A simple blog of large model inference

Weight

The LLMs we commonly use today are almost exclusively built on the Decoder-only architecture.

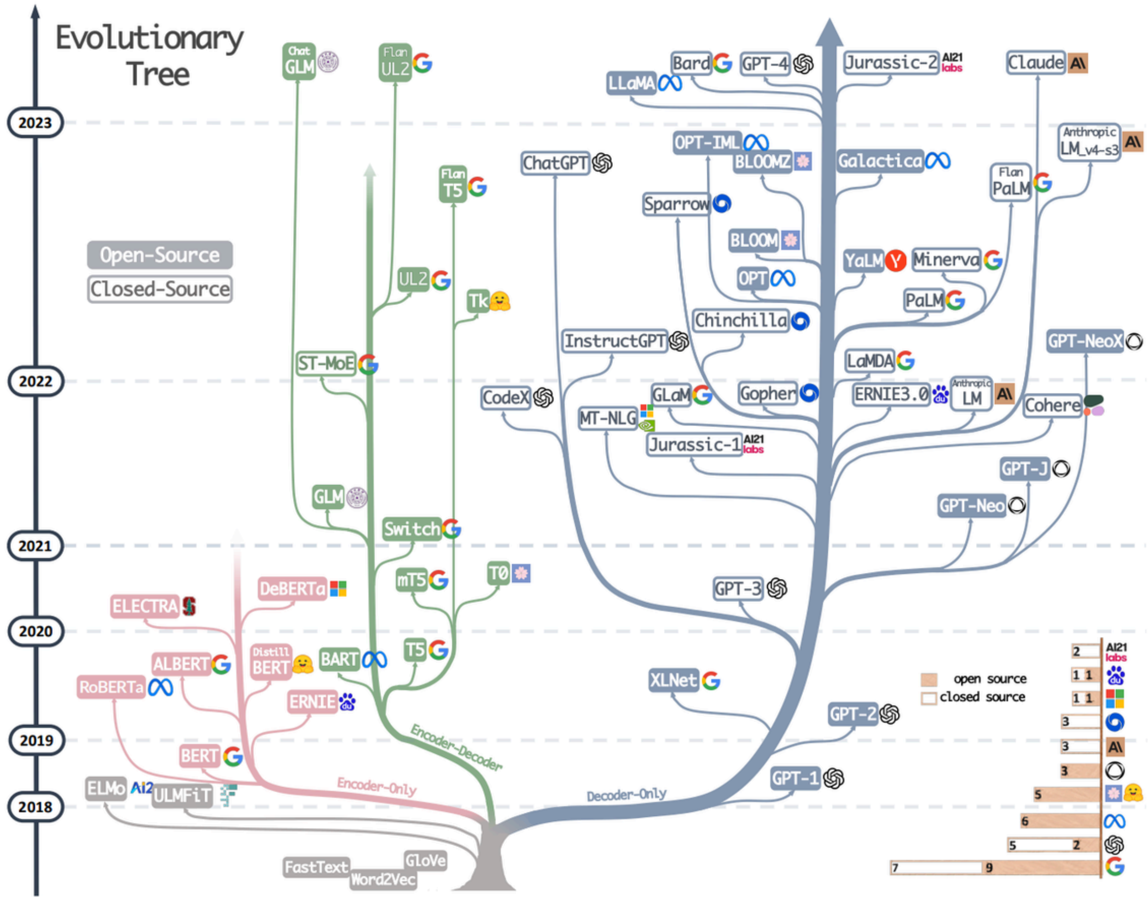


Fig.1.The evolutionary tree of modern LLMs[1]

The Transformer block in the Decoder-only architecture is illustrated in the following figure.

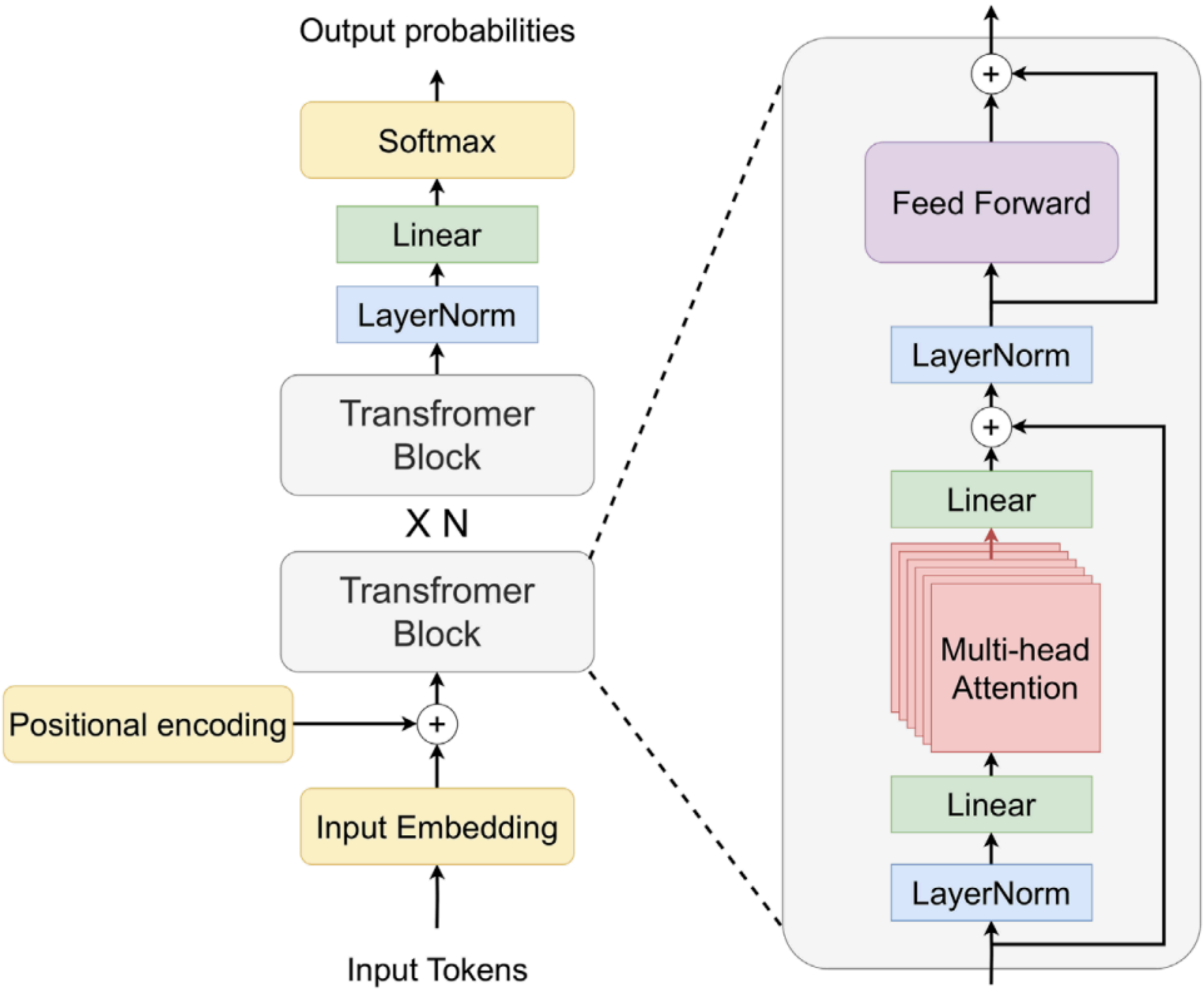


Fig.2.Decoder-only Transformer architecture[2]

First, let's calculate the parameters of the attention module. Its structure is as follows, involving four matrices: Q, K, V for the dot-product attention and the O matrix for the linear transformation after dot-product attention.

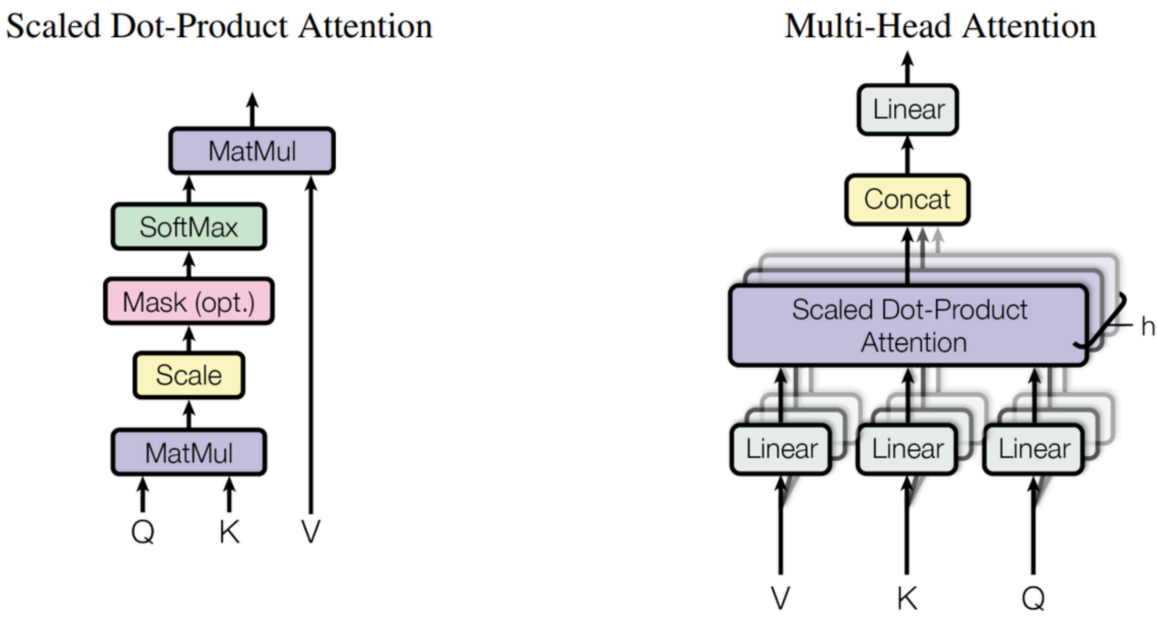


Fig.3. Multi-Head Attention[3]

Denote the hidden dimension of the transformer by h_1 .Given the weight matrices of a transformer layer by $w_q, w_k.w_v, w_o \in R^{h_1 \times h_1}$ .The size of the multi-head attention mechanism module is $n\_bytes \times 4 \times {h_1}^2$,where n_bytes indicate the number of bytes per param; for float32s, this is 4, for float16s, this is 2, etc.

The second part is the FFN (Feed Forward Network), which is essentially composed of two linear layers:

$$\mathrm{FFN}(x) = f_{relu}\left(0, xW_1 + b_1\right) W_2 + b_2$$

The hidden dimension of the second MLP layer by h_2 (typically four times the size of h_1). So,the size of FFN is $n\_bytes \times 2h_1h_2$.

Denote the total number of transformer layers by l ,the total weight of a LLM is

$$n\_bytes \times \left(4{h_1}^2 + 2h_1h_2\right)$$

(We ignore the embedding layer(s), which is relatively small)

Flops counting

This part is primarily referenced from [6].

> How many flops in a matmul?

> The computation for a matrix-vector multiplication is $2mn$ for $A \in \mathbb{R}^{m \times n}, b \in \mathbb{R}^n$ .A matrix-matrix is $2mnp$ for $A \in \mathbb{R}^{m \times n}, B \in \mathbb{R}^{n \times p}$.

If we consider only the calculation for K and V with one token, the total memory required is $n\_bytes \times 2lh_1{}^2 + n_{token} \times h_1$,and the flops are $n_{token} \times 2 \cdot 2lh_1{}^2$. Therefore, if we use half-precision (float16), the numbers for just the kv weights and computations are equal.If we perform inference using an A100 GPU, it has a FP16 Tensor Core performance of 312 TFLOPS and a bandwidth of 1555 GB/s.The difference between them is 208 times! We assume (correctly, this has been very well optimised) that we can start the computations while we load the weights.This means that if we're going to compute kv for one token, it'll take the same amount of time to compute for up to 208 tokens.

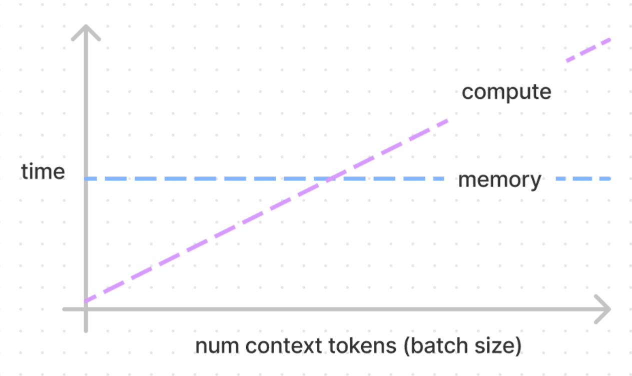


Fig.4.The number of tokens leads to different bounds.

KV Cache

Because the decoder works in an auto-regressive fashion,and will inference token by token.

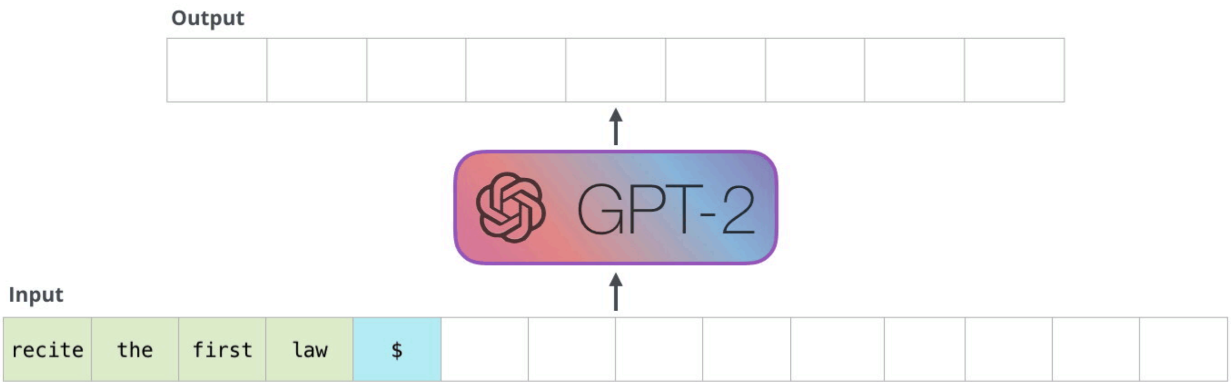
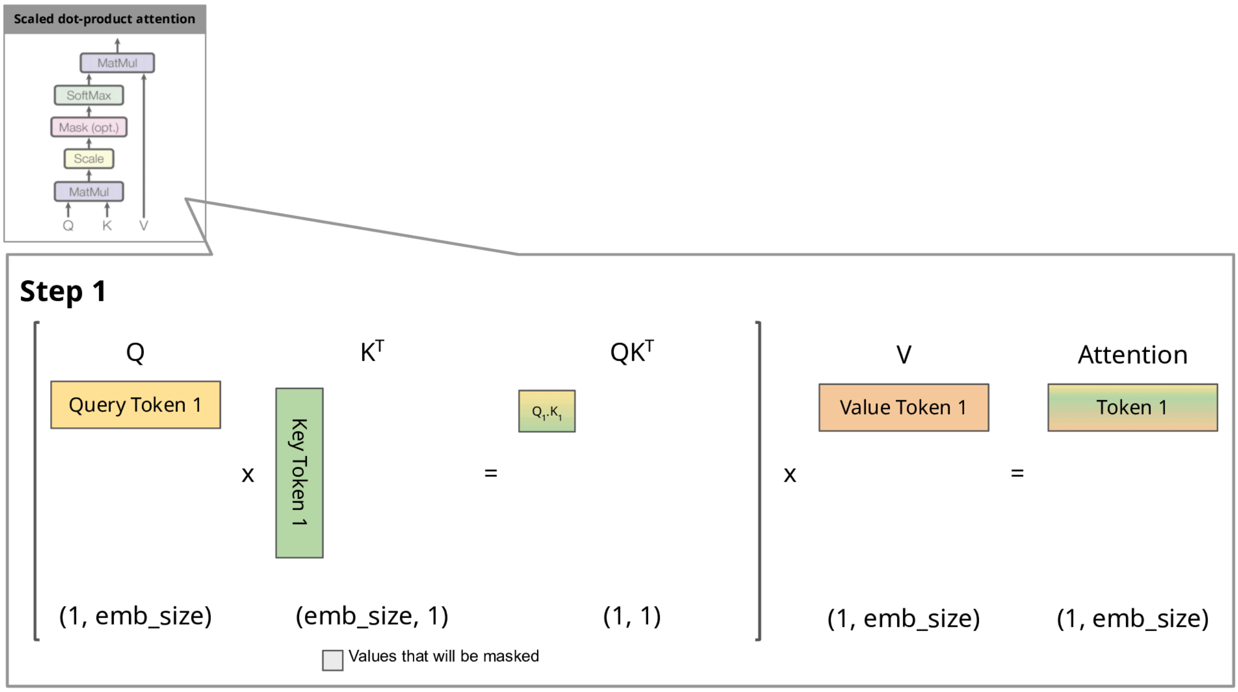


Fig.5.Auto-regreessive[4]

This autoregressive behavior repeats some operations and redundantly computes the K and V values generated by earlier tokens:



Zoom-in! (simplified without Scale and Softmax)

Fig.6.Step-by-step visualization of the scaled dot-product attention in the decoder[4]

Since the decoder is causal (i.e., the attention of a token only depends on its preceding tokens), at each generation step we are recalculating the same previous token attention, when we actually just want to calculate the attention for the new token.

This is where KV comes into play. By caching the previous Keys and Values, we can focus on only calculating the attention for the new token.

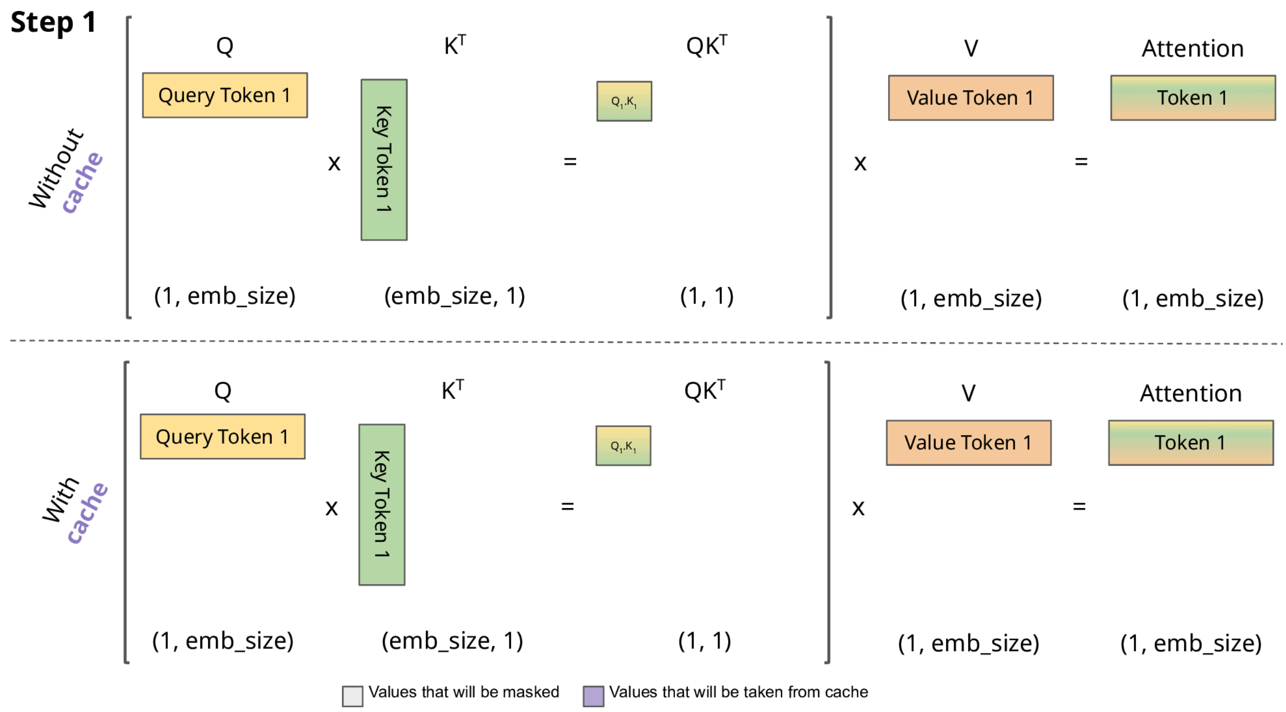


Fig.7.Comparison of scaled dot-product attention with and without KV caching[4]

Why is this optimization important? As seen in the picture above, the matrices obtained with KV caching are way smaller, which leads to faster matrix multiplications. The only downside is that it needs more RAM to cache the Key and Value states.

So let's calculate the memory of KV cache.Denote the the input sequence(prompt) length by s , the output sequence length by n ,and the batch size by b ,The total number of bytes to store the KV cache in peak is $n\_bytes \times 2 \times blh_1\,(s+n)$.

In the setting of FlexGen[5], the OPT-175B model (l = 96, h_1 = 12288, h_2 = 49152) takes 325 GB. With a batch size of b = 512, an input sequencelength s = 512, and an output sequence length of n = 32, the total memory required to store the KV cache is 1.2 TB,which is 3.8× the model weights, making the KV cache a new bottleneck of large-batch high-throughput inference.

FLOPs-bound vs Memory-bound

This part is primarily referenced from [7].

In addition to the analysis above, we also face a more severe memory-bound issue, especially with operations like Softmax.

The operations in a Transformer can be categorized into three types[7]:

Tensor Contractions: These are matrix-matrix multiplications (MMMs), batched MMMs, and in principle could include arbitrary tensor contractions.

Statistical Normalizations: These are operators such as softmax and layer normalization. These are less computeintensive than tensor contractions, and involve one or more reduction operation, the result of which is then applied via a map. This compute pattern means that data layout and vectorization is important for operator performance.

Element-wise Operators: These are the remaining operators: biases, dropout, activations, and residual connections.

Table 1. Proportions for operator classes in PyTorch.

Operator class	% flop	% Runtime
△ Tensor contraction	99.80	61.0
□ Stat. normalization	0.17	25.5
○ Element-wise	0.03	13.5

Table A.1. Flop analysis for BERT encoder layer. △ – tensor contraction, □ – statistical normalization, ○ – element-wise. MHA operators are filled black. We bold whichever is greater, % peak (compute-bound) or MUE (memory-bound). The speedup is computed for kernels in isolation, overall speedup may be different due to measurement overheads.

			Input	Output	PyTorch			Ours				
	Operator	Gflop	(1e6)	(1e6)	Gflop	Time (μs)	% peak	Time (μs)	% peak	MUE	Speedup	Kernel
Forward	▲ Q, K, V	25.770	7.34	12.58	25.782	333	56.2	306	**61.2**	12	1.08	—
	● Input bias	0.013	12.59	12.58	0.025	90	0.4	66	0.5	**78**	1.35	AIB
	▲ QK^T	4.295	8.39	33.55	4.329	189	16.5	143	21.8	**50**	1.32	—
	■ Scaled softmax	0.201	33.55	100.66	0.956	453	1.3	433	1.3	**32**	1.04	SM
	▲ Gamma	4.295	37.75	4.19	8.598	142	21.9	160	**19.4**	6	0.88	—
	▲ Out	8.590	5.24	4.19	8.686	136	45.9	120	**52**	10	1.13	—
	● Output bias	0.004	4.20	4.19	0.008	34	0.4					
	○ Dropout	0.004	4.19	8.39	0.014	37	0.3	102	0.1	**42**	1.68	DRLN
	○ Residual	0.004	8.39	4.19	0.008	36	0.3					
	□ LayerNorm	0.029	4.20	4.19	0.052	63	1.3					
	△ Linear	34.360	8.39	16.78	34.377	451	55.4	402	**62.1**	12	1.12	—
	○ Bias	0.017	16.78	16.78	0.034	116	0.4					
	○ ReLU	—	16.78	16.78	—	112	0	183	0.3	**76**	1.90	BRD
	○ Dropout	0.017	16.78	33.55	0.052	120	0.4					
	△ Linear	34.360	20.97	4.19	34.456	449	55.6	369	**67.6**	6	1.21	—
	○ Bias	0.004	4.20	4.19	0.008	35	0.3					
	○ Dropout	0.004	4.19	8.39	0.014	37	0.3	101	0.1	**43**	1.70	BDRLN
	○ Residual	0.004	8.39	4.19	0.008	37	0.3					
	□ LayerNorm	0.029	8.39	4.19	0.052	63	1.3					

We can observe that softmax occupies most of the computation time, and the Memory Usage Efficiency (MUE) value indicates that it is memory-bound.

There are currently many approaches aimed at optimizing memory to enhance the performance of large models, such as FlashAttention[8],vLLM[9]

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