Lecture 13:

Transformer Architecture

Ho-min Park

homin.park@ghent.ac.kr

powersimmani@gmail.com

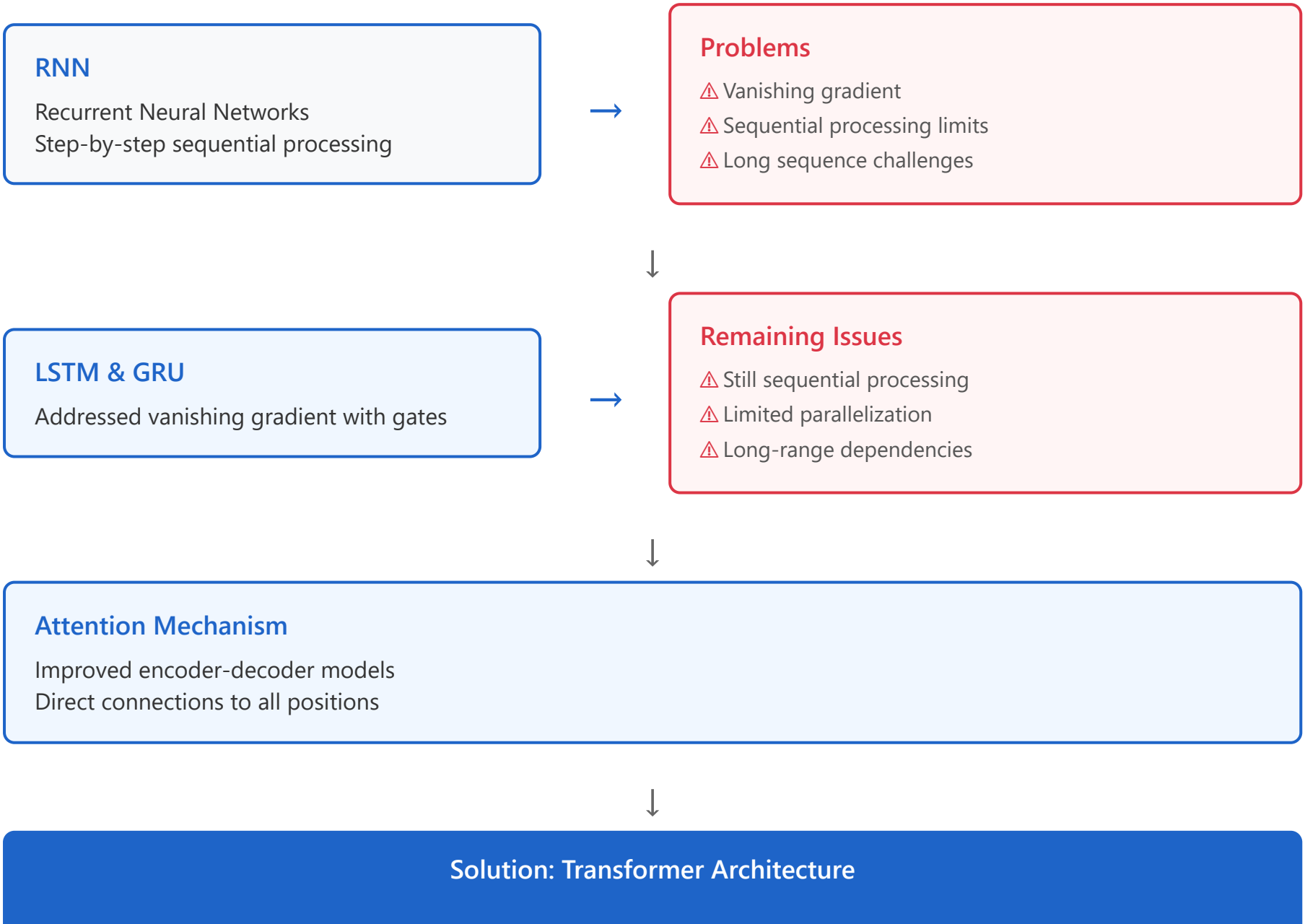
Lecture Contents

Part 7: Applications and Next Steps

Part 1/7:

Introduction & Motivation

1. Review of Last Lesson
2. The Emergence and Impact of Transformers


RNN
Recurrent Neural Networks
Step-by-step sequential processing
Problems
⚠ Vanishing gradient
⚠ Sequential processing limits
⚠ Long sequence challenges
LSTM & GRU
Addressed vanishing gradient with gates
Remaining Issues
⚠ Still sequential processing
⚠ Limited parallelization
⚠ Long-range dependencies
Attention Mechanism
Improved encoder-decoder models
Direct connections to all positions
Solution: Transformer Architecture

