Transformers

Machine Learning Course - CS-433
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EPFL

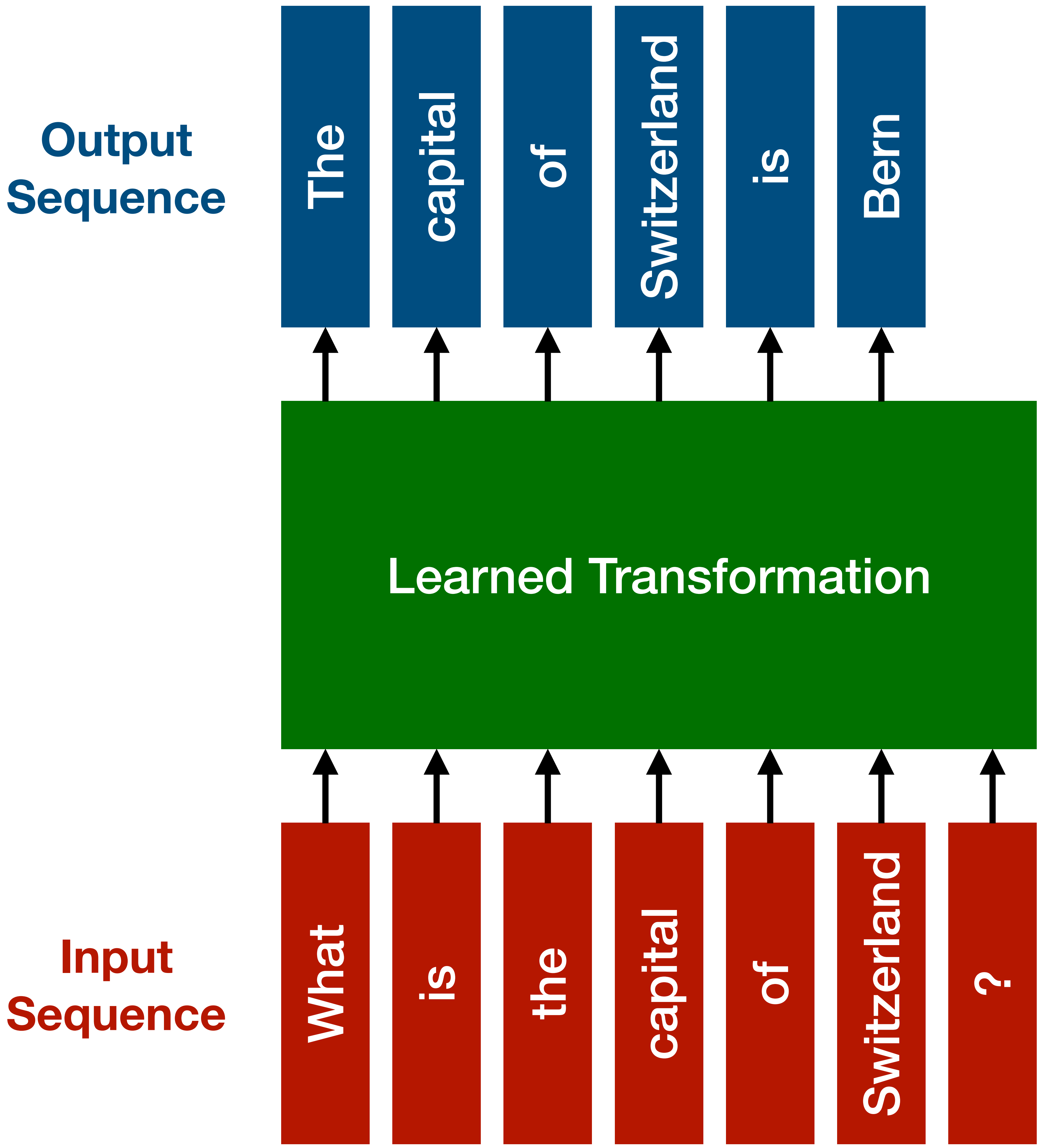
Sequence-to-Sequence Transformations

Sequence-to-Sequence Transformations

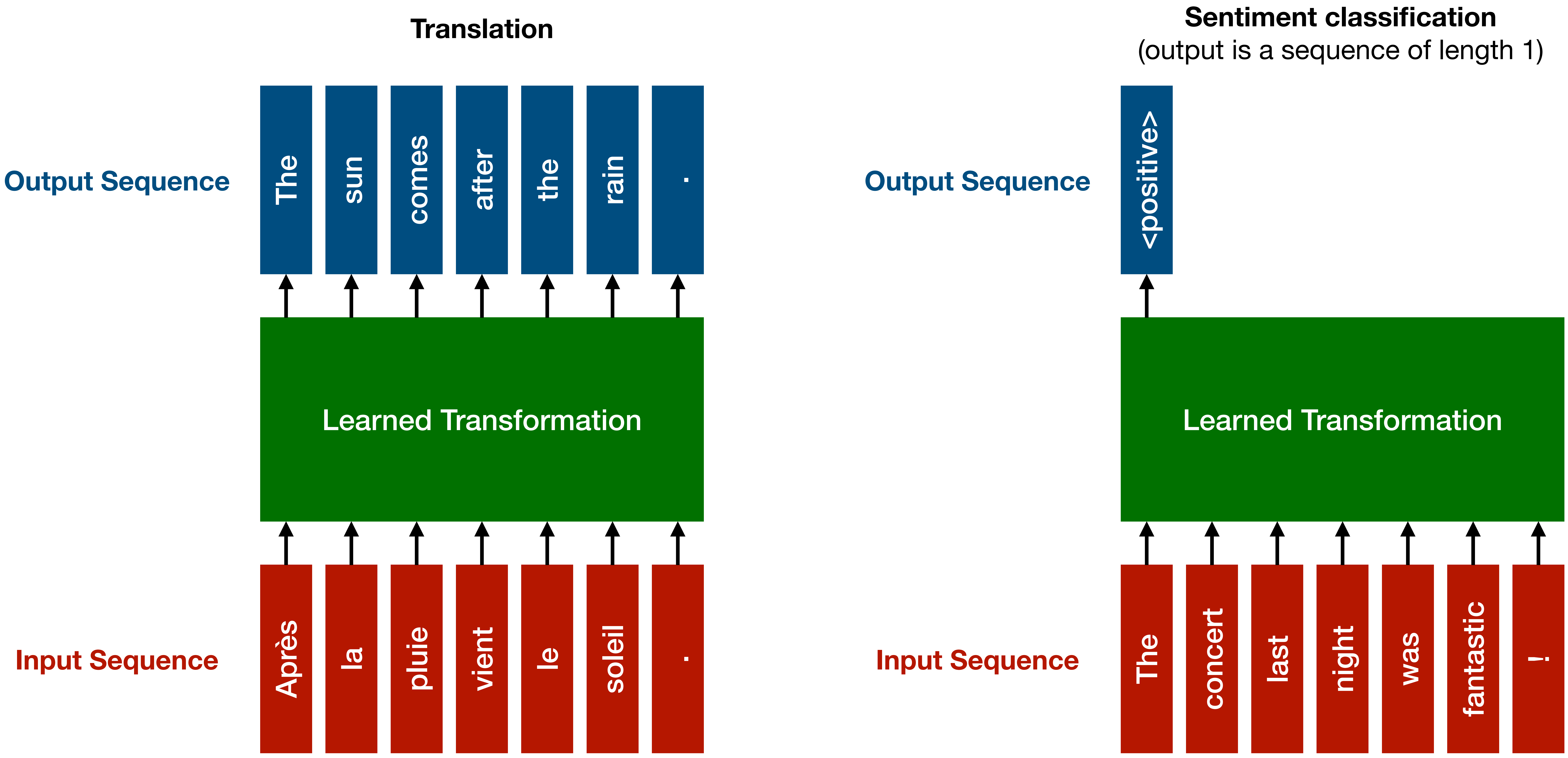
- Many interesting problems in ML can be expressed as **mapping one sequence to another**

- **Example**: chatbots like ChatGPT
  - Input: question (word sequence)
  - Output: answer (word sequence)

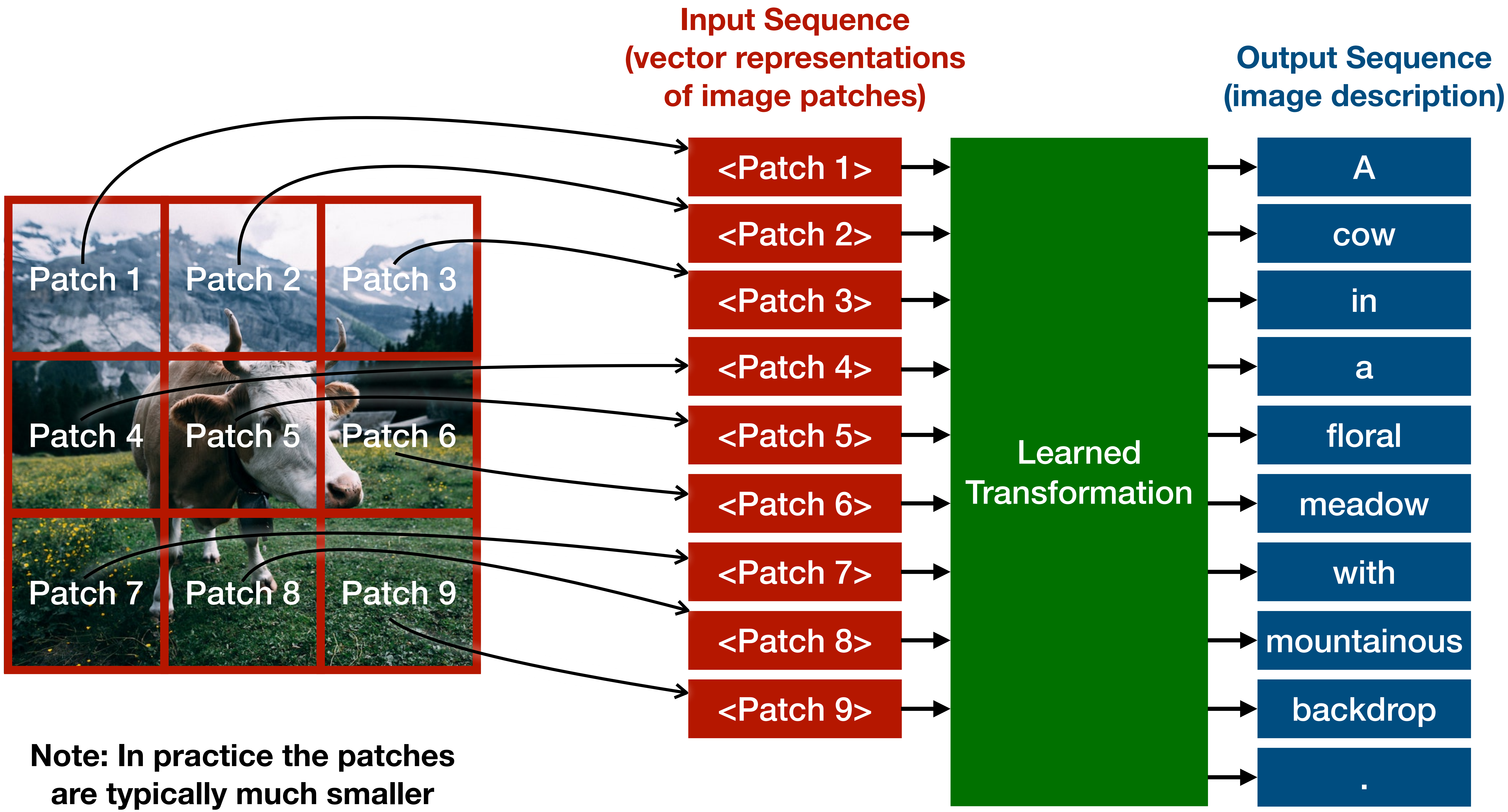
- Input and output sequences can represent various types of data: words, images, speech, proteins, time series, etc.



The sequence-to-sequence framework is very general

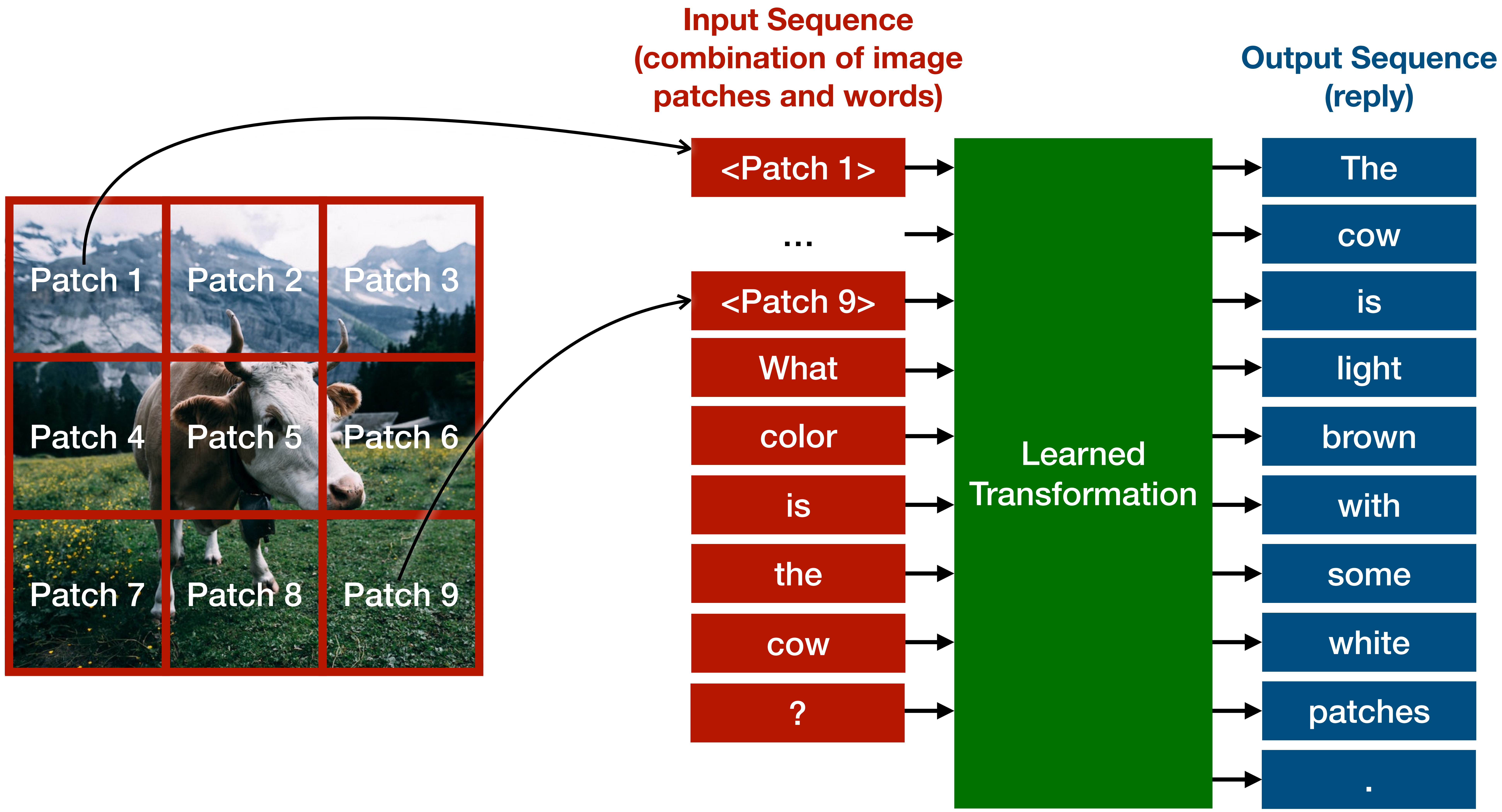


Images can also be represented as sequences



Note: In practice the patches are typically much smaller

Sequences can be multimodal (image + text)



