ECE 57000 Assignment 7 Exercise

Your Name:

Objective: Build different transformer components and test them.

In [1]:
```
import numpy as np
import string
import time
import torch
import pdb
import math
import torch.nn as nn
from torch.autograd import Variable
from torch.nn import functional as F
np.random.seed(124)
```

NOTE: In this assignment, we will use the convention of having the batch dimension first so tensors will have shapes of `(N, L, D)` where `N` is the batch dimension, `L` is the max sequence length, and `D` is the feature dimension.

The default in PyTorch is for the sequence dimension to be first, i.e., `(L, N, D)` but most functions in PyTorch can be altered to make the batch dimension to be first by using `batch_first=True`, see for example the arguments for `torch.nn.LSTM`.

Exercise 1: Positional Encoder (20 points)

The positional encoder is a simple function that takes a 3D tensor of shape (batch_size, sequence_length, encoding_size), i.e., `(N, L, D)`, and returns a 3D tensor of the same shape where positional encoding embedding has been added. The positional encoder is a function of the position of the token in the sequence. The positional encoder is defined as:

$$PE_{(pos,2i)} = \sin(pos/10000^{2i/d_{model}})$$

$$PE_{(pos,2i+1)} = \cos(pos/10000^{2i/d_{model}})$$

where pos is the position and i is the dimension. That is, each dimension of the positional encoding corresponds to a sinusoid. The wavelengths form a geometric progression from 2π to $10000 \cdot 2\pi$.

In practice, the positional encoding is added to the embedding vector. This is done by first creating a tensor of shape (1, sequence_length, d_model) and then adding it to the embedding vector. This ensures that the positional encoding is added to every element in the batch via broadcasting.

Hints:

- If done correctly the output of the code below should look like:
```
torch.Size([1, 4, 512])
False
input_pe: tensor([0.0100, 0.0200, 0.0300, 0.0400, 0.0500])
output_pe: tensor([0.2263, 1.4525, 0.6788, 1.9051, 1.1314])
input_pe: tensor([0.0100, 0.0200, 0.0300, 0.0400, 0.0500])
output_pe: tensor([1.0677, 1.0222, 1.4808, 1.5285, 1.8931])
input_pe: tensor([5.0800, 5.0900, 5.1000, 5.1100, 5.1200])
output_pe: tensor([115.9473, 115.1735, 116.3998, 115.6261, 116.8524])
```

In [11]:
```python
class PositionalEncoder(nn.Module):
    def __init__(self, d_model, max_seq_len = 80):
        super().__init__()
        self.d_model = d_model

        # create constant 'pe' matrix with values dependant on
        # pos and i
        pe = torch.zeros(max_seq_len, d_model)

        #### YOUR CODE HERE ####
        # Loop over the positions and the embedding dimensions
        # and calculate the positional encoding for each dimension
        # and position
        # If you want extra challenge, try to do this without loops.

        for pos in range(max_seq_len):
          for i in range(0, d_model, 2):
            pe[pos, i] = math.sin(pos / (10000**(i/self.d_model)))
            pe[pos, i + 1] = math.cos(pos / (10000**(i/self.d_model)))


        #### END YOUR CODE ####

        pe = pe.unsqueeze(0)
        # Register this as something to keep when saving a model
        #  but that is not a learnable parameter
        self.register_buffer('pe', pe)


    def forward(self, x):
        # make embeddings relatively larger than pe
        x = x * math.sqrt(self.d_model)
        # add constant positional encoding to embedding
        seq_len = x.size(1)
        x = x + Variable(self.pe[:,:seq_len], requires_grad=False)
        return x

pe = PositionalEncoder(512)
input_pe = torch.arange(1, 513)*0.01
input_pe = input_pe.repeat(1, 4, 1).float()

output_pe = pe(input_pe)
```

```
print(output_pe.shape)

# check the difference between the two embeddings
print(torch.equal(input_pe, output_pe)) # They should not be equal after adding positi
print(f"input_pe: {input_pe[0, 0, 0:5]} \noutput_pe: {output_pe[0, 0, 0:5]}")
print(f"input_pe: {input_pe[0, 1, 0:5]} \noutput_pe: {output_pe[0, 1, 0:5]}")
print(f"input_pe: {input_pe[0, 2, -5:]} \noutput_pe: {output_pe[0, 2, -5:]}")
```

```
torch.Size([1, 4, 512])
False
input_pe: tensor([0.0100, 0.0200, 0.0300, 0.0400, 0.0500])
output_pe: tensor([0.2263, 1.4525, 0.6788, 1.9051, 1.1314])
input_pe: tensor([0.0100, 0.0200, 0.0300, 0.0400, 0.0500])
output_pe: tensor([1.0677, 0.9929, 1.5007, 1.4748, 1.9333])
input_pe: tensor([5.0800, 5.0900, 5.1000, 5.1100, 5.1200])
output_pe: tensor([115.9473, 115.1738, 116.3998, 115.6263, 116.8524])
```

