CS440/ECE448 Spring 2024

MP09: Transformer

The first thing you need to do is to download mp09.zip. Unlike several previous MPs, you will need to complete the code in several .py files

This file (`mp09_notebook.ipynb`) will walk you through the whole MP, giving you instructions and debugging tips as you go.

Throughout this MP, you will implement many of the operations in the Transformer architecture. The implementation will mostly follow the instructions in the original paper "Attention is All You Need" by Vaswani et al, 2017. (https://arxiv.org/abs/1706.03762). Much of the class structures and code have already been completed for you, and you are only required to fill in the missing parts as instructed by the comments in the code and in this notebook.

Table of Contents

Code structure

The repository, once unzipped, is structured like this:

```
├─ data - Folder that contains either synthetic or real data
and the expected outputs, for use by the tests.
│
├─ tests - Folder that contains tests used by grade.py
│
├─ mha.py - Implements multi-head attention; you need to
implement some part of it
│
├─ pe.py - Implements positional encoding; you need to
implement some part of it
│
├─ encoder.py - Implements the Transformer encoder layer and
the encoder; you need to implement some part of it
│
```

```
  ├─ decoder.py - Implements the Transformer decoder layer and
the decoder; you need to implement some part of it.
  |
  ├─ transformer.py - Implements the Transformer decoder layer
and the decoder; you need to implement some part of it
  |
  ├─ grade.py - Launches some tests on the visible data and
their expected output given to you
  |
  ├─ trained_de_en_state_dict.pt - A trained Transformer
encoder-decoder checkpoint for checking your implementation.
```

We suggest that you create a new environment with Python 3.10 for this MP to avoid conflict with other versions of PyTorch and its dependencies that you might already have installed before in your current Python environment; if you use Anaconda, you can do this by

`conda create -n transformer_mp_torch_2.0.1 python=3.10`

`conda activate transformer_mp_torch_2.0.1`

Then, in this environment,

For OSX, run `pip install torch==2.0.1`

For Linux and Windows, run `pip install torch==2.0.1 --index-url https://download.pytorch.org/whl/cpu`

Then you can install the rest of the dependencies with

`pip install gradescope-utils`

`pip install editdistance`

`pip install numpy`

`pip install jupyterlab`

You can now re-open this notebook by launching `jupyter lab` in the newly created environment.

Note: for our provided visible test output to match yours, you must specify the PyTorch version of `torch==2.0.1`. Otherwise, local testing may show small discrepancies, such as if you use another version of PyTorch. The GradeScope auto-grader will NOT show any discrepancies as it shall be able to generate test outputs (on the hidden set) automatically.

Multi-head Attention

The multi-head attention mechanism forms the backbone of Transformer encoder and decoder layers. The paper summarizes the operation of Multi-head attention as:

$$\begin{aligned}\mathrm{MultiHead}(Q,K,V) &= \mathrm{Concat}(\mathrm{head}_1,\ldots,\ \mathrm{head}_{\mathrm{h}})W^O \\ \text{where head } &= \mathrm{Attention}\left(QW_i^Q, KW_i^K, VW_i^V\right)\end{aligned}$$

In essence, the multi-head attention module takes three inputs, the query matrix (Q), the key matrix (K), and the value matrix (V). Q, K, V goes through h different linear transformations, resulting in QW_i^Q, KW_i^K, VW_i^V for $i \in \{1, \cdots h\}$. For simplicity, we will assume that $Q \in \mathbb{R}^{T_q \times d_{model}}$, $K \in \mathbb{R}^{T_k \times d_{model}}$, $V \in \mathbb{R}^{T_k \times d_{model}}$, $W_i^Q \in \mathbb{R}^{d_{model} \times d_k}$, $W_i^K \in \mathbb{R}^{d_{model} \times d_k}$, $W_i^V \in \mathbb{R}^{d_{model} \times d_k}$ and $d_k \times h = d_{model}$.

For each different set of $Q_i := QW_i^Q$, $K_i := KW_i^K$, $V_i := VW_i^V$, scaled-dot product attention is computed as:

$$\mathrm{Attention}(Q_i, K_i, V_i) = \mathrm{softmax}\left(\frac{Q_i K_i^T}{\sqrt{d_k}}\right)V_i$$

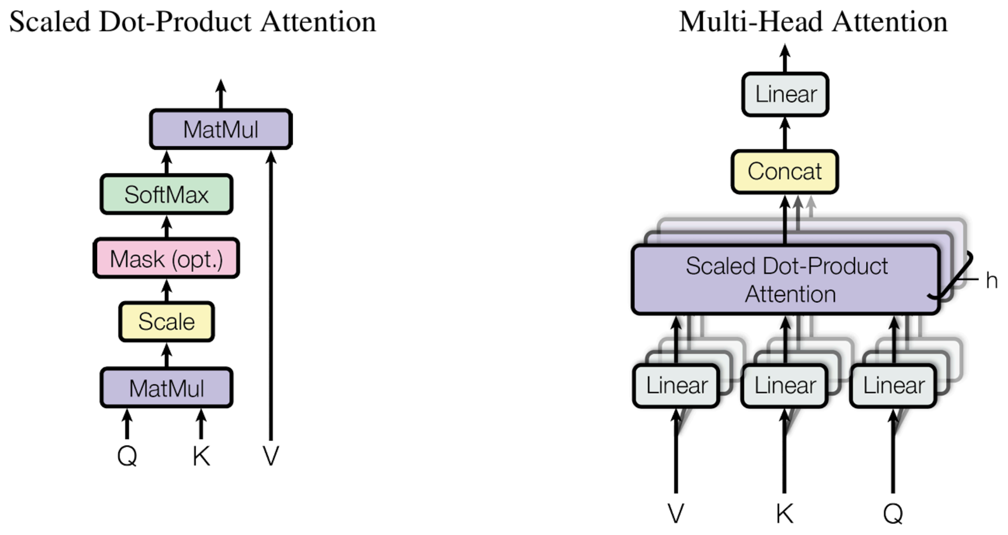
where d_k is the dimension of the individual attention heads.

Finally, $\mathrm{Attention}(Q_i, K_i, V_i)$ from different heads i are concatenated, and the concatenated result goes through another linear transformation $W^O \in \mathbb{R}^{d_{model} \times d_{model}}$.

The figure from pg.4 of the paper shows an illustration of the operations involved.

In [13]:
```
from IPython.display import Image
Image("img/mha.PNG")
```

Out[13]:



In `mha.py`, you will need to implement two functions: `def compute_mh_qkv_transformation(self, Q, K, V)` and `def compute_scaled_dot_product_attention(self, query, key, value, key_padding_mask = None, attention_mask = None)` in the class `class MultiHeadAttention(nn.Module)`. They will be combined in `def forward(self, query, key, value, key_padding_mask = None, attention_mask = None)` to implement the entire operations involved in the multi-head attention mechanism. The model parameters, especially W^Q, W^K, W^V, and W^O, are defined and given in `def __init__(self, d_model, num_heads)`, and should not be modified. You should not import other helpers not already given to you.

Note:

1. W^Q, W^K, and W^V are not defined as separate `nn.Linear` objects in `class MultiHeadAttention(nn.Module)`. In `def compute_mh_qkv_transformation(self, Q, K, V)`, you need to use `torch.Tensor.contiguous().view()` to reshape the last dimension from a single dimension of size `d_model` to two dimensions `num_heads x d_k` (hint: the reverse operation has been defined at the last line of `def compute_scaled_dot_product_attention(self, query, key, value, key_padding_mask = None, attention_mask = None)`, already given to you), and then use `torch.Tensor.transpose()` to get the expected output shape.
2. In `def compute_scaled_dot_product_attention(self, query, key, value, key_padding_mask = None, attention_mask = None)`, you will also need to correctly apply the masking operations. There are two different masks, the `key_padding_mask` and the `attention_mask`. Both are used to disallow attention to certain regions of the input. Please read the function definitions to figure out how to use them.

In [4]:
```
from mha import MultiHeadAttention
help(MultiHeadAttention.compute_mh_qkv_transformation)
```

```
Help on function compute_mh_qkv_transformation in module mha:

compute_mh_qkv_transformation(self, Q, K, V)
    Transform query, key and value using W_q, W_k, W_v and split

    Input:
        Q (torch.Tensor) - Query tensor of size B x T_q x d_model.
        K (torch.Tensor) - Key tensor of size B x T_k x d_model.
        V (torch.Tensor) - Value tensor of size B x T_v x d_model. Note that T
_k = T_v.

    Output:
        q (torch.Tensor) - Transformed query tensor B x num_heads x T_q x d_k.
        k (torch.Tensor) - Transformed key tensor B x num_heads x T_k x d_k.
        v (torch.Tensor) - Transformed value tensor B x num_heads x T_v x d_k.
Note that T_k = T_v
        Note that d_k * num_heads = d_model
```

In [6]:
```
help(MultiHeadAttention.compute_scaled_dot_product_attention)
```

```
Help on function compute_scaled_dot_product_attention in module mha:

compute_scaled_dot_product_attention(self, query, key, value, key_padding_mask
=None, attention_mask=None)
    This function calculates softmax(Q K^T / sqrt(d_k))V for the attention hea
ds; further, a key_padding_mask is given so that padded regions are not attend
ed, and an attention_mask is provided so that we can disallow attention for so
me part of the sequence
    Input:
    query (torch.Tensor) - Query; torch tensor of size B x num_heads x T_q x d
_k, where B is the batch size, T_q is the number of time steps of the query (a
ka the target sequence), num_head is the number of attention heads, and d_k is
the feature dimension;

    key (torch.Tensor) - Key; torch tensor of size B x num_head x T_k x d_k, w
here in addition, T_k is the number of time steps of the key (aka the source s
equence);

    value (torch.Tensor) - Value; torch tensor of size B x num_head x T_v x d_
k; where in addition, T_v is the number of time steps of the value (aka the so
urce sequence);, and we assume d_v = d_k
    Note: We assume T_k = T_v as the key and value come from the same source i
n the Transformer implementation, in both the encoder and the decoder.

    key_padding_mask (None/torch.Tensor) - If it is not None, then it is a tor
ch.IntTensor/torch.LongTensor of size B x T_k, where for each key_padding_mask
[b] for the b-th source in the batch, the non-zero positions will be ignored a
s they represent the padded region during batchify operation in the dataloader
(i.e., disallowed for attention) while the zero positions will be allowed for
attention as they are within the length of the original sequence

    attention_mask (None/torch.Tensor) - If it is not None, then it is a torc
h.IntTensor/torch.LongTensor of size 1 x T_q x T_k or B x T_q x T_k, where aga
in, T_q is the length of the target sequence, and T_k is the length of the sou
rce sequence. An example of the attention_mask is used for decoder self-attent
ion to enforce auto-regressive property during parallel training; suppose the
maximum length of a batch is 5, then the attention_mask for any input in the b
atch will look like this for each input of the batch.
    0 1 1 1 1
    0 0 1 1 1
    0 0 0 1 1
    0 0 0 0 1
    0 0 0 0 0
    As the key_padding_mask, the non-zero positions will be ignored and disall
owed for attention while the zero positions will be allowed for attention.


    Output:
    x (torch.Tensor) - torch tensor of size B x T_q x d_model, which is the at
tended output
```

If you believe you have implemented it correctly, you can run python.grade.py to see if you have passed the tests related to `mha.py`. We have defined four tests (out of 10, including 2 for EC) that you should have passed: `test_mha_no_mask`, which tests the basic operation of `mha.py` without masking involved, `test_mha_key_padding_mask`, which, in addtion, tests `mha.py` with `key_padding_mask`, `test_mha_key_padding_mask_attention_mask`, which, in addtion, tests `mha.py` with `key_padding_mask` and `attention_mask`, and `test_mha_different_query_and_key`, which tests `mha.py` with query and key (value) of different length in the temporal dimension.

