From Transformer to GPT

The Original Transformer

The original Transformer architecture (Vaswani et al., 2017) was designed for sequence-to-sequence tasks and uses an **Encoder-Decoder** framework.

- Encoder: Maps an input sequence to a contextualized representation.
- Decoder: Produces outputs token-by-token using the encoder output and previously generated tokens.
- **Self-Attention**: Mechanism for learning dependencies within a sequence.
- Transformer: Fully relies on self-attention in both encoder and decoder for translation tasks.

Probabilistic Formulation:

$$P(Y \mid X) = \prod_{t} P(Y_t \mid Y_{< t}, X)$$

Evolving to a GPT

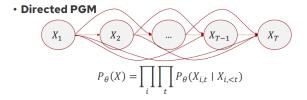
GPT simplifies the Transformer by dropping the encoder and using a decoder-only model to model input sequences:

$$P(X) = \prod_{t} P(X_t \mid X_{< t})$$

Objective:

$$\max_{\theta} \sum_{i} \sum_{t} \log P_{\theta}(X_{i,t} \mid X_{i,< t})$$

This enforces causal structure over the input, forming a directed probabilistic graphical model.



Writing a GPT

Model Configuration

```
import torch
torch.manual_seed(1337)

# Training hyperparameters
batch_size = 16
max_iters = 5000
eval_interval = 100
learning_rate = 1e-3
eval_iters = 200
```

```
from gpt_config import GPTConfig
config = GPTConfig(
   block_size = 8,
   device = 'cuda' if torch.cuda.is_available() else 'cpu',
   n_{embd} = 64,
   n_{head} = 4,
   n_{ayer} = 4,
   dropout = 0.0
Load and Encode Dataset
with open('input.txt', 'r', encoding='utf-8') as f:
   text = f.read()
chars = sorted(list(set(text)))
config.vocab_size = len(chars)
stoi = { ch:i for i,ch in enumerate(chars) }
itos = { i:ch for i,ch in enumerate(chars) }
encode = lambda s: [stoi[c] for c in s]
decode = lambda 1: ''.join([itos[i] for i in 1])
Train/Test Split and Block Sampling
data = torch.tensor(encode(text), dtype=torch.long)
n = int(0.9*len(data))
train_data = data[:n]
val_data = data[n:]
x = train_data[:config.block_size]
y = train_data[1:config.block_size+1]
for t in range(config.block_size):
   context = x[:t+1]
   target = y[t]
   print(f"For input {context}, target is: {target}")
Helper Functions
def get_batch(split):
   data = train_data if split == 'train' else val_data
   ix = torch.randint(len(data) - config.block_size, (batch_size,))
   x = torch.stack([data[i:i+config.block_size] for i in ix])
   y = torch.stack([data[i+1:i+config.block_size+1] for i in ix])
   return x.to(config.device), y.to(config.device)
@torch.no_grad()
def estimate_loss():
   out = {}
   model.eval()
```

for split in ['train', 'val']:

```
losses = torch.zeros(eval_iters)
for k in range(eval_iters):
    X, Y = get_batch(split)
    logits, loss = model(X, Y)
    losses[k] = loss.item()
    out[split] = losses.mean()
model.train()
return out
```

Training the Model

```
from gpt_zero import GPT
model = GPT(config)
m = model.to(config.device)
print(sum(p.numel() for p in m.parameters())/1e6, 'M parameters')
optimizer = torch.optim.AdamW(model.parameters(), lr=learning_rate)
for iter in range(max_iters):
    if iter % eval_interval == 0 or iter == max_iters - 1:
       losses = estimate_loss()
       print(f"step {iter}: train loss {losses['train']:.4f}, val loss {losses['val']:.4f}")
   xb, yb = get_batch('train')
   logits, loss = model(xb, yb)
   optimizer.zero_grad(set_to_none=True)
    loss.backward()
   optimizer.step()
context = torch.zeros((1, 1), dtype=torch.long, device=config.device)
print(decode(m.generate(context, max_new_tokens=2000)[0].tolist()))
```

Training Output

```
Model Size: 0.208961 M parameters

Sample Output (Shakespeare-like):

WARWICK:

Yeart, their to you's my 'tcknow your turrothose...

ROMEO:

Wwell-Bethal,

Be lords!
```

Scaling from "GPT" to GPT-4

Overview

This section summarizes the evolution of the GPT family, from a simple, scratch-built model to GPT-4. Each stage reflects major increases in model size, dataset quality, training techniques, and inference strategies.

