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

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Background

Vision Transformer (ViT) is an innovative image classification model proposed in 2021. It is breaking away from the dominant role of traditional CNNs in image processing.

CNNs: Relies on convolution operations.

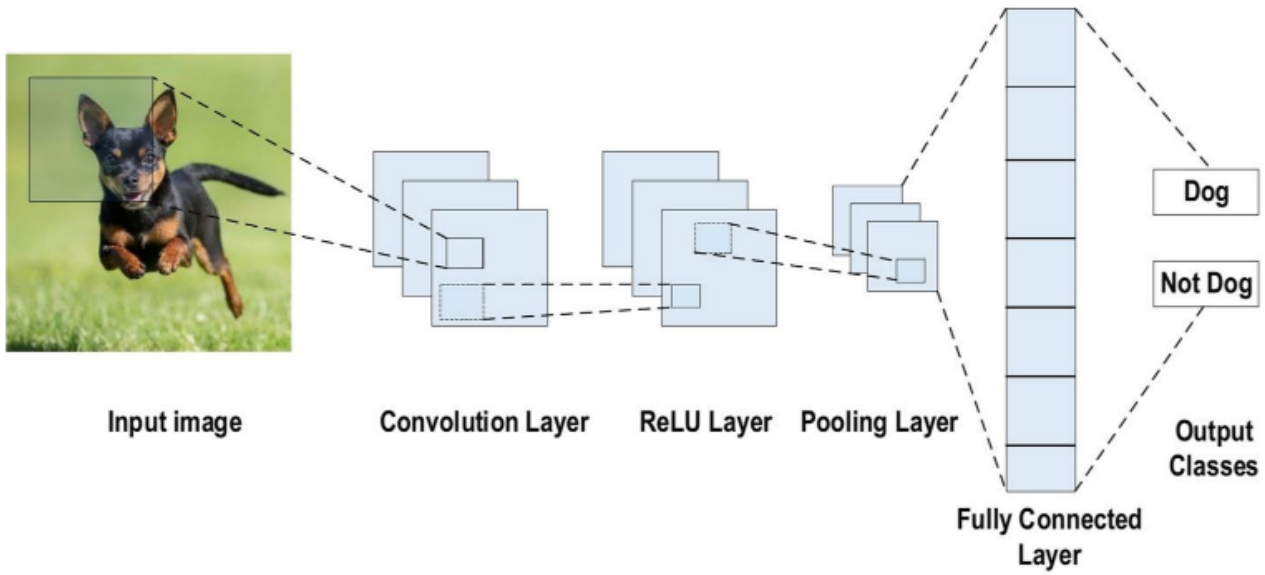


Figure: An example of CNNs architecture for image classification [1].

