Transformer with PyTorch

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Contents

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 $\mathbf{V}$:

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

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:

$$\begin{aligned}
\implies \mathbf{q}\mathbf{K}^\top &= \begin{bmatrix} \underbrace{\mathbf{q}\mathbf{k}_1^\top}_{\in\mathbb{R}} & \cdots & \underbrace{\mathbf{q}\mathbf{k}_m^\top}_{\in\mathbb{R}} \end{bmatrix} \\
\implies A(\mathbf{q}, \mathbf{K}, \mathbf{V}) &\equiv \text{softmax}(\mathbf{q}\mathbf{K}^\top)\mathbf{V} \\
&= \text{softmax}\big(\begin{bmatrix} \mathbf{q}\mathbf{k}_1^\top & \ldots & \mathbf{q}\mathbf{k}_m^\top \end{bmatrix} \big) \begin{bmatrix} - & \mathbf{v}_1 & - \\ - & \ldots & - \\ - & \mathbf{v}_m & - \end{bmatrix} \\
&= \sum_{i=1}^{m} \underbrace{\frac{\exp[\mathbf{q}\mathbf{k}_i^\top]}{\sum_j \exp[\mathbf{q}\mathbf{k}_j^\top]}}_{\mathbf{a}_i} \mathbf{v}_i \\
&\in \mathbb{R}^{d_\mathbf{v}}
\end{aligned} \tag{2}$$

1.2 Scaled Dot-Product Attention (SDPA)

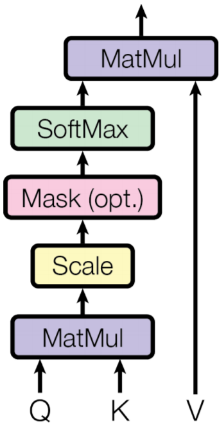
the problem starts as d_k becomes larger, variance of $\mathbf{q}\mathbf{k}^\top$ increases. Then as a result, some dot product values gets very large, with exp(.), softmax $\mathbf{p}$ gets peaky! Remember derivative of cross-entropy between softmax p and y is:

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

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:

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



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

1.3 in the case of "seq2seq with attention"

we have:

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

where 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 $\mathbf{h}_i \mathbf{z}_j^\top$:

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

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:

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

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

$$\implies \mathbf{Q}\mathbf{K}^\top = \begin{bmatrix} \mathbf{q}_1\mathbf{k}_1^\top & \dots & \mathbf{q}_1\mathbf{k}_m^\top \\ \dots & \dots & \dots \\ \mathbf{q}_n\mathbf{k}_1^\top & \dots & \mathbf{q}_n\mathbf{k}_m^\top \end{bmatrix} \tag{8}$$

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

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

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 $\mathbf{V}$.

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

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:

$$\mathbf{Q} = \mathbf{XW}_Q, \quad \mathbf{K} = \mathbf{XW}_K, \quad \mathbf{V} = \mathbf{XW}_V \tag{11}$$

and let:

$$m = n = T \tag{12}$$

we achieved self-attention, in summary:

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

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

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:

$$\mathbf{Y} = \underbrace{\mathrm{concat}(\mathbf{O}_1, \ldots, \mathbf{O}_h)}_{T \times d_{\mathrm{model}}} \underbrace{\mathbf{W}_O}_{d_{\mathrm{model}} \times d_{\mathrm{model}}} \tag{14}$$

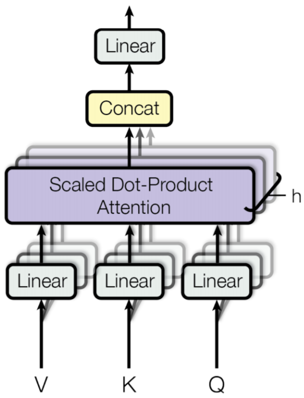


Figure 1: Multi-head Attention

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:

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

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

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

$$
\begin{aligned}
h &\equiv n_{\text{heads}} \\
d_k &= \mathrm{d}_v = d_h \\
d_h \times h &\equiv \mathrm{d}_{\text{model}}
\end{aligned} \tag{16}
$$

and the code has a few definitions:

```python
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:

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

```python
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:
```

1. 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).

$$\left[\underbrace{\begin{bmatrix} - & \mathbf{y}_1 & - \\ & \vdots & \\ - & \mathbf{y}_T & - \end{bmatrix}}_{T \times d_{\text{model}}}\right] \tag{18}$$

The column dimesion 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:

$$\mathbf{Q} = \mathbf{X}\mathbf{W}_Q, \quad \mathbf{K} = \mathbf{X}\mathbf{W}_K, \quad \mathbf{V} = \mathbf{X}\mathbf{W}_V \tag{19}$$

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

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

```
        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:

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

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

after running the above code, each $\mathbf{Q}, \mathbf{K}, \mathbf{V}$ matrix is still having their heads together in a big matrix, so we need to chop them up into separate heads:

2. now we split the $\mathbf{QKV}$ single large matrix into each separate $\mathbf{Q}, \mathbf{K}, \mathbf{V}$ 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 $\mathbf{Q}$, $\mathbf{K}$ and $\mathbf{V}$, 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:

$$\mathbf{Q} = \begin{bmatrix} \underbrace{\begin{bmatrix} \underbrace{\begin{bmatrix} - & \mathbf{q}_1 & - \\ - & \dots & - \\ - & \mathbf{q}_T & - \end{bmatrix}}_{\mathbf{Q}_{(1)}:\, T\times d_k} & \dots & \underbrace{\begin{bmatrix} - & \mathbf{q}_1 & - \\ - & \dots & - \\ - & \mathbf{q}_T & - \end{bmatrix}}_{\mathbf{Q}_{(h)}:\, T\times d_k} \end{bmatrix}}_{T\times d_{\text{model}}} \end{bmatrix} \mathbf{K} = \begin{bmatrix} \underbrace{\begin{bmatrix} \underbrace{\begin{bmatrix} - & \mathbf{k}_1 & - \\ - & \dots & - \\ - & \mathbf{k}_T & - \end{bmatrix}}_{\mathbf{K}_{(1)}:\, T\times d_k} & \dots & \underbrace{\begin{bmatrix} - & \mathbf{k}_1 & - \\ - & \dots & - \\ - & \mathbf{k}_T & - \end{bmatrix}}_{\mathbf{K}_{(h)}:\, T\times d_k} \end{bmatrix}}_{T\times d_{\text{model}}} \end{bmatrix}$$
$$\mathbf{V} = \begin{bmatrix} \underbrace{\begin{bmatrix} \underbrace{\begin{bmatrix} - & \mathbf{v}_1 & - \\ - & \dots & - \\ - & \mathbf{v}_T & - \end{bmatrix}}_{\mathbf{V}_{(1)}:\, T\times d_v} & \dots & \underbrace{\begin{bmatrix} - & \mathbf{v}_1 & - \\ - & \dots & - \\ - & \mathbf{v}_T & - \end{bmatrix}}_{\mathbf{V}_{(h)}:\, T\times d_v} \end{bmatrix}}_{T\times d_{\text{model}}} \end{bmatrix} \tag{22}$$

where we remind ourselves that:

$$\begin{aligned} h &\equiv n_{\text{heads}} \\ d_h \times h &= \mathrm{d}_{\text{model}} \end{aligned} \tag{23}$$

