Milestone Project 2

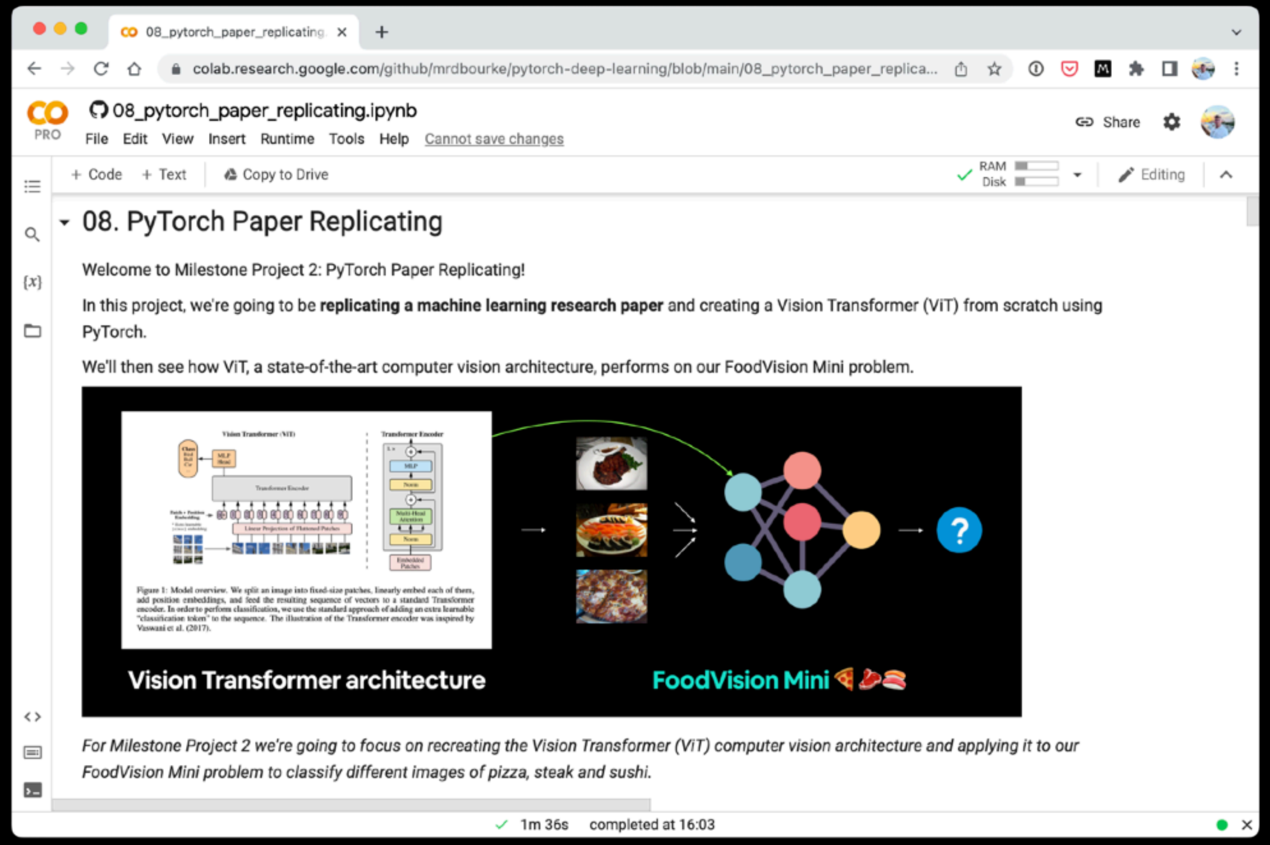
Paper Replicating with

PyTorch

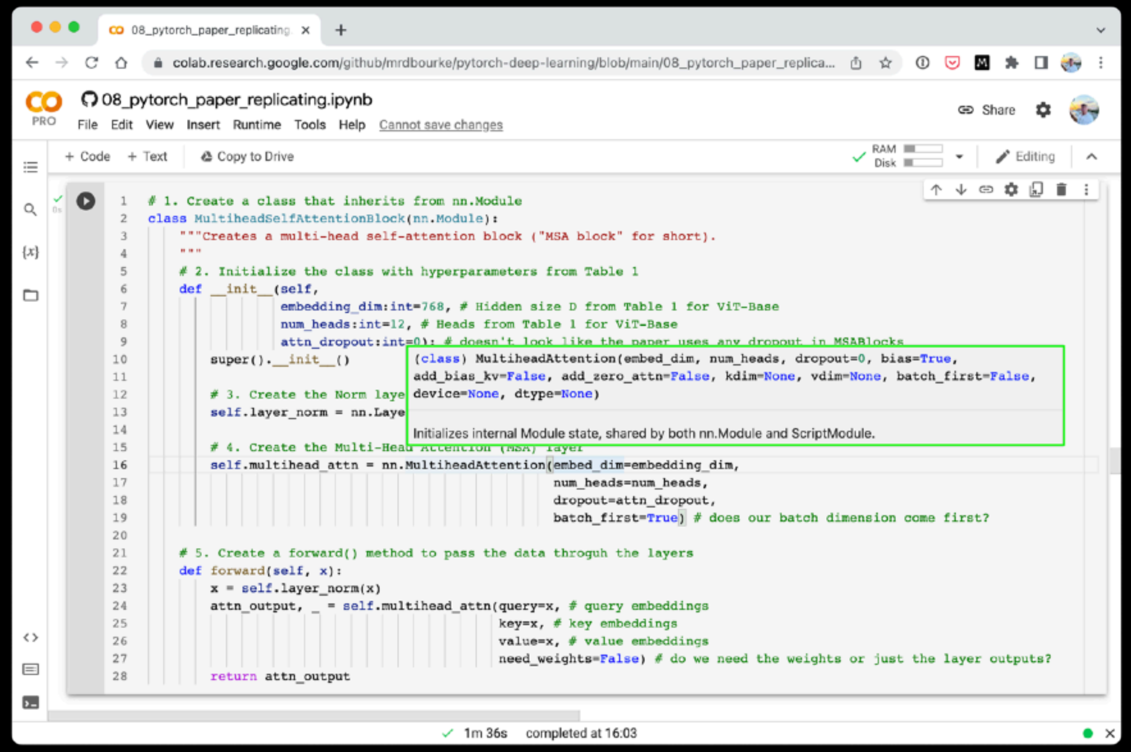
Where can you get help?

"If in doubt, run the code"

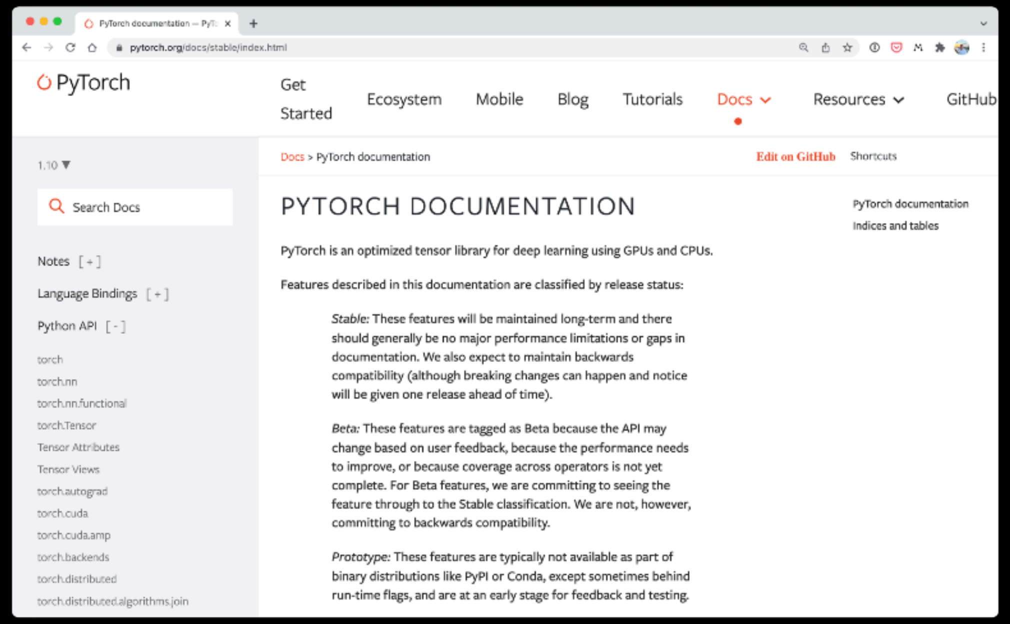
- Follow along with the code

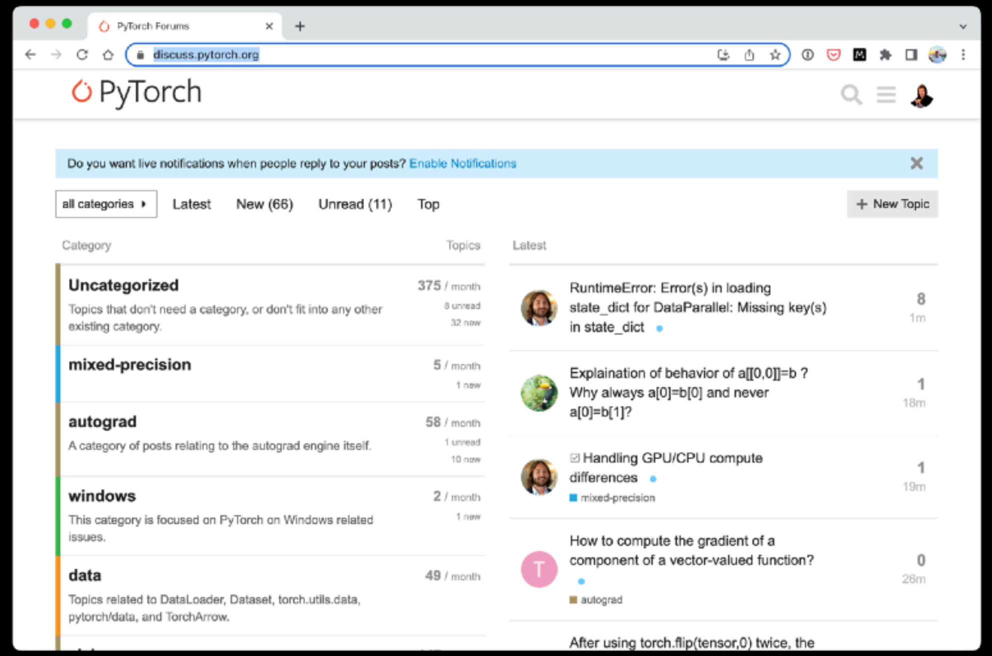


- Try it for yourself
- Press SHIFT + CMD + SPACE to read the docstring

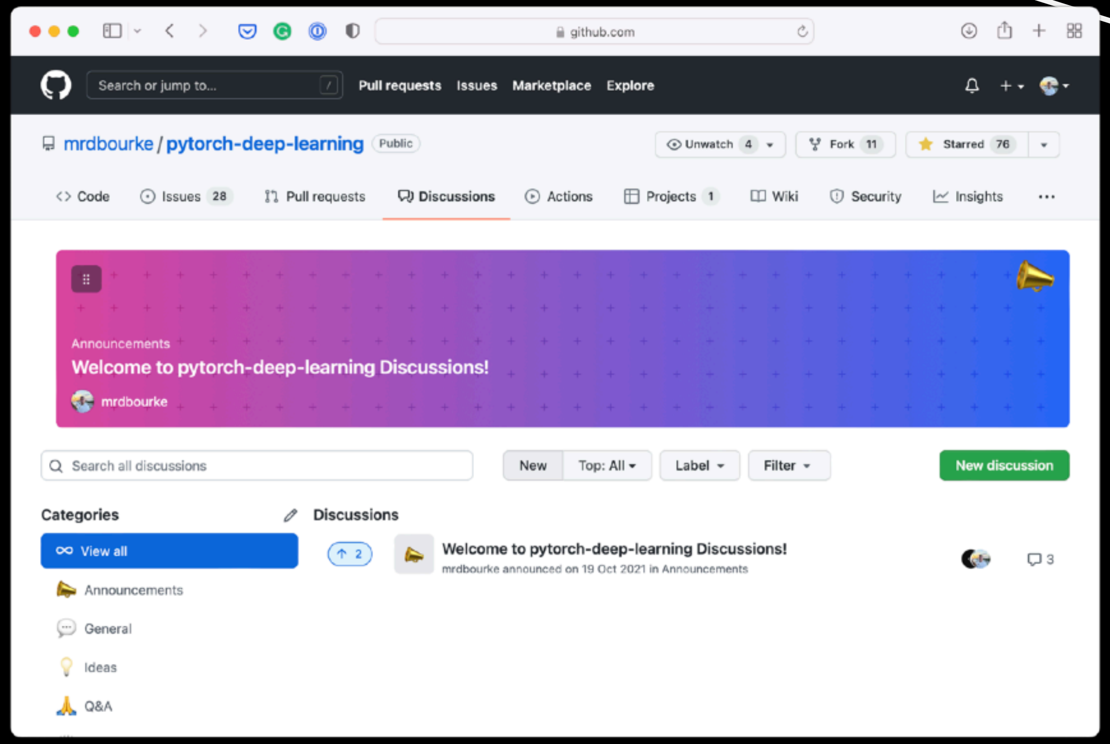


- Search for it





- Try again
- Ask



https://www.github.com/mrdbourke/pytorch-deep-learning/discussions

“What is machine learning research paper replicating?”

Turning research into usable code.

What is paper replicating?


Published as a conference paper at ICLR 2021

AN IMAGE IS WORTH 16X16 WORDS: TRANSFORMERS FOR IMAGE RECOGNITION AT SCALE

Alexey Dosovitskiy[∗,†], Lucas Beyer[∗], Alexander Kolesnikov[∗], Dirk Weissenborn[∗], Xiaohua Zhai[∗], Thomas Unterthiner, Mostafa Dehghani, Matthias Minderer, Georg Heigold, Sylvain Gelly, Jakob Uszkoreit, Neil Houlsby[∗,†]
[∗]equal technical contribution, [†]equal advising
Google Research, Brain Team
{adosovitskiy, neilhoulsby}@google.com

ABSTRACT

While the Transformer architecture has become the de-facto standard for natural language processing tasks, its applications to computer vision remain limited. In vision, attention is either applied in conjunction with convolutional networks, or used to replace certain components of convolutional networks while keeping their overall structure in place. We show that this reliance on CNNs is not necessary and a pure transformer applied directly to sequences of image patches can perform very well on image classification tasks. When pre-trained on large amounts of data and transferred to multiple mid-sized or small image recognition benchmarks (ImageNet, CIFAR-100, VTAB, etc.), Vision Transformer (ViT) attains excellent results compared to state-of-the-art convolutional networks while requiring substantially fewer computational resources to train.[1]

1 INTRODUCTION

Self-attention-based architectures, in particular Transformers (Vaswani et al., 2017), have become the model of choice in natural language processing (NLP). The dominant approach is to pre-train on a large text corpus and then fine-tune on a smaller task-specific dataset (Devlin et al., 2019). Thanks to Transformers' computational efficiency and scalability, it has become possible to train models of unprecedented size, with over 100B parameters (Brown et al., 2020; Lepikhin et al., 2020). With the models and datasets growing, there is still no sign of saturating performance.

In computer vision, however, convolutional architectures remain dominant (LeCun et al., 1989; Krizhevsky et al., 2012; He et al., 2016). Inspired by NLP successes, multiple works try combining CNN-like architectures with self-attention (Wang et al., 2018; Carion et al., 2020), some replacing the convolutions entirely (Ramachandran et al., 2019; Wang et al., 2020a). The latter models, while theoretically efficient, have not yet been scaled effectively on modern hardware accelerators due to the use of specialized attention patterns. Therefore, in large-scale image recognition, classic ResNet-like architectures are still state of the art (Mahajan et al., 2018; Xie et al., 2020; Kolesnikov et al., 2020).

Source: https://arxiv.org/pdf/2010.11929.pdf (ViT paper)

Machine learning paper

Cooking recipe

What is paper replicating?

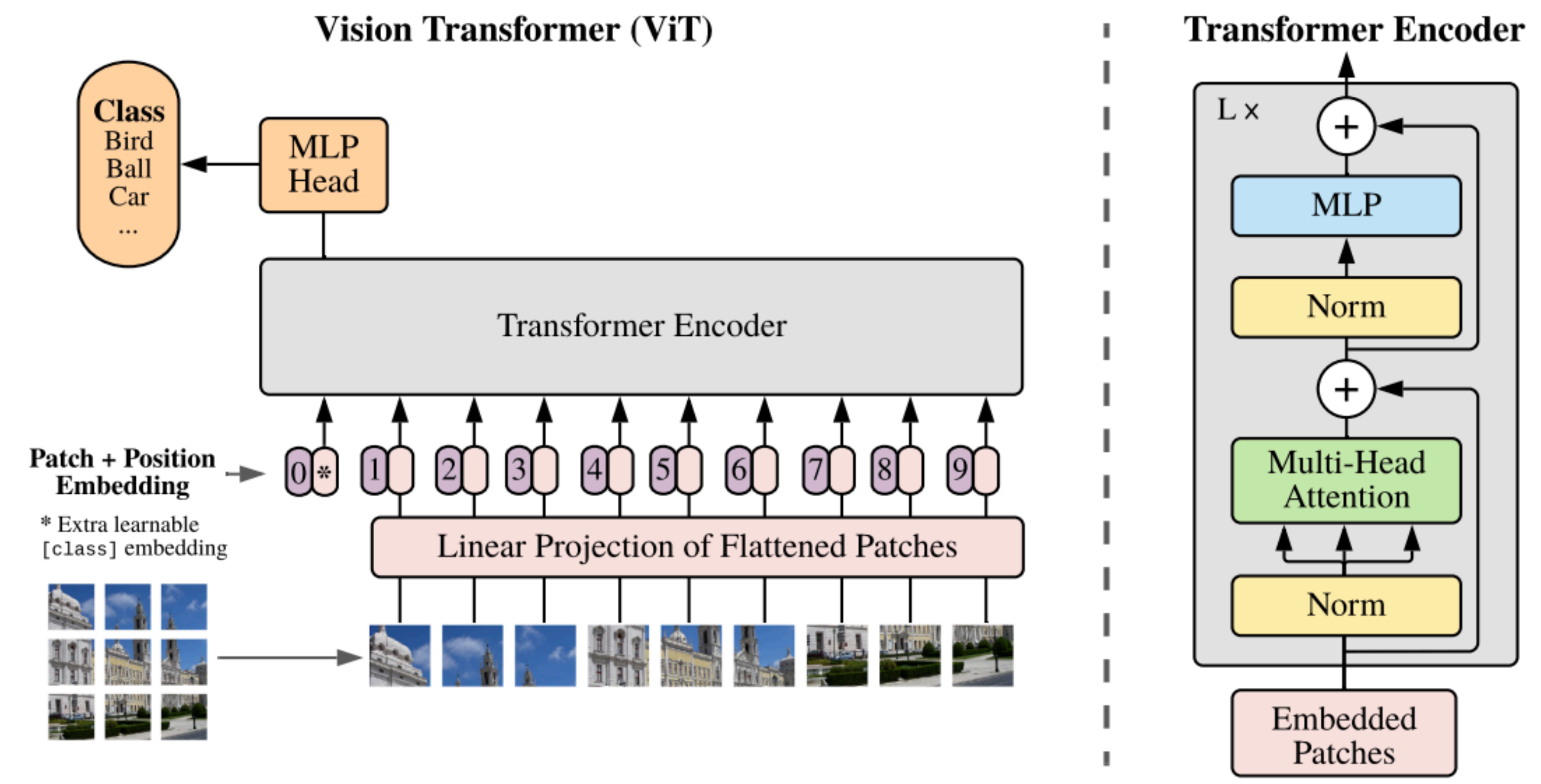


Figure 1: Model overview. We split an image into fixed-size patches, linearly embed each of them, add position embeddings, and feed the resulting sequence of vectors to a standard Transformer encoder. In order to perform classification, we use the standard approach of adding an extra learnable "classification token" to the sequence. The illustration of the Transformer encoder was inspired by Vaswani et al. (2017).

$$\mathbf{z}_0 = [\mathbf{x}_{\text{class}};\, \mathbf{x}_p^1\mathbf{E};\, \mathbf{x}_p^2\mathbf{E}; \cdots;\, \mathbf{x}_p^N\mathbf{E}] + \mathbf{E}_{pos}, \qquad \mathbf{E} \in \mathbb{R}^{(P^2 \cdot C)\times D},\, \mathbf{E}_{pos} \in \mathbb{R}^{(N+1)\times D} \tag{1}$$

$$\mathbf{z'}_\ell = \mathrm{MSA}(\mathrm{LN}(\mathbf{z}_{\ell-1})) + \mathbf{z}_{\ell-1}, \qquad \ell = 1 \ldots L \tag{2}$$

$$\mathbf{z}_\ell = \mathrm{MLP}(\mathrm{LN}(\mathbf{z'}_\ell)) + \mathbf{z'}_\ell, \qquad \ell = 1 \ldots L \tag{3}$$

$$\mathbf{y} = \mathrm{LN}(\mathbf{z}_L^0) \tag{4}$$

The Transformer encoder (Vaswani et al., 2017) consists of alternating layers of multiheaded self-attention (MSA, see Appendix A) and MLP blocks (Eq. 2, 3). Layernorm (LN) is applied before every block, and residual connections after every block (Wang et al., 2019; Baevski & Auli, 2019).

