From Attention to Transformers

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Impact of Attention and Transformers

The "T" in ChatGPT

They are the driving force of LLMs, AlphaFold, (and almost everything else in neural networks)

Impact across fields:

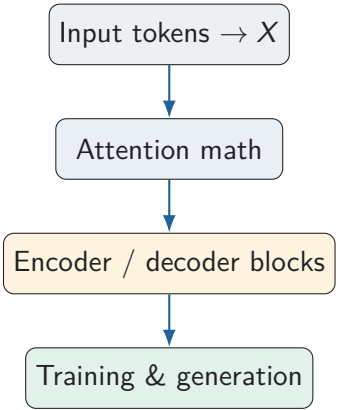
- Natural language processing
- Vision
- Protein structure prediction
- Materials modeling

Agenda and Roadmap

Core idea

Attention is the computational primitive; the Transformer is the architecture built around it.

- Start with a sequence of token embeddings.
- Build Q, K, and V from linear projections.
- Use attention to compute every-to-every interactions.
- Wrap that mechanism with residual paths, normalization, and MLPs.
- Add masking and caching to make decoding practical.



Notation and shapes

Single sequence view (used to explain attention)

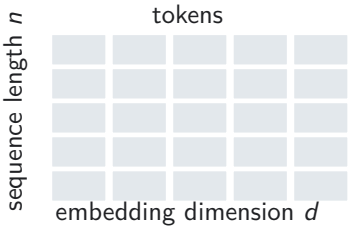
$$X \in \mathbb{R}^{n \times d_x}$$

- n: sequence length
- d_x: token embedding dimension

Batched Transformer view

$$X \in \mathbb{R}^{B \times n \times d_{model}}$$

- B: batch size
- same attention math, with an extra leading batch dimension



Throughout the deck, dimensions are the quickest way to see what a tensor means.

Step 1: build Q, K, and V

Start with token matrix

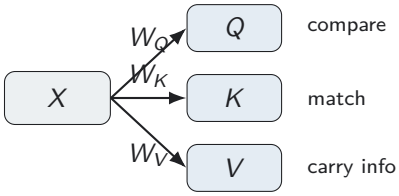
$$X \in \mathbb{R}^{n \times d_{model}}$$

Project it three different ways:

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

$$Q, K \in \mathbb{R}^{n \times d_k}, \qquad V \in \mathbb{R}^{n \times d_v}$$

- same n: still one row per token
- new feature spaces: each projection has a different role
- attention uses Q and K to decide weights, then applies them to V



Step 2: raw attention scores are $QK^\top$

Before softmax, attention forms the raw score matrix

$$S = QK^\top$$

Shape check:

$$Q \in \mathbb{R}^{n \times d_k}, \qquad K^\top \in \mathbb{R}^{d_k \times n} \qquad \Longrightarrow \qquad S \in \mathbb{R}^{n \times n}$$

Each entry is a dot product:

$$S_{ij} = q_i \cdot k_j$$

- row i: scores produced by query token i
- column j: how strongly key token j matches
- these are **logits**, not probabilities yet

raw attention logits $S = QK^\top$

keys

queries

$$\begin{array}{c|cccc} & & & & \\ \hline & q_1 k_1^\top & q_1 k_2^\top & \cdots & q_1 k_n^\top \\ & q_2 k_1^\top & q_2 k_2^\top & \cdots & q_2 k_n^\top \\ & \vdots & \vdots & \ddots & \vdots \\ & q_n k_1^\top & q_n k_2^\top & \cdots & q_n k_n^\top \end{array}$$

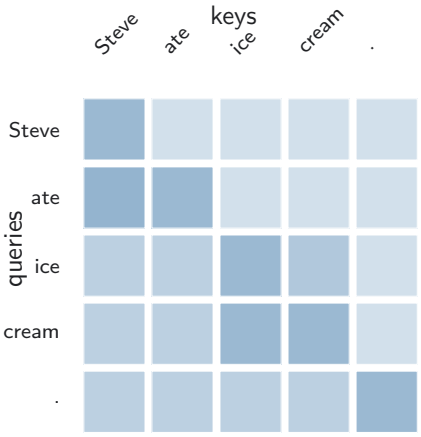
Why the raw score matrix is $n \times n$

