An Image is Worth 16x16 Words: Transformers for Image Recognition at Scale

DEEP LEARNING BASED ANOMALY DETECTION MODELING (GEK6207.01-00)
Coding practice

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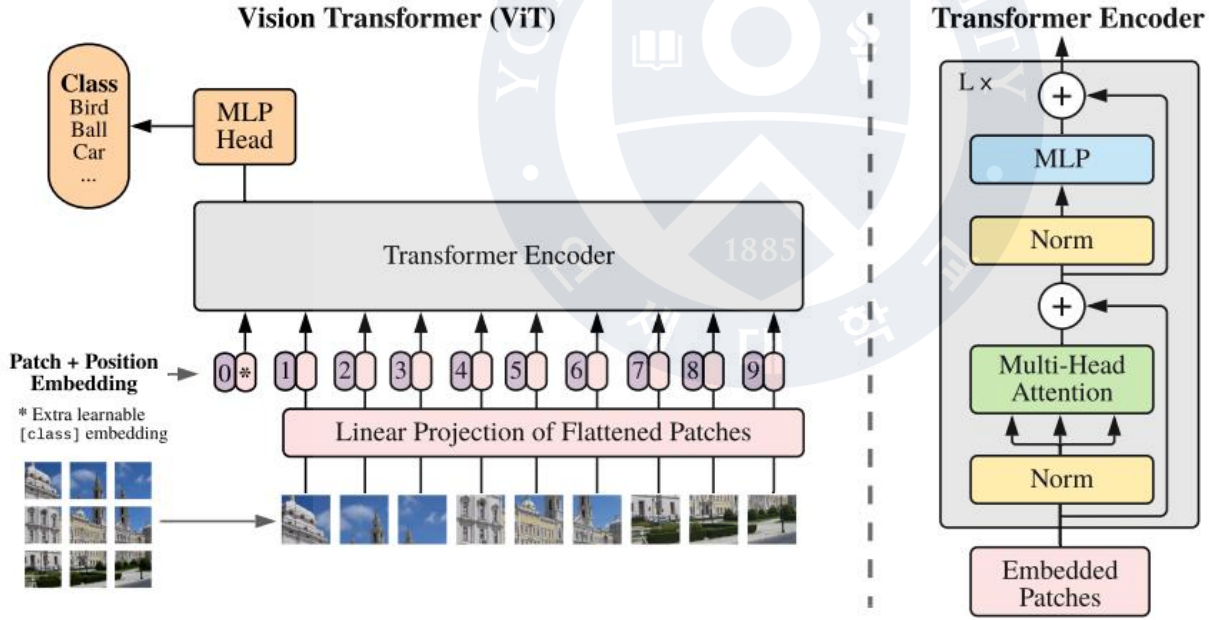
2 Vision Transformer

What is a ViT?

The Vision Transformer (ViT) is a novel deep learning architecture for image classification. Unlike traditional convolutional neural networks (CNNs), ViT adopts a transformer-based model originally designed for natural language processing.
ViT divides input images into fixed-size patches,captures global context through Transformer Encoder.
This approach eliminates the need for conv layers, allowing ViT to efficiently handle long-range dependencies in images.



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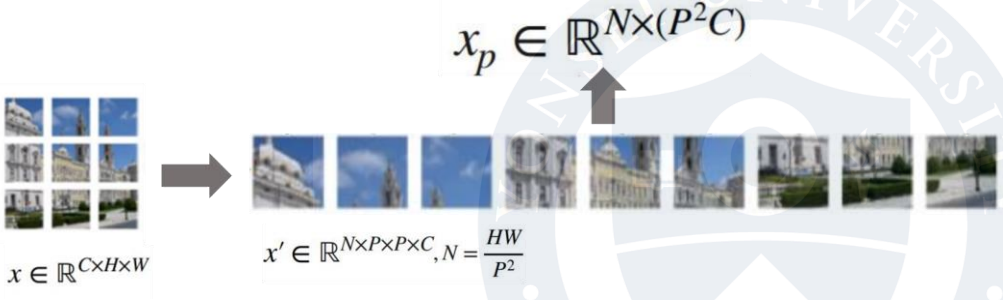
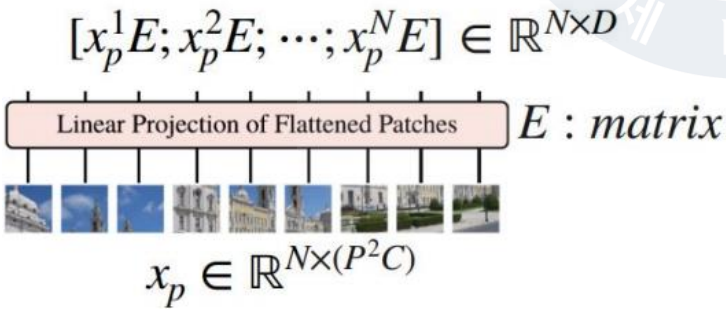
ViT Process

Step 1. Given an image (x), the image is divided into N patches of size PxP to construct a patch sequence set (x_p).



