Transformers

CoE197Z/EE298Z (Deep Learning)

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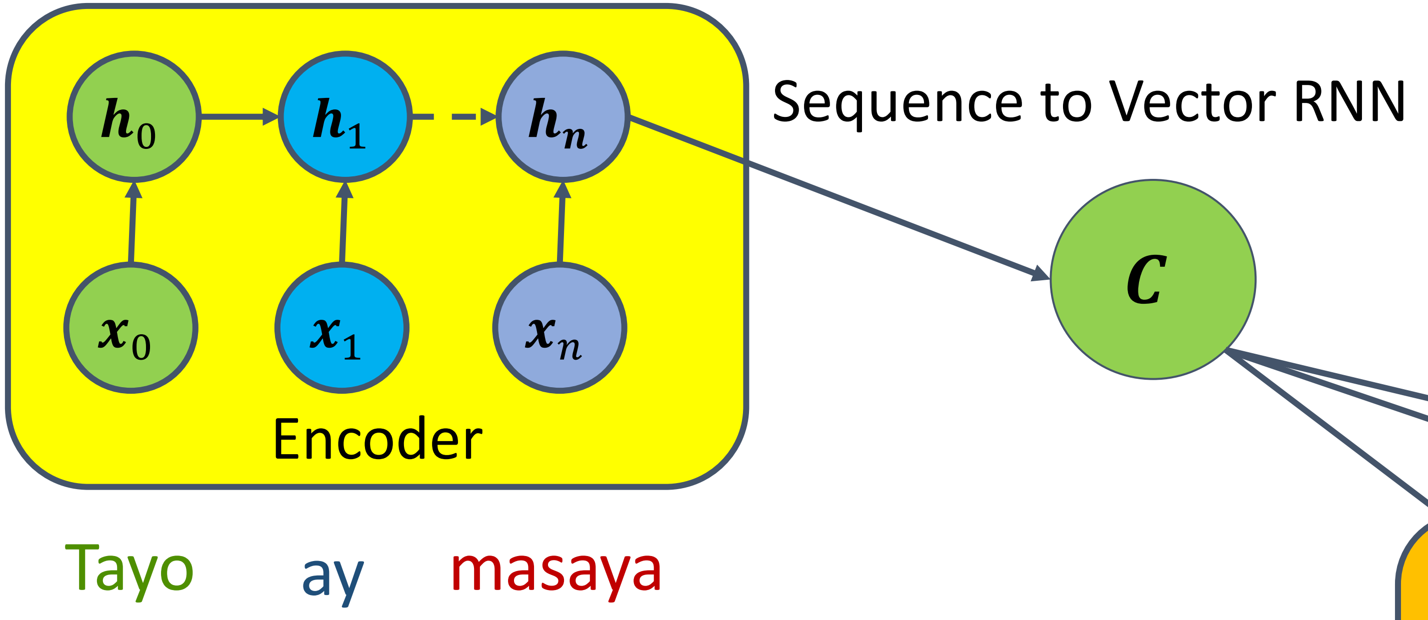
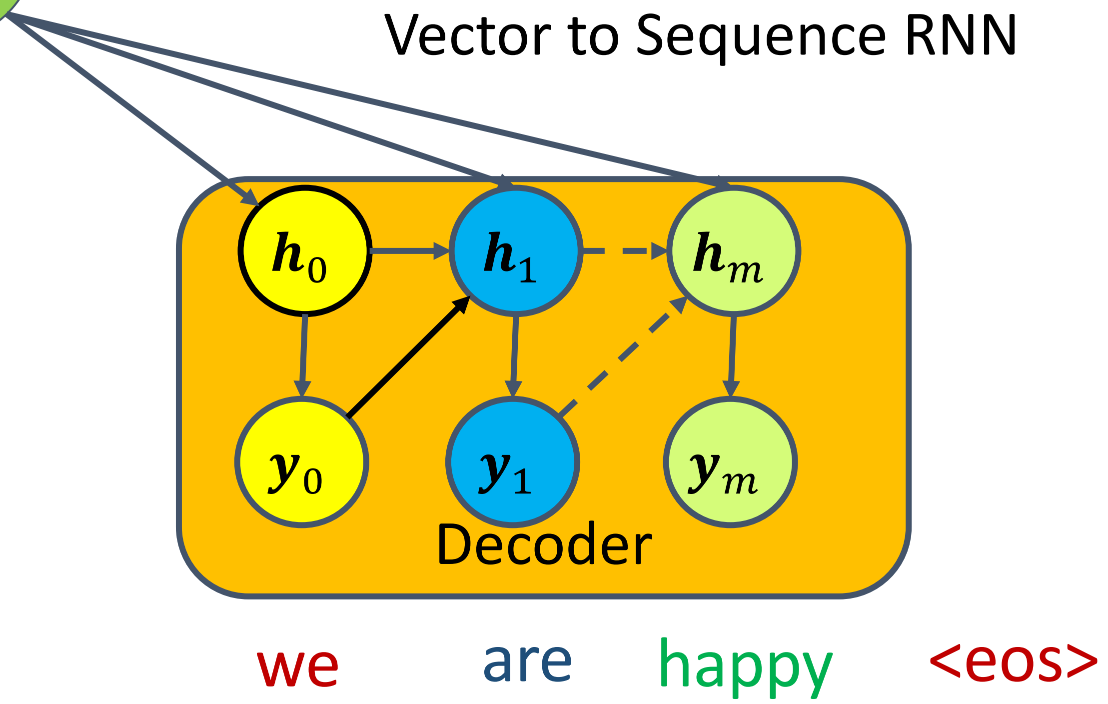
Encoder-Decoder Sequence-to-Sequence



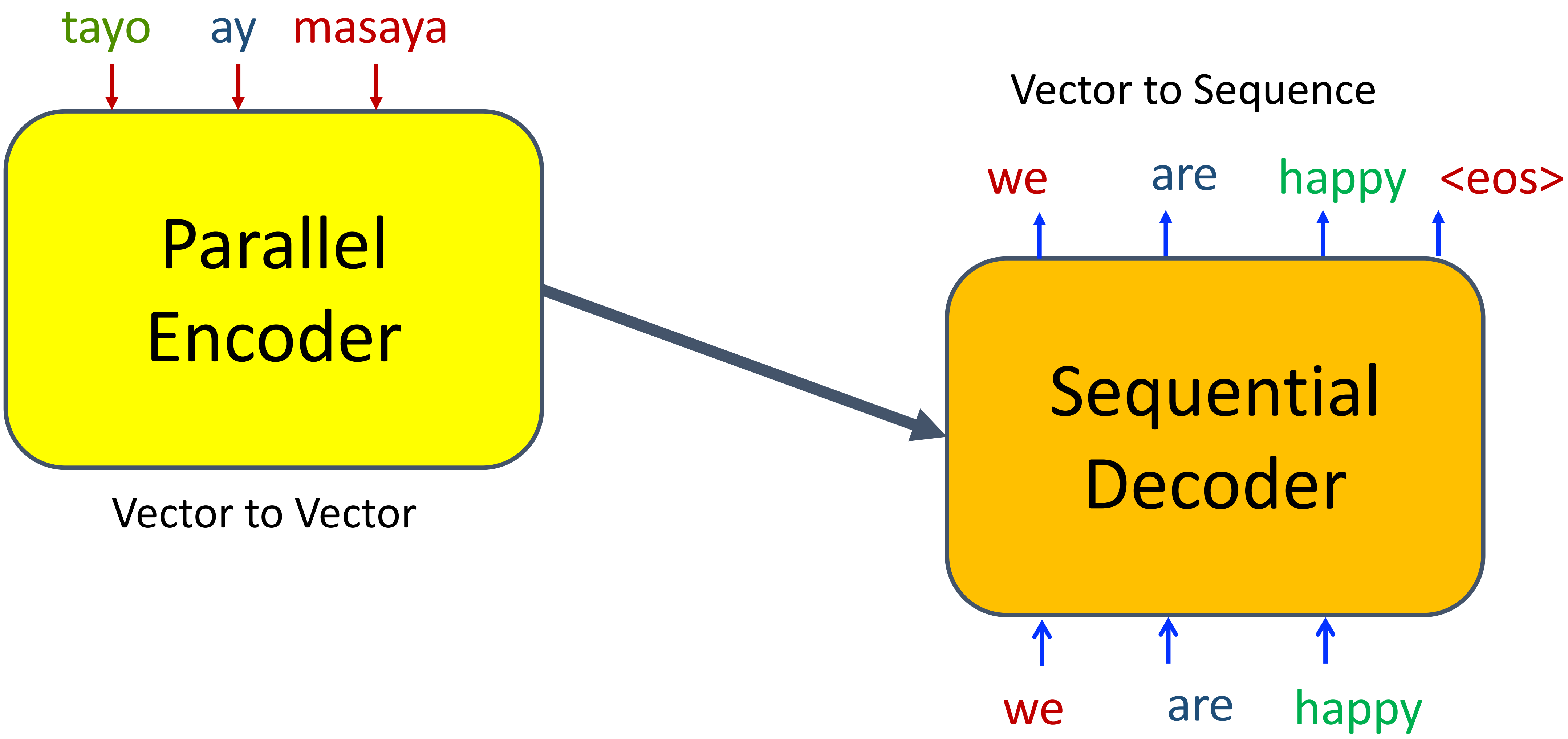


Input to Encoder has length n
$\boldsymbol{C}$ is the context summarized by h_n
Output of Decoder has length m
In general $n \neq m$

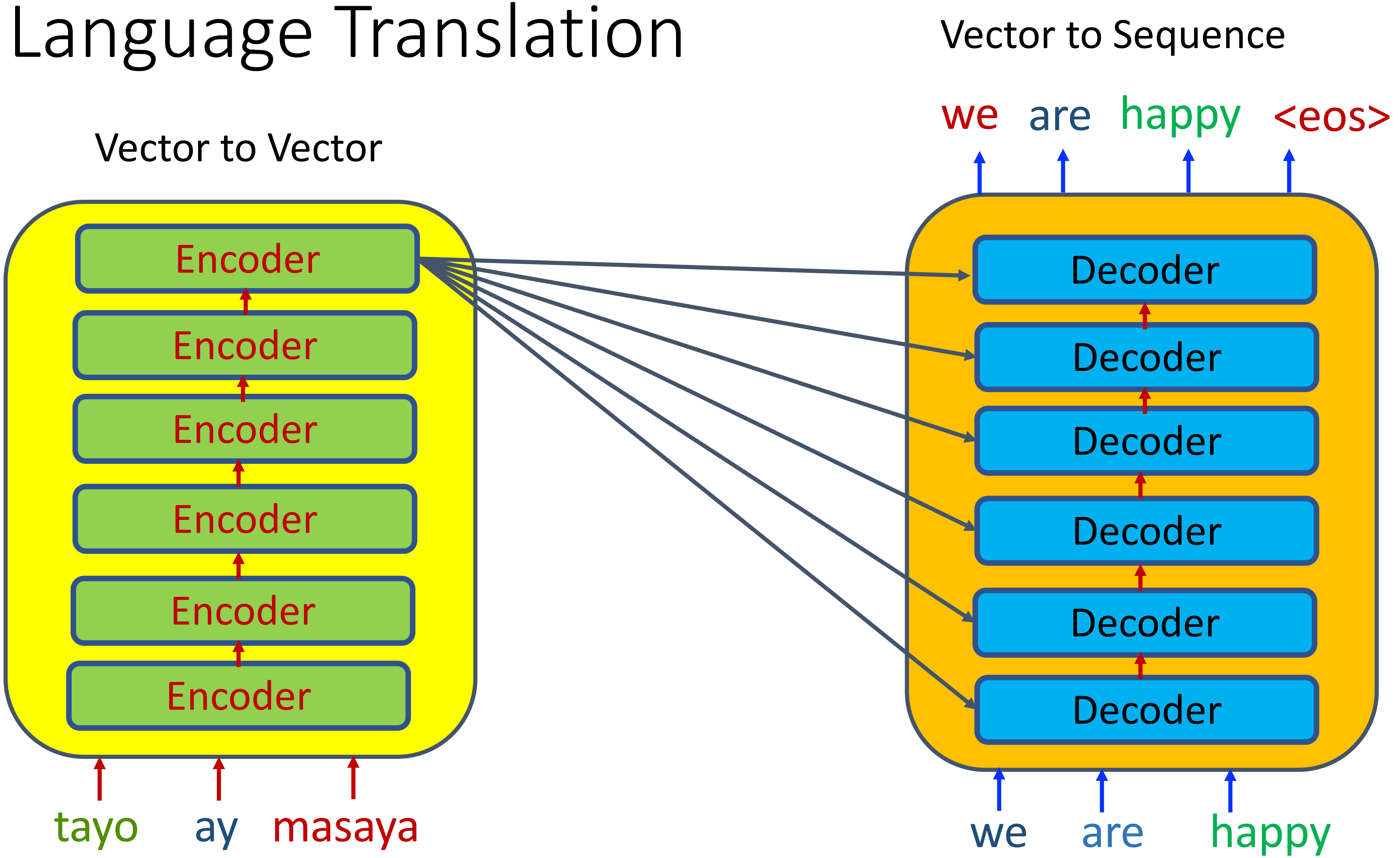
seq2seq

RNN	**Transformer**
Serial Difficult to parallelize Uni-directional Bi-directional version is much slower Susceptible to catastrophic forgetting Slow	Parallel Bidirectional Not susceptible to catastrophic forgetting Fast

