Transformers

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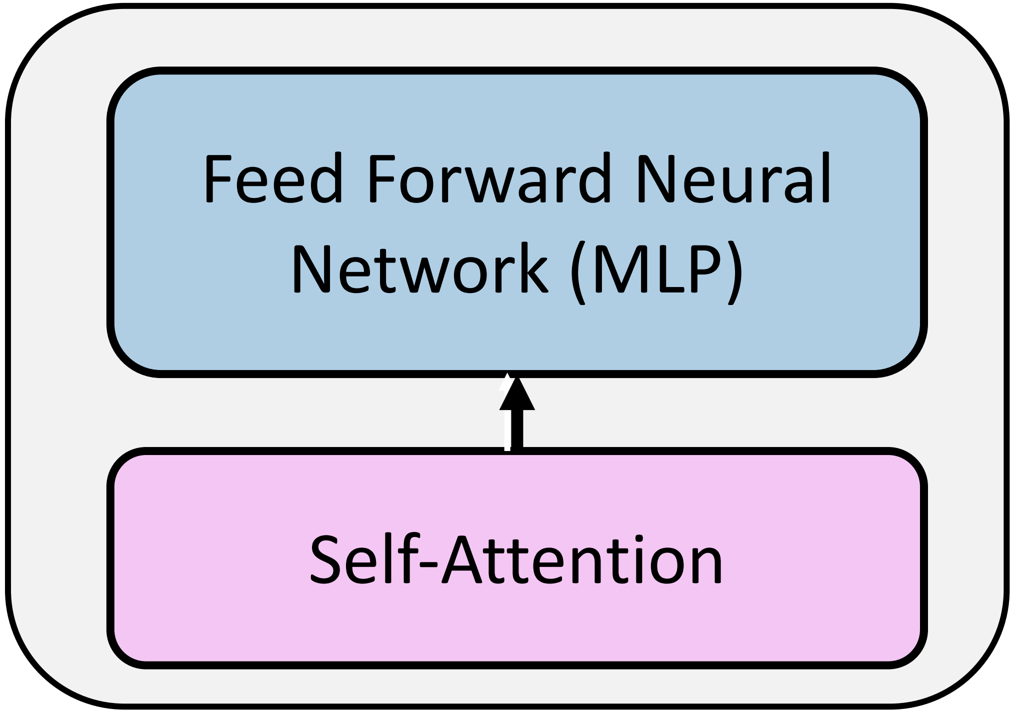
Transformer Encoder/Decoder Unit Details

