Exercise 11 Part 1: Self-Attention

Summer Semester 2024

Author: Stefan Baumann (stefan.baumann@lmu.de)

Task: Implement Self-Attention

In this exercise, you will implement multi-head self-attention for a 2D sequence of tokens (shape B D H W) yourself using **only basic functions (no pre-made attention implementations!)**. You're allowed to use simple functions such as, e.g., torch.bmm(), torch.nn.functional.softmax(), ... and simple modules such as torch.nn.Linear.

Usage of functions provided by the einops library (such as einops.rearrange()) is also allowed and encouraged (but completely optional!), as it allows writing the code in a nice and concise way by specifying operations across axes of tensors as strings instead of relying on dimension indices. A short introduction into einops is available at

https://nbviewer.org/github/arogozhnikov/einops/blob/master/docs/1-einops-basics.ipynb.

```
import math
import torch
import torch.nn as nn
import torch.nn.functional as F
# Optional
import einops
device = 'mps' if torch.backends.mps.is available() else ('cuda' if
torch.cuda.is available() else 'cpu')
print(f'Using device "{device}".')
Using device "mps".
class SelfAttention2d(nn.Module):
    def init (
        self,
        embed dim: int = 256,
        head dim: int = 32,
        value dim: int = 32,
        num heads: int = 8,
    ):
        """Multi-Head Self-Attention Module with 2d token input &
output
           Allows the model to jointly attend to information from
different representation subspaces.
        Args:
```

```
embed dim (int, optional): Dimension of the tokens at the
input & output (total dimensions of model). Defaults to 256.
            head dim (int, optional): Per-head dimension of guery &
kev. Defaults to 32.
            value dim (int, optional): Per-head dimension of values
(total number of features for values). Defaults to 32.
            num heads (int, optional): Number of parallel attention
heads. Defaults to 6.
        super(). init ()
        self.embed dim = embed dim
        self.head \overline{dim} = head \overline{dim}
        self.value dim = value dim
        self.num heads = num heads
        # Define linear layers for q/k/v/output
        self.q = nn.Linear(embed dim, num heads * head dim)
        self.k = nn.Linear(embed_dim, num_heads * head_dim)
        self.v = nn.Linear(embed dim, num heads * value dim)
        self.out = nn.Linear(num_heads * value_dim, embed dim)
        self.softmax = nn.Softmax(dim=-1)
        self.scale = 1 / math.sqrt(self.head dim) # Scaling factor
for attention logits 1/sqrt(head dim)
        self.init weights()
    def forward(self, x: torch.Tensor) -> torch.Tensor:
        """Forward of multi-head self-attention
           The convention is that each head's part in q/k/v is
contiquous.
           i.e., if you want to get the guery for head 0, it's at
q[..., :head dim], head 1 is at <math>q[..., head dim:2*head dim]...
        Args:
            x (torch.Tensor): Input tensor of shape (B, D, H, W)
(batch, embedding dimension, height, width)
        Returns:
            torch.Tensor: Output tensor of shape (B, D, H, W) (batch,
embedding dimension, height, width)
        B, D, H, W = x.shape # Batch size, Channels, Height, Width
                                # Number of tokens
        N = H * W
        # Reshape input to (B, N, D) for linear projections
        x_{flat} = x.reshape(B, D, N).permute(0, 2, 1) # Shape: (B, N, 1)
D)
```

```
# linear projections for q, k, v
        Q = self.q(x flat)
        K = self.k(x flat)
        V = self.v(x flat)
        # Reshape and transpose to split heads
        Q = Q.reshape(B, N, self.num_heads, self.head_dim).permute(0,
2, 1, 3) # Shape: (B, H, N, head_dim)
        K = K.reshape(B, N, self.num_heads, self.head_dim).permute(0,
2, 1, 3) # Shape: (B, H, N, head dim)
        V = V.reshape(B, N, self.num_heads, self.value_dim).permute(0,
2, 1, 3) # Shape: (B, H, N, value dim)
        # Compute attention scores with scaling of attention logits by
1/sqrt(head dim)
        attn scores = Q @ K.transpose(-2, -1) * self.scale
        attn probs = self.softmax(attn scores)
        # Apply attention to values
        attn output = attn probs @ V
        # Concatenate heads and reshape to (B, N, D)
        if self.head dim > 1:
            attn output = attn output.permute(0, 2, 1,
3).contiguous().view(B, N, -1)
        else:
            attn output = attn output.squeeze(-1)
        # Apply output linear layer
        out = self.out(attn output)
        # Reshape back to (B, D, H, W)
        out = out.permute(\frac{0}{2}, \frac{1}{2}).view(B, D, H, W)
        return out
    def init weights(self):
        for m in [self.q, self.k, self.v, self.out]:
            nn.init.xavier uniform (m.weight)
            nn.init.zeros (m.bias)
# Unit Test (single-head) DO NOT CHANGE!
with torch.no grad():
    layer = SelfAttention2d(embed dim=256, head dim=256,
value dim=256, num heads=1).to(device)
    x = torch.randn((4, 256, 24, 24), device=device)
    res layer = layer(x)
    layer ref = nn.MultiheadAttention(layer.embed dim,
```

```
layer.num heads).to(device)
    layer ref.load state dict({ 'in proj weight':
torch.cat([layer.q.weight, layer.k.weight, layer.v.weight]),
'out proj.weight': layer.out.weight }, strict=False)
    res ref = layer ref(*[x.view(*x.shape[:2], -1).permute(2, 0, 1)] *
3)[0].permute(1, 2, 0).view(*x.shape)
    assert torch.allclose(res layer, res ref, rtol=1e-2, atol=1e-5),
'Single-head attention result incorrect.'
# Unit Test (multi-head) DO NOT CHANGE!
with torch.no grad():
    layer = SelfAttention2d().to(device)
    x = torch.randn((4, 256, 24, 24), device=device)
    res layer = layer(x)
    layer ref = nn.MultiheadAttention(layer.embed dim,
layer.num heads).to(device)
    layer_ref.load_state_dict({ 'in_proj_weight':
torch.cat([layer.q.weight, layer.k.weight, layer.v.weight]),
'out proj.weight': layer.out.weight }, strict=False)
    res_ref = layer_ref(*[x.view(*x.shape[:2], -1).permute(2, 0, 1)] *
3)[0].permute(1, 2, 0).view(*x.shape)
    assert torch.allclose(res layer, res ref, rtol=1e-2, atol=1e-5),
'Multi-head attention result incorrect.'
print('All tests passed.')
All tests passed.
```