Step 2. Through linear projection, each patch of x_p is transformed into D dimensions.



$x_p^i \in \mathbb{R}^{P^2C}, E \in \mathbb{R}^{(P^2C)\times D}$

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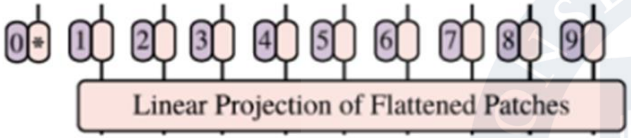
ViT Process

Step 3. Add a class token(X_{cls}) to X_pE and perform positional embedding.



$$[x_p^1E; x_p^2E; \cdots; x_p^NE] \in \mathbb{R}^{N\times D} \Rightarrow [x_{cls}; x_p^1E; x_p^2E; \cdots; x_p^NE] \in \mathbb{R}^{(N+1)\times D}$$

$$z_0 = [x_{cls}; x_p^1E; x_p^2E; \cdots; x_p^NE] + E_{pos} \in \mathbb{R}^{(N+1)\times D}$$

Class token: A trainable vector, when passed through the encoder, serves as the representation vector for the image.

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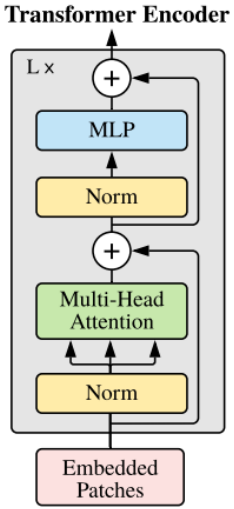
ViT Process

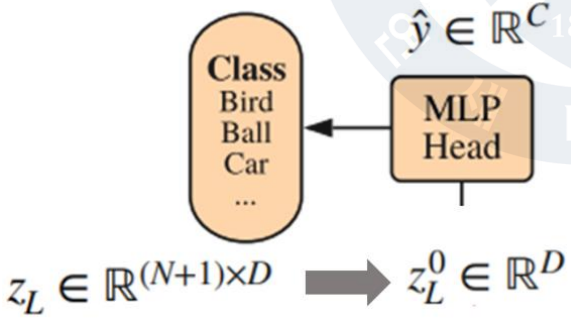
Step 4. Forward z_0 into the Transformer Encoder and perform Multi-Head Self Attention (MSA).

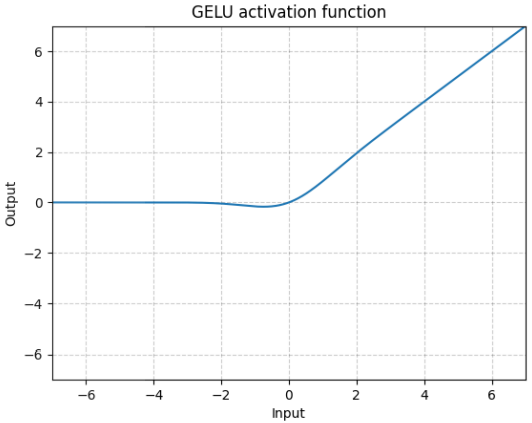
$$z'_l = MSA(LN(z_{l-1})) + z_{l-1}$$

$$z_l = MLP(LN(z'_l)) + z'_l \qquad l = 1,2,\cdots,L$$



Step 5. Classify the class of the image by forwarding the class token, which represents the image, into the MLP.





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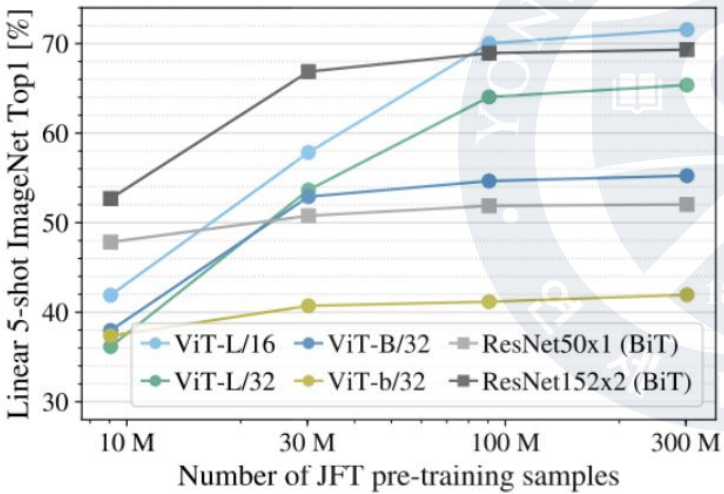
Experiments

Transformers lack some of the inductive biases inherent to CNNs, such as translation equivariance and locality, therefore do not generalize well when trianed on insufficient amounts of data.