Operations: Linear, Layer Norm, Activation, Tensor Multiply/Add, Softmax



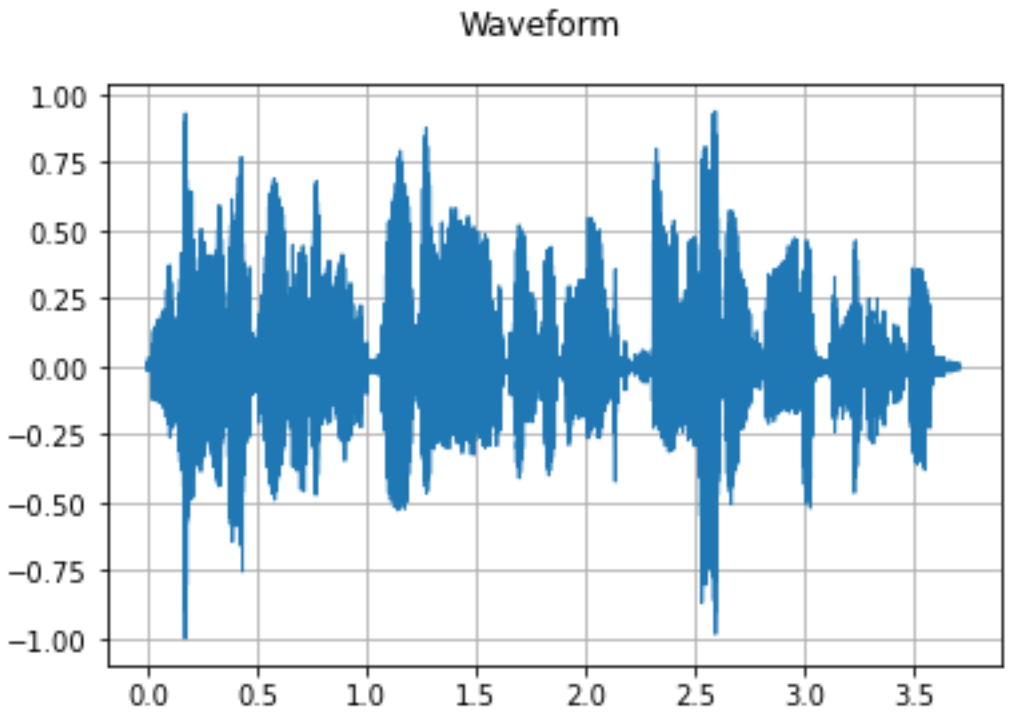
Encoder Block

Types of data that transformers can process

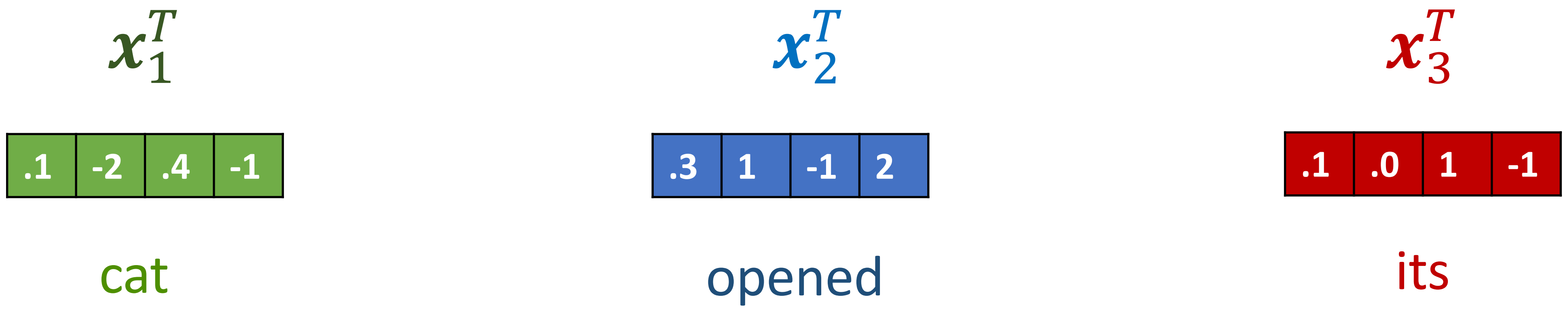
Any

Wikipedia
The Free Encyclopedia

COCO 2017 Keypoint Detection Task

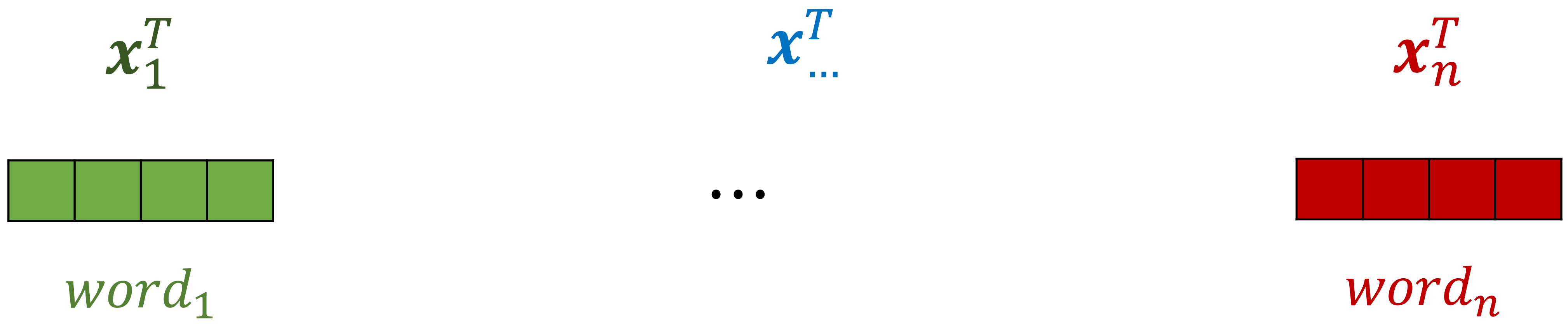


Input Embedding is an $n - dim$ vector



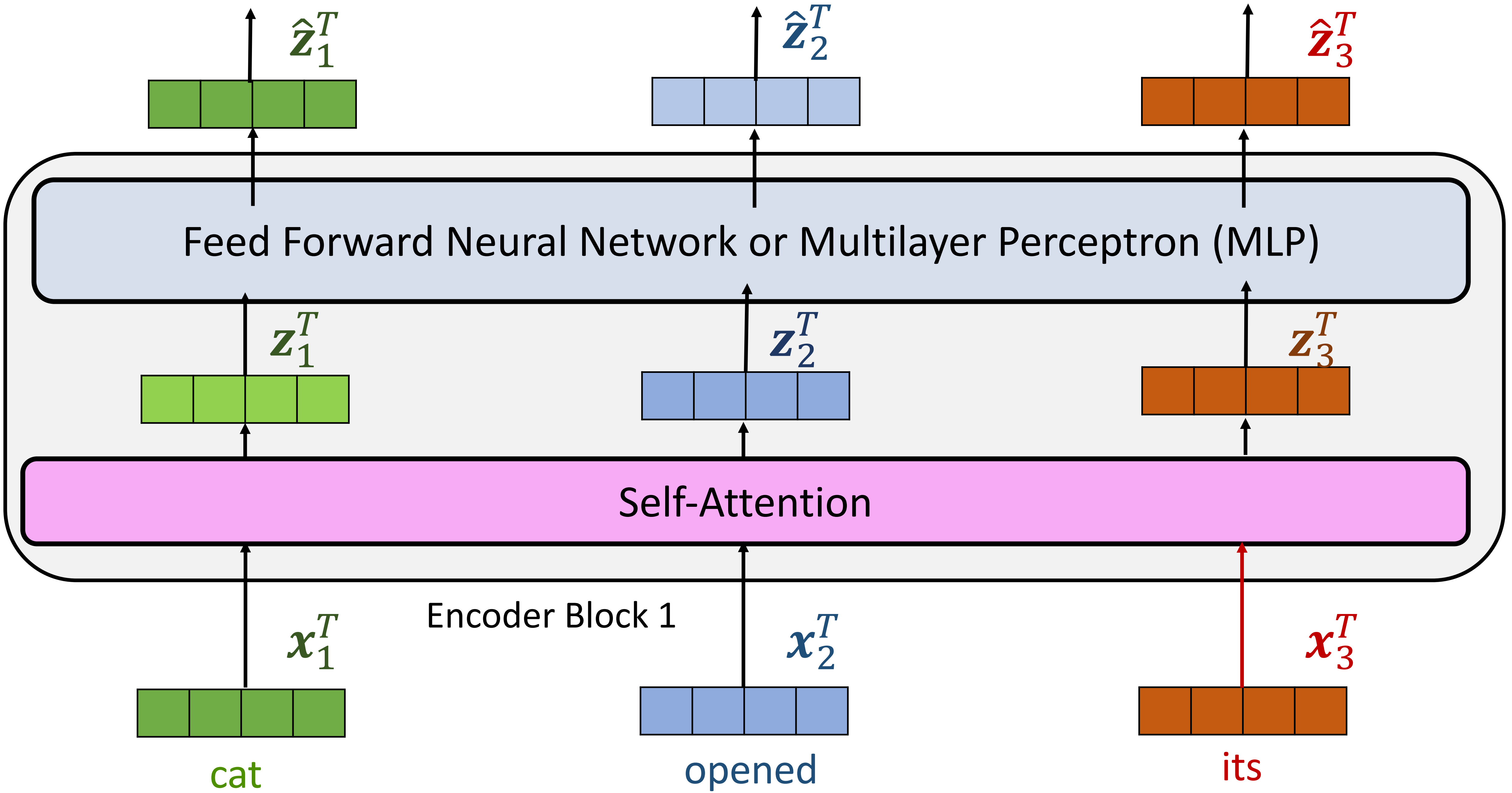
Example: Each word is converted into a 512-dim embedding vector.
In the simple example above, it is 4-dim.

The Length of the Input is $\boldsymbol{n}$

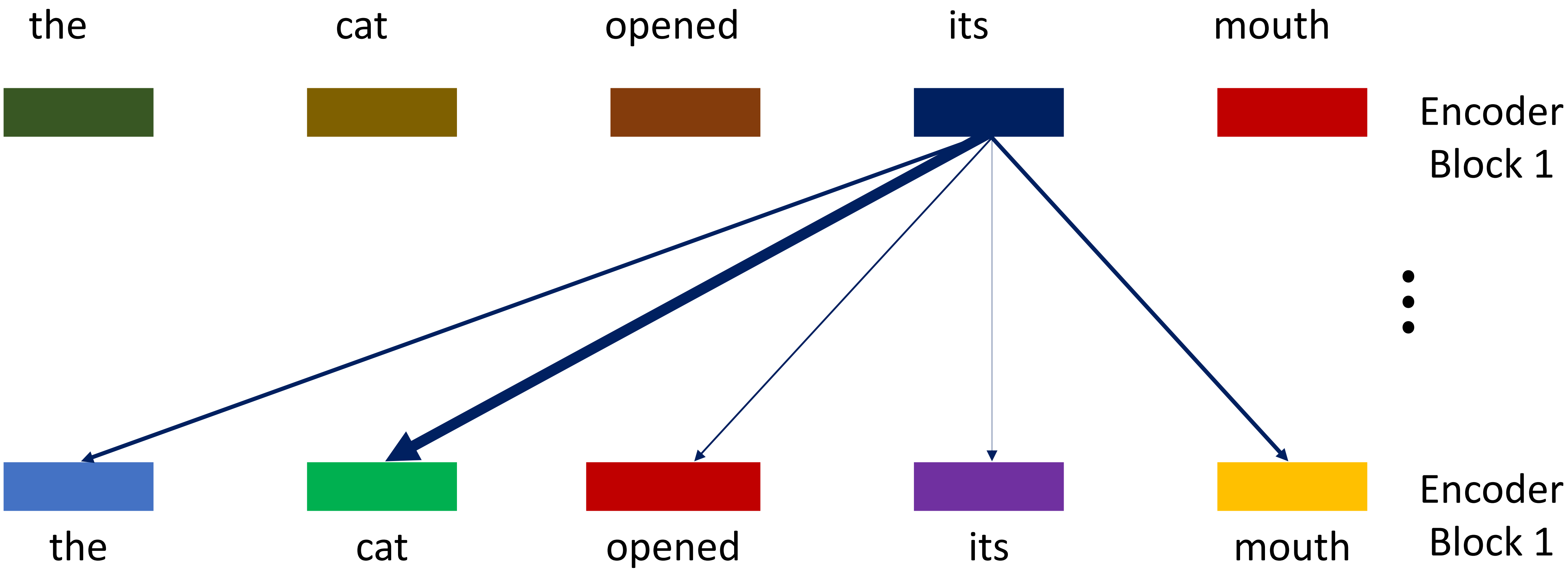


Example: n could be the maximum possible length of a sentence.

Encoder with Latent Variables $\boldsymbol{z}_i$



Attention between 2 words



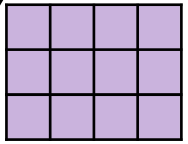
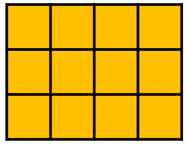
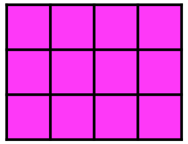
Attention as measured by the width of the arrow

$Query \quad Key \quad Value$

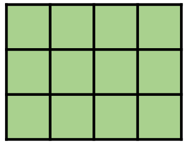
$$Attention(Q, K, V) = softmax\left(\frac{QK^T}{\sqrt{d_k}}\right)V$$

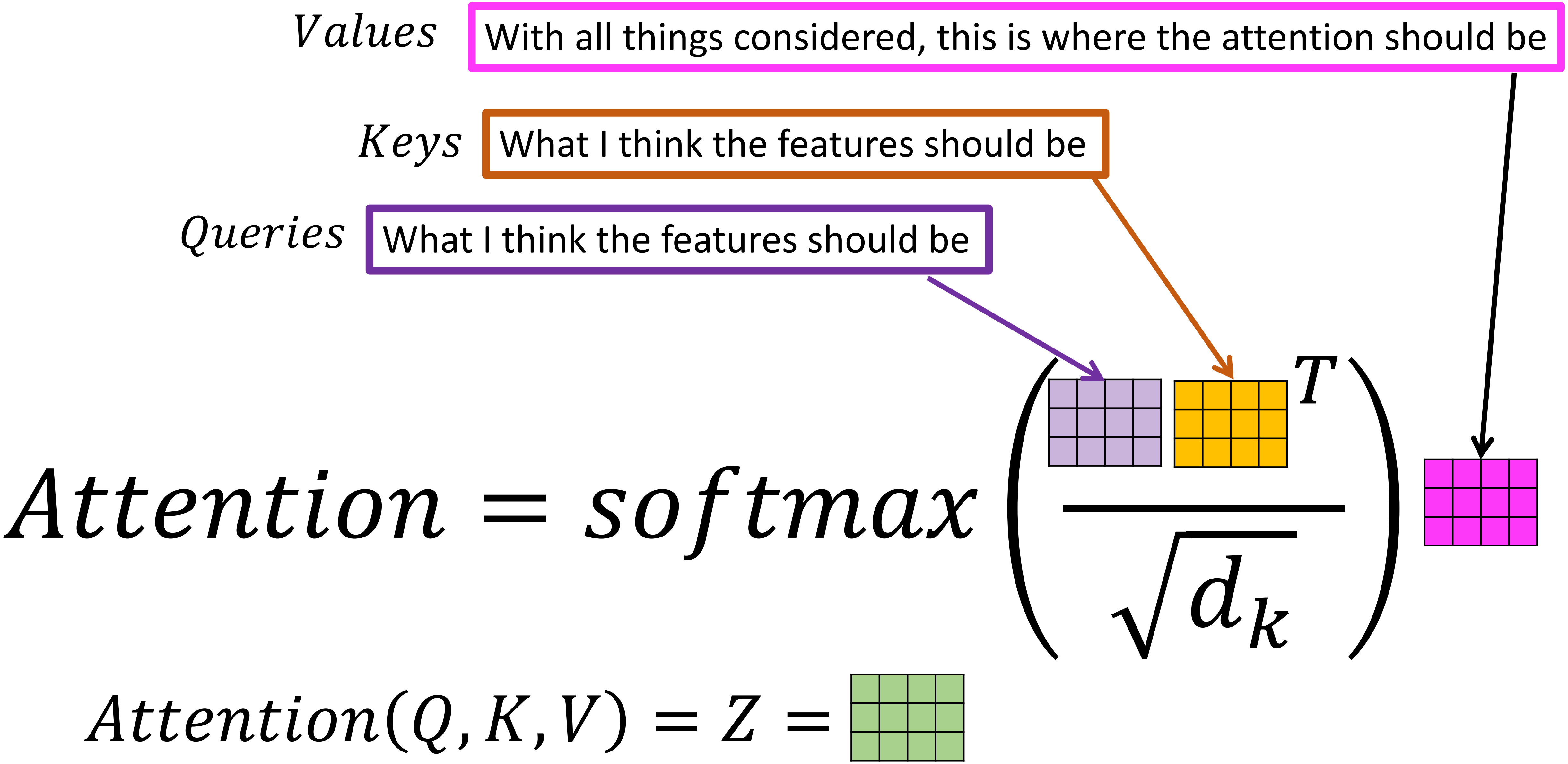
d_k is keys/queries dim (e.g. 4)