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

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

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

$$\begin{bmatrix} \mathbf{Q}_{(1)}\mathbf{K}_{(1)}^\top & \dots & \mathbf{Q}_{(h)}\mathbf{K}_{(h)}^\top \end{bmatrix} \tag{24}$$

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

```
att = att / (self.head_dim ** 0.5)
```

where we obtained:

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

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

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

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

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

```
att = F.softmax(att, dim=-1)
att = self.attn_dropout(att)
```

$$\begin{bmatrix} \underbrace{\begin{bmatrix} \text{softmax}\left(\begin{bmatrix} \frac{\mathbf{q}_1^{(1)}\mathbf{k}_1^{(1)\top}}{\sqrt{d_h}} & \dots & -\infty \end{bmatrix}\right) \\ \vdots \\ \text{softmax}\left(\begin{bmatrix} \frac{\mathbf{q}_T^{(1)}\mathbf{k}_1^{(1)\top}}{\sqrt{d_h}} & \dots & \frac{\mathbf{q}_T^{(1)}\mathbf{k}_T^{(1)\top}}{\sqrt{d_h}} \end{bmatrix}\right) \end{bmatrix}}_{\text{softmax}\left(\frac{\mathbf{Q}^{(1)}\mathbf{K}^{(1)\top}}{\sqrt{d_h}}\right)} & \dots & \underbrace{\begin{bmatrix} \text{softmax}\left(\begin{bmatrix} \frac{\mathbf{q}_1^{(h)}\mathbf{k}_1^{(h)\top}}{\sqrt{d_h}} & \dots & -\infty \end{bmatrix}\right) \\ \vdots \\ \text{softmax}\left(\begin{bmatrix} \frac{\mathbf{q}_T^{(h)}\mathbf{k}_1^{(h)\top}}{\sqrt{d_h}} & \dots & \frac{\mathbf{q}_T^{(h)}\mathbf{k}_T^{(h)\top}}{\sqrt{d_h}} \end{bmatrix}\right) \end{bmatrix}}_{\text{softmax}\left(\frac{\mathbf{Q}^{(h)}\mathbf{K}^{(h)\top}}{\sqrt{d_h}}\right)} \end{bmatrix} \tag{27}$$

7. apply weighted sum to the values:

```
# Weighted sum of values
y = att @ v  # (B, n_heads, T, head_dim)
```

where we obtained:

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

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:

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

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
```

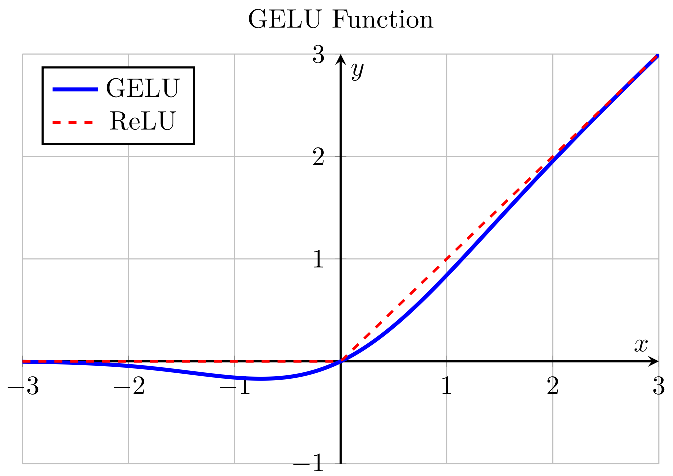
one can see that the final output is a tensor of shape B, T, d_{model}.

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:

```python
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.



The mathematical definition involves the Cumulative Distribution Function (CDF) of the Gaussian (Normal) distribution, often denoted as $\Phi(x)$.
the advantage of GELU over ReLU is that it is smoother and has a better gradient flow.

$$\mathrm{GELU}(x) = x \cdot \Phi(x) \tag{30}$$

In simpler terms:
Output=Input $\times$ (Probability that a normal distribution value is less than Input)

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.

$$\begin{bmatrix}[0 & 1 & 2 & \dots & T-1]\end{bmatrix} \tag{31}$$

```
        # 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
```

In above code, F.cross_entropy() function expects inputs expects the shape: (Total_Number_of_Predictions, Number_of_Classes). However, the current shape is (B, T, vocab_size), where vocab_size is the number of classes.