Parallel processing + Effective long-range dependencies

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

Revolutionary Architecture for Deep Learning

Core Innovation

⚡ **Eliminated recurrence entirely**
Enabled full parallelization

📈 **Massive dataset training**
Efficient at scale

🎯 **State-of-the-art performance**
Across multiple benchmarks

🏗️ Foundation Models

GPT, BERT, and modern LLMs

💬 NLP Revolution

Translation • Summarization
Question Answering • Generation

🌐 Beyond NLP

Vision Transformers (ViT)
Audio Processing • Multimodal AI

✨ Impact

New era of AI capabilities
Industry-wide transformation

Transformer Architecture

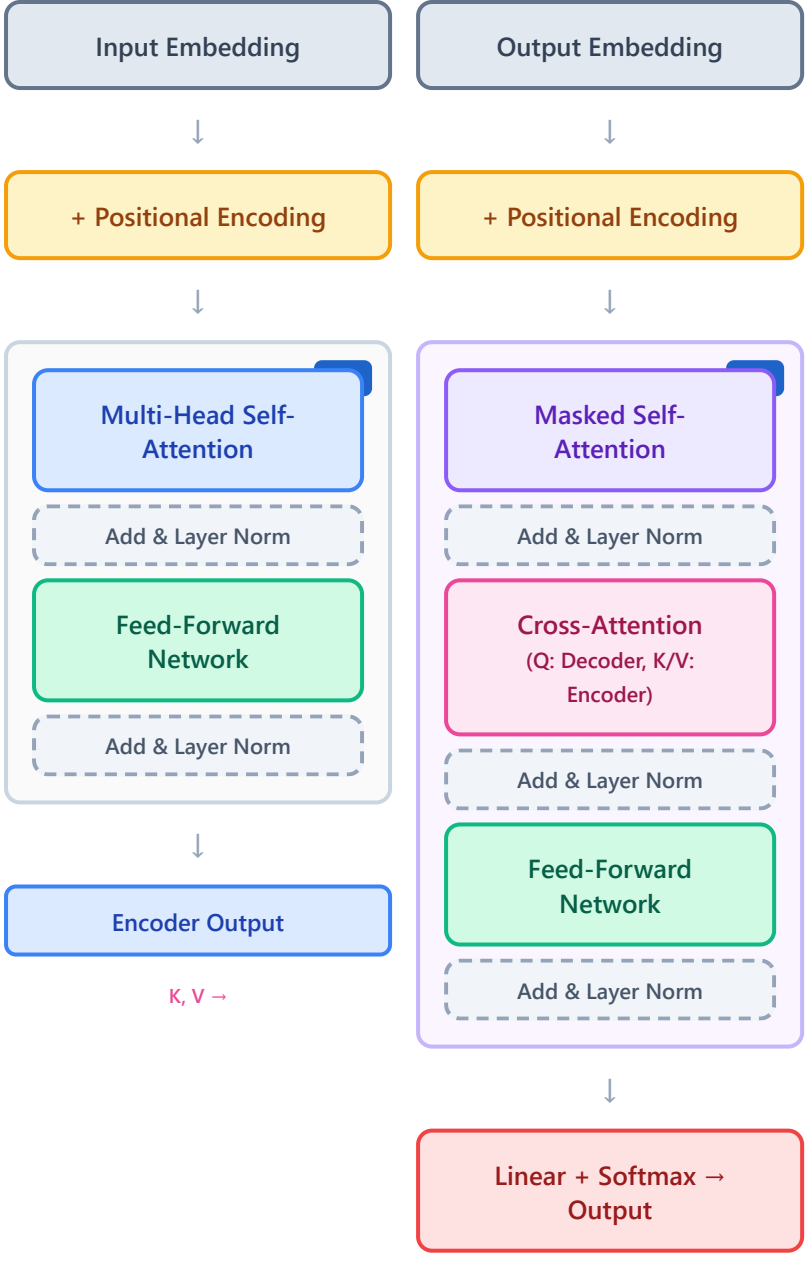
Key Components & Structure

Encoder

Decoder

🔍 Self-Attention

🔀 Multi-Head



Each position attends to all positions, capturing contextual relationships

Parallel attention heads learn diverse representations

Positional Encoding

Injects sequence order using sinusoidal functions

Feed-Forward

Position-wise MLP with two linear layers + ReLU

Add & Norm

Residual connections + Layer Normalization for stable training

Cross-Attention

Decoder queries (Q) attend to Encoder's keys (K) and values (V)

Part 2/7:

Self-Attention Mechanism

3. RNN Attention vs. Self-Attention
4. Query, Key, and Value Concepts
5. Self-Attention Computation Process (1/2)
6. Self-Attention Computation Process (2/2)
7. Self-Attention Matrix Operations

RNN Attention vs. Self-Attention

Aspect	RNN Attention	Self-Attention
Source	Query from decoder, Keys/Values from encoder	All from the same sequence
Processing	Sequential processing	Parallel processing
Relationships	Limited to current step	Captures relationships between all positions
Complexity	$O(n)$ per step	$O(n^2)$ total

Key Advantage

Self-attention enables parallelization and better long-range dependency modeling

Query, Key, and Value Concepts

Query (Q)

What information am I looking for?

Key (K)

What information do I contain?

Value (V)

The actual information I store

Database Analogy

Query matches **Keys** to retrieve **Values**

Linear Projections

1. Each token generates Q, K, V
2. Through learned transformations:

$$Q = XW_Q$$

$$K = XW_K$$

$$V = XW_V$$

3. Projection matrices **learned during training**

> **X** = Input token embeddings
> $\mathbf{W_Q}$, $\mathbf{W_K}$, $\mathbf{W_V}$ = Trainable weight matrices

Numerical Example: Computing Q, K, V

Input Token Embeddings (X)

5 tokens × 3 dimensions

```
X = [
   [1.0, 0.5, 0.2],   # Token 1
   [0.3, 1.2, 0.8],   # Token 2
   [0.7, 0.4, 1.1],   # Token 3
   [1.5, 0.9, 0.3],   # Token 4
   [0.6, 1.3, 0.7]    # Token 5
]
```

W_Q (Query)

```
[[ 1.0, 0.0, 0.5],
 [ 0.5, 1.0, 0.0],
 [ 0.0, 0.5, 1.0]]
```

W_K (Key)

```
[[ 0.8, 0.2, 0.3],
 [ 0.3, 0.9, 0.1],
 [ 0.2, 0.1, 0.8]]
```

W_V (Value)

```
[[ 1.0, 0.3, 0.2],
 [ 0.2, 1.0, 0.4],
 [ 0.1, 0.3, 1.0]]
```

Matrix Multiplication

$Q = XW_Q$

```
[[1.25, 0.60, 0.70],
 [0.90, 1.60, 0.95],
 [0.90, 0.95, 1.45],
 [1.95, 1.05, 1.05],
 [1.25, 1.65, 1.00]]
```

$K = XW_K$

```
[[0.99, 0.67, 0.51],
 [0.76, 1.22, 0.85],
 [0.90, 0.61, 1.13],
 [1.53, 1.14, 0.78],
 [1.01, 1.36, 0.87]]
```

$V = XW_V$

```
[[1.12, 0.86, 0.60],
 [0.62, 1.53, 1.34],
 [0.89, 0.94, 1.40],
 [1.71, 1.44, 0.96],
 [0.93, 1.69, 1.34]]
```

Key Insight

Each of the 5 tokens now has its own:

- **Query vector** (what it's looking for)
- **Key vector** (what it contains)
- **Value vector** (its actual information)

These will be used in the attention mechanism to determine which tokens should attend to which!

Positional Encoding Methods

Sinusoidal
Original Transformer

```
PE(pos, 2i) = sin(pos / 10000^(2i/d))
PE(pos, 2i+1) = cos(pos / 10000^(2i/d))
```

✓ **Any length** sequences

Learned
BERT Approach

```
Trainable embedding matrix:
PE ∈ ℝ^(max_len × d_model)
```

✓ **Task-optimized**

Relative
T5, Transformer-XL

```
Relative distances:
distance = pos_i - pos_j
```

✓ **Best relationships**

📊 Attention Calculation Example

Attention Scores = QK^T

	T1	T2	T3	T4	T5
T1	1.29	1.46	1.27	1.44	1.41
T2	1.46	2.17	1.89	1.57	1.80
T3	1.27	1.89	2.38	1.79	2.05
T4	1.44	1.57	1.79	1.86	1.83
T5	1.41	1.80	2.05	1.83	1.94

Scaled Scores = $QK^T / \sqrt{d_k}$

	T1	T2	T3	T4	T5
T1	0.74	0.84	0.73	0.83	0.81
T2	0.84	1.25	1.09	0.91	1.04
T3	0.73	1.09	1.37	1.03	1.18
T4	0.83	0.91	1.03	1.07	1.06
T5	0.81	1.04	1.18	1.06	1.12

🎯 Attention Weights after Softmax (First Row)

Token 1	Token 2	Token 3	Token 4	Token 5
0.190	0.210 ⬆	0.188 ⬇	0.208	0.204

Token 1 attends **most to Token 2 (0.210)** and **least to Token 3 (0.188)**

Self-Attention Computation Process (2/2)

From Attention Weights to Context-Aware Representations

5

Apply Attention Weights to Values

Multiply attention weights with value vectors

```
Weighted Values = Attention × V
```

↓

6

Sum Weighted Values

Aggregate weighted values for each position

```
Output = Σ (Attention × V)
```

↓

🎯 Output

Context-Aware Representation for Each Token

Each output embedding contains information from entire sequence

⚡ **Parallel**
computation for all positions simultaneously

🔄 **Differentiable**
end-to-end for backpropagation

🌐 **Global context**
in every output representation

💡 Numerical Example (Continued)

📋 **Recap from Part 1:**

We computed attention weights using softmax on scaled scores.
Now we'll use these weights to create context-aware representations.