Transformers

What is a Transformer?

$$f : sequence \rightarrow sequence$$

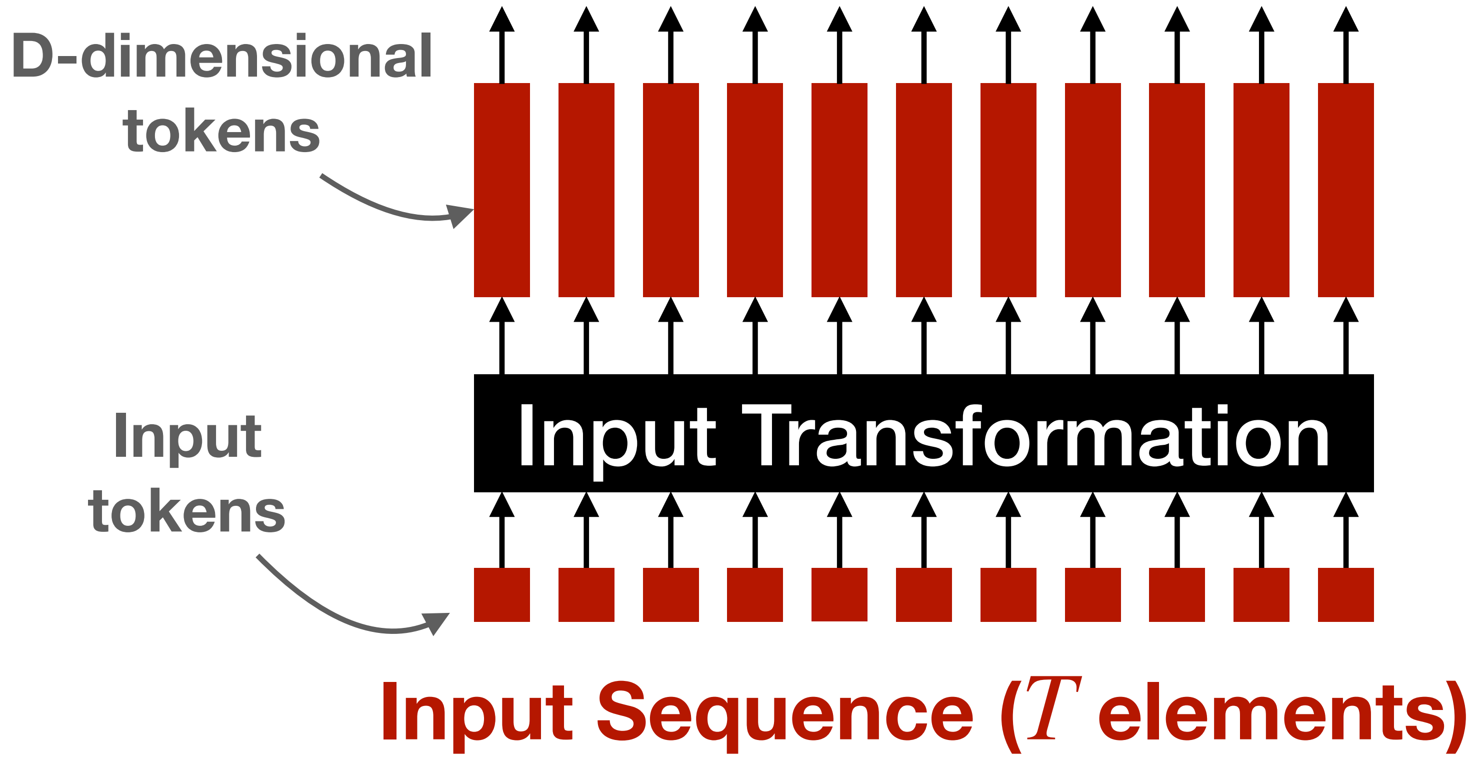
(using **self-attention**)

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**

Overview of 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



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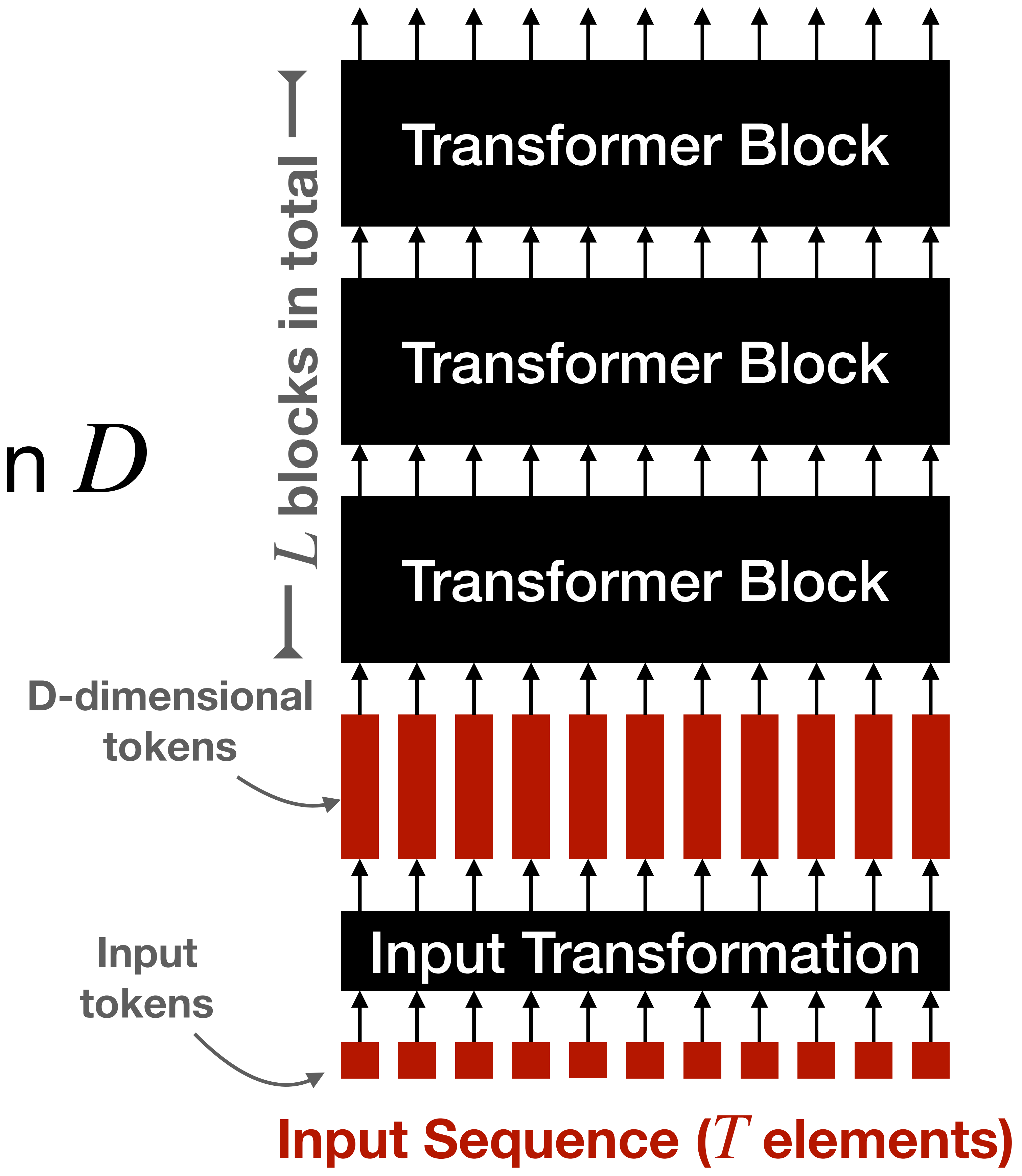
Transformer block: transforms a sequence of T vectors of dimension D into a new sequence of T vectors of dimension D using **self-attention** and **MLP sub-blocks**



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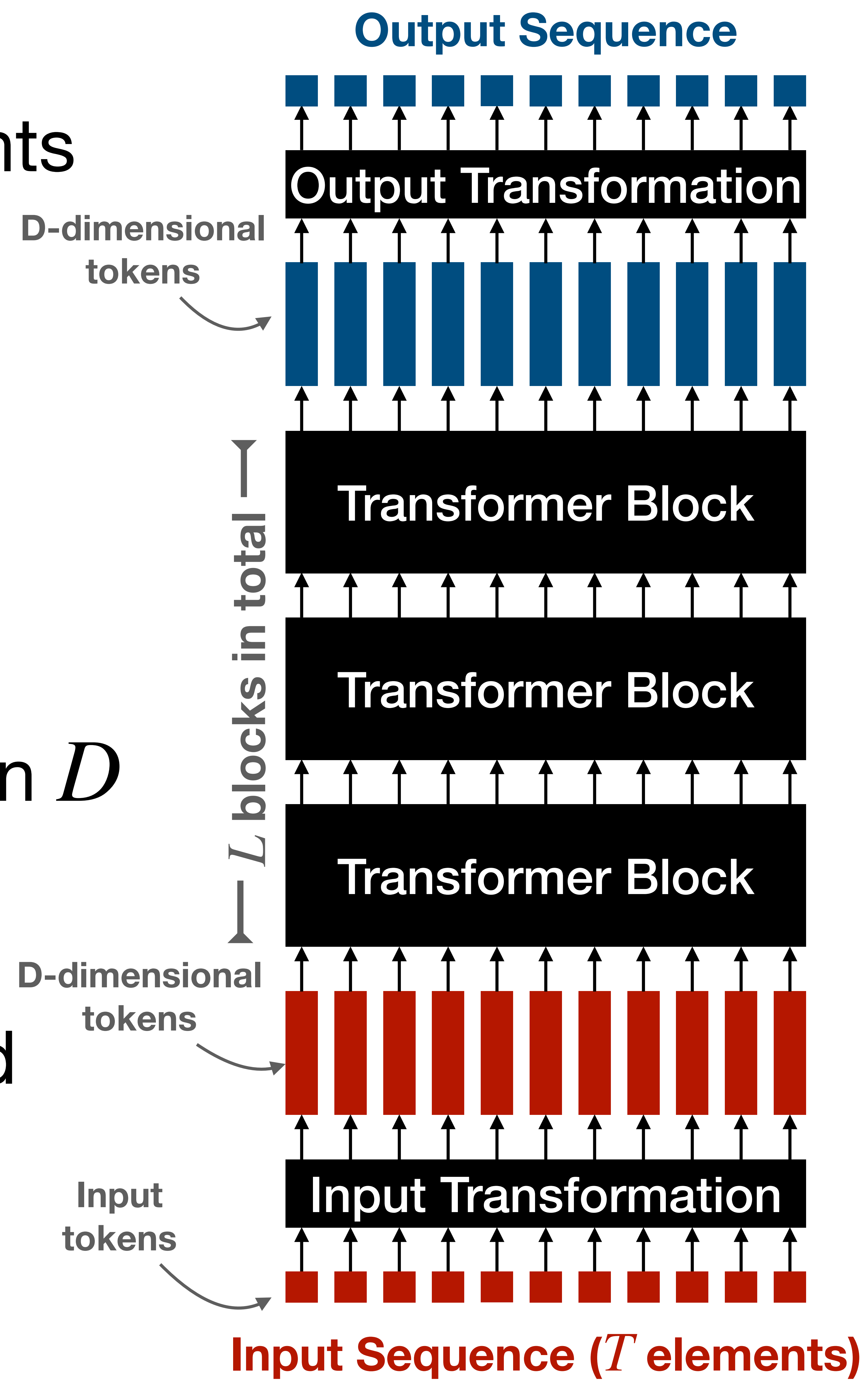
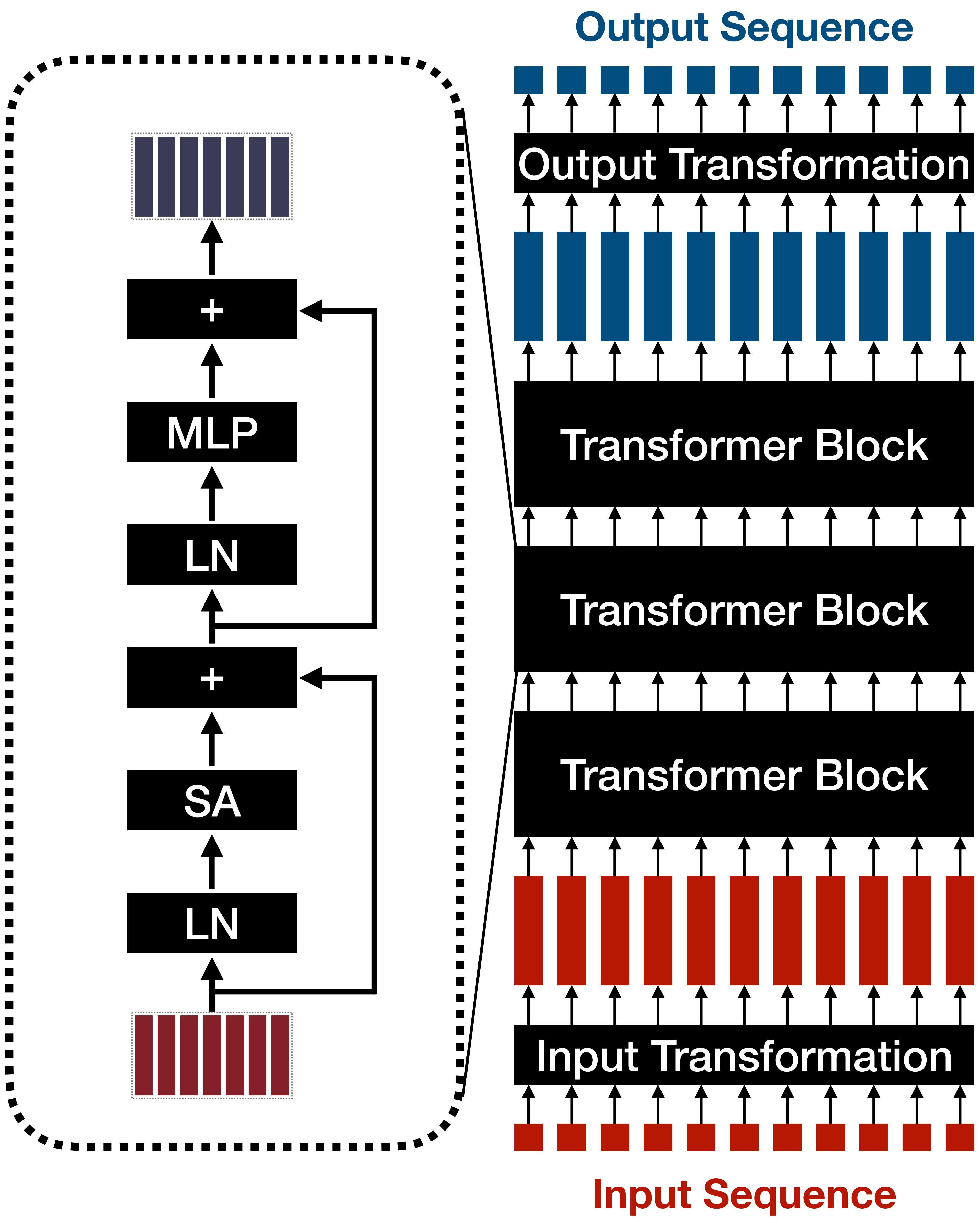
Output transformation: converts the vectors to the desired output format (e.g., single-element sequence for classification, multiple-element sequence of words)



