Problem 1

(a)

Substituting $\mathbf{h}_1 = \mathbf{W}_x\mathbf{x}_1$:

$$\mathbf{h}_2 = \mathbf{W}_h\mathbf{h}_1 + \mathbf{W}_x\mathbf{x}_2$$

$$\mathbf{h}_2 = \mathbf{W}_h\mathbf{W}_x\mathbf{x}_1 + \mathbf{W}_x\mathbf{x}_2$$

Substituting $\mathbf{h}_2$:

$$\mathbf{y}_2 = \phi_y(\mathbf{W}_y\mathbf{h}_2)$$

$$\mathbf{y}_2 = \phi_y(\mathbf{W}_y\mathbf{W}_h\mathbf{W}_x\mathbf{x}_1 + \mathbf{W}_y\mathbf{W}_x\mathbf{x}_2)$$

(b)

Substituting $\mathbf{h}_2 = \mathbf{W}_h\mathbf{W}_x\mathbf{x}_1 + \mathbf{W}_x\mathbf{x}_2$:

$$\mathbf{h}_3 = \mathbf{W}_h\mathbf{h}_2 + \mathbf{W}_x\mathbf{x}_3$$

$$\mathbf{h}_3 = \mathbf{W}_h(\mathbf{W}_h\mathbf{W}_x\mathbf{x}_1 + \mathbf{W}_x\mathbf{x}_2) + \mathbf{W}_x\mathbf{x}_3$$

$$\mathbf{h}_3 = \mathbf{W}_h^2\mathbf{W}_x\mathbf{x}_1 + \mathbf{W}_h\mathbf{W}_x\mathbf{x}_2 + \mathbf{W}_x\mathbf{x}_3$$

substituting $\mathbf{h}_3$:

$$\mathbf{y}_3 = \phi_y(\mathbf{W}_y\mathbf{h}_3)$$

$$\mathbf{y}_3 = \phi_y(\mathbf{W}_y\mathbf{W}_h^2\mathbf{W}_x\mathbf{x}_1 + \mathbf{W}_y\mathbf{W}_h\mathbf{W}_x\mathbf{x}_2 + \mathbf{W}_y\mathbf{W}_x\mathbf{x}_3)$$

(C)

$$\mathbf{h}_T = \mathbf{W}_h \mathbf{h}_{T-1} + \mathbf{W}_x \mathbf{x}_T$$

By recursively substituting $\mathbf{h}_{T-1}, \mathbf{h}_{T-2}, \ldots, \mathbf{h}_1$, we get:

$$\mathbf{h}_T = \mathbf{W}_h^{T-1} \mathbf{W}_x \mathbf{x}_1 + \mathbf{W}_h^{T-2} \mathbf{W}_x \mathbf{x}_2 + \cdots + \mathbf{W}_h \mathbf{W}_x \mathbf{x}_{T-1} + \mathbf{W}_x \mathbf{x}_T$$

$$\mathbf{h}_T = \sum_{i=1}^{T} \mathbf{W}_h^{T-i} \mathbf{W}_x \mathbf{x}_i$$

$$\mathbf{y}_T = \phi_y \left(\mathbf{W}_y \sum_{i=1}^{T} \mathbf{W}_h^{T-i} \mathbf{W}_x \mathbf{x}_i \right)$$

(d)

In an RNN, the contribution of the first input $\mathbf{x}_1$ to the hidden state $\mathbf{h}_T$ and the output $\mathbf{y}_T$ is given by:

$$\mathbf{h}_T = \sum_{i=1}^{T} \mathbf{W}_h^{T-i} \mathbf{W}_x \mathbf{x}_i$$

For the first input $\mathbf{x}_1$, its contribution to $\mathbf{h}_T$ is:

$$\mathbf{W}_h^{T-1} \mathbf{W}_x \mathbf{x}_1$$

If we decompose the matrix $\mathbf{W}_h$ using its eigenvalues and eigenvectors, we have:

$$\mathbf{W}_h = \mathbf{P} \mathbf{\Lambda} \mathbf{P}^{-1}$$

where $\mathbf{\Lambda}$ is the diagonal matrix containing the eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ of $\mathbf{W}_h$. Hence, the expression for $\mathbf{W}_h^{T-1}$ becomes:

$$\mathbf{W}_h^{T-1} = \mathbf{P} \mathbf{\Lambda}^{T-1} \mathbf{P}^{-1}$$

In $\mathbf{\Lambda}^{T-1}$, the eigenvalues are raised to the power of $T-1$, i.e.,

$$\mathbf{\Lambda}^{T-1} = \operatorname{diag}(\lambda_1^{T-1}, \lambda_2^{T-1}, \ldots, \lambda_n^{T-1})$$

If the eigenvalues λ_i of $\mathbf{W}_h$ are less than 1 (which is often the case for neural network parameters), then as T increases, λ_i^{T-1} tends to 0. Thus, the contribution of the first input $\mathbf{x}_1$ to $\mathbf{h}_T$ and $\mathbf{y}_T$ diminishes exponentially with T.

(e)

RNN

$$\mathbf{h}_T = \mathbf{W}_h \mathbf{h}_{T-1} + \mathbf{W}_x \mathbf{x}_T$$

At each timestep, the computation only involves $\mathbf{h}_{T-1}$ and $\mathbf{x}_T$, takes $O(1)$

There are T steps in total, so the computation cost is linear to $T : O(T)$

Self-attention Layer

Pair-wise inner product takes the dot product between query and key -- $O(T^2 d)$

Softmax over the square matrix -- $O(T^2)$

Matrix Multiplication of $\mathbf{A}$ and $\mathbf{V}$ -- $O(T^2)$

The total cost is $O(T^2)$

RNN VS Transformer

With sufficient parallel hardware, a forward pass on a transformer will generally be faster than on an RNN. Although transformers have a higher memory and time complexity than RNN, but transformers can be fully parallelized across all tokens, order information is maintained by positional encoding while RNNs must process sequentially, waiting for each hidden state to be calculated before moving to the next. This makes transformers more efficient on parallel hardware.

(f)

If memory constraints are manageable, I would choose a transformer, as RNNs suffer from vanishing gradient problems and cannot be parallelized effectively. Transformers handle long-range dependencies better and can fully utilize parallel hardware for long sequences.

