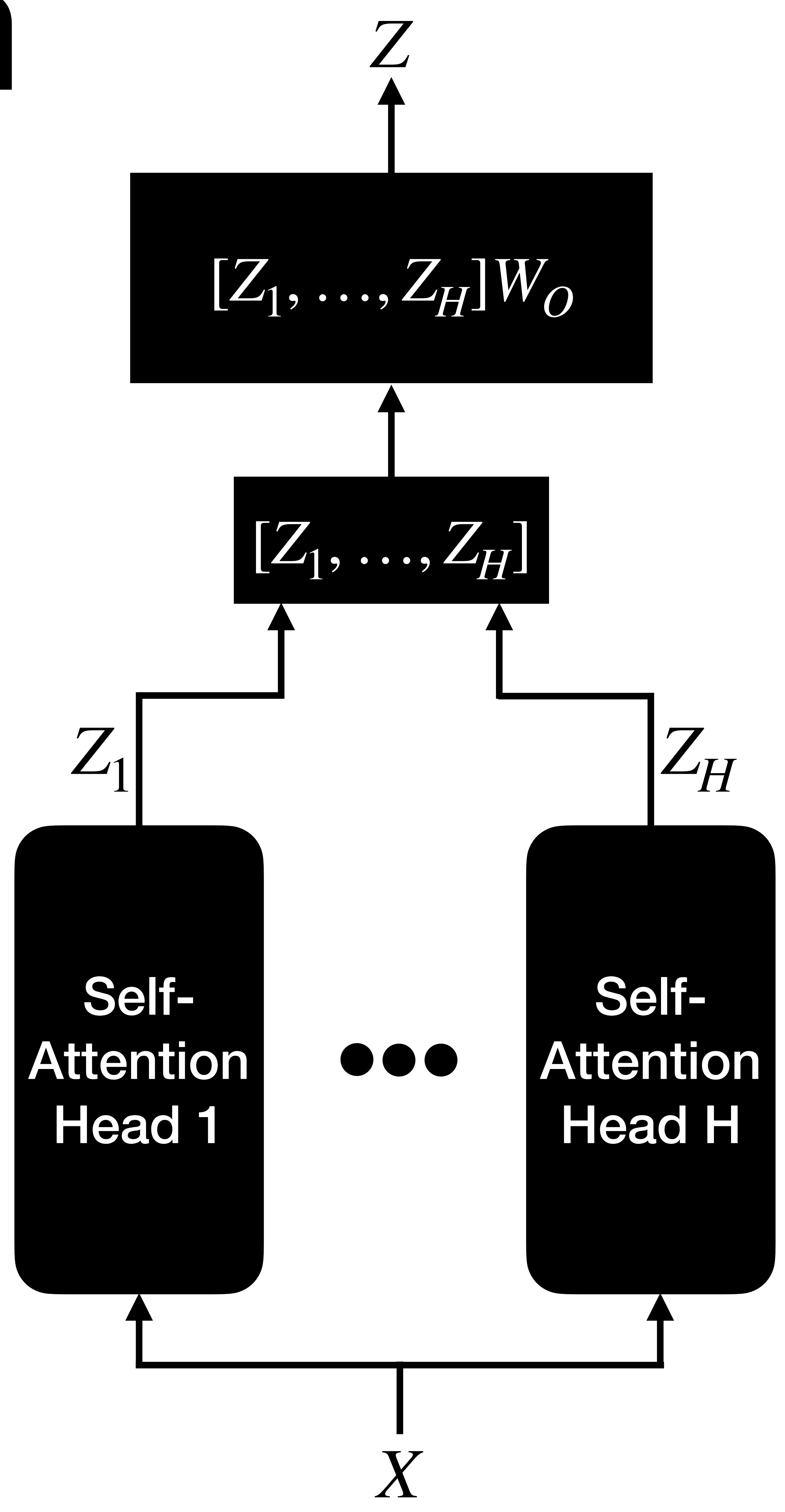
$$Z_h = \mathrm{softmax}\left(\frac{XW_{Q,h}W_{K,h}^{\top}X^{\top}}{\sqrt{D_K}}\right)XW_{V,h}$$

$$W_{V,h} \in \mathbb{R}^{D\times D_V},\ W_{K,h} \in \mathbb{R}^{D\times D_K},\ W_{Q,h} \in \mathbb{R}^{D\times D_K}$$

- The final output is obtained by concatenating head-outputs and applying a linear transformation

