LLM NOTES

A PREPRINT

August 22, 2025

Contents

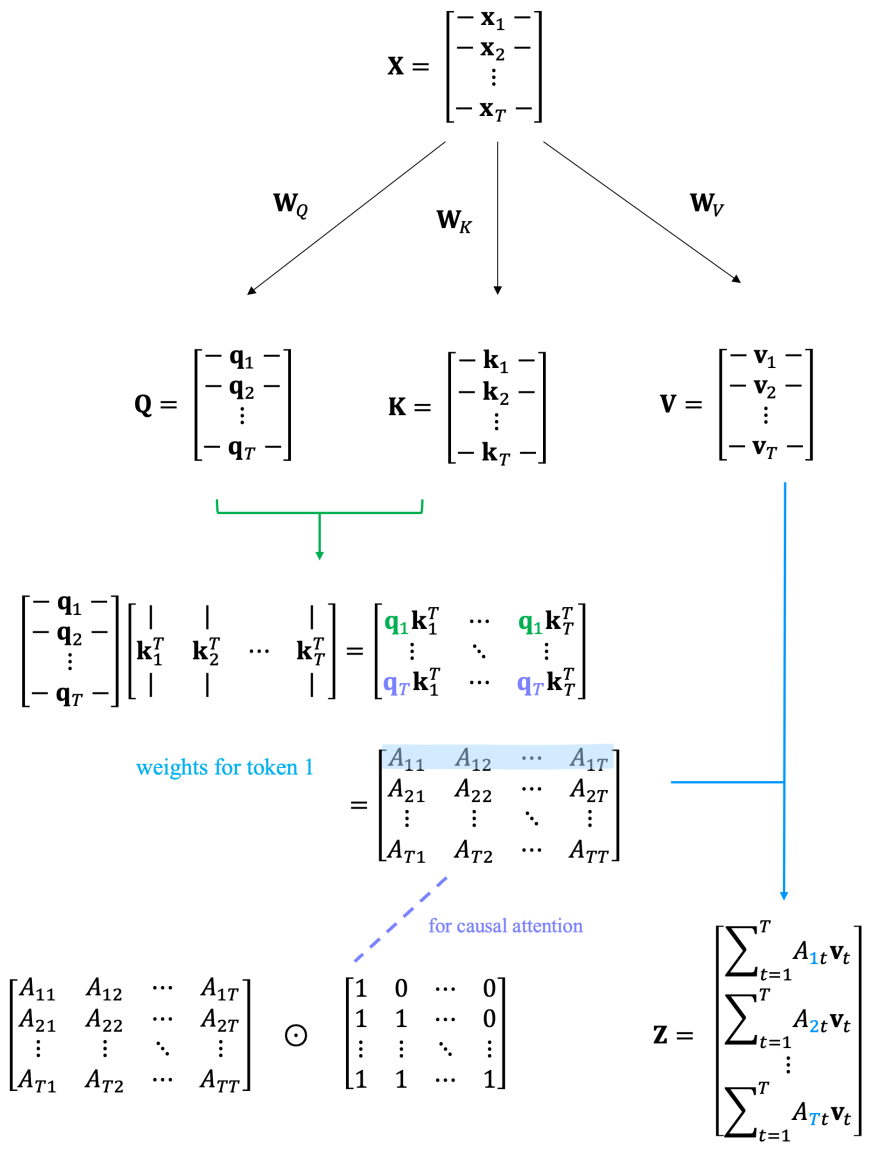
1 Common component

1.1 Self Attention

Given input $\boldsymbol{X} \in \mathbb{R}^{T\times D}$ where T is the sequence length and D is the embedding dimension, we have

$$\boldsymbol{Q} = \boldsymbol{X}\boldsymbol{W}_Q \in \mathbb{R}^{T\times d_k} \quad \boldsymbol{K} = \boldsymbol{X}\boldsymbol{W}_K \in \mathbb{R}^{T\times d_k} \quad \boldsymbol{V} = \boldsymbol{X}\boldsymbol{W}_V \in \mathbb{R}^{T\times d_v} \tag{1}$$