Problem 2

(d)

To adapt transformers for continuous inputs like audio and images, the data can be divided into patches or frames, which act as "tokens." These tokens are flattened and projected into embeddings, with positional encodings added to retain order. This allows transformers to capture both local and global relationships through self-attention, similar to how they handle discrete token sequences.

Problem 3

(b)

To handle arbitrarily long inputs, we can use sinusoidal positional encodings such as SIREN instead of learned embeddings. Sinusoidal functions are periodic and continuous, allowing them to generate unique positional values for any token position without needing a fixed embedding table. This ensures that the model can encode positions for sequences of any length, as the functions can always compute a position, avoiding the limitations of predefined positional embeddings.

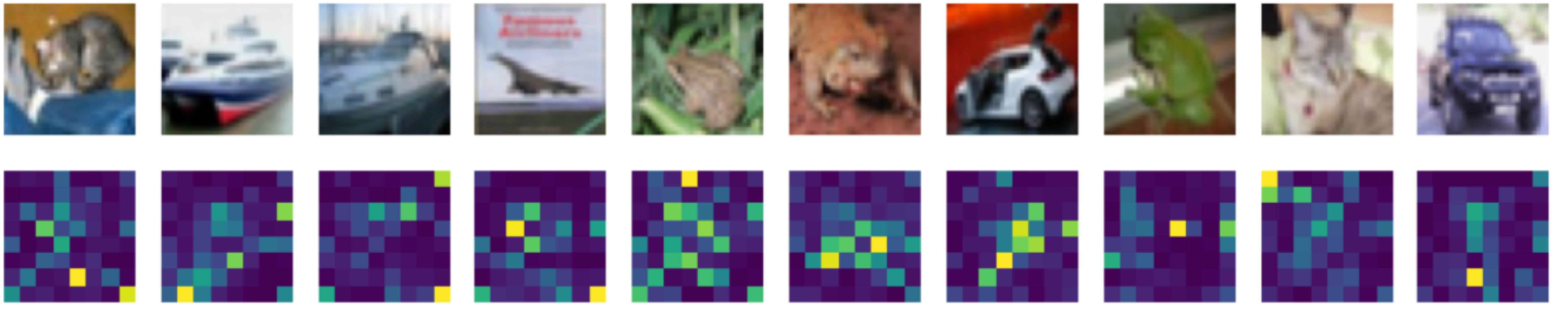
(c)

Train Epoch: 9, Loss: 0.4039117162513733, Acc: 0.875360000038147

Val Epoch: 9, Loss: 1.3148666219711305, Acc: 0.5961

(d)

The Attention Heatmaps



Observation

The attention heatmaps are visualizing how the class token (averaged over all heads and layers) is attending to different patches of the image. Since the class token is used to aggregate information for classification, the highlighted patches in the heatmap indicate the regions the model is focusing on to make its decision.

In the heatmaps, attention is concentrated on specific patches for most images, meaning that the model focuses only on certain parts of the image for classification. In the second image of a ship, the highlighted area in the attention heatmap roughly correspond to the main body of the ship.This suggests the model is learning to focus on meaningful parts of the image for classification.

The attention patterns vary across images, meaning the model adjusts its attention depending on the content of the image. For instance, images with larger or more complex subjects might have a more spread-out attention, while images with smaller or simpler subjects may have a more concentrated attention.

(e)

- CNNs, with their inductive biases for translation invariance, perform well on small datasets by efficiently learning local patterns with fewer data. In contrast, ViTs rely on global attention without these biases, making them more flexible but data-hungry. ViTs typically require larger datasets or extensive pretraining to learn meaningful patterns due to their lack of built-in biases.
- CNNs inherently capture spatial hierarchies through convolutional layers, allowing them to handle varying image sizes by down-sampling and preserving local patterns. ViTs, on the other hand, depend on fixed patch sizes and positional encodings, which makes them less adaptable to images of different sizes unless explicitly designed to adjust positional encodings like using periodical functions as discussed in former question.

Problem 4

(e)

Because autoregressive generation is sequential, predicting one token at a time where each step depends on the previous one, making it hard to parallelize. In contrast, training processes all tokens in parallel, allowing for faster computation by fully utilizing the GPU.

(f)

In the early epochs, the generated text tends to be repetitive, with outputs like "I, I, I, I" due to the model's initial reliance on simple patterns. As training progresses, the model learns better language structure, reducing repetition and producing more meaningful, contextually relevant sentences.

(g)

```
<START> KING RICHARD III : Why , I have a man ? I have not a word ? what is a man ? I will I am a man ? I am I will be a man . I am a man ? What , I will not be a man
```

(h)

Greedy decoding always selects the token with the highest probability at each step, which can lead to degenerate sequences, particularly when the highest-probability tokens are repeated frequently.Nucleus sampling select tokens from a dynamically sized subset whose cumulative probability exceeds a threshold. This allows the model to consider more diverse but still likely tokens, breaking the repetitive patterns. The trade-off is that it introduces some randomness which may result in lower-quality outputs. Besides it can be slower compared to greedy decoding.

(i)

KV caching technique speeds up generation by storing previously computed key-value pairs, so the model doesn't have to recompute attention for all tokens each time a new token is generated. Instead, it only computes attention for the new token, reducing the computational complexity from quadratic to linear as sequences grow.

```python
import torch
import torch.nn as nn
from typing import Tuple, Union, Optional, List
import torchvision
import torchvision.transforms as transforms
import matplotlib.pyplot as plt
import numpy as np


# a utility for calculating running average
class AverageMeter:
    def __init__(self):
        self.num = 0
        self.tot = 0

    def update(self, val: float, sz: float):
        self.num += val * sz
        self.tot += sz

    def calculate(self) -> float:
        return self.num / self.tot
```

