

NATURAL LANGUAGE PROCESSING

Attention mechanisms & Transformer architecture

Modern NLP Foundations & Chatbot development

Learning objectives

1

Understand the motivation and mechanics of Attention mechanism in Seq2Seq models

2

Master Self-Attention with Query, Key, Value framework and Scaled Dot-Product

3

Explain Multi-Head Attention and why multiple heads improve performance

4

Understand Transformer architecture: Encoder, Decoder, Positional Encoding

5

Build Chatbots using attention-based models and modern LLM architectures

6

Evaluate and deploy conversational AI systems with proper metrics

Session agenda

Part 1

Attention mechanisms: a review

Seq2Seq recap, attention core idea, score functions

Part 2

Self-Attention & Multi-head

Q, K, V framework, scaled dot-product, multiple heads

Part 3

Transformer architecture

Positional encoding, encoder-decoder, BERT/GPT/T5

Part 4

Chatbot development

NLU pipeline, intent & slots, dialogue state tracking

Part 5

Implementation & Evaluation

HuggingFace, metrics, common pitfalls

Part 6

Lab & Final Assignment

Hands-on exercises, project requirements

Attention mechanisms: A review

From Seq2Seq bottleneck to dynamic context

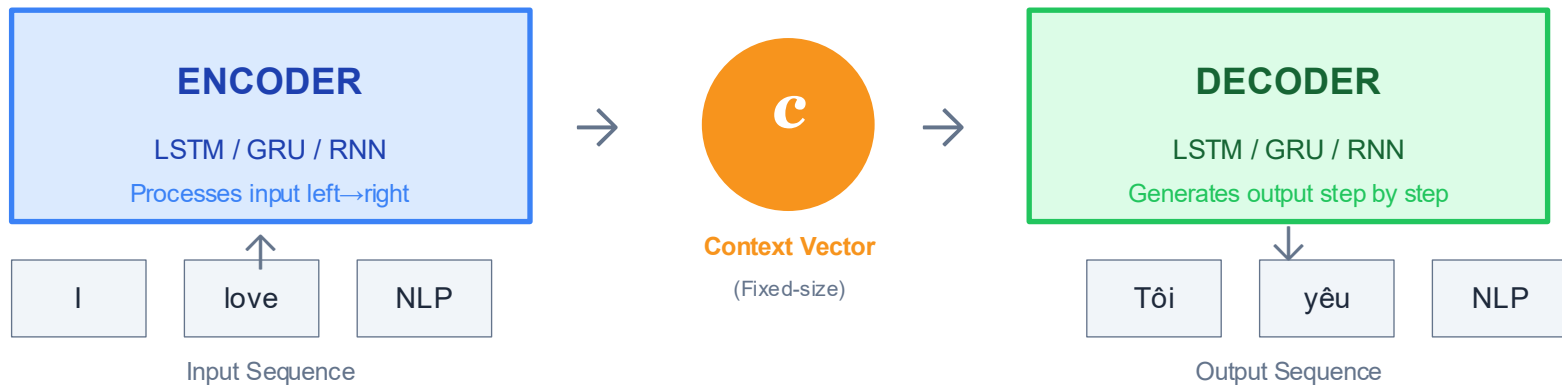
Seq2Seq Architecture Recap

The Bottleneck Problem

Attention Score Functions

Context Vector Computation

Recap: Seq2Seq (Encoder-Decoder) architecture



Key Equations

Encoder: $h_t = f(x_t, h_{t-1})$

Context: $c = h_t(\text{final hidden state})$

Decoder: $s_t = g(y_{t-1}, s_{t-1}, c)$

Applications

Machine Translation (EN→VN)

Text Summarization

Chatbots & Dialogue Systems

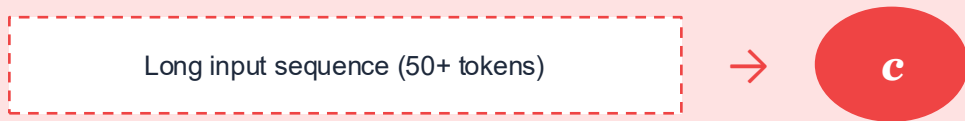
Question Answering

The Bottleneck problem in Seq2Seq

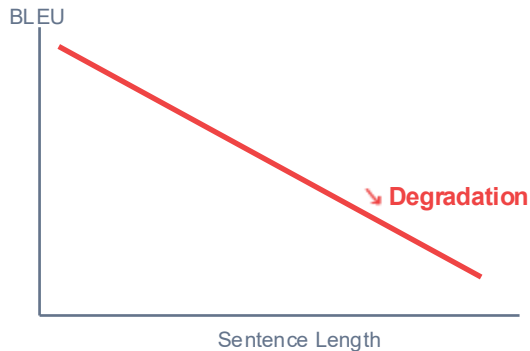
The Problem

The entire input sequence is compressed into a single fixed-size vector c .

For long sequences, this causes severe information loss!



Performance vs Sentence Length



Key Insight

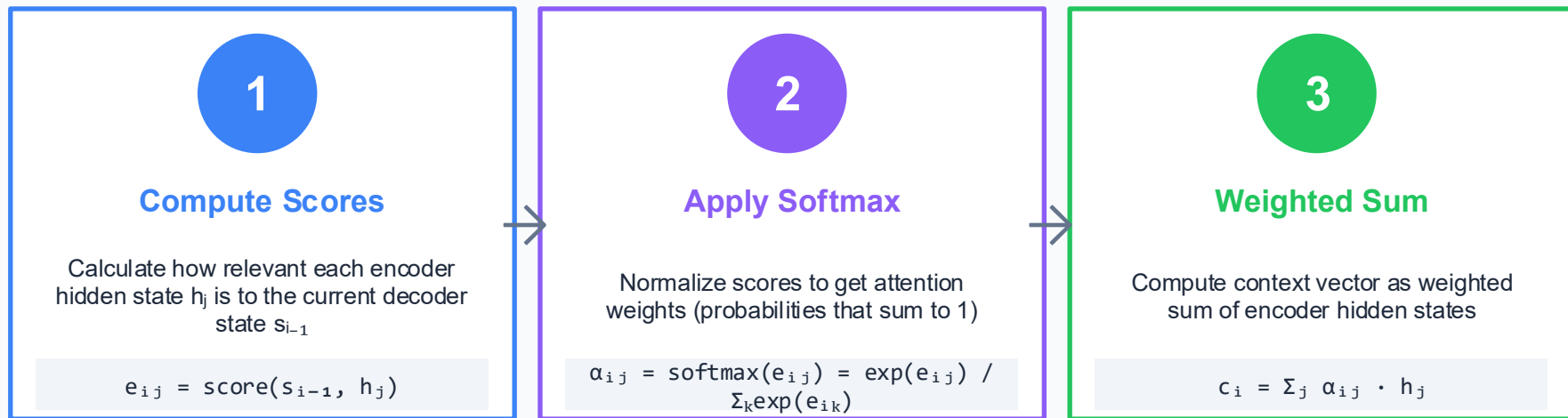
When translating a word, we don't need ALL input information — just the relevant parts! This observation leads to the Attention mechanism.

Solution: Attention Mechanism

Instead of using one fixed context vector, dynamically focus on different parts of the input at each decoding step.

Attention: The core idea

At each decoding step, compute a weighted combination of ALL encoder hidden states based on their relevance to the current output.



Human Intuition

I love machine learning



Focus on relevant words → Tôi yêu học máy

Attention score functions

Different ways to compute relevance score between decoder state s_{i-1} and encoder hidden state h_j :

Dot Product

(Luong, 2015)

$$\text{score}(s, h) = s^T h$$

✓ Pros:

Simple, fast, no parameters

✗ Cons:

Requires same dimensions

General (Bilinear)

(Luong, 2015)

$$\text{score}(s, h) = s^T W_a h$$

✓ Pros:

Learnable, flexible

✗ Cons:

Needs $d \times d$ parameter matrix

Concat (Additive)

(Bahdanau, 2014)

$$\text{score} = v_a^T \tanh(W_a[s; h])$$

✓ Pros:

Most expressive

✗ Cons:

Slower, more parameters

Transformer uses Scaled Dot-Product: divides by $\sqrt{d_k}$ to prevent softmax saturation

Attention weights: step-by-step

$$\alpha_{ij} = \text{softmax}(e_{ij}) = \exp(e_{ij}) / \sum_k \exp(e_{ik})$$

Example: Translating "I love machine learning" → "Tôï ..."

Step 1: Compute raw scores (dot product)

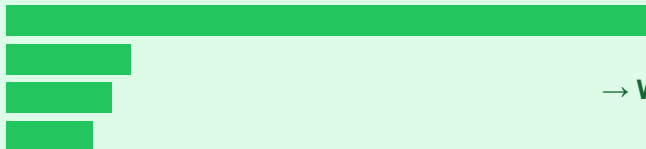
$e_{11} = s_0 \cdot h_1 = 2.1$ ("I")
 $e_{12} = s_0 \cdot h_2 = 0.5$ ("love")
 $e_{13} = s_0 \cdot h_3 = 0.3$ ("machine")
 $e_{14} = s_0 \cdot h_4 = 0.1$ ("learning")

Step 2: Apply softmax

$\exp(2.1)=8.17$, $\exp(0.5)=1.65$
 $\exp(0.3)=1.35$, $\exp(0.1)=1.11$
Sum = 12.28

Step 3: Attention weights (normalized probabilities)

I	$\alpha = 0.67$
love	$\alpha = 0.13$
machine	$\alpha = 0.11$
learning	$\alpha = 0.09$



→ When generating "Tôï", model focuses 67% on "I"

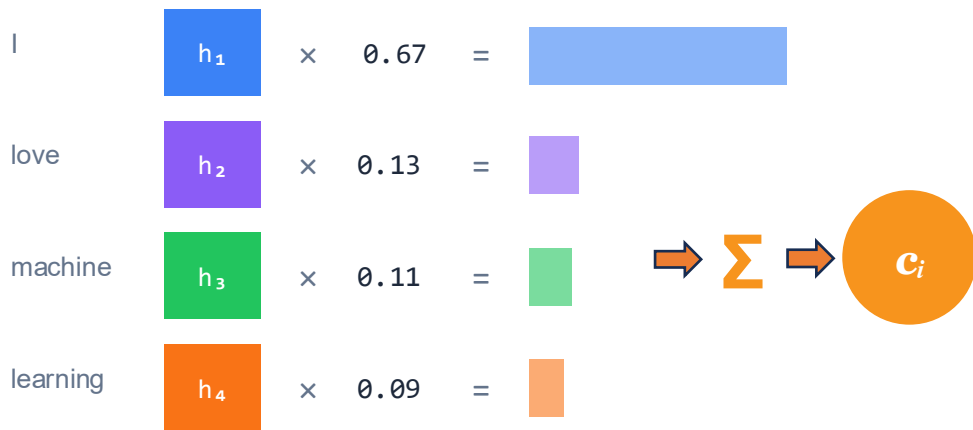
Key Properties: $\alpha_{ij} \in [0,1]$ • $\sum_j \alpha_{ij} = 1$

- Higher weight = more relevance
- Differentiable!