- ImageNet, 1K classes, 1.3M images
- ImageNet-21k, 21K classes, 14M images
- JFT, 18K classes, 303M images

ImageNet-21k or JFT (pre-training) -> ImageNet (fine-tuning)

We find that large scale training trumps inductive bias.

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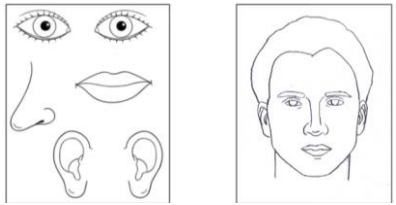
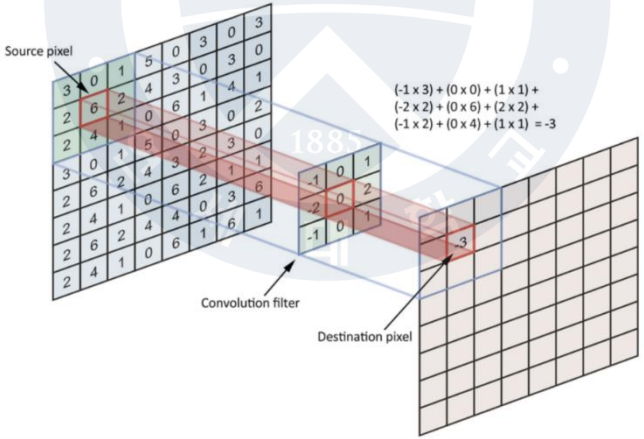
Inductive bias

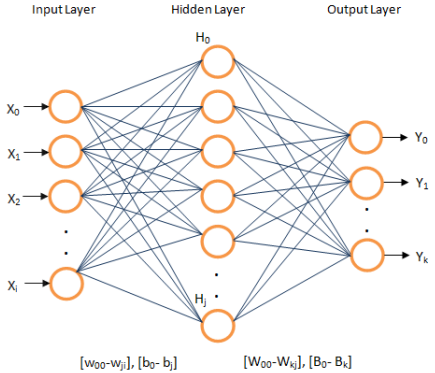
A set of assumptions used to predict outputs accurately for inputs that the model encounters for the first time.

- **Locality:** It is possible to extract features within a specific region of an image simply by checking at it.

- **Translation equivariance:** If the input position changes, the output also transforms to the corresponding position.







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Dataset

CIFAR-10

- CIFAR-10 is a dataset that consists of 60,000 color images, each with a size of 32x32 pixels.
- These images are divided into 10 distinct classes, and each class contains 6,000 images.
- The dataset is balanced, meaning that there are an equal number of images for each class.
- The dataset is split into two subsets: a training set and a test set.
- The training set contains 50,000 images (5,000 images per class), while the test set consists of 10,000 images (1,000 images per class).

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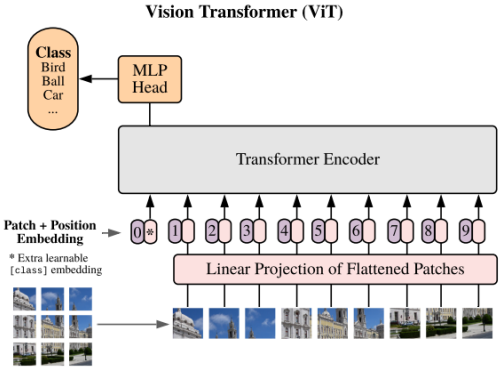

Patch Embedding

In [81]:

```python
class PatchEmbedding(nn.Module):
    def __init__(self, in_channels: int = 3, patch_size: int = 8, emb_size: int = 128):
        self.patch_size = patch_size
        super().__init__()
        self.projection = nn.Sequential(
            # break-down the image in s1 x s2 patches and flat them
            Rearrange('b c (h s1) (w s2) -> b (h w) (s1 s2 c)', s1=patch_size, s2=patch_size),
            nn.Linear(patch_size * patch_size * in_channels, emb_size)
        )

    def forward(self, x: Tensor) -> Tensor:
        x = self.projection(x) # [b d hw]
        x = x.permute(0,2,1) # [b hw d]
        return x
```

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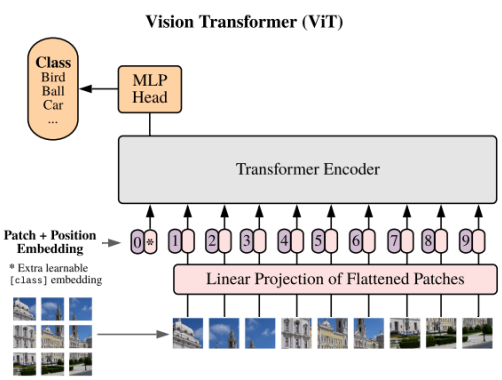
Positional Embedding