Problem 2: Implement a Transformer

Part 2.A

```python
class AttentionHead(nn.Module):
    def __init__(self, dim: int, n_hidden: int):
        # dim: the dimension of the input
        # n_hidden: the dimension of the keys, queries, and values

        super().__init__()

        self.W_K = nn.Linear(dim, n_hidden)  # W_K weight matrix
        self.W_Q = nn.Linear(dim, n_hidden)  # W_Q weight matrix
        self.W_V = nn.Linear(dim, n_hidden)  # W_V weight matrix
        self.n_hidden = n_hidden

    def forward(
        self, x: torch.Tensor, attn_mask: Optional[torch.Tensor]
    ) -> Tuple[torch.Tensor, torch.Tensor]:
        # x                the inputs. shape: (B x T x dim)
        # attn_mask        an attention mask. If None, ignore. If not None, then mask[b, i, j]
        #                  contains 1 if (in batch b) token i should attend on token j and 0
        #                  otherwise. shape: (B x T x T)
        #
        # Outputs:
        # attn_output      the output of performing self-attention on x. shape: (Batch x Num_tokens x n_hidden)
        # alpha            the attention weights (after softmax). shape: (B x T x T)
        #

        out, alpha = None, None
        # TODO: Compute self attention on x.
        #       (1) First project x to the query Q, key K, value V.
        #       (2) Then compute the attention weights alpha as:
        #                  alpha = softmax(QK^T/sqrt(n_hidden))
        #           Make sure to take into account attn_mask such that token i does not attend on token
        #           j if attn_mask[b, i, j] == 0. (Hint, in such a case, what value should you set the weight
        #           to before the softmax so that after the softmax the value is 0?)
        #       (3) The output is a linear combination of the values (weighted by the alphas):
        #                  out = alpha V
        #       (4) return the output and the alpha after the softmax

        # ======= Answer START ========

        query = self.W_Q(x)
        key = self.W_K(x)
        value = self.W_V(x)
        scores = torch.matmul(query, key.transpose(-2, -1)) / self.n_hidden**0.5
        if attn_mask is not None:
            attn_mask = attn_mask.to(scores.device)
```

```
            scores = scores.masked_fill(attn_mask == 0, float("-inf"))
        alpha = torch.softmax(scores, dim=-1)
        attn_output = torch.matmul(alpha, value)

        # ======= Answer  END ========

        return attn_output, alpha
```

Part 2.B

```
class MultiHeadedAttention(nn.Module):
    def __init__(self, dim: int, n_hidden: int, num_heads: int):
        # dim: the dimension of the input
        # n_hidden: the hidden dimenstion for the attention layer
        # num_heads: the number of attention heads
        super().__init__()

        # TODO: set up your parameters for multi-head attention. You should initialize
        #       num_heads attention heads (see nn.ModuleList) as well as a linear layer
        #       that projects the concatenated outputs of each head into dim
        #       (what size should this linear layer be?)

        # ======= Answer START ========
        self.num_heads = num_heads
        self.n_hidden = n_hidden
        self.attn_heads = nn.ModuleList(
            [AttentionHead(dim=dim, n_hidden=n_hidden) for _ in range(num_heads)]
        )
        self.project_layer = nn.Linear(num_heads * n_hidden, dim)

        # ======= Answer  END ========

    def forward(
        self, x: torch.Tensor, attn_mask: Optional[torch.Tensor]
    ) -> Tuple[torch.Tensor, torch.Tensor]:
        # x                the inputs. shape: (B x T x dim)
        # attn_mask        an attention mask. If None, ignore. If not None, then mask[b, i, j]
        #                  contains 1 if (in batch b) token i should attend on token j and 0
        #                  otherwise. shape: (B x T x T)
        #
        # Outputs:
        # attn_output      the output of performing multi-headed self-attention on x.
        #                  shape: (B x T x dim)
        # attn_alphas      the attention weights of each of the attention heads.
        #                  shape: (B x Num_heads x T x T)

        attn_output, attn_alphas = None, None

        # TODO: Compute multi-headed attention. Loop through each of your attention heads
        #       and collect the outputs. Concatenate them together along the hidden dimension,
        #       and then project them back into the output dimension (dim). Return both
        #       the final attention outputs as well as the alphas from each head.

        # ======= Answer START ========

        outputs = []
        alphas = []
        for attn_layer in self.attn_heads:
            output, alpha = attn_layer(x=x, attn_mask=attn_mask)
            outputs.append(output)  # output (B, T, n_hidden)
            alphas.append(alpha)  # alpha (B, T, T)

        attn_output = torch.cat(outputs, dim=-1)  # (B,T,Num_heads*n_hidden)
        attn_alphas = torch.stack(alphas, dim=1)  # (B,Num_heads,T,T)
        attn_output = self.project_layer(attn_output)  # (B,Num_heads,dim)

        # ======= Answer END ========
        return attn_output, attn_alphas
```

Part 2.C

```
# these are already implemented for you!


class FFN(nn.Module):
    def __init__(self, dim: int, n_hidden: int):

        # dim       the dimension of the input

        # n_hidden  the width of the linear layer

        super().__init__()

        self.net = nn.Sequential(
            nn.LayerNorm(dim),
            nn.Linear(dim, n_hidden),
            nn.GELU(),
            nn.Linear(n_hidden, dim),
        )

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

        # x         the input. shape: (B x T x dim)

        # Outputs:

        # out       the output of the feed-forward network: (B x T x dim)
        return self.net(x)


class AttentionResidual(nn.Module):
    def __init__(self, dim: int, attn_dim: int, mlp_dim: int, num_heads: int):

        # dim       the dimension of the input

        # attn_dim  the hidden dimension of the attention layer

        # mlp_dim   the hidden layer of the FFN

        # num_heads the number of heads in the attention layer
        super().__init__()

        self.attn = MultiHeadedAttention(dim, attn_dim, num_heads)

        self.ffn = FFN(dim, mlp_dim)

    def forward(
        self, x: torch.Tensor, attn_mask: torch.Tensor
    ) -> Tuple[torch.Tensor, torch.Tensor]:

        # x                the inputs. shape: (B x T x dim)

        # attn_mask        an attention mask. If None, ignore. If not None, then mask[b, i, j]

        #                  contains 1 if (in batch b) token i should attend on token j and 0

        #                  otherwise. shape: (B x T x T)

        #

        # Outputs:

        # attn_output      shape: (B x T x dim)

        # attn_alphas      the attention weights of each of the attention heads.

        #                  shape: (B x Num_heads x T x T)

        attn_out, alphas = self.attn(x=x, attn_mask=attn_mask)

        x = attn_out + x

        x = self.ffn(x) + x
        return x, alphas

class Transformer(nn.Module):
    def __init__(
```

```
        self, dim: int, attn_dim: int, mlp_dim: int, num_heads: int, num_layers: int
    ):
        # dim       the dimension of the input
        # attn_dim  the hidden dimension of the attention layer
        # mlp_dim   the hidden layer of the FFN
        # num_heads the number of heads in the attention layer
        # num_layers the number of attention layers.
        super().__init__()

        # TODO: set up the parameters for the transformer!
        #       You should set up num_layers of AttentionResiduals
        #       nn.ModuleList will be helpful here.

        # ======= Answer START ========
        self.attn_net = nn.ModuleList(
            [
                AttentionResidual(
                    dim=dim, attn_dim=attn_dim, mlp_dim=mlp_dim, num_heads=num_heads
                )
                for _ in range(num_layers)
            ]
        )

        # ======= Answer END ========

    def forward(
        self, x: torch.Tensor, attn_mask: torch.Tensor, return_attn=False
    ) -> Tuple[torch.Tensor, Optional[torch.Tensor]]:
        # x                the inputs. shape: (B x T x dim)
        # attn_mask        an attention mask. Pass this to each of the AttentionResidual layers!
        #                  shape: (B x T x T)
        #
        # Outputs:
        # attn_output      shape: (B x T x dim)
        # attn_alphas      If return_attn is False, return None. Otherwise return the attention weights
        #                  of each of each of the attention heads for each of the layers.
        #                  shape: (B x Num_layers x Num_heads x T x T)

        output, collected_attns = None, None

        # TODO: Implement the transformer forward pass! Pass the input successively through each of the
        # AttentionResidual layers. If return_attn is True, collect the alphas along the way.

        # ======= Answer START ========
        attn_alphas = []
        for attn_res in self.attn_net:
            x, alphas = attn_res(x=x, attn_mask=attn_mask)
            attn_alphas.append(alphas)
        output = x
        if return_attn:
            collected_attns = torch.stack(attn_alphas, dim=1)

        # ======= Answer END ========

        return output, collected_attns
```