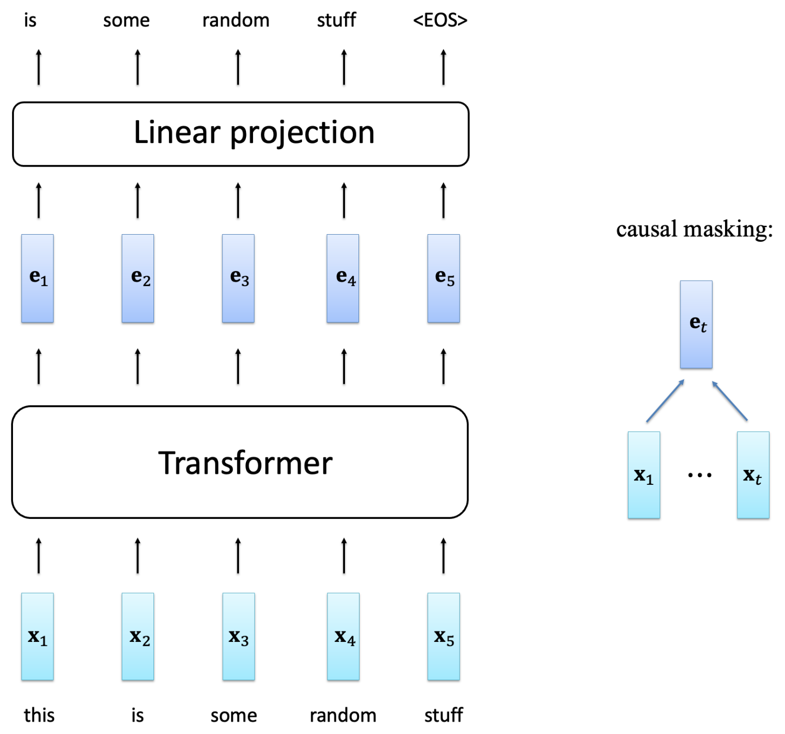
$$\text{Attn}(\boldsymbol{Q},\boldsymbol{K},\boldsymbol{V}) = \text{softmax}\left(\frac{\boldsymbol{Q}\boldsymbol{K}^\top}{\sqrt{d_k}}\right)\boldsymbol{V} \tag{2}$$


$\mathbf{X} = [\mathbf{x}_1; \mathbf{x}_2; \vdots; \mathbf{x}_T]$
$\mathbf{W}_Q$
$\mathbf{W}_K$
$\mathbf{W}_V$
$\mathbf{Q} = [\mathbf{q}_1; \mathbf{q}_2; \vdots; \mathbf{q}_T]$
$\mathbf{K} = [\mathbf{k}_1; \mathbf{k}_2; \vdots; \mathbf{k}_T]$
$\mathbf{V} = [\mathbf{v}_1; \mathbf{v}_2; \vdots; \mathbf{v}_T]$
$[\mathbf{q}_1; \mathbf{q}_2; \vdots; \mathbf{q}_T][\mathbf{k}_1^T \; \mathbf{k}_2^T \cdots \mathbf{k}_T^T] = [\mathbf{q}_1\mathbf{k}_1^T \cdots \mathbf{q}_1\mathbf{k}_T^T; \vdots \ddots \vdots; \mathbf{q}_T\mathbf{k}_1^T \cdots \mathbf{q}_T\mathbf{k}_T^T]$
weights for token 1
$= [A_{11}\; A_{12} \cdots A_{1T}; A_{21}\; A_{22} \cdots A_{2T}; \vdots; A_{T1}\; A_{T2} \cdots A_{TT}]$
for causal attention
$[A_{11}\; A_{12} \cdots A_{1T}; A_{21}\; A_{22} \cdots A_{2T}; \vdots; A_{T1}\; A_{T2} \cdots A_{TT}] \odot [1\; 0 \cdots 0; 1\; 1 \cdots 0; \vdots; 1\; 1 \cdots 1]$
$\mathbf{Z} = [\sum_{t=1}^T A_{1t}\mathbf{v}_t; \sum_{t=1}^T A_{2t}\mathbf{v}_t; \vdots; \sum_{t=1}^T A_{Tt}\mathbf{v}_t]$

1.2 Causal Masking & Unsupervised Pretraining

Given an input with size $[B, T, D]$, for each $[T, D]$, it is a sentence itself, like "this is some random stuff" shown below. To do efficient training, now for each token in the sentence, the transformer needs to predict its next token. This is done by using causal masking:

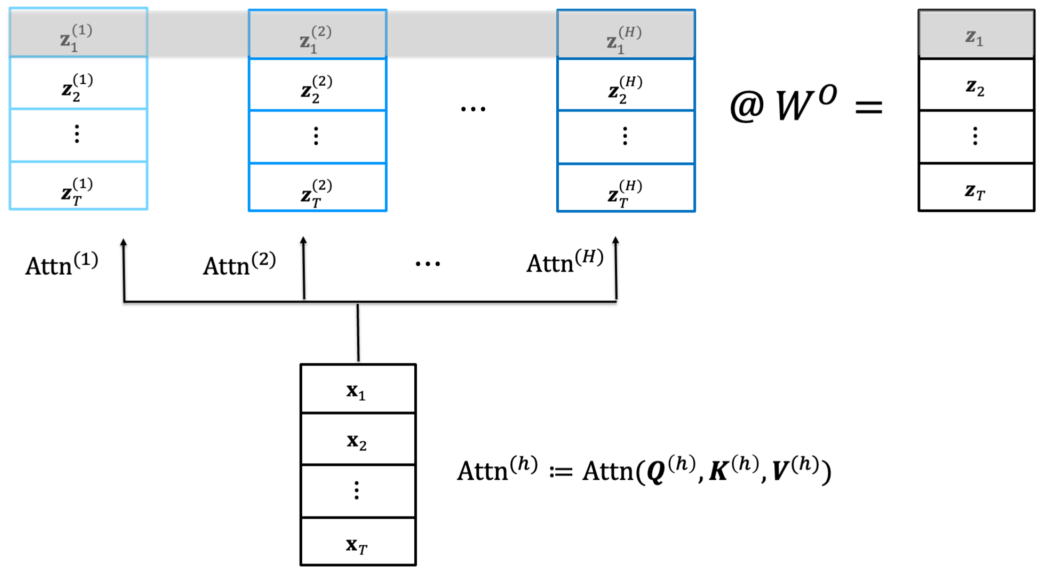
for t-th token, it is only allowed to look at $\boldsymbol{x}_{1:t}$.