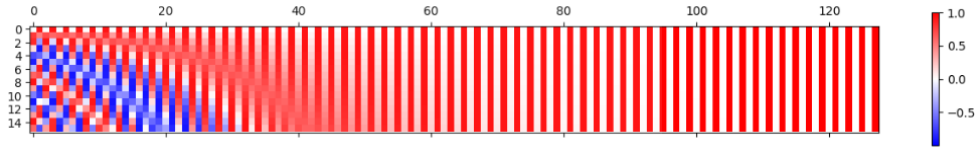
$$PE_{(pos,2i)} = sin(pos/10000^{2i/d_{\text{model}}})$$
$$PE_{(pos,2i+1)} = cos(pos/10000^{2i/d_{\text{model}}})$$



In [83]:

```
pos_num = 16
d_model = 128

# all positions of tokens
posses = np.arange(pos_num) # [0, 1, ..., 14, 15] (size: pos_num = 16)

# exponent of 10000
i = np.arange(d_model)//2 # [0, 0, 1, 1, ...., 63, 63] (size: d_model = 128)
two_i = 2*i # [0, 0, 2, 2, ...., 126, 126]
exponent = two_i/d_model # [0, 0, 0.00x, 0.00x, ...., 0.9xx, 0.9x]

# fraction = positions / 10000^exponent
denominator = np.power(10000, exponent) # [1, 1, ..., 9xxx, 9xxx] (size: d_model = 128)
fraction = posses[:, np.newaxis] / denominator # shape: pos_num x d_model = 16 x 128

# even index of PE vector -> sin(fraction) = sin(pos/10000^exponent)
# odd index of PE vector -> cos(fraction) = cos(pos/10000^exponent)
pos_emb = np.zeros((pos_num, d_model))
pos_emb[:, 0::2] = np.sin(fraction[:, 0::2]) # shape: 16 x 64
pos_emb[:, 1::2] = np.cos(fraction[:, 1::2]) # shape: 16 x 64
print(pos_emb.shape)
```

(16, 128)



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Multi-head Self Attention (MSA)

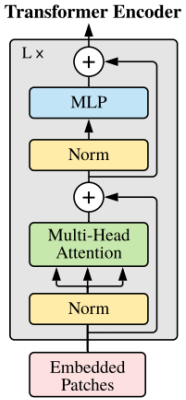
In [88]:

```python
class MultiheadAttention(nn.Module):
    def __init__(self, emb_size: int = 128, num_heads: int = 4, dropout: float = 0):
        super().__init__()
        self.num_heads = num_heads
        self.embed_dim = emb_size
        self.head_dim = int(emb_size / num_heads)
        self.query = nn.Linear(emb_size, emb_size)
        self.key = nn.Linear(emb_size, emb_size)
        self.value = nn.Linear(emb_size, emb_size)
        self.dropout = nn.Dropout(dropout)

    def forward(self, x):
        batch_size = x.size(0)
        q = self.query(x) # [b, n, d], n=hw+1
        k = self.key(x)
        v = self.value(x)
        q = q.view(batch_size, -1, self.num_heads, self.head_dim).permute(0,2,1,3) # [b, h, n, d/h]
        k = k.view(batch_size, -1, self.num_heads, self.head_dim).permute(0,2,3,1) # k.t
        v = v.view(batch_size, -1, self.num_heads, self.head_dim).permute(0,2,1,3)

        scaling = self.head_dim ** (1/2)
        attention = torch.softmax(q @ k / scaling, dim=-1) # [b, h, n, n]
        x = self.dropout(attention) @ v # [b, h, n, d/h]
        x = x.permute(0,2,1,3).reshape(batch_size, -1, self.embed_dim) # [b, n, d]

        return x, attention
```



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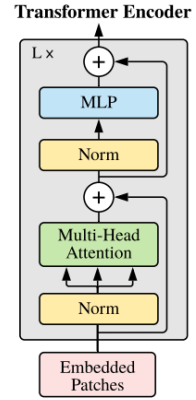

MLP

In [91]:
```python
class MLP(nn.Sequential):
    def __init__(self, emb_size: int, expansion: int = 4, drop_p: float = 0.):
        super().__init__()
        self.mlp = nn.Sequential(
            nn.Linear(emb_size, expansion * emb_size),
            nn.GELU(),
            nn.Dropout(drop_p),
            nn.Linear(expansion * emb_size, emb_size),
        )

    def forward(self, x):
        return self.mlp(x)
```

Residual Connection

In [89]:
```python
class ResidualAdd1(nn.Module):
    def __init__(self, fn):
        super().__init__()
        self.fn = fn

    def forward(self, x):
        res = x
        x, attention = self.fn(x)
        x += res
        return x, attention
```

In [90]:
```python
class ResidualAdd2(nn.Module):
    def __init__(self, fn):
        super().__init__()
        self.fn = fn

    def forward(self, x):
        res = x
        x = self.fn(x)
        x += res
        return x
```