Test your transformer implementation here

```
def perform_transformer_test_cases():
    num_tokens = 100
    batch_size = 10
    dim = 64
    num_layers = 4
    num_heads = 2
    dummy_model = Transformer(
        dim=dim, attn_dim=32, mlp_dim=dim, num_heads=num_heads, num_layers=num_layers
    ).cuda()

    inp = torch.randn(batch_size, num_tokens, dim).cuda()

    # test case 1 regular forward pass
    print("Test Case 1")
    with torch.no_grad():
        output, alpha = dummy_model(inp, attn_mask=None)
        assert alpha is None
```

```python
        assert output.shape == (
            batch_size,
            num_tokens,
            dim,
        ), f"wrong output shape {output.shape}"

    # test case 2 collect attentions
    print("Test Case 2")
    with torch.no_grad():
        output, alpha = dummy_model(inp, attn_mask=None, return_attn=True)
        assert output.shape == (
            batch_size,
            num_tokens,
            dim,
        ), f"wrong output shape {output.shape}"
        assert alpha.shape == (
            batch_size,
            num_layers,
            num_heads,
            num_tokens,
            num_tokens,
        ), f"wrong alpha shape {alpha.shape}"

    print("Test Case 3")
    # test case 3 with attention mask
    attn_mask = torch.zeros(batch_size, num_tokens, num_tokens).cuda()
    attn_mask[:, torch.arange(num_tokens), torch.arange(num_tokens)] = 1
    attn_mask[:, torch.arange(num_tokens)[1:], torch.arange(num_tokens)[:-1]] = 1
    with torch.no_grad():
        output, alpha = dummy_model(inp, attn_mask=attn_mask, return_attn=True)
        print("Attention mask pattern", attn_mask[0])
        print("Alpha pattern", alpha[0, 0, 0])
        assert torch.all(alpha.permute(1, 2, 0, 3, 4)[:, :, attn_mask == 0] == 0).item()

    print("Test Case 4")
    # test case 4 creates a causal mask where each token can only attend to previous tokens and itself
    causal_mask = (
        torch.tril(torch.ones(num_tokens, num_tokens))
        .unsqueeze(0)
        .repeat(batch_size, 1, 1)
    )  # Shape: (B, T, T)

    with torch.no_grad():
        output, alpha = dummy_model(inp, attn_mask=causal_mask, return_attn=True)
        # Verify the causal mask
        for b in range(batch_size):
            for l in range(num_layers):
                for h in range(num_heads):
                    attn_weights = alpha[b, l, h]  # Shape: (T, T)
                    # Positions where j > i should have zero attention weights
                    # We can create a boolean mask for j > i
                    future_mask = torch.triu(
                        torch.ones(num_tokens, num_tokens), diagonal=1
                    ).bool()  # Shape: (T, T)
                    # Extract attention weights for future positions
                    future_attn = attn_weights[future_mask]
                    # Assert that these weights are close to zero
                    assert torch.all(
                        future_attn < 1e-6
                    ), f"Causal mask violated in batch {b}, layer {l}, head {h}"


perform_transformer_test_cases()
```

```
Test Case 1
Test Case 2
Test Case 3
Attention mask pattern tensor([[1., 0., 0.,  ..., 0., 0., 0.],
        [1., 1., 0.,  ..., 0., 0., 0.],
        [0., 1., 1.,  ..., 0., 0., 0.],
        ...,
        [0., 0., 0.,  ..., 1., 0., 0.],
        [0., 0., 0.,  ..., 1., 1., 0.],
        [0., 0., 0.,  ..., 0., 1., 1.]], device='cuda:0')
Alpha pattern tensor([[1.0000, 0.0000, 0.0000,  ..., 0.0000, 0.0000, 0.0000],
        [0.5219, 0.4781, 0.0000,  ..., 0.0000, 0.0000, 0.0000],
        [0.0000, 0.6204, 0.3796,  ..., 0.0000, 0.0000, 0.0000],
        ...,
```

```
        [0.0000, 0.0000, 0.0000,  ..., 0.7375, 0.0000, 0.0000],
        [0.0000, 0.0000, 0.0000,  ..., 0.5805, 0.4195, 0.0000],
        [0.0000, 0.0000, 0.0000,  ..., 0.0000, 0.6439, 0.3561]],
       device='cuda:0')
Test Case 4
```