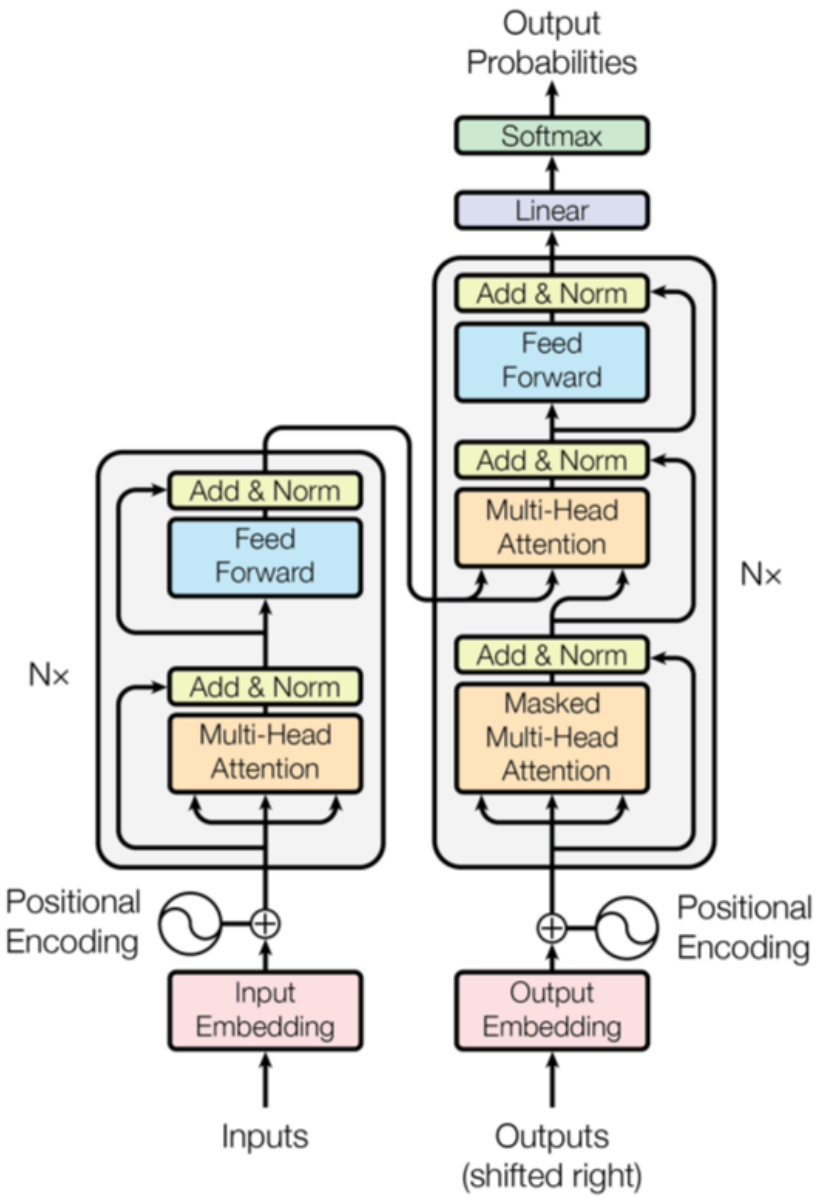
Vision Transformer (ViT): Transformer $\xrightarrow{\text{apply}}$ Image regconition

1. Inspired by the Transformer scaling successes in NLP, they experiment with applying a standard Transformer directly to images, with the fewest possible modifications.
2. Treat image patches the same way as tokens (words) in an NLP application.

A transformer is a deep learning architecture that was developed by researchers at Google and is based on the multi-head attention mechanism, which was proposed in the 2017 paper "Attention Is All You Need" [2].

