

Transformers Architecture

From Self-Attention to Large-Scale Foundation Models

Introduction

The Transformer architecture revolutionized AI by replacing recurrence with self-attention, enabling parallelization and long-context understanding. It is the foundation of models like GPT, BERT, and Vision Transformers.

Historical Evolution

Pre-transformer era relied on RNNs and LSTMs, which struggled with long dependencies. The paper 'Attention Is All You Need' (Vaswani et al., 2017) introduced self-attention as a new paradigm. Andrej Karpathy's implementations (minGPT, nanoGPT) demonstrate this architecture end-to-end.

High-Level Overview

The transformer consists of: 1. Embedding Layer, 2. Positional Encoding, 3. Multi-Head Self-Attention, 4. Feed Forward Network, 5. Layer Normalization & Residuals. Variants include Encoder-Only (BERT), Decoder-Only (GPT), and Encoder-Decoder (T5).

Self-Attention Mechanism

Each token is projected into three vectors: Query (Q), Key (K), and Value (V). Attention is computed as $\text{Softmax}(QK^T / \sqrt{d_k}) \times V$. This allows each token to attend to all others simultaneously. Multi-head attention runs this process multiple times in parallel to learn richer relationships.

Code Example (from Karpathy's nanoGPT)

```
import torch.nn as nn
self.attn = nn.MultiheadAttention(embed_dim, num_heads, dropout=0.1)
attn_output, _ = self.attn(x, x, x)
```

Positional Encoding

Transformers lack recurrence, so position must be injected explicitly. Original sinusoidal encoding: $PE(pos, 2i) = \sin(pos/10000^{(2i/d)})$, $PE(pos, 2i+1) = \cos(pos/10000^{(2i/d)})$. Learned embeddings (as used in GPT) are now common for efficiency.

Transformer Encoder Block

Each encoder layer includes:

- Multi-Head Self-Attention
- Add & Norm
- Feed Forward Network (two linear layers with ReLU/GELU)
- Another Add & Norm. Residual connections stabilize deep networks and improve

gradient flow.

Decoder Block

Decoder has masked self-attention to prevent looking at future tokens. If used in seq2seq tasks, cross-attention attends over encoder outputs. GPT-style models use only the decoder block with causal masks.

Feed Forward Network (FFN)

Typically two linear layers with nonlinearity: $\text{FFN}(x) = \max(0, xW_1 + b_1)W_2 + b_2$. Hidden layer is usually 4x embedding size. This step enables non-linear transformations between attention layers.

Layer Normalization & Residual Connections

Add & Norm pattern ensures training stability. Residuals help maintain information across layers; normalization prevents exploding gradients.

Training and Parallelization

Transformers are trained on large corpora using teacher forcing. Self-attention allows full-sequence parallelism, enabling massive scaling on GPUs/TPUs. Techniques like gradient checkpointing, mixed precision, and distributed training (e.g., DeepSpeed) are key for efficiency.

Karpathy's Perspective

Karpathy emphasizes simplicity — building transformers from scratch using PyTorch to understand each component. His minGPT repository breaks the model into a few hundred lines for clarity. He advocates for inspecting attention matrices and understanding gradients intuitively.

Optimization Insights (From Stanford CS25)

Stanford's course highlights scaling laws (model size \propto performance), and shows how compute efficiency and dataset curation critically impact downstream generalization.

Variants & Extensions

- Vision Transformers (ViT) – treat image patches as tokens
- Efficient Transformers – Linformer, Performer, Reformer
- Mixture-of-Experts (MoE) – sparse activation of sub-models
- Retrieval-Augmented Transformers – integrate external knowledge bases

Applications Beyond NLP

Transformers are now used in vision, audio, biology (AlphaFold), time series forecasting, and multi-modal learning. Stanford CS25 demos illustrate unified architectures for text, image, and reinforcement learning tasks.

Strengths & Limitations

Strengths:

- Parallelism in training
- Captures long-range dependencies
- Generalizes across domains

Limitations:

- Quadratic complexity with sequence length
- Data and compute intensive
- Lack of inductive bias for spatial data

Implementation Pseudocode (Simplified)

```
def transformer_block(x):  
    q,k,v = linear(x), linear(x), linear(x)  
    attn = softmax(q@k.T/sqrt(d))*v  
    x = x + attn  
    x = layer_norm(x)  
    ff = relu(linear(x))  
    return layer_norm(x + ff)
```

Efficiency Improvements

Recent methods include:

- Sparse attention (Longformer, BigBird)
- Low-rank factorization
- Quantization and pruning
- Flash Attention (optimized CUDA kernels)

These reduce compute cost and memory footprint.

Scaling Laws & Large Models

Empirical scaling laws (OpenAI, DeepMind): performance improves predictably with data, compute, and parameters. This motivates large models like GPT-4 and PaLM. However, diminishing returns appear beyond optimal scaling regimes.

Explainability and Visualization

Attention heatmaps reveal which tokens the model focuses on. Layer-wise relevance propagation and attribution methods help interpret transformer behavior.

Future of Transformer Architecture

Expect hybrid designs combining CNNs, Graph Networks, and Transformers. Focus areas: efficiency, interpretability, and domain adaptation for edge deployment.

Summary

Transformers unify sequence modeling through attention. From Karpathy's minimalist GPT to Stanford's multi-domain applications, the architecture continues to evolve. Mastering attention mechanics and optimization is key to building next-gen AI systems.

Q&A; / Discussion

Prompt: How would you design a transformer variant for edge deployment while balancing accuracy, size, and latency?