Context vector computation

$$c_i = \sum_j \alpha_{ij} \cdot h_j \quad (\text{Weighted sum of encoder hidden states})$$

Visual: How context vector is computed



Numerical Example

If each h_j is a 3-dim vector:

$$h_1 = [0.2, 0.8, 0.1]$$

$$h_2 = [0.5, 0.3, 0.2]$$

$$h_3 = [0.1, 0.4, 0.9]$$

$$h_4 = [0.3, 0.1, 0.7]$$

$$c = 0.67 \times h_1 + 0.13 \times h_2 + 0.11 \times h_3 + 0.09 \times h_4$$

$$c = [0.24, 0.62, 0.24]$$

→ Dominated by h_1 ("I")

Key: Context vector c_i is DIFFERENT for each decoder step — dynamically adapts to what's being generated!

Attention visualization: alignment matrix

Attention Alignment Matrix (EN → VN)

	I	love	machine	learning
Tôi	0.90	0.05	0.03	0.02
yêu	0.05	0.85	0.05	0.05
học	0.02	0.08	0.45	0.45
máy	0.02	0.03	0.50	0.45

Interpretation

"Tôi" → "I" (0.90)

"yêu" → "love" (0.85)

"học máy" → "machine" + "learning"
(multi-word alignment!)

Benefits

- Interpretable alignments
- Debug translation errors
- Understand model behavior
- Detect attention issues

Multi-word alignment: "machine learning" → "học máy" — attention handles this naturally!

Cross-attention vs Self-attention

Cross-Attention

Used in: Seq2Seq, Encoder-Decoder



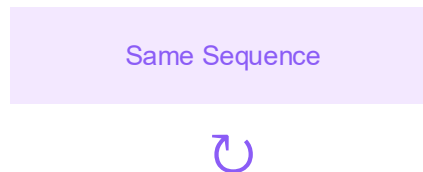
Key points:

- Query: from decoder (target)
- Key, Value: from encoder (source)
- Connects TWO sequences
- Used for translation alignment

`score(decoderstate, encoderstate)`

Self-Attention

Used in: Transformers, BERT, GPT



Key points:

- Q, K, V all from SAME sequence
- Each position attends to all others
- Captures internal relationships
- Foundation of Transformers

`score(positioni, positionj)`

Key: Cross = between sequences | Self = within same sequence. Transformer uses BOTH!

Why Self-attention for NLP?

RNN/LSTM Limitations

- Sequential processing: $O(n)$ steps
- Long-range dependencies hard
- Cannot parallelize training
- Vanishing gradients for long seq

Self-Attention Advantages

- Parallel processing: $O(1)$ steps
- Direct connection to any position
- Fully parallelizable on GPU
- Constant path length

Example: "The cat sat on the mat because it was tired"

Self-attention directly connects "it" → "cat" in 1 step. RNN needs 5 steps to propagate this information.

Summary: Attention Mechanisms

1

Bottleneck Problem

Fixed context vector loses info for long sequences

2

Attention Solution

Dynamically focus on relevant input parts per step

3

Score Functions

Dot Product, General, Concat to compute relevance

4

Attention Weights

Softmax gives probability distribution over inputs

5

Self-Attention

Each position attends to all positions in same sequence

Essential Formulas

Score Functions:

Dot: $s^T h$

General: $s^T W_a h$

Concat: $v_a^T \tanh(W_a [s; h])$

Attention Weight:

$\alpha_{ij} = \text{softmax}(e_{ij})$

Context Vector:

$c_i = \sum_j \alpha_{ij} \cdot h_j$

Self-attention & Multi-head attention

The foundation of transformer architecture

Query, Key, Value Framework

Scaled Dot-Product Attention

Why Scale by $\sqrt{d_k}$?

Multi-Head Attention

Parameter Analysis & Dimensions

Introducing Query, Key, Value (Q, K, V)

Self-Attention uses three learned projections of the input: Query (Q), Key (K), and Value (V)



Query

"What am I looking for?"

Represents the current position's question to ask other positions



Key

"What do I contain?"

Represents information each position advertises about itself



Value

"What do I provide?"

The actual content to be retrieved when a query matches a key

Attention Flow:



matches



→ score →

softmax →

retrieve



→ **Output**

Database analogy: understanding Q, K, V

Think of attention as a "soft" database lookup — instead of exact matching, we use similarity scores

Traditional Database Lookup

Query: `SELECT value WHERE key = 'cat'`

Key	Value
dog	[0.2, 0.8, 0.1]
cat	[0.9, 0.3, 0.5]
bird	[0.1, 0.6, 0.7]

Result: Exact match → [0.9, 0.3, 0.5]

Binary: either 0 or 1 (match/no match)

Attention (soft lookup)

Query: "kitten" (similar to cat)

Key	Score	Value
dog	0.2	[0.2, 0.8, 0.1]
cat	0.7	[0.9, 0.3, 0.5]
bird	0.1	[0.1, 0.6, 0.7]

Result: Weighted sum of all values

$$= 0.2 \times v_1 + 0.7 \times v_2 + 0.1 \times v_3$$

Continuous: soft weights $\in [0, 1]$

Attention is differentiable — we can learn Q, K, V through backpropagation!

Creating Q, K, V: linear projections

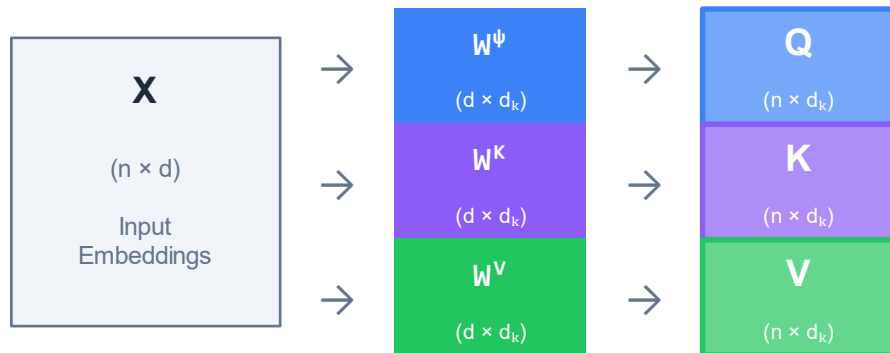
$$Q = X \cdot W^Q$$

$$K = X \cdot W^K$$

$$V = X \cdot W^V$$

Where X is the input sequence, and W^Q, W^K, W^V are learnable weight matrices

Visual: How Q, K, V are created from input X



Dimensions

n = sequence length
 d = input embedding dimension
 d_k = key/query dimension
 d_v = value dimension

Typically: $d_k = d_v = d/h$
(h = number of heads)

Same input X → Different projections

W matrices are **LEARNED** during training

Self-Attention: each position attends to all

In self-attention, Q, K, V all come from the SAME sequence — each position can attend to every other position

Example: "The cat sat on the mat because it was tired"



"it" attends to "cat" (coreference)

Self-Attention Matrix (simplified):

	cat	sat	it	was
cat	0.9	0.1	0.0	0.0
sat	0.3	0.5	0.1	0.1
it	0.7	0.1	0.1	0.1
was	0.2	0.2	0.3	0.4

← "it" strongly attends to "cat" (0.7)

Why Self-Attention Works

- Captures long-range dependencies
- Resolves coreference (it → cat)
- Parallel computation (no RNN!)
- Learns multiple relationships

Scaled dot-product attention

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

The core formula of Transformer attention — memorize this!