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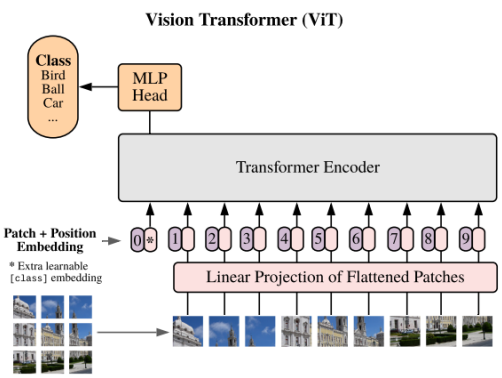


Transformer Encoder Block

In [92]:
```
class TransformerEncoderBlock(nn.Sequential):
    def __init__(self,
                 emb_size: int = 128,
                 drop_p = 0.,
                 forward_expansion: int = 4,
                 forward_drop_p: float = 0.,
                 ** kwargs):
        super().__init__()

        self.work1 = ResidualAdd1(nn.Sequential(
                                nn.LayerNorm(emb_size),
                                MultiheadAttention(emb_size, **kwargs)))
        self.work2 = ResidualAdd2(nn.Sequential(
                                nn.LayerNorm(emb_size),
                                MLP(emb_size, expansion=forward_expansion, drop_p=forward_drop_p),
                                nn.Dropout(drop_p)))

    def forward(self, x):
        x, attention = self.work1(x)
        x = self.work2(x)
        return x, attention
```

Vision Transformer

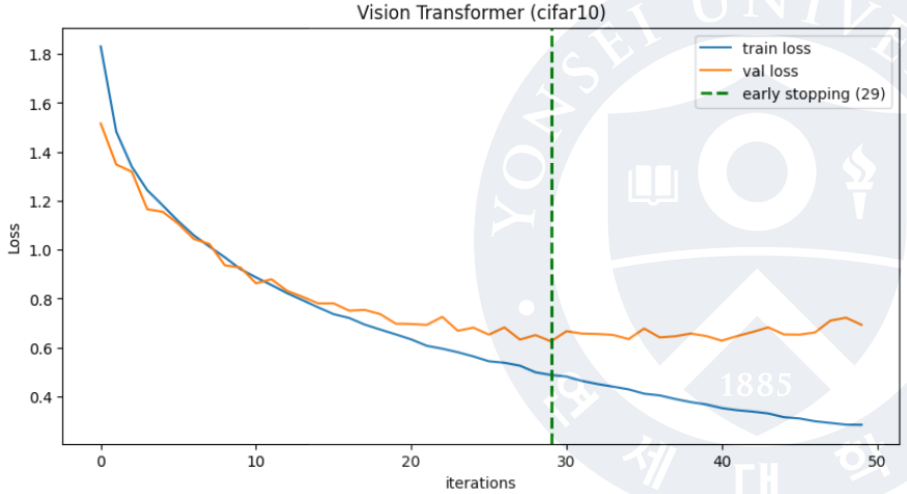
In [94]:
```
class VisionTransformer(nn.Sequential):
    def __init__(self, patch_size: int = 8, emb_size: int = 128, num_layers: int = 12, num_heads: int = 4, n_classes: int = 10, cpu=Fal
        super().__init__()
        self.patchembedding = PatchEmbedding(patch_size=patch_size, emb_size=emb_size, cpu=cpu)
        self.transformer = nn.ModuleList([TransformerEncoderBlock(emb_size=emb_size, num_heads=num_heads) for _ in range(num_layers)])
        self.mlp_head = nn.Sequential(nn.LayerNorm(emb_size),
                                      nn.Linear(emb_size, n_classes))

    def forward(self, x):
        x = self.patchembedding(x)
        for layer in self.transformer:
            x, attention = layer(x)
        x = self.mlp_head(x[:,0])
        return x, attention
```

2 Vision Transformer

Training Setting and Loss

- Loss graph



· To extract the best performance among 50 epochs, `early stopping` was employed.
· In this experiment, the validation set and the test set are the same.
· The best model can be confirmed through `weight/cifar_vit_pe_conv.pth`.

- **Model**
  · patch size: 4x4
  · embedding size: 192
  · num layers: 12
  · num classes: 10
  · num heads: 12
- **Training**
  · batch size: 256
  · num epoch: 50
  · optimizer: Adam (lr=0.001, weight_decay=5e-5)
  · data augmentation: RandomCrop(32, padding=4), RandomHorizontalFlip()

$$CE = -\sum_{i}^{C} t_i log(f(s)_i)$$

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Accuracy

ViT Basic	ViT PE	ViT PE & Conv
75.03 %	76.05 %	**78.55** %

- `ViT Basic` : positional encoding with Training, patch embedding with FC layer.
- `ViT PE` : positional encoding without Training, patch embedding with FC layer.
- `ViT PE & Conv` : position encoding without Training, patch embedding with Conv2d.

1. Creating Positional Encoding vectors can make the training of the model more challenging.
2. Inductive bias is crucial in small datasets.