In the end, for each data in the batch, it will have T prediction assuming there's no padding. So in the end, we average $B \times T$ cross entropy loss.

1.3 Multi-Head Attention

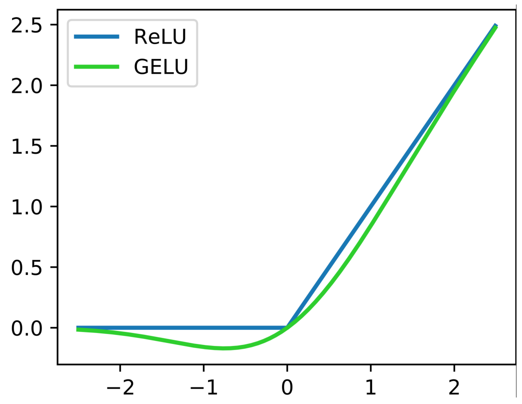
In multi-head attention, input $\boldsymbol{X}$ is first passed through H self-attention layer in parallel. Then, the output from each head is concatenated together and fused by a linear projection



1.4 Activation Functions

ReLU $f(x) = \max(0, x)$

GeLU $f(x) = x\Phi(x)$, $\Phi(x)$ is the CDF of Gaussian



GLU (gated activations) Vanilla MLP in transformer has the path

$$\boldsymbol{x} = \text{fc1}(\boldsymbol{x}; \boldsymbol{W}_1) \tag{3}$$
$$\boldsymbol{x} = \text{activation}(\boldsymbol{x}) \quad \text{(simple non-linear function, no parameter)}$$
$$\boldsymbol{x} = \text{fc2}(\boldsymbol{x}; \boldsymbol{W}_2) \tag{4}$$

GLU and its variants combine the first fully connected layer and the activation function together:

$$\boldsymbol{x} = \text{activation}(\boldsymbol{x}; \boldsymbol{W}, \boldsymbol{V}) \tag{5}$$
$$\boldsymbol{x} = \text{fc2}(\boldsymbol{x}; \boldsymbol{W}_2) \tag{6}$$

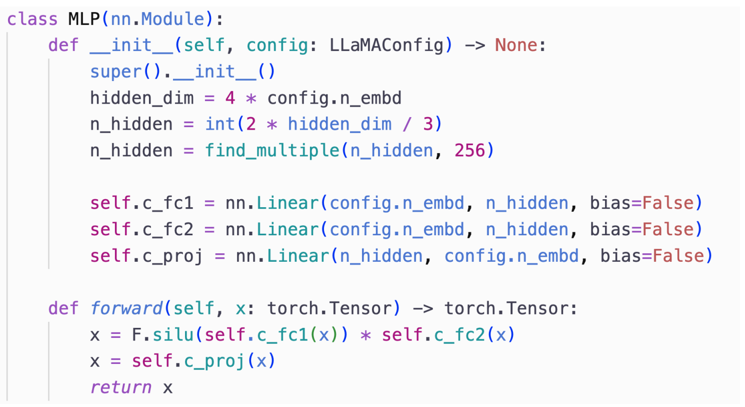
where

$$\text{GLU}(\boldsymbol{x}, \boldsymbol{W}, \boldsymbol{V}) = \sigma(x\boldsymbol{W}) \odot (\boldsymbol{x}\boldsymbol{V}) \tag{7}$$
$$\text{GeGLU}(\boldsymbol{x}, \boldsymbol{W}, \boldsymbol{V}) = \text{GELU}(\boldsymbol{x}\boldsymbol{W}) \odot (\boldsymbol{x}\boldsymbol{V}) \tag{8}$$
$$\text{SwiGLU}(\boldsymbol{x}, \boldsymbol{W}, \boldsymbol{V}) = \text{Swish}_1(\boldsymbol{x}\boldsymbol{W}) \odot (\boldsymbol{x}\boldsymbol{V}) \tag{9}$$

where $\text{Swish}_\beta(\boldsymbol{x}) = \boldsymbol{x}\sigma(\beta\boldsymbol{x})$, *i.e.*, $\text{Swish}_1(\boldsymbol{x}) = \boldsymbol{x}\sigma(\boldsymbol{x})$. Sigmoid is applied element-wise on the matrix.

Here since the gating part is element-wise, it allows the MLP to filter out unimportant features for each input. To make sure the computation cost is still more or less the same as vanilla MLP, the hidden dimension is usually sized down a bit.