Formula Breakdown

Q

Query matrix ($n \times d_k$) — what each position is looking for

K

Key matrix ($n \times d_k$) — what each position contains

V

Value matrix ($n \times d_v$) — actual content to retrieve

QK^T

Attention scores matrix ($n \times n$) — similarity between all pairs

$\sqrt{d_k}$

Scaling factor — prevents softmax saturation (explained next)

softmax

Normalizes scores to probabilities (rows sum to 1)

Output Dimensions: $(n \times n) \times (n \times d_v) = (n \times d_v)$ — same shape as V, but with attended information

Why Scale by $\sqrt{d_k}$? preventing gradient vanishing

Problem Without Scaling

For high d_k (e.g., 64), the dot product QK^T grows very large:

If $q, k \sim N(0,1)$, then:
 $q \cdot k$ has variance = d_k

For $d_k = 64$:
Variance = 64, Std = 8

Large values → **Softmax saturates** → **Gradients vanish!**

Solution: Scale by $\sqrt{d_k}$

Dividing by $\sqrt{d_k}$ normalizes the variance:

$$\text{Var}(q \cdot k / \sqrt{d_k}) = d_k / d_k = 1$$

For $d_k = 64$:
 $\sqrt{64} = 8$
New Variance = 1, Std = 1

Stable softmax → **Healthy gradients** → **Better training!**

Softmax Behavior Comparison

Without scaling (scores = [8, 4, 0, -4]):

0.982	0.018	0.000	0.000
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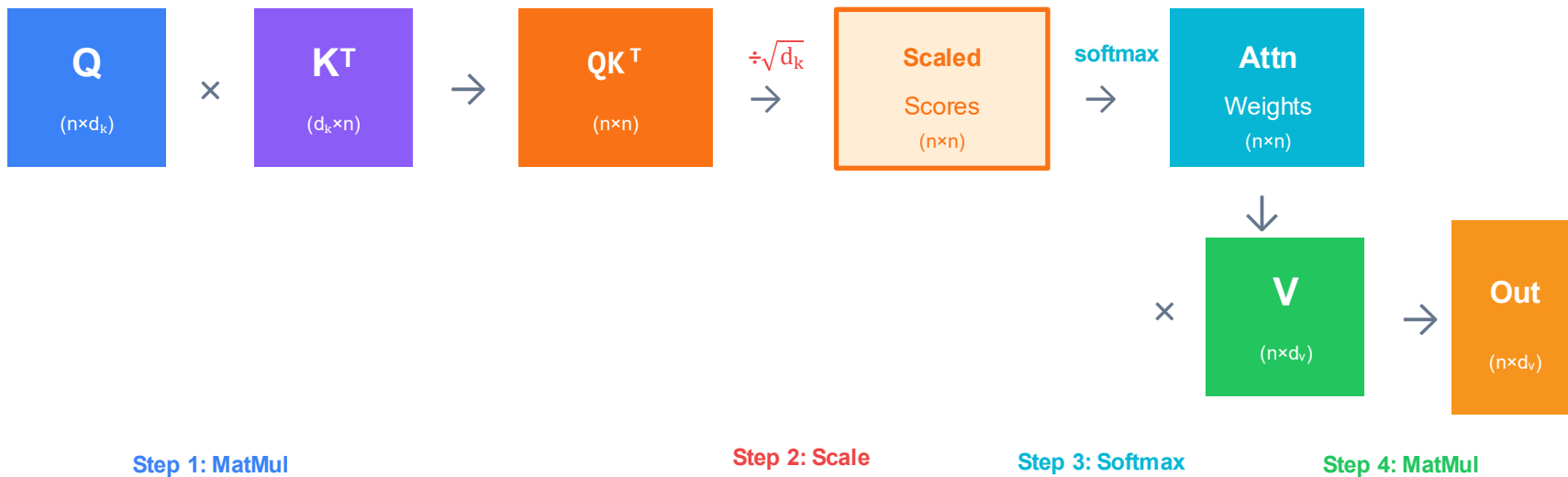
→ Almost one-hot! Gradients ≈ 0

With scaling (scores = [1, 0.5, 0, -0.5]):

0.39	0.24	0.14	0.09
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→ Smooth distribution, healthy gradients!

Scaled dot-product: computation flow



Example

Input: "I love NLP" with $d_k = 4$

Q (3×4)

I: [1, 0, 1, 0]
love: [0, 1, 1, 0]
NLP: [1, 1, 0, 1]

K (3×4)

I: [1, 1, 0, 0]
love: [0, 1, 1, 1]
NLP: [1, 0, 1, 1]

V (3×4)

I: [0.1, 0.2, 0.3, 0.4]
love: [0.5, 0.6, 0.7, 0.8]
NLP: [0.9, 1.0, 1.1, 1.2]

Step 1: QK^T (raw scores)

	I	love	NLP
I:	[1,	1,	2]
love:	[1,	2,	1]
NLP:	[1,	2,	2]

Step 2: $\div \sqrt{4} = \div 2$

	I	love	NLP
I:	[0.5,	0.5,	1.0]
love:	[0.5,	1.0,	0.5]
NLP:	[0.5,	1.0,	1.0]

Step 3: Softmax (each row)

	I	love	NLP
I:	[0.27,	0.27,	0.45]
love:	[0.24,	0.40,	0.24]
NLP:	[0.21,	0.35,	0.35]

Step 4: $\text{Attn} \times V = \text{Output}$

I: [0.57, 0.66, 0.75, 0.84]
love: [0.48, 0.56, 0.64, 0.72]
NLP: [0.54, 0.62, 0.70, 0.78]

Weighted combination of V rows!

Multi-head attention: Why multiple heads?

Single Head Limitation

One attention head can only learn ONE type of relationship:

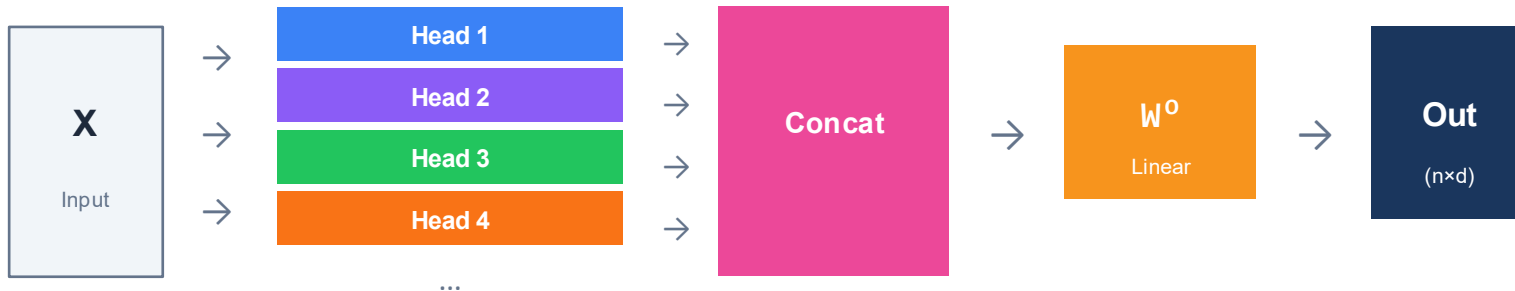
- Maybe it learns syntax
- OR maybe semantics
- OR maybe position
- But NOT all at once!

Multi-Head Solution

Run multiple attention heads in parallel, each learning different relationships:

- Head 1: syntactic structure
- Head 2: coreference
- Head 3: semantic similarity
- Concatenate all insights!

Multi-Head Architecture



Different heads learn different aspects: syntax, semantics, coreference, position — then combine them!

Multi-Head Attention: the formula

$$\text{MultiHead}(Q, K, V) = \text{Concat}(\text{head}_1, \dots, \text{head}_h) \cdot W^O$$

$$\text{where } \text{head}_i = \text{Attention}(Q \cdot W_i^Q, K \cdot W_i^K, V \cdot W_i^V)$$

h = number of heads (typically 8 or 12)

Understanding Each Component

W_i^Q, W_i^K, W_i^V	Projection matrices for head i	$(d \times d_k), (d \times d_k), (d \times d_v)$
head_i	Output of attention head i	$(n \times d_v)$
$\text{Concat}(\dots)$	Concatenate all head outputs	$(n \times h \cdot d_v)$
W^O	Output projection matrix	$(h \cdot d_v \times d)$

Insight

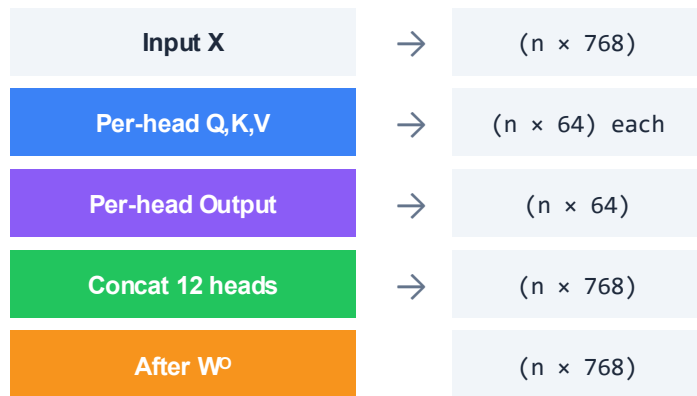
Each head has its own W^Q, W^K, W^V matrices, allowing it to learn different patterns!

BERT-base: $d=768, h=12, d_k=d_v=64$ | GPT-2: $d=768, h=12, d_k=d_v=64$ | GPT-3: $d=12288, h=96, d_k=d_v=128$

Parameter & dimension analysis

Example: BERT-base configuration — $d = 768$, $h = 12$ heads, $d_k = d_v = 64$

Dimension Flow



Why $d_k = d/h = 768/12 = 64$?

Concat restores original dim!

