

Transformer with PyTorch

Richard Xu

December 15, 2025

1 Dot-Product Attention (DPA)

1.1 single query \mathbf{q}

The very famous paper, “Attention Is All You Need” (Google) [1] introduced the concept of attention, which is a key component of the Transformer architecture

We are given a single query vector \mathbf{q} , and matrix of keys \mathbf{K} and values \mathbf{V} :

$$\mathbf{q} \equiv \underbrace{\begin{bmatrix} - & \mathbf{q} & - \end{bmatrix}}_{\in \mathbb{R}^{1 \times d_k}} \quad \mathbf{K} \equiv \underbrace{\begin{bmatrix} - & \mathbf{k}_1 & - \\ - & \dots & - \\ - & \mathbf{k}_m & - \end{bmatrix}}_{\in \mathbb{R}^{m \times d_k}} \quad \mathbf{V} \equiv \underbrace{\begin{bmatrix} - & \mathbf{v}_1 & - \\ - & \dots & - \\ - & \mathbf{v}_m & - \end{bmatrix}}_{\in \mathbb{R}^{m \times d_v}} \quad (1)$$

and let $(\mathbf{q}, \mathbf{K}, \mathbf{V})$ be tuples. Bear in mind that in Eq.(1), \mathbf{q} is a row vector. This is to conform with Eq.(7), where all the $\mathbf{Q}, \mathbf{K}, \mathbf{V}$ have each element expressed as a row vector.

the Dot-Product Attention (DPA) is defined as:

$$\begin{aligned} \implies \mathbf{qK}^\top &= \begin{bmatrix} \underbrace{\mathbf{qk}_1^\top}_{\in \mathbb{R}} & \dots & \underbrace{\mathbf{qk}_m^\top}_{\in \mathbb{R}} \end{bmatrix} \\ \implies A(\mathbf{q}, \mathbf{K}, \mathbf{V}) &\equiv \text{softmax}(\mathbf{qK}^\top)\mathbf{V} \\ &= \text{softmax}\left(\begin{bmatrix} \mathbf{qk}_1^\top & \dots & \mathbf{qk}_m^\top \end{bmatrix}\right) \begin{bmatrix} - & \mathbf{v}_1 & - \\ - & \dots & - \\ - & \mathbf{v}_m & - \end{bmatrix} \\ &= \sum_{i=1}^m \underbrace{\frac{\exp[\mathbf{qk}_i^\top]}{\sum_j \exp[\mathbf{qk}_j^\top]}}_{\mathbf{a}_i} \mathbf{v}_i \\ &\in \mathbb{R}^{d_v} \end{aligned} \quad (2)$$

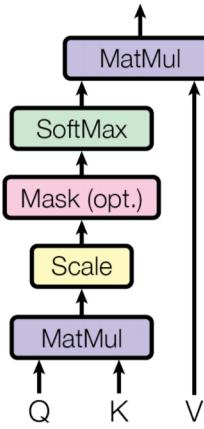
1.2 Scaled Dot-Product Attention (SDPA)

the problem starts as d_k becomes larger, variance of \mathbf{qK}^\top increases. hen as a result, some dot product values gets very large, with $\exp(\cdot)$, softmax \mathbf{p} gets peaky! Remember derivative of cross-entropy between softmax \mathbf{p} and \mathbf{y} is:

$$\begin{aligned} \mathbf{C}(\mathbf{z}) &= -\sum_{k=1}^K y_k [\log(p_k)] = -\sum_{k=1}^K y_k \left[\log \left(\frac{\exp^{z_k}}{\sum_l \exp^{z_l}} \right) \right] \\ \implies \frac{\mathbf{C}(\mathbf{z})}{\partial \mathbf{z}} &= (\mathbf{p} - \mathbf{y}) \end{aligned} \quad (3)$$

with a peaky softmax, lots of element in gradient vector $\frac{\mathbf{C}(\mathbf{z})}{\partial \mathbf{z}}$ are zero!
the solution then becomes that of scaling by length of d_k :

$$A(\mathbf{Q}, \mathbf{K}, \mathbf{V}) = \text{softmax} \left(\frac{\mathbf{Q}\mathbf{K}^\top}{\sqrt{d_k}} \right) \mathbf{V} \quad (4)$$



“mask (opt.)” is only used at decoder during training

1.3 in the case of “seq2seq with attention”

we have:

$$\begin{aligned} \mathbf{q} &\equiv \mathbf{h}_i \\ \mathbf{k}_i &= \mathbf{v}_i = \mathbf{z}_i \\ \implies A(\mathbf{q}, \mathbf{K}, \mathbf{V}) &\equiv A(\mathbf{h}_i, \mathbf{Z}, \mathbf{Z}) = c_i \end{aligned} \quad (5)$$

where c_i is our conditional or context vector. In order to confirm the notation in Eq.(1), we have assumed \mathbf{h}_i to be a row vector, so instead of $\mathbf{h}_i^\top \mathbf{z}_j$, we express it as $\mathbf{h}_i \mathbf{z}_j^\top$:

$$a_{ij} = \frac{\exp(e_{i,j})}{\sum_{t=1}^m \exp(e_{i,t})} = \frac{\exp(\mathbf{h}_i \mathbf{z}_j^\top)}{\sum_{t=1}^m \exp(\mathbf{h}_i \mathbf{z}_t^\top)} \quad (6)$$

1.4 multiple queries

now we have multiple $\mathbf{Q} = \{\mathbf{q}_i\}$, e.g., N words in the decoder, we now have \mathbf{Q} , \mathbf{K} and \mathbf{V} expressed as:

$$\mathbf{Q} \equiv \underbrace{\begin{bmatrix} - & \mathbf{q}_1 & - \\ - & \dots & - \\ - & \mathbf{q}_n & - \end{bmatrix}}_{n \times d_k} \quad \mathbf{K} \equiv \underbrace{\begin{bmatrix} - & \mathbf{k}_1 & - \\ - & \dots & - \\ - & \mathbf{k}_m & - \end{bmatrix}}_{m \times d_k} \quad \mathbf{V} \equiv \underbrace{\begin{bmatrix} - & \mathbf{v}_1 & - \\ - & \dots & - \\ - & \mathbf{v}_m & - \end{bmatrix}}_{m \times d_v} \quad (7)$$

$A(\mathbf{Q}, \mathbf{K}, \mathbf{V}) = \text{softmax}(\mathbf{Q}\mathbf{K}^\top)\mathbf{V}$ can be expressed as follows:

$$\Rightarrow \mathbf{Q}\mathbf{K}^\top = \begin{bmatrix} \mathbf{q}_1\mathbf{k}_1^\top & \dots & \mathbf{q}_1\mathbf{k}_m^\top \\ \dots & \dots & \dots \\ \mathbf{q}_n\mathbf{k}_1^\top & \dots & \mathbf{q}_n\mathbf{k}_m^\top \end{bmatrix} \quad (8)$$

in the case of self attention, where $m = n$, then $\mathbf{Q}\mathbf{K}^\top$ is a square matrix of $n \times n$.

$$\begin{aligned} \Rightarrow \mathbf{O} &\equiv \text{softmax}(\mathbf{Q}\mathbf{K}^\top)\mathbf{V} \\ &= \mathbf{A}\mathbf{V} \\ &= \underbrace{\begin{bmatrix} \text{softmax}([\mathbf{q}_1\mathbf{k}_1^\top \dots \mathbf{q}_1\mathbf{k}_m^\top]) \\ \vdots \\ \text{softmax}([\mathbf{q}_n\mathbf{k}_1^\top \dots \mathbf{q}_n\mathbf{k}_m^\top]) \end{bmatrix}}_{n \times m} \underbrace{\begin{bmatrix} - & \mathbf{v}_1 & - \\ - & \dots & - \\ - & \mathbf{v}_m & - \end{bmatrix}}_{m \times d_v} \\ &= \underbrace{\begin{bmatrix} \sum_{i=1}^m \underbrace{\frac{\exp[\mathbf{q}_1\mathbf{k}_i^\top]}{\sum_j \exp[\mathbf{q}_1\mathbf{k}_j^\top]}}_{\text{row vector } 1 \text{ in } \mathbb{R}^{d_v}} \mathbf{v}_i \\ \vdots \\ \sum_{i=1}^m \underbrace{\frac{\exp[\mathbf{q}_n\mathbf{k}_i^\top]}{\sum_j \exp[\mathbf{q}_n\mathbf{k}_j^\top]}}_{\text{row vector } n \text{ in } \mathbb{R}^{d_v}} \mathbf{v}_i \end{bmatrix}}_{n \times d_v} \quad (9) \end{aligned}$$

looking at the i -th row of \mathbf{A} , i.e., \mathbf{a}_i , it can be expressed as a weighted sum of the rows of \mathbf{V} .

$$\mathbf{a}_i\mathbf{V} = [a_{i,1} \dots a_{i,m}] \begin{bmatrix} - & \mathbf{v}_1 & - \\ \vdots & \ddots & \vdots \\ - & \mathbf{v}_m & - \end{bmatrix} = \sum_{i=1}^m a_{i,j} \mathbf{v}_i \quad (10)$$

The output \mathbf{O} 's dimension has number of row to be the same as \mathbf{Q} , and column dimension to be d_V . This means that it has the number of elements of \mathbf{Q} , and each element is the same dimension as \mathbf{v}_i .

2 Self-attention and Multi-head Attention

The Transformer architecture uses multi-head attention, which is a key component of the Transformer architecture. Generally, input vectors are $(\mathbf{Q}, \mathbf{K}, \mathbf{V})$

When we let:

$$\mathbf{Q} = \mathbf{X}\mathbf{W}_Q, \quad \mathbf{K} = \mathbf{X}\mathbf{W}_K, \quad \mathbf{V} = \mathbf{X}\mathbf{W}_V \quad (11)$$

and let:

$$m = n = T \quad (12)$$

we achieved self-attention, in summary:

1. for each head i , linear transform \mathbf{X} into several lower dimensional spaces via projection matrices $\mathbf{W}_i^q, \mathbf{W}_i^k, \mathbf{W}_i^v$ to obtain:

$$\mathbf{O}^{(i)} = \text{SDPA}(\mathbf{X}\mathbf{W}_Q^{(i)}, \mathbf{X}\mathbf{W}_K^{(i)}, \mathbf{X}\mathbf{W}_V^{(i)}) \quad (13)$$

2. each iteration i correspond to one “layer” of the [“linear”, “Scaled Dot-Product Attention”] on the figure 1
3. then concatenate to produce output:

with multi-head attention, we have multiple \mathbf{O}_i s therefore, we need to mix them together:

$$\mathbf{Y} = \underbrace{\text{concat}(\mathbf{O}_1, \dots, \mathbf{O}_h)}_{T \times d_{\text{model}}} \underbrace{\mathbf{W}_O}_{d_{\text{model}} \times d_{\text{model}}} \quad (14)$$

