EE-508: Hardware Foundations for Machine Learning

Transformers – Part 2

University of Southern California

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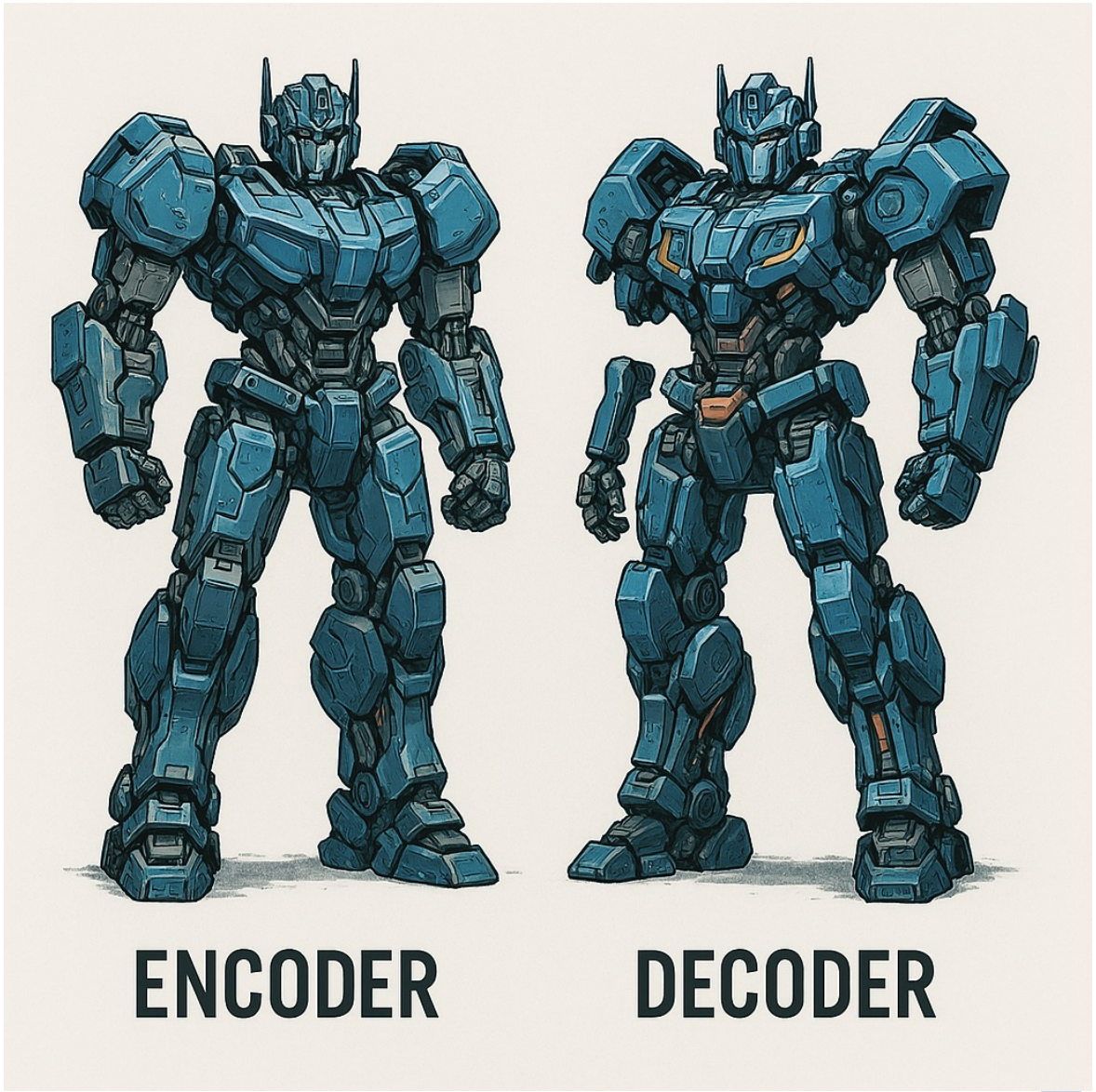
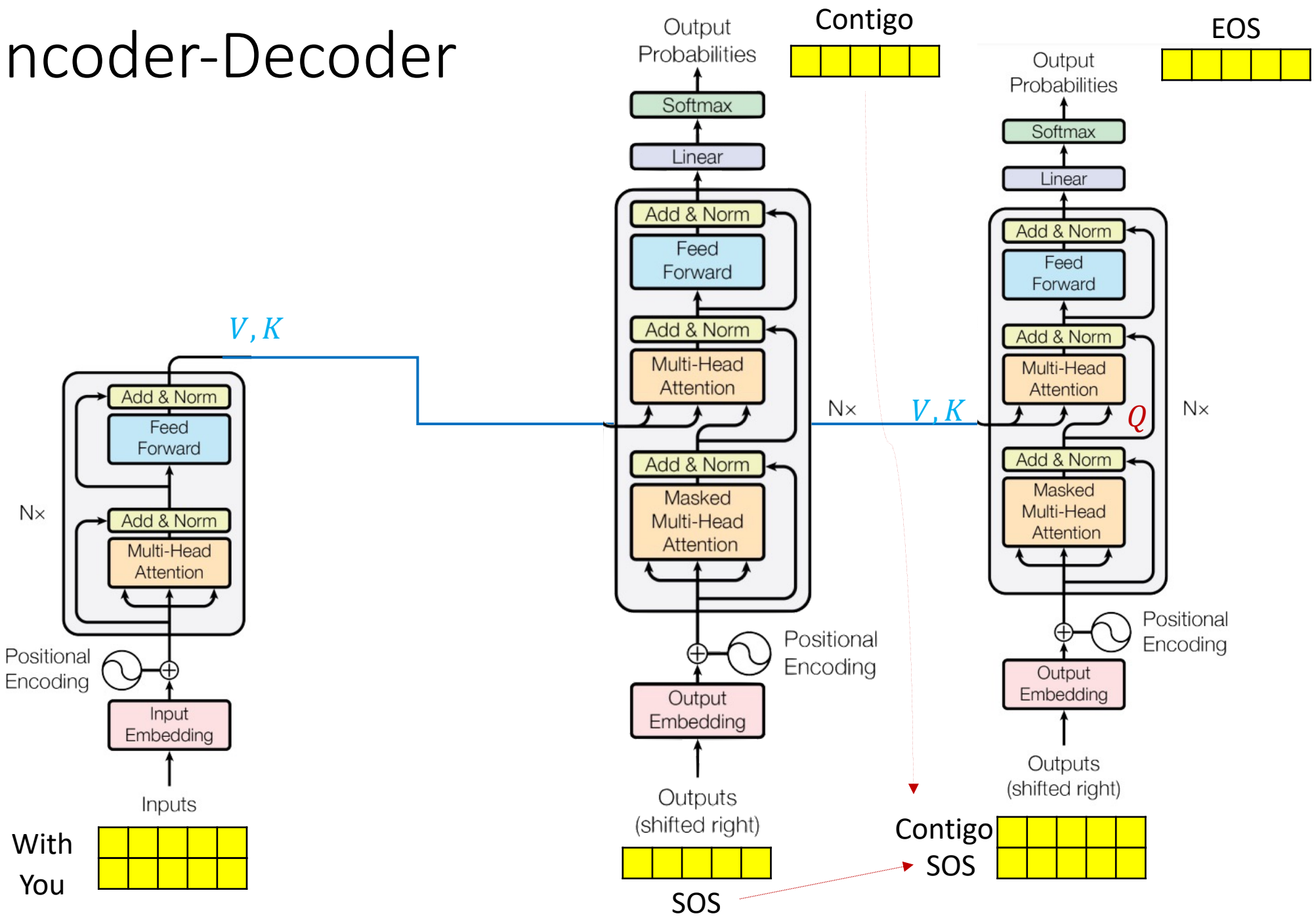
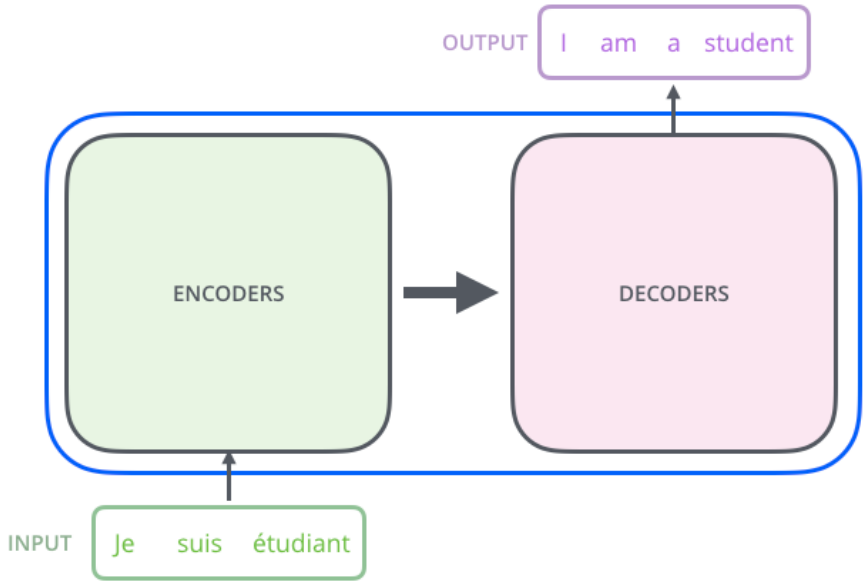
Instructors:
Arash Saifhashemi


ENCODER
DECODER

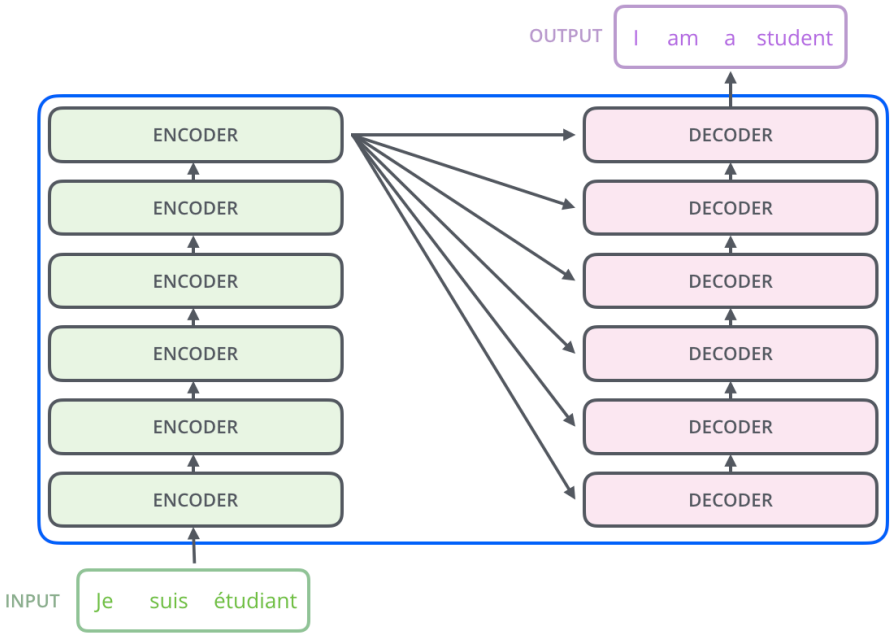
Encoder-Decoder



Encoder-Decoder Summary



Encoder-decoder structure for translation



Stacked encoders and decoders and attention connections

Source: https://jalammar.github.io/illustrated-transformer/

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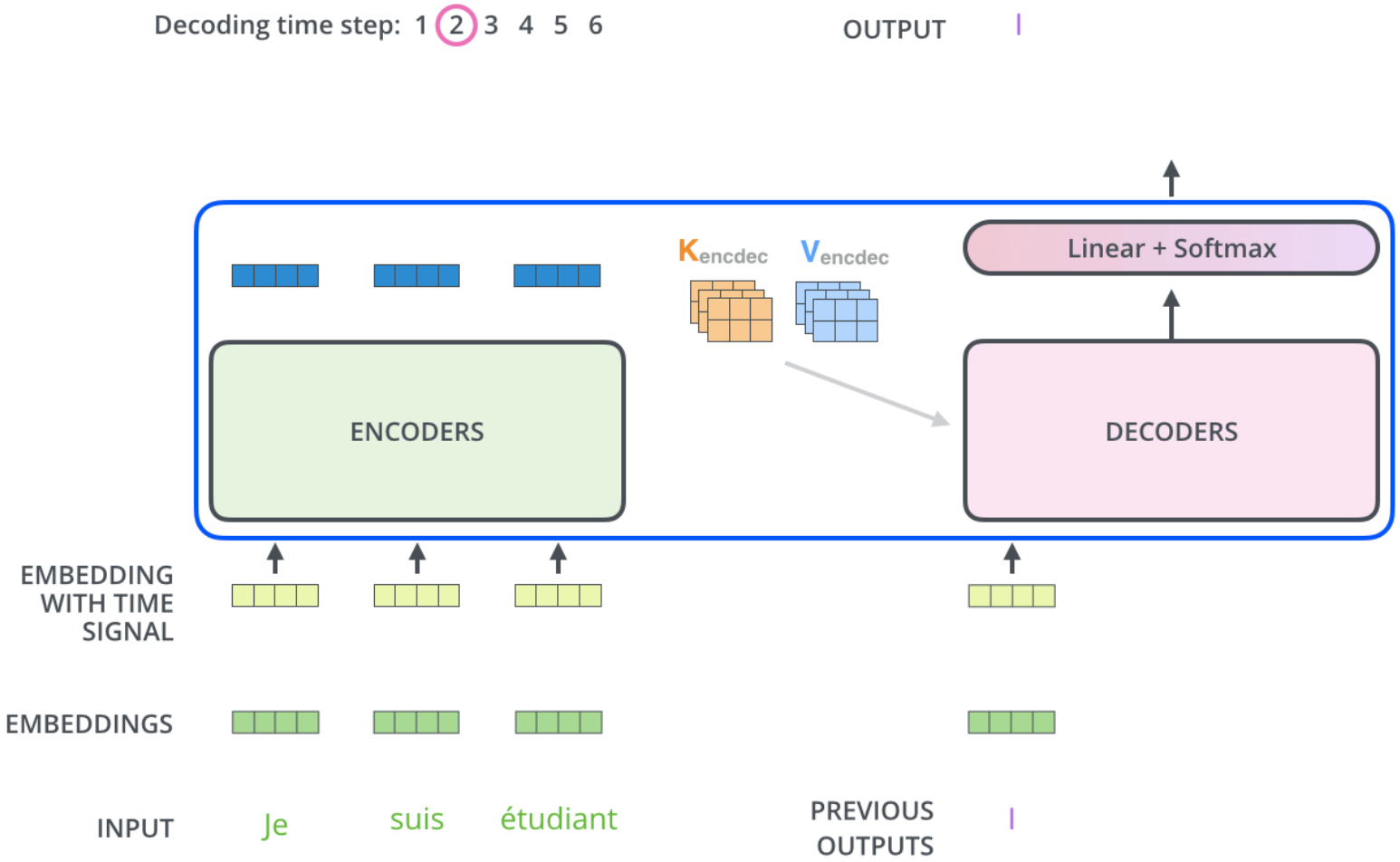

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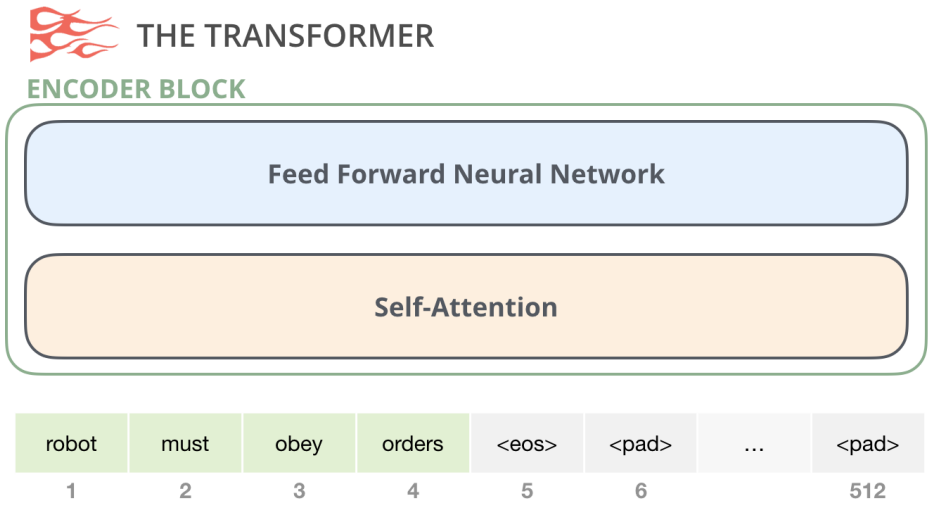
The Evolution of the Transformer Block

"...robot must obey orders given by human beings, except where such orders would conflict with the First Law"



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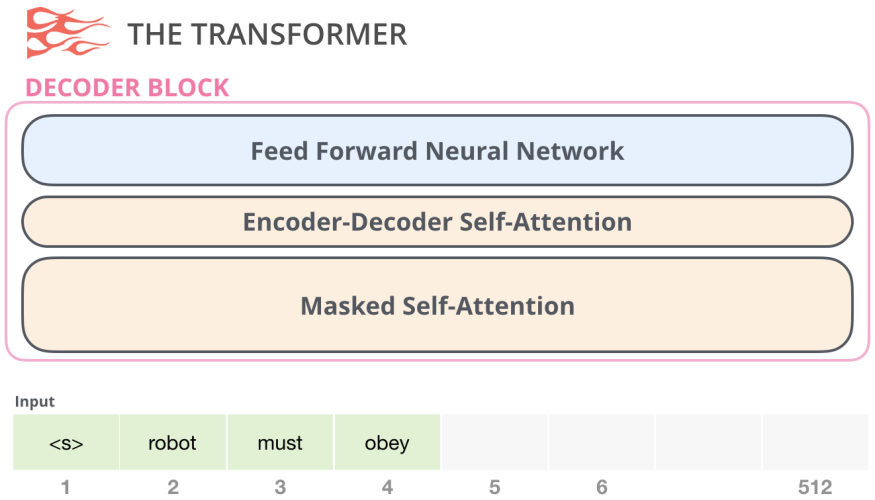

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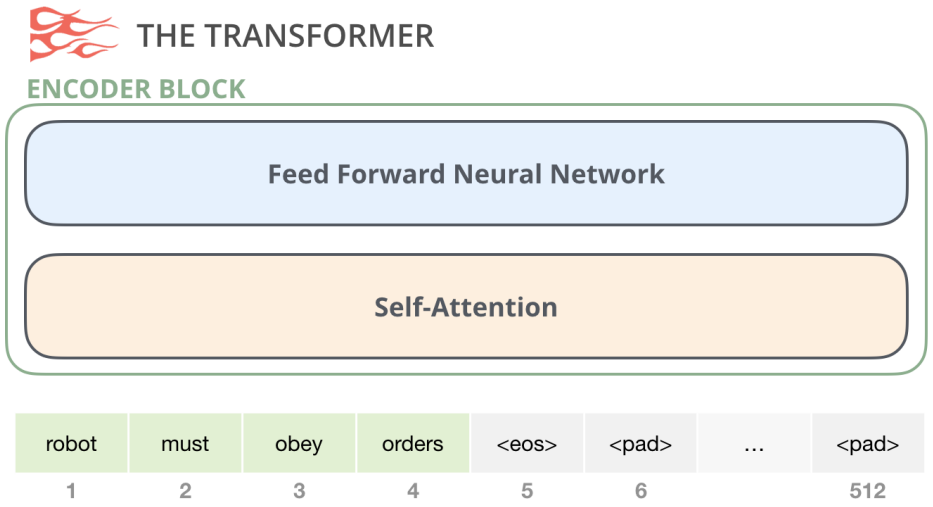