Introduction

Transformer - NLP



Vision Transformation - ViT

Model Overview

Split image into patches → Embedding → Transformer encoder

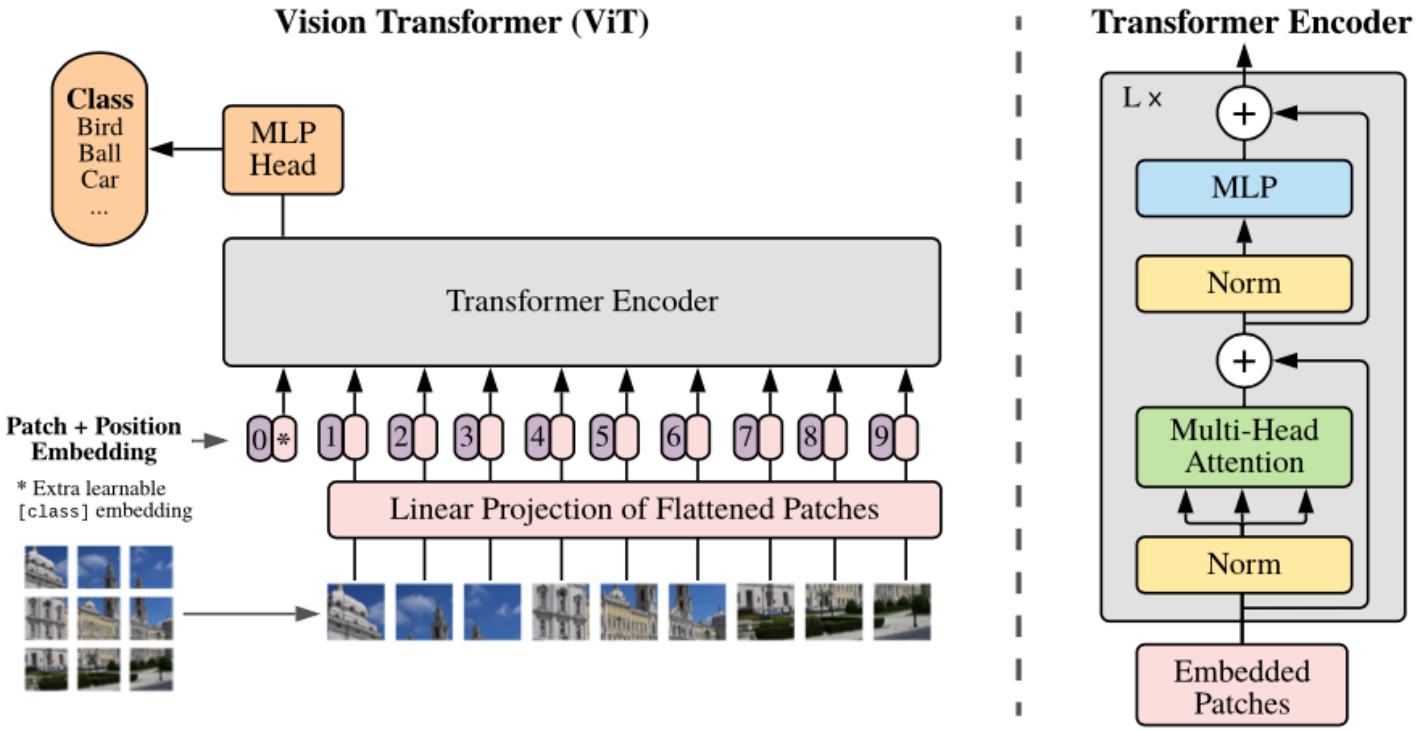


Figure: Model Overview

Vision Transformation - ViT

Method - Reshape Image

Reshape the image $x \in \mathbb{R}^{H \times W \times C}$ into a sequence of flattened 2D patches $x_p \in \mathbb{R}^{N \times (P^2 \cdot C)}$, 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.

Figure: Image Reshaping

Vision Transformation - ViT

Method - Patch Embedding

Patch embedding:

Flatten the patches and map to D dimensions with a trainable linear projection.

$$z_0 = [x_{\text{class}};\ x_p^1\mathbf{E};\ x_p^2\mathbf{E};\ \ldots;\ x_p^N\mathbf{E}] + \mathbf{E}_{pos}$$

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

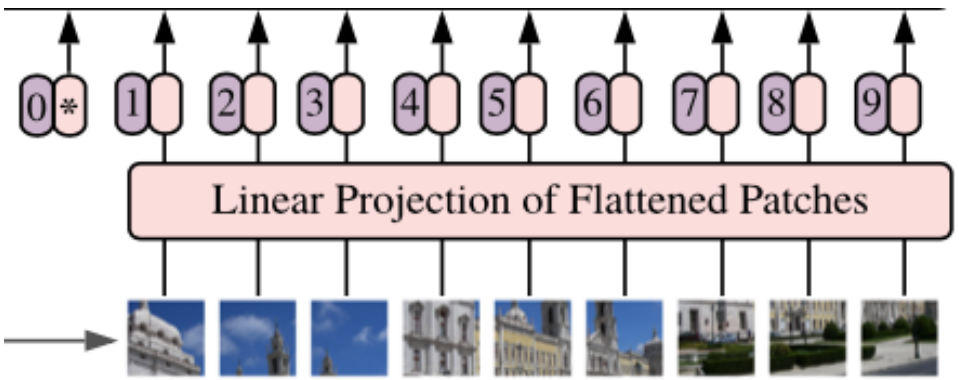


Figure: Patch Embedding

Vision Transformation - ViT

Method

- **Inductive Bias** Vision Transformer has much less image-specific inductive bias than CNNs. Only MLP layers are local and translationally equivariant, while the self-attention layers are global. Resolution adjustments and patch extraction are the only inductive biases introduced manually.
- **Hybrid Architecture** The input sequence can be formed from feature maps of a CNN. In this hybrid model, the patch embedding projection **E** is applied to patches extracted from a CNN feature map.