Exercise 11 Part 2: Vision Transformers

Summer Semester 2024

Author: Stefan Baumann (stefan.baumann@lmu.de)

Task: Implement & Train a ViT

Refer to the lecture and the original ViT paper (*AN IMAGE IS WORTH 16X16 WORDS: TRANSFORMERS FOR IMAGE RECOGNITION AT SCALE*, Dosovitskiy et al., 2020) for details. The naming of the hyperparameters is as in the aforementioned paper.

Similar to Part 1, you're expected to implement each block yourself, although you're allowed to use blocks like torch.nn.MultiheadAttention, torch.nn.Linear, etc. Implement the blocks as in the original ViT paper. No usage of things such as full pre-made FFN/self-attention blocks or full transformer implementations like

torchvision.models.vision_transformer.VisionTransformer is allowed for this exercise. You're expected to do full vectorized implementations in native PyTorch (again, einops is allowed) without relying on Python for loops for things such as patching etc.

Some relevant details:

- For simplicity of implementation, we will use a randomly (Gaussian with mean 0 and variance 1) initialized *learnable* positional embedding, not a Fourier/sinusoidal one.
- Don't forget about all of the layer norms!
- Consider the batch_first attribute of nn.MultiheadAttention, should you use that class
- We'll make the standard assumption that $dim_{\text{head}} = dim_{\text{hidden}}/N_{\text{heads}}$

```
import torch
import torch.nn as nn
import torch.nn.functional as F
import torchvision.transforms as T
from torchvision.datasets import CIFAR10
from torch.utils.data import DataLoader
import matplotlib.pyplot as plt
from tqdm.auto import tqdm

# Optional
import einops

device = 'mps' if torch.backends.mps.is_available() else ('cuda' if
torch.cuda.is_available() else 'cpu')
print(f'Using device "{device}".')

Using device "mps".
```

```
/Users/janinaalicamattes/miniforge3/envs/pytorch-py11/lib/python3.11/
site-packages/tqdm/auto.py:21: TqdmWarning: IProgress not found.
Please update jupyter and ipywidgets. See
https://ipywidgets.readthedocs.io/en/stable/user install.html
  from .autonotebook import tgdm as notebook tgdm
class ResidualModule(nn.Module):
    def __init__(
            self,
            inner module: nn.Module
        ):
        super().__init__()
        self.inner module = inner module
    def forward(self, x: torch.Tensor) -> torch.Tensor:
        return x + self.inner module(x)
class FeedForwardBlock(nn.Module):
    """ FeedForwardBlock class for the MLP of a transformer block in
the Transformer Encoder.
        The linear MLP layers are local and translationally
equivariant,
        while the self-attention layers are global and permutation
invariant.
        Aras:
            hidden size (int): Hidden size of the model.
            mlp size (int): Size of the MLP.
            p dropout (float): Dropout probability.
        Returns:
            torch. Tensor: Output tensor of the feedforward block.
    0.00
    def __init__(
            self,
            hidden size: int,
            mlp_size: int,
            p dropout: float
        ):
        super(). init ()
        self.dropout = p dropout
        self.hidden size = hidden size # kept fixed
        self.mlp size = mlp size
        self.linear1 = nn.Linear(self.hidden size, self.mlp size)
        self.dropout1 = nn.Dropout(self.dropout)
        self.gelu = nn.GELU()
        self.linear2 = nn.Linear(self.mlp size, self.hidden size)
        self.dropout2 = nn.Dropout(self.dropout)
```

```
def forward(self, x: torch.Tensor) -> torch.Tensor:
        x = self.linear1(x)
        x = self.gelu(x)
        x = self.dropout1(x)
        x = self.linear2(x)
        x = self.dropout2(x)
        return x
class SelfAttentionTransformerBlock(nn.Module):
    """ SelfAttentionTransformerBlock class for the transformer block
in the Transformer Encoder.
        The linear MLP layers are local and translationally
        while the self-attention layers are global and permutation
invariant.
        Args:
            hidden size (int): Hidden size of the model.
            n heads (int): Number of heads in the multi-head self-
attention.
            p dropout (float): Dropout probability.
        Returns:
            torch. Tensor: Output tensor of the transformer block.
    0.00
    def __init (
            self,
            hidden size: int,
            n heads: int,
            p dropout: float
        ):
        super(). init ()
        self.hidden size = hidden size
        self.n heads = n heads
        self.p_dropout = p_dropout
        self.mlp size = self.hidden size * 4 # Standard in the
literature
        # Layer normalization
        self.norm1 = nn.LayerNorm(self.hidden size)
        self.norm2 = nn.LayerNorm(self.hidden size)
        # Multi-head self-attention
        self.mha = nn.MultiheadAttention(self.hidden size,
self.n heads, dropout=p dropout, batch first=True)
        # MLP block
        self.mlp = FeedForwardBlock(self.hidden size, self.mlp size,
```

```
self.p dropout)
        # Dropout
        self.dropout = nn.Dropout(self.p dropout)
    def forward(self, x: torch.Tensor) -> torch.Tensor:
        # Residual connection
        residual = x
        # Self-attention (global and permutation invariant)
        x = self.norm1(x)