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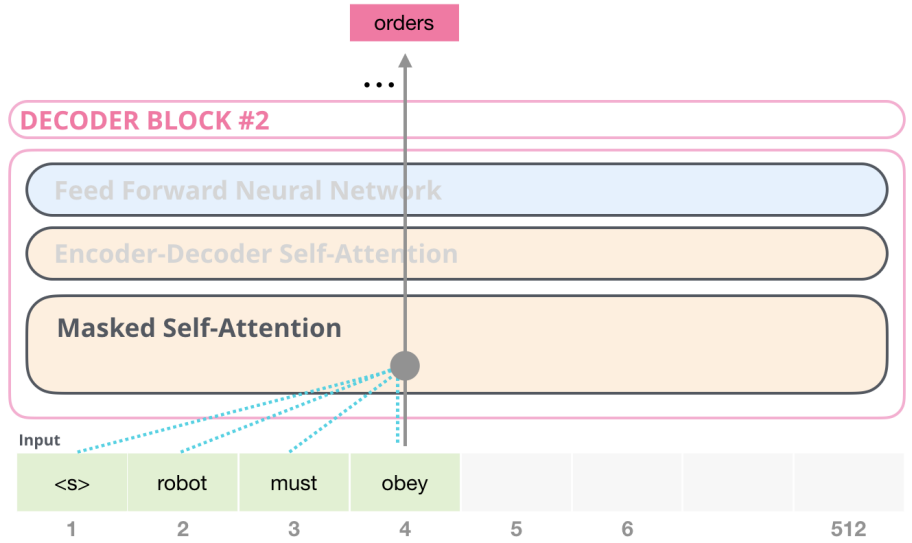

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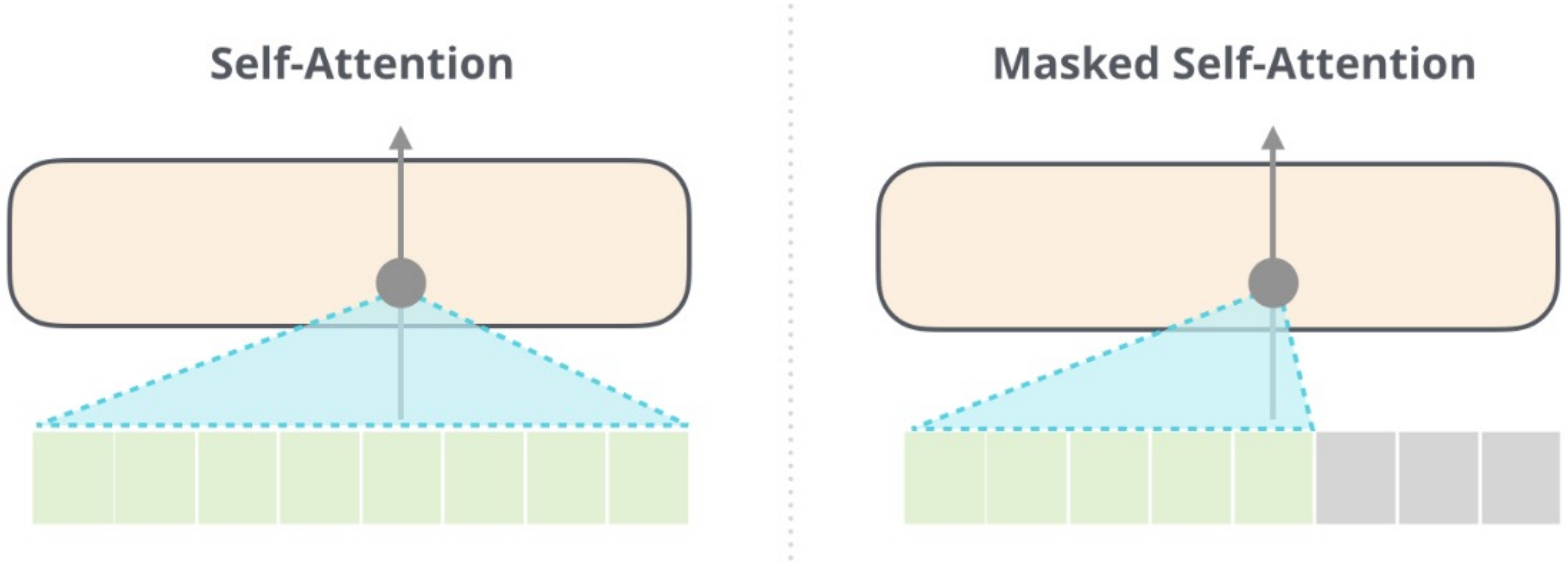

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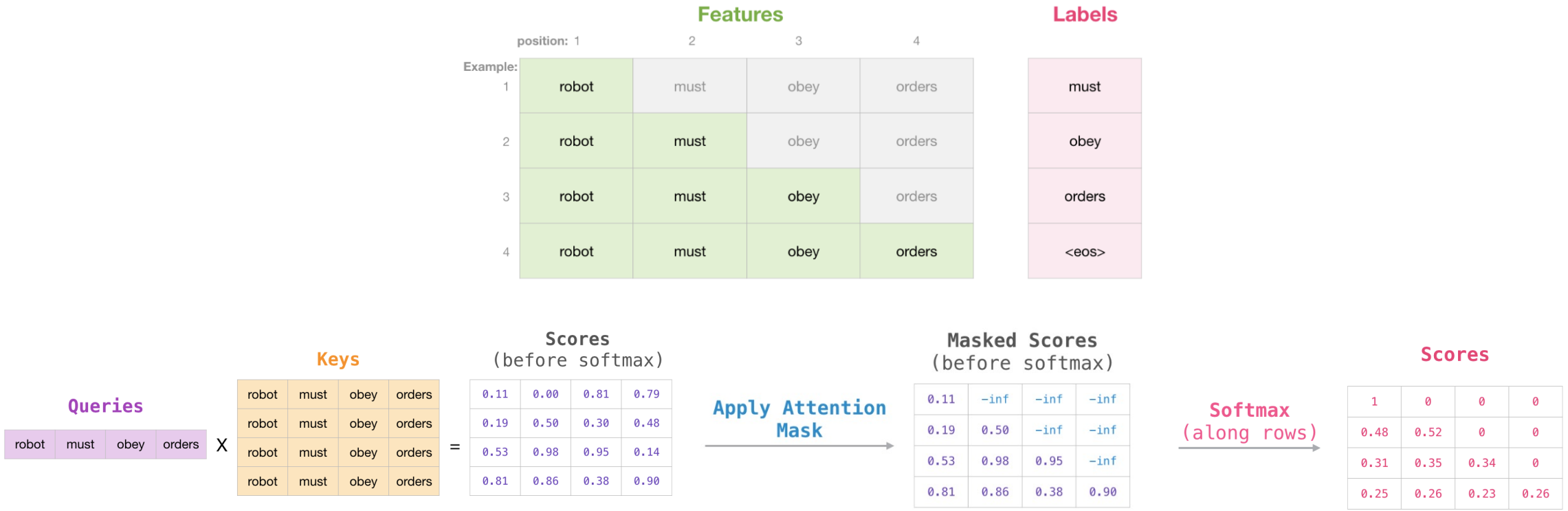

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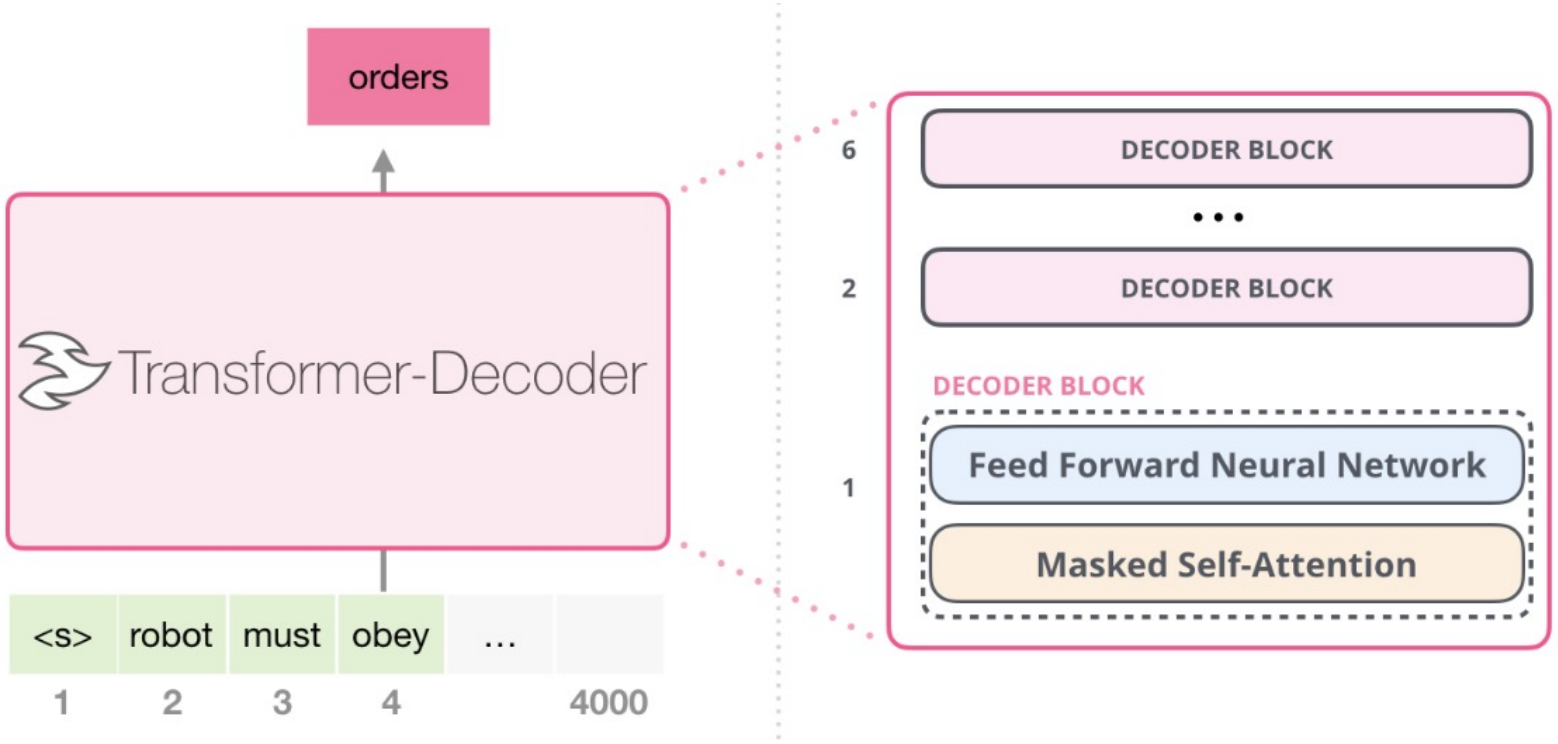
The Decoder Only Block



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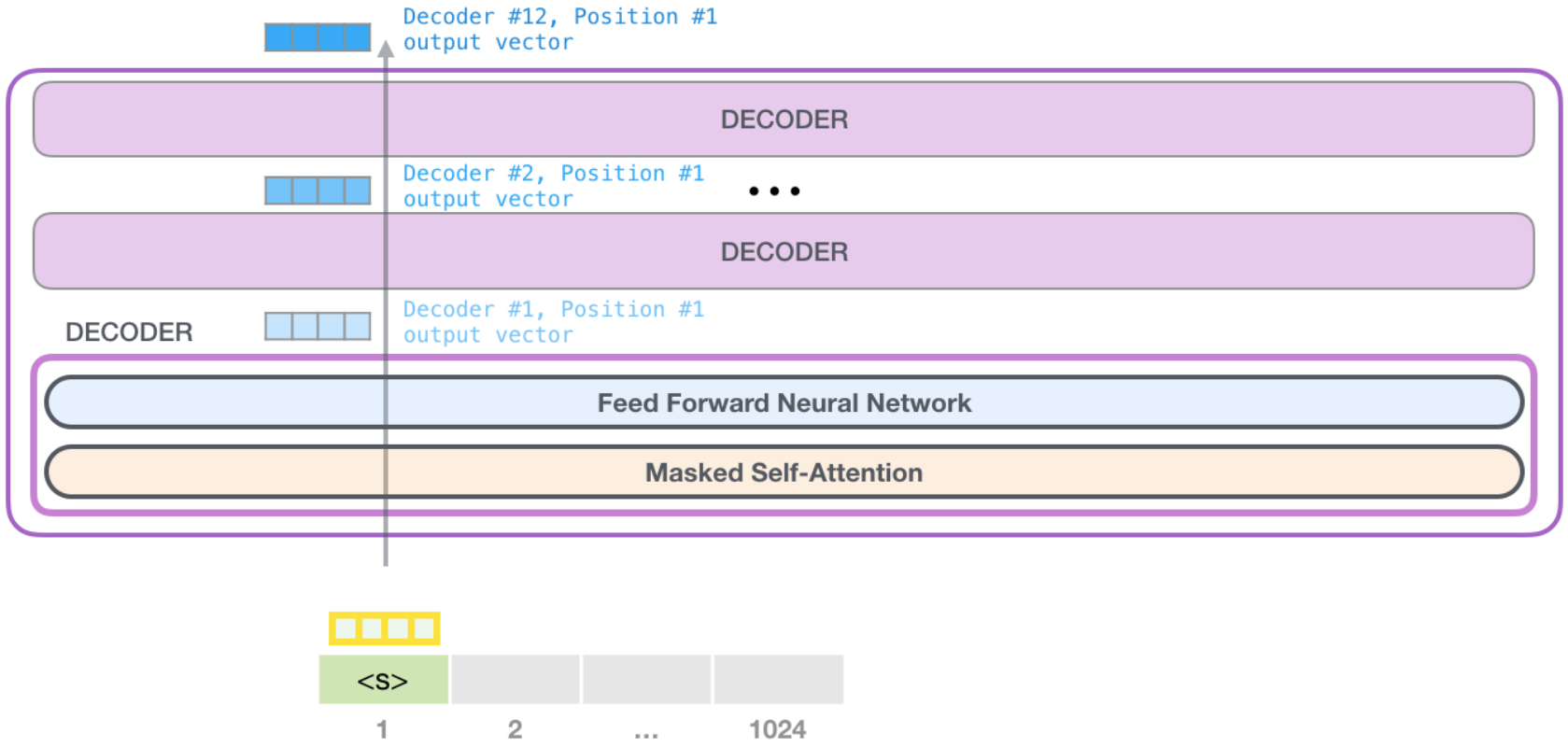
The Output is Still Embedding



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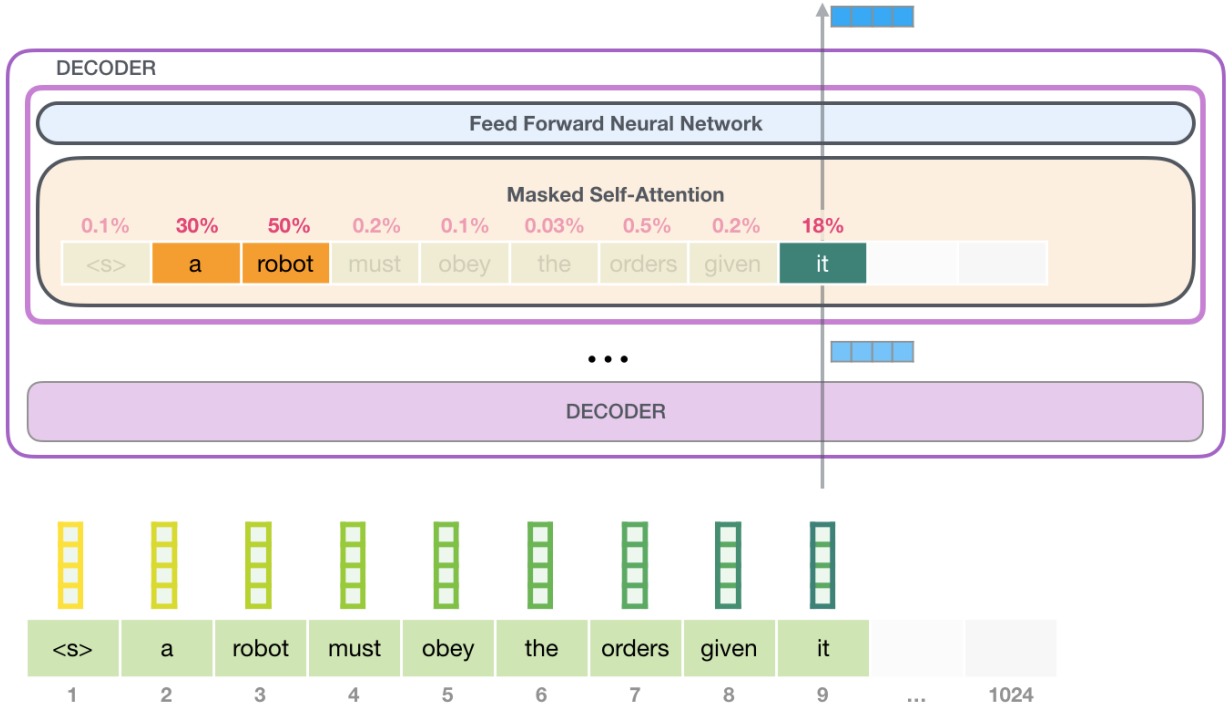
Masked Self Attention



The self-attention layer in the top block is paying attention to “a robot” when it processes the word “it”. The vector it will pass to its neural network is a sum of the vectors for each of the three words multiplied by their scores.

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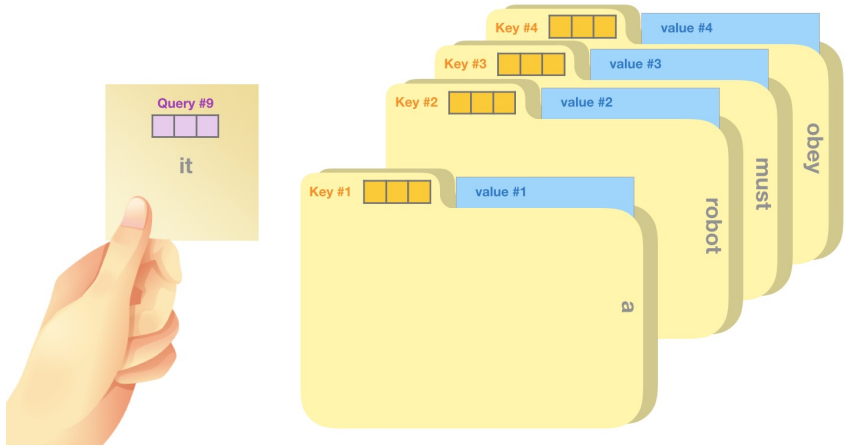
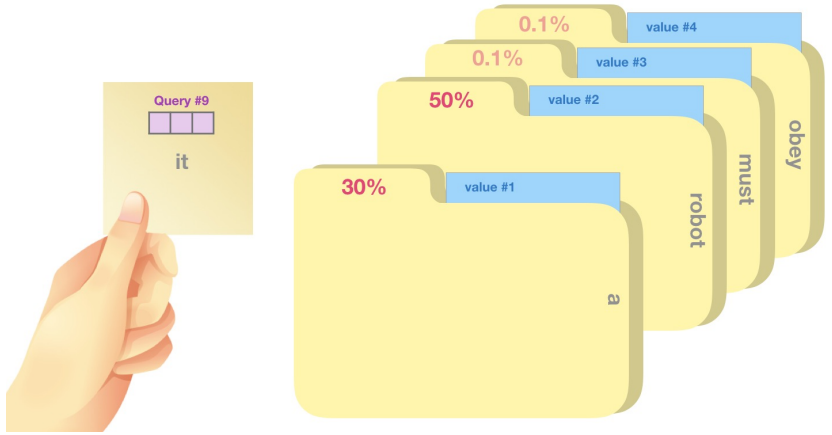
Remember K,V,Q from Database Analogy





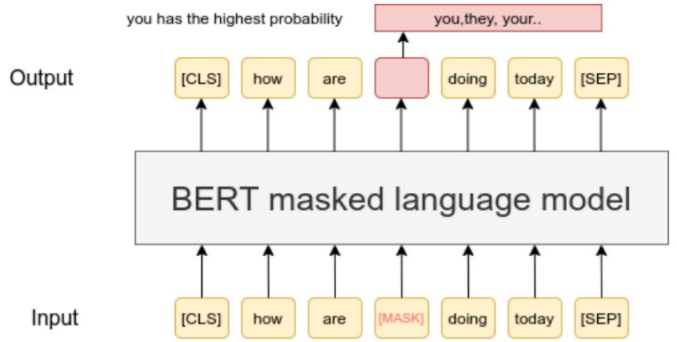
Second Law of Robotics

A robot must obey the orders given **it** by human beings except where **such orders** would conflict with the **First Law**.

