

Transformer — Zero to Hero: Complete Technical Manual

Exhaustive explanation, diagrams, numeric examples, and PyTorch-style appendix

Intended coverage: fundamentals → attention → multi-head → residuals → FFN → layernorm → pos enc → KV cache → training/decoding → implementation notes

How to use this manual

This document is structured to teach every concept from first principles, then present the exact formulas and implementation notes you need to write bug-free code. Key results are boxed. Diagrams are simplified for robustness and clarity. A numerical worked example shows attention computed step-by-step (digit-by-digit) to remove any ambiguity.

1 Prerequisites: linear algebra and probability refresher

We assume basic familiarity with vectors, matrices and common operations. Quick recap:

- A vector $v \in \mathbb{R}^d$ is a column of d numbers. A matrix $A \in \mathbb{R}^{m \times n}$ maps $\mathbb{R}^n \rightarrow \mathbb{R}^m$ via Ax .
- Matrix multiplication: $(AB)_{ij} = \sum_k A_{ik}B_{kj}$.
- Transpose: A^\top flips rows/columns.
- Dot product: for $u, v \in \mathbb{R}^d$, $u \cdot v = u^\top v = \sum_{i=1}^d u_i v_i$.
- Softmax (row-wise): for vector $z \in \mathbb{R}^n$,

$$\text{softmax}(z)_i = \frac{e^{z_i}}{\sum_{j=1}^n e^{z_j}}.$$

Numerically stable trick: subtract the max before exponentiating: $\text{softmax}(z) = \text{softmax}(z - \max(z))$.

Notation used throughout:

- N — sequence length (tokens).
- d — model (embedding) dimension.
- H — number of attention heads.
- d_{head} — per-head dimensionality (so typically $d = H \cdot d_{\text{head}}$).
- d_{ff} — hidden dimension of the position-wise feedforward network.
- $X \in \mathbb{R}^{N \times d}$ — token embeddings for a full sequence.

2 High-level architecture

A single (decoder-only) Transformer layer block processes token embeddings through:

LayerNorm → MultiHeadAttention (masked) → Residual add → LayerNorm → FFN → Residual add.

In equation (pre-layernorm variant):

$$y_1 = x + \text{MultiHead}(\text{LayerNorm}(x)), \quad y = y_1 + \text{FFN}(\text{LayerNorm}(y_1)).$$

2.1 What each piece does (plain English)

- **Embedding:** map token IDs to vectors.
- **Positional encoding:** inject token position information into embeddings.
- **Multi-head attention:** each token can “read” information from other tokens via learned queries/keys/values.
- **Residual connections:** add the input to outputs to preserve low-level signal and ease training.
- **LayerNorm:** normalize vector components per token for stable optimization.
- **FFN:** position-wise MLP to increase representation power.

3 Attention: full derivation and implementation

3.1 Intuition

A token forms a *query* that asks “what I want to fetch from the context”. Each context token exposes a *key* describing what it contains and a *value* describing what to pass on. Attention scores measure query-key similarity; softmax weights values to produce the output.

3.2 Scaled dot-product attention (single head)

Given $X \in \mathbb{R}^{N \times d}$. Learn three projections:

$$W_Q, W_K, W_V \in \mathbb{R}^{d \times d_{\text{head}}}.$$

Compute:

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

so $Q, K, V \in \mathbb{R}^{N \times d_{\text{head}}}$.

Scores matrix (unnormalized):

$$S = QK^\top \in \mathbb{R}^{N \times N}, \quad S_{ij} = Q_i \cdot K_j.$$

Scale and add optional mask M :

$$\tilde{S} = \frac{S}{\sqrt{d_{\text{head}}}} + M.$$

Row-wise softmax:

$$A = \text{softmax}(\tilde{S}) \quad (\text{apply softmax to each row of } \tilde{S}).$$

Attention output:

$$\text{Attention}(Q, K, V) = AV \in \mathbb{R}^{N \times d_{\text{head}}}.$$

Why scale by $\sqrt{d_{\text{head}}}$? Dot products grow in magnitude with dimension; dividing stabilizes the softmax input, preventing extreme probabilities that kill gradients.