Problem 3: Vision Transformer

Part 3.A

```
class PatchEmbed(nn.Module):
    """Image to Patch Embedding"""

    def __init__(self, img_size: int, patch_size: int, nin: int, nout: int):
        # img_size       the width and height of the image. you can assume that
        #                the images will be square
        # patch_size     the width of each square patch. You can assume that
        #                img_size is divisible by patch_size
        # nin            the number of input channels
        # nout           the number of output channels

        super().__init__()
        assert img_size % patch_size == 0

        self.img_size = img_size
        self.num_patches = (img_size // patch_size) ** 2
        # TODO Set up parameters for the Patch Embedding
        # ======= Answer START ========
        self.patch_size = patch_size
        self.conv2d = nn.Conv2d(
            in_channels=nin,
            out_channels=nout,
            kernel_size=patch_size,
            stride=patch_size,
        )

        # ======= Answer END ========

    def forward(self, x: torch.Tensor):
        # x        the input image. shape: (B, nin, Height, Width)
        #
        # Output
        # out      the patch embeddings for the input. shape: (B, num_patches, nout)

        # TODO: Implement the patch embedding. You want to split up the image into
        # square patches of the given patch size. Then each patch_size x patch_size
        # square should be linearly projected into an embedding of size nout.
        #
        # Hint: Take a look at nn.Conv2d. How can this be used to perform the
        #       patch embedding?
        out = None

        # ======= Answer START ========
        x = self.conv2d(x)  # (B,nout,sqrt(num_patch),sqrt(num_patch))
        x = x.flatten(start_dim=2, end_dim=-1)  # (B,nout,num_patches,)
        out = x.transpose(1, 2)  # (B, num_patches, nout)

        # ======= Answer END ========

        return out
```

Part 3.B

```
class VisionTransformer(nn.Module):
    def __init__(
        self,
        n_channels: int,
        nout: int,
        img_size: int,
        patch_size: int,
        dim: int
```

```
        dim: int,
        attn_dim: int,
        mlp_dim: int,
        num_heads: int,
        num_layers: int,
    ):
        # n_channels       number of input image channels
        # nout             desired output dimension
        # img_size         width of the square image
        # patch_size       width of the square patch
        # dim              embedding dimension
        # attn_dim         the hidden dimension of the attention layer
        # mlp_dim          the hidden layer dimension of the FFN
        # num_heads        the number of heads in the attention layer
        # num_layers       the number of attention layers.
        super().__init__()
        self.patch_embed = PatchEmbed(
            img_size=img_size, patch_size=patch_size, nin=n_channels, nout=dim
        )  # out (B, num_patches, nout)
        self.pos_E = nn.Embedding(
            (img_size // patch_size) ** 2, dim
        )  # positional embedding matrix

        self.cls_token = nn.Parameter(torch.randn(1, 1, dim))  # learned class embedding
        self.transformer = Transformer(
            dim=dim,
            attn_dim=attn_dim,
            mlp_dim=mlp_dim,
            num_heads=num_heads,
            num_layers=num_layers,
        )

        self.head = nn.Sequential(nn.LayerNorm(dim), nn.Linear(dim, nout))

    def forward(
        self, img: torch.Tensor, return_attn=False
    ) -> Tuple[torch.Tensor, Optional[torch.Tensor]]:
        # img          the input image. shape: (B, nin, img_size, img_size)
        # return_attn  whether to return the attention alphas
        #
        # Outputs
        # out          the output of the vision transformer. shape: (B, nout)
        # alphas       the attention weights for all heads and layers. None if return_attn is False, otherwise
        #              shape: (B, num_layers, num_heads, num_patches + 1, num_patches + 1)

        # generate embeddings
        embs = self.patch_embed(img)  # patch embedding (B, num_patches, nout)
        B, T, _ = embs.shape
        pos_ids = torch.arange(T).expand(B, -1).to(embs.device)
        embs += self.pos_E(pos_ids)  # positional embedding

        cls_token = self.cls_token.expand(len(embs), -1, -1)  # (B,1,dim)
        x = torch.cat([cls_token, embs], dim=1)

        x, alphas = self.transformer(x, attn_mask=None, return_attn=return_attn)
        out = self.head(x)[:, 0]  # select cls_token
        return out, alphas
```

Part 3.C

```
# set up the dataset and dataloader

MEAN = [0.4914, 0.4822, 0.4465]
STD = [0.2470, 0.2435, 0.2616]
img_transform = transforms.Compose(
    [
        transforms.ToTensor(),
        transforms.Normalize(mean=MEAN, std=STD),
    ]
)
inv_transform = transforms.Compose(
    [
        transforms.Normalize(mean=[0.0, 0.0, 0.0], std=1 / np.array(STD)),
        transforms.Normalize(mean=-np.array(MEAN), std=[1.0, 1.0, 1.0]),
        transforms.ToPILImage(),
```

```
    ]
)


train_dataset = torchvision.datasets.CIFAR10(
    train=True, root="data", transform=img_transform, download=True
)
val_dataset = torchvision.datasets.CIFAR10(
    train=False, root="data", transform=img_transform
)
train_dataloader = torch.utils.data.DataLoader(
    train_dataset, batch_size=256, shuffle=True, num_workers=10
)
val_dataloader = torch.utils.data.DataLoader(
    val_dataset, batch_size=256, shuffle=False, num_workers=10
)
```

```
Downloading https://www.cs.toronto.edu/~kriz/cifar-10-python.tar.gz to data\cifar-10-python.tar.gz
100%|██████████| 170498071/170498071 [00:04<00:00, 35028052.55it/s]
Extracting data\cifar-10-python.tar.gz to data
```

```
# set up the model and optimizer

import torch.optim as optim

model = VisionTransformer(
    n_channels=3,
    nout=10,
    img_size=32,
    patch_size=4,
    dim=128,
    attn_dim=64,
    mlp_dim=128,
    num_heads=3,
    num_layers=6,
).cuda()

criterion = nn.CrossEntropyLoss()


NUM_EPOCHS = 10
optimizer = optim.AdamW(model.parameters(), lr=0.001)
scheduler = optim.lr_scheduler.CosineAnnealingLR(optimizer, T_max=NUM_EPOCHS)


# evaluate the model
def evaluate_cifar_model(model, criterion, val_loader):
    is_train = model.training
    model.eval()
    with torch.no_grad():
        loss_meter, acc_meter = AverageMeter(), AverageMeter()
        for img, labels in val_loader:
            # move all img, labels to device (cuda)
            img = img.cuda()
            labels = labels.cuda()
            outputs, _ = model(img)
            loss_meter.update(criterion(outputs, labels).item(), len(img))
            acc = (outputs.argmax(-1) == labels).float().mean().item()
            acc_meter.update(acc, len(img))
    model.train(is_train)
    return loss_meter.calculate(), acc_meter.calculate()


# Time Estimate: less than 5 minutes on T4 GPU
# train the model
import tqdm

for epoch in range(NUM_EPOCHS):  #
    loss_meter = AverageMeter()
    acc_meter = AverageMeter()
    for img, labels in tqdm.tqdm(train_dataloader):
        img, labels = img.cuda(), labels.cuda()

        optimizer.zero_grad()

        outputs, _ = model(img)
        loss = criterion(outputs, labels)
```

```
        loss_meter.update(loss.item(), len(img))
        acc = (outputs.argmax(-1) == labels).float().mean().item()
        acc_meter.update(acc, len(img))
        loss.backward()
        optimizer.step()
    scheduler.step()
    print(
        f"Train Epoch: {epoch}, Loss: {loss_meter.calculate()}, Acc: {acc_meter.calculate()}"
    )
    if epoch % 10 == 0:
        val_loss, val_acc = evaluate_cifar_model(model, criterion, val_dataloader)
        print(f"Val Epoch: {epoch}, Loss: {val_loss}, Acc: {val_acc}")

val_loss, val_acc = evaluate_cifar_model(model, criterion, val_dataloader)
print(f"Val Epoch: {epoch}, Loss: {val_loss}, Acc: {val_acc}")
print("Finished Training")
```