It is expected, for now, for the other six tests to either fail or error out.

In [3]:
```
!python grade.py
```

```
EEE....FEE
======================================================================
ERROR: test_encoder_decoder_predictions (test_visible.TestStep.test_encoder_de
coder_predictions)
----------------------------------------------------------------------
Traceback (most recent call last):
  File "/mnt/c/Users/junru/Downloads/transformer_mp/src_test/tests/test_visibl
e.py", line 311, in test_encoder_decoder_predictions
    output = model(src = src, tgt = trg, src_lengths = src_lengths, tgt_length
s = trg_lengths)
             ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
^^^^^^^^^^^^^^^^
  File "/home/jerome-ni/anaconda3/envs/test_transformer_mp_torch_2.0.1/lib/pyt
hon3.11/site-packages/torch/nn/modules/module.py", line 1501, in _call_impl
    return forward_call(*args, **kwargs)
           ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
  File "/mnt/c/Users/junru/Downloads/transformer_mp/src_test/transformer.py",
line 230, in forward
    enc_output, src_padding_mask = self.forward_encoder(src, src_lengths)
                                   ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
  File "/mnt/c/Users/junru/Downloads/transformer_mp/src_test/transformer.py",
line 155, in forward_encoder
    src_embedded = self.dropout(self.positional_encoding(self.encoder_embeddin
g(src)))
                   ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
^^^^^^^^
  File "/home/jerome-ni/anaconda3/envs/test_transformer_mp_torch_2.0.1/lib/pyt
hon3.11/site-packages/torch/nn/modules/module.py", line 1501, in _call_impl
    return forward_call(*args, **kwargs)
           ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
  File "/home/jerome-ni/anaconda3/envs/test_transformer_mp_torch_2.0.1/lib/pyt
hon3.11/site-packages/torch/nn/modules/dropout.py", line 59, in forward
    return F.dropout(input, self.p, self.training, self.inplace)
           ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
  File "/home/jerome-ni/anaconda3/envs/test_transformer_mp_torch_2.0.1/lib/pyt
hon3.11/site-packages/torch/nn/functional.py", line 1252, in dropout
    return _VF.dropout_(input, p, training) if inplace else _VF.dropout(input,
p, training)
                                                            ^^^^^^^^^^^^^^^^^^
^^^^^^^^^^^^^
TypeError: dropout(): argument 'input' (position 1) must be Tensor, not NoneTy
pe

======================================================================
ERROR: test_encoder_decoder_states (test_visible.TestStep.test_encoder_decoder
_states)
----------------------------------------------------------------------
Traceback (most recent call last):
  File "/mnt/c/Users/junru/Downloads/transformer_mp/src_test/tests/test_visibl
e.py", line 365, in test_encoder_decoder_states
    output = model(src = src, tgt = trg, src_lengths = src_lengths, tgt_length
s = trg_lengths)
             ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
^^^^^^^^^^^^^^^^
  File "/home/jerome-ni/anaconda3/envs/test_transformer_mp_torch_2.0.1/lib/pyt
hon3.11/site-packages/torch/nn/modules/module.py", line 1501, in _call_impl
    return forward_call(*args, **kwargs)
           ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
  File "/mnt/c/Users/junru/Downloads/transformer_mp/src_test/transformer.py",
line 230, in forward
```

```
    enc_output, src_padding_mask = self.forward_encoder(src, src_lengths)
                                   ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
  File "/mnt/c/Users/junru/Downloads/transformer_mp/src_test/transformer.py",
line 155, in forward_encoder
    src_embedded = self.dropout(self.positional_encoding(self.encoder_embeddin
g(src)))
                   ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
^^^^^^^^
  File "/home/jerome-ni/anaconda3/envs/test_transformer_mp_torch_2.0.1/lib/pyt
hon3.11/site-packages/torch/nn/modules/module.py", line 1501, in _call_impl
    return forward_call(*args, **kwargs)
           ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
  File "/home/jerome-ni/anaconda3/envs/test_transformer_mp_torch_2.0.1/lib/pyt
hon3.11/site-packages/torch/nn/modules/dropout.py", line 59, in forward
    return F.dropout(input, self.p, self.training, self.inplace)
           ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
  File "/home/jerome-ni/anaconda3/envs/test_transformer_mp_torch_2.0.1/lib/pyt
hon3.11/site-packages/torch/nn/functional.py", line 1252, in dropout
    return _VF.dropout_(input, p, training) if inplace else _VF.dropout(input,
p, training)
                                                            ^^^^^^^^^^^^^^^^^^
^^^^^^^^^^^^^
TypeError: dropout(): argument 'input' (position 1) must be Tensor, not NoneTy
pe

======================================================================
ERROR: test_encoder_output (test_visible.TestStep.test_encoder_output)
----------------------------------------------------------------------
Traceback (most recent call last):
  File "/mnt/c/Users/junru/Downloads/transformer_mp/src_test/tests/test_visibl
e.py", line 272, in test_encoder_output
    output_encoder, _ = model.forward_encoder(src = src, src_lengths = src_len
gths)
                        ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
^^^^^
  File "/mnt/c/Users/junru/Downloads/transformer_mp/src_test/transformer.py",
line 155, in forward_encoder
    src_embedded = self.dropout(self.positional_encoding(self.encoder_embeddin
g(src)))
                   ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
^^^^^^^^
  File "/home/jerome-ni/anaconda3/envs/test_transformer_mp_torch_2.0.1/lib/pyt
hon3.11/site-packages/torch/nn/modules/module.py", line 1501, in _call_impl
    return forward_call(*args, **kwargs)
           ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
  File "/home/jerome-ni/anaconda3/envs/test_transformer_mp_torch_2.0.1/lib/pyt
hon3.11/site-packages/torch/nn/modules/dropout.py", line 59, in forward
    return F.dropout(input, self.p, self.training, self.inplace)
           ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
  File "/home/jerome-ni/anaconda3/envs/test_transformer_mp_torch_2.0.1/lib/pyt
hon3.11/site-packages/torch/nn/functional.py", line 1252, in dropout
    return _VF.dropout_(input, p, training) if inplace else _VF.dropout(input,
p, training)
                                                            ^^^^^^^^^^^^^^^^^^
^^^^^^^^^^^^^
TypeError: dropout(): argument 'input' (position 1) must be Tensor, not NoneTy
pe

======================================================================
ERROR: test_decoder_inference_cache_extra_credit (test_visible_ec.TestStep.tes
t_decoder_inference_cache_extra_credit)
----------------------------------------------------------------------
Traceback (most recent call last):
  File "/mnt/c/Users/junru/Downloads/transformer_mp/src_test/tests/test_visibl
e_ec.py", line 162, in test_decoder_inference_cache_extra_credit
    output_list, decoder_cache = model.inference(src = src, src_lengths = src_
lengths, max_output_length = MAX_INFERENCE_LENGTH)
                                 ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
  File "/mnt/c/Users/junru/Downloads/transformer_mp/src_test/transformer.py",
line 254, in inference
    enc_output, _ = self.forward_encoder(src, src_lengths)
                    ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
  File "/mnt/c/Users/junru/Downloads/transformer_mp/src_test/transformer.py",
line 155, in forward_encoder
    src_embedded = self.dropout(self.positional_encoding(self.encoder_embeddin
g(src)))
                   ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
^^^^^^^^
  File "/home/jerome-ni/anaconda3/envs/test_transformer_mp_torch_2.0.1/lib/pyt
hon3.11/site-packages/torch/nn/modules/module.py", line 1501, in _call_impl
    return forward_call(*args, **kwargs)
           ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
  File "/home/jerome-ni/anaconda3/envs/test_transformer_mp_torch_2.0.1/lib/pyt
hon3.11/site-packages/torch/nn/modules/dropout.py", line 59, in forward
    return F.dropout(input, self.p, self.training, self.inplace)
           ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
  File "/home/jerome-ni/anaconda3/envs/test_transformer_mp_torch_2.0.1/lib/pyt
hon3.11/site-packages/torch/nn/functional.py", line 1252, in dropout
    return _VF.dropout_(input, p, training) if inplace else _VF.dropout(input,
p, training)
                                                            ^^^^^^^^^^^^^^^^^^
^^^^^^^^^^^^^
TypeError: dropout(): argument 'input' (position 1) must be Tensor, not NoneTy
pe

======================================================================
ERROR: test_decoder_inference_outputs_extra_credit (test_visible_ec.TestStep.t
est_decoder_inference_outputs_extra_credit)
----------------------------------------------------------------------
Traceback (most recent call last):
  File "/mnt/c/Users/junru/Downloads/transformer_mp/src_test/tests/test_visibl
e_ec.py", line 109, in test_decoder_inference_outputs_extra_credit
    output_list, decoder_cache = model.inference(src = src, src_lengths = src_
lengths, max_output_length = MAX_INFERENCE_LENGTH)
                                 ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
  File "/mnt/c/Users/junru/Downloads/transformer_mp/src_test/transformer.py",
line 254, in inference
    enc_output, _ = self.forward_encoder(src, src_lengths)
                    ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
  File "/mnt/c/Users/junru/Downloads/transformer_mp/src_test/transformer.py",
line 155, in forward_encoder
    src_embedded = self.dropout(self.positional_encoding(self.encoder_embeddin
g(src)))
                   ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
^^^^^^^^
  File "/home/jerome-ni/anaconda3/envs/test_transformer_mp_torch_2.0.1/lib/pyt
hon3.11/site-packages/torch/nn/modules/module.py", line 1501, in _call_impl
    return forward_call(*args, **kwargs)
```

```
             ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
  File "/home/jerome-ni/anaconda3/envs/test_transformer_mp_torch_2.0.1/lib/pyt
hon3.11/site-packages/torch/nn/modules/dropout.py", line 59, in forward
    return F.dropout(input, self.p, self.training, self.inplace)
             ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
  File "/home/jerome-ni/anaconda3/envs/test_transformer_mp_torch_2.0.1/lib/pyt
hon3.11/site-packages/torch/nn/functional.py", line 1252, in dropout
    return _VF.dropout_(input, p, training) if inplace else _VF.dropout(input,
p, training)
                                                            ^^^^^^^^^^^^^^^^^^
^^^^^^^^^^^^^
TypeError: dropout(): argument 'input' (position 1) must be Tensor, not NoneTy
pe

======================================================================
FAIL: test_pe (test_visible.TestStep.test_pe)
----------------------------------------------------------------------
Traceback (most recent call last):
  File "/mnt/c/Users/junru/Downloads/transformer_mp/src_test/tests/test_visibl
e.py", line 236, in test_pe
    self.assertAlmostEqual(torch.sum(torch.abs(pe.pe - self.pe_test_data["p
e"])).item(), 0, places = 4, msg='Positional Encoding has incorrect encoding e
ntries')
AssertionError: 270.70733642578125 != 0 within 4 places (270.70733642578125 di
fference) : Positional Encoding has incorrect encoding entries

----------------------------------------------------------------------
Ran 10 tests in 1.604s

FAILED (failures=1, errors=5)
```

Positional Encoding

In order for the model to make use of the order of the sequence, some information about the relative or absolute position of the tokens in the sequence must be injected into the input embeddings at the bottoms of the encoder and decoder stacks. These positional encodings have the same dimension d_{model} as the embeddings and the rest of the encoder and decoder modules. The original paper defines a simple positional encoding as sine and cosine functions of different frequencies:

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

where pos is the position and i is an index into the dimension d_{model} (i.e., $i \in \{0, 1, \cdots, d_{model}\}$). That is, each dimension of the positional encoding corresponds to a sinusoid. The wavelengths form a geometric progression from 2π to $10000 \times 2\pi$.