Parameter Count

Per head (W^Q, W^K, W^V):

$$3 \times (768 \times 64) = 147,456$$

All 12 heads:

$$12 \times 147,456 = 1,769,472$$

Output W^O :

$$768 \times 768 = 589,824$$

Total: ~2.36M params

Model Comparison

Model	d	h	$d_k = d/h$	MHA Params
BERT-base	768	12	64	2.36M
GPT-2	768	12	64	2.36M
GPT-3 (175B)	12288	96	128	603M

What different attention heads learn

Research has shown that different heads specialize in different linguistic patterns (Clark et al., 2019)

Syntactic Heads

Attend to grammatical structure

e.g., subject→verb, noun→adjective

Positional Heads

Attend to nearby positions

e.g., previous token, next token

Coreference Heads

Link pronouns to entities

e.g., "it" → "the cat"

Semantic Heads

Attend to related meanings

e.g., "bank" → "money", "river"

Example: "The cat sat on the mat because it was tired"

Head 3 (Coreference): "it" strongly attends to "cat" (0.72) | Head 7 (Positional): "sat" attends to "cat" (0.45) | Head 11 (Syntactic): "tired" attends to "was" (0.68)

Summary: self-attention & multi-Head

1

Q, K, V Framework

Query asks, Key advertises, Value provides content

2

Scaled Dot-Product

Attention = $\text{softmax}(QK^T/\sqrt{d_k}) \cdot V$

3

Why $\sqrt{d_k}$ Scaling

Prevents gradient vanishing from softmax saturation

4

Multi-Head Attention

Multiple heads learn different relationship types

5

Dimension Analysis

$d_k = d/h$ ensures output matches input dimension

Formulas

Linear Projections:

$$Q = XW^Q, K = XW^K, V = XW^V$$

Scaled Dot-Product:

$$\text{Attn} = \text{softmax}(QK^T/\sqrt{d_k})V$$

Multi-Head:

$$\text{MHA} = \text{Concat}(\text{heads})W^O$$

Typical Config:

$$d=768, h=12, d_k=64$$

Transformer architecture

"Attention Is All You Need" (Vaswani et al., 2017)

The architecture that revolutionized NLP and AI

Why Transformers? RNN vs Self-Attention

Positional Encoding — Adding Position Information

Encoder Block — Self-Attention + FFN

Decoder Block — Masked Attention + Cross-Attention

BERT vs GPT vs T5 — Architectural Variants

Why transformers? From RNN to self-attention

RNN/LSTM Problems

Sequential Processing

Must process tokens one-by-one, $O(n)$ steps

Long-Range Dependencies

Information decays over distance

No Parallelization

Cannot utilize GPU parallelism

Vanishing Gradients

Hard to train on long sequences



Transformer Solutions

Parallel Processing

All positions computed simultaneously

Direct Connections

Any token can attend to any other in $O(1)$

Full GPU Utilization

Matrix operations are highly parallel

Stable Gradients

Residual connections + LayerNorm

Key Innovation: Replace recurrence entirely with Self-Attention — "Attention Is All You Need"

Training Speed: Transformer trains ~10x faster than RNN on same data (due to parallelization)

Original paper: Achieved SOTA on WMT EN→DE translation in 3.5 days on 8 GPUs (vs weeks for RNN)

Positional Encoding: Why is it needed?

The Problem: Self-Attention is Position-Agnostic!

Self-attention treats input as a SET, not a SEQUENCE. Without position info, "dog bites man" = "man bites dog"!

Example: Position matters for meaning!



Same words, different order → Completely different meaning!

Solution: Add Positional Encoding to Input Embeddings



Positional Encoding: sinusoidal formulas

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

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

pos = position in sequence (0, 1, 2, ...), i = dimension index (0 to d/2-1), d = model dimension

Why sinusoidal functions?

1. Unique encoding per position

Each position has distinct pattern

2. Bounded values [-1, 1]

Won't dominate embeddings

3. Relative positions learnable

$\text{PE}(\text{pos}+k)$ is linear function of $\text{PE}(\text{pos})$

4. Generalizes to longer sequences

Can extrapolate beyond training length

different wavelengths

Dimension 0-1 (i=0):

wavelength = $2\pi \approx 6.28$

→ Changes rapidly with position

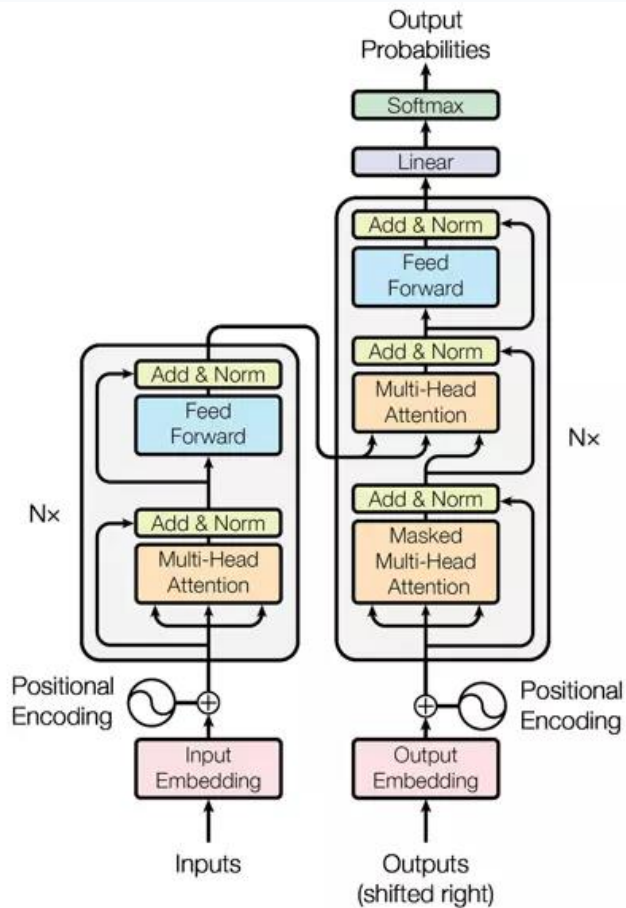
Dimension d-2, d-1 (i=d/2-1):

wavelength = $2\pi \times 10000 \approx 62,832$

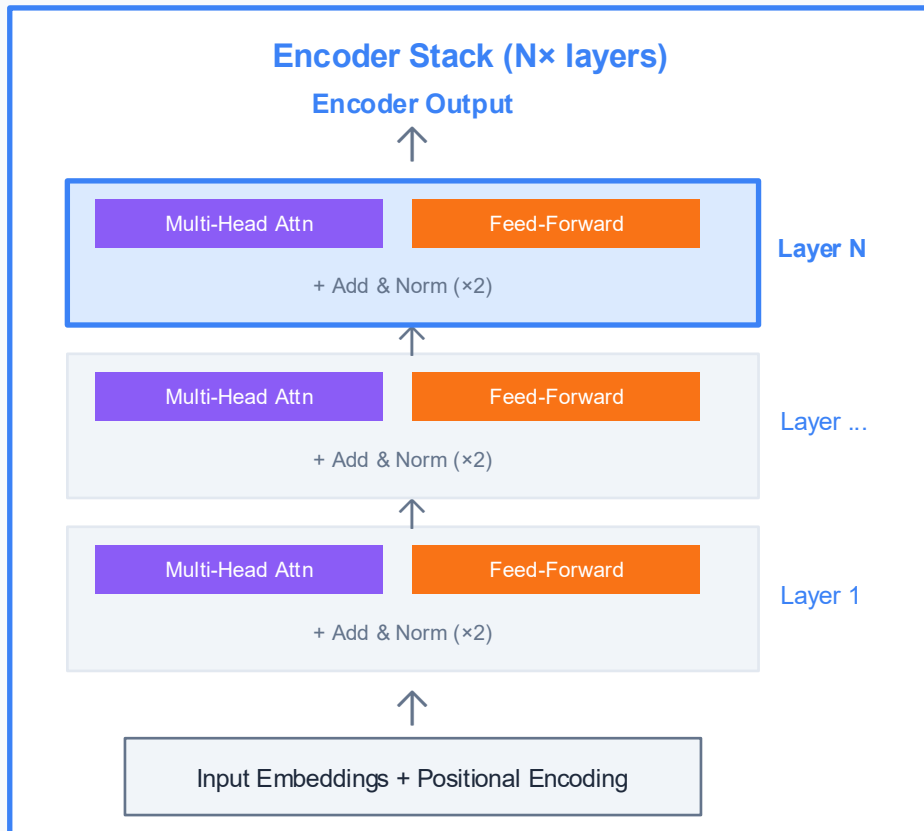
→ Changes very slowly

This creates a spectrum from fine-grained to coarse-grained position information!

Transformer architecture



Transformer Encoder: Overview



Each Encoder Layer Contains:

1. Multi-Head Self-Attention

Each position attends to all positions in the input

2. Add & Normalize

Residual connection + Layer Normalization

3. Feed-Forward Network

Two linear layers with ReLU activation

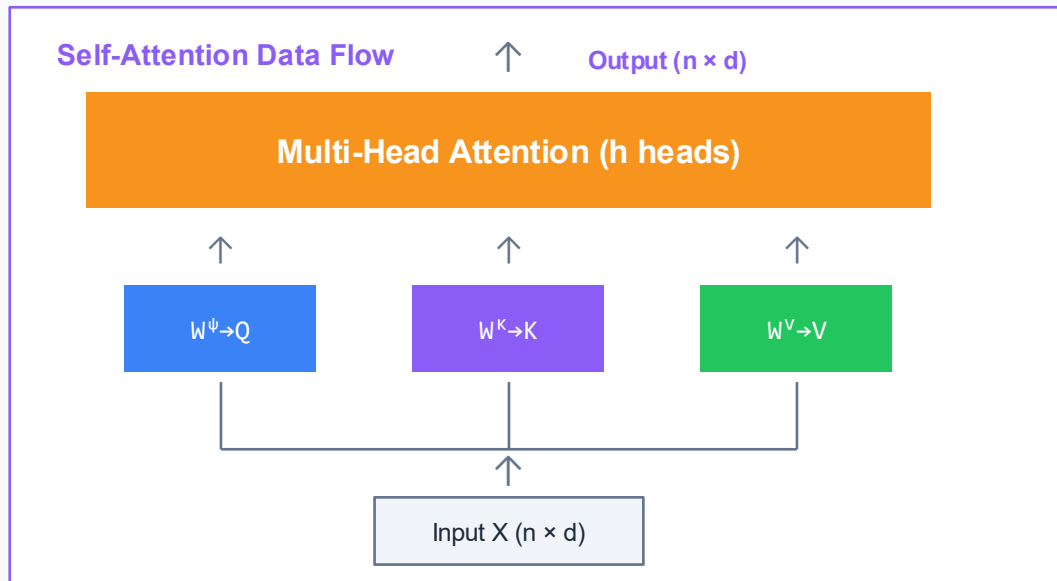
4. Add & Normalize

Another residual + LayerNorm

BERT-base: N=12, GPT-2: N=12, GPT-3: N=96

Encoder: Self-Attention Sub-Layer

$\text{SelfAttn}(X) = \text{MultiHead}(Q=X, K=X, V=X)$ — All from same input!