Attention Weights Matrix (5×5) - After Softmax:

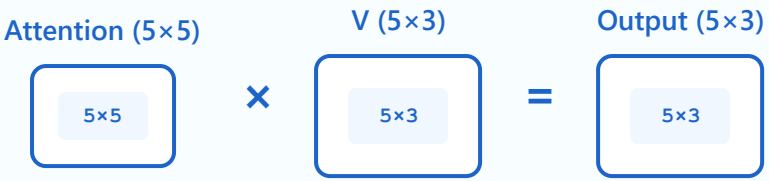
0.182	0.204	0.207	0.192	0.198
0.170	0.279	0.222	0.173	0.186
0.162	0.206	0.272	0.184	0.208
0.188	0.213	0.224	0.219	0.215
0.178	0.212	0.239	0.204	0.244

Each row sums to 1.0 and represents how much each token attends to others

Value Matrix V (5×3) - Same as X in our example:

1.0	0.5	0.2
0.8	1.2	0.3
0.6	0.9	1.1
1.1	0.4	0.7
0.9	0.7	0.8

⑤ Weighted Values = Attention × V (Matrix Multiplication):



⑥ Final Output Matrix (5×3) - Context-Aware Embeddings:

0.87	0.74	0.59
0.83	0.88	0.58
0.83	0.78	0.68
0.88	0.73	0.63
0.84	0.78	0.70

Each row is a new embedding that incorporates information from all tokens

🎯 Token 1's Output Example

Original embedding:

1.0 0.5 0.2

Context-aware embedding:

0.87 0.74 0.59

✓ *The output is a weighted combination of all tokens' values*
✓ *Token 1 now "knows about" the entire sequence context*
✓ *Different attention patterns → Different contextual representations*

💭 How Token 1's Output was Computed:

Output[1] = 0.182×[1.0, 0.5, 0.2] + 0.204×[0.8, 1.2, 0.3] + 0.207×[0.6, 0.9, 1.1] + 0.192×[1.1, 0.4, 0.7] + 0.198×[0.9, 0.7, 0.8]
= [0.87, 0.74, 0.59]

This is a weighted average where weights come from attention scores!

Self-Attention Matrix Operations

Input	→	`(batch_size, seq_len, d_model)`
Q, K, V	→	`(batch_size, seq_len, d_k)`
Scores	→	`(batch_size, seq_len, seq_len)`
Output	→	`(batch_size, seq_len, d_k)`

GPU Parallelization

Matrix multiplication enables **efficient GPU computation**

Memory Requirement

$O(n^2)$ for sequence length **n**

Efficiency Trade-off

Speed vs **Memory**

Input/Output Attention Scores (seq_len × seq_len) Final Output

Computation Example

`seq_len = 5` `d_model = 3` `d_k = 3` `batch_size = 1`

1 Input Embeddings (X)

X: Input sequence with 5 tokens

```
[[0.5, 0.8, 0.3], ← Token 1
[0.2, 0.6, 0.9], ← Token 2
[0.7, 0.4, 0.1], ← Token 3
[0.3, 0.9, 0.5], ← Token 4
[0.6, 0.2, 0.8]] ← Token 5
```

Shape: (5, 3) = (seq_len, d_model)

2 Linear Projections: Q = XW_Q, K = XW_K, V = XW_V

Q (Query Matrix)

```
[[0.6, 0.4, 0.5],
[0.3, 0.7, 0.2],
[0.5, 0.3, 0.6],
[0.4, 0.8, 0.3],
[0.7, 0.2, 0.4]]
```

Shape: (5, 3) = (seq_len, d_k)

K (Key Matrix)

```
[[0.4, 0.6, 0.3],
[0.5, 0.4, 0.7],
[0.3, 0.5, 0.4],
[0.6, 0.3, 0.5],
[0.2, 0.7, 0.6]]
```

Shape: (5, 3) = (seq_len, d_k)

V (Value Matrix)

```
[[0.7, 0.3, 0.5],
[0.4, 0.6, 0.2],
[0.6, 0.4, 0.7],
[0.5, 0.7, 0.3],
[0.3, 0.5, 0.8]]
```

Shape: (5, 3) = (seq_len, d_k)

3 Compute Attention Scores: QK^T / √d_k

$$\text{Scores} = Q \times K^T / \sqrt{d\_k} = Q \times K^T / \sqrt{3} \approx Q \times K^T / 1.732$$

QK^T: Raw attention scores (before scaling)

```
[[0.67, 0.71, 0.58, 0.69, 0.64], ← Token 1 attending to all tokens
[0.52, 0.49, 0.44, 0.51, 0.53], ← Token 2 attending to all tokens
[0.61, 0.67, 0.54, 0.63, 0.56], ← Token 3 attending to all tokens
[0.68, 0.73, 0.59, 0.69, 0.70], ← Token 4 attending to all tokens
[0.50, 0.58, 0.48, 0.55, 0.48]] ← Token 5 attending to all tokens
```

Shape: (5, 5) = (seq_len, seq_len) - Critical $O(n^2)$ memory!

⚠ **Key Point:** This 5×5 attention score matrix is where the $O(n^2)$ memory complexity comes from. For sequence length n=5, we need 25 values. For n=1000, we'd need 1,000,000 values!

4 Apply Softmax (row-wise normalization)

Attention Weights (after softmax)

```
[[0.189, 0.204, 0.176, 0.201, 0.190], ← Sum = 1.0
[0.203, 0.199, 0.192, 0.201, 0.205], ← Sum = 1.0
[0.194, 0.205, 0.188, 0.199, 0.194], ← Sum = 1.0
[0.197, 0.208, 0.185, 0.197, 0.203], ← Sum = 1.0
[0.196, 0.208, 0.189, 0.201, 0.196]] ← Sum = 1.0
```

Shape: (5, 5) - Each row sums to 1.0 (probability distribution)

5 Compute Weighted Sum: Attention_Weights × V

$$\text{Output} = \text{Softmax}(QK^T / \sqrt{d\_k}) \times V$$

Final Output (context-aware representations)

```
[[0.50, 0.50, 0.50], ← Updated Token 1
[0.50, 0.50, 0.50], ← Updated Token 2
[0.50, 0.50, 0.50], ← Updated Token 3
[0.50, 0.50, 0.50], ← Updated Token 4
[0.50, 0.50, 0.50]] ← Updated Token 5
```

Shape: (5, 3) = (seq_len, d_k) - Same as input!

✅ **Result:** Each token now has a context-aware representation that incorporates information from all other tokens through the attention mechanism.

Matrix Shape Summary

Input X: (5, 3) = (seq_len, d_model)

Q, K, V: (5, 3) each = (seq_len, d_k)

Scores QK^T: (5, 5) = (seq_len, seq_len) ← $O(n^2)$ bottleneck!

Output: (5, 3) = (seq_len, d_k)

Part 3/7:

Multi-Head Attention

8. Why is Multi-Head Necessary?
9. Multi-Head Attention Architecture
10. Multi-Head Operation Example
11. Multi-Head Attention Implementation Points

Why is Multi-Head Attention Necessary?