2.1 Detailed implementation

2.1.1 class CausalSelfAttention(nn.Module)

```
class CausalSelfAttention(nn.Module):
```

this class defines the causal self-attention mechanism, the smallest unit of the Transformer architecture. We know that if we have h heads, then when we put multiple heads together, we have:

$$\begin{aligned} \mathbf{Q} &= \underbrace{\begin{bmatrix} - & \mathbf{x}_1 & - \\ - & \dots & - \\ - & \mathbf{x}_T & - \end{bmatrix}}_{T \times d_{\text{model}}} \underbrace{\begin{bmatrix} \mathbf{W}_Q^{(1)} & \dots & \mathbf{W}_Q^{(h)} \\ d_{\text{model}} \times d_k & & d_{\text{model}} \times d_k \end{bmatrix}}_{d_{\text{model}} \times d_{\text{model}}} = \underbrace{\begin{bmatrix} \mathbf{Q}^{(1)} & \dots & \mathbf{Q}^{(h)} \\ T \times d_k & & T \times d_k \end{bmatrix}}_{T \times d_{\text{model}}} \\ \mathbf{K} &= \underbrace{\begin{bmatrix} - & \mathbf{x}_1 & - \\ - & \dots & - \\ - & \mathbf{x}_T & - \end{bmatrix}}_{T \times d_{\text{model}}} \underbrace{\begin{bmatrix} \mathbf{W}_K^{(1)} & \dots & \mathbf{W}_K^{(h)} \\ d_{\text{model}} \times d_k & & d_{\text{model}} \times d_k \end{bmatrix}}_{d_{\text{model}} \times d_{\text{model}}} = \underbrace{\begin{bmatrix} \mathbf{K}^{(1)} & \dots & \mathbf{K}^{(h)} \\ T \times d_k & & T \times d_k \end{bmatrix}}_{T \times d_{\text{model}}} \end{aligned} \quad (15)$$

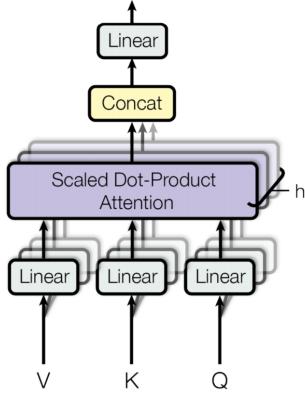


Figure 1: Multi-head Attention

note that this also corresponds to the B, T, C format (after adding the batch dimension B). where,

$$\begin{aligned} h &\equiv n_{\text{heads}} \\ d_k = d_v &= d_h \\ d_h \times h &\equiv d_{\text{model}} \end{aligned} \tag{16}$$

and the code has a few definitions:

```
def __init__(self, d_model: int, n_heads: int, dropout: float, max_seq_len: int):
    super().__init__()
    assert d_model % n_heads == 0
    self.n_heads = n_heads
    self.head_dim = d_model // n_heads # per-head dimensionality

    # Single projection that produces query, key, and value in one matmul
    self.qkv = nn.Linear(d_model, 3 * d_model)
    # Final projection after concatenating heads
    self.proj = nn.Linear(d_model, d_model)
    self.attn_dropout = nn.Dropout(dropout)
    self.resid_dropout = nn.Dropout(dropout)
```

Precompute variable mask matrix and store lower-triangular mask of shape $(1, 1, T, T)$, so it can be broadcasted over (B, h, T, T) :

for example, for $T = 5$, we have:

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 & 1 \end{bmatrix} \tag{17}$$

```
mask = torch.tril(torch.ones(max_seq_len, max_seq_len))
mask = mask.view(1, 1, max_seq_len, max_seq_len)
```

2.1.2 Step of each Transformer Layer

```
def forward(self, x: torch.Tensor) -> torch.Tensor:
```

- At the conclusion of each Transformer layer, we have the output \mathbf{Y} of shape (B, T, C) , where it looks like (assume $B = 1$). See Eq.(29).

$$\underbrace{\begin{bmatrix} - & \mathbf{y}_1 & - \\ & \vdots & \\ - & \mathbf{y}_T & - \end{bmatrix}}_{T \times d_{\text{model}}} \quad (18)$$

The column dimension is $h \times d_v$, which is also the size of the input vector \mathbf{x}_t . It can be thought as the “essential” form of the qkv matrix.

Now, we need to perform:

$$\mathbf{Q} = \mathbf{XW}_Q, \quad \mathbf{K} = \mathbf{XW}_K, \quad \mathbf{V} = \mathbf{XW}_V \quad (19)$$

to obtain the following single large matrix before splitting into $\mathbf{Q}, \mathbf{K}, \mathbf{V}$ matrices, we still assume $B = 1$.

$$\underbrace{\begin{bmatrix} -\mathbf{q}_1^{(1)} & \dots & -\mathbf{q}_1^{(h)} & -\mathbf{k}_1^{(1)} & \dots & -\mathbf{k}_1^{(h)} & -\mathbf{v}_1^{(1)} & \dots & -\mathbf{v}_1^{(h)} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ -\mathbf{q}_T^{(1)} & \dots & -\mathbf{q}_T^{(h)} & -\mathbf{k}_T^{(1)} & \dots & -\mathbf{k}_T^{(h)} & -\mathbf{v}_T^{(1)} & \dots & -\mathbf{v}_T^{(h)} \end{bmatrix}}_{T \times (d_{\text{model}} \times 3)} \quad (20)$$

```
B, T, C = x.size() # batch, time, channels
qkv = self.qkv(x)
```

after running the following code, we split the (B, T, C) format into (B, T, h, d_v) , i.e., the big multi-head matrix containing all $\mathbf{Q}, \mathbf{K}, \mathbf{V}$ into separate $\mathbf{Q}, \mathbf{K}, \mathbf{V}$ matrices:

$$\underbrace{\begin{bmatrix} - & \mathbf{q}_1^{(1)} & - & \dots & - & \mathbf{q}_1^{(h)} & - \\ & \vdots & & \ddots & & \vdots & \\ - & \mathbf{q}_T^{(1)} & - & \dots & - & \mathbf{q}_T^{(h)} & - \end{bmatrix}}_{T \times d_{\text{model}}} \underbrace{\begin{bmatrix} - & \mathbf{k}_1^{(1)} & - & \dots & - & \mathbf{k}_1^{(h)} & - \\ & \vdots & & \ddots & & \vdots & \\ - & \mathbf{k}_T^{(1)} & - & \dots & - & \mathbf{k}_T^{(h)} & - \end{bmatrix}}_{T \times d_{\text{model}}} \underbrace{\begin{bmatrix} - & \mathbf{v}_1^{(1)} & - & \dots & - & \mathbf{v}_1^{(h)} & - \\ & \vdots & & \ddots & & \vdots & \\ - & \mathbf{v}_T^{(1)} & - & \dots & - & \mathbf{v}_T^{(h)} & - \end{bmatrix}}_{T \times d_{\text{model}}} \quad (21)$$

```
q, k, v = qkv.split(C, dim=2) # each of shape (B, T, C)
```

2. now we split the **QKV** single large matrix into each separate **Q, K, V** matrices:

```
def reshape_heads(t: torch.Tensor) -> torch.Tensor:
    # Reshape to (B, n_heads, T, head_dim) for parallel head
    # computation
    return t.view(B, T, self.n_heads, self.head_dim).transpose(1, 2)

# (B, n_heads, T, head_dim)
q = reshape_heads(q)
k = reshape_heads(k)
v = reshape_heads(v)
```

after running the above code, it has split up **Q, K** and **V**, so that each will be in the form of for simplicity let $B = 1$, and we would like to have the structure to look like:

$$\mathbf{Q} = \underbrace{\begin{bmatrix} - & \mathbf{q}_1 & - \\ - & \dots & - \\ - & \mathbf{q}_T & - \end{bmatrix}}_{\mathbf{Q}_{(1)}: T \times d_k} \dots \underbrace{\begin{bmatrix} - & \mathbf{q}_1 & - \\ - & \dots & - \\ - & \mathbf{q}_T & - \end{bmatrix}}_{\mathbf{Q}_{(h)}: T \times d_k} \quad \mathbf{K} = \underbrace{\begin{bmatrix} - & \mathbf{k}_1 & - \\ - & \dots & - \\ - & \mathbf{k}_T & - \end{bmatrix}}_{\mathbf{K}_{(1)}: T \times d_k} \dots \underbrace{\begin{bmatrix} - & \mathbf{k}_1 & - \\ - & \dots & - \\ - & \mathbf{k}_T & - \end{bmatrix}}_{\mathbf{K}_{(h)}: T \times d_k}$$

$$\mathbf{V} = \underbrace{\begin{bmatrix} - & \mathbf{v}_1 & - \\ - & \dots & - \\ - & \mathbf{v}_T & - \end{bmatrix}}_{\mathbf{V}_{(1)}: T \times d_v} \dots \underbrace{\begin{bmatrix} - & \mathbf{v}_1 & - \\ - & \dots & - \\ - & \mathbf{v}_T & - \end{bmatrix}}_{\mathbf{V}_{(h)}: T \times d_v} \quad (22)$$

where we remind ourselves that:

$$h \equiv n_{\text{heads}} \quad (23)$$

$$d_h \times h = d_{\text{model}}$$

3. we then apply $\mathbf{Q}\mathbf{K}^\top$:

```
att = (q @ k.transpose(-2, -1)) # (B, n_heads, T, T)
```

note the above code does not perform $\mathbf{Q}\mathbf{K}^\top$, after **Q** and **K** are concatenated from all the heads, but rather it performs $\mathbf{Q}\mathbf{K}^\top$ for each head, i.e., broadcasted matrix multiplication:

$$\left[\mathbf{Q}_{(1)} \mathbf{K}_{(1)}^\top \quad \dots \quad \mathbf{Q}_{(h)} \mathbf{K}_{(h)}^\top \right] \quad (24)$$

4. we then scale by $1/\sqrt{d_h}$:

$$\text{att} = \text{att} / (\text{self.head_dim} ** 0.5)$$

where we obtained:

$$\left[\frac{\mathbf{Q}_{(1)} \mathbf{K}_{(1)}^\top}{\sqrt{d_h}} \dots \frac{\mathbf{Q}_{(h)} \mathbf{K}_{(h)}^\top}{\sqrt{d_h}} \right] = \underbrace{\begin{bmatrix} \frac{\mathbf{q}_1^{(1)} \mathbf{k}_1^{(1)\top}}{\sqrt{d_h}} & \dots & \frac{\mathbf{q}_1^{(1)} \mathbf{k}_T^{(1)\top}}{\sqrt{d_h}} \\ \vdots & \ddots & \vdots \\ \frac{\mathbf{q}_T^{(1)} \mathbf{k}_1^{(1)\top}}{\sqrt{d_h}} & \dots & \frac{\mathbf{q}_T^{(1)} \mathbf{k}_T^{(1)\top}}{\sqrt{d_h}} \end{bmatrix}}_{\frac{\mathbf{Q}^{(1)} \mathbf{K}^{(1)\top}}{\sqrt{d_h}}} \dots \underbrace{\begin{bmatrix} \frac{\mathbf{q}_1^{(h)} \mathbf{k}_1^{(h)\top}}{\sqrt{d_h}} & \dots & \frac{\mathbf{q}_1^{(h)} \mathbf{k}_T^{(h)\top}}{\sqrt{d_h}} \\ \vdots & \ddots & \vdots \\ \frac{\mathbf{q}_T^{(h)} \mathbf{k}_1^{(h)\top}}{\sqrt{d_h}} & \dots & \frac{\mathbf{q}_T^{(h)} \mathbf{k}_T^{(h)\top}}{\sqrt{d_h}} \end{bmatrix}}_{\mathbf{Q}^{(h)} \mathbf{K}^{(h)\top}} \quad (25)$$