$$Attention = softmax\left(\frac{\text{[Q]}\ \text{[K]}^T}{\sqrt{d_k}}\right)\text{[V]}$$

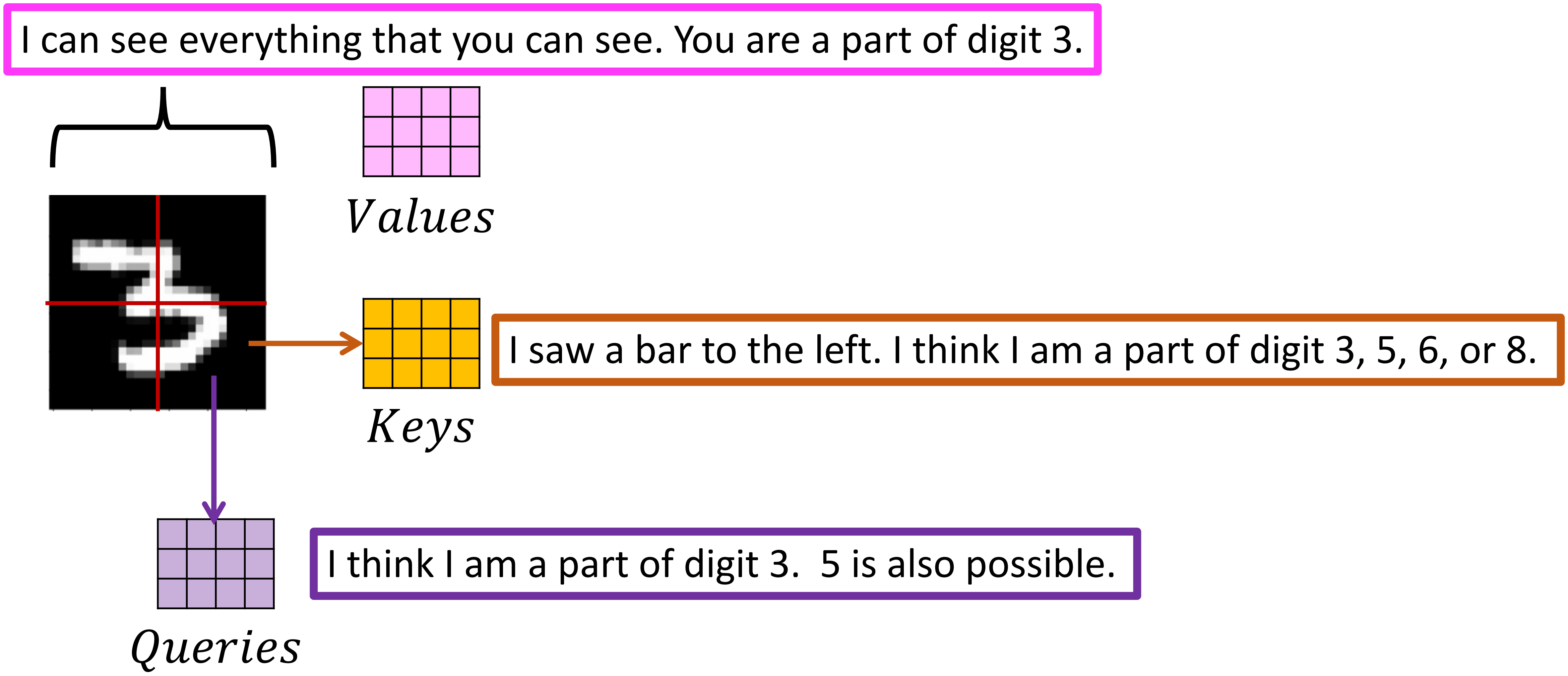




$$Attention(Q, K, V) = Z =$$



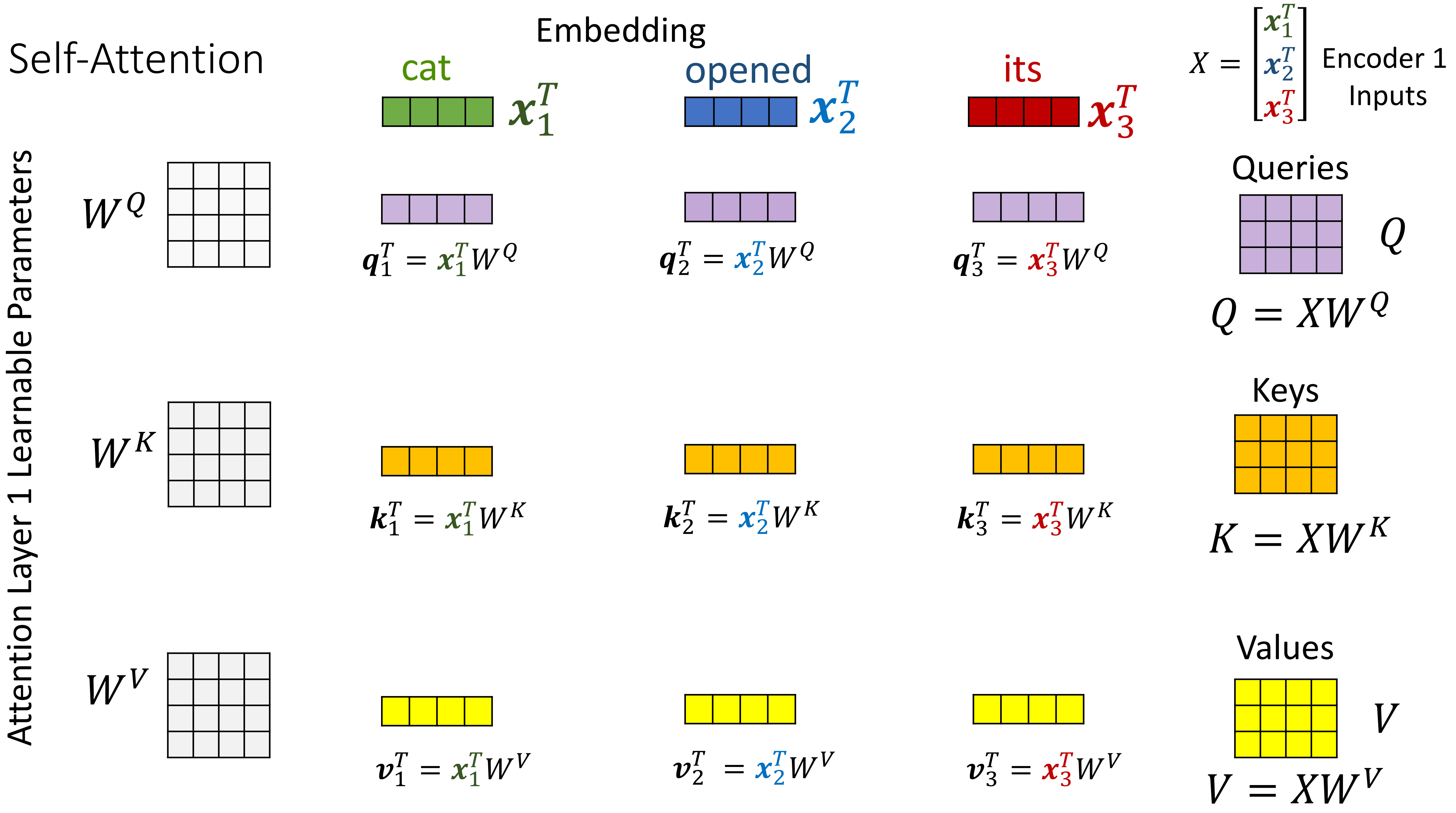

Values
With all things considered, this is where the attention should be
Keys
What I think the features should be
Queries
What I think the features should be
Attention = softmax
T
d_k
Attention(Q, K, V) = Z =