Single Head

- **Limited representation capacity**
- Single attention pattern only
- Cannot capture multiple relationship types simultaneously

Single Attention Head

Multi-Head

- Different heads learn different patterns
- Some heads capture **syntax**, others **semantics**
- Attend to different positions for different purposes
- Empirically improves performance significantly

Head 1	Head 2	Head 3	Head 4
Head 5	Head 6	Head 7	Head 8

Analogy: Similar to multiple CNN filters capturing different features

Expressiveness

Increases model power without excessive parameters

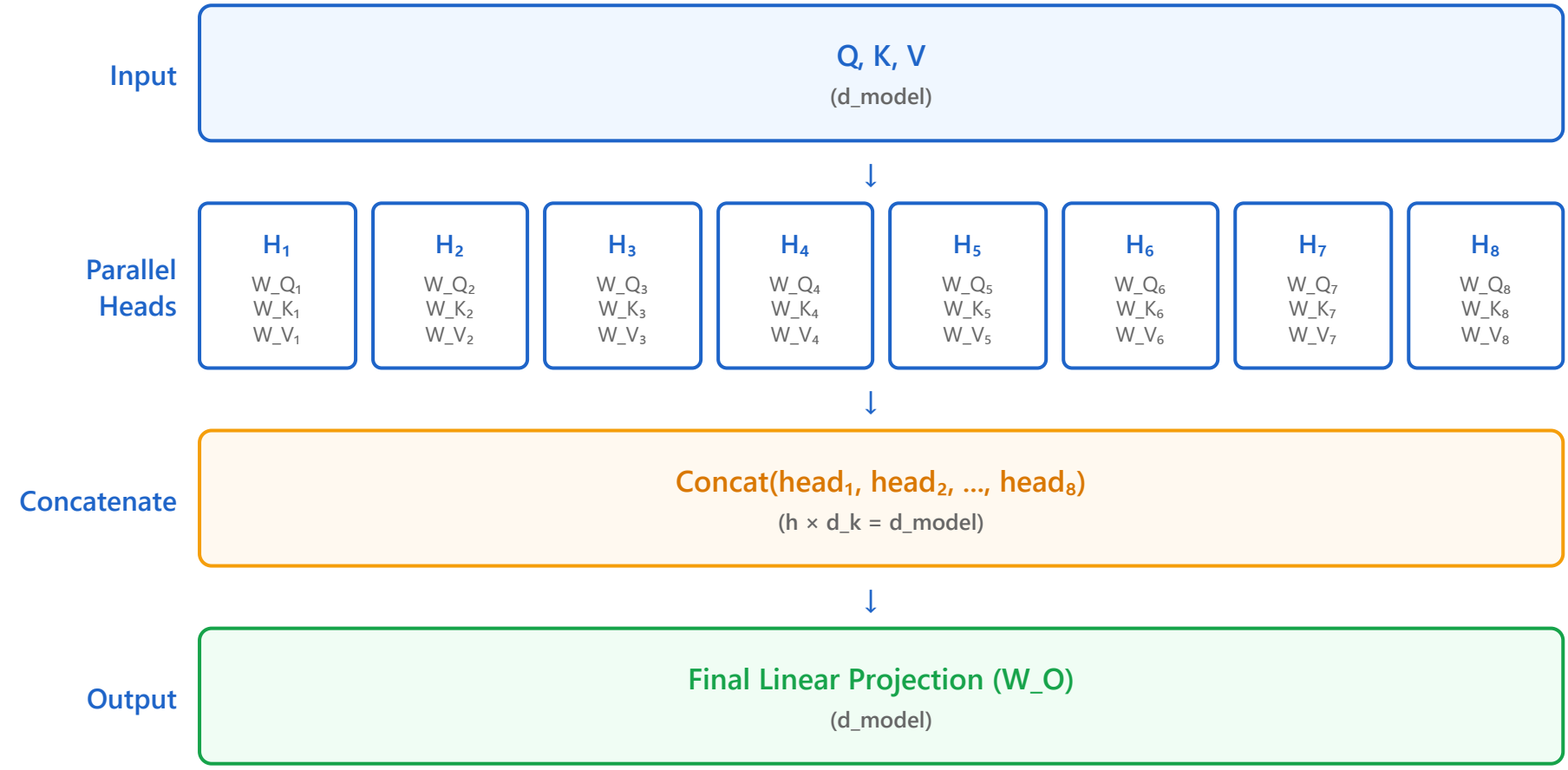
Diversity

Multiple perspectives on the same input

Performance

Empirically proven improvements

Multi-Head Attention Architecture



Configuration

Typically **h = 8** heads

Head dimension: **d_k = d_model / h**

Parameters

Each head: separate W_Q, W_K, W_V

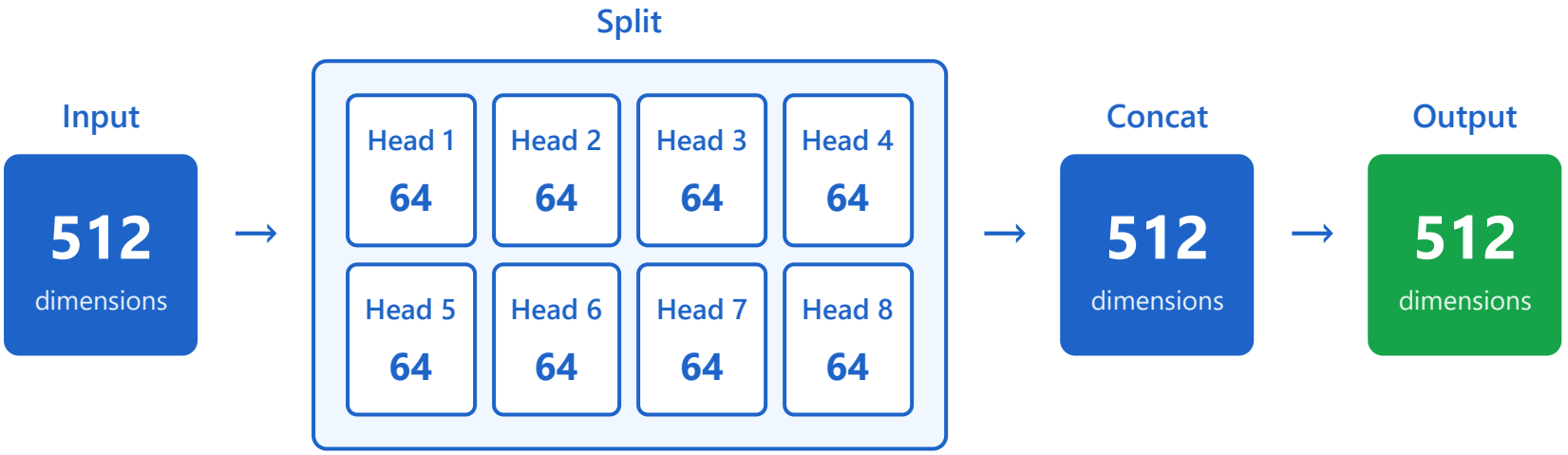
Total params ≈ single large head

Formula

$$\text{MultiHead}(Q,K,V) = \text{Concat}(\text{head}_1, \ldots, \text{head}_h)W_O$$

Multi-Head Operation Example

Configuration: **d_model = 512**, **h = 8** heads → Each head: **d_k = 64** dimensions



8 × 64 = 512 | Each head learns different attention patterns **independently**

🎯 Each head learns **different patterns** independently

⚡ Computational cost **distributed** across heads

🚀 **Parallelized** efficiently on modern hardware

Detailed Calculation Example

Setup: **d_model = 4**, **h = 2** heads, **sequence length = 8** → Each head: **d_k = 2** dimensions

Input Matrix X

Shape: (8, 4) - [sequence length × d_model]

```
token 1: [0.2, 0.5, 0.1, 0.8]
token 2: [0.3, 0.7, 0.4, 0.2]
token 3: [0.6, 0.1, 0.9, 0.5]
token 4: [0.4, 0.8, 0.3, 0.7]
token 5: [0.7, 0.2, 0.6, 0.4]
token 6: [0.5, 0.6, 0.2, 0.9]
token 7: [0.8, 0.3, 0.5, 0.1]
token 8: [0.1, 0.9, 0.7, 0.6]
```

Weight Matrices (per head)

