Transformers and ViT

CSE 849 Deep Learning Spring 2025

Zijun Cui

Project 3

• It requires considerable time from your end.

Plan ahead and Start early.

Class Schedule Update

• We will begin *Generative Modeling* immediately after the *Transformer* lectures. Topics on *Graph Neural Networks* will be moved to the end of the course. This change ensures that you learn about *Diffusion Models* in time for Project 4.

3/24	17 Transformer and ViT We are here	18 Transformer Case Study: LLMs
3/31	19 Probabilistic Deep Learning and Generative modeling	20 Generative Modeling
4/7	21 Diffusion Models 1	22 Diffusion Models 2 Project 4 Out; Project 3 Due
4/14	23 Diffusion Models Applications and Bayesian Deep Learning	24 Bayesian Deep Learning and Deep PGM
4/21	25 Graph Neural Network	No Class
4/28	Final Exam Week	Final Exam Week Project 4 Due on Wednesday, April 30 th .

I plan to have **no**class on

Thursday, April

24, to give you

more time to focus

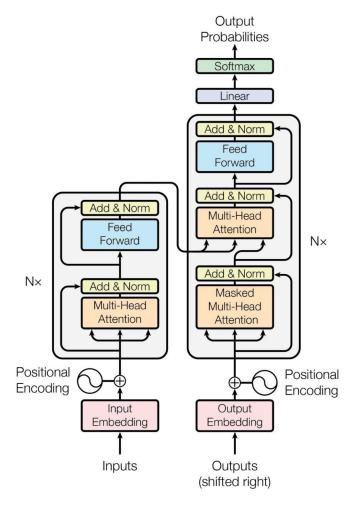
on Project 4

I have updated syllabus in Piazza accordingly.

Now let's continue from the last lecture and finish Transformer Architecture

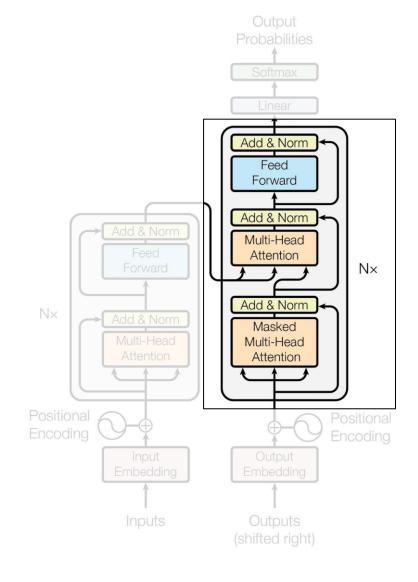
- ✓ Tokenization
- ✓ Input Embeddings
- **✓** Position Encodings
- ✓ Query, Key, & Value
- ✓ Attention
- ✓ Self Attention
- ✓ Multi-Head Attention
- √ Feed Forward
- ✓ Add & Norm
- ✓ Encoders

- Masked Attention
- Encoder Decoder Attention
- Linear
- Softmax
- Decoders
- Encoder-Decoder Models



Encoder Decoder Attention

Encoder Decoder Attention? Add & Norm



Input Norm(Z')

Encoder Decoder Attention

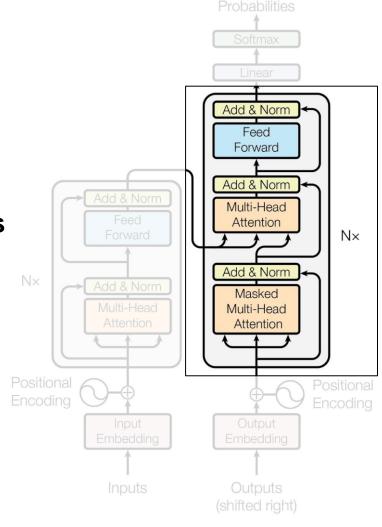
Encoder

Decoder

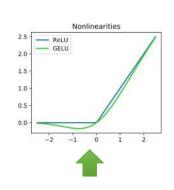
Keys from **Encoder Outputs**Values from **Encoder Outputs**

Queries from **Decoder Inputs**

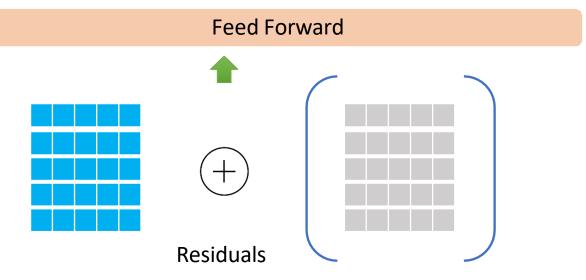
NOTE: Every decoder block receives the same FINAL encoder output

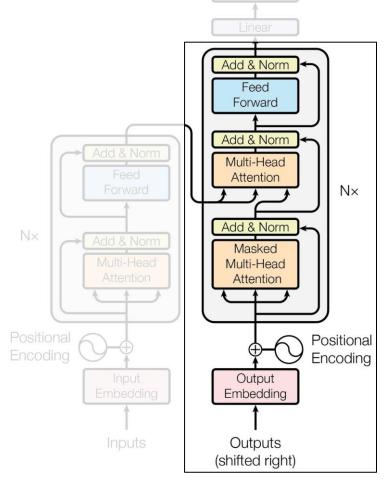


Encoder Decoder Attention



- Non Linearity
- Complex Relationships
- Learn from each other





Add n Norm Decoder Self Attn

Norm(Z'')

Decoder

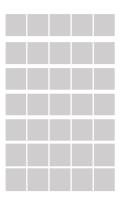
DECODER

.