5. we apply a causal mask to the attention matrix, so that each word can only attend to the previous words:

$$\# \text{ Apply causal mask so position } t \text{ cannot attend to positions } > t \\ \text{att} = \text{att}. \text{masked_fill}(\text{self}. \text{mask}[:, :, :T, :T] == 0, \text{float}(' -inf'))$$

$$\left[\begin{bmatrix} \frac{\mathbf{q}_1^{(1)} \mathbf{k}_1^{(1)\top}}{\sqrt{d_h}} & \dots & -\infty \\ \vdots & \ddots & \vdots \\ \frac{\mathbf{q}_T^{(1)} \mathbf{k}_1^{(1)\top}}{\sqrt{d_h}} & \dots & \frac{\mathbf{q}_T^{(1)} \mathbf{k}_T^{(1)\top}}{\sqrt{d_h}} \end{bmatrix} \dots \begin{bmatrix} \frac{\mathbf{q}_1^{(h)} \mathbf{k}_1^{(h)\top}}{\sqrt{d_h}} & \dots & -\infty \\ \vdots & \ddots & \vdots \\ \frac{\mathbf{q}_T^{(h)} \mathbf{k}_1^{(h)\top}}{\sqrt{d_h}} & \dots & \frac{\mathbf{q}_T^{(h)} \mathbf{k}_T^{(h)\top}}{\sqrt{d_h}} \end{bmatrix} \right] \quad (26)$$

6. apply row-wise softmax to the attention matrix:

$$\text{att} = \text{F.softmax}(\text{att}, \text{dim}=-1) \\ \text{att} = \text{self.attn_dropout}(\text{att})$$

$$\left[\begin{bmatrix} \text{softmax}\left(\left[\frac{\mathbf{q}_1^{(1)} \mathbf{k}_1^{(1)\top}}{\sqrt{d_h}} \dots -\infty\right]\right) \\ \vdots \\ \text{softmax}\left(\left[\frac{\mathbf{q}_T^{(1)} \mathbf{k}_1^{(1)\top}}{\sqrt{d_h}} \dots \frac{\mathbf{q}_T^{(1)} \mathbf{k}_T^{(1)\top}}{\sqrt{d_h}}\right]\right) \end{bmatrix} \dots \begin{bmatrix} \text{softmax}\left(\left[\frac{\mathbf{q}_1^{(h)} \mathbf{k}_1^{(h)\top}}{\sqrt{d_h}} \dots -\infty\right]\right) \\ \vdots \\ \text{softmax}\left(\left[\frac{\mathbf{q}_T^{(h)} \mathbf{k}_1^{(h)\top}}{\sqrt{d_h}} \dots \frac{\mathbf{q}_T^{(h)} \mathbf{k}_T^{(h)\top}}{\sqrt{d_h}}\right]\right) \end{bmatrix} \right] \quad (27)$$

7. apply weighted sum to the values:

$$\# \text{ Weighted sum of values} \\ \text{y} = \text{att} @ \text{v} \# (\text{B}, \text{n_heads}, \text{T}, \text{head_dim})$$

where we obtained:

$$\underbrace{\left[\begin{array}{cccc} \text{softmax} \left(\frac{\mathbf{Q}^{(1)} \mathbf{K}^{(1)\top}}{\sqrt{d_h}} \right) \mathbf{V}^{(1)} & \dots & \text{softmax} \left(\frac{\mathbf{Q}^{(h)} \mathbf{K}^{(h)\top}}{\sqrt{d_h}} \right) \mathbf{V}^{(h)} \end{array} \right]}_{T \times d_{\text{model}}} \quad (28)$$

8. transform the output back to the original dimension B, T, C , where `contiguous()` is a method that returns a contiguous tensor.

```
# (B, n_heads, T, head_dim) -> (B, T, n_heads, head_dim)
y = y.transpose(1, 2)
y = y.contiguous()
# Reassemble heads: (B, T, C)
y = y.view(B, T, C)
```

know that:

$$\underbrace{\left[\begin{array}{ccc} - & \mathbf{y}_1 & - \\ & \vdots & \\ - & \mathbf{y}_T & - \end{array} \right]}_{T \times d_{\text{model}}} = \underbrace{\left[\begin{array}{ccccc} - & \mathbf{o}_1^{(1)} & - & \dots & - \\ - & \dots & - & & \\ - & \mathbf{o}_T^{(1)} & - & & \\ \hline \mathbf{O}_{(1)}: & T \times d_h & & & \end{array} \right]}_{T \times d_{\text{model}}} \dots \underbrace{\left[\begin{array}{ccccc} - & \mathbf{o}_1^{(h)} & - & \dots & - \\ - & \dots & - & & \\ - & \mathbf{o}_T^{(h)} & - & & \\ \hline \mathbf{O}_{(h)}: & T \times d_h & & & \end{array} \right]}_{T \times d_{\text{model}}} \underbrace{\mathbf{W}_O}_{d_{\text{model}} \times d_{\text{model}}} \quad (29)$$

$$= \underbrace{\left[\begin{array}{ccccc} - & \mathbf{o}_1^{(1)} & - & \dots & - & \mathbf{o}_1^{(h)} & - \\ & \vdots & & \ddots & & \vdots & \\ - & \mathbf{o}_T^{(1)} & - & \dots & - & \mathbf{o}_T^{(h)} & - \end{array} \right]}_{T \times d_{\text{model}}} \underbrace{\mathbf{W}_O}_{d_{\text{model}} \times d_{\text{model}}}$$

each row of \mathbf{y}_i can be determined independently and in parallel.

9. we then perform a final linear projection on the concatenated heads:

```
# Final linear projection on the concatenated heads
y = self.resid_dropout(self.proj(y)) # resid_dropout is the residual
# dropout
return y
```

one can see that the final output is a tensor of shape B, T, d_{model} .

2.1.3 class TransformerBlock(nn.Module)

The following is the code for Pre-norm Transformer block with attention followed by an MLP, where the `CausalSelfAttention()` is from the previous section:

```

class TransformerBlock(nn.Module):
    def __init__(self, d_model: int, n_heads: int, d_ff: int, dropout: float,
                 max_seq_len: int):
        super().__init__()
        # Pre-layernorm improves optimization stability in autoregressive LMs
        self.ln1 = nn.LayerNorm(d_model)
        self.attn = CausalSelfAttention(d_model, n_heads, dropout, max_seq_len)
        self.ln2 = nn.LayerNorm(d_model)
        # Feed-forward network (position-wise MLP)
        self.mlp = nn.Sequential(
            nn.Linear(d_model, d_ff),
            nn.GELU(),
            nn.Dropout(dropout),
            nn.Linear(d_ff, d_model),
            nn.Dropout(dropout),
        )
    def forward(self, x: torch.Tensor) -> torch.Tensor:
        # Attention sub-layer with residual connection
        x = x + self.attn(self.ln1(x))
        # MLP sub-layer with residual connection
        x = x + self.mlp(self.ln2(x))
        return x

```

$x = x + f(x)$ is the residual connection. and `nn.GELU()` is the activation function.

2.1.4 class TransformerLM(nn.Module)

```

class TransformerLM(nn.Module):
    """Causal language model built from Transformer blocks."""

    def __init__(self, config: ModelConfig):
        super().__init__()
        self.config = config
        # Token and positional embeddings are summed to form the input stream
        self.token_emb = nn.Embedding(config.vocab_size, config.d_model)
        self.pos_emb = nn.Embedding(config.max_seq_len, config.d_model)
        self.drop = nn.Dropout(config.dropout)
        # Stack of identical Transformer blocks
        self.blocks = nn.ModuleList([
            TransformerBlock(config.d_model, config.n_heads, config.d_ff, config
                            .dropout, config.max_seq_len)
            for _ in range(config.n_layers)
        ])
        # Final layernorm before projecting to vocabulary logits
        self.ln_f = nn.LayerNorm(config.d_model)
        # LM head ties to embedding size but does not share weights here
        self.lm_head = nn.Linear(config.d_model, config.vocab_size, bias=False)

    def forward(self, idx: torch.Tensor, targets: Optional[torch.Tensor] = None)
        :

```

```

"""Forward pass producing next-token logits and optional cross-entropy
loss.

Parameters
-----
idx : torch.Tensor
    Token indices of shape (B, T).
targets : Optional[torch.Tensor]
    Target indices of shape (B, T). If provided, a token-level
    cross-entropy loss is computed and returned.

Returns
-----
Tuple[torch.Tensor, Optional[torch.Tensor]]
    - logits: (B, T, vocab_size)
    - loss: scalar loss if targets is provided, else None
"""

B, T = idx.shape
# Ensure sequence length fits within the configured context window
assert T <= self.config.max_seq_len

# Positions 0..T-1 for current sequence length
pos = torch.arange(0, T, dtype=torch.long, device=idx.device).unsqueeze
(0)

```

this is to create a tensor of shape $(1, T)$ with values from 0 to $T-1$. We call the `unsqueeze(0)` to add a batch dimension, so that it can be broadcasted over the batch dimension when adding to the token embeddings.

$$[[0 \ 1 \ 2 \ \dots \ T-1]] \quad (30)$$

```

# Embed tokens and positions, then apply dropout
x = self.token_emb(idx) + self.pos_emb(pos)
x = self.drop(x)

# Pass through the stack of Transformer blocks
for blk in self.blocks:
    x = blk(x)

# Final normalization and projection to vocabulary
x = self.ln_f(x)
logits = self.lm_head(x)

# Compute token-level cross-entropy if targets are given
loss = None
if targets is not None:
    loss = F.cross_entropy(logits.view(-1, logits.size(-1)), targets.
        view(-1))
return logits, loss

```

```

@torch.no_grad()
def generate(self, idx: torch.Tensor, max_new_tokens: int) -> torch.Tensor:
    """Greedy-free sampling generation from the language model.

    Iteratively samples `max_new_tokens` next tokens by:
    - conditioning on the last `max_seq_len` tokens
    - computing logits for the next position
    - sampling from the softmax distribution
    - appending the sampled token to the context

    Parameters
    -----
    idx : torch.Tensor
        Initial context token indices of shape (B, T0).
    max_new_tokens : int
        Number of new tokens to sample and append.

    Returns
    -----
    torch.Tensor
        Extended token indices of shape (B, T0 + max_new_tokens).
    """
    self.eval()
    for _ in range(max_new_tokens):
        # Restrict conditioning length to model's maximum context window
        # only the last self.config.max_seq_len tokens are used to condition
        # the generation, as they are the most recent tokens
        idx_cond = idx[:, -self.config.max_seq_len:]
        logits, _ = self(idx_cond)
        # Select logits for the last time step (the next token prediction)
        logits = logits[:, -1, :]
        probs = F.softmax(logits, dim=-1)
        # Multinomial sampling allows for non-greedy, stochastic generation
        next_id = torch.multinomial(probs, num_samples=1)
        # Append sampled token and continue
        idx = torch.cat((idx, next_id), dim=1)
    return idx