In `pe.py`, you will need to fill in the missing code to calculate the positional encoding, `self.pe`, in `def __init__(self, d_model, max_seq_length)` and implement the function `def forward(x)` in the class `class PositionalEncoding(nn.Module)`.

Note:

1. For better numerical accuracy, it is recommended that you make use of:

$$\frac{1}{10000}^{\frac{2i}{d_{model}}} = \exp^{2i\times(-\frac{\log(10000)}{d_{model}})}$$

2. We assume that the input `x` in `def forward(x)` will always be smaller than the `max_seq_length`, so you can safely slice into `self.pe`

If you believe you have implemented everything in this section correctly, you can run `python.grade.py` to see if you have passed the test related to `pe.py`. We have defined one test for `pe.py` that you should have passed: `test_pe`, which initializes a `PositionalEncoding` object, test to see if you have filled in `self.pe` correctly, and if the `def forward(x)` works with some random test data.

It is expected, for now, for the other five tests to either fail or error out (assuming you passed the four tests for `mha.py` already)

In [4]:
```
!python grade.py
```

```
EEF.....EE
======================================================================
ERROR: test_encoder_decoder_predictions (test_visible.TestStep.test_encoder_de
coder_predictions)
----------------------------------------------------------------------
Traceback (most recent call last):
  File "/mnt/c/Users/junru/Downloads/transformer_mp/src_test/tests/test_visibl
e.py", line 311, in test_encoder_decoder_predictions
    output = model(src = src, tgt = trg, src_lengths = src_lengths, tgt_length
s = trg_lengths)
             ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
^^^^^^^^^^^^^^^^
  File "/home/jerome-ni/anaconda3/envs/test_transformer_mp_torch_2.0.1/lib/pyt
hon3.11/site-packages/torch/nn/modules/module.py", line 1501, in _call_impl
    return forward_call(*args, **kwargs)
           ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
  File "/mnt/c/Users/junru/Downloads/transformer_mp/src_test/transformer.py",
line 233, in forward
    dec_output = self.forward_decoder(enc_output, src_padding_mask, tgt, tgt_l
engths)
                 ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
^^^^^^^
  File "/mnt/c/Users/junru/Downloads/transformer_mp/src_test/transformer.py",
line 208, in forward_decoder
    return dec_output
           ^^^^^^^^^^
NameError: name 'dec_output' is not defined

======================================================================
ERROR: test_encoder_decoder_states (test_visible.TestStep.test_encoder_decoder
_states)
----------------------------------------------------------------------
Traceback (most recent call last):
  File "/mnt/c/Users/junru/Downloads/transformer_mp/src_test/tests/test_visibl
e.py", line 365, in test_encoder_decoder_states
    output = model(src = src, tgt = trg, src_lengths = src_lengths, tgt_length
s = trg_lengths)
             ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
^^^^^^^^^^^^^^^^
  File "/home/jerome-ni/anaconda3/envs/test_transformer_mp_torch_2.0.1/lib/pyt
hon3.11/site-packages/torch/nn/modules/module.py", line 1501, in _call_impl
    return forward_call(*args, **kwargs)
           ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
  File "/mnt/c/Users/junru/Downloads/transformer_mp/src_test/transformer.py",
line 233, in forward
    dec_output = self.forward_decoder(enc_output, src_padding_mask, tgt, tgt_l
engths)
                 ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
^^^^^^^
  File "/mnt/c/Users/junru/Downloads/transformer_mp/src_test/transformer.py",
line 208, in forward_decoder
    return dec_output
           ^^^^^^^^^^
NameError: name 'dec_output' is not defined

======================================================================
ERROR: test_decoder_inference_cache_extra_credit (test_visible_ec.TestStep.tes
t_decoder_inference_cache_extra_credit)
----------------------------------------------------------------------
Traceback (most recent call last):
  File "/mnt/c/Users/junru/Downloads/transformer_mp/src_test/tests/test_visibl
e_ec.py", line 162, in test_decoder_inference_cache_extra_credit
    output_list, decoder_cache = model.inference(src = src, src_lengths = src_
lengths, max_output_length = MAX_INFERENCE_LENGTH)
                                 ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
  File "/mnt/c/Users/junru/Downloads/transformer_mp/src_test/transformer.py",
line 274, in inference
    tgt_embedded = self.dropout(self.positional_encoding(self.decoder_embeddin
g(tgt)))

^^^
NameError: name 'tgt' is not defined

======================================================================
ERROR: test_decoder_inference_outputs_extra_credit (test_visible_ec.TestStep.t
est_decoder_inference_outputs_extra_credit)
----------------------------------------------------------------------
Traceback (most recent call last):
  File "/mnt/c/Users/junru/Downloads/transformer_mp/src_test/tests/test_visibl
e_ec.py", line 109, in test_decoder_inference_outputs_extra_credit
    output_list, decoder_cache = model.inference(src = src, src_lengths = src_
lengths, max_output_length = MAX_INFERENCE_LENGTH)
                                 ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
  File "/mnt/c/Users/junru/Downloads/transformer_mp/src_test/transformer.py",
line 274, in inference
    tgt_embedded = self.dropout(self.positional_encoding(self.decoder_embeddin
g(tgt)))

^^^
NameError: name 'tgt' is not defined

======================================================================
FAIL: test_encoder_output (test_visible.TestStep.test_encoder_output)
----------------------------------------------------------------------
Traceback (most recent call last):
  File "/mnt/c/Users/junru/Downloads/transformer_mp/src_test/tests/test_visibl
e.py", line 279, in test_encoder_output
    self.assertAlmostEqual(torch.sum(torch.abs(ref_enc_item - enc_item)).item
(), 0, places = 4, msg=f'The encoder output for the sample #{item_idx} in the
batch #{it_idx} is not correct')
AssertionError: 646.3253784179688 != 0 within 4 places (646.3253784179688 diff
erence) : The encoder output for the sample #0 in the batch #0 is not correct

----------------------------------------------------------------------
Ran 10 tests in 1.817s

FAILED (failures=1, errors=4)
```

Transformer Encoder

The Transformer Encoder consists of a stack of Transformer encoder layers. Each encoder layer has two sets of sub-layer operations, applied one set after another. The first set involves the multi-head self-attention mechanism, and the second set involves a simple, position-wise, fully connected feed-forward network. In the paper, for each of the two sub-layer operation sets, a dropout operation is immediately applied to the output of the sub-layer, followed by a residual connection around each of the two sub-layers, followed by layer normalization. That is, let x denote the input to the sub-layer, the output of each sub-layer is $\mathrm{LayerNorm}(x + \mathrm{DropOut}(\mathrm{Sublayer}(x)))$, where $\mathrm{Sublayer}(x)$ is the function implemented by the sub-layer itself.

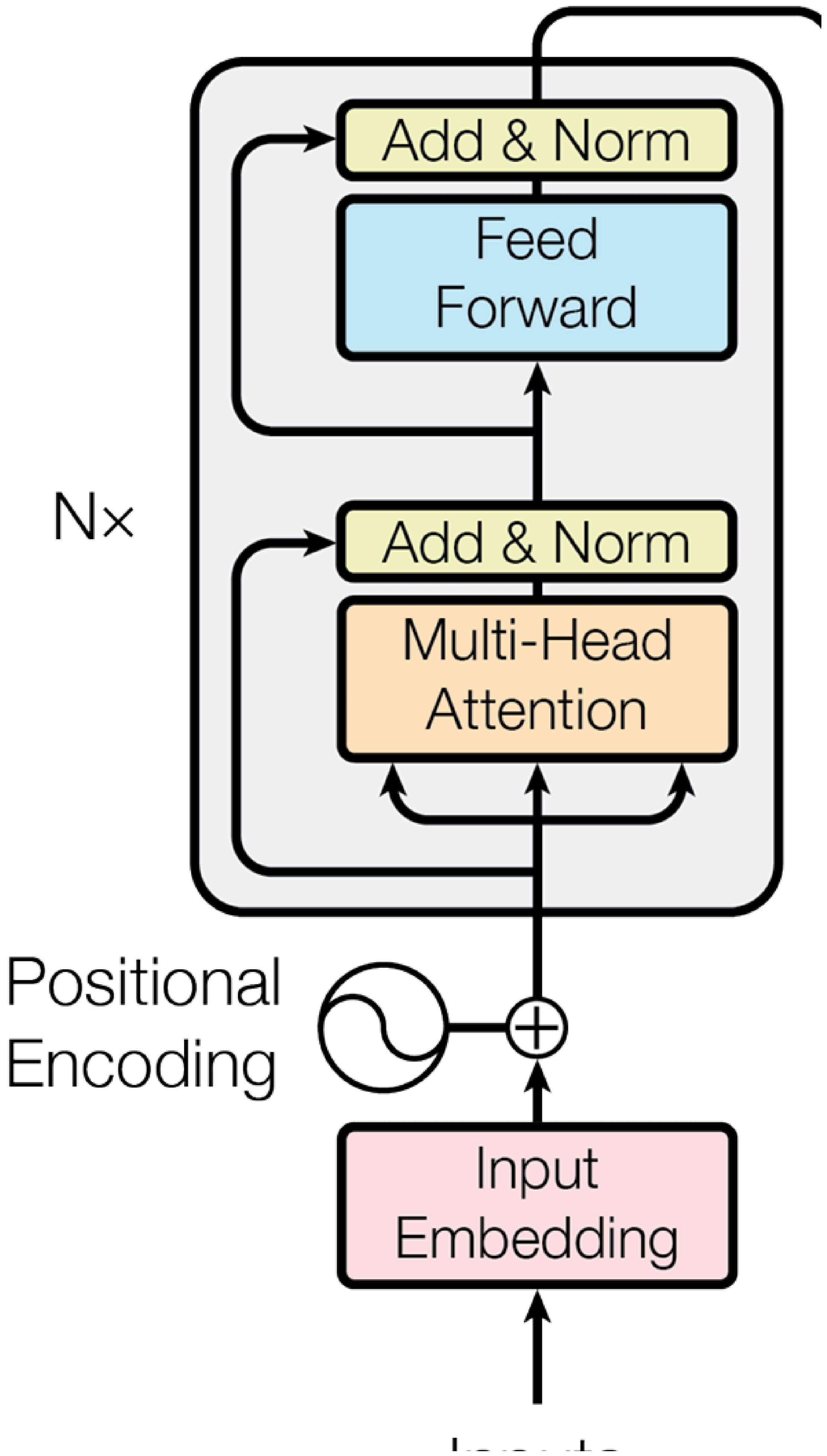
For the first $\mathrm{Sublayer}(x)$, the encoder multi-head self-attention mechanism, all of the keys, values, and queries come from the same place, and are either the encoder input (for the first layer), or the output of the previous layer (for subsequent layers). Each position in the encoder self-attention mechanism can attend to all positions in the previous layer of the encoder (or input for the first layer). Note that in the actual implementation, if we are padding each source input in the batch to the same length, we still need to use a mask to avoid the encoder self-attention mechanism from attending to position beyond the original input length.