Word	Value vector	Score	Value X Score
<s>		0.001	
a		0.3	
robot		0.5	
must		0.002	
obey		0.001	
the		0.0003	
orders		0.005	
given		0.002	
it		0.19	
		Sum:	

Understanding vs Generation

- **BERT = encoder-only (understanding)**
  - **Input:**
    "A robot may not [MASK] a human being."
  - **Output (prediction):**
    "*injure*"
  - BERT is trained to fill in masked words based on full sentence context. It sees both left and right of [MASK].
- **GPT = decoder-only (generation)**
  - **Input:**
    "A robot may not"
  - **Generated Output (token-by-token):**
    "injure" → "a" → "human" → "being" ...
  - GPT-2 generates the next token using only the previous ones.



Applications of BERT

Text Classification

Sentiment analysis, topic classification

The movie was [great]

↓

Positive

Question Answering (QA)

Input: passage + question

Einstein was born in Germany.

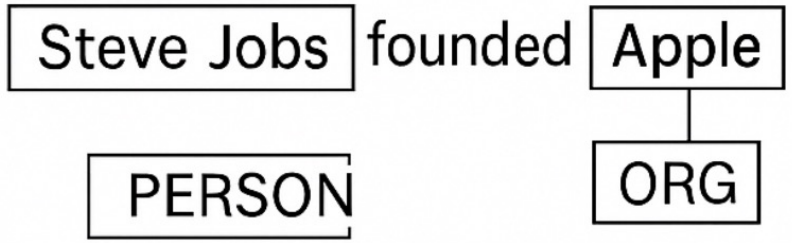
Q: Where was Einstein born?

↓

Germany

Named Entity Recognition

Label words as people, places, organizations



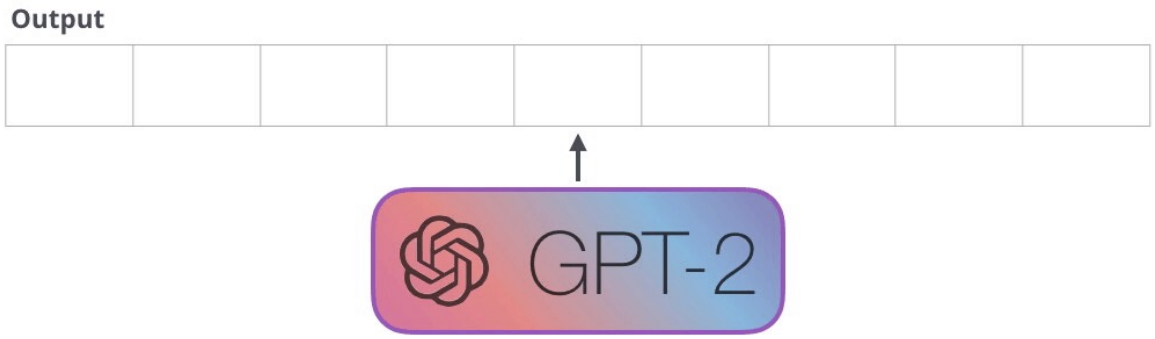
Coreference Resolution

Figuring out what pronouns refer to

John helped Tom because he was late.

he = John?

How Does the Decoder Work?



In the auto-regressive generation of the decoder, given an input the model predicts the next token, and then taking the combined input in the next step the next prediction is made.

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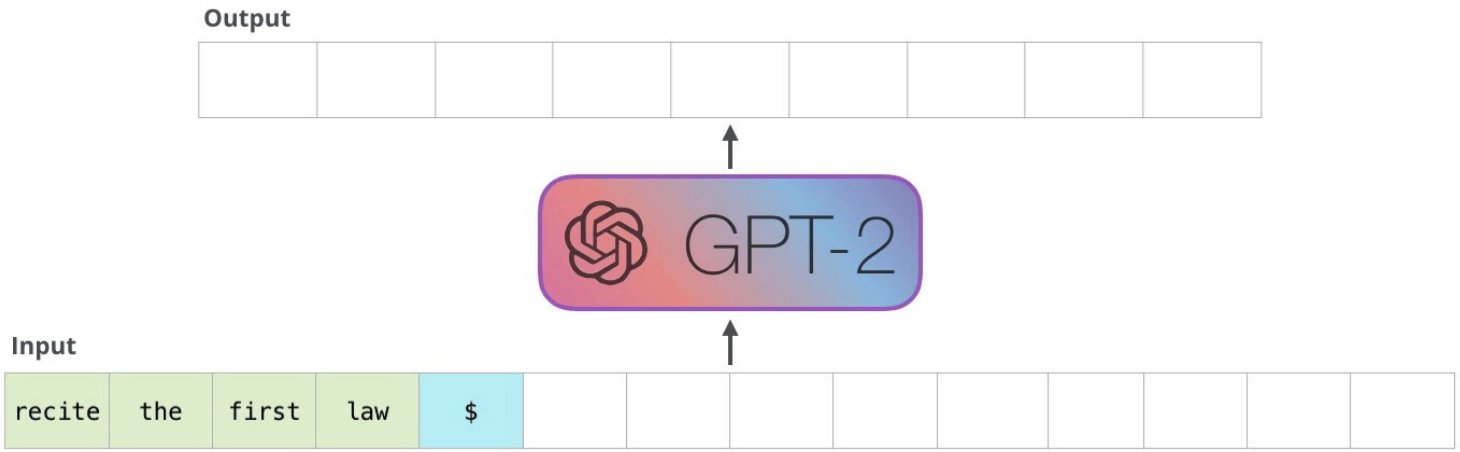

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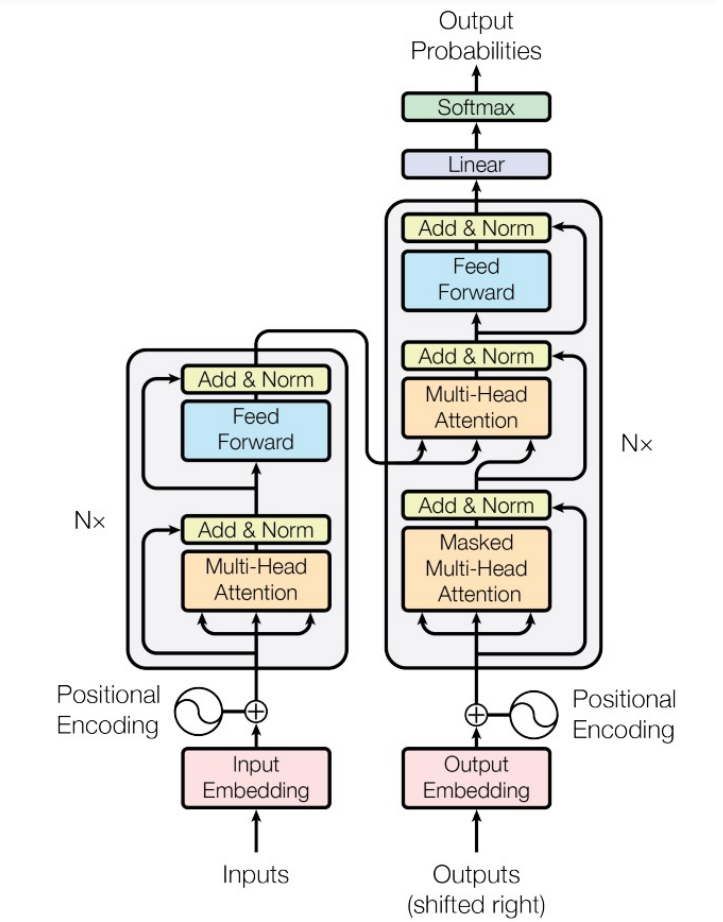
Understanding KV Caching in Transformers

- **Transformer Inference Basics**
  - **Autoregressive Generation**
    - Transformers generate text step-by-step (autoregressively).
    - To predict the *next* token, the model uses *all* previous tokens as input.
  - **Example:**
    1. Input: *[CLS] The cat sat* -> Predict: **on**
    2. Input: *[CLS] The cat sat **on*** -> Predict: **the**
    3. Input: *[CLS] The cat sat on **the*** -> Predict: **mat**
  - Each prediction step involves a full pass through the Transformer layers.



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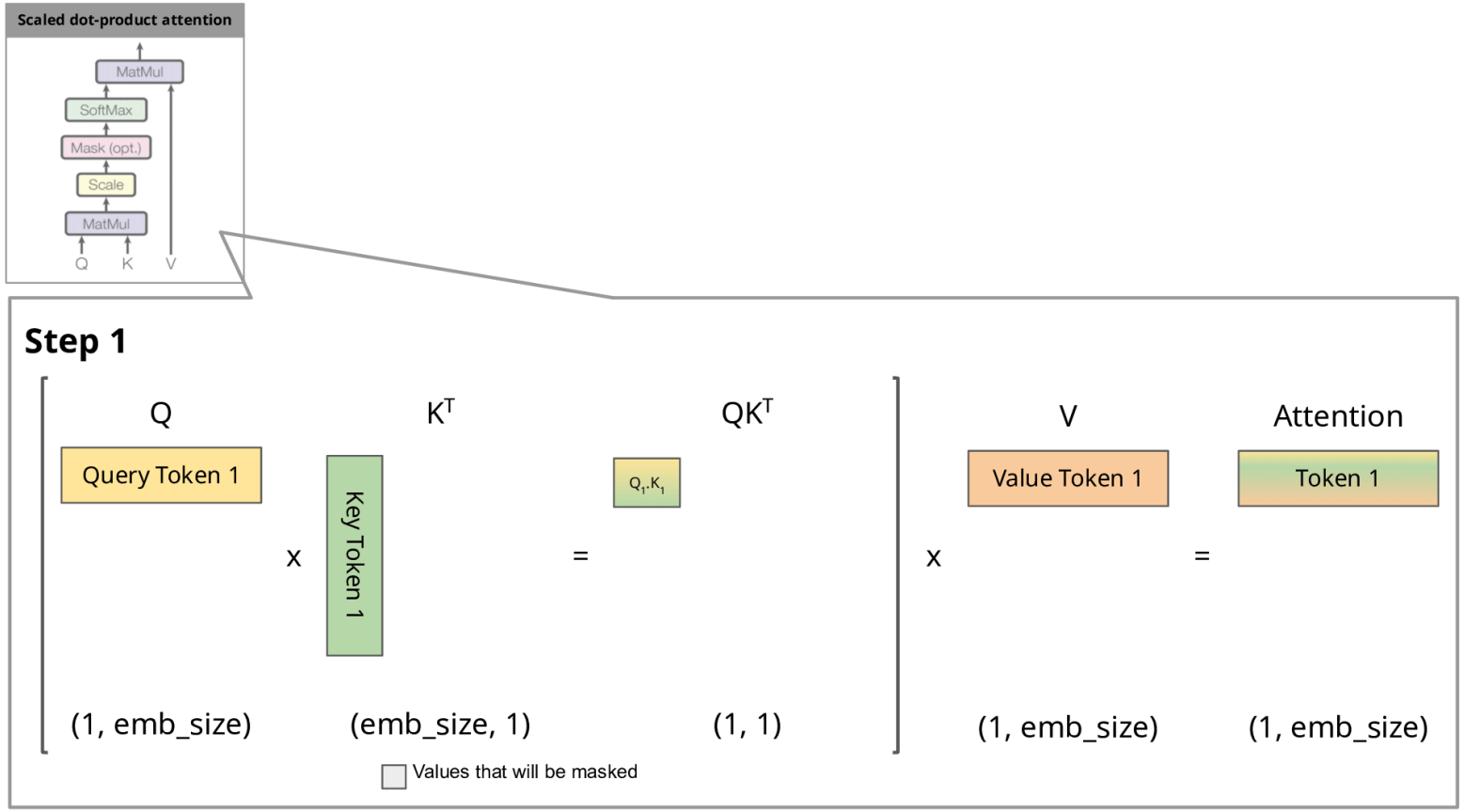

Zoom-in! (simplified without Scale and Softmax)

Step-by-step visualization of the scaled dot-product attention in the decoder. emb_size means embedding size.

(Image source: https://medium.com/@joaolages/kv-caching-explained-276520203249)

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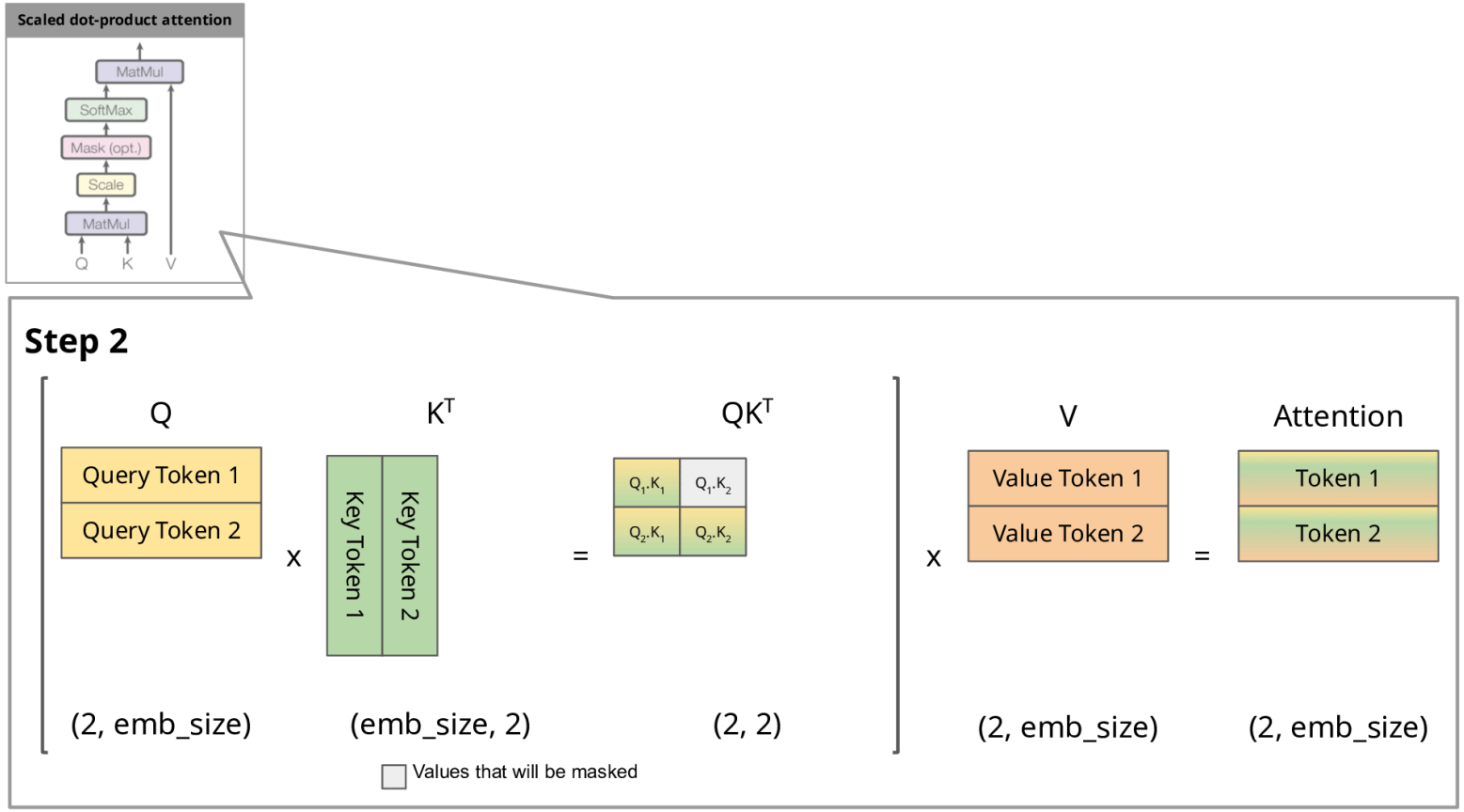

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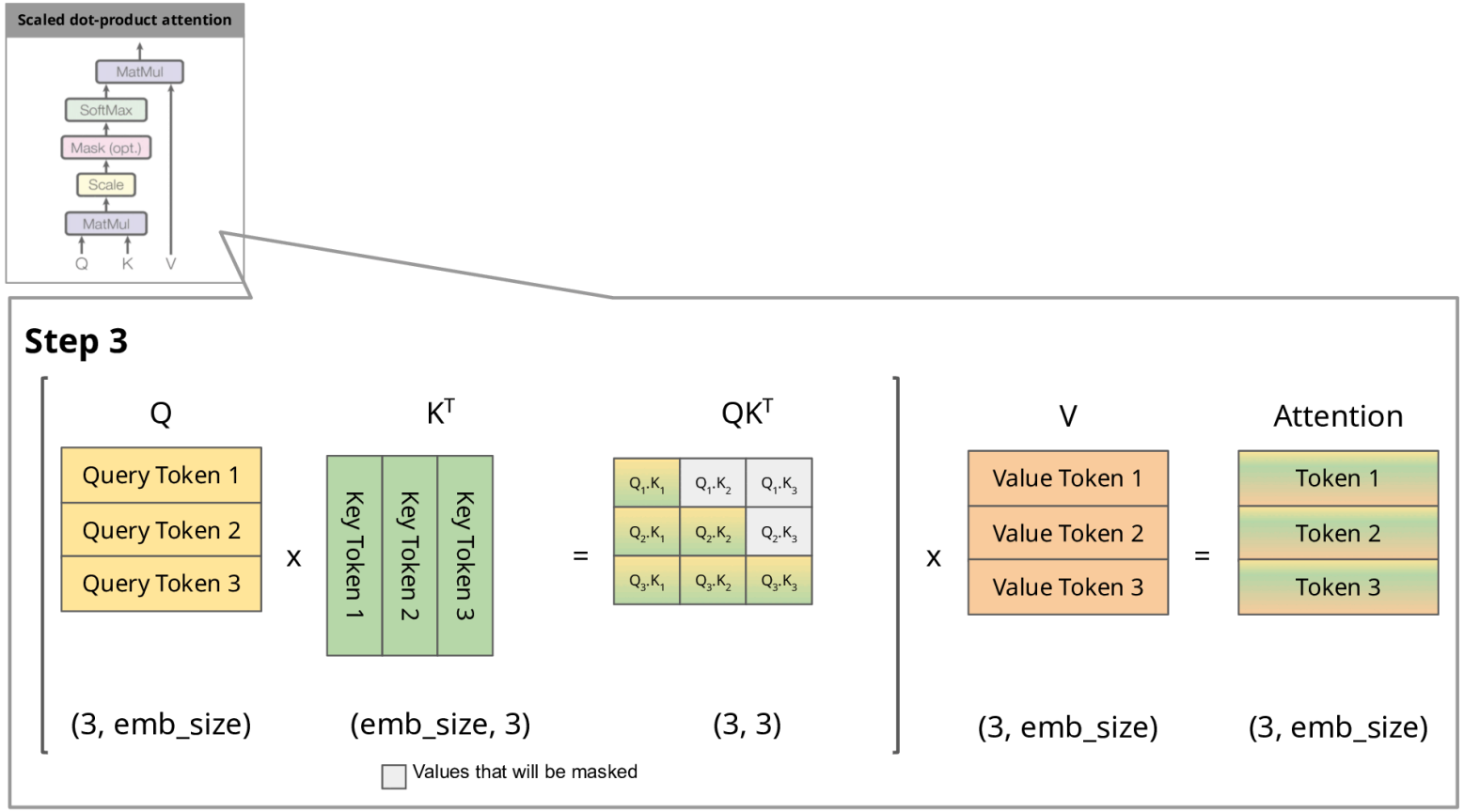