Code wise, SwiGLU looks like this



```python
class MLP(nn.Module):
    def __init__(self, config: LLaMAConfig) -> None:
        super().__init__()
        hidden_dim = 4 * config.n_embd
        n_hidden = int(2 * hidden_dim / 3)
        n_hidden = find_multiple(n_hidden, 256)

        self.c_fc1 = nn.Linear(config.n_embd, n_hidden, bias=False)
        self.c_fc2 = nn.Linear(config.n_embd, n_hidden, bias=False)
        self.c_proj = nn.Linear(n_hidden, config.n_embd, bias=False)

    def forward(self, x: torch.Tensor) -> torch.Tensor:
        x = F.silu(self.c_fc1(x)) * self.c_fc2(x)
        x = self.c_proj(x)
        return x
```

Figure 1: SwiGLU

2 Inference Specific

2.1 KV-Cache

Causal masking is used during training to prevent the model from looking into future tokens to cheat. During inference, technically we don't really need to mask things as there is no way for the model to cheat. But the causal mask is still kept to preserve the same computation pattern as training.

Apart from allowing us to use the model as it is, causal masking during inference also allows us to reuse things. Let's look at the pipeline of generating:

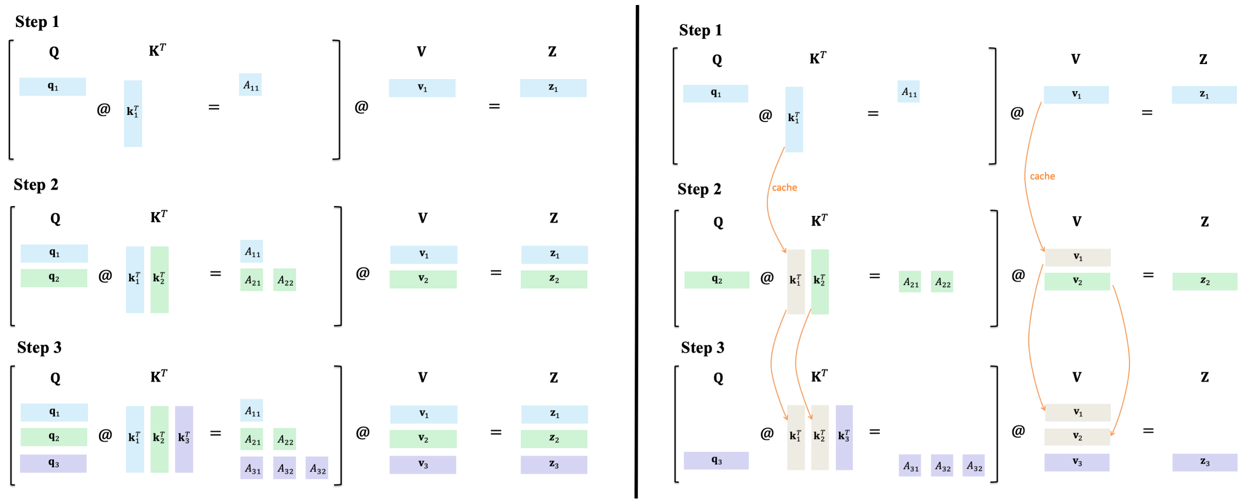


Figure 2: Left: no cache. Right: KV cache. Coloured parts are the actual computation.

KV-cache is built on this two observations:

- At each time step t, due to causal masking $\boldsymbol{k}_{<t}$ and $\boldsymbol{v}_{<t}$ will remain the same
- To predict <token$_{t+1}$> we only need embedding of <token$_t$>.

Therefore, we can make prediction efficiently by drop redundant and unnecessary computation. At each time step t, we will only compute

$$\boldsymbol{q}_t, \boldsymbol{k}_t, \boldsymbol{v}_t \tag{10}$$

instead of $\boldsymbol{q}_{1:t}, \boldsymbol{k}_{1:t}, \boldsymbol{v}_{1:t}$.

