COMS4995W32
Applied Machine Learning

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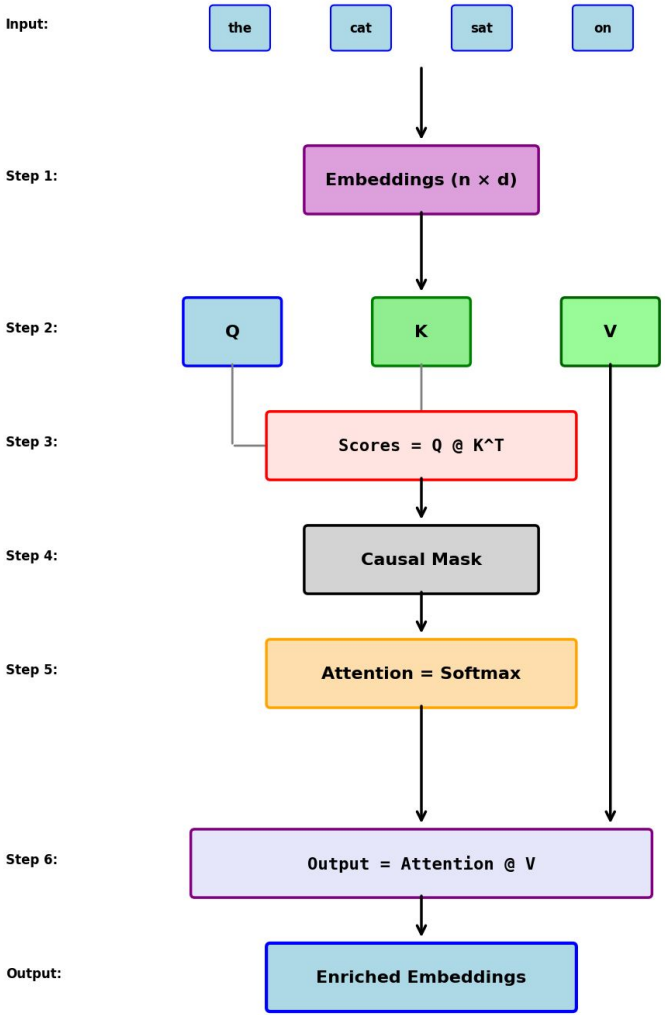
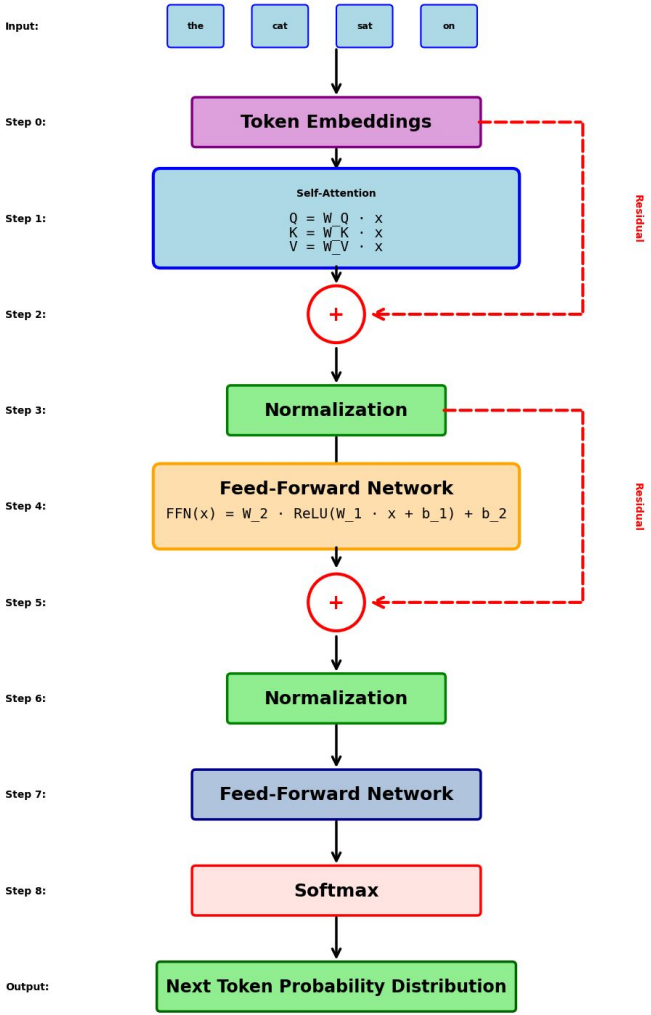
Columbia University | Fall 2025

Transformer++

Recap on Transformer


Input:
the
cat
sat
on
Step 1:
Embeddings (n × d)
Step 2:
Q
K
V
Step 3:
Scores = Q @ K^T
Step 4:
Causal Mask
Step 5:
Attention = Softmax
Step 6:
Output = Attention @ V
Output:
Enriched Embeddings



🤖 Attention is All You Need

Agenda++ 📃

- Positional Encoding & Masking
- Multi-head Self-Attention
- Normalization & Optimization
- Model Family
- Decoding Strategies
- Research Frontiers

Positional Encoding

Why Position Matters 🤔

Transformer treats all tokens in parallel → no notion of order

Think of it as giving every token a "position tag"

- Just like labeling words 1, 2, 3, … in a sentence

2 main strategies:

- Absolute: encode position directly (e.g., sinusoidal)
- Relative: express distance between tokens (e.g., RoPE)

Classic Sinusoidal Encoding 🔢

Position embeddings are deterministic sine and cosine functions

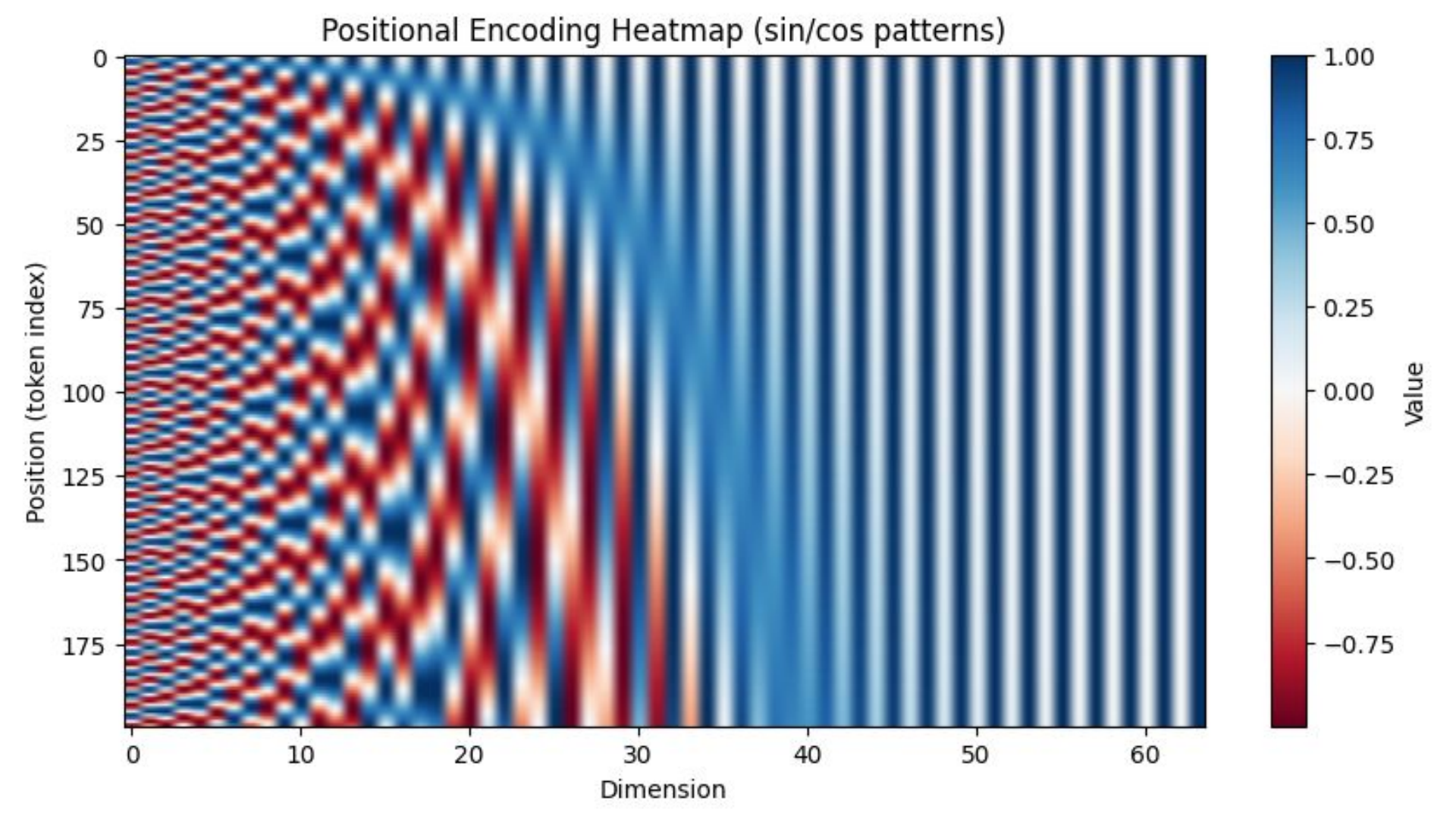
For a token at position `t`:

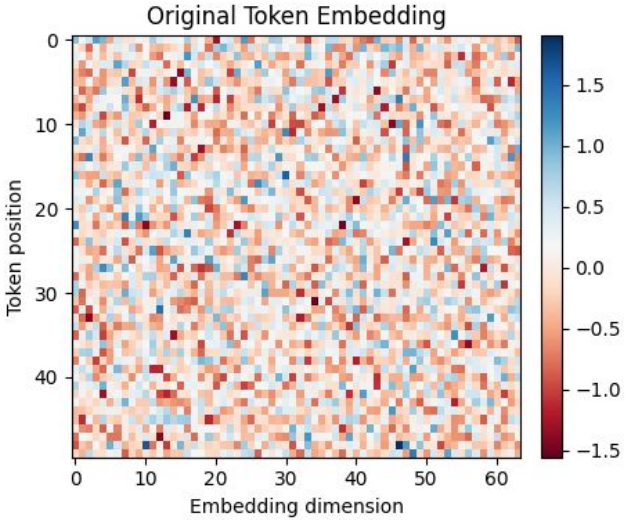
Even dimensions → PE(t, 2i) = sin(t / (10000 ^ (2i / d_model)))

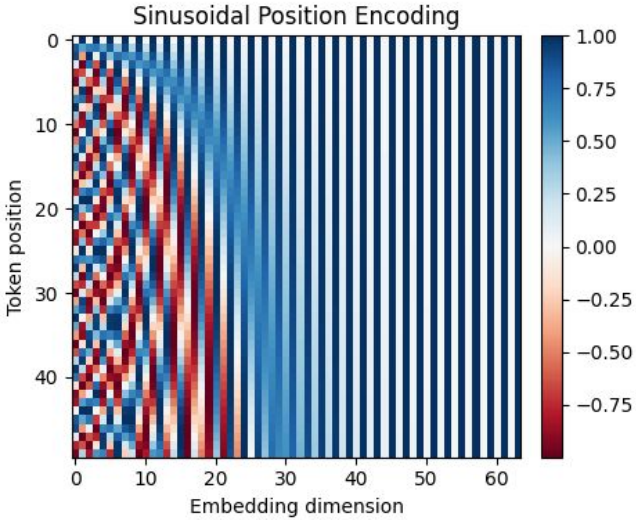
Odd dimensions → PE(t, 2i+1) = cos(t / (10000 ^ (2i / d_model)))

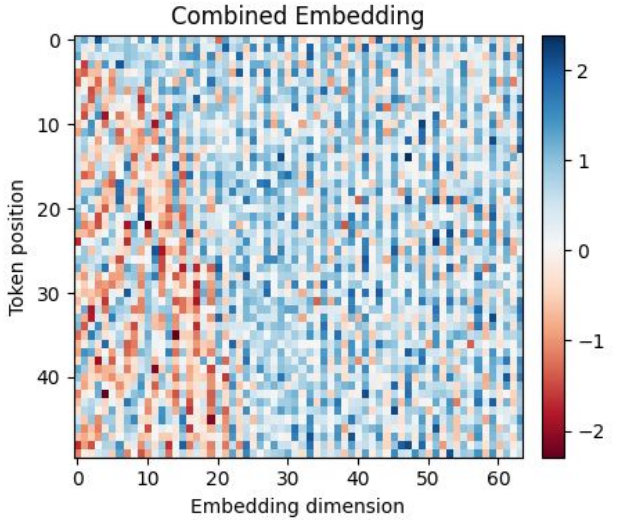
Continuous and smooth → generalizes to unseen positions

Limitation: fixed frequency range, weaker for very long sequences


Positional Encoding Heatmap (sin/cos patterns)
Position (token index)
0
25
50
75
100
125
150
175
0
10
20
30
40
50
60
Dimension
Value
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75


Original Token Embedding
Token position
Embedding dimension
0
10
20
30
40
50
60
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5


Sinusoidal Position Encoding
Token position
Embedding dimension
0
10
20
30
40
50
60
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75


Combined Embedding
Token position
Embedding dimension
0
10
20
30
40
50
60
2
1
0
−1
−2

Rotary Position Embedding (RoPE) 🔄

Idea: Instead of giving each token a fixed position number, RoPE rotates token representations in a smooth way across the sequence

How it works:

- Each token's query (Q) and key (K) vectors are placed on tiny 2-D circles
- As position increases, we rotate these vectors a little more each time
- Close tokens = small rotation difference → easy to attend
- Distant tokens = larger rotation difference → harder to attend

Used in LLaMA, ChatGPT, Gemini, and most modern LLMs

$$\textit{Attention Score}_{1,3} = \begin{bmatrix} q_{11} & q_{12} & q_{13} & q_{14} & q_{15} & q_{16} \end{bmatrix} \cdot \begin{bmatrix} \cos 2\theta_a & -\sin 2\theta_a & 0 & 0 & 0 & 0 \\ \sin 2\theta_a & \cos 2\theta_a & 0 & 0 & 0 & 0 \\ 0 & 0 & \cos 2\theta_b & -\sin 2\theta_b & 0 & 0 \\ 0 & 0 & \sin 2\theta_b & \cos 2\theta_b & 0 & 0 \\ 0 & 0 & 0 & 0 & \cos 2\theta_c & -\sin 2\theta_c \\ 0 & 0 & 0 & 0 & \sin 2\theta_c & \cos 2\theta_c \end{bmatrix} \cdot \begin{bmatrix} k_{31} \\ k_{32} \\ k_{33} \\ k_{34} \\ k_{35} \\ k_{36} \end{bmatrix} =$$

$$= \begin{bmatrix} q_{11} & q_{12} \end{bmatrix} \cdot \begin{bmatrix} \cos 2\theta_a & -\sin 2\theta_a \\ \sin 2\theta_a & \cos 2\theta_a \end{bmatrix} \cdot \begin{bmatrix} k_{31} \\ k_{32} \end{bmatrix} + \begin{bmatrix} q_{13} & q_{13} \end{bmatrix} \cdot \begin{bmatrix} \cos 2\theta_b & -\sin 2\theta_b \\ \sin 2\theta_b & \cos 2\theta_b \end{bmatrix} \cdot \begin{bmatrix} k_{33} \\ k_{34} \end{bmatrix} + \begin{bmatrix} q_{15} & q_{16} \end{bmatrix} \cdot \begin{bmatrix} \cos 2\theta_c & -\sin 2\theta_c \\ \sin 2\theta_c & \cos 2\theta_c \end{bmatrix} \cdot \begin{bmatrix} k_{35} \\ k_{36} \end{bmatrix} = a_{13}$$

Multi-Head Attention

Motivation

A single attention head can only flow one type of information

Multi-head attention allows flowing various information in parallel

Intuitively:

→ Each head = one “expert” view of the data

→ Together = an ensemble of perspectives working in parallel

Stabilizes training through feature diversity

Mechanism

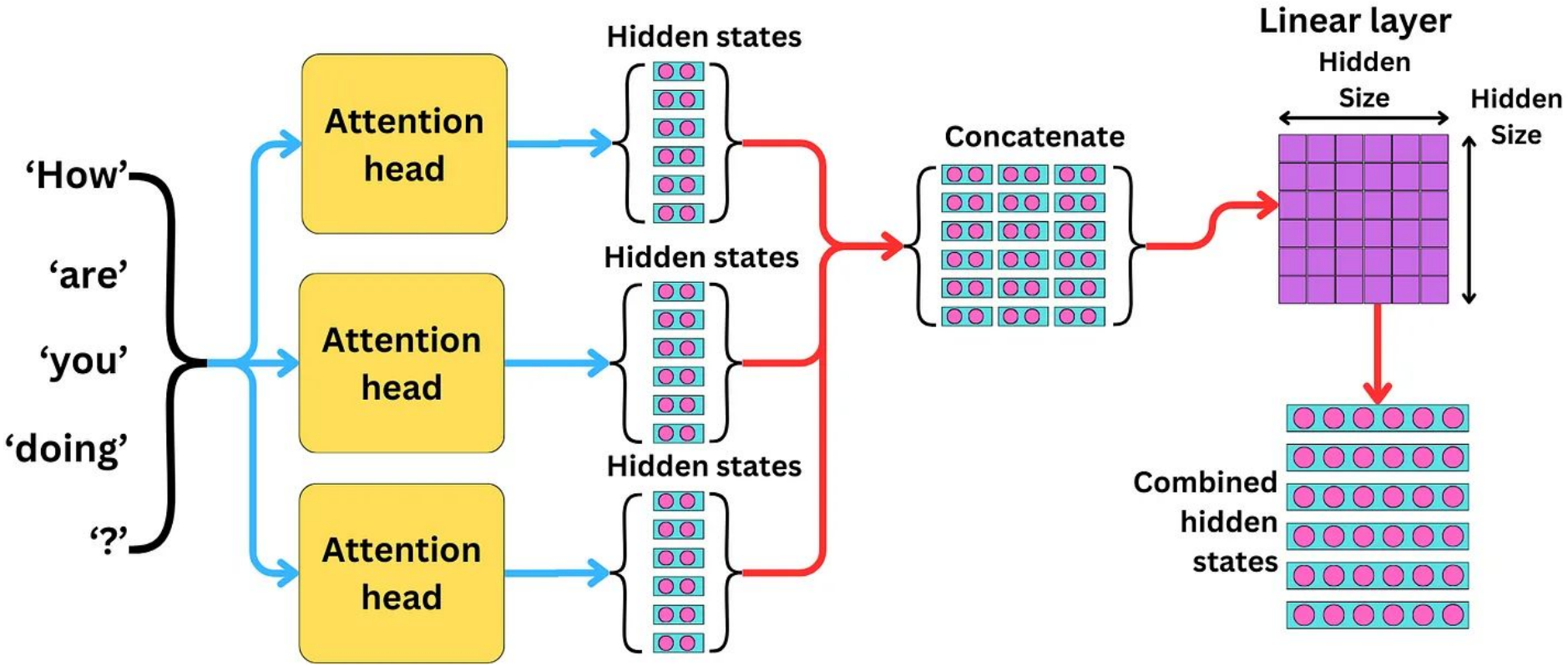
Split the hidden dimension (d_model) into h smaller parts (one per head):

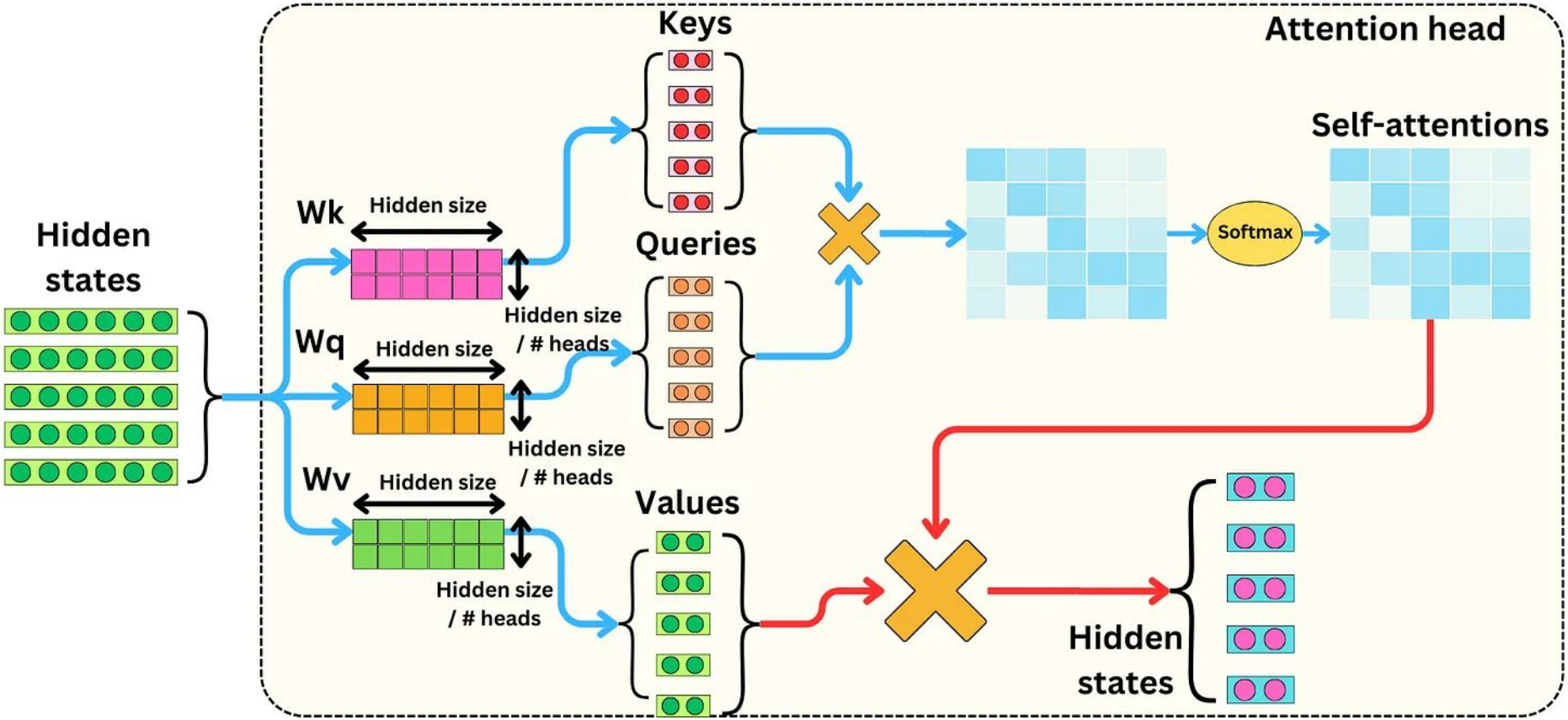
$$d\_h = d\_model // h$$

Each head performs self-attention independently:

$$Attention(Q, K, V) = softmax((QK^T) / sqrt(d\_h)) \times V$$

Concatenate all head outputs and project back to d_model


'How'
'are'
'you'
'doing'
'?'
Attention head
Attention head
Attention head
Hidden states
Hidden states
Hidden states
Concatenate
Linear layer
Hidden Size
Hidden Size
Combined hidden states


Attention head
Keys
Queries
Values
Wk
Wq
Wv
Hidden size
Hidden size / # heads
Hidden states
Self-attentions
Softmax
Hidden states

Normalization & Optimization

To Make Training Stable 

Problem

Very deep networks → gradients explode or vanish → unstable training

Solution

Residual connections + Normalization keep signal flow smooth and balanced

[Residual connections] carries the original signal forward/backward

[Normalization] scales activations, so each layer receives consistent inputs

LayerNorm

Given a token's hidden vector $x = [x_1, x_2, \ldots, x\_d]$

Compute mean and variance:

$$\mu = \text{mean}(x)$$

$$\sigma^2 = \text{mean}((x - \mu)^2)$$

Normalize each feature:

$$LN(x) = \gamma * (x - \mu) / \text{sqrt}(\sigma^2 + \varepsilon) + \beta$$

where γ and β are learnable scale and shift parameters

RMSNorm

Compute root mean square (RMS):

