### Milestone Project 2 Paper Replicating with



# O PyTorch

# Where can you get help?

- Follow along with the code
- Try it for yourself
- Press SHIFT + CMD + SPACE to read the docstring
- Search for it
- Try again
- Ask

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







### "If in doubt, run the code"

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# "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<sup>\*,†</sup>, Lucas Beyer<sup>\*</sup>, Alexander Kolesnikov<sup>\*</sup>, Dirk Weissenborn<sup>\*</sup>, Xiaohua Zhai<sup>\*</sup>, Thomas Unterthiner, Mostafa Dehghani, Matthias Minderer, Georg Heigold, Sylvain Gelly, Jakob Uszkoreit, Neil Houlsby<sup>\*,†</sup> <sup>\*</sup>equal technical contribution, <sup>†</sup>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.<sup>1</sup>

### 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:** <u>https://arxiv.org/pdf/2010.11929.pdf</u> (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).

$\mathbf{z}_0 = [\mathbf{x}_{ ext{class}};\mathbf{x}_p^1\mathbf{E};\mathbf{x}_p^2\mathbf{E};\cdots;\mathbf{x}_p^N\mathbf{E}] + \mathbf{E}_{pos},$	$\mathbf{E} \in \mathbb{R}^{(P^2 \cdot C) \times D},  \mathbf{E}_{pos} \in \mathbb{R}^{(N+1) \times D}$	(1)
$\mathbf{z'}_{\ell} = \mathrm{MSA}(\mathrm{LN}(\mathbf{z}_{\ell-1})) + \mathbf{z}_{\ell-1},$	$\ell = 1 \dots L$	(2)
$\mathbf{z}_{\ell} = \mathrm{MLP}(\mathrm{LN}(\mathbf{z}'_{\ell})) + \mathbf{z}'_{\ell},$	$\ell = 1 \dots L$	(3)
$\mathbf{y} = \mathrm{LN}(\mathbf{z}_L^0)$		(4)

The Transformer encoder (Vaswani et al., 2017) consists of alternating layers of multiheaded selfattention (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