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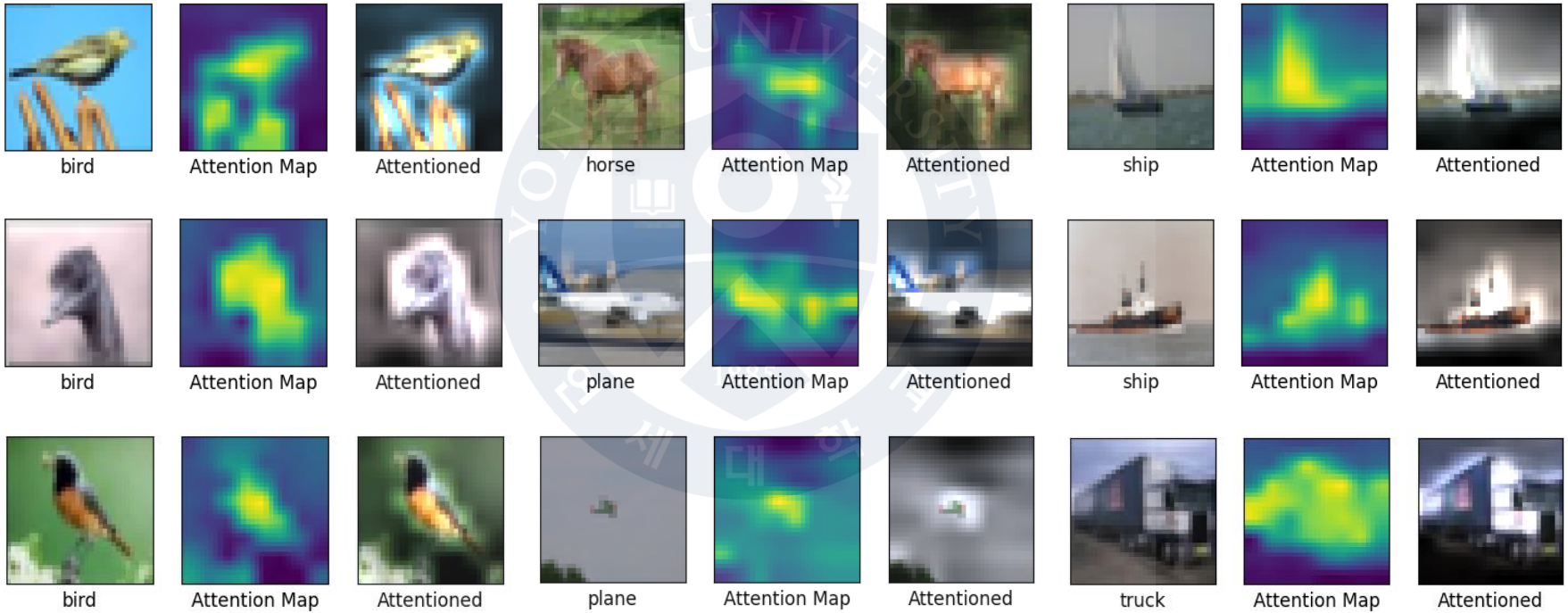
Visualization



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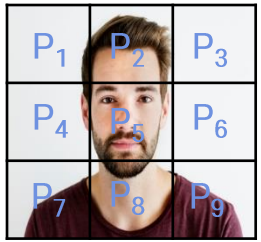
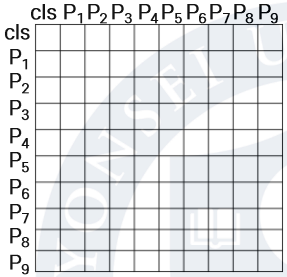
How to Visualize?



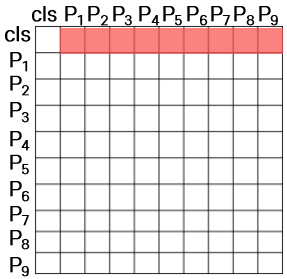
Image(30x30) to 9 patches

ViT

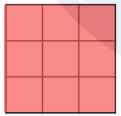


Attention Matrix (10x10)

Class token: A trainable vector, when passed through the encoder, serves as the representation vector for the image.

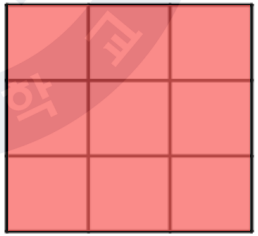


Normalize & Unflatten



3x3

Resizing



30x30

indicating where the model is focusing on in the image through the cls token portion of the attention map.