Therefore, we transform the logits to have the shape ($B \times T$, vocab_size), and the targets to have the shape ($B \times T$).

```
    @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).
```

```python
        """
        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, $\mathbf{K}$ and $\mathbf{V}$ must be the same thing. For example,

1. Text-to-image Cross-Attention:

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

2. Image-to-text Cross-Attention:

$$\begin{aligned} \mathbf{K} \text{ and } \mathbf{V} \text{ are image embedding} \\ \mathbf{Q} \text{ is text embedding} \end{aligned} \tag{33}$$

3 Recent Developments

3.1 $\mathbf{K} - \mathbf{V}$ caching

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

$$\mathbf{QK}^\top = \begin{bmatrix} \mathbf{q}_1\mathbf{k}_1^\top & \dots & \mathbf{q}_1\mathbf{k}_T^\top \\ \vdots & \ddots & \vdots \\ \mathbf{q}_T\mathbf{k}_1^\top & \dots & \mathbf{q}_T\mathbf{k}_T^\top \end{bmatrix} \tag{34}$$

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

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

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:

$$
\begin{bmatrix}
\mathbf{q}_1\mathbf{k}_1^\top & - & - & - \\
\vdots & \ddots & \vdots & \vdots \\
\mathbf{q}_T\mathbf{k}_1^\top & \dots & \mathbf{q}_T\mathbf{k}_T^\top & - \\
\mathbf{q}_{T+1}\mathbf{k}_1^\top & \dots & \mathbf{q}_{T+1}\mathbf{k}_T^\top & \mathbf{q}_{T+1}\mathbf{k}_{T+1}^\top
\end{bmatrix}
=
\begin{bmatrix}
\underbrace{\mathbf{Q}\mathbf{K}^\top}_{\text{lower triangular}} & - \\
\mathbf{q}_{T+1}\mathbf{K}^\top & \mathbf{q}_{T+1}\mathbf{k}_{T+1}^\top
\end{bmatrix}
\tag{36}
$$

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):

$$
\begin{bmatrix}
\frac{\exp(\mathbf{q}_1\mathbf{k}_1^\top)}{\exp(\mathbf{q}_1\mathbf{k}_1^\top)}\mathbf{v}_1 \\
\frac{\exp(\mathbf{q}_2\mathbf{k}_1^\top)}{\exp(\mathbf{q}_2\mathbf{k}_1^\top)+\exp(\mathbf{q}_2\mathbf{k}_2^\top)}\mathbf{v}_1 + \frac{\exp(\mathbf{q}_2\mathbf{k}_2^\top)}{\exp(\mathbf{q}_2\mathbf{k}_1^\top)+\exp(\mathbf{q}_2\mathbf{k}_2^\top)}\mathbf{v}_2 \\
\frac{\exp(\mathbf{q}_3\mathbf{k}_1^\top)}{\exp(\mathbf{q}_3\mathbf{k}_1^\top)+\exp(\mathbf{q}_3\mathbf{k}_2^\top)+\exp(\mathbf{q}_3\mathbf{k}_3^\top)}\mathbf{v}_1 + \frac{\exp(\mathbf{q}_3\mathbf{k}_2^\top)}{\exp(\mathbf{q}_3\mathbf{k}_1^\top)+\exp(\mathbf{q}_3\mathbf{k}_2^\top)+\exp(\mathbf{q}_3\mathbf{k}_3^\top)}\mathbf{v}_2 + \frac{\exp(\mathbf{q}_3\mathbf{k}_3^\top)}{\exp(\mathbf{q}_3\mathbf{k}_1^\top)+\exp(\mathbf{q}_3\mathbf{k}_2^\top)+\exp(\mathbf{q}_3\mathbf{k}_3^\top)}\mathbf{v}_3 \\
\vdots \\
\sum_{i=1}^{T}\frac{\exp(\mathbf{q}_T\mathbf{k}_i^\top)}{\sum_{j=1}^{T}\exp(\mathbf{q}_T\mathbf{k}_j^\top)}\mathbf{v}_i \\
\sum_{i=1}^{T+1}\frac{\exp(\mathbf{q}_{T+1}\mathbf{k}_i^\top)}{\sum_{j=1}^{T+1}\exp(\mathbf{q}_{T+1}\mathbf{k}_j^\top)}\mathbf{v}_i
\end{bmatrix}
\tag{37}
$$

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.

3.2 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:

$$
\begin{aligned}
\mathbf{C}_{K,V} &= \mathbf{X}\mathbf{W}_{\downarrow K,V} \\
&= \underbrace{\begin{bmatrix} - & \mathbf{x}_1 & - \\ - & \dots & - \\ - & \mathbf{x}_T & - \end{bmatrix}}_{T\times d_{\text{model}}}
\underbrace{\begin{bmatrix} \mathbf{w}_{1,1} & \dots & \mathbf{w}_{1,576} \\ \vdots & \ddots & \vdots \\ \mathbf{w}_{7168,1} & \dots & \mathbf{w}_{7168,576} \end{bmatrix}}_{d_{\text{model}}\times 576}
\end{aligned}
\tag{38}
$$

where $\mathbf{C}_{K,V}$ is the "common" part of the latent representation of the sentence for both $\mathbf{K}$ and $\mathbf{V}$. They are also the same for all heads. This is why this quantity is referred to directly, instead of having $\mathbf{X}\mathbf{W}_{\downarrow K,V}$.

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

$$
\begin{array}{lcl}
\text{traditional} & & \text{multi-head latent attention} \\[1em]
\mathbf{Q}^{(i)} = \mathbf{X}\mathbf{W}_Q^{(i)} & \rightarrow & \underbrace{\mathbf{Q}^{(i)}}_{T\times 128} = \mathbf{X} \underbrace{\mathbf{W}_Q^{(i)}}_{7168\times 128} \\
\mathbf{K}^{(i)} = \mathbf{X}\mathbf{W}_K^{(i)} & \rightarrow & \underbrace{\mathbf{K}^{(i)}}_{T\times 128} = \mathbf{X} \underbrace{\mathbf{W}_{\downarrow K,V}}_{d_{\text{model}}\times 576} \underbrace{\mathbf{W}_{\uparrow K}^{(i)}}_{576\times 128} = \underbrace{\mathbf{C}_{K,V}}_{T\times 576} \underbrace{\mathbf{W}_{\uparrow K}^{(i)}}_{576\times 128} \\
\mathbf{V}^{(i)} = \mathbf{X}\mathbf{W}_V^{(i)} & \rightarrow & \underbrace{\mathbf{V}^{(i)}}_{T\times 128} = \mathbf{X} \underbrace{\mathbf{W}_{\downarrow K,V}}_{d_{\text{model}}\times 576} \underbrace{\mathbf{W}_{\uparrow V}^{(i)}}_{576\times 128} = \underbrace{\mathbf{C}_{K,V}}_{T\times 576} \underbrace{\mathbf{W}_{\uparrow V}^{(i)}}_{576\times 128}
\end{array}
\tag{39}
$$

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

$$
\begin{aligned}
\mathbf{W}_K^{(i)} &\longrightarrow \mathbf{W}_{\downarrow K,V}\ \mathbf{W}_{\uparrow K}^{(i)} \\
\mathbf{K}^{(i)} &\longrightarrow \mathbf{X}\mathbf{W}_{\downarrow K,V}\ \mathbf{W}_{\uparrow K}^{(i)}
\end{aligned}
\tag{40}
$$

substitute:

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

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

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

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

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

$$
\begin{aligned}
&\begin{bmatrix} - & \mathbf{x}_1 & - \\ - & \dots & - \\ - & \mathbf{x}_T & - \end{bmatrix} [\mathbf{W}_{\downarrow K,V}] = \text{cache} \\
\implies &\begin{bmatrix} - & \mathbf{x}_1 & - \\ - & \dots & - \\ - & \mathbf{x}_T & - \\ \color{red}- & \color{red}\mathbf{x}_{T+1} & \color{red}- \end{bmatrix} [\mathbf{W}_{\downarrow K,V}] = \begin{bmatrix} \text{cache} \\ \color{red}\mathbf{x}_{T+1}\mathbf{W}_{\downarrow K,V} \end{bmatrix}
\end{aligned} \tag{43}
$$

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

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

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.

3.3 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))
```

$$\begin{aligned} i &= \begin{bmatrix} 0 & 2 & 4 & \dots & d_v - 2 \end{bmatrix} \\ \text{freqs} &= \underbrace{\begin{bmatrix} \frac{1}{\theta^{0/d_h}} & \frac{1}{\theta^{2/d_h}} & \frac{1}{\theta^{4/d_h}} & \dots & \frac{1}{\theta^{(d_h-2)/d_h}} \end{bmatrix}}_{1\times(d_h/2)} \end{aligned} \tag{47}$$