Vision Transformation - ViT

Method - Fine-Tuning and Higher Resolution

- Pre-training is done on large datasets; fine-tuning adapts ViT for downstream tasks.
- The pre-trained prediction head is removed, replaced with a new $D \times K$ feedforward layer.
- When fine-tuning at a higher resolution:
  - Keep the patch size constant, increasing the sequence length.
  - Perform 2D interpolation of position embeddings to adapt to the new resolution.
- ViT can handle arbitrary sequence lengths, but pre-trained position embeddings may lose meaning.

Experiments

Setup

Datasets: ILSVRC-2012 ImageNet; ImageNet-21; JFT
Benchmark tasks: original validation labels; ReaL labels; CIFAR-10/100; Oxford-IIIT Pets; Oxford Flowers-102; 19-task VTAB classification suite.
ViT: Base, Large, Huge Models. (Ex. ViT-L/16 $\sim$ "Large" variant with 16 $\times$ 16 input patch size) Configurations based on BERT. Smaller patch size are more computational expensive.
Baseline CNNs: ResNet; replaced Batch Normalization layer with Group Normalization.
Hybrid: Intermediate feature maps from CNN to ViT with patch size $= 1$.

Experiments

Setup

Training

Optimizer: Adam ($\beta_1 = 0.9$, $\beta_2 = 0.999$)
Batch Size: 4096
Weight Decay: 0.1 (for improved transfer learning)
Learning Rate: Linear warmup & decay

Fine-Tuning

Optimizer: SGD with momentum
Batch Size: 512
Averaging: Polyak Averaging (factor = 0.9999) for improved generalization.

Metrics

Few-Shot Accuracy: Regularized least-squares regression that maps training image to $\{-1, 1\}^K$ target vectors
Fine-Tuning Accuracy: Performance after fine-tuning on downstream tasks.

Comparison

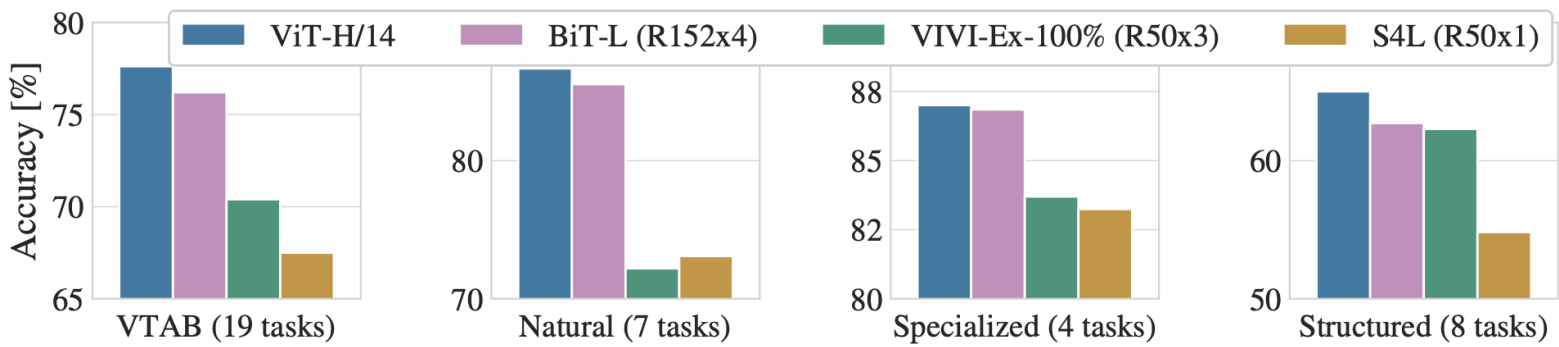
ViT-H/14 & ViT-L/16 vs.Big Transfer & Noisy Student

Result Overview

- **ViT-L/16** (pre-trained on JFT-300M) **outperforms BiT-L** on all tasks while using fewer computational resources.
- **ViT-H/14** (pre-trained on JFT-300M) shows improved performance, especially on challenging datasets like ImageNet, but also requires less compute than previous SOTA.
- **ViT-L/16** (pre-trained on ImageNet-21k) delivers strong performance across tasks and is resource-efficient. (as a controlled study for different architectures)