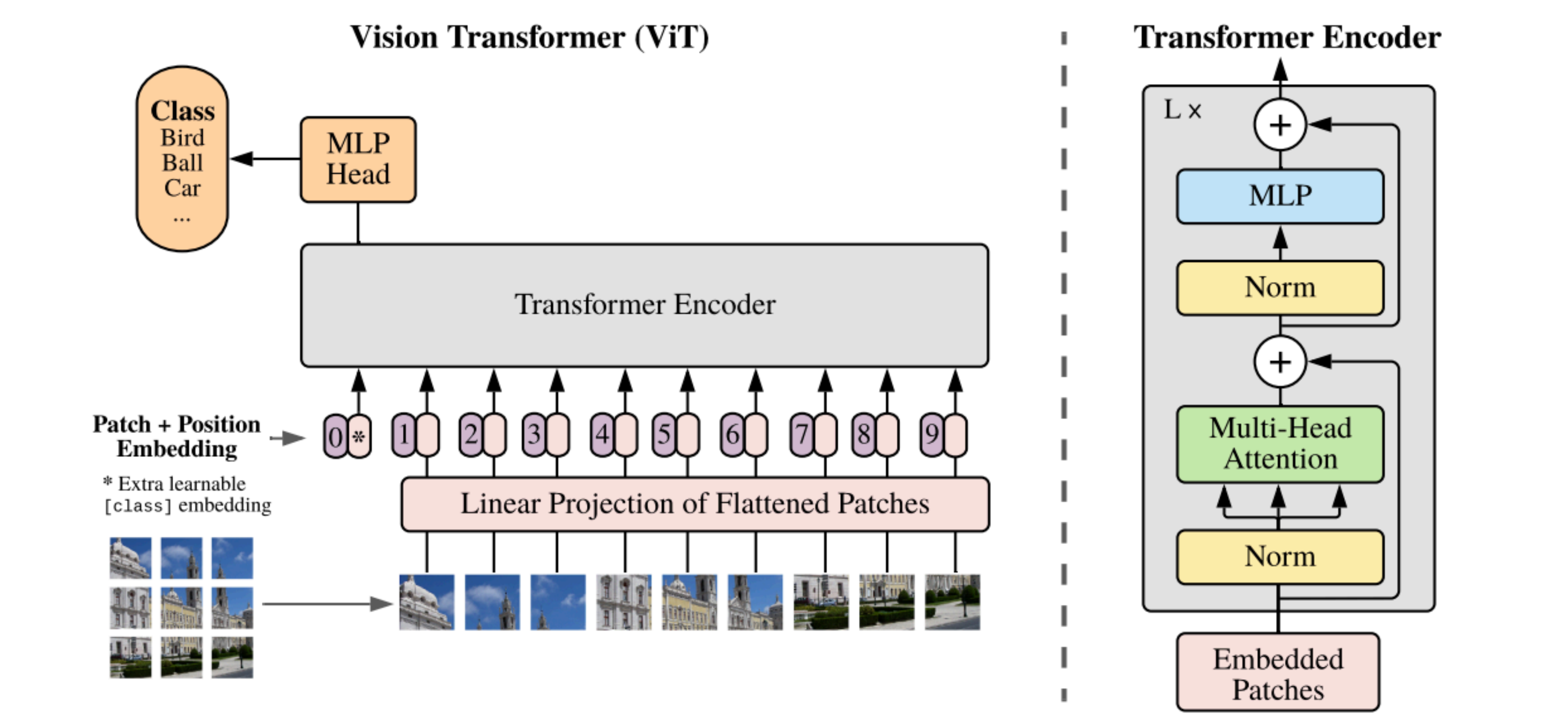
Source: ViT paper

```python
import torch as nn

class ViT(nn.Module):
    """Creates a Vision Transformer architecture with ViT-Base hyperparameters by default."""
    def __init__(self,
                 img_size:int=224, # Training resolution from Table 3 in ViT paper
                 in_channels:int=3, # Number of channels in input image
                 patch_size:int=16, # Patch size
                 num_transformer_layers:int=12, # Layers from Table 1 for ViT-Base
                 embedding_dim:int=768, # Hidden size D from Table 1 for ViT-Base
                 mlp_size:int=3072, # MLP size from Table 1 for ViT-Base
                 num_heads:int=12, # Heads from Table 1 for ViT-Base
                 num_classes:int=1000): # Default for ImageNet but can customize this
        super().__init__()

        self.patch_embedding = PatchEmbedding(in_channels=in_channels,
                                              patch_size=patch_size,
                                              embedding_dim=embedding_dim)

        self.transformer_enedoder = nn.Sequential(*[TransformerEncoderBlock(embedding_dim=embedding_dim,
                                                                            num_heads=num_heads,
                                                                            mlp_size=mlp_size) for _ in range(num_transformer_layers)])

        self.classifier = nn.Sequential(
            nn.Linear(in_features=embedding_dim, out_features=num_classes)
        )

    def forward(self, x):
        x = self.patch_embedding(x)
        x = self.transformer_enedoder(x)
        return self.classifier(x[:, 0])

# Create ViT
vit = ViT()
```

Images + math + text

Usable code

Terminology



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Source: ViT paper

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

Alexey Dosovitskiy*,†, Lucas Beyer*, Alexander Kolesnikov*, Dirk Weissenborn*, Xiaohua Zhai*, Thomas Unterthiner, Mostafa Dehghani, Matthias Minderer, Georg Heigold, Sylvain Gelly, Jakob Uszkoreit, Neil Houlsby*,†
*equal technical contribution, †equal advising
Google Research, Brain Team
{adosovitskiy, neilhoulsby}@google.com

Abstract

While the Transformer architecture has become the de-facto standard for natural language processing tasks, its applications to computer vision remain limited. In vision, attention is either applied in conjunction with convolutional networks, or used to replace certain components of convolutional networks while keeping their overall structure in place. We show that this reliance on CNNs is not necessary and a pure transformer applied directly to sequences of image patches can perform very well on image classification tasks. When pre-trained on large amounts of data and transferred to multiple mid-sized or small image recognition benchmarks (ImageNet, CIFAR-100, VTAB, etc.), Vision Transformer (ViT) attains excellent results compared to state-of-the-art convolutional networks while requiring substantially fewer computational resources to train.[1]

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Vision Transformer (ViT) architecture

ViT paper

“Why replicate machine learning research papers?”

1. It’s fun… and…

```
Machine Learning Engineer*
----

1. Download a paper
2. Implement it
3. Keep doing this until you have skills
```

- George Hotz, founder of comma.ai

*Machine Learning Engineering also involves building infrastructure around your models/ data preprocessing steps

“What is a machine learning research paper?”

Anatomy of a research paper*

(and many other kinds of scientific papers)

Section	What is it?
Abstract	An **overview/summary** of the paper's main findings/contributions.
Introduction	What's the paper's **main problem**? And details of previous methods used to try and solve it.
Method	What **steps did the researchers take** when conducting their research? For example, what model(s), data sources, training setups were used?
Results	What are the **outcomes** of the paper? If a new type of model or training setup was used, how did the results of findings compare to previous works? (this is where experiment tracking comes in handy)
Conclusion	What are the **limitations** of the suggested methods? What are some next steps for the research community?
References	What **resources/other papers** did the researchers look at to build their own body of work?
Appendix	Are there any **extra resources/findings** to look at that weren't included in any of the above sections?

*This structure is quite fluid. It's more of a general guide than a required outline.

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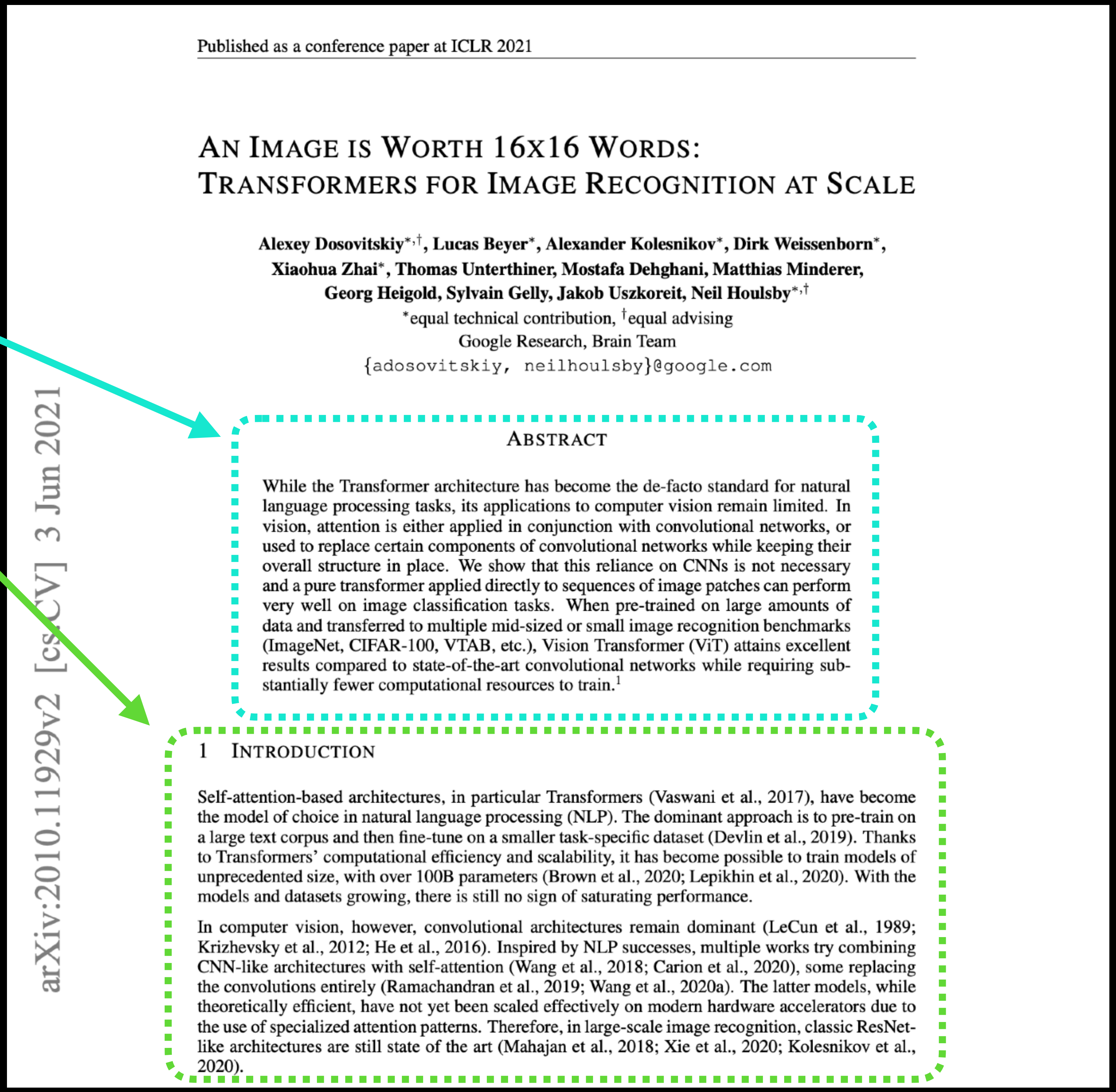

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*equal technical contribution, †equal advising

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arXiv:2010.11929v2 [cs.CV] 3 Jun 2021

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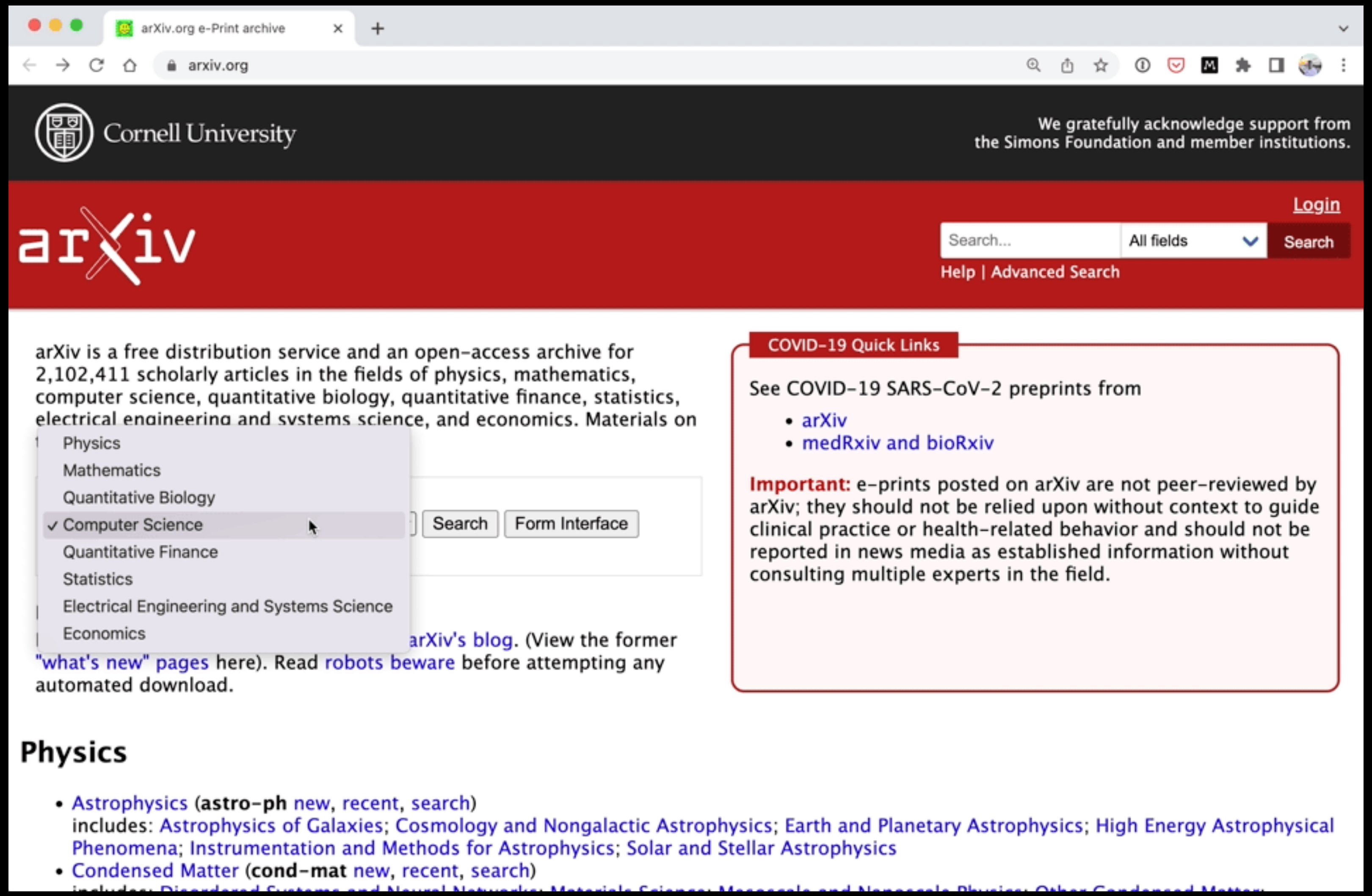
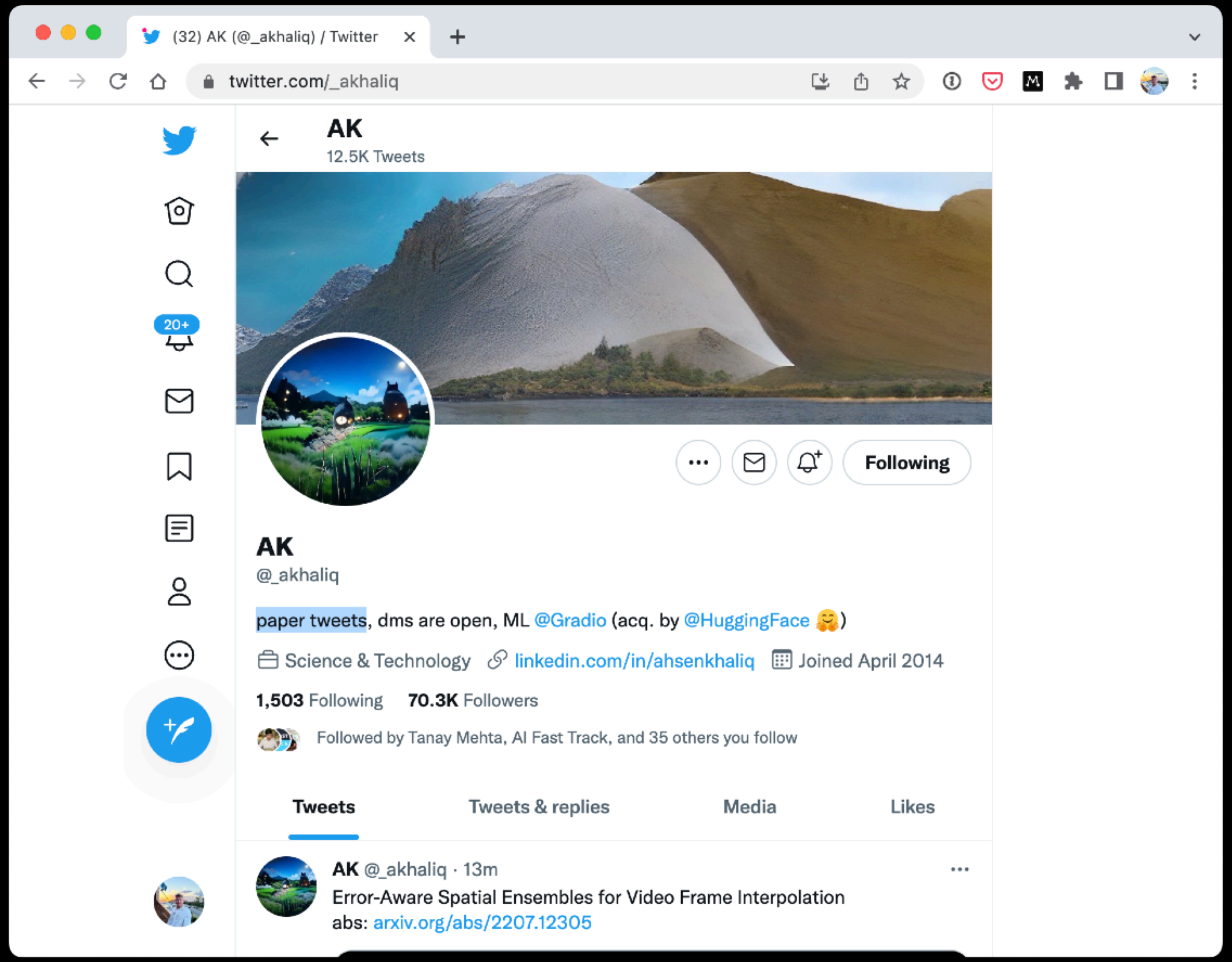
ViT paper

“Where can you find machine learning research papers?”