Key Points

Bidirectional Attention

Each position can see ALL other positions (past and future)

No Masking in Encoder

Unlike decoder, encoder sees full sequence

Parallel Computation

All n positions computed simultaneously

Context Mixing

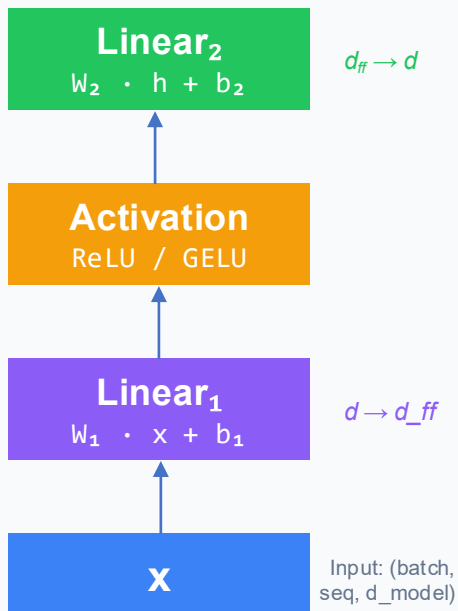
Each output is a mix of all inputs

Output shape is same as input ($n \times d$) — this allows stacking multiple encoder layers!

Encoder: Feed-Forward Network (FFN)

$$\text{FFN}(x) = \max(0, x \cdot W_1 + b_1) \cdot W_2 + b_2$$

= $\text{ReLU}(x \cdot W_1 + b_1) \cdot W_2 + b_2$ (Two linear layers with ReLU in between)



Key Properties

Expansion then Compression

$d \rightarrow d_{\text{ff}}$ (expand) $\rightarrow d$ (compress)
Typically $d_{\text{ff}} = 4d$ (e.g., 768 \rightarrow 3072)

Position-wise

Same FFN applied to each position
No interaction between positions

Non-linearity

ReLU adds non-linear transformation
(GELU used in BERT/GPT)

Parameters: $W_1 (d \times d_{\text{ff}}) + W_2 (d_{\text{ff}} \times d) + \text{biases} \approx 2 \times d \times d_{\text{ff}}$

BERT-base: $768 \times 3072 \times 2 \approx 4.7\text{M}$ params per layer $\times 12$ layers = 56M params (just for FFN!)

Activation functions in FFN

ReLU (Original Transformer)

$$\text{ReLU}(x) = \max(0, x)$$

Simple, fast, but "dead neurons" issue

Used in: Original Transformer (2017)

GELU (Modern)

$$\begin{aligned}\text{GELU}(x) &= x \cdot P(X \leq x) = x \cdot \Phi(x) \\ &= 0.5x(1 + \tanh\left(\sqrt{\frac{2}{\pi}}(x + 0.044715x^3)\right))\end{aligned}$$

Used in: BERT, GPT, most modern LLMs

SwiGLU (Modern LLMs: LLaMA, Mistral, Qwen)

$$\text{SwiGLU}(x, W, V, b, c) = \text{Swish}(xW+b) \odot (xV+c)$$

where $\text{Swish}(x) = x \cdot \sigma(x)$

Evolution: ReLU (2017) → GELU (2018) → SwiGLU (2020+)

Layer Normalization & Residual Connections

Layer Normalization

$$\text{LN}(x) = \gamma \cdot (x - \mu) / \sigma + \beta$$

$\mu = \text{mean}(x)$, $\sigma = \text{std}(x)$, γ and β are learned

Why Layer Norm (not Batch Norm)?

- Normalize across features (d dimension)
- Independent of batch size
- Works with variable sequence lengths
- More stable for sequence models

Residual Connections

$$\text{Output} = x + \text{SubLayer}(x)$$

Why Residual Connections?

- Gradient flows directly (skip connection)
- Enables training very deep networks
- Model can learn "do nothing" easily
- Proven in ResNet (He et al., 2015)

Combined: Add & Norm (Post-LN Transformer)

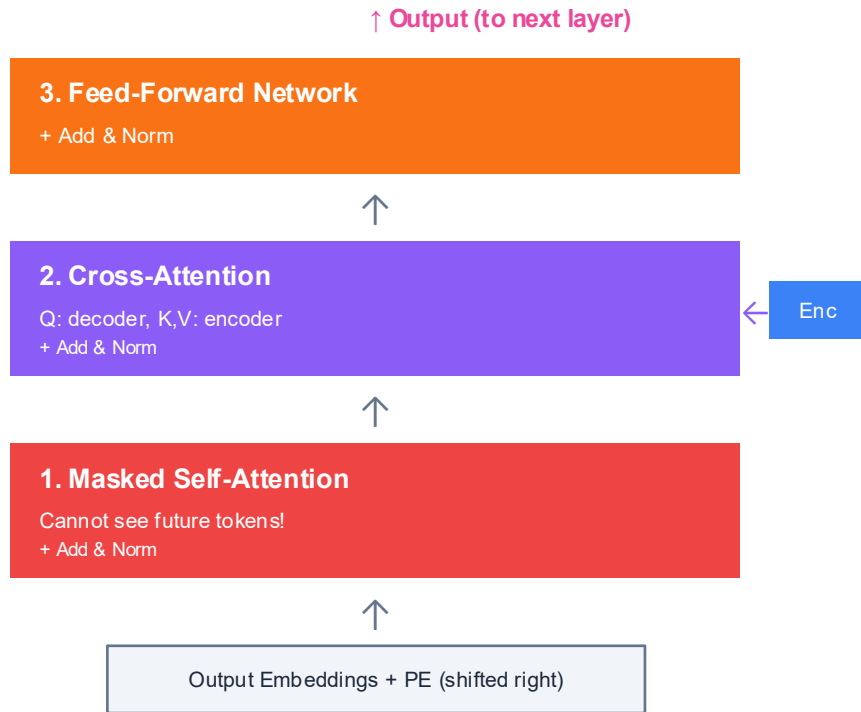
$$\text{output} = \text{LayerNorm}(x + \text{SubLayer}(x))$$

Applied twice in each encoder layer: once after Self-Attention, once after FFN

Pre-LN: $\text{LN}(x) + \text{SubLayer}(\text{LN}(x))$ — more stable for deep models

Transformer Decoder: Overview

Decoder Layer Structure



Decoder has 3 Sub-layers

- 1 Masked Self-Attention**
Attend to previous output tokens only (causal)
- 2 Cross-Attention**
Attend to encoder output (source sequence)
- 3 Feed-Forward Network**
Same as encoder FFN (position-wise)

Each sub-layer has Add & Norm:
 $\text{output} = \text{LayerNorm}(x + \text{Sublayer}(x))$

Decoder: Masked Self-Attention

Problem: At inference, decoder generates tokens one-by-one — it cannot see future tokens!

Causal Mask (Lower Triangular)

	<s>	I	love	NLP
<s>	1	$-\infty$	$-\infty$	$-\infty$
I	1	1	$-\infty$	$-\infty$
love	1	1	1	$-\infty$
NLP	1	1	1	1

 = can attend  = masked ($-\infty \rightarrow \text{softmax}=0$)

Masked Attention Formula

$$\text{Attn} = \text{softmax}((QK^T + M) / \sqrt{d_k}) \cdot V$$

where $M[i,j] = 0$ if $j \leq i$, else $-\infty$

$\text{softmax}(-\infty) = 0$, so future tokens get zero weight!

Generation Example

Step 1: Generate "I"

→ sees only <start>

Step 2: Generate "love"

→ sees <start>, "I"

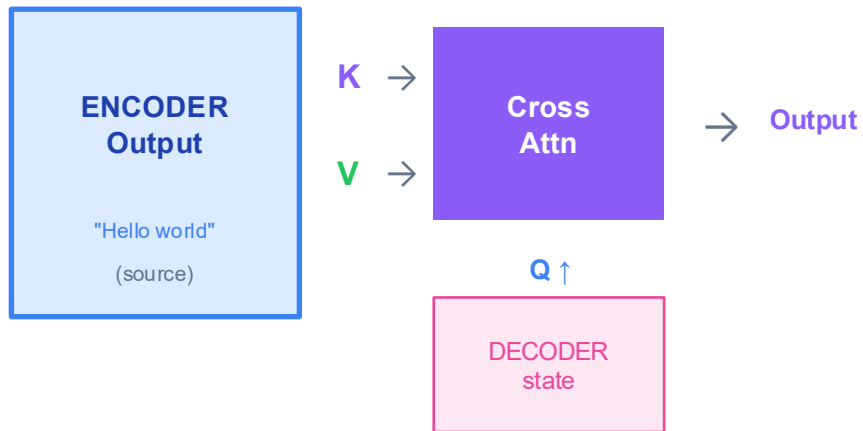
Step 3: Generate "NLP"

→ sees <start>, "I", "love"

Decoder: Cross-Attention

$$\text{CrossAttn}(Q_{\text{dec}}, K_{\text{enc}}, V_{\text{enc}}) = \text{softmax}(Q_{\text{dec}} \cdot K_{\text{enc}}^T / \sqrt{d_k}) \cdot V_{\text{enc}}$$

Cross-Attention Data Flow



How Cross-Attention Works

Q comes from Decoder

"What info do I need to generate the next target word?"