W_Q - Query Weight

Shape: (4, 2)

W_K - Key Weight

Shape: (4, 2)

W_V - Value Weight

Shape: (4, 2)

Step-by-Step Calculation Process

Step 1: Split Input into 2 Heads

X_{head1} = X[:, 0:2] → Shape: (8, 2) - first 2 dimensions

X_{head2} = X[:, 2:4] → Shape: (8, 2) - last 2 dimensions

Step 2: Compute Q, K, V for Each Head

Head 1:

$Q_1 = X_{head1} \times W_{Q1}$ → (8, 2) × (2, 2) = (8, 2)

$K_1 = X_{head1} \times W_{K1} \rightarrow (8, 2) \times (2, 2) = \mathbf{(8, 2)}$

$V_1 = X_{head1} \times W_{V1} \rightarrow (8, 2) \times (2, 2) = \mathbf{(8, 2)}$

Step 3: Calculate Attention Scores

$Scores_1 = (Q_1 \times K_1^T) / \sqrt{d_k}$

$= (8, 2) \times (2, 8) / \sqrt{2} = \mathbf{(8, 8)}$

Step 4: Apply Softmax & Compute Output

$Attention_1 = softmax(Scores_1) \rightarrow (8, 8)$

$Output_1 = Attention_1 \times V_1 \rightarrow (8, 8) \times (8, 2) = \mathbf{(8, 2)}$

Step 5: Concatenate Head Outputs

$MultiHead = Concat(Output_1, Output_2)$

$= Concat[(8, 2), (8, 2)] = \mathbf{(8, 4)}$

Step 6: Final Linear Projection

$Final\ Output = MultiHead \times W_O$

$= (8, 4) \times (4, 4) = \mathbf{(8, 4)}$

Key Insight: Each head processes **2 dimensions** independently, learning different attention patterns. Final output maintains original **(8, 4)** shape.

Multi-Head Attention Implementation Points

Initialization & Configuration

Projection Matrices
Initialize with **appropriate scaling**

Head Dimensions
Use **same d_k** across all heads for simplicity

Regularization & Stability

Dropout
Apply after **attention weights** and **final output**

Layer Normalization
Typically after multi-head attention

Residual Connections
Help **gradient flow**

Optimization

Long Sequences
Consider **linear attention variants** for efficiency

✓ Efficient computation strategies

Best Practices

- Consistent head dimensions
- Proper normalization placement
- Efficient memory management

Key Trade-off

More heads increase model capacity but require **higher computational cost** — balance based on task requirements

Part 4/7:

Positional Encoding

12. The Need for Positional Information
13. Positional Encoding Methods
14. Positional Encoding Visualization

The Need for Positional Information

⚠ Core Problem

Self-attention is **permutation invariant**
Without position information, word order is ignored!

"cat ate mouse" = "mouse ate cat"

RNN Approach

- **Inherently encodes position** through sequential processing
- Position is implicit in the processing order
- No additional mechanism needed

Transformer Approach

- Parallel processing = **no inherent position**
- Needs **explicit positional information**
- Critical: Word order is crucial for meaning

Solution

Positional encodings must be added to input embeddings **before the first layer**

Positional Encoding Methods

Sinusoidal

Original Transformer

```
PE(pos, 2i) =
sin(pos / 10000^(2i/d_model))
```

```
PE(pos, 2i+1) =
cos(pos / 10000^(2i/d_model))
```

✓ Advantages

- 🎯 Works for **unseen sequence lengths**
- 📐 Deterministic pattern
- ♾️ Generalizes to any length

Learned

BERT Approach

```
Trainable embedding
matrix:

PE ∈ ℝ^(max_len × d_model)
```

✓ Advantages

- 🎯 **Better for fixed-length** tasks
- 📊 Task-specific optimization
- 🔧 Learned during training

Relative

T5, Transformer-XL

```
Encodes relative
distances between
positions:

distance = pos_i - pos_j
```

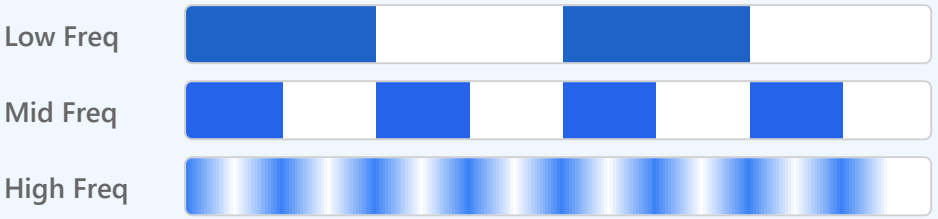
✓ Advantages

- 🎯 **Captures relationships** better
- 📏 Distance-based encoding
- 🌐 Position-invariant patterns

Sinusoidal	Learned	Relative
✓ Any length	✓ Task-optimized	✓ Best relationships

Positional Encoding Visualization

Frequency Patterns Across Dimensions



Unique Patterns

Each position has **unique encoding pattern**

Smooth Gradient

Allows model to learn **relative positions**

Multiple Frequencies

Different frequencies for different dimensions

Low Frequencies

Capture **global position**
Overall sequence location

High Frequencies

Capture **local position**
Fine-grained distinctions

Magnitude Balance

Magnitude **comparable** to embedding values

Element-wise addition to token embeddings | Preserves both semantic and positional information

Calculation Example (d_model=4, max_len=8)

Formula

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

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

Token Embeddings | Positional Encoding | Final Input

X (8×4)					PE (8×4)					X + PE (8×4)			
0.5	-0.3	0.8	-0.2	+	0.00	1.00	0.00	1.00	=	0.50	0.70	0.80	0.80
-0.1	0.7	0.2	0.4		0.84	0.54	0.01	1.00		0.74	1.24	0.21	1.40
0.9	-0.5	-0.3	0.6		0.91	-0.42	0.02	1.00		1.81	-0.92	-0.28	1.60
0.3	0.4	-0.7	0.1		0.14	-0.99	0.03	1.00		0.44	-0.59	-0.67	1.10
-0.6	0.2	0.5	-0.4		-0.76	-0.66	0.04	1.00		-1.36	-0.46	0.54	0.60
0.7	-0.8	0.1	0.3		-0.96	0.28	0.05	1.00		-0.26	-0.52	0.15	1.30
-0.2	0.6	-0.4	0.8		-0.28	0.96	0.06	1.00		-0.48	1.56	-0.34	1.80
0.4	-0.1	0.9	-0.5		0.66	0.75	0.07	0.99		1.06	0.65	0.97	0.49

Key Insight: Each position gets a unique sinusoidal pattern. Lower dimensions (0,1) use high frequency for fine-grained position, while higher dimensions (2,3) use low frequency for global position.