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

$$\text{freqs} = \underbrace{\begin{bmatrix} \frac{1}{\theta^{0}} & \frac{1}{\theta^{2}} & \frac{1}{\theta^{4}} & \dots & \frac{1}{\theta^{d_h-2}} \end{bmatrix}}_{1\times(d_h/2)} \tag{48}$$

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:

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

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

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

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

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

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

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

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

```
        # 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
```

$\mathbf{Q}'_{even} =$

$$\underbrace{\begin{bmatrix} q_{0,0}\text{cos}(\frac{0}{\theta^0}) - q_{0,1}\text{sin}(\frac{0}{\theta^0}) & q_{0,2}\text{cos}(\frac{0}{\theta^2}) - q_{0,3}\text{sin}(\frac{0}{\theta^2}) & \dots & q_{0,d_h-2}\text{cos}(\frac{0}{\theta^{d_h-2}}) - q_{0,d_h-1}\text{sin}(\frac{0}{\theta^{d_h-2}}) \\ q_{1,0}\text{cos}(\frac{1}{\theta^0}) - q_{1,1}\text{sin}(\frac{1}{\theta^0}) & q_{1,2}\text{cos}(\frac{1}{\theta^2}) - q_{1,3}\text{sin}(\frac{1}{\theta^2}) & \dots & q_{1,d_h-2}\text{cos}(\frac{1}{\theta^{d_h-2}}) - q_{1,d_h-1}\text{sin}(\frac{1}{\theta^{d_h-2}}) \\ \vdots & \vdots & \ddots & \vdots \\ q_{T-2,0}\text{cos}(\frac{T-2}{\theta^0}) - q_{T-2,1}\text{sin}(\frac{T-2}{\theta^0}) & q_{T-2,2}\text{cos}(\frac{T-2}{\theta^2}) - q_{T-2,3}\text{sin}(\frac{T-2}{\theta^2}) & \dots & q_{T-2,d_h-2}\text{cos}(\frac{T-2}{\theta^{d_h-2}}) - q_{T-2,d_h-1}\text{sin}(\frac{T-2}{\theta^{d_h-2}}) \\ q_{T-1,0}\text{cos}(\frac{T-1}{\theta^0}) - q_{T-1,1}\text{sin}(\frac{T-1}{\theta^0}) & q_{T-1,2}\text{cos}(\frac{T-1}{\theta^2}) - q_{T-1,3}\text{sin}(\frac{T-1}{\theta^2}) & \dots & q_{T-1,d_h-2}\text{cos}(\frac{T-1}{\theta^{d_h-2}}) - q_{T-1,d_h-1}\text{sin}(\frac{T-1}{\theta^{d_h-2}}) \end{bmatrix}}_{T\times(d_h/2)} \tag{53}$$

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

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

$\mathbf{Q}'_{odd} =$

$$\underbrace{\begin{bmatrix} q_{0,0}\text{sin}(\frac{0}{\theta^0}) + q_{0,1}\text{cos}(\frac{0}{\theta^0}) & q_{0,2}\text{sin}(\frac{0}{\theta^2}) + q_{0,3}\text{cos}(\frac{0}{\theta^2}) & \dots & q_{0,d_h-2}\text{sin}(\frac{0}{\theta^{d_h-2}}) + q_{0,d_h-1}\text{cos}(\frac{0}{\theta^{d_h-2}}) \\ q_{1,0}\text{sin}(\frac{1}{\theta^0}) + q_{1,1}\text{cos}(\frac{1}{\theta^0}) & q_{1,2}\text{sin}(\frac{1}{\theta^2}) + q_{1,3}\text{cos}(\frac{1}{\theta^2}) & \dots & q_{1,d_h-2}\text{sin}(\frac{1}{\theta^{d_h-2}}) + q_{1,d_h-1}\text{cos}(\frac{1}{\theta^{d_h-2}}) \\ \vdots & \vdots & \ddots & \vdots \\ q_{T-2,0}\text{sin}(\frac{T-2}{\theta^0}) + q_{T-2,1}\text{cos}(\frac{T-1}{\theta^0}) & q_{T-2,2}\text{sin}(\frac{T-1}{\theta^2}) + q_{T-2,3}\text{cos}(\frac{T-1}{\theta^2}) & \dots & q_{T-2,d_h-2}\text{sin}(\frac{T-1}{\theta^{d_h-2}}) + q_{T-2,d_h-1}\text{cos}(\frac{T-1}{\theta^{d_h-2}}) \\ q_{T-1,0}\text{sin}(\frac{T-1}{\theta^0}) + q_{T-1,1}\text{cos}(\frac{T-1}{\theta^0}) & q_{T-1,2}\text{sin}(\frac{T-1}{\theta^2}) + q_{T-1,3}\text{cos}(\frac{T-1}{\theta^2}) & \dots & q_{T-1,d_h-2}\text{sin}(\frac{T-1}{\theta^{d_h-2}}) + q_{T-1,d_h-1}\text{cos}(\frac{T-1}{\theta^{d_h-2}}) \end{bmatrix}}_{T\times(d_h/2)} \tag{55}$$

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

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

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 addtion 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 addtion of the two red terms will be a $2-d$ rotation by $\frac{1}{\theta^2}$ radians.