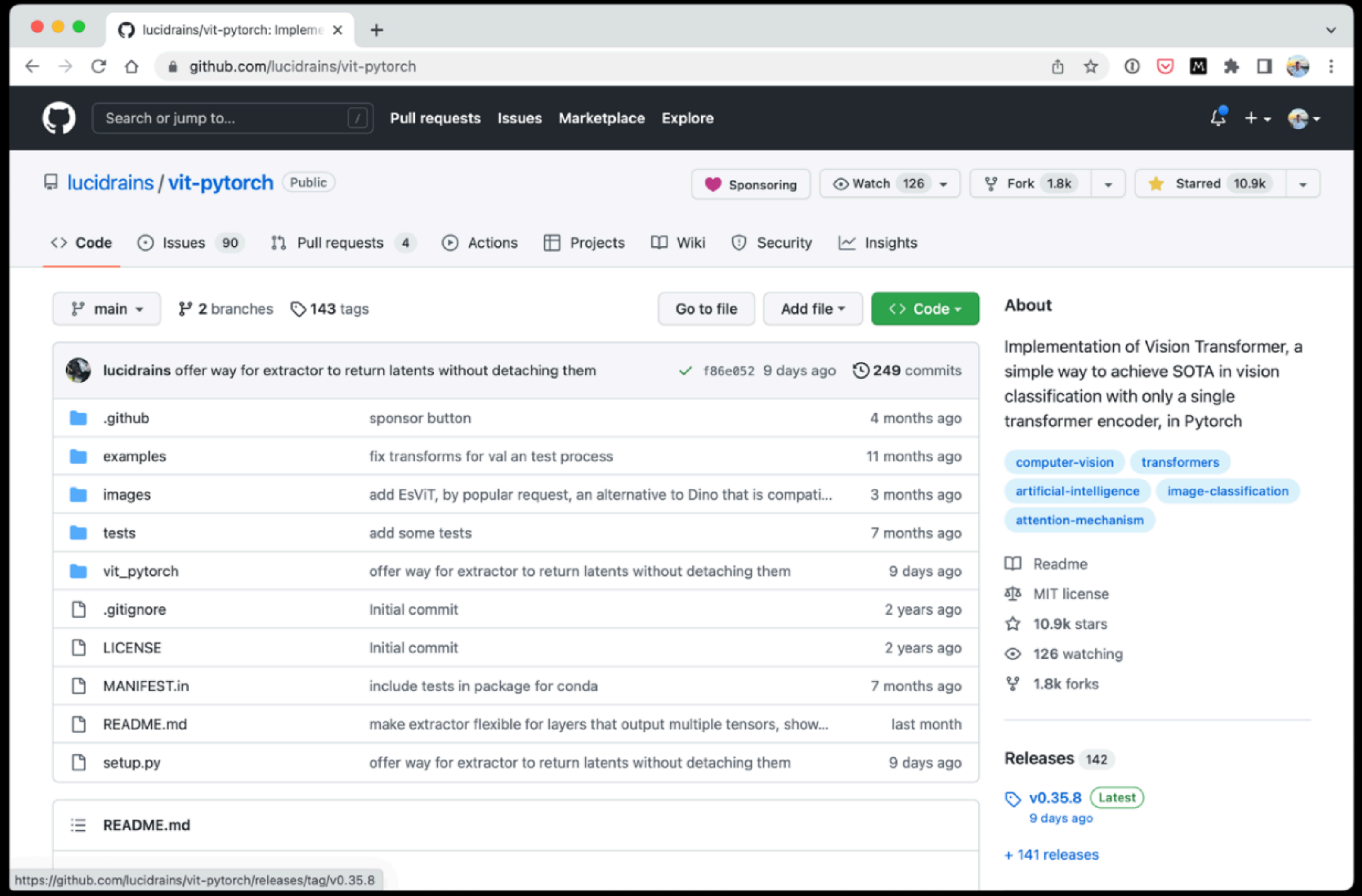
Finding machine learning papers
(and code)



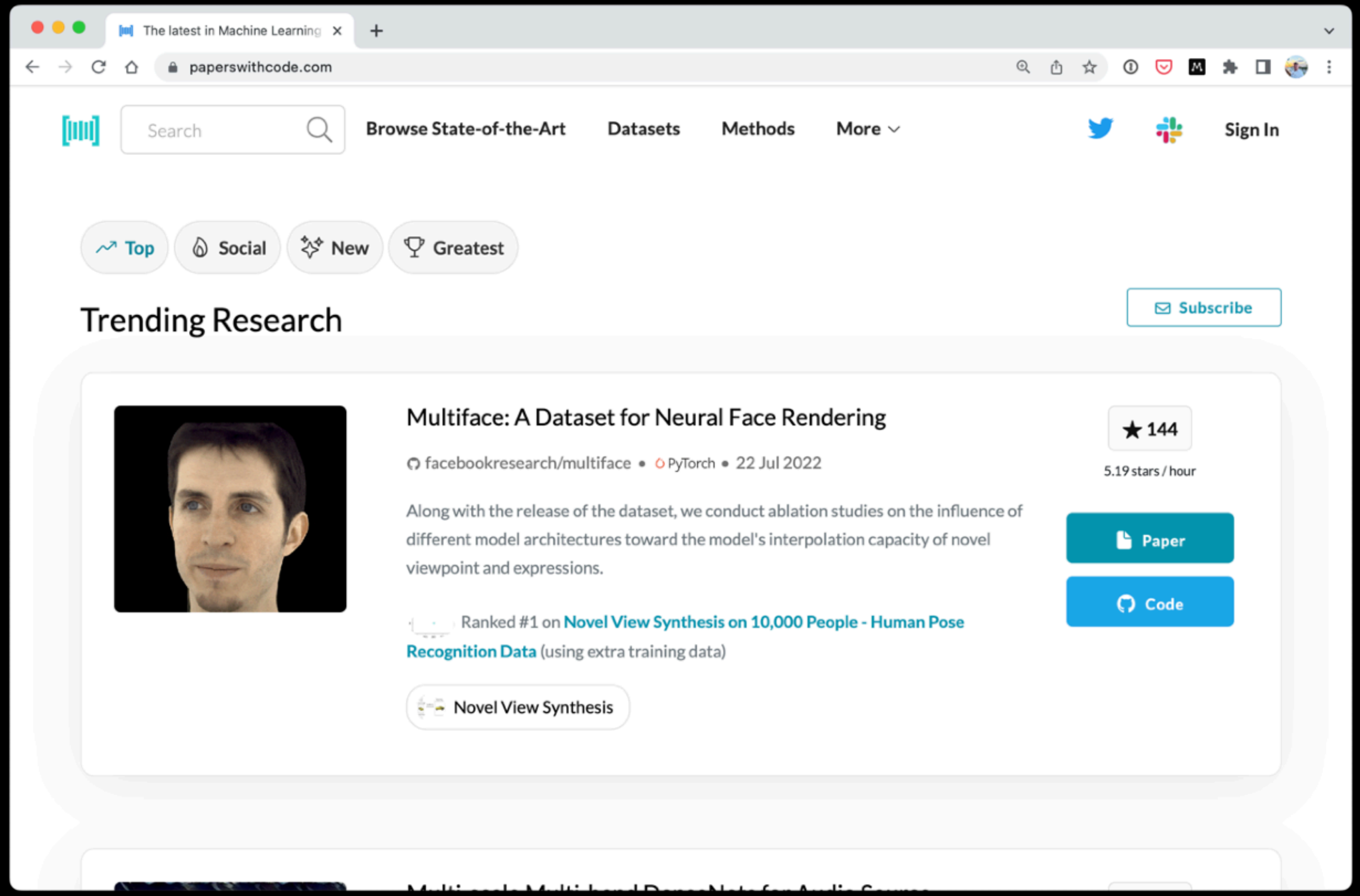
Source: https://arxiv.org/



Source: AK Twitter



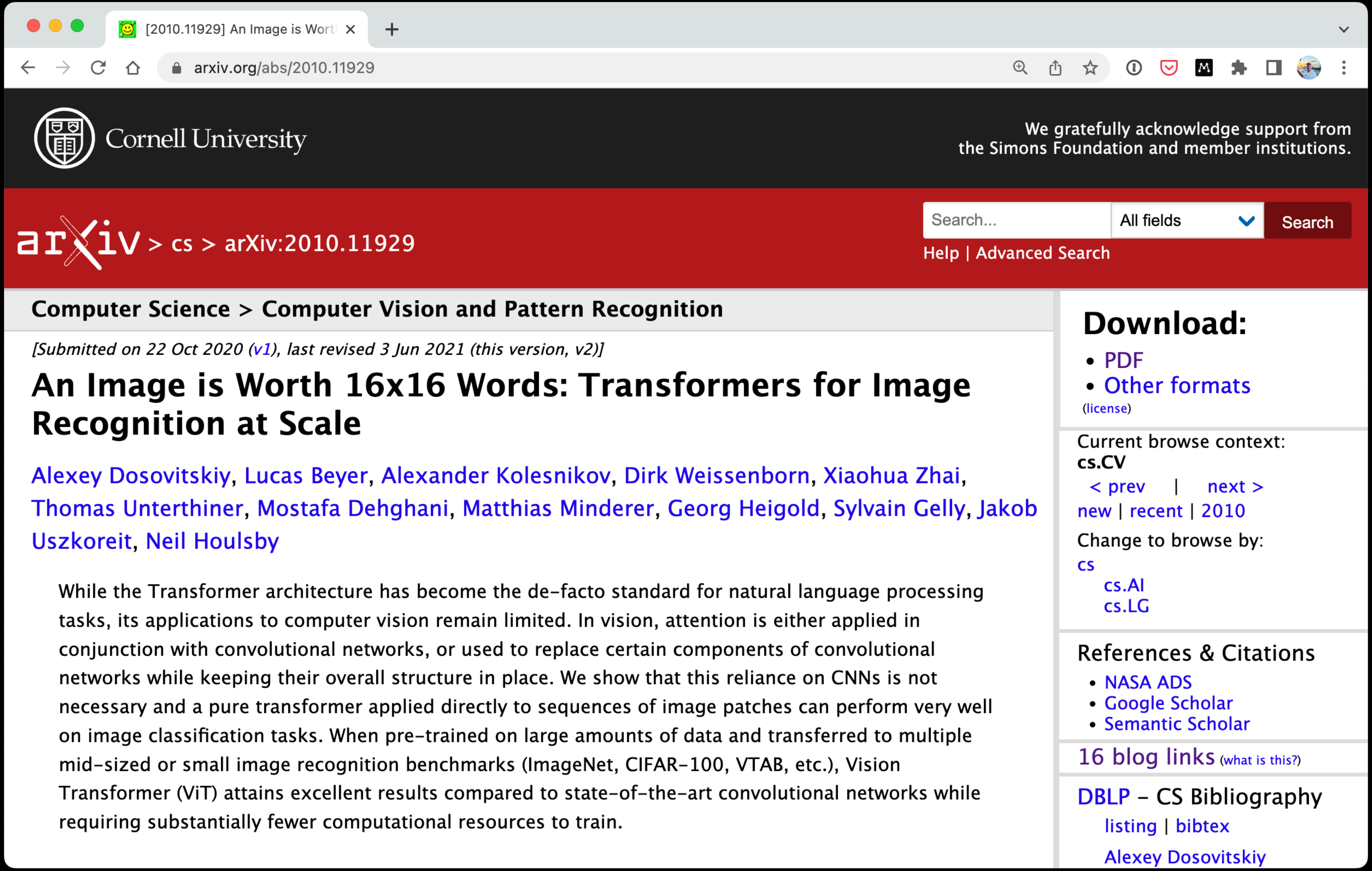
Source: https://github.com/lucidrains/vit-pytorch



Source: https://paperswithcode.com/

What we're doing

Replicating the **Vision Transformer** paper (ViT paper)



Source: ViT paper

Machine Learning vs. Deep Learning

(common algorithms)

- Random forest
- Gradient boosted models
- Naive Bayes
- Nearest neighbour
- Support vector machine
- ...many more

(since the advent of deep learning these are often referred to as "shallow algorithms")

- Neural networks
- Fully connected neural network
- Convolutional neural network
- Recurrent neural network
- Transformer
- ...many more

What we're focused on building (with PyTorch)

(depending how you represent your problem, many algorithms can be used for both)

Structured data ⟷ **Unstructured data**

Machine Learning vs. Deep Learning

(common algorithms)

Source: Photo by John Tubelleza

- Neural networks
- Fully connected neural network
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- ...many more

What we're focused on building (with PyTorch)

Unstructured data

Machine Learning vs. Deep Learning
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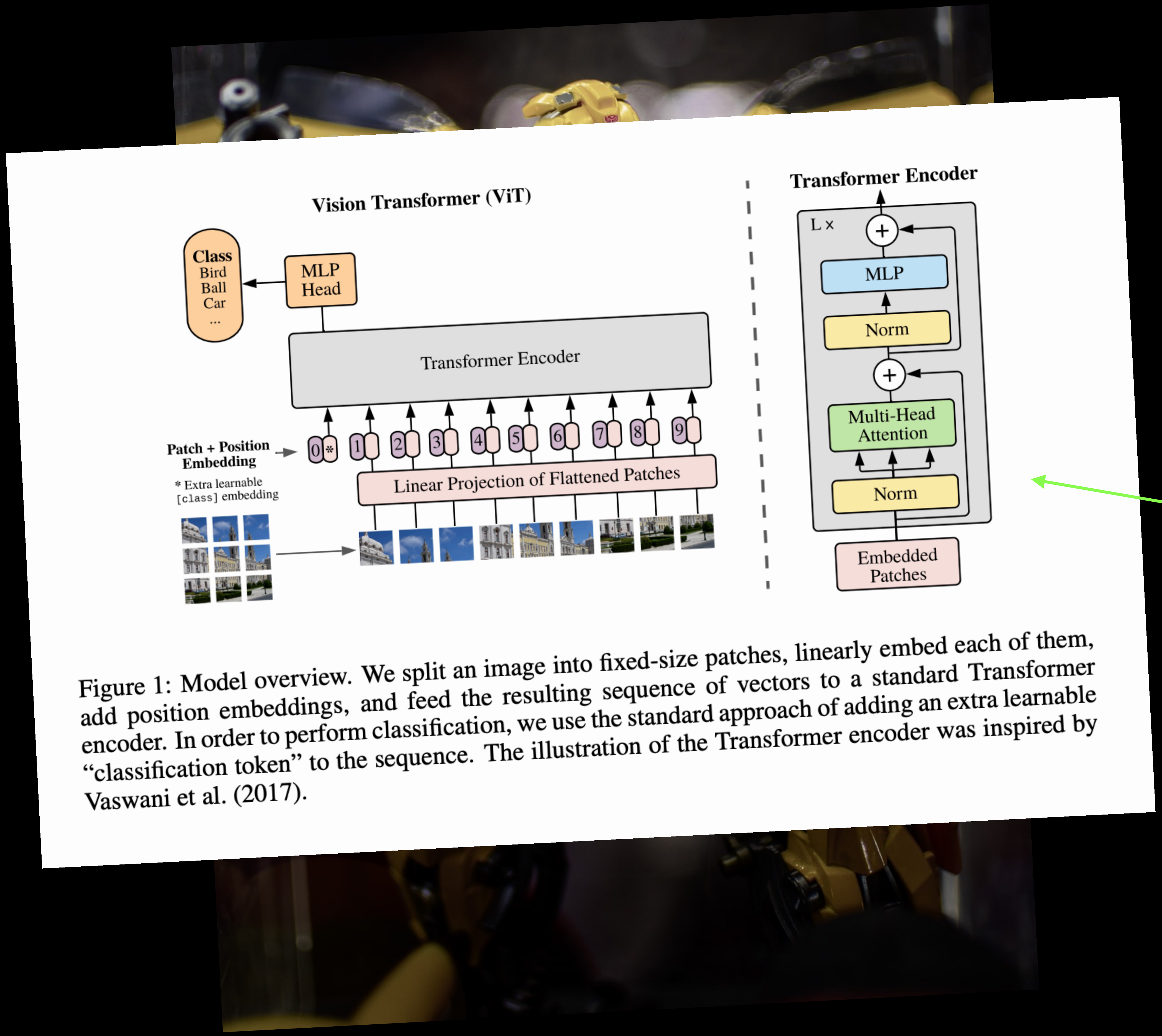