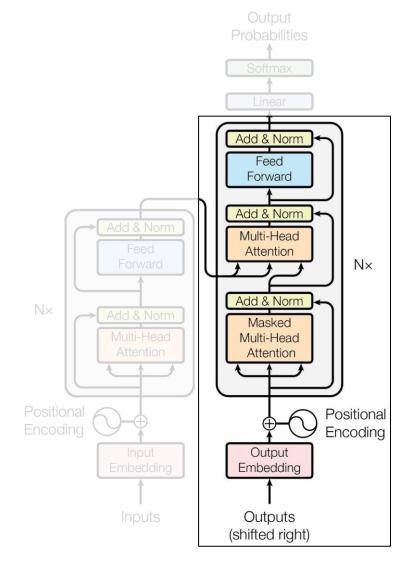
DECODER

DECODER

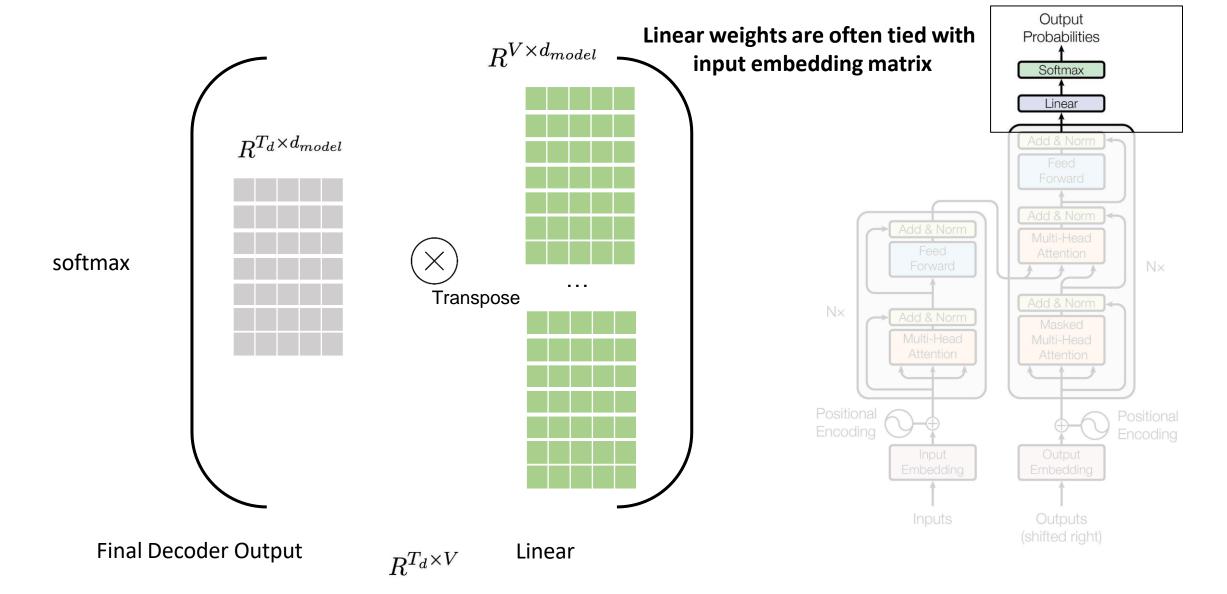
 $R^{T_d \times d_{model}}$



Decoder output

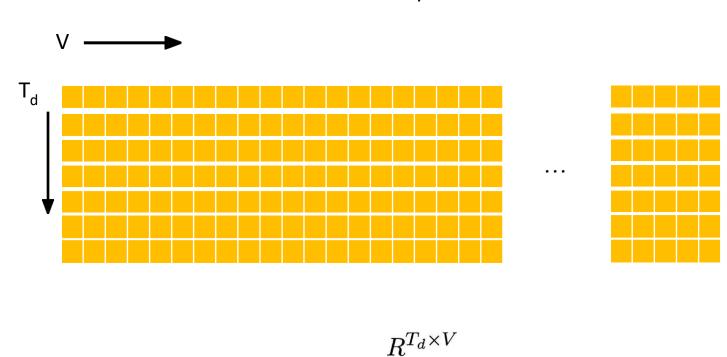


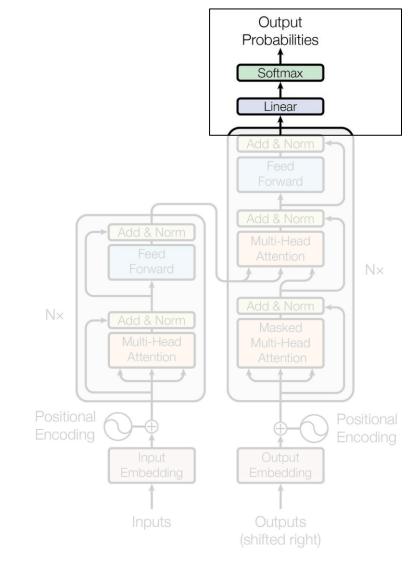
Linear



Softmax

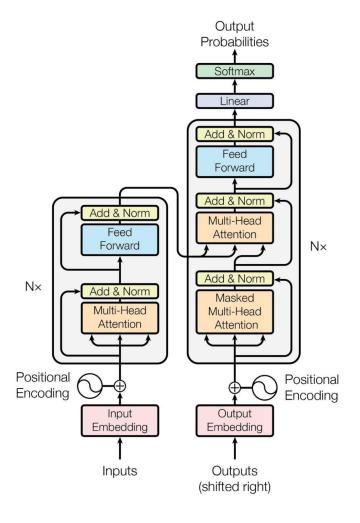
Output Probabilities

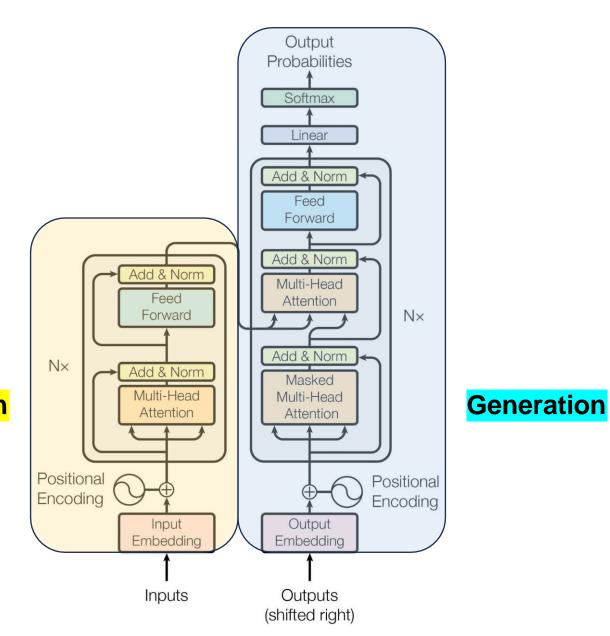




- ✓ Tokenization
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- **✓** Decoders
- Encoder-Decoder Models

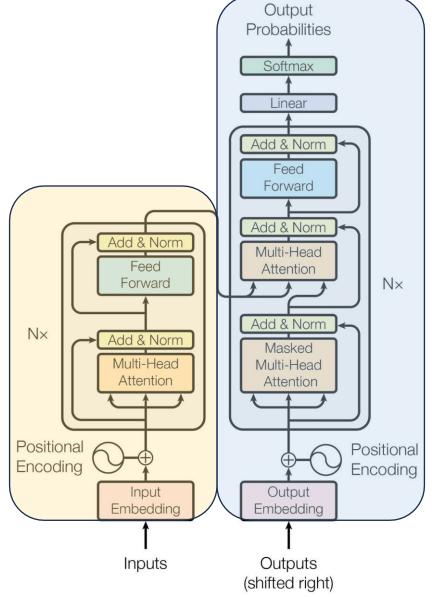




Representation

Input – input tokens
Output – hidden states

Representation



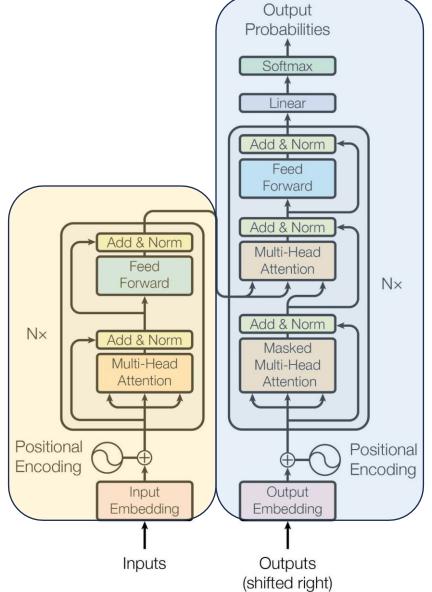
Input – output tokens and hidden states

Output – output tokens

Input – input tokensOutput – hidden states

Model can see all timesteps

Representation



Input – output tokens and hidden states

Output – output tokens

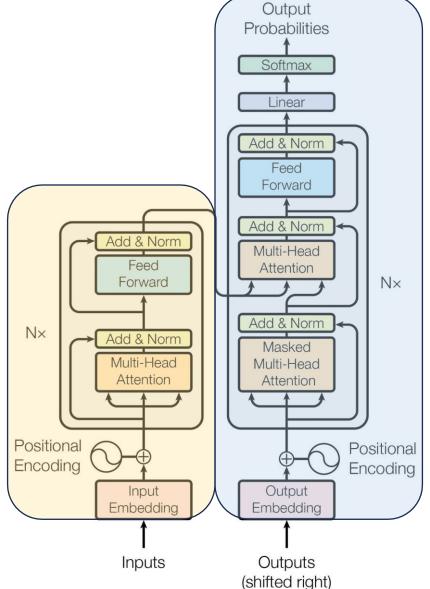
Model can only see previous timesteps

Input – input tokensOutput – hidden states

Model can see all timesteps

Does not usually output tokens, so no inherent auto-regressivity

Representation



Input – output tokens and hidden states

Output – output tokens

Model can only see previous timesteps

Model is auto-regressive with previous timesteps' outputs

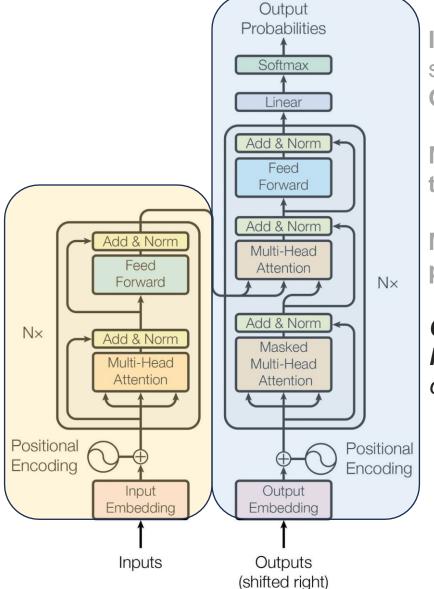
Input – input tokens
Output – hidden states

Model can see all timesteps

Does not usually output tokens, so no inherent auto-regressivity

Can also be adapted to generate tokens by appending a module that maps hidden state dimensionality to vocab size

Representation



Input – output tokens and hidden states

Output – output tokens

Model can only see previous timesteps

Model is auto-regressive with previous timesteps' outputs

Can also be adapted to generate hidden states by looking before token outputs

- ✓ Tokenization
- ✓ Input Embeddings
- **✓** Position Encodings
- ✓ Query, Key, & Value
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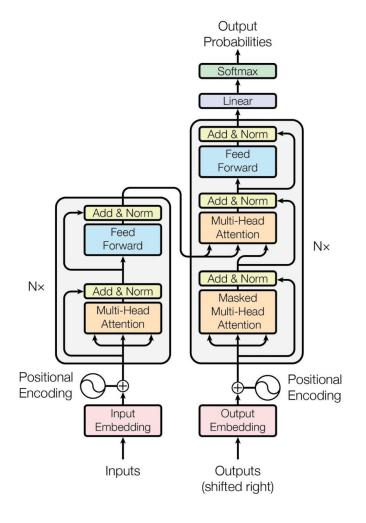
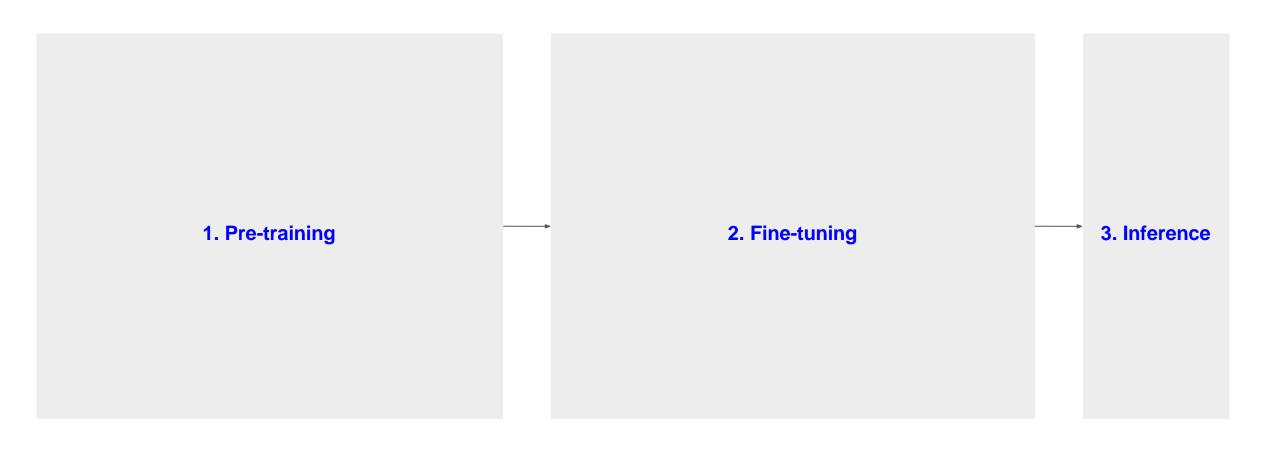
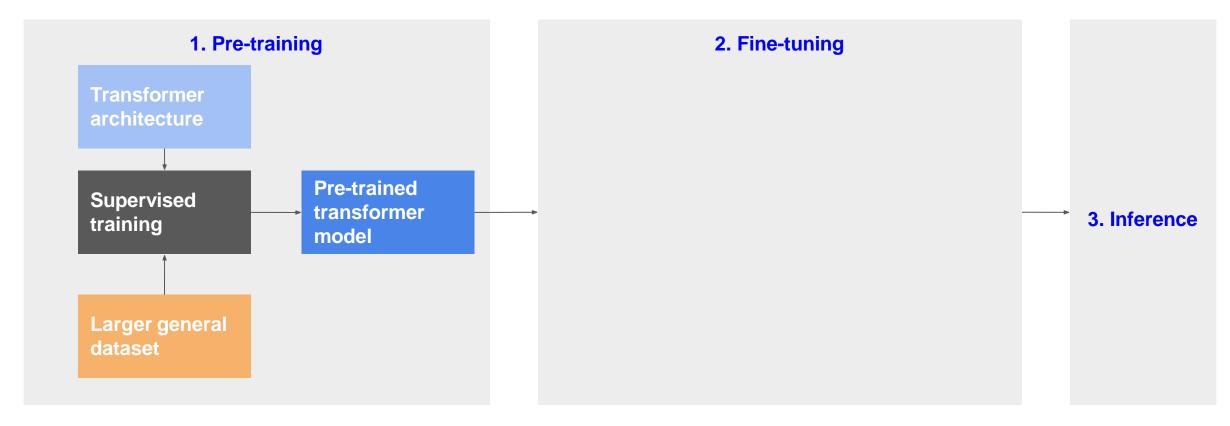