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

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:

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

```
    # 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.

3.4 Decoupled RoPE

we have, given h heads:

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

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:

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

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:

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

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, note that the following, we changed from right multiplication to left multiplication:

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

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

$$\boldsymbol{o}_t = \begin{bmatrix}\boldsymbol{o}_{t,1} & \boldsymbol{o}_{t,2} & \dots & \boldsymbol{o}_{t,h}\end{bmatrix} \tag{63}$$

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

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

by letting: $\boldsymbol{c}_t^Q = \boldsymbol{W}_{\downarrow Q}\ \mathbf{x}_t, \quad \boldsymbol{c}_t^Q \in \mathbb{R}^{d_\text{C}}$, we have:

$$\begin{aligned}\boldsymbol{q}_t^{(i)} &= \begin{bmatrix}(\underbrace{\boldsymbol{W}_{\uparrow Q}^{(i)}}_{d_h \times d_C}\ \underbrace{\boldsymbol{W}_{\downarrow Q}}_{d_C \times d_\text{model}}\ \mathbf{x}_t) & \text{RoPE}(\underbrace{\boldsymbol{W}_{(R)Q}^{(i)}}_{d_h^R \times d_C}\ \underbrace{\boldsymbol{W}_{\downarrow Q}}_{d_C \times d_\text{model}}\ \mathbf{x}_t)\end{bmatrix} \\ &= \underbrace{\begin{bmatrix}\boldsymbol{W}_{\uparrow Q}^{(i)}\ \boldsymbol{c}_Q^t & \text{RoPE}(\boldsymbol{W}_{(R)Q}^{(i)}\ \boldsymbol{c}_Q^t)\end{bmatrix}}_{(d_h + d_h^R) \times 1}\end{aligned} \tag{65}$$

you see that $\mathbf{q}_t^{(i)}$ has two parts, each projecting the hidden state $\mathbf{x}_t$ into a different space by matrices $\boldsymbol{W}_{\uparrow Q}^{(i)}$ and $\boldsymbol{W}_{(R)Q}^{(i)}$. Similiarly, by letting: $\boldsymbol{c}_{K,V}^t = \boldsymbol{W}_{\downarrow K,V}\ \mathbf{x}_t, \quad \boldsymbol{c}_{K,V}^t \in \mathbb{R}^{d_\text{C}}$, we have:

$$\begin{aligned}\boldsymbol{k}_s^{(i)} &= \begin{bmatrix}(\underbrace{\boldsymbol{W}_{\uparrow K}^{(i)}}_{d_h \times d_C}\ \underbrace{\boldsymbol{W}_{\downarrow K,V}}_{d_C \times d_\text{model}}\ \mathbf{x}_s) & \text{RoPE}(\underbrace{\boldsymbol{W}_{(R)K}^{(i)}}_{d_h^R \times d_C}\ \underbrace{\boldsymbol{W}_{\downarrow K,V}}_{d_C \times d_\text{model}}\ \mathbf{x}_s)\end{bmatrix} \\ &= \underbrace{\begin{bmatrix}\boldsymbol{W}_{\uparrow K}^{(i)}\ \boldsymbol{c}_{K,V}^s & \text{RoPE}(\boldsymbol{W}_{(R)K}^{(i)}\ \boldsymbol{c}_{K,V}^s)\end{bmatrix}}_{(d_h + d_h^R) \times 1}\end{aligned} \tag{66}$$

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

$$\begin{aligned}\boldsymbol{v}_t^C &= \underbrace{\boldsymbol{W}_{\uparrow V}^{(i)}}_{d_h \times d_C}\ \underbrace{\boldsymbol{W}_{\downarrow K,V}}_{d_C \times d_\text{model}}\ \underbrace{\boldsymbol{x}_t}_{d_\text{model} \times 1} \\ &= \underbrace{\boldsymbol{W}_{\uparrow V}^{(i)}}_{d_h \times d_C}\ \underbrace{\boldsymbol{c}_{K,V}^t}_{d_C \times 1}\end{aligned} \tag{67}$$

during inference, we have the following steps:

- for the t-th token, we compute:

$$q_t^{(i)} = \left[W_{\uparrow Q}^{(i)} \, c_Q^t \quad \mathrm{RoPE}(W_{(R)Q}^{(i)} \, c_Q^t) \right] \tag{68}$$

  here, nothing needs to be cached.

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

$$k_s^{(i)} = \left[W_{\uparrow K}^{(i)} \, c_{K,V}^s \quad \mathrm{RoPE}(W_{(R)K}^{(i)} \, c_{K,V}^s) \right] \tag{69}$$

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

  - $c_{K,V}^t = W_{\downarrow K,V} \, h_t$
  - $k_{(R)t}^{(i)} = \mathrm{RoPE}(W_{(R)K}^{(i)} \, c_{K,V}^t)$

3.5 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 q_t and the previous key 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., $\{q_{t,j}^I\}_{j=1}^{H^I}$, and a set of key vectors per head, i.e., $\{k_{s,j}^I\}_{j=1}^{H^I}$. However, to save computation, the key vector is shared across all the index heads, i.e., $k_{s,j}^I$ is the same for all $j = 1, 2, \ldots, H^I$. So we can simply use k_s^I for all the index heads.

$$I_{t,s} = \sum_{j=1}^{H_I} w_{t,j}^I \cdot \mathrm{ReLU}(q_{t,j}^I \cdot k_s^I) \tag{70}$$

which can be thought as the average attention (across all the index heads) between the current query q_t and the previous key 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 $q_{t,j}^I$ and k_s^I are 128.