2.2 Multi-Query Attention

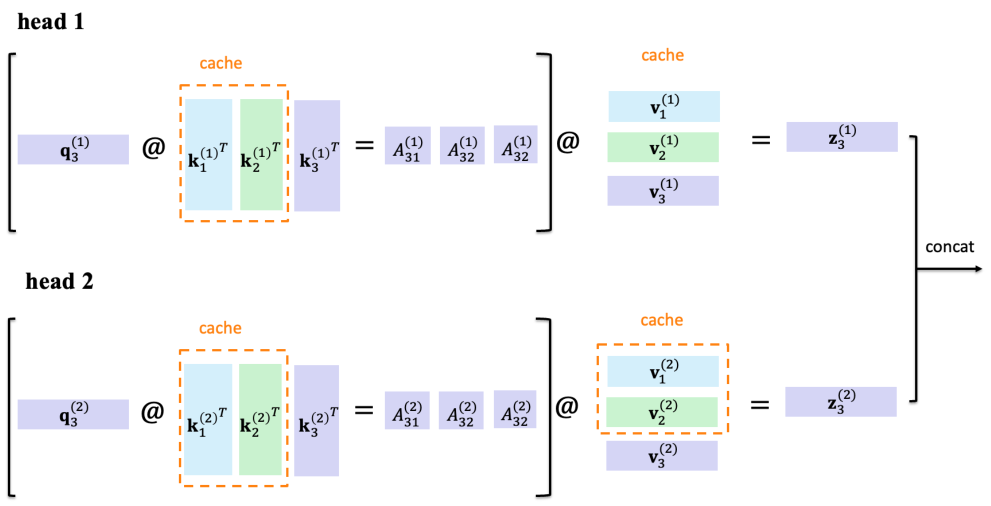
In KV-cache, at time step t, the past $t-1$ keys and values are cached, which corresponds to $2 * n_h * (t-1) * h_s$ memory. When t gets larger, storing them all on a single GPU will be impossible and the loading will slow things down.

The idea of multi-query attention (MQA) is quite simple. In MHA, different heads have different query, key and value projection matrix. In MQA, the key and value projection matrics will be shared across all heads, only query project matrix will be different:

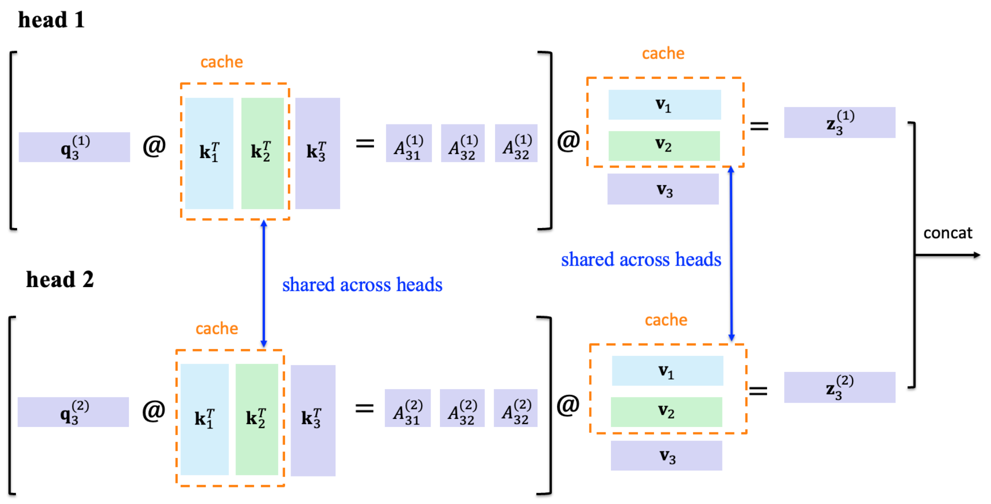
$$\begin{array}{ll} \text{MHA} & \text{MQA} \\ \boldsymbol{Q}^{(h)} = \boldsymbol{W}_Q^{(h)}\boldsymbol{X} & \boldsymbol{Q}^{(h)} = \boldsymbol{W}_Q^{(h)}\boldsymbol{X} \\ \boldsymbol{K}^{(h)} = \boldsymbol{W}_K^{(h)}\boldsymbol{X} & \boldsymbol{K}^{(h)} = \boldsymbol{W}_K\boldsymbol{X} \quad \text{(shared across heads)} \\ \boldsymbol{V}^{(h)} = \boldsymbol{W}_V^{(h)}\boldsymbol{X} & \boldsymbol{V}^{(h)} = \boldsymbol{W}_V\boldsymbol{X} \quad \text{(shared across heads)} \end{array} \tag{11}$$

This way, we only need to store one set of KV-cache and share it across all heads.