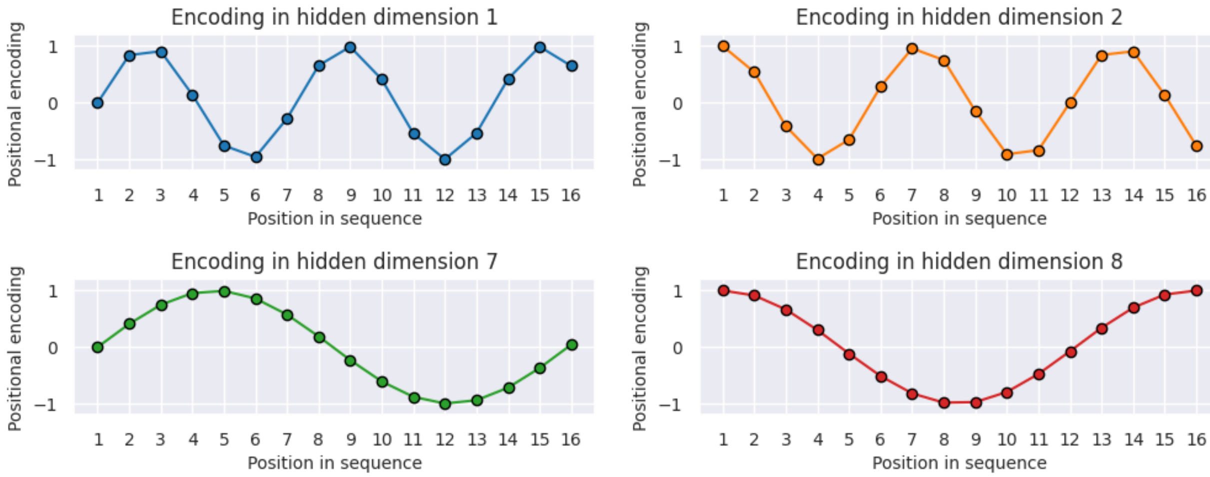
To understand the positional encoding, we will generate an image of the positional encoding over the hidden dimensionality and position in a sequence. Below we visualize the positional encoding (encoding_size = 64) for the hidden dimensions 1, 2, 7 and 8 where sine and cosine waves with different wavelengths encode the position in the hidden dimensions.

In [12]:

```
import seaborn as sns
import matplotlib.pyplot as plt

p_encode = PositionalEncoder(64)
pe = p_encode.pe.squeeze().T.cpu().numpy()

sns.set_theme()
fig, ax = plt.subplots(2, 2, figsize=(12,4))
dims = [1, 2, 7, 8]
ax = [a for a_list in ax for a in a_list]
for i in range(len(ax)):
    ax[i].plot(np.arange(1,17), pe[dims[i]-1,:16], color=f'C{i}', marker="o", markersi
    ax[i].set_title(f"Encoding in hidden dimension {dims[i]}")
    ax[i].set_xlabel("Position in sequence", fontsize=10)
    ax[i].set_ylabel("Positional encoding", fontsize=10)
    ax[i].set_xticks(np.arange(1,17))
    ax[i].tick_params(axis='both', which='major', labelsize=10)
    ax[i].tick_params(axis='both', which='minor', labelsize=8)
    ax[i].set_ylim(-1.2, 1.2)
fig.subplots_adjust(hspace=0.8)
sns.reset_orig()
plt.show()
```