$$Z = [Z_1, \ldots, Z_H]W_O$$

where $W_O \in \mathbb{R}^{HD_V\times D}$ is learned via backpropagation



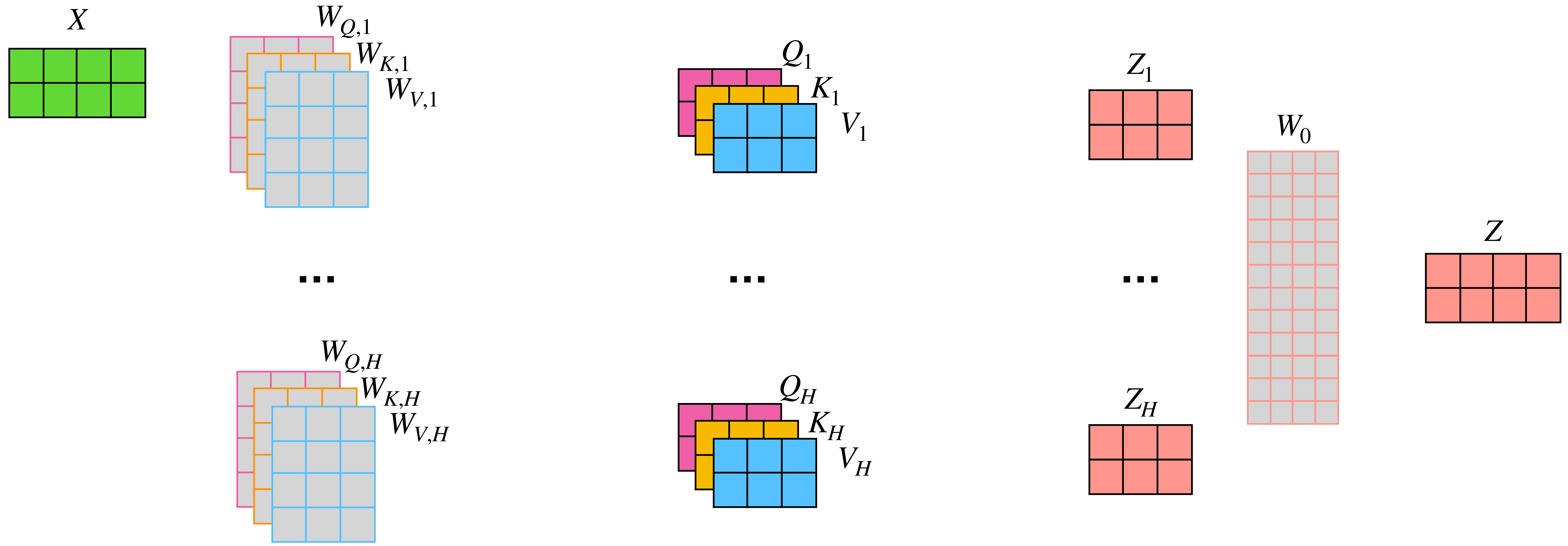
Multi-Head Self-Attention: recap

1) Input

2) Split into H heads
We multiply X by weight matrices

3) Calculate attention using the resulting Q_h, K_h, V_h matrices

4) Concatenate the resulting matrices Z_h and multiply by W_0 to obtain the final output Z of the self-attention layer



Illustrations borrowed from The Illustrated Transformer

Positional Information in Transformers

- **Attention by itself does not account for the order of input**
- **But in practice, the input order matters:**

  "She prefers cats to dogs" ≠ "She prefers dogs to cats"
- **Solution**: incorporate a positional encoding in the network which is a function from the position to a feature vector $pos : \{1, \ldots, T\} \rightarrow \mathbb{R}^D$
- **The most basic choice** is to add a positional embedding W_{pos} corresponding to each token's position t to the input embedding. $W_{pos} \in \mathbb{R}^{D \times T}$ is learned via backpropagation along with the other parameters
- Numerous hand-crafted positional encodings exist (active area of research!)