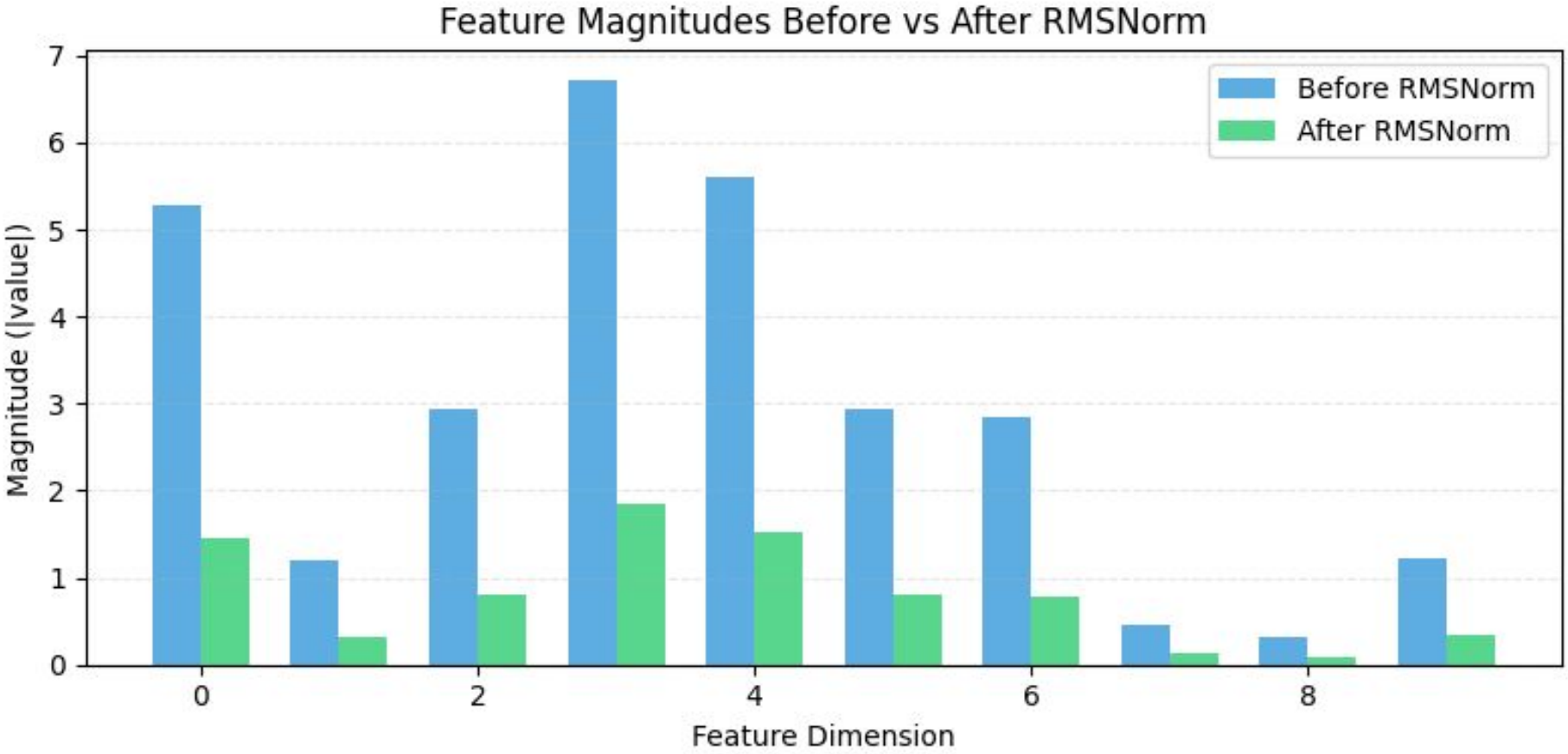
$$\text{rms}(x) = \text{sqrt}(\text{mean}(x^2))$$

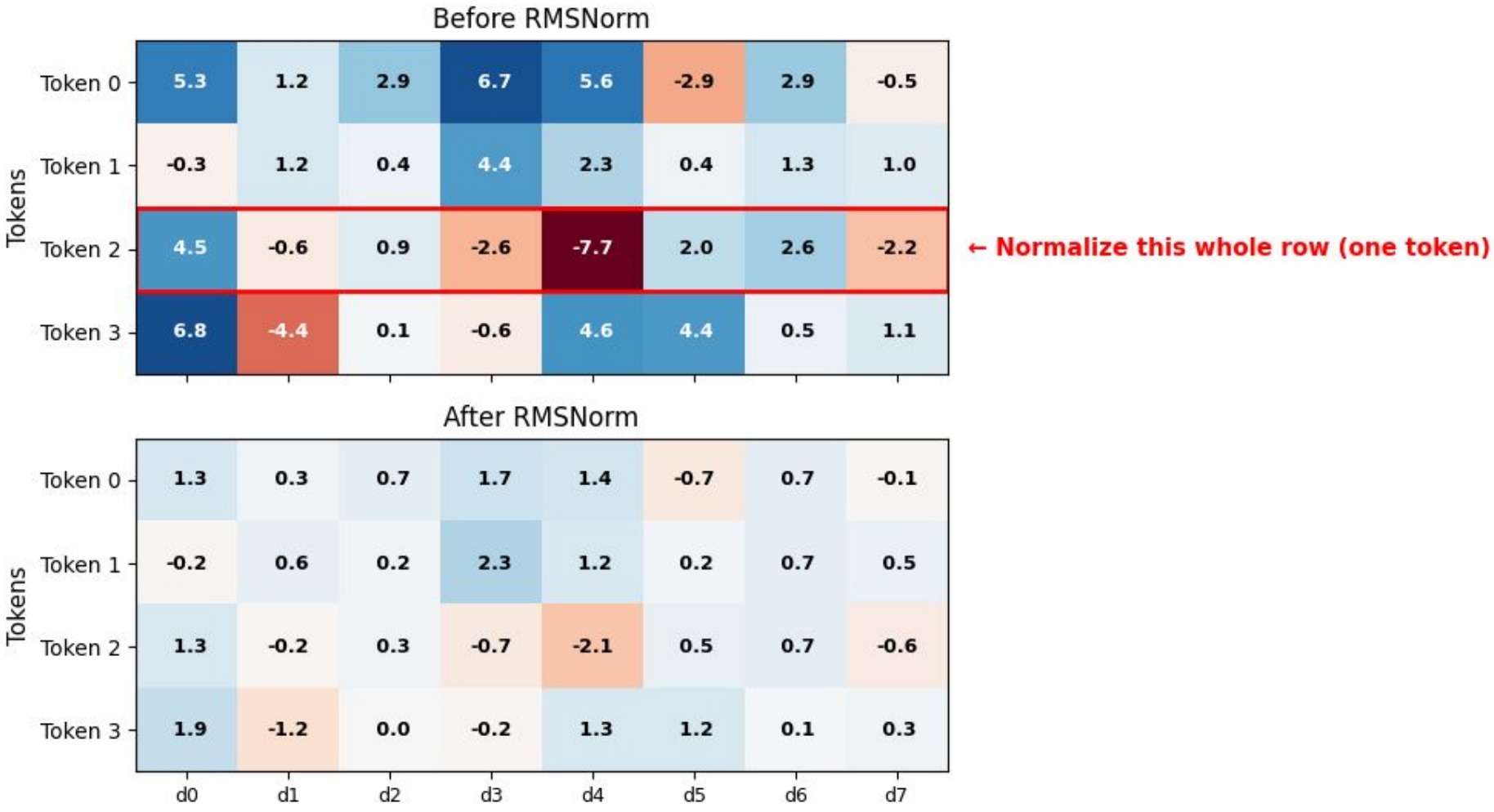
Normalize by magnitude only:

$$\text{RMSNorm}(x) = \gamma * x / (\text{rms}(x) + \varepsilon)$$

Key difference:

- LayerNorm centers by mean and scales by std → more accurate
- RMSNorm skips mean subtraction → faster, nearly identical stability


Feature Magnitudes Before vs After RMSNorm
Before RMSNorm
After RMSNorm
Magnitude (|value|)
Feature Dimension
0
1
2
3
4
5
6
7
0
2
4
6
8


Before RMSNorm
Tokens
Token 0
Token 1
Token 2
Token 3
5.3 1.2 2.9 6.7 5.6 -2.9 2.9 -0.5
-0.3 1.2 0.4 4.4 2.3 0.4 1.3 1.0
4.5 -0.6 0.9 -2.6 -7.7 2.0 2.6 -2.2
6.8 -4.4 0.1 -0.6 4.6 4.4 0.5 1.1
← Normalize this whole row (one token)
After RMSNorm
Tokens
Token 0
Token 1
Token 2
Token 3
1.3 0.3 0.7 1.7 1.4 -0.7 0.7 -0.1
-0.2 0.6 0.2 2.3 1.2 0.2 0.7 0.5
1.3 -0.2 0.3 -0.7 -2.1 0.5 0.7 -0.6
1.9 -1.2 0.0 -0.2 1.3 1.2 0.1 0.3
d0 d1 d2 d3 d4 d5 d6 d7