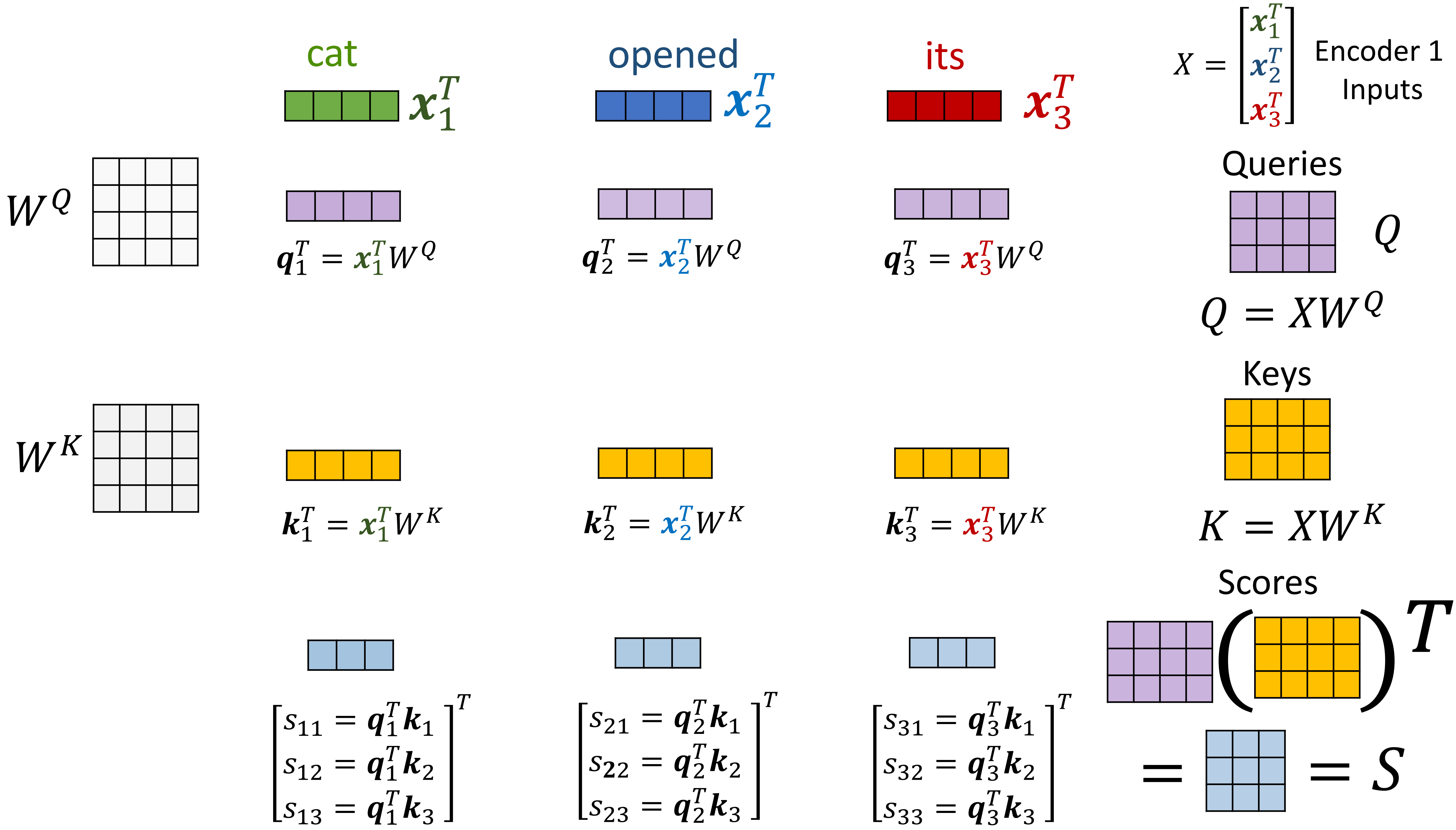
Consider an Attention Layer Examining a Digit



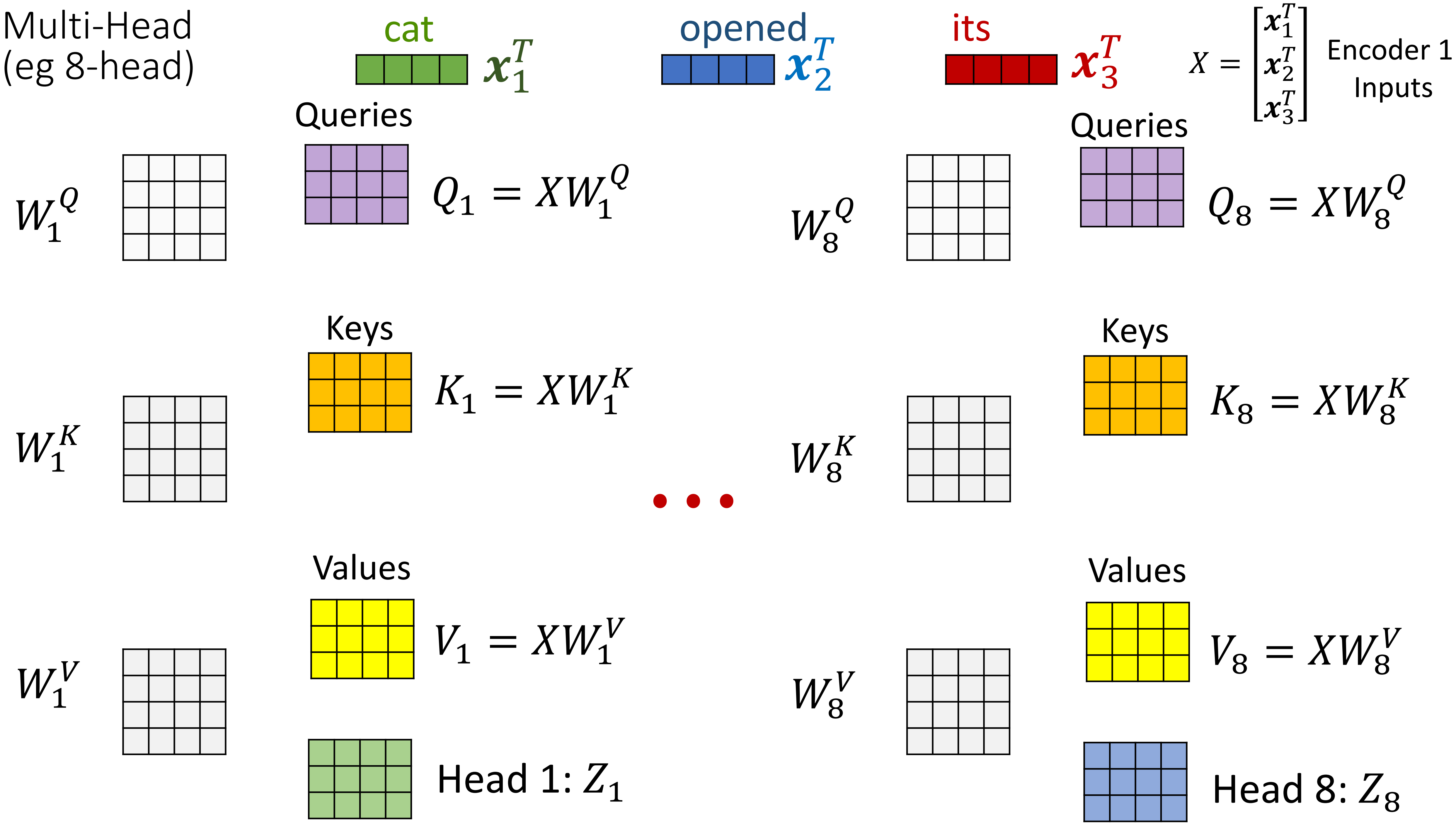
Example: Let us focus on the lower-right patch only