```

2.2 Cross-Attention

If we were to perform cross-attention, **K** and **V** must be the same thing. For example,

1. Text-to-image Cross-Attention:

$$\begin{aligned} \mathbf{K} \text{ and } \mathbf{V} &\text{ are text embedding} \\ \mathbf{Q} &\text{ is image embedding} \end{aligned} \tag{31}$$

2. Image-to-text Cross-Attention:

$$\begin{aligned} \mathbf{K} \text{ and } \mathbf{V} &\text{ are image embedding} \\ \mathbf{Q} &\text{ is text embedding} \end{aligned} \tag{32}$$

3 $\mathbf{K} - \mathbf{V}$ caching

looking at $\mathbf{Q}\mathbf{K}^\top$, imagine in a self-attention scenario, where the current sentence length is T , and $m = n = T$, then $\mathbf{Q}\mathbf{K}^\top$ is a square matrix of $T \times T$, where we have:

$$\mathbf{Q}\mathbf{K}^\top = \begin{bmatrix} \mathbf{q}_1\mathbf{k}_1^\top & \dots & \mathbf{q}_1\mathbf{k}_T^\top \\ \vdots & \ddots & \vdots \\ \mathbf{q}_T\mathbf{k}_1^\top & \dots & \mathbf{q}_T\mathbf{k}_T^\top \end{bmatrix} \tag{33}$$

let's say we have a new word w_{T+1} to be added to the sentence, then we have:

$$\begin{bmatrix} \mathbf{q}_1\mathbf{k}_1^\top & \dots & \mathbf{q}_1\mathbf{k}_T^\top & \mathbf{q}_1\mathbf{k}_{T+1}^\top \\ \vdots & \ddots & \vdots & \vdots \\ \mathbf{q}_T\mathbf{k}_1^\top & \dots & \mathbf{q}_T\mathbf{k}_T^\top & \mathbf{q}_T\mathbf{k}_{T+1}^\top \\ \mathbf{q}_{T+1}\mathbf{k}_1^\top & \dots & \mathbf{q}_{T+1}\mathbf{k}_T^\top & \mathbf{q}_{T+1}\mathbf{k}_{T+1}^\top \end{bmatrix} = \begin{bmatrix} \mathbf{Q}\mathbf{K}^\top & \mathbf{Q}\mathbf{k}_{T+1}^\top \\ \mathbf{q}_{T+1}\mathbf{K}^\top & \mathbf{q}_{T+1}\mathbf{k}_{T+1}^\top \end{bmatrix} \tag{34}$$

From here, one sees that in generic matrix multiplication, one needs to cache both \mathbf{K} and \mathbf{Q} . However, the matrix masks out the upper triangular part of the matrix, i.e., it looks like this:

$$\begin{bmatrix} \mathbf{q}_1\mathbf{k}_1^\top & - & - & - \\ \vdots & \ddots & \vdots & \vdots \\ \mathbf{q}_T\mathbf{k}_1^\top & \dots & \mathbf{q}_T\mathbf{k}_T^\top & - \\ \mathbf{q}_{T+1}\mathbf{k}_1^\top & \dots & \mathbf{q}_{T+1}\mathbf{k}_T^\top & \mathbf{q}_{T+1}\mathbf{k}_{T+1}^\top \end{bmatrix} = \begin{bmatrix} \underbrace{\mathbf{Q}\mathbf{K}^\top}_{\text{lower triangular}} & - \\ \mathbf{q}_{T+1}\mathbf{K}^\top & \mathbf{q}_{T+1}\mathbf{k}_{T+1}^\top \end{bmatrix} \tag{35}$$

One can see the newly added row (no new column is added) in the above matrix, requires \mathbf{q}_{T+1} , \mathbf{k}_{T+1} and \mathbf{K} . This means that \mathbf{K} needs to be cached.

Again looking at Eq.(9):

$$\left[\begin{array}{c} \frac{\exp(\mathbf{q}_1\mathbf{k}_1^\top)}{\exp(\mathbf{q}_1\mathbf{k}_1^\top)} \mathbf{v}_1 \\ \frac{\exp(\mathbf{q}_2\mathbf{k}_1^\top)}{\exp(\mathbf{q}_2\mathbf{k}_1^\top) + \exp(\mathbf{q}_2\mathbf{k}_2^\top)} \mathbf{v}_1 + \frac{\exp(\mathbf{q}_2\mathbf{k}_2^\top)}{\exp(\mathbf{q}_2\mathbf{k}_1^\top) + \exp(\mathbf{q}_2\mathbf{k}_2^\top)} \mathbf{v}_2 \\ \frac{\exp(\mathbf{q}_3\mathbf{k}_1^\top)}{\exp(\mathbf{q}_3\mathbf{k}_1^\top) + \exp(\mathbf{q}_3\mathbf{k}_2^\top) + \exp(\mathbf{q}_3\mathbf{k}_3^\top)} \mathbf{v}_1 + \frac{\exp(\mathbf{q}_3\mathbf{k}_2^\top)}{\exp(\mathbf{q}_3\mathbf{k}_1^\top) + \exp(\mathbf{q}_3\mathbf{k}_2^\top) + \exp(\mathbf{q}_3\mathbf{k}_3^\top)} \mathbf{v}_2 + \frac{\exp(\mathbf{q}_3\mathbf{k}_3^\top)}{\exp(\mathbf{q}_3\mathbf{k}_1^\top) + \exp(\mathbf{q}_3\mathbf{k}_2^\top) + \exp(\mathbf{q}_3\mathbf{k}_3^\top)} \mathbf{v}_3 \\ \vdots \\ \sum_{i=1}^T \frac{\exp(\mathbf{q}_T\mathbf{k}_i^\top)}{\sum_{j=1}^T \exp(\mathbf{q}_T\mathbf{k}_j^\top)} \mathbf{v}_i \\ \sum_{i=1}^{T+1} \frac{\exp(\mathbf{q}_{T+1}\mathbf{k}_i^\top)}{\sum_{j=1}^{T+1} \exp(\mathbf{q}_{T+1}\mathbf{k}_j^\top)} \mathbf{v}_i \end{array} \right] \tag{36}$$

the last row in the above matrix contains the newly added row, where all \mathbf{v}_i are needed for computation and hence they need to be cached.

3.0.1 Multi-head latent attention

say we have sentence of length T , and we have each word represented by a $d = 7168$ dimensional vector. Then we can have:

$$\begin{aligned} \mathbf{L}_{K,V} &= \mathbf{X} \mathbf{W}_{\downarrow K,V} \\ &= \underbrace{\begin{bmatrix} - & \mathbf{x}_1 & - \\ - & \dots & - \\ - & \mathbf{x}_T & - \end{bmatrix}}_{T \times d_{\text{model}}} \underbrace{\begin{bmatrix} \mathbf{w}_{1,1} & \dots & \mathbf{w}_{1,576} \\ \vdots & \ddots & \vdots \\ \mathbf{w}_{7168,1} & \dots & \mathbf{w}_{7168,576} \end{bmatrix}}_{d_{\text{model}} \times 576} \end{aligned} \quad (37)$$

where $\mathbf{L}_{K,V}$ is the “common” part of the latent representation of the sentence for both \mathbf{K} and \mathbf{V} .

normally, in the case of self-attention, one should have, $\mathbf{Q} = \mathbf{X} \mathbf{W}_Q$, $\mathbf{K} = \mathbf{X} \mathbf{W}_K$, $\mathbf{V} = \mathbf{X} \mathbf{W}_V$, but in here, we are having:

traditional	multi-head latent attention
-------------	-----------------------------

$$\begin{array}{lll} \mathbf{Q} = \mathbf{X} \mathbf{W}_Q & \rightarrow & \underbrace{\mathbf{Q}}_{T \times 128} = \mathbf{X} \underbrace{\mathbf{W}_Q}_{7168 \times 128} \\ \mathbf{K} = \mathbf{X} \mathbf{W}_K & \rightarrow & \underbrace{\mathbf{K}}_{T \times 128} = \mathbf{X} \underbrace{\mathbf{W}_{\downarrow K,V}}_{d_{\text{model}} \times 576} \underbrace{\mathbf{W}_{\uparrow K}}_{576 \times 128} = \underbrace{\mathbf{L}_{K,V}}_{T \times 576} \underbrace{\mathbf{W}_{\uparrow K}}_{576 \times 128} \\ \mathbf{V} = \mathbf{X} \mathbf{W}_V & \rightarrow & \underbrace{\mathbf{V}}_{T \times 128} = \mathbf{X} \underbrace{\mathbf{W}_{\downarrow K,V}}_{d_{\text{model}} \times 576} \underbrace{\mathbf{W}_{\uparrow V}}_{576 \times 128} = \underbrace{\mathbf{L}_{K,V}}_{T \times 576} \underbrace{\mathbf{W}_{\uparrow V}}_{576 \times 128} \end{array} \quad (38)$$

making $\mathbf{W}_{\downarrow K,V}$ to be common for all heads for both \mathbf{K} and \mathbf{V} . Therefore only a smaller $\mathbf{W}_{\uparrow K}$ and $\mathbf{W}_{\uparrow V}$ need to be trained per head for both \mathbf{K} and \mathbf{V} . This means that:

$$\begin{aligned} \mathbf{W}_K &\longrightarrow \mathbf{W}_{\downarrow K,V} \mathbf{W}_{\uparrow K} \\ \mathbf{K} = \mathbf{W}_K &\longrightarrow \mathbf{X} \mathbf{W}_{\downarrow K,V} \mathbf{W}_{\uparrow K} \end{aligned} \quad (39)$$

substitute:

$$\begin{aligned} \mathbf{Q} \mathbf{K}^\top &= \mathbf{X} \mathbf{W}_Q (\mathbf{X} \mathbf{W}_{\downarrow K,V} \mathbf{W}_{\uparrow K})^\top \\ &= \mathbf{X} \mathbf{W}_Q ((\mathbf{X} \mathbf{W}_{\downarrow K,V}) \mathbf{W}_{\uparrow K})^\top \\ &= \underbrace{\mathbf{X}}_{T \times d_{\text{model}}} \underbrace{(\mathbf{W}_Q \mathbf{W}_{\uparrow K}^\top)}_{d_{\text{model}} \times 576} \underbrace{(\mathbf{X} \mathbf{W}_{\downarrow K,V})^\top}_{576 \times T} \end{aligned} \quad (40)$$

$$\begin{aligned}
\mathbf{QK}^\top &= \mathbf{XW}_Q(\mathbf{X W}_{\downarrow K,V} \mathbf{W}_{\uparrow K})^\top \\
&= \mathbf{XW}_Q((\mathbf{X W}_{\downarrow K,V}) \mathbf{W}_{\uparrow K})^\top \\
&= \underbrace{\mathbf{X}_{T \times d_{\text{model}}}}_{d_{\text{model}} \times 576} \underbrace{(\mathbf{W}_Q \mathbf{W}_{\uparrow K}^\top)}_{576 \times 576} \underbrace{(\mathbf{X W}_{\downarrow K,V})^\top}_{576 \times T}
\end{aligned} \tag{41}$$