Step 3, MHA

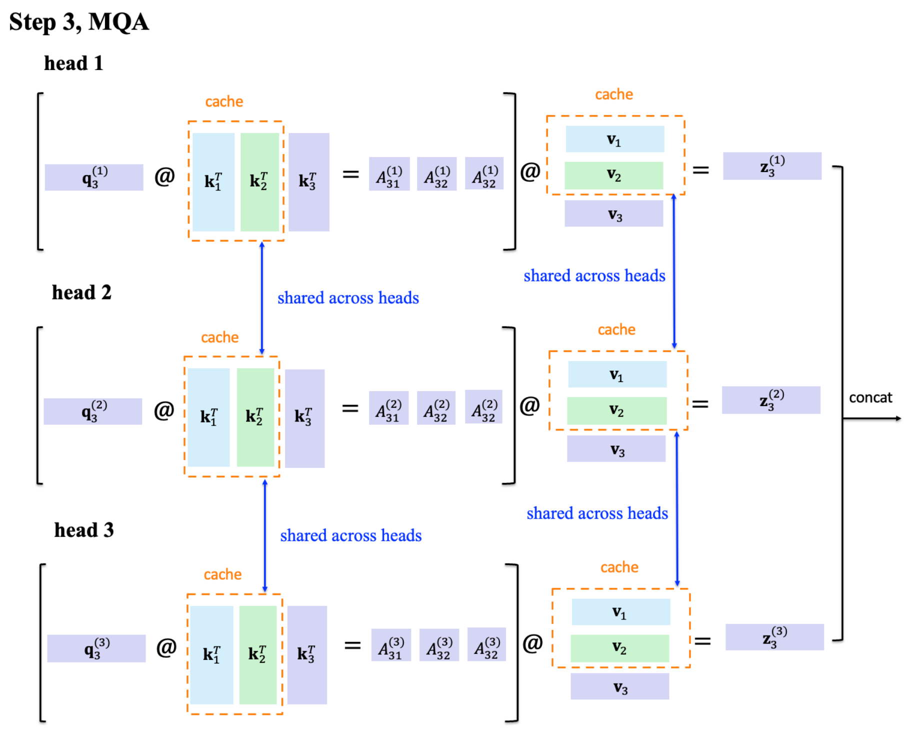


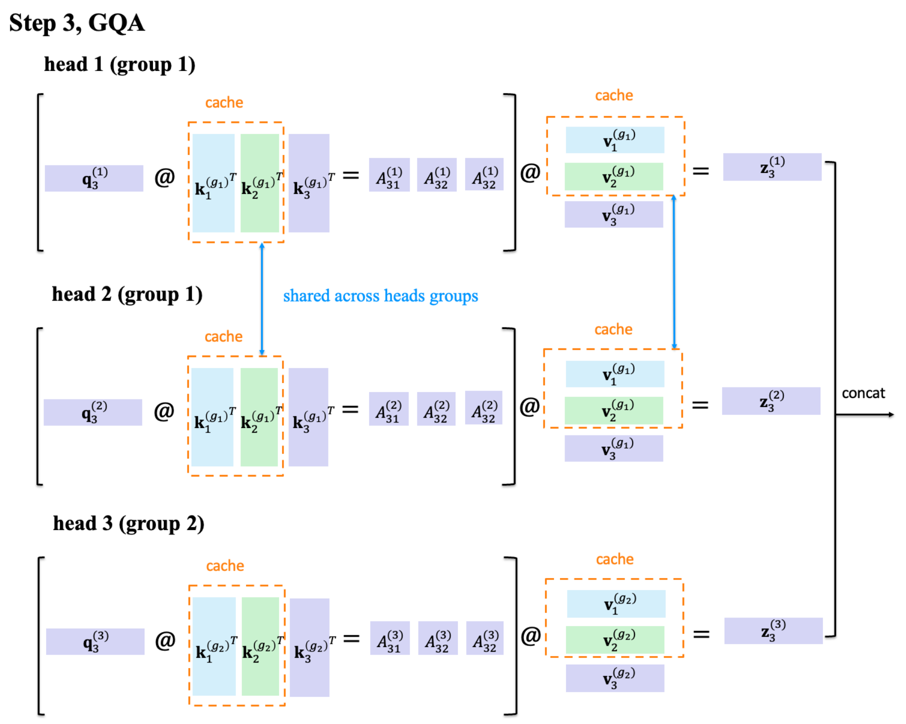
Step 3, MQA



2.3 Grouped-Query Attention

Sharing the key and value projection across all attention heads might be too brutal, in grouped-query attention, $\boldsymbol{W}_K$ and $\boldsymbol{W}_V$ are shared in grouped heads. So basically different groups have different $\boldsymbol{K}$ and $\boldsymbol{V}$.


Step 3, MQA
head 1
head 2
head 3
cache
shared across heads
concat
$\mathbf{q}_3^{(1)}$ @ $\mathbf{k}_1^T$ $\mathbf{k}_2^T$ $\mathbf{k}_3^T$ = $A_{31}^{(1)}$ $A_{32}^{(1)}$ $A_{32}^{(1)}$ @ $\mathbf{v}_1$ $\mathbf{v}_2$ $\mathbf{v}_3$ = $\mathbf{z}_3^{(1)}$
$\mathbf{q}_3^{(2)}$ @ $\mathbf{k}_1^T$ $\mathbf{k}_2^T$ $\mathbf{k}_3^T$ = $A_{31}^{(2)}$ $A_{32}^{(2)}$ $A_{32}^{(2)}$ @ $\mathbf{v}_1$ $\mathbf{v}_2$ $\mathbf{v}_3$ = $\mathbf{z}_3^{(2)}$
$\mathbf{q}_3^{(3)}$ @ $\mathbf{k}_1^T$ $\mathbf{k}_2^T$ $\mathbf{k}_3^T$ = $A_{31}^{(3)}$ $A_{32}^{(3)}$ $A_{32}^{(3)}$ @ $\mathbf{v}_1$ $\mathbf{v}_2$ $\mathbf{v}_3$ = $\mathbf{z}_3^{(3)}$