### Images + math + text

•••

# Create ViT vit = ViT()

### 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])
```

### Usable code



# Terminology



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### Source: <u>ViT paper</u>

### Vision Transformer (ViT) architecture

Published as a conference paper at ICLR 2021

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\*equal technical contribution, <sup>†</sup>equal advising Google Research, Brain Team {adosovitskiy, neilhoulsby}@google.com

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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.<sup>1</sup>

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**Source:** <u>https://arxiv.org/pdf/2010.11929.pdf</u> (ViT paper)

### ViT paper

arXiv:2010.11929v2 [cs.CV] 3 Jun 202

# "Why replicate machine learning research papers?"

1. It's fun... and...

### 59 Machine Learning Engineer 60 \_\_\_\_ 61 62 1. Download a paper 2. Implement it 63 Keep doing this until you have skills 64

- George Hotz, founder of <u>comma.ai</u>

\*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

Abstract	An <b>overview</b> ,
Introduction	What's the paper's <b>main p</b>
Method	What <b>steps did the researchers</b>
Results	What are the <b>outcomes</b> of the results of findings compare t
Conclusion	What are the <b>limitations</b> of <sup>.</sup>
References	What <b>resources/other p</b> a
Appendix	Are there any <b>extra resources</b>

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

### What is it?

**/summary** of the paper's main findings/contributions.

problem? And details of previous methods used to try and solve it.

take when conducting their research? For example, what model(s), data sources, training setups were used?

e paper? If a new type of model or training setup was used, how did the o previous works? (this is where experiment tracking comes in handy)

the suggested methods? What are some next steps for the research community?

**apers** did the researchers look at to build their own body of work?

**/findings** to look at that weren't included in any of the above sections?







# Anatomy of a research paper\*

Section	What is it?
Abstract	An <b>overview/summary</b> of the paper's main findings/co
Introduction	What's the paper's <b>main problem</b> ? And details of previous m and solve it.
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Conclusion	What are the <b>limitations</b> of the suggested methods? What an for the research community?
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3 Jun 202

CS

arXiv:2010.11929v2

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# "Where can you find machine learning research papers?"

### Finding machine learning papers (and code)

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← → C △ ▲ arxiv.org	Q Ó 🌣 🛈 😾 🛤 🖬 🚳 🗄
Cornell University	We gratefully acknowledge support from the Simons Foundation and member institutions
arXiv	Login Search All fields ✓ Search Help   Advanced Search
arXiv is a free distribution service and an open-access archive for 2,102,411 scholarly articles in the fields of physics, mathematics, computer science, quantitative biology, quantitative finance, statistics, electrical engineering and systems science, and economics. Materials on Physics Mathematics Quantitative Biology Computer Science Quantitative Finance Statistics Electrical Engineering and Systems Science Economics arXiv's blog. (View the former "what's new" pages here). Read robots beware before attempting any automated download.	COVID-19 Quick Links See COVID-19 SARS-CoV-2 preprints from • arXiv • medRxiv and bioRxiv Important: e-prints posted on arXiv are not peer-reviewed by arXiv; they should not be relied upon without context to guide clinical practice or health-related behavior and should not be reported in news media as established information without consulting multiple experts in the field.
Physics	

- Astrophysics (astro-ph new, recent, search)
- includes: Astrophysics of Galaxies; Cosmology and Nongalactic Astrophysics; Earth and Planetary Astrophysics; High Energy Astrophysical Phenomena; Instrumentation and Methods for Astrophysics; Solar and Stellar Astrophysics
- · Condensed Matter (cond-mat new, recent, search)

### Source: <u>https://arxiv.org/</u>

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3 main - 3 2 branches (> 143 tag)	Go to file Add file -	<> Code -	About
Iucidrains offer way for extractor to re	eturn latents without detaching them 🗸 f86e052 9 days ago 🕤	249 commits	Implementation of Vision Transformer, a simple way to achieve SOTA in vision classification with only a single
github	sponsor button	4 months ago	transformer encoder, in Pytorch
examples	fix transforms for val an test process	11 months ago	computer-vision transformers
images	add EsViT, by popular request, an alternative to Dino that is compati	3 months ago	artificial-intelligence image-classification
tests	add some tests	7 months ago	attention-mechanism
vit_pytorch	offer way for extractor to return latents without detaching them	9 days ago	🛱 Readme
