Architecture of ML Systems (AMLS)
07 LLM Training and Inference

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Last update: Jun 05, 2025

Announcements / Org

- **#1 Hybrid & Video Recording**
  - Hybrid lectures (in-person, zoom) with optional attendance
    https://tu-berlin.zoom.us/j/9529634787?pwd=R1ZsN1M3SC9BOU1OcFdmem9zT202UT09
  - Zoom **video recordings**, links from website
    https://mboehm7.github.io/teaching/ss25_amls/index.htm

- **#2 Projects & Exercises**
  - **Submission deadline: Jul 15 EOD**
  - Get started, use the office hour (Tue 4pm-5.30), and mentor meetings

~3 ECTS → 90h

Categories of Execution Strategies

Batch
SIMD/ SPMD

Independent Tasks
MIMD

Mini-batch, Federated, RL

Self-supervised, supervised, RL

05_a Data-Parallel Execution

05_b Task-Parallel Execution

06 Parameter Servers
(data, model)

07 LLM Training
(dense, MoE)

08 Hybrid Execution and HW Accelerators

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09 Caching, Partitioning, Indexing, and Compression

Agenda

- Basics and Terminology
- LLM Data Preprocessing
- LLM Pre-Training
- LLM Post-Training and Fine-Tuning
- LLM Inference

Basics and Terminology

Large Language Models (LLMs) Overview

- **Tokens/Words x_i**
  - Sequence of characters, n-grams, or words; **dictionary defined upfront**
  - The larger the tokens, the more efficient but the less effective

```
(AMLS, is, an, easy, course)
```

- **LLMs as Generate AI**
  - **Probability distribution** $p(x_1, \ldots, x_L)$
  - Generative models $X_{1:L} \sim p(x_1, \ldots, x_L)$

- **Autoregressive LLMs**
  - Sequential product of conditional token probabilities (by chain rule)
  - $p(x_1, \ldots, x_L) = p(x_1) * p(x_2|x_1) * p(x_3|x_2,x_1) * \ldots$

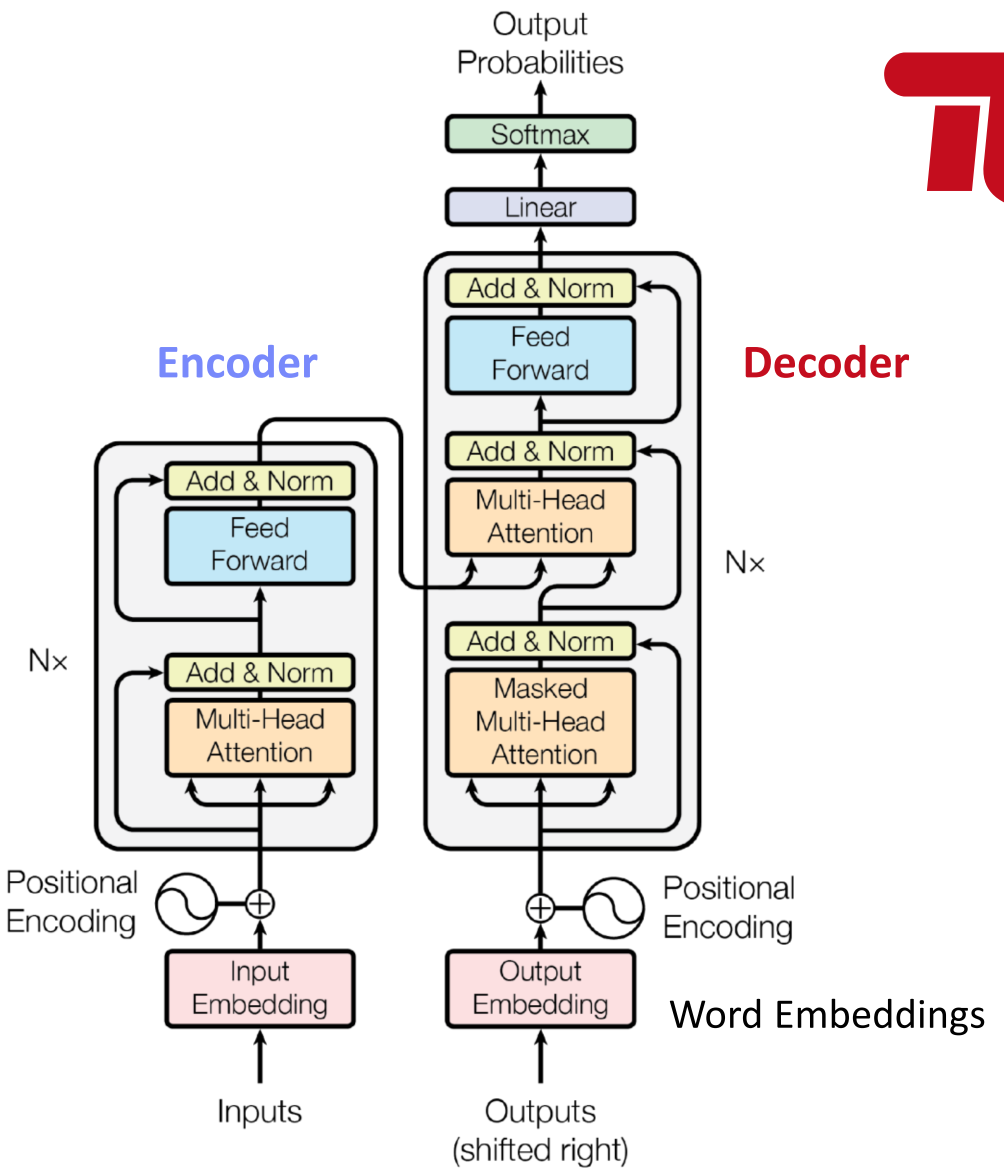
```
p(AMLS)
* p(is|AMLS)
* p(an|AMLS,is)
* p(easy|AMLS,is,an)
* p(course|AMLS,is,an,easy)
= 0.7
```

Transformer Model Architecture

- **Encoder-Decoder Structure**
  - **Encoder:** maps sequence of symbols (x_1, …, x_n) to continuous representation (z_1, …, z_n)
  - **Decoder:** maps sequence (z_1, …, z_n) sequentially to output symbol sequence (y_1, …, y_n)

- **Additional Features**
  - Stacked self-attention and fully-connected layers
  - **Residual connections** and layer normalization
  - **Masked self-attention** in decoder to ensure model uses only tokens before position i

[Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N. Gomez, Lukasz Kaiser, Illia Polosukhin: Attention is All you Need. **NeurIPS 2017**]

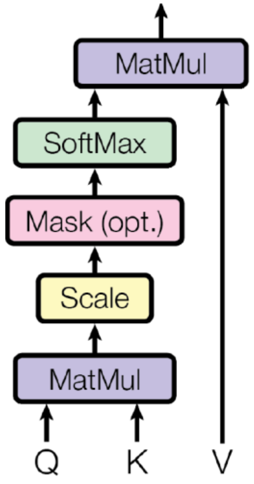


Transformer Model Architecture, cont.

[Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N. Gomez, Lukasz Kaiser, Illia Polosukhin: Attention is All you Need. **NeurIPS 2017**]

- **Basic Attention Block (Self-Attention)**
  - Mapping of a queries **Q** (search terms) and keys **K** (context words) / values **V** (modification of query) pairs to output
  - **Scaled dot-product attention** (divided by sqrt(d_k))

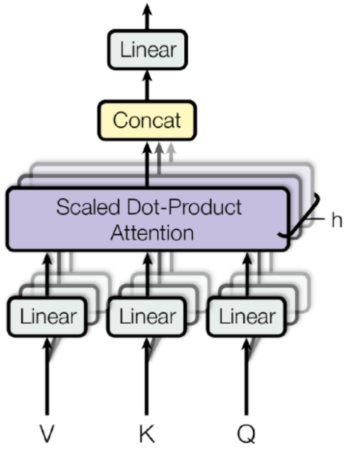
$$\mathrm{Attention}(Q, K, V) = \mathrm{softmax}(\frac{QK^T}{\sqrt{d_k}})V$$



size d_k size d_v

- **Multi-head Attention Block**
  - **Project queries, keys, values h times** with different linear projections
  - Attend to information from different subspaces

$$\mathrm{MultiHead}(Q, K, V) = \mathrm{Concat}(\mathrm{head}_1, ..., \mathrm{head}_h)W^O$$
$$\text{where } \mathrm{head_i} = \mathrm{Attention}(QW_i^Q, KW_i^K, VW_i^V)$$



- **Cross Attention**
  - Two sequences (in **Decoder**)
    - Key and value vectors from input sequence
    - Query vectors from output sequence

Dense vs Mixture of Experts (MoE) Models

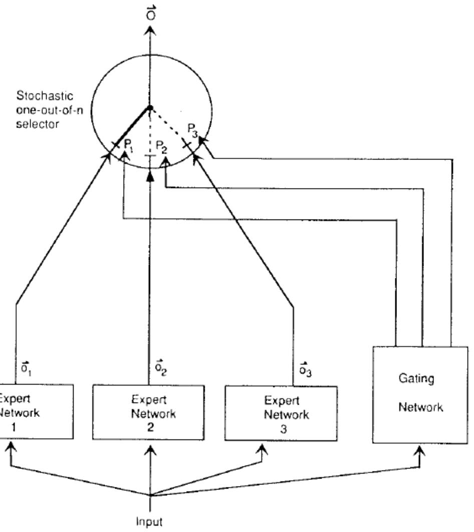
- **Dense Models**
  - Stack of transformer layers (e.g., 16 - 128), **all parameters active during inference**
  - E.g., GPT-2 and GPT-3 (sparse transformer)

[Tom B. Brown et al: Language Models are Few-Shot Learners. CoRR abs/2005.14165 (2020), GPT-3]

Model Name	n_{params}	n_{layers}	d_{model}	n_{heads}	d_{head}	Batch Size	Learning Rate
GPT-3 Small	125M	12	768	12	64	0.5M	6.0×10^{-4}
GPT-3 Medium	350M	24	1024	16	64	0.5M	3.0×10^{-4}
GPT-3 Large	760M	24	1536	16	96	0.5M	2.5×10^{-4}
GPT-3 XL	1.3B	24	2048	24	128	1M	2.0×10^{-4}
GPT-3 2.7B	2.7B	32	2560	32	80	1M	1.6×10^{-4}
GPT-3 6.7B	6.7B	32	4096	32	128	2M	1.2×10^{-4}
GPT-3 13B	13.0B	40	5140	40	128	2M	1.0×10^{-4}
GPT-3 175B or "GPT-3"	175.0B	96	12288	96	128	3.2M	0.6×10^{-4}

- **Mixture of Experts**
  - Ensemble of specialized models (experts)
  - Router / **gating network selects top-K experts**
  - E.g., DeepSeek-V3 (8+1 out of 256), [GPT-4]

[DeepSeek-AI: DeepSeek-V3 Technical Report, **2025**, https://arxiv.org/pdf/2412.19437]



[Robert A. Jacobs, Michael I. Jordan, Steven J. Nowlan, Geoffrey E. Hinton: Adaptive Mixtures of Local Experts. **Neural Comput. 3(1), 1991**]

[Michael I. Jordan, Robert A. Jacobs: Hierarchies of Adaptive Experts. **NeurIPS 1991**]

LLM Training and Inference Workflow

Data Collection	Data Pre-processing (tokenize)	Pre-Training (multiple phases)	Post-Training / Fine-Tuning	LLM Inference
Crawl the Internet	Train Tokenizer (e.g., common subsequences)	Train LLM on very large data corpus	Fine-tune model on high-quality and/or user data	Test-time compute

LLM Data Preprocessing

Stanford ENGINEERING

[Stanford CS229 Machine Learning, Yann Dubois:
Building Large Language Models (LLMs),
https://www.youtube.com/watch?v=9vM4p9NN0Ts]

Data Sources

- **#1 Web Crawling**
  - Download websites from public internet
  - Common crawl **250 billion websites**, 2-5 billion new / month
  - Other sources: Project Gutenberg (books), Stack Exchange (code), Wikipedia, Newspapers (see **law suites**), LeetCode (code)
- **#2 Text Extraction**
  - From HTML and PDF (remove meta data)
- **#3 Filtering**
  - Remove undesirable content (e.g., outliers, backlist, low quality)
  - Remove duplicates (within and across documents)
- **#4 Composition**
  - Mix categories of data (e.g., source code, entertainment, text books)
  - Synthetic and multi-modal data