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: maps each token ID $i \in \{1,\ldots,N_{vocab}\}$ into a real-valued vector $\mathbf{w}_i \in \mathbb{R}^D$:

- Token embeddings: $[\mathbf{w}_0, \mathbf{w}_{5124}, \mathbf{w}_{1029}, \mathbf{w}_{645}, \mathbf{w}_{3001}, \mathbf{w}_{6931}, \mathbf{w}_{7330}, \mathbf{w}_{10}]$

➡The whole input sequence of T tokens leads to an input matrix $X = \begin{bmatrix} \mathbf{w}_0 \\ \mathbf{w}_{5124} \\ \vdots \\ \mathbf{w}_{10} \end{bmatrix} \in \mathbb{R}^{T \times D}$

Notation: Throughout this lecture, all vectors will be treated as row vectors.

Text Token Embeddings - Learning

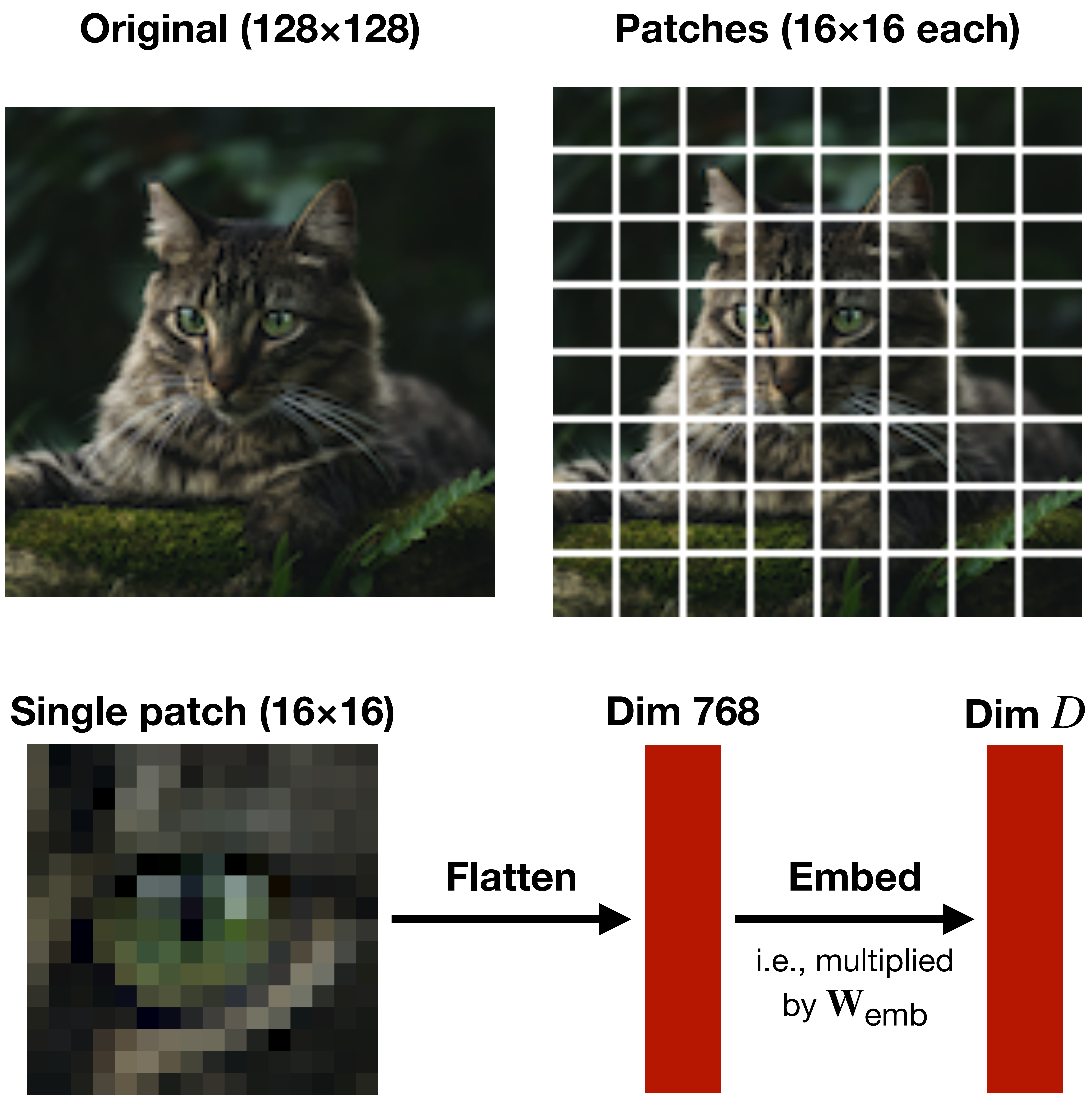
- The matrix $W_{\text{emb}} = \begin{bmatrix} \mathbf{w}_1 \\ \vdots \\ \mathbf{w}_{N_{vocab}} \end{bmatrix} \in \mathbb{R}^{N_{vocab} \times D}$ is learned via backpropagation, along with all other transformer parameters
- This can be seen as a matrix multiplication:

$$X = \begin{bmatrix} \mathbf{e}_{i_1} \\ \vdots \\ \mathbf{e}_{i_T} \end{bmatrix} W_{\text{emb}} \quad (\text{since } \mathbf{e}_i W_{\text{emb}} = (W_{\text{emb}})_{i,:} = \mathbf{w}_i)$$

- The tokenizer procedure is typically fixed in advance and not learned

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 $W_{\text{emb}} \in \mathbb{R}^{768 \times D}$ which is shared for all inputs
- Learn W_{emb} through backpropagation, along with all other transformer parameters
- The whole input sequence of T embedded patches leads to an input matrix $X \in \mathbb{R}^{T \times D}$



Self-attention

What is Self-attention?

$$A : tokens \rightarrow tokens$$

(using a **weighted average**)

Reminder: a token is simply a real-valued vector

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

Self-Attention

Define K, Q, V from the **same** input sequence $X \in \mathbb{R}^{T \times D}$

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

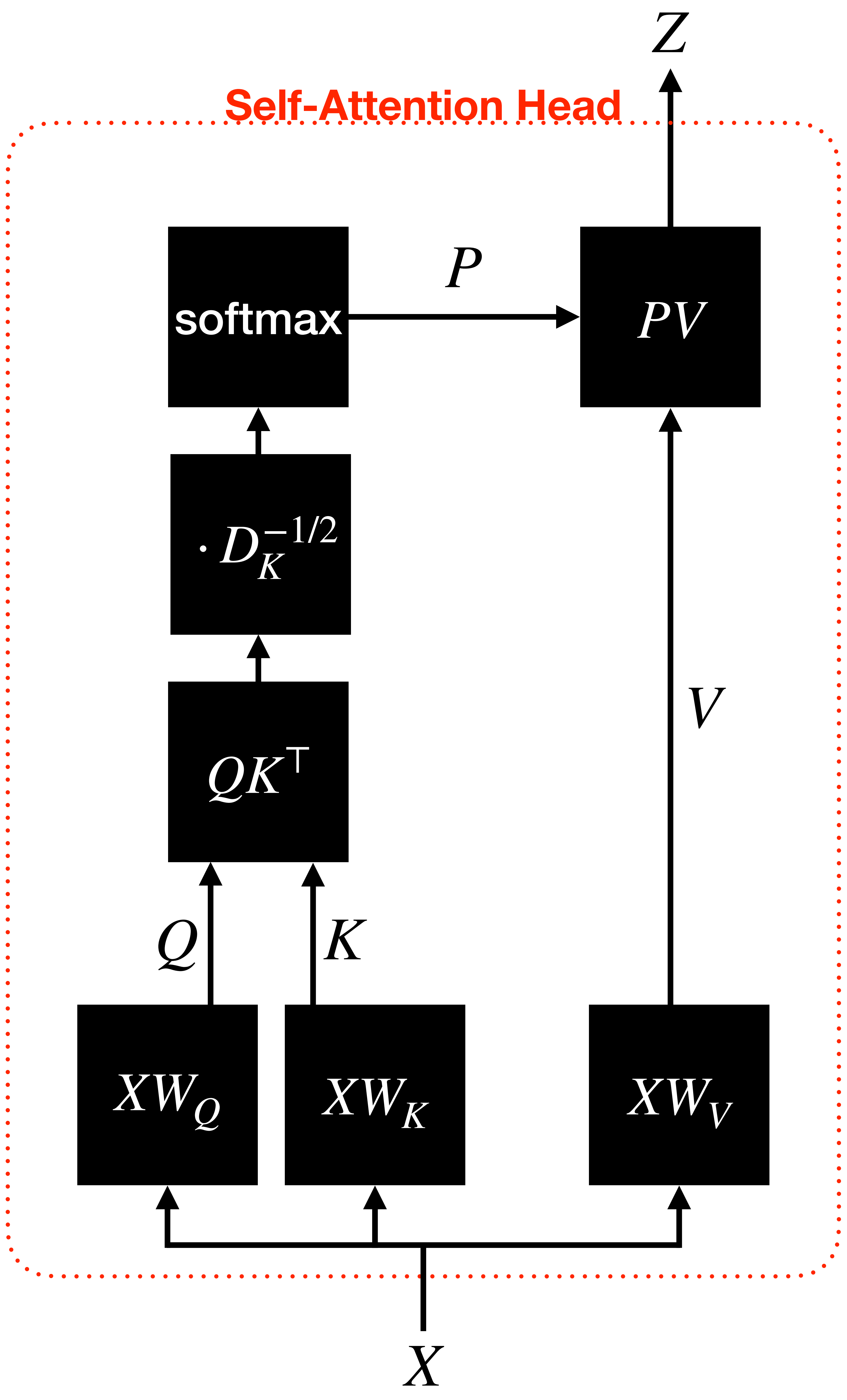
➡ $W_K, W_Q \in \mathbb{R}^{D \times D_K}$, $W_V \in \mathbb{R}^{D \times D_V}$ are parameters

The output of self-attention is then given by:

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

➡ $\text{softmax}(\,\cdot\,)$ is applied row-wise

➡ Quadratic computational complexity $O(T^2)$



Attention as a Weighted Average

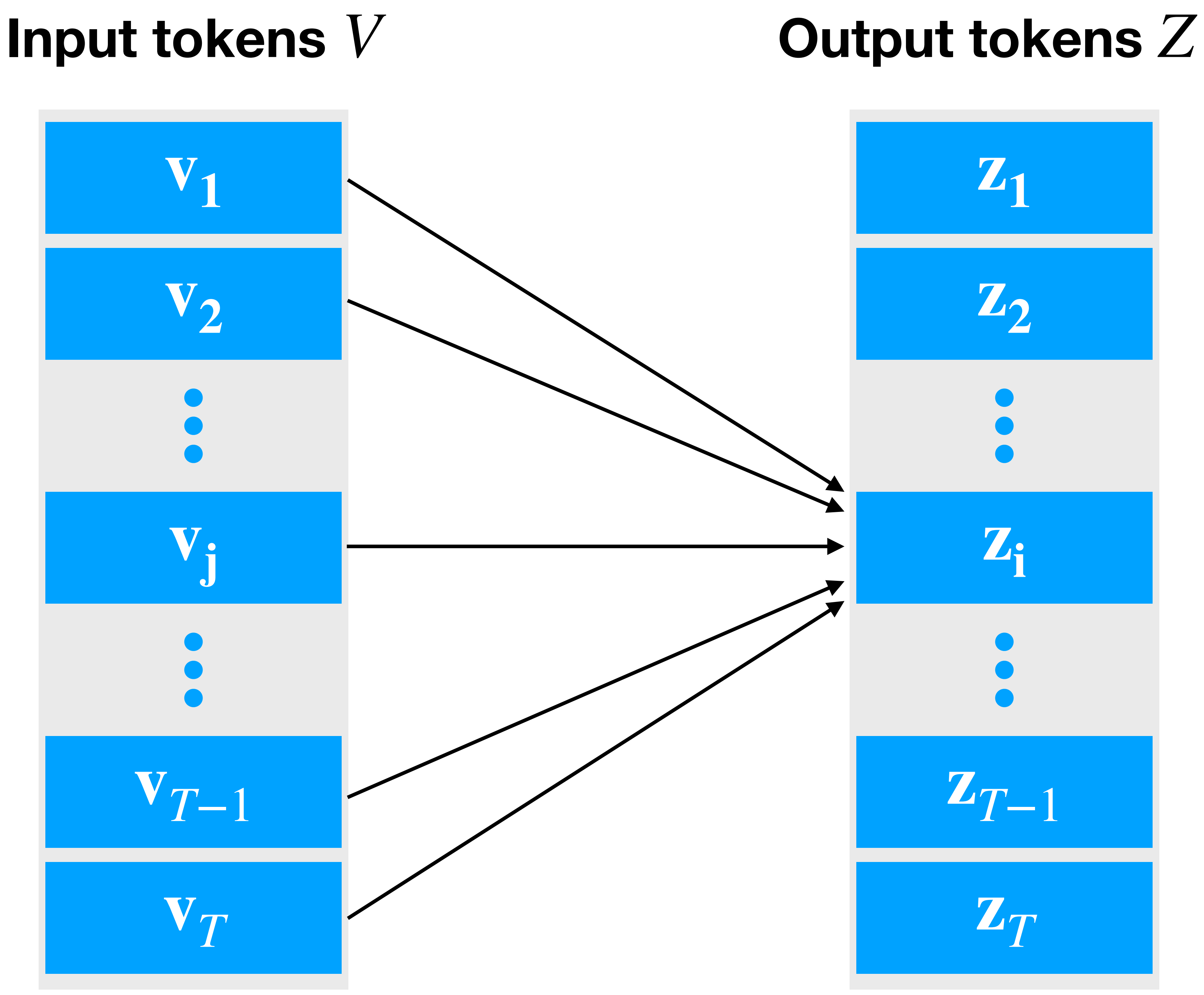
Notation: throughout this lecture, the j-th **rows** of V and Z are denoted by $\mathbf{v}_j$ and $\mathbf{z}_j$