        x = self.mha(x, x, x)[0]
        x = self.dropout(x)
        # Residual connection
        x = x + residual
        # Residual connection
        residual = x
        # MLP (local and translationally equivariant)
        x = self.norm2(x)
        x = self.mlp(x)
        x = self.dropout(x)
        # Residual connection
        x = x + residual
        return x
class VisionTransformer(nn.Module):
    def __init__(
            self.
            in channels: int = 3,
            patch size: int = 4,
            image size: int = 32,
            layers: int = 6,
            hidden size: int = 256,
            mlp\_size: int = 512,
            n heads: int = 8,
            num classes: int = 10,
            p dropout: float = 0.2,
        ):
        super().__init__()
        self.in channels = in channels
        self.patch size = patch size
        self.image_size = image_size
        self.layers = layers
        self.hidden size = hidden size
```

```
self.mlp size = mlp size
        self.n heads = n heads
        self.num_classes = num_classes
        self.p dropout = p dropout
        # ----- Transformer Encoder -----
        # Image patches / token
        self.num patches = (self.image size // self.patch size) ** 2 #
Number of patches (L) or tokens
        self.patch_dim = self.in_channels * (self.patch size ** 2) #
Dimension of the patch after flattening (D)
        # Patch embedding - linear projection of the patches
        self.patch_embed = nn.Linear(self.patch_dim, self.hidden_size)
        # Positional encoding - learnable positional embeddings
        self.pos embed = nn.Parameter(torch.randn(1, self.num patches
+ 1, hidden size))
        # CLS token - classification token
        self.cls token = nn.Parameter(torch.zeros(1, 1,
self.hidden size))
        # Transformer blocks
        self.transformer_blocks = nn.Sequential(*[
            SelfAttentionTransformerBlock(self.hidden size,
self.n heads, self.p dropout)
           for _ in range(self.layers)
        1)
        # Dropout
        self.dropout = nn.Dropout(self.p_dropout)
        # ----- Classification head -----
        self.norm = nn.LayerNorm(self.hidden size)
        self.classification head = nn.Linear(self.hidden size,
self.num classes)
        # Initialize weights
        self. init weights()
    def init weights(self):
```

```
# Initialize weights
        self.apply(self. init layer weights)
    def _init_layer_weights(self, m):
        # Initialize weights of the model
        if isinstance(m, nn.Linear):
            nn.init.xavier_uniform_(m.weight)
            if m.bias is not None:
                nn.init.zeros_(m.bias)
        elif isinstance(m, nn.LayerNorm):
            nn.init.ones_(m.weight)
            nn.init.zeros (m.bias)
    def patchify(self, x: torch.Tensor) -> torch.Tensor:
        """Takes an image tensor of shape (B, C, H, W) and transforms
it to a sequence of patches (B, L, D), with a learnable linear
projection after flattening,
        and a standard additive positional encoding applied. Note that
the activations in (Vision) Transformer implementations are
        typically passed around in channels- last layout, different
from typical PyTorch norms.
        The linear projection of flattened image patches produces
lower-dimensional linear embddings from flattened patches and adds
positional embeddings.
       Args:
            x (torch.Tensor): Input tensor of shape (B, C, H, W)
        Returns:
            torch. Tensor: Embedded patch sequence tensor with
positional encodings applied and shape (B, L, D)
        B, C, H, W = x.shape
        # Reshape and flatten the image patches
        x = x.reshape(B, C, H // self.patch_size, self.patch_size, W
// self.patch size, self.patch size)
        x = x.permute(0, 2, 4, 1, 3, 5).contiguous()
                                                                  #
Size: (B, H, W, C, patch_size, patch_size)
        x = x.view(B, -1, C * self.patch size * self.patch size) #
Size: (B, L, D) with D: C * patch_size * patch_size
        # Linear projection of the patches
        x = self.patch embed(x)
        # Add positional embeddings
        x = x + self.pos embed[:, 1:, :]
```

```
# Add CLS token
        cls token = self.cls token.expand(B, -1, -1)
        x = torch.cat((cls_token, x), dim=1)
        # Add positional embeddings for the CLS token
        x[:, 0, :] = x[:, 0, :] + self.pos_embed[:, 0, :]
        return x
    def forward(self, x: torch.Tensor) -> torch.Tensor:
        """Takes an image tensor of shape (B, C, H, W), applies
patching, a standard ViT
           and then an output projection of the CLS token
           to finally create a class logit prediction of shape (B,
N cls)
       Args:
            x (torch.Tensor): Input tensor of shape (B, C, H, W)
        Returns:
            torch. Tensor: Output logits of shape (B, N cls)
        # Patchify input image + pos embeddings
        x = self.patchify(x)
        # Apply dropout
        x = self.dropout(x)
        # Transformer blocks
        x = self.transformer blocks(x)
        # Classification head
        x = self.norm(x[:, 0])
                                           # select only the learned
CLS token with Size: (B, D)
        x = self.classification_head(x)
        return x
```