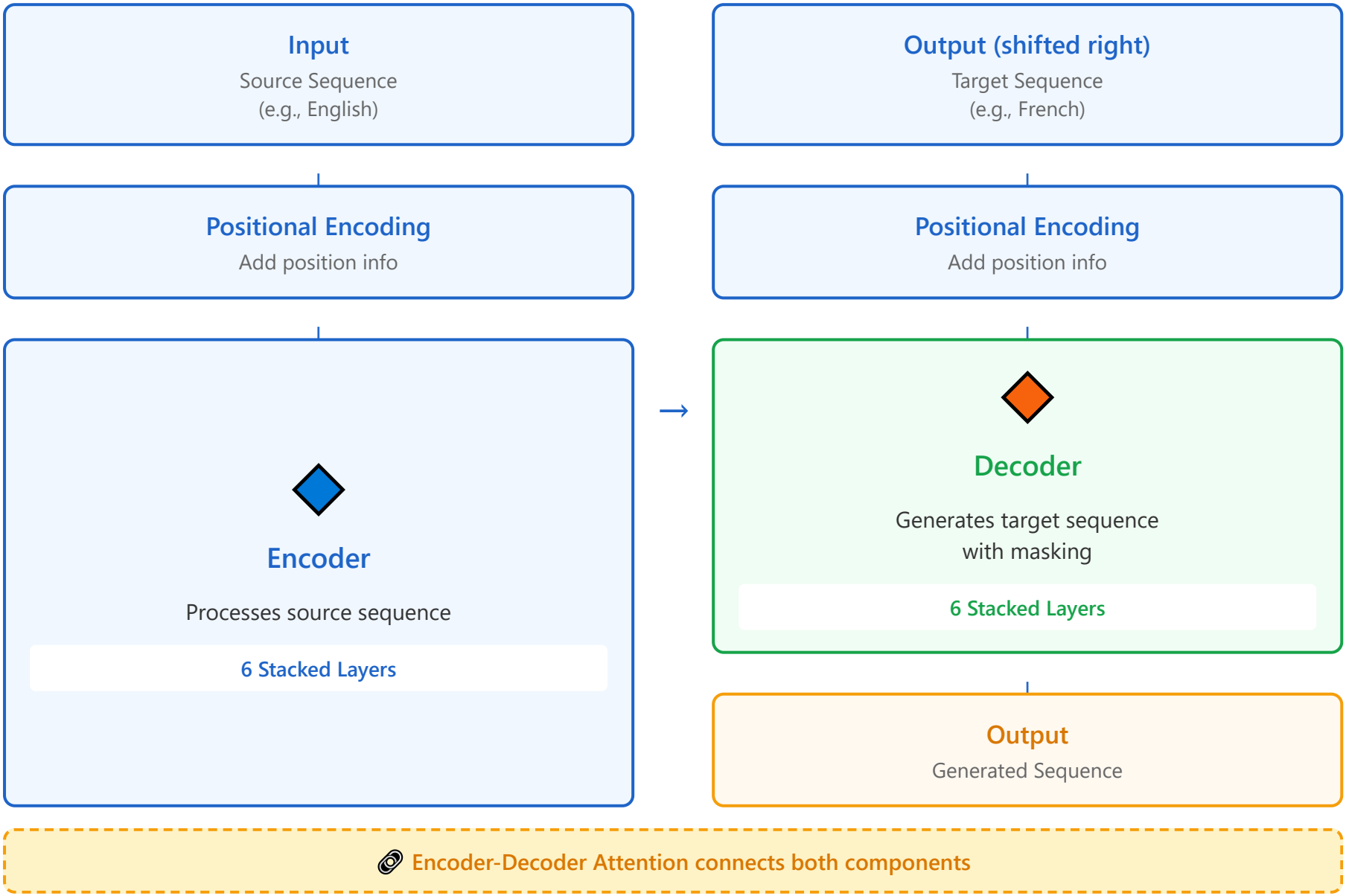
Part 5/7:

Transformer Architecture

15. Overall Transformer Structure
16. Detailed Analysis of the Encoder
17. Detailed Analysis of the Decoder
18. Feed-Forward Network & Layer Normalization
19. Training vs. Inference

Overall Transformer Structure

Encoder-Decoder Architecture for Sequence-to-Sequence Tasks



Identical layers
with different parameters

Seq2Seq tasks
Translation, Summarization

Decoder uses
masking for causality

Detailed Computation Example

Step-by-step process with actual dimensions (d_model = 4, sequence length = 8)

Step 1: Input Embedding

Source (English): "I love deep learning very much !"

Tokenization: [I, love, deep, learning, very, much, !, <PAD>] → 8 tokens

Embedding Matrix: Vocabulary × d_model → Each token → 4D vector

```
X_embedded (8 × 4) =
[[0.2, 0.5, -0.3, 0.8],  # I
 [0.1, -0.4, 0.6, 0.3],  # love
 [-0.5, 0.2, 0.4, -0.1], # deep
 [0.3, 0.7, -0.2, 0.5],  # learning
 [0.4, -0.3, 0.1, 0.6],  # very
 [-0.2, 0.5, 0.3, -0.4], # much
 [0.6, 0.1, -0.5, 0.2],  # !
 [0.0, 0.0, 0.0, 0.0]]   # <PAD>
```

Step 2: Positional Encoding

Add position information using sin/cos functions:

PE(pos, 2i) = sin(pos / 10000^(2i/d_model))

PE(pos, 2i+1) = cos(pos / 10000^(2i/d_model))

```
PE (8 × 4) =
[[0.00, 1.00, 0.00, 1.00],  # pos 0
 [0.84, 0.54, 0.01, 1.00],  # pos 1
```

```
 [0.91, -0.42, 0.02, 1.00], # pos 2
 [0.14, -0.99, 0.03, 1.00], # pos 3
 [-0.76, -0.65, 0.04, 1.00], # pos 4
 [-0.96, 0.28, 0.05, 1.00],  # pos 5
 [-0.28, 0.96, 0.06, 1.00],  # pos 6
 [0.66, 0.75, 0.07, 0.99]]   # pos 7

X_input (8 × 4) = X_embedded + PE
[[0.20, 1.50, -0.30, 1.80],
 [0.94, 0.14, 0.61, 1.30],
 [0.41, -0.22, 0.42, 0.90],
 [0.44, -0.29, -0.17, 1.50],
 [-0.36, -0.95, 0.14, 1.60],
 [-1.16, 0.78, 0.35, 0.60],
 [0.32, 1.06, -0.44, 1.20],
 [0.66, 0.75, 0.07, 0.99]]
```

🔷 Step 3: Encoder Self-Attention (Layer 1)

Multi-Head Attention computation:

1) Linear projections (d_k = d_model / num_heads = 4 / 2 = 2 per head):

```
W_Q (4 × 4), W_K (4 × 4), W_V (4 × 4)
Q = X_input @ W_Q → (8 × 4)
K = X_input @ W_K → (8 × 4)
V = X_input @ W_V → (8 × 4)
```

2) Attention scores:

```
Scores = Q @ K^T / √d_k → (8 × 8)
// Example scores (showing first 4×4 block):
[[2.3, 0.8, 1.2, 1.5, ...],
 [0.8, 2.1, 0.9, 1.3, ...],
```

```
 [1.2, 0.9, 2.5, 1.1, ...],
 [1.5, 1.3, 1.1, 2.2, ...]]

Attention = softmax(Scores) → (8 × 8)
// Softmax normalizes each row to sum to 1
[[0.35, 0.08, 0.12, 0.15, ...], # I attends to all
 [0.10, 0.31, 0.11, 0.16, ...], # love attends to all
 [0.13, 0.09, 0.41, 0.12, ...], # deep attends to all
 ...]
```

3) Apply attention to values:

```
Output = Attention @ V → (8 × 4)
// Each token representation is now context-aware
```

🔄 Step 4: Add & Norm + Feed-Forward

1) Residual connection and Layer Normalization:

```
X1 = LayerNorm(X_input + Attention_output) → (8 × 4)
```

2) Feed-Forward Network (expand to d_ff = 16, then back to 4):

```
FFN(x) = W_2 @ ReLU(W_1 @ x + b_1) + b_2
W_1: (4 × 16), W_2: (16 × 4)

FFN_output = FFN(X1) → (8 × 4)
X_encoder1 = LayerNorm(X1 + FFN_output) → (8 × 4)
```

