

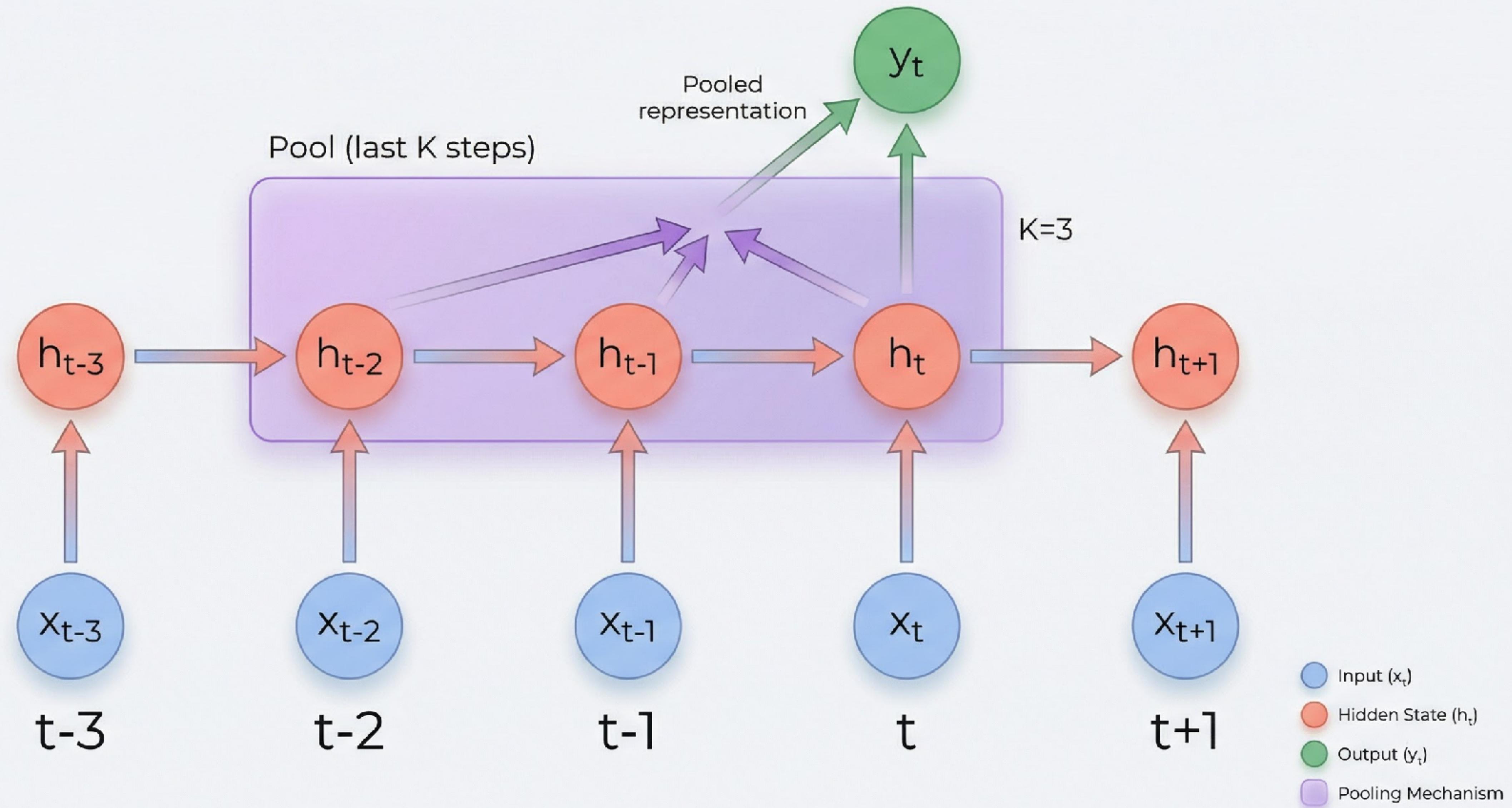
# **Deep Learning (1470)**

**Randall Balestriero**

**Class 13: Transformers**

# Recap!

# Recurrent Neural Network with Pooling