As the architecture scaled, so did the model's capabilities—enabling GPT to move from character-level toy outputs to world-class language generation and multimodal reasoning.

Glossary of Key Terms

- Tokenizer: Breaks input text into smaller units. GPT evolved from character-level to Byte-Pair Encoding (BPE), and later to multimodal tokenization.
- ReLU / GELU: Activation functions that determine how neurons in the model fire. GELU is smoother and generally performs better in transformers.
- Embedding Dimension: Size of the vector used to represent each token.
- Attention Heads: Parallel attention mechanisms in each transformer block that allow the model to focus on different parts of the input simultaneously.
- Context Length: Maximum number of tokens the model can consider at once.
- Parameters: Total number of learnable weights in the model. Higher parameter counts generally allow for more expressive power.
- Training Dataset: Text corpus used to train the model. Increased in size and diversity across versions.
- Optimizer: Algorithm used to adjust the model weights during training. Adam is widely used, often with modifications like learning rate warmup and weight decay.
- Sampling Strategy: Method for generating output text. Greedy selects the highest-probability token each time, while top-k introduces diversity.
- Mixture-of-Experts (MoE): A sparsely activated architecture where only subsets of the model are used per input, improving scalability.
- RLHF: Reinforcement Learning from Human Feedback—a training method that aligns model outputs with human preferences.

From "GPT" to GPT-1

- Architecture
 - Tokenizer: Characters \rightarrow Byte-Pair Encoding (BPE)
 - Activation: ReLU \rightarrow GELU
 - Weight Sharing: Tied input/output embeddings
 - Scale (117M params):
 - * Layers: $4 \rightarrow 12$
 - * Attention heads: $4 \rightarrow 12$
 - * Context length: $32 \rightarrow 512$
 - * Vocabulary: $65 \rightarrow 40,000$ tokens
 - * Embedding dim: $64 \rightarrow 768$

• Training

- Dataset: TinyShakespeare (1MB) \rightarrow BookCorpus (5GB)
- Initialization/normalization: Default \rightarrow Tuned
- Optimizer: Adam \rightarrow Adam + warmup + weight decay

• Inference

- Sampling: Greedy \rightarrow Top-k

From GPT-1 to GPT-2

- Architecture (1.5B params max):
 - Layers: $12 \rightarrow 48$
 - Heads: $12 \rightarrow 25$
 - Embedding dim: $768 \rightarrow 1600$
 - Context length: $512 \rightarrow 1024$
 - Vocab size: $40k \rightarrow 50k$ tokens
- Training: BookCorpus (5GB) → WebText (40GB)

From GPT-2 to GPT-3

- Architecture (1.5B \rightarrow 175B params):
 - Layers: $48 \rightarrow 96$
 - Heads: $25 \rightarrow 96$
 - Embedding dim: $1600 \rightarrow 12,288$
 - Context length: $1024 \rightarrow 2048$
- Training: WebText (40GB) \rightarrow Common Crawl + books, code, etc. (\sim 570GB)

From GPT-3 to GPT-4

- Architecture:
 - Likely incorporates Mixture-of-Experts (MoE)
 - Tokenizer expanded for multimodal inputs (e.g., images)
 - Scale:
 - * Parameters: 175B \rightarrow estimated >1T
 - * Context length: 2048 \rightarrow 128,000 tokens
- Training:
 - Data sources: WebText + books, Wikipedia, code, etc. $(\sim 570\text{GB})$ → much larger, proprietary dataset (details undisclosed)

- Reported training data: \sim 13 trillion tokens (\sim 50TB)
- Alignment: Reinforcement learning from human feedback (RLHF) + system-level safety mechanisms

Mixture of Experts (MoE)

Core Idea: Instead of using a single feedforward layer (FFN) at each transformer block, MoE introduces multiple "expert" FFNs and uses a routing mechanism to dynamically select a subset for each input.