Transformer



Language Translation

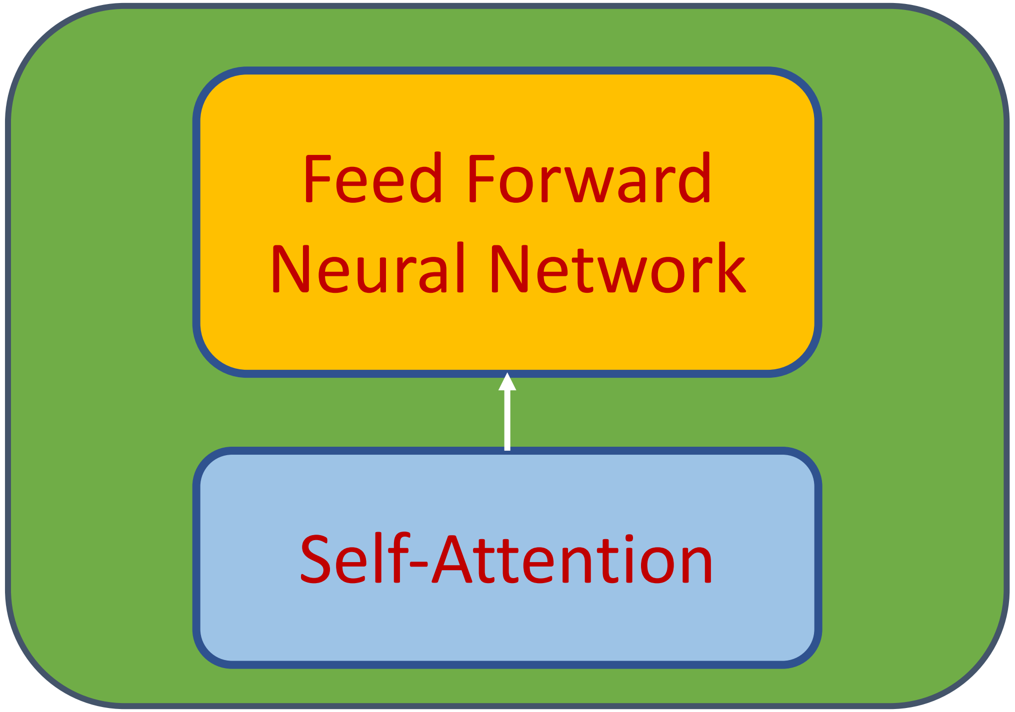


Transformer Encoder Unit Details

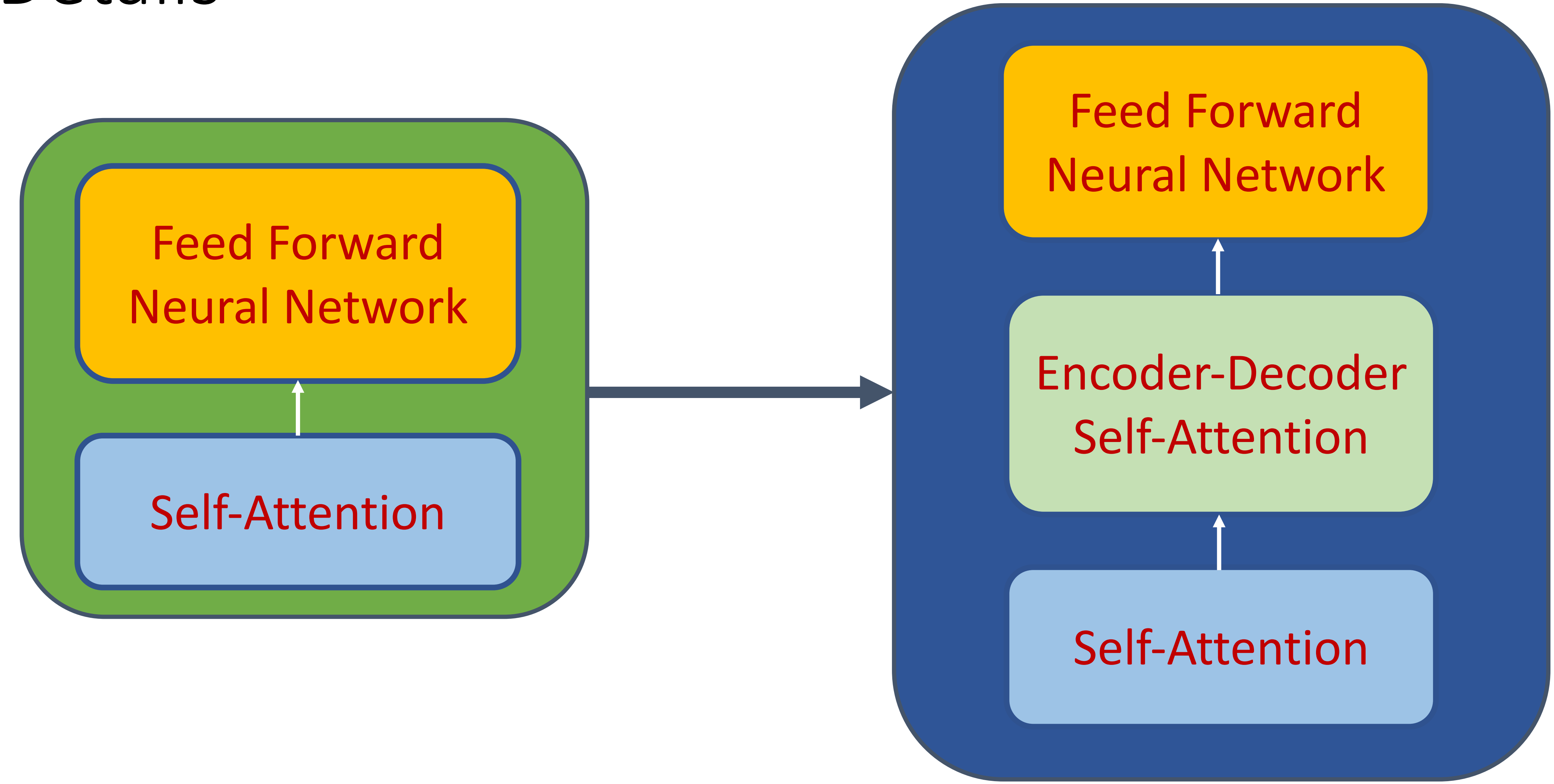
No recurrence (No RNN)

No CNN

Operations: Linear, Norm, Matrix Multiply, Dot Product, Softmax



Transformer Encoder and Decoder Unit Details



Input Embedding is an $n-dim$ vector

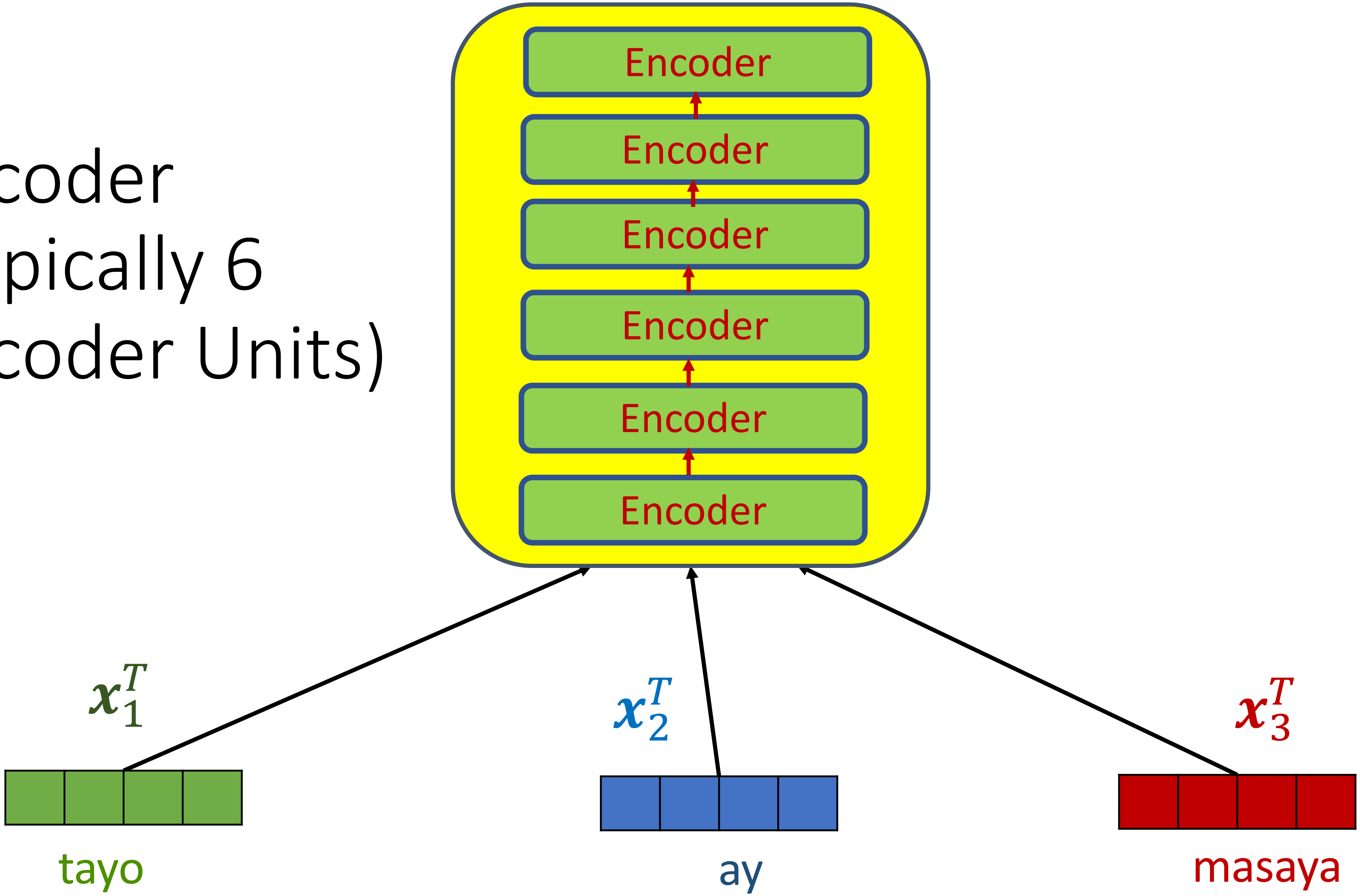
$\boldsymbol{x}_1^T$ = [.1, -2, .4, -1] — tayo

$\boldsymbol{x}_2^T$ = [.3, 1, -1, 2] — ay

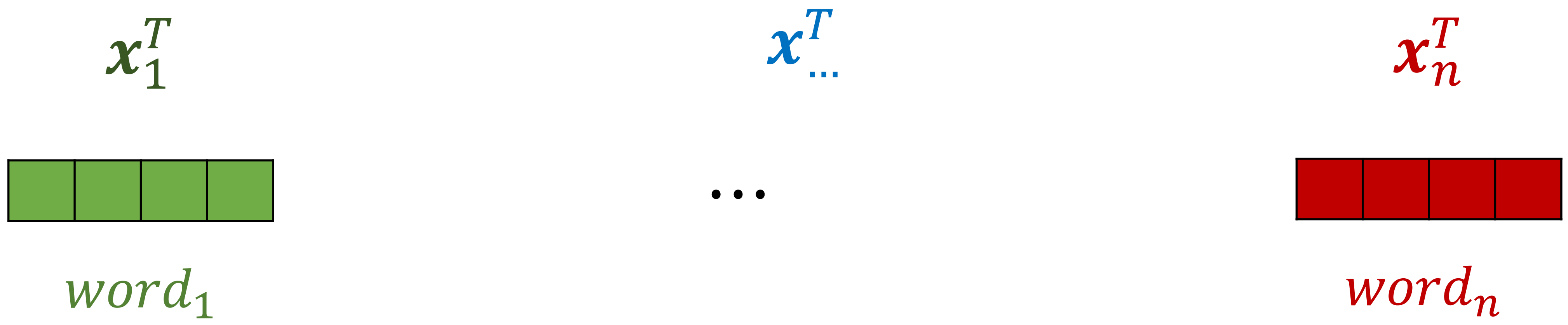
$\boldsymbol{x}_3^T$ = [.1, .0, 1, -1] — masaya

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

Encoder (Typically 6 Encoder Units)