🗅 .gitignore	Initial commit	2 years ago	MIT license
	Initial commit	2 years ago	<ul> <li>126 watching</li> </ul>
MANIFEST.in	include tests in package for conda	7 months ago	양 1.8k forks
C README.md	make extractor flexible for layers that output multiple tensors, show	last month	
🗅 setup.py	offer way for extractor to return latents without detaching them	9 days ago	Releases 142
i≡ README.md			<ul> <li>v0.35.8 (Latest)</li> <li>9 days ago</li> <li>+ 141 releases</li> </ul>

**Source:** <u>https://github.com/lucidrains/vit-pytorch</u>



Source: <a href="https://paperswithcode.com/">https://paperswithcode.com/</a>









Source: ViT paper

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

# Machine Learning vs. Deep Learning (common algorithms)

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

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

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

Structured data +

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

What we're focused on building (with PyTorch)

**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 (common algorithms)



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: Photo by John Tubelleza

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- ...many more

What we're focused on building (with PyTorch)

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### Vision Transformer architecture



### FoodVision Mini 🝕 🌽 🍣



















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?

### 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.

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

### Batch size = 4096

Source: ViT paper



# Inputs, outputs, layers and blocks







# ViT Overview: Inputs and Outputs





# ViT Overview: Inputs and Outputs



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: <u>ViT paper</u> Figure 1

 $\begin{aligned} \mathbf{z}_0 &= [\mathbf{x}_{\text{class}}; \, \mathbf{x}_p^1 \mathbf{E}; \, \mathbf{x}_p^2 \mathbf{E}; \cdots; \, \mathbf{x}_p^N \mathbf{E}] + \mathbf{E}_{pos}, \\ \mathbf{z}'_{\ell} &= \text{MSA}(\text{LN}(\mathbf{z}_{\ell-1})) + \mathbf{z}_{\ell-1}, \\ \mathbf{z}_{\ell} &= \text{MLP}(\text{LN}(\mathbf{z}'_{\ell})) + \mathbf{z}'_{\ell}, \end{aligned}$  $\mathbf{y} = LN(\mathbf{z}_L^0)$ 

 $\mathbf{E} \in \mathbb{R}^{(P^2 \cdot C) \times D}, \, \mathbf{E}_{pos} \in \mathbb{R}^{(N+1) \times D}$  $\ell = 1 \dots L$  $\ell = 1 \dots L$ 

The Transformer encoder (Vaswani et al., 2017) consists of alternating layers of multiheaded selfattention (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: <u>ViT paper</u> section 3.1





### Vit Overview: Workflow visualize, visualize, visualize!



### **Original image**



# Paper reading tip: math to text

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Similar to BERT's [class] token, we prepend a learnable embedding to the sequence of embedded patches ( $v_0^0 = x_{thin}$ ), whose state at the output of the Transformer encoder ( $v_0^0$ ) serves as the image representation y (Eq. 4). Both during gene-training and fine-tuning time and by a single linear layer at fine-tuning time. Position embeddings are added to the patch embeddings to retain positional information. We use standard learnable 1D position embeddings (Appendix D.4). The resulting sequence of embedding vectors serves as input to the encoder. The Transformer encoder (Vaswari 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).			SNIPS $( \mathbf{x} \text{ Search your Snips} )$ $( \mathbf{x} \text{ Search your Snips} )$ $( \mathbf{x} = (\mathbf{x}_{min}; \mathbf{x}_{i}^{1}\mathbf{E}; \mathbf{x}_{i}^{2}\mathbf{E}; \cdots; \mathbf{x}_{i}^{N}\mathbf{E}] + \mathbf{E}_{pmin},  \mathbf{E} \in \mathbb{R}^{(p^{k}C)\times D}, \mathbf{E}_{pmin} \in \mathbb{R}^{(N+1)\times D}  (1)$ $(\mathbf{x} = MLP(LN(\mathbf{x}_{i}(t_{i})) + \mathbf{x}_{i-1},  \mathbf{E} = 1L  (2)$ $(\mathbf{x} = MLP(LN(\mathbf{x}_{i}(t_{i})) + \mathbf{x}_{i-1},  \mathbf{E} = 1L  (3)$ $(\mathbf{x} = MLP(LN(\mathbf{x}_{i}(t_{i})) + \mathbf{x}_{i-1},  \mathbf{E} = \mathbf{L} \cdot \mathbf{L}  (3)$ $(\mathbf{x} = MLP(LN(\mathbf{x}_{i}(t_{i})) + \mathbf{x}_{i-1},  \mathbf{E} = 1L  (3)$ $(\mathbf{x} = \mathbf{L} \cdot \mathbf{L} \mathbf{x} = \mathbf{L} \cdot \mathbf{L}  \mathbf{L}$	<pre>vit-paper-demo</pre>
			Similar to BERT's [class] token, we prepend a learnable embedding to the sequence of embedded patches $\{x_{D}^{0}\} = x_{class}\}$ , whose state at the output of the Transformer encoder $\{x_{D}^{0}\}$ serves as the image representation y (Eq. 4). Both during pre-training and fine-tuning, a classification beak is attached to $x_{D}^{0}$ . 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. 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. The Transformer encoder (Vaswani et al., 2017) consists of alternating layers of multiheaded self-attention (NSA, see Appendix A) 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).	\mathbf{y} &=\operatorname{LN}\left(z \end{aligned} &

Source: <u>mathpix.com</u>, see a <u>live demo</u>