For the second $\mathrm{Sublayer}(x)$, the position-wise, fully-connected feed-forward network, the network is applied to each position separately and identically. This consists of two linear transformations with a ReLU activation in between, as $\mathrm{FFN}(x) = \max\left(0, xW_1 + b_1\right) W_2 + b_2$, where for the inner layer, $W_1 \in \mathbb{R}^{d_{model} \times d_{ff}}$, $b_1 \in \mathbb{R}^{d_{ff}}$ and for the outer layer, $W_2 \in \mathbb{R}^{d_{ff} \times d_{model}}$, $b_2 \in \mathbb{R}^{d_{model}}$.

The figure below from pg. 3 of the original paper shows the Transformer encoder architecture.

In [14]:
```
from IPython.display import Image
Image("img/encoder.PNG")
```

```
Out[14]:
```


Add & Norm
Feed Forward
Nx
Add & Norm
Multi-Head Attention
Positional Encoding
Input Embedding

In `encoder.py`, you will need to complete the `def forward(self, x,self_attn_padding_mask = None)` defined in the class `class TransformerEncoderLayer(nn.Module)`, which implements a single layer in the Transformer encoder. In `def __init__(self, embedding_dim, ffn_embedding_dim, num_attention_heads, dropout_prob)`, we have already pre-defined some model submodules and hyperparameters as:

```
self.embedding_dim - This is the model dimension, aka d_model

self.self_attn  - Build the self-attention mechanism using
MultiHeadAttention implemented earlier

self.self_attn_layer_norm - Layer norm for the self-attention
layer's output

self.activation_fn - The ReLU activation for position-wise
feed-forward network

self.fc1 - The parameters will be used for W_1 and b_1 in the
position-wise feed-forward network

self.fc2 - The parameters will be used for W_2 and b_2 in the
position-wise feed-forward network

self.dropout - The DropOut regularization module to be applied
immediately after self-attention module and FFN module
```

As described earlier, in `def forward(self, x,self_attn_padding_mask = None)`, you are simply asked to implement:

$$\text{LayerNorm}(x + \text{DropOut}(\text{Self-Attention}(x)))$$

followed by

$$\text{LayerNorm}(x + \text{DropOut}(\text{FFN}(x)))$$

where $\text{FFN}(x) = \max\left(0, xW_1 + b_1\right) W_2 + b_2$.

You should use all the model parameters already given to you in `class TransformerEncoderLayer(nn.Module)`, and should not need to define or use other parameters or helper functions.

The entire Transformer encoder has already been implemented for you, which simply stacks the Transformer Encoder Layer implemented earlier together to form a Transformer

Encoder. Please read the `class TransformerEncoder(nn.Module)` in `encoder.py` as you will need to invoke its `forward` function later.

In [5]:
```python
from encoder import TransformerEncoder, TransformerEncoderLayer
help(TransformerEncoderLayer.forward)
```

```
Help on function forward in module encoder:

forward(self, x, self_attn_padding_mask=None)
    Applies the self attention module + Dropout + Add & Norm operation, and th
e position-wise feedforward network + Dropout + Add & Norm operation. Note tha
t LayerNorm is applied after the self-attention, and another time after the ff
n modules, similar to the original Transformer implementation.

    Input:
        x (torch.Tensor) - input tensor of size B x T x embedding_dim from the
encoder input or the previous encoder layer; serves as input to the Transforme
rEncoderLayer's self attention mechanism.

        self_attn_padding_mask (None/torch.Tensor) - If it is not None, then i
t is a torch.IntTensor/torch.LongTensor of size B x T, where for each self_att
n_padding_mask[b] for the b-th source in the batch, the non-zero positions wil
l be ignored as they represent the padded region during batchify operation in
the dataloader (i.e., disallowed for attention) while the zero positions will
be allowed for attention as they are within the length of the original sequenc
e

    Output:
        x (torch.Tensor) - the encoder layer's output, of size B x T x embeddi
ng_dim, after the self attention module + Dropout + Add & Norm operation, and
the position-wise feedforward network + Dropout + Add & Norm operation.
```

To finish your Transformer encoder (after reading the implementation in `class TransformerEncoder(nn.Module)`), you now need to implement the `def forward_encoder(self, src, src_lengths)` in `class Transformer(nn.Module)`, which is defined in `transformer.py`. The `__init__(self, src_vocab_size, tgt_vocab_size, sos_idx, eos_idx, d_model, num_heads, num_layers, d_ff, max_seq_length, dropout_prob)` defines some model submodules and hyperparameters that are related to `forward_encoder` as:

```
self.encoder_embedding - Encoder input embedding that converts
discrete tokens into continuous vectors; this will be already
invoked for you in forward_encoder to get the encoder's input
src_embedded.

self.positional_encoding - Positional Encoding used by the
Transformer encoder; this will be already invoked for you in
forward_encoder to get the encoder's input src_embedded.

self.encoder - Creates an instance of TransformerEncoder.

self.dropout - For applying additional dropout after positional
```

```
encoding; this will be already invoked for you in
forward_encoder to get the encoder's input src_embedded.
```

All you need to do in `def forward_encoder(self, src, src_lengths)` is to create the padding mask for the encoder input correctly, and get the output from the `TransformerEncoder` correctly. You will find the helper function `def length_to_padding_mask(lengths, device="cpu", dtype=torch.long)` to be useful for creating the padding mask (aka `encoder_padding_mask`, or `self_attn_padding_mask`).

In [8]:
```
help(TransformerEncoder.forward)
```

```
Help on function forward in module encoder:

forward(self, x, encoder_padding_mask=None)
    Applies the encoder layers in self.layers one by one, followed by an optio
nal output layer if it exists

    Input:
        x (torch.Tensor) - input tensor of size B x T x embedding_dim; input t
o the TransformerEncoderLayer's self attention mechanism

        encoder_padding_mask (None/torch.Tensor) - If it is not None, then it
is a torch.IntTensor/torch.LongTensor of size B x T, where for each encoder_pa
dding_mask[b] for the b-th source in the batch, the non-zero positions will be
ignored as they represent the padded region during batchify operation in the d
ataloader (i.e., disallowed for attention) while the zero positions will be al
lowed for attention as they are within the length of the original sequence

    Output:
        x (torch.Tensor) - the Transformer encoder's output, of size B x T x e
mbedding_dim, if output layer is None, or of size B x T x output_layer_size, i
f there is an output layer.
```

In [10]:
```
from transformer import Transformer, length_to_padding_mask
help(Transformer.forward_encoder)
```

```
Help on function forward_encoder in module transformer:

forward_encoder(self, src, src_lengths)
    Applies the Transformer encoder to src, where each sequence in src has bee
n padded to the max(src_lengths)

    Input:
        src (torch.Tensor) - Encoder's input tensor of size B x T_e x d_model

        src_lengths (torch.Tensor) - A 1D iterable of Long/Int of length B, wh
ere the b-th length in src_lengths corresponds to the actual length of src[b]
(beyond that is the pre-padded region); T_e = max(src_lengths)

    Output:
        enc_output (torch.Tensor) - the Transformer encoder's output, of size
B x T_e x d_model

        src_padding_mask (torch.Tensor) - the encoder_padding_mask/key_padding
_mask used by the Transformer encoder's self-attention; this should be created
from src_lengths
```

In [11]:
```
help(length_to_padding_mask)
```

```
Help on function length_to_padding_mask in module transformer:

length_to_padding_mask(lengths, device='cpu', dtype=torch.int64)
    Convert a list/1D tensor/1D array of length in to padding masks used by th
e encoder and the decoder's attention mechanism

    For example, length_to_padding_mask([3, 4, 5]) will return a torch.tensor
of dtype, on the device, as:
    [[0, 0, 0, 1, 1],
     [0, 0, 0, 0, 1],
     [0, 0, 0, 0, 0]]

    Input:
        lengths (List/torch.Tensor/np.array) - a 1D iterable List/torch.Tenso
r/np.array
        device (str/torch.Tensor.device): where the return tensor will be loca
ted, say, "cpu" or "cuda" or torch.Tensor.device
        dtype (torch.dtype) - result dtype

    Output:
        ret (torch.Tensor) - a padding mask of size len(lengths) x max(length
s), with non-zero positions indicating locations out of bounds , of "dtype", o
n the "device"
```

If you believe you have implemented everything in this section correctly, you can run `python.grade.py` to see if you have passed the test related to the Transformer encoder implementation, assuming ALL your previous tests have passed. We have defined one test for checking your Transformer encoder implementation that you should have passed: `test_encoder_output`, which initializes a `Transformer` object, loads the model weights from a de-en neural machine translation checkpoint `trained_de_en_state_dict.pt`, and invokes the `forward_encoder` function on some German sentences (that are converted to discrete index sequences) to check against the intermediate encoder output pre-generated by our implementation.

It is expected, for now, for the other four tests to either fail or error out (assuming you passed the four tests for `mha.py`, and the one test for `pe.py` already)

Note: if you are getting a very small error that causes you to fail the test, please double-check that you have the correct torch version installed. Our outputs on the visible set are pre-generated using `Python 3.10` and `torch== 2.0.1`, so at the very least you need to make sure that you are using `torch==2.0.1` for this. It has been known that newer or older PyTorch versions may have slightly different implementations of the same internal module, and result in slightly different computed results. If in doubt, you can also submit to GradeScope for testing. The auto-grader on GradeScope will NOT have this issue, as the solutions will be generated during the submission with the same platform and package versions as your implementation will use, but your code will be tested on the hidden set instead.

```
In [12]: !python grade.py
```

```
EE......EE
======================================================================
ERROR: test_encoder_decoder_predictions (test_visible.TestStep.test_encoder_de
coder_predictions)
----------------------------------------------------------------------
Traceback (most recent call last):
  File "/mnt/c/Users/junru/Downloads/transformer_mp/src_test/tests/test_visibl
e.py", line 311, in test_encoder_decoder_predictions
    output = model(src = src, tgt = trg, src_lengths = src_lengths, tgt_length
s = trg_lengths)
             ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
^^^^^^^^^^^^^^^^
  File "/home/jerome-ni/anaconda3/envs/test_transformer_mp_torch_2.0.1/lib/pyt
hon3.11/site-packages/torch/nn/modules/module.py", line 1501, in _call_impl
    return forward_call(*args, **kwargs)
           ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
  File "/mnt/c/Users/junru/Downloads/transformer_mp/src_test/transformer.py",
line 233, in forward
    dec_output = self.forward_decoder(enc_output, src_padding_mask, tgt, tgt_l
engths)
                 ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
^^^^^^^
  File "/mnt/c/Users/junru/Downloads/transformer_mp/src_test/transformer.py",
line 208, in forward_decoder
    return dec_output
           ^^^^^^^^^^
NameError: name 'dec_output' is not defined

======================================================================
ERROR: test_encoder_decoder_states (test_visible.TestStep.test_encoder_decoder
_states)
----------------------------------------------------------------------
Traceback (most recent call last):
  File "/mnt/c/Users/junru/Downloads/transformer_mp/src_test/tests/test_visibl
e.py", line 365, in test_encoder_decoder_states
    output = model(src = src, tgt = trg, src_lengths = src_lengths, tgt_length
s = trg_lengths)
             ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
^^^^^^^^^^^^^^^^
  File "/home/jerome-ni/anaconda3/envs/test_transformer_mp_torch_2.0.1/lib/pyt
hon3.11/site-packages/torch/nn/modules/module.py", line 1501, in _call_impl
    return forward_call(*args, **kwargs)
           ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
  File "/mnt/c/Users/junru/Downloads/transformer_mp/src_test/transformer.py",
line 233, in forward
    dec_output = self.forward_decoder(enc_output, src_padding_mask, tgt, tgt_l
engths)
                 ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
^^^^^^^
  File "/mnt/c/Users/junru/Downloads/transformer_mp/src_test/transformer.py",
line 208, in forward_decoder
    return dec_output
           ^^^^^^^^^^
NameError: name 'dec_output' is not defined

======================================================================
ERROR: test_decoder_inference_cache_extra_credit (test_visible_ec.TestStep.tes
t_decoder_inference_cache_extra_credit)
----------------------------------------------------------------------
Traceback (most recent call last):
  File "/mnt/c/Users/junru/Downloads/transformer_mp/src_test/tests/test_visibl
e_ec.py", line 162, in test_decoder_inference_cache_extra_credit
    output_list, decoder_cache = model.inference(src = src, src_lengths = src_
lengths, max_output_length = MAX_INFERENCE_LENGTH)
                                 ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
  File "/mnt/c/Users/junru/Downloads/transformer_mp/src_test/transformer.py",
line 274, in inference
    tgt_embedded = self.dropout(self.positional_encoding(self.decoder_embeddin
g(tgt)))

^^^
NameError: name 'tgt' is not defined

======================================================================
ERROR: test_decoder_inference_outputs_extra_credit (test_visible_ec.TestStep.t
est_decoder_inference_outputs_extra_credit)
----------------------------------------------------------------------
Traceback (most recent call last):
  File "/mnt/c/Users/junru/Downloads/transformer_mp/src_test/tests/test_visibl
e_ec.py", line 109, in test_decoder_inference_outputs_extra_credit
    output_list, decoder_cache = model.inference(src = src, src_lengths = src_
lengths, max_output_length = MAX_INFERENCE_LENGTH)
                                 ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
  File "/mnt/c/Users/junru/Downloads/transformer_mp/src_test/transformer.py",
line 274, in inference
    tgt_embedded = self.dropout(self.positional_encoding(self.decoder_embeddin
g(tgt)))

^^^
NameError: name 'tgt' is not defined

----------------------------------------------------------------------
Ran 10 tests in 1.876s

FAILED (errors=4)
```