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Appendix

Patch Embedding *[Positional Encoding with Training]*

In [28]:

```python
class PatchEmbedding(nn.Module):
    def __init__(self, in_channels: int = 3, img_size: int = 32, patch_size: int = 8, emb_size: int = 128):
        self.patch_size = patch_size
        super().__init__()
        self.projection = nn.Sequential(
            # break-down the image in s1 x s2 patches and flat them
            Rearrange('b c (h s1) (w s2) -> b (h w) (s1 s2 c)', s1=patch_size, s2=patch_size),
            nn.Linear(patch_size * patch_size * in_channels, emb_size)
        )

        # cls token
        self.cls_token = nn.Parameter(torch.randn(1, 1, emb_size)) # [1, 1, d]
        # pos encoding
        self.positions = nn.Parameter(torch.randn((img_size // patch_size) **2 + 1, emb_size)) # [hw+1, d]

    def forward(self, x: Tensor) -> Tensor:
        b, _, _, _ = x.shape
        x = self.projection(x) # [b, hw, d]
        cls_tokens = repeat(self.cls_token, '1 1 d -> b 1 d', b=b) # [b, 1, d]

        x = torch.concat([cls_tokens, x], dim=1) # [b, hw+1, d]
        x += self.positions
        return x
```

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Appendix

Patch Embedding *[Positional Encoding with Untraining]*

In [86]:

```python
class PatchEmbedding(nn.Module):
    def __init__(self, in_channels: int = 3, img_size: int = 32, patch_size: int = 8, emb_size: int = 128, cpu=False):
        super().__init__()
        self.patch_size = patch_size

        self.projection = nn.Sequential(
            # break-down the image in s1 x s2 patches and flat them
            Rearrange('b c (h s1) (w s2) -> b (h w) (s1 s2 c)', s1=patch_size, s2=patch_size),
            nn.Linear(patch_size * patch_size * in_channels, emb_size)
        )

        # cls token
        self.cls_token = nn.Parameter(torch.randn(1, 1, emb_size)) # [1, 1, d]
        # pos encoding
        hw_plus_one = (img_size // patch_size) **2 + 1
        self.positions = PE(pos_num=hw_plus_one, d_model=emb_size, cpu=cpu) # [hw+1, d]

    def forward(self, x: Tensor) -> Tensor:
        b, _, _, _ = x.shape
        x = self.projection(x) # [b, hw, d]
        cls_tokens = repeat(self.cls_token, '1 1 d -> b 1 d', b=b) # [b, 1, d]

        x = torch.concat([cls_tokens, x], dim=1) # [b, hw+1, d]
        x += self.positions
        return x
```

In [85]:

```python
def PE(pos_num, d_model, cpu=False):
    posses = np.arange(pos_num)

    i = np.arange(d_model)//2
    exponent = 2*i/d_model
    pos_emb = posses[:, np.newaxis] / np.power(10000, exponent)

    pos_emb[:, 0::2] = np.sin(pos_emb[:, 0::2])
    pos_emb[:, 1::2] = np.cos(pos_emb[:, 1::2])

    if cpu:
        pos_emb = torch.from_numpy(pos_emb)
    else:
        pos_emb = torch.from_numpy(pos_emb).to("cuda")

    return pos_emb
```

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Appendix

Patch Embedding *[Patch Embedding with Convolution]*

In [170…

```python
class PatchEmbedding(nn.Module):
    def __init__(self, in_channels: int = 3, img_size: int = 32, patch_size: int = 8, emb_size: int = 128, cpu=False):
        super().__init__()
        self.patch_size = patch_size

        self.projection = nn.Sequential(
            nn.Conv2d(in_channels, emb_size, kernel_size=patch_size, stride=patch_size),
            Rearrange('b d h w -> b d (h w)')
        )

        # cls token
        self.cls_token = nn.Parameter(torch.randn(1, 1, emb_size)) # [1, 1, d]
        # pos encoding
        hw_plus_one = (img_size // patch_size) **2 + 1
        self.positions = PE(pos_num=hw_plus_one, d_model=emb_size, cpu=cpu) # [hw+1, d]

    def forward(self, x: Tensor) -> Tensor:
        b, _, _, _ = x.shape
        x = self.projection(x) # [b d hw]
        x = x.permute(0,2,1) # [b hw d]
        cls_tokens = repeat(self.cls_token, '1 1 d -> b 1 d', b=b) # [b, 1, d]

        x = torch.concat([cls_tokens, x], dim=1) # [b, hw+1, d]
        x += self.positions
        return x
```

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Appendix

Visualization

```
1. Create a single row vector by averaging 'num_head' row vectors. (using average attention weights)
2. Convert the row vector (1x64) into a 2D matrix (8x8).
3. Resize the matrix to the original image size (32x32).
4. Perform min-max normalization on the matrix. (scaling values to range between 0 and 1)
5. Multiply the matrix with the original image. (incorporating the focused area into the original image)
6. Multiply the resulting matrix by 2 and visualize it. (amplifying the representation of the focused area)
```

```python
# 이미지 시각화
num = 0
img = images[num].to(device)
mean=(0.4914, 0.4822, 0.4465)
std=(0.2023, 0.1994, 0.2010)
show_img = img.clone()
for i in range(3):
    show_img[i] = show_img[i] * std[i] + mean[i]
show_img = show_img.cpu().permute(1,2,0)

fig = plt.figure(figsize=(10, 5))
ax = fig.add_subplot(1, 5, 1)
ax.axes.get_xaxis().set_visible(False)
ax.axes.get_yaxis().set_visible(False)
ax.imshow(show_img)
ax.text(0.5, -0.15, f'{classes[predicted[num]]}', transform=ax.transAxes, fontsize=12, ha='center')
```

```python
# 어텐션 맵 시각화
output, attention = net(img.unsqueeze(0)) # [1, h, n, n]

sum_heatmap = np.zeros(shape=(32,32), dtype=np.float32)
for i in range(num_heads):
    attn_heatmap = attention[0, i, 0, 1:].reshape((8, 8)).detach().cpu().numpy() # cls_token row of attn map
    attn_heatmap = cv2.resize(attn_heatmap,(32,32))
    sum_heatmap += attn_heatmap
avg_heatmap = sum_heatmap / num_heads
avg_heatmap = (avg_heatmap - avg_heatmap.min()) / (avg_heatmap.max() - avg_heatmap.min())

ax = fig.add_subplot(1, 5, 2)
ax.axes.get_xaxis().set_visible(False)
ax.axes.get_yaxis().set_visible(False)
ax.imshow(avg_heatmap)
ax.text(0.5, -0.15, 'Attention Map', transform=ax.transAxes, fontsize=12, ha='center')
```