Table of contents

- **✓** The Transformer Architecture
- 1. Pre-training and Fine-tuning
- 2. Transformer Applications
- 3. Case study Large Language Models

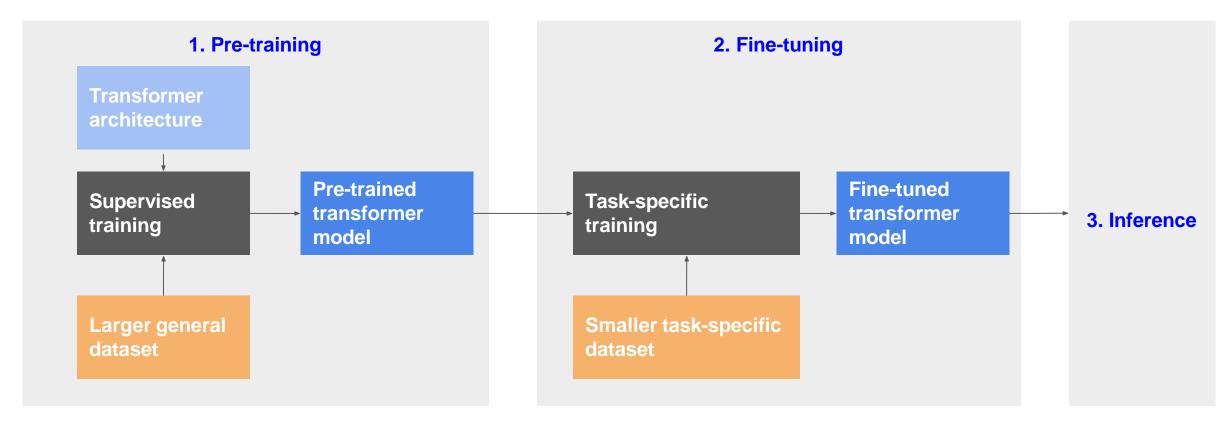






Lots of data, learn general things. May serve as a parameter initialization.

Usually requires significant computational resources and time.



Lot's of data, learn general things. May serve as a parameter initialization.

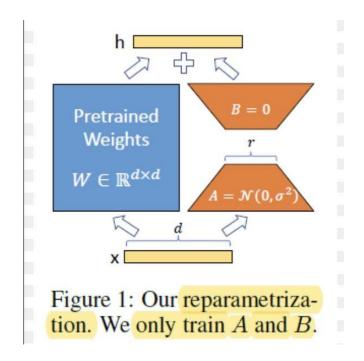
Usually requires significant computational resources and time.

Adaptation to the specific task.

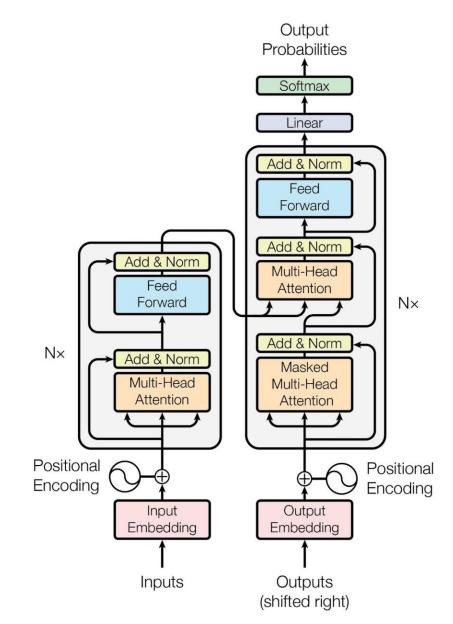
Potentially less computationally intensive.

Parameter-Efficient Fine-Tuning Techniques

LoRA (Lower-Rank Adaptation)



LoRA: https://arxiv.org/abs/2106.09685 BitFit: https://arxiv.org/abs/2106.10199

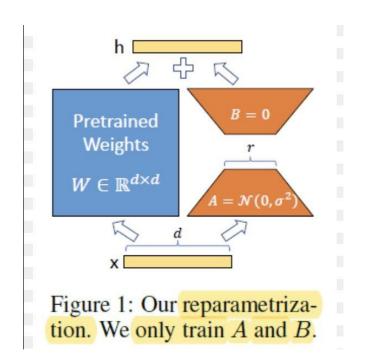


Parameter-Efficient Fine-Tuning Techniques

Can be applied to:

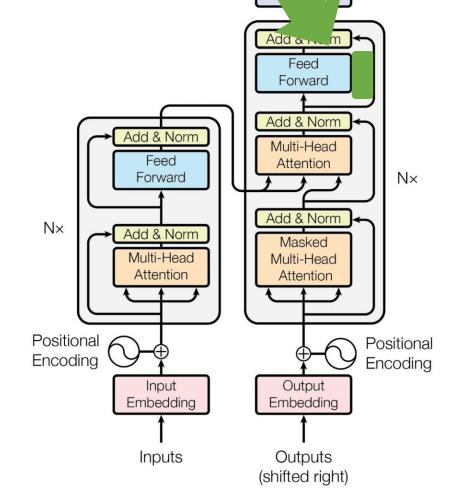
- 1.Attention layers (Q/K/V projections)
- 2.Feed-forward layers (as shown)
- 3. Anywhere with large linear projections

LoRA (Lower-Rank Adaptation)



$$\mathbf{Q}^{m,\ell}(\mathbf{x}) = \mathbf{W}_q^{m,\ell}\mathbf{x} + \mathbf{b}_q^{m,\ell}$$
 $\mathbf{K}^{m,\ell}(\mathbf{x}) = \mathbf{W}_k^{m,\ell}\mathbf{x} + \mathbf{b}_k^{m,\ell}$
 $\mathbf{V}^{m,\ell}(\mathbf{x}) = \mathbf{W}_v^{m,\ell}\mathbf{x} + \mathbf{b}_v^{m,\ell}$

Finetune only the additive bis terms b



Output

obabilities

LoRA: https://arxiv.org/abs/2106.09685 BitFit: https://arxiv.org/abs/2106.10199

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- **✓** The Transformer Architecture
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Output Probabilities Softmax Linear Add & Norm Feed Forward Add & Norm Add & Norm Multi-Head Feed Attention Forward N× Add & Norm $N \times$ Add & Norm Masked Multi-Head Multi-Head Attention Attention Positional Positional Encoding Encoding Output Input Embedding Embedding Outputs Inputs (shifted right)

Generation / Decoder

Representation / Encoder

Data Modalities

- ✓ Language
- Vision
- Audio
- ... and many other modalities (e.g., biological/physiological signals, etc.)
- Multimodal (>2 data modalities)

Computer Vision

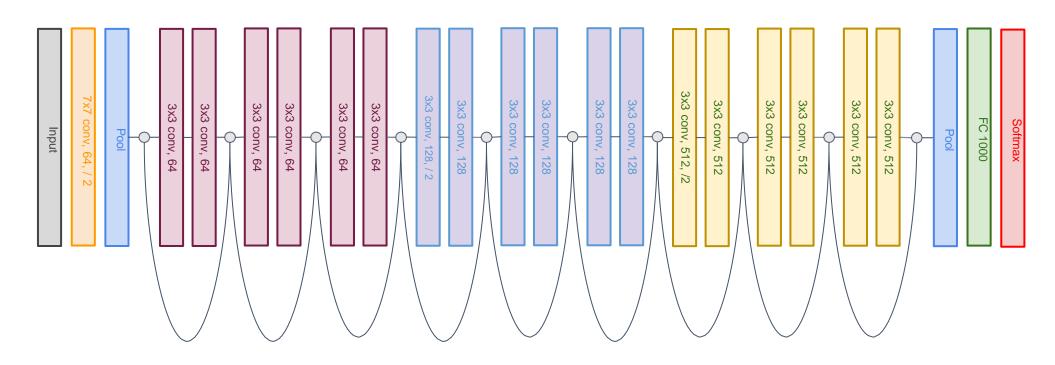
- 1. In computer vision convolutional architectures remain largely dominant.
- 2. Inspired by NLP successes, multiple works try introducing combining CNN-like architectures with self-attention or replacing the convolutions entirely.
- 3. However, they faced challenges with performance and scaling.
- 4. Key breakthrough Vision Transformer (ViT) released in 2020