Transformer Decoder

The Transformer Decoder consists of a stack of Transformer decoder layers. Each decoder layer has three sets of sub-layer operations, applied one set after another. The first set involves the decoder multi-head self-attention mechanism, the second set involves multi-head encoder-decoder attention mechanism, and the third set involves a simple, position-wise, fully connected feed-forward network. A dropout operation is immediately applied to the output of the sub-layer, followed by a residual connection around each of the two sub-layers, followed by layer normalization. That is, let x denote the input to the sub-layer, the output of each sub-layer is $\mathrm{LayerNorm}(x + \mathrm{DropOut}(\mathrm{Sublayer}(x)))$, where $\mathrm{Sublayer}(x)$ is the function implemented by the sub-layer itself.

For the first $\mathrm{Sublayer}(x)$, the decoder multi-head self-attention mechanism, all of the keys, values, and queries come from the same place, and are either the decoder input (for the first layer) or the output of the previous decoder layer (for subsequent layers). However, unlike encoder self-attention, we prevent each temporal position in the temporal dimension from attending to subsequent positions. We have already taken care of this scenario with the `attention_mask` argument in the `forward` function of the `MultiHeadAttention` module. This masking ensures that the predictions for position $i + 1$ can depend only on the known outputs at positions up to and including i. If we are padding each decoder input in the batch to the same length, we still need to use a mask to additionally avoid the decoder self-attention mechanism from attending to positions beyond the original input length.

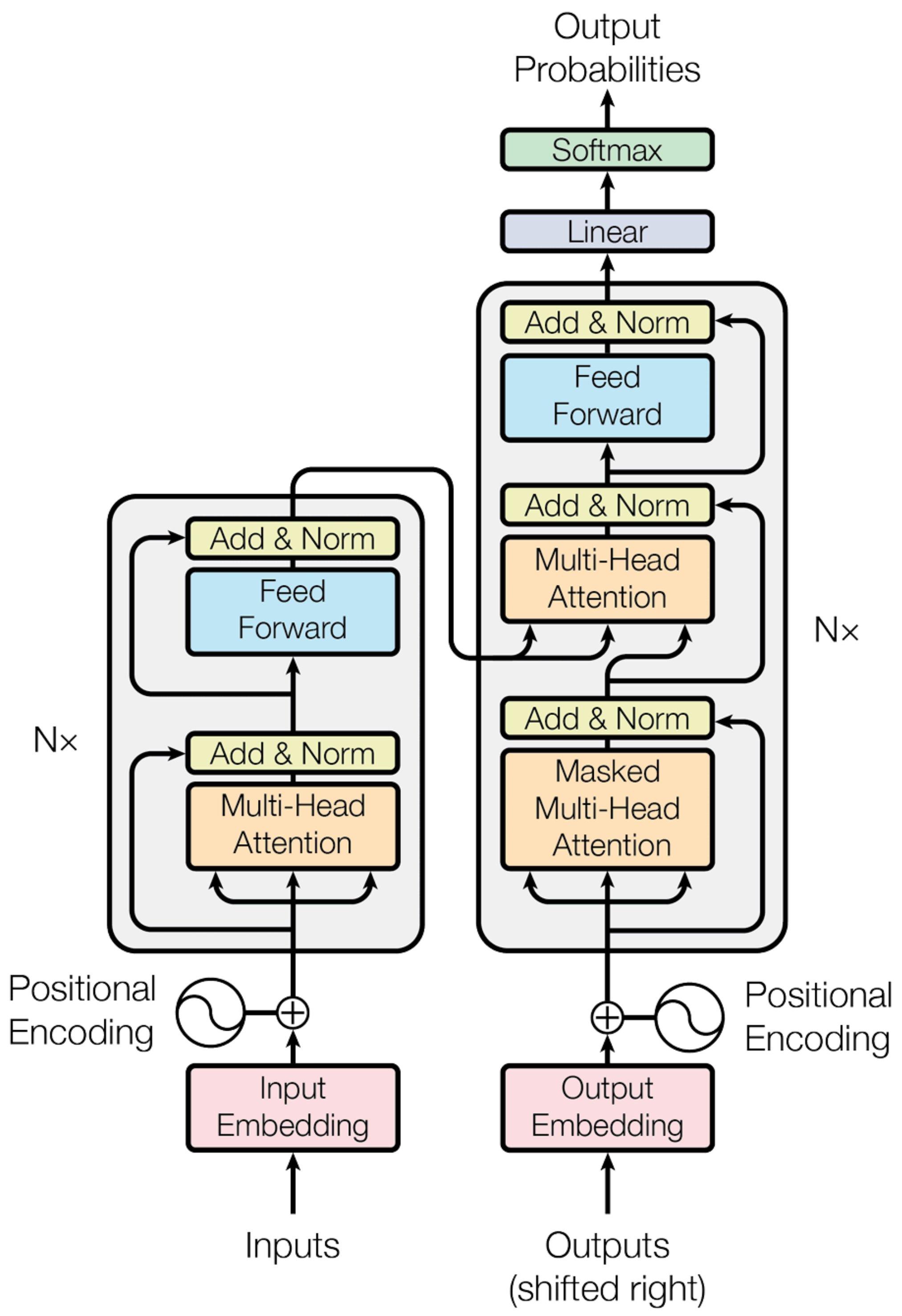
For the second $\text{Sublayer}(x)$, the encoder-decoder multi-head attention mechanism, the queries come from the previous decoder layer, and the memory keys and values come from the output of the encoder. This allows every position in the decoder to attend to all positions in the input sequence. We still need to use a mask to avoid attending to positions beyond the original input sequence length.

For the third $\text{Sublayer}(x)$, the position-wise, fully-connected feed-forward network, the network is applied to each position separately and identically. This consists of two linear transformations with a ReLU activation in between, as $\text{FFN}(x) = \max\left(0, xW_1 + b_1\right) W_2 + b_2$, where for the inner layer, $W_1 \in \mathbb{R}^{d_{model} \times d_{ff}}$, $b_1 \in \mathbb{R}^{d_{ff}}$ and for the outer layer, $W_2 \in \mathbb{R}^{d_{ff} \times d_{model}}$, $b_2 \in \mathbb{R}^{d_{model}}$.

The figure below from pg. 3 of the original paper shows the entire Transformer encoder-decoder architecture, as part of the encoder-decoder attention module's input comes from the Transformer encoder.

In [15]:
```
from IPython.display import Image
Image("img/encoder_decoder.PNG")
```

Out[15]:



In `decoder.py`, you will need to complete the `def forward(self, x, encoder_out = None, encoder_padding_mask = None, self_attn_padding_mask = None,self_attn_mask = None)` defined in the class `class TransformerDecoderLayer(nn.Module)`, which implements a single decoder layer in the Transformer decoder. In `def __init__(self, embedding_dim, ffn_embedding_dim, num_attention_heads, dropout_prob, no_encoder_attn=False)`, we have already pre-defined some model submodules and hyperparameters as:

```
self.embedding_dim - This is the model dimension, aka d_model

self.self_attn  - Build the decoder self-attention mechanism
using MultiHeadAttention implemented earlier

self.self_attn_layer_norm - Layer norm for the decoder self-
attention layer's output

self.encoder_attn - If an encoder-decoder architecture is
built, we build the encoder-decoder attention using
MultiHeadAttention implemented earlier

self.encoder_attn_layer_norm - Layer norm for the encoder-
decoder attention layer's output

self.activation_fn - The ReLU activation for position-wise
feed-forward network

self.fc1 - The parameters will be used for W_1 and b_1 in the
position-wise feed-forward network

self.fc2 - The parameters will be used for W_2 and b_2 in the
position-wise feed-forward network

self.dropout - The DropOut regularization module to be applied
immediately after self-attention module, encoder-decoder
attention module and FFN module
```

As described earlier, in `def forward(self, x, encoder_out = None, encoder_padding_mask = None, self_attn_padding_mask = None,self_attn_mask = None)`, you are simply asked to implement:

$$x = \text{LayerNorm}(x + \text{DropOut}(\text{Decoder-Self-Attention}(x)))$$

followed by

$$x = \text{LayerNorm}(x + \text{DropOut}(\text{Encoder-Decoder-Attention}(x, \mathit{encoder\_out})))$$

followed by

$$x = \text{LayerNorm}(x + \text{DropOut}(\text{FFN}(x)))$$

where $\text{FFN}(x) = \max(0, xW_1 + b_1)\, W_2 + b_2$.

You should use all the model parameters already given to you in `class TransformerDecoderLayer(nn.Module)`, and should not need to define or use other parameters or helper functions.

The entire Transformer decoder has already been implemented for you, which simply stacks the TransformerDecoderLayer implemented earlier together to form a TransformerDecoder.

Please read the `class TransformerDecoder(nn.Module)` in `decoder.py` as you will need to invoke its `forward` function later.