Architecture

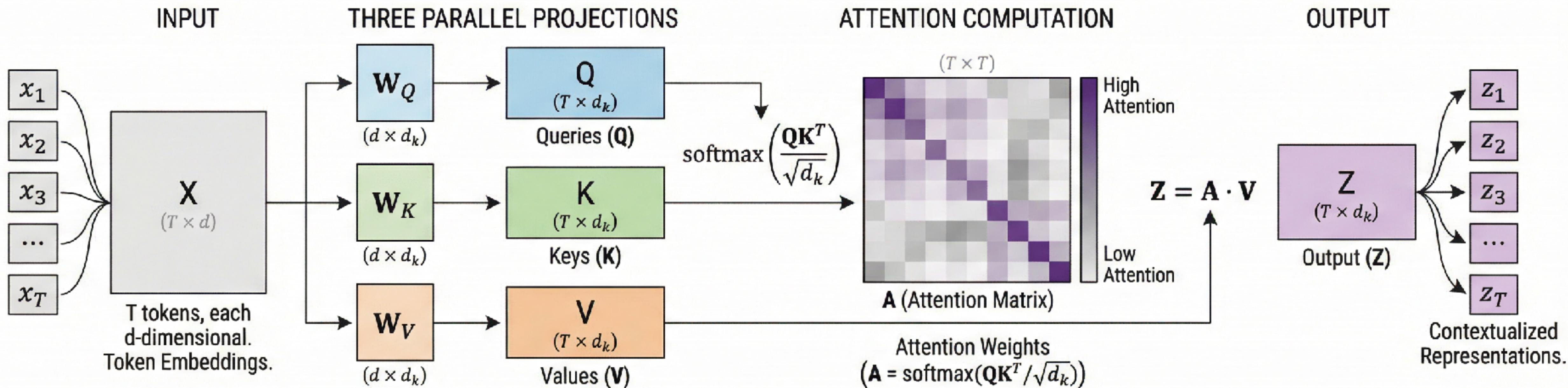


# Transformers anyone?

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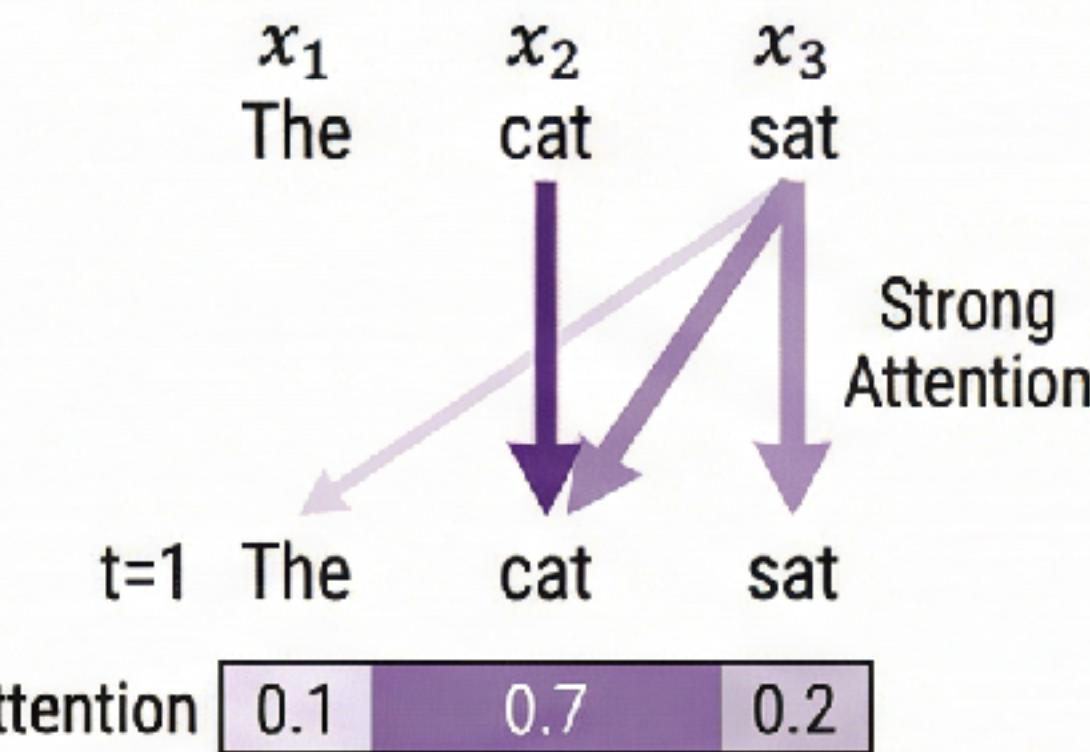