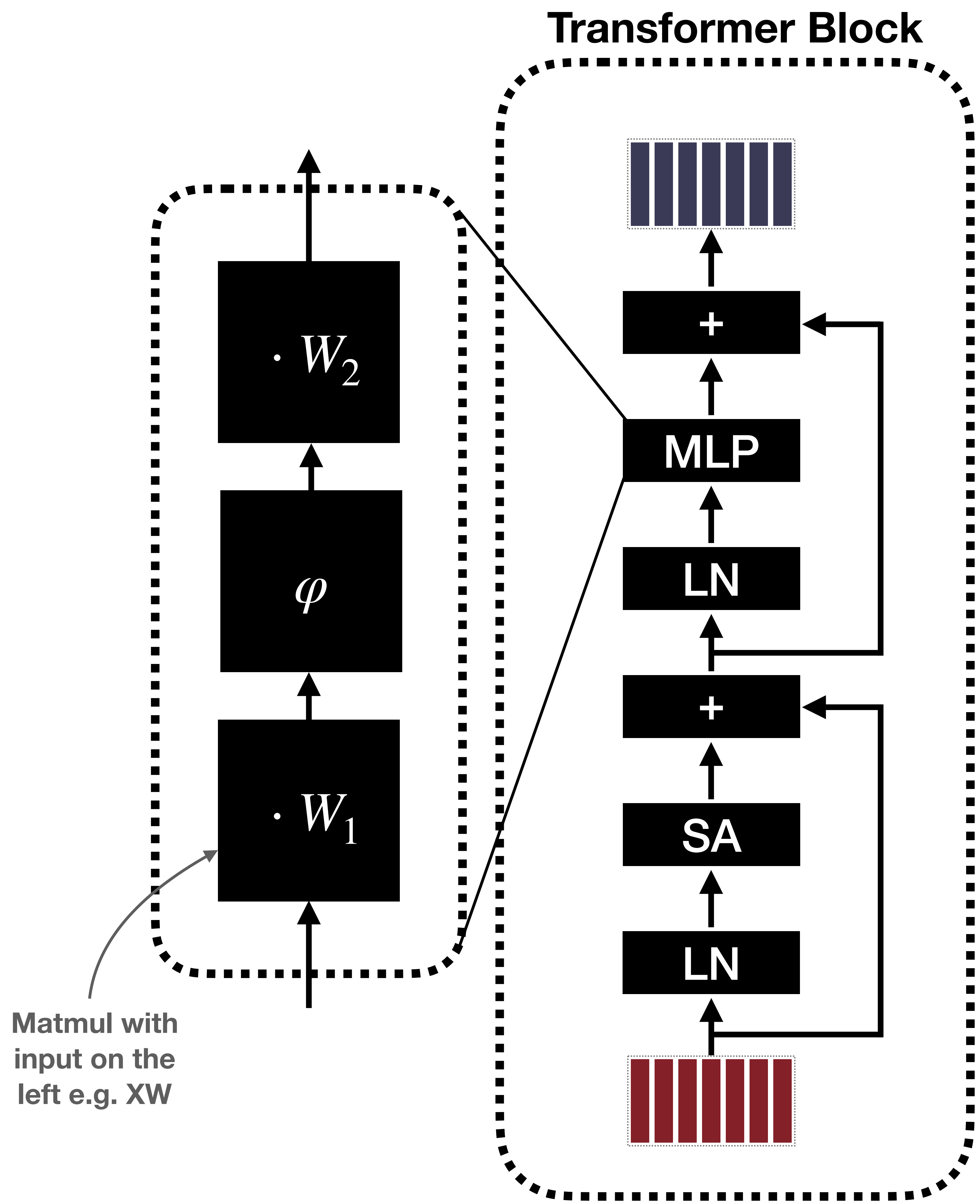
MLP

Mixing Information within Tokens

- **MLP** mixes information within each token
- Apply the same transformation to each token independently:

$$MLP(X) = \varphi(XW_1)W_2$$

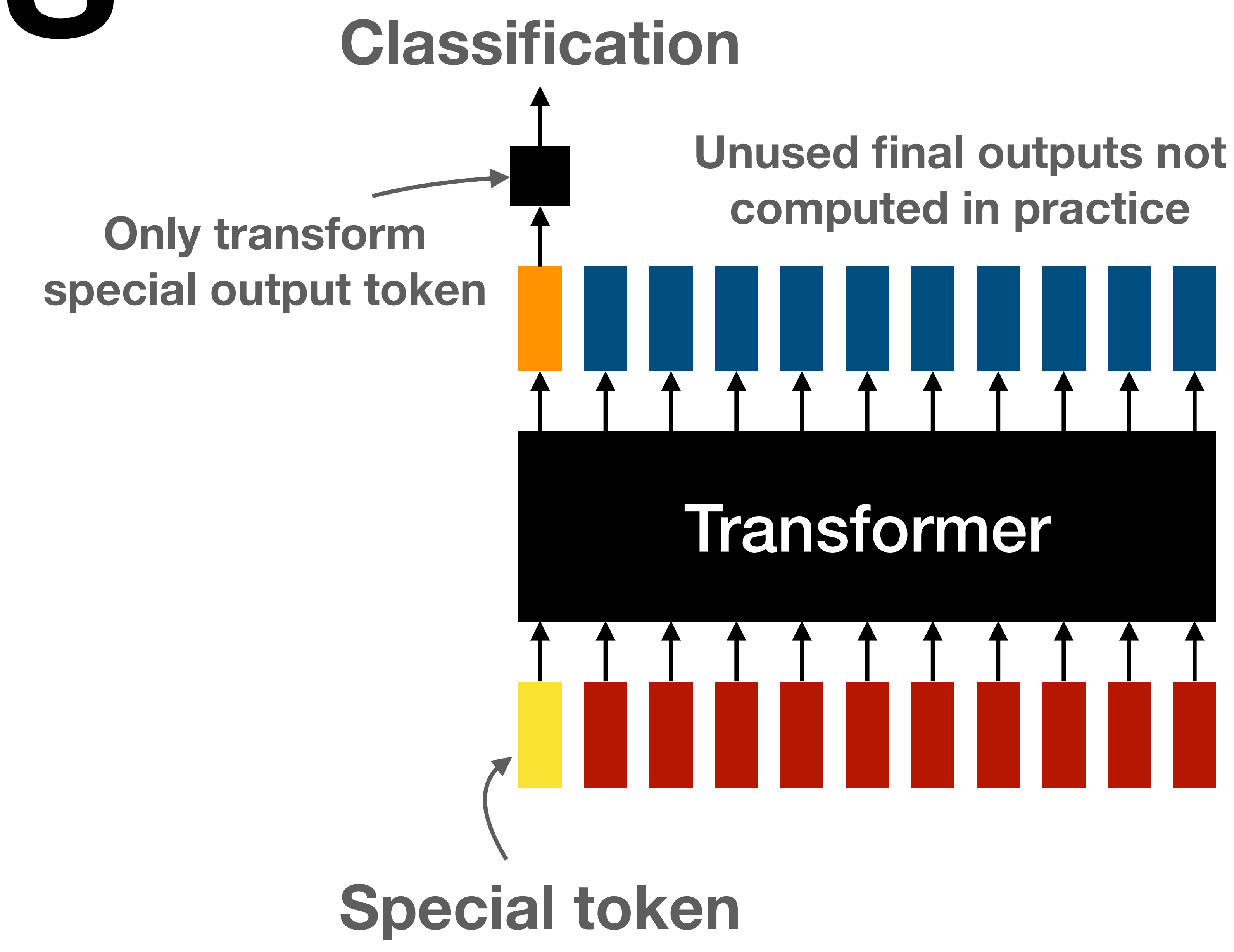
- Matrices $W_1, W_2 \in \mathbb{R}^{D \times D}$ learned via backprop
- Non-linearity φ in between (e.g., ReLU or GeLU)
- The model may also include learned bias terms