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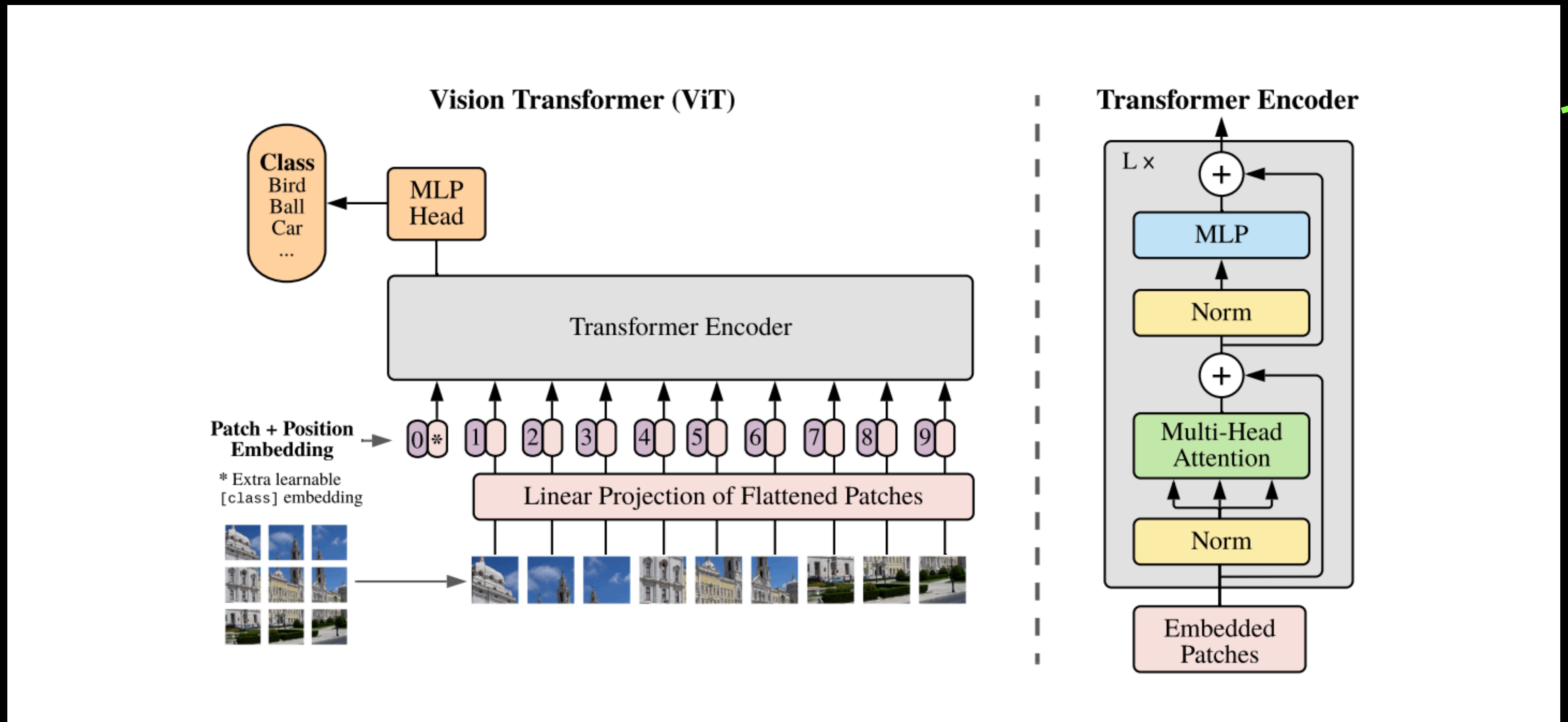
What we're doing



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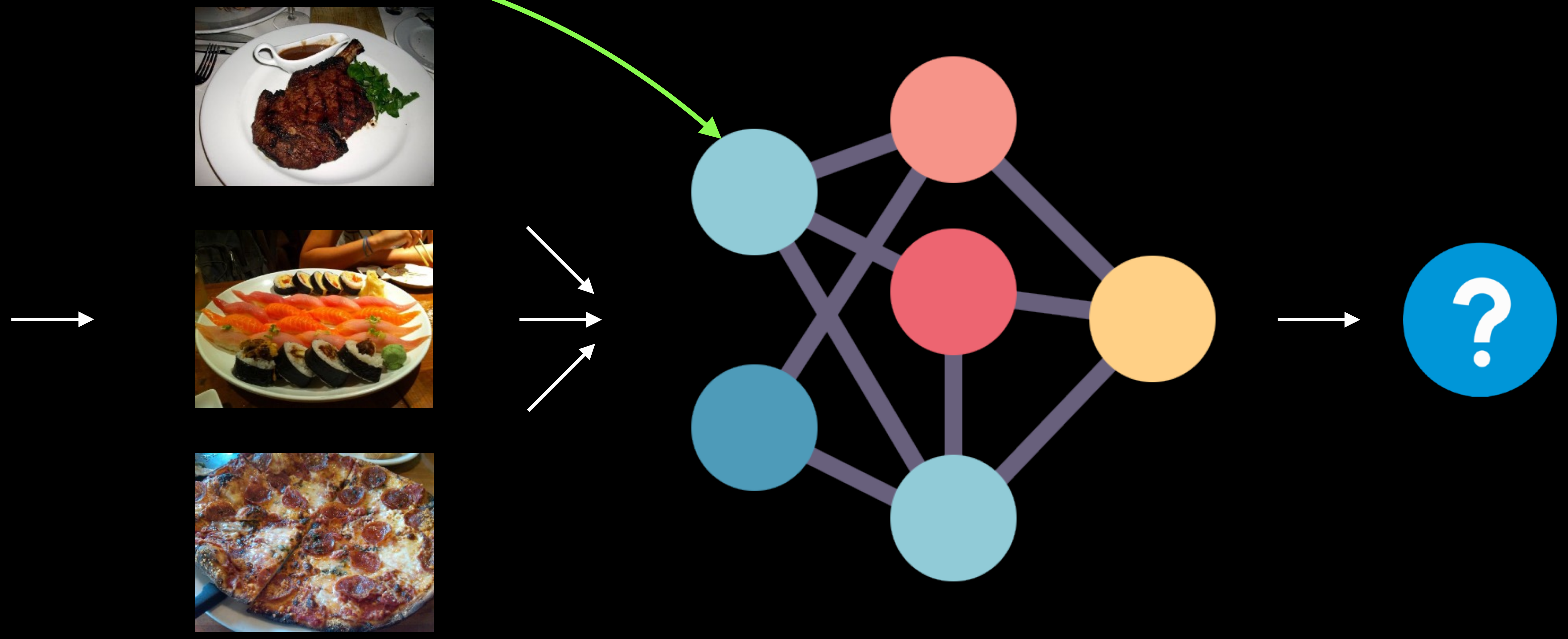
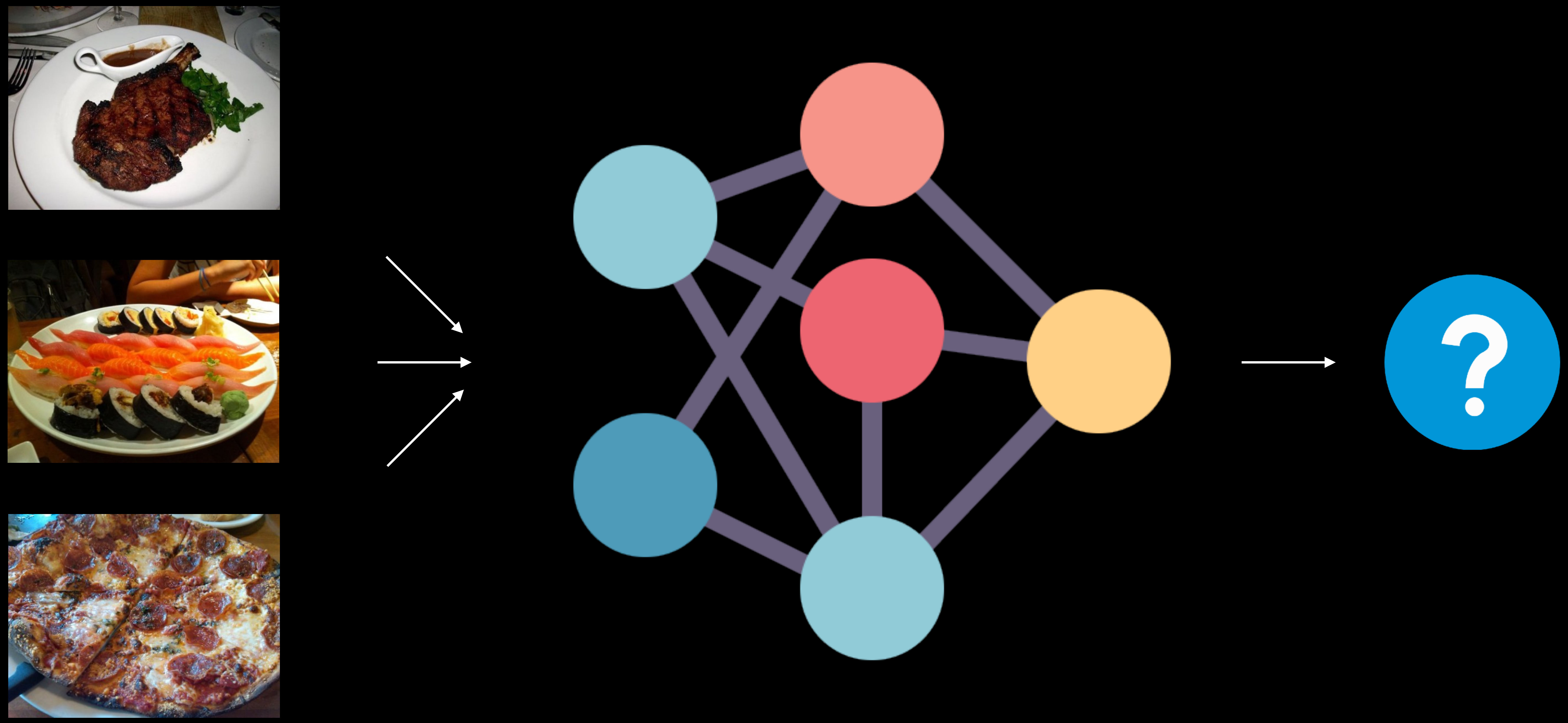


Vision Transformer architecture

FoodVision Mini 🍕🥩🍣

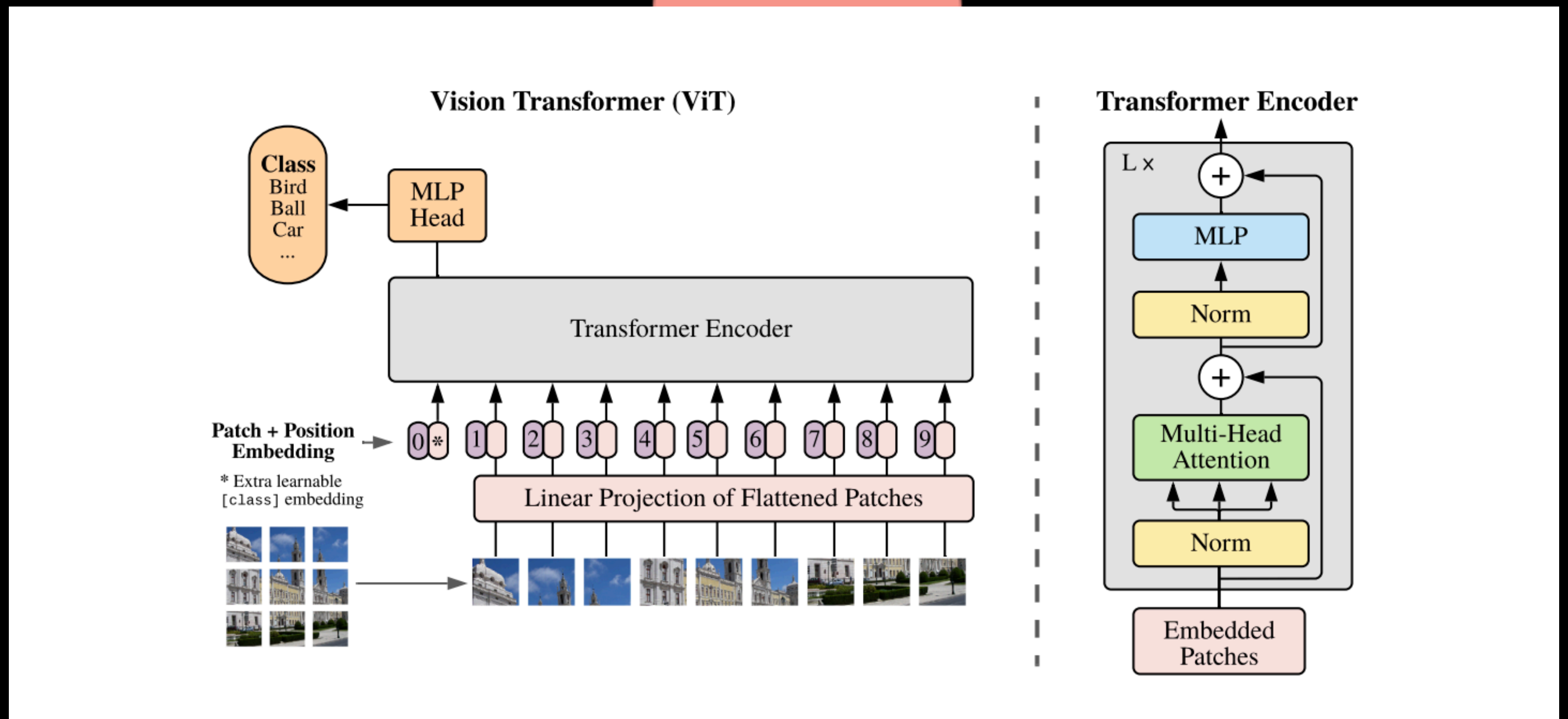
What we’re doing



FoodVision Mini 🍕🥩🍣

What we're doing

Original ViT Architecture



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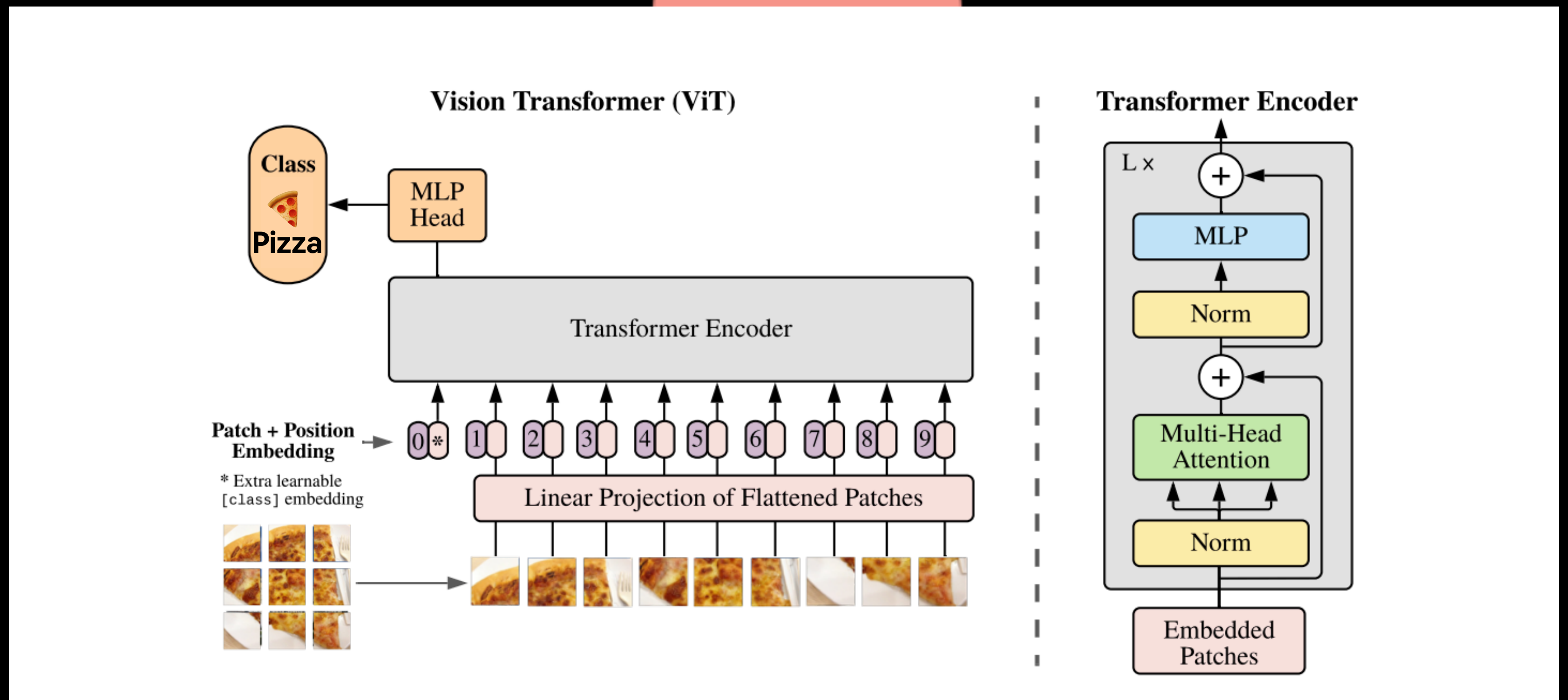
Source: ViT paper

FoodVision Mini 🍕🥩🍣

What we're doing

ViT adapted to FoodVision Mini



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FoodVision Mini 🍕🥩🍣

What we're going to cover

(broadly)

- Getting setup (importing previously written code)
- Introduce machine learning paper replicating with PyTorch
- Replicating ViT for FoodVision Mini 🍕🥩🍣
- Training a custom ViT
- Feature extraction with a pretrained ViT

(we'll be cooking up lots of code!)

How: 👩‍🍳 👩‍🔬

Let’s code!