```
\text {class }};
thbf{x}_{p}^{2}
{N}
, & & \mathbf{E} \in
t) \times D},
(N+1) \times D} \\
```

```
orname{LN}\left(\math
}_{\ell-1}, & & \ell=1
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```
orname{<mark>LN</mark>}\left(\math
athbf{<mark>z}_</mark>{\ell}^{\prime}
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```
z}_{L}^{0}\right) & &
```

STANDARD

### Magic!

- $egin{aligned} \mathbf{z}_0 &= ig[\mathbf{x}_{ ext{class}}\,;\mathbf{x}_p^1\mathbf{E};\mathbf{x}_p^2\mathbf{E};\cdots;\mathbf{x}_p^N\mathbf{E}ig] + \mathbf{E}_{pos}, \ \mathbf{z}_\ell' &= ext{MSA}( ext{LN}(\mathbf{z}_{\ell-1})) + \mathbf{z}_{\ell-1}, \ \mathbf{z}_\ell &= ext{MLP}ig( ext{LN}ig(\mathbf{z}_\ell'ig)ig) + \mathbf{z}_\ell', \ \mathbf{y} &= ext{LN}ig(\mathbf{z}_L^0ig) \end{aligned}$
- $\mathbf{E} \in \mathbb{R}^{\left(P^2 \cdot C
  ight) imes D}, \mathbf{E}_{pos} \in \mathbb{R}^{(N+1) imes D} \ \ell = 1 \dots L \ \ell = 1 \dots L$

# Equation 1: The Patch 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).

### Image size = (H, W, C) $\rightarrow$ (N\_Patches, (P<sup>2</sup> • C))

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

 $\mathbf{z}_0 = [\mathbf{x}_{class}; \, \mathbf{x}_p^1 \mathbf{E}; \, \mathbf{x}_p^2 \mathbf{E}; \cdots; \, \mathbf{x}_p^N \mathbf{E}] + \mathbf{E}_{pos},$  $\mathbf{z}'_{\ell} = \mathrm{MSA}(\mathrm{LN}(\mathbf{z}_{\ell-1})) + \mathbf{z}_{\ell-1},$  $\mathbf{z}_{\ell} = \mathrm{MLP}(\mathrm{LN}(\mathbf{z}'_{\ell})) + \mathbf{z}'_{\ell},$  $\mathbf{y} = LN(\mathbf{z}_L^0)$ 

$$\mathbf{E} \in \mathbb{R}^{(P^2 \cdot C) \times D}, \ \mathbf{E}_{pos} \in \mathbb{R}^{(N+1) \times D}$$
$$\ell = 1 \dots L$$
$$\ell = 1 \dots L$$

### 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.

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







# Equation 1: The Patch Embedding



$$\mathbf{z}_{0} = [\mathbf{x}_{\text{class}}; \mathbf{x}_{p}^{1}\mathbf{E}; \mathbf{x}_{p}^{2}\mathbf{E}; \cdots; \mathbf{x}_{p}^{N}\mathbf{E}] + \mathbf{E}_{pos}, \qquad \mathbf{E} \in \mathbb{R}^{(P^{2} \cdot C) \times D}, \quad \mathbf{E}_{pos} \in \mathbb{R}^{(N+1) \times D}$$
(1)  
$$\mathbf{z}_{\ell} = \text{MSA}(\text{LN}(\mathbf{z}_{\ell-1})) + \mathbf{z}_{\ell-1}, \qquad \ell = 1 \dots L$$
(2)  
$$\mathbf{z}_{\ell} = \text{MLP}(\text{LN}(\mathbf{z}_{\ell})) + \mathbf{z}_{\ell}', \qquad \ell = 1 \dots L$$
(3)

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

```
# 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).

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

$$\begin{aligned} \mathbf{z}_0 &= [\mathbf{x}_{\text{class}}; \, \mathbf{x}_p^1 \mathbf{E}; \, \mathbf{x}_p^2 \mathbf{E}; \cdots; \, \mathbf{x}_p^N \mathbf{E}] + \mathbf{E}_{pos}, \\ \mathbf{z}'_{\ell} &= \text{MSA}(\text{LN}(\mathbf{z}_{\ell-1})) + \mathbf{z}_{\ell-1}, \\ \mathbf{z}_{\ell} &= \text{MLP}(\text{LN}(\mathbf{z}'_{\ell})) + \mathbf{z}'_{\ell}, \\ \mathbf{y} &= \text{LN}(\mathbf{z}_L^0) \end{aligned}$$

 $\mathbf{E} \in \mathbb{R}^{(P^2 \cdot C) \times D}, \, \mathbf{E}_{pos} \in \mathbb{R}^{(N+1) \times D}$  $\ell = 1 \dots L$  $\ell = 1 \dots L$ 

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



# Equation 1: The Class Token

### Sequence of patch embeddings

# Create the class token embedding class\_token = nn.Parameter(torch.ones(batch\_size, 1, embedding\_dimension), requires\_grad=True) # make embedding learnable