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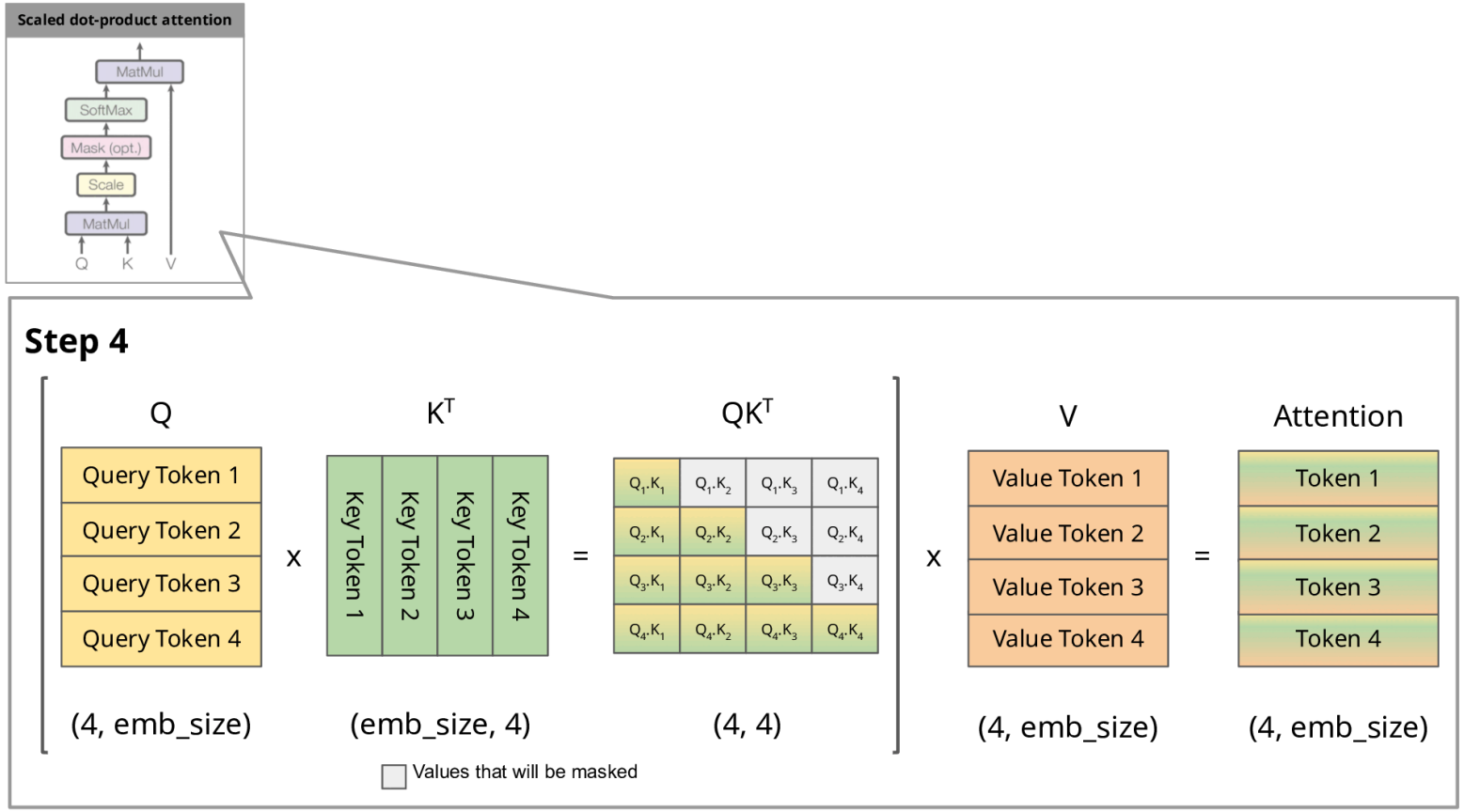

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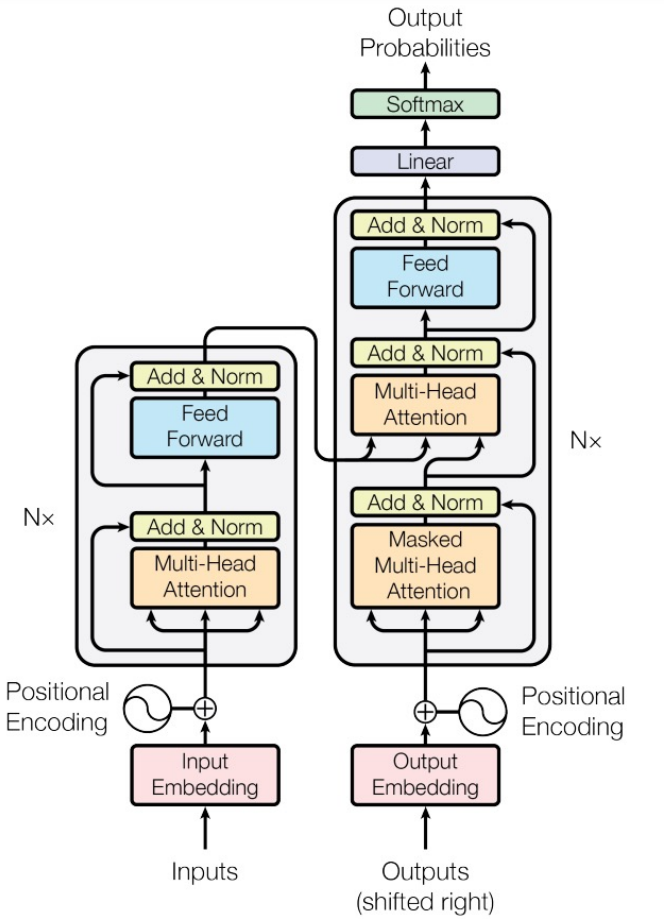
The Challenge: No Cache

- **What happens without caching?**
  - Every calculation is repeated for the *entire growing sequence* at each step.
  - Embeddings, Positional Encodings, Q/K/V projections, Attention Scores, FFNs... everything!
- **Example (Predicting Token 4: "mat"):**
  - Input: `The cat sat on`
  - Calculations involve interactions of all token pairs
- **Example (Predicting Token 5):**
  - Input: `The cat sat on` **`the`**
  - *All* previous interactions are recalculated, PLUS new ones:
  - **Highly inefficient!**



The cat sat on

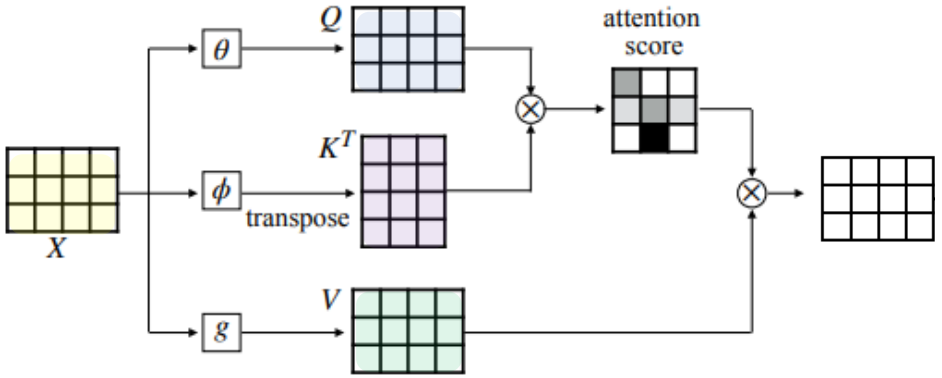
The cat sat on the

Solution: KV Cache

$$\text{Attention}(Q, K, V) = \text{Softmax}\left(\frac{QK^\top}{\sqrt{d}}\right)V$$

- **What Can We Reuse?**
  - In the attention mechanism, the **Key (K)** and **Value (V)** vectors for a token depend *only* on that token's input representation (at that layer).
  - They don't change based on which token is *querying* them.
- **The KV Cache:**
  - Store (cache) the calculated **K** and **V** vectors for all previous tokens in each layer.

The cat, the cute little white one, sat on the mat and it



Role of Cache

$$\text{Attention}(Q, K, V) = \text{Softmax}\left(\frac{QK^\top}{\sqrt{d}}\right)V$$

- **Optimized Calculation Flow**
  1. Calculate Q, K, V only for the *newest* input token.
  2. Retrieve the cached K and V vectors for *all previous* tokens.
  3. Combine the new K/V with the cached K/V.
  4. Calculate attention scores *only* for the new token's Q against *all* K's (cached + new).
  5. Compute the weighted sum using *all* V's (cached + new).
  6. Update the cache by adding the new K and V.

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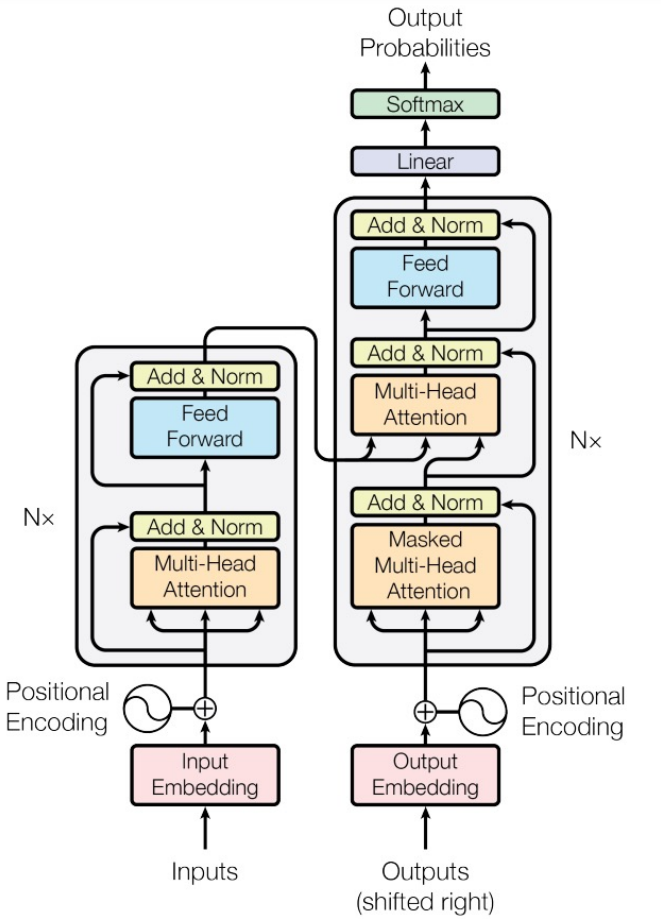
- **Example (Predicting Token 5 with Cache):**
  - `The cat sat on` **`the`**
  - Input: Only process token 4 (the). Calculate: $Q_4 = W_Q \cdot x_4, \quad K_4 = W_K \cdot x_4, \quad V_4 = W_V \cdot x_4$
  - Retrieve Cache $[K_0, K_1, K_2, K_3]$, $[V_0, V_1, V_2, V_3]$:
  - Attention: Calculate Q_4 interacting with $[K_0, K_1, K_2, K_3]$
  - Output: Weighted sum using $[V_0, V_1, V_2, V_3]$:
  - Update Cache: Store K_4, V_4.

$$\text{Scores: } \alpha_i = \text{softmax}\left(\frac{Q_4 \cdot K_i^T}{\sqrt{d_k}}\right), \quad i \in \{1, 2, 3, 4\}$$

- **Much faster:** Only 1 Q vector calculation and 1 x N attention instead of N x N.

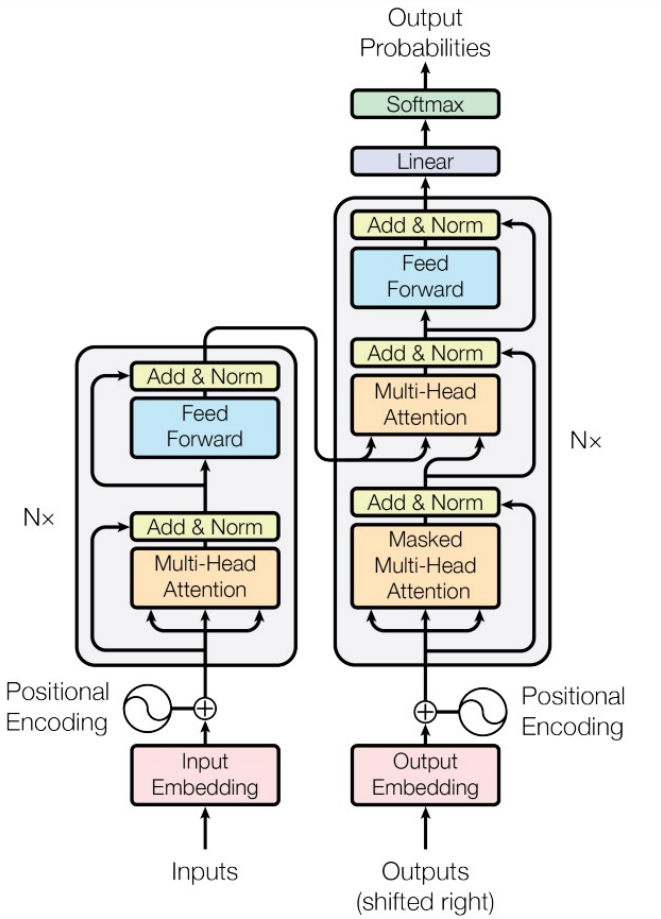
How KV Cache Works

- **Encoding Position Information**
  - Transformers need to know the order of tokens.
- **Traditional Absolute Encodings:** (e.g., Sinusoidal, Learned Embeddings)
  - Add a unique vector based on the token's *absolute position* (1st, 2nd, 3rd...) directly to the token embedding.
  - $Input = TokenEmbedding + PositionalEncoding(absolute\_position)$

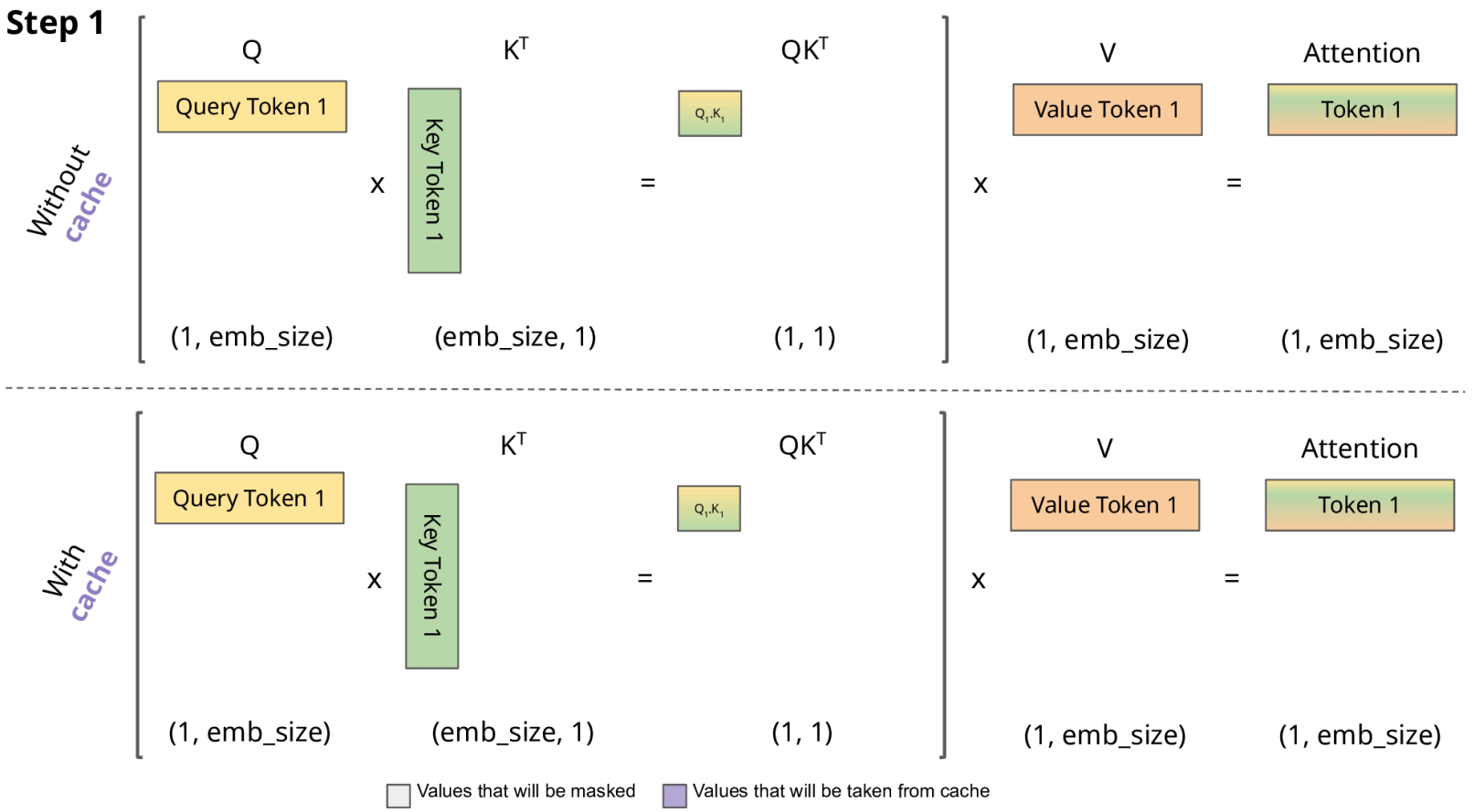


Caching with Absolute Encodings

- **How it Works:**
  - The K and V vectors are calculated from embeddings that *already include* absolute positional information.
  - KV Caching **still works** perfectly fine. You cache these position-infused K and V vectors.
- **Subtlety:**
  - The cached K and V vectors have the *absolute position* information "baked in".
  - Attention scores implicitly depend on these absolute positions.
  - The model must learn to interpret **relative positioning** (m-n) from vectors that have **absolute positions** (m and n) baked into them.