Exercise 2: Scaled Dot-Product Attention (30 points)

In this exercise, you will implement a version of attention used in transformers. The key difference from the one described in class is that the attention scores (pre-softmax) are scaled by a factor of $\frac{1}{\sqrt{d_k}}$, where d_k is the dimension of the keys (and the queries):

$$A(Q, K, V) = \text{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right)V$$

where $Q \in \mathbb{R}^{L \times d_k}$, $K \in \mathbb{R}^{L \times d_k}$, and $V \in \mathbb{R}^{L \times d_v}$, where d_v is the dimension of the values. The softmax is across the column dimension. The output of attention should be a matrix $A \in \mathbb{R}^{L \times d_v}$.

Additionally, we will implement a **batched version** of this that can be used for multiple sequences at the same time. To do this, you will need to use the following **batched** version(s) of matrix multiplication either `torch.bmm` or `torch.matmul` for both the QK^T and the product of the attention matrix and V. We recommend that you use `torch.bmm` as it is more explicit.

Hint:

- You will need to transpose the matrices in the `k` tensor. Specifically, you will need to swap the last and second to last dimension so that it has shape (batch_size, d_k, seq_len). One way to do this is via the `transpose` function.
- If done correctly, the output should be like below:
```
Is shape of output correct? True
Is shape of att_values correct? True
Do attention values sum to 1? True
Output check (first):
tensor([-1.3709, -0.6827,  0.3234,  0.8677, -0.1474, -0.9653, -0.7344,
0.8126,
        0.1219,  0.3224,  0.6257, -0.0958, -0.1664, -0.0667, -0.2810,
0.3068,
```

```
      -0.7030, -0.6719,  0.4364, -1.0071,  0.3534,  0.3160,  0.0326,
-0.7315,
      -0.5165])
Output check (last):
tensor([-0.2094,  1.3784,  0.2855, -0.1716,  0.1597, -0.6656,  0.3981,
-0.9903,
      -0.6043, -0.6398,  0.0563, -1.5367, -0.0225, -0.8317,  0.0572,
0.2014,
       0.1324, -0.4563,  0.3832,  0.1051,  0.0653, -0.2076,  0.6225,
-0.4946,
      -0.2935])
Is the implementation similar to Pytorch implementation? True
```