Comparison

	Ours-JFT (ViT-H/14)	Ours-JFT (ViT-L/16)	Ours-I21k (ViT-L/16)	BiT-L (ResNet152x4)	Noisy Student (EfficientNet-L2)
ImageNet	**88.55** ± 0.04	87.76 ± 0.03	85.30 ± 0.02	87.54 ± 0.02	88.4/88.5*
ImageNet ReaL	**90.72** ± 0.05	90.54 ± 0.03	88.62 ± 0.05	90.54	90.55
CIFAR-10	**99.50** ± 0.06	99.42 ± 0.03	99.15 ± 0.03	99.37 ± 0.06	–
CIFAR-100	**94.55** ± 0.04	93.90 ± 0.05	93.25 ± 0.05	93.51 ± 0.08	–
Oxford-IIIT Pets	**97.56** ± 0.03	97.32 ± 0.11	94.67 ± 0.15	96.62 ± 0.23	–
Oxford Flowers-102	99.68 ± 0.02	**99.74** ± 0.00	99.61 ± 0.02	99.63 ± 0.03	–
VTAB (19 tasks)	**77.63** ± 0.23	76.28 ± 0.46	72.72 ± 0.21	76.29 ± 1.70	–
TPUv3-core-days	2.5k	0.68k	0.23k	9.9k	12.3k



Scaling Study

Goal

- Evaluate transfer performance from JFT-300M vs. pre-training cost for different models.

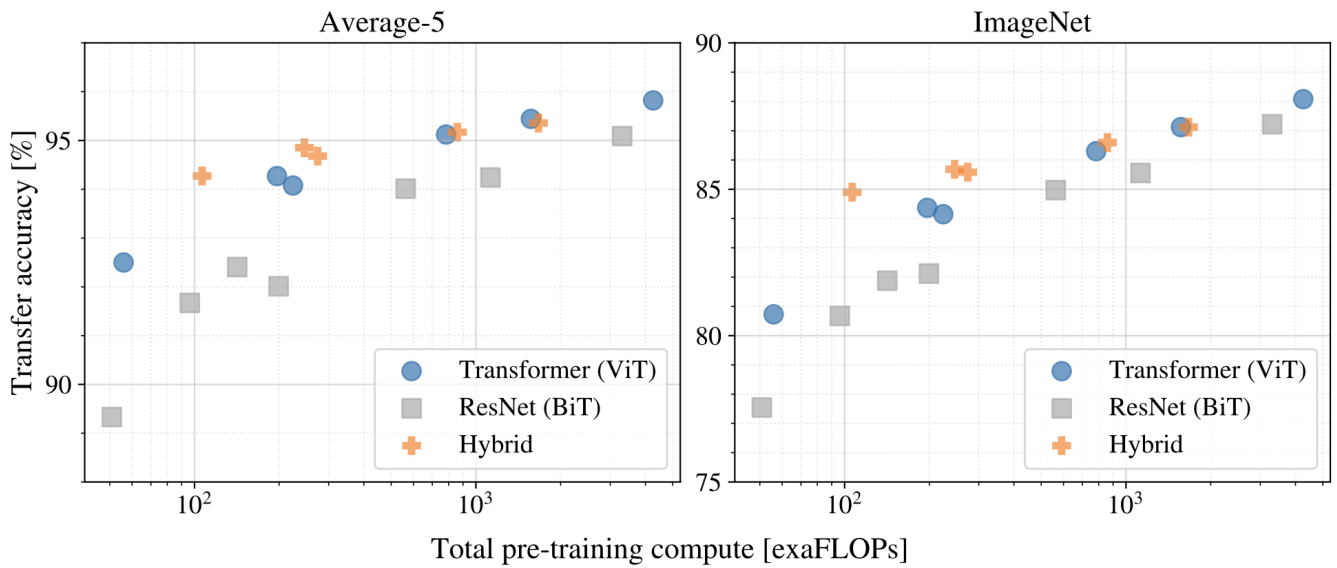
Model Set

- 7 ResNets: R50x1, R50x2, R101x1, R152x1, R152x2 (7 epochs), R152x2, R200x3 (14 epochs)
- 6 ViTs: ViT-B/32, B/16, L/32, L/16 (7 epochs), L/16, H/14 (14 epochs)
- 5 Hybrids: Combos of ResNet + ViT models (7 epochs for smaller, 14 for larger models)