Self-Attention

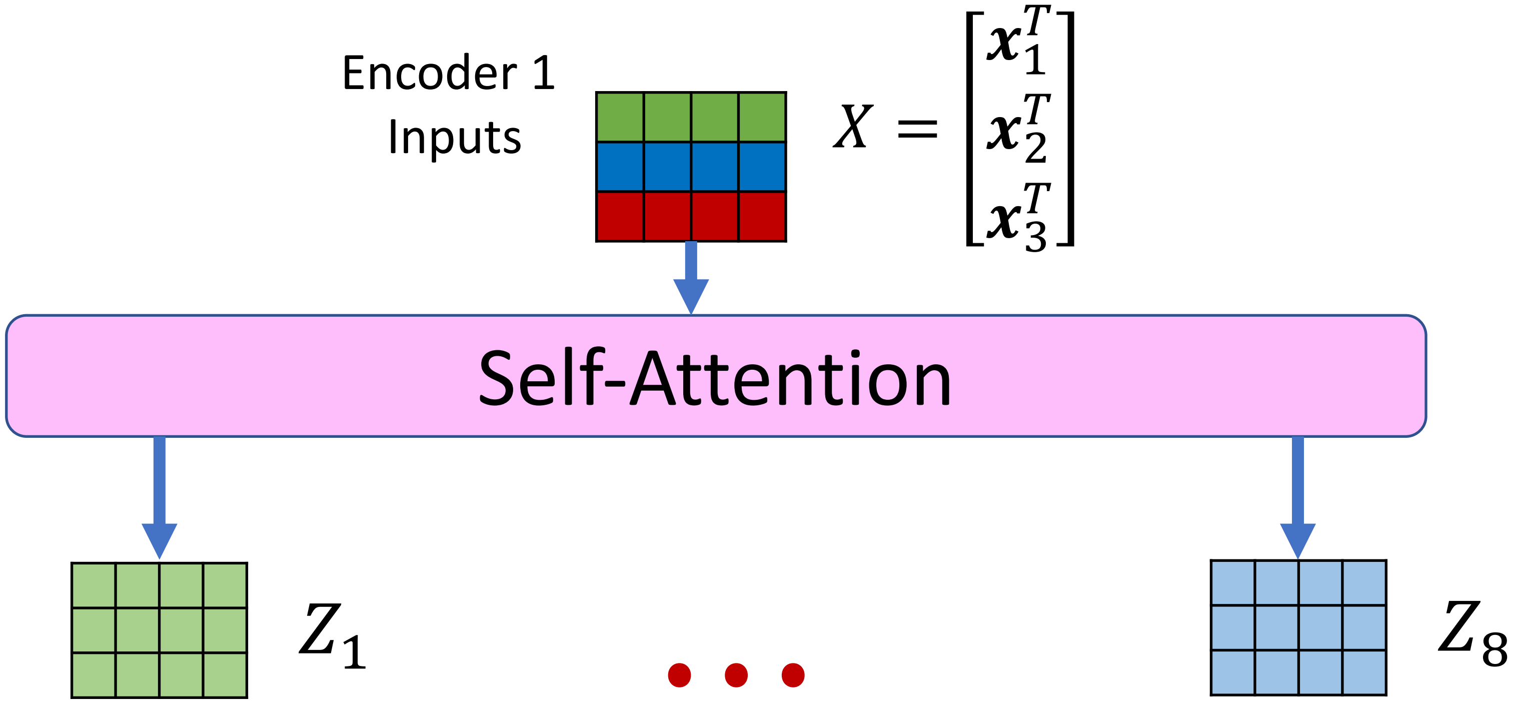




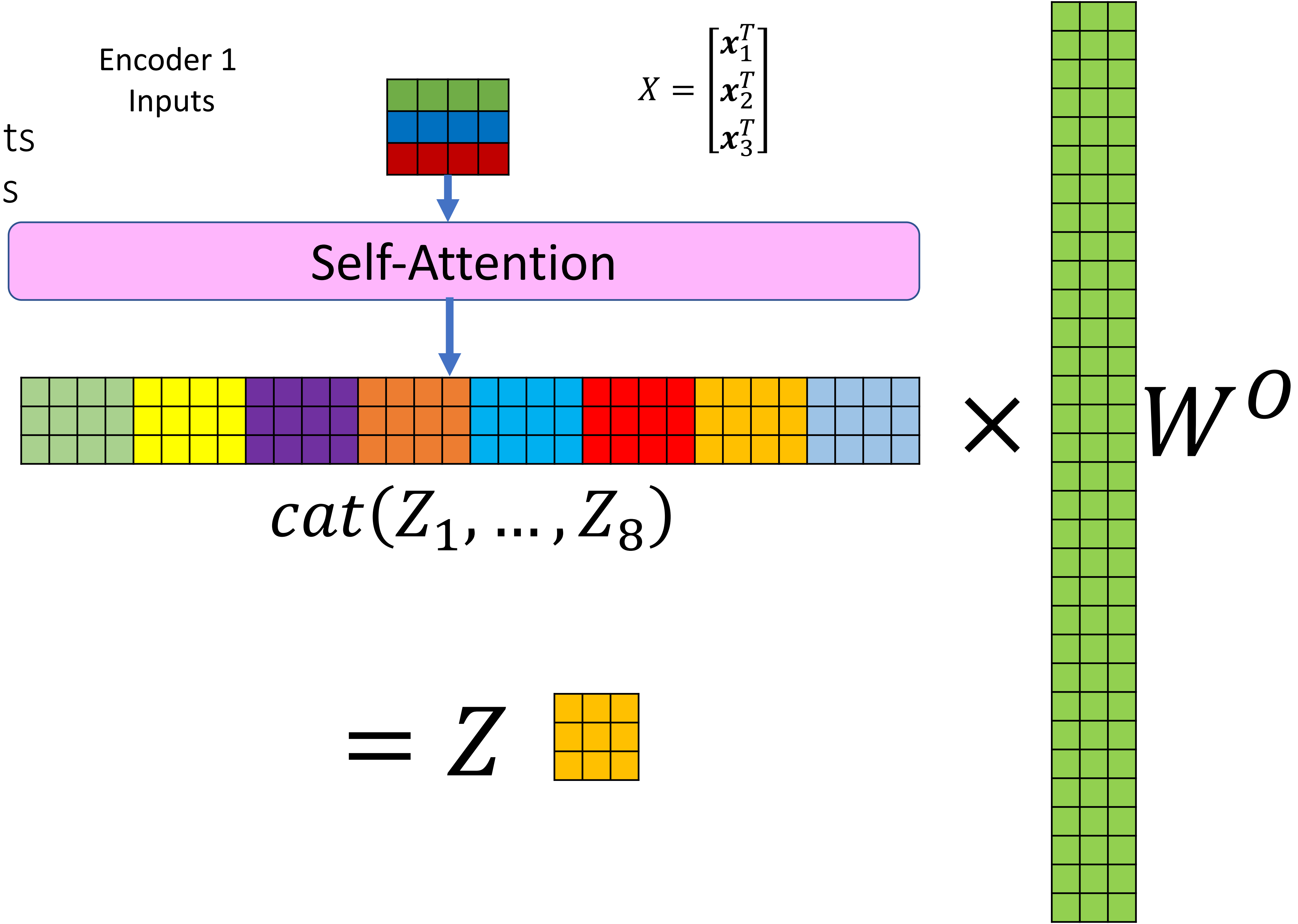
cat
opened
its
$\boldsymbol{x}_1^T$
$\boldsymbol{x}_2^T$
$\boldsymbol{x}_3^T$
$X = \begin{bmatrix} \boldsymbol{x}_1^T \\ \boldsymbol{x}_2^T \\ \boldsymbol{x}_3^T \end{bmatrix}$
Encoder 1 Inputs
W^Q
$\boldsymbol{q}_1^T = \boldsymbol{x}_1^T W^Q$
$\boldsymbol{q}_2^T = \boldsymbol{x}_2^T W^Q$
$\boldsymbol{q}_3^T = \boldsymbol{x}_3^T W^Q$
Queries
Q
$Q = XW^Q$
W^K
$\boldsymbol{k}_1^T = \boldsymbol{x}_1^T W^K$
$\boldsymbol{k}_2^T = \boldsymbol{x}_2^T W^K$
$\boldsymbol{k}_3^T = \boldsymbol{x}_3^T W^K$
Keys
$K = XW^K$
$\begin{bmatrix} s_{11} = \boldsymbol{q}_1^T \boldsymbol{k}_1 \\ s_{12} = \boldsymbol{q}_1^T \boldsymbol{k}_2 \\ s_{13} = \boldsymbol{q}_1^T \boldsymbol{k}_3 \end{bmatrix}^T$
$\begin{bmatrix} s_{21} = \boldsymbol{q}_2^T \boldsymbol{k}_1 \\ s_{22} = \boldsymbol{q}_2^T \boldsymbol{k}_2 \\ s_{23} = \boldsymbol{q}_2^T \boldsymbol{k}_3 \end{bmatrix}^T$
$\begin{bmatrix} s_{31} = \boldsymbol{q}_3^T \boldsymbol{k}_1 \\ s_{32} = \boldsymbol{q}_3^T \boldsymbol{k}_2 \\ s_{33} = \boldsymbol{q}_3^T \boldsymbol{k}_3 \end{bmatrix}^T$
Scores
T
$= S$


Multi-Head
(eg 8-head)
cat
$\boldsymbol{x}_1^T$
opened
$\boldsymbol{x}_2^T$
its
$\boldsymbol{x}_3^T$
$X = \begin{bmatrix} \boldsymbol{x}_1^T \\ \boldsymbol{x}_2^T \\ \boldsymbol{x}_3^T \end{bmatrix}$
Encoder 1
Inputs
Queries
W_1^Q
$Q_1 = XW_1^Q$
Keys
W_1^K
$K_1 = XW_1^K$
Values
W_1^V
$V_1 = XW_1^V$
Head 1: Z_1
Queries
W_8^Q
$Q_8 = XW_8^Q$
Keys
W_8^K
$K_8 = XW_8^K$
Values
W_8^V
$V_8 = XW_8^V$
Head 8: Z_8