In [38]:

```python
def attention(q, k, v):
    '''
    Inputs:
    q: query vector of shape (batch_size, seq_len, d_k)
    k: key vector of shape (batch_size, seq_len, d_k)
    v: value vector of shape (batch_size, seq_len, d_v)

    Returns:
    output: attention weighted sum of the value vectors
        of shape (batch_size, seq_len, d_k)
    scores: attention weights of shape (batch_size, seq_len, seq_len)
    '''
    d_k = k.size(-1)
    assert d_k == q.size(-1), 'q and k should have the same dimensionality'
    d_v = v.size(-1)

    #### YOUR CODE HERE ####

    k_T = k.transpose(-2,-1)
    scores = torch.bmm(q, k_T) / (d_k**0.5)
    att_values = F.softmax(scores, dim = -1)
    output = torch.bmm(att_values, v)


    #### END YOUR CODE ####

    return output, att_values

# test the attention function with some random values
torch.manual_seed(42)  # Do not change random seed
q = torch.randn(2, 5, 512)
k = torch.randn(2, 5, 512)
v = torch.randn(2, 5, 256)

output, att_values = attention(q, k, v)
print(f"Is shape of output correct? {output.shape == v.shape}")
print(f"Is shape of att_values correct? {att_values.shape == torch.Size([q.shape[0], q
print(f"Do attention values sum to 1? {torch.allclose(torch.sum(att_values, dim=-1), t

# Last 25 values of last sample and last token
print(f"Output check (first): \n{output[0,0,:25]}")
print(f"Output check (last): \n{output[-1,-1,-25:]}")

# Compare with Pytorch Implementation
out = F.scaled_dot_product_attention(q,k,v)
```

```
print(f'Is the implementation similar to Pytorch implementation?'
      f' {torch.allclose(output, out, atol=1e-3, rtol=1)}')
```

```
Is shape of output correct? True
Is shape of att_values correct? True
Do attention values sum to 1? True
Output check (first):
tensor([-1.3709, -0.6827,  0.3234,  0.8677, -0.1474, -0.9653, -0.7344,  0.8126,
         0.1219,  0.3224,  0.6257, -0.0958, -0.1664, -0.0667, -0.2810,  0.3068,
        -0.7030, -0.6719,  0.4364, -1.0071,  0.3534,  0.3160,  0.0326, -0.7315,
        -0.5165])
Output check (last):
tensor([-0.2094,  1.3784,  0.2855, -0.1716,  0.1597, -0.6656,  0.3981, -0.9903,
        -0.6043, -0.6398,  0.0563, -1.5367, -0.0225, -0.8317,  0.0572,  0.2014,
         0.1324, -0.4563,  0.3832,  0.1051,  0.0653, -0.2076,  0.6225, -0.4946,
        -0.2935])
Is the implementation similar to Pytorch implementation? True
```

Exercise 3: Attention modules (50 points)

Task 1: Self-attention module

Implement a self-attention module that takes in `x` and computes `q`, `k`, `v` internally using 3 linear layers. Then, use your function from above to compute the output and attention and return it. The attention module should take as constructor parameters the `input_dim`, `key_dim`, and the `output_dim`.

Your output should look like the following:

```
input shape: torch.Size([4, 10, 512])
output shape: torch.Size([4, 10, 512])
Input:
tensor([-0.1988, -0.3060,  0.6383,  0.5713,  1.2769])
Output:
tensor([ 8.6836e-02, -4.1725e-02, -2.5798e-01, -9.6712e-02,  3.0079e-
05],
       grad_fn=<SliceBackward>)

Does the module exhibit permutation-equivaraince? True
The following two lines should be the same:
tensor([ 0.1849,  0.3706,  0.1488,  0.0898,  0.2528,  0.4277,
0.4572,  0.1172,
         0.0893, -0.2081], grad_fn=<SliceBackward>)
tensor([ 0.1849,  0.3706,  0.1488,  0.0898,  0.2528,  0.4277,
0.4572,  0.1172,
         0.0893, -0.2081], grad_fn=<SliceBackward>)
```