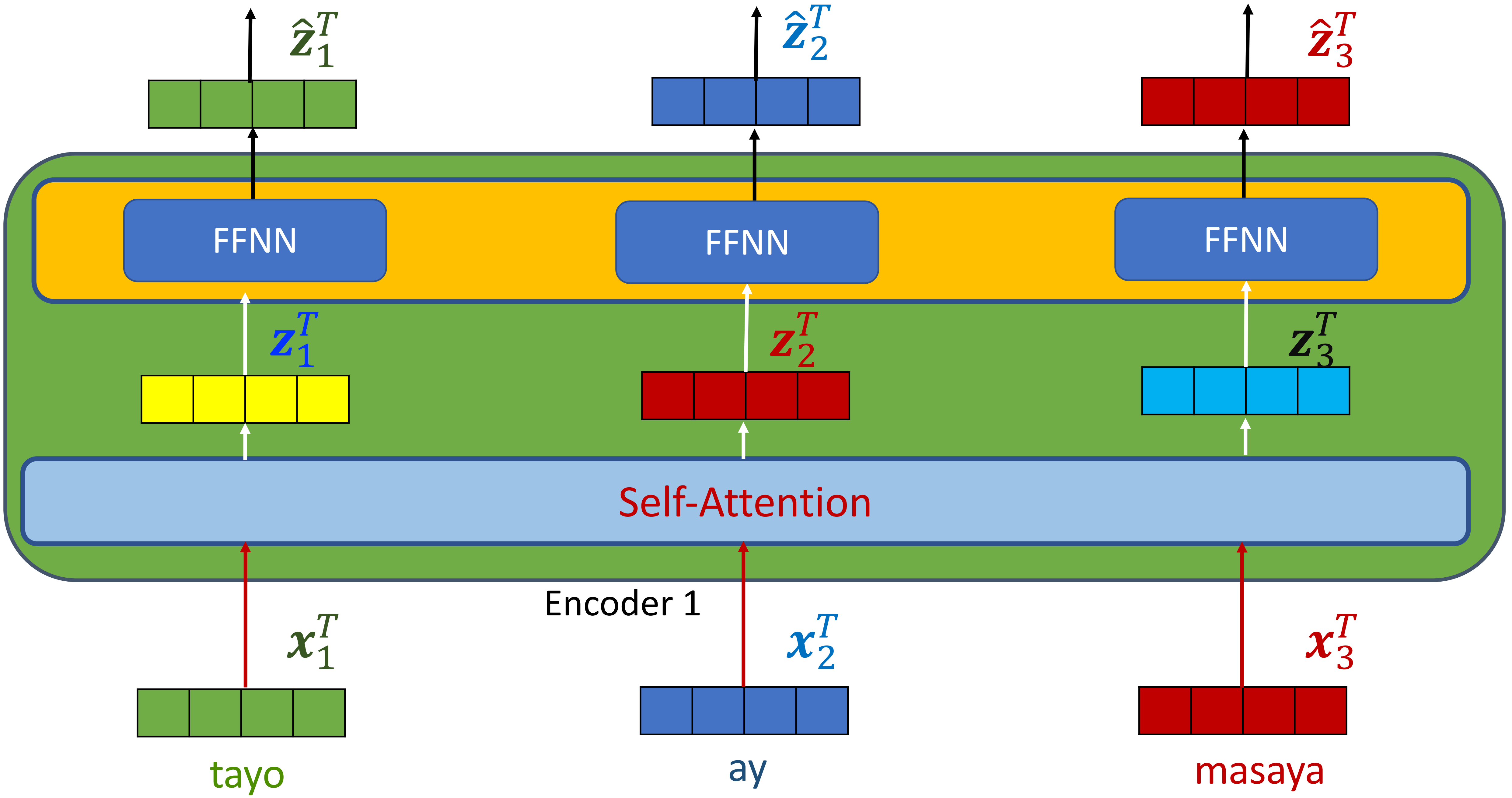


The Length of the Input is $\boldsymbol{n}$

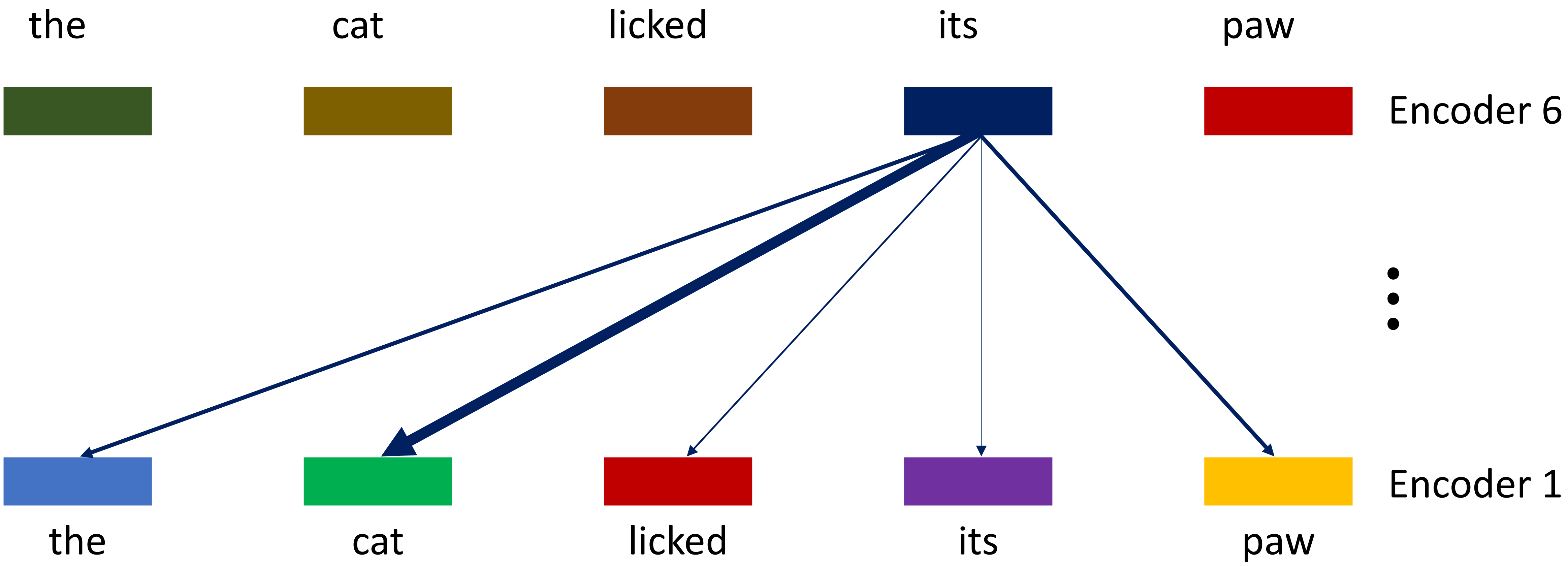


Example: n could be the maximum possible length of a sentence.

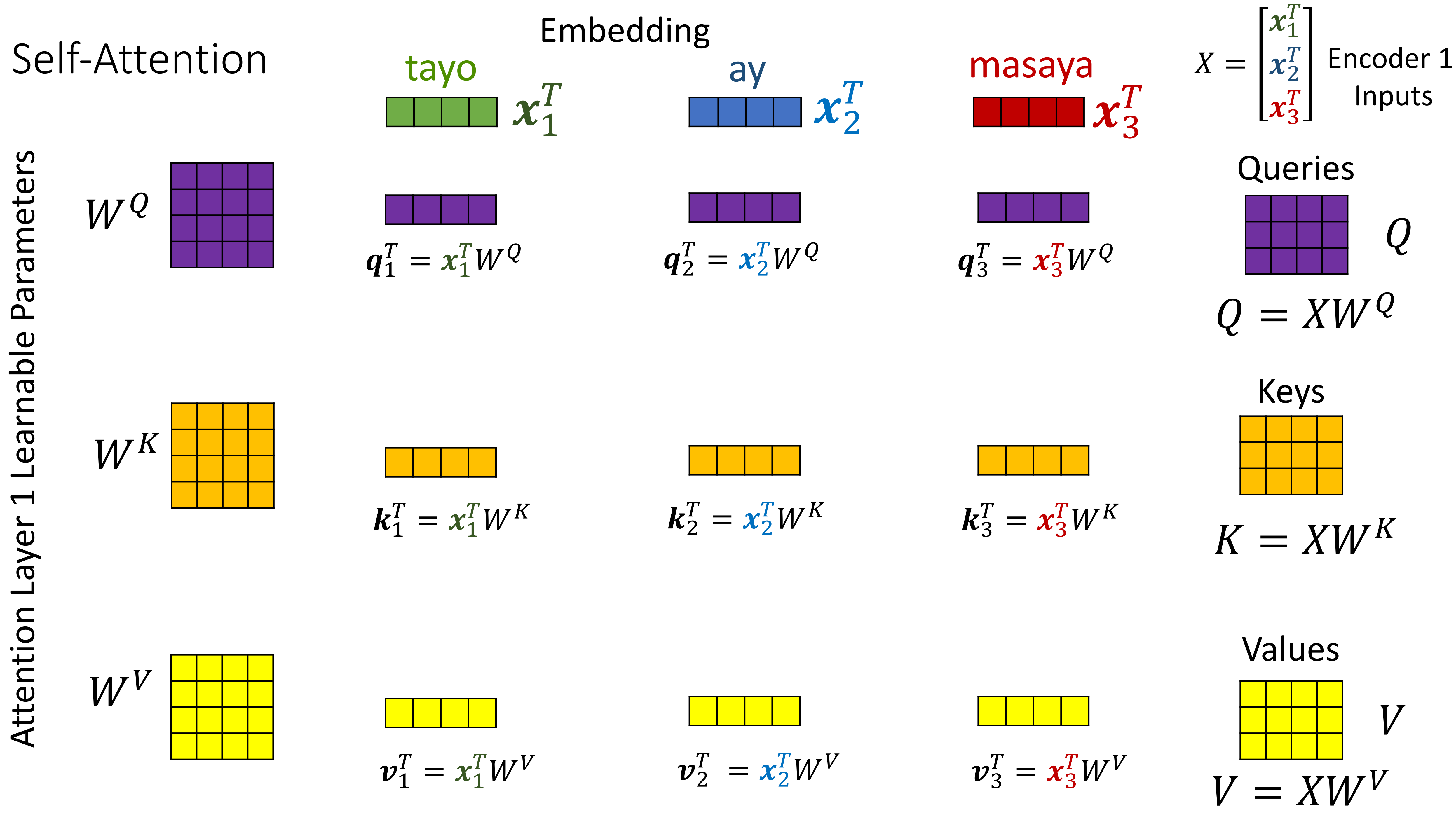
Encoder with Latent Variables $\boldsymbol{z}_i$

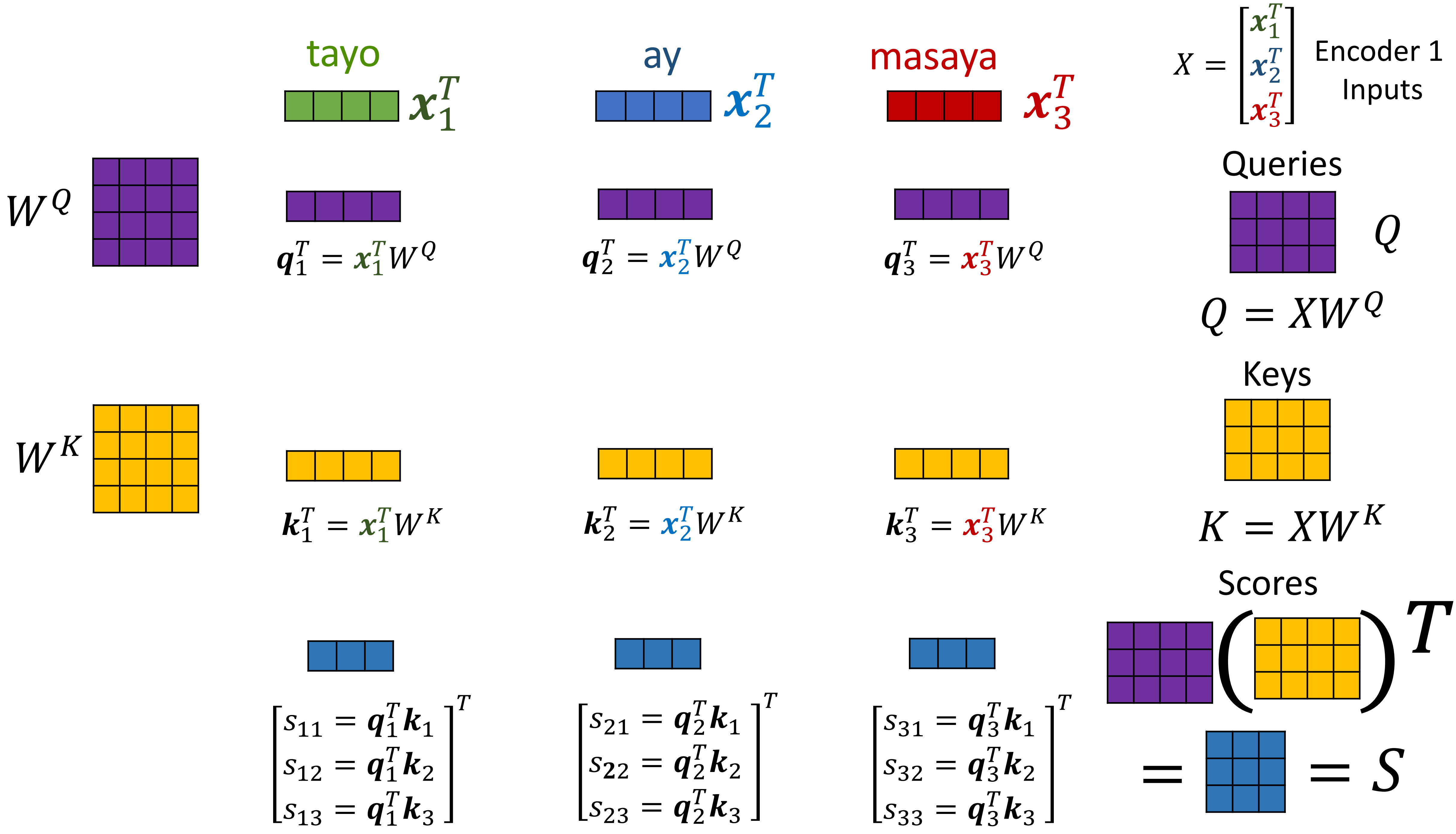


Attention between 2 words



Attention as measured by the width of the arrow

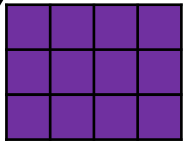
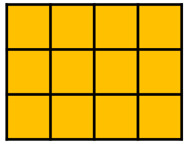
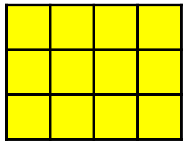

Self-Attention
Embedding
tayo
ay
masaya
x_1^T
x_2^T
x_3^T
$X = \begin{bmatrix} x_1^T \\ x_2^T \\ x_3^T \end{bmatrix}$
Encoder 1 Inputs
Attention Layer 1 Learnable Parameters
W^Q
W^K
W^V
$q_1^T = x_1^T W^Q$
$q_2^T = x_2^T W^Q$
$q_3^T = x_3^T W^Q$
Queries
Q
$Q = XW^Q$
$k_1^T = x_1^T W^K$
$k_2^T = x_2^T W^K$
$k_3^T = x_3^T W^K$
Keys
$K = XW^K$
$v_1^T = x_1^T W^V$
$v_2^T = x_2^T W^V$
$v_3^T = x_3^T W^V$
Values
V
$V = XW^V$

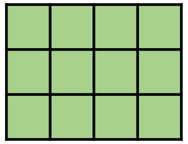


tayo
ay
masaya
x_1^T
x_2^T
x_3^T
$X = \begin{bmatrix} x_1^T \\ x_2^T \\ x_3^T \end{bmatrix}$
Encoder 1 Inputs
W^Q
$q_1^T = x_1^T W^Q$
$q_2^T = x_2^T W^Q$
$q_3^T = x_3^T W^Q$
Queries
Q
$Q = XW^Q$
W^K
$k_1^T = x_1^T W^K$
$k_2^T = x_2^T W^K$
$k_3^T = x_3^T W^K$
Keys
$K = XW^K$
$\begin{bmatrix} s_{11} = q_1^T k_1 \\ s_{12} = q_1^T k_2 \\ s_{13} = q_1^T k_3 \end{bmatrix}^T$
$\begin{bmatrix} s_{21} = q_2^T k_1 \\ s_{22} = q_2^T k_2 \\ s_{23} = q_2^T k_3 \end{bmatrix}^T$
$\begin{bmatrix} s_{31} = q_3^T k_1 \\ s_{32} = q_3^T k_2 \\ s_{33} = q_3^T k_3 \end{bmatrix}^T$
Scores
$(\ )^T$
$= \ = S$

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

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

$Attention = softmax\Bigg($   $^T \Big/ \sqrt{d_k}\Bigg)$ 

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

Values When all things considered, what my outputs should be

Keys What others think my outputs should be

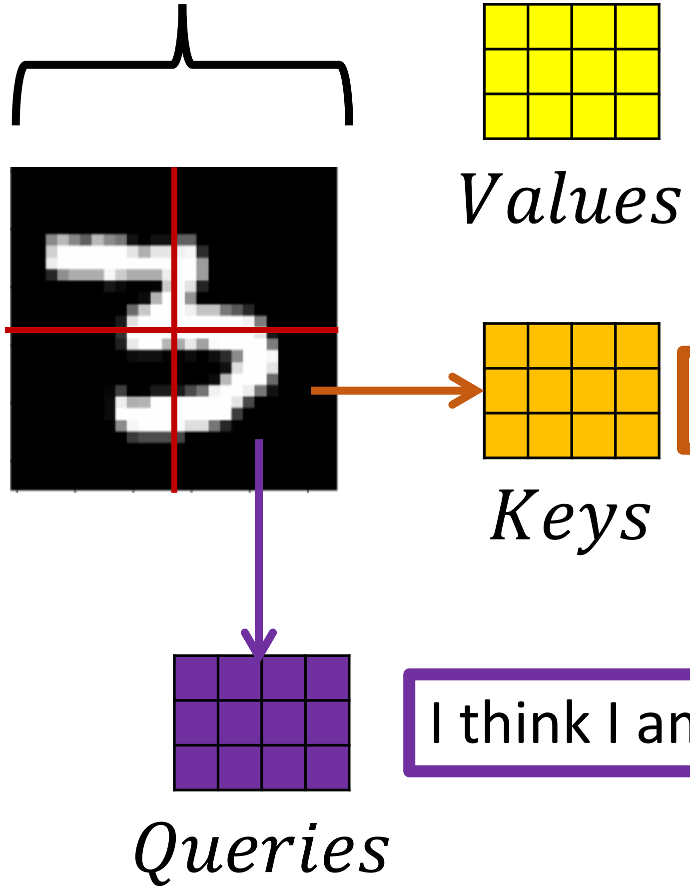
Queries What I think my outputs should be

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

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

Consider an Attention Layer Examining a Digit

Quiet! I can see everything that you can see. My friend, you are a part of digit 3.