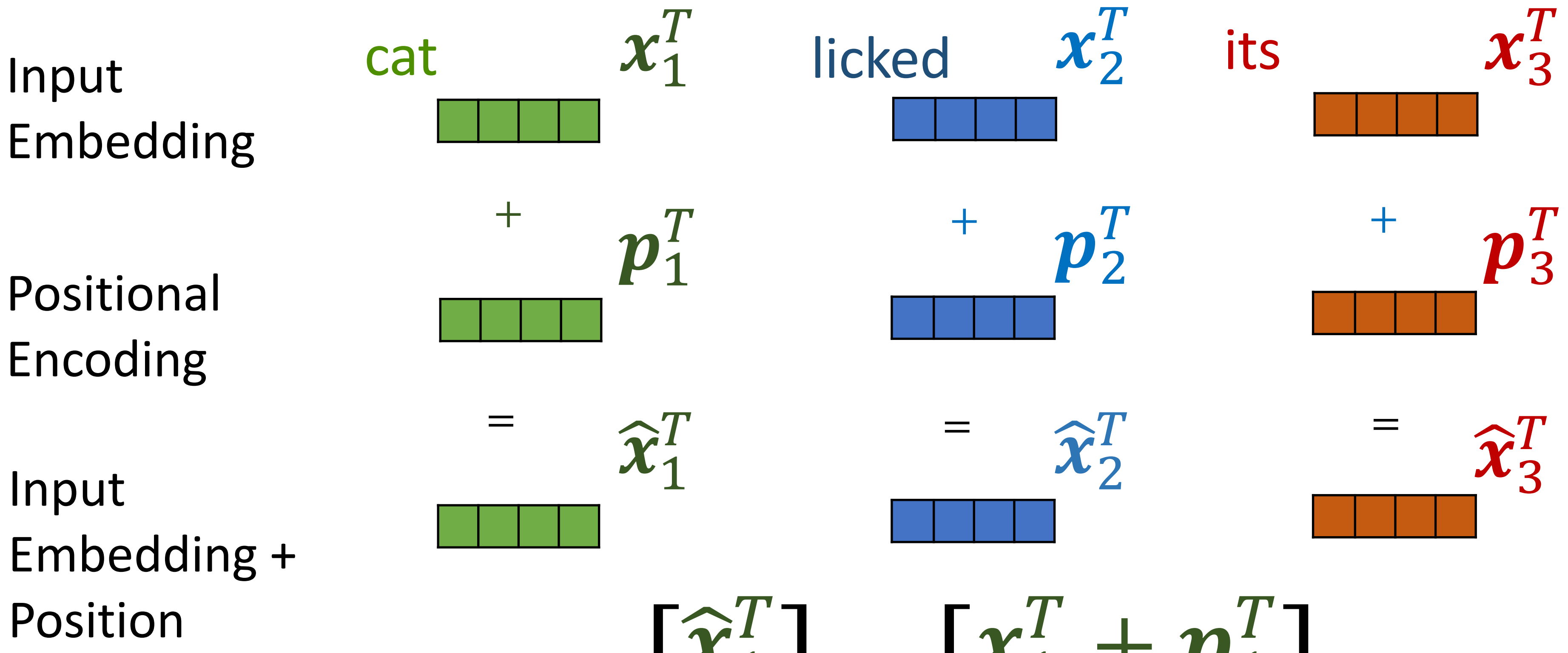
Multi-Head
(eg 8-head)



Multi-Head
(eg 8-head)
Merge Outputs
Apply Weights



Adding Position Info to Inputs



$$\hat{X} = \begin{bmatrix} \widehat{\boldsymbol{x}}_1^T \\ \widehat{\boldsymbol{x}}_2^T \\ \widehat{\boldsymbol{x}}_3^T \end{bmatrix} = \begin{bmatrix} \boldsymbol{x}_1^T + \boldsymbol{p}_1^T \\ \boldsymbol{x}_2^T + \boldsymbol{p}_2^T \\ \boldsymbol{x}_3^T + \boldsymbol{p}_3^T \end{bmatrix}$$

Positional Encoding

$$PE_{(pos,2i)} = \sin\left(\frac{pos}{10000^{\frac{2i}{d_k}}}\right) \quad dim = 2i \;\; is\ even$$

$$PE_{(pos,2i+1)} = \cos\left(\frac{pos}{10000^{\frac{2i}{d_k}}}\right) \quad dim = 2i+1 \;\; is\ odd$$

$pos = 0,1, \dots n_{pos-1}$

$dim = 0,1, \dots n_{dim-1}$

Other positional encoding methods: learnable

Positional Encoding Matrix with d=4, n=100

Sequence	Index of token, k	i=0	i=0	i=1	i=1
I	0	$P_{00}=\sin(0)$ = 0	$P_{01}=\cos(0)$ = 1	$P_{02}=\sin(0)$ = 0	$P_{03}=\cos(0)$ = 1
am	1	$P_{10}=\sin(1/1)$ = 0.84	$P_{11}=\cos(1/1)$ = 0.54	$P_{12}=\sin(1/10)$ = 0.10	$P_{13}=\cos(1/10)$ = 1.0
a	2	$P_{20}=\sin(2/1)$ = 0.91	$P_{21}=\cos(2/1)$ = -0.42	$P_{22}=\sin(2/10)$ = 0.20	$P_{23}=\cos(2/10)$ = 0.98
Robot	3	$P_{30}=\sin(3/1)$ = 0.14	$P_{31}=\cos(3/1)$ = -0.99	$P_{32}=\sin(3/10)$ = 0.30	$P_{33}=\cos(3/10)$ = 0.96

Positional Encoding Matrix for the sequence 'I am a robot'

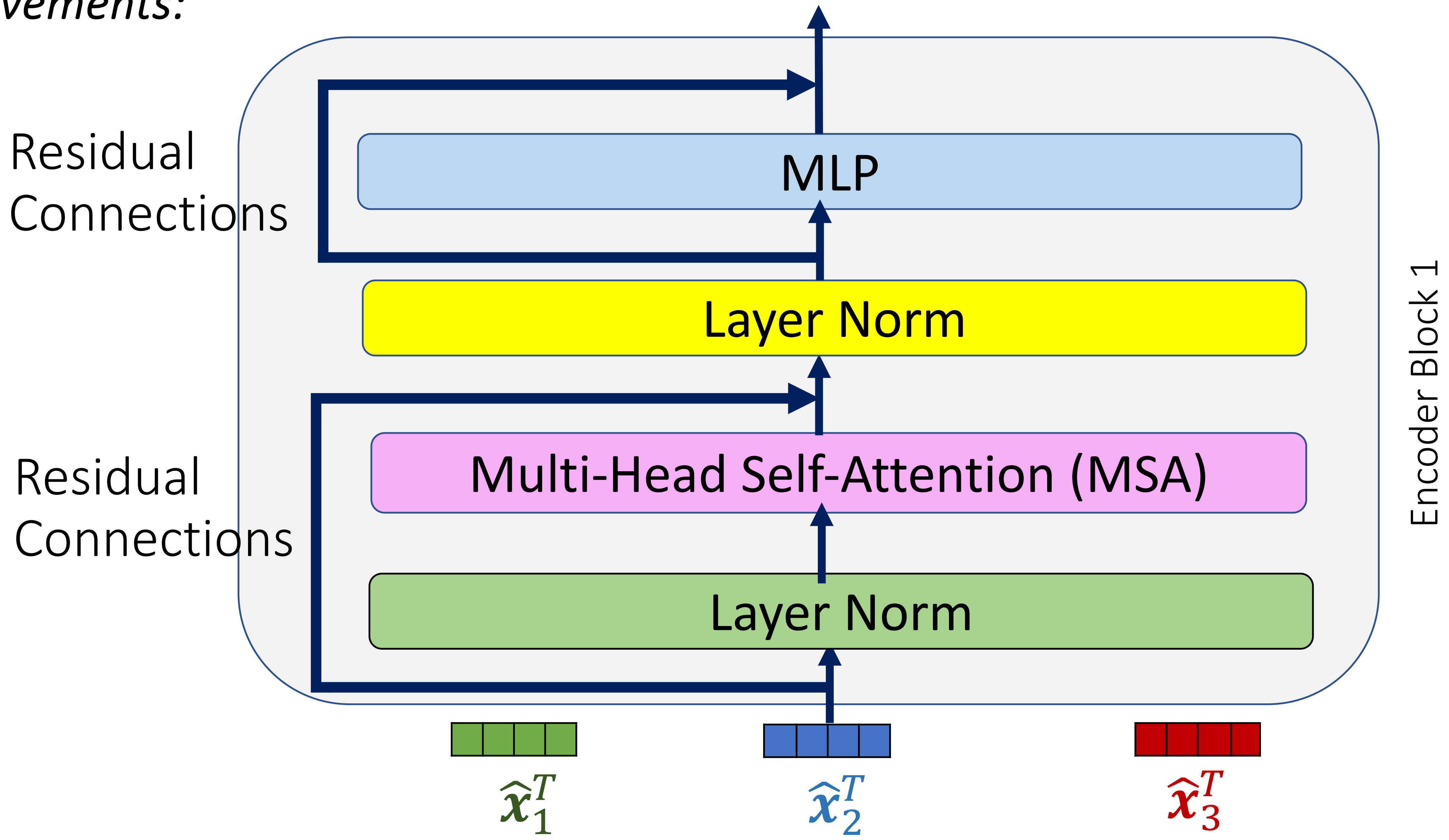
Positional Encoding

i

k

	0	0		n
0	$\sin\left(\frac{0}{10000^{\frac{2(0)}{d_k}}}\right)$	$\cos\left(\frac{0}{10000^{\frac{2(1)}{d_k}}}\right)$		
1	$\sin\left(\frac{1}{10000^{\frac{2(0)}{d_k}}}\right)$	$\cos\left(\frac{0}{10000^{\frac{2(1)}{d_k}}}\right)$		
2				

Improvements:



Layer Normalization vs Batch Normalization

$$\mu = \frac{1}{d}\sum_{i}^{d} x_i$$

$$\sigma^2 = \frac{1}{d}\sum_{i}^{d} (x_i - \mu)^2$$

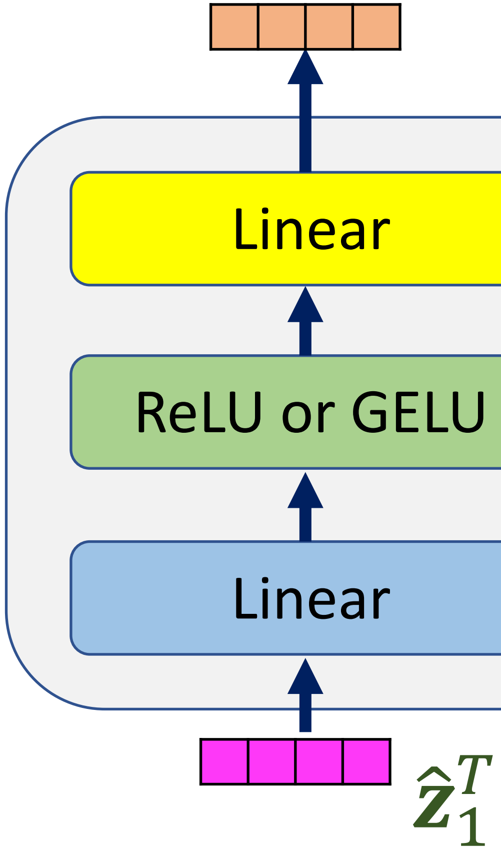
$$\hat{x}_i = \frac{x_i - \mu}{\sqrt{\sigma^2 + \epsilon}}$$

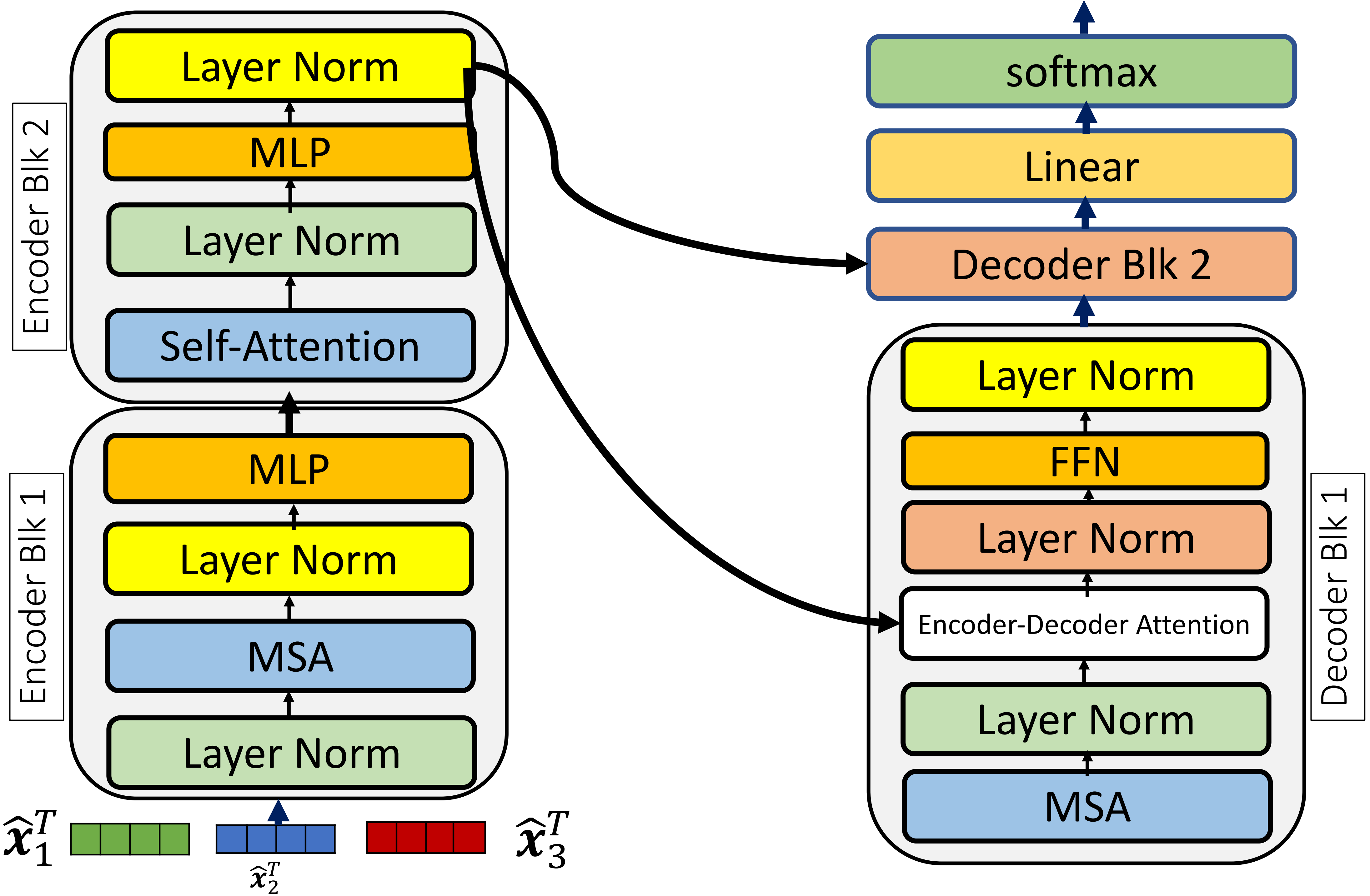
- Batch Normalization – d is across the entire batch
- Layer Normalization - d is across the layer

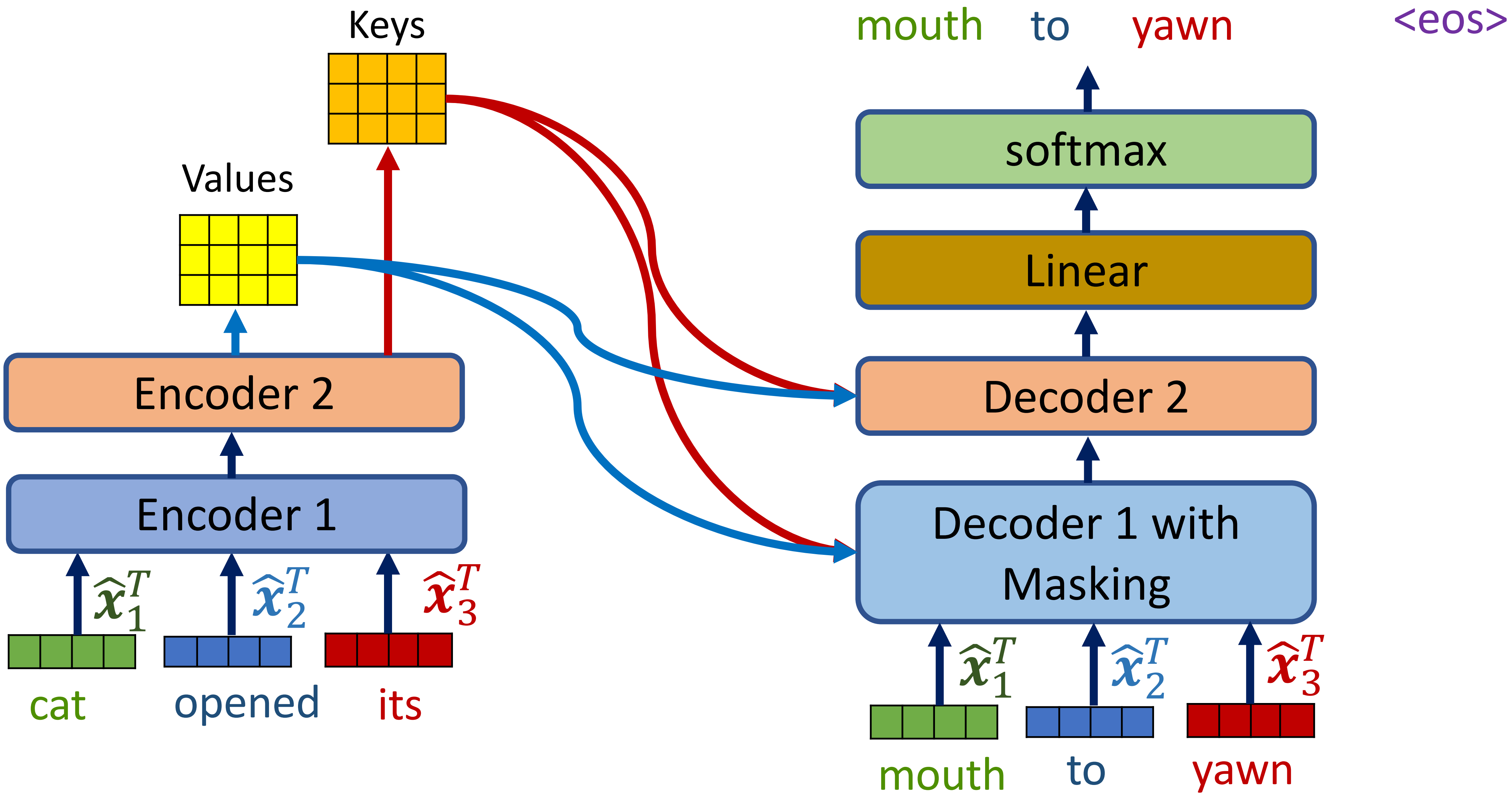
$\hat{x}_i$ is the normalized feature

FFN: Feed Forward Neural Network (MLP)

$$MLP(x) = \max(0, xW_1 + b_1)W_2 + b_2$$




Layer Norm
MLP
Layer Norm
Self-Attention
Encoder Blk 2
MLP
Layer Norm
MSA
Layer Norm
Encoder Blk 1
$\hat{x}_1^T$
$\hat{x}_2^T$
$\hat{x}_3^T$
softmax
Linear
Decoder Blk 2
Layer Norm
FFN
Layer Norm
Encoder-Decoder Attention
Layer Norm
MSA
Decoder Blk 1



Masking prevents Decoder 1 from seeing the future.
Decoder 1 relies only on the previous outputs.