→ Repeat this process for 6 encoder layers
→ Final encoder output: (8 × 4)

Step 5: Decoder Input & Masked Self-Attention

Target (French): "<BOS> J' aime l' apprentissage profond <PAD>"
Shifted right: [<BOS>, J', aime, l', apprentissage, profond, <PAD>, <PAD>]

After embedding + positional encoding: Y_input (8 × 4)

Masked Self-Attention:

```
Mask prevents attending to future tokens:
[[1, 0, 0, 0, 0, 0, 0, 0],  # <BOS> only sees itself
 [1, 1, 0, 0, 0, 0, 0, 0],  # J' sees <BOS>, J'
 [1, 1, 1, 0, 0, 0, 0, 0],  # aime sees up to aime
 [1, 1, 1, 1, 0, 0, 0, 0],  # l' sees up to l'
 [1, 1, 1, 1, 1, 0, 0, 0],  # apprentissage
 [1, 1, 1, 1, 1, 1, 0, 0],  # profond
 [1, 1, 1, 1, 1, 1, 1, 0],  # <PAD>
 [1, 1, 1, 1, 1, 1, 1, 1]]  # <PAD>

Masked_Attention_output → (8 × 4)
```

Step 6: Encoder-Decoder Cross-Attention

Query from decoder, Key & Value from encoder:

```
Q = Decoder_output @ W_Q → (8 × 4)  # from decoder
K = Encoder_output @ W_K → (8 × 4)  # from encoder
V = Encoder_output @ W_V → (8 × 4)  # from encoder

Cross_Attention = softmax(Q @ K^T / √d_k) @ V
// Decoder attends to ALL encoder positions
// This allows decoder to "look at" the source sentence
```

```
Cross_Attention_output → (8 × 4)
```

📤 Step 7: Final Output & Prediction

After 6 decoder layers:

```
Decoder_final_output → (8 × 4)
```

Linear projection to vocabulary size (e.g., 10,000):

```
Logits = Decoder_output @ W_output → (8 × 10000)
Probabilities = softmax(Logits) → (8 × 10000)
```

For each position, pick highest probability token:

```
Position 0: P("J'") = 0.92 → output "J'"
Position 1: P("aime") = 0.87 → output "aime"
Position 2: P("l'") = 0.91 → output "l'"
Position 3: P("apprentissage") = 0.84 → output "apprentissage"
Position 4: P("profond") = 0.89 → output "profond"
Position 5: P("<EOS>") = 0.95 → output "<EOS>" (stop)

Final Translation: "J' aime l' apprentissage profond"
```

🎯 Key Dimensional Flow Summary

Input tokens (8) → Embedding (8×4) → +PE (8×4) →
Encoder layers (8×4 maintained) → Encoder output (8×4) →

Decoder input (8×4) → Decoder layers (8×4 maintained) →

Linear projection (8×4 → 8×10000) → Softmax → Predictions (8×10000)

Detailed Analysis of the Encoder

Single Encoder Layer

1

Multi-Head Self-Attention

Captures relationships between all positions

+ Residual → Layer Norm

2

Feed-Forward Network

Position-wise transformation

+ Residual → Layer Norm

This structure is **repeated 6 times** (stacked layers)
Each layer has **different parameters**

Residual Connections

Around **each sub-layer** to help gradient flow

Layer Normalization

Applied **after each sub-layer** for stability

Same Structure

All layers share **identical structure** but have different parameters

Output dimension **preserved** throughout:
d_model = 512

Detailed Analysis of the Decoder

Single Decoder Layer (3 Sub-layers)

1. **Masked Multi-Head Self-Attention**
   Prevents attending to future positions

+ Residual → Layer Norm

2. **Encoder-Decoder Attention (Cross-Attention)**
   Q from decoder, K & V from encoder output

+ Residual → Layer Norm

3. **Feed-Forward Network**
   Position-wise transformation

+ Residual → Layer Norm

6 stacked layers with residual connections and layer normalization throughout

Masking
Prevents attending to future positions during training

Cross-Attention
Uses encoder output as Keys and Values

Residual Connections
Around all sub-layers for gradient flow

Layer Normalization
Applied throughout for stability

Comparison
Decoder has 3 sub-layers vs Encoder's 2 sub-layers

Feed-Forward Network & Layer Normalization

Feed-Forward Network (FFN)

$$FFN(x) = \max(0, xW_1 + b_1)W_2 + b_2$$

Input	Hidden	Output
d_model (512)	→ 4×d_model (2048)	→ d_model (512)

- Two **linear transformations** with **ReLU activation**
- Hidden dimension typically **4× d_model** (e.g., 2048)
- Applied **identically to each position** separately (position-wise)

Layer Normalization

Normalization
Normalizes across **feature dimension**

Training Benefits
Stabilizes training and speeds convergence

Application
Applied after each sub-layer with residual connections

Placement Strategy
Post-LN vs **Pre-LN**
affects training dynamics

Training vs. Inference

Training Mode
Teacher Forcing

- **Parallel processing** of all target tokens simultaneously
- **Masking** ensures causality (no future information leakage)
- Ground truth tokens used as input for next positions
- **Fast & efficient** - entire sequence at once

Processing Mode

ALL → ALL

Inference Mode
Autoregressive Generation

- **Token-by-token** autoregressive generation
- Each **generated token** becomes input for next step
- **Beam search** or sampling for generation strategies
- **KV-caching** improves inference efficiency

Processing Mode

ONE → ONE

Speed	Processing	Input Source

Training: Parallelizable
Inference: Sequential

Training: All at once
Inference: Step by step

Training: Ground truth
Inference: Generated

Computational Examples

🔬 Interactive Transformer Explainer - Try it yourself!

🎓 Training Mode: Parallel Processing

Input sequence: `["I", "love", "deep", "learning", "and", "AI", "research", "!"]`
Hidden dimension: `d = 4`

Step 1: All tokens processed simultaneously

Input Embeddings (8×4)

```
I:          [0.2, 0.5, -0.1, 0.3]
love:       [0.8, -0.2, 0.4, 0.1]
deep:       [-0.3, 0.6, 0.2, 0.5]
learning:   [0.4, 0.1, -0.5, 0.7]
and:        [0.1, -0.4, 0.3, -0.2]
AI:         [0.9, 0.3, -0.1, 0.6]
```

```
research:    [-0.2, 0.7, 0.4, -0.3]
!:           [0.5, -0.1, 0.6, 0.2]
```

↓ Transformer Layer with Causal Masking

Output Hidden States (8×4)

```
h₁ :         [0.25, 0.48, -0.12, 0.35]   ← attends to position 1 only
h₂ :         [0.52, 0.15, 0.18, 0.28]    ← attends to positions 1-2
h₃ :         [0.18, 0.42, 0.08, 0.45]    ← attends to positions 1-3
h₄ :         [0.38, 0.22, -0.15, 0.58]   ← attends to positions 1-4
h5:          [0.22, -0.08, 0.25, 0.12]   ← attends to positions 1-5
h6:          [0.68, 0.28, 0.05, 0.52]    ← attends to positions 1-6
h7:          [0.15, 0.55, 0.32, -0.08]   ← attends to positions 1-7
h8:          [0.42, 0.18, 0.48, 0.25]    ← attends to positions 1-8
```

✓ All 8 hidden states computed in **ONE forward pass** (parallel)
✓ Causal masking prevents each position from attending to future positions