- T **input and output tokens**: $V \in \mathbb{R}^{T \times D_V}, Z \in \mathbb{R}^{T \times D_V}$
- Outputs are a **weighted average** of the inputs:

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

- Weighting coefficients $P \in [0,1]^{T \times T}$ form valid probability distributions over the input tokens:

➡ $\sum_{j=1}^{T} p_{i,j} = 1$ (i.e., each row sums to one)



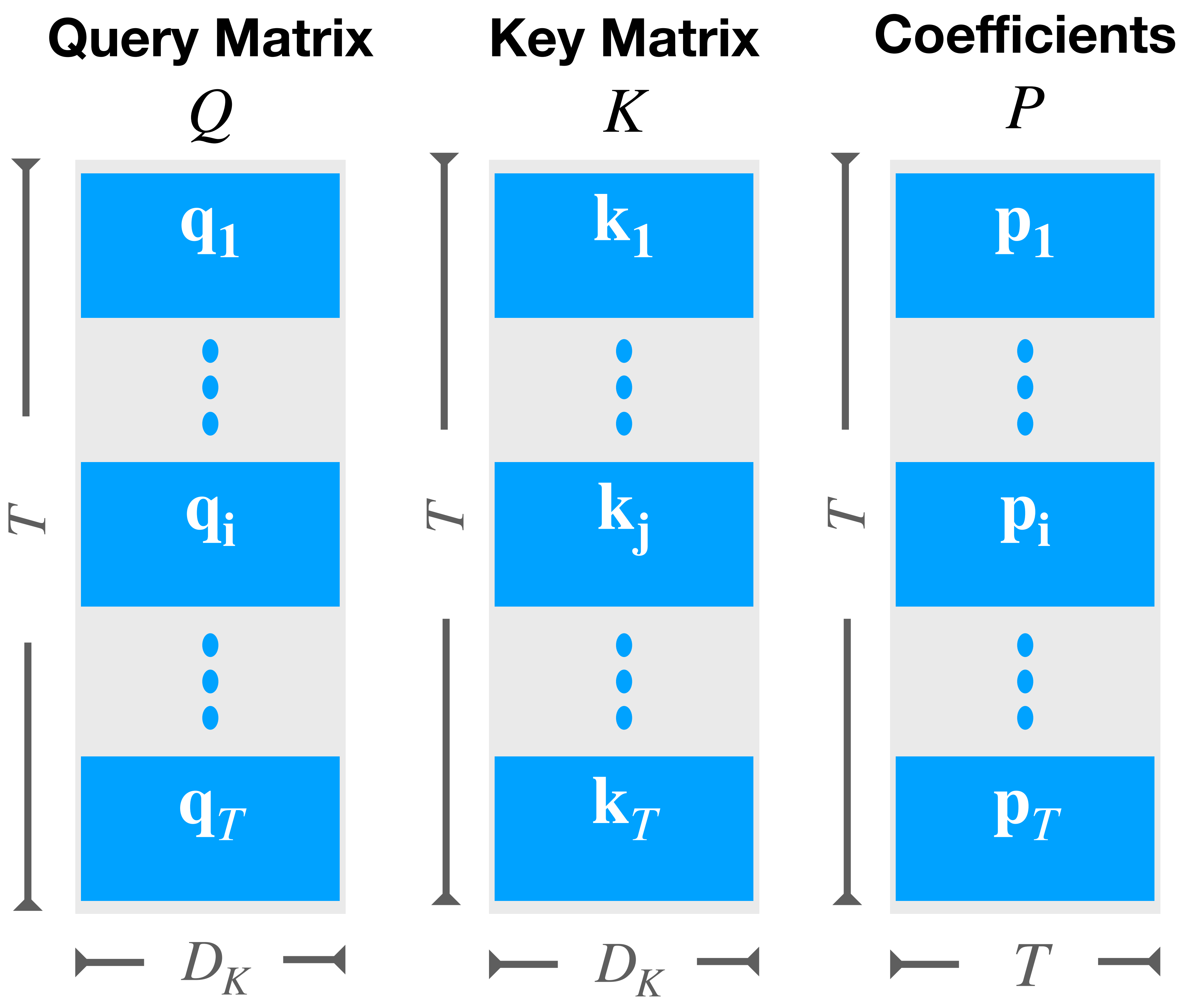
The Weighting Coefficients P

- **Query tokens** $Q \in \mathbb{R}^{T \times D_K}$ (one query per output token)
- **Key tokens** $K \in \mathbb{R}^{T \times D_K}$ (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 the temperature by $\sqrt{D_K}$) to obtain a probability distribution
- This can be expressed as:

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

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

The softmax is applied on each row *independently*



Computation complexity:

$$O(T \times T)$$

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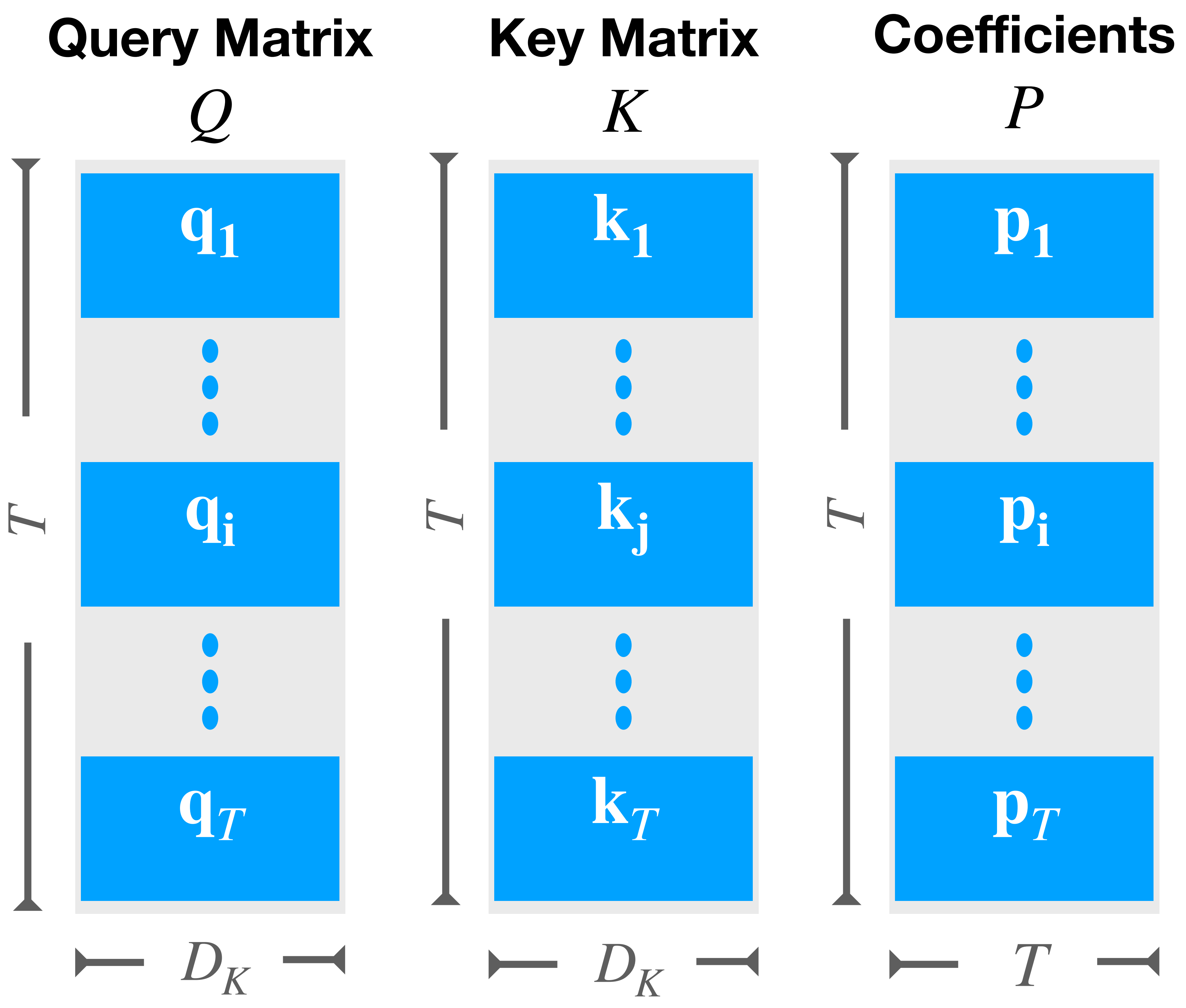


In some applications, **causal masking** is used:

Sum until position i: $p_{i,j} = \dfrac{\exp\left(\mathbf{q}_i \mathbf{k}_j^\top / \sqrt{D_K}\right)}{\sum_{t=1}^{i} \exp\left(\mathbf{q}_i \mathbf{k}_t^\top / \sqrt{D_K}\right)}$ for $j \leq i$ and $p_{i,j} = 0$ otherwise

Mask before softmax: $P = \text{softmax}\left(M + \dfrac{QK^\top}{\sqrt{D_K}}\right)$

where $M \in \mathbb{R}^{T \times T}$ is the matrix $M_{ij} = -\infty$ for $j > i$ and $M_{i,j} = 0$ otherwise

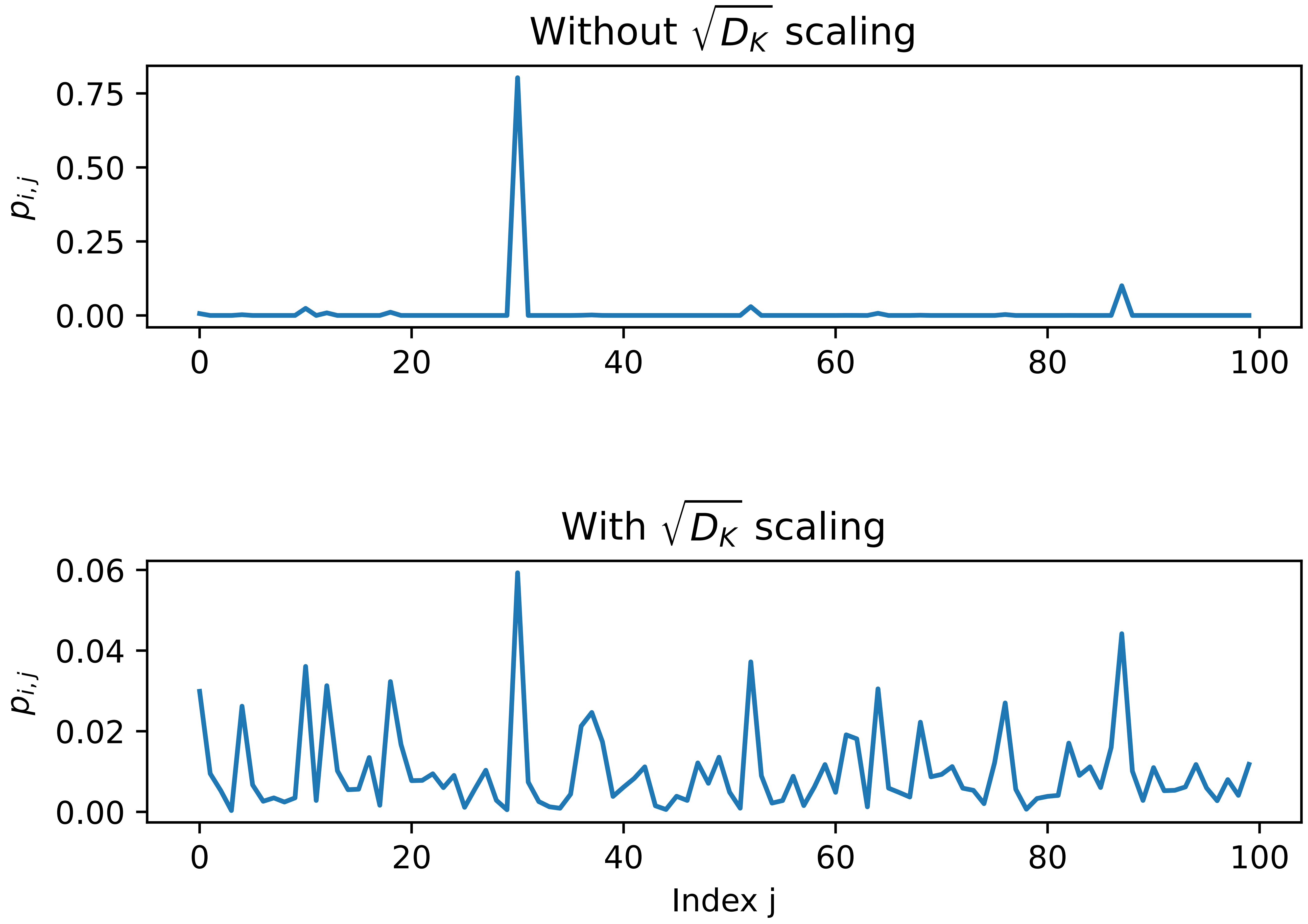
Computation complexity:

$O(T \times T)$

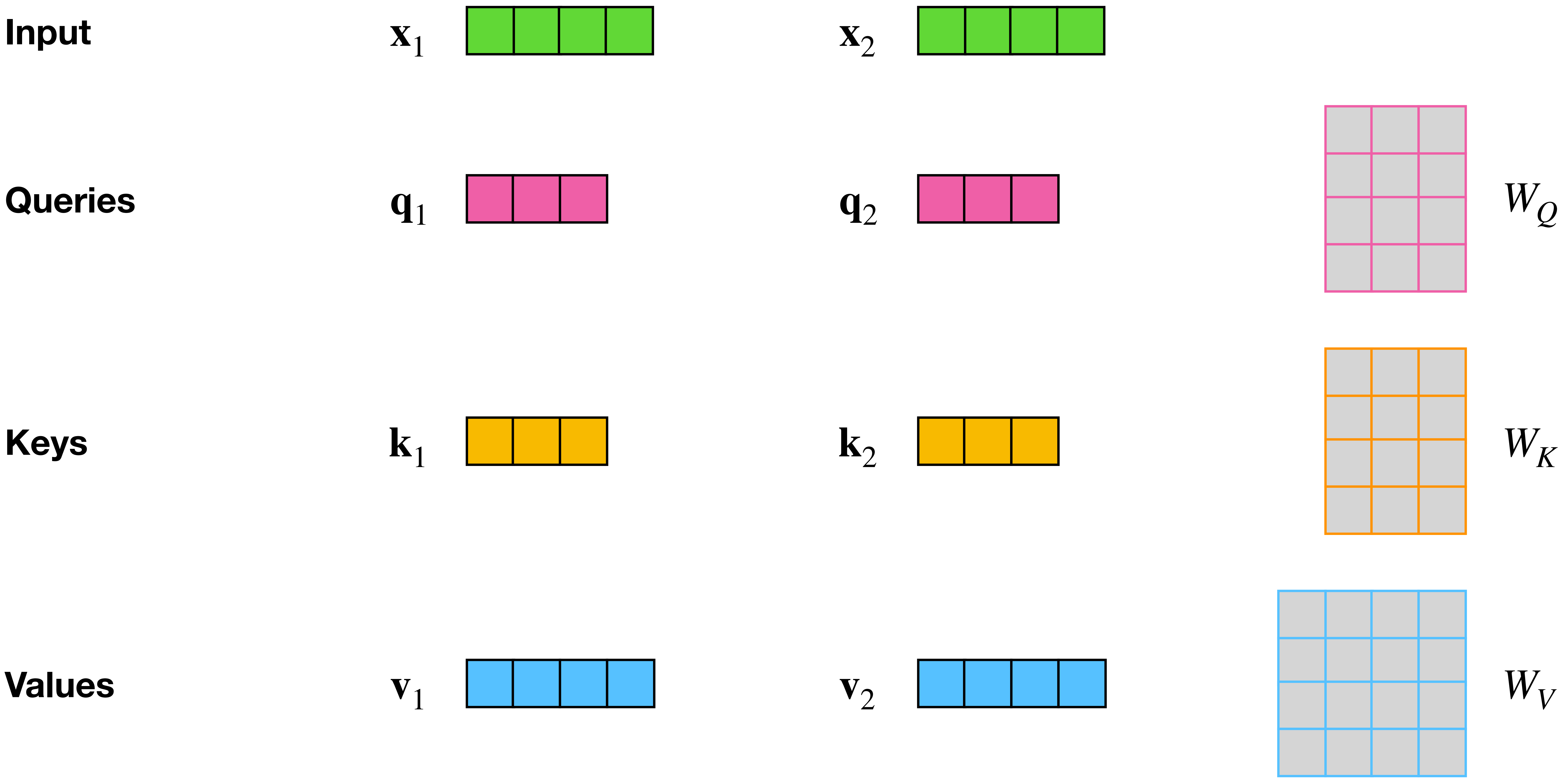
Why Use the $1/\sqrt{D_K}$ Scaling?

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

- **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: Step-by-Step

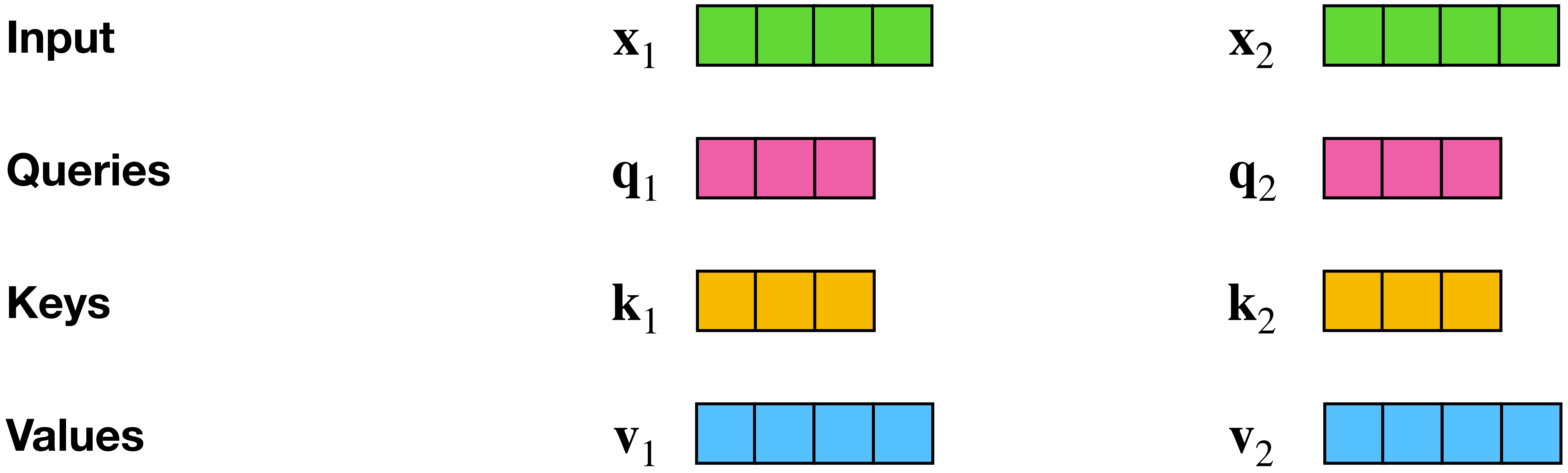


$$\boxed{\begin{aligned} Q &= XW_Q \\ K &= XW_K \\ V &= XW_V \end{aligned}}$$

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

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

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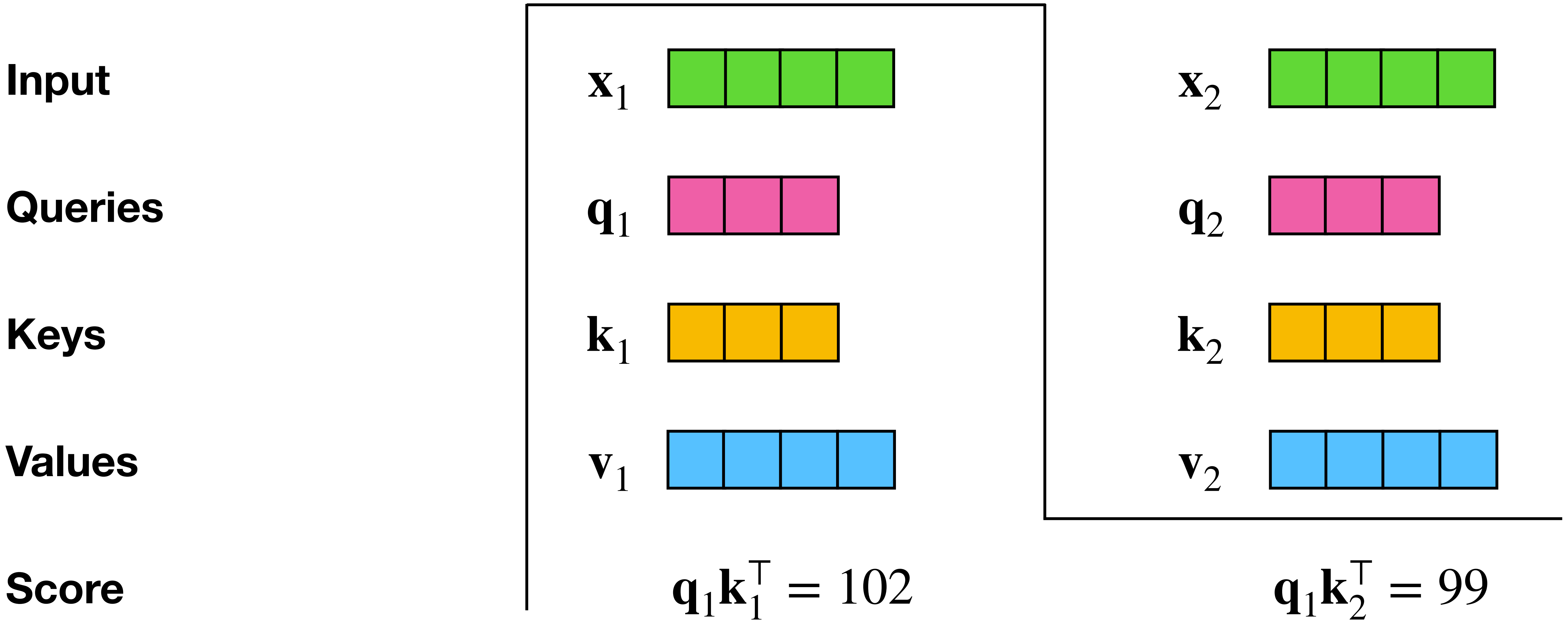
Self-Attention: Step-by-Step



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	$\mathbf{x}_1$	$\mathbf{x}_2$
Queries	$\mathbf{q}_1$	$\mathbf{q}_2$
Keys	$\mathbf{k}_1$	$\mathbf{k}_2$
Values	$\mathbf{v}_1$	$\mathbf{v}_2$
Score	$\mathbf{q}_1\mathbf{k}_1^\top = 102$	$\mathbf{q}_1\mathbf{k}_2^\top = 99$
Divide by $\sqrt{D_K}$	$\frac{\mathbf{q}_1\mathbf{k}_1^\top}{\sqrt{D_K}} = 58.9$	$\frac{\mathbf{q}_1\mathbf{k}_2^\top}{\sqrt{D_K}} = 57.2$
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

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Softmax	$p_{1,1} = 0.85$	$p_{1,2} = 0.15$
Softmax*Value	$p_{1,1}\mathbf{v}_1$	$p_{1,2}\mathbf{v}_2$
Sum	$\mathbf{z}_1$	$\mathbf{z}_2$

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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Sum	$\mathbf{z}_1$	$\mathbf{z}_2$

$$\boxed{Z = \text{softmax}\left(\frac{XW_QW_K^\top X^\top}{\sqrt{D_K}}\right)XW_V}$$

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:

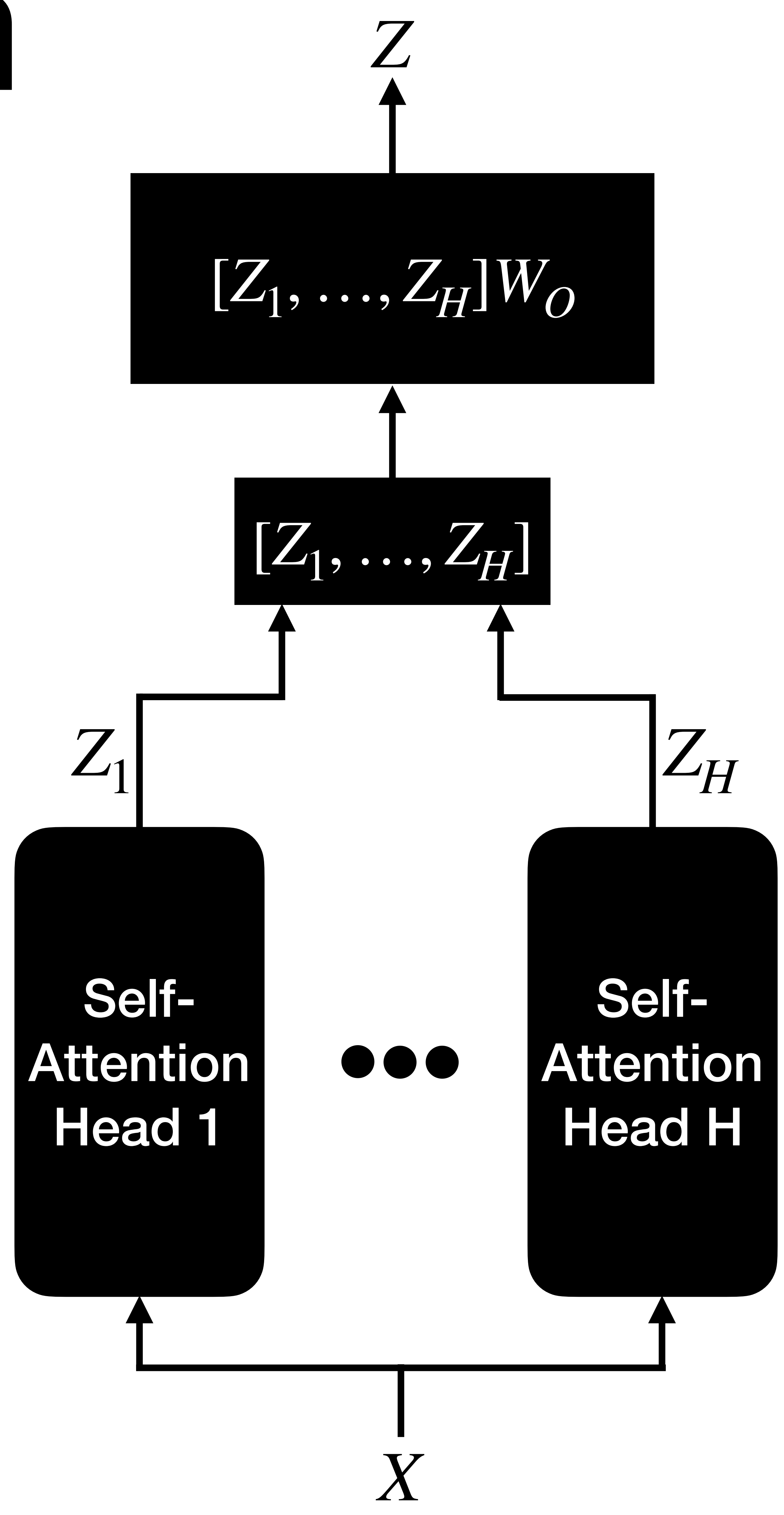
$$Z_h = \text{softmax}\left(\frac{XW_{Q,h}W_{K,h}^\top X^\top}{\sqrt{D_K}}\right)XW_{V,h}$$