Image size and batch size

Models	Dataset	Epochs	Base LR	LR decay	Weight decay	Dropout
ViT-B/{16,32}	JFT-300M	7	$8 \cdot 10^{-4}$	linear	0.1	0.0
ViT-L/32	JFT-300M	7	$6 \cdot 10^{-4}$	linear	0.1	0.0
ViT-L/16	JFT-300M	7/14	$4 \cdot 10^{-4}$	linear	0.1	0.0
ViT-H/14	JFT-300M	14	$3 \cdot 10^{-4}$	linear	0.1	0.0
R50x{1,2}	JFT-300M	7	10^{-3}	linear	0.1	0.0
R101x1	JFT-300M	7	$8 \cdot 10^{-4}$	linear	0.1	0.0
R152x{1,2}	JFT-300M	7	$6 \cdot 10^{-4}$	linear	0.1	0.0
R50+ViT-B/{16,32}	JFT-300M	7	$8 \cdot 10^{-4}$	linear	0.1	0.0
R50+ViT-L/32	JFT-300M	7	$2 \cdot 10^{-4}$	linear	0.1	0.0
R50+ViT-L/16	JFT-300M	7/14	$4 \cdot 10^{-4}$	linear	0.1	0.0
ViT-B/{16,32}	ImageNet-21k	90	10^{-3}	linear	0.03	0.1
ViT-L/{16,32}	ImageNet-21k	30/90	10^{-3}	linear	0.03	0.1
ViT-$*$	ImageNet	300	$3 \cdot 10^{-3}$	cosine	0.3	0.1

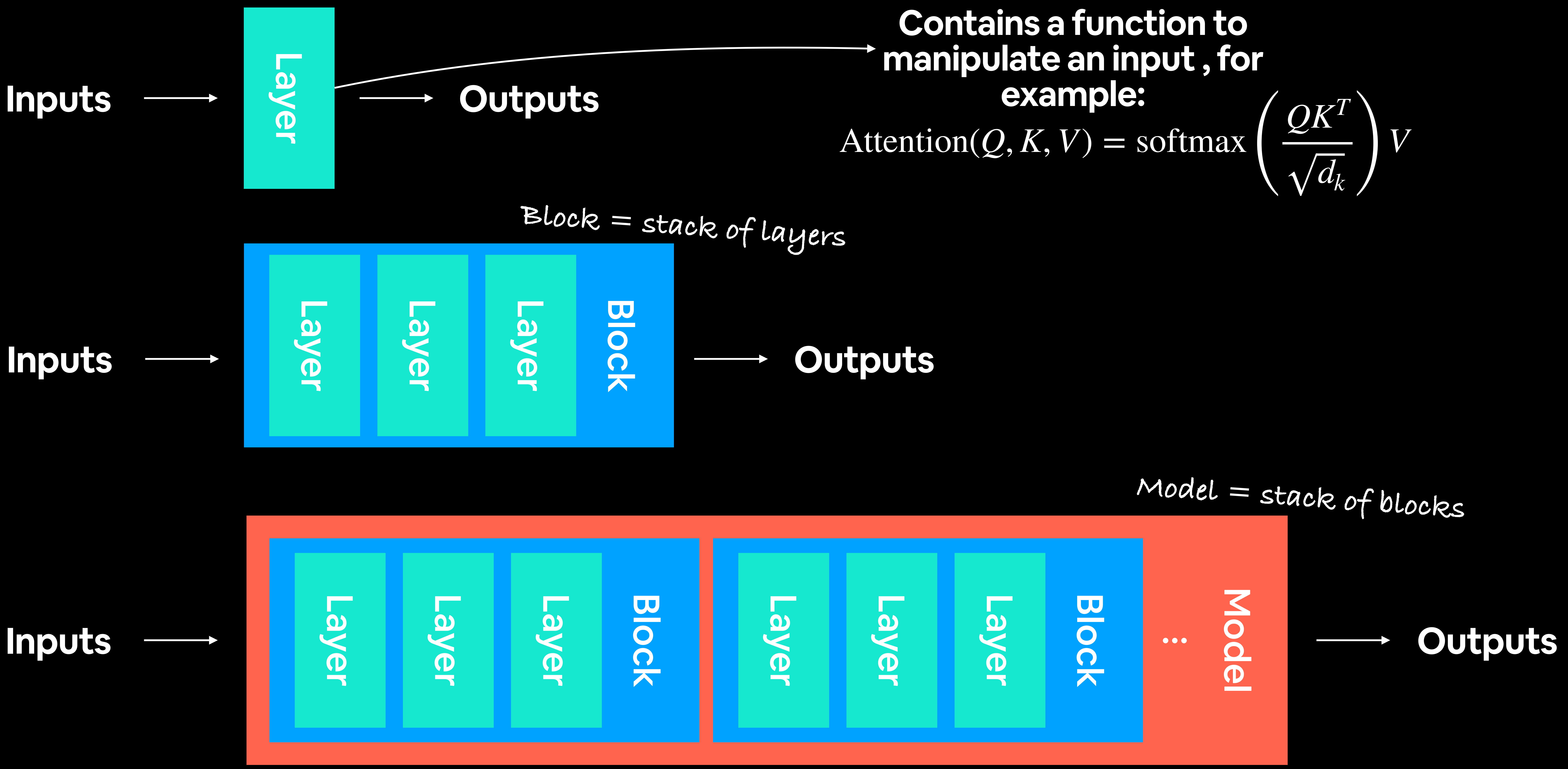
Table 3: Hyperparameters for training. All models are trained with a batch size of 4096 and learning rate warmup of 10k steps. For ImageNet we found it beneficial to additionally apply gradient clipping at global norm 1. Training resolution is 224.

Batch size = 4096

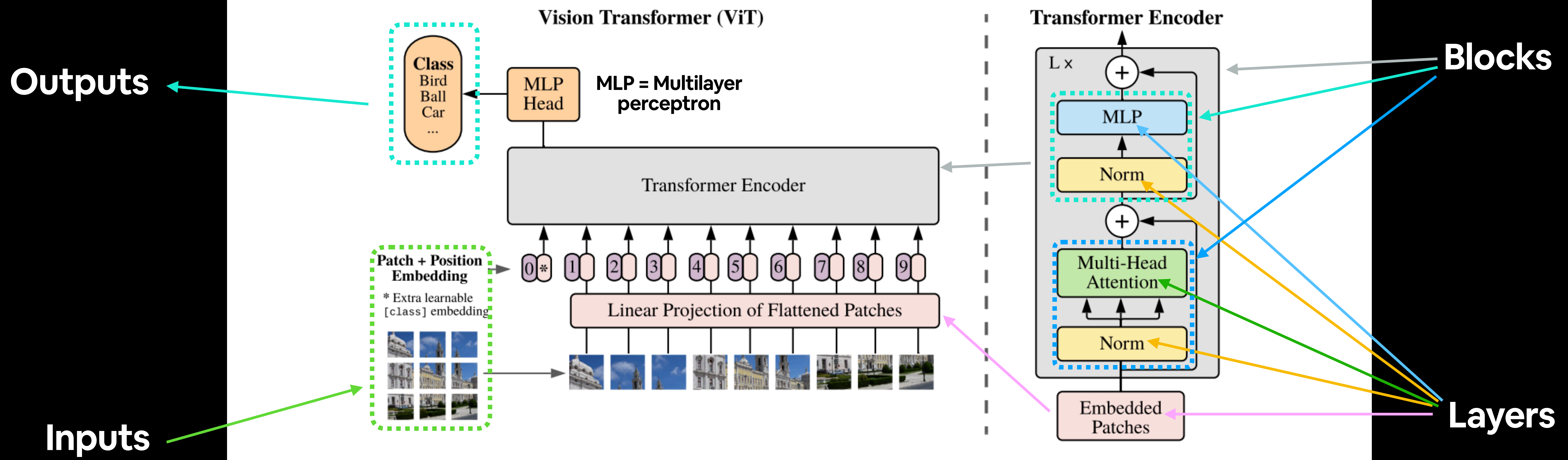
Source: ViT paper

Image size = 224x224 (height=224, width=224)

Inputs, outputs, layers and blocks



ViT Overview: Inputs and Outputs



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Source: ViT paper

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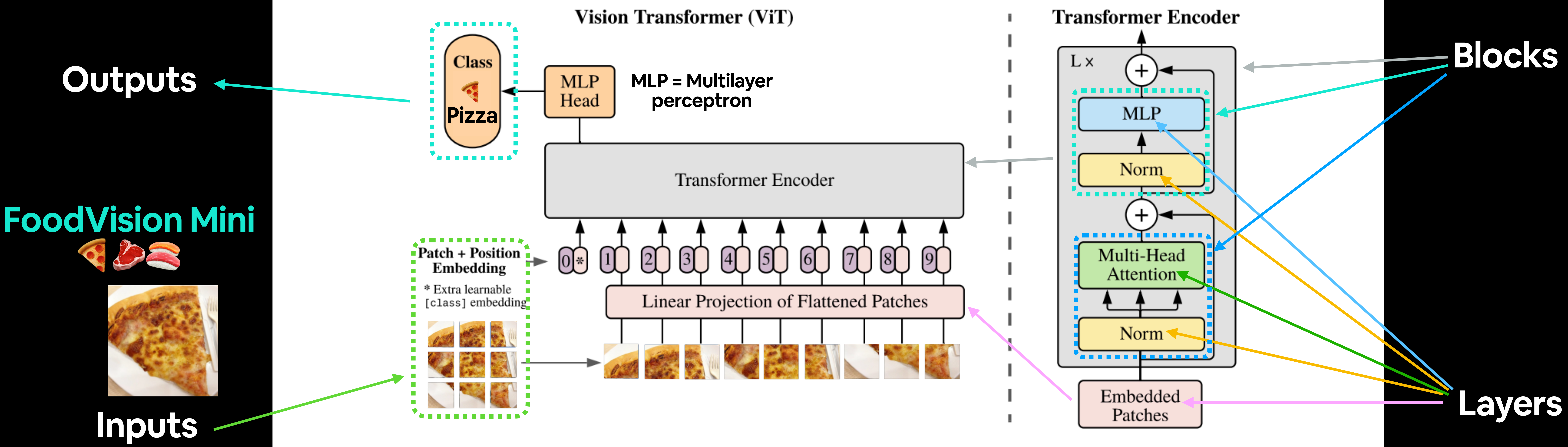

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Source: ViT paper

ViT Overview: Four Equations

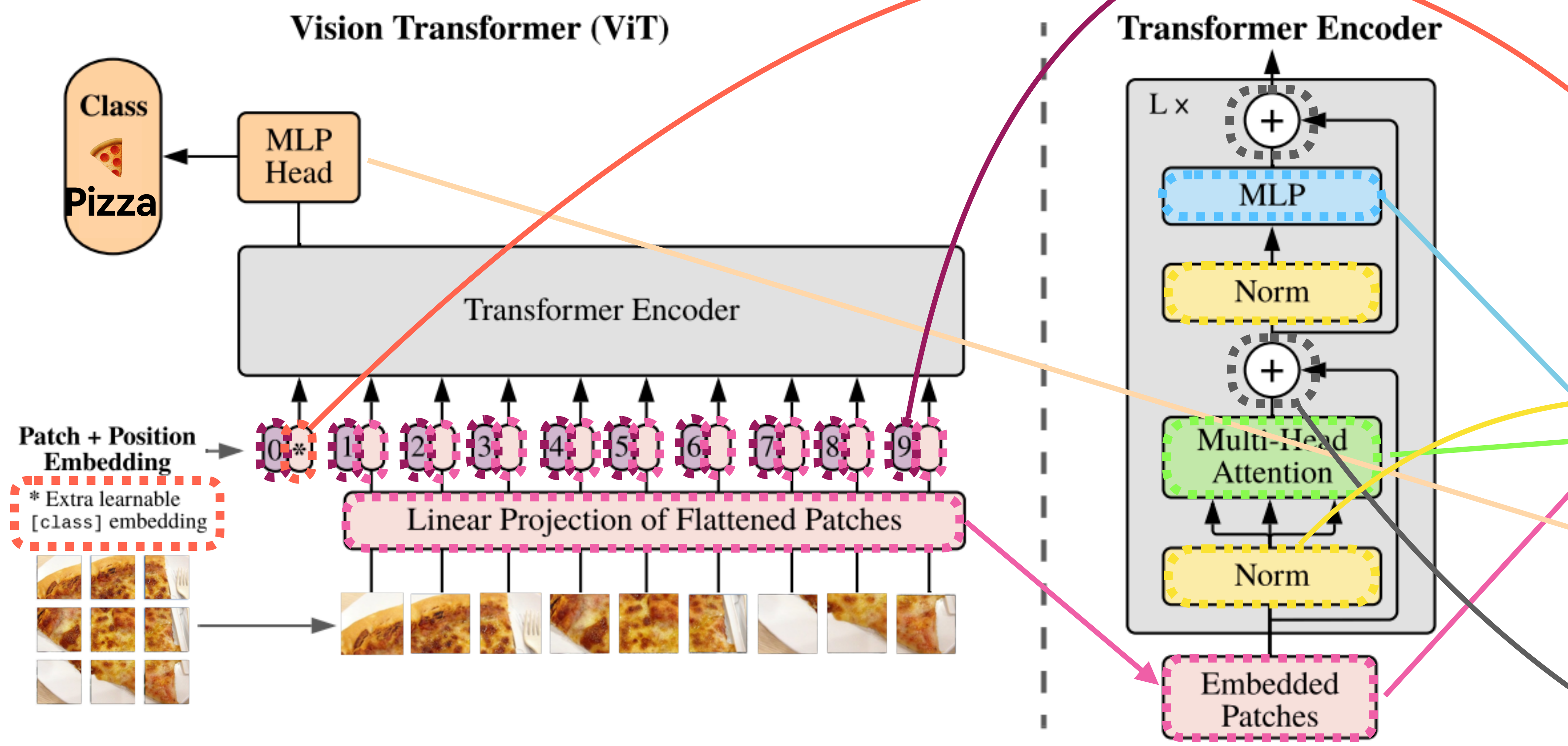


Figure 1: Model overview. We split an image into fixed-size patches, linearly embed each of them, add position embeddings, and feed the resulting sequence of vectors to a standard Transformer encoder. In order to perform classification, we use the standard approach of adding an extra learnable "classification token" to the sequence. The illustration of the Transformer encoder was inspired by Vaswani et al. (2017).

Source: ViT paper Figure 1

$$\mathbf{z}_0 = [\mathbf{x}_{\text{class}}; \mathbf{x}_p^1\mathbf{E}; \mathbf{x}_p^2\mathbf{E}; \cdots; \mathbf{x}_p^N\mathbf{E}] + \mathbf{E}_{pos}, \qquad \mathbf{E} \in \mathbb{R}^{(P^2 \cdot C)\times D},\ \mathbf{E}_{pos} \in \mathbb{R}^{(N+1)\times D} \tag{1}$$

$$\mathbf{z}'_\ell = \text{MSA}(\text{LN}(\mathbf{z}_{\ell-1})) + \mathbf{z}_{\ell-1}, \qquad \ell = 1 \ldots L \tag{2}$$

$$\mathbf{z}_\ell = \text{MLP}(\text{LN}(\mathbf{z}'_\ell)) + \mathbf{z}'_\ell, \qquad \ell = 1 \ldots L \tag{3}$$

$$\mathbf{y} = \text{LN}(\mathbf{z}_L^0) \tag{4}$$

The Transformer encoder (Vaswani et al., 2017) consists of alternating layers of multiheaded self-attention (MSA, see Appendix A) and MLP blocks (Eq. 2, 3). Layernorm (LN) is applied before every block, and residual connections after every block (Wang et al., 2019; Baevski & Auli, 2019).

Source: ViT paper section 3.1

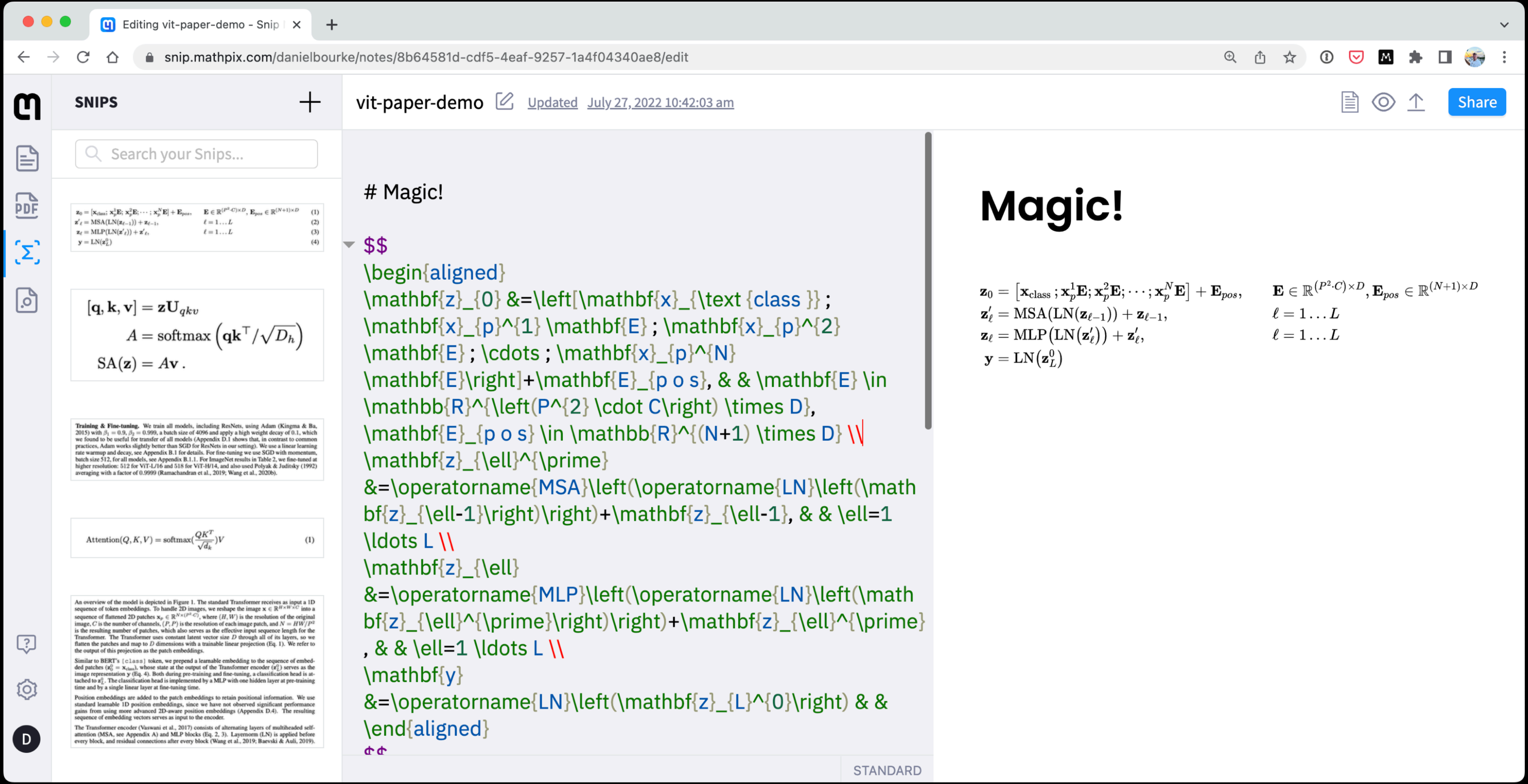
ViT Overview: Workflow

visualize, visualize, visualize!