🎯 Inference Mode: Autoregressive Generation

Starting prompt: `["I", "love"]`
Target: Generate next 3 tokens

Hidden dimension: $d = 4$

Step 1: Process ["I", "love"] → Generate "deep"

Input Embeddings:

```
I: [0.2, 0.5, -0.1, 0.3]
love: [0.8, -0.2, 0.4, 0.1]
```

→

Output Hidden State:

h_2 : [0.52, 0.15, 0.18, 0.28]

Generated: **"deep"**

Step 2: Process ["I", "love", "deep"] → Generate "learning"

Input Embeddings:

```
I: [0.2, 0.5, -0.1, 0.3]
love: [0.8, -0.2, 0.4, 0.1]
deep: [-0.3, 0.6, 0.2, 0.5]
```

→

Output Hidden State:

h_3 : [0.18, 0.42, 0.08, 0.45]

Generated: **"learning"**

Step 3: Process ["I", "love", "deep", "learning"] → Generate "and"

Input Embeddings:

```
I: [0.2, 0.5, -0.1, 0.3]
love: [0.8, -0.2, 0.4, 0.1]
deep: [-0.3, 0.6, 0.2, 0.5]
learning: [0.4, 0.1, -0.5, 0.7]
```

→

Output Hidden State:

h_4 : [0.38, 0.22, -0.15, 0.58]

Generated: **"and"**

✓ Each token requires a **separate forward pass** (sequential)
✓ Previously generated tokens become input for next step
✓ Context grows at each step: 2 tokens → 3 tokens → 4 tokens

📊 Computation Comparison

Training	VS	Inference
1 forward pass		**3 forward passes**
8 tokens → 8 hidden states		2→3→4 tokens sequentially
Matrix operation (8×4)		Growing context each step
All positions in parallel		One token at a time

Part 6/7:

Implementation Tips

20. Masking Implementation
21. Learning Stabilization Techniques
22. Hyperparameter Guide

Masking Implementation

Padding Mask

Ignore padding tokens in attention

- Shape: **(batch_size, 1, 1, seq_len)**
- Marks which positions are actual tokens vs padding

1	1	1	0	0

Look-Ahead Mask (Causal)

Prevent attending to future tokens

- **Upper triangular matrix** of -inf values
- Ensures causality during decoding

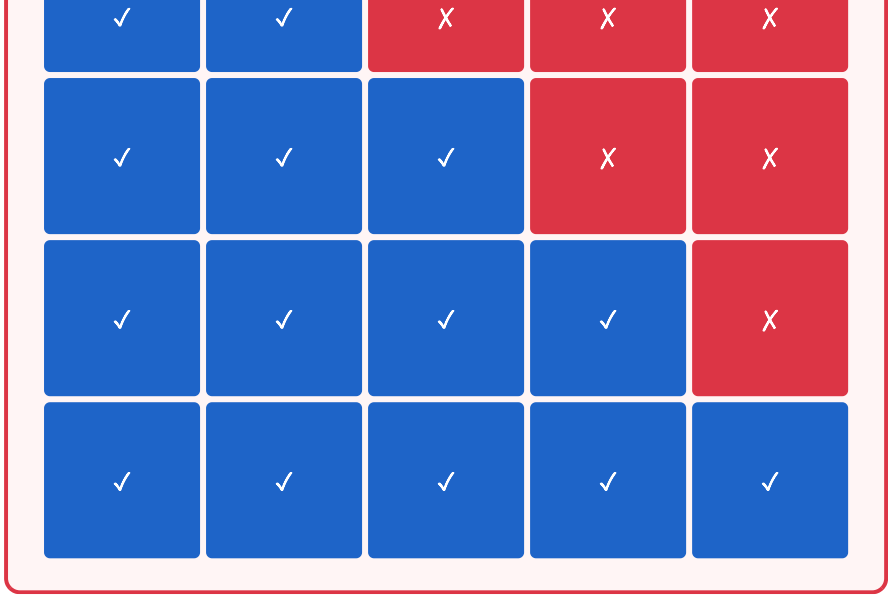
✓	✗	✗	✗	✗

Application Timing

Applied **before softmax** in attention calculation

Mask Values

Use **-inf** for masked positions (becomes 0 after softmax)



Combined Masks

Multiple masks combined using
element-wise OR operation

⚠

Proper masking is crucial for correct model behavior

Learning Stabilization Techniques

Learning Rate Warmup

Gradually increase learning rate initially to stabilize training

```
lr = d_model^(-0.5) × min(step^(-0.5), step × warmup^(-1.5))
```

Label Smoothing

Reduces **overconfidence** in predictions

- ✓ Typical value: **ε = 0.1**
- ✓ Improves generalization

Gradient Clipping

Prevents **exploding gradients** during training

- ✓ Caps gradient norm at threshold
- ✓ Ensures training stability

Dropout

Regularization through random neuron dropout

- ✓ Applied to **attention weights**
- ✓ Applied to **FFN outputs**

Weight Initialization

Proper initialization for stable gradients

- ✓ **Xavier** initialization
- ✓ **He** initialization

Mixed Precision Training

Uses **FP16** for faster computation

- ✓ Reduces memory usage
- ✓ Speeds up training

🎓 Training Best Practices

Combine these techniques for **stable and efficient training** of Transformer models

Hyperparameter Guide

Parameter	Base Model	Large Model
d_model	512	1024
Layers (N)	6	12+
Attention Heads (h)	8	16
d_ff (FFN hidden)	2048	4096
Dropout Rate	0.1	0.1

Warmup Steps
4000 steps (typical)

Batch Size
As large as GPU memory allows

Adam Optimizer

β_1 = 0.9

β_2 = 0.98

ε = 10^{-9}

Base model suitable for most tasks
Large model for complex problems

Part 7/7:

Applications & Next Steps

23. Transformer Applications
24. Summary and Next Steps

Transformer Applications Across Domains

Natural Language Processing

- **GPT** - Text generation
- **BERT** - Language understanding
- **T5** - Text-to-text framework

Machine Translation

- High-quality translation systems

Near human-level performance

Computer Vision

- **ViT** - Vision Transformers
- **DINO** - Self-supervised learning
- **CLIP** - Vision-language models

Speech Processing

- **Whisper** - Speech transcription
- Audio generation systems

Multimodal AI

- **DALL-E** - Text-to-image
- **GPT-4** - Multi-capability AI
- **Flamingo** - Text + Image

Time Series

- **Temporal Fusion Transformer**
- Forecasting and prediction

Code Generation

Biology & Science

- **GitHub Copilot** - AI pair programming
- **AlphaCode** - Competitive programming

- **AlphaFold2**
- Protein structure prediction

Summary and Next Steps

Key Concepts

- **Self-Attention** Mechanism
- **Multi-Head** Attention
- **Positional Encoding**

Advantages

- **Parallelization** - Fast training
- **Long-range dependencies** - Global context
- **Flexibility** - Multiple domains

Challenges

- Quadratic complexity $O(n^2)$
- Large memory requirements

Next Steps

1. **Next Lecture**
   Advanced topics: Sparse attention, Linear attention
2. **Efficient Transformers**
   Explore Reformer, Linformer, Performer
3. **Practice**
   Implement a mini-Transformer from scratch
4. **Explore Libraries**
   Hugging Face Transformers library

Recommended Reading

"Attention Is All You Need" paper

Vaswani et al., 2017

Thank you

Ho-min Park

homin.park@ghent.ac.kr

powersimmani@gmail.com