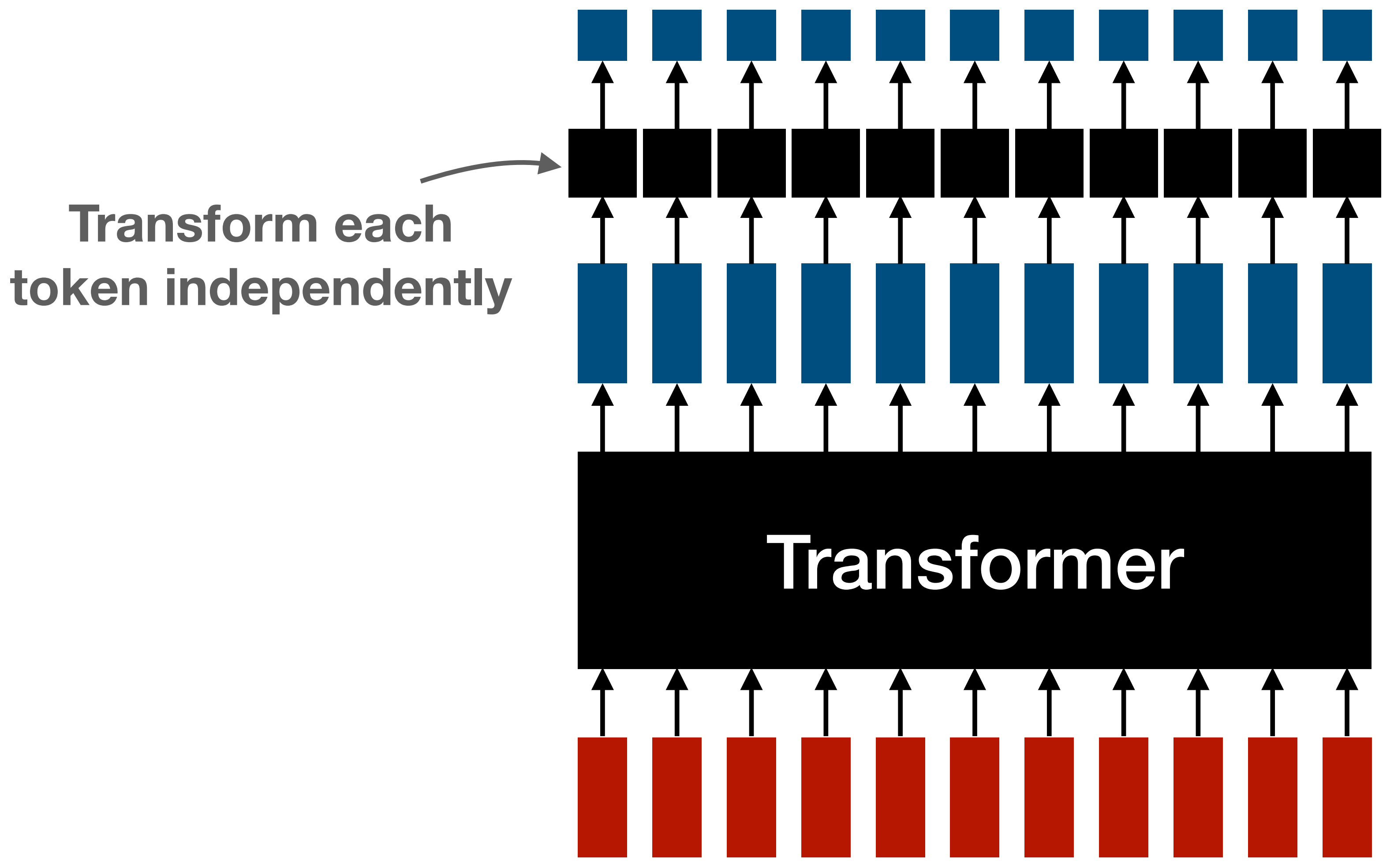


Output Transformations

Output Transformations

- We obtain the output from the final transformer block
- Output transformation is typically simple: linear transformation or a small MLP
- The specifics are highly dependent on the task:
  - **Single output** (e.g., sequence-level classification): apply an output transformation to a special task-specific input token or to the average of all tokens
  - **Multiple outputs** (e.g., per-token classification): apply an output transformation to each token independently