- Remember that although we have different $\mathbf{W}_{\uparrow K}$ for each head, $(\mathbf{W}_Q \mathbf{W}_{\uparrow K}^\top)$ can be computed first only once, before they multiple with \mathbf{X} (and $(\mathbf{X} \mathbf{W}_{\downarrow K,V})$) during inference time for each variable length \mathbf{X} . This means that we do not need to store \mathbf{W}_Q and $\mathbf{W}_{\uparrow K}$ separately, but rather we can store $\mathbf{W}_Q \mathbf{W}_{\uparrow K}^\top$ once. It's like having a new \mathbf{W}_Q

In terms of caching, assumed that at the length of T words, we have cached $\mathbf{X}(\mathbf{W}_Q \mathbf{W}_{\uparrow K}^\top)$ and $\mathbf{XW}_{\downarrow K,V}$. Then after adding a new word, i.e., \mathbf{X}_{T+1} , we can just compute one more row of the matrix $\mathbf{X}_{T+1}\mathbf{W}_Q\mathbf{W}_{\uparrow K}$ and $\mathbf{X}_{T+1}\mathbf{W}_{\downarrow K,V}$ and append it to the cache, i.e.,

$$\begin{aligned}
&\left[\begin{array}{ccc} - & \mathbf{x}_1 & - \\ - & \dots & - \\ - & \mathbf{x}_T & - \end{array} \right] [(\mathbf{W}_Q \mathbf{W}_{\uparrow K}^\top)] = \text{cache} \\
\implies &\left[\begin{array}{ccc} - & \mathbf{x}_1 & - \\ - & \dots & - \\ - & \mathbf{x}_T & - \\ - & \mathbf{x}_{T+1} & - \end{array} \right] [(\mathbf{W}_Q \mathbf{W}_{\uparrow K}^\top)] = \left[\begin{array}{c} \text{cache} \\ \mathbf{x}_{T+1}(\mathbf{W}_Q \mathbf{W}_{\uparrow K}^\top) \end{array} \right]
\end{aligned} \tag{42}$$

the same applies to $\mathbf{XW}_{\downarrow K,V}$, i.e.,

$$\begin{aligned}
&\left[\begin{array}{ccc} - & \mathbf{x}_1 & - \\ - & \dots & - \\ - & \mathbf{x}_T & - \end{array} \right] [\mathbf{W}_{\downarrow K,V}] = \text{cache} \\
\implies &\left[\begin{array}{ccc} - & \mathbf{x}_1 & - \\ - & \dots & - \\ - & \mathbf{x}_T & - \\ - & \mathbf{x}_{T+1} & - \end{array} \right] [\mathbf{W}_{\downarrow K,V}] = \left[\begin{array}{c} \text{cache} \\ \mathbf{x}_{T+1}\mathbf{W}_{\downarrow K,V} \end{array} \right]
\end{aligned} \tag{43}$$

Now, let's look at the output of the multi-head attention:

$$\begin{aligned}
\mathbf{Y} &= \underbrace{\begin{bmatrix} - & \mathbf{y}_1 & - \\ & \vdots & \\ - & \mathbf{y}_T & - \end{bmatrix}}_{T \times d_{\text{model}}} = \underbrace{\text{concat}(\mathbf{O}_1, \dots, \mathbf{O}_h)}_{T \times (d_h \times h)} \underbrace{\mathbf{W}_O}_{d_{\text{model}} \times d_{\text{model}}} \\
&= \left[\text{softmax}\left(\frac{\mathbf{Q}_{(1)} \mathbf{K}_{(1)}^\top}{\sqrt{d_h}}\right) \mathbf{V}_{(1)} \quad \dots \quad \text{softmax}\left(\frac{\mathbf{Q}_{(h)} \mathbf{K}_{(h)}^\top}{\sqrt{d_h}}\right) \mathbf{V}_{(h)} \right] \mathbf{W}_O \\
&= [\mathbf{O}_{(1)} \mathbf{V}_{(1)} \quad \dots \quad \mathbf{O}_{(h)} \mathbf{V}_{(h)}] \mathbf{W}_O \\
&= \underbrace{[\mathbf{O}_{(1)} \quad \dots \quad \mathbf{O}_{(h)}]}_{T \times d_h} \underbrace{\begin{bmatrix} \mathbf{V}_{(1)} & \dots & \mathbf{0} \\ d_h \times d_h & & \\ \vdots & \ddots & \vdots \\ \mathbf{0} & \dots & \mathbf{V}_{(h)} \\ d_h \times d_h & & \end{bmatrix}}_{d_h \times d_h} \underbrace{\begin{bmatrix} \mathbf{W}_O^{1:d_h, 1:d_{\text{model}}} \\ d_h \times d_{\text{model}} \\ \vdots \\ \mathbf{W}_O^{d_h \times (h-1)+1:d_{\text{model}}, 1:d_{\text{model}}} \\ d_h \times d_{\text{model}} \end{bmatrix}}_{d_h \times d_{\text{model}}} \\
&= \underbrace{[\mathbf{O}_{(1)} \quad \dots \quad \mathbf{O}_{(h)}]}_{T \times d_{\text{model}}} \underbrace{\begin{bmatrix} \mathbf{V}_{(1)} \mathbf{W}_O^{1:d_h, 1:d_{\text{model}}} \\ d_h \times d_{\text{model}} \\ \vdots \\ \mathbf{V}_{(h)} \mathbf{W}_O^{d_h \times (h-1)+1:d_{\text{model}}, 1:d_{\text{model}}} \\ d_h \times d_{\text{model}} \end{bmatrix}}_{d_{\text{model}} \times d_{\text{model}}} \tag{44}
\end{aligned}$$

now that we replaced \mathbf{W}_V with $\mathbf{W}_{\downarrow K, V} \mathbf{W}_{\uparrow V}$, we can have:

$$\mathbf{V} = \underbrace{\mathbf{X}}_{T \times d_{\text{model}}} \underbrace{\mathbf{W}_{\downarrow K, V}}_{d_{\text{model}} \times 576} \underbrace{\mathbf{W}_{\uparrow V}}_{576 \times d_h} \tag{45}$$

therefore, we can have each \mathbf{V} , for example $\mathbf{V}_{(1)}$ as

$$\mathbf{V}_{(1)} \mathbf{W}_O^{1:d_h, 1:d_{\text{model}}} = \underbrace{\mathbf{X}}_{T \times d_{\text{model}}} \underbrace{\mathbf{W}_{\downarrow K, V}}_{d_{\text{model}} \times 576} \underbrace{\mathbf{W}_{\uparrow V}}_{576 \times d_h} \underbrace{\mathbf{W}_O^{1:d_h, 1:d_{\text{model}}}}_{d_h \times d_{\text{model}}} \tag{46}$$

we already computed $\mathbf{X} \mathbf{W}_{\downarrow K, V}$ as $\mathbf{L}_{K, V}$, and we can also pre-compute $\mathbf{W}_{\uparrow V} \mathbf{W}_O^{1:d_h, 1:d_{\text{model}}}$ as single matrix, instead of storing $\mathbf{W}_{\uparrow V}$ and $\mathbf{W}_O^{1:d_h, 1:d_{\text{model}}}$ separately.

Finally, we have \mathbf{Y} as the output of the multi-head attention layer.

4 Rotary Embedding RoPE

From the paper, [2], here is the RoPE Python code implementation:

```

class RotaryEmbedding(nn.Module):
    def __init__(self, head_dim=64, rope_theta=100000):
        super().__init__()
        self.head_dim = head_dim
        self.rope_theta = rope_theta

    def forward(self, x):
        # x shape: [batch, num_heads, seq_len, head_dim]

```

```

# Compute frequencies
i = torch.arange(0, self.head_dim, 2)
freqs = 1.0 / (self.rope_theta ** (i / self.head_dim))

```

$$i = [0 \ 2 \ 4 \ \dots \ d_v - 2]$$

$$\text{freqs} = \underbrace{\left[\frac{1}{\theta^{0/d_h}} \ \frac{1}{\theta^{2/d_h}} \ \frac{1}{\theta^{4/d_h}} \ \dots \ \frac{1}{\theta^{(d_h-2)/d_h}} \right]}_{1 \times (d_h/2)} \quad (47)$$

to avoid notational clutter, we write θ^{t/d_h} as θ^t for short.

$$\text{freqs} = \underbrace{\left[\frac{1}{\theta^0} \ \frac{1}{\theta^2} \ \frac{1}{\theta^4} \ \dots \ \frac{1}{\theta^{d_h-2}} \right]}_{1 \times (d_h/2)} \quad (48)$$

this is in the decreasing frequency order.

```

# Compute angles for all positions
pos = torch.arange(x.shape[2])
angles = torch.outer(pos, freqs)

```

since x shape is (batch, num_heads, T, head_dim), therefore x.shape[2] is the seq_len, i.e., T . Therefore, we have:

$$\begin{aligned} \text{angles} &= \begin{bmatrix} 0 \times \frac{1}{\theta^0} & 0 \times \frac{1}{\theta^2} & 0 \times \frac{1}{\theta^4} & \dots & 0 \times \frac{1}{\theta^{d_h-2}} \\ 1 \times \frac{1}{\theta^0} & 1 \times \frac{1}{\theta^2} & 1 \times \frac{1}{\theta^4} & \dots & 1 \times \frac{1}{\theta^{d_h-2}} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ (T-1) \times \frac{1}{\theta^0} & (T-1) \times \frac{1}{\theta^2} & (T-1) \times \frac{1}{\theta^4} & \dots & (T-1) \times \frac{1}{\theta^{d_h-2}} \end{bmatrix} \\ &= \underbrace{\begin{bmatrix} \frac{0}{\theta^0} & \frac{0}{\theta^2} & \frac{0}{\theta^4} & \dots & \frac{0}{\theta^{d_h-2}} \\ \frac{1}{\theta^0} & \frac{1}{\theta^2} & \frac{1}{\theta^4} & \dots & \frac{1}{\theta^{d_h-2}} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \frac{T-1}{\theta^0} & \frac{T-1}{\theta^2} & \frac{T-1}{\theta^4} & \dots & \frac{T-1}{\theta^{d_h-2}} \end{bmatrix}}_{T \times (d_h/2)} \end{aligned} \quad (49)$$

for each t^{th} token, there is a corresponding frequency for each feature, i.e., $\frac{t}{\theta^0}, \frac{t}{\theta^2}, \frac{t}{\theta^4}, \dots, \frac{t}{\theta^{d_h-2}}$

```
# Precompute sin/cos
cos = torch.cos(angles)
sin = torch.sin(angles)
cos = cos.unsqueeze(0).unsqueeze(0)
sin = sin.unsqueeze(0).unsqueeze(0)
```