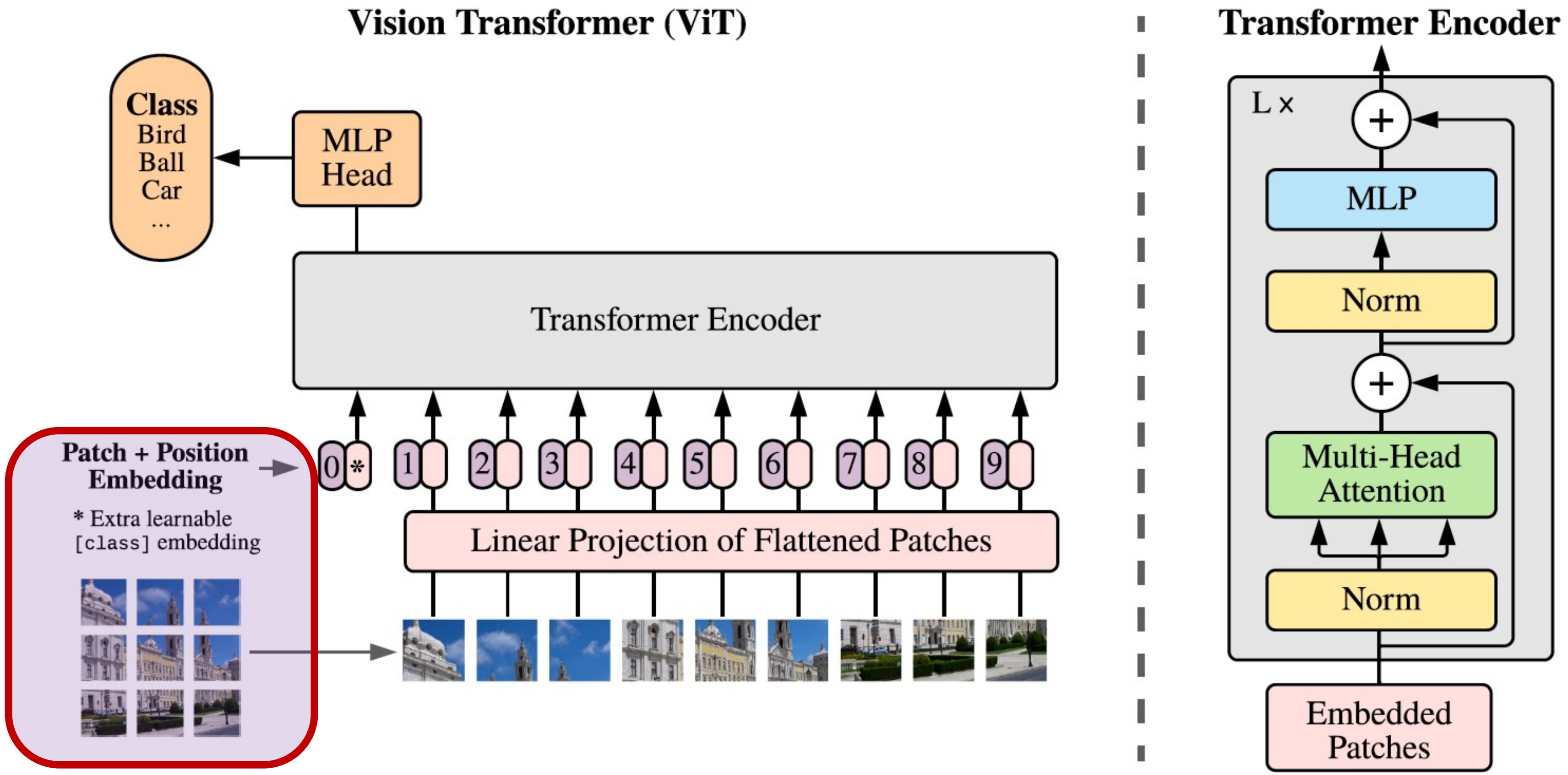


Figure 1: Model overview. We split an image into fixed-size patches, linearly embed each of them, add position embeddings to the resulting sequence of vectors, and feed the patches to a standard Transformer encoder. In order to perform classification, we use the standard approach of adding an extra learnable "classification token" to the sequence. The illustration of the Transformer encoder was inspired by Vaswani et al. (2017).

AN IMAGE IS WORTH 16X16 WORDS:
TRANSFORMERS FOR IMAGE RECOGNITION AT SCALE, ICLR 2021

Inductive Bias

Transformers lack some inductive biases inherent to CNNs, such as translation equivariance and scale invariance (w/ maxpool), and therefore do not generalize well when trained on insufficient amounts of data.

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

References

Vaswani, Ashish, et al. "Attention is all you need." *Advances in neural information processing systems*. 2017.

Dosovitskiy, Alexey, et al. "An image is worth 16x16 words: Transformers for image recognition at scale." *arXiv preprint arXiv:2010.11929* (2020). ICLR 2021.

Illustrated Transformer, http://jalammar.github.io/illustrated-transformer/

Transformers from Scratch, http://peterbloem.nl/blog/transformers

Transformer Family, https://lilianweng.github.io/lil-log/2020/04/07/the-transformer-family.html

In Summary

Transformers could be the most important breakthrough in the recent history of deep learning

Transformers have been used to produce state-of-the-art performances in language, vision, audio, and multi-modal domains

Expect more development in this field in the near future

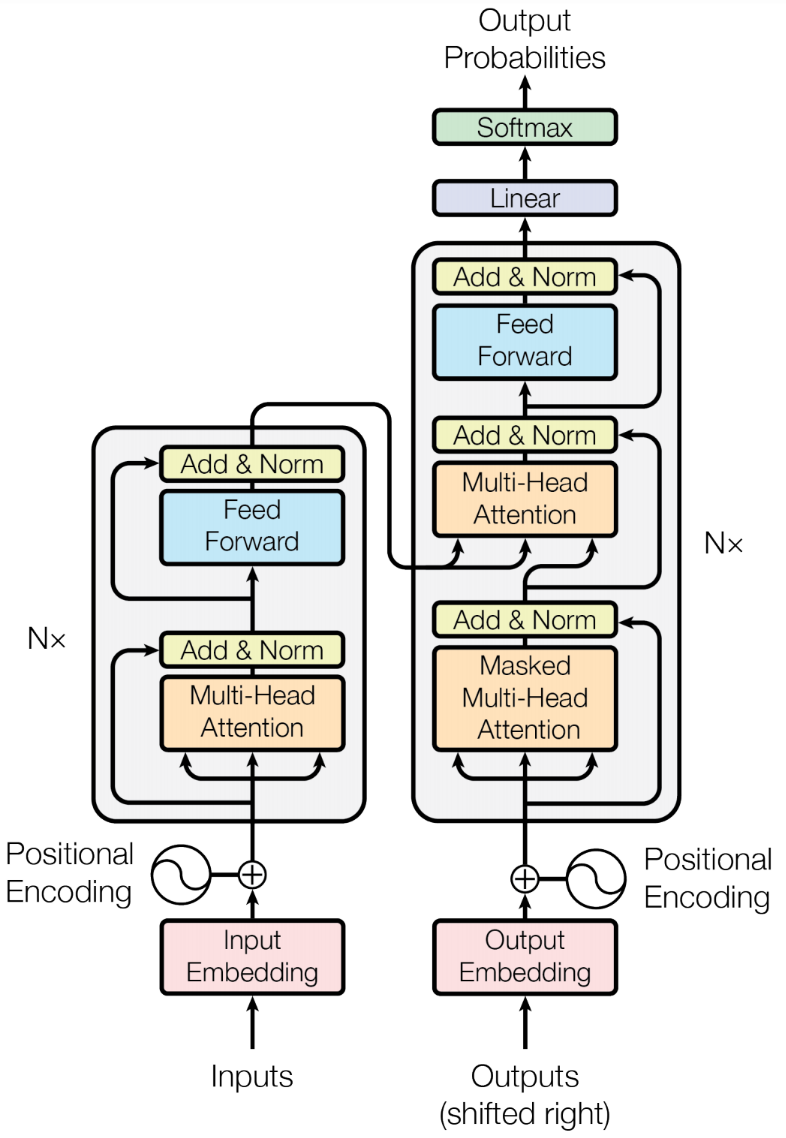


Figure 1: The Transformer - model architecture.

Vaswani, Ashish, et al. "Attention is all you need." *Advances in neural information processing systems*. 2017.

Code demo is next