K, V come from Encoder

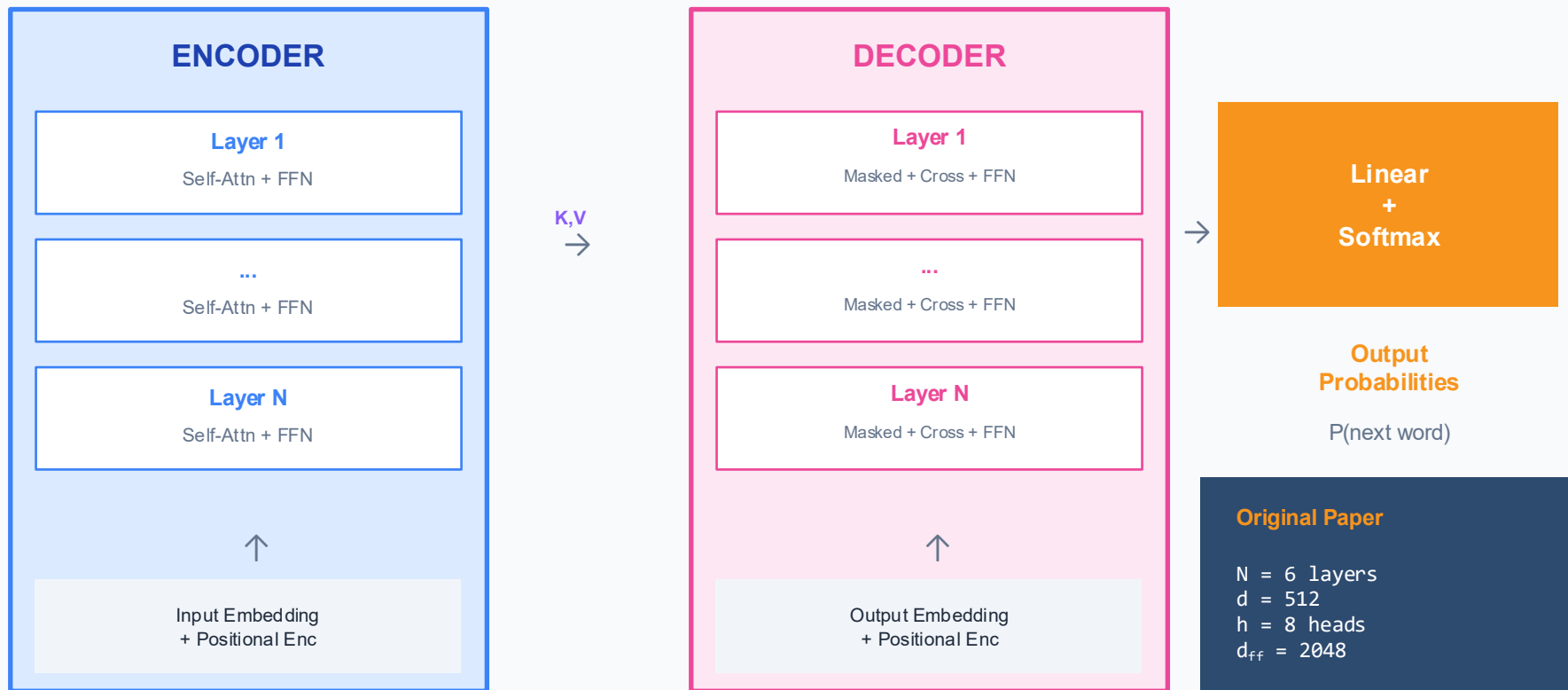
"Here's the source sentence context for you to use."

Result

Decoder focuses on relevant source words when generating each target word

Translation: "Hello world" → "Xin chào thế giới" — when generating "chào", decoder attends strongly to "Hello"

Transformer Architecture



Encoder: bidirectional self-attention | Decoder: masked self-attention + cross-attention to encoder

Transformer variants: BERT vs GPT vs T5

BERT

(2018, Google)

Bidirectional Encoder

Architecture

Encoder-only

Attention

Bidirectional

Pre-training

MLM + NSP

Best for

Classification, NER, QA

Encoder

GPT

(2018-2023, OpenAI)

Generative Pre-trained

Architecture

Decoder-only

Attention

Causal (left→right)

Pre-training

Next token prediction

Best for

Text generation, Chat

Decoder

T5

(2019, Google)

Text-to-Text Transfer

Architecture

Encoder-Decoder

Attention

Enc: bi, Dec: causal

Pre-training

Span corruption

Best for

Translation, Summary

Enc

→

Dec

Modern trend: Decoder-only (GPT-style) dominates for generation; Encoder-only (BERT) for understanding tasks

Training Transformers: key considerations

Training Setup

Optimizer: AdamW

$\beta_1=0.9$, $\beta_2=0.98$, weight decay=0.01

Learning Rate Schedule:

Warmup + Linear/Cosine decay

Regularization:

Dropout (0.1)

Model Size Comparison

Model	Params	Layers	d_model	Heads	Training Data
BERT-base	110M	12	768	12	16GB
GPT-2	1.5B	48	1600	25	40GB
GPT-3	175B	96	12288	96	570GB
LLaMA 2	70B	80	8192	64	2T tokens
GPT-4	~1.8T*	?	?	?	~13T tokens*

* Estimated/rumored

Summary: transformer architecture

1

Positional Encoding

Sinusoidal functions add position info to embeddings

2

Encoder Block

Self-Attention + FFN + Add&Norm (bidirectional)

3

Decoder Block

Masked Self-Attn + Cross-Attn + FFN (causal)

4

Residual + LayerNorm

Enable deep networks with stable gradients

5

BERT/GPT/T5

Encoder-only / Decoder-only / Encoder-Decoder variants

Formulas

Positional Encoding:

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

FFN:

$$FFN(x) = \text{ReLU}(xw_1 + b_1)w_2 + b_2$$

Add & Norm:

$$\text{LayerNorm}(x + \text{Sublayer}(x))$$

Masked Attention:

$$M[i, j] = 0 \text{ if } j \leq i \text{ else } -\infty$$

Chatbot development

From rule-based to LLM-powered Conversational AI

Chatbot Types & Architecture

NLU Pipeline: Intent & Slot Filling

Dialogue State Tracking

LLM-based Chatbots & RAG

Implementation with HuggingFace

What is a Chatbot?

A chatbot is a software application that simulates human conversation through text or voice interactions

Core Components of a Chatbot System

NLU

Natural Language Understanding

Parse user input → intent + entities

DM

Dialogue Management

Track state, decide next action

NLG

Natural Language Generation

Generate human-like responses

KB

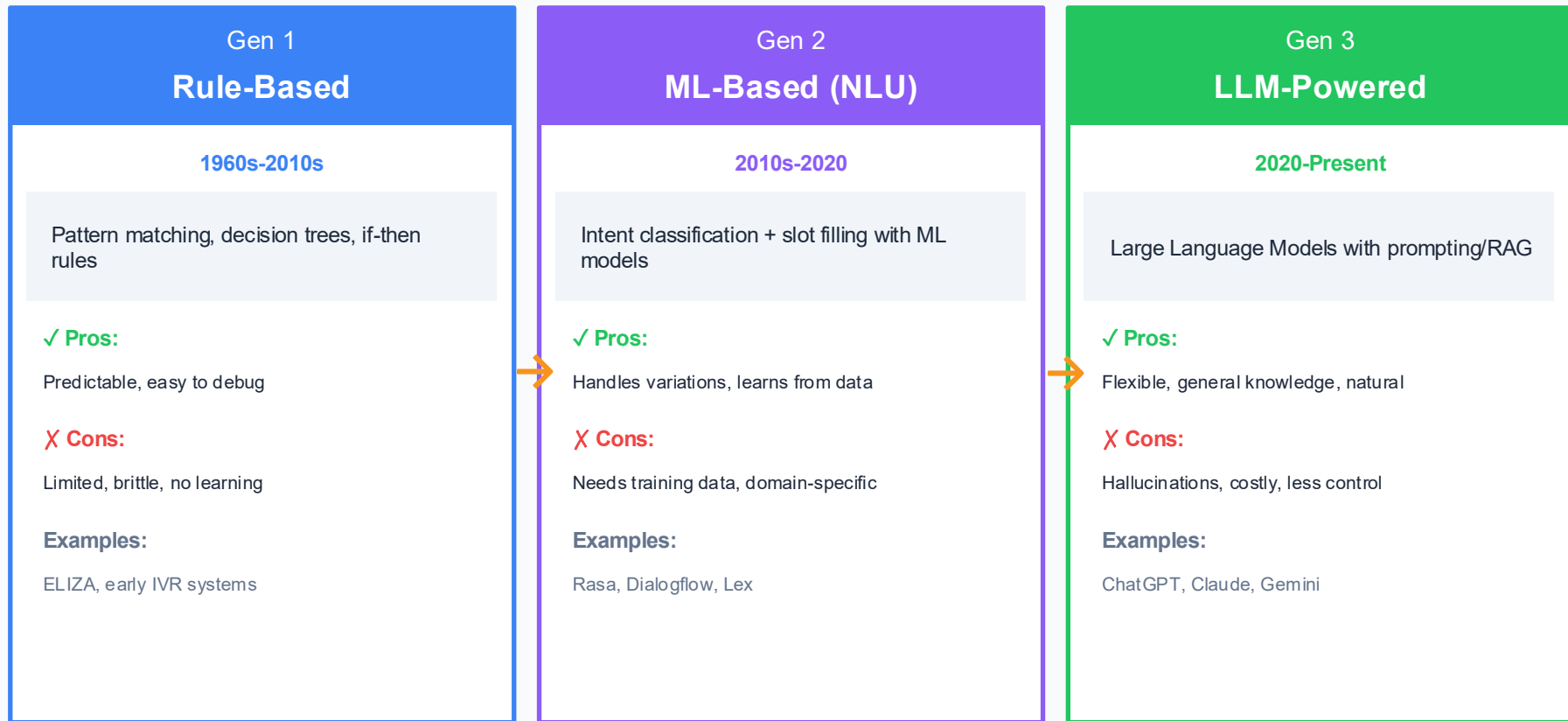
Knowledge Base

Store facts, FAQs, business logic

Common Use Cases

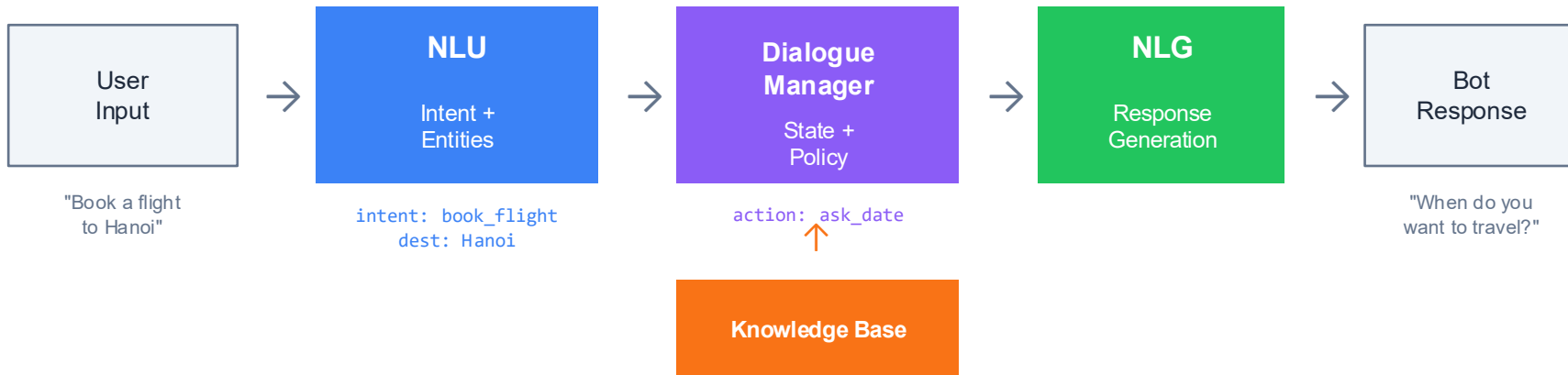
- Customer Support
- E-commerce
- Healthcare
- Banking
- Education
- Entertainment