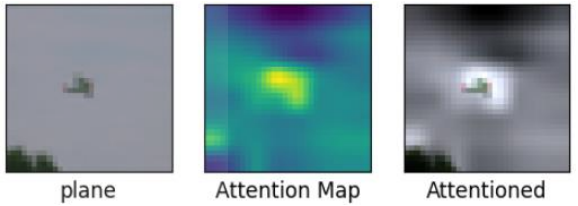
(1,2,3)

(4)

```python
# 어텐션된 이미지 시각화
attn_img = show_img.clone().detach()
attn_img[:,:,0] = (attn_img[:,:,0]*avg_heatmap)*2
attn_img[:,:,1] = (attn_img[:,:,1]*avg_heatmap)*2
attn_img[:,:,2] = (attn_img[:,:,2]*avg_heatmap)*2

ax = fig.add_subplot(1, 5, 3)
ax.axes.get_xaxis().set_visible(False)
ax.axes.get_yaxis().set_visible(False)
ax.imshow(attn_img)
ax.text(0.5, -0.15, 'Attentioned', transform=ax.transAxes, fontsize=12, ha='center')
```

(5,6)



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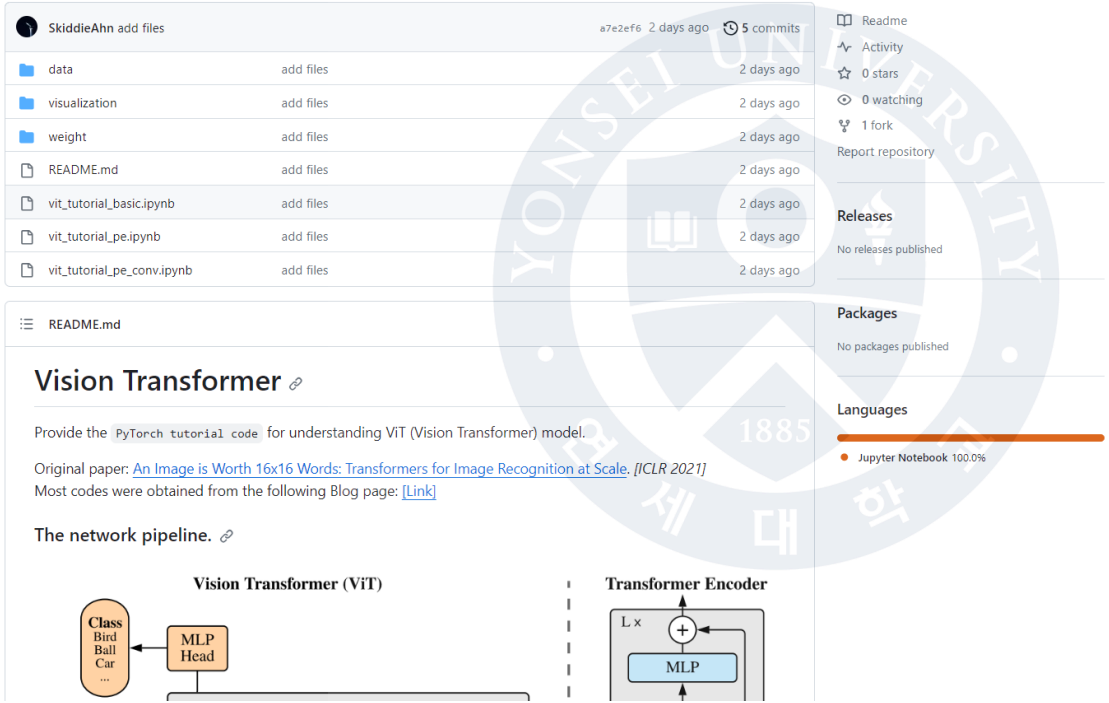
Github Code



https://github.com/ad-yonsei/Code-Vision-Transformer

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References

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Thank You

Vision Transformer - coding practice

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