Step 3, GQA
head 1 (group 1)
head 2 (group 1)
head 3 (group 2)
cache
shared across heads groups
concat
$\mathbf{q}_3^{(1)}$ @ $\mathbf{k}_1^{(g_1)T}$ $\mathbf{k}_2^{(g_1)T}$ $\mathbf{k}_3^{(g_1)T}$ = $A_{31}^{(1)}$ $A_{32}^{(1)}$ $A_{32}^{(1)}$ @ $\mathbf{v}_1^{(g_1)}$ $\mathbf{v}_2^{(g_1)}$ $\mathbf{v}_3^{(g_1)}$ = $\mathbf{z}_3^{(1)}$
$\mathbf{q}_3^{(2)}$ @ $\mathbf{k}_1^{(g_1)T}$ $\mathbf{k}_2^{(g_1)T}$ $\mathbf{k}_3^{(g_1)T}$ = $A_{31}^{(2)}$ $A_{32}^{(2)}$ $A_{32}^{(2)}$ @ $\mathbf{v}_1^{(g_1)}$ $\mathbf{v}_2^{(g_1)}$ $\mathbf{v}_3^{(g_1)}$ = $\mathbf{z}_3^{(2)}$
$\mathbf{q}_3^{(3)}$ @ $\mathbf{k}_1^{(g_2)T}$ $\mathbf{k}_2^{(g_2)T}$ $\mathbf{k}_3^{(g_2)T}$ = $A_{31}^{(3)}$ $A_{32}^{(3)}$ $A_{32}^{(3)}$ @ $\mathbf{v}_1^{(g_2)}$ $\mathbf{v}_2^{(g_2)}$ $\mathbf{v}_3^{(g_2)}$ = $\mathbf{z}_3^{(3)}$

3 Positional Embedding

3.1 RoPE

Once and for all vs add all the time In vanilla position embedding, it adds a vector at the beginning of the NN once and for all. The positional encoding might get lost in deep networks. If we look at the computation in transformer, the position only matters in the attention score computation. So RoPE encode position into query and key vector in every attention layer instead.

Absolute position vs relative position Another thing RoPE did is encode the *relative* position. The idea is, for a given word when computing its attention score, only the relative position between this word and other word should matter. Specifically, if we add the position into the computation of query and key computation:

$$\boldsymbol{q}_m \triangleq f_q(\boldsymbol{x}_m, m), \qquad \boldsymbol{k}_n \triangleq f_k(\boldsymbol{x}_n, n) \tag{12}$$

Then the attention score (which is an inner product) should only depends on the word embeddings $\boldsymbol{x}_m$, $\boldsymbol{x}_n$ and their relative position $m - n$:

$$\boldsymbol{q}_m^T \boldsymbol{k}_n = \langle f_q(\boldsymbol{x}_m, m), f_k(\boldsymbol{x}_n, n)\rangle = g(\boldsymbol{x}_m, \boldsymbol{x}_n, m - n) \tag{13}$$

One simple choice for $f_{\{q,k\}}(\boldsymbol{x}_m, m)$ is rotate them:

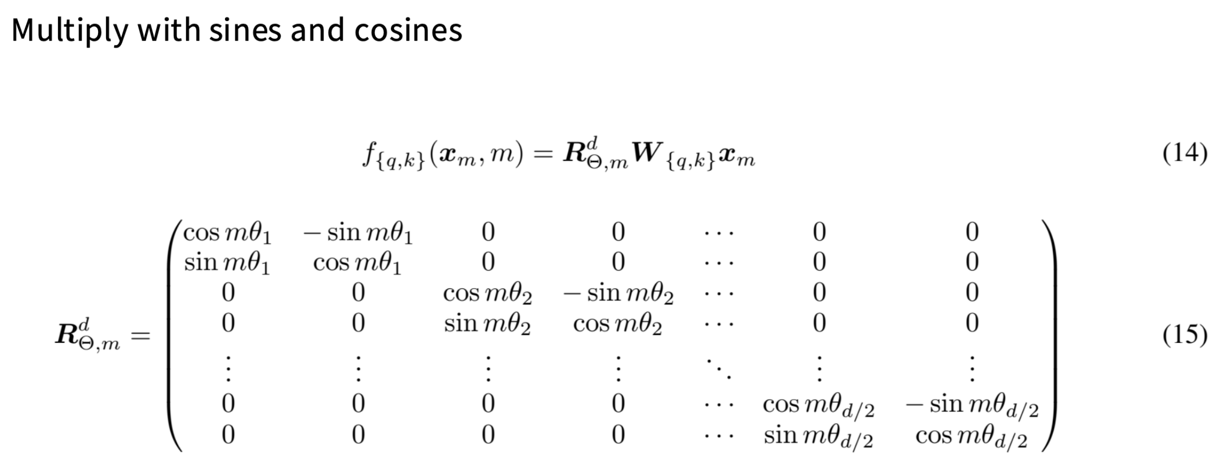
$$f_{\{q,k\}}(\boldsymbol{x}_m, m) = \boldsymbol{R}(m)\boldsymbol{W}_{\{q,k\}}\boldsymbol{x}_m \tag{14}$$

where $\boldsymbol{R}(m)$ is a rotation matrix whose angle depends on m.