Pre-LN vs Post-LN 🔁

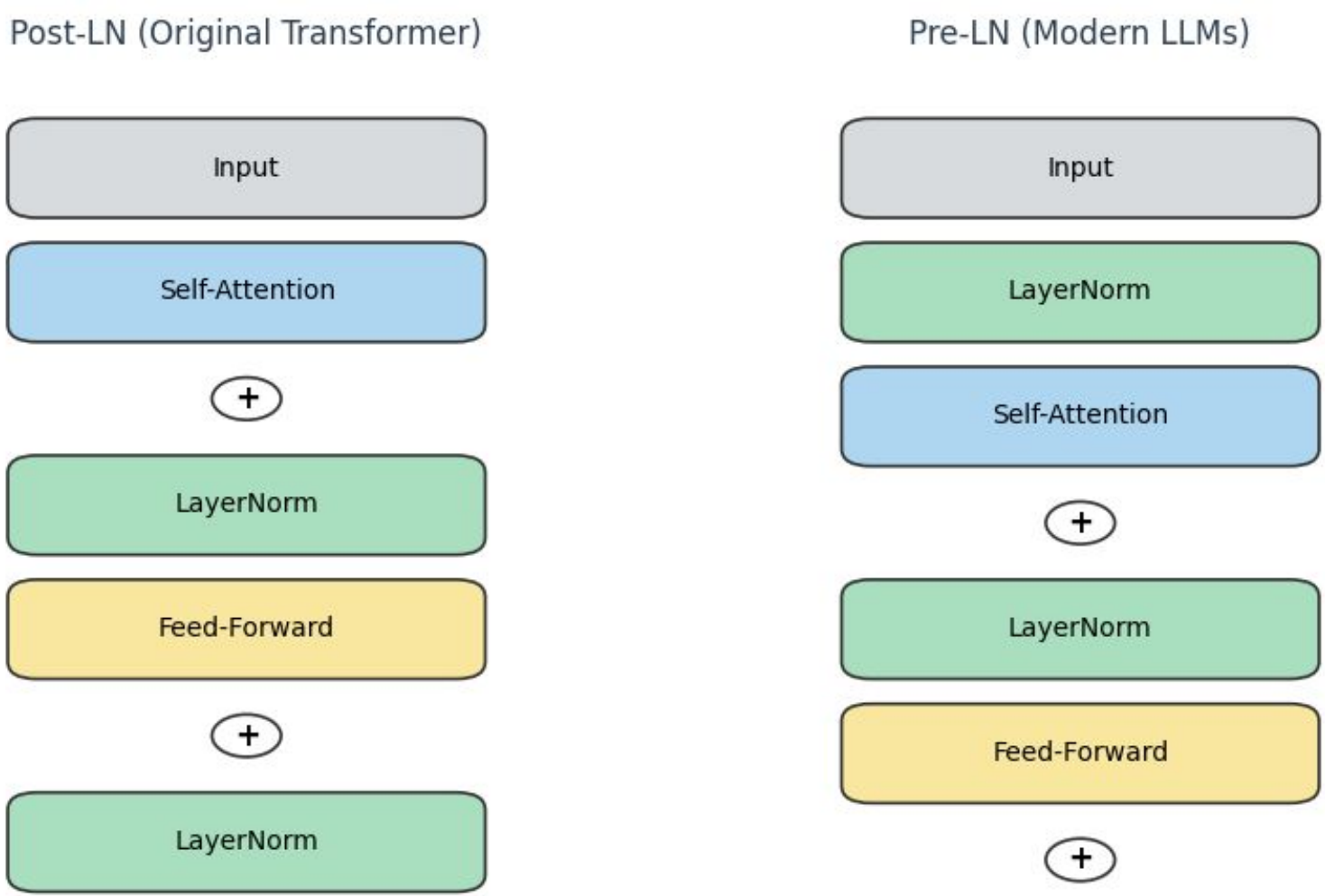
Post-LN (original Transformer): LayerNorm after each attention + residual

- Decent quality, but hard to train deep models

Pre-LN (modern LLMs): LayerNorm before attention + feed-forward

- Keeps activations within a stable range before large matrix multiplications
- Prevents softmax saturation by controlling the scale of Q and K vectors
- Makes training converge faster and more reliably

  Adopted by most modern LLMs: GPT, LLaMA, PaLM, Mistral……


Post-LN (Original Transformer)
Input
Self-Attention
+
LayerNorm
Feed-Forward
+
LayerNorm
Pre-LN (Modern LLMs)
Input
LayerNorm
Self-Attention
+
LayerNorm
Feed-Forward
+

More Tricks ⚡

AdamW (with weight decay on non-sparse weights)

→ Adam + decoupled weight decay → smoother convergence, better generalization

Learning rate warm-up + cosine decay

→ Gradually increases LR early to prevent divergence, then smoothly decays to stabilize convergence

Gradient clipping

→ Caps extreme gradient values to prevent sudden parameter spikes and exploding updates

Gradient accumulation

→ Accumulates gradients over multiple micro-batches to simulate a larger effective batch size

Takeaways 💡

✅ Modern LLM De-facto Setup:

Pre-LN + RMSNorm + AdamW + LR Warm-up

Model Family

From Building Blocks to Model Families

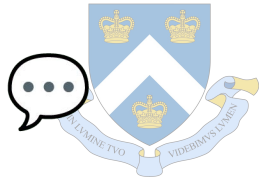
The same Transformer block can act very differently depending on:

- Masking pattern – what each token can “see”
- Training objective – what the model is asked to predict

These choices define 3 major model families:

- Decoder-only → generates text step by step
- Encoder-only → understands full context
- Encoder-Decoder → translates one sequence into another

Decoder-only Family – Language Model (LM)



Mask: Causal → token t can observe only tokens < t

Objective: Predict next token → P(token□ | tokens(1…□-1))

Usage:

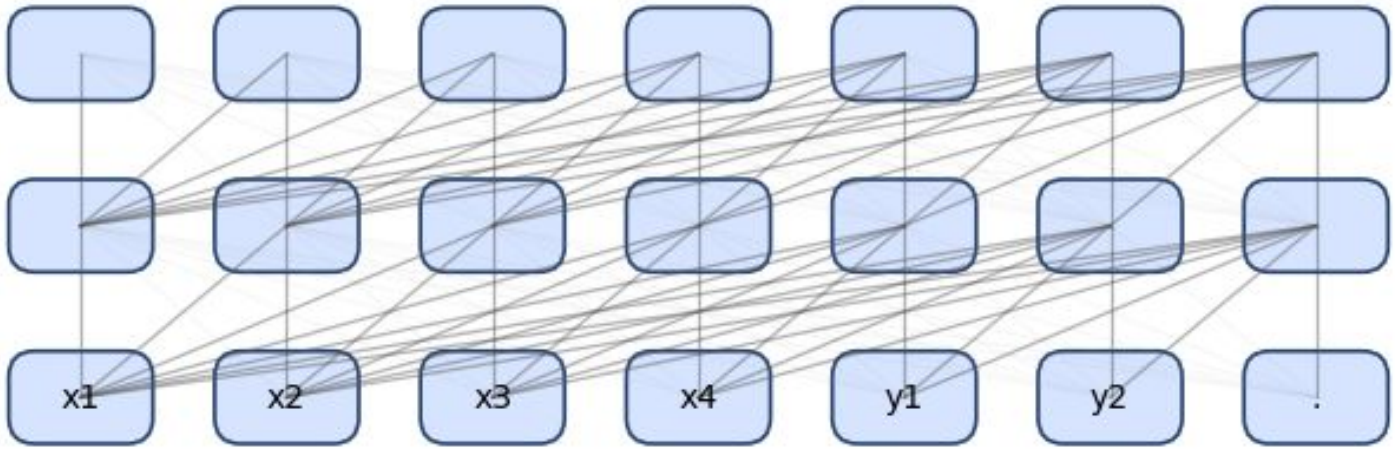
- Natural language generation (chatbots, storytelling)
- Code generation and completion (Copilot, Claude)

Examples:

GPT-2 / GPT-3 / GPT-4, LLaMA, Gemini, Mistral….

Decoder-only

causal self-attention



Encoder-only Family – Masked Language Model (MLM)

Mask: Full attention → all tokens can attend bidirectionally

Objective: Predict randomly masked tokens using both-sided context

Usage:

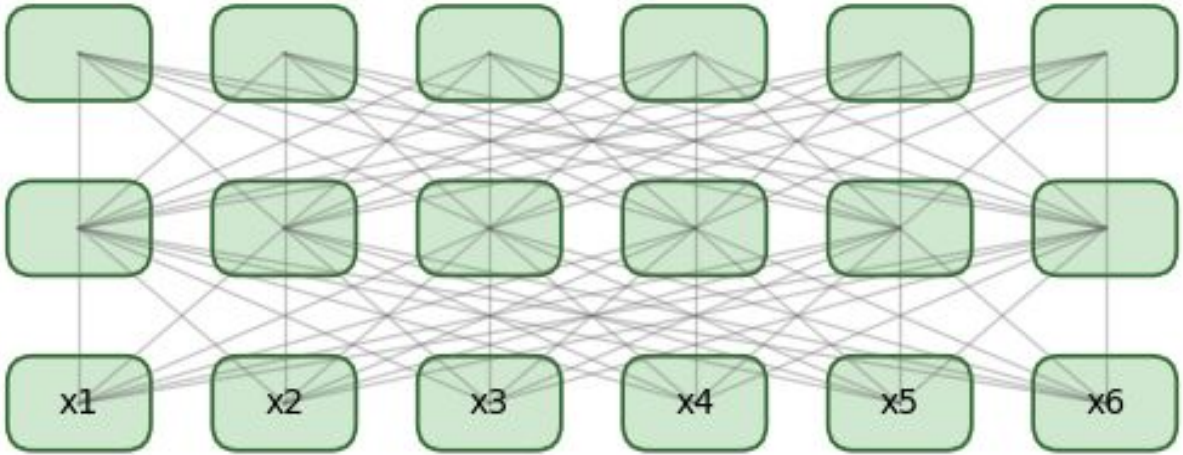
- Text classification (sentiment, topic)
- Retrieval and ranking (semantic search, dense embeddings)