# SINGLE HEAD SELF-ATTENTION MECHANISM



## CONCRETE EXAMPLES OF ATTENTION PATTERNS FOR LANGUAGE MODELING

EXAMPLE 1 (t=3): Short Sentence



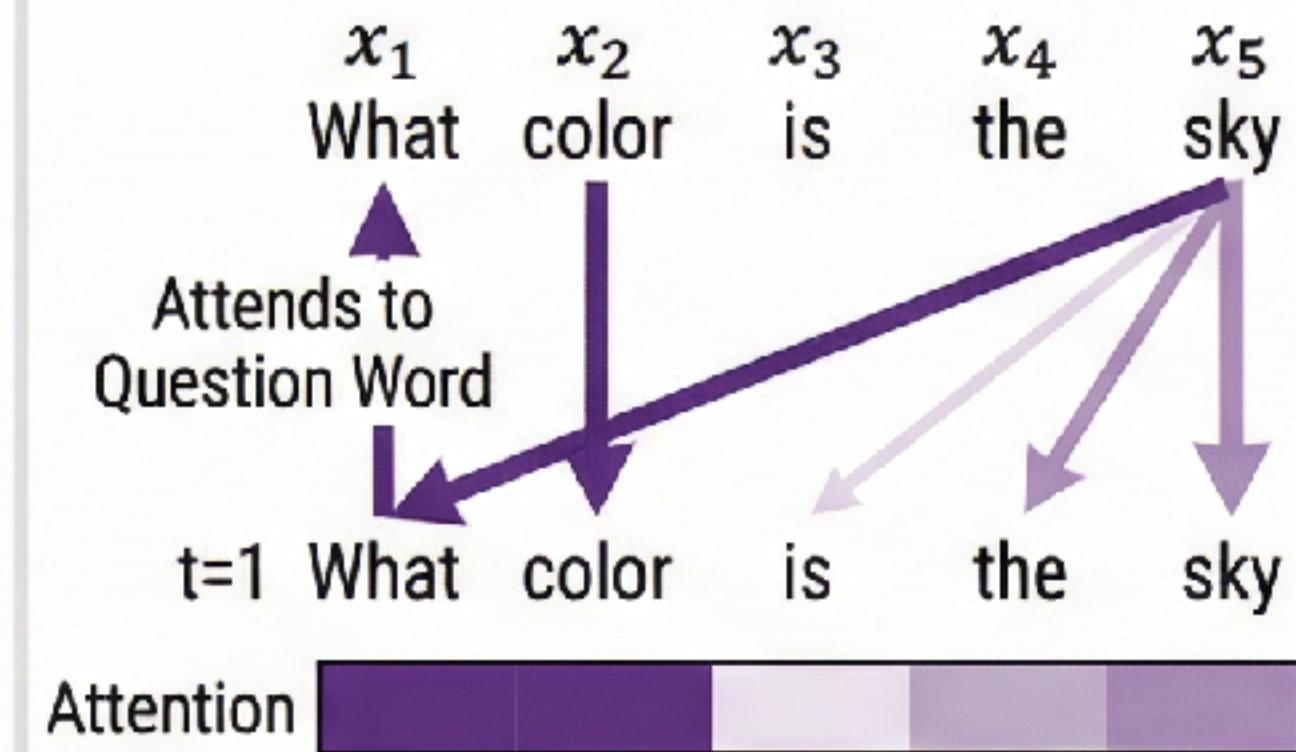
Position t=3 ("sat") attends strongly to "cat" (the subject).

EXAMPLE 2 (t=15): Long-range Dependency



Sparse attention; Position t=15 ("sat") attends to "cat" despite distance.

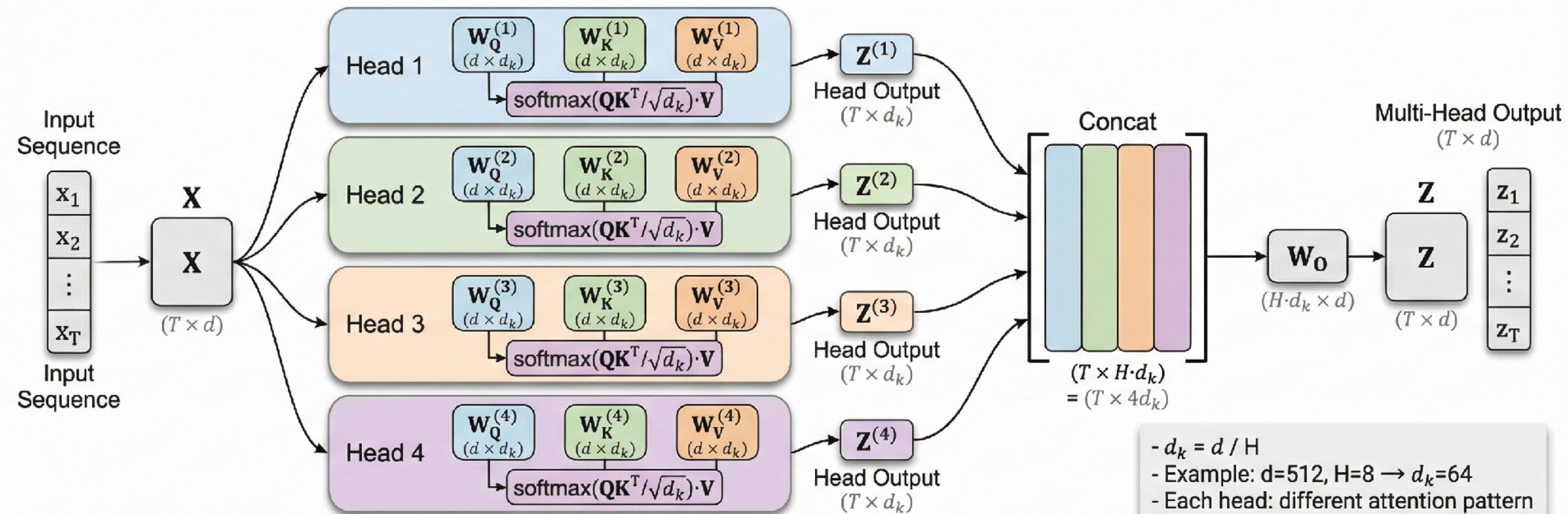
EXAMPLE 3 (Question): Question Answering



Position t=5 ("sky") attends back to "What" and "color" to form the answer.