Shut up! You can't be a part of digit 5. I saw a bar to the left.

I think I am a part of digit 5

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

Multi-Head
(eg 8-head)

tayo $\boldsymbol{x}_1^T$

ay $\boldsymbol{x}_2^T$

masaya $\boldsymbol{x}_3^T$

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

$K_8 = XW_8^K$

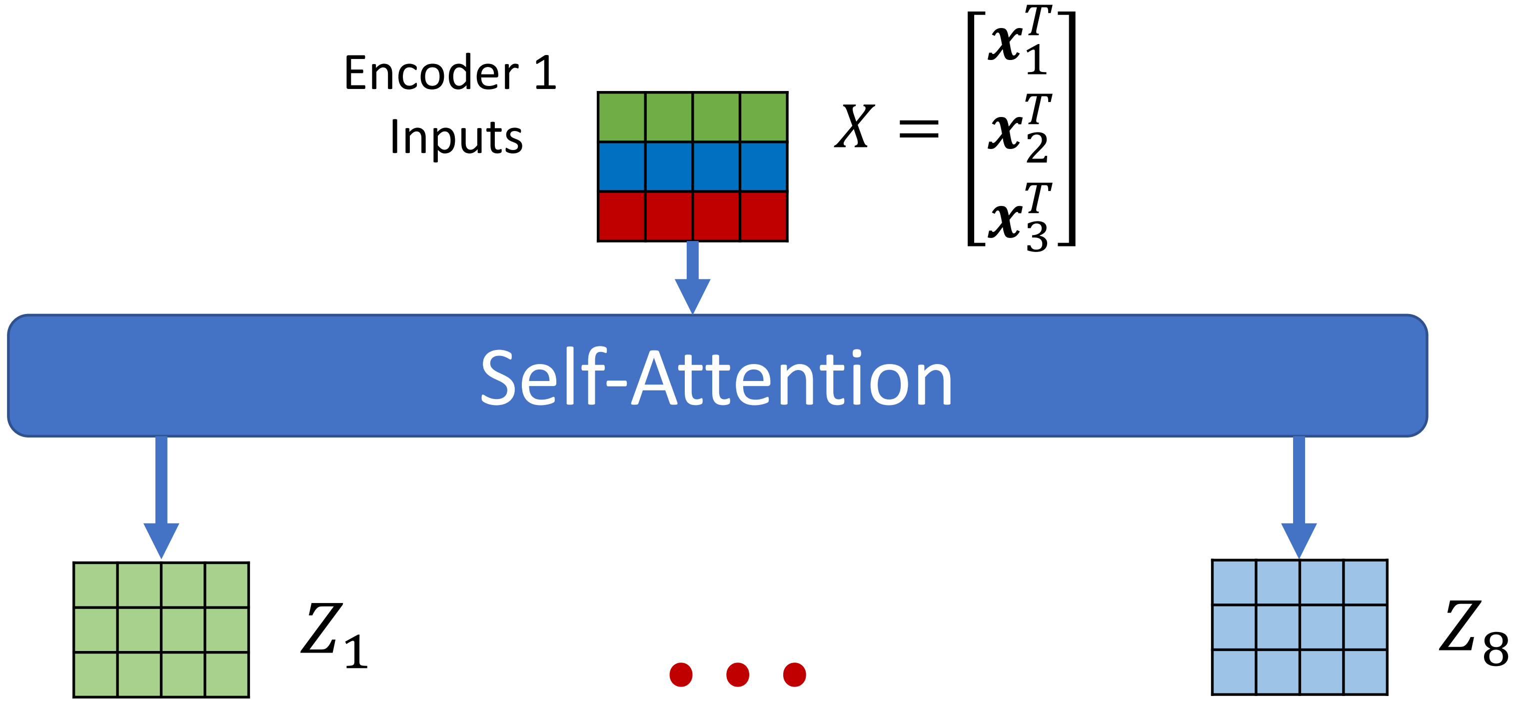
Values

W_8^V

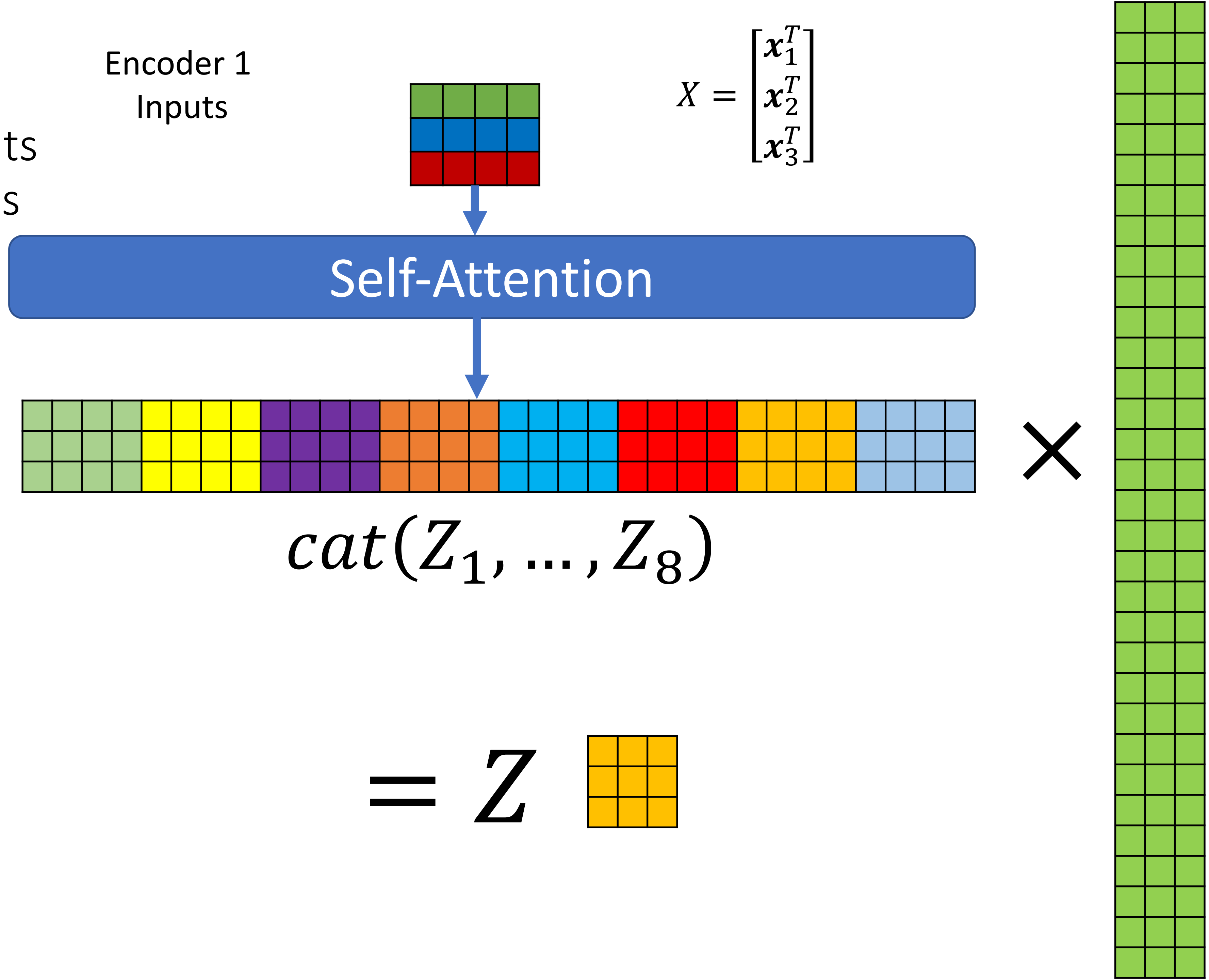
$V_8 = XW_8^V$

Head 8: Z_8

Multi-Head
(eg 8-head)



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



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

$$cat(Z_1, \ldots, Z_8) \times W^O$$

$$= Z$$

Adding Position Info to Inputs

	tayo	ay	masaya
Input Embedding	$\boldsymbol{x}_1^T$	$\boldsymbol{x}_2^T$	$\boldsymbol{x}_3^T$
	+	+	+
Positional Encoding	$\boldsymbol{p}_1^T$	$\boldsymbol{p}_2^T$	$\boldsymbol{p}_3^T$
	=	=	=
Input Embedding + Position	$\widehat{\boldsymbol{x}}_1^T$	$\widehat{\boldsymbol{x}}_2^T$	$\widehat{\boldsymbol{x}}_3^T$

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

Positional Encoding

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

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

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

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

Other positional encoding methods: learnable

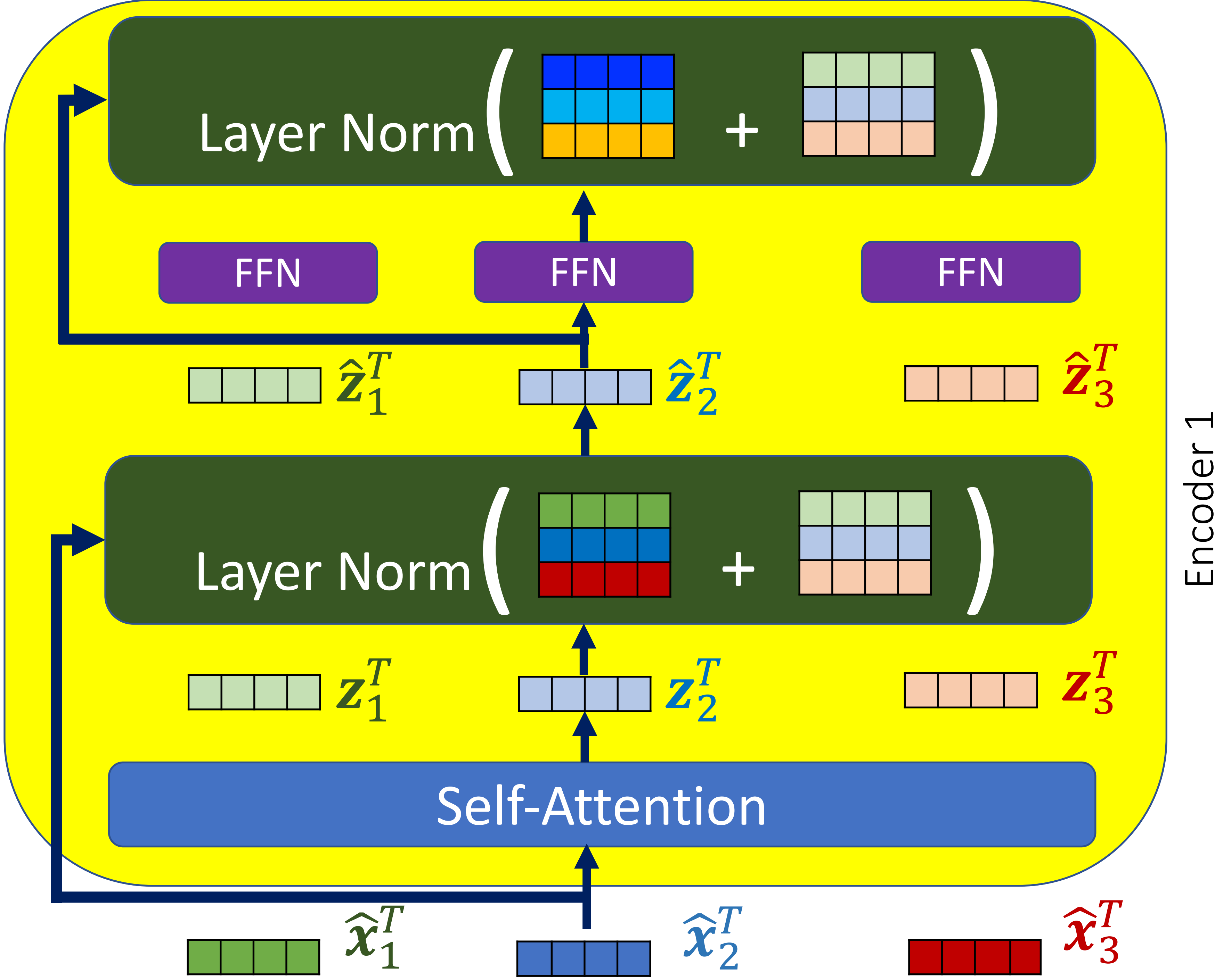
Assuming $n_{pos-1} = 2, n_{dim-1} = 3, d_k = 4$

pos	dim			
	0	1	2	3
0	$\sin\left(\frac{0}{10000^{0/4}}\right)$	$\cos\left(\frac{0}{10000^{0/4}}\right)$	$\sin\left(\frac{0}{10000^{2/4}}\right)$	$\cos\left(\frac{0}{10000^{2/4}}\right)$
1	$\sin\left(\frac{1}{10000^{0/4}}\right)$	$\cos\left(\frac{1}{10000^{0/4}}\right)$	$\sin\left(\frac{1}{10000^{2/4}}\right)$	$\cos\left(\frac{1}{10000^{2/4}}\right)$
2	$\sin\left(\frac{2}{10000^{0/4}}\right)$	$\cos\left(\frac{2}{10000^{0/4}}\right)$	$\sin\left(\frac{2}{10000^{2/4}}\right)$	$\cos\left(\frac{2}{10000^{2/4}}\right)$

Improvements:

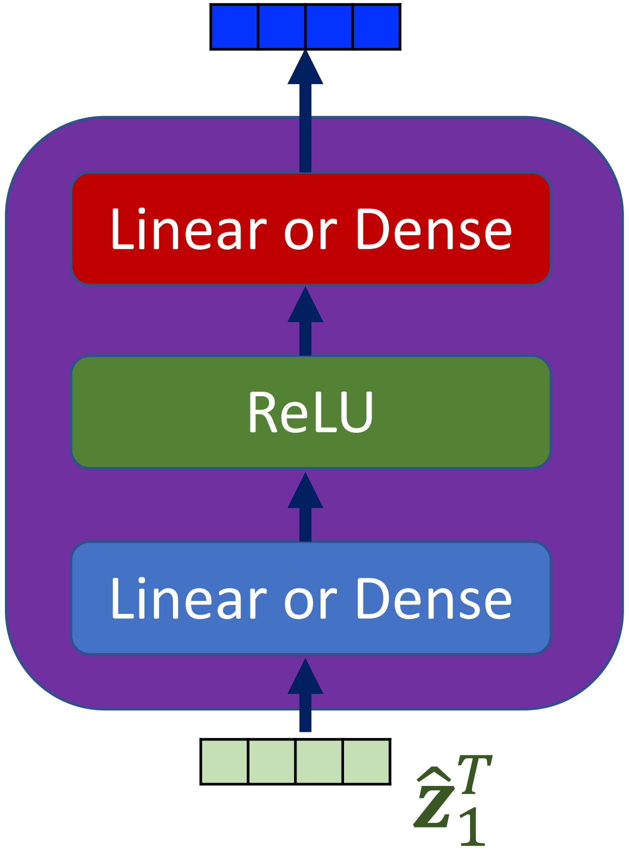
Residual Connections

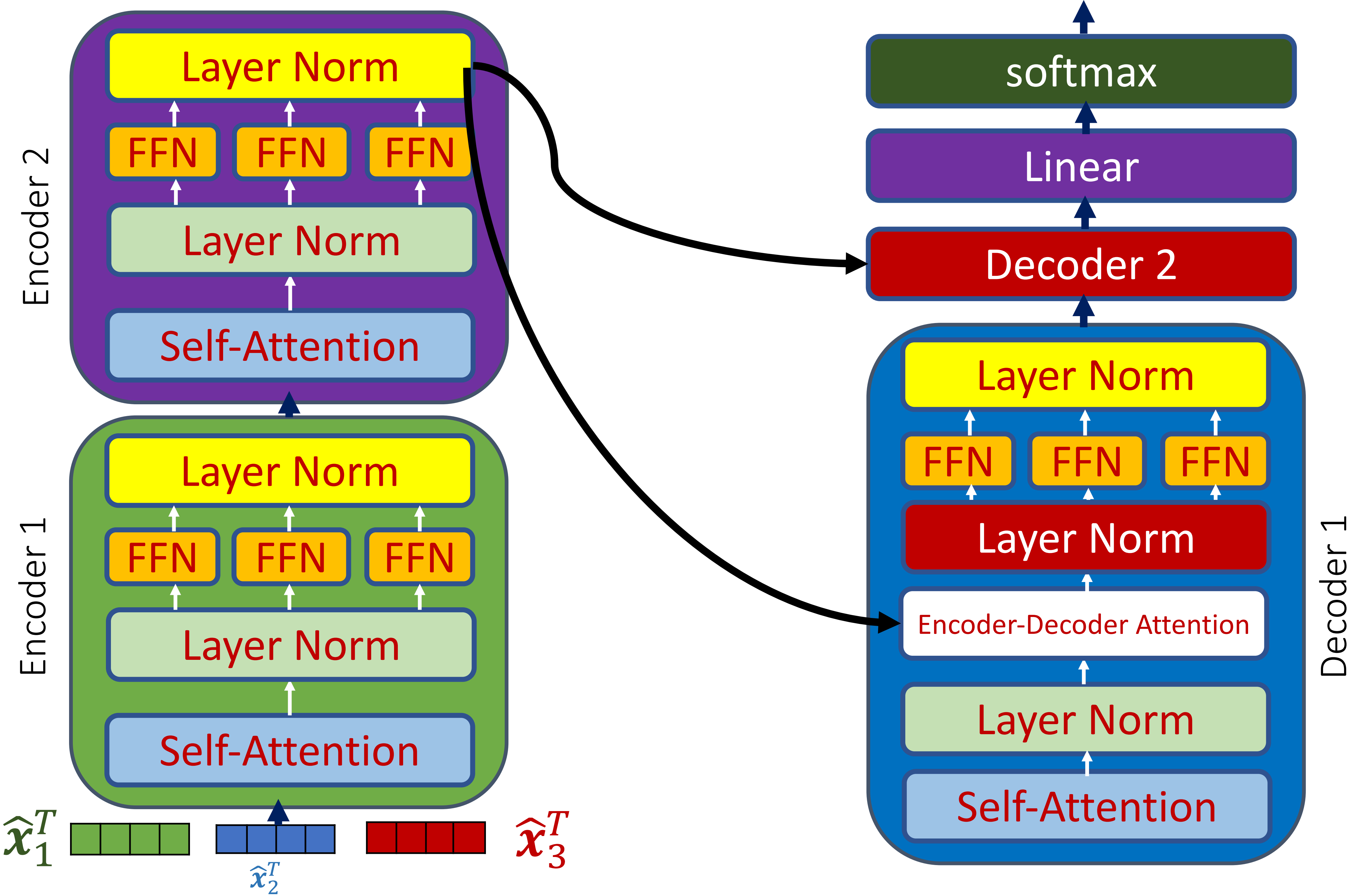
Layer Norm



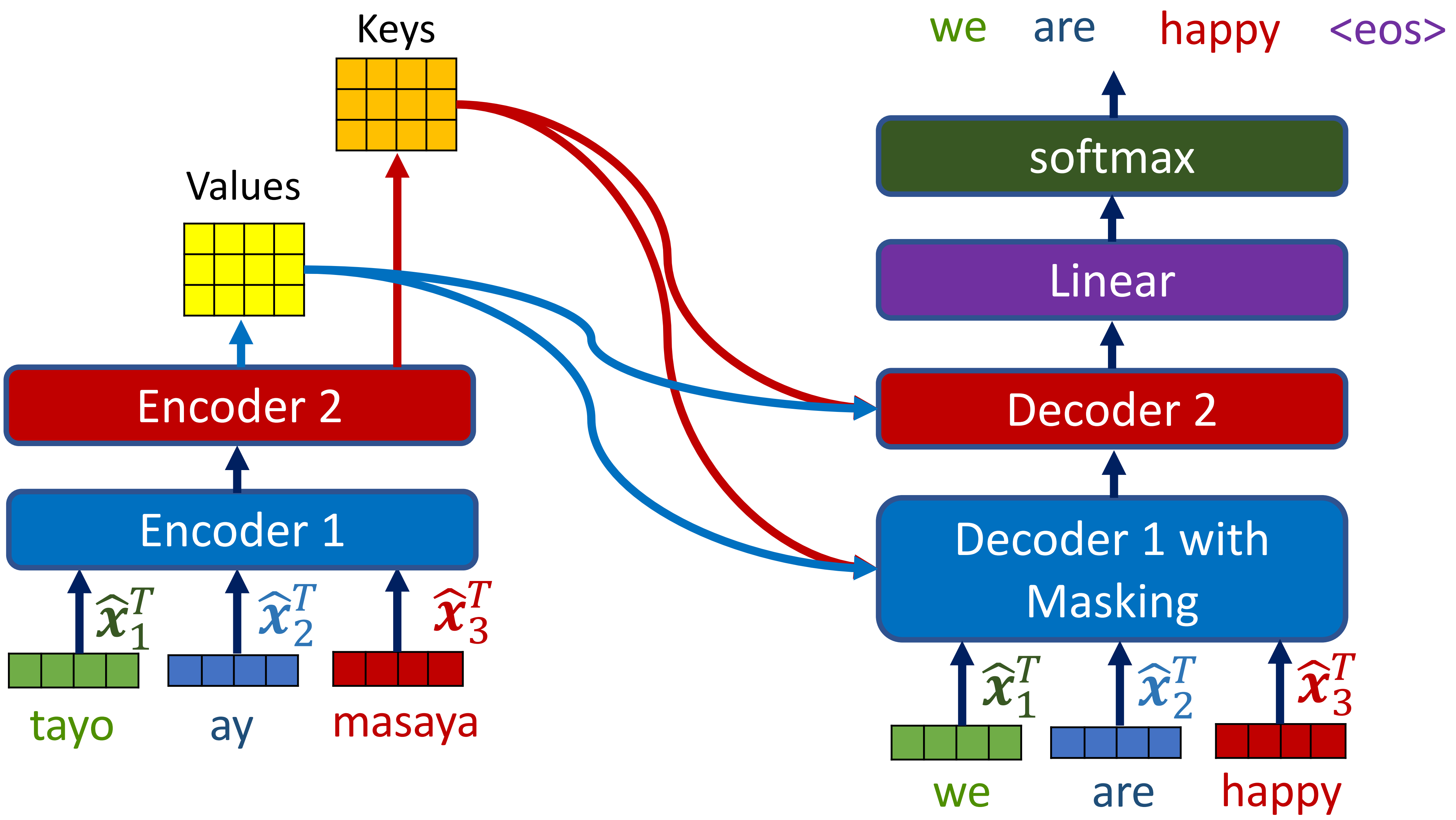
FFN: Feed Forward Neural Network (MLP)

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





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



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

Vision Transformer

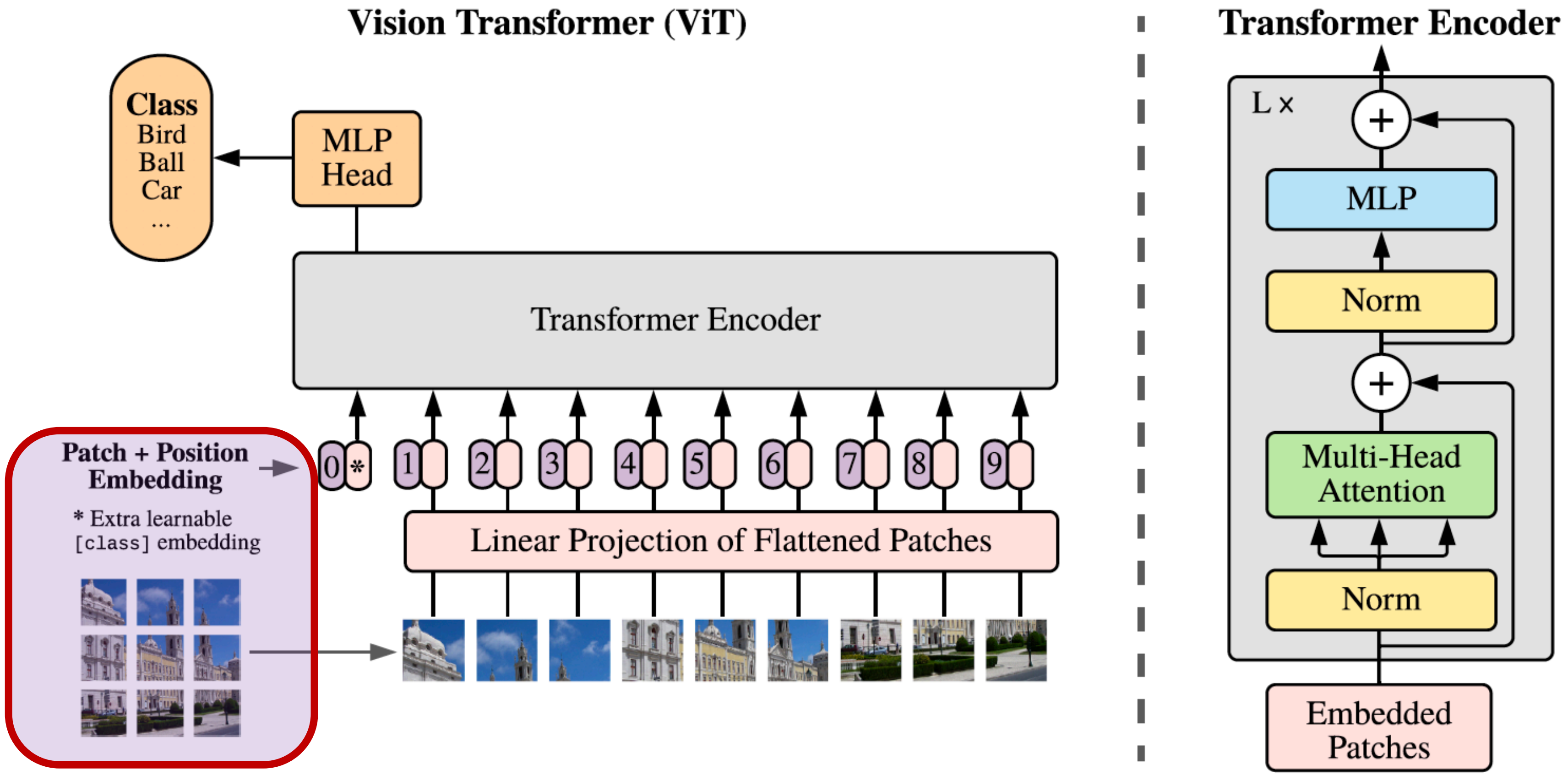
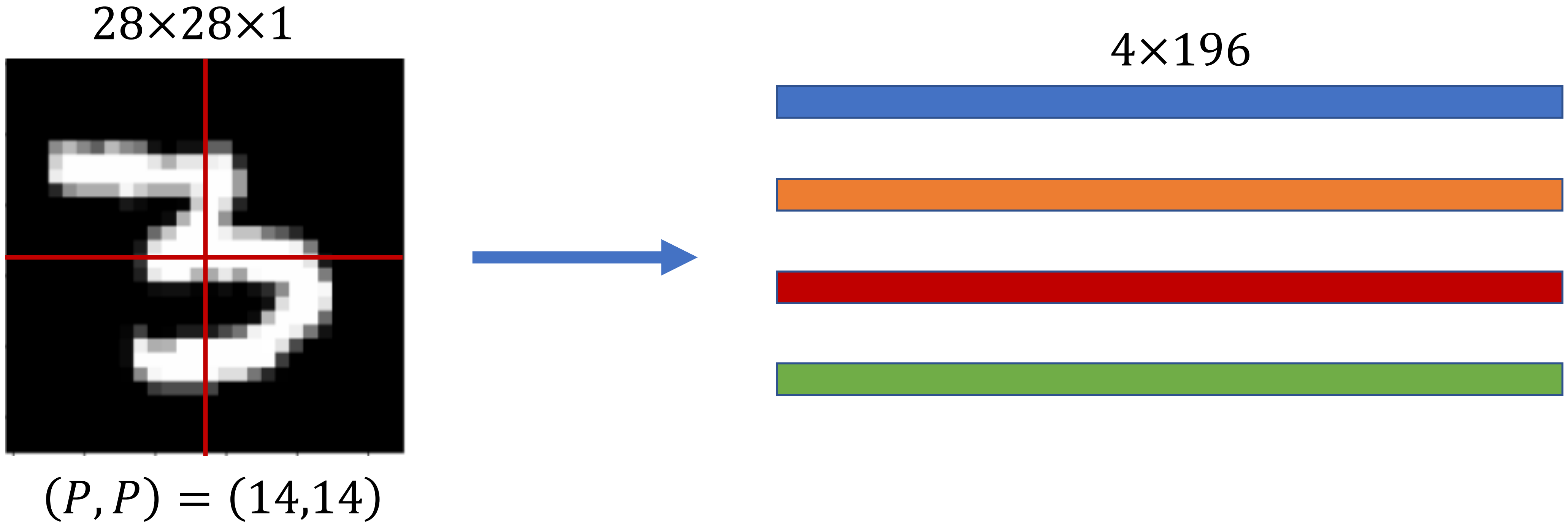