Use Attention / Transformers for Vision

- -- Earlier attempts
- -- Vision Transformer (ViT)

Idea #1: Add attention to existing CNNs

Start from standard CNN architecture (e.g. ResNet)

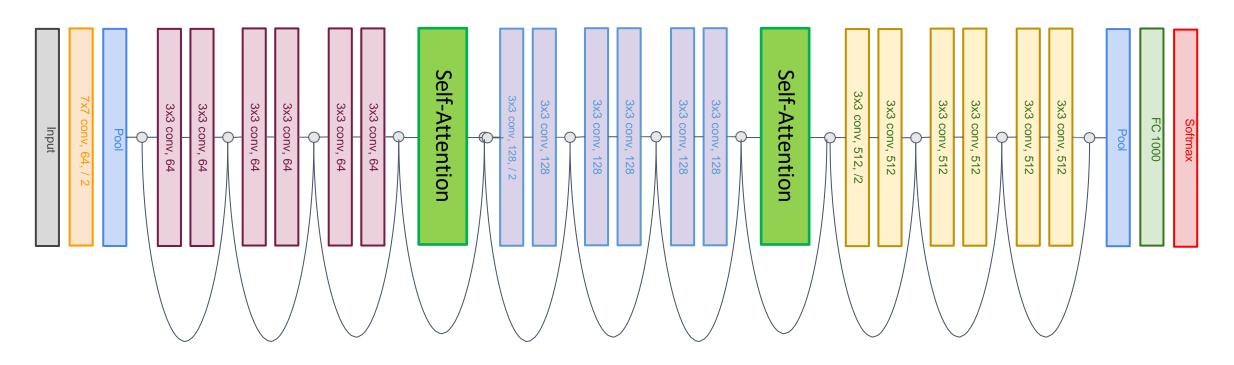


Zhang et al, "Self-Attention Generative Adversarial Networks", ICML 2018 Wang et al, "Non-local Neural Networks", CVPR 2018

Idea #1: Add attention to existing CNNs

Start from standard CNN architecture (e.g. ResNet)

Add Self-Attention blocks between existing ResNet blocks

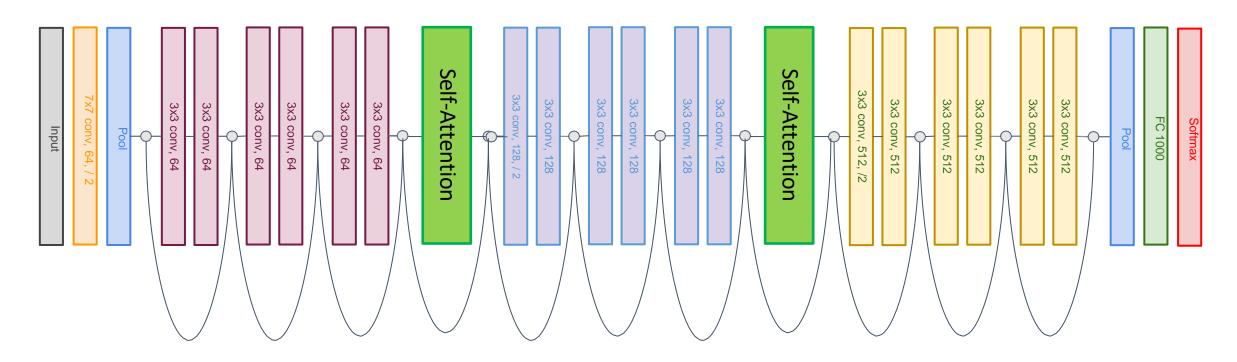


Zhang et al, "Self-Attention Generative Adversarial Networks", ICML 2018 Wang et al, "Non-local Neural Networks", CVPR 2018

Idea #1: Add attention to existing CNNs

Model is still a CNN! Start from standard CNN architecture (e.g. ResNet) Can we replace

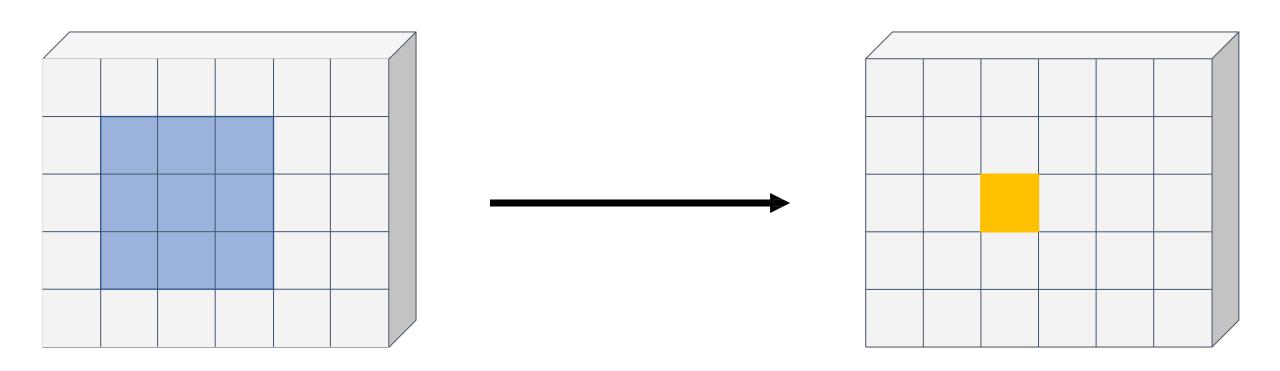
convolution entirely? Add Self-Attention blocks between existing ResNet blocks



Zhang et al, "Self-Attention Generative Adversarial Networks", ICML 2018 Wang et al, "Non-local Neural Networks", CVPR 2018

Idea #2: Replace Convolution with "Local Attention"

Convolution: Output at each position is inner product of conv kernel with receptive field in input

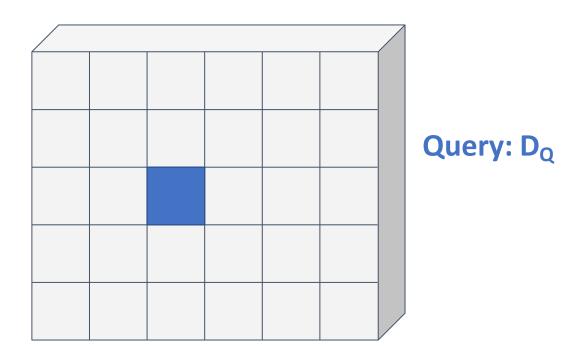


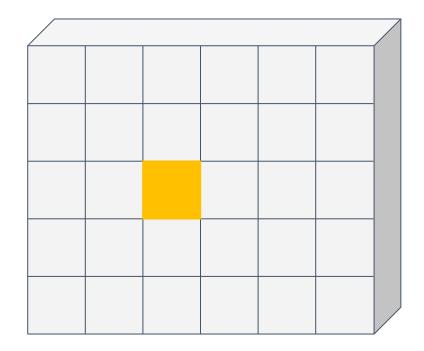
Hu et al, "Local Relation Networks for Image Recognition", ICCV 2019;

Ramachandran et al, "Stand-Alone Self-Attention in Vision Models", NeurIPS 2019

Idea #2: Replace Convolution with "Local Attention"

Map center of receptive field to query





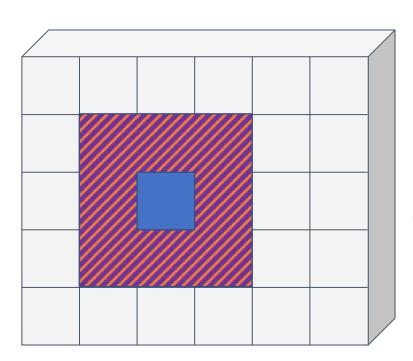
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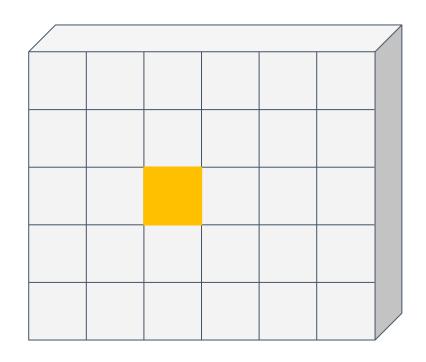
Map each element in receptive field to key and value



Query: D_Q

Keys: R x R x D_Q

Values: R x R x C'



Hu et al, "Local Relation Networks for Image Recognition", ICCV 2019;