Examples:

BERT, RoBERTa, SpanBERT, ALBERT……

Encoder-only

bi-directional self-attention



Encoder-Decoder Family – Seq2Seq Denoising

Mask:

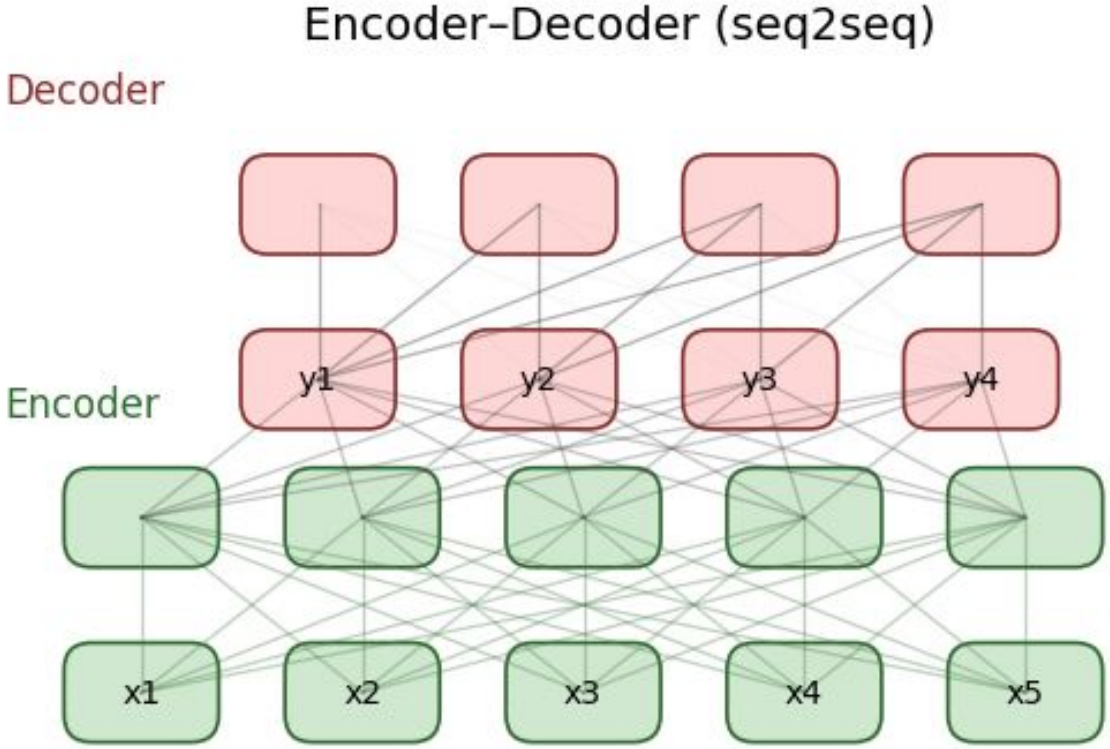
- Encoder → Full attention (understanding input)
- Decoder → Causal mask (generate token by token)
- Cross-attention → connects decoder queries to encoder outputs

Usage:

- Machine translation
- Image → text generation

Examples:

- T5, BART, mT5, MarianMT……


Encoder–Decoder (seq2seq)
Decoder
Encoder
y1
y2
y3
y4
x1
x2
x3
x4
x5

Takeaways 🧠

Free text corpus → Decoder-only (Language Modeling)

- No paired data, just raw text
- Train to predict the next token - learns grammar, style, and coherence

Feature learning or retrieval → Encoder-only (Masked LM)

- Focus on deep understanding, not generation
- Learns contextual embeddings for classification or search

Labeled input/output pairs → Encoder–Decoder (Seq2Seq)

- Each input has a corresponding target (translation, summarization)
- Model learns conditional mapping P(output | input)

Decoding Strategies

Decoding Controls the Model's Voice 🎯

The model outputs a probability distribution over the vocabulary at every step

Decoding = the decision rule for turning probabilities into actual words

This choice directly affects:

- Quality → coherence, grammatical correctness
- Diversity → creativity, surprise, and variability

Different decoding strategies can completely change tone and creativity

Decoding Controls the Model's Voice 🎯

Greedy decoding

- Always picks the most probable next token

Beam search

- Keeps several candidate sequences and expands the best-scoring ones

Sampling (Top-k / Top-p)

- Randomly sample from the most likely tokens

Greedy Decoding 🧩

Always pick the token with the highest probability at each step

At step t, choose:

$$y_t = \text{argmax } P(y \mid y_1, y_2, \ldots, y_{t-1})$$

The next token y_t is appended to the sequence, then repeats

Fast and deterministic → same prompt always yields the same output

Can fall into repetitive loops if top token probability dominates

Best for short factual answers or structured text generation

Beam Search 🌲

Keeps multiple candidate sequences (beams) at each step

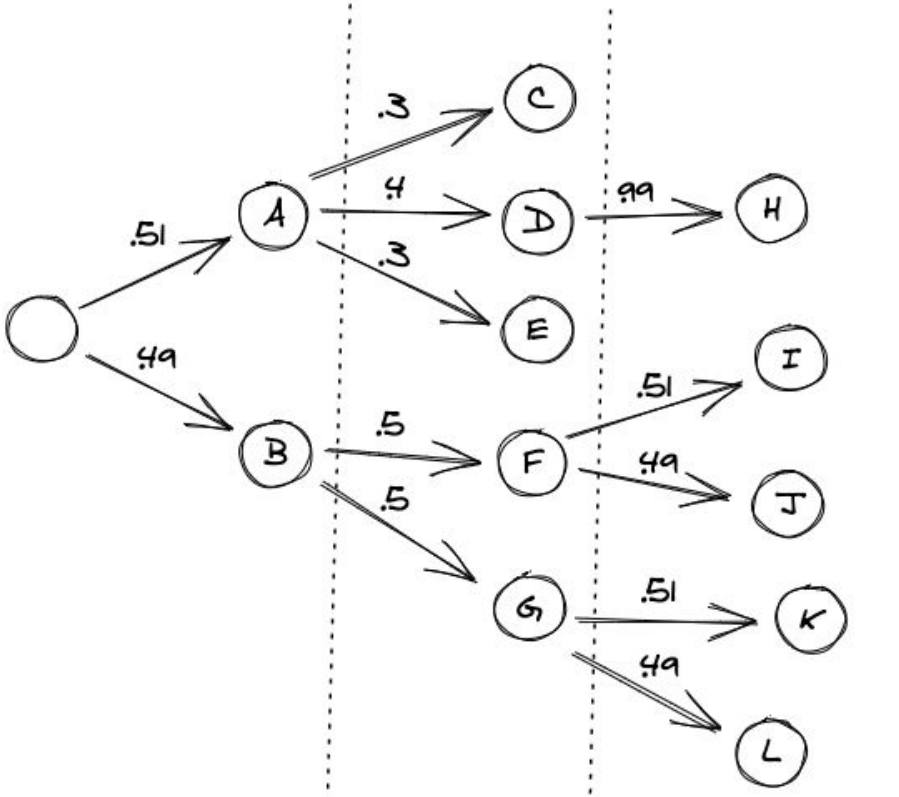
At step `t`, select top_beam sequences with the highest cumulative log-probability:

$$\text{Score}(y\_1, \ldots, y\_t) = \Sigma \log P(y\_t \mid y\_1, \ldots, y\_t\text{-}1, x)$$