In [17]:
```
from decoder import TransformerDecoder, TransformerDecoderLayer
help(TransformerDecoderLayer.forward)
```

```
Help on function forward in module decoder:

forward(self, x, encoder_out=None, encoder_padding_mask=None, self_attn_paddin
g_mask=None, self_attn_mask=None)
    Applies the self attention module + Dropout + Add & Norm operation, the en
coder-decoder attention + Dropout + Add & Norm operation (if self.encoder_attn
is not None), and the position-wise feedforward network + Dropout + Add & Norm
operation. Note that LayerNorm is applied after the self-attention operation,
after the encoder-decoder attention operation and another time after the ffn m
odules, similar to the original Transformer implementation.

    Input:
        x (torch.Tensor) - input tensor of size B x T_d x embedding_dim from t
he decoder input or the previous encoder layer, where T_d is the decoder's tem
poral dimension; serves as input to the TransformerDecoderLayer's self attenti
on mechanism.

        encoder_out (None/torch.Tensor) - If it is not None, then it is the ou
tput from the TransformerEncoder as a tensor of size B x T_e x embedding_dim,
where T_e is the encoder's temporal dimension; serves as part of the input to
the TransformerDecoderLayer's self attention mechanism (hint: which part?).

        encoder_padding_mask (None/torch.Tensor) - If it is not None, then it
is a torch.IntTensor/torch.LongTensor of size B x T_e, where for each encoder_
padding_mask[b] for the b-th source in the batched tensor encoder_out[b], the
non-zero positions will be ignored as they represent the padded region during
batchify operation in the dataloader (i.e., disallowed for attention) while th
e zero positions will be allowed for attention as they are within the length o
f the original sequence

        self_attn_padding_mask (None/torch.Tensor) - If it is not None, then i
t is a torch.IntTensor/torch.LongTensor of size B x T_d, where for each self_a
ttn_padding_mask[b] for the b-th source in the batched tensor x[b], the non-ze
ro positions will be ignored as they represent the padded region during batchi
fy operation in the dataloader (i.e., disallowed for attention) while the zero
positions will be allowed for attention as they are within the length of the o
riginal sequence

        self_attn_mask (None/torch.Tensor) - If it is not None, then it is a t
orch.IntTensor/torch.LongTensor of size 1 x T_d x T_d or B x T_d x T_d. It is
used for decoder self-attention to enforce auto-regressive property during par
allel training; suppose the maximum length of a batch is 5, then the attention
_mask for any input in the batch will look like this for each input of the bat
ch.
        0 1 1 1 1
        0 0 1 1 1
        0 0 0 1 1
        0 0 0 0 1
        0 0 0 0 0
        The non-zero positions will be ignored and disallowed for attention wh
ile the zero positions will be allowed for attention.

    Output:
        x (torch.Tensor) - the decoder layer's output, of size B x T_d x embed
ding_dim, after the self attention module + Dropout + Add & Norm operation, th
e encoder-decoder attention + Dropout + Add & Norm operation (if self.encoder_
attn is not None), and the position-wise feedforward network + Dropout + Add &
Norm operation.
```

To finish your Transformer decoder (after reading the implementation in `class TransformerDecoder(nn.Module)`), you now need to implement the `def forward_decoder(self, enc_output, src_padding_mask, tgt, tgt_lengths)` in `class Transformer(nn.Module)`, which is defined in `transformer.py`. The `__init__(self, src_vocab_size, tgt_vocab_size, sos_idx, eos_idx, d_model, num_heads, num_layers, d_ff, max_seq_length, dropout_prob)` defines some model submodules and hyperparameters that are related to `forward_decoder` as:

```
self.decoder_embedding - Decoder input embedding that converts
discrete tokens into continuous vectors; this will be already
invoked for you in forward_decoder to get the decoder's input
tgt_embedded.

self.positional_encoding - Positional Encoding used by the
Transformer decoder; this will be already invoked for you in
forward_decoder to get the decoder's input tgt_embedded.

self.decoder - Creates an instance of TransformerDecoder.

self.dropout - For applying additional dropout after positional
encoding; this will be already invoked for you in
forward_decoder to get the decoder's input tgt_embedded.

self.sos_idx - Every encoder and decoder sequence starts with
this token index (useful in extra-credit)
self.eos_idx - Every encoder and decoder sequence ends with
this token index (useful in extra-credit)
```

All you need to do in `def forward_decoder(self, enc_output, src_padding_mask, tgt, tgt_lengths)` is to a. create the padding mask and the attention mask for the decoder input correctly; b. pass the `tgt_embedded`, which is your decoder (target) sequence input, `enc_output` and `src_padding_mask`, which are return values from your `forward_encoder`, into the `forward` call of `TransformerDecoder` object; c. return the decoder output.

You will find the helper function `def length_to_padding_mask(lengths, device="cpu", dtype=torch.long)` to be useful for creating the padding mask for padded decoder input (aka `self_attn_padding_mask`). You will find the helper function `def subsequent_mask(size, device="cpu", dtype=torch.long)` to be useful for creating the additional decoder auto-regressive mask for self-attention (aka `self_attn_mask`).

In [18]:
```
help(TransformerDecoder.forward)
```

```
Help on function forward in module decoder:

forward(self, x, decoder_padding_mask=None, decoder_attention_mask=None, encod
er_out=None, encoder_padding_mask=None)
    Applies the encoder layers in self.layers one by one, followed by an optio
nal output layer if it exists

    Input:
        x (torch.Tensor) - input tensor of size B x T_d x embedding_dim; input
to the TransformerDecoderLayer's self attention mechanism

        decoder_padding_mask (None/torch.Tensor) - If it is not None, then it
is a torch.IntTensor/torch.LongTensor of size B x T_d, where for each decoder_
padding_mask[b] for the b-th source in the batched tensor x[b], the non-zero p
ositions will be ignored as they represent the padded region during batchify o
peration in the dataloader (i.e., disallowed for attention) while the zero pos
itions will be allowed for attention as they are within the length of the orig
inal sequence

        decoder_attention_mask (None/torch.Tensor) - If it is not None, then i
t is a torch.IntTensor/torch.LongTensor of size 1 x T_d x T_d or B x T_d x T_
d. It is used for decoder self-attention to enforce auto-regressive property d
uring parallel training; suppose the maximum length of a batch is 5, then the
attention_mask for any input in the batch will look like this for each input o
f the batch.
        0 1 1 1 1
        0 0 1 1 1
        0 0 0 1 1
        0 0 0 0 1
        0 0 0 0 0
        The non-zero positions will be ignored and disallowed for attention wh
ile the zero positions will be allowed for attention.

        encoder_out (None/torch.Tensor) - If it is not None, then it is the ou
tput from the TransformerEncoder as a tensor of size B x T_e x embedding_dim,
where T_e is the encoder's temporal dimension; serves as part of the input to
the TransformerDecoderLayer's self attention mechanism (hint: which part?).

        encoder_padding_mask (None/torch.Tensor) - If it is not None, then it
is a torch.IntTensor/torch.LongTensor of size B x T_e, where for each encoder_
padding_mask[b] for the b-th source in the batch, the non-zero positions will
be ignored as they represent the padded region during batchify operation in th
e dataloader (i.e., disallowed for attention) while the zero positions will be
allowed for attention as they are within the length of the original sequence

    Output:
        x (torch.Tensor) - the Transformer decoder's output, of size B x T_d x
embedding_dim, if output layer is None, or of size B x T_d x output_layer_siz
e, if there is an output layer.
```

In [19]:

```
help(Transformer.forward_decoder)
```

```
Help on function forward_decoder in module transformer:

forward_decoder(self, enc_output, src_padding_mask, tgt, tgt_lengths)
    Applies the Transformer decoder to tgt and enc_output (possibly as used du
ring training to obtain the next token prediction under teacher-forcing), wher
e sequences in enc_output are associated with src_padding_mask, and each seque
nce in tgt has been padded to the max(tgt_lengths)

    Input:
        enc_output (torch.Tensor) - the Transformer encoder's output, of size
B x T_e x d_model

        src_padding_mask (torch.Tensor) - the encoder_padding_mask/key_padding
_mask associated with enc_output. It is a torch.IntTensor/torch.LongTensor of
size B x T_e, where for each src_padding_mask[b] for the b-th source in the ba
tched tensor enc_output[b], the non-zero positions will be ignored as they rep
resent the padded region during batchify operation in the dataloader (i.e., di
sallowed for attention) while the zero positions will be allowed for attention
as they are within the length of the original sequence

        tgt (torch.Tensor) - Decoder's input tensor of size B x T_d x d_model

        tgt_lengths (torch.Tensor) - A 1D iterable of Long/Int of length B, wh
ere the b-th length in tgt_lengths corresponds to the actual length of tgt[b]
(beyond that is the pre-padded region); T_d = max(tgt_lengths)


    Output:
        dec_output (torch.Tensor) - the Transformer's final output from the de
coder of size B x T_d x tgt_vocab_size, as there is an output layer.
```

In [21]:
```python
from transformer import subsequent_mask
help(subsequent_mask)
```

```
Help on function subsequent_mask in module transformer:

subsequent_mask(size, device='cpu', dtype=torch.int64)
    Create mask for subsequent steps size x size; this may be useful for creat
ing decoder attention masks for parallel auto-regressive training.

    subsequent_mask(3) will return a torch.tensor of dtype, on the device, as:
    [[0, 1, 1],
     [0, 0, 1],
     [0, 0, 0]]

    Input:
        size (int) - size of mask
        device (str/torch.Tensor.device): where the return tensor will be loca
ted, say, "cpu" or "cuda" or torch.Tensor.device
        dtype (torch.dtype) - result dtype

    Output:
        torch.Tensor - mask for subsequent steps with shape as size x size, of
"dtype", on the "device"
```

If you believe you have implemented everything in this section correctly, you can run `python.grade.py` to see if you have passed the test related to the Transformer decoder implementation, assuming ALL your previous tests have passed. We have defined two tests that you should have passed: `test_encoder_decoder_predictions`, which initializes a `Transformer` object, loads the model weights from a de-en neural machine translation checkpoint `trained_de_en_state_dict.pt`, and invokes the `forward_decoder` function on some German sentences (that are converted to discrete index sequences), which, conditioned on previous tokens in the parallel English sentences, predicts the next tokens in English. We take your next token prediction outputs of the unpadded regions to check against the next token predictions pre-generated by our implementation. This test will also throw an error if the next token prediction accuracy does not match ours, which indicates some major bugs. The second test, `test_encoder_decoder_states,` works similarly, except that we are checking your pre-softmax output layer states from the decoder instead of discrete predictions.

It is expected, for now, for the other two tests to either fail or error out, as they are for extra credit (assuming you passed the four tests for `mha.py`, the one test for `pe.py`, and the one test for your Transformer encoder implementation).

Note: if you are getting a very small error that causes you to fail the test, please double-check that you have the correct torch version installed. Our outputs on the visible set are pre-generated using `Python 3.10` and `torch== 2.0.1`, so at the very least you need to make sure that you are using `torch==2.0.1` for this. It has been known that newer or older PyTorch versions may have slightly different implementations of the same internal module, and result in slightly different computed results. If in doubt, you can also submit to GradeScope for testing. The auto-grader on GradeScope will NOT have this issue, as the solutions will be generated during the submission with the same platform and package versions as your implementation will use, but your code will be tested on the hidden set instead.