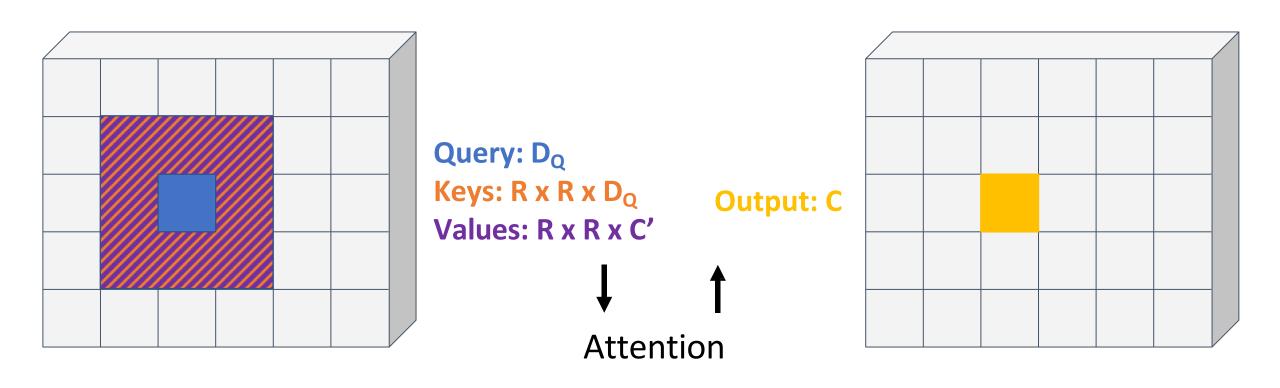
Ramachandran et al, "Stand-Alone Self-Attention in Vision Models", NeurIPS 2019

Idea #2: Replace Convolution with "Local Attention"

Map center of receptive field to query

Map each element in receptive field to key and value

Compute output using attention



Hu et al, "Local Relation Networks for Image Recognition", ICCV 2019;

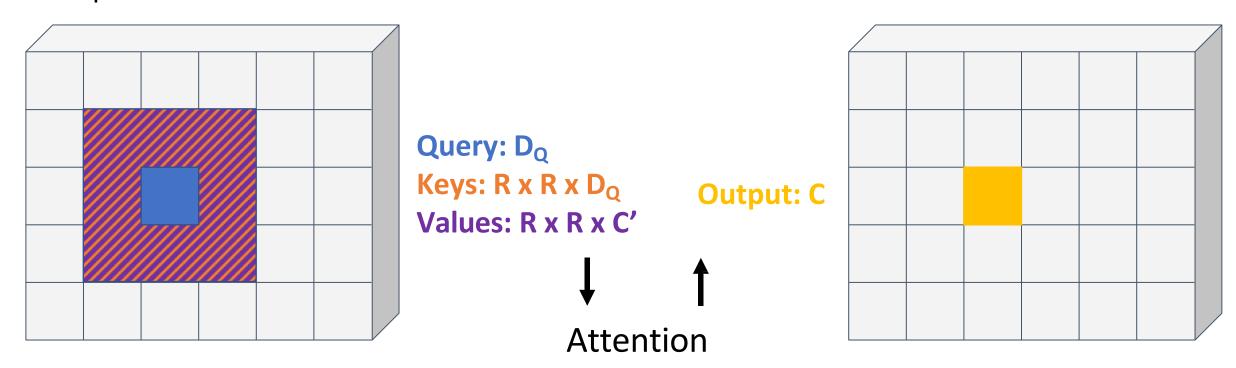
Idea #2: Replace Convolution with "Local Attention"

Map center of receptive field to query

Map each element in receptive field to key and value

Compute output using attention

Replace all conv in ResNet with local attention



Lots of tricky details, hard to implement, only marginally better than ResNets

Hu et al, "Local Relation Networks for Image Recognition", ICCV 2019;

Ramachandran et al, "Stand-Alone Self-Attention in Vision Models", NeurIPS 2019

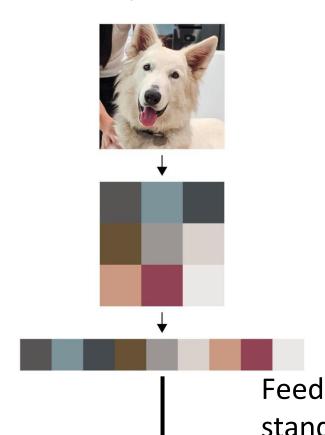
Idea #3: Standard Transformer on Pixels

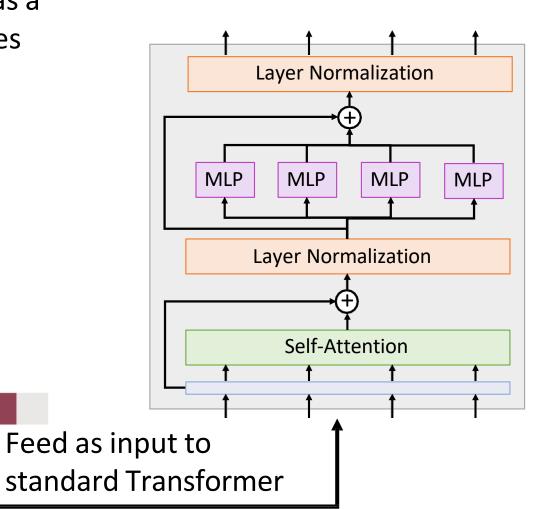
Treat an image as a set of pixel values **Layer Normalization** MLP MLP MLP MLP **Layer Normalization Self-Attention** Feed as input to standard Transformer

Chen et al, "Generative Pretraining from Pixels", ICML 2020

Idea #3: Standard Transformer on Pixels

Treat an image as a set of pixel values





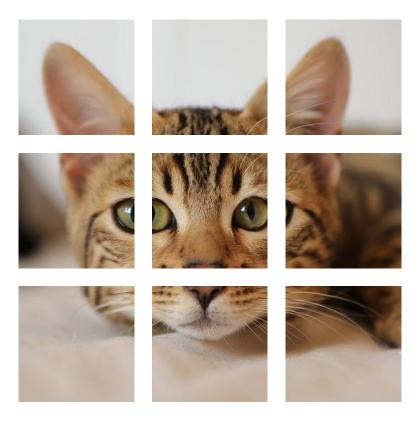
Problem: Memory use!

R x R image needs R⁴ elements per attention matrix

R=128, 48 layers, 16 heads per layer takes 768GB of memory for attention matrices for a single example...

Chen et al, "Generative Pretraining from Pixels", ICML 2020





N input patches, each of shape 3x16x16













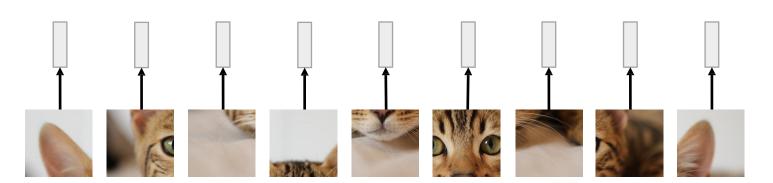


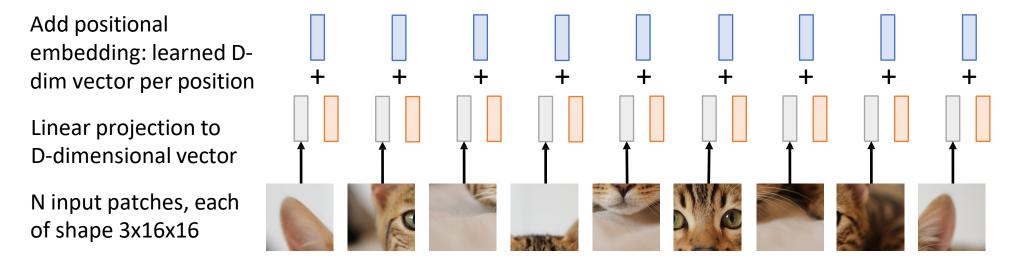


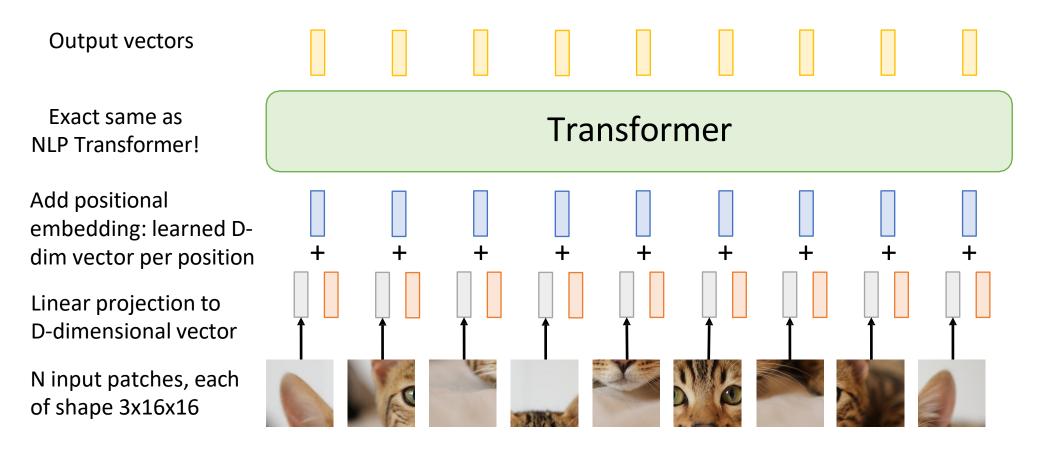


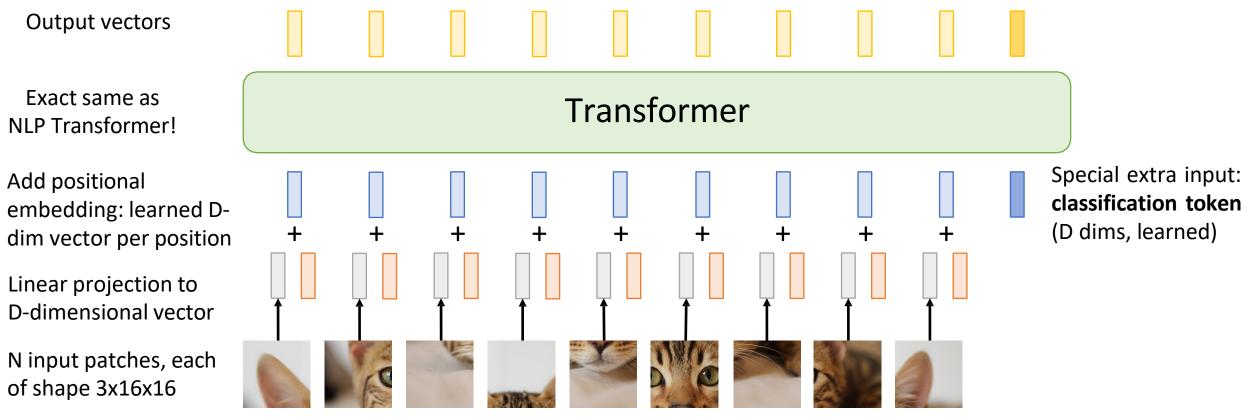
Linear projection to D-dimensional vector