- $w_{t,j}^I$: A learnable scalar weight. This is particuarlly 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 $\boldsymbol{q}_{t,j}^I$ and $\boldsymbol{k}_s^I$, therefore, a orthognal projection is used to project the query and key vectors to prevent them to be too cencenrated at some values, for example, $\boldsymbol{q}_{t,j}^I = \begin{bmatrix} 0.01 & 0.98 & \dots & 0.01 \end{bmatrix}^\top$.

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

$$(\mathbf{U}\boldsymbol{q})^\top(\mathbf{U}\boldsymbol{k}) = \boldsymbol{q}^\top\boldsymbol{k} \tag{71}$$

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

4 Flash Attention

this is from the paper [4]:

4.1 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:

$$\begin{aligned}
&m_0 = -\infty \\
&\text{for } 1 \le i \le N \text{ do} \\
&\quad m_i = \max(m_{i-1}, x_i) \\
&\text{return } m_N
\end{aligned} \tag{72}$$

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:

$$\begin{aligned}
&d_0 = 0 \\
&\text{for } 1 \le i \le N \text{ do} \\
&\quad d_i = d_{i-1} + \exp^{x_i - m_N} \\
&\text{return } d_N
\end{aligned} \tag{73}$$

3. loop 3: normalize the logits:

$$\begin{aligned}
&\text{for } 1 \le i \le N \text{ do} \\
&\quad a_i = \frac{\exp^{x_i - m_N}}{d_N} \\
&\text{return } \{a_i\}_{i=1}^N
\end{aligned} \tag{74}$$

4.2 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:

$$
\begin{aligned}
d_i &= \sum_{j=1}^{i} \exp^{x_j - m_N} \\
&= \underbrace{\sum_{j=1}^{i-1} \exp^{x_j - m_N}}_{d_{i-1}} + \exp^{x_i - m_N} \\
&= d_{i-1} + \exp^{x_i - m_N}
\end{aligned}
\tag{75}
$$

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

$$
d_0 = 0 \quad \text{and} \quad d_i = d_{i-1} + \exp^{x_i - m_N} \tag{76}
$$

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:

$$
d'_{i} = \sum_{j=1}^{i} \exp^{x_j - m_{i}} \tag{77}
$$

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.(77), 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).

$$
d'_i = \underbrace{\sum_{j=1}^{i-1} \exp^{x_j - m_i}}_{\neq d'_{i-1}} + \exp^{x_i - m_i} \tag{78}
$$

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

$$
\begin{aligned}
d'_i &= \sum_{j=1}^{\color{red}{i-1}} \exp^{x_j - m_i} + \exp^{x_i - m_i} \\
&= \Big(\sum_{j=1}^{i-1} \exp^{x_j - m_i}\Big) \underbrace{\exp^{m_{i-1}} \exp^{-m_{i-1}}}_{\text{dummy variable}} + \exp^{x_i - m_i} \qquad \text{perform} \times \exp^{m_{i-1}} \exp^{-m_{i-1}} \\
&= \Big(\sum_{j=1}^{i-1} \exp^{x_j - \color{red}{m_{i-1}}}\Big) \exp^{m_{i-1}} \exp^{-\color{blue}{m_i}} + \exp^{x_i - m_i} \qquad \text{sawp the red and blue terms} \\
&= \underbrace{\Big(\sum_{j=1}^{i-1} \exp^{x_j - \color{red}{m_{i-1}}}\Big)}_{\mathrm{d}'_{i-1}} \exp^{m_{i-1} - m_i} + \exp^{x_i - m_i} \\
&= d'_{i-1} \exp^{m_{i-1} - m_i} + \exp^{x_i - m_i}
\end{aligned}
\tag{79}
$$

therefore, we can have the algorithm to be:

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

$$
\begin{aligned}
& m_0 = -\infty \\
& d_0 = 0 \\
& \text{for } 1 \le i \le N \text{ do} \\
& \quad m_i = \max(m_{i-1}, x_i) \\
& \quad d_i = d_{i-1} \exp^{m_{i-1} - m_i} + \exp^{x_i - m_i} \\
& \text{return } m_N, d_N
\end{aligned}
\tag{80}
$$

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

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

$$
\begin{aligned}
& \text{for } 1 \le i \le N \text{ do} \\
& \quad a_i = \frac{\exp^{x_i - m_N}}{d_N} \\
& \text{return } \{a_i\}_{i=1}^{N}
\end{aligned}
\tag{81}
$$

   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.

4.3 online attention

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

$$
\begin{aligned}
\mathbf{q}\mathbf{K}^\top &= \begin{bmatrix}\mathbf{q}\mathbf{k}_1^\top & \dots & \mathbf{q}\mathbf{k}_m^\top\end{bmatrix} \\
\implies \mathbf{o} &= \text{softmax}(\mathbf{q}\mathbf{K}^\top)\mathbf{V} \\
&= \begin{bmatrix}\text{softmax}\big(\begin{bmatrix}\mathbf{q}\mathbf{k}_1^\top & \dots & \mathbf{q}\mathbf{k}_m^\top\end{bmatrix}\big)\end{bmatrix} \begin{bmatrix} - & \mathbf{v}_1 & - \\ - & \dots & - \\ - & \mathbf{v}_m & - \end{bmatrix} \\
&= \sum_{i=1}^{N} \frac{\exp[\mathbf{q}\mathbf{k}_i^\top]}{\sum_j \exp[\mathbf{q}\mathbf{k}_j^\top]}\mathbf{v}_i \\
&= \sum_{i=1}^{N} a_i \mathbf{v}_i
\end{aligned}
\tag{82}
$$

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

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

$$
\begin{aligned}
& m_0 = -\infty \\
& d_0 = 0 \\
& \text{for } 1 \le i \le N \text{ do} \\
& \quad \color{red}{x_i = q_i \mathbf{k}_i^\top} \\
& \quad m_i = \max(m_{i-1}, x_i) \\
& \quad d_i = d_{i-1} \exp^{m_{i-1}-m_i} + \exp^{x_i - m_i} \\
& \text{return } m_N, d_N
\end{aligned}
\tag{83}
$$

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

$$
\begin{aligned}
& \mathbf{o}_0 = \mathbf{0} \\
& \text{for } 1 \le i \le N \text{ do} \\
& \quad a_i = \frac{\exp^{x_i - m_N}}{d_N} \\
& \quad \color{red}{\mathbf{o}_i = \mathbf{o}_{i-1} + a_i \mathbf{v}_i}
\end{aligned}
\qquad\qquad
\begin{aligned}
& \mathbf{o}_0 = \mathbf{0} \\