Interpretation

Each row corresponds to one query token.
Each column corresponds to one key token.
The entry S_{ij} tells us how strongly token i matches token j **before normalization**.

$$S = QK^\top \in \mathbb{R}^{n \times n}$$

- every token compares against every token
- one row = one token asking about all other tokens
- values need not be symmetric



Step 3: scale the logits, then apply row-wise softmax

Raw attention scores:

$$S = QK^\top$$

Scaled scores:

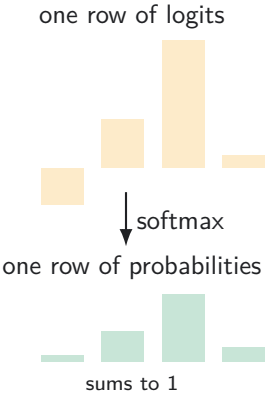
$$\widetilde{S} = \frac{QK^\top}{\sqrt{d_k}}$$

Normalized attention weights:

$$A = \mathrm{softmax}\left(\widetilde{S}\right)$$

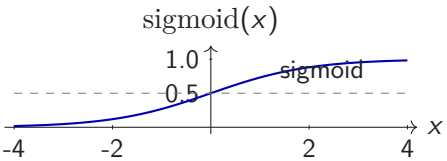
Softmax is applied row-wise, so each row becomes a distribution:

$$A_{ij} \geq 0, \qquad \sum_j A_{ij} = 1$$



Sigmoid vs. Softmax

$$\sigma(x) = \frac{1}{1 + e^{-x}} (sigmoid) \qquad \sigma(x)_i = \frac{e^{x_i}}{\sum_j e^{x_j}} (softmax)$$



- **Sigmoid** acts on a single scalar
- **Softmax** acts on a vector quantity
- Sigmoid maps one value into the range $(0, 1)$
- Softmax turns a vector into a probability distribution (sum to 1)
- In attention, **softmax** is used so each row of attention weights sums to 1

Why divide by $\sqrt{d_k}$, and why softmax after that?

What goes wrong without scaling

As d_k grows, raw dot products tend to grow in variance. Large logits make softmax very sharp, so one token dominates and the rest get almost zero weight.

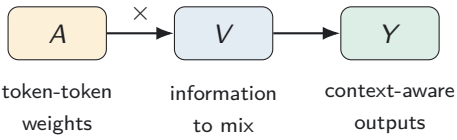
$$S = QK^\top, \qquad \widetilde{S} = \frac{S}{\sqrt{d_k}}, \qquad A = \mathrm{softmax}(\widetilde{S})$$

- $\sqrt{d_k}$ keeps logits in a reasonable range
- softmax then converts each row into a probability distribution
- this preserves graded, every-to-every interactions
- avoids attention becoming one-hot

Step 4: use attention weights to mix the values

Once we have attention weights A, we apply them to the value matrix:

$$Y = AV$$



For token i:

$$y_i = \sum_{j=1}^{n} A_{ij} v_j$$

- row i of A says how much token i should use each value vector
- same number of tokens in, same number of tokens out

$$A \in \mathbb{R}^{n \times n}, \qquad V \in \mathbb{R}^{n \times d_v} \qquad \Longrightarrow \qquad Y \in \mathbb{R}^{n \times d_v}$$

Attention pipeline: logits → weights → outputs

The whole computation can be read in three stages:

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

$$S = QK^\top$$

$$A = \text{softmax}\left(\frac{S}{\sqrt{d_k}}\right)$$

$$Y = AV$$

- S: raw compatibility logits
- A: normalized attention weights
- Y: mixed, context-aware token representations