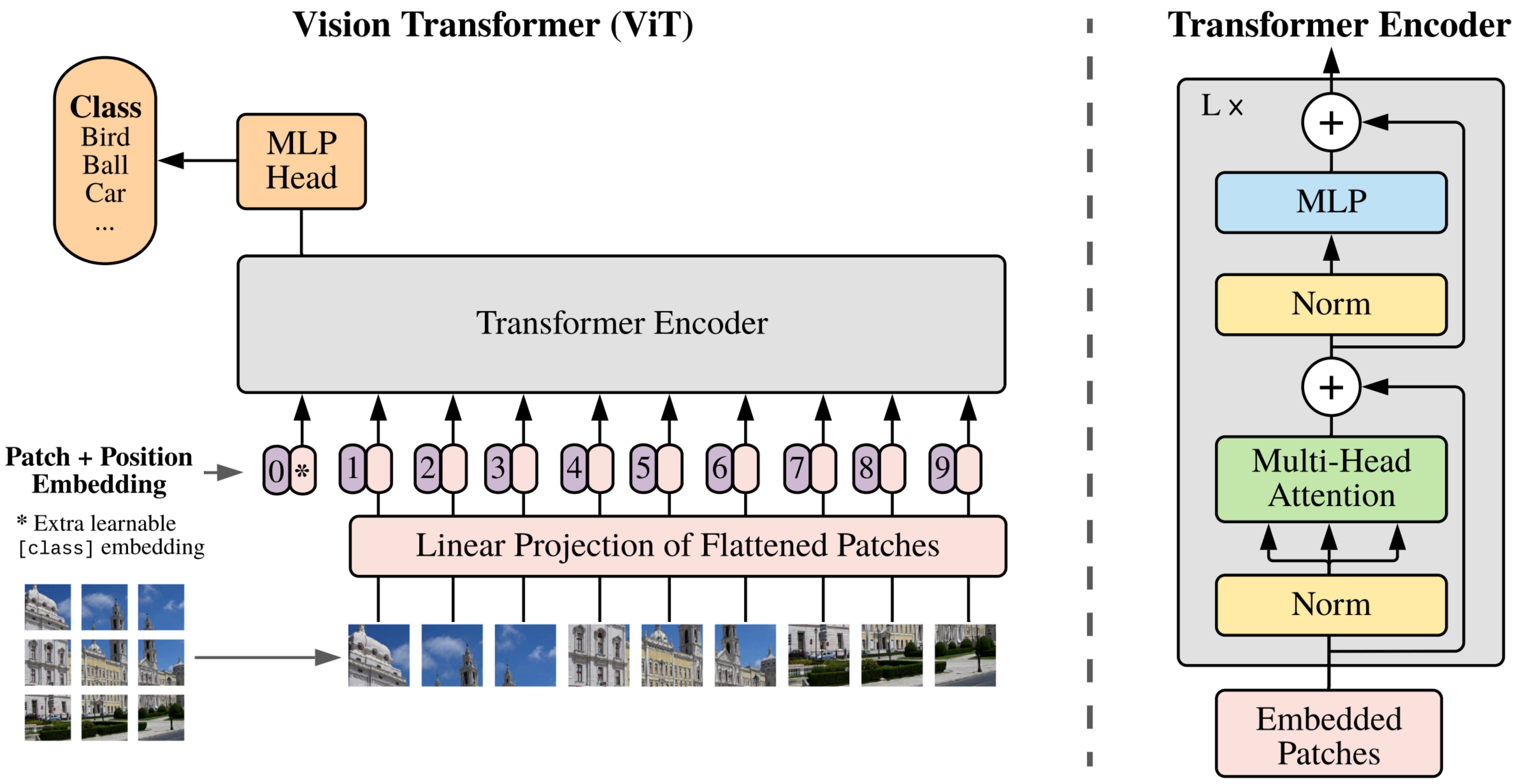




Putting the pieces together: Vision Transformers

Vision Transformer Architecture

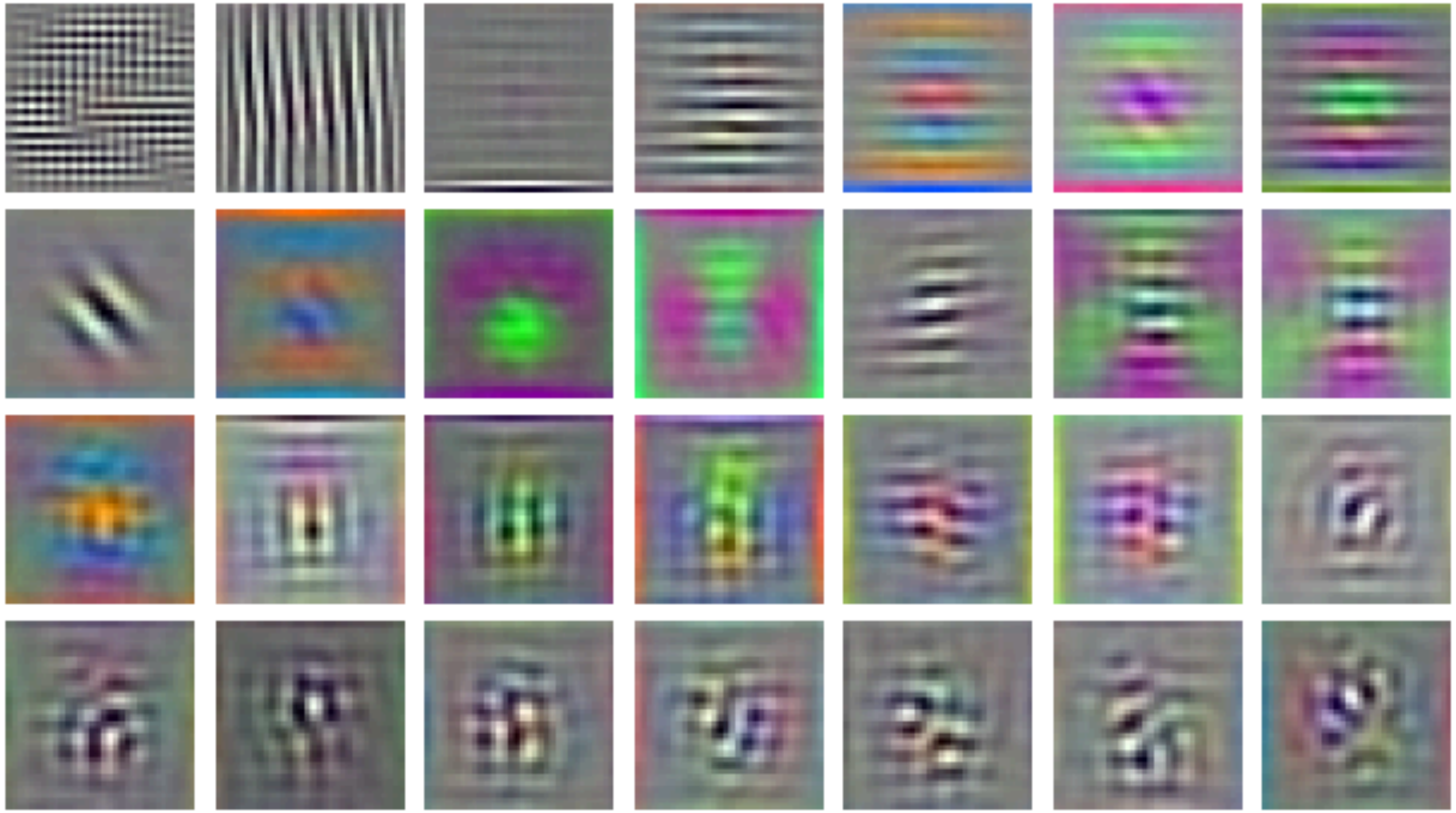
- **Simple architecture**: number of features D is constant across all layers. There is no use of padding, pooling, or strides.
- Self-attention is **more general** than convolution and can potentially express it
- The receptive field is the **whole image** after just one self-attention layer
- ViTs require more data than CNNs due to their reduced inductive bias in extracting local features
- However, ViTs become competitive with CNNs after **large-scale pretraining**



$$
\begin{aligned}
\mathbf{z}_0 &= [\mathbf{x}_\text{class};\, \mathbf{x}^1_p\mathbf{E};\, \mathbf{x}^2_p\mathbf{E};\, \cdots;\, \mathbf{x}^N_p\mathbf{E}] + \mathbf{E}_{pos}, && \mathbf{E} \in \mathbb{R}^{(P^2\cdot C)\times D},\ \mathbf{E}_{pos} \in \mathbb{R}^{(N+1)\times D} \\
\mathbf{z'}_\ell &= \text{MSA}(\text{LN}(\mathbf{z}_{\ell-1})) + \mathbf{z}_{\ell-1}, && \ell = 1\ldots L \\
\mathbf{z}_\ell &= \text{MLP}(\text{LN}(\mathbf{z'}_\ell)) + \mathbf{z'}_\ell, && \ell = 1\ldots L \\
\mathbf{y} &= \text{LN}(\mathbf{z}^0_L)
\end{aligned}
$$

Source: An Image is Worth 16x16 Words: Transformers for Image Recognition at Scale (ICLR 2020)

What do ViTs learn: embedding layer



The first 28 principal components of the embedding layer applied on patches

Source: An Image is Worth 16x16 Words: Transformers for Image Recognition at Scale (ICLR 2020)