3.3 Mask M for autoregressive decoding



For decoder-only models (causal LM), future positions must be blocked:

$$M_{ij} = \begin{cases} 0 & j \leq i, \\ -\infty & j > i. \end{cases}$$

In practice, use a large negative constant (e.g., $-1e9$) for numerical compatibility.

4 Multi-head attention: math and shapes

- For each head $h = 1, \dots, H$, have independent projections $W_Q^{(h)}, W_K^{(h)}, W_V^{(h)} \in \mathbb{R}^{d \times d_{\text{head}}}$.
- Compute head outputs: $\text{head}_h = \text{Attention}(XW_Q^{(h)}, XW_K^{(h)}, XW_V^{(h)}) \in \mathbb{R}^{N \times d_{\text{head}}}$.
- Concatenate heads: $[\text{head}_1 \parallel \dots \parallel \text{head}_H] \in \mathbb{R}^{N \times (Hd_{\text{head}})}$.
- Final linear projection: multiply by $W_O \in \mathbb{R}^{Hd_{\text{head}} \times d}$ to produce $\mathbb{R}^{N \times d}$.

5 Residual stream and layer normalization

5.1 Residual connections

If a sub-layer computes $F(x)$, the residual update is $x \leftarrow x + F(x)$. This keeps identity paths and makes gradient flow easier.

5.2 Layer Normalization (LayerNorm)

For a token vector $x \in \mathbb{R}^d$:

$$\mu = \frac{1}{d} \sum_{i=1}^d x_i, \quad \sigma = \sqrt{\frac{1}{d} \sum_{i=1}^d (x_i - \mu)^2 + \epsilon},$$
$$\text{LayerNorm}(x) = \gamma \frac{x - \mu}{\sigma} + \beta,$$

with learnable $\gamma, \beta \in \mathbb{R}^d$.

Pre-norm vs post-norm: apply LayerNorm before sublayers (pre-norm) for improved stability in deep models. Many modern implementations use pre-norm.

6 Position-wise Feedforward Network (FFN)

Function applied independently to each position:

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

Typical: $W_1 \in \mathbb{R}^{d_{\text{ff}} \times d}$, $W_2 \in \mathbb{R}^{d \times d_{\text{ff}}}$, with $d_{\text{ff}} \approx 4d$ typical.

Activations: GeLU or SwiGLU are common and perform better than ReLU in practice.

7 Token embeddings and positional encodings

- **Token Embedding matrix** $E \in \mathbb{R}^{|V| \times d}$. Token ids \rightarrow row vectors.
- **Positional Encoding** options:
 1. Learned positional embeddings $P \in \mathbb{R}^{L \times d}$ (where L is maximum length), added: $X \leftarrow X + P$.
 2. Sinusoidal encodings (original): deterministic functions of position.

8 KV cache for fast autoregressive inference

At inference time, recomputing K, V for all previous tokens every step is wasteful. Cache K and V per layer and head, append new K, V at each step, then attention uses cached K, V plus current Q . This reduces compute from $O(N^2)$ to $O(N)$ per generated token at each step for the newly computed projections (but memory increases as $O(N)$ per layer).

9 Numerical worked example: attention computed step-by-step

We show a full numeric example, small and explicit. All arithmetic is listed.

Setup

Choose:

$$N = 3 \quad (3 \text{ tokens}), \quad d = 4, \quad d_{\text{head}} = 2, \quad H = 1 \quad (\text{single head for clarity}).$$

Input embeddings $X \in \mathbb{R}^{3 \times 4}$:

$$X = \begin{pmatrix} 1 & 0 & 2 & 1 \\ 0 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix}.$$

Projection matrices (small integer values for clarity):

$$W_Q = \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 1 \\ 0 & 1 \end{pmatrix}, \quad W_K = \begin{pmatrix} 0 & 1 \\ 1 & 0 \\ 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad W_V = \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

Step 1: compute $Q = XW_Q$

Compute each row of Q as $X_i \cdot W_Q$.