Encoder block = attention + residual + norm + FFN

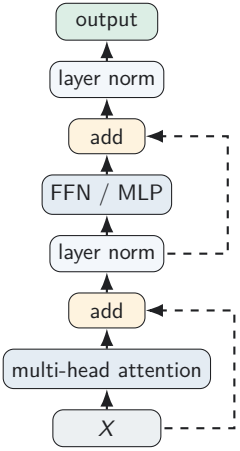
$$\tilde{X} = X + \mathrm{MHA}(X)$$

$$X' = \mathrm{LayerNorm}(\tilde{X})$$

$$\hat{X} = X' + \mathrm{FFN}(X')$$

$$X_{out} = \mathrm{LayerNorm}(\hat{X})$$

- residuals preserve information and help gradients flow
- layer norm stabilizes the feature scale per token
- FFN mixes information within each token after attention mixed information across tokens



LayerNorm and FFN: what happens inside a block

LayerNorm per token

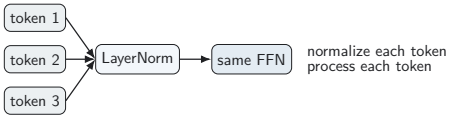
For batched data $X \in \mathbb{R}^{B \times n \times d_{model}}$, normalize each token independently across its feature dimension:

$$\text{LayerNorm}(x) = \gamma \odot \frac{x - \mu}{\sigma + \varepsilon} + \beta$$

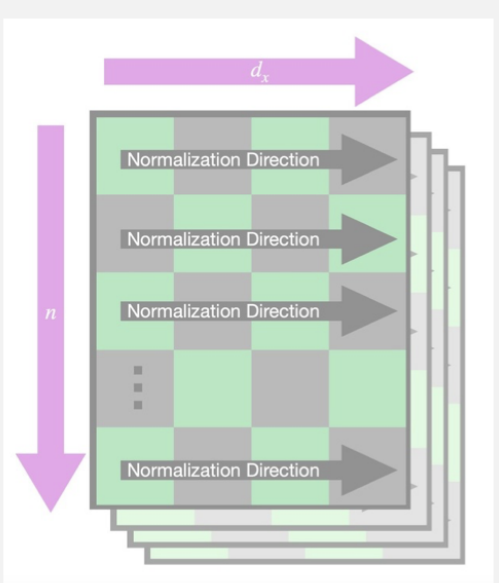
Feed-forward network per token

$$\text{FFN}(x) = W_2\, \sigma(W_1 x + b_1) + b_2$$

Same weights are reused at every token position.



LayerNorm


d_x
n
Normalization Direction
Normalization Direction
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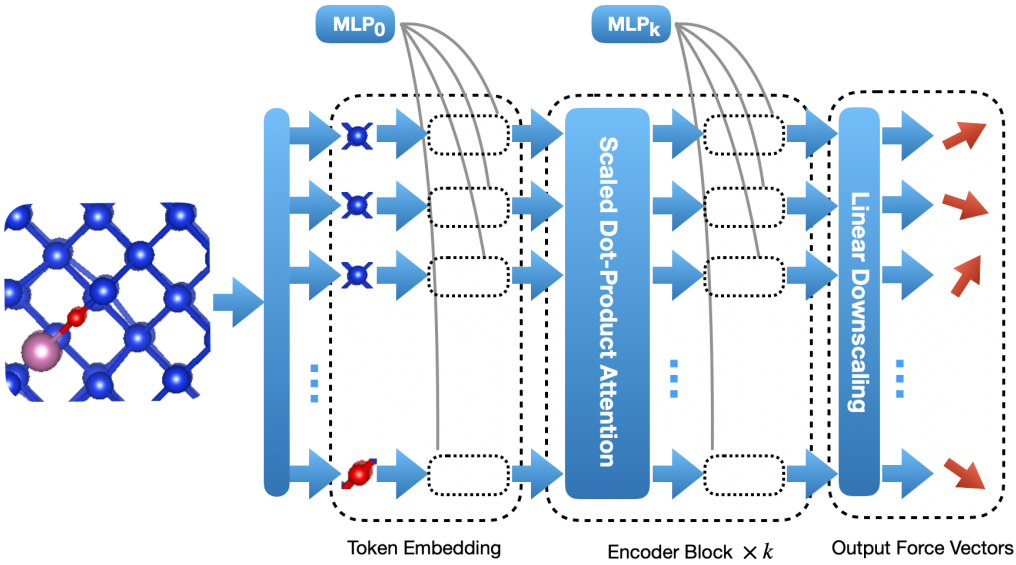
Normalization Direction