Original image

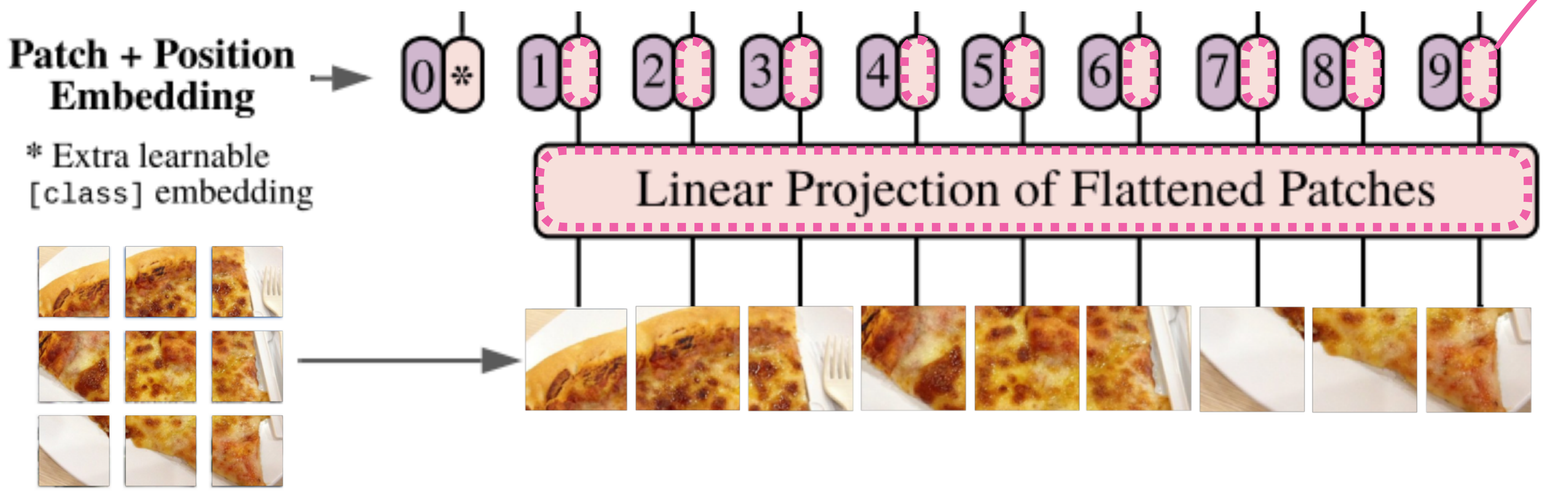
FoodVision Mini 🍕🥩🍣

Paper reading tip: math to text



Source: mathpix.com, **see a** live demo

Equation 1: The Patch Embedding



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3.1 Vision Transformer (ViT)

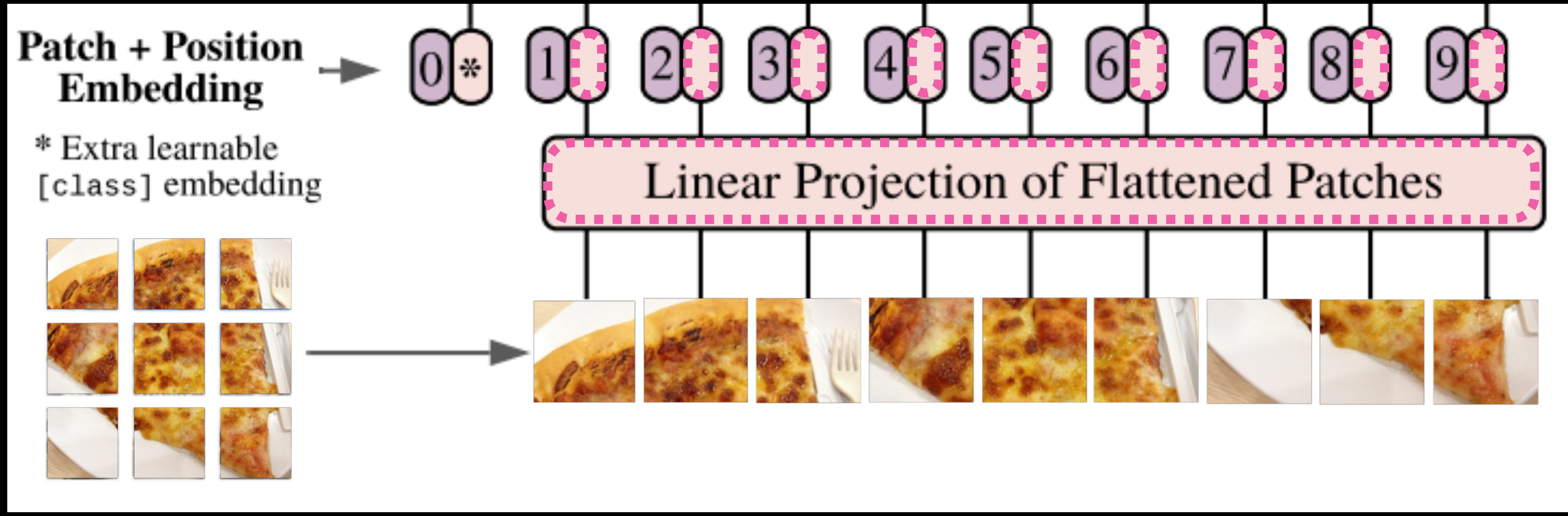
An overview of the model is depicted in Figure 1. The standard Transformer receives as input a 1D sequence of token embeddings. To handle 2D images, we reshape the image $\mathbf{x} \in \mathbb{R}^{H\times W\times C}$ into a sequence of flattened 2D patches $\mathbf{x}_p \in \mathbb{R}^{N\times(P^2\cdot C)}$, where (H, W) is the resolution of the original image, C is the number of channels, (P, P) is the resolution of each image patch, and $N = HW/P^2$ is the resulting number of patches, which also serves as the effective input sequence length for the Transformer. The Transformer uses constant latent vector size D through all of its layers, so we flatten the patches and map to D dimensions with a trainable linear projection (Eq. 1). We refer to the output of this projection as the patch embeddings.

Image size = `(H, W, C) -> (N_Patches, (P² • C))`

Embedding size (D) = 768 (ViT-Base)

For example, patch size = 16 (ViT-Base) :
`(224, 224, 3) -> (196, 768)`

Equation 1: The Patch Embedding



$$\mathbf{z}_0 = [\mathbf{x}_{\text{class}}; \mathbf{x}_p^1\mathbf{E}; \mathbf{x}_p^2\mathbf{E}; \cdots; \mathbf{x}_p^N\mathbf{E}] + \mathbf{E}_{pos}, \quad \mathbf{E} \in \mathbb{R}^{(P^2 \cdot C)\times D}, \mathbf{E}_{pos} \in \mathbb{R}^{(N+1)\times D} \quad (1)$$

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$$\mathbf{y} = \text{LN}(\mathbf{z}_L^0) \quad (4)$$

```python
# 1. Create a class which subclasses nn.Module
class PatchEmbedding(nn.Module):
    """Turns a 2D input image into a 1D sequence learnable embedding vector.

    Args:
        in_channels (int): Number of color channels for the input images. Defaults to 3.
        patch_size (int): Size of patches to convert input image into. Defaults to 16.
        embedding_dim (int): Size of embedding to turn image into. Defaults to 768.
    """
    # 2. Initialize the class with appropriate variables
    def __init__(self,
                 in_channels:int=3,
                 patch_size:int=16,
                 embedding_dim:int=768): # same as ViT-Base
        super().__init__()

        # 3. Create a layer to turn an image into patch embeddings
        self.patcher = nn.Conv2d(in_channels=in_channels,
                                 out_channels=embedding_dim,
                                 kernel_size=patch_size,
                                 stride=patch_size,
                                 padding=0)

        # 4. Create a layer to flatten the patch feature maps into a single dimension
        self.flatten = nn.Flatten(start_dim=2, # only flatten the feature map dimensions
                                  end_dim=3)

    # 5. Define the forward method
    def forward(self, x):
        x_patched = self.patcher(x)
        x_flattened = self.flatten(x_patched)

        # 6. Make sure the output shape has the right order
        return x_flattened.permute(0, 2, 1) # [batch_size, P^2•C, N] -> [batch_size, N, P^2•C]
```

Equation 1: The Class Token

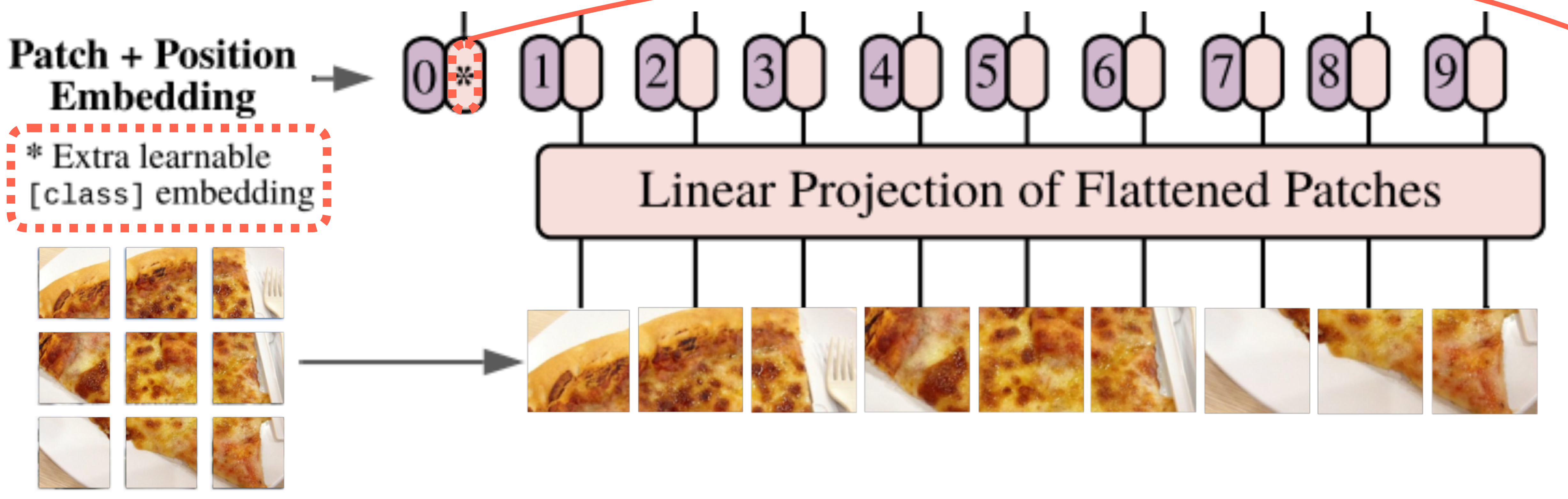

Figure 1: Model overview. We split an image into fixed-size patches, linearly embed each of them, add position embeddings, and feed the resulting sequence of vectors to a standard Transformer encoder. In order to perform classification, we use the standard approach of adding an extra learnable "classification token" to the sequence. The illustration of the Transformer encoder was inspired by Vaswani et al. (2017).

$$\mathbf{z}_0 = [\boxed{\mathbf{x}_\text{class}}; \mathbf{x}_p^1\mathbf{E}; \mathbf{x}_p^2\mathbf{E}; \cdots; \mathbf{x}_p^N\mathbf{E}] + \mathbf{E}_{pos}, \qquad \mathbf{E} \in \mathbb{R}^{(P^2 \cdot C) \times D},\ \mathbf{E}_{pos} \in \mathbb{R}^{(N+1) \times D} \tag{1}$$

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$$\mathbf{y} = \text{LN}(\mathbf{z}_L^0) \tag{4}$$

Similar to BERT's [class] token, we prepend a learnable embedding to the sequence of embedded patches ($\mathbf{z}_0^0 = \mathbf{x}_\text{class}$), whose state at the output of the Transformer encoder ($\mathbf{z}_L^0$) serves as the image representation $\mathbf{y}$ (Eq. 4). Both during pre-training and fine-tuning, a classification head is attached to $\mathbf{z}_L^0$. The classification head is implemented by a MLP with one hidden layer at pre-training time and by a single linear layer at fine-tuning time.

Prepend a learnable class embedding token to the 0 index of the patch embedding

Equation 1: The Class Token

Sequence of patch embeddings

```
tensor([[[-0.3714,  0.0556, -0.1053,  ...,  0.2598, -0.1740,  0.1473],
         [-0.4294,  0.0788, -0.1078,  ...,  0.2671, -0.1797,  0.1644],
         [-0.4774,  0.0965, -0.1198,  ...,  0.3465, -0.1918,  0.1432],
         ...,
         [-0.1749,  0.0247, -0.0610,  ...,  0.1185, -0.0448,  0.0451],
         [-0.1679,  0.0264, -0.0745,  ...,  0.1182, -0.0693,  0.0623],
         [-0.0631, -0.0043, -0.0612,  ...,  0.0553, -0.0460,  0.0837]]],
       grad_fn=<PermuteBackward0>)
```

Shape: [1, 196, 786], [batch_size, number_of_patches, embedding_dimension]

Create learnable class token and prepend it to patch embeddings

```
# Create the class token embedding
class_token = nn.Parameter(torch.ones(batch_size, 1, embedding_dimension),
                           requires_grad=True) # make embedding learnable

# Add the class token embedding to the front of the patch embedding
patch_embedded_image_with_class_embedding = torch.cat((class_token, patch_embedded_image),
                                                      dim=1) # concat on first dimension
```

Patch embeddings with learnable class token

```
tensor([[[ 1.0000,  1.0000,  1.0000,  ...,  1.0000,  1.0000,  1.0000],
         [-0.3714,  0.0556, -0.1053,  ...,  0.2598, -0.1740,  0.1473],
         [-0.4294,  0.0788, -0.1078,  ...,  0.2671, -0.1797,  0.1644],
         ...,
         [-0.1749,  0.0247, -0.0610,  ...,  0.1185, -0.0448,  0.0451],
         [-0.1679,  0.0264, -0.0745,  ...,  0.1182, -0.0693,  0.0623],
         [-0.0631, -0.0043, -0.0612,  ...,  0.0553, -0.0460,  0.0837]]],
       grad_fn=<CatBackward0>)
```

Learnable class token prepended

Shape: [1, 197, 786], [batch_size, number_of_patches + class_token, embedding_dimension]

Equation 1: The Position Embedding

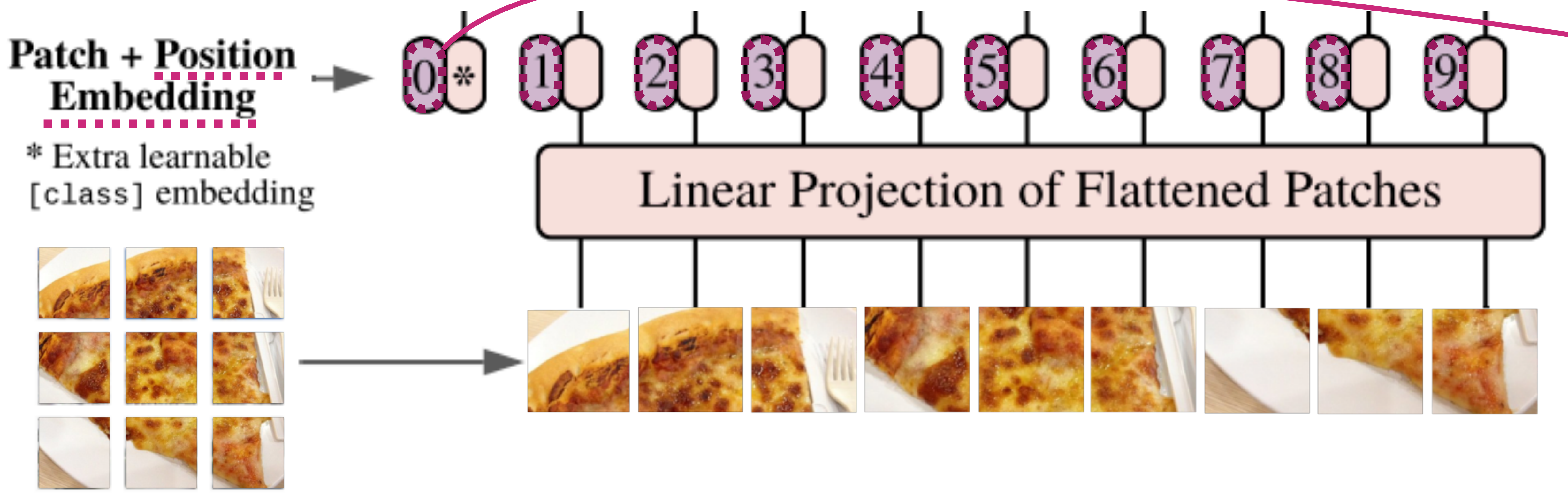

Figure 1: Model overview. We split an image into fixed-size patches, linearly embed each of them, add position embeddings, and feed the resulting sequence of vectors to a standard Transformer encoder. In order to perform classification, we use the standard approach of adding an extra learnable "classification token" to the sequence. The illustration of the Transformer encoder was inspired by Vaswani et al. (2017).

Position Embeddings Shape:
[num_patches+1, embedding_dimension]
(+1 is for the class_token)

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$$\mathbf{y} = \mathrm{LN}(\mathbf{z}_L^0) \tag{4}$$

Position embeddings are added to the patch embeddings to retain positional information. We use standard learnable 1D position embeddings, since we have not observed significant performance gains from using more advanced 2D-aware position embeddings (Appendix D.4). The resulting sequence of embedding vectors serves as input to the encoder.

Add a **learnable 1D set of position embeddings** to [class_token, patch embedding]

Equation 1: The Position Embedding

Patch embeddings with learnable class token

Learnable class token prepended

```
tensor([[[ 1.0000,  1.0000,  1.0000,  ...,  1.0000,  1.0000,  1.0000],
         [-0.3714,  0.0556, -0.1053,  ...,  0.2598, -0.1740,  0.1473],
         [-0.4294,  0.0788, -0.1078,  ...,  0.2671, -0.1797,  0.1644],
         ...,
         [-0.1749,  0.0247, -0.0610,  ...,  0.1185, -0.0448,  0.0451],
         [-0.1679,  0.0264, -0.0745,  ...,  0.1182, -0.0693,  0.0623],
         [-0.0631, -0.0043, -0.0612,  ...,  0.0553, -0.0460,  0.0837]]],
       grad_fn=<CatBackward0>)
```

Shape: [1, 197, 786], [batch_size, number_of_patches + class_token, embedding_dimension]

Create position embeddings and add to patch embeddings with learnable class token

```
# Create the learnable 1D position embedding
position_embedding = nn.Parameter(torch.ones(1, number_of_patches+1, embedding_dimension),
                                  requires_grad=True) # make sure it's learnable

# Add the position embedding to the patch and class token embedding
patch_and_position_embedding = patch_embedded_image_with_class_embedding + position_embedding
```

Patch embeddings with learnable class token and position embeddings

Values all changed thanks to position embeddings

```
tensor([[[2.0000, 2.0000, 2.0000,  ..., 2.0000, 2.0000, 2.0000],
         [0.6286, 1.0556, 0.8947,  ..., 1.2598, 0.8260, 1.1473],
         [0.5706, 1.0788, 0.8922,  ..., 1.2671, 0.8203, 1.1644],
         ...,
         [0.8251, 1.0247, 0.9390,  ..., 1.1185, 0.9552, 1.0451],
         [0.8321, 1.0264, 0.9255,  ..., 1.1182, 0.9307, 1.0623],
         [0.9369, 0.9957, 0.9388,  ..., 1.0553, 0.9540, 1.0837]]],
       grad_fn=<AddBackward0>)
```

Shape: [1, 197, 786], [batch_size, number_of_patches + class_token, embedding_dimension]

Equation 1: Putting it all together

```python
# 1. Set patch size
patch_size = 16

# 2. Print shape of original image tensor and get the image dimensions
print(f"Image tensor shape: {image.shape}")
height, width = image.shape[1], image.shape[2]

# 3. Get image tensor and add batch dimension
x = image.unsqueeze(0)
print(f"Input image with batch dimension shape: {x.shape}")

# 4. Create patch embedding layer
patch_embedding_layer = PatchEmbedding(in_channels=3, # number of color channels in image
                                       patch_size=patch_size,
                                       embedding_dim=768) # from Table 1 for ViT-Base

# 5. Pass image through patch embedding layer
patch_embedding = patch_embedding_layer(x)
print(f"Patching embedding shape: {patch_embedding.shape}")

# 6. Create class token embedding
batch_size = patch_embedding.shape[0]
embedding_dimension = patch_embedding.shape[-1]
class_token = nn.Parameter(torch.ones(batch_size, 1, embedding_dimension),
                           requires_grad=True) # make sure it's learnable
print(f"Class token embedding shape: {class_token.shape}")

# 7. Prepend class token embedding to patch embedding
patch_embedding_class_token = torch.cat((class_token, patch_embedding), dim=1)
print(f"Patch embedding with class token shape: {patch_embedding_class_token.shape}")

# 8. Create position embedding
number_of_patches = int((height * width) / patch_size**2)
position_embedding = nn.Parameter(torch.ones(1, number_of_patches+1, embedding_dimension),
                                  requires_grad=True) # make sure it's learnable

# 9. Add position embedding to patch embedding with class token
patch_and_position_embedding = patch_embedding_class_token + position_embedding
print(f"Patch and position embedding shape: {patch_and_position_embedding.shape}")
```