### **Create learnable class token and** prepend it to patch embeddings

Patch embeddings with learnable class token



Shape: [1, 197, 786], [batch\_size, number\_of\_patches + class\_token, embedding\_dimension]

•••						
tensor([[[-0.3	714, 0.0556,	-0.1053,	,	0.2598,	-0.1740,	0.1473],
[-0.4	294, 0.0788,	-0.1078,	,	0.2671,	-0.1797,	0.1644],
[-0.4	774, 0.0965,	-0.1198,	,	0.3465,	-0.1918,	0.1432],
···,						
[-0.1	749, 0.0247,	-0.0610,	,	0.1185,	-0.0448,	0.0451],
[-0.1	679, 0.0264,	-0.0745,	,	0.1182,	-0.0693,	0.0623],
[-0.0	631, -0.0043,	-0.0612,	,	0.0553,	-0.0460,	0.0837]]],
grad_fn	= <permutebackw< td=""><td>ard0&gt;)</td><td></td><td></td><td></td><td></td></permutebackw<>	ard0>)				
pe: [1, 196, 7	86], [batch_	size, num	nber_c	of_patc	hes, embe	edding dimen

```
# 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
```

# **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).

 $\mathbf{E} \in \mathbb{R}^{(P^2 \cdot C) \times D}, \, \mathbf{E}_{pos} \in \mathbb{R}^{(N+1) \times D}$  $\mathbf{z}_0 = [\mathbf{x}_{\text{class}}; \, \mathbf{x}_p^1 \mathbf{E}; \, \mathbf{x}_p^2 \mathbf{E}; \cdots; \, \mathbf{x}_p^N \mathbf{E}] + \mathbf{E}_{pos},$  $\mathbf{z}'_{\ell} = \mathrm{MSA}(\mathrm{LN}(\mathbf{z}_{\ell-1})) + \mathbf{z}_{\ell-1},$  $\ell = 1 \dots L$  $\mathbf{z}_{\ell} = \mathrm{MLP}(\mathrm{LN}(\mathbf{z}'_{\ell})) + \mathbf{z}'_{\ell},$  $\ell = 1 \dots L$  $\mathbf{y} = LN(\mathbf{z}_L^0)$ 

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

**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

				Ceurnaol	e class toke
tensor([[[ 1.0000, [-0.3714,	1.0000, 1.0000 0.0556, -0.1053	),, 1. 3,, 0.	0000, 1.0000, 2598, -0.1740,	1.0000], Prej 0.1473],	pended
[-0.4294,	0.0788, -0.1078	3,, 0.	2671, -0.1797,	0.1644],	
[-0.1749,	0.0247, -0.0610	),, 0.	1185, -0.0448,	0.0451],	
[-0.1679, [-0.0631, grad_fn= <cat< td=""><td>-0.0043, -0.0745 -0.0043, -0.0612 Backward0&gt;)</td><td>9,, 0. 2,, 0.</td><td>0553, -0.0460,</td><td>0.0823], 0.0837]]],</td><td></td></cat<>	-0.0043, -0.0745 -0.0043, -0.0612 Backward0>)	9,, 0. 2,, 0.	0553, -0.0460,	0.0823], 0.0837]]],	

Shape: [1, 197, 786], [batch\_size, number\_of\_patches + class\_token, embedding\_dimension]

