

2025 USA-NA-AIO Round 2, Problem 2, Part 5

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May 2025

Part 5 (10 points, coding task)

In this part, you are asked to build your own multi-head attention module that subclasses `nn.Module`.

- For simplicity, we ignore any masking. That is, each position in an attending sequence attends to all positions in a being attended sequence.
- In your code, you do not need to worry about whether your code is efficient in an autoprogressive token generation process when your module is used in inference in a GPT-like task.

That is, if we use your code in a GPT-like task to autoprogressively generate tokens, it is totally fine if you repeatedly generate the same key and value at a given position rather than more efficiently storing their values in cache.

- The class name is `MyMHA`.
- Attributes:
 - `D_1` : Dimension of a hidden state/token in an attending sequence.
 - `D_2` : Dimension of a hidden state/token in a being attended sequence.
 - `D_v` : Dimension of a value vector.
 - `D_qk` : Dimension of a query/key vector.
 - `H` : Number of heads.

- W_Q : A linear module whose weights is a query-projection matrix. The shape should be consistant with your answer in Part 2. No bias.
 - W_K : A linear module whose weights is key-projection matrix. The shape should be consistant with your answer in Part 2. No bias.
 - W_V : A linear module whose weights is value-projection matrix. The shape should be consistant with your answer in Part 2. No bias.
 - W_O : A linear module whose weights is an out-projection matrix. The shape should be consistant with your answer in Part 4. No bias.
- Method `__init__` :
 - Inputs
 - D_1
 - D_2
 - D_{qk}
 - D_v
 - H
 - Outputs
 - None
 - What to do inside this method
 - Initialize attribute values
 - Method `forward` :

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- Inputs:
 - An attending sequence (tensor) with shape (B, L_1, D_1)
 - A being addended sequence (tensor) with shape (B, L_2, D_2)
- Outputs
 - Post-out-projection outputs with shape (B, L_1, D_1)
- What to do inside this method
 - Compute the outputs
 - After each operation, add a comment on the tensor shape
 - **Do not use any loop**

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WRITE YOUR SOLUTION HERE

```
class MyMHA(nn.Module):
    def __init__(self, D_1, D_2, D_qk, D_v, H):
        super().__init__()
        self.D_1 = D_1
        self.D_2 = D_2
        self.D_qk = D_qk
        self.D_v = D_v
        self.H = H

        self.W_Q = nn.Linear(in_features=D_1, out_features=H*D_qk, bias=False)
        self.W_K = nn.Linear(in_features=D_2, out_features=H*D_qk, bias=False)
        self.W_V = nn.Linear(in_features=D_2, out_features=H*D_v, bias=False)
        self.W_O = nn.Linear(in_features=H*D_v, out_features=D_1, bias=False)
```

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```

def forward(self, x, y):
    B = x.shape[0] # batch size
    L_1 = x.shape[1] # the length of sequence x
    L_2 = y.shape[1] # the length of sequence y

    Q = self.W_Q(x) # shape: (B,L_1,H*D_qk)
    K = self.W_K(y) # shape: (B,L_2,H*D_qk)
    V = self.W_V(y) # shape: (B,L_2,H*D_v)

    Q = Q.reshape(B,L_1,self.H,self.D_qk) # shape: (B,L_1,H,D_qk)
    K = K.reshape(B,L_2,self.H,self.D_qk) # shape: (B,L_2,H,D_qk)
    V = V.reshape(B,L_2,self.H,self.D_v) # shape: (B,L_2,H,D_v)

    Q = Q.permute(0,2,1,3) # shape: (B,H,L_1,D_qk)
    K = K.permute(0,2,1,3) # shape: (B,H,L_2,D_qk)
    V = V.permute(0,2,1,3) # shape: (B,H,L_2,D_v)

    logits = Q @ K.transpose(-2,-1) / (self.D_qk**0.5) # shape: (B,H,L_1,L_2)
    alpha = torch.softmax(logits, dim=-1) # shape: (B,H,L_1,L_2)

    O = alpha @ V # shape: (B,H,L_1,D_v)

    O = O.permute(0,2,1,3) # shape: (B,L_1,H,D_v)
    O = O.reshape(B,L_1,self.H*self.D_v) # shape: (B,L_1,H*D_v)
    return self.W_O(O) # shape: (B,L_1,D_1)

"""
END OF THIS PART """

```

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