Row 1: $X_1 = (1, 0, 2, 1)$.

$$Q_{1,1} = 1 \cdot 1 + 0 \cdot 0 + 2 \cdot 1 + 1 \cdot 0 = 1 + 0 + 2 + 0 = 3.$$

$$Q_{1,2} = 1 \cdot 0 + 0 \cdot 1 + 2 \cdot 1 + 1 \cdot 1 = 0 + 0 + 2 + 1 = 3.$$

So row 1 of Q is $(3, 3)$.

Row 2: $X_2 = (0, 1, 0, 1)$.

$$Q_{2,1} = 0 \cdot 1 + 1 \cdot 0 + 0 \cdot 1 + 1 \cdot 0 = 0.$$

$$Q_{2,2} = 0 \cdot 0 + 1 \cdot 1 + 0 \cdot 1 + 1 \cdot 1 = 0 + 1 + 0 + 1 = 2.$$

So row 2: $(0, 2)$.

Row 3: $X_3 = (1, 1, 1, 0)$.

$$Q_{3,1} = 1 \cdot 1 + 1 \cdot 0 + 1 \cdot 1 + 0 \cdot 0 = 1 + 0 + 1 + 0 = 2.$$

$$Q_{3,2} = 1 \cdot 0 + 1 \cdot 1 + 1 \cdot 1 + 0 \cdot 1 = 0 + 1 + 1 + 0 = 2.$$

Row 3: $(2, 2)$.

Thus

$$Q = \begin{pmatrix} 3 & 3 \\ 0 & 2 \\ 2 & 2 \end{pmatrix}.$$

Step 2: compute $K = XW_K$

Row 1: $X_1 = (1, 0, 2, 1)$.

$$K_{1,1} = 1 \cdot 0 + 0 \cdot 1 + 2 \cdot 1 + 1 \cdot 0 = 0 + 0 + 2 + 0 = 2.$$

$$K_{1,2} = 1 \cdot 1 + 0 \cdot 0 + 2 \cdot 0 + 1 \cdot 1 = 1 + 0 + 0 + 1 = 2.$$

Row 1: $(2, 2)$.

Row 2: $X_2 = (0, 1, 0, 1)$.

$$K_{2,1} = 0 \cdot 0 + 1 \cdot 1 + 0 \cdot 1 + 1 \cdot 0 = 0 + 1 + 0 + 0 = 1.$$

$$K_{2,2} = 0 \cdot 1 + 1 \cdot 0 + 0 \cdot 0 + 1 \cdot 1 = 0 + 0 + 0 + 1 = 1.$$

Row 2: $(1, 1)$.

Row 3: $X_3 = (1, 1, 1, 0)$.

$$K_{3,1} = 1 \cdot 0 + 1 \cdot 1 + 1 \cdot 1 + 0 \cdot 0 = 0 + 1 + 1 + 0 = 2.$$

$$K_{3,2} = 1 \cdot 1 + 1 \cdot 0 + 1 \cdot 0 + 0 \cdot 1 = 1 + 0 + 0 + 0 = 1.$$

Row 3: $(2, 1)$.

So

$$K = \begin{pmatrix} 2 & 2 \\ 1 & 1 \\ 2 & 1 \end{pmatrix}.$$

Step 3: compute $V = XW_V$

Row 1: $X_1 = (1, 0, 2, 1)$.

$$V_{1,1} = 1 \cdot 1 + 0 \cdot 0 + 2 \cdot 0 + 1 \cdot 1 = 1 + 0 + 0 + 1 = 2.$$

$$V_{1,2} = 1 \cdot 0 + 0 \cdot 1 + 2 \cdot 1 + 1 \cdot 0 = 0 + 0 + 2 + 0 = 2.$$

Row 1: $(2, 2)$.

Row 2: $X_2 = (0, 1, 0, 1)$.

$$V_{2,1} = 0 \cdot 1 + 1 \cdot 0 + 0 \cdot 0 + 1 \cdot 1 = 0 + 0 + 0 + 1 = 1.$$

$$V_{2,2} = 0 \cdot 0 + 1 \cdot 1 + 0 \cdot 1 + 1 \cdot 0 = 0 + 1 + 0 + 0 = 1.$$

Row 2: $(1, 1)$.