Diagram 1: MoE Routing Mechanism

- A router analyzes each input token and assigns it to the most relevant expert(s).
- Only a small subset of experts (e.g., 1 or 2 out of 4) is activated per token.
- This allows for *sparse computation*, reducing the cost while increasing model capacity.

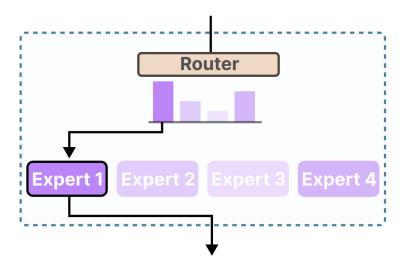
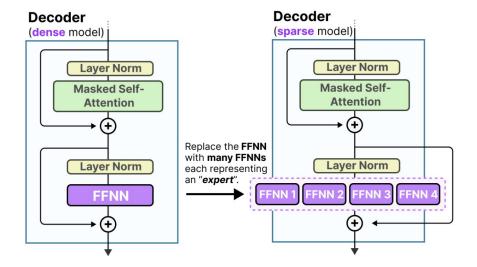


Diagram 2: MoE in Transformer Decoders

- In a standard transformer (left), each token passes through a single FFN after self-attention.
- In an MoE transformer (right), this FFN is replaced with many parallel FFNs (the experts).
- The router selects a few experts to process the token, and the outputs are combined.
- Result: Higher model capacity with the same or lower computational cost at inference time.



Mixture of Experts: Probabilistic View

Key Idea: Model the output as a weighted sum of predictions from multiple expert networks.

• Let

$$P(Y \mid X) = \sum_{m} g_{m}(X) \cdot P_{m}(Y \mid X)$$

where:

- $-P_m(Y \mid X)$: prediction from expert m
- $g_m(X)$: gating function output (i.e., weight) for expert m
- Subject to constraints:

$$\sum_{m} g_m(X) = 1, \text{ and } g_m(X) \ge 0 \quad \forall m, X$$

ensuring a valid probability distribution over experts.

- A gating network computes $g_m(X)$, deciding how much each expert contributes based on the input.
- The **stochastic selector** uses these weights to sample or activate experts probabilistically.
- This framework can be trained via the **EM algorithm**, where:
 - E-step estimates expert responsibilities $g_m(X)$
 - M-step updates expert and gating parameters

MoE: A Unifying Framework for Ensembles

Let the predictive distribution be modeled as:

$$P(Y \mid X) = \sum_{m} g_{m}(X) \cdot P_{m}(Y \mid X)$$

- Mixture of Experts: $g_m(X)$ is a learned gating function.
- Bagging: $g_m(X) = \frac{1}{M}$ is a uniform weight across experts.
- Boosting: $g_m(X) = \alpha_m$ is a fixed expert-specific weight, constant across inputs.

MoE: Error Analysis

Let:

$$P(Y \mid X) = \sum_{m} g_{m}(X) \cdot P_{m}(Y \mid X)$$

Define the expected prediction (mean function) of the ensemble:

$$\bar{f}(x) := \mathbb{E}[Y \mid X = x] = \sum_{m} g_m(x) f_m(x)$$

Compare two types of errors:

• Ensemble error:

$$\epsilon(x) := (Y - \bar{f}(x))^2$$

• Average expert error:

$$\bar{\epsilon}(x) := \frac{1}{M} \sum_{m} (Y - f_m(x))^2$$

Key question: Will minimizing ensemble error $\epsilon(x)$ also minimize average expert error $\bar{\epsilon}(x)$?