Scaling Study

A controlled scaling study - performance on JFT-300M

- **ViTs outperform ResNets:** ViTs use 2-4× less compute to achieve the same performance across 5 datasets.
- **Hybrids outperform ViTs at small budgets:** Hybrids are better at lower computational budgets, but this advantage diminishes as model size increases.
- **ViTs don't saturate:** Performance continues to improve without significant saturation in the tested range.



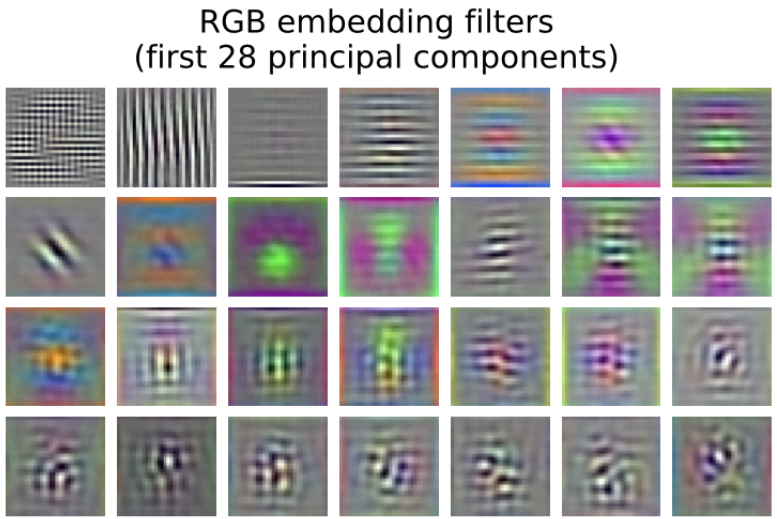
Internal Representation

1. **Projection and Embedding**

- **First Layer:** The Vision Transformer (ViT) linearly projects flattened image patches into a lower-dimensional space.

$$z_0 = [X_{class}\,; x_p^1 E;\ x_p^2 E; ...;\ x_p^N E] + E_{pos},$$
$$\mathrm{E} \in \mathbb{R}^{(P^2 \cdot C) \times D},\ E_{pos} \in \mathbb{R}^{(N+1) \times D}$$

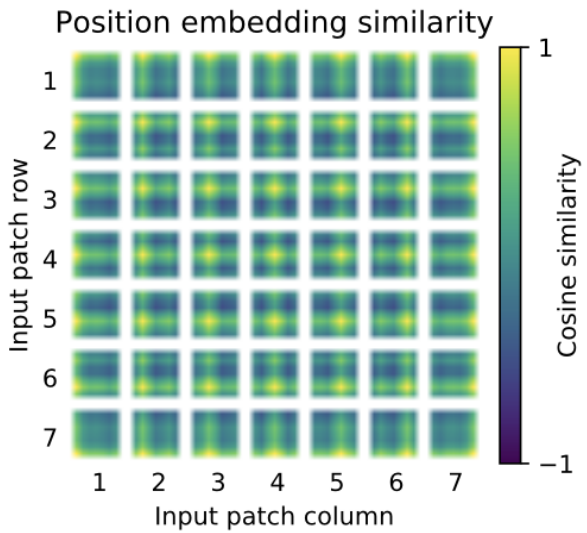
- **Embedding Filters:** The top principal components of the learned embeddings resemble basis functions for capturing fine details within each image patch.