Types of Chatbots: Evolution



Traditional Chatbot architecture (pipeline)

Task-Oriented Chatbot Pipeline



Key Concepts in Pipeline Architecture

Intent: What the user wants (e.g., book_flight, cancel_order)

Dialogue State: Current conversation context and filled slots

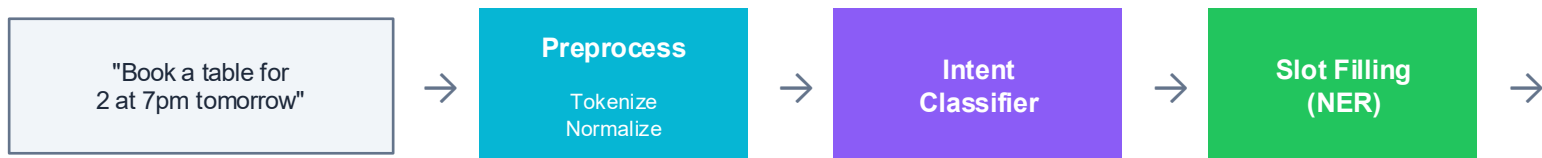
Entity/Slot: Key information (e.g., destination=Hanoi, date=tomorrow)

Policy: Rules/model deciding what action to take next

NLU Pipeline: From text to structured data

NLU transforms unstructured user text into structured representation that machines can process

NLU Processing Pipeline



Structured Output:

```
{
  intent: "book_table",
  slots: { num_people: "2", time: "7pm", date: "tomorrow" }
}
```

Intent Classification

Multi-class classification: Map input to one of predefined intents (book_table, cancel, etc.)

Slot Filling (NER)

Sequence labeling: Extract entities and their types (date, time, location, quantity, etc.)

Intent classification: models & methods

Intent Classification = Text Classification → Map user utterance to one of N predefined intent classes

Classification Methods Comparison

Traditional ML

Models:

SVM, Naive Bayes, RF

Features:

TF-IDF, n-grams, BoW

✓ Fast, interpretable

✗ Need feature engineering

Deep Learning

Models:

CNN, LSTM, BiLSTM

Features:

Word embeddings

✓ Learn features automatically

✗ Need more data

Transformers

Models:

BERT, RoBERTa, DistilBERT

Features:

Contextual embeddings

✓ SOTA accuracy, transfer learning

✗ Compute intensive

Modern Approach: BERT-based Intent Classification

[CLS] text



BERT



[CLS]
embed



Linear



Softmax



P(intent)

Fine-tune BERT on your intent dataset — typically 90%+ accuracy with few hundred examples!

Slot Filling: Named Entity Recognition

Slot Filling = Sequence Labeling → Assign a label to each token in the input sequence

BIO Tagging Scheme Example

Tokens:	Book	a	flight	to	Ha	Noi	tomorrow	at	3pm
Labels:	O	O	O	O	B-LOC	I-LOC	B-DATE	O	B-TIME

B = Begin, I = Inside, O = Outside entity

Slot Filling Models

BiLSTM-CRF

Bidirectional LSTM + Conditional Random Field for sequence constraints

BERT + Linear

BERT encoder + linear layer per token, fine-tuned end-to-end

Joint Model

Single model for intent + slots sharing encoder (multi-task learning)

Dialogue State Tracking (DST)

DST maintains a structured representation of the conversation: what slots have been filled, what's still needed

Example Conversation

User: I want to book a restaurant

→ intent: book_restaurant

Bot: What cuisine do you prefer?

User: Vietnamese food please

→ cuisine: vietnamese

Bot: For how many people?

User: 4 people, tomorrow night

→ num_people: 4, date: tomorrow, time: night

Current Dialogue State

```
{
  intent: "book_restaurant",
  slots: {
    cuisine: "vietnamese",
    num_people: 4,
    date: "tomorrow",
    time: "night",
    location: null // unfilled
  },
  turn_count: 3
}
```

Next Action: location is null → Ask "Where would you like to dine?" OR use default location

LLM-based Chatbots: the new paradigm

Shift: From pipeline components to single powerful model that handles NLU + DM + NLG together!

Traditional Pipeline

User Input → NLU → DM → NLG → Response

- Separate models for each component
- Need training data for each task
- Errors propagate through pipeline
- Limited to predefined intents/slots

LLM-Based Approach

User Input → LLM (+ context) → Response

- Single model handles everything
- Few-shot or zero-shot learning
- Flexible, handles new scenarios
- Natural, human-like responses



Key Technologies for LLM Chatbots

RAG

Retrieval-Augmented Generation

Fine-tuning

Adapt LLM to your domain

Prompting

In-context learning

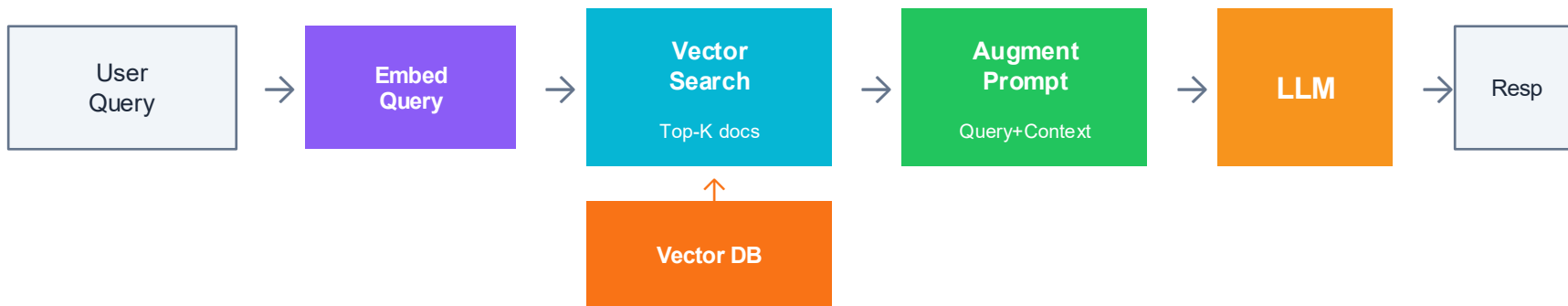
Guardrails

Safety & constraints

RAG: Retrieval-Augmented Generation

RAG = Retrieve relevant documents + Augment prompt with context + Generate response with LLM

RAG Pipeline Architecture



RAG Benefits

- Up-to-date knowledge
- Reduced hallucinations
- Domain-specific answers

Popular Tools

- Vector DBs: Pinecone, Chroma, Weaviate
- Frameworks: LangChain, LlamaIndex

Fine-tuning vs Prompting: When to Use What?

Fine-tuning

What:

Train model weights on your data

When to use:

- Specific domain/style needed
- Have labeled training data (1k+)
- Need consistent behavior

Pros:

Better performance on specific tasks

Cons:

Costly, needs data, may overfit

Prompting (In-Context Learning)

What:

Guide model via instructions/examples

When to use:

- Quick prototyping
- Limited/no training data
- Need flexibility

Pros:

Fast iteration, no training needed

Cons:

Limited by context window, variable

Decision Guide

Start with prompting → If not enough, try RAG → If still not enough, fine-tune → For best results, combine all!

Prompt engineering for Chatbots

System Prompt Structure

Role:

You are a helpful customer support agent for TechCorp...

Instructions:

Answer questions about products. Be polite. Ask clarifying questions if needed...

Constraints:

Do not discuss competitors. Do not make promises about refunds...

Format:

Keep responses under 100 words. Use bullet points for lists...

Examples:

User: How do I reset? Assistant: To reset your device, go to Settings > Reset...

Best Practices

- Be specific and clear
- Use delimiters (###, """)
- Give examples (few-shot)
- Specify output format
- Test edge cases
- Iterate and refine

Advanced Techniques

Chain-of-Thought: Step-by-step reasoning

Self-Consistency: Multiple paths, vote

ReAct: Reason + Act iteratively

Reflection: Self-critique & improve

Chatbot evaluation metrics

Task-Specific Metrics

Intent Classification

Accuracy, F1-score, Precision, Recall

Slot Filling (NER)

Entity-level F1, Span-level accuracy

Dialogue Success

Task completion rate, # turns to complete

Response Quality Metrics

BLEU:

N-gram overlap with reference (translation)

ROUGE:

Recall-oriented for summarization

BERTScore:

Semantic similarity using BERT embeddings

Perplexity:

How well model predicts responses

Human Evaluation (Most Important!)