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

```
# 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}")</pre>



(1)
 (2)
 (3)
 (4)

### Equation 2: The MSA Block MSA = Multí-Head Self Attention



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).



The Transformer encoder (Vaswani et al., 2017) consists of alternating layers of multiheaded selfattention (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 2: The MSA Block** MSA = Multí-Head Self Attention



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).

> **q** = query k = key v = value

$$\begin{aligned} \mathbf{z}_{0} &= [\mathbf{x}_{\text{class}}; \, \mathbf{x}_{p}^{1} \mathbf{E}; \, \mathbf{x}_{p}^{2} \mathbf{E}; \cdots; \, \mathbf{x}_{p}^{N} \mathbf{E}] + \mathbf{E}_{pos}, & \mathbf{E} \in \mathbb{R}^{(P^{2} \cdot C) \times D}, \, \mathbf{E}_{pos} \in \mathbb{R}^{(N+1) \times D} \\ \mathbf{z}_{\ell} &= \mathrm{MLP}(\mathrm{LN}(\mathbf{z}_{\ell-1})) + \mathbf{z}_{\ell-1}, & \ell = 1 \dots L \\ \mathbf{z}_{\ell} &= \mathrm{MLP}(\mathrm{LN}(\mathbf{z}_{\ell})) + \mathbf{z}_{\ell}', & \ell = 1 \dots L \\ \mathbf{y} &= \mathrm{LN}(\mathbf{z}_{L}^{0}) \end{aligned}$$

The Transformer encoder (Vaswani et al., 2017) consists of alternating layers of multiheaded selfattention (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).

### 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  $z \in \mathbb{R}^{N \times D}$ , we compute a weighted sum over all values y in the sequence. The attention weights  $A_{ij}$  are based on the pairwise similarity between two elements of the sequence and their respective query  $q^i$  and key  $k^j$  representations.

$$\begin{split} \left[ \mathbf{q}, \mathbf{k}, \mathbf{v} \right] &= \mathbf{z} \mathbf{U}_{qkv} & \mathbf{U}_{qkv} \in \mathbb{R}^{D \times 3D_h}, \\ A &= \operatorname{softmax} \left( \mathbf{q} \mathbf{k}^\top / \sqrt{D_h} \right) & A \in \mathbb{R}^{N \times N}, \\ \operatorname{SA}(\mathbf{z}) &= A \mathbf{v} \,. \end{split}$$

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.

$$MSA(\mathbf{z}) = [SA_1(z); SA_2(z); \cdots; SA_k(z)] \mathbf{U}_{msa} \qquad \mathbf{U}_{msa} \in \mathbb{R}^{k \cdot D_h \times D}$$









### Equation 2: The MSA Block MSA = Multí-Head Self Attention

### 

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
```





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: The MLP Block** MLP = Multilayer Perceptron

Equation 3 = "MLP block"

$\mathbf{z}_0 = [\mathbf{x}_{ ext{class}};\mathbf{x}_p^1\mathbf{E};\mathbf{x}_p^2\mathbf{E};\cdots;\mathbf{x}_p^N\mathbf{E}] + \mathbf{E}_{pos},$	$\mathbf{E} \in \mathbb{R}^{(P^2 \cdot C) \times D},  \mathbf{E}_{pos} \in \mathbb{R}^{(N+1) \times D}$
$\mathbf{z}'_{\ell} = \mathrm{MSA}(\mathrm{LN}(\mathbf{z}_{\ell-1})) + \mathbf{z}_{\ell-1},$	$\ell = 1 \dots L$
$\mathbf{z}_{\ell} = \mathrm{MLP}(\mathrm{LN}(\mathbf{z}'_{\ell})) + \mathbf{z}'_{\ell},$	$\ell = 1 \dots L$
$\mathbf{y} = \mathrm{LN}(\mathbf{z}_L^0)$	

The Transformer encoder (Vaswani et al., 2017) consists of alternating layers of multiheaded selfattention (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

```
•••
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

 $\mathbf{E} \in \mathbb{R}^{(P^2 \cdot C) \times D}, \, \mathbf{E}_{pos} \in \mathbb{R}^{(N+1) \times D}$  $\mathbf{z}_0 = [\mathbf{x}_{ ext{class}}; \, \mathbf{x}_p^1 \mathbf{E}; \, \mathbf{x}_p^2 \mathbf{E}; \cdots; \, \mathbf{x}_p^N \mathbf{E}] + \mathbf{E}_{pos},$  $\mathbf{z'}_{\ell} = \mathrm{MSA}(\mathrm{LN}(\mathbf{z}_{\ell-1})) + \mathbf{z}_{\ell-1}, \qquad \ell = 1 \dots L$  $\mathbf{z}_{\ell} = \mathrm{MLP}(\mathrm{LN}(\mathbf{z'}_{\ell})) + \mathbf{z'}_{\ell},$  $\mathbf{y} = LN(\mathbf{z}_L^0)$ 

The Transformer encoder (Vaswani et al., 2017) consists of alternating layers of multiheaded selfattention (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



```
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
```