Internal Representation

2. **Learned Position Embedding**

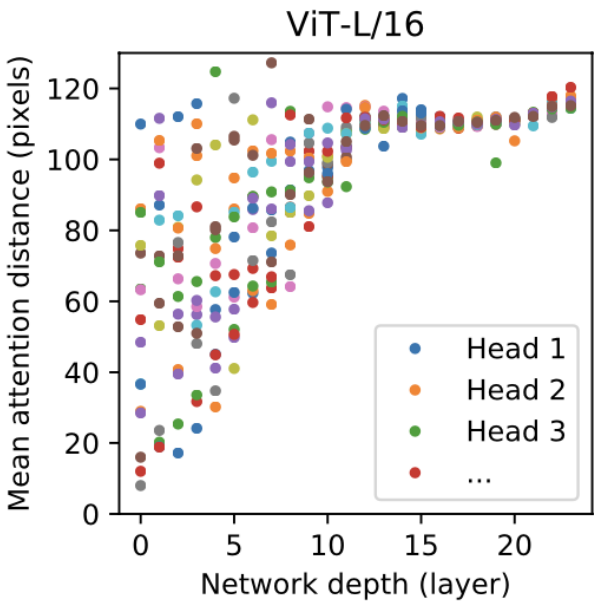
- **Spatial Distance:** Patches closer in space tend to have more similar position embeddings.
- **Row/Column Structure:** Patches in the same row or column have similar embeddings.
- **Sinusoidal Structure:** Apparent in larger grids, explaining why 2D-aware hand-crafted embeddings don't improve performance

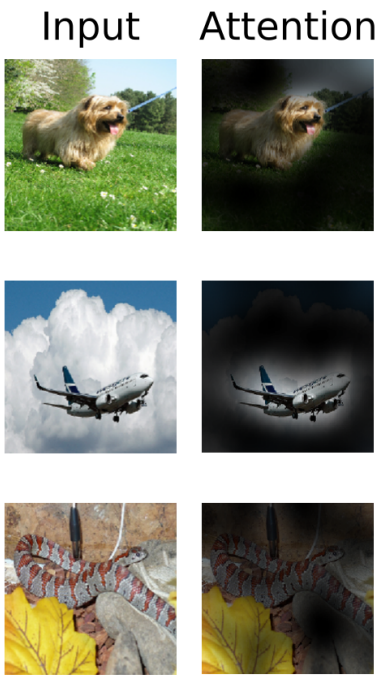


Internal Representation

3. **Self Attention**

- **Global Integration via Self-Attention:** ViT uses self-attention to integrate information across the entire image, even in the lowest layers.
- **Attention Distance:** The average distance across which information is integrated (similar to receptive field in CNNs)





Self-Attention

A popular building block for neural architectures.

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

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

$$A = \text{softmax}(\boldsymbol{q}\boldsymbol{k}^\top / \sqrt{D_h}) \qquad A \in \mathbb{R}^{N \times N}$$

$$SA(\boldsymbol{z}) = A\boldsymbol{v}$$

Conclusion

- **Direct application of Transformer**: Apply standard Transformer encoders to images by treating images as a sequence of patches with minimal image-specific inductive biases.
- **Pre-training Success:** This strategy works surprisingly well when coupled with pre-training on large datasets.
- **Computational Efficiency:** ViT offers strong performance with relatively low pre-training cost.

Quiz

Quiz 1: Match each feature with the correct model (CNN or ViT).

Feature	Model
(A) Uses Self-attention mechanism (Transformers) to process images	_____
(B) Use convolutional filter slides across the image and extracts features	_____
(C) Treat images as sequences of patches	_____
(D) Works well even with small datasets	_____
(E) Needs large datasets	_____
(F) Requires positional encodings to retain spatial information	_____

Quiz 2: In patch embedding process, if the flattened 2D patches is $x_p = \begin{pmatrix} 1 & 2 \\ 1 & 1 \end{pmatrix}$ and the linear projection matrix is $\mathbf{E} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 4 & 4 \end{pmatrix}$, what is $x_p^2\mathbf{E}$ after patch embedding?

$$\text{Hint:} \quad z_0 = [x_{\text{class}};\ x_p^1\mathbf{E};\ x_p^2\mathbf{E}; \ldots;\ x_p^N\mathbf{E}] + \mathbf{E}_{pos}$$

References

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