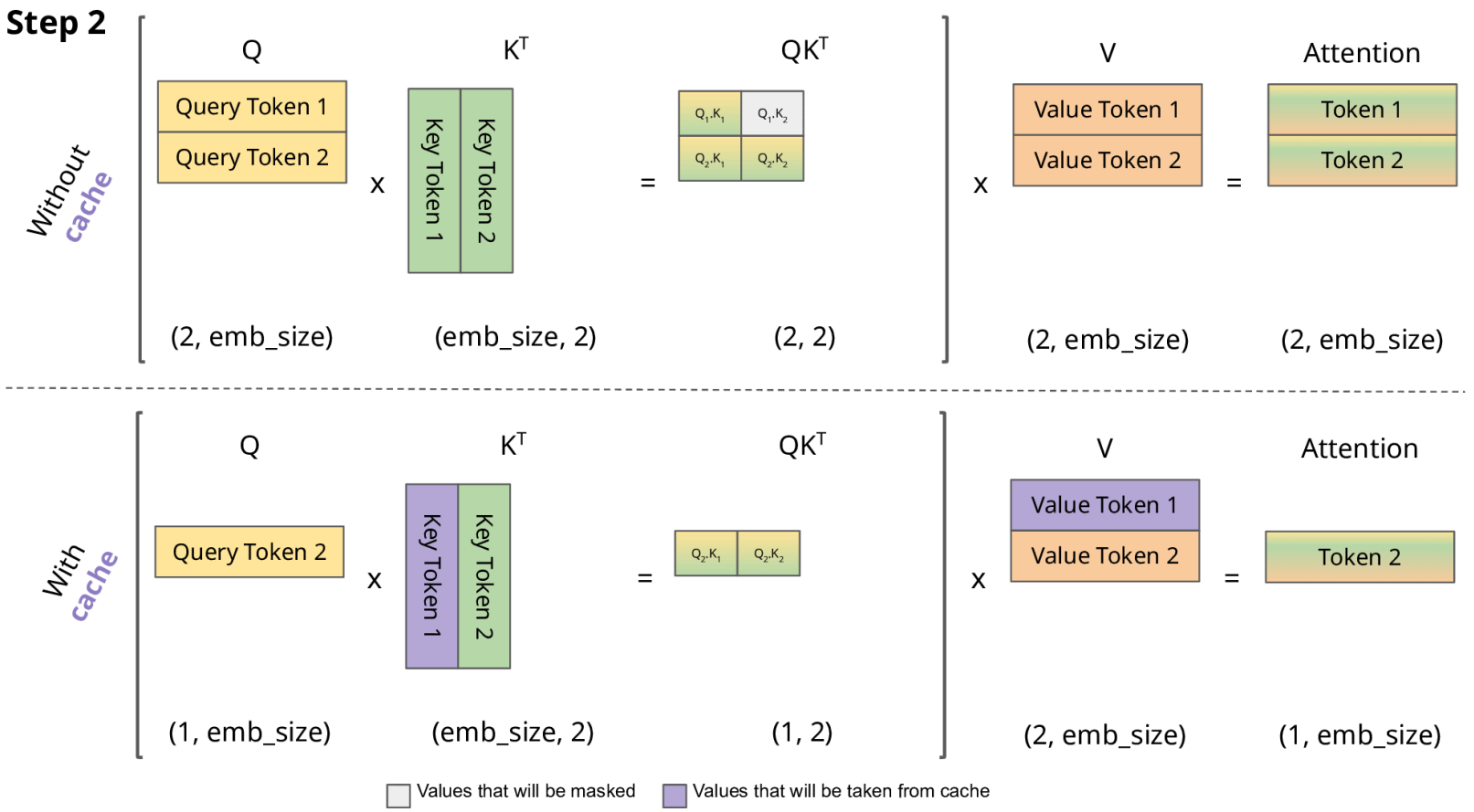
Caching Key and Value



- Pro: Matrix multiplication would be simpler (smaller size)
- Con: We need extra memory per token!

(Image source: https://medium.com/@joaolages/kv-caching-explained-276520203249)

Caching Key and Value



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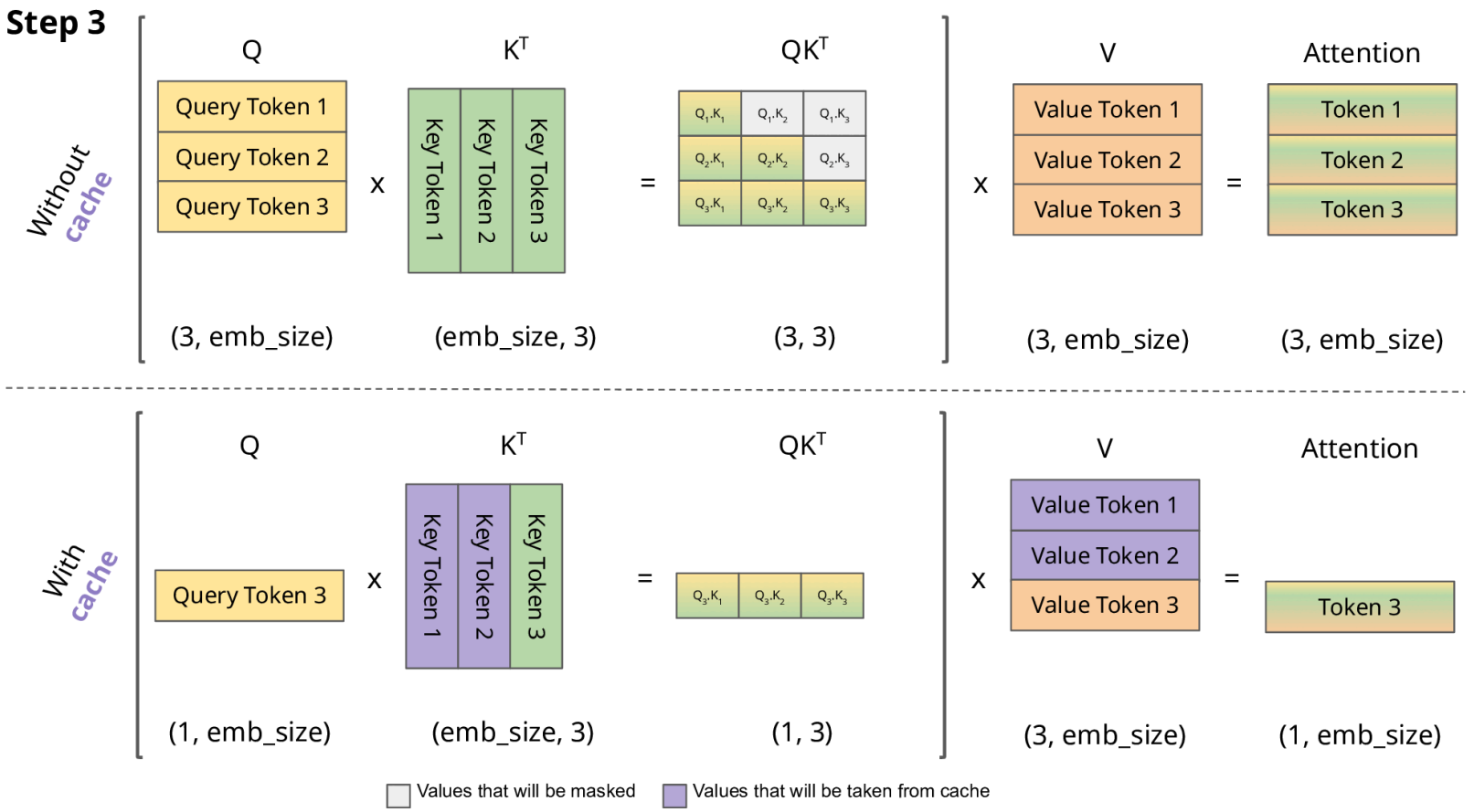

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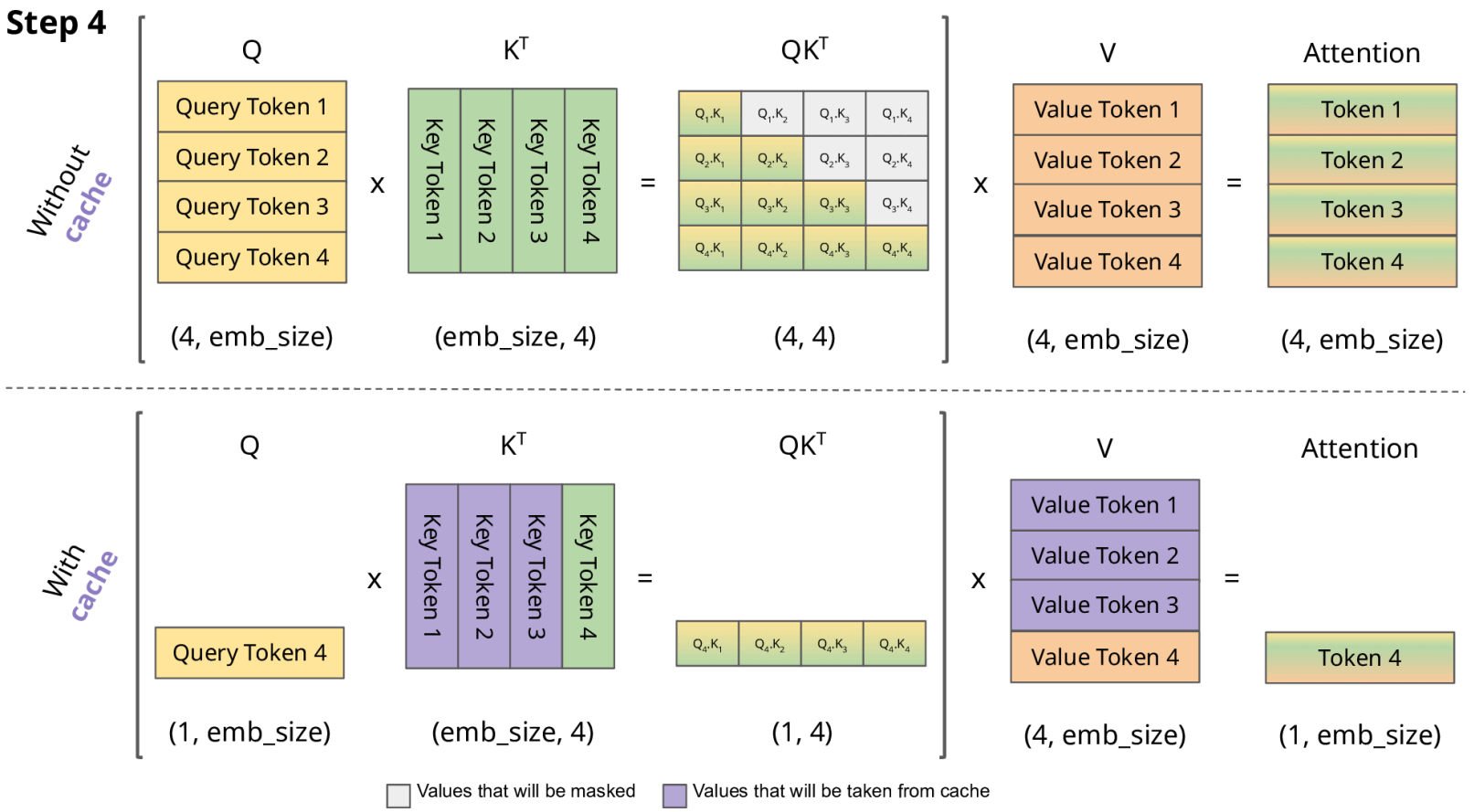

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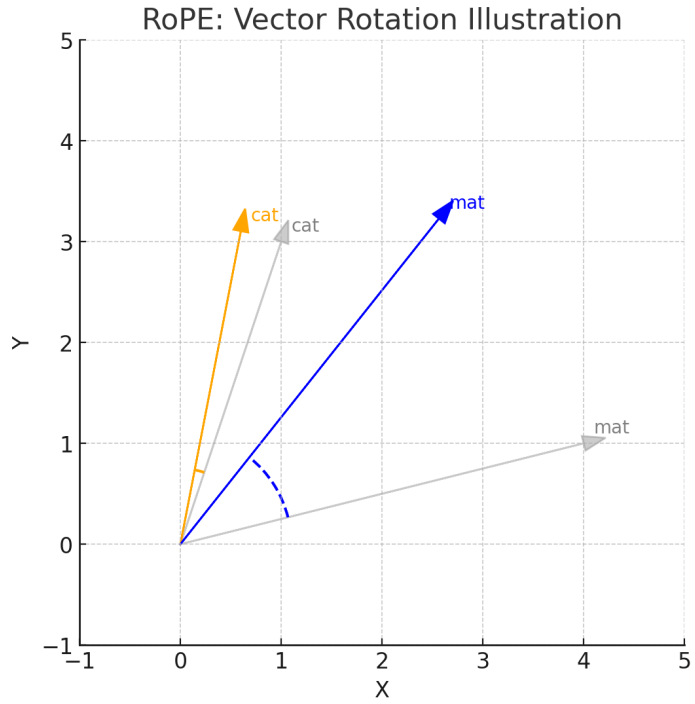
Introducing RoPE

- **Rotary Positional Embedding (RoPE)**
  - A different way to encode position.
  - Doesn't *add* positional vectors to embeddings.
  - Instead, it *rotates* the Q and K vectors based on their position *after* projection, just before the attention dot-product.
- **Key Property:**
  - The attention score for tokens at positions m,n
    - $(RotatedQ(m).\ RotatedK(n)^T)$
      - (T stands for transpose)
    - depends mathematically only on the original Q/K content and the *relative distance* (m - n), not the absolute positions m and n.

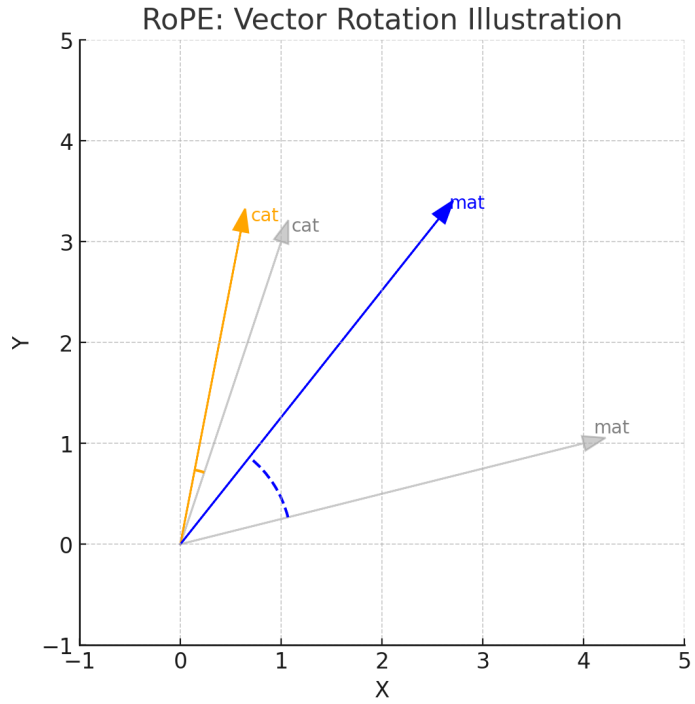


The **cat** sat on the **mat**

Each word is rotated to encode position

RoPE & Caching Advantage

- **Simpler, More Elegant Caching**
  - Calculate base Q, K, V from token embeddings (no positional info added).
  - Cache these **"pure content" K and V vectors**.
- During attention calculation for a new token at position m:
  - Retrieve cached K's (from positions n).
  - *Dynamically* apply RoPE rotation to the new Q using position m.
  - *Dynamically* apply RoPE rotation to the cached K's using their original positions n.
  - Calculate dot products.
- Cache the *un-rotated*, pure K and V for the new token.
- **Advantage:**
  - Cached state (K, V) is position-agnostic.
  - Relative position information is applied "on-the-fly" during attention.
  - Conceptually cleaner, directly models relative positions.

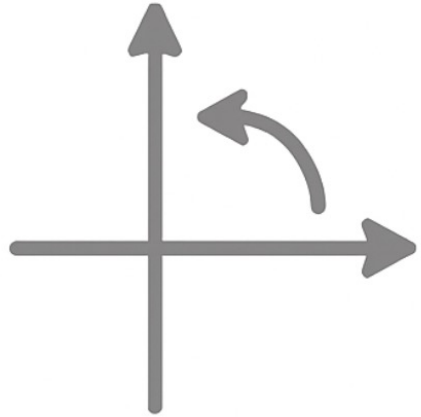


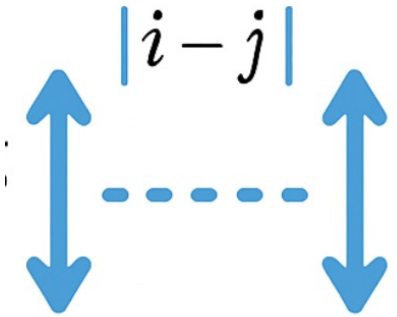
The **cat** sat on the **mat**

Each word is rotated to encode position

RoPE: Rotary Positional Embedding

- **Efficient & Scalable:**
  - RoPE encodes position via rotation, which avoids adding embeddings and works natively within attention.
- **Better Generalization:**
  - Encodes **relative** positions, preserving meaning across contexts and longer sequences.
- **Modern Default:**
  - Used in LLaMA, GPT-NeoX, and other advanced models for high-performance language modeling.





Multi-Head Latent Attention (MLA) in DeepSeek-V3

- MLA (Multi-Head Latent Attention) is a **low-rank compressed version of standard attention**.
- It is designed to:
  - **Reduce KV cache memory** during inference.
  - **Reduce query activation memory** during training.
  - **Match performance** of standard Multi-Head Attention (MHA), but more efficiently.

Remember in Standard Transformer...

- You have access to the **entire input sequence** at once (e.g., 1024 tokens), so you compute attention like this:
  - One big matrix multiplication.
  - Parallel computation across all tokens.
  - Training is fast and fully batched.

$$\text{Attention}(Q, K, V) = \text{Softmax}\left(\frac{QK^\top}{\sqrt{d}}\right)V$$

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- You have access to the **entire input sequence** at once (e.g., 1024 tokens), so you compute attention like this:
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$$\text{Attention}(Q, K, V) = \text{Softmax}\left(\frac{QK^\top}{\sqrt{d}}\right)V$$

- But during inference (Generation):
  - Now you're generating **one token at a time**, e.g., for text completion or chat.
- **But recomputing all $K_1 ... K_t$ every time would be slow.**
  - So instead, we:
  - **Cache** $K_1, K_2, ..., K_{t-1}$ and $V_1, V_2, ..., V_{t-1}$
  - Only compute K_t and V_t once
  - Append to the cache
  - Use the cache to compute:

$$\text{Attention}(Q_t, [K_1, ..., K_t], [V_1, ..., V_t])$$

What is KV Caching? Why Optimize It?

- In autoregressive generation:
  - You compute attention one token at a time.
  - You must **cache all previous K and V vectors** for fast computation.
- **Standard Transformer:**
  - K/V stored in full dimension → **expensive**.
- **MLA:**
  - Only cache:
    - c_t^{KV} (compressed key-value vector)
    - $k_t^{(R)}$ (positional key)
  - Reconstruct actual keys/values **on-the-fly** using these small vectors.
- **Result:** Much smaller KV cache → faster inference, lower memory.