COMMON CRAWL

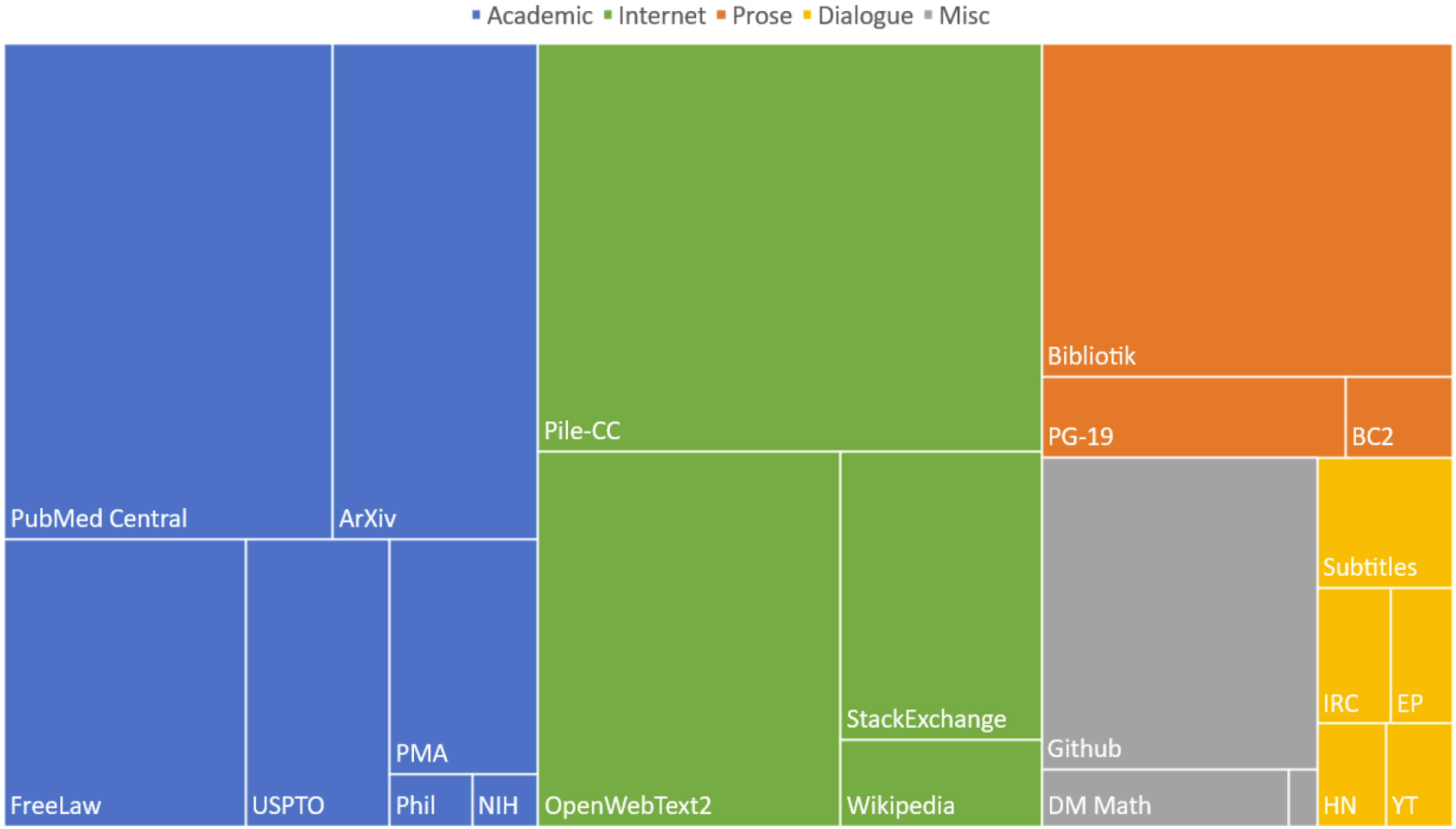
[https://commoncrawl.org/]

[Dong Huang, Yuhao Qing, Weiyi Shang, Heming Cui, Jie Zhang: EffiBench: Benchmarking the Efficiency of Automatically Generated Code. **NeurIPS 2024**]

~15T Tokens
(usually 1 epoch)

Data Sources, cont.

- **Composition of the Pile by Category**



[Leo Gao et al: The Pile: An 800GB Dataset of Diverse Text for Language Modeling. CoRR abs/2101.00027, 2021, https://arxiv.org/pdf/2101.00027]

Tokenization

- **Purpose**
  - Split input strings into sequence of tokens
  - Robustness to typos and different languages (more general than words)

`(AML, Sis, ane, asy, cou, rse)`

- **Common Approach**
  - Often **Token := 3-4 characters** (n-grams), sometimes longer words or individual characters
  - **Special handling of numbers** (single digit vs full number) **and source code** (handling indentation)

- **Byte-Pair Encoding (BPE)**
  - Large text corpus, start with single characters
  - **Merge common pairs** of tokens into token
  - **Repeat** until num merges / dictionary size

Algorithm 1 Learn BPE operations

```
import re, collections

def get_stats(vocab):
  pairs = collections.defaultdict(int)
  for word, freq in vocab.items():
    symbols = word.split()
    for i in range(len(symbols)-1):
      pairs[symbols[i],symbols[i+1]] += freq
  return pairs

def merge_vocab(pair, v_in):
  v_out = {}
  bigram = re.escape(' '.join(pair))
  p = re.compile(r'(?<!\S)' + bigram + r'(?!\S)')
  for word in v_in:
    w_out = p.sub(''.join(pair), word)
    v_out[w_out] = v_in[word]
  return v_out

vocab = {'l o w </w>' : 5, 'l o w e r </w>' : 2,
         'n e w e s t </w>':6, 'w i d e s t </w>':3}
num_merges = 10
for i in range(num_merges):
  pairs = get_stats(vocab)
  best = max(pairs, key=pairs.get)
  vocab = merge_vocab(best, vocab)
  print(best)
```

[Rico Sennrich, Barry Haddow, Alexandra Birch: Neural Machine Translation of Rare Words with Subword Units. **ACL 2016**]

[Taku Kudo, John Richardson: SentencePiece: A simple and language independent subword tokenizer... **EMNLP 2018** (Gemini)]]

Positional Embeddings

[https://cyrilzakka.github.io/llm-playbook/nested/fixed-pos-embed.html]

- **Challenge**
  - Transformers/self-attention by themselves **invariant to permutations** of input sequences
  - Positional embeddings combine **word embeddings and token positions**
- **Fixed Positional Embeddings**
  - Absolute positional encoding, which requires fixed sequence length or scaling; token pos, embedding index i, embedding dim d
  - Add positional embedding to word embedding of input token
  - **Example: Sinusoidal Positional Encoding**

even i: $$PE_{(\mathrm{pos},\ 2\mathrm{i})} = \sin\left(\frac{\mathrm{pos}}{10000^{\frac{2i}{d}}}\right)$$

odd i: $$PE_{(\mathrm{pos},\ 2\mathrm{i}+1)} = \cos\left(\frac{\mathrm{pos}}{10000^{\frac{2i}{d}}}\right)$$

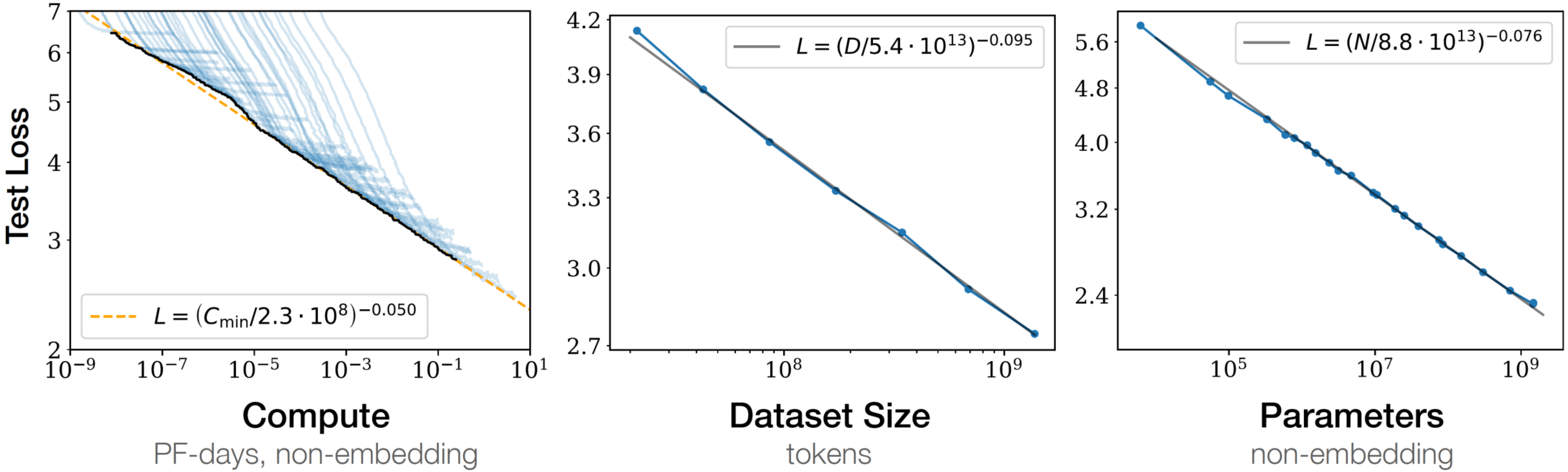
[https://medium.com/autonomous-agents/math-behind-positional-embeddings-in-transformer-models-921db18b0c28]

- **Rotary Positional Embedding (RoPE)**
  - Relative positional encoding
  - **Rotate queries and keys** with rotation relative to position in sequence

LLM Pre-Training

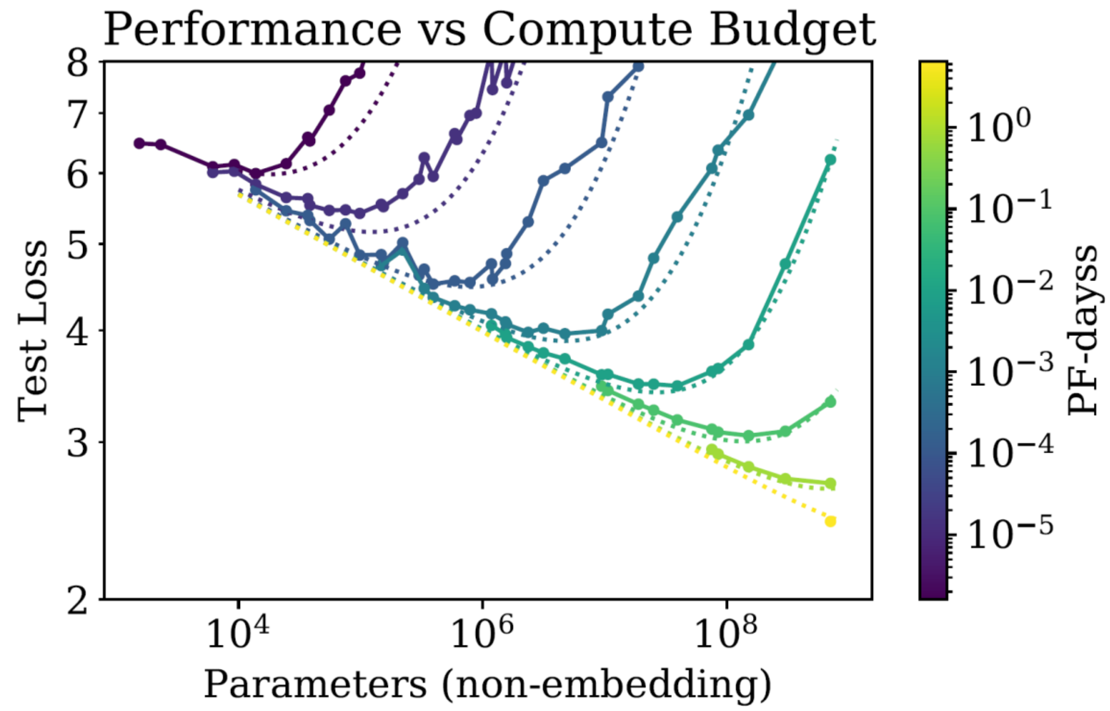
Scaling Laws

- **Predictable Performance w/ increasing Compute / Data Size / #Parameters**

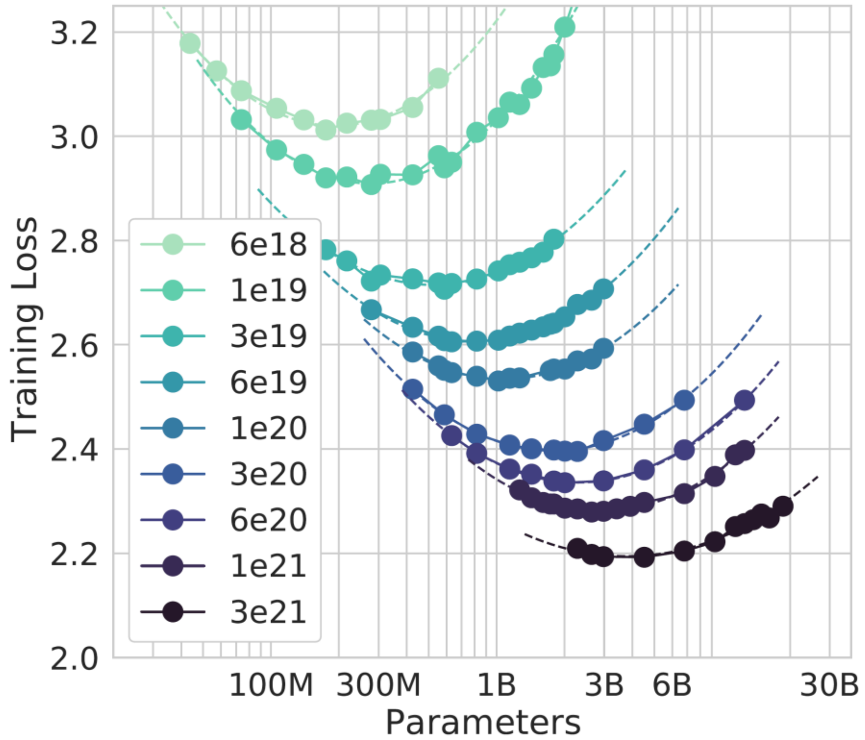


[Jared Kaplan et al: Scaling Laws for Neural Language Models. CoRR abs/2001.08361, **2020**, https://arxiv.org/pdf/2001.08361]

Scaling Laws, cont.



IsoFLOP Curves



[Jared Kaplan et al: Scaling Laws for Neural Language Models. CoRR abs/2001.08361, **2020**]

OpenAI

[Jordan Hoffmann et al.: Training Compute-Optimal Large Language Models. CoRR abs/2203.15556, 2022, https://arxiv.org/pdf/2203.15556]

DeepMind

Training Regimes

[DeepSeek-AI: DeepSeek-V3 Technical Report, **2025**, https://arxiv.org/pdf/2412.19437]

- **Data/Model Selection**
  - Given a fixed FLOPs budget, select model size & # training tokens
  - Training range of models → Fit curve for scaling
- **Pre-Training**
  - Train selected model in single-pass over data
  - **State-of-the-art: 15T tokens**; e.g., DeepSeek-V3: 14.8T tokens
- **Context-Length Extensions**
  - Phase 1: max context length extended to **32K tokens**
  - Phase 2: max context length extended to **128K tokens**
- **Fine-Tuning**
  - Overfitting on high-quality data, **Supervised Fine-Tuning** (SFT)
  - Reinforcement Learning (RL); **RL from Human Feedback** (RLFH)

Models and Training Cost

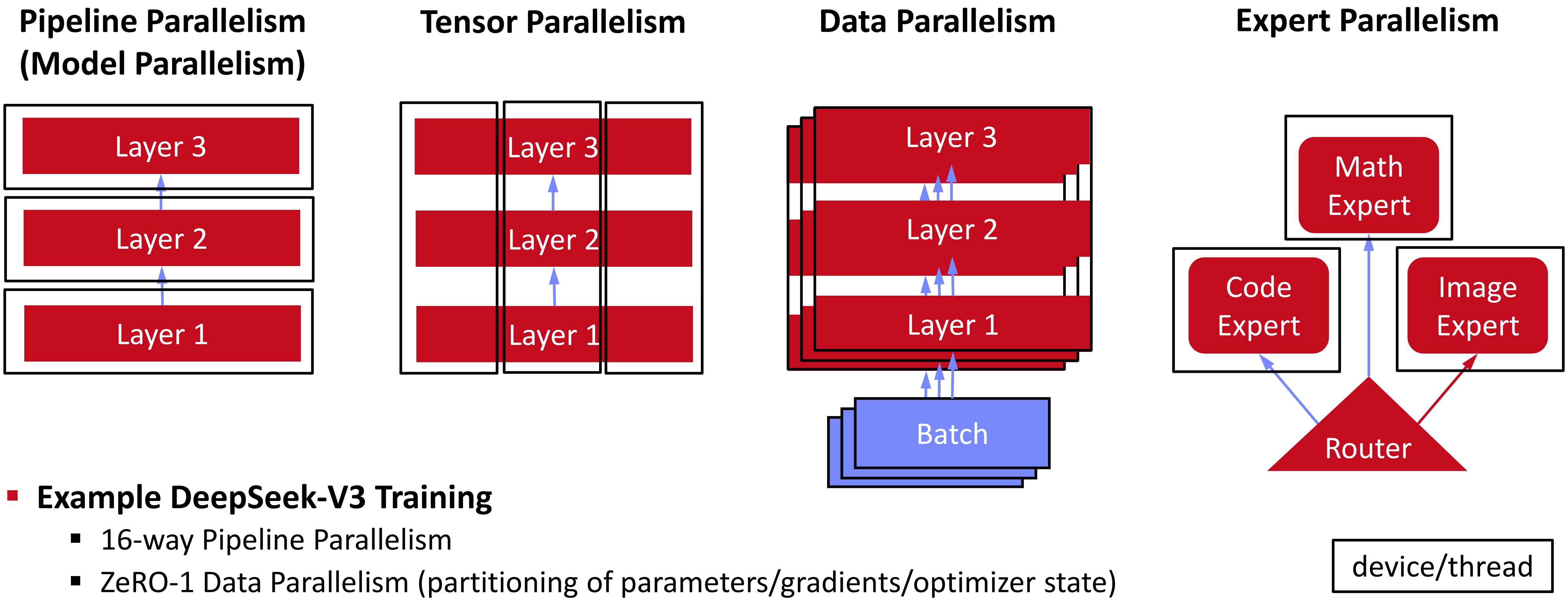
- **OpenAI GPT**
  - GPT-3: **4.5M USD**, GPT-4: **100M USD**
- **Google Gemini**
  - Gemini 1.0 Ultra: **192M USD**
- **Meta Llama**
  - Llama-3.1: **170M USD**
- **DeepSeek**
  - DeepSeek-V3: **5.3M USD**
- **Mistral**
  - Mistral Large: 41M USD
- **X Grok**
  - Grok-2: **107M USD**

[https://www.wired.com/story/openai-ceo-sam-altman-the-age-of-giant-ai-models-is-already-over/]

[https://www.visualcapitalist.com/the-surging-cost-of-training-ai-models/]

Training Costs	Pre-Training	Context Extension	Post-Training	Total
in H800 GPU Hours	2664K	119K	5K	2788K
in USD	$5.328M	$0.238M	$0.01M	$5.576M

Employed Types of Parallelism



- **Example DeepSeek-V3 Training**
  - 16-way Pipeline Parallelism
  - ZeRO-1 Data Parallelism (partitioning of parameters/gradients/optimizer state)
  - 64-way Expert Parallelism on 8 nodes

Sparse Transformers (e.g., GPT-3)

[Rewon Child, Scott Gray, Alec Radford, Ilya Sutskever: Generating Long Sequences with Sparse Transformers, CoRR 2019, https://arxiv.org/pdf/1904.10509]

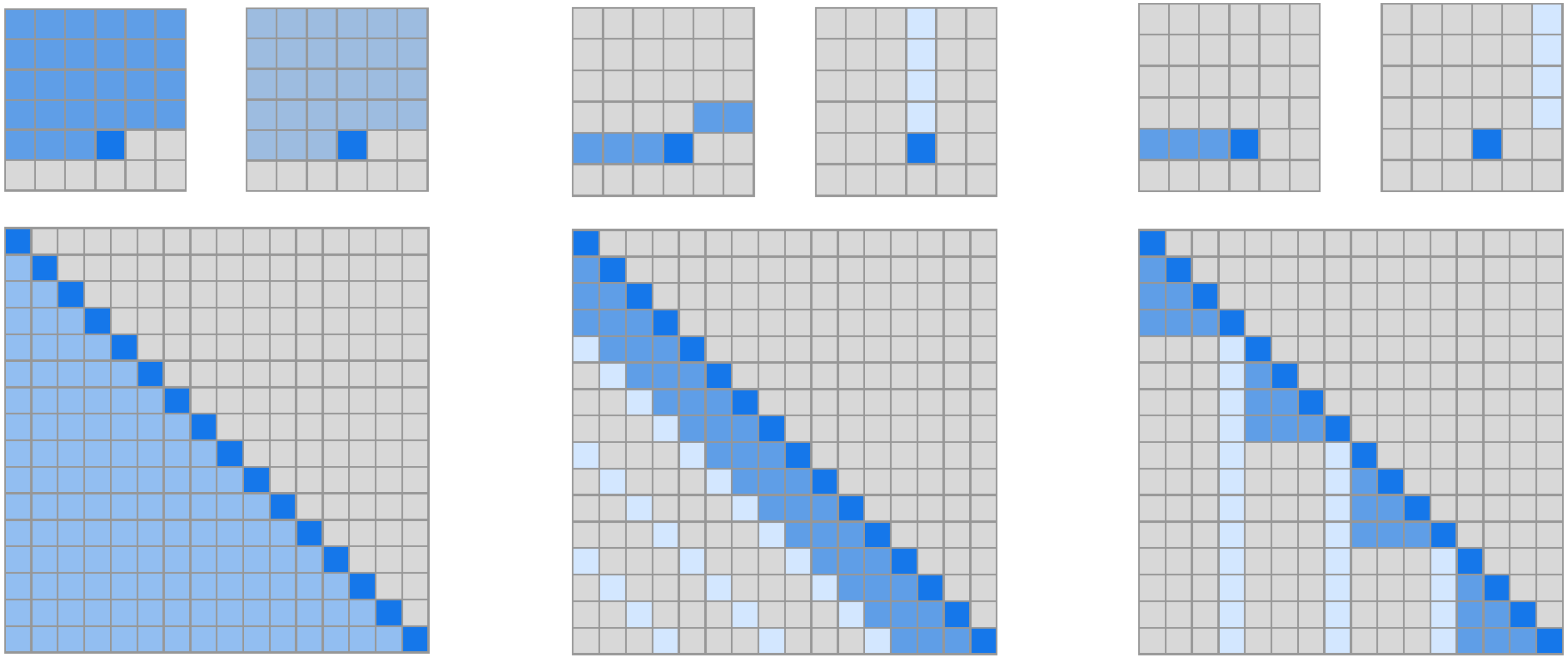
Transformer
O(n^2 * d)

Sparse Transformer
Strided

O(n * √n * d)

Sparse Transformer
Fixed/Blocked

Current Position (Query)

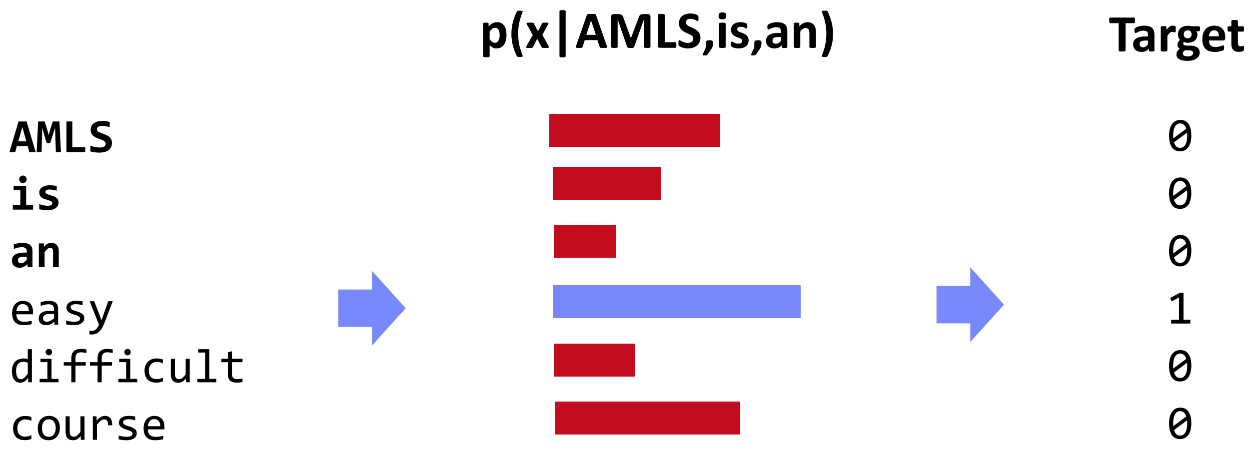


Attention Positions

LLM Post-Training and Fine-Tuning

Training Objective and Losses

- **Objective: Classify next token (multi-class classification)**
  - Cross-entropy loss
  - **Min –log(p(x))**



Types of Post-Training

- **#1 Foundation Model Fine-Tuning**
  - Fine-tuning for specific **high-quality data** (e.g., Wikipedia), and **tasks** (e.g., coding) through feedback
  - **Overfitting** to high-quality data

- **#2 Model Distillation and Quantization**
  - Transferring knowledge from **large teacher model** to **small student model**
  - **Goal:** reduce inference costs / resource requirements (# layers, model dim, attention heads)
  - **Example:** Llama 3.2 (09/2024): 90B, 11B, 3B, 1B parameters + FP32 / FP16 / UINT8 quantized variants

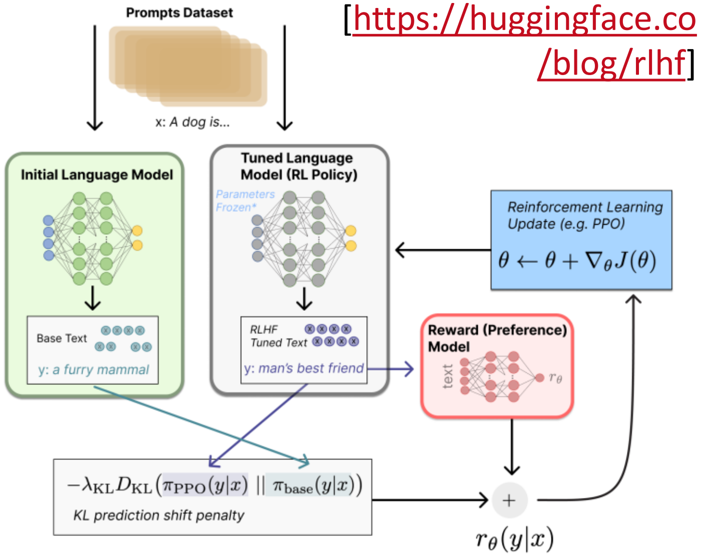
- **#3 User-level Fine-Tuning**
  - Specialize the LLM through user- and domain-specific data
  - Create model variants (**pro:** effectiveness, **con:** number of models)

SFT and RLHF

- **Supervised Fine-Tuning (SFT)**
  - Fine-tune LLM with language modeling (next word prediction) and desired output (human feedback)
  - Example prompts and expected answers (free form text) → **limited by human ability / costs**
  - **Example:** GPT-3 → ChatGPT

- **Reinforcement Learning from Human Feedback (RLHF)**
  - Aks fine-tuned LLM to generate two different answers
    → **humans ranks the answers**
  - #1 Train Reward Model **RM** for classifying preferences
  - #2 Proximal Policy Optimization (PPO) with **RM**
  - Freeze model parameters and **LoRA Low-Rank Adaptation** for LLMs

[https://huggingface.co/blog/rlhf]



[Edward J. Hu, Yelong Shen, Phillip Wallis, Zeyuan Allen-Zhu, Yuanzhi Li, Shean Wang, Lu Wang, Weizhu Chen: **LoRA:** Low-Rank Adaptation of Large Language Models. **ICLR 2022**]

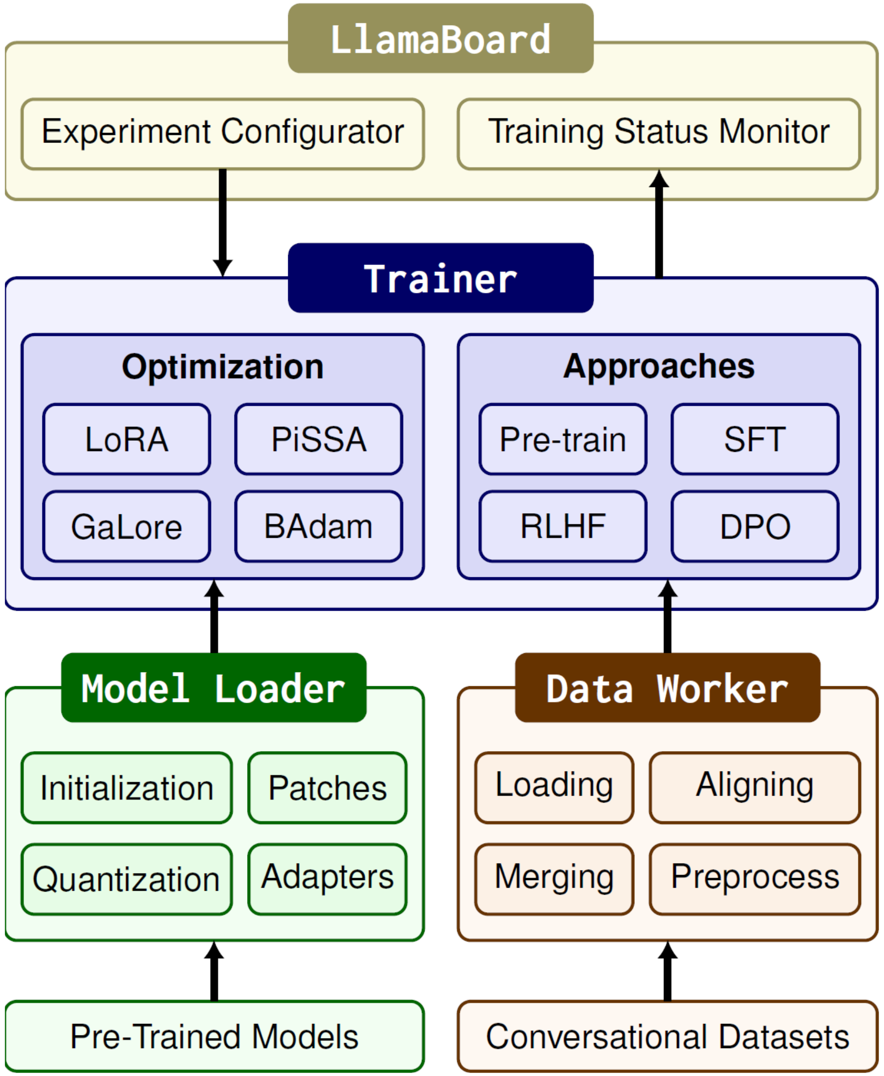
$$h = W_0 x + \Delta W x = W_0 x + BAx$$

User-Level Fine-Tuning Tools

- **Example LlamaFactory**

	LlamaFactory	FastChat	LitGPT	LMFlow	Open-Instruct
LoRA	✓	✓	✓	✓	✓
QLoRA	✓	✓	✓	✓	✓
DoRA	✓				
LoRA+	✓				
PiSSA	✓				
GaLore	✓	✓		✓	✓
BAdam	✓				
Flash attention	✓	✓	✓	✓	✓
S^2 attention	✓				
Unsloth	✓		✓		
DeepSpeed	✓	✓	✓	✓	✓
SFT	✓	✓	✓	✓	✓
RLHF	✓			✓	
DPO	✓				✓
KTO	✓				
ORPO	✓				

[Yaowei Zheng, Richong Zhang, Junhao Zhang, Yanhan Ye, Zheyan Luo, Yongqiang Ma: LlamaFactory: Unified Efficient Fine-Tuning of 100+ Language Models. CoRR abs/2403.13372 (2024), https://arxiv.org/pdf/2403.13372]



LLM Inference

Prompting Strategies

- **#1 Zero-shot**
  - General question answering and task processing, often via **prompt templates**
  - **No provided examples**, best effort results
- **#2 Few-shot**
  - Give **general instruction and few examples**; one-shot as an extreme case (“human instruction”)
  - LLM executes task while considering the pattern of examples
- **DSPy**
  - Programmatic, compositional interaction with LLMs

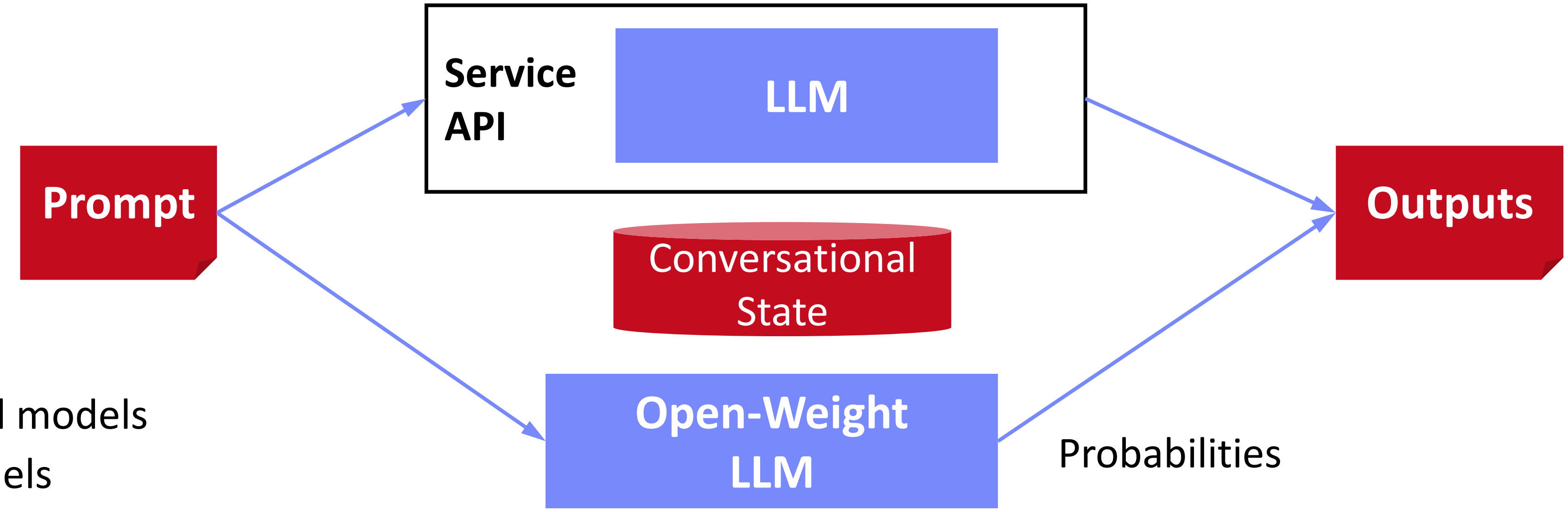
[https://github.com/stanfordnlp/dspy]

- **Jail Breaking**
  - Append special prefixed/suffixes for getting refused answers from LLM
  - **Example:** optimized **suffix search for probability of “Sure”**

[Maksym Andriushchenko, Francesco Croce, Nicolas Flammarion: Jailbreaking Leading Safety-Aligned LLMs with Simple Adaptive Attacks. **CoRR 2024** https://arxiv.org/pdf/2404.02151v4]

LLM Inference Overview

- **Overview**



- **Model Variants**
  - Large and small models
  - Quantized models

- **Service API Costs**
  - Billed by input/output tokens
  - GPT-4.1: 2/8$ per 1M input/output tokens; **0.5$ / 1M cached input tokens**
  - GPT-4.1-mini: 0.4/1.6$ per 1M input/output tokens; **0.1$ / 1M cached input tokens**

LLM Offline and Online Inference

Easy, fast, and cheap LLM serving for everyone

[https://docs.vllm.ai/en/stable/getting_started/examples/basic.html#]

- **vLLM: LLM Inference and Serving**
  - Management of attention key/value cache
  - Batching of incoming requests, eviction mechanisms
  - HuggingFace models and hardware accelerators

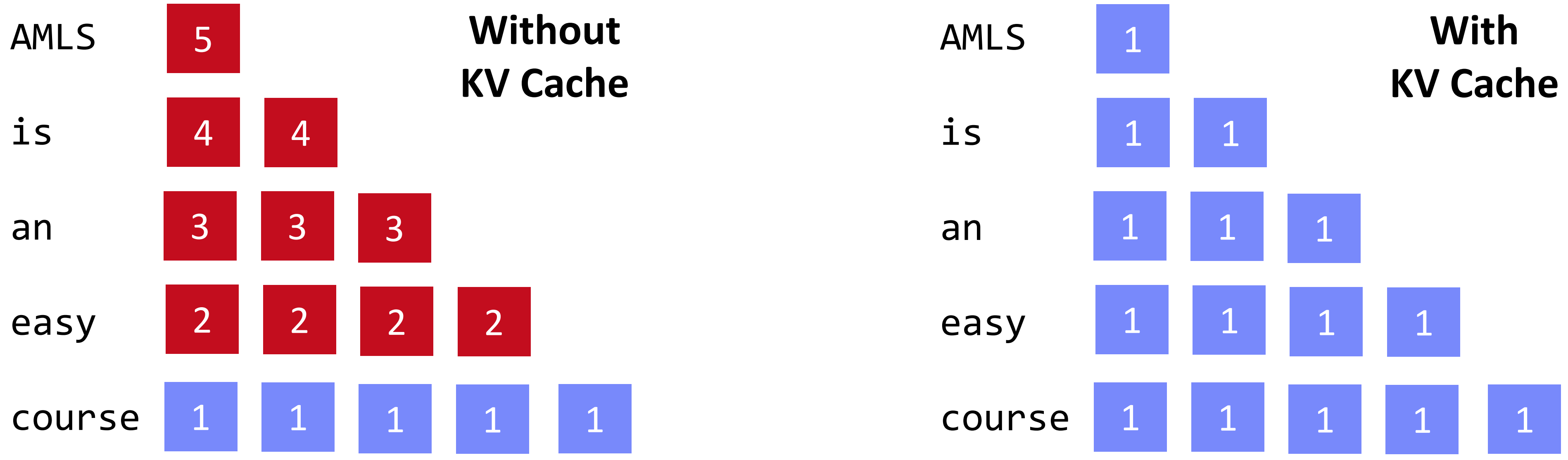
```python
from vllm import LLM, SamplingParams

# Sample prompts.
prompts = [
    "Hello, my name is",
    "The president of the United States is",
    "The capital of France is",
    "The future of AI is",
]
# Create a sampling params object.
sampling_params = SamplingParams(
  temperature=0.8, top_p=0.95)
...
```

```python
# Create an LLM.
llm = LLM(model="facebook/opt-125m")
# Generate texts from the prompts (RequestOutput)
outputs = llm.generate(prompts, sampling_params)
# Print the outputs.
print("\nGenerated Outputs:\n" + "-" * 60)
for output in outputs:
    prompt = output.prompt
    generated_text = output.outputs[0].text
    print(f"Prompt:    {prompt!r}")
    print(f"Output:    {generated_text!r}")
    print("-" * 60)
```

Key-Value (KV) Caching

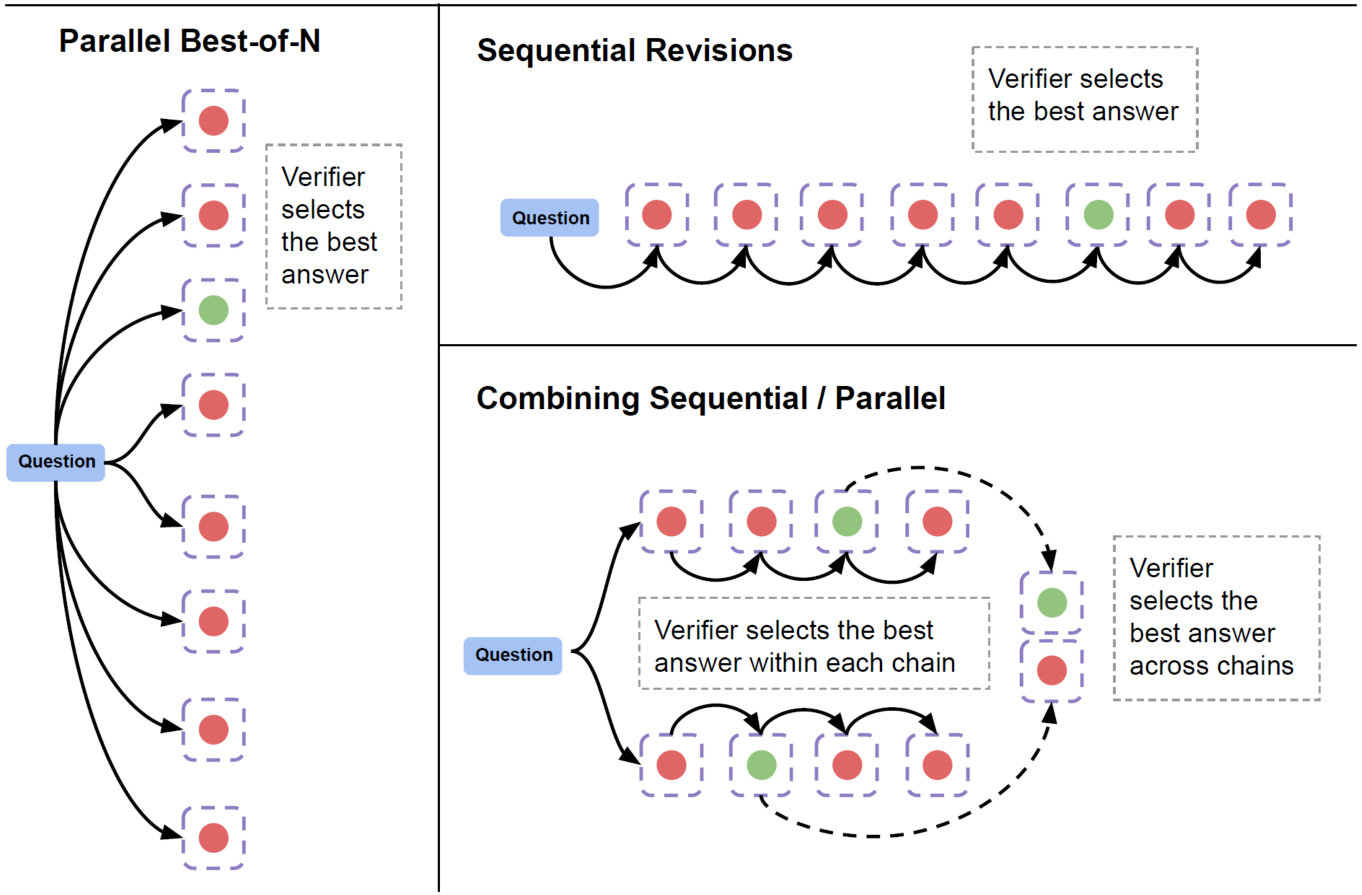
- **Basic Idea**
  - For every token, compute squared attention to all previous tokens → **large overlap**
  - Establish KV cache to **compute rows of keys/values just ones**



Test-Time Compute

- **Overview: Leverage multiple LLM invocations for improved accuracy at expense of compute costs**

[Charlie Snell, Jaehoon Lee, Kelvin Xu, Aviral Kumar: Scaling LLM Test-Time Compute Optimally can be More Effective than Scaling Model Parameters. CoRR abs/2408.03314 (2024) https://arxiv.org/pdf/2408.03314]



Summary & QA

- **Basics and Terminology**
- **LLM Data Preprocessing**
- **LLM Pre-Training**
- **LLM Post-Training and Fine-Tuning**
- **LLM Inference**

- **Next Lectures** (Part A)
  - **08 Hybrid Execution and HW Accelerators** [Jun 12]
  - **09 Caching, Partitioning, Indexing and Compression** [Jun 19]