Row 3: $X_3 = (1, 1, 1, 0)$.

$$V_{3,1} = 1 \cdot 1 + 1 \cdot 0 + 1 \cdot 0 + 0 \cdot 1 = 1 + 0 + 0 + 0 = 1.$$

$$V_{3,2} = 1 \cdot 0 + 1 \cdot 1 + 1 \cdot 1 + 0 \cdot 0 = 0 + 1 + 1 + 0 = 2.$$

Row 3: $(1, 2)$.

So

$$V = \begin{pmatrix} 2 & 2 \\ 1 & 1 \\ 1 & 2 \end{pmatrix}.$$

Step 4: compute score matrix $S = QK^\top$

We compute $S_{ij} = Q_i \cdot K_j$.

Row 1 dot row 1:

$$S_{11} = (3, 3) \cdot (2, 2) = 3 \cdot 2 + 3 \cdot 2 = 6 + 6 = 12.$$

Row 1 dot row 2:

$$S_{12} = (3, 3) \cdot (1, 1) = 3 + 3 = 6.$$

Row 1 dot row 3:

$$S_{13} = (3, 3) \cdot (2, 1) = 3 \cdot 2 + 3 \cdot 1 = 6 + 3 = 9.$$

So first row of S : $(12, 6, 9)$.

Row 2: $Q_2 = (0, 2)$.

$$S_{21} = (0, 2) \cdot (2, 2) = 0 \cdot 2 + 2 \cdot 2 = 4.$$

$$S_{22} = (0, 2) \cdot (1, 1) = 0 + 2 = 2.$$

$$S_{23} = (0, 2) \cdot (2, 1) = 0 + 2 = 2.$$

Row 2: $(4, 2, 2)$.

Row 3: $Q_3 = (2, 2)$.

$$S_{31} = (2, 2) \cdot (2, 2) = 4 + 4 = 8.$$

$$S_{32} = (2, 2) \cdot (1, 1) = 2 + 2 = 4.$$

$$S_{33} = (2, 2) \cdot (2, 1) = 4 + 2 = 6.$$

Row 3: $(8, 4, 6)$.

Thus

$$S = \begin{pmatrix} 12 & 6 & 9 \\ 4 & 2 & 2 \\ 8 & 4 & 6 \end{pmatrix}.$$

Step 5: scale scores by $\sqrt{d_{\text{head}}}$

Here $d_{\text{head}} = 2$. Thus $\sqrt{2} = 1.4142135623730951$ (we'll keep 8–9 digits for clarity).

Divide every entry by $\sqrt{2}$:

First row:

$$\tilde{S}_{11} = \frac{12}{\sqrt{2}} \approx 8.48528137, \quad \tilde{S}_{12} = \frac{6}{\sqrt{2}} \approx 4.24264069, \quad \tilde{S}_{13} = \frac{9}{\sqrt{2}} \approx 6.36396103.$$

Second row:

$$\tilde{S}_{21} = \frac{4}{\sqrt{2}} \approx 2.82842712, \quad \tilde{S}_{22} = \frac{2}{\sqrt{2}} \approx 1.41421356, \quad \tilde{S}_{23} = \frac{2}{\sqrt{2}} \approx 1.41421356.$$

Third row:

$$\tilde{S}_{31} = \frac{8}{\sqrt{2}} \approx 5.65685425, \quad \tilde{S}_{32} = \frac{4}{\sqrt{2}} \approx 2.82842712, \quad \tilde{S}_{33} = \frac{6}{\sqrt{2}} \approx 4.24264069.$$

Step 6: softmax (row-wise) — compute probabilities

We compute softmax on each row. For numerical stability subtract the row max first.

Row 1: values (8.48528137, 4.24264069, 6.36396103). Max is 8.48528137. Subtract:

$$(0, -4.24264068, -2.12132034).$$

Exponentiate:

$$e^0 = 1, \quad e^{-4.24264068} \approx 0.014332, \quad e^{-2.12132034} \approx 0.119019.$$

Sum: $1 + 0.014332 + 0.119019 \approx 1.133351$.