Compute Base content

$$\boxed{\mathbf{c}_t^{KV}} = W^{DKV}\mathbf{h}_t,$$

$\mathbf{h}_t$: hidden state at time t

W^{DKV}: projection matrix

$\mathbf{c}_t^{KV}$: base content vector for key/value processing

Compute Multi-head Content Keys

$$\boxed{\mathbf{c}_t^{KV}} = W^{DKV}\mathbf{h}_t,$$

$$[\mathbf{k}_{t,1}^C; \mathbf{k}_{t,2}^C; \ldots; \mathbf{k}_{t,n_h}^C] = \mathbf{k}_t^C = W^{UK}\mathbf{c}_t^{KV},$$

- Project content vector into keys for each attention head
- Split into n_h heads

Compute Rotary Key Vector

$$\boxed{\mathbf{c}_t^{KV}} = W^{DKV}\mathbf{h}_t,$$

$$[\mathbf{k}_{t,1}^C; \mathbf{k}_{t,2}^C; \ldots; \mathbf{k}_{t,n_h}^C] = \mathbf{k}_t^C = W^{UK}\mathbf{c}_t^{KV},$$

$$\boxed{\mathbf{k}_t^R} = \mathrm{RoPE}(W^{KR}\mathbf{h}_t),$$

- Apply RoPE to a different projection of the hidden state
- This gives a **position-aware** key embedding (shared or per-head)

Final Key Vector per Head

$$\boxed{\mathbf{c}_t^{KV}} = W^{DKV}\mathbf{h}_t,$$

$$[\mathbf{k}_{t,1}^C; \mathbf{k}_{t,2}^C; \ldots; \mathbf{k}_{t,n_h}^C] = \mathbf{k}_t^C = W^{UK}\mathbf{c}_t^{KV},$$

$$\boxed{\mathbf{k}_t^R} = \mathrm{RoPE}(W^{KR}\mathbf{h}_t),$$

$$\mathbf{k}_{t,i} = [\mathbf{k}_{t,i}^C; \mathbf{k}_t^R],$$

For each attention head i, the key is a **concatenation** of:

- Head-specific content key $\mathbf{k}_{t,i}^C$
- Shared rotary positional component $\mathbf{k}_t^R$

Compute Multi-head Values

$$\boxed{\mathbf{c}_t^{KV}} = W^{DKV}\mathbf{h}_t,$$
$$[\mathbf{k}_{t,1}^C; \mathbf{k}_{t,2}^C; \ldots; \mathbf{k}_{t,n_h}^C] = \mathbf{k}_t^C = W^{UK}\mathbf{c}_t^{KV},$$
$$\boxed{\mathbf{k}_t^R} = \mathrm{RoPE}(W^{KR}\mathbf{h}_t),$$
$$\mathbf{k}_{t,i} = [\mathbf{k}_{t,i}^C; \mathbf{k}_t^R],$$
$$[\mathbf{v}_{t,1}^C; \mathbf{v}_{t,2}^C; \ldots; \mathbf{v}_{t,n_h}^C] = \mathbf{v}_t^C = W^{UV}\mathbf{c}_t^{KV},$$

- Values are derived from the same $\mathbf{c}_t^{KV}$
- One projection matrix per head

Multi-Head Latent Attention

$$\boxed{\mathbf{c}_t^{KV}} = W^{DKV}\mathbf{h}_t,$$

$$[\mathbf{k}_{t,1}^C; \mathbf{k}_{t,2}^C; \ldots; \mathbf{k}_{t,n_h}^C] = \mathbf{k}_t^C = W^{UK}\mathbf{c}_t^{KV},$$

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$$[\mathbf{v}_{t,1}^C; \mathbf{v}_{t,2}^C; \ldots; \mathbf{v}_{t,n_h}^C] = \mathbf{v}_t^C = W^{UV}\mathbf{c}_t^{KV},$$

Compressing K,Q,V

- **Why Compress?**
  - Original vector is 4096D → storing this for every token in long sequences is costly.
  - Compressed vector is only 128D → **less memory** and **faster inference**.
  - In DeepSeek-V3, **only c_t^{KV} and $k_t^{(R)}$ are cached** (not the full key/value), saving even more space.

$$c_t^{KV} = W^{DKV} h_t, \quad W^{DKV} \in \mathbb{R}^{128 \times 4096}$$

Then:

- Up-project to **keys**:

$$\mathbf{k}_t^C = W^{UK} \mathbf{c}_t^{KV}$$

- Up-project to **values**:

$$\mathbf{v}_t^C = W^{UV} \mathbf{c}_t^{KV}$$

$$\boxed{\mathbf{c}_t^{KV}} = W^{DKV} \mathbf{h}_t,$$

$$[\mathbf{k}_{t,1}^C; \mathbf{k}_{t,2}^C; \ldots; \mathbf{k}_{t,n_h}^C] = \mathbf{k}_t^C = W^{UK} \mathbf{c}_t^{KV},$$

$$\boxed{\mathbf{k}_t^R} = \mathrm{RoPE}(W^{KR} \mathbf{h}_t),$$

$$\mathbf{k}_{t,i} = [\mathbf{k}_{t,i}^C; \mathbf{k}_t^R],$$

$$[\mathbf{v}_{t,1}^C; \mathbf{v}_{t,2}^C; \ldots; \mathbf{v}_{t,n_h}^C] = \mathbf{v}_t^C = W^{UV} \mathbf{c}_t^{KV},$$

What is Low-Rank Compression?

- **In standard attention:**
  - Queries (Q), Keys (K), and Values (V) are **direct linear projections** of the hidden state $h_t \in \mathbb{R}^d$ (where d is large, e.g., 4096).
- **In MLA:**
  - Instead of projecting full-size Q, K, V, we **first reduce the dimensionality**:
  - The compressed version of the hidden state vector, $h_t = c_t \in \mathbb{R}^{d^c}$, where $d^c \ll d$ (e.g., 128 instead of 4096)
  - This is called **low-rank compression**.
- **Why?**
  - It saves:
    - Memory for storing K/V during inference.
    - Activation memory for Q during training.

$$\boxed{\mathbf{c}_t^{KV}} = W^{DKV}\mathbf{h}_t,$$
$$[\mathbf{k}_{t,1}^C; \mathbf{k}_{t,2}^C; \ldots; \mathbf{k}_{t,n_h}^C] = \mathbf{k}_t^C = W^{UK}\mathbf{c}_t^{KV},$$
$$\boxed{\mathbf{k}_t^R} = \mathrm{RoPE}(W^{KR}\mathbf{h}_t),$$
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$$[\mathbf{v}_{t,1}^C; \mathbf{v}_{t,2}^C; \ldots; \mathbf{v}_{t,n_h}^C] = \mathbf{v}_t^C = W^{UV}\mathbf{c}_t^{KV},$$

How Compression Works in DeepSeek:

- **Start with full hidden state** $h_t \in \mathbb{R}^{4096}$.
- **Apply a down-projection matrix**:

$$\mathbf{k}_t = W^K \mathbf{h}_t \qquad \mathbf{v}_t = W^V \mathbf{h}_t$$

Standard MHA

Requires caching **both K and V** per token

$$c_t^{KV} = W^{DKV} h_t, \quad W^{DKV} \in \mathbb{R}^{128 \times 4096}$$

Then:

- Up-project to **keys**:

$$\mathbf{k}_t^C = W^{UK} \mathbf{c}_t^{KV}$$

- Up-project to **values**:

$$\mathbf{v}_t^C = W^{UV} \mathbf{c}_t^{KV}$$

Multi Latent Attention (MLA)

Only c_t^{KV} is cached — saving memory

Multi-Head Latent Attention (MLA)

(1) Compress hidden state for keys/values

$$\mathbf{c}_t^{KV} = W^{DKV}\mathbf{h}_t$$

(2) Up-project to get per-head keys

$$[\mathbf{k}_{t,1}^C, \mathbf{k}_{t,2}^C, ..., \mathbf{k}_{t,n_h}^C] = \mathbf{k}_t^C = W^{UK}\mathbf{c}_t^{KV}$$

(3) Compute positional keys with RoPE

$$[\mathbf{k}_{t,1}^R, \mathbf{k}_{t,2}^R, ..., \mathbf{k}_{t,n_h}^R] = \mathbf{k}_t^R = \mathrm{RoPE}(W^{KR}\mathbf{h}_t)$$

(4) Final key per head = content + position

$$\mathbf{k}_{t,i} = [\mathbf{k}_{t,i}^C; \mathbf{k}_{t,i}^R]$$

(5) Up-project to get per-head values

$$[\mathbf{v}_{t,1}^C, \mathbf{v}_{t,2}^C, ..., \mathbf{v}_{t,n_h}^C] = \mathbf{v}_t^C = W^{UV}\mathbf{c}_t^{KV}$$

Symbol	Description
$\mathbf{h}_t \in \mathbb{R}^d$	Hidden state at time step `t`
d	Embedding dimension
n_h	Number of attention heads
d_h	Dimension per head (`d = n_h × d_h`)
$d_c \ll d$	Compressed dimension
$\mathbf{c}_t^{KV} \in \mathbb{R}^{d_c}$	Compressed latent for keys & values
$W^{DKV} \in \mathbb{R}^{d_c \times d}$	Down-projection matrix
$W^{UK}, W^{UV} \in \mathbb{R}^{d_h n_h \times d_c}$	Up-projection matrices for keys and values
$W^{KR} \in \mathbb{R}^{d_h n_h \times d}$	Projects hidden state for RoPE
$\mathrm{RoPE}(\cdot)$	Rotary Positional Embedding
$\mathbf{k}_t^C, \mathbf{k}_t^R \in \mathbb{R}^{d_h n_h}$	Content and positional keys
$\mathbf{k}_{t,i} \in \mathbb{R}^{2d_h}$	Final key for head `i` (concatenation)
$\mathbf{v}_t^C \in \mathbb{R}^{d_h n_h}$	Values for all heads

Why it's called "latent"

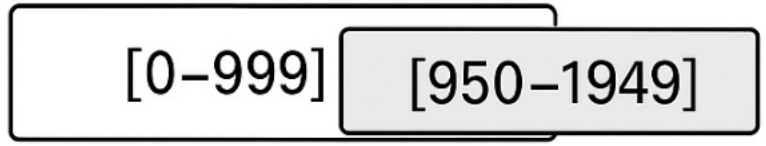
- Latent refers to **"Intermediate, hidden representations** in a neural network
  - Not directly observable, but inferred from data
  - Capture **abstract features**, patterns, or concepts
- MLA
  - h_t Hidden state — a latent vector encoding all context learned so far
  - C_t^{KV} Latent content vector — not directly observable, used internally to compute attention
  - Key, Value vectors: Latent because they represent how to relate tokens — not exposed directly
- **Other examples in ML**
  - **Latent space** in autoencoders (compressed internal representation)
  - **Latent variables** in probabilistic models (e.g. topic distributions in LDA)

Long Sequences

- Transformers have **quadratic time & memory** complexity: $O(n^2)$
  - Sequences like **books, code, or genomes** can be **10k+ tokens**
  - Solution: **Split into chunks** to fit in memory and allow parallelization
- **Naive Chunking:**
  - Input split into non-overlapping blocks : [Token 0–999], [1000–1999], etc.
  - **Problem:**
    - **No attention across chunks**
    - Tokens **lose access to global context**
    - Model can't relate distant concepts

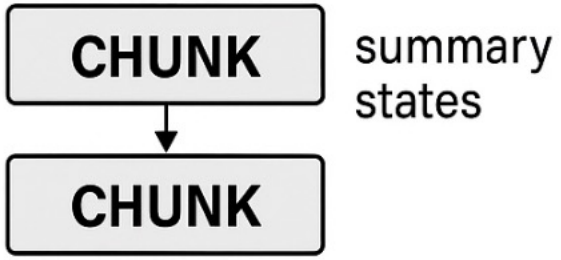
Solutions to Preserve Context

- **Overlapping Chunks**
  - Add **token overlap** between chunks
  - Example: [0–999], [950–1949]
  - Preserves partial context

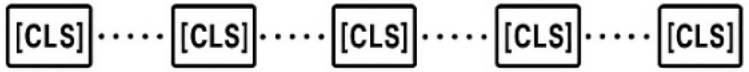


Add token overlap between chunks
Example: [0–999], [950–1949]
Preserves partial context

- **Recurrent Memory**
  - Pass **summary states** across chunks (Transformer-XL)
  - Maintains long-term dependencies

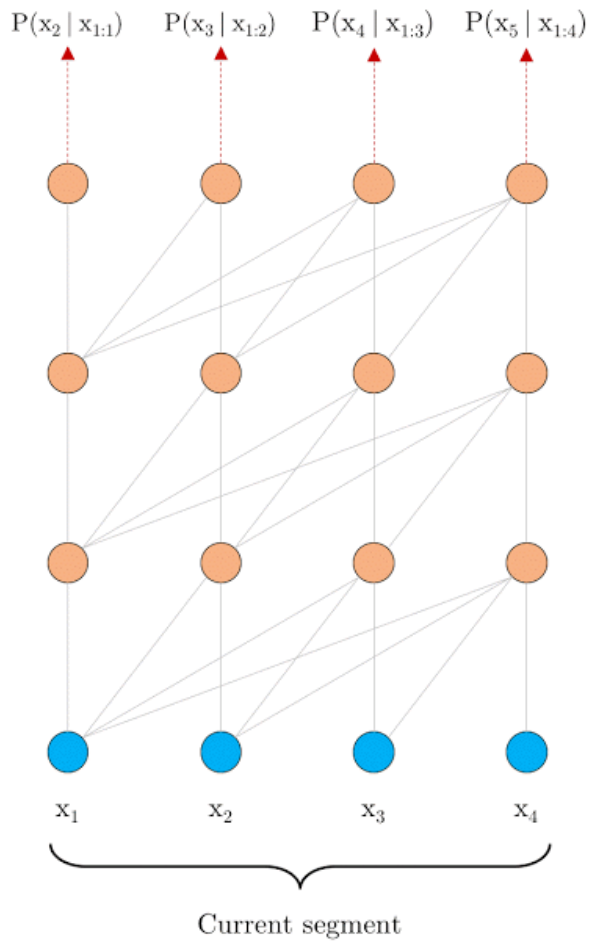


- **Sparse or Global Attention**
  - Use **special tokens** that attend across chunks (e.g., [CLS] tokens in Longformer/BigBird)
  - Global views with local efficiency

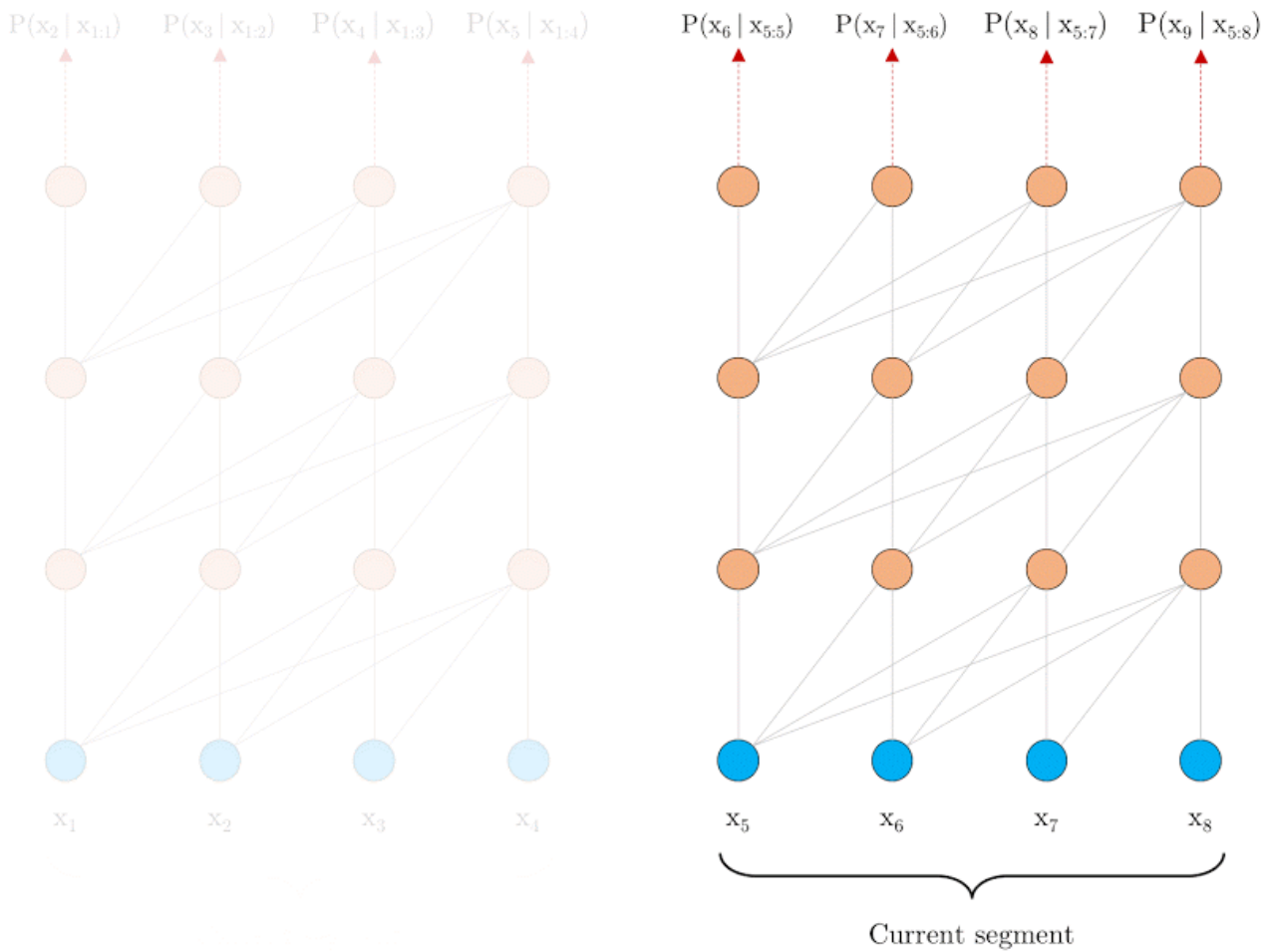


The Problem: Limited Context in Transformers

- Standard Transformers process sequences in fixed-length segments.
- No information flow between segments during training.
- Leads to:
  - Inability to capture long-range dependencies.
  - Context fragmentation during evaluation.
  - Inefficient evaluation.



Vanilla Transformer with a fixed-length context at training time.