& \text{for } 1 \le i \le N \text{ do} \\
& \quad \color{red}{\mathbf{o}_i = \mathbf{o}_{i-1} + \frac{\exp^{x_i - m_N}}{d_N}}\mathbf{v}_i
\end{aligned}
\tag{84}
$$

note that we can apply the same trick as Eq.(77) to the second loop:

$$
\begin{aligned}
\mathbf{o}_i &= \sum_{i=1}^{N} \frac{\exp^{x_i - m_N}}{d'_N}\mathbf{v}_i \\
\mathbf{o}'_i &= \sum_{j=1}^{i} \frac{\exp^{x_j - \color{red}{m_i}}}{\color{red}{d'_i}}\mathbf{v}_j
\end{aligned}
\tag{85}
$$

where we have $\mathbf{o}_N = \mathbf{o}'_N$. Apply the same track as Eq.(77), we have:

$$
\begin{aligned}
\mathbf{o}'_i &= \sum_{j=1}^{i} \frac{\exp^{x_j - m_i}}{d'_i} \mathbf{v}_j \\
&= (\sum_{j=1}^{i-1} \frac{\exp^{x_j - m_i}}{d'_i} \mathbf{v}_j) + \frac{\exp^{x_i - m_i}}{d'_i} \mathbf{v}_i \\
&= \underbrace{(\sum_{j=1}^{i-1} \frac{\exp^{x_j - m_i}}{d'_i} \mathbf{v}_j)}_{\neq \mathbf{o}_{i-1}} \frac{d'_{i-1}}{d'_{i-1}} \frac{\exp^{m_{i-1}}}{\exp^{m_{i-1}}} + \frac{\exp^{x_i - m_i}}{d'_i} \mathbf{v}_i \\
&= \underbrace{(\sum_{j=1}^{i-1} \frac{\exp^{x_j - m_{i-1}}}{d'_{i-1}} \mathbf{v}_j)}_{= \mathbf{o}_{i-1}} \frac{d'_{i-1}}{d'_i} \frac{\exp^{m_i}}{\exp^{m_{i-1}}} + \frac{\exp^{x_i - m_i}}{d'_i} \mathbf{v}_i \\
&= \mathbf{o}_{i-1} \frac{d'_{i-1}}{d'_i} \frac{\exp^{m_i}}{\exp^{m_{i-1}}} + \frac{\exp^{x_i - m_i}}{d'_i} \mathbf{v}_i
\end{aligned}
\tag{86}
$$

4.3.1 final algorithm

everything comes down to just a single loop:

$$
\begin{aligned}
& m_0 = -\infty \\
& d_0 = 0 \\
& \mathbf{o}_0 = \mathbf{0} \\
& \text{for } 1 \leq i \leq N \text{ do} \\
& \quad x_i = q_i \mathbf{k}_i^\top \\
& \quad m_i = \max(m_{i-1}, x_i) \\
& \quad d_i = d_{i-1} \exp^{m_{i-1} - m_i} + \exp^{x_i - m_i} \\
& \quad \mathbf{o}_i = \mathbf{o}_{i-1} \frac{d_{i-1}}{d_i} \frac{\exp^{m_i}}{\exp^{m_{i-1}}} + \frac{\exp^{x_i - m_i}}{d_i} \mathbf{v}_i \\
& \text{return } \mathbf{o}_N
\end{aligned}
\tag{87}
$$

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

5 Manifold-Constrained Hyper-Connections (mHC)

imagine that at layer l, we have multiple streams of input vectors, $\mathbf{x}_l^{(1)}, \mathbf{x}_l^{(2)}, \mathbf{x}_l^{(3)}, \mathbf{x}_l^{(4)}$, we can aggregate them together to form a single vector, where each $\mathbf{x}_l^{(i)} \in \mathbb{R}^d$:

$$
\mathbf{X}_l = \begin{bmatrix} - & \mathbf{x}_l^{(1)} & - \\ - & \mathbf{x}_l^{(2)} & - \\ \vdots & \vdots & \vdots \\ - & \mathbf{x}_l^{(n)} & - \end{bmatrix} \tag{88}
$$

1. Aggregation Streams:

   now we need a parameter vector to aggregate the streams:

$$
\mathcal{H}_l^{\text{pre}} = \begin{bmatrix} \alpha_l^{(1)} & \alpha_l^{(2)} & \dots & \alpha_l^{(n)} \end{bmatrix} \in \mathbb{R}^{1 \times n} \tag{89}
$$

   We can have the pre-aggregated vector:

$$
\mathbf{x}_l^{\text{pre}} = \mathcal{H}_l^{\text{pre}} \mathbf{X}_l \tag{90}
$$

   where $\mathbf{x}_l^{\text{pre}} \in \mathbb{R}^{1 \times d}$, i.e., a row vector. this is the same as computing the sum of the streams, i.e.,

$$
\mathbf{x}_l^{\text{pre}} = \sum_{i=1}^{n} \alpha_l^{(i)} \mathbf{x}_l^{(i)} \tag{91}
$$

2. neural network:

$$
\mathcal{F}_{W_l}(\mathbf{x}_l^{\text{pre}}) = \begin{bmatrix} \bar{z}_{l,1} & \bar{z}_{l,2} & \dots & \bar{z}_{l,d} \end{bmatrix} \tag{92}
$$

   this is the main neural network that we need, and its still only performed on a single stream, as it is the most expensive operation.

3. Expand Streams:

   We need another set of parameters to expand the stream:

$$
\mathcal{H}_l^{\text{post}} = \begin{bmatrix} \beta_l^{(1)} & \beta_l^{(2)} & \dots & \beta_l^{(n)} \end{bmatrix}^\top \in \mathbb{R}^{n \times 1} \tag{93}
$$

   then the expanded streams are:

$$
\begin{aligned}
\mathbf{Z}_l &= \mathcal{H}_l^{\text{post}} \mathcal{F}_{W_l}(\mathbf{x}_l^{\text{pre}}) \\
&= \begin{bmatrix} \beta_l^{(1)} \\ \beta_l^{(2)} \\ \vdots \\ \beta_l^{(n)} \end{bmatrix} \begin{bmatrix} \bar{z}_{l,1} & \bar{z}_{l,2} & \dots & \bar{z}_{l,d} \end{bmatrix}
\end{aligned} \tag{94}
$$

4. Mix Streams:
   here we have another set of parameters to mix the streams $\mathcal{H}_l^{\text{res}} \in \mathbb{R}^{n \times n}$:

$$\begin{aligned} \mathbf{H}_l &= \mathcal{H}_l^{\text{res}} \, \mathbf{X}_l \\ \text{where } \mathbf{H}_l &\in \mathbb{R}^{n \times d} \end{aligned} \tag{95}$$

   then the mixed streams are:

$$\mathbf{x}_{l+1} = \mathbf{H}_l + \mathbf{Z}_l \tag{96}$$

Putting them all together, we have:

$$\mathbf{x}_{l+1} = \mathcal{H}_l^{\text{res}} \, \mathbf{x}_l + \mathcal{H}_l^{\text{post}} \big(\mathcal{F}_{W_l} \big(\mathcal{H}_l^{\text{pre}} \, \mathbf{x}_l \big) \big) \tag{97}$$

5.1 issue with the implementation

looking at the residual connection, we have:

$$\begin{aligned} \mathbf{x}_L &= \underbrace{\mathbf{x}_{L-1}} + \underbrace{\mathcal{F}_{W_{L-1}}(\mathbf{x}_{L-1})}_{\text{don't apply recursion}} \\ &= \underbrace{\mathbf{x}_{L-2} + \mathcal{F}_{W_{L-2}}(\mathbf{x}_{L-2})} + \mathcal{F}_{W_{L-1}}(\mathbf{x}_{L-1}) \\ &= \mathbf{x}_{L-3} + \mathcal{F}_{W_{L-3}}(\mathbf{x}_{L-3}) + \mathcal{F}_{W_{L-2}}(\mathbf{x}_{L-2}) + \mathcal{F}_{W_{L-1}}(\mathbf{x}_{L-1}) \\ &\vdots \\ &= \mathbf{x}_l + \sum_{i=l}^{L-1} \mathcal{F}_{W_i}(\mathbf{x}_i). \end{aligned} \tag{98}$$

You see that the first term is the identity mapping, which prevents gradient vanishing and exploding, i.e, $\frac{\partial \mathbf{x}_L}{\partial \mathbf{x}_l} = 1 + \text{some terms}$.

now we turn our attention to the hyper-connections:

$$
\begin{aligned}
\mathbf{x}_L &= \mathcal{H}^{\mathrm{res}}_{L-1}\,\underline{\mathbf{x}_{L-1}} + \mathcal{H}^{\mathrm{post}}_{L-1}\big(\mathcal{F}_{W_{L-1}}\big(\mathcal{H}^{\mathrm{pre}}_{L-1}\,\mathbf{x}_{L-1}\big)\big) \\
&= \mathcal{H}^{\mathrm{res}}_{L-1}\,\underbrace{\big(\mathcal{H}^{\mathrm{res}}_{L-2}\,\mathbf{x}_{L-2} + \mathcal{H}^{\mathrm{post}}_{L-2}\big(\mathcal{F}_{W_{L-2}}\big(\mathcal{H}^{\mathrm{pre}}_{L-2}\,\mathbf{x}_{L-2}\big)\big)\big)}_{\mathbf{x}_{L-1}} + \mathcal{H}^{\mathrm{post}}_{L-1}\big(\mathcal{F}_{W_{L-1}}\big(\mathcal{H}^{\mathrm{pre}}_{L-1}\,\mathbf{x}_{L-1}\big)\big) \\
&= \mathcal{H}^{\mathrm{res}}_{L-1}\,\mathcal{H}^{\mathrm{res}}_{L-2}\,\underline{\mathbf{x}_{L-2}} + \mathcal{H}^{\mathrm{res}}_{L-1}\,\mathcal{H}^{\mathrm{post}}_{L-2}\big(\mathcal{F}_{W_{L-2}}\big(\mathcal{H}^{\mathrm{pre}}_{L-2}\,\mathbf{x}_{L-2}\big)\big) + \mathcal{H}^{\mathrm{post}}_{L-1}\big(\mathcal{F}_{W_{L-1}}\big(\mathcal{H}^{\mathrm{pre}}_{L-1}\,\mathbf{x}_{L-1}\big)\big) \\
&= \mathcal{H}^{\mathrm{res}}_{L-1}\,\mathcal{H}^{\mathrm{res}}_{L-2}\,\underbrace{\big(\mathcal{H}^{\mathrm{res}}_{L-3}\,\mathbf{x}_{L-3} + \mathcal{H}^{\mathrm{post}}_{L-3}\big(\mathcal{F}_{W_{L-3}}\big(\mathcal{H}^{\mathrm{pre}}_{L-3}\,\mathbf{x}_{L-3}\big)\big)\big)}_{\mathbf{x}_{L-2}} \\
&\qquad + \mathcal{H}^{\mathrm{res}}_{L-1}\,\mathcal{H}^{\mathrm{post}}_{L-2}\big(\mathcal{F}_{W_{L-2}}\big(\mathcal{H}^{\mathrm{pre}}_{L-2}\,\mathbf{x}_{L-2}\big)\big) + \mathcal{H}^{\mathrm{post}}_{L-1}\big(\mathcal{F}_{W_{L-1}}\big(\mathcal{H}^{\mathrm{pre}}_{L-1}\,\mathbf{x}_{L-1}\big)\big) \\
&= \mathcal{H}^{\mathrm{res}}_{L-1}\,\mathcal{H}^{\mathrm{res}}_{L-2}\,\mathcal{H}^{\mathrm{res}}_{L-3}\,\mathbf{x}_{L-3} \\
&\qquad + \mathcal{H}^{\mathrm{res}}_{L-1}\,\mathcal{H}^{\mathrm{res}}_{L-2}\,\underbrace{\mathcal{H}^{\mathrm{post}}_{L-3}\big(\mathcal{F}_{W_{L-3}}\big(\mathcal{H}^{\mathrm{pre}}_{L-3}\,\mathbf{x}_{L-3}\big)\big)} + \mathcal{H}^{\mathrm{res}}_{L-1}\,\underbrace{\mathcal{H}^{\mathrm{post}}_{L-2}\big(\mathcal{F}_{W_{L-2}}\big(\mathcal{H}^{\mathrm{pre}}_{L-2}\,\mathbf{x}_{L-2}\big)\big)} + \underbrace{\mathcal{H}^{\mathrm{post}}_{L-1}\big(\mathcal{F}_{W_{L-1}}\big(\mathcal{H}^{\mathrm{pre}}_{L-1}\,\mathbf{x}_{L-1}\big)}\\
&\qquad\vdots \\
&= \left(\prod_{i=1}^{L-l} \mathcal{H}^{\mathrm{res}}_{L-i}\right)\mathbf{x}_l + \sum_{i=1}^{L-1}\left(\prod_{j=1}^{L-1-i} \mathcal{H}^{\mathrm{res}}_{L-j}\right)\underbrace{\mathcal{H}^{\mathrm{post}}_{i}\,\mathcal{F}_{W_i}\big(\mathcal{H}^{\mathrm{pre}}_{i}\,\mathbf{x}_i\big)}\,.
\end{aligned}
\tag{99}
$$

5.2 need $\mathcal{H}^{\mathrm{res}}_l$ to be doubly stochastic

we no longer have the identity mapping, i.e., $\frac{\partial \mathbf{x}_L}{\partial \mathbf{x}_l} \neq 1$, as we now have:

$$
\left(\prod_{i=1}^{L-l} \mathcal{H}^{\mathrm{res}}_{L-i}\right)\mathbf{x}_l \tag{100}
$$

However, if we can make sure that at each layer, $\mathcal{H}^{\mathrm{res}}_l$ is a doubly stochastic matrix, i.e., $\mathcal{H}^{\mathrm{res}}_l \in \mathbb{R}^{n\times n}$ and then the product of two doubly stochastic matrices is also a doubly stochastic matrix, one can be shown in the followig example of matrix multiplication:

$$
\mathbf{AB} = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}\begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{bmatrix} = \begin{bmatrix} a_{11}b_{11} + a_{12}b_{21} & a_{11}b_{12} + a_{12}b_{22} \\ a_{21}b_{11} + a_{22}b_{21} & a_{21}b_{12} + a_{22}b_{22} \end{bmatrix} \tag{101}
$$

you see that the row sum:

$$
a_{11}b_{11} + a_{12}b_{21} + a_{11}b_{12} + a_{12}b_{22} = a_{11}(b_{11} + b_{12}) + a_{12}(b_{21} + b_{22}) = 1 \tag{102}
$$

likewise, the column sum:

$$
a_{11}b_{11} + a_{12}b_{21} + a_{21}b_{11} + a_{22}b_{21} = b_{11}(a_{11} + a_{21}) + b_{21}(a_{12} + a_{22}) = 1 \tag{103}
$$

in addition, the $\|\mathcal{H}^{\mathrm{res}}_l\|_2 = 1$, i.e., the maximum eigenvalue of $\mathcal{H}^{\mathrm{res}}_l$ is 1.
This step can be achieved by Sinkhorn-Knopp algorithm.

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