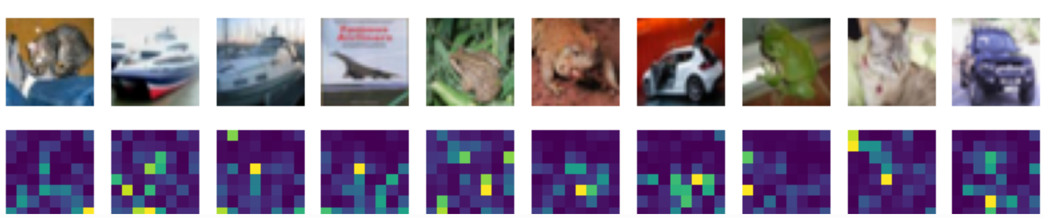
```
100%|██████████| 196/196 [00:35<00:00,  5.55it/s]
Train Epoch: 0, Loss: 1.6804874281692506, Acc: 0.38952
Val Epoch: 0, Loss: 1.5092397380828857, Acc: 0.4563
100%|██████████| 196/196 [00:29<00:00,  6.57it/s]
Train Epoch: 1, Loss: 1.3700932378387451, Acc: 0.5073200000381469
100%|██████████| 196/196 [00:44<00:00,  4.45it/s]
Train Epoch: 2, Loss: 1.2277209970474243, Acc: 0.55962
100%|██████████| 196/196 [00:29<00:00,  6.68it/s]
Train Epoch: 3, Loss: 1.116184849205017, Acc: 0.59924
100%|██████████| 196/196 [00:28<00:00,  6.76it/s]
Train Epoch: 4, Loss: 1.0049517052459718, Acc: 0.640800000038147
100%|██████████| 196/196 [00:29<00:00,  6.72it/s]
Train Epoch: 5, Loss: 0.8878362503242493, Acc: 0.6823200000190734
100%|██████████| 196/196 [00:29<00:00,  6.75it/s]
Train Epoch: 6, Loss: 0.7388031967544556, Acc: 0.7391800000572205
100%|██████████| 196/196 [00:28<00:00,  6.87it/s]
Train Epoch: 7, Loss: 0.594149854593277, Acc: 0.7941600000572204
100%|██████████| 196/196 [00:28<00:00,  6.90it/s]
Train Epoch: 8, Loss: 0.46669787870407103, Acc: 0.8454
100%|██████████| 196/196 [00:28<00:00,  6.93it/s]
Train Epoch: 9, Loss: 0.39107312546730044, Acc: 0.877840000038147
Val Epoch: 9, Loss: 1.3601046726226806, Acc: 0.5931
Finished Training
```

Part 3.D

```
for val_batch in val_dataloader:
    break

model.eval()
with torch.no_grad():
    img, labels = val_batch
    img = img.cuda()
    outputs, attns = model(img, return_attn=True)

fig, ax = plt.subplots(2, 10, figsize=(10, 2))
for i in range(10):
    flattened_attns = (
        attns.flatten(1, 2)[:, :, 0, 1:].mean(1).reshape(-1, 8, 8).cpu().numpy()
    )
    ax[0, i].imshow(inv_transform(img[i]))
    ax[1, i].imshow(flattened_attns[i])
    ax[0, i].axis(False)
    ax[1, i].axis(False)
```



Problem 4: Dialogue GPT

```
!pip install wget
```

```
import wget
import os

if not os.path.exists("input.txt"):
    wget.download(
        "https://raw.githubusercontent.com/karpathy/char-rnn/master/data/tinyshakespeare/input.txt"
    )
```

```
with open("input.txt", "r") as f:
    raw_text = f.read()
all_dialogues = raw_text.split("\n\n")
```

```
import nltk
from nltk.tokenize import word_tokenize

nltk.download("punkt", download_dir="nltk_data")
```

```
[nltk_data] Downloading package punkt to nltk_data...
[nltk_data]   Package punkt is already up-to-date!
True
```

```
nltk.data.path.append("./nltk_data")
```