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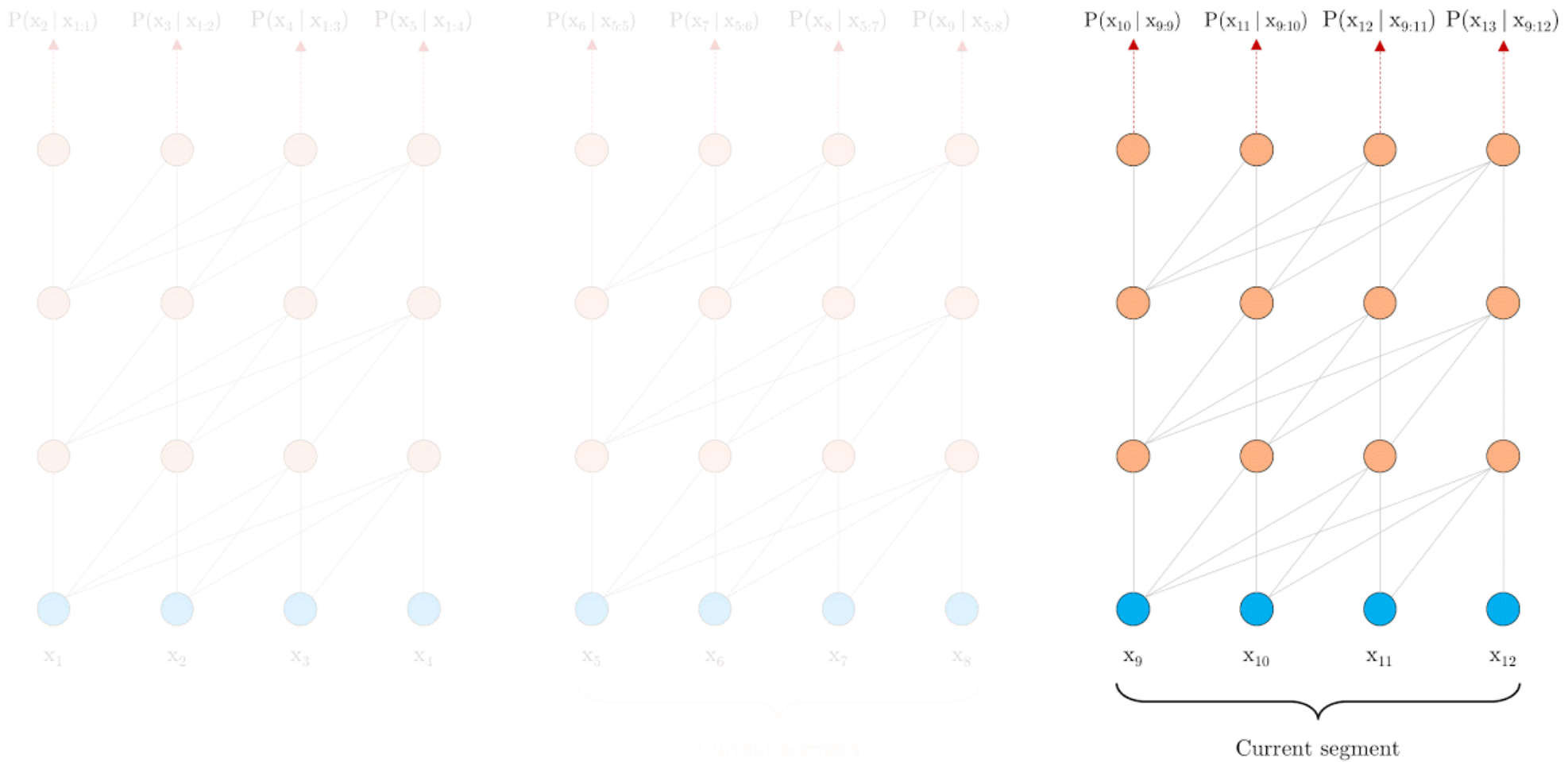

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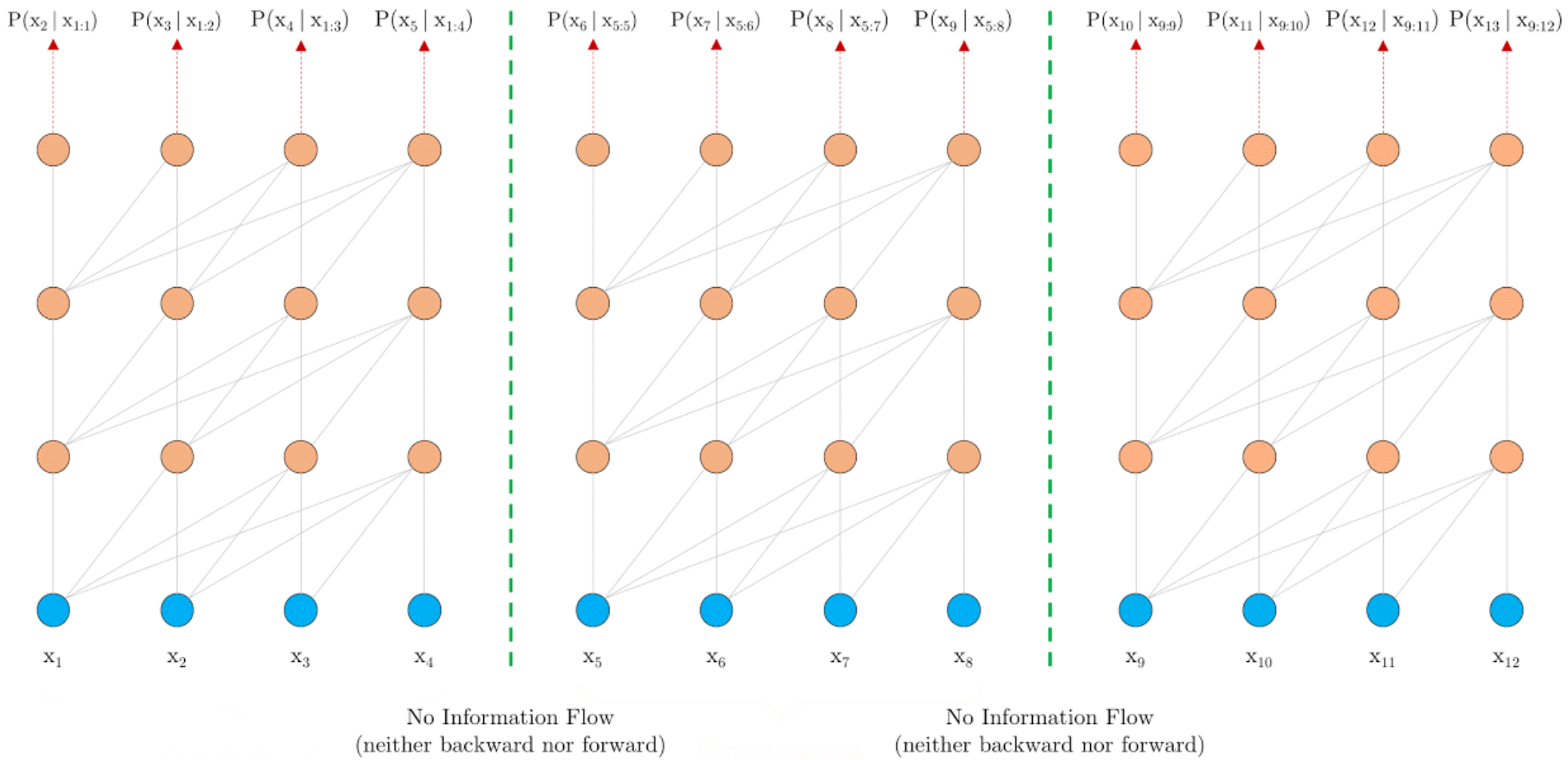

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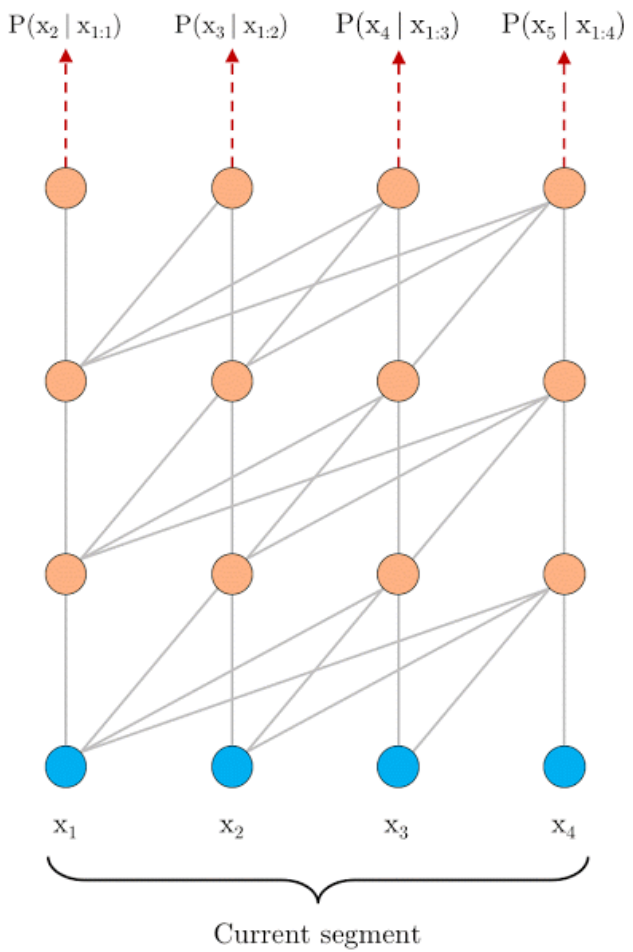
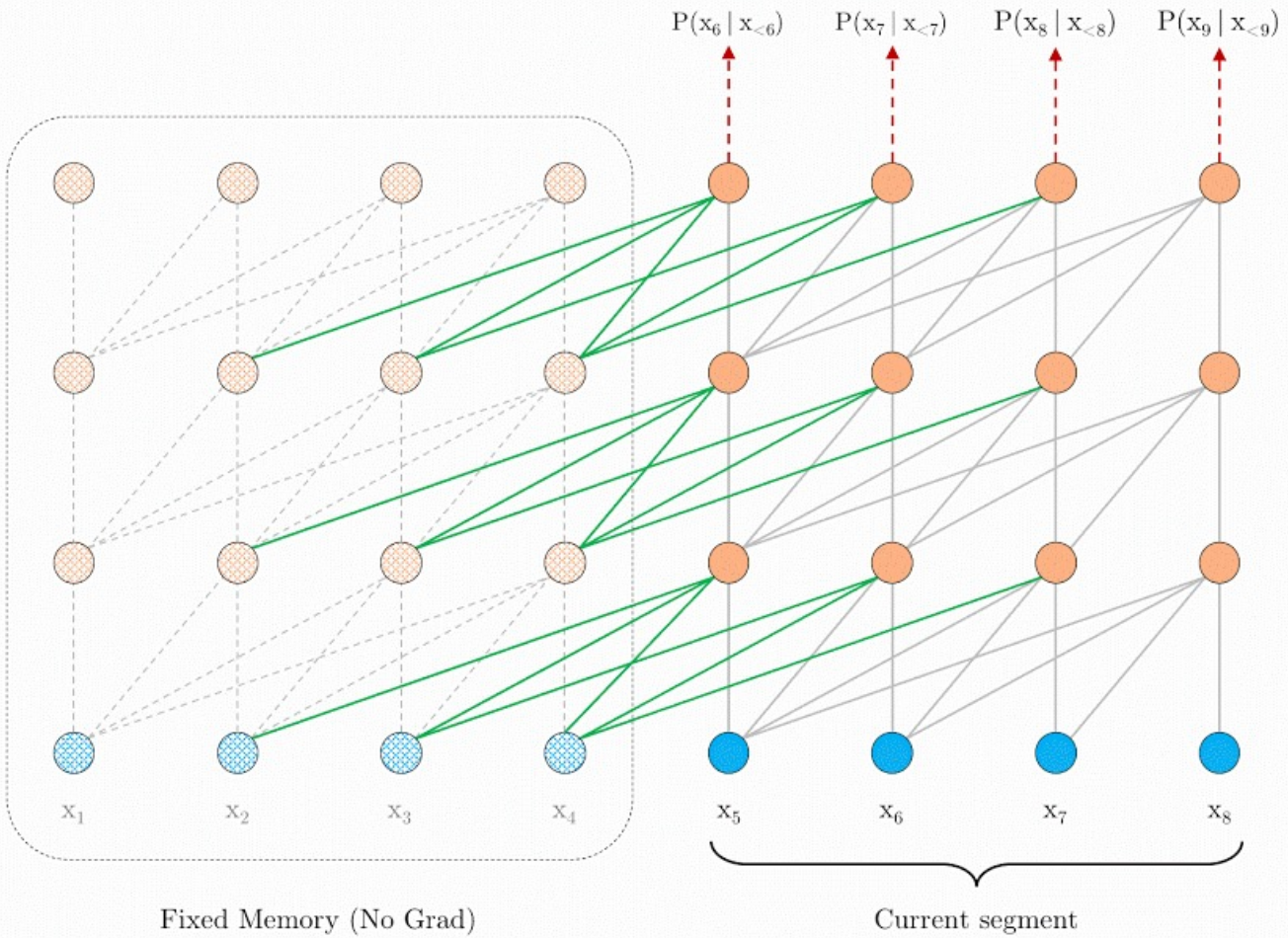


Transformer-XL with segment-level recurrence at training time.

Improve Transformer's ability to model **long-term dependencies** by **reusing hidden states from previous segments**.



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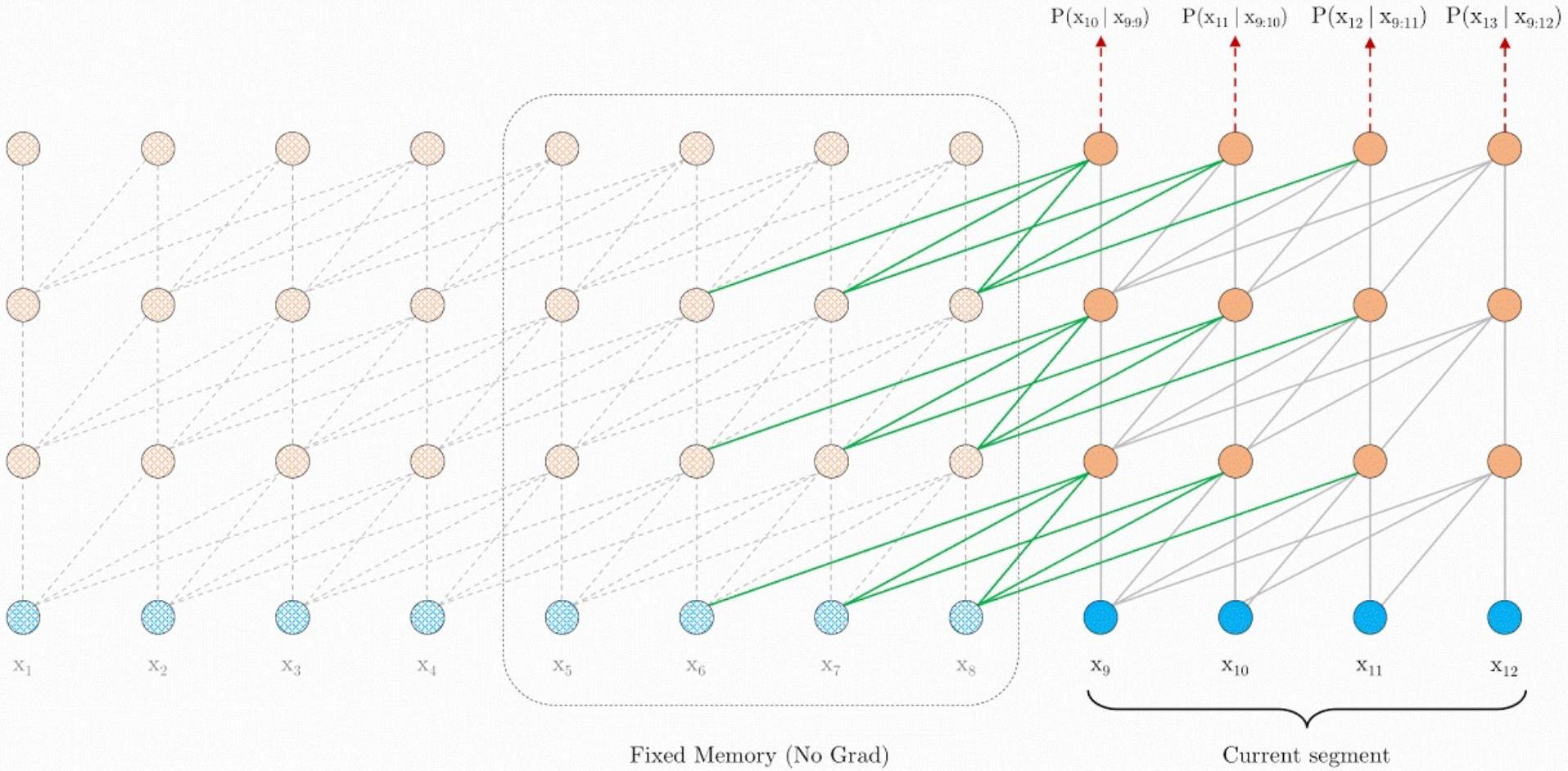

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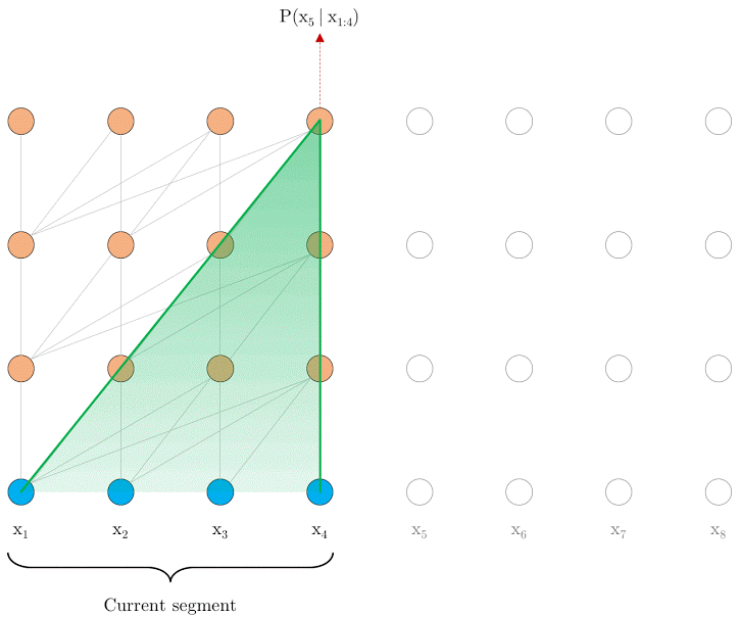
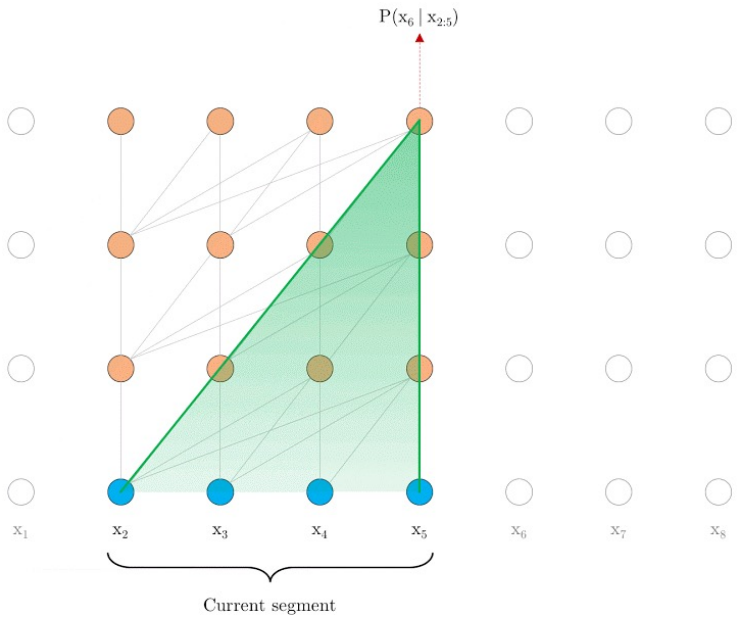


Vanilla Transformer with a fixed-length context at evaluation time.