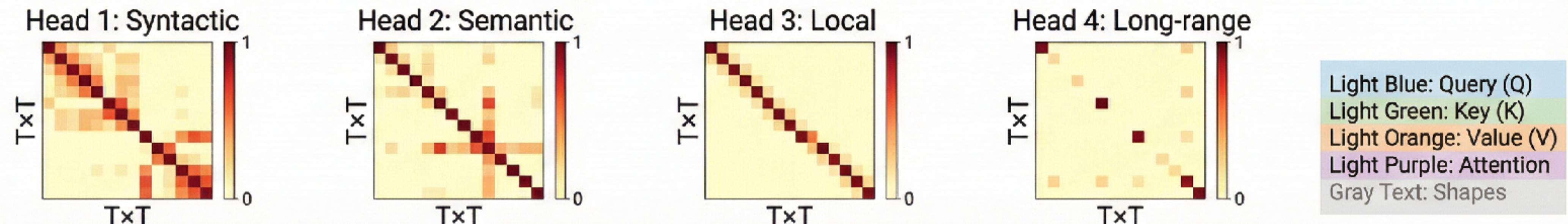
**COLOR LEGEND:** Light Blue = Queries (Q), Light Green = Keys (K) = Values (V) = Output (Z) & Attention Weights = Low Attention = High Attention

# Multi-Head Self-Attention



$$\text{MultiHead}(X) = \text{Concat}(\text{head}_1, \text{head}_2, \dots, \text{head}_H) \cdot W_O \quad \text{where } \text{head}_h = \text{Attention}(XW_Q^{(h)}, XW_K^{(h)}, XW_V^{(h)})$$

**Why Multiple Heads?**



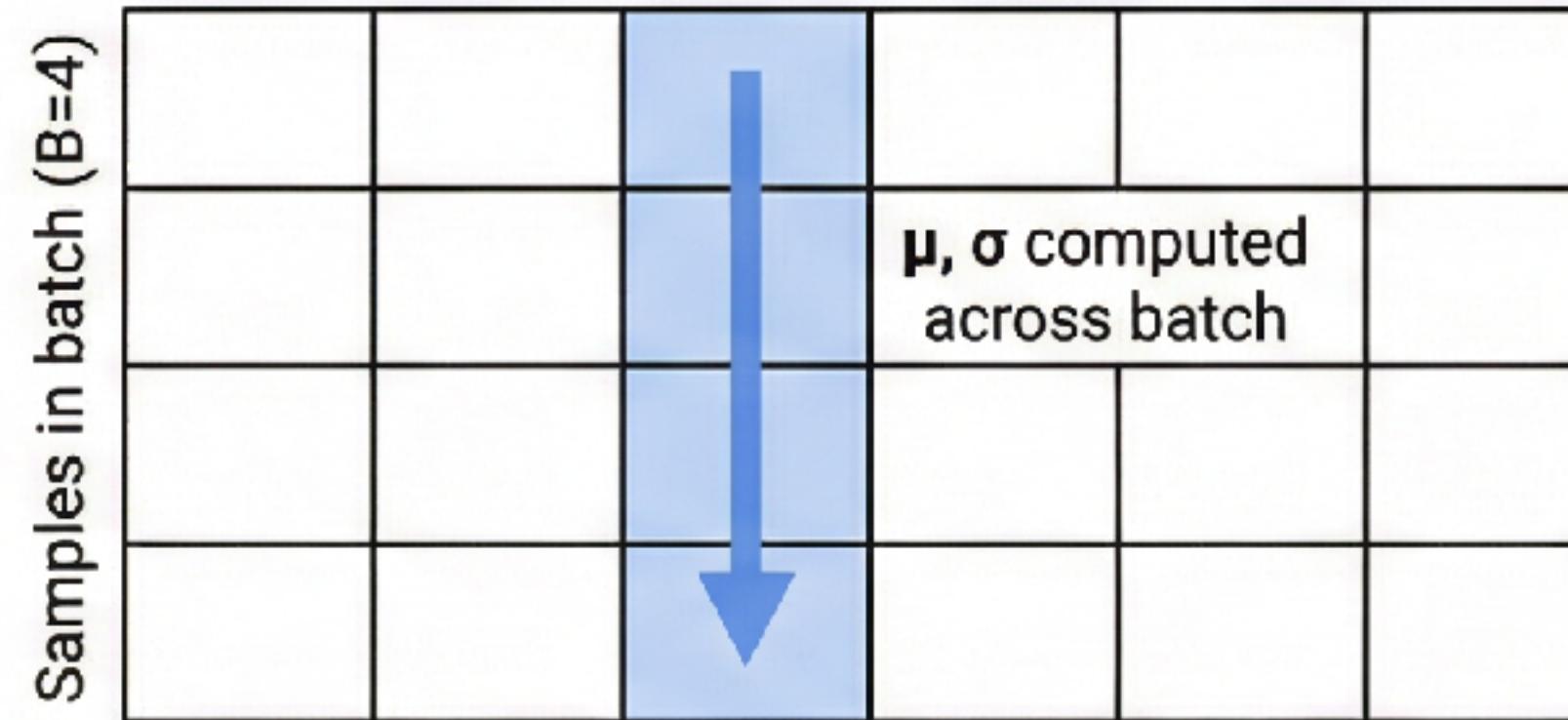
**Break: Remember batch-norm?**

# Batch Normalization vs Layer Normalization

Why transformers use LayerNorm

## BATCH NORMALIZATION

(Batch/Tokens x Features)