Softmax row 1:

$$A_1 = \left(\frac{1}{1.133351}, \frac{0.014332}{1.133351}, \frac{0.119019}{1.133351} \right) \approx (0.88164541, 0.01266889, 0.10568570).$$

Row 2: values (2.82842712, 1.41421356, 1.41421356). Max is 2.82842712. Subtract:

$$(0, -1.41421356, -1.41421356).$$

Exponentiate:

$$e^0 = 1, \quad e^{-1.41421356} \approx 0.243144, \quad e^{-1.41421356} \approx 0.243144.$$

Sum: $1 + 0.243144 + 0.243144 \approx 1.486288$.

Softmax row 2:

$$A_2 \approx (0.6728418, 0.1635791, 0.1635791).$$

Row 3: values (5.65685425, 2.82842712, 4.24264069). Max is 5.65685425. Subtract:

$$(0, -2.82842712, -1.41421356).$$

Exponentiate:

$$e^0 = 1, \quad e^{-2.82842712} \approx 0.059015, \quad e^{-1.41421356} \approx 0.243144.$$

Sum: $1 + 0.059015 + 0.243144 \approx 1.302159$.

Softmax row 3:

$$A_3 \approx (0.76791794, 0.04538836, 0.18669370).$$

So the attention matrix A (rows sum to 1) is approximately:

$$A \approx \begin{pmatrix} 0.88164541 & 0.01266889 & 0.10568570 \\ 0.67284180 & 0.16357910 & 0.16357910 \\ 0.76791794 & 0.04538836 & 0.18669370 \end{pmatrix}.$$

Step 7: final head output AV

Multiply A (3x3) by V (3x2) to get output (3x2).

Compute row 1:

$$\text{out}_1 = 0.88164541 \cdot V_1 + 0.01266889 \cdot V_2 + 0.10568570 \cdot V_3.$$

Recall $V_1 = (2, 2)$, $V_2 = (1, 1)$, $V_3 = (1, 2)$.

Compute first component:

$$\text{out}_{1,1} = 0.88164541 \cdot 2 + 0.01266889 \cdot 1 + 0.10568570 \cdot 1 = 1.76329082 + 0.01266889 + 0.10568570 = 1.88164541.$$

Second component:

$$\text{out}_{1,2} = 0.88164541 \cdot 2 + 0.01266889 \cdot 1 + 0.10568570 \cdot 2 = 1.76329082 + 0.01266889 + 0.21137140 = 1.98733111.$$

Row 1 output: (1.88164541, 1.98733111).

Row 2:

$$\text{out}_2 = 0.67284180 \cdot V_1 + 0.16357910 \cdot V_2 + 0.16357910 \cdot V_3.$$

First component:

$$= 0.67284180 \cdot 2 + 0.16357910 \cdot 1 + 0.16357910 \cdot 1 = 1.3456836 + 0.1635791 + 0.1635791 = 1.6728418.$$

Second component:

$$= 0.67284180 \cdot 2 + 0.16357910 \cdot 1 + 0.16357910 \cdot 2 = 1.3456836 + 0.1635791 + 0.3271582 = 1.8364209.$$

Row 2 output: (1.6728418, 1.8364209).

Row 3:

$$\text{out}_3 = 0.76791794 \cdot V_1 + 0.04538836 \cdot V_2 + 0.18669370 \cdot V_3.$$

First component:

$$= 0.76791794 \cdot 2 + 0.04538836 \cdot 1 + 0.18669370 \cdot 1 = 1.53583588 + 0.04538836 + 0.18669370 = 1.76791794.$$

Second component:

$$= 0.76791794 \cdot 2 + 0.04538836 \cdot 1 + 0.18669370 \cdot 2 = 1.53583588 + 0.04538836 + 0.37338740 = 1.95461164.$$

Row 3 output: (1.76791794, 1.95461164).

So final head output:

$$\text{Attention}(Q, K, V) \approx \begin{pmatrix} 1.88164541 & 1.98733111 \\ 1.67284180 & 1.83642090 \\ 1.76791794 & 1.95461164 \end{pmatrix}.$$

Summary of numeric example: Every intermediate matrix (Q, K, V, S, \tilde{S}, A) is shown and the arithmetic is fully expanded. This demonstrates exactly how to compute attention for small toy values and can be used to unit-test an implementation.