Figure 1: Model overview. We split an image into fixed-size patches, linearly embed each of them, add position embeddings to the resulting sequence of vectors, and feed the patches to a standard Transformer encoder. In order to perform classification, we use the standard approach of adding an extra learnable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

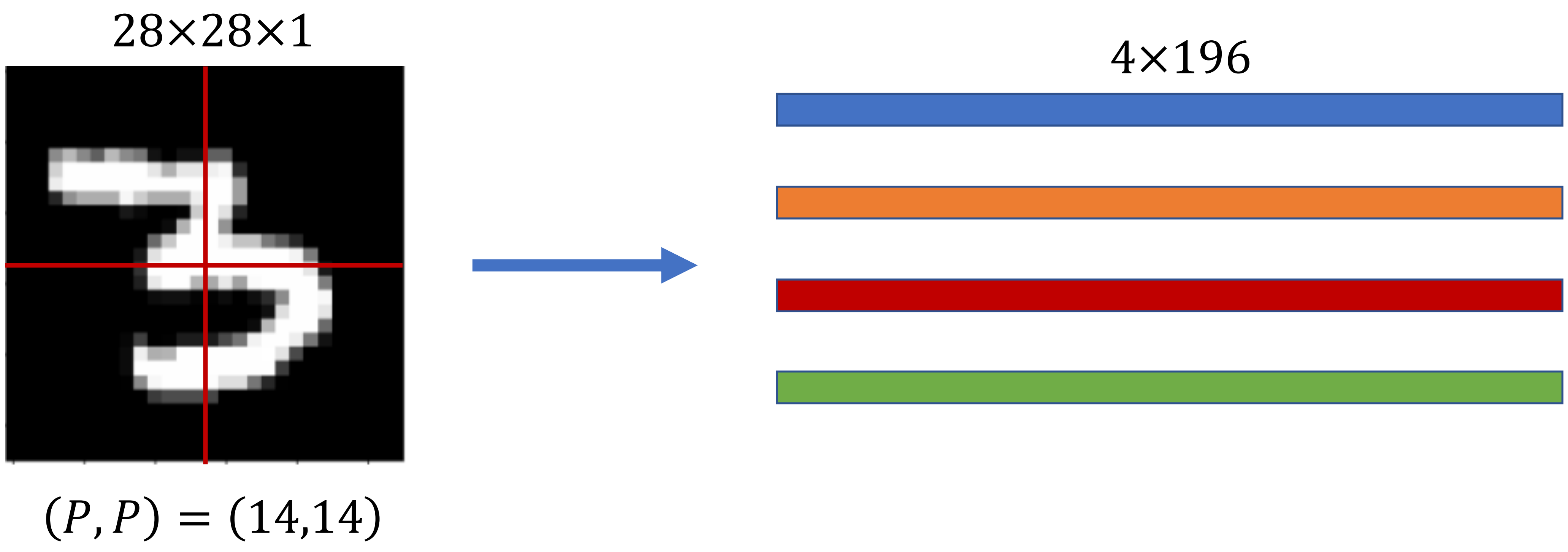
AN IMAGE IS WORTH 16X16 WORDS:
TRANSFORMERS FOR IMAGE RECOGNITION AT SCALE, ICLR 2021 Submission

```python
class ViT(nn.Module):
    def __init__(self, *, image_size, patch_size, num_classes, dim, depth, heads, mlp_dim, channels = 3):
        super().__init__()
        assert image_size % patch_size == 0, 'image dimensions must be divisible by the patch size'
        num_patches = (image_size // patch_size) ** 2
        patch_dim = channels * patch_size ** 2

        self.patch_size = patch_size

        self.pos_embedding = nn.Parameter(torch.randn(1, num_patches + 1, dim))
        self.patch_to_embedding = nn.Linear(patch_dim, dim)
        self.cls_token = nn.Parameter(torch.randn(1, 1, dim))
        self.transformer = Transformer(dim, depth, heads, mlp_dim)

        self.to_cls_token = nn.Identity()
```

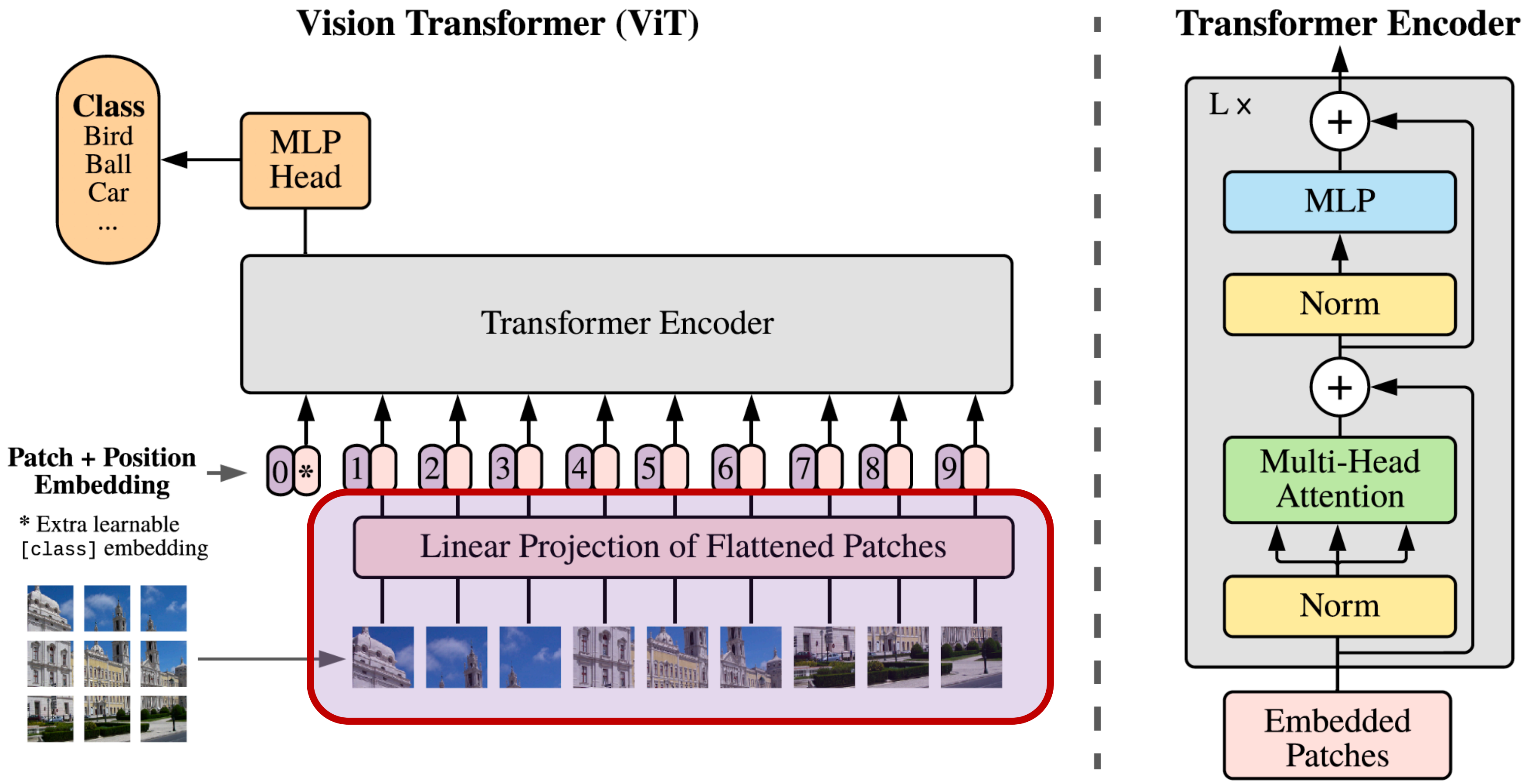


3.1 VISION TRANSFORMER (VIT)

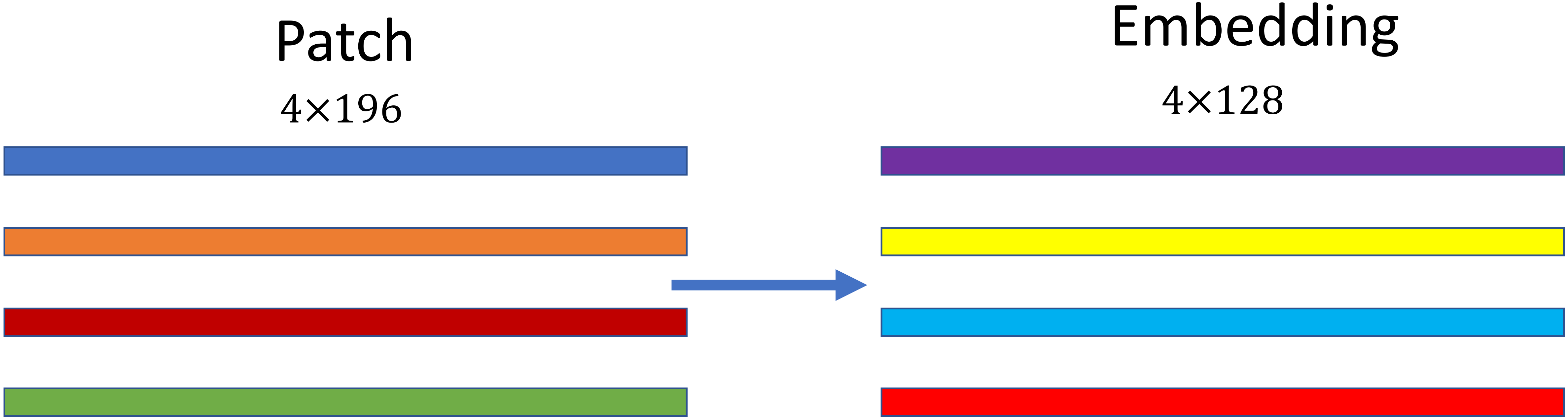
Our Transformer for images follows the architecture designed for NLP. Figure 1 depicts the setup. The standard Transformer receives as input a 1D sequence of token embeddings. To handle 2D images, we reshape the image $\mathbf{x} \in \mathbb{R}^{H \times W \times C}$ into a sequence of flattened 2D patches $\mathbf{x}_p \in \mathbb{R}^{N \times (P^2 \cdot C)}$. (H, W) is the resolution of the original image and (P, P) is the resolution of each image patch. $N = HW/P^2$ is then the effective sequence length for the Transformer. The Transformer uses constant widths through all of its layers, so a trainable linear projection maps each vectorized patch to the model dimension D (Eq. 1), the output of which we refer to as our patch embeddings.




```python
def forward(self, img, mask = None):
    p = self.patch_size

    x = rearrange(img, 'b c (h p1) (w p2) -> b (h w) (p1 p2 c)', p1 = p, p2 = p)
```




```python
    self.patch_to_embedding = nn.Linear(patch_dim, dim)
def forward(self, img, mask = None):
    p = self.patch_size

    x = rearrange(img, 'b c (h p1) (w p2) -> b (h w) (p1 p2 c)', p1 = p, p2 = p)
    x = self.patch_to_embedding(x)
```




```python
self.patch_to_embedding = nn.Linear(patch_dim, dim)
```

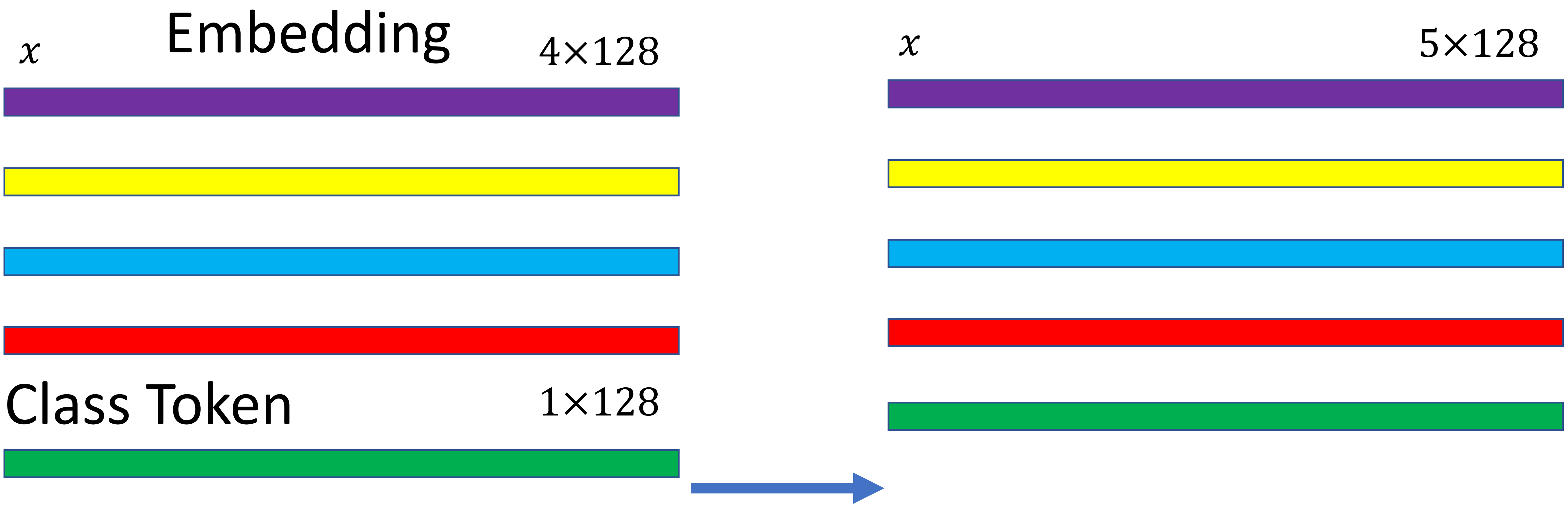
$$\mathbf{z}_0 = [\mathbf{x}_{\text{class}};\, \mathbf{x}_p^1\mathbf{E};\, \mathbf{x}_p^2\mathbf{E};\, \cdots;\, \mathbf{x}_p^N\mathbf{E}] + \mathbf{E}_{pos}, \qquad \mathbf{E} \in \mathbb{R}^{(P^2 \cdot C) \times D},\, \mathbf{E}_{pos} \in \mathbb{R}^{(N+1) \times D}$$