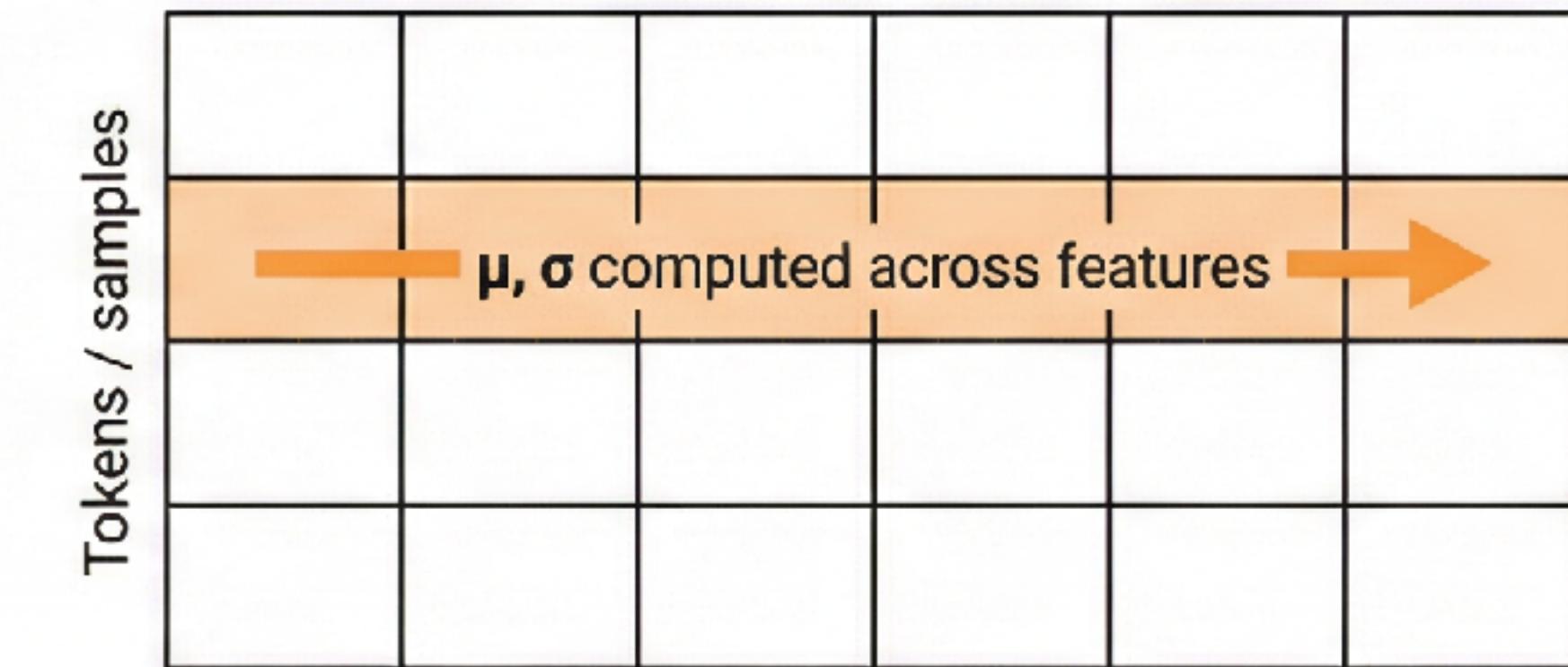
### Batch Normalization

$$\hat{x} = \frac{x - \mu_B}{\sigma_B}$$

Per feature, across batch

## LAYER NORMALIZATION

(Batch/Tokens x Features)



### Layer Normalization

$$\hat{x} = \frac{x - \mu_d}{\sigma_d}$$

Per token, across features

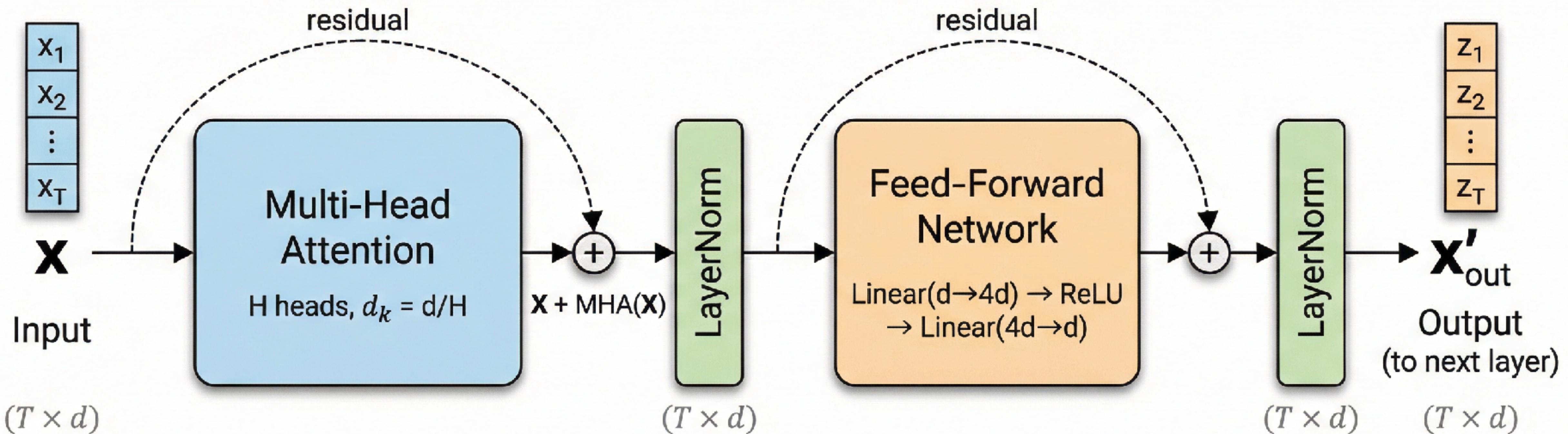
	Batch Norm	Layer Norm
Normalizes	Across batch (↓)	Across features (→)
Statistics	Per feature	Per token
Batch size 1	✗ Fails	✓ Works
Train=Inference	✗ Different	✓ Same
Transformers	✗ Not used	✓ Standard