Part 4.A

```
def tokenize(s):
    return word_tokenize(s)


class MyTokenizer:
    def __init__(self, raw_text: str):
        # raw_text     contains the text from which we will build our vocabulary

        self.start = "<START>"  # token that starts every example
        self.pad = "<PAD>"  # token used to pad examples to the same length
        self.unk = "<UNK>"  # token used if encountering a word not in our vocabulary

        vocab = np.unique(tokenize(raw_text))  # use nltk tokenizer
        vocab = np.concatenate([np.array([self.start, self.pad, self.unk]), vocab])

        self.vocab = vocab  # array of tokens in order
        self.tok_to_id = {w: i for i, w in enumerate(vocab)}  # mapping of token to ID
        self.vocab_size = len(self.vocab)  # size of vocabulary

    def encode(self, s: str) -> torch.Tensor:
        # s           input string
        #
        # Output
        # id_tensor   a tensor of token ids, starting with the start token.t

        id_tensor = None

        # TODO: tokenize the input using word_tokenize. Return a tensor
        # of the token ids, starting with the token id for the start token.
        # ============ ANSWER START ===========
        tokens = tokenize(s)
        token_ids = [self.tok_to_id[self.start]]
        token_ids += [
            self.tok_to_id.get(token, self.tok_to_id[self.unk]) for token in tokens
        ]
        id_tensor = torch.tensor(token_ids)

        # ============ ANSWER END =============

        return id_tensor

    def decode(self, toks: torch.Tensor) -> str:
        # toks         a list of token ids
        #
```

```
        # Output
        # decoded_str  the token ids decoded back into a string (join with a space)

        decoded_str = None

        # TODO: convert the token ids back to the actual corresponding words.
        # Join the tokens with a space and return the full string
        # ============ ANSWER START ===========
        tokens = [self.vocab[token_id] for token_id in toks]
        decoded_str = " ".join(tokens)

        # ============ ANSWER END =============

        return decoded_str

    def pad_examples(self, tok_list: List[torch.Tensor]) -> torch.Tensor:
        # Pads the tensors to the right with the pad token so that they are the same length.
        #
        # tok_list       a list of tensors containing token ids (maybe of different lengths)
        #
        # Output
        # padded_tokens  shape: (len(tok_list), max length within tok_list)
        return torch.nn.utils.rnn.pad_sequence(
            tok_list, batch_first=True, padding_value=self.tok_to_id[self.pad]
        )


tok = MyTokenizer(raw_text)


# tokenizer test cases
input_string = "KING RICHARD III:\nSay that I did all this for love of her."
enc = tok.encode(input_string)
print(enc)
dec = tok.decode(enc)
print(dec)
assert dec == "<START> KING RICHARD III : Say that I did all this for love of her ."
```

```
tensor([    0,  1593,  2182,  1481,   223,  2343, 12742,  1476,  5704,  3319,
        12795,  6848,  8727,  9608,  7655,   221])
<START> KING RICHARD III : Say that I did all this for love of her .
```

Part 4.B

```
class DialogueDataset:
    def __init__(self, tokenizer: MyTokenizer, lines: List[str], max_N: int):
        # tokenizer    an instance of MyTokenizer
        # lines        a list of strings. each element in an example in the dataset
        # max_N        the maximum number of tokens allowed per example. More than this will be truncated
        self.lines = lines
        self.tokenizer = tokenizer
        self.max_N = max_N

    def __len__(self) -> int:
        return len(self.lines)

    def __getitem__(self, idx: int) -> torch.Tensor:
        # returns the example at int encoded by the tokenizer
        # truncates the example if it is more than max_N tokens
        return self.tokenizer.encode(self.lines[idx])[: self.max_N]


def collate_fn(examples: List[torch.Tensor]):
    # examples        a batch of tensors containing token ids (maybe of different lengths)
    # Outputs a dictionary containing
    #   input_ids     a single tensor with all of the examples padded (from the right) to the max
    #                 length within the batch. shape:(B, max length within examples)
    #   input_mask    a tensor indicating which tokens are padding and should be ignored. 0 if padding
    #                 and 1 if not. shape: (B, max length within examples)
    new_input_ids = tok.pad_examples(examples)
    attn_mask = torch.ones(new_input_ids.shape)
    attn_mask[new_input_ids == tok.tok_to_id[tok.pad]] = 0
    return {"input_ids": tok.pad_examples(examples), "input_mask": attn_mask}
```

```
ds = DialogueDataset(tok, all_dialogues, max_N=200)
training_dl = torch.utils.data.DataLoader(ds, batch_size=64, collate_fn=collate_fn)
```

```
# take a look at an example of an element from the training dataloader
for batch in training_dl:
    print(batch)
    print(batch["input_ids"].shape)
    break
```

```
{'input_ids': tensor([[   0, 1151,  708,  ...,    1,    1,    1],
        [   0,  323,  223,  ...,    1,    1,    1],
        [   0, 1151,  708,  ...,    1,    1,    1],
        ...,
        [   0, 1733,  223,  ...,    1,    1,    1],
        [   0, 1151, 2385,  ...,    1,    1,    1],
        [   0, 1733,  223,  ...,    1,    1,    1]]), 'input_mask': tensor([[1., 1., 1.,  ..., 0., 0., 0.],
        [1., 1., 1.,  ..., 0., 0., 0.],
        [1., 1., 1.,  ..., 0., 0., 0.],
        ...,
        [1., 1., 1.,  ..., 0., 0., 0.],
        [1., 1., 1.,  ..., 0., 0., 0.],
        [1., 1., 1.,  ..., 0., 0., 0.]])}
torch.Size([64, 200])
```