In [47]:
```
class SelfAttention(nn.Module):
    def __init__(self, input_dim, key_dim, output_dim):
        super().__init__()
        #### YOUR CODE HERE ####
```

```
        self.linear_q = nn.Linear(input_dim, key_dim)
        self.linear_k = nn.Linear(input_dim, key_dim)
        self.linear_v = nn.Linear(input_dim, output_dim)

        #### END YOUR CODE ####

    def forward(self, x):
        '''
        `x` has shape (batch_dim, sequence_length, input_dim) or (N, L, D_in)

        The output should have shape (batch_dim, sequence_length, output_dim) or (N, L
        '''
        #### YOUR CODE HERE ####

        q = self.linear_q(x)
        k = self.linear_k(x)
        v = self.linear_v(x)

        output, att_values = attention(q,k,v)

        #### END YOUR CODE ####

        return output

# test the self-attention module with some random values
torch.manual_seed(48)
input_dim = 512
key_dim = 64
output_dim = 512
self_attn = SelfAttention(input_dim, key_dim, output_dim)
x = torch.randn(4, 10, 512)
output = self_attn(x)
print(f"input shape: {x.shape}")
print(f"output shape: {output.shape}")
print(f'Input: \n{x[0,0,:5]}\nOutput: \n{output[0,0,:5]}\n')

# For self-attention, let’s check the “permutation-equivariant” property,
# i.e., permute the input sequence and check if the output sequence is also permuted b
# This is a nice sanity check that self-attention is working properly.
random_permutation = torch.randperm(x.size(1))
reverse_permutation = torch.zeros_like(random_permutation)
reverse_permutation[random_permutation] = torch.arange(len(random_permutation))
assert torch.all(x[:, random_permutation, :][:, reverse_permutation, :] == x), 'invers

x_prime = x[:, random_permutation, :] # Permute input
output_prime = self_attn(x_prime)
output_prime_permuted = output_prime[:, reverse_permutation, :]  # Reverse permutatior
print(f'Does the module exhibit permutation-equivaraince?'
      f' {torch.allclose(output, output_prime_permuted, atol=1e-5, rtol=1)}')
print(f'The following two lines should be the same:')
print(output[-1,-1,:10])
print(output_prime_permuted[-1,-1,:10])
```

```
input shape: torch.Size([4, 10, 512])
output shape: torch.Size([4, 10, 512])
Input:
tensor([-0.1988, -0.3060,  0.6383,  0.5713,  1.2769])
Output:
tensor([ 8.6836e-02, -4.1725e-02, -2.5798e-01, -9.6712e-02,  3.0022e-05],
       grad_fn=<SliceBackward0>)

Does the module exhibit permutation-equivaraince? True
The following two lines should be the same:
tensor([ 0.1849,  0.3706,  0.1488,  0.0898,  0.2528,  0.4277,  0.4572,  0.1172,
         0.0893, -0.2081], grad_fn=<SliceBackward0>)
tensor([ 0.1849,  0.3706,  0.1488,  0.0898,  0.2528,  0.4277,  0.4572,  0.1172,
         0.0893, -0.2081], grad_fn=<SliceBackward0>)
```

Task 2: Cross Attention module

For cross attention, there will be an first input `x` that will correspond to the query and a second input `y` that will correspond to the keys and values. (In self-attention, `x` and `y` were equal). This should be the same basic idea except that there is a linear layer to compute `q` from `x` and linear layers to compute `k` and `v` from `y`.

The output should look like the following:

```
input shape x and y: torch.Size([3, 10, 512]), torch.Size([3, 10,
256])
output shape: torch.Size([3, 10, 128])
x
tensor([-0.0385,  0.9773, -1.4370,  0.8719, -2.1034, -0.2877,
0.3034, -1.9151,
         1.1799,  0.6151])
y
tensor([-2.1565,  0.2397,  0.5872,  0.3950, -0.6114,  0.3489,
-0.3467,  0.2792,
        -1.2541,  0.4053])
output
tensor([-0.1544,  0.0847,  0.2329,  0.0549, -0.1424,  0.0711,
0.0105, -0.2139,
        -0.0208, -0.1942], grad_fn=<SliceBackward>)
```