LayerNorm: each token normalized independently → perfect for variable-length sequences & autoregressive generation

$$\text{LayerNorm}(x) = \gamma \cdot \frac{(x - \mu)}{\sqrt{\sigma^2 + \epsilon}} + \beta$$

# Transformer Layer

Stacked Nx times



**Self-Attention Sublayer:**

$$\mathbf{X}' = \text{LayerNorm}(\mathbf{X} + \text{MultiHeadAttention}(\mathbf{X}))$$

**Feed-Forward Sublayer:**

$$\mathbf{X}'' = \text{LayerNorm}(\mathbf{X}' + \text{FFN}(\mathbf{X}'))$$

$$\text{FFN}(\mathbf{x}) = \mathbf{W}_2 \cdot \text{ReLU}(\mathbf{W}_1 \mathbf{x} + \mathbf{b}_1) + \mathbf{b}_2$$

$d$  = model dim (512, 768)

$d_{ff} = 4d$  (2048, 3072)

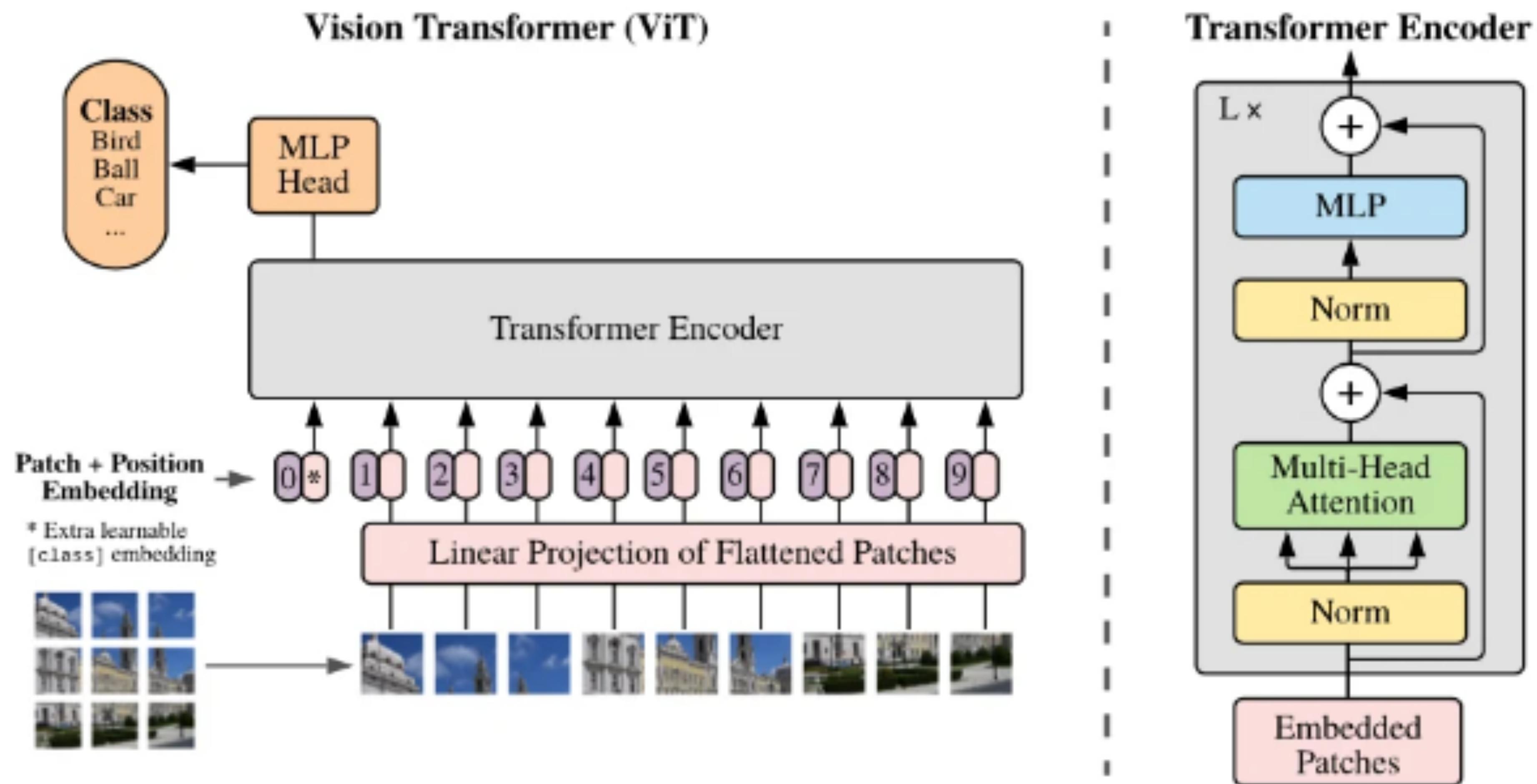
$H$  = heads (8, 12)