$$\cos = \left[\begin{bmatrix} \cos\left(\frac{0}{\theta^0}\right) & \cos\left(\frac{0}{\theta^2}\right) & \cos\left(\frac{0}{\theta^4}\right) & \dots & \cos\left(\frac{0}{\theta^{d_h-2}}\right) \\ \cos\left(\frac{1}{\theta^0}\right) & \cos\left(\frac{1}{\theta^2}\right) & \cos\left(\frac{1}{\theta^4}\right) & \dots & \cos\left(\frac{1}{\theta^{d_h-2}}\right) \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \cos\left(\frac{T-1}{\theta^0}\right) & \cos\left(\frac{T-1}{\theta^2}\right) & \cos\left(\frac{T-1}{\theta^4}\right) & \dots & \cos\left(\frac{T-1}{\theta^{d_h-2}}\right) \end{bmatrix} \right] \quad (50)$$

$$\sin = \left[\begin{bmatrix} \sin\left(\frac{0}{\theta^0}\right) & \sin\left(\frac{0}{\theta^2}\right) & \sin\left(\frac{0}{\theta^4}\right) & \dots & \sin\left(\frac{0}{\theta^{d_h-2}}\right) \\ \sin\left(\frac{1}{\theta^0}\right) & \sin\left(\frac{1}{\theta^2}\right) & \sin\left(\frac{1}{\theta^4}\right) & \dots & \sin\left(\frac{1}{\theta^{d_h-2}}\right) \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \sin\left(\frac{T-1}{\theta^0}\right) & \sin\left(\frac{T-1}{\theta^2}\right) & \sin\left(\frac{T-1}{\theta^4}\right) & \dots & \sin\left(\frac{T-1}{\theta^{d_h-2}}\right) \end{bmatrix} \right] \quad (51)$$

```
# Split into pairs
x_even = x[:, :, 0::2]
x_odd = x[:, :, 1::2]
```

for example, if x is \mathbf{Q} , then we have:

$$\mathbf{Q}_{even} = \begin{bmatrix} q_{0,0} & q_{0,2} & q_{0,4} & \dots & q_{0,d_h-2} \\ q_{1,0} & q_{1,2} & q_{1,4} & \dots & q_{1,d_h-2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ q_{T-1,0} & q_{T-1,2} & q_{T-1,4} & \dots & q_{T-1,d_h-2} \end{bmatrix} \mathbf{Q}_{odd} = \begin{bmatrix} q_{0,1} & q_{0,3} & q_{0,5} & \dots & q_{0,d_h-1} \\ q_{1,1} & q_{1,3} & q_{1,5} & \dots & q_{1,d_h-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ q_{T-1,1} & q_{T-1,3} & q_{T-1,5} & \dots & q_{T-1,d_h-1} \end{bmatrix} \quad (52)$$

```
# Apply rotation (broadcasting cos/sin across batch and heads)
x_even_new = x_even * cos - x_odd * sin
x_odd_new = x_even * sin + x_odd * cos
```

$$\mathbf{Q}'_{even} = \underbrace{\begin{bmatrix} q_{0,0}\cos\left(\frac{0}{\theta^0}\right) - q_{0,1}\sin\left(\frac{0}{\theta^0}\right) & q_{0,2}\cos\left(\frac{0}{\theta^2}\right) - q_{0,3}\sin\left(\frac{0}{\theta^2}\right) & \dots & q_{0,d_h-2}\cos\left(\frac{0}{\theta^{d_h-2}}\right) - q_{0,d_h-1}\sin\left(\frac{0}{\theta^{d_h-2}}\right) \\ q_{1,0}\cos\left(\frac{1}{\theta^0}\right) - q_{1,1}\sin\left(\frac{1}{\theta^0}\right) & q_{1,2}\cos\left(\frac{1}{\theta^2}\right) - q_{1,3}\sin\left(\frac{1}{\theta^2}\right) & \dots & q_{1,d_h-2}\cos\left(\frac{1}{\theta^{d_h-2}}\right) - q_{1,d_h-1}\sin\left(\frac{1}{\theta^{d_h-2}}\right) \\ \vdots & \vdots & \ddots & \vdots \\ q_{T-2,0}\cos\left(\frac{T-2}{\theta^0}\right) - q_{T-2,1}\sin\left(\frac{T-2}{\theta^0}\right) & q_{T-2,2}\cos\left(\frac{T-2}{\theta^2}\right) - q_{T-2,3}\sin\left(\frac{T-2}{\theta^2}\right) & \dots & q_{T-2,d_h-2}\cos\left(\frac{T-2}{\theta^{d_h-2}}\right) - q_{T-2,d_h-1}\sin\left(\frac{T-2}{\theta^{d_h-2}}\right) \\ q_{T-1,0}\cos\left(\frac{T-1}{\theta^0}\right) - q_{T-1,1}\sin\left(\frac{T-1}{\theta^0}\right) & q_{T-1,2}\cos\left(\frac{T-1}{\theta^2}\right) - q_{T-1,3}\sin\left(\frac{T-1}{\theta^2}\right) & \dots & q_{T-1,d_h-2}\cos\left(\frac{T-1}{\theta^{d_h-2}}\right) - q_{T-1,d_h-1}\sin\left(\frac{T-1}{\theta^{d_h-2}}\right) \end{bmatrix}}_{T \times (d_h/2)} \quad (53)$$

each $(t, j)^{\text{th}}$ element is of the form, for $t = 0, 1, \dots, T - 1$ and $j = 0, 1, \dots, (d_h/2) - 1$:

$$q'_{t,j} = q_{t,2j}\cos\left(\frac{t}{\theta^j}\right) - q_{t,2j+1}\sin\left(\frac{t}{\theta^j}\right) \quad (54)$$

$$\mathbf{Q}'_{odd} = \underbrace{\begin{bmatrix} q_{0,0}\sin\left(\frac{0}{\theta^0}\right) + q_{0,1}\cos\left(\frac{0}{\theta^0}\right) & q_{0,2}\sin\left(\frac{0}{\theta^2}\right) + q_{0,3}\cos\left(\frac{0}{\theta^2}\right) & \dots & q_{0,d_h-2}\sin\left(\frac{0}{\theta^{d_h-2}}\right) + q_{0,d_h-1}\cos\left(\frac{0}{\theta^{d_h-2}}\right) \\ q_{1,0}\sin\left(\frac{1}{\theta^0}\right) + q_{1,1}\cos\left(\frac{1}{\theta^0}\right) & \color{red}{q_{1,2}\sin\left(\frac{1}{\theta^2}\right) + q_{1,3}\cos\left(\frac{1}{\theta^2}\right)} & \dots & q_{1,d_h-2}\sin\left(\frac{1}{\theta^{d_h-2}}\right) + q_{1,d_h-1}\cos\left(\frac{1}{\theta^{d_h-2}}\right) \\ \vdots & \vdots & \ddots & \vdots \\ q_{T-2,0}\sin\left(\frac{T-2}{\theta^0}\right) + q_{T-2,1}\cos\left(\frac{T-1}{\theta^0}\right) & q_{T-2,2}\sin\left(\frac{T-1}{\theta^2}\right) + q_{T-2,3}\cos\left(\frac{T-1}{\theta^2}\right) & \dots & q_{T-2,d_h-2}\sin\left(\frac{T-1}{\theta^{d_h-2}}\right) + q_{T-2,d_h-1}\cos\left(\frac{T-1}{\theta^{d_h-2}}\right) \\ q_{T-1,0}\sin\left(\frac{T-1}{\theta^0}\right) + q_{T-1,1}\cos\left(\frac{T-1}{\theta^0}\right) & q_{T-1,2}\sin\left(\frac{T-1}{\theta^2}\right) + q_{T-1,3}\cos\left(\frac{T-1}{\theta^2}\right) & \dots & q_{T-1,d_h-2}\sin\left(\frac{T-1}{\theta^{d_h-2}}\right) + q_{T-1,d_h-1}\cos\left(\frac{T-1}{\theta^{d_h-2}}\right) \end{bmatrix}}_{T \times (d_h/2)} \quad (55)$$

each $(t, j)^{\text{th}}$ element is of the form, for $t = 0, 1, \dots, T - 1$ and $j = 0, 1, \dots, (d_h/2) - 1$:

$$q'_{t,j} = q_{t,2j}\sin\left(\frac{t}{\theta^j}\right) + q_{t,2j+1}\cos\left(\frac{t}{\theta^j}\right) \quad (56)$$

One can see that the addition of the corresponding even and odd elements will be a $2 - d$ rotation by each corresponding θ with different frequency. For example, the addition of the two blue terms will be a $2 - d$ rotation by θ^2 with frequency 1, i.e., by $\frac{1}{\theta^2}$ radians, and the addition of the two red terms will be a $2 - d$ rotation by $\frac{1}{\theta^2}$ radians.

$$\begin{bmatrix} q'_{1,2} \\ q'_{1,3} \end{bmatrix} = \begin{bmatrix} \cos\left(\frac{1}{\theta^2}\right) & -\sin\left(\frac{1}{\theta^2}\right) \\ \sin\left(\frac{1}{\theta^2}\right) & \cos\left(\frac{1}{\theta^2}\right) \end{bmatrix} \begin{bmatrix} q_{1,2} \\ q_{1,3} \end{bmatrix} = \begin{bmatrix} q_{1,2}\cos\left(\frac{1}{\theta^2}\right) - q_{1,3}\sin\left(\frac{1}{\theta^2}\right) \\ q_{1,2}\sin\left(\frac{1}{\theta^2}\right) + q_{1,3}\cos\left(\frac{1}{\theta^2}\right) \end{bmatrix} \quad (57)$$

or more generally, for each token t , and each feature block $(2i, 2i+1)$ (i.e., the i^{th} feature block after we stack them together in the next step), we have:

$$\begin{aligned} [q'_{t,2i} \quad q'_{t,2i+1}] &= [q_{t,2i}\cos\left(\frac{t}{\theta^2}\right) - q_{t,2i+1}\sin\left(\frac{t}{\theta^2}\right) \quad q_{t,2i}\sin\left(\frac{t}{\theta^2}\right) + q_{t,2i+1}\cos\left(\frac{t}{\theta^2}\right)] \\ &= [q_{t,2i} \quad q_{t,2i+1}] R\left(\frac{t}{\theta^2}\right) \end{aligned} \quad (58)$$

```
# Interleave back
x_rotated = torch.stack([x_even_new, x_odd_new], dim=-1)
x_rotated = x_rotated.flatten(-2, -1)
return x_rotated
```

`torch.stack([], dim=-1)` will stack the \mathbf{Q}'_{even} , of size $(T, (d_v/2))$, and \mathbf{Q}'_{odd} , of size $(T, (d_v/2))$, along the last dimension (hence creating a new dimension of size 2) so that the result is a tensor of shape $(T, (d_v/2), 2)$, and then the `flatten(-2, -1)` will flatten the last two dimensions, so that the result is a tensor of shape (T, d_v) , which is the same as the original \mathbf{Q} tensor.