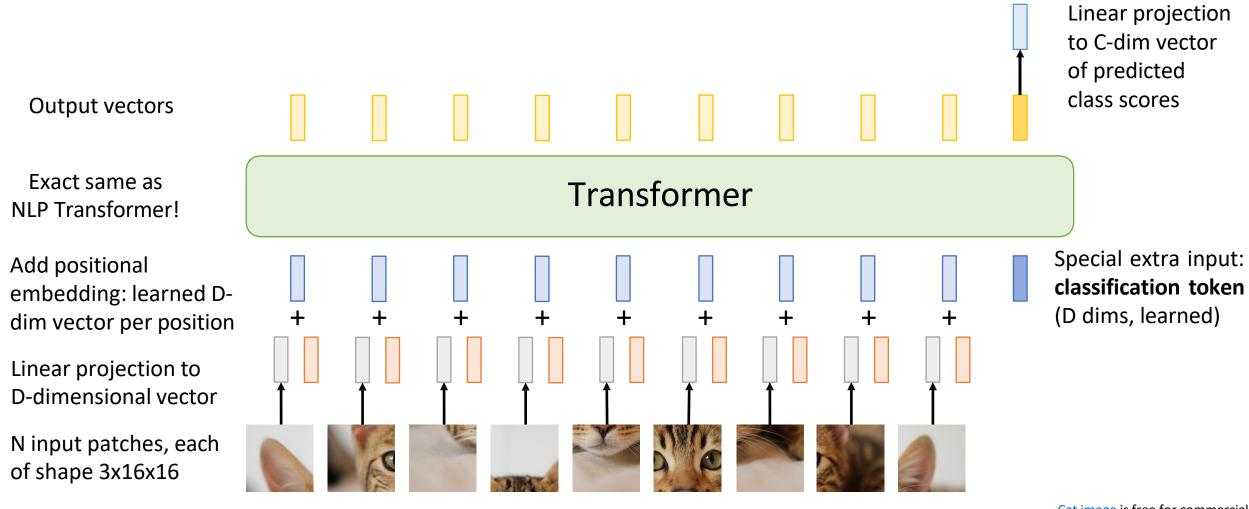
N input patches, each of shape 3x16x16

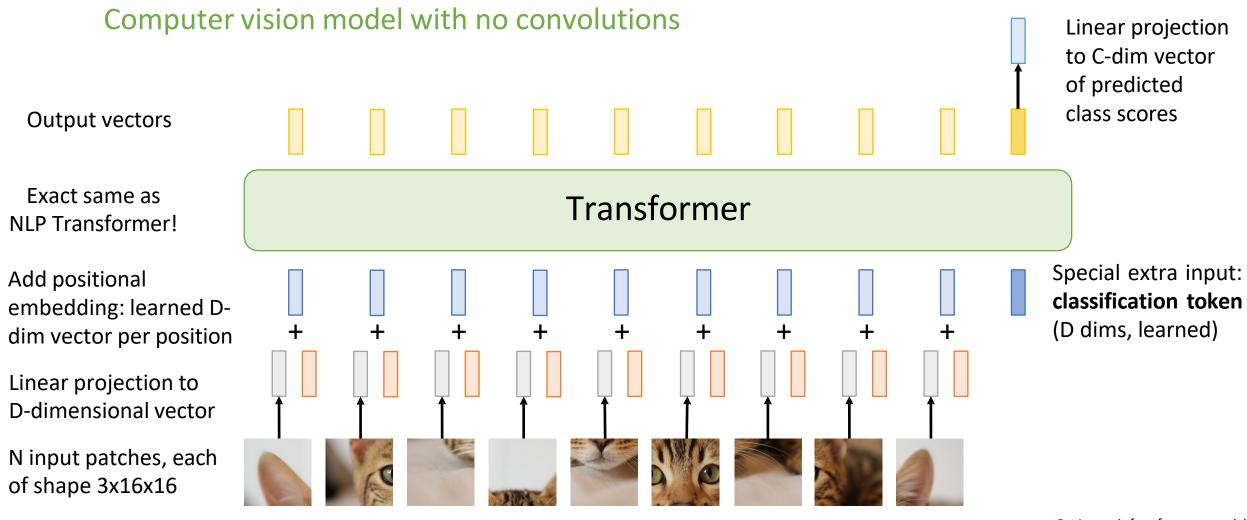


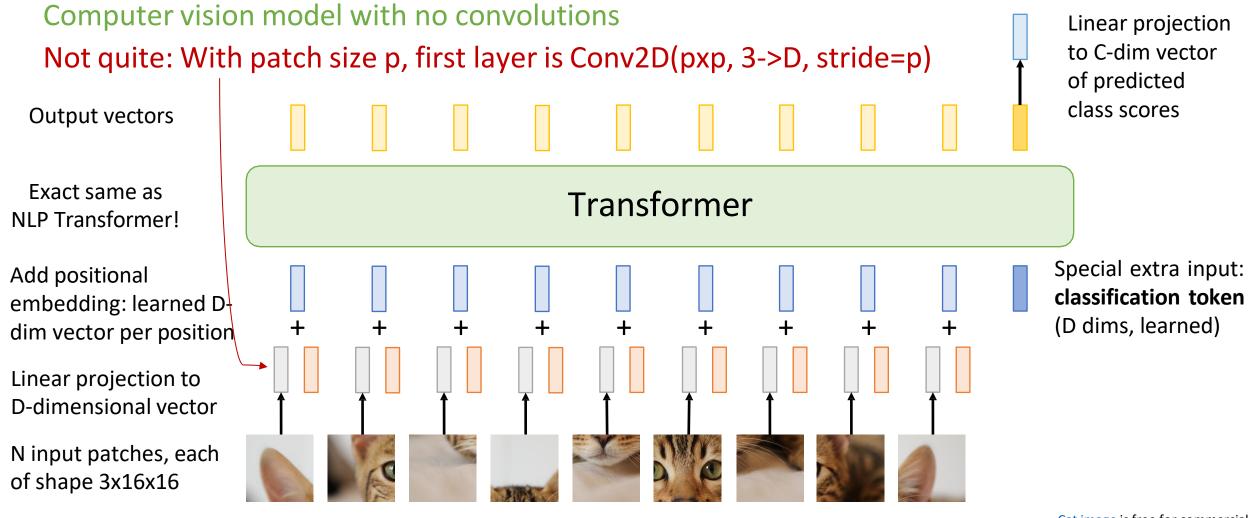


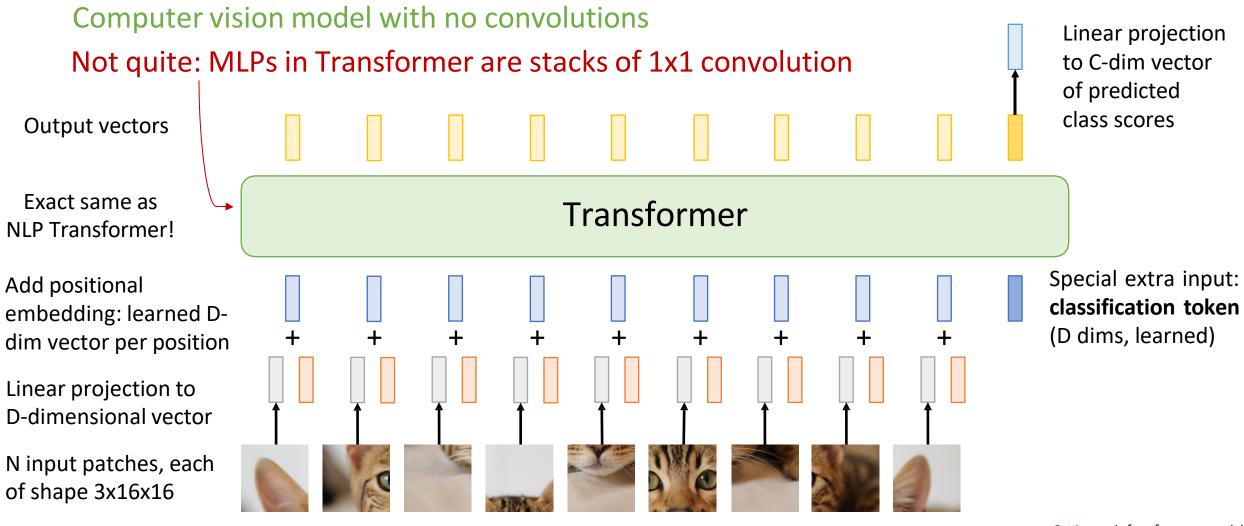












(drop classification token here for simplicity)

In practice: take 224x224 input image, divide into 14x14 grid of 16x16 pixel patches (or 16x16 grid of 14x14 patches)

Each attention matrix has $14^4 = 38,416$ entries, takes 150 KB (or 65,536 entries, takes 256 KB)

Linear projection to C-dim vector of predicted class scores

Output vectors





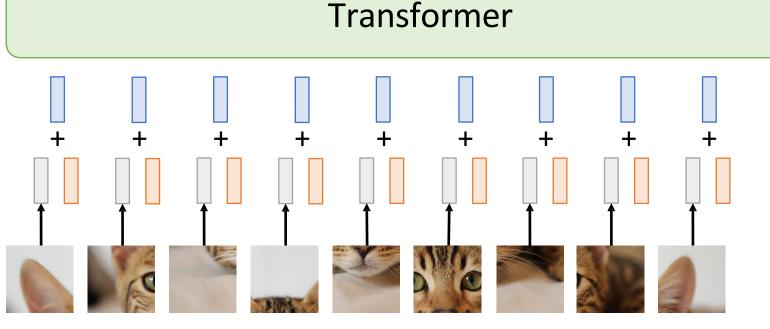


Exact same as NLP Transformer!