Light Blue: Attention Components

Light Green: LayerNorm

Light Orange: Feed-Forward Network

# Vision Transformers!



**Break: efficient implementation  
for sequence modeling?**

# Causal Self-Attention

Masked attention for autoregressive models (GPT, LLaMA, etc.)

## THE PROBLEM

The **cat sat on the**

↑  
The cat sat on the  
Left-to-right generation

When predicting token  $t$ , we can  
ONLY see tokens  $1, 2, \dots, t-1$

Token 5 cannot see  
future tokens 6, 7, ...

## FULL ATTENTION MATRIX

$Q \cdot K^T$				
$x_1$	$x_2$	$x_3$	$x_4$	$x_5$
$s_{11}$	$s_{12}$	$s_{13}$	$s_{14}$	$s_{15}$
$s_{21}$	$s_{22}$	$s_{23}$	$s_{24}$	$s_{25}$
$s_{31}$	$s_{32}$	$s_{33}$	$s_{34}$	$s_{35}$
$s_{41}$	$s_{42}$	$s_{43}$	$s_{44}$	$s_{45}$
$s_{51}$	$s_{52}$	$s_{53}$	$s_{54}$	$s_{55}$

Raw scores:  $Q \cdot K^T / \sqrt{d_k}$   
( $T \times T$ )

## THE CAUSAL MASK

<span style="background-color: green;">■</span>	<span style="background-color: red;">■</span>	<span style="background-color: green;">■</span>	<span style="background-color: green;">■</span>	<span style="background-color: green;">■</span>
0	$-\infty$	$-\infty$	$-\infty$	$-\infty$
0	0	$-\infty$	$-\infty$	$-\infty$
0	0	0	$-\infty$	$-\infty$
0	0	0	0	$-\infty$
0	0	0	0	0

Causal Mask  $M$

## MASKED SCORES

$x_1$	$x_2$	$x_3$	$x_4$	$x_5$
$s_{11}$	$-\infty$	$-\infty$	$-\infty$	$-\infty$
$s_{21}$	$s_{22}$	$-\infty$	$-\infty$	$-\infty$
$s_{31}$	$s_{32}$	$s_{33}$	$-\infty$	$-\infty$
$s_{41}$	$s_{42}$	$s_{43}$	$s_{44}$	$-\infty$
$s_{51}$	$s_{52}$	$s_{53}$	$s_{54}$	$s_{55}$

Masked Scores

## AFTER SOFTMAX

Upper triangle is exactly 0 ( $e^{-\infty} = 0$ )				
1.0	0	0	0	0
0.3	0.7	0	0	0
0.1	0.6	0.3	0	0
0.1	0.2	0.4	0.3	0
0.1	0.1	0.3	0.2	0.3

Each row sums to 1

Attention weights  
 $A = \text{softmax}(\text{masked scores})$

Row  $t$  only has non-zero  
weights for positions  $\leq t$

## KEY INSIGHT - PARALLELISM

### Sequential Generation (Inference)

Step 1:  $x_1$   
Step 2:  $x_1 \rightarrow$  predict  $x_2 \rightarrow$  predict  $x_3 \rightarrow x_1, x_2, x_3 \rightarrow$  predict  $x_4$   
Step 3:  $x_5$  (attend to  $x_1$  only) (attend to  $x_1, x_2$ ) (attend to  $x_1, x_2, x_3$ )  
...

$T$  sequential steps



Masking enables parallel training  
while maintaining causal property

### Parallel Training

All  $T$  positions computed simultaneously  
Single matrix multiplication with mask  
Same result as sequential, but parallel!

1 parallel step (same result!)