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

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

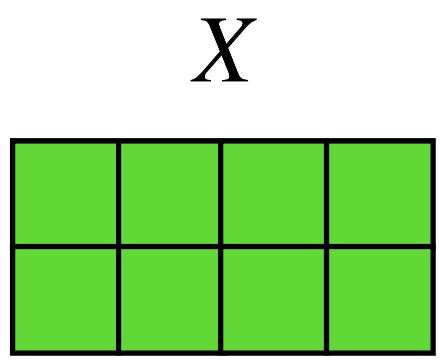
$$Z = [Z_1, \ldots, Z_H]W_O$$

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

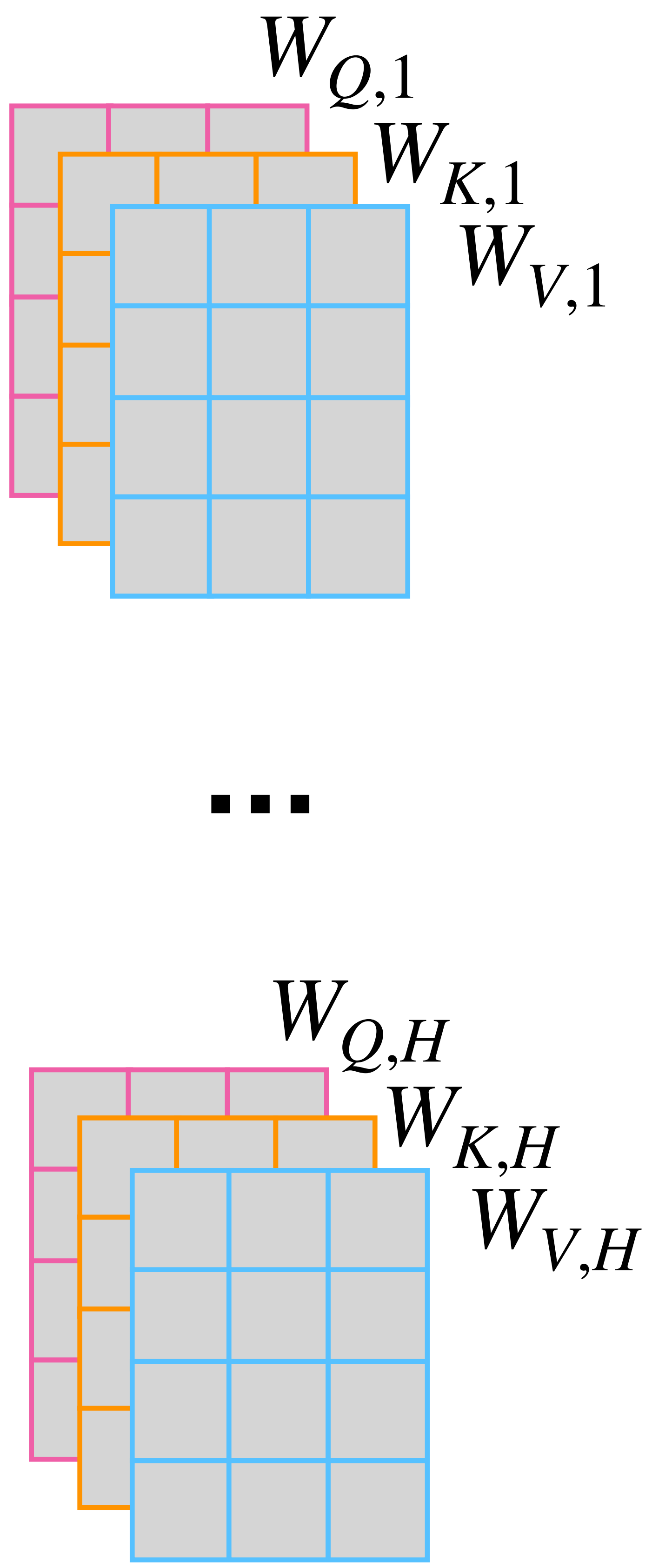


Multi-Head Self-Attention: recap

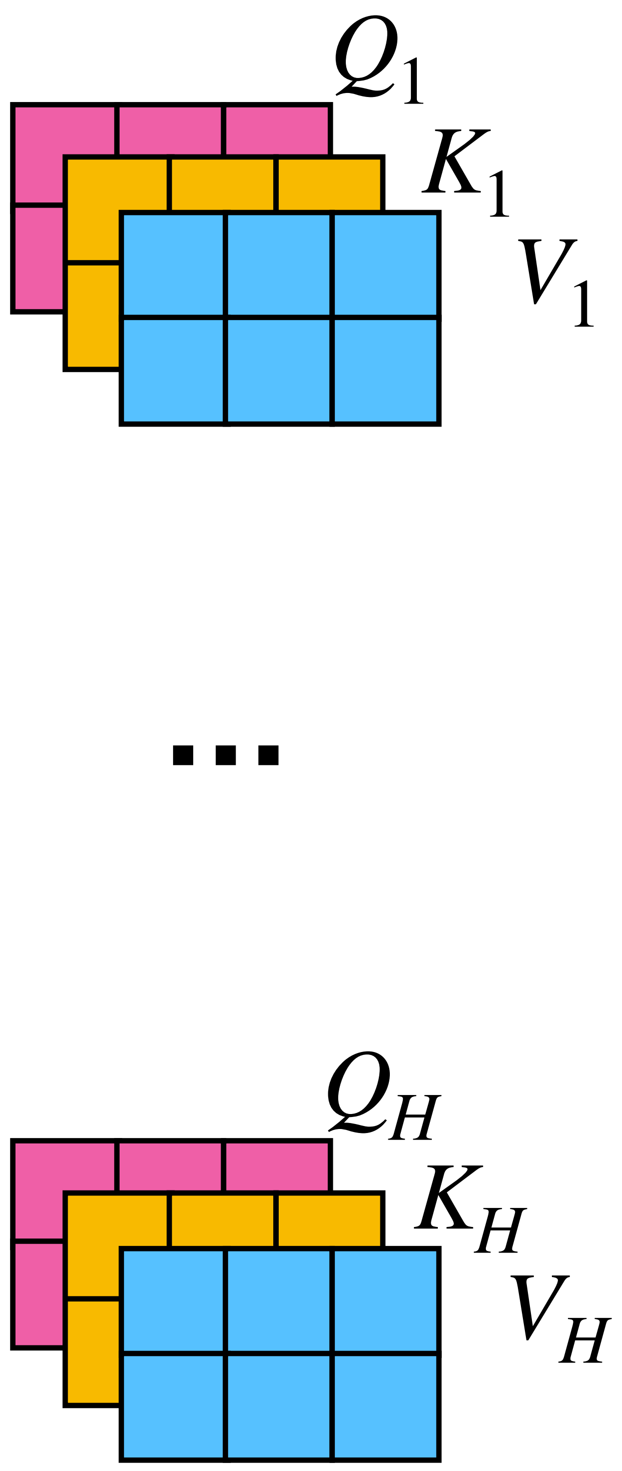
1) Input



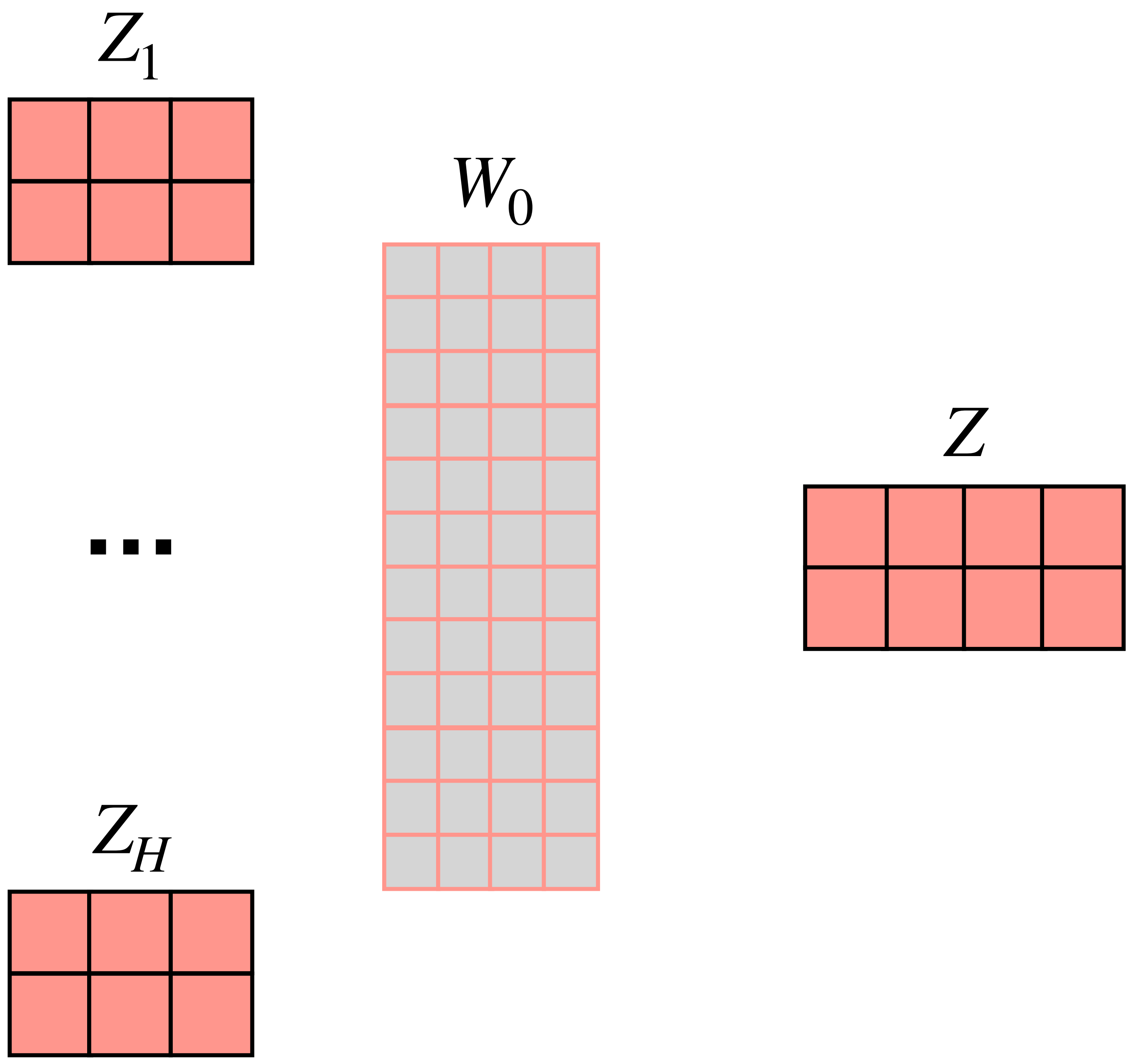
2) Split into H heads
We multiply X by weight matrices



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

Attention does not account for the order of input

For a permutation matrix $R \in \{0,1\}^{T \times T}$ we have:

$$Z_R = \text{softmax}\left(\frac{RXW_Q W_K^\top X^\top R^\top}{\sqrt{D_K}}\right) RXW_V$$

Permute every X in original formula

$$= R\text{softmax}\left(\frac{XW_Q W_K^\top X^\top R^\top}{\sqrt{D_K}}\right) RXW_V$$

Since softmax is computed row-wise

$$= R\text{softmax}\left(\frac{XW_Q W_K^\top X^\top}{\sqrt{D_K}}\right) R^\top RXW_V$$

Reordering the terms in the softmax sum does not affect the output

$$= RPR^{-1}RXW_V$$

For a permutation matrix: transpose=inverse

$$= RPXW_V$$

Which is equivalent to a permutation of the original output $Z = PV$

Positional Information in Transformers

- **In practice, the input order matters:**
  "She prefers cats to dogs" $\neq$ ***"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 : $\{1,\ldots,T\} \to \mathbb{R}^D$

- **The most basic choice** is to add a positional embedding W_{pos} corresponding to each token's position t to the input embedding. $W_{\text{pos}} \in \mathbb{R}^{T\times D}$ is learned via backpropagation along with the other parameters:

$$X = \begin{bmatrix} \mathbf{e}_{i_1} \\ \vdots \\ \mathbf{e}_{i_T} \end{bmatrix} W_{\text{emb}} + \begin{bmatrix} \mathbf{e}_1 \\ \vdots \\ \mathbf{e}_T \end{bmatrix} W_{\text{pos}}$$

- Numerous hand-crafted positional encodings exist (active area of research!)

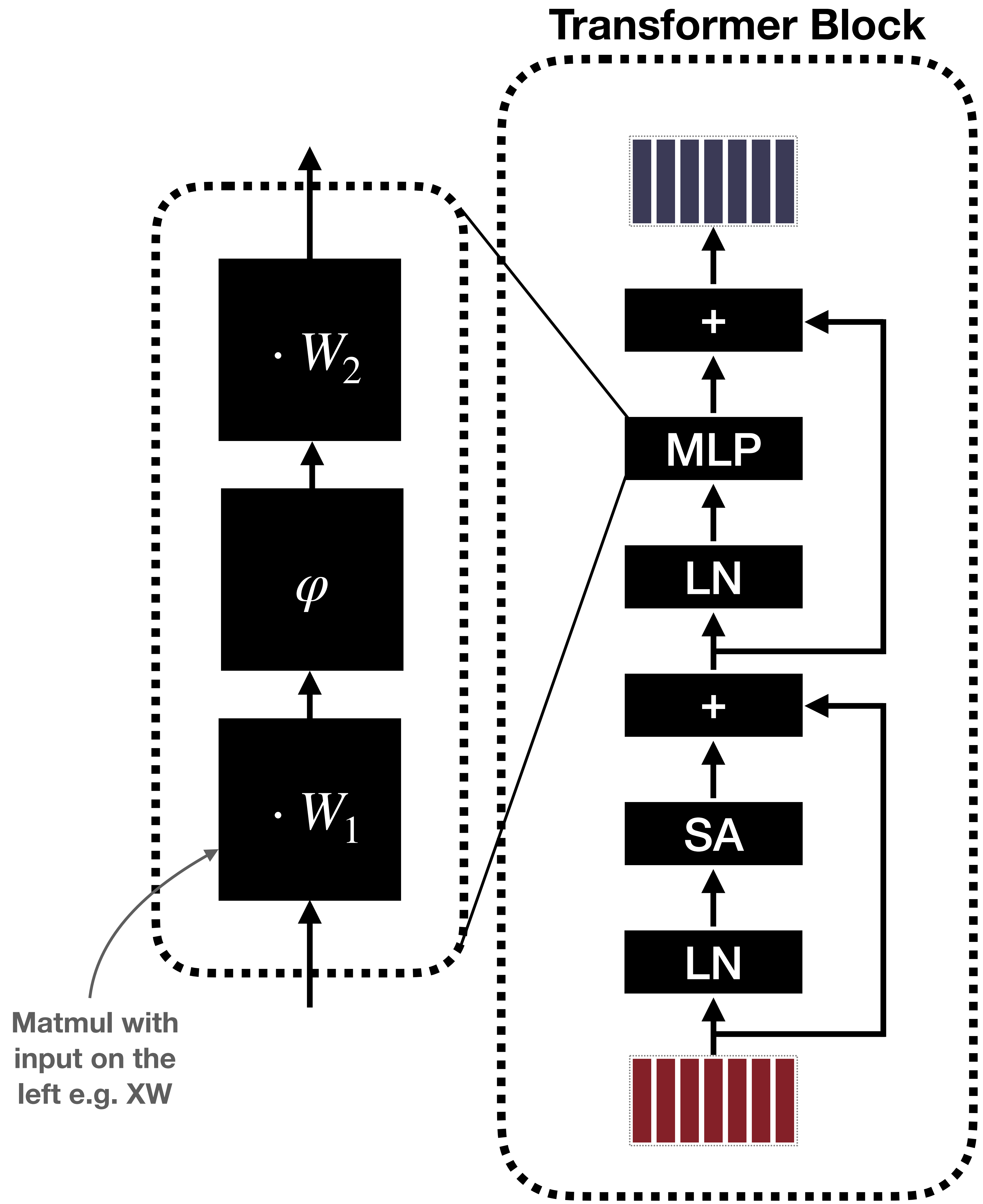
MLP

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



Mixing Information within Tokens

- **MLP** mixes information within each token

The same MLP is applied to each token:

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

$$\iff$$

$$MLP(\mathbf{x}_t) = \varphi(\mathbf{x}_t W_1)W_2, \text{ for each token } \mathbf{x}_1, \ldots, \mathbf{x}_T$$

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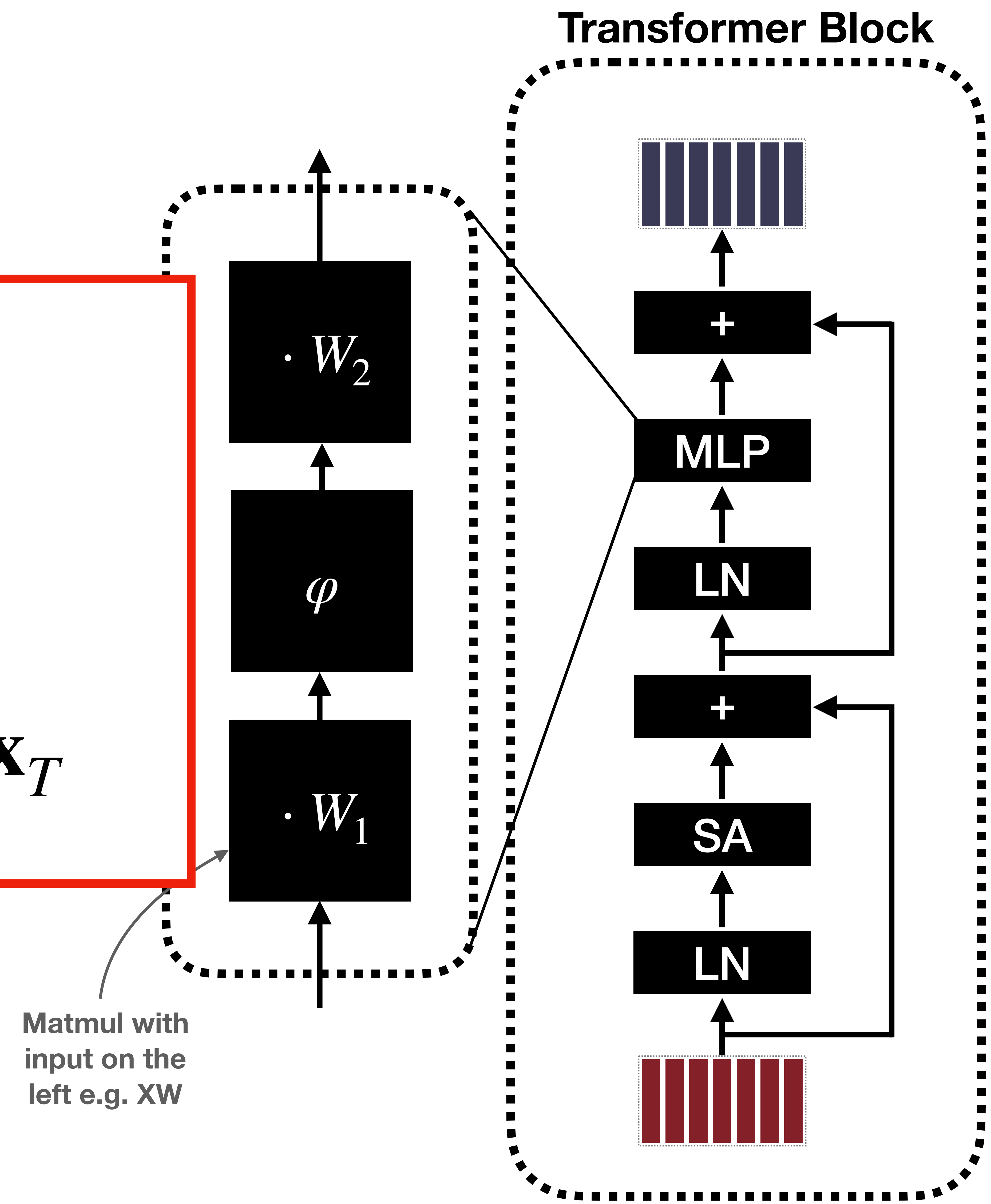
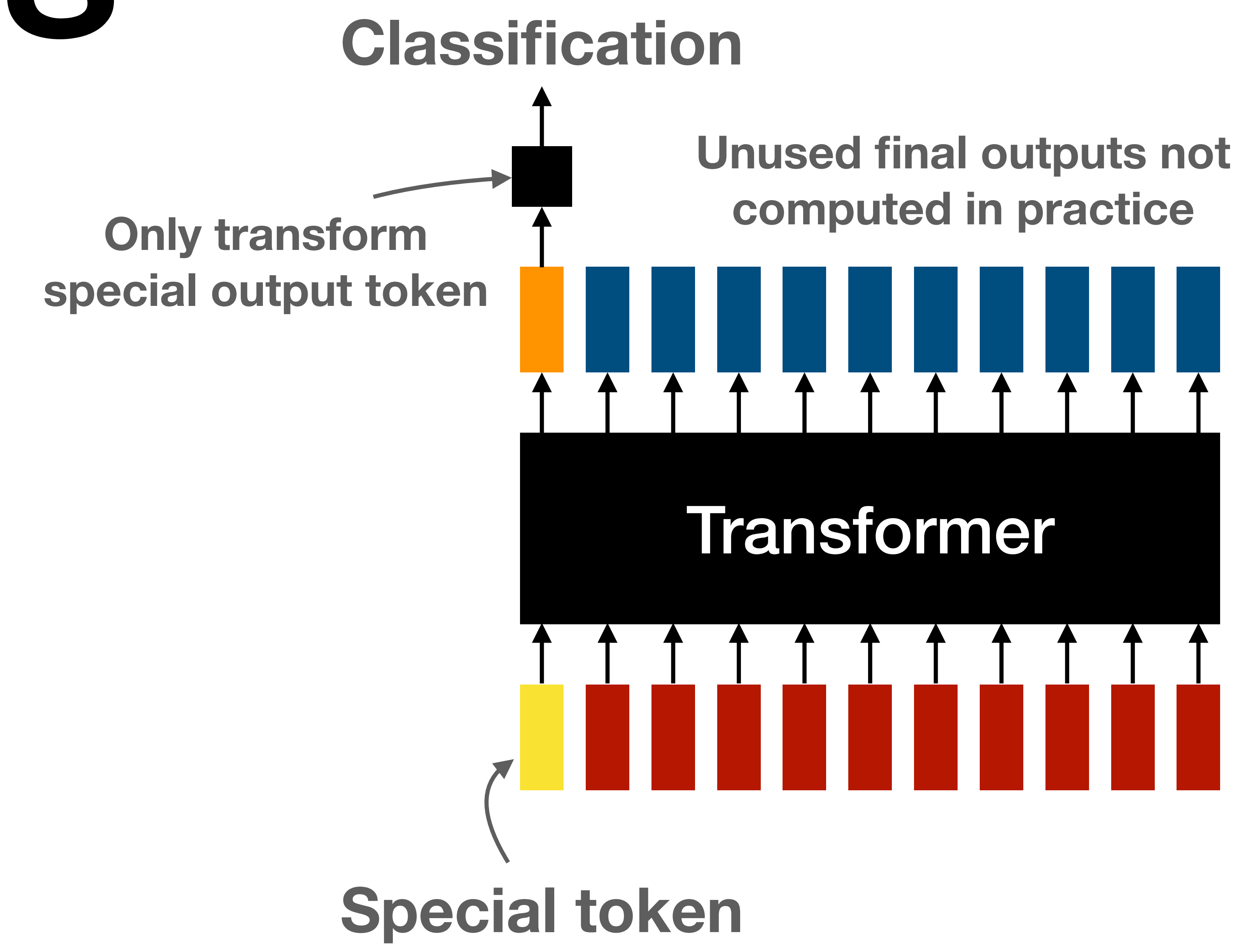
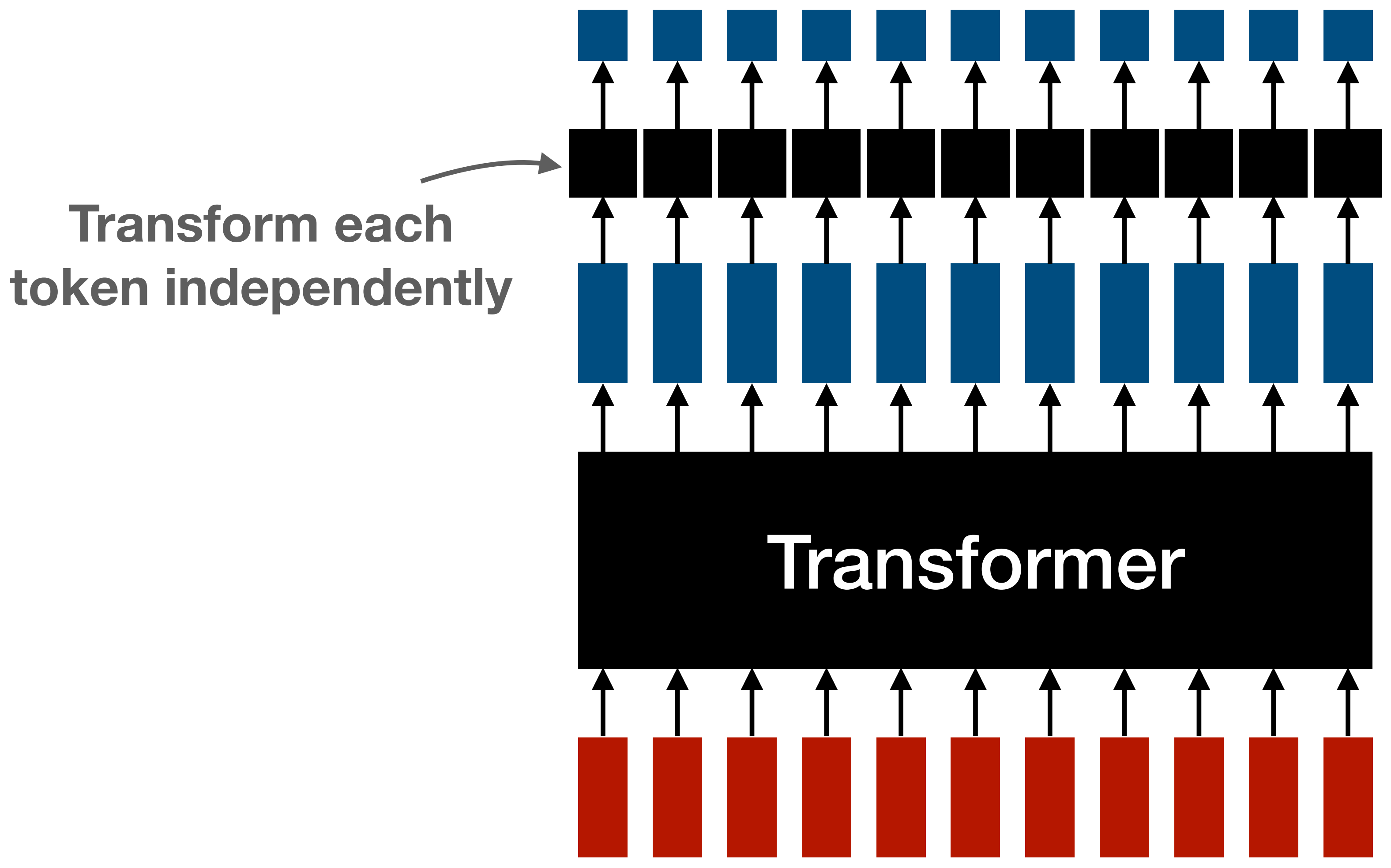