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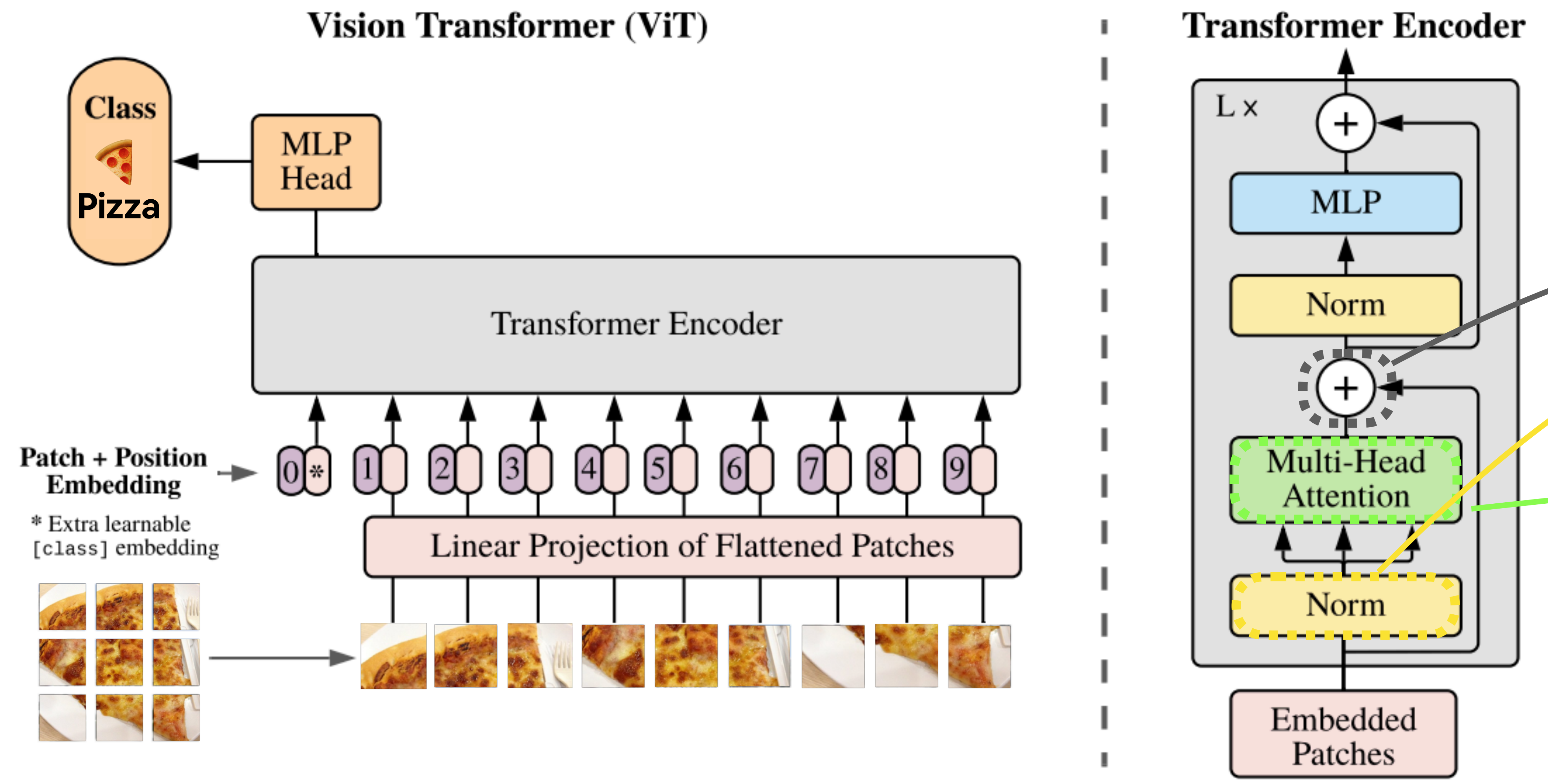
Equation 2: The MSA Block

MSA = Multi-Head Self Attention



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Equation 2 = "MSA block"

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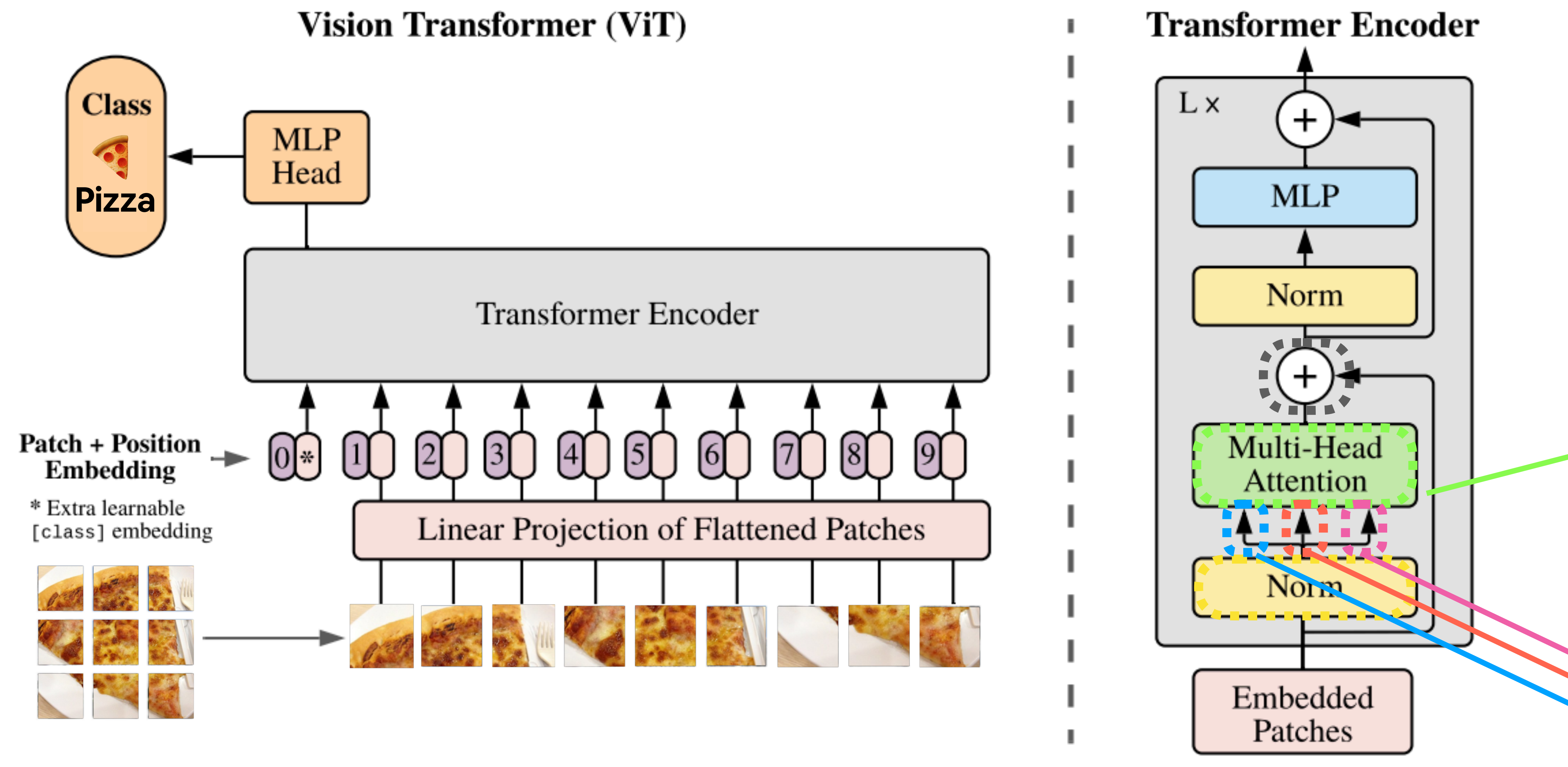

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A MULTIHEAD SELF-ATTENTION From "Attention is all you need" paper

Standard **qkv** self-attention (SA, Vaswani et al. (2017)) is a popular building block for neural architectures. For each element in an input sequence $\mathbf{z} \in \mathbb{R}^{N\times D}$, we compute a weighted sum over all values $\mathbf{v}$ in the sequence. The attention weights A_{ij} are based on the pairwise similarity between two elements of the sequence and their respective query $\mathbf{q}^i$ and key $\mathbf{k}^j$ representations.

$$[\mathbf{q}, \mathbf{k}, \mathbf{v}] = \mathbf{z}\mathbf{U}_{qkv} \qquad \mathbf{U}_{qkv} \in \mathbb{R}^{D\times 3D_h}, \tag{5}$$

$$A = \text{softmax}\left(\mathbf{q}\mathbf{k}^\top/\sqrt{D_h}\right) \qquad A \in \mathbb{R}^{N\times N}, \tag{6}$$

$$\text{SA}(\mathbf{z}) = A\mathbf{v}\,. \tag{7}$$

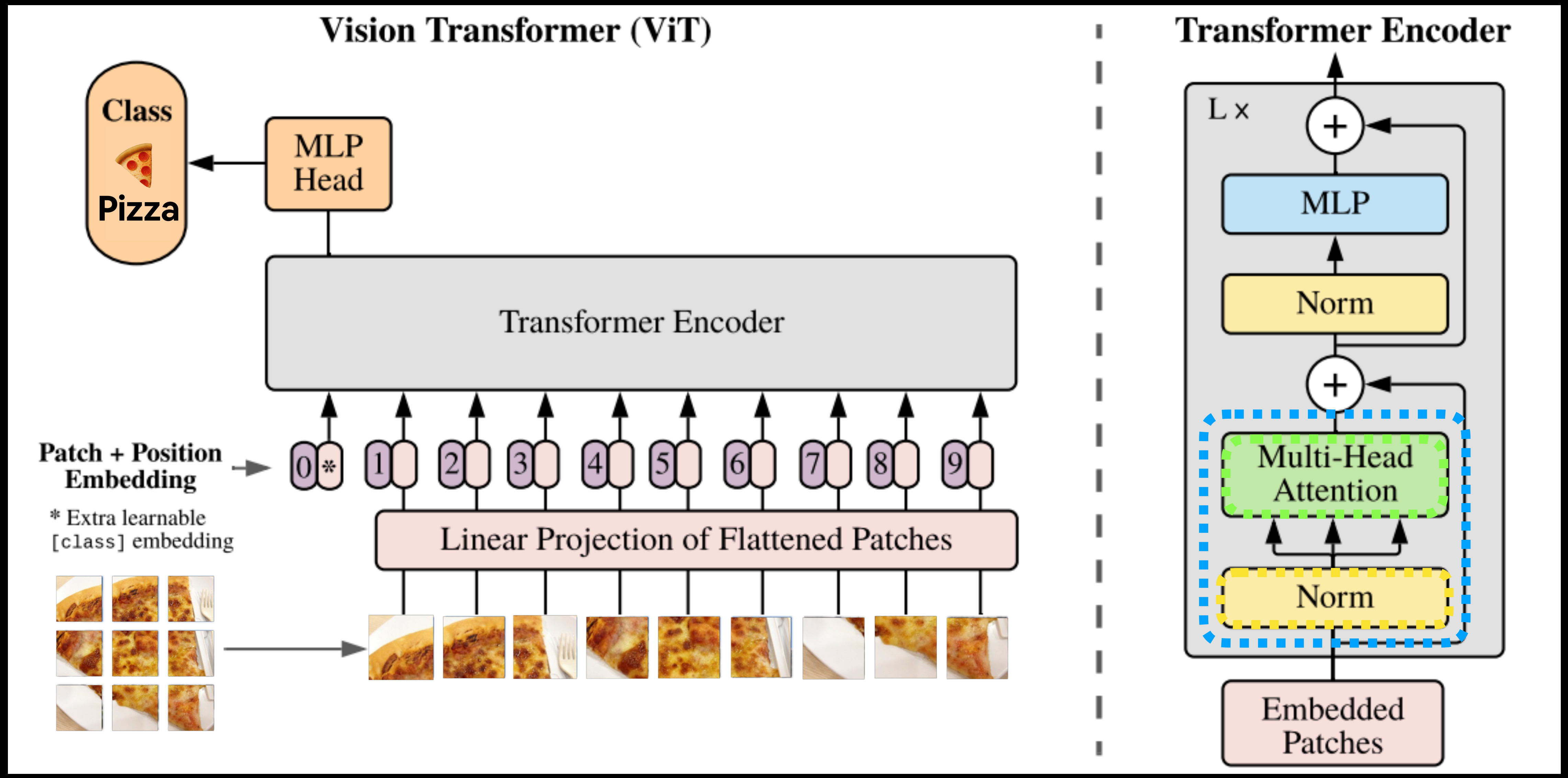
Multihead self-attention (MSA) is an extension of SA in which we run k self-attention operations, called "heads", in parallel, and project their concatenated outputs. To keep compute and number of parameters constant when changing k, D_h (Eq. 5) is typically set to D/k.

$$\text{MSA}(\mathbf{z}) = [\text{SA}_1(z); \text{SA}_2(z); \cdots; \text{SA}_k(z)]\,\mathbf{U}_{msa} \qquad \mathbf{U}_{msa} \in \mathbb{R}^{k\cdot D_h\times D} \tag{8}$$

q = query
k = key
v = value

Equation 2: The MSA Block

MSA = Multi-Head Self Attention



$$\mathbf{z}_0 = [\mathbf{x}_{\text{class}};\, \mathbf{x}_p^1\mathbf{E};\, \mathbf{x}_p^2\mathbf{E};\cdots;\, \mathbf{x}_p^N\mathbf{E}] + \mathbf{E}_{pos}, \qquad \mathbf{E} \in \mathbb{R}^{(P^2\cdot C)\times D},\ \mathbf{E}_{pos} \in \mathbb{R}^{(N+1)\times D} \quad (1)$$

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$$\mathbf{y} = \mathrm{LN}(\mathbf{z}_L^0) \quad (4)$$

```python
from torch import nn

# 1. Create a class that inherits from nn.Module
class MultiheadSelfAttentionBlock(nn.Module):
    """Creates a multi-head self-attention block ("MSA block" for short).
    """
    # 2. Initialize the class with hyperparameters from Table 1
    def __init__(self,
                 embedding_dim:int=768, # Hidden size D from Table 1 for ViT-Base
                 num_heads:int=12, # Heads from Table 1 for ViT-Base
                 attn_dropout:int=0): # doesn't look like the paper uses any dropout in MSABlocks
        super().__init__()

        # 3. Create the Norm layer (LN)
        self.layer_norm = nn.LayerNorm(normalized_shape=embedding_dim)

        # 4. Create the Multi-Head Attention (MSA) layer
        self.multihead_attn = nn.MultiheadAttention(embed_dim=embedding_dim,
                                                    num_heads=num_heads,
                                                    dropout=attn_dropout,
                                                    batch_first=True) # batch dimension first?

    # 5. Create a forward() method to pass the data through the layers
    def forward(self, x):
        x = self.layer_norm(x)
        attn_output, _ = self.multihead_attn(query=x, # query embeddings
                                             key=x, # key embeddings
                                             value=x, # value embeddings
                                             need_weights=False) # only get layer outputs
        return attn_output
```

Equation 3: The MLP Block

MLP = Multilayer Perceptron

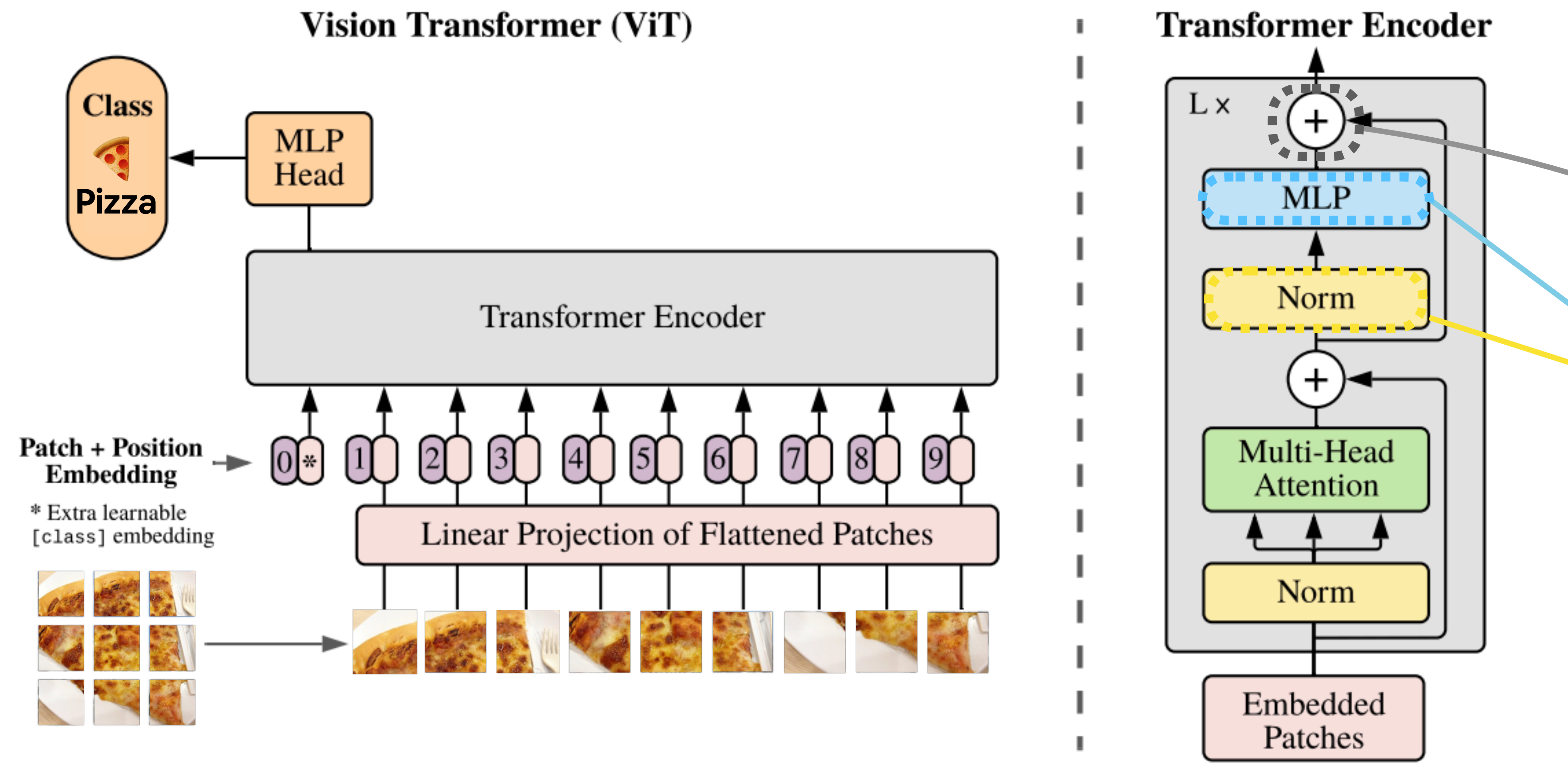


Figure 1: Model overview. We split an image into fixed-size patches, linearly embed each of them, add position embeddings, and feed the resulting sequence of vectors to a standard Transformer encoder. In order to perform classification, we use the standard approach of adding an extra learnable "classification token" to the sequence. The illustration of the Transformer encoder was inspired by Vaswani et al. (2017).