10 Backprop intuition (concise)

Attention is differentiable everywhere (softmax is smooth). Gradients flow through:

$$\frac{\partial \mathcal{L}}{\partial W_Q}, \frac{\partial \mathcal{L}}{\partial W_K}, \frac{\partial \mathcal{L}}{\partial W_V},$$

via chain-rule through $A = \text{softmax}(\frac{QK^\top}{\sqrt{d_k}} + M)$ and AV . Pay attention that softmax Jacobian is dense per row: efficient implementations avoid naive Jacobian and instead use matrix-vector identities.

11 Implementation notes and gotchas

- **Compute multi-head efficiently:** compute Q, K, V with single linear layers producing shape $[N, H, d_{\text{head}}]$ by a single matmul and reshape, rather than separate loops for heads.
- **Masking and fp16:** use a large finite negative number (e.g., $-1e9$) for mask to avoid producing NaN in fp16 when exponentiating $-\infty$.
- **Stable softmax:** subtract max per row before exponentiating.

- **Tied embeddings:** tying input embeddings E and output linear projection (transposed) saves memory and sometimes improves generalization.
- **Pre-norm recommended:** for deep stacks (hundreds of layers), pre-norm (LayerNorm before sublayer) is more stable.
- **KV cache memory:** each layer caches $K, V \in \mathbb{R}^{T \times d_{\text{head}}}$ per head. For long contexts this can be memory-heavy.

12 PyTorch-style pseudocode (concise, clear shapes)

```
# INPUT:
# x: Tensor of shape (batch, seq_len, d)
# mask: Tensor of shape (batch, seq_len, seq_len) with 0 where allowed, -1e9 where blocked

# single linear to get QKV, then reshape
qkv = linear_qkv(x) # (batch, seq_len, 3*d)
qkv = qkv.view(batch, seq_len, 3, H, d_head)
qkv = qkv.permute(2, 0, 3, 1, 4) # (3, batch, H, seq_len, d_head)
Q, K, V = qkv[0], qkv[1], qkv[2] # each (batch, H, seq_len, d_head)

# compute scores
scores = torch.matmul(Q, K.transpose(-2,-1)) # (batch, H, seq_len, seq_len)
scores = scores / math.sqrt(d_head)
scores = scores + mask # broadcasting mask
attn = torch.softmax(scores, dim=-1) # along last dim

# weighted sum
out = torch.matmul(attn, V) # (batch, H, seq_len, d_head)
out = out.permute(0, 2, 1, 3).contiguous().view(batch, seq_len, d)
out = linear_out(out) # (batch, seq_len, d)
```

13 Decoding and sampling strategies (short)

- **Greedy:** pick argmax each step.
- **Temperature:** divide logits by temperature τ before softmax.
- **Top-k:** restrict to top-k logits.
- **Top-p (nucleus):** restrict to smallest set whose cumulative prob $\geq p$.

14 Putting it all together: the full decoder-only block (diagram)



15 Advanced topics (brief pointers)

- **Sparse attention** (local/blockwise) for very long sequences.
- **Relative positional encodings** for better generalization to unseen lengths.
- **Mixture of Experts** to scale model capacity efficiently.
- **Efficient kernels / flash attention** to reduce memory bandwidth and runtime.

Appendix A — Summary cheat-sheet

- $Q = XW_Q, K = XW_K, V = XW_V$.
- $S = QK^\top, \tilde{S} = S/\sqrt{d_k} + M$.
- $A = \text{softmax}(\tilde{S})$ row-wise.
- $\text{head} = AV, \text{MultiHead} = \text{Concat}(\text{heads})W_O$.
- FFN: $W_2 \sigma(W_1 x + b_1) + b_2$.

If you want: I can now

1. Expand the PyTorch pseudocode into a full runnable script (training loop, loss, optimizer, data batching).
2. Produce a version of this manual optimized for printing (larger diagrams, two-column layout).
3. Add a section "Debugging checklist" with unit tests and tiny code assertions (e.g., check shapes, row sums of attention equal 1, masking tests).

Tell me which and I'll produce it immediately.