Class Token

1×128

Similar to BERT's `[class]` token, we prepend a learnable embedding to the sequence of embedded patches ($\mathbf{z}_0^0 = \mathbf{x}_{\text{class}}$), whose state at the output of the Transformer encoder ($\mathbf{z}_0^L$) serves as the

```
    self.cls_token = nn.Parameter(torch.randn(1, 1, dim))

def forward(self, img, mask = None):
    p = self.patch_size

    x = rearrange(img, 'b c (h p1) (w p2) -> b (h w) (p1 p2 c)', p1 = p, p2 = p
    x = self.patch_to_embedding(x)

    cls_tokens = self.cls_token.expand(img.shape[0], -1, -1)
```




```python
x = torch.cat((cls_tokens, x), dim=1)
```

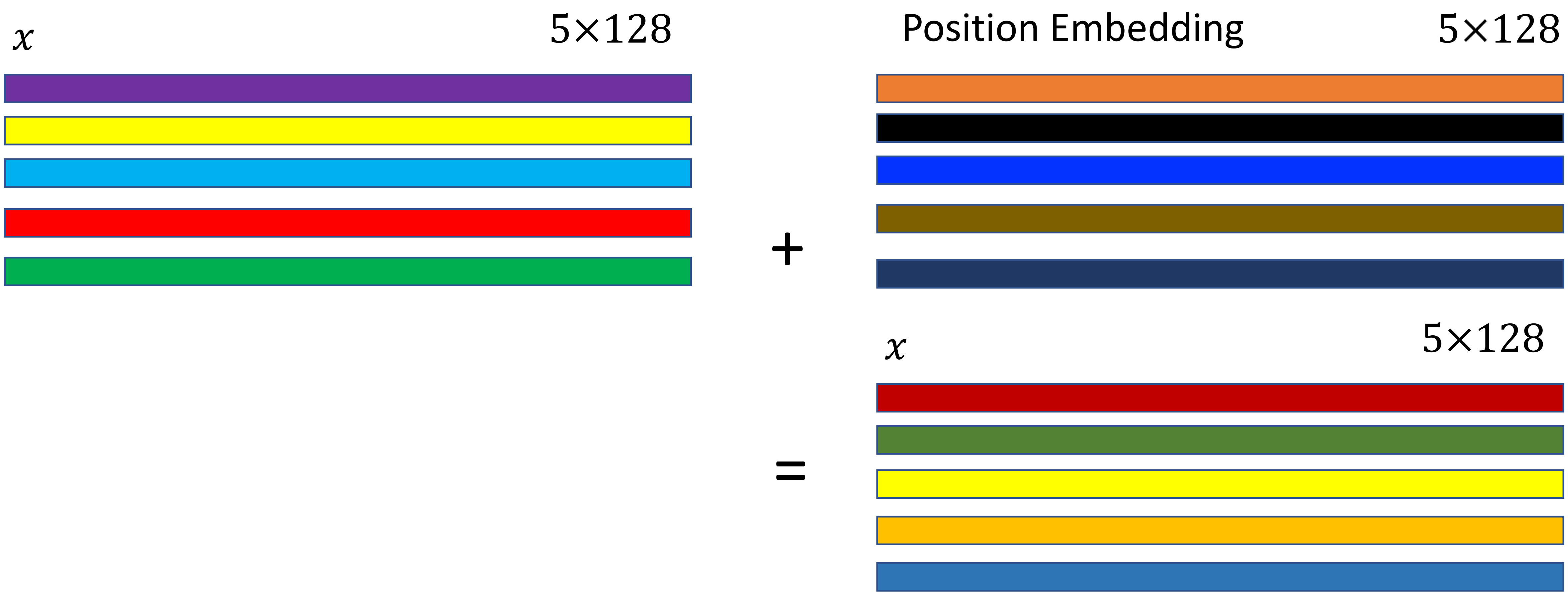
$$\mathbf{z}_0 = [\mathbf{x}_{\text{class}};\, \mathbf{x}_p^1\mathbf{E};\, \mathbf{x}_p^2\mathbf{E};\, \cdots;\, \mathbf{x}_p^N\mathbf{E}] + \mathbf{E}_{pos},$$

```python
def forward(self, img, mask = None):
    p = self.patch_size

    x = rearrange(img, 'b c (h p1) (w p2) -> b (h w) (p1 p2 c)', p1 = p, p2 = p)
    x = self.patch_to_embedding(x)

    cls_tokens = self.cls_token.expand(img.shape[0], -1, -1)
    x = torch.cat((cls_tokens, x), dim=1)
```

Position Embedding

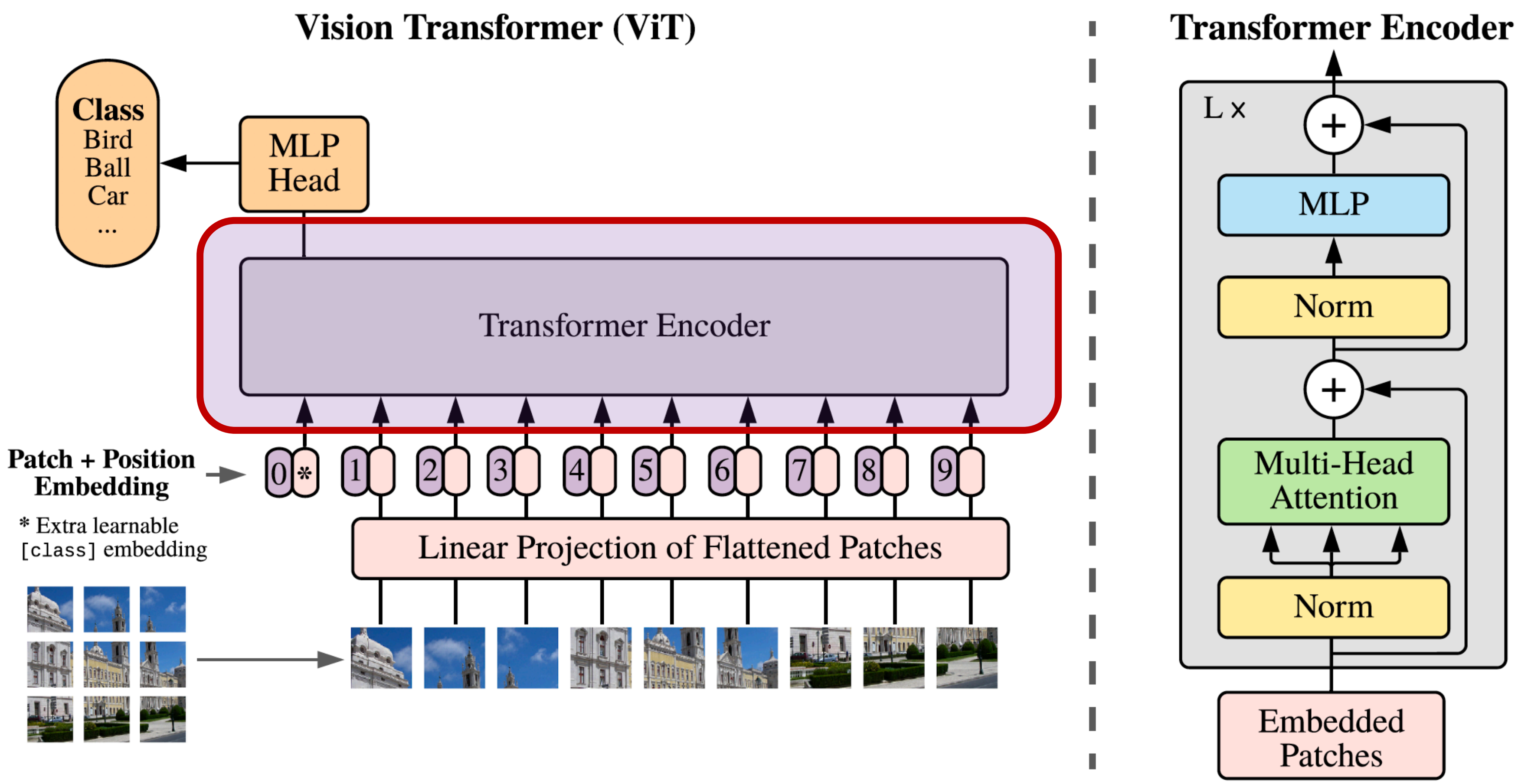
Position embeddings are added to the patch embeddings to retain positional information. We explore different 2D-aware variants of position embeddings (Appendix C.3) without any significant gains over standard 1D position embeddings. The joint embedding serves as input to the encoder.

```
self.pos_embedding = nn.Parameter(torch.randn(1, num_patches + 1, dim))
```

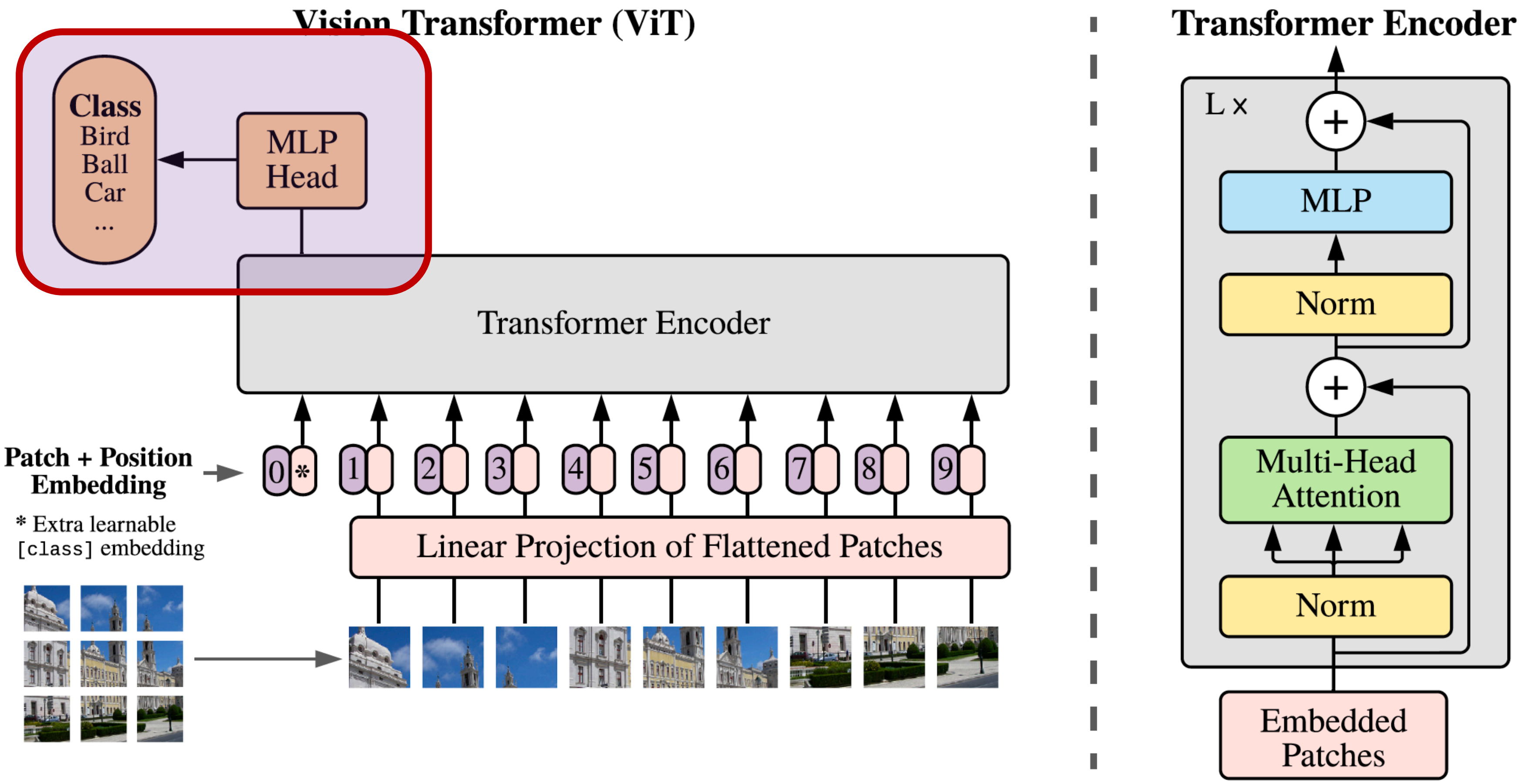


$$\mathbf{z}_0 = [\mathbf{x}_{\text{class}};\, \mathbf{x}_p^1\mathbf{E};\, \mathbf{x}_p^2\mathbf{E};\, \cdots;\, \mathbf{x}_p^N\mathbf{E}] + \mathbf{E}_{pos}, \qquad \mathbf{E} \in \mathbb{R}^{(P^2\cdot C)\times D},\, \mathbf{E}_{pos} \in \mathbb{R}^{(N+1)\times D}$$

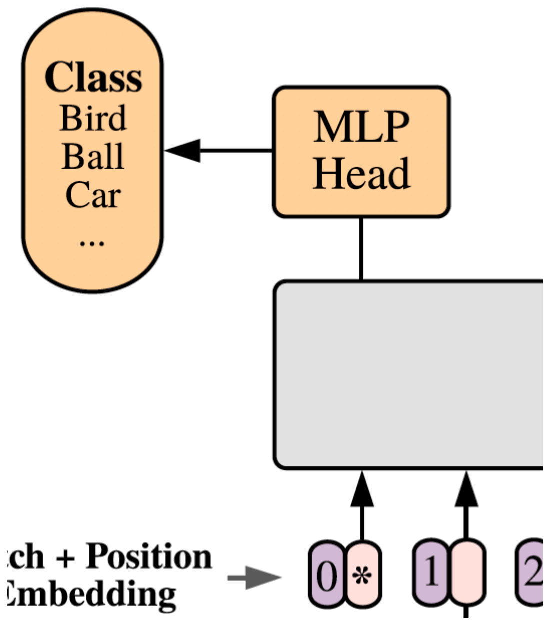
```
x += self.pos_embedding
```




```
x = self.transformer(x, mask)
```




```python
x = self.to_cls_token(x[:, 0])
return self.mlp_head(x)
```




```
self.mlp_head = nn.Sequential(
    nn.Linear(dim, mlp_dim),
    nn.GELU(),
    nn.Linear(mlp_dim, num_classes)
)
```

image representation $\mathbf{y}$ (Eq. 4). Both during pre-training and fine-tuning, the classification head is attached to $\mathbf{z}_L^0$.

```
x = self.to_cls_token(x[:, 0])
return self.mlp_head(x)
```

```python
def forward(self, img, mask = None):
    p = self.patch_size

    x = rearrange(img, 'b c (h p1) (w p2) -> b (h w) (p1 p2 c)', p1 = p, p2 = p)
    x = self.patch_to_embedding(x)

    cls_tokens = self.cls_token.expand(img.shape[0], -1, -1)
    x = torch.cat((cls_tokens, x), dim=1)
    x += self.pos_embedding
    x = self.transformer(x, mask)

    x = self.to_cls_token(x[:, 0])
    return self.mlp_head(x)
```