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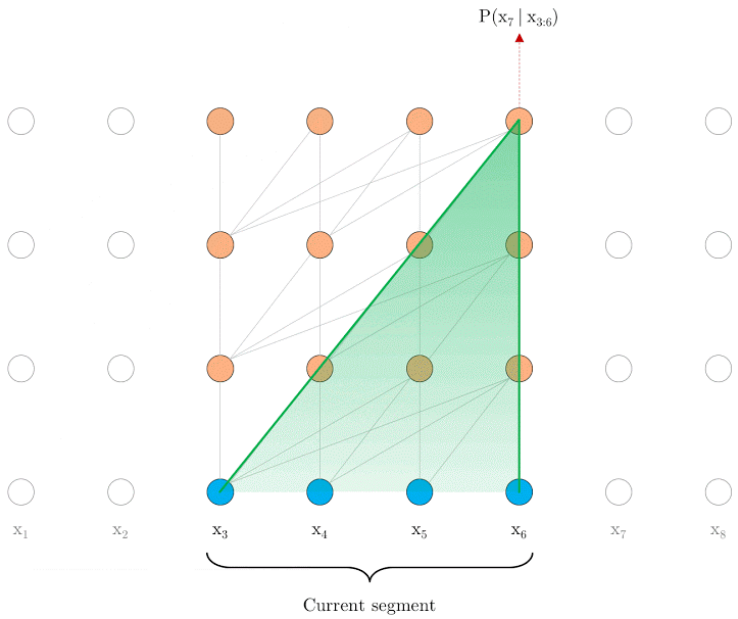

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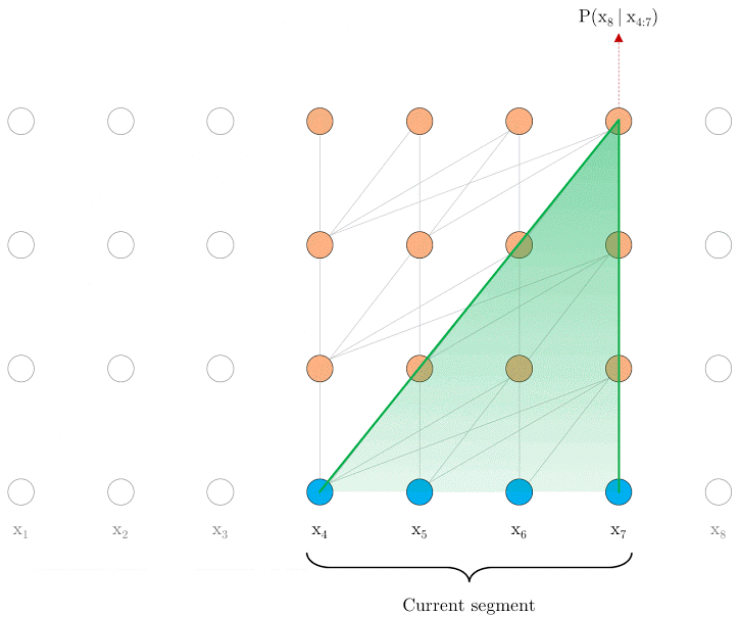

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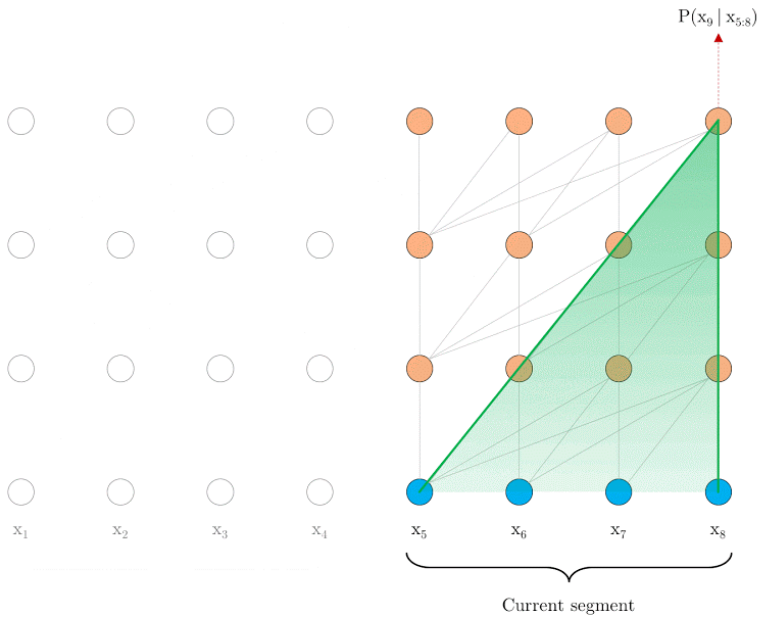

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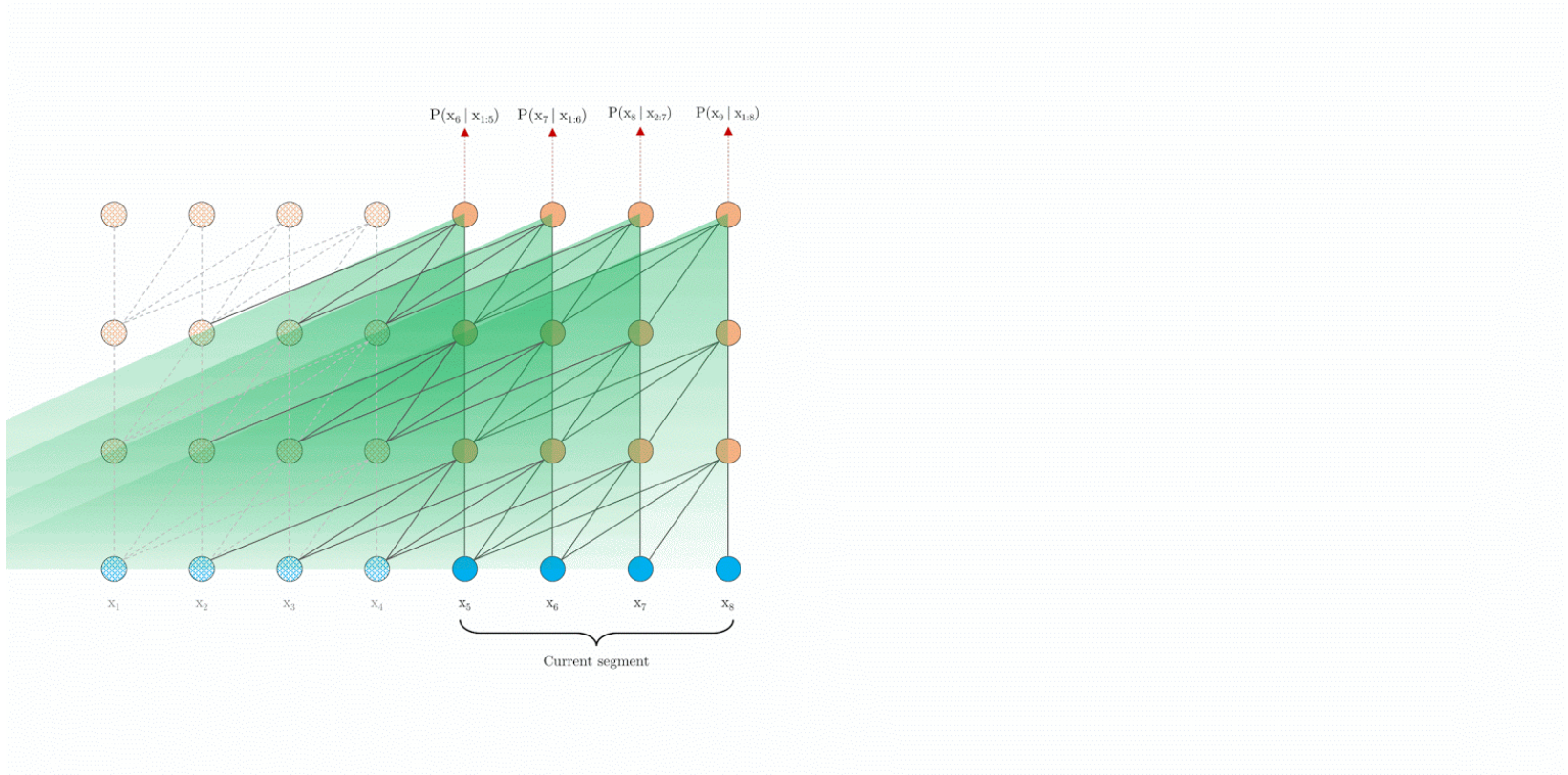
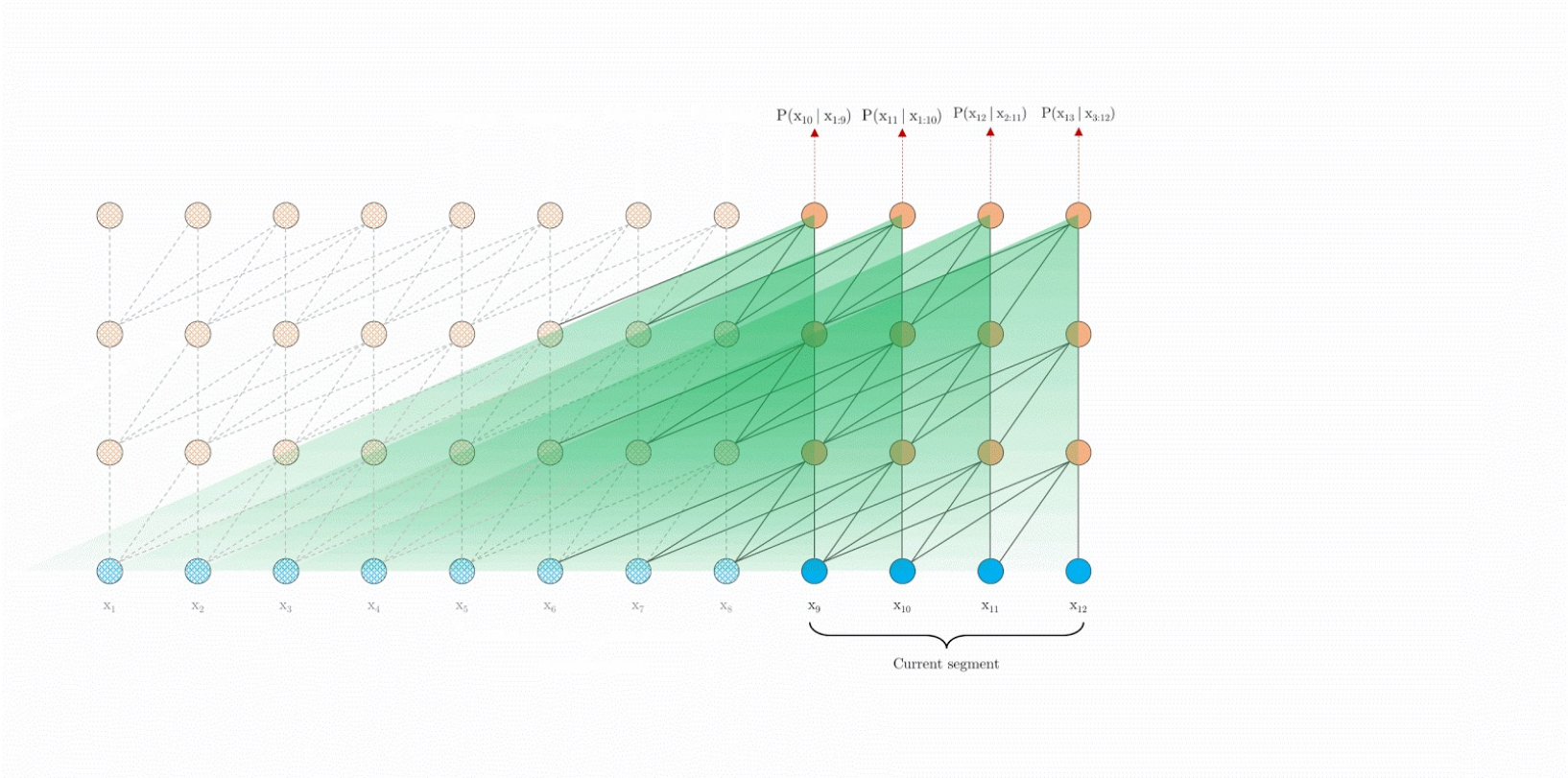


Transformer-XL with segment-level recurrence at evaluation time.



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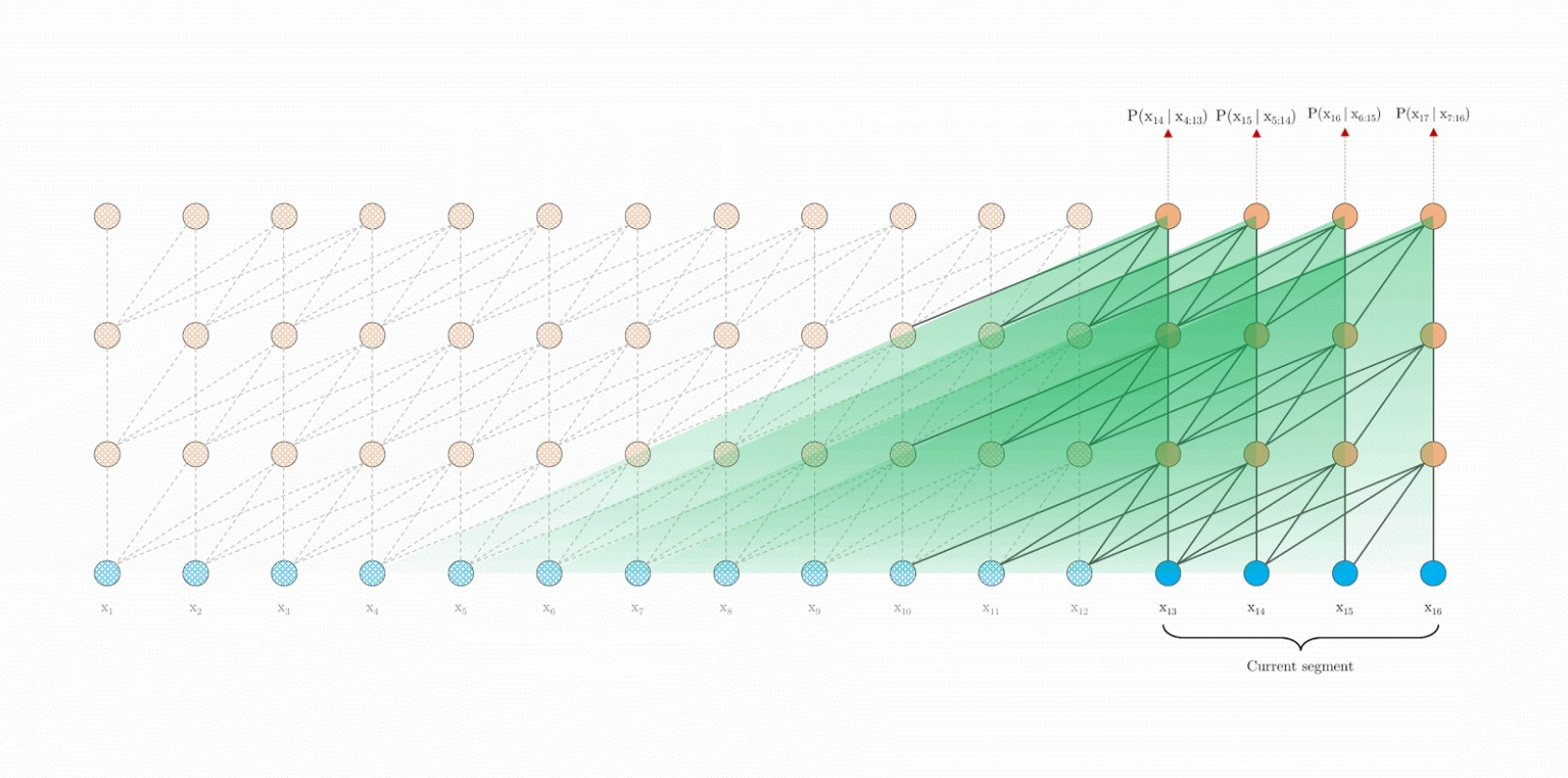

Transformer-XL with segment-level recurrence at evaluation time.

Relative Positional Encoding

- In long sequences, we **divide data into fixed-length segments** during training/inference. For example:
  - Segment 1: tokens $x_0, x_1, \ldots, x_9$
  - Segment 2: tokens $x_{10}, x_{11}, \ldots, x_{19}$
- **Segments shift when we move to the next chunk of input**, like in streaming text or large documents.
- **Problem with absolute positions:**
  - Segment 1: token x0 has absolute position 0
  - Segment 2: token x10 has absolute position 0 **again**, if we reset every segment
  - This breaks the continuity of attention across segments

For example, consider an old segment with contextual positions [0, 1, 2, 3]. When a new segment is processed, we have positions [0, 1, 2, 3, 0, 1, 2, 3] for the two segments combined, where the semantics of each position id is incoherent through out the sequence.

Relative Positional Encoding

- **Core Idea:** Instead of encoding absolute position (i), encode the *relative distance* (i-j) between the query token (i) and the key token (j).
- **Consistency:** The distance between two tokens remains the same regardless of which segment they appear in or which states are being reused.
  - Encodes "How far away is token j from token i?"

The quick brown fox jumps over the lazy dog

Absolute 4 5 8

Relative

jump to fox: 1
jump to lazy: -3

Relative Positional Encoding Used in Transformer-XL

- x_i, x_j: input token vectors at positions i, j
- W_Q, W_K, W_R: learnable projection matrices
- r_{i-j}: **sinusoidal embedding** of relative distance $i - j$ (non-learnable)
- u, v: trainable global vectors (shared across tokens)

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

$$Q = XW_Q, K = XW_K, V = XW_V$$

$$A_{i,j} = Q_i \cdot K_j^T = (x_i W_Q)(x_j W_K)^T$$

Score between query xi and key xj

$$A_{i,j} = \underbrace{x_i^T W_Q^T W_K x_j}_{\text{content-to-content}} + \underbrace{x_i^T W_Q^T W_R r_{i-j}}_{\text{content-to-position}} + \underbrace{u^T W_K x_j}_{\text{global content bias}} + \underbrace{v^T W_R r_{i-j}}_{\text{global position bias}}$$

Standard query-key interaction

Query attends to relative position embedding

Bias based on key content

Bias based on position offset

Content to Content Attention

- **What it is:**
  - The standard dot product between the query and key.
  - Captures the similarity between token xi (query) and token xj (key).
- **Role:**
  - Purely based on **token content**.
  - Found in the original Transformer.

$$A_{i,j} = \underbrace{x_i^T W_Q^T W_K x_j}_{\text{content-to-content}} + \underbrace{x_i^T W_Q^T W_R r_{i-j}}_{\text{content-to-position}} + \underbrace{u^T W_K x_j}_{\text{global content bias}} + \underbrace{v^T W_R r_{i-j}}_{\text{global position bias}}$$

Content-to-Position Attention

- **What it is:**
  - r_{i-j} represents the **relative distance** between i and j.
  - We project both the query and the relative position embedding, then take their dot product.
  - Allows the query to attend to **relative positions**, not absolute.
  - Crucial for enabling consistent attention when segments shift or memory is reused.
  - Same r would be used even if segment started at a different index.

$i-j$	dim 0 (sin)	dim 1 (cos)	dim 2 (sin)	dim 3 (cos)	dim 4 (sin)	dim 5 (cos)
-3	-0.1411	-0.9900	-0.2939	-0.9558	-0.4339	-0.9010
-2	-0.0900	-0.9959	-0.1960	-0.9807	-0.2963	-0.9551
-1	-0.0475	-0.9988	-0.1036	-0.9946	-0.1581	-0.9874
0	0.0000	1.0000	0.0000	1.0000	0.0000	1.0000
+1	0.0475	0.9988	0.1036	0.9946	0.1581	0.9874
+2	0.0900	0.9959	0.1960	0.9807	0.2963	0.9551
+3	0.1411	0.9900	0.2939	0.9558	0.4339	0.9010

$$A_{i,j} = \underbrace{x_i^T W_Q^T W_K x_j}_{\text{content-to-content}} + \underbrace{x_i^T W_Q^T W_R r_{i-j}}_{\text{content-to-position}} + \underbrace{u^T W_K x_j}_{\text{global content bias}} + \underbrace{v^T W_R r_{i-j}}_{\text{global position bias}}$$

Global Content Bias

- **What it is:**
  - u is a **learned global content bias vector**, shared across all queries.
  - Computes a bias based on the **key token's content** xj.
- **Role:**
  - Adds a fixed influence based on **what the key is**, not on the query.
  - Helps stabilize attention scores.

$$A_{i,j} = \underbrace{x_i^T W_Q^T W_K x_j}_{\text{content-to-content}} + \underbrace{x_i^T W_Q^T W_R r_{i-j}}_{\text{content-to-position}} + \underbrace{u^T W_K x_j}_{\text{global content bias}} + \underbrace{v^T W_R r_{i-j}}_{\text{global position bias}}$$

Global Position Bias

- **What it is:**
  - v is a **learned global position bias vector**.
  - Applied to the relative position embedding r_{i-j} .
- **Role:**
  - Adds a fixed bias for each **relative position** (e.g., -1, 0, +2).
  - Helps encode structural inductive bias — e.g., maybe recent tokens are more important.

$$A_{i,j} = \underbrace{x_i^T W_Q^T W_K x_j}_{\text{content-to-content}} + \underbrace{x_i^T W_Q^T W_R r_{i-j}}_{\text{content-to-position}} + \underbrace{u^T W_K x_j}_{\text{global content bias}} + \underbrace{v^T W_R r_{i-j}}_{\text{global position bias}}$$