In [51]:

```python
class CrossAttention(nn.Module):
    def __init__(self, x_input_dim, y_input_dim, key_dim, output_dim):
        super().__init__()
        #### YOUR CODE HERE ####
        self.linear_q = nn.Linear(x_input_dim, key_dim)
        self.linear_k = nn.Linear(y_input_dim,key_dim)
        self.linear_v = nn.Linear(y_input_dim, output_dim)


        #### END YOUR CODE ####

    def forward(self, x, y):
        #### YOUR CODE HERE ####
        q = self.linear_q(x)
```

```
        k = self.linear_k(y)
        v = self.linear_v(y)

        output, att_weight = attention(q,k,v)

        #### END YOUR CODE ####

        return output

# test the attention module with some random values
torch.manual_seed(14)
x_input_dim = 512
y_input_dim = 256
key_dim = 64
output_dim = 128
cross_attn = CrossAttention(x_input_dim, y_input_dim, key_dim, output_dim)
x = torch.randn(3, 10, x_input_dim)
y = torch.randn(3, 10, y_input_dim)
output = cross_attn(x, y)
print(f"input shape x and y: {x.shape}, {y.shape}")
print(f"output shape: {output.shape}")
print(f'x\n{x[0,0,:10]}')
print(f'y\n{y[0,0,:10]}')
print(f'output\n{output[0,0,:10]}')
```

```
input shape x and y: torch.Size([3, 10, 512]), torch.Size([3, 10, 256])
output shape: torch.Size([3, 10, 128])
x
tensor([-0.0385,  0.9773, -1.4370,  0.8719, -2.1034, -0.2877,  0.3034, -1.9151,
         1.1799,  0.6151])
y
tensor([-2.1565,  0.2397,  0.5872,  0.3950, -0.6114,  0.3489, -0.3467,  0.2792,
        -1.2541,  0.4053])
output
tensor([-0.1544,  0.0847,  0.2329,  0.0549, -0.1424,  0.0711,  0.0105, -0.2139,
        -0.0208, -0.1942], grad_fn=<SliceBackward0>)
```

Task 3: Multi-headed self-attention module

Multi-headed self-attention merely passes the the input to each attention module, concatenates all the outputs, and then applies a linear layer to get the final output. Implement multi-headed attention below.

Output should look like:

```
input shape: torch.Size([3, 10, 256])
output shape: torch.Size([3, 10, 32])
x
tensor([ 0.7195, -0.3636,  1.3771,  0.3482, -0.0604, -0.3034,
-0.0698,  0.2131,
         -0.9736, -0.4651])
output
tensor([ 0.2290, -0.0350,  0.0918, -0.1069, -0.1679, -0.1939,
-0.2167,  0.1841,
          0.0546,  0.1668], grad_fn=<SliceBackward>)
```

In [67]:
```
class MultiHeadedAttention(nn.Module):
    def __init__(self, attn_modules, final_output_dim):
        super().__init__()
        #### YOUR CODE HERE ####
        # 1) Save the attn_modules as a nn.ModuleList
        # 2) Setup a linear layer
        #   Hint for 2: Need to compute the concatenated dimensionality to
        #   setup linear layer by extracting the output dimension from each
        #   attention module.

        self.module_list = nn.ModuleList()
        self.module_list.extend(attn_modules)
        output_dim = 0



        for module in self.module_list:
            output_dim += module.linear_v.out_features

        self.linear = nn.Linear(output_dim, final_output_dim)



        #### END YOUR CODE ####

    def forward(self, x):
        #### YOUR CODE HERE ####
        # 1) Concatenate outputs of each self-attention module
        # 2) Apply final linear layer


        output = torch.cat([module(x) for module in self.module_list], dim = -1)
        output = self.linear(output)

        #### END YOUR CODE ####

        return output

# test the multi-headed attention module with some random values
torch.manual_seed(10)
input_dim = 256
key_dim = 128
output_dim = 64
final_output_dim = 32
num_heads = 8
attn_modules = [SelfAttention(input_dim, key_dim, output_dim//num_heads) for _ in rang
multi_attn = MultiHeadedAttention(attn_modules, final_output_dim)

x = torch.randn(3, 10, input_dim)
output = multi_attn(x)
print(f"input shape: {x.shape}")
print(f"output shape: {output.shape}")
print(f'x\n{x[0,0,:10]}\noutput\n{output[0,0,:10]}')
```

```
input shape: torch.Size([3, 10, 256])
output shape: torch.Size([3, 10, 32])
x
tensor([ 0.7195, -0.3636,  1.3771,  0.3482, -0.0604, -0.3034, -0.0698,  0.2131,
        -0.9736, -0.4651])
output
tensor([ 0.2290, -0.0350,  0.0918, -0.1069, -0.1679, -0.1939, -0.2167,  0.1841,
         0.0546,  0.1668], grad_fn=<SliceBackward0>)
```

(Optional, ungraded) Masked attention module

Try to implement the masked attention module for the decoder in a transformer.

In [ ]:

```

```