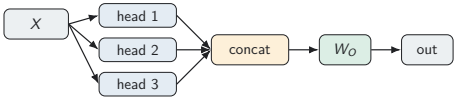
Transformer encoder



Multi-head attention: one mechanism, many subspaces

$$\text{head}_i = \text{softmax}\left(\frac{Q_i K_i^\top}{\sqrt{d_k}}\right) V_i \qquad i = 1, \ldots, h$$

$$\text{MHA}(X) = \text{Concat}(\text{head}_1, \ldots, \text{head}_h) W_O$$



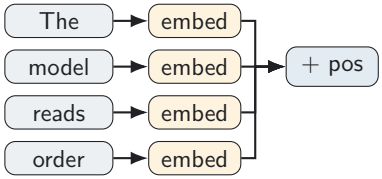
- split d_{model} across h heads, usually with $d_k = d_{model}/h$
- each head can specialize to a different interaction pattern
- concatenate the heads, then project back to d_{model}

Decoders and LLMs

Input stage: embeddings and positional information

- Transformers operate on sequences of continuous vectors.
- Native data is tokenized into discrete units, then embedded into $\mathbb{R}^{d_{model}}$.
- Positional encoding is added so the model can tell tokens apart by order.

$$X_0 = E(\text{tokens}) + P$$



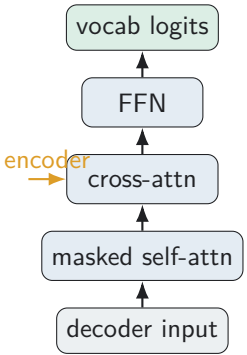
Why this matters

Pure attention is permutation-equivariant. Without positional information, the model sees a bag of tokens rather than an ordered sequence.

Decoder block: what changes

1. masked self-attention on decoder tokens
2. residual + layer norm
3. cross-attention to encoder outputs (if an encoder exists)
4. residual + layer norm
5. FFN, then projection to vocabulary logits

$$X \in \mathbb{R}^{B\times n\times d_{model}} \quad \rightarrow \quad XW_V \in \mathbb{R}^{B\times n\times |\mathcal{V}|}$$



Decoder-only models

Skip cross-attention entirely. Masked self-attention + FFN is enough for next-token prediction.

What the decoder is trained to do

Given a sequence:

`Steve went to the store`

The decoder is trained with a shifted input:

input: ⟨*sos*⟩ `Steve went to the store`

target: `Steve went to the store` ⟨*eos*⟩

What each position learns

- ⟨*sos*⟩ → Steve
- ⟨*sos*⟩ `Steve` → went
- ⟨*sos*⟩ `Steve went` → to
- ...

Key idea

The model always predicts the **next token given the full prefix**.

- not pairwise ("Steve → went")
- always **prefix → next token**

From decoder outputs to next-token probabilities

Decoder output:

$$X \in \mathbb{R}^{B \times n \times d_{model}}$$

Project to vocabulary:

$$Z = XW_{out} \in \mathbb{R}^{B \times n \times |\mathcal{V}|}$$

- each position produces logits over the vocabulary

Convert to probabilities:

$$P = \text{softmax}(Z)$$

We only use the **last position**: $P(x_t \mid x_{1:t-1})$

Interpretation

- logits = unnormalized scores
- softmax = probability distribution
- size = vocabulary size

Key detail

The distribution is conditioned on **all previous tokens**.

Autoregressive generation (inference loop)

Start with:

$$[\langle sos \rangle]$$

Loop:

1. Run decoder on current sequence
2. Take logits at **last position**
3. Compute probabilities with softmax
4. **Sample or argmax** next token
5. Append token to sequence

Repeat until:

- $\langle eos \rangle$ is produced
- or max length reached

Example

- $\langle sos \rangle \rightarrow$ Steve
- $\langle sos \rangle$ Steve $\rightarrow$ went
- $\langle sos \rangle$ Steve went $\rightarrow$ to

Key idea

Each prediction becomes part of the next input.