Equation 3 = "MLP block"

$$\mathbf{z}_0 = [\mathbf{x}_{\text{class}};\, \mathbf{x}_p^1\mathbf{E};\, \mathbf{x}_p^2\mathbf{E};\cdots;\, \mathbf{x}_p^N\mathbf{E}] + \mathbf{E}_{pos}, \qquad \mathbf{E} \in \mathbb{R}^{(P^2\cdot C)\times D},\ \mathbf{E}_{pos} \in \mathbb{R}^{(N+1)\times D} \tag{1}$$

$$\mathbf{z}'_\ell = \mathrm{MSA}(\mathrm{LN}(\mathbf{z}_{\ell-1})) + \mathbf{z}_{\ell-1}, \qquad \ell = 1 \ldots L \tag{2}$$

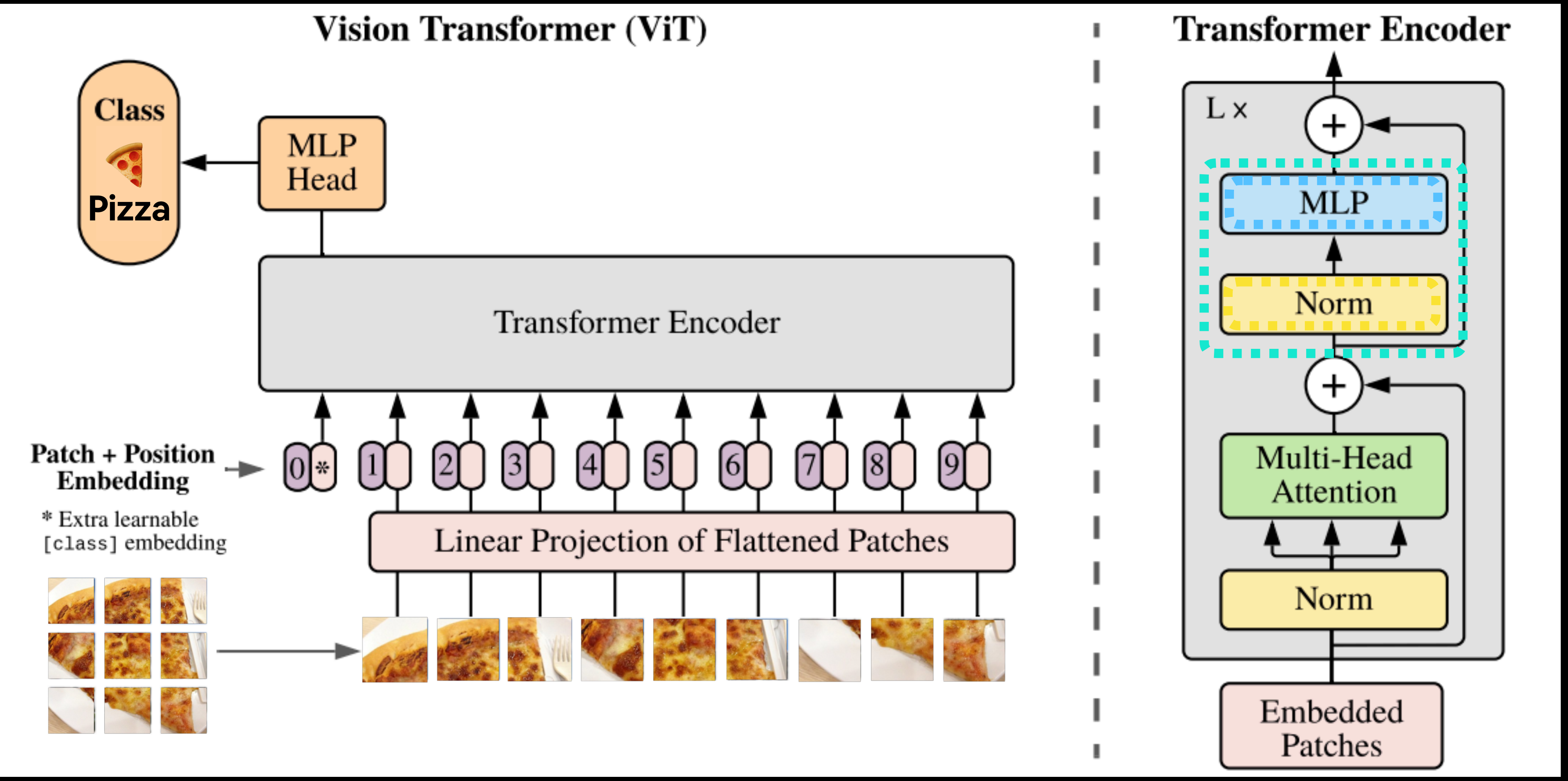
$$\mathbf{z}_\ell = \mathrm{MLP}(\mathrm{LN}(\mathbf{z}'_\ell)) + \mathbf{z}'_\ell, \qquad \ell = 1 \ldots L \tag{3}$$

$$\mathbf{y} = \mathrm{LN}(\mathbf{z}_L^0) \tag{4}$$

The Transformer encoder (Vaswani et al., 2017) consists of alternating layers of multiheaded self-attention (MSA, see Appendix A) and MLP blocks (Eq. 2, 3). Layernorm (LN) is applied before every block, and residual connections after every block (Wang et al., 2019; Baevski & Auli, 2019).

Equation 3: The MLP Block

MLP = Multilayer perceptron



$$\mathbf{z}_0 = [\mathbf{x}_{\text{class}};\, \mathbf{x}_p^1\mathbf{E};\, \mathbf{x}_p^2\mathbf{E};\cdots;\, \mathbf{x}_p^N\mathbf{E}] + \mathbf{E}_{pos}, \qquad \mathbf{E}\in\mathbb{R}^{(P^2\cdot C)\times D},\ \mathbf{E}_{pos}\in\mathbb{R}^{(N+1)\times D} \qquad (1)$$

$$\mathbf{z}'_\ell = \text{MSA}(\text{LN}(\mathbf{z}_{\ell-1})) + \mathbf{z}_{\ell-1}, \qquad \ell = 1\ldots L \qquad (2)$$

$$\mathbf{z}_\ell = \text{MLP}(\text{LN}(\mathbf{z}'_\ell)) + \mathbf{z}'_\ell, \qquad \ell = 1\ldots L \qquad (3)$$

$$\mathbf{y} = \text{LN}(\mathbf{z}_L^0) \qquad (4)$$

```python
from torch import nn

# 1. Create a class that inherits from nn.Module
class MLPBlock(nn.Module):
    """Creates a layer normalized multilayer perceptron block ("MLP block" for short)."""
    # 2. Initialize the class with hyperparameters from Table 1 and Table 3
    def __init__(self,
                 embedding_dim:int=768, # Hidden Size D from Table 1 for ViT-Base
                 mlp_size:int=3072, # MLP size from Table 1 for ViT-Base
                 dropout:int=0.1): # Dropout from Table 3 for ViT-Base
        super().__init__()

        # 3. Create the Norm layer (LN)
        self.layer_norm = nn.LayerNorm(normalized_shape=embedding_dim)

        # 4. Create the Multilayer perceptron (MLP) layer(s)
        self.mlp = nn.Sequential(
            nn.Linear(in_features=embedding_dim,
                      out_features=mlp_size),
            nn.GELU(), # "The MLP contains two layers with a GELU non-linearity (section 3.1)."
            nn.Dropout(p=dropout),
            nn.Linear(in_features=mlp_size, # same in_features as out_features of layer above
                      out_features=embedding_dim), # take back to embedding_dim
            nn.Dropout(p=dropout) # "Dropout, when used, is applied after every dense layer.."
        )

    # 5. Create a forward() method to pass the data through the layers
    def forward(self, x):
        x = self.layer_norm(x)
        x = self.mlp(x)
        return x
```

The Transformer Encoder

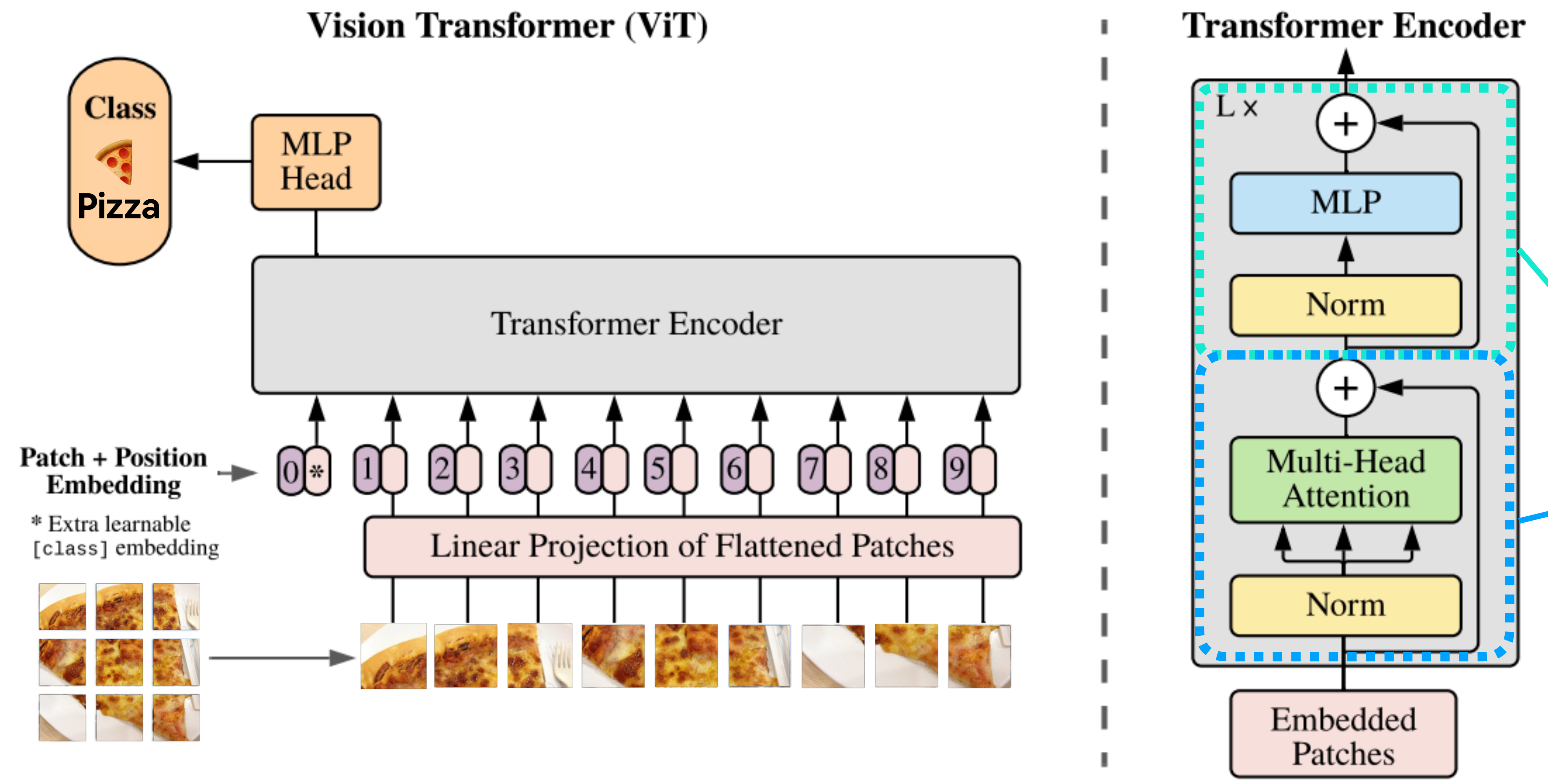


Figure 1: Model overview. We split an image into fixed-size patches, linearly embed each of them, add position embeddings, and feed the resulting sequence of vectors to a standard Transformer encoder. In order to perform classification, we use the standard approach of adding an extra learnable "classification token" to the sequence. The illustration of the Transformer encoder was inspired by Vaswani et al. (2017).

Transformer Encoder = Alternating layers of equation 2 and 3

$$\mathbf{z}_0 = [\mathbf{x}_{\text{class}};\, \mathbf{x}_p^1\mathbf{E};\, \mathbf{x}_p^2\mathbf{E};\, \cdots;\, \mathbf{x}_p^N\mathbf{E}] + \mathbf{E}_{pos}, \qquad \mathbf{E} \in \mathbb{R}^{(P^2 \cdot C)\times D},\, \mathbf{E}_{pos} \in \mathbb{R}^{(N+1)\times D} \tag{1}$$

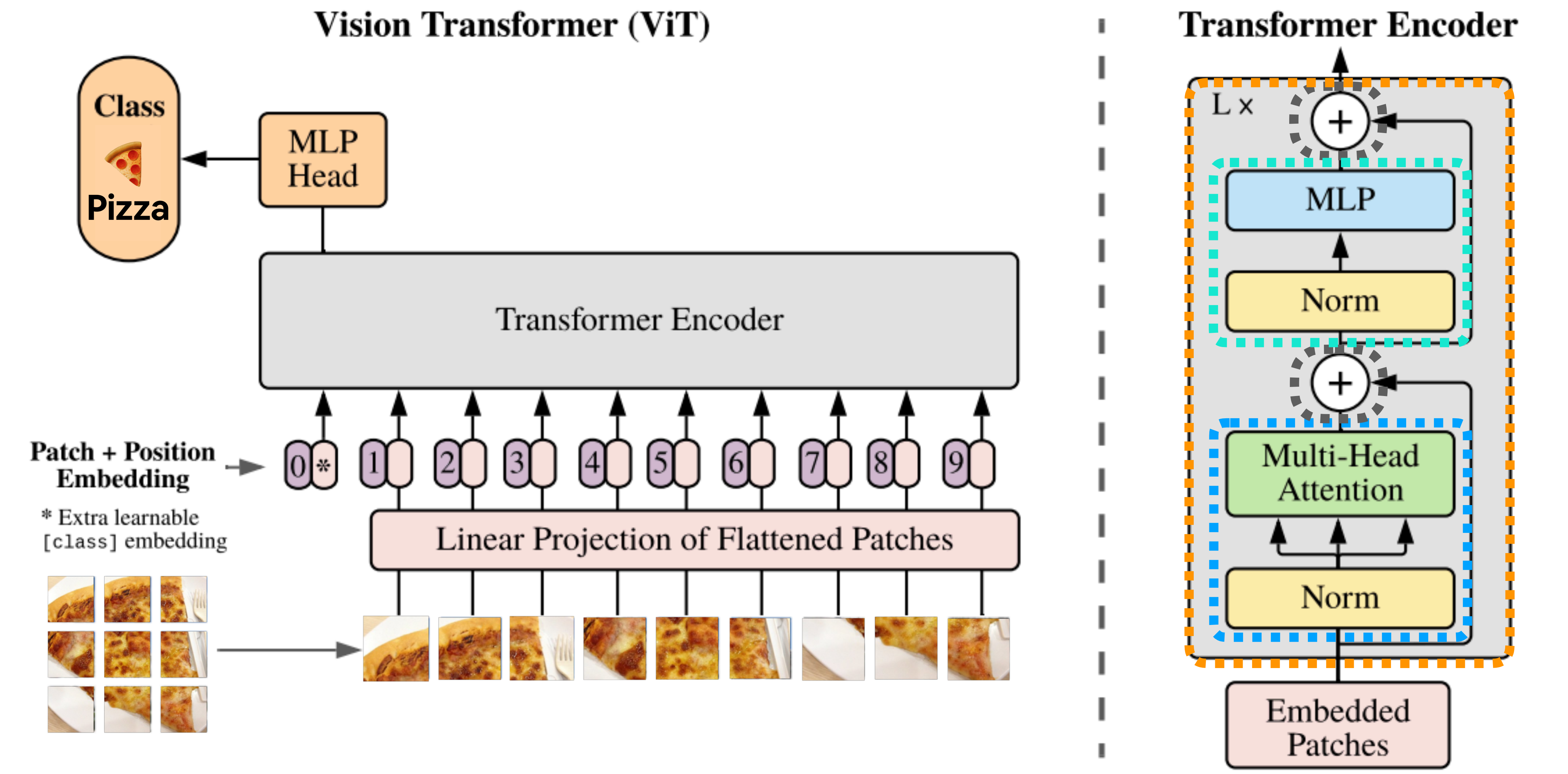
$$\mathbf{z}'_\ell = \mathrm{MSA}(\mathrm{LN}(\mathbf{z}_{\ell-1})) + \mathbf{z}_{\ell-1}, \qquad \ell = 1 \ldots L \tag{2}$$

$$\mathbf{z}_\ell = \mathrm{MLP}(\mathrm{LN}(\mathbf{z}'_\ell)) + \mathbf{z}'_\ell, \qquad \ell = 1 \ldots L \tag{3}$$

$$\mathbf{y} = \mathrm{LN}(\mathbf{z}_L^0) \tag{4}$$

The Transformer encoder (Vaswani et al., 2017) consists of alternating layers of multiheaded self-attention (MSA, see Appendix A) and MLP blocks (Eq. 2, 3). Layernorm (LN) is applied before every block, and residual connections after every block (Wang et al., 2019; Baevski & Auli, 2019).

The Transformer Encoder



$$\mathbf{z}_0 = [\mathbf{x}_{\text{class}};\, \mathbf{x}_p^1\mathbf{E};\, \mathbf{x}_p^2\mathbf{E};\, \cdots;\, \mathbf{x}_p^N\mathbf{E}] + \mathbf{E}_{pos}, \qquad \mathbf{E} \in \mathbb{R}^{(P^2\cdot C)\times D},\ \mathbf{E}_{pos} \in \mathbb{R}^{(N+1)\times D} \tag{1}$$

$$\mathbf{z}'_\ell = \text{MSA}(\text{LN}(\mathbf{z}_{\ell-1})) + \mathbf{z}_{\ell-1}, \qquad \ell = 1 \ldots L \tag{2}$$

$$\mathbf{z}_\ell = \text{MLP}(\text{LN}(\mathbf{z}'_\ell)) + \mathbf{z}'_\ell, \qquad \ell = 1 \ldots L \tag{3}$$

$$\mathbf{y} = \text{LN}(\mathbf{z}_L^0) \tag{4}$$

```python
from torch import nn

# 1. Create a class that inherits from nn.Module
class TransformerEncoderBlock(nn.Module):
    """Creates a Transformer Encoder block."""
    # 2. Initialize the class with hyperparameters from Table 1 and Table 3
    def __init__(self,
                 embedding_dim:int=768, # Hidden size D from Table 1 for ViT-Base
                 num_heads:int=12, # Heads from Table 1 for ViT-Base
                 mlp_size:int=3072, # MLP size from Table 1 for ViT-Base
                 mlp_dropout:int=0.1, # Dropout for dense layers from Table 3 for ViT-Base
                 attn_dropout:int=0): # Dropout for attention layers
        super().__init__()

        # 3. Create MSA block (equation 2)
        self.msa_block = MultiheadSelfAttentionBlock(embedding_dim=embedding_dim,
                                                     num_heads=num_heads,
                                                     attn_dropout=attn_dropout)

        # 4. Create MLP block (equation 3)
        self.mlp_block =  MLPBlock(embedding_dim=embedding_dim,
                                   mlp_size=mlp_size,
                                   dropout=mlp_dropout)

    # 5. Create a forward() method
    def forward(self, x):

        # 6. Create residual connection for MSA block (add the input to the output)
        x =  self.msa_block(x) + x

        # 7. Create residual connection for MLP block (add the input to the output)
        x = self.mlp_block(x) + x

        return x
```