4.1 Decoupled RoPE

we have, given h heads:

$$\begin{aligned} \mathbf{Y}^{(i)} &= \text{softmax} \left(\frac{1}{\sqrt{d_k}} \underbrace{\mathbf{X}_{T \times d_{\text{model}}}}_{d_{\text{model}} \times 128} \underbrace{\mathbf{W}_Q^{(i)}}_{128 \times 576} \underbrace{\mathbf{W}_{\uparrow K}^{(i)\top} (\mathbf{X} \mathbf{W}_{\downarrow K,V})^\top}_{576 \times T} \right) \underbrace{\mathbf{X}_{T \times 576}}_{T \times 576} \underbrace{\mathbf{W}_{\downarrow K,V}}_{576 \times d_v} \underbrace{\mathbf{W}_{\uparrow V}^{(i)}}_{d_v \times d_{\text{model}}} \underbrace{\mathbf{W}_O^{(i-1) \times d_v + 1:i \times d_v, 1:d_{\text{model}}}}_{d_v \times d_{\text{model}}} \\ \mathbf{Y} &= \sum_{i=1}^h \mathbf{Y}^{(i)} \end{aligned} \quad (59)$$

when we have multiple heads, the output is the same size, except there are multiple of $\mathbf{Y}^{(i)}$ added together.

Here is something about RoPE, let's take the terms inside the softmax function, and remove the $\frac{1}{\sqrt{d_k}}$ term, we have:

$$\underbrace{\mathbf{X}_{T \times d_{\text{model}}}}_{d_{\text{model}} \times 128} \underbrace{\mathbf{W}_Q^{(i)}}_{128 \times 576} \underbrace{\mathbf{W}_{\uparrow K}^{(i)\top} (\mathbf{X} \mathbf{W}_{\downarrow K,V})^\top}_{576 \times T} \quad (60)$$

Since RoPE is applied to the \mathbf{Q} and \mathbf{K} matrices, where there is not a single RoPE matrix for all the tokens, i.e., we do not have something like:

$$\underbrace{\mathbf{X}_{T \times d_{\text{model}}}}_{d_{\text{model}} \times 128} \underbrace{\mathbf{W}_Q^{(i)}}_{128 \times 576} \underbrace{\mathbf{R}^{(i)\top} \mathbf{R}^{(i)}}_{128 \times 576} \underbrace{\mathbf{W}_{\uparrow K}^{(i)\top} (\mathbf{X} \mathbf{W}_{\downarrow K,V})^\top}_{576 \times T} \quad (61)$$

For this reason, we may consider a decoupled RoPE mechanism, where we have two separate part of each row of \mathbf{Q} and \mathbf{K} matrices, i.e., we break up \mathbf{q}_t and \mathbf{k}_t into two parts, one is the part that does not involve RoPE (of a larger dimension), and the other is the part that involves RoPE (of a smaller dimension).

For each head i , and each token t , we have:

$$\mathbf{k}_t^C = \mathbf{W}_{\uparrow K}^{(i)} \mathbf{c}_t^{KV}, \quad \mathbf{v}_t^C = \mathbf{W}_{\uparrow V}^{(i)} \mathbf{c}_t^{KV} \quad (62)$$

for the t -th token, we have the following concatenation of outputs:

$$\mathbf{o}_t = [\mathbf{o}_{t,1} \quad \mathbf{o}_{t,2} \quad \dots \quad \mathbf{o}_{t,h}] \quad (63)$$

which is the weighted sum of \mathbf{v}_j^C for $j = 1, 2, \dots, t$, responding to a specific query \mathbf{q}_t , we now drop the head index i for simplicity:

$$\mathbf{o}_t = \sum_{j=1}^t \text{Softmax} \left(\frac{\mathbf{q}_t^\top \mathbf{k}_j}{\sqrt{d_h + d_h^R}} \right) \mathbf{v}_j^C \quad (64)$$

by letting: $\mathbf{c}_t^Q = \mathbf{W}_{\downarrow Q} \mathbf{h}_t$, $\mathbf{c}_t^Q \in \mathbb{R}^{d_C}$, we have:

$$\begin{aligned}\mathbf{q}_t &= \left[\underbrace{\left(\mathbf{W}_{\uparrow Q} \quad \mathbf{W}_{\downarrow Q} \quad \mathbf{h}_t \right)}_{d_h \times d_C \quad d_C \times d_{\text{model}}} \quad \text{RoPE}(\underbrace{\mathbf{W}_Q^R \quad \mathbf{W}_{\downarrow Q}}_{d_h^R \times d_C \quad d_C \times d_{\text{model}}} \quad \mathbf{h}_t) \right] \\ &= \underbrace{\left[\mathbf{W}_{\uparrow Q} \mathbf{c}_t^Q \quad \text{RoPE}(\mathbf{W}_Q^R \mathbf{c}_t^Q) \right]}_{(d_h + d_h^R) \times 1}\end{aligned}\tag{65}$$

you see that \mathbf{q}_t has two parts, each projecting the hidden state \mathbf{h}_t into a different space by matrices $\mathbf{W}_{\uparrow Q}$ and \mathbf{W}_Q^R . Similiarly, by letting: $\mathbf{c}_t^{KV} = \mathbf{W}_{\downarrow K} \mathbf{h}_t$, $\mathbf{c}_t^{KV} \in \mathbb{R}^{d_C}$, we have:

$$\begin{aligned}\mathbf{k}_j &= \left[\underbrace{\left(\mathbf{W}_{\uparrow K} \quad \mathbf{W}_{\downarrow K} \quad \mathbf{h}_j \right)}_{d_h \times d_C \quad d_C \times d_{\text{model}}} \quad \text{RoPE}(\underbrace{\mathbf{W}_K^R \quad \mathbf{W}_{\downarrow K}}_{d_h^R \times d_C \quad d_C \times d_{\text{model}}} \quad \mathbf{h}_j) \right] \\ &= \underbrace{\left[\mathbf{W}_{\uparrow K} \mathbf{c}_j^{KV} \quad \text{RoPE}(\mathbf{W}_K^R \mathbf{c}_j^{KV}) \right]}_{(d_h + d_h^R) \times 1}\end{aligned}\tag{66}$$

$$\begin{aligned}\mathbf{k}_t &= \left[\mathbf{W}_{\uparrow K} \mathbf{c}_t^{KV} \quad \text{RoPE}(\mathbf{W}_K^R \mathbf{c}_t^{KV}) \right] \in \mathbb{R}^{d_h + d_h^R} \\ \text{where } \mathbf{W}_{\uparrow K} &\in \mathbb{R}^{d_h \times d_C}, \quad \mathbf{W}_K^R \in \mathbb{R}^{d_h^R \times d_C}\end{aligned}\tag{67}$$

now we look at the value \mathbf{v}_t^C , we have:

$$\begin{aligned}\mathbf{v}_t^C &= \underbrace{\mathbf{W}_{\uparrow V}}_{d_h \times d_C} \quad \underbrace{\mathbf{W}_{\downarrow KV}}_{d_C \times d_{\text{model}}} \quad \underbrace{\mathbf{h}_t}_{d_{\text{model}} \times 1} \\ &= \underbrace{\mathbf{W}_{\uparrow V}}_{d_h \times d_C} \quad \underbrace{\mathbf{c}_t^{KV}}_{d_C \times 1}\end{aligned}\tag{68}$$

during inference, we have the following steps:

- for the t -th token, we compute:

$$\mathbf{q}_t = \left[\mathbf{W}_{\uparrow Q} \mathbf{c}_t^Q \quad \text{RoPE}(\mathbf{W}_Q^R \mathbf{c}_t^Q) \right]\tag{69}$$

here, nothing needs to be cached.

- and for each of the j -th token, $\forall j \in \{1, 2, \dots, t-1\}$, we have:

$$\mathbf{k}_j = \left[\mathbf{W}_{\uparrow K} \mathbf{c}_j^{KV} \quad \text{RoPE}(\mathbf{W}_K^R \mathbf{c}_j^{KV}) \right]\tag{70}$$

the things in the cache are the red parts, i.e.,

- $\mathbf{c}_t^{KV} = \mathbf{W}_{\downarrow KV} \mathbf{h}_t$
- $\mathbf{k}_t^R = \text{RoPE}(\mathbf{W}_K^R \mathbf{c}_t^{KV})$

4.1.1 Lightening Indexer

As the number of tokens t increases, it became too computationally expensive to compute all the attention weights for each token $j \leq t$ with the current token t , therefore, we need a lightening indexer to handle this.

Deepseek [3] computes the current query \mathbf{q}_t and the previous key \mathbf{k}_s to decide which query-key pair to use for the attention calculation. Now since we have H^I to indicate the number of index head. (in the paper, $H^I = 64$). Therefore, we have a set of query vectors per head, i.e., $\{\mathbf{q}_{t,j}^I\}_{j=1}^{H^I}$, and a set of key vectors per head, i.e., $\{\mathbf{k}_{s,j}^I\}_{j=1}^{H^I}$. However, to save computation, the key vector is shared across all the index heads, i.e., $\mathbf{k}_{s,j}^I$ is the same for all $j = 1, 2, \dots, H^I$. So we can simply use \mathbf{k}_s^I for all the index heads.

$$I_{t,s} = \sum_{j=1}^{H_I} w_{t,j}^I \cdot \text{ReLU}(\mathbf{q}_{t,j}^I \cdot \mathbf{k}_s^I) \quad (71)$$

which can be thought as the average attention (across all the index heads) between the current query \mathbf{q}_t and the previous key \mathbf{k}_s .

- Note that H^I is smaller than number of heads used in the main attention, i.e., h . $H^I = 64$ in the paper.
- The dimensions of both $\mathbf{q}_{t,j}^I$ and \mathbf{k}_s^I are 128.
- $w_{t,j}^I$: A learnable scalar weight. This is particularly important as it's learnable parameter!
- Using ReLU activation instead of softmax is beneficial for throughput optimization (FP8 implementation).

Since lower precision is used for both $\mathbf{q}_{t,j}^I$ and \mathbf{k}_s^I , therefore, a orthogonal projection is used to project the query and key vectors to prevent them to be too concentrated at some values, for example, $\mathbf{q}_{t,j}^I = [0.01 \ 0.98 \ \dots \ 0.01]^\top$.

Knowing that by applying an orthogonal projection \mathbf{U} , between \mathbf{q} and \mathbf{k} , their dot product is preserved:

$$(\mathbf{U}\mathbf{q})^\top(\mathbf{U}\mathbf{k}) = \mathbf{q}^\top\mathbf{k} \quad (72)$$

but the projection \mathbf{U} can make both \mathbf{q} and \mathbf{k} to have the values more spread out separately.