Training vs inference (why they differ)

Training (teacher forcing)

- full sequence given at once
- predictions made at all positions
- parallel computation

$$[\langle sos \rangle, x_1, x_2, x_3] \to [x_1, x_2, x_3, x_4]$$

Inference (generation)

- no ground truth future tokens
- must generate step-by-step
- sequential loop

$$\begin{aligned} [\langle sos \rangle] &\to x_1 \\ [\langle sos \rangle, x_1] &\to x_2 \\ [\langle sos \rangle, x_1, x_2] &\to x_3 \\ &\vdots \end{aligned}$$

Consequence

Errors can compound over time.

Cross-attention and causal masking

Cross-attention

Use different sources for queries vs. keys/values:

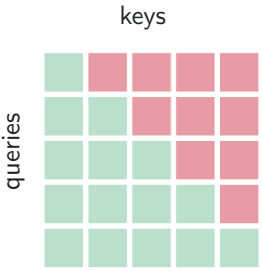
$$Q = X_{dec} W_Q, \qquad K = X_{enc} W_K, \qquad V = X_{enc} W_V$$

The decoder asks questions; the encoder provides the memory to read from.

Causal masking

Prevent token t from attending to future tokens $> t$ by adding a mask before softmax.

$$A = \text{softmax}\left(\frac{QK^\top + M}{\sqrt{d_k}} \right)$$



green: allowed
red: masked future

Autoregressive decoding with KV cache

At time step t, only the new token needs fresh projections:

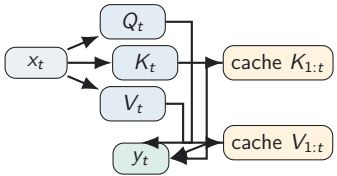
$$Q_t = x_t W_Q, \qquad K_t = x_t W_K, \qquad V_t = x_t W_V$$

Cache all previous keys and values, then append the new ones:

$$K_{1:t} \in \mathbb{R}^{B\times h\times t\times d_k}, \qquad V_{1:t} \in \mathbb{R}^{B\times h\times t\times d_v}$$

$$A_t = \mathrm{softmax}\left(\frac{Q_t K_{1:t}^\top}{\sqrt{d_k}}\right), \qquad y_t = A_t V_{1:t}$$

- softmax now runs over the t past positions
- caching avoids recomputing old K and V every step



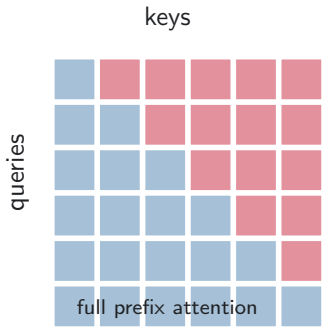
Prefill phase: full triangular attention

During the prompt (prefill), we process the entire sequence at once:

$$A = \text{softmax}\left(\frac{QK^\top + M}{\sqrt{d_k}}\right)$$

- Q, K, V computed for **all tokens**
- causal mask M removes future tokens
- produces a **lower triangular attention matrix**

cost: $O(n^2)$



Naive autoregressive decoding (no cache)

At each step t, we would recompute everything:

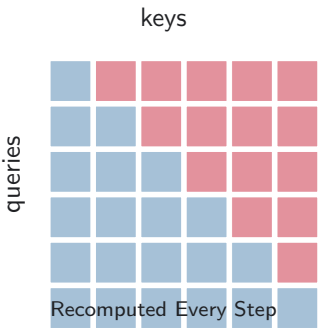
$$Q_{1:t}, K_{1:t}, V_{1:t}$$

- recompute attention over entire prefix
- repeated work for earlier tokens

total cost: $O(n^2)$ per step $\Rightarrow O(n^3)$

Key inefficiency

We keep recomputing the same K and V for past tokens.