In [22]:
```
!python grade.py
```

```
........EE
======================================================================
ERROR: test_decoder_inference_cache_extra_credit (test_visible_ec.TestStep.tes
t_decoder_inference_cache_extra_credit)
----------------------------------------------------------------------
Traceback (most recent call last):
  File "/mnt/c/Users/junru/Downloads/transformer_mp/src_test/tests/test_visibl
e_ec.py", line 162, in test_decoder_inference_cache_extra_credit
    output_list, decoder_cache = model.inference(src = src, src_lengths = src_
lengths, max_output_length = MAX_INFERENCE_LENGTH)
                                 ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
  File "/mnt/c/Users/junru/Downloads/transformer_mp/src_test/transformer.py",
line 274, in inference
    tgt_embedded = self.dropout(self.positional_encoding(self.decoder_embeddin
g(tgt)))

^^^
NameError: name 'tgt' is not defined

======================================================================
ERROR: test_decoder_inference_outputs_extra_credit (test_visible_ec.TestStep.t
est_decoder_inference_outputs_extra_credit)
----------------------------------------------------------------------
Traceback (most recent call last):
  File "/mnt/c/Users/junru/Downloads/transformer_mp/src_test/tests/test_visibl
e_ec.py", line 109, in test_decoder_inference_outputs_extra_credit
    output_list, decoder_cache = model.inference(src = src, src_lengths = src_
lengths, max_output_length = MAX_INFERENCE_LENGTH)
                                 ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
  File "/mnt/c/Users/junru/Downloads/transformer_mp/src_test/transformer.py",
line 274, in inference
    tgt_embedded = self.dropout(self.positional_encoding(self.decoder_embeddin
g(tgt)))

^^^
NameError: name 'tgt' is not defined

----------------------------------------------------------------------
Ran 10 tests in 2.064s

FAILED (errors=2)
```

Submission

For submission onto GradeScope, make sure you are uploading all relevant Python modules onto Gradescope. Again, these are:

```
mha.py
pe.py
encoder.py
decoder.py
transformer.py
```

Extra Credit: Auto-regressive Decoding During Inference

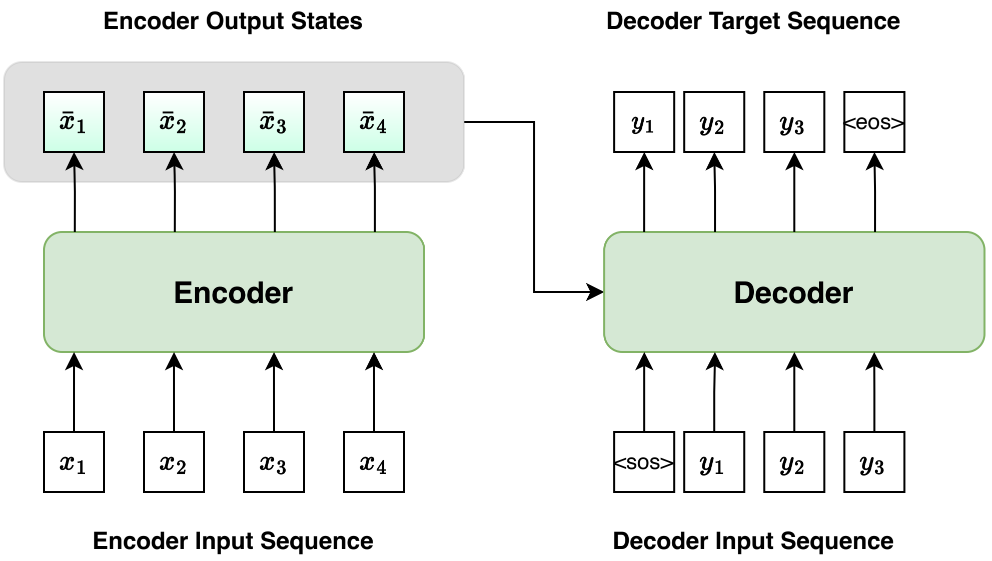
In the main part of the MP, we implemented the `forward` function of the Transformer decoder. The previous implementation is mainly used in training. During training, when we are given paired source and target sequences, we feed the source sequence into the encoder, we feed the entire target sequence as the decoder's input, and we predict the left-shifted target sequence with the decoder auto-regressive attention mask applied (conditioned on the encoder's output). Hence, we call this training routine "teacher-forcing".

This is depicted in the following figure, where we use $[x_1, x_2, x_3, x_4]$ to indicate the source sequence and $[y_1, y_2, y_3]$ to indicate the paired target sequence, as one would find in most sequence-to-sequence parallel datasets. We introduce the $< sos >$ token as the start-of-sentence sentinel and the $< eos >$ token as the end-of-sentence sentinel. Note that with our decoder auto-regressive attention mask implemented earlier (and passed to the decoder during training), when predicting y_1, besides the entire encoder states $[\bar{x}_1, \bar{x}_2, \bar{x}_3, \bar{x}_4]$, it can only access the decoder states of $< sos >$ for decoder self-attention; when predicting y_2, besides the entire encoder states $[\bar{x}_1, \bar{x}_2, \bar{x}_3, \bar{x}_4]$, it can only access the decoder states of $< sos >$ and y_1 for decoder self-attention; when predicting y_3, besides the entire encoder states $[\bar{x}_1, \bar{x}_2, \bar{x}_3, \bar{x}_4]$, it can only access the decoder states of $< sos >$, y_1 and y_2 for decoder self-attention; when predicting $< eos >$, besides the entire encoder states $[\bar{x}_1, \bar{x}_2, \bar{x}_3, \bar{x}_4]$, it can access the decoder states of $< sos >$, y_1, y_2 and y_3 for decoder self-attention.

Note that even if the decoder were to make a mistake after the output layer during training, and suppose that it predicts y_2 as $\tilde{y}_2$, when predicting y_3, the decoder prediction is still conditioned on the decoder states generated by $< sos >$, y_1 and y_2, instead of $< sos >$, y_1 and $\tilde{y}_2$. This is where the name "teacher-forcing" came from.

```
In [25]: from IPython.display import SVG
         SVG("img/encoder_decoder_teacher_forcing.SVG")
```

Out[25]:



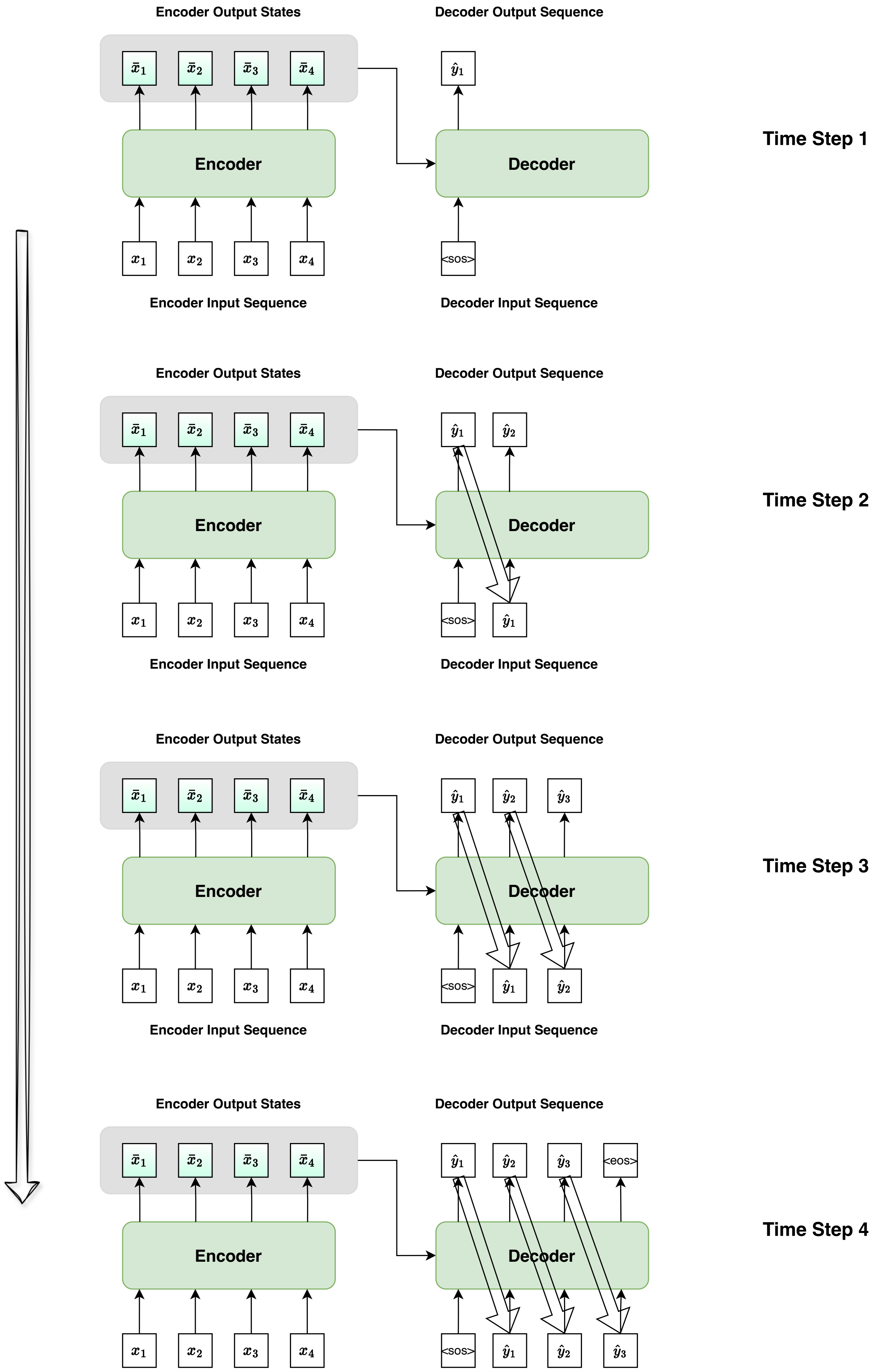
After training the encoder-decoder model, one shall use it for inference by providing the model with just the source sequence $[x_1, x_2, x_3, x_4]$. Now we must put the decoder in the truly auto-regressive mode. To do so, the decoder must work in a step-by-step fashion, by conditioning the prediction for time step $T+1$ on the predicted tokens from $t = 1, 2, \cdots, T$ as:

```
enc_out = Encoder([x_1,..., x_H])

y_hat = [sos]

While the last token of y_hat is not eos:

    y_hat_i =  Decoder(y_hat, enc_out)

    Append y_hat_i to the end of y_hat

return y_hat
```

which is depicted by the following figure.

In [26]:
```python
from IPython.display import SVG
SVG("img/encoder_decoder_inference.SVG")
```

Out[26]:


Encoder Output States
Decoder Output Sequence
$\bar{x}_1$ $\bar{x}_2$ $\bar{x}_3$ $\bar{x}_4$
$\hat{y}_1$ $\hat{y}_2$ $\hat{y}_3$ <eos>
Encoder
Decoder
x_1 x_2 x_3 x_4
<sos>
Encoder Input Sequence
Decoder Input Sequence
Time Step 1
Time Step 2
Time Step 3
Time Step 4

Encoder Input Sequence **Decoder Input Sequence**

To complete the extra credit, you will need to complete the missing code in three functions.

The first function is `def forward_one_step_ec(self, x, encoder_out = None, encoder_padding_mask = None, self_attn_padding_mask = None, self_attn_mask = None, cache = None)` in `class TransformerDecoderLayer(nn.Module)`, within `decoder.py`. Please read the function helper and the comments within.