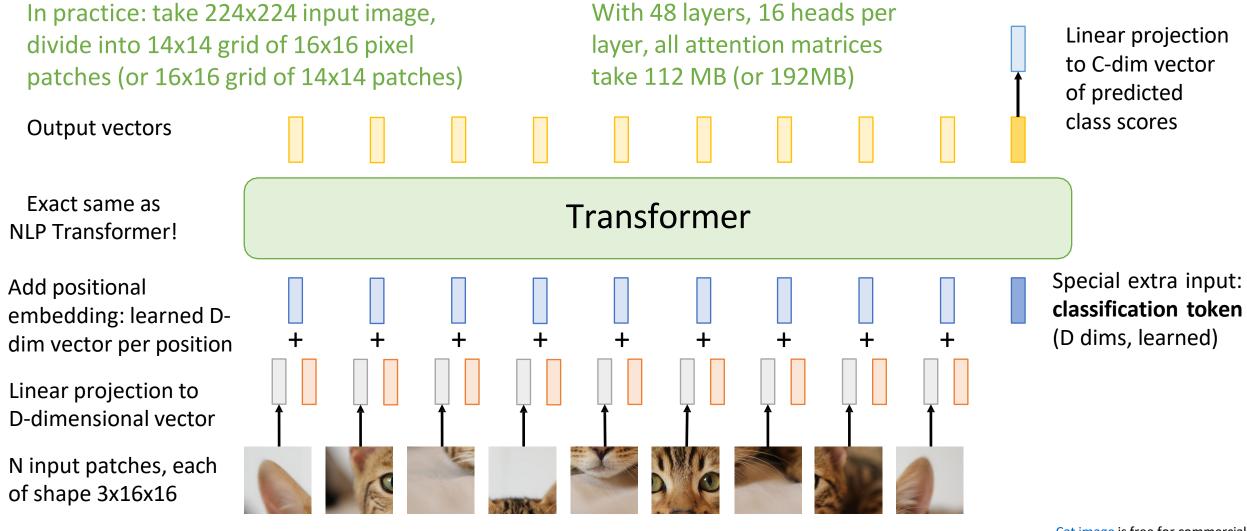
Add positional embedding: learned D-dim vector per position

Linear projection to D-dimensional vector

N input patches, each of shape 3x16x16

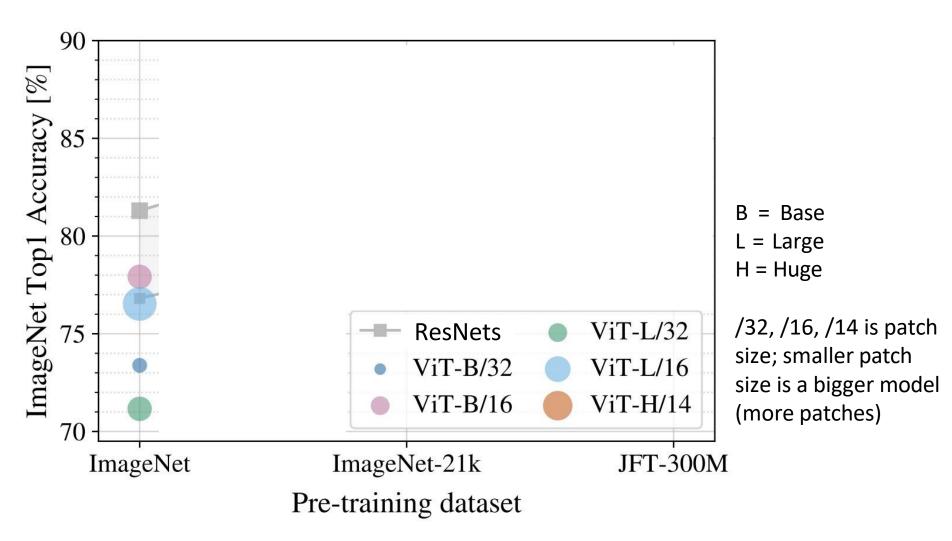


Special extra input: classification token (D dims, learned)



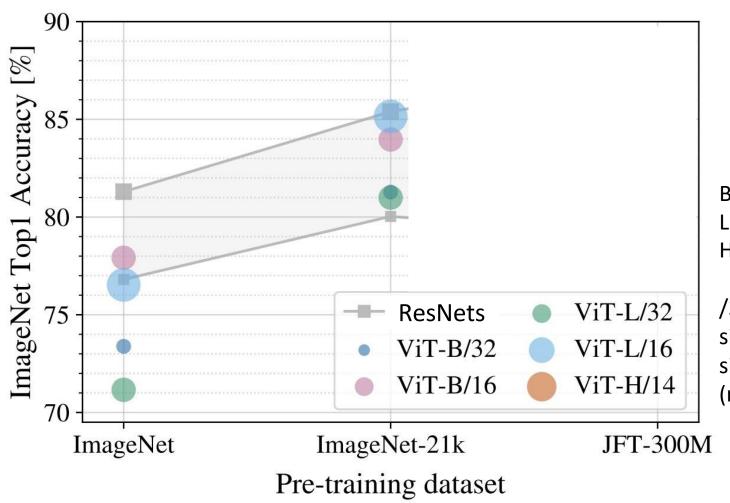
Recall: ImageNet dataset has 1k categories, 1.2M images

When trained on ImageNet, ViT models perform worse than ResNets



ImageNet-21k has 14M images with 21k categories

If you pretrain on ImageNet-21k and fine-tune on ImageNet, ViT does better: big ViTs match big ResNets



B = Base

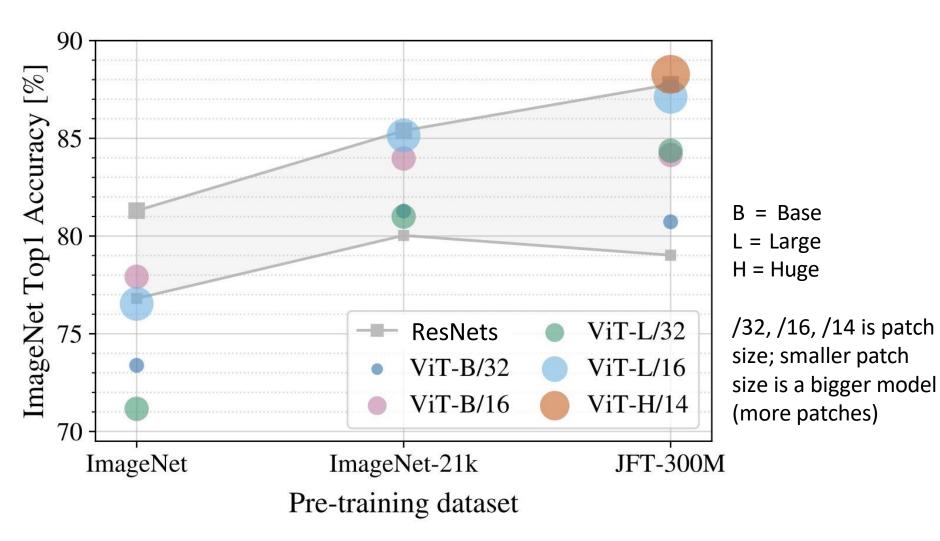
L = Large

H = Huge

/32, /16, /14 is patch size; smaller patch size is a bigger model (more patches)

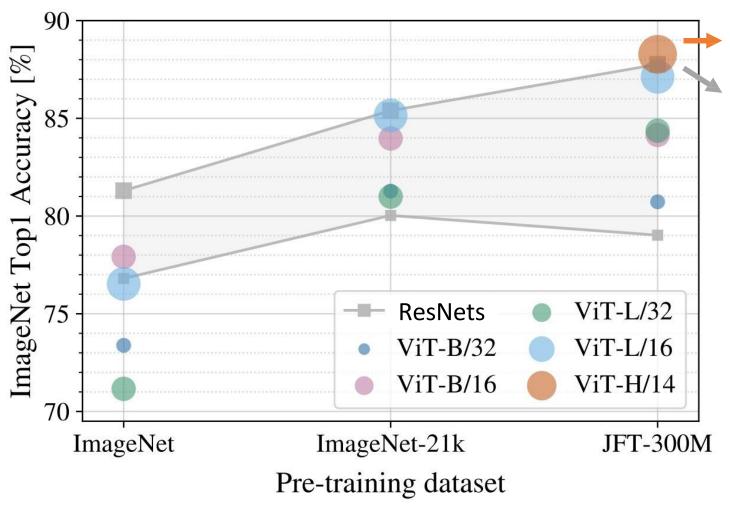
JFT-300M is an internal Google dataset with 300M labeled images

If you pretrain on JFT and finetune on ImageNet, large ViTs outperform large ResNets



JFT-300M is an internal Google dataset with 300M labeled images

If you pretrain on JFT and finetune on ImageNet, large ViTs outperform large ResNets