Transformer

$$\mathbf{z}'_\ell = \mathrm{MSA}(\mathrm{LN}(\mathbf{z}_{\ell-1})) + \mathbf{z}_{\ell-1}, \qquad \ell = 1 \ldots L$$

$$\mathbf{z}_\ell = \mathrm{MLP}(\mathrm{LN}(\mathbf{z}'_\ell)) + \mathbf{z}'_\ell, \qquad \ell = 1 \ldots L$$

$$\mathbf{y} = \mathrm{LN}(\mathbf{z}_L^0)$$

```
class Transformer(nn.Module):
    def __init__(self, dim, depth, heads, mlp_dim):
        super().__init__()
        self.layers = nn.ModuleList([])
        for _ in range(depth):
            self.layers.append(nn.ModuleList([
                Residual(PreNorm(dim, Attention(dim, heads = heads))),
                Residual(PreNorm(dim, FeedForward(dim, mlp_dim)))
            ]))
    def forward(self, x, mask = None):
        for attn, ff in self.layers:
            x = attn(x, mask = mask)
            x = ff(x)
        return x
```

Residual

```python
class Residual(nn.Module):
    def __init__(self, fn):
        super().__init__()
        self.fn = fn
    def forward(self, x, **kwargs):
        return self.fn(x, **kwargs) + x
```

Layer Norm

```python
class PreNorm(nn.Module):
    def __init__(self, dim, fn):
        super().__init__()
        self.norm = nn.LayerNorm(dim)
        self.fn = fn
    def forward(self, x, **kwargs):
        return self.fn(self.norm(x), **kwargs)
```

Feed Forward (MLP)

```python
class FeedForward(nn.Module):
    def __init__(self, dim, hidden_dim):
        super().__init__()
        self.net = nn.Sequential(
            nn.Linear(dim, hidden_dim),
            nn.GELU(),
            nn.Linear(hidden_dim, dim)
        )
    def forward(self, x):
        return self.net(x)
```

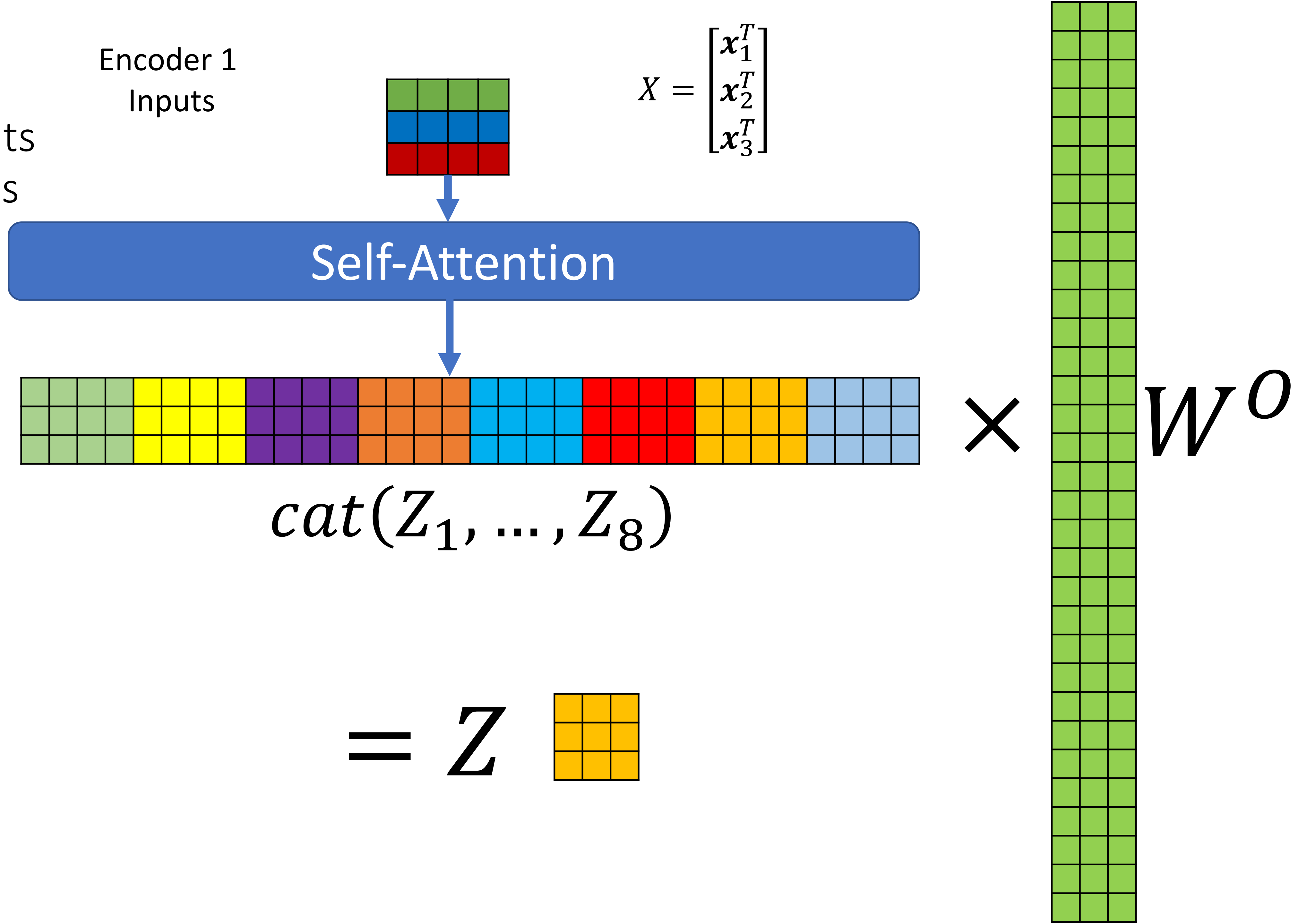
Attention

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

```
class Attention(nn.Module):
    def __init__(self, dim, heads = 8):
        super().__init__()
        self.heads = heads
        self.scale = dim ** -0.5

        self.to_qkv = nn.Linear(dim, dim * 3, bias = False)
        self.to_out = nn.Linear(dim, dim)
    def forward(self, x, mask = None):
        b, n, _, h = *x.shape, self.heads
        qkv = self.to_qkv(x)
        q, k, v = rearrange(qkv, 'b n (qkv h d) -> qkv b h n d', qkv = 3, h = h)

        dots = torch.einsum('bhid,bhjd->bhij', q, k) * self.scale
```

$$\frac{QK^T}{\sqrt{d_k}}$$

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



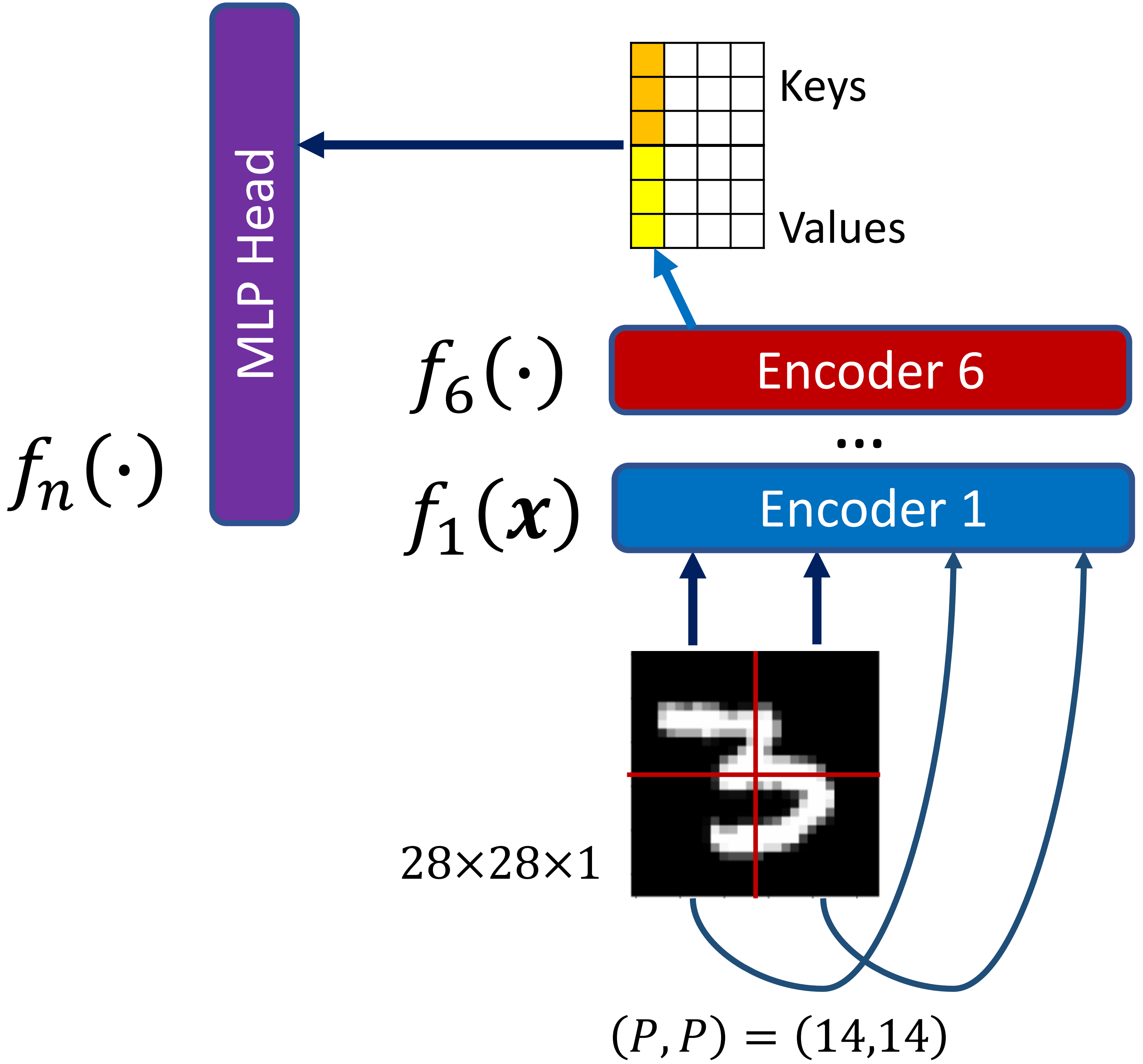
$$Attention(Q,K,V) = softmax\left(\frac{QK^T}{\sqrt{d_k}}\right)V$$

```
attn = dots.softmax(dim=-1)

out = torch.einsum('bhij,bhjd->bhid', attn, v)
out = rearrange(out, 'b h n d -> b n (h d)')
out =  self.to_out(out)
return out
```

$$\times W^O = Z$$

$$cat(Z_1, \ldots, Z_8)$$

Function composition



Inductive Bias

Transformers lack some inductive biases inherent to CNNs, such as translation equivariance and locality, 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.

CNN Model on MNIST: ~99.2% 15mins to train on CPU

Transformer Model on MNIST: ~98.2% 7mins to train on CPU

References

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

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

https://github.com/lucidrains/vit-pytorch

In Summary

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

Transformer has been used to produce state-of-the-art performances in NLP and vision

Expect more development in this field in the near future

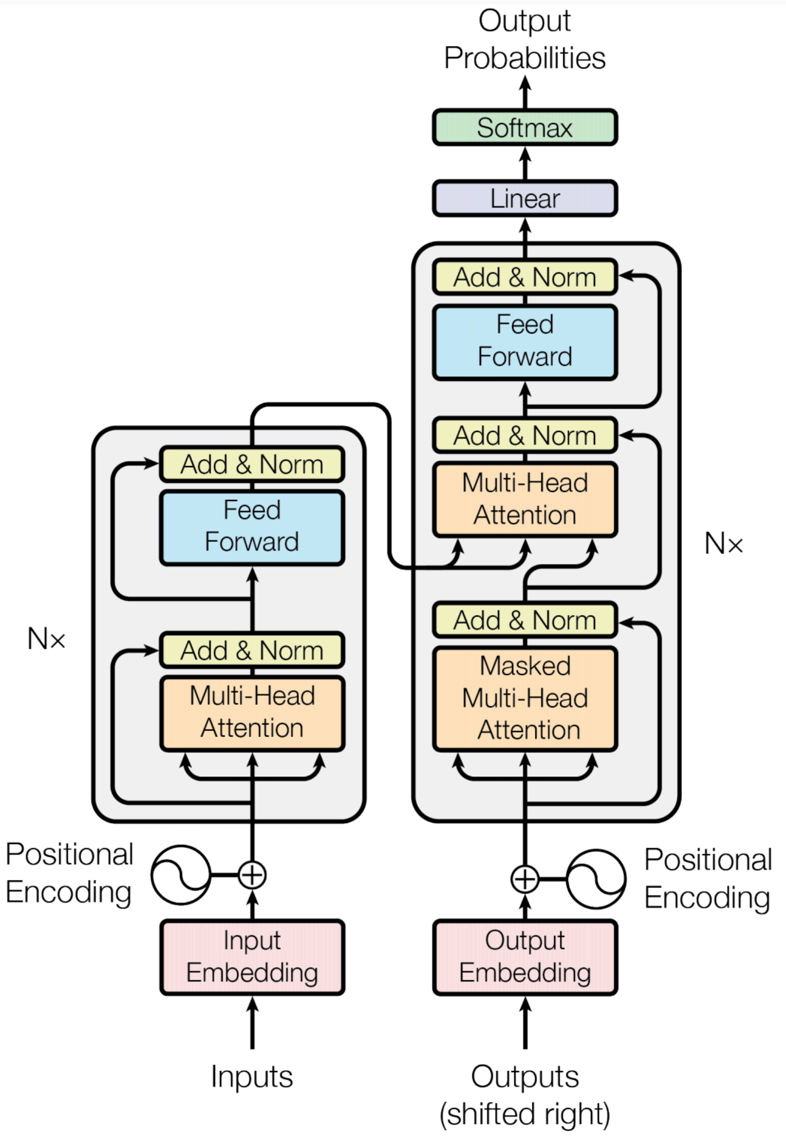


Figure 1: The Transformer - model architecture.

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