MoE: Diversity vs. Error

Recall:

• Ensemble error: $\epsilon(x) = (Y - \bar{f}(x))^2$

• Average expert error: $\bar{\epsilon}(x) = \frac{1}{M} \sum_{m} (Y - f_m(x))^2$

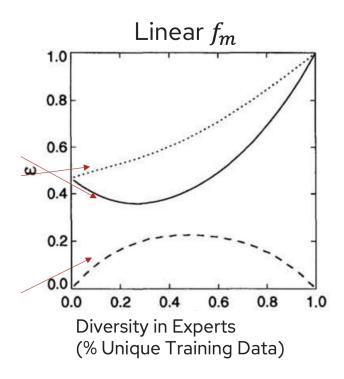
Graphical Insight:

• As diversity among experts increases (x-axis = % unique training data per expert):

 $-\epsilon(x)$ (solid line): Ensemble error is minimized at moderate diversity.

 $-\bar{\epsilon}(x)$ (dotted line): Average expert error increases with diversity.

- Dashed line: Represents disagreement (variance) between experts' outputs.



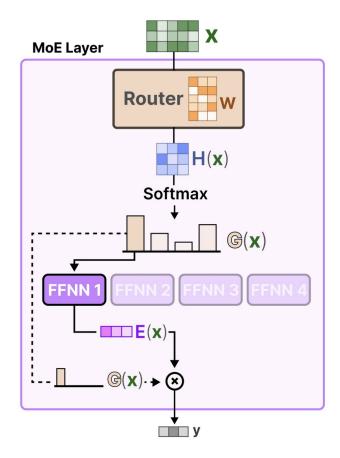
Interpretation:

- Expert predictions can individually overfit, but if their errors are uncorrelated, the ensemble prediction can be robust and accurate.
- Key intuition: Diverse (even slightly overfitted) experts cancel out each other's errors when averaged.
- Mild overfitting or purposeful variation among experts improves ensemble generalization.

MoE in Large Language Models (LLMs)

MoE Layer Structure:

- Input X is passed through a **router**, which outputs activations $\mathbf{H}(x)$.
- The router computes softmax scores G(x), representing how much to weight each expert.
- A small number of experts (e.g., top-1 or top-2) are activated based on G(x).
- Only the selected FFNNs are evaluated; their outputs E(x) are weighted by G(x) and aggregated into the final output y.



Implications for Serving:

- Efficiency: Sparse activation means only a few experts need to be loaded and executed per token, reducing compute and memory.
- Scalability: Enables use of massive models without needing to evaluate all parameters at once.

Implications for Training:

- Over-specialization: Without proper regularization, some experts dominate while others are underused.
- Trade-off with scale: As shown in the plot, more experts (e.g., 128) can reduce training loss but may hurt validation performance due to overfitting or imbalance.

Empirical Insight:

- Validation loss increases for larger expert counts, indicating a generalization gap.
- Solution approaches may include load balancing, expert dropout, or routing noise.

Summary Tables

From Transformer to GPT

Component	Transformer	GPT
Architecture	Encoder-decoder (full)	Decoder-only
Attention	Full self-attention	Masked (causal) self-attention
Positional encoding	Sinusoidal (original)	Learned positional embeddings
Output	Task-specific	Next-token prediction
Training objective	Flexible (e.g., translation)	Language modeling (autoregressive)
Inference	Depends on task	Greedy / sampling for text gen

From GPT-1 to GPT-4

Architecture:

- Scale: Broad range; largest grew from 1.5B $\rightarrow > \! 1 \mathrm{T}$ parameters

- Context length: $512 \rightarrow 128,000$

- Layers: $12 \rightarrow > 96$

- Attention heads: 12 $\rightarrow >\!96$

- Embedding dimension: $768 \rightarrow >12,288$

- Vocabulary size: $40k \rightarrow >50k$ tokens

• Tokenizer: Supports multimodal inputs (e.g., images)

• Architecture includes: Mixture-of-Experts (MoE)

Training:

• Dataset: BookCorpus (5GB) \rightarrow Private corpus of 13T tokens (\sim 50TB)

• Alignment: Reinforcement learning from human feedback (RLHF)