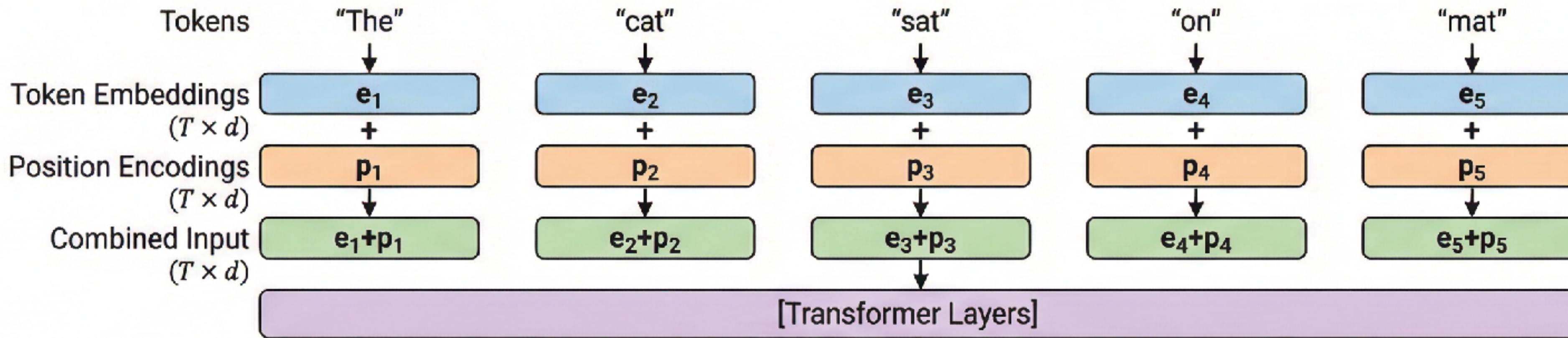
Causal Attention: 
$$\mathbf{A} = \text{softmax}\left(\frac{\mathbf{Q} \cdot \mathbf{K}^T + \mathbf{M}}{\sqrt{d_k}}\right)$$
 
$$\mathbf{Z} = \mathbf{A} \cdot \mathbf{V}$$
 where  $M_{ij} = 0$  if  $j \leq i$ , else  $-\infty$

# Break: How to encode position?

# Positional Encodings

Injecting position information into the transformer

## SECTION 1: WHERE TO ADD



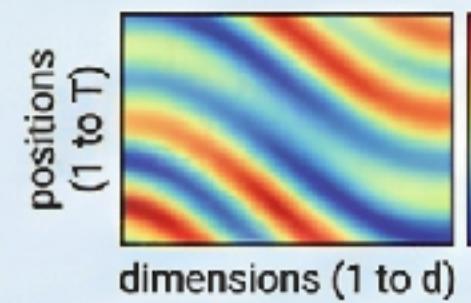
Position encoding added to token embeddings **BEFORE** transformer layers

## SECTION 2: TYPES OF POSITIONAL ENCODINGS

### Sinusoidal (Original Transformer)

$$\text{PE}(pos, 2i) = \sin\left(\frac{pos}{10000^{2i/d}}\right)$$

$$\text{PE}(pos, 2i+1) = \cos\left(\frac{pos}{10000^{2i/d}}\right)$$



- Fixed (not learned)
- Deterministic
- Can extrapolate to longer sequences

### Learned (BERT, GPT-2)

$$\mathbf{P} \in \mathbb{R}^{T_{\max} \times d}$$

"Lookup table of learnable vectors"

$$\begin{matrix} \mathbf{P}_1 \\ \mathbf{P}_2 \\ \vdots \\ \mathbf{P}_T \end{matrix} \quad (T_{\max} \times d)$$

- Learned during training
- More flexible
- Limited to max sequence length  $T_{\max}$

### Relative (Transformer-XL, T5)

"Encode relative distance  $(i - j)$  not absolute position"  
 $a_{ij}$  depends on  $(i - j)$

$$\begin{matrix} -2 & -2 & & & \\ -1 & -1 & -2 & & \\ 0 & 0 & -1 & -2 & \\ +1 & +1 & 0 & -1 & \\ +2 & +2 & +2 & 0 & \end{matrix}$$

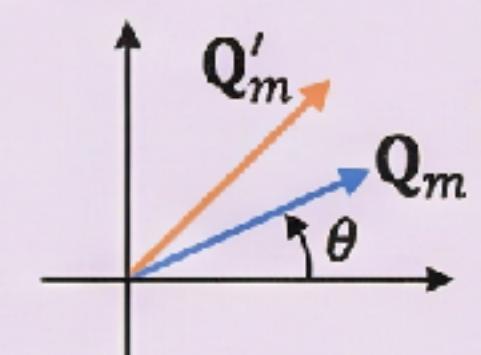
- Captures relative distance
- Better for long sequences
- Added in attention computation

### RoPE / Rotary (LLaMA, GPT-NeoX)

"Rotate  $\mathbf{Q}$  and  $\mathbf{K}$  vectors based on position"

$$\mathbf{Q}'_m = \mathbf{R}_m \cdot \mathbf{Q}_m$$

$$\mathbf{K}'_n = \mathbf{R}_n \cdot \mathbf{K}_n$$



- Applied to  $\mathbf{Q}, \mathbf{K}$  in attention
- Relative position via rotation
- Extrapolates well

## SECTION 3: VISUAL COMPARISON

Method	Where Added	Learned?	Extrapolation
Sinusoidal	Input	No	✓ Good
Learned	Input	Yes	✗ Limited
Relative	Attention	Yes	✓ Good
RoPE	$\mathbf{Q}, \mathbf{K}$	No	✓ Good

### Input to transformer:

$$\mathbf{X} = \text{TokenEmbed(tokens)} + \text{PositionEncode(positions)}$$

### For sinusoidal:

$$\text{PE}(t, 2i) = \sin\left(\frac{t}{10000^{2i/d}}\right) \quad \text{PE}(t, 2i+1) = \cos\left(\frac{t}{10000^{2i/d}}\right)$$

## EQUATIONS BOX

See you Monday!