Output Transformations

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

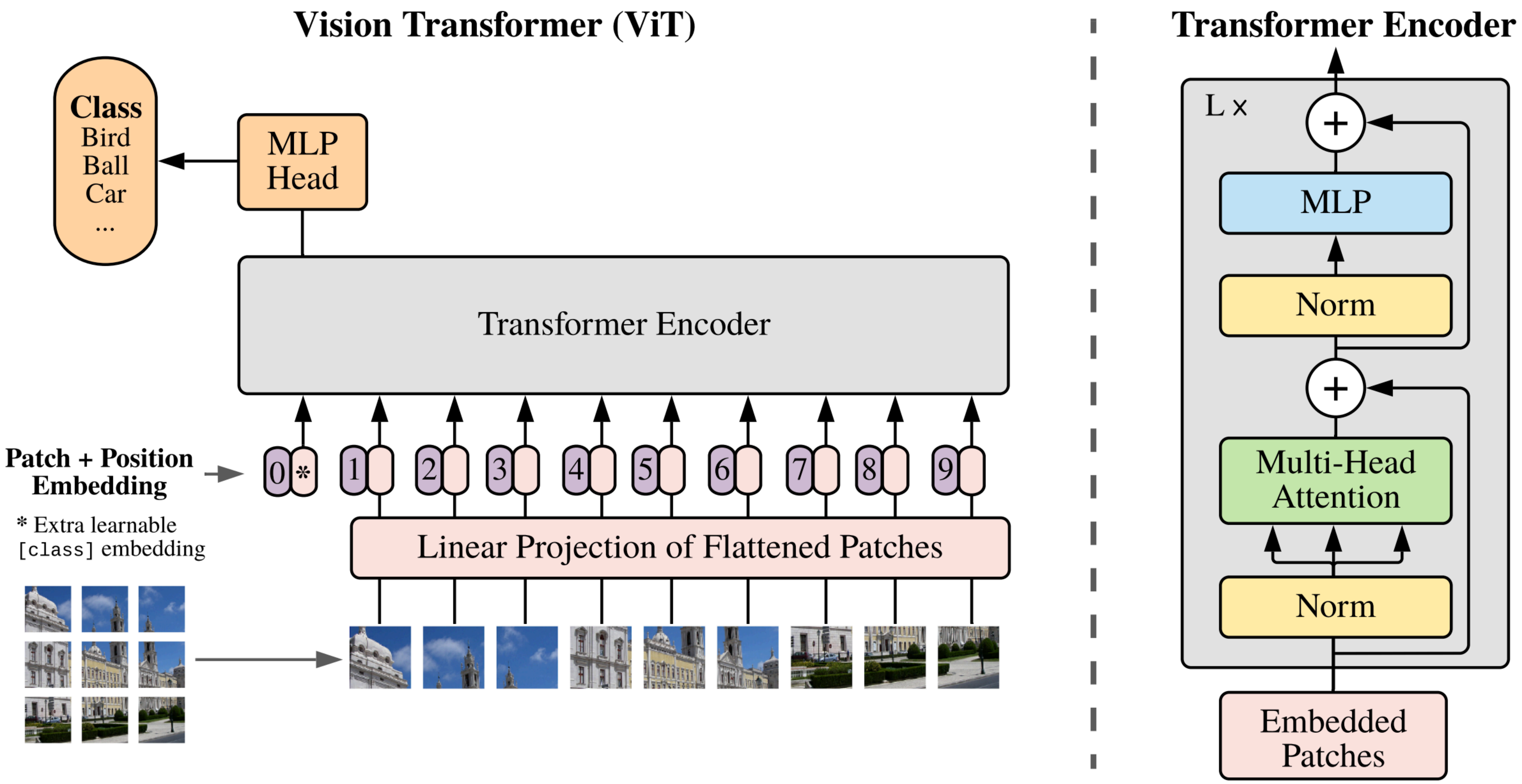




Putting the pieces together: Vision Transformers

Vision Transformer Architecture

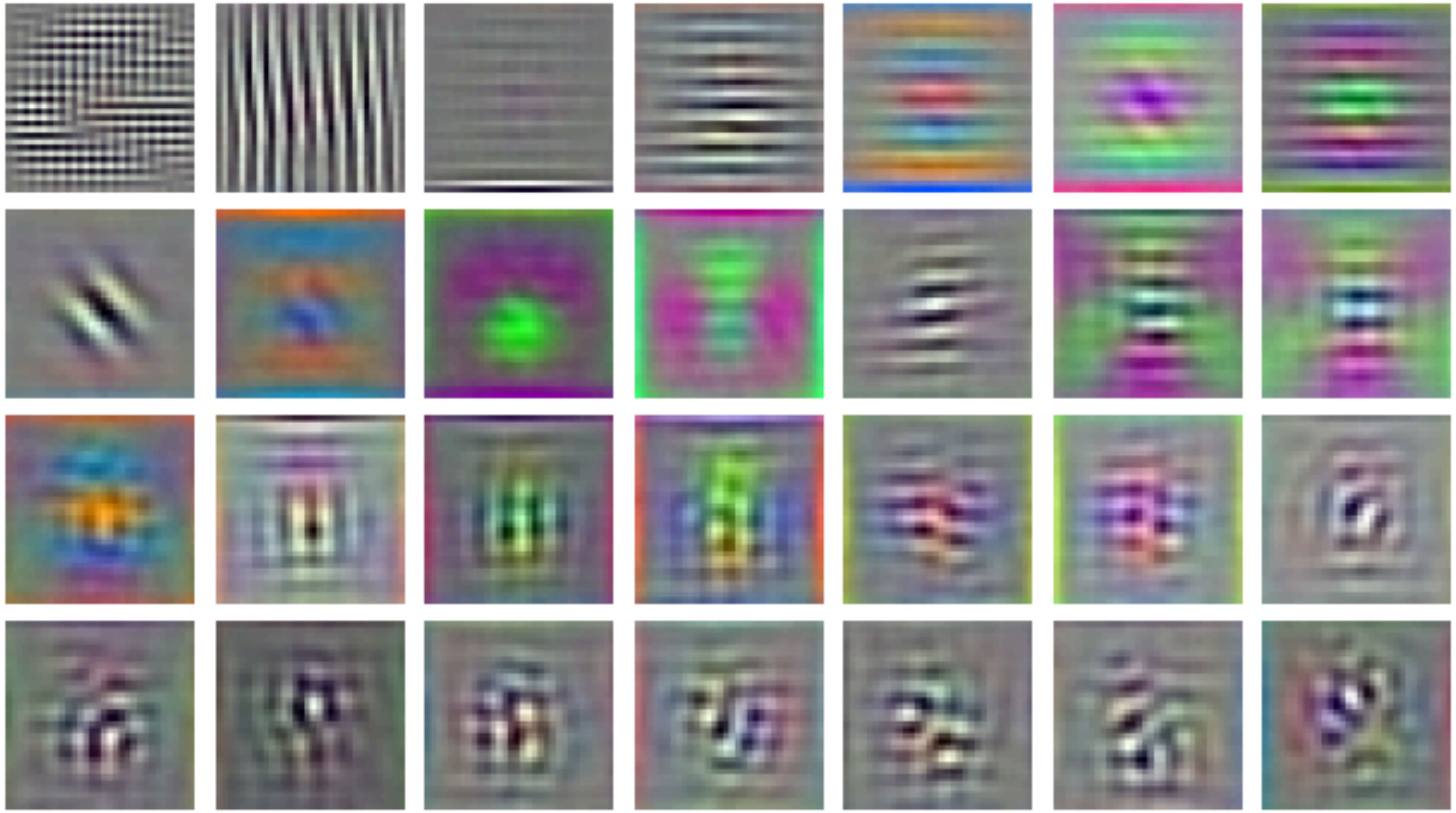
- **Simple architecture**: number of features D is constant across all layers. There is no use of padding, pooling, or strides.
- Self-attention is **more general** than convolution and can express it
- The receptive field is the **whole image** after just one self-attention layer
- ViTs require more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



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

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

What do ViTs learn: embedding layer



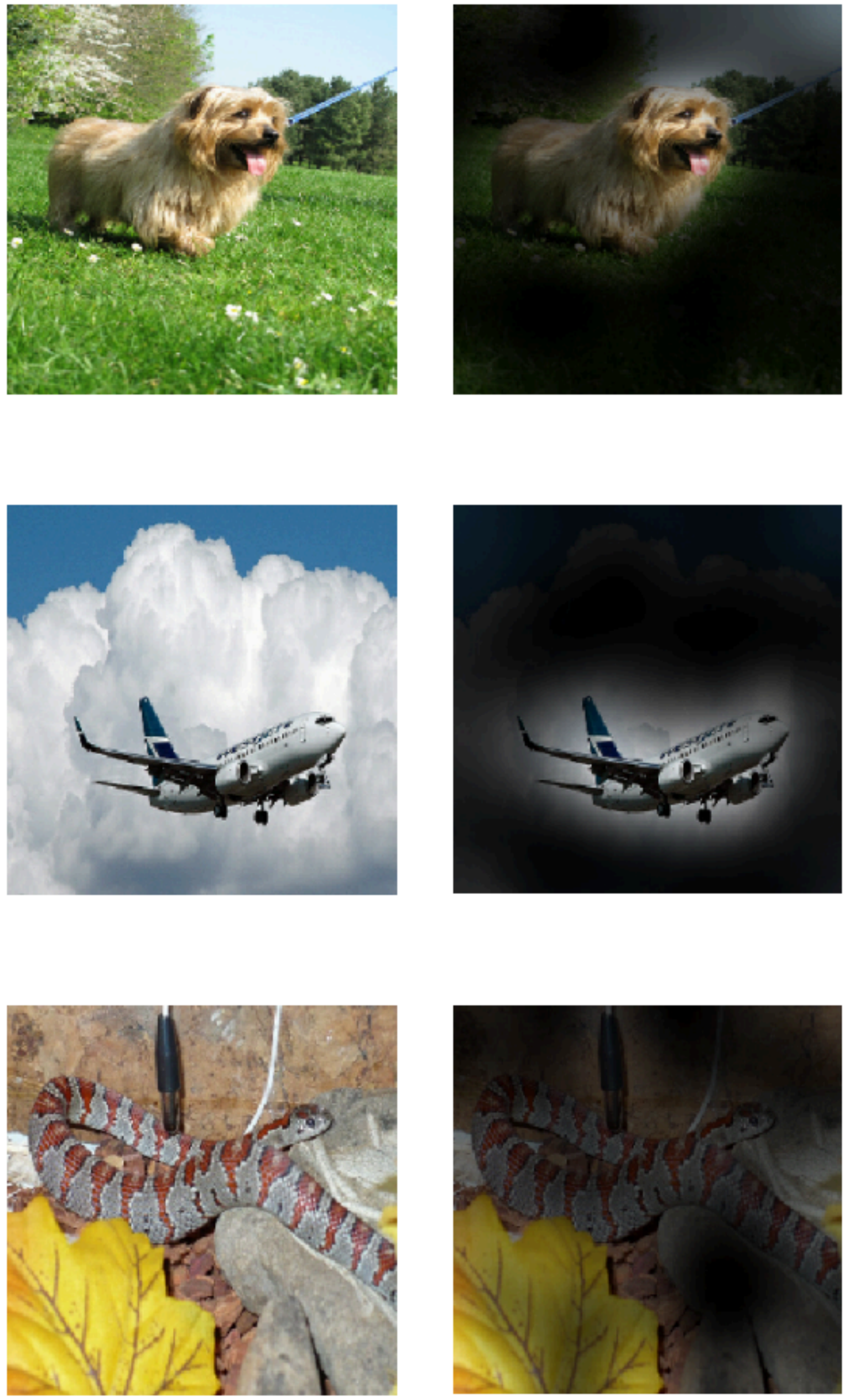
The first 28 principal components of the embedding layer applied on patches

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

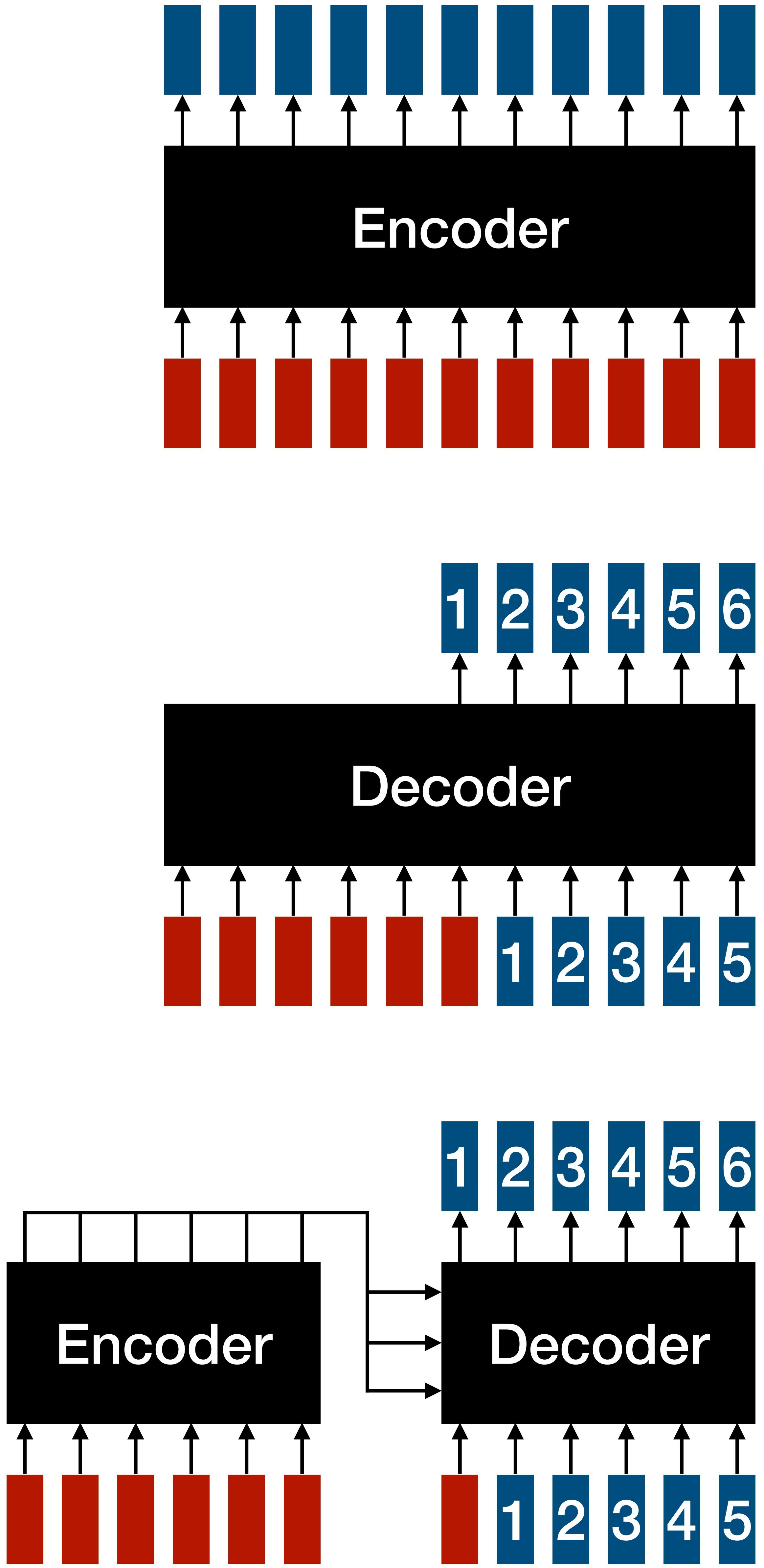


Source: An Image is Worth 16x16 Words: Transformers for Image Recognition at Scale (ICLR 2020)

The Big Picture and Takeaways

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 $\mathbf{x}_{t+1} \sim \mathit{softmax}(f(\mathbf{x}_1, \ldots, \mathbf{x}_t))$ 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 sequence 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)