KV caching: from quadratic to linear decoding

Instead of recomputing everything:

$$K_{1:t} = [K_{1:t-1}, K_t], \quad V_{1:t} = [V_{1:t-1}, V_t]$$

Only compute:

$$Q_t = x_t W_Q$$

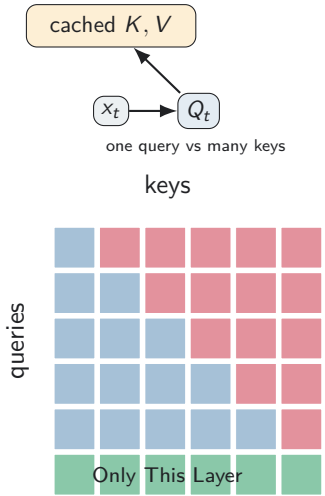
Then:

$$A_t = \text{softmax}\left(\frac{Q_t K_{1:t}^\top}{\sqrt{d_k}}\right)$$

$$y_t = A_t V_{1:t}$$

- attend over cached keys/values
- only one new query per step

cost per step: $O(t) \quad \Rightarrow \quad O(n)$



How context is built across layers

In a **single isolated layer**, Q, K, and V are just separate linear projections of the same input:

$$Q^{(l)} = X^{(l)} W_Q^{(l)}, \qquad K^{(l)} = X^{(l)} W_K^{(l)}, \qquad V^{(l)} = X^{(l)} W_V^{(l)}$$

Within that one layer, Q does **not** directly modify K or V. The dependency appears because Transformers are **stacks of layers**.

The chain reaction

1. **Layer 1 input:** raw token embeddings
2. **Layer 1 attention:** $Q^{(1)}$ and $K^{(1)}$ determine which tokens interact
3. **Layer 1 output:** tokens become *contextualized*
4. **Layer 2 input:** that contextualized output becomes the new input

So if token i uses its query to attend to nearby context in Layer 1, that context gets mixed into its output representation. By Layer 2, the new K and V are built from a representation that already knows more about the sentence.

Why Layer 1 queries matter for the KV cache

Let $X^{(l)}$ be the input to layer l. The attention output is

$$Z^{(l)} = \text{softmax}\left(\frac{Q^{(l)}(K^{(l)})^\top}{\sqrt{d_k}}\right) V^{(l)}$$

and this becomes the next layer's input:

$$X^{(l+1)} = Z^{(l)}$$

Why $Q^{(l)}$ matters

The query affects the **attention weights**, which determine how much of each value vector gets mixed into the output $Z^{(l)}$.

Since the next layer is built from that output,

$$K^{(l+1)} = X^{(l+1)} W_K^{(l+1)}, \qquad V^{(l+1)} = X^{(l+1)} W_V^{(l+1)}$$

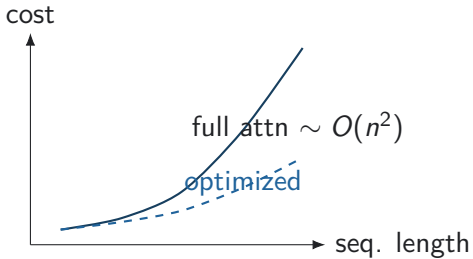
the Keys and Values in later layers inherit the effects of earlier attention.

Efficiency and common modern variants

Why efficiency matters

Full self-attention computes n^2 token-token interactions. Long contexts make both memory and compute expensive.

- FlashAttention: better memory/computation scheduling
- Multi-query attention: cheaper KV storage
- Ring / distributed variants: help large-scale multi-GPU training
- low-rank, sparse, or Nyström-style approximations: reduce cost of mixing. SSMs also may be used.



Takeaways

1. Attention computes weighted information exchange across tokens.
2. The $n \times n$ map is the heart of the mechanism: who reads from whom.
3. Scaling, masking, and multi-head structure make the primitive numerically stable and expressive.
4. A Transformer block wraps attention with residual paths, normalization, and a token-wise FFN.
5. Decoder training and inference differ: teacher forcing is parallel; generation is sequential and cache-heavy.

Attention is the operation. Transformers are the system built around it.