Part 4.C

```
embs = torch.ones((32, 100, 128))
B, T, _ = embs.shape
pos_ids = torch.arange(T).expand(B, -1)
print(pos_ids)
pos_E = nn.Embedding(200, 128)
print(pos_E)
pos_E(pos_ids).shape
```

```
tensor([[ 0,  1,  2,  ..., 97, 98, 99],
        [ 0,  1,  2,  ..., 97, 98, 99],
        [ 0,  1,  2,  ..., 97, 98, 99],
        ...,
        [ 0,  1,  2,  ..., 97, 98, 99],
        [ 0,  1,  2,  ..., 97, 98, 99],
        [ 0,  1,  2,  ..., 97, 98, 99]])
Embedding(200, 128)
torch.Size([32, 100, 128])
```

```
class DialogueGPT(nn.Module):
    def __init__(
        self,
        vocab_size: int,
        max_N: int,
        dim: int,
        attn_dim: int,
        mlp_dim: int,
        num_heads: int,
        num_layers: int,
    ):
        # vocab_size       size of the vocabulary
        # max_N            maximum number of tokens allowed to appear in 1 example
        # dim              embedding dimension
        # attn_dim         the hidden dimension of the attention layer
        # mlp_dim          the hidden layer dimension of the FFN
        # num_heads        the number of heads in the attention layer
        # num_layers       the number of attention layers.

        super().__init__()

        # TODO: set up the token embedding and positional embeddings
        #       Hint, use nn.Embedding
        # =========== ANSWER START ============
        self.token_embed = nn.Embedding(vocab_size, dim)
        self.pos_embed = nn.Embedding(max_N, dim)

        # =========== ANSWER END =============

        self.transformer = Transformer(
```

```
            dim=dim,
            attn_dim=attn_dim,
            mlp_dim=mlp_dim,
            num_heads=num_heads,
            num_layers=num_layers,
        )

        self.head = nn.Sequential(nn.LayerNorm(dim), nn.Linear(dim, vocab_size))

    def forward(
        self, input_ids: torch.Tensor, return_attn=False
    ) -> Tuple[torch.Tensor, Optional[torch.Tensor]]:
        # input_ids     a batch of input ids (right padded). shape: (B x T)
        # return_attn   whether to return the attention weights
        #
        # Output
        # out           the logit vector (B x T x V)
        # alphas        the attention weights if return_attn is True. Otherwise None shape: (B, num_layers, num_heads, T, T)

        embs = None

        # TODO: retrieve the token embeddings for the input_ids.
        #       Add to the token embeddings the positional embeddings.
        #       Store the combined embedding in embs
        # ============ ANSWER START ============
        B, T = input_ids.shape
        token_embeds = self.token_embed(input_ids)  # (B,T,dim)
        pos_ids = (
            torch.arange(T, device=input_ids.device).unsqueeze(0).expand(B, -1)
        )  #  (B,T)
        pos_embeds = self.pos_embed(pos_ids)  # (B,T,dim)
        embs = pos_embeds + token_embeds  # (B,T,dim)

        # ============ ANSWER END ============

        causal_attn_mask = None

        # TODO: Create the causal attention mask, which should be of size (B, T, T)
        #       Remember that the causal attention mask is lower triangular (all tokens only
        #       depend on themselves and the tokens before them).
        # .      Store the mask in causal_attn_mask
        # Hint: check out torch.tril
        # ============ ANSWER START ============
        causal_attn_mask = torch.tril(torch.ones(T, T, device=input_ids.device))
        causal_attn_mask = causal_attn_mask.unsqueeze(0).expand(B, -1, -1)

        # ============ ANSWER END ==============

        x, alphas = self.transformer(
            embs, attn_mask=causal_attn_mask, return_attn=return_attn
        )
        out = self.head(x)
        return out, alphas

    def generate(self, input_ids, num_tokens):
        # you can assume batch size 1
        with torch.no_grad():
            for i in range(num_tokens):
                out, _ = self.forward(input_ids)
                new_token = torch.argmax(out[:, [-1]], -1)
                input_ids = torch.cat([input_ids, new_token], dim=1)
        return input_ids
```

Part 4.D

```
class DialogueLoss(nn.Module):
    def __init__(self):
        super().__init__()
        self.criterion = nn.CrossEntropyLoss(reduction="none")

    def forward(
        self, logits: torch.Tensor, input_ids: torch.Tensor, inp_mask: torch.Tensor
    ):
        # logits      the logits produced by DialogueGPT. shape: (B x T x V)
```

```
        # input_ids   the token ids. shape: (B x T)
        # inp_mask    a 0/1 mask of which tokens are padding tokens and should be ignored. shape: (B x T)

        # TODO: Implement the language model loss. For logits[i], we want to supervise the i+1 token_id
        # with the cross entropy loss. We thus will not supervise the start token (input_ids[0]) or use
        # the last logit vector (logits[-1]). Return the average of the losses for each token in the batch,
        # making sure to ignore tokens corresponding to the padding (use inp_mask).

        # ============ ANSWER START ============
        pred = logits[:, :-1, :]  # B,T-1,V
        gt = input_ids[:, 1:]  # B,T-1
        pred = pred.permute(0, 2, 1)  # B,V,T-1
        print(f"preded logits size {pred.shape}")
        print(f"input id size {gt.shape}")
        loss = self.criterion(pred, gt)
        inp_mask = inp_mask[:, 1:]
        loss = loss * inp_mask
        loss = torch.sum(loss) / torch.sum(inp_mask)

        # ============ ANSWER END ==============
        return loss
```

Part 4.F

```
import torch.optim as optim

model = DialogueGPT(
    vocab_size=tok.vocab_size,
    max_N=200,
    dim=128,
    attn_dim=64,
    mlp_dim=128,
    num_heads=3,
    num_layers=6,
).cuda()
criterion = DialogueLoss()

NUM_EPOCHS = 80


optimizer = optim.AdamW(
    model.parameters(), lr=0.0001, weight_decay=0
)  # implement in homework
scheduler = optim.lr_scheduler.CosineAnnealingLR(optimizer, T_max=NUM_EPOCHS)


# Time estimate: around 30 minutes on T4 GPU
# Training
import tqdm

for epoch in range(NUM_EPOCHS):  # loop over the dataset multiple times
    loss_meter = AverageMeter()
    for inp_dict in tqdm.tqdm(training_dl):
        # get the inputs; data is a list of [inputs, labels]
        inp_ids, inp_mask = inp_dict["input_ids"], inp_dict["input_mask"]
        inp_ids = inp_ids.cuda()
        inp_mask = inp_mask.cuda()
        # zero the parameter gradients
        optimizer.zero_grad()

        # forward + backward + optimize
        outputs, _ = model(input_ids=inp_ids)
        loss = criterion(outputs, inp_ids, inp_mask)
        loss_meter.update(loss.item(), len(inp_dict["input_ids"]))
        loss.backward()
        optimizer.step()
    scheduler.step()

    # print example
    inp = tok.encode("").unsqueeze(0).cuda()
    print(tok.decode(model.generate(inp, 10)[0].cpu()))

    print(
        f"Train Epoch: {epoch}, Loss: {loss_meter.calculate():0.4f}, LR: {scheduler.get_last_lr()[0]}"
    )
```

Show hidden output

Part 4.G

```
inp = tok.encode("").unsqueeze(0).cuda()
print(tok.decode(model.generate(inp, 50)[0].cpu()))
```

```
<START> KING RICHARD III : Why , I have a man ? I have not a word ? what is a man ? I will I am a man ? I am I will be a man . I am a ma
```