Produces more coherent and complete results than greedy decoding

Lower randomness → less diversity, slower inference

Works best for translation, summarization, and other structured tasks



Greedy: A

Beam: A, B

Greedy: AD

Beam: BF, BG

Greedy: ADH

Beam: BFI, BG,K

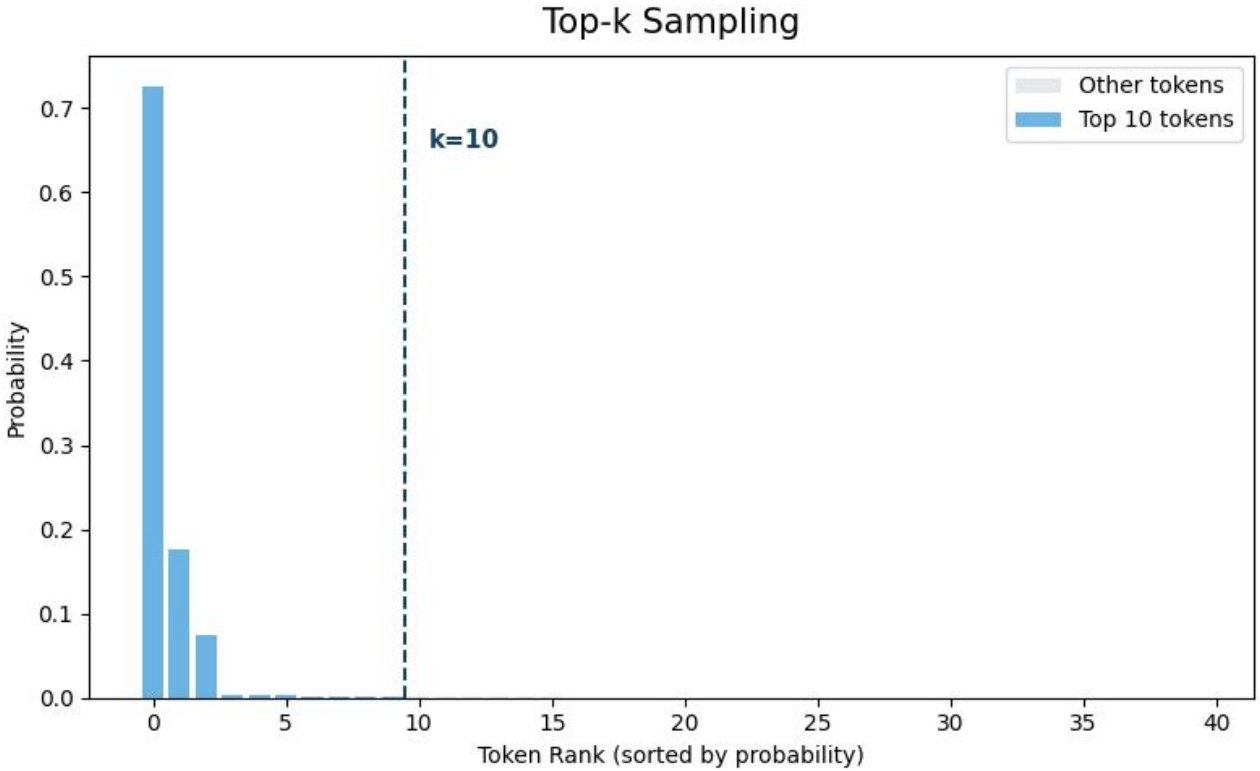
Sampling Methods (Top-k and Top-p) 🎲

Top-k: sample from the k most probable tokens (e.g., k = 50)

Top-p (Nucleus): dynamically sample from the smallest set whose probabilities sum ≥ p (e.g., p = 0.9)

Introduces controlled randomness → more natural and varied outputs

Sampling Methods (Top-k) 🎲



Takeaways 🧠

Greedy decoding → safe, focused, and deterministic

- Always picks the top token → consistent but can repeat or lack creativity

Beam search → structured and globally optimized

- Evaluates multiple candidate paths → improves coherence, often used in translation or summarization

Sampling (Top-k / Top-p) → diverse and expressive

- Introduces controlled randomness → more natural, creative responses at the cost of stability

Research Frontier

Long-Context

Long-Context Transformers 📏

Problem

Standard attention cost is $O(n^2)$ → too slow for long documents or sessions

Motivation

- Modern LLMs need to reason across 10k+ tokens: long conversations, multi-document reasoning, full-context summarization
- Long context enables more natural interactions and persistent memory

Common solutions

Sliding-Window attention, Sparse attention

Sliding Window Attention

Divides long sequences into local chunks (windows)

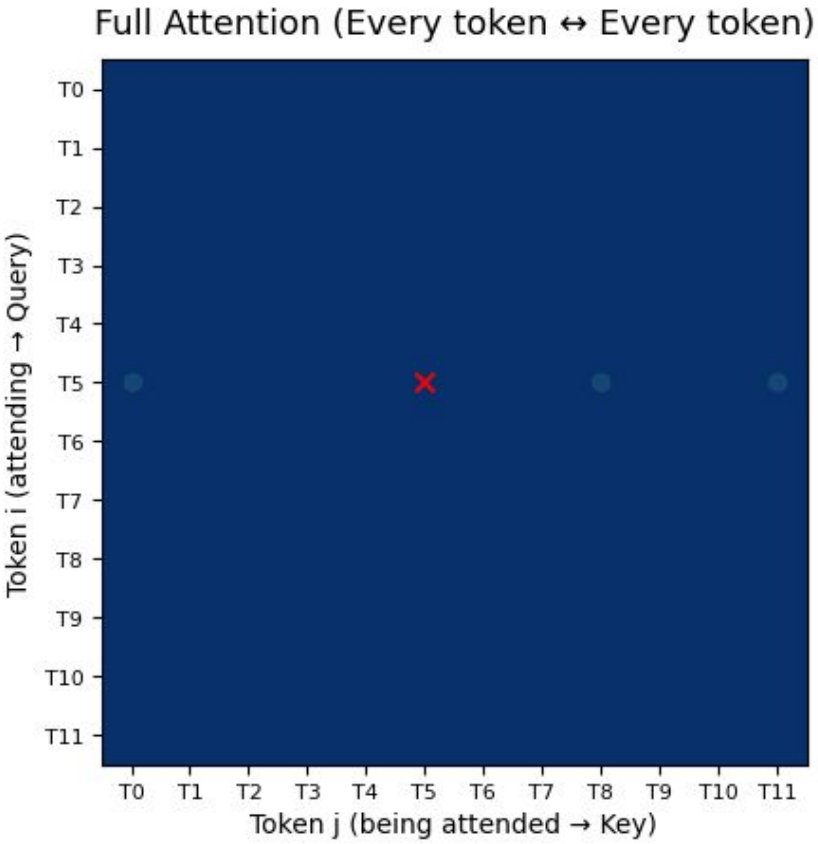
Each token attends only to nearby tokens within a fixed window size

Windows may overlap slightly to preserve continuity across boundaries

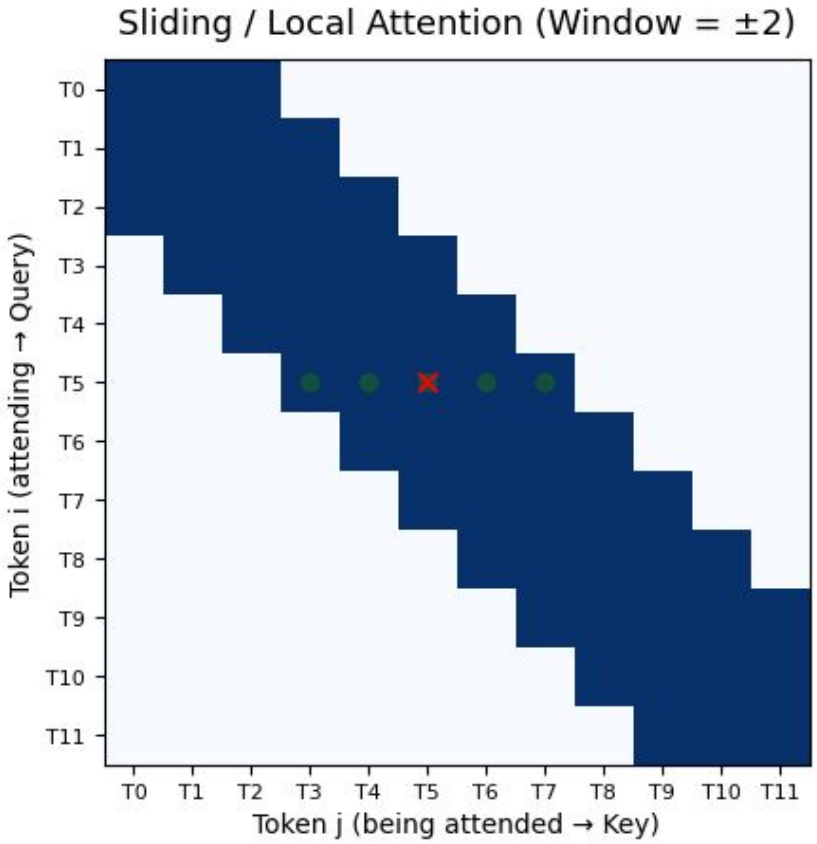
Great for long documents - balances efficiency and context

Used in models like Longformer, Transformer-XL, LLaMA……

Each token attends to ALL others → O(n²)



Each token attends only nearby tokens → O(n·w)



FlashAttention ⚡

Core Idea:

- Standard attention connects every token with every other token → $O(n^2)$ cost
- Sparse attention keeps only the important links — making it much faster

How It Works:

- Local pattern: each token attends only to its neighbors
- Global pattern: a few special tokens (e.g., [CLS], separators) can see everything → summarize or broadcast information
- Random / Strided pattern: connect to a few distant tokens → let the model “jump” occasionally for long-range info

Evaluating Long Context Models 🔎

Benchmarks

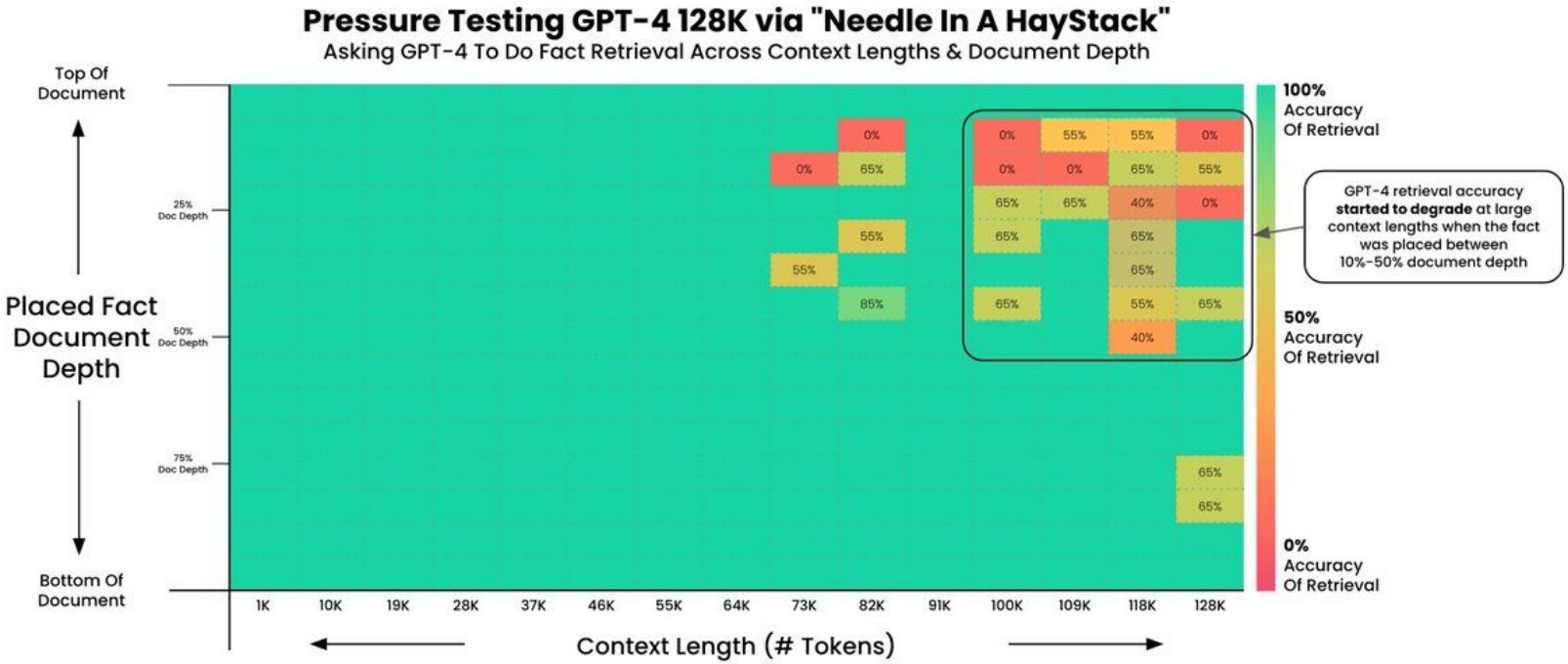
Needle-in-a-Haystack: insert a single fact in thousands of irrelevant tokens

What to Measure

Retrieval Accuracy: can the model locate the right span or entity inside 10k+ tokens?

Faithful Generation: does it use retrieved information correctly without hallucinating?

Evaluating Long Context Models 🔍



Goal: Test GPT-4 Ability To Retrieve Information From Large Context Windows

A fact was placed within a document. GPT-4 (1106-preview) was then asked to retrieve it. The output was evaluated for accuracy.
This test was run at 15 different document depths (top > bottom) and 15 different context lengths (1K >128K tokens).
2x tests were run for larger contexts for a larger sample size.

Mixture-of-Experts (MoE)

Mixture-of-Experts (MoE) 🧠

Each token activates only a small subset (top-k) of experts

Greatly increases capacity without raising compute cost

Router network decides which experts process each token

Experts are trained jointly and specialize on different patterns

Used in Switch Transformer,Mixtral, Llama and recent scalable LLMs

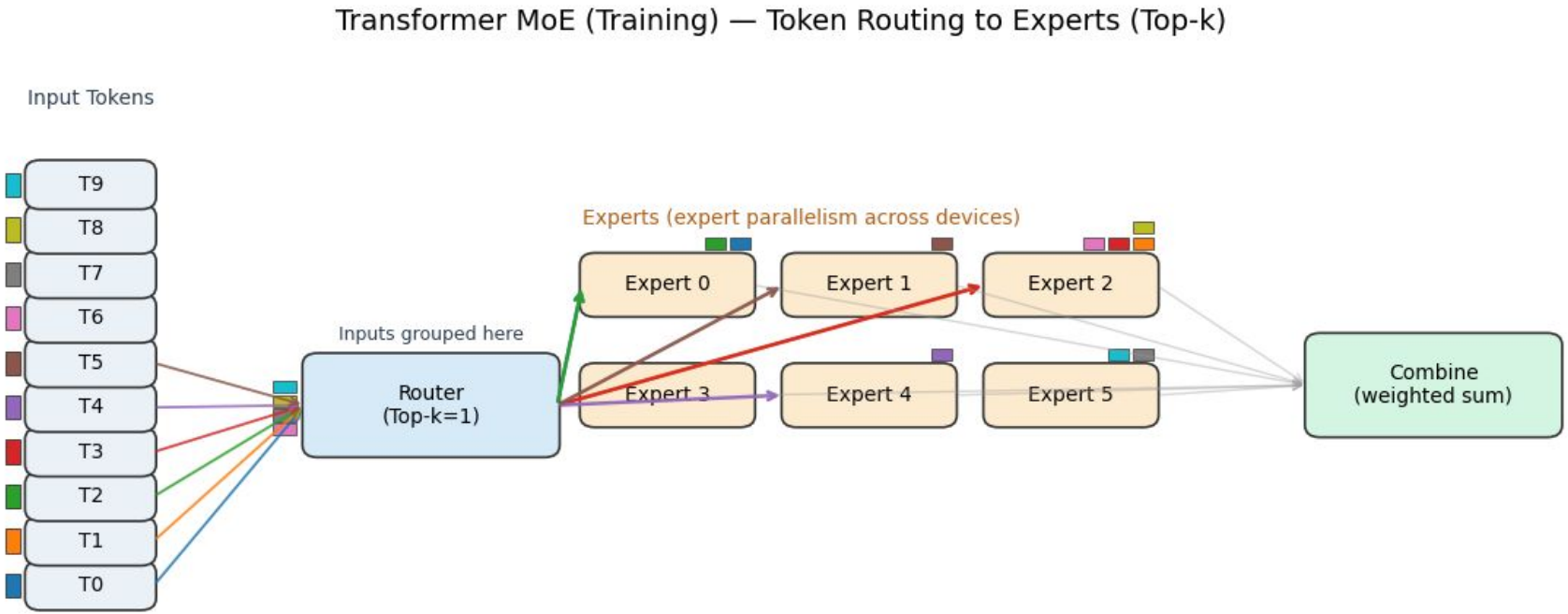
Routing and Balancing ⚖️

Router predicts which experts to use for each token

- Predicts which experts each token should use (usually top-1 or top-2)
- Implemented as a lightweight gating network - outputs routing probabilities

Load balancing loss prevents all tokens from choosing same experts

- Ensures tokens are distributed evenly across experts
- Prevents “expert collapse,” where all tokens pick the same expert


Transformer MoE (Training) — Token Routing to Experts (Top-k)
Input Tokens
T9
T8
T7
T6
T5
T4
T3
T2
T1
T0
Inputs grouped here
Router
(Top-k=1)
Experts (expert parallelism across devices)
Expert 0
Expert 1
Expert 2
Expert 3
Expert 4
Expert 5
Combine
(weighted sum)

Research Trend – Modular Reasoning Systems

MoE encourages specialization

- Each expert implicitly learns to handle specific domains (math, reasoning)

Goal: scalable systems that can grow capacity by adding new experts without retraining the entire model

Example directions:

- Task-aware expert activation (activate “math” or “code” experts)
- Hierarchical MoE – group experts into thematic clusters
- Continual learning with plug-in experts