ViT: 2.5k TPU-v3 core days of training

ResNet: 9.9k TPU-v3 core days of training

ViTs make more efficient use of GPU / TPU hardware (matrix multiply is more hardware-friendly than conv)

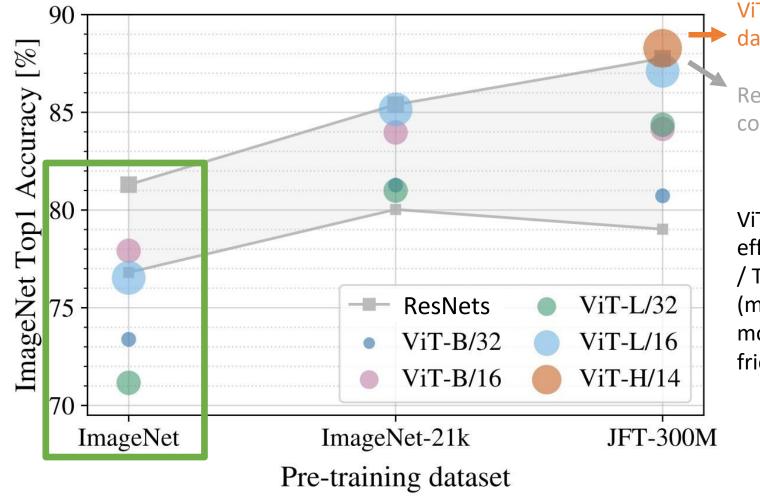
How can we

improve the

performance

of ViT models

on ImageNet?



ViT: 2.5k TPU-v3 core days of training

ResNet: 9.9k TPU-v3 core days of training

ViTs make more efficient use of GPU / TPU hardware (matrix multiply is more hardware-friendly than conv)

Regularization for ViT models:

- Weight Decay
- Stochastic Depth
- Dropout (in FFN layers of Transformer)

Data Augmentation for ViT models:

- MixUp
- RandAugment

Steiner et al, "How to train your ViT? Data, Augmentation, and Regularization in Vision Transformers", arXiv 2021

Regularization for ViT models:

- Weight Decay
- **Stochastic Depth**
- Dropout (in FFN layers of Transformer)

Data Augmentation for ViT models:

- MixUp
- RandAugment

ImageNet-1k, 300ep Hybrid models: No regularization Regularization 0.1 ResNet blocks, then ViT blocks RTi 69 71 ViT models: Ti/16 Ti = Tiny S/32 70 S = SmallS/1676 B = BaseL = Large B/3263 69 **R26S** Original Paper: B/16 70 76 77.9 76.53 L/16 69 R50L 70 Adding regularization is heavy2 med1 (almost) always helpful

More augmentation

med1

Steiner et al, "How to train your ViT? Data, Augmentation, and Regularization in Vision Transformers", arXiv 2021



- Weight Decay
- Stochastic Depth
- Dropout (in FFN layers of Transformer)

Data Augmentation for ViT

models:

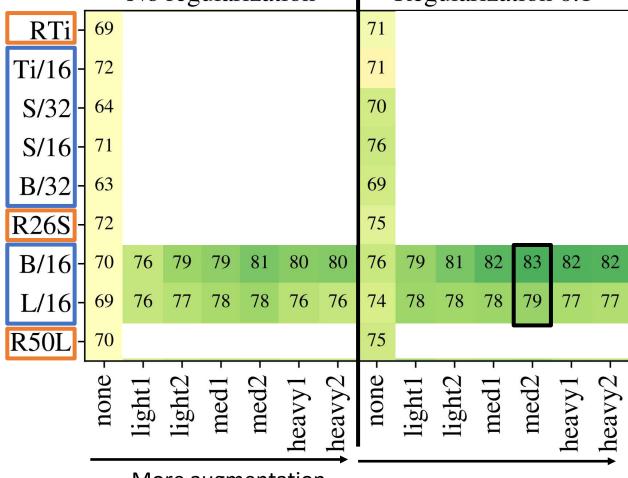
- MixUp

RandAugment

Hybrid models: ResNet blocks, then ViT blocks ViT models: Ti = Tiny S = SmallB = BaseL = Large Original Paper: 77.9 76.53 Regularization + Augmentation gives big improvements over original results

ImageNet-1k, 300ep

No regularization Regularization 0.1



More augmentation

Steiner et al, "How to train your ViT? Data, Augmentation, and Regularization in Vision Transformers", arXiv 2021

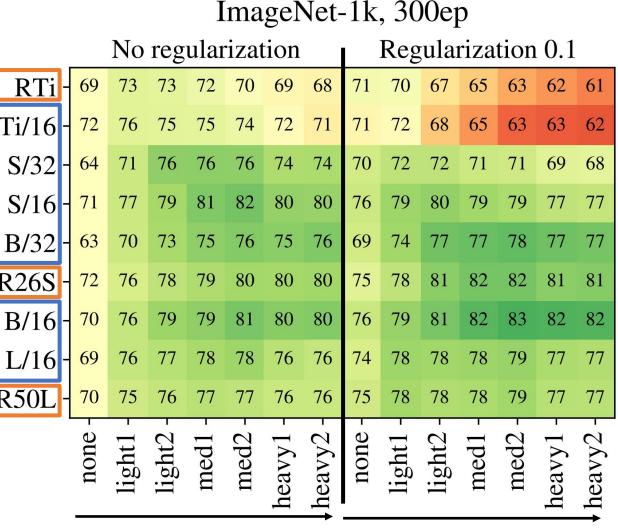
Regularization for ViT models:

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Data Augmentation for ViT models:

- MixUp
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Hybrid models: ResNet blocks, then ViT blocks RTi ViT models: Ti/16 Ti = Tiny S/32 S = SmallS/16 B = BaseL = Large B/32**R26S** Original Paper: B/16 77.9 76.53 L/1669 Lots of other R50L patterns in full results



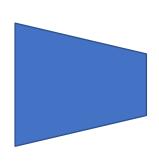
More augmentation

Steiner et al, "How to train your ViT? Data, Augmentation, and Regularization in Vision Transformers", arXiv 2021

Improving ViT: Distillation

Step 1: Train a <u>teacher</u>
CNN on ImageNet





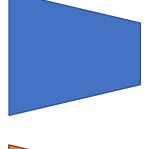
$$\begin{array}{c} P(\text{cat}) = 0.9 \\ P(\text{dog}) = 0.1 \end{array} \longrightarrow \begin{array}{c} \text{Cross} \\ \text{Entropy} \\ \text{Loss} \end{array} \longrightarrow \begin{array}{c} \text{GT label:} \\ \text{Cat} \end{array}$$

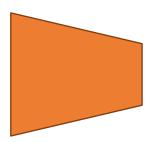
Step 2: Train a

student ViT to match
ImageNet predictions
from the teacher CNN
(and match GT labels)









$$P(cat) = 0.1$$

$$P(dog) = 0.9$$

$$P(cat) = 0.2$$

$$P(cat) = 0.2$$

$$P(dog) = 0.8$$

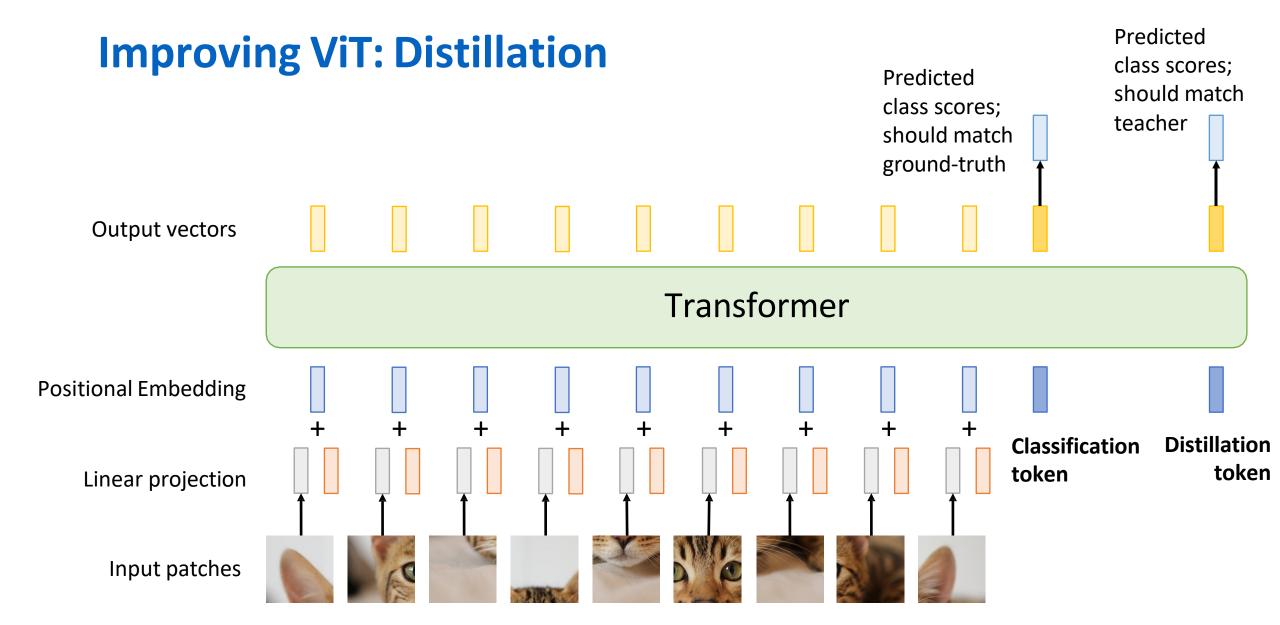
$$P(cat) = 0.2$$

$$P(dog) = 0.8$$

$$P(cat) = 0.2$$