5 Flash Attention

this is from the paper [4]:

5.1 traditional softmax algorithm

The algorithm for computing softmax is as follows, given there is a logit set $\{x_i\}_{i=1}^N$, where each $x_i \in \mathbb{R}$. We need three separate loops to compute the softmax output:

1. loop 1: compute the maximum value in the logit set:

```

 $m_0 = -\infty$ 
for  $1 \leq i \leq N$  do
 $m_i = \max(m_{i-1}, x_i)$ 
return  $m_N$ 

```

(73)

2. loop 2: compute the sum of the exponential of the logits after we obtained m_N which is the maximum value in the logit set:

```

 $d_0 = 0$ 
for  $1 \leq i \leq N$  do
 $d_i = d_{i-1} + \exp^{x_i - m_N}$ 
return  $d_N$ 

```

(74)

3. loop 3: normalize the logits:

```

for  $1 \leq i \leq N$  do
 $a_i = \frac{\exp^{x_i - m_N}}{d_N}$ 
return  $\{a_i\}_{i=1}^N$ 

```

(75)

5.2 online softmax algorithm

now looking at the second loop, in essence, at the i -th iteration, it is computing the sum of the exponential of the logits from 1 to i :

$$\begin{aligned}
d_i &= \sum_{j=1}^i \exp^{x_j - m_N} \\
&= \underbrace{\sum_{j=1}^{i-1} \exp^{x_j - m_N}}_{d_{i-1}} + \exp^{x_i - m_N} \\
&= d_{i-1} + \exp^{x_i - m_N}
\end{aligned}$$
(76)

with the initial condition $d_0 = 0$, the above can also be expressed as:

$$d_0 = 0 \quad \text{and} \quad d_i = d_{i-1} + \exp^{x_i - m_N}$$
(77)

However, the above cannot be combined with the first loop, because of the m_N term. Therefore, instead of subtracting a “global” maximum value m_N , we subtract a “intermediate” maximum value m_i up to the i -th iteration:

$$d'_{\textcolor{red}{i}} = \sum_{j=1}^{\textcolor{red}{i}} \exp^{x_j - m_i} \quad (78)$$

at the completion of the entire loop, we have $d'_N = d_N$, even though $d_i \neq d'_i \quad \forall i \neq N$ in general. However, if we do the same trick as Eq.(78), however, the first term is not equal to $d'_{i-1} = \sum_{j=1}^{i-1} \exp^{x_j - m_{i-1}}$, i.e., you cannot write the sum as, (a term only contain sum up to $i-1$ terms d_{i-1}) + (a term only contain x_i term).

$$d'_i = \underbrace{\sum_{j=1}^{\textcolor{red}{i}-1} \exp^{x_j - m_i} + \exp^{x_i - m_i}}_{\neq d'_{i-1}} \quad (79)$$

but we can make it so, by adding and subtracting a dummy variable:

$$\begin{aligned} d'_i &= \sum_{j=1}^{\textcolor{red}{i}-1} \exp^{x_j - m_i} + \exp^{x_i - m_i} \\ &= \left(\sum_{j=1}^{\textcolor{red}{i}-1} \exp^{x_j - m_i} \right) \underbrace{\exp^{m_{i-1}} \exp^{-m_{i-1}}}_{\text{dummy variable}} + \exp^{x_i - m_i} \quad \text{perform } \times \exp^{m_{i-1}} \exp^{-m_{i-1}} \\ &= \left(\sum_{j=1}^{\textcolor{red}{i}-1} \exp^{x_j - \textcolor{red}{m}_{i-1}} \right) \exp^{m_{i-1}} \exp^{-\textcolor{blue}{m}_i} + \exp^{x_i - m_i} \quad \text{sawp the red and blue terms} \quad (80) \\ &= \underbrace{\left(\sum_{j=1}^{\textcolor{red}{i}-1} \exp^{x_j - \textcolor{red}{m}_{i-1}} \right)}_{d'_{i-1}} \exp^{m_{i-1} - m_i} + \exp^{x_i - m_i} \\ &= d'_{i-1} \exp^{m_{i-1} - m_i} + \exp^{x_i - m_i} \end{aligned}$$

therefore, we can have the algorithm to be:

1. loop 1: compute the maximum value in the logit set:

```

 $m_0 = -\infty$ 
 $d_0 = 0$ 
for  $1 \leq i \leq N$  do
   $m_i = \max(m_{i-1}, x_i)$ 
   $d_i = d_{i-1} \exp^{m_{i-1} - m_i} + \exp^{x_i - m_i}$ 
return  $m_N, d_N$ 

```

(81)

we also changed $d'_i \rightarrow d_i$ to simplify the notation.

2. loop 2: same as loop 3 in the traditional softmax algorithm:

$$\begin{aligned}
 & \text{for } 1 \leq i \leq N \text{ do} \\
 & \quad a_i = \frac{\exp^{x_i - m_N}}{d_N} \\
 & \quad \text{return } \{a_i\}_{i=1}^N
 \end{aligned} \tag{82}$$

since we are not perform “reduce” operation, such as sum, max, etc., as in here, we compute each a_i individually, we cannot combine it with the first loop.

5.3 online attention

looking at the single \mathbf{q} row matrix form, where we have:

$$\begin{aligned}
 \mathbf{qK}^\top &= [\mathbf{qk}_1^\top \dots \mathbf{qk}_m^\top] \\
 \implies \mathbf{o} &= \text{softmax}(\mathbf{qK}^\top) \mathbf{V} \\
 &= [\text{softmax}([\mathbf{qk}_1^\top \dots \mathbf{qk}_m^\top])] \begin{bmatrix} - & \mathbf{v}_1 & - \\ - & \dots & - \\ - & \mathbf{v}_m & - \end{bmatrix} \\
 &= \sum_{i=1}^N \frac{\exp[\mathbf{qk}_i^\top]}{\sum_j \exp[\mathbf{qk}_j^\top]} \mathbf{v}_i \\
 &= \sum_{i=1}^N a_i \mathbf{v}_i
 \end{aligned} \tag{83}$$

taking a particular row of the above, $\mathbf{x} = \mathbf{qK}^\top$, where $x_i = \mathbf{qk}_i^\top$ is an element of \mathbf{x} :

1. loop 1: compute the maximum value in the logit set:

$$\begin{aligned}
 m_0 &= -\infty \\
 d_0 &= 0 \\
 &\text{for } 1 \leq i \leq N \text{ do} \\
 &\quad \color{red}{x_i = q_i k_i^\top} \\
 &\quad m_i = \max(m_{i-1}, x_i) \\
 &\quad d_i = d_{i-1} \exp^{m_{i-1} - m_i} + \exp^{x_i - m_i} \\
 &\quad \text{return } m_N, d_N
 \end{aligned} \tag{84}$$

2. loop 2: adding $\mathbf{o} = \sum_{i=1}^N a_i \mathbf{v}_i$ to the second loop:

$$\begin{aligned}
& \mathbf{o}_0 = \mathbf{0} \\
& \text{for } 1 \leq i \leq N \text{ do} \\
& \quad a_i = \frac{\exp^{x_i - m_N}}{d_N} \\
& \quad \mathbf{o}_i = \mathbf{o}_{i-1} + a_i \mathbf{v}_i
\end{aligned}
\quad
\begin{aligned}
& \mathbf{o}_0 = \mathbf{0} \\
& \text{for } 1 \leq i \leq N \text{ do} \\
& \quad \mathbf{o}_i = \mathbf{o}_{i-1} + \frac{\exp^{x_i - m_N}}{d_N} \mathbf{v}_i
\end{aligned} \tag{85}$$

note that we can apply the same trick as Eq.(78) to the second loop:

$$\begin{aligned}
\mathbf{o}_i &= \sum_{i=1}^N \frac{\exp^{x_i - m_N}}{d'_N} \mathbf{v}_i \\
\mathbf{o}'_i &= \sum_{j=1}^i \frac{\exp^{x_j - \mathbf{m}_i}}{d'_i} \mathbf{v}_j
\end{aligned} \tag{86}$$

where we have $\mathbf{o}_N = \mathbf{o}'_N$. Apply the same track as Eq.(78), we have:

$$\begin{aligned}
\mathbf{o}'_i &= \sum_{j=1}^i \frac{\exp^{x_j - \mathbf{m}_i}}{d'_i} \mathbf{v}_j \\
&= \left(\sum_{j=1}^{i-1} \frac{\exp^{x_j - m_i}}{d'_i} \mathbf{v}_j \right) + \frac{\exp^{x_i - m_i}}{d'_i} \mathbf{v}_i \\
&= \underbrace{\left(\sum_{j=1}^{i-1} \frac{\exp^{x_j - m_i}}{d'_i} \mathbf{v}_j \right)}_{\neq \mathbf{o}_{i-1}} \frac{d'_{i-1}}{d'_i} \frac{\exp^{m_{i-1}}}{\exp^{m_{i-1}}} + \frac{\exp^{x_i - m_i}}{d'_i} \mathbf{v}_i \\
&= \underbrace{\left(\sum_{j=1}^{i-1} \frac{\exp^{x_j - m_{i-1}}}{d'_{i-1}} \mathbf{v}_j \right)}_{=\mathbf{o}_{i-1}} \frac{d'_{i-1}}{d'_i} \frac{\exp^{m_i}}{\exp^{m_{i-1}}} + \frac{\exp^{x_i - m_i}}{d'_i} \mathbf{v}_i \\
&= \mathbf{o}_{i-1} \frac{d'_{i-1}}{d'_i} \frac{\exp^{m_i}}{\exp^{m_{i-1}}} + \frac{\exp^{x_i - m_i}}{d'_i} \mathbf{v}_i
\end{aligned} \tag{87}$$

5.3.1 final algorithm

everything comes down to just a single loop:

```

 $m_0 = -\infty$ 
 $d_0 = 0$ 
 $\mathbf{o}_0 = \mathbf{0}$ 
for  $1 \leq i \leq N$  do
     $x_i = q_i \mathbf{k}_i^\top$  (88)
     $m_i = \max(m_{i-1}, x_i)$ 
     $d_i = d_{i-1} \exp^{m_{i-1} - m_i} + \exp^{x_i - m_i}$ 
     $\mathbf{o}_i = \mathbf{o}_{i-1} \frac{d_{i-1}}{d_i} \frac{\exp^{m_i}}{\exp^{m_{i-1}}} + \frac{\exp^{x_i - m_i}}{d_i} \mathbf{v}_i$ 
return  $\mathbf{o}_N$ 

```

again, we changed $d'_i \rightarrow d_i$ and $\mathbf{o}'_i \rightarrow \mathbf{o}_i$ to simplify the notation.

References

- [1] Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N Gomez, Łukasz Kaiser, and Illia Polosukhin, “Attention is all you need,” Advances in neural information processing systems, vol. 30, 2017.
- [2] Jianlin Su, Murtadha Ahmed, Yu Lu, Shengfeng Pan, Wen Bo, and Yunfeng Liu, “Roformer: Enhanced transformer with rotary position embedding,” Neurocomputing, vol. 568, pp. 127063, 2024.
- [3] Aixin Liu, Aoxue Mei, Bangcai Lin, Bing Xue, Bingxuan Wang, Bingzheng Xu, Bochao Wu, Bowei Zhang, Chaofan Lin, Chen Dong, et al., “Deepseek-v3. 2: Pushing the frontier of open large language models,” arXiv preprint arXiv:2512.02556, 2025.
- [4] Tri Dao, Dan Fu, Stefano Ermon, Atri Rudra, and Christopher Ré, “Flashattention: Fast and memory-efficient exact attention with io-awareness,” Advances in neural information processing systems, vol. 35, pp. 16344–16359, 2022.