In [29]:
```
help(TransformerDecoderLayer.forward_one_step_ec)
```

```
Help on function forward_one_step_ec in module decoder:

forward_one_step_ec(self, x, encoder_out=None, encoder_padding_mask=None, self
_attn_padding_mask=None, self_attn_mask=None, cache=None)
    Applies the self attention module + Dropout + Add & Norm operation, the en
coder-decoder attention + Dropout + Add & Norm operation (if self.encoder_attn
is not None), and the position-wise feedforward network + Dropout + Add & Norm
operation, but for just a single time step at the last time step. Note that La
yerNorm is applied after the self-attention operation, after the encoder-decod
er attention operation and another time after the ffn modules, similar to the
original Transformer implementation.

    Input:
        x (torch.Tensor) - input tensor of size B x T_d x embedding_dim from t
he decoder input or the previous encoder layer, where T_d is the decoder's tem
poral dimension; serves as input to the TransformerDecoderLayer's self attenti
on mechanism. You need to correctly slice x in the function below so that it i
s only calculating a one-step (one frame in length in the temporal dimension)
decoder output of the last time step.

        encoder_out (None/torch.Tensor) - If it is not None, then it is the ou
tput from the TransformerEncoder as a tensor of size B x T_e x embedding_dim,
where T_e is the encoder's temporal dimension; serves as part of the input to
the TransformerDecoderLayer's self attention mechanism (hint: which part?).

        encoder_padding_mask (None/torch.Tensor) - If it is not None, then it
is a torch.IntTensor/torch.LongTensor of size B x T_e, where for each encoder_
padding_mask[b] for the b-th source in the batched tensor encoder_out[b], the
non-zero positions will be ignored as they represent the padded region during
batchify operation in the dataloader (i.e., disallowed for attention) while th
e zero positions will be allowed for attention as they are within the length o
f the original sequence

        self_attn_padding_mask (None/torch.Tensor) - If it is not None, then i
t is a torch.IntTensor/torch.LongTensor of size B x T_d, where for each self_a
ttn_padding_mask[b] for the b-th source in the batched tensor x[b], the non-ze
ro positions will be ignored as they represent the padded region during batchi
fy operation in the dataloader (i.e., disallowed for attention) while the zero
positions will be allowed for attention as they are within the length of the o
riginal sequence. If it is not None, then you need to correctly slice it in th
e function below so that it is corresponds to the self_attn_padding_mask for c
alculating a one-step (one frame in length in the temporal dimension) decoder
output of the last time step.

        self_attn_mask (None/torch.Tensor) - If it is not None, then it is a t
orch.IntTensor/torch.LongTensor of size 1 x T_d x T_d or B x T_d x T_d. It is
used for decoder self-attention to enforce auto-regressive property during par
allel training; suppose the maximum length of a batch is 5, then the attention
_mask for any input in the batch will look like this for each input of the bat
ch.
        0 1 1 1 1
        0 0 1 1 1
        0 0 0 1 1
        0 0 0 0 1
        0 0 0 0 0
        The non-zero positions will be ignored and disallowed for attention wh
ile the zero positions will be allowed for attention. If it is not None, then
you need to correctly slice it in the function below so that it is corresponds
to the self_attn_padding_mask for calculating a one-step (one frame in length
in the temporal dimension) decoder output of the last time step.
```

```
        cache (torch.Tensor) - the output from this decoder layer previously c
omputed up until the previous time step before the last; hence it is of size B
x (T_d-1) x embedding_dim. It is to be concatenated with the single time-step
output calculated in this function before being returned


    Returns:
        x (torch.Tensor) - Output tensor B x T_d x embedding_dim, which is a c
oncatenation of cache (previously computed up until the previous time step bef
ore the last) and the newly computed one-step decoder output for the last time
step.
```

It is very similar to the `forward(self, x, encoder_out=None, encoder_padding_mask=None, self_attn_padding_mask=None, self_attn_mask=None)` in `class TransformerDecoderLayer(nn.Module)`, except for a few things:

1. While `x` is still an input tensor of size (B, T_d, embedding_dim), when calculating the decoder self-attention, you need to slice the input `x` and the input masks so that the last frame `ag_x` of shape (B , 1 ,embedding_dim) shall attend to all temporal dimensions of `x`, and the output of decoder self-attention, encoder-decoder attention, and position-wise feedforward network are all of the shape (B , 1 ,embedding_dim).
2. It has an extra input argument called `cache`. This is the decoder layer output for the current decoder layer computed until and including the previous time step. Hence, the temporal dimension is one less than the temporal dimension of the decoder input argument `x`. Once you have computed the layer output of the current time step, you need to concatenate your computed one-frame-length output of size (B , 1 ,embedding_dim) to the temporal dimension of `cache`, and return it as the return value.

The second function you need to write is `def forward_one_step_ec(self, x, decoder_padding_mask = None, decoder_attention_mask = None, encoder_out = None, encoder_padding_mask = None, cache = None)` in `class TransformerDecoder(nn.Module)`, within `decoder.py`. Please read the function helper and the comments within.

In [38]:
```
import decoder
import importlib
importlib.reload(decoder)
help(decoder.TransformerDecoder.forward_one_step_ec)
```

```
Help on function forward_one_step_ec in module decoder:

forward_one_step_ec(self, x, decoder_padding_mask=None, decoder_attention_mask
=None, encoder_out=None, encoder_padding_mask=None, cache=None)
    Forward one step.

    Input:
        x (torch.Tensor) - input tensor of size B x T_d x embedding_dim; input
to the TransformerDecoderLayer's self attention mechanism

        decoder_padding_mask (None/torch.Tensor) - If it is not None, then it
is a torch.IntTensor/torch.LongTensor of size B x T_d, where for each decoder_
padding_mask[b] for the b-th source in the batched tensor x[b], the non-zero p
ositions will be ignored as they represent the padded region during batchify o
peration in the dataloader (i.e., disallowed for attention) while the zero pos
itions will be allowed for attention as they are within the length of the orig
inal sequence

        decoder_attention_mask (None/torch.Tensor) - If it is not None, then i
t is a torch.IntTensor/torch.LongTensor of size 1 x T_d x T_d or B x T_d x T_
d. It is used for decoder self-attention to enforce auto-regressive property d
uring parallel training; suppose the maximum length of a batch is 5, then the
attention_mask for any input in the batch will look like this for each input o
f the batch.
        0 1 1 1 1
        0 0 1 1 1
        0 0 0 1 1
        0 0 0 0 1
        0 0 0 0 0
        The non-zero positions will be ignored and disallowed for attention wh
ile the zero positions will be allowed for attention.

        encoder_out (None/torch.Tensor) - If it is not None, then it is the ou
tput from the TransformerEncoder as a tensor of size B x T_e x embedding_dim,
where T_e is the encoder's temporal dimension; serves as part of the input to
the TransformerDecoderLayer's self attention mechanism (hint: which part?).

        encoder_padding_mask (None/torch.Tensor) - If it is not None, then it
is a torch.IntTensor/torch.LongTensor of size B x T_e, where for each encoder_
padding_mask[b] for the b-th source in the batch, the non-zero positions will
be ignored as they represent the padded region during batchify operation in th
e dataloader (i.e., disallowed for attention) while the zero positions will be
allowed for attention as they are within the length of the original sequence

        cache (None/List[torch.Tensor]) -  If it is not None, then it is a lis
t of cache tensors of each decoder layer calculated until and including the pr
evious time step; hence, if it is not None, then each tensor in the list is of
size B x (T_d-1) x embedding_dim; the list length is equal to len(self.layer
s), or the number of decoder layers.

    Output:
        y (torch.Tensor) -  Output tensor from the Transformer decoder consist
ing of a single time step, of size B x 1 x embedding_dim, if output layer is N
one, or of size B x 1 x output_layer_size, if there is an output layer.

        new_cache (List[torch.Tensor]) -  List of cache tensors of each decode
r layer for use by the auto-regressive decoding of the next time step; each te
nsor is of size B x T_d x embedding_dim; the list length is equal to len(self.
layers), or the number of decoder layers.
```

It is very similar to `forward(self, x, decoder_padding_mask = None, decoder_attention_mask = None, encoder_out = None, encoder_padding_mask = None)` in `class TransformerDecoder(nn.Module)`, except for a few things:

1. Instead of calling into the `forward` function of `TransformerDecoderLayer`, you need to call into the `forward_one_step_ec` that you just completed for `TransformerDecoderLayer`.
2. The output of this function is a tuple `(y, new_cache)`. `y` is a single output frame in the temporal dimension. To correctly return `new_cache,` you need to store a list of layer outputs of (B, T_d, embedding_dim) as returned by each decoder layer separately so that this `new_cache` can be used by the function caller (immediately described below) for auto-regressive decoding the next time step (and, of course, the `new_cache` returned by this next call into `forward_one_step_ec` for the next time step would be (B, T_d + 1, embedding_dim))

The last function you need to complete is `def inference(self, src, src_lengths, max_output_length)` in `class Transformer(nn.Module)`, within `transformer.py`. Most of the function has been completed for you. The only things you need to figure out is to initialize `tgt`, the starting decoder input sequence, to extend your decoder predictions, and when to break out of the decoding loop. We assume that every output sequence starts with `self.sos` and end with `self.eos`. Please refer to the figure and the pseudo-code for auto-regressive inference at the start of this section.

In [39]:
```
help(Transformer.inference)
```

```
Help on function inference in module transformer:

inference(self, src, src_lengths, max_output_length)
    Applies the entire Transformer encoder-decoder to src and target, possibly
as used during inference to auto-regressively obtain the next token; each sequ
ence in src has been padded to the max(src_lengths)
    Input:
        src (torch.Tensor) - Encoder's input tensor of size B x T_e x d_model

        src_lengths (torch.Tensor) - A 1D iterable of Long/Int of length B, wh
ere the b-th length in src_lengths corresponds to the actual length of src[b]
(beyond that is the pre-padded region); T_e = max(src_lengths)


    Output:
        decoded_list (List(torch.Tensor) - a list of auto-regressively obtaine
d decoder output token predictions; the b-th item of the decoded_list should b
e the output from src[b], and each of the sequence predictions in decoded_list
is of a possibly different length.

        decoder_layer_cache_list (List(List(torch.Tensor))) - a list of decode
r_layer_cache; the b-th item of the decoded_layer_cache_list should be the dec
oder_layer_cache for the src[b], which itself is a list of torch.Tensor, as re
turned by self.decoder.forward_one_step_ec (see the function definition there
for more details) when the auto-regressive inference ends for src[b].
```

If you believe you have implemented everything in this section correctly, you can run `python.grade.py` to see if you have passed the test related to the extra credit auto-regressive inference implementation, assuming ALL your previous tests have passed. We have defined two tests that you should have passed: `test_decoder_inference_outputs_extra_credit`, which initializes a `Transformer` object, loads the model weights from a de-en neural machine translation checkpoint `trained_de_en_state_dict.pt`, and invokes the `inference` function on some German sentences (that are converted to discrete index sequences), which auto-regressively decodes the English translation (that are in the form of discrete index sequences). We take your `decoded_list` returned by `inference` to check against our decoded results pre-generated by our implementation. This test will also throw an error if the normalized edit distance, or error rate computed against ground-truth English translations, does not match ours, which indicates some major bugs. The second test, `test_decoder_inference_cache_extra_credit,` works similarly, except that we are checking the `decoder_layer_cache_list` returned by `inference` function, which is a more careful examination of whether your auto-regressive inference has been implemented correctly.

Note: if you are getting a very small error that causes you to fail the test, please double-check that you have the correct torch version installed. Our outputs on the visible set are pre-generated using `Python 3.10` and `torch== 2.0.1`, so at the very least you need to make sure that you are using `torch==2.0.1` for this. It has been known that newer or older PyTorch versions may have slightly different implementations of the same internal module, and result in slightly different computed results. If in doubt, you can also submit to

GradeScope for testing. The auto-grader on GradeScope will NOT have this issue, as the solutions will be generated during the submission with the same platform and package versions as your implementation will use, but your code will be tested on the hidden set instead.

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In [41]: !python grade.py
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..........
----------------------------------------------------------------------
Ran 10 tests in 3.391s

OK
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