Training

Do not modify this code! You are free to modify the four parameters in the first block, although no modifications should be necessary to achieve >70% validation accuracy with a correct transformer implementation.

```
DATASET_CACHE_DIR = './data'
BATCH_SIZE = 128
LR = 3e-4
N_EPOCHS = 50
```

```
transforms val = T.Compose([
    T.ToTensor(),
    T.Normalize([0.49139968, 0.48215841, 0.44653091], [0.24703223,
0.24348513. 0.261587841).
transforms train = T.Compose([
    T.RandomHorizontalFlip(),
    T.RandomResizedCrop((32, 32), scale=(0.8, 1.0), ratio=(0.9, 1.1)),
    T.ToTensor(),
    T.Normalize([0.49139968, 0.48215841, 0.44653091], [0.24703223,
0.24348513, 0.26158784]),
model = VisionTransformer().to(device)
optim = torch.optim.Adam(model.parameters(), lr=LR)
loss fn = nn.CrossEntropyLoss()
dataloader train = DataLoader(CIFAR10(root=DATASET CACHE DIR,
train=True, download=True, transform=transforms_train),
batch size=BATCH SIZE, shuffle=True, drop last=True, num workers=4)
dataloader val = DataLoader(CIFAR10(root=DATASET CACHE DIR,
train=False, download=True, transform=transforms val),
batch size=BATCH SIZE, shuffle=False, drop last=False, num workers=4)
train losses = []
val accs = []
for i epoch in range(N EPOCHS):
    for i step, (images, labels) in (pbar :=
tqdm(enumerate(dataloader train), desc=f'Training (Epoch {i epoch +
1}/{N EPOCHS})')):
        optim.zero grad()
        loss = loss fn(model(images.to(device)), labels.to(device))
        loss.backward()
        optim.step()
        # Some logging
        loss val = loss.detach().item()
        train losses.append(loss val)
        pbar.set_postfix({ 'loss': loss_val } | ({ 'val_acc':
val accs[-1] } if len(val accs) > 0 else { }))
    # Validation every epoch
    with torch.no grad():
        n_total, n correct = 0, 0
        for i step, (images, labels) in (pbar :=
tqdm(enumerate(dataloader val), desc='Validating')):
            predicted = model(images.to(device)).argmax(dim=-1)
            n correct += (predicted.cpu() ==
labels).float().sum().item()
```

```
n total += labels.shape[0]
        val accs.append(n correct / n total)
        print(f'Validation accuracy: {val accs[-1]:.3f}')
plt.figure(figsize=(6, 3))
plt.subplot(121)
plt.plot(train losses)
plt.xlabel('Steps')
plt.ylabel('Training Loss')
plt.subplot(122)
plt.plot(val accs)
plt.xlabel('Epochs')
plt.ylabel('Validation Accuracy')
plt.tight layout()
plt.show()
Downloading https://www.cs.toronto.edu/~kriz/cifar-10-python.tar.gz to
./data/cifar-10-python.tar.gz
100% | 170498071/170498071 [00:03<00:00, 48744481.98it/s]
Extracting ./data/cifar-10-python.tar.gz to ./data
/usr/local/lib/python3.10/dist-packages/torch/utils/data/
dataloader.py:558: UserWarning: This DataLoader will create 4 worker
processes in total. Our suggested max number of worker in current
system is 2, which is smaller than what this DataLoader is going to
create. Please be aware that excessive worker creation might get
DataLoader running slow or even freeze, lower the worker number to
avoid potential slowness/freeze if necessary.
 warnings.warn( create warning msg(
Files already downloaded and verified
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Validation accuracy: 0.469
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```

```
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ion minor":0}
Validation accuracy: 0.519
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Validation accuracy: 0.545
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ion minor":0}
Validation accuracy: 0.541
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Validation accuracy: 0.566
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Validation accuracy: 0.562
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Validation accuracy: 0.596
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ion minor":0}
Validation accuracy: 0.600
```

```
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ion minor":0}
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ion minor":0}
Validation accuracy: 0.598
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ion minor":0}
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ion minor":0}
Validation accuracy: 0.610
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ion minor":0}
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Validation accuracy: 0.618
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Validation accuracy: 0.614
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ion minor":0}
Validation accuracy: 0.629
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ion minor":0}
Validation accuracy: 0.636
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ion minor":0}
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```

```
Validation accuracy: 0.645
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ion minor":0}
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Validation accuracy: 0.652
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