Fluency

Is the response grammatically correct and natural? [1-5]

Relevance

Does it address the user's question/request? [1-5]

Helpfulness

Did it actually help the user achieve their goal? [1-5]

Safety

Is the response appropriate and harmless? [Yes/No]

Common pitfalls & solutions

❌ Hallucinations

LLM generates plausible but false information

✓ Use RAG, add fact-checking, constrain outputs

❌ Context Loss

Bot forgets earlier conversation turns

✓ Include conversation history in prompt, use memory

❌ Off-topic Responses

Bot responds to irrelevant or harmful requests

✓ Add guardrails, intent filtering, safety checks

❌ Inconsistent Persona

Bot's personality/knowledge varies across turns

✓ Strong system prompt, fine-tuning, testing

❌ Latency Issues

Slow response times frustrate users

✓ Use smaller models, caching, streaming responses

❌ Handling Errors

Bot crashes or gives unhelpful error messages

✓ Graceful fallbacks, human handoff, logging

Summary: Chatbot Development

1

Chatbot Types

Rule-based → ML/NLU → LLM-powered evolution

2

NLU Pipeline

Intent classification + Slot filling + Dialogue state

3

LLM Chatbots

Single model for NLU+DM+NLG, more flexible

4

RAG

Retrieve context + Augment prompt + Generate

5

Prompt Engineering

Role, instructions, constraints, format, examples

Tools & Frameworks

Models:

BERT, GPT, LLaMA, Mistral

Libraries:

HuggingFace, LangChain

Platforms:

Rasa, Dialogflow, Amazon Lex

Vector DBs:

Pinecone, Chroma, Weaviate

Evaluation

Measuring Success

Automatic Evaluation Metrics (BLEU, ROUGE, BERTScore)

Human Evaluation Frameworks

A/B Testing & Online Evaluation

Standard Benchmarks & Datasets

Hands-on Implementation Lab

Why evaluation matters

"You can't improve what you don't measure" — Evaluation guides development, deployment, and iteration

Automatic Metrics

What:

Computed automatically from outputs

Examples:

BLEU, ROUGE, F1, BERTScore

Pros:

Fast, scalable, reproducible

Human Evaluation

What:

Human judges rate quality

Examples:

Likert scales, A/B preference

Pros:

Captures nuance, real quality

Online Evaluation

What:

Real user behavior metrics

Examples:

Task success, engagement, CTR

Pros:

Real-world performance

Evaluation Pipeline: Offline (Auto + Human) → Online A/B Test → Production Monitoring

Best practice: Use automatic metrics for fast iteration, human eval for quality gates, online metrics for deployment decisions

Automatic Evaluation Metrics

BLEU (Bilingual Evaluation Understudy)

$$\text{BLEU} = \text{BP} \times \exp(\sum w_n \log p_n)$$

p_n = n-gram precision

BP = brevity penalty (penalizes short outputs)

Typically BLEU-4 uses $n = 1, 2, 3, 4$

ROUGE (Recall-Oriented Understudy)

$$\text{ROUGE-N} = |\text{matched n-grams}| / |\text{ref n-grams}|$$

ROUGE-1: unigram recall

ROUGE-2: bigram recall

ROUGE-L: longest common subsequence

F1 Score (Intent & Slot Evaluation)

$$\text{F1} = 2 \times (P \times R) / (P + R)$$

P = Precision = $TP / (TP + FP)$

R = Recall = $TP / (TP + FN)$

Use macro/micro F1 for multi-class

BERTScore (Semantic Similarity)

$$\text{BERTScore} = \text{cosine_sim}(\text{BERT}(\text{cand}), \text{BERT}(\text{ref}))$$

Uses BERT embeddings for semantic matching

Captures meaning even with different wording

More robust than n-gram metrics

Use: BLEU for translation | ROUGE for summarization | F1 for classification/NER | BERTScore for open-ended generation

Human Evaluation Framework

Human evaluation is the gold standard — automatic metrics don't capture all aspects of quality

Common Evaluation Dimensions

Fluency	Is the response grammatically correct and natural?	[1-5]
Relevance	Does it address the user's actual question?	[1-5]
Correctness	Is the information factually accurate?	[1-5]
Helpfulness	Did it help achieve the user's goal?	[1-5]
Safety	Is it appropriate and harmless?	[Yes/No]

Evaluation Methods

Likert Scale Rating

Rate each response 1-5

Pairwise Comparison

"Which response is better?"

Best-Worst Scaling

Pick best & worst from N options

Side-by-Side (SxS)

Compare A vs B directly

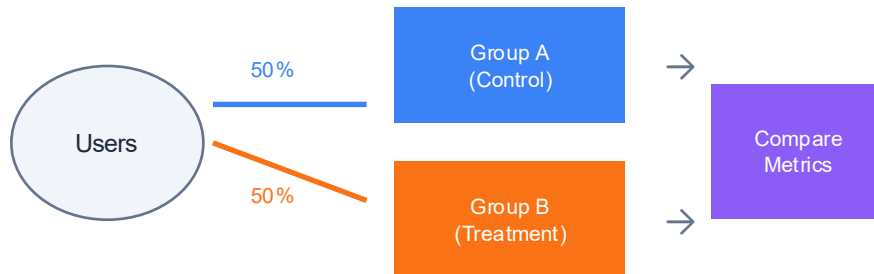
Best Practices

- Use 3+ annotators per item
- Calculate inter-annotator agreement ($\text{Kappa} \geq 0.6$)
- Randomize order
- Blind to system identity
- Clear guidelines + examples

A/B Testing & Online Evaluation

A/B Testing: Compare two versions with real users to make data-driven decisions

A/B Test Setup



Key Metrics to Track:

- Task completion rate
- User satisfaction (thumbs up/down)
- Session length, # of turns
- Fallback/error rate

Statistical Considerations

Sample Size

Need enough users for significance
(typically 1000+ per variant)

Statistical Significance

$p\text{-value} < 0.05$ (95% confidence)

Effect Size

How big is the improvement?
Cohen's d, relative lift %

Decision Framework

B significantly better → Deploy B | No significant difference → Consider cost/complexity | B worse → Keep A, investigate why

Standard Benchmarks & Datasets

NLU Benchmarks

GLUE/SuperGLUE General language understanding

SNIPS Intent classification + slot filling

ATIS Airline travel domain NLU

MultiWOZ Multi-domain dialogue state

CoNLL-2003 Named Entity Recognition

Generation Benchmarks

PersonaChat Persona-based conversation

DailyDialog Daily life conversations

Wizard of Wikipedia Knowledge-grounded dialogue

ConvAI2 Open-domain chatbot challenge

MT-Bench Multi-turn LLM evaluation

LLM Leaderboards & Evaluation Suites

LMSYS Chatbot Arena Human preference voting, ELO ranking

HELM Stanford holistic LLM evaluation

Open LLM Leaderboard HuggingFace benchmark suite

AlpacaEval GPT-4 based automatic evaluation

Summary: Evaluation & Implementation

1

Automatic Metrics

BLEU, ROUGE, F1, BERTScore — fast & scalable

2

Human Evaluation

Fluency, relevance, helpfulness — gold standard

3

A/B Testing

Real users, statistical significance, data-driven decisions

4

Benchmarks

SNIPS, MultiWOZ, MT-Bench — standardized comparison

Key Formulas

BLEU:

$$BP \times \exp(\sum w_n \log p_n)$$

F1 Score:

$$2 \times (P \times R) / (P + R)$$

BERTScore:

$$\text{cosine}(\text{BERT}(c), \text{BERT}(r))$$

Kappa (Agreement):

$$(p_o - p_e) / (1 - p_e)$$

Assignment & Summary

Build Your Own Transformer-based Chatbot

Assignment: Build a transformer chatbot

Final Project: End-to-End Chatbot Development

Apply Attention, Transformers, and NLU concepts to build a working chatbot system

Learning Objectives

- Understand Transformer architecture in practice
- Implement intent classification with BERT
- Build slot filling / NER system
- Design dialogue management logic
- Evaluate using appropriate metrics
- Document and present your work

Team Formation

- Individual or teams of 2-3 students
- Larger teams require proportionally larger scope
- Clear contribution statement required

Session summary

Part 1

Introduction & Attention

Seq2Seq bottleneck, Attention mechanism basics

Part 2

Self-Attention & Multi-Head

Q,K,V framework, Scaled dot-product, MHA

Part 3

Transformer Architecture

Positional encoding, Encoder, Decoder, BERT/GPT/T5

Part 4

Chatbot Development

NLU pipeline, Intent+Slot, RAG, Prompt engineering

Part 5

Evaluation & Implementation

BLEU, ROUGE, F1, Human eval, A/B testing, Lab

Part 6

Assignment & Summary

Project requirements

Key formulas review

Attention Mechanisms

Scaled Dot-Product:

$$\text{Attn}(Q, K, V) = \text{softmax}(QK^T / \sqrt{d_k}) \cdot V$$

Multi-Head Attention:

$$\text{MHA} = \text{Concat}(\text{head}_1, \dots, \text{head}_n) \cdot W^O$$

Linear Projections:

$$Q = XW^Q, \quad K = XW^K, \quad V = XW^V$$

Positional Encoding:

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

Transformer Components

Feed-Forward Network:

$$\text{FFN}(x) = \text{ReLU}(xW_1 + b_1)W_2 + b_2$$

Layer Normalization:

$$\text{LN}(x) = \gamma \cdot (x - \mu) / \sigma + \beta$$

Residual Connection:

$$\text{output} = \text{LayerNorm}(x + \text{Sublayer}(x))$$

Masked Attention:

$$M[i, j] = 0 \text{ if } j \leq i, \text{ else } -\infty$$

Evaluation Metrics

BLEU: $BP \times \exp(\sum w_n \log p_n)$

F1 Score: $2 \times (P \times R) / (P + R)$

ROUGE-N: $| \text{matched n-grams} | / | \text{ref n-grams} |$

BERTScore: $\text{cosine}(\text{BERT}(\text{cand}), \text{BERT}(\text{ref}))$