- The embedding layer: edge/color detectors similar to first-layer convolutions

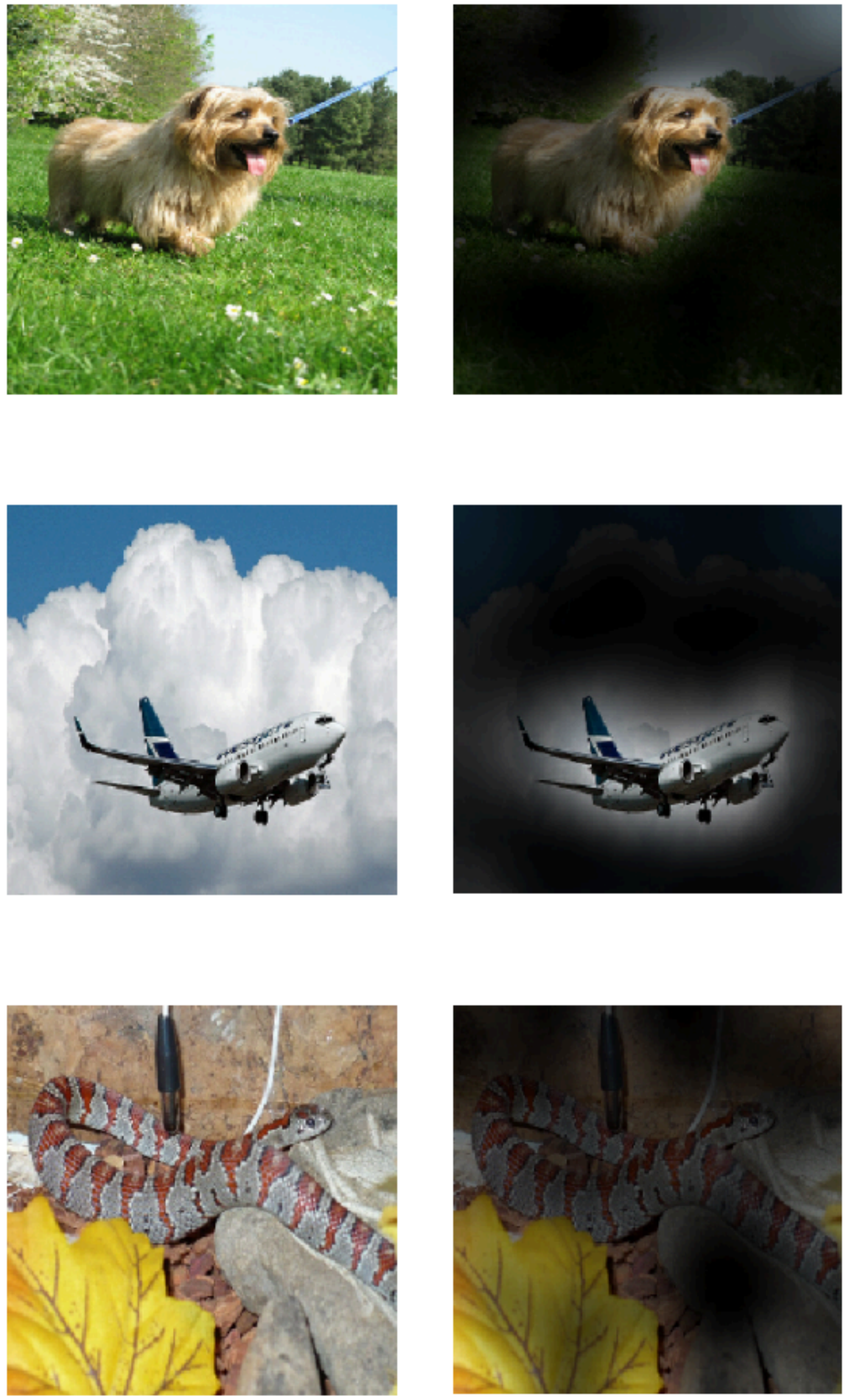
What do ViTs learn: attention

- The input-dependent attention weights can be visualized and manually inspected

- We show here one particular method known as Attention Rollout: where the attention weights are averaged across all heads and the resulting weight matrices of all layers are multiplied together

- This accounts for the mixing of attention across tokens through all layers

- In many cases, the model attends to image regions that are **semantically relevant** for classification



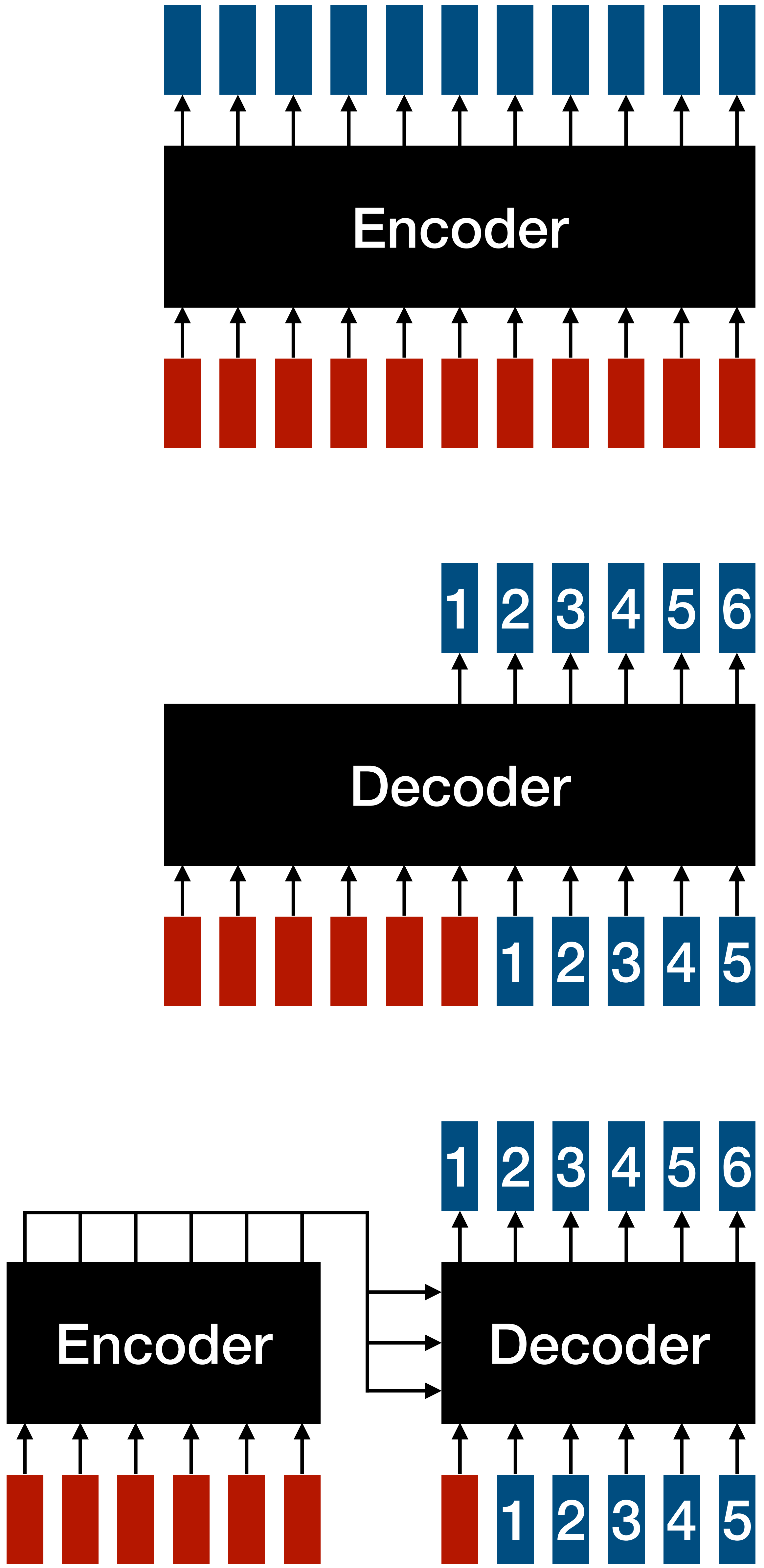
Source: An Image is Worth 16x16 Words: Transformers for Image Recognition at Scale (ICLR 2020)

The Big Picture and Takeaways

Encoders and Decoders

The transformer architecture can be used in different ways

- **Encoders** (e.g., classification):
  - They produce a fixed output size and process all inputs simultaneously
- **Decoders** (e.g., ChatGPT):
  - **Auto-regressively sample** the next token as $x_{t+1} \sim softmax(f(x_1, \ldots, x_t))$ and use it as **new input token**
  - Capable of generating responses of arbitrary length
- **Encoder-decoder** (e.g., translation):
  - First encode the whole input (e.g., in one language) and then decode to token by token (e.g., in a different language)



Transformers: Big Picture

- **Everything can be seen as a token, hence transformers are applicable across any modality**
- **CNNs can also be used for text processing, but transformers excel at capturing long-range dependencies** (as an example, the latest GPT-4 model can process up to 128k input tokens, equivalent to ~300 pages of text).
- **Self-attention scales quadratically with token length**, making it computationally expensive for large volumes of text or numerous patches—active area of research
- **However, self-attention is highly parallelizable**, which is advantageous for multi-GPU or multi-node training setups
- Transformers are now the **preferred method** for both text and vision applications
- **Emergent abilities at scale**: few-shot learning (aka in-context learning from a few example) and zero-short learning (e.g., you can ask ChatGPT any question without prior training on the task)

Recap

- **Transformers** iteratively map sequences to sequences using the self-attention mechanism
- The whole architecture is remarkably simple:
  - **Self-attention blocks** mix the information **between** tokens
  - **MLP blocks** mix the information **within** each token
- Transformers excel at modeling long-range dependencies
- Different architectures are possible (e.g., ChatGPT is decoder-only, but neural translation typically employs an encoder-decoder)
- Transformers have become a **universal architecture** for almost any type of data modality; they perform exceptionally well when given enough pretraining data

Additional Resources

If you want to learn more about attention and transformers:

- **The Illustrated Transformer**: https://jalammar.github.io/illustrated-transformer/ (a good step-by-step guide with detailed illustrations)

- **The blog of Lilian Weng (OpenAI)**: https://lilianweng.github.io/posts/2018-06-24-attention/ (from 2018 but covers well the history of the attention mechanism and its different versions)

- **CS231n: Deep Learning for Computer Vision (Stanford)**: http://cs231n.stanford.edu/slides/2023/lecture_9.pdf (more on positional encodings, masked self-attention, general attention, discussion of recurrent neural networks)

- **Minimal implementation of GPT-2**: https://github.com/karpathy/nanoGPT/ (some things are just clearer in code)