Define $\widetilde{\boldsymbol{q}}_m = \boldsymbol{W}_q \boldsymbol{x}_m$ and $\widetilde{\boldsymbol{k}}_m = \boldsymbol{W}_k \boldsymbol{x}_m$, now we have

$$(\boldsymbol{R}(m)\boldsymbol{W}_q\boldsymbol{x}_m)^T(\boldsymbol{R}(n)\boldsymbol{W}_k\boldsymbol{x}_n) = \widetilde{\boldsymbol{q}}_m^T \boldsymbol{R}(m)^T \boldsymbol{R}(n) \widetilde{\boldsymbol{k}}_n = \widetilde{\boldsymbol{q}}_m^T \boldsymbol{R}(n-m) \widetilde{\boldsymbol{k}}_n \tag{15}$$

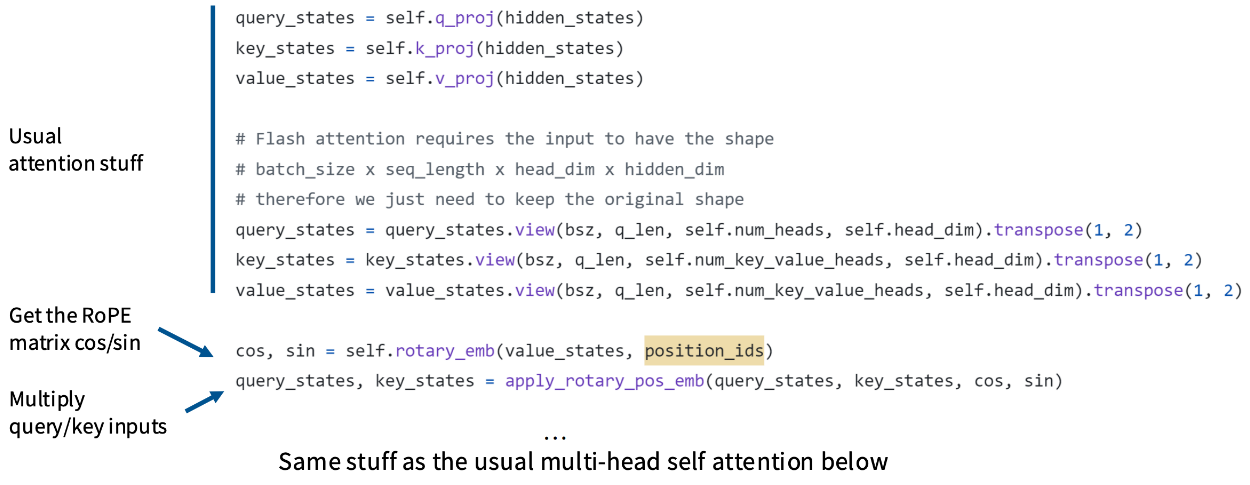
Because rotation in higher dimension than 2D is not deterministic, it does a funky thing to split query vector in a bunch of 2D pairs, and then rotate them each.



Multiply with sines and cosines

$$f_{\{q,k\}}(\boldsymbol{x}_m, m) = \boldsymbol{R}^d_{\Theta,m}\boldsymbol{W}_{\{q,k\}}\boldsymbol{x}_m \tag{14}$$

$$\boldsymbol{R}^d_{\Theta,m} = \begin{pmatrix} \cos m\theta_1 & -\sin m\theta_1 & 0 & 0 & \cdots & 0 & 0 \\ \sin m\theta_1 & \cos m\theta_1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & \cos m\theta_2 & -\sin m\theta_2 & \cdots & 0 & 0 \\ 0 & 0 & \sin m\theta_2 & \cos m\theta_2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & \cos m\theta_{d/2} & -\sin m\theta_{d/2} \\ 0 & 0 & 0 & 0 & \cdots & \sin m\theta_{d/2} & \cos m\theta_{d/2} \end{pmatrix} \tag{15}$$


Usual attention stuff
Get the RoPE matrix cos/sin
Multiply query/key inputs
Same stuff as the usual multi-head self attention below

```python
query_states = self.q_proj(hidden_states)
key_states = self.k_proj(hidden_states)
value_states = self.v_proj(hidden_states)

# Flash attention requires the input to have the shape
# batch_size x seq_length x head_dim x hidden_dim
# therefore we just need to keep the original shape
query_states = query_states.view(bsz, q_len, self.num_heads, self.head_dim).transpose(1, 2)
key_states = key_states.view(bsz, q_len, self.num_key_value_heads, self.head_dim).transpose(1, 2)
value_states = value_states.view(bsz, q_len, self.num_key_value_heads, self.head_dim).transpose(1, 2)

cos, sin = self.rotary_emb(value_states, position_ids)
query_states, key_states = apply_rotary_pos_emb(query_states, key_states, cos, sin)

...
```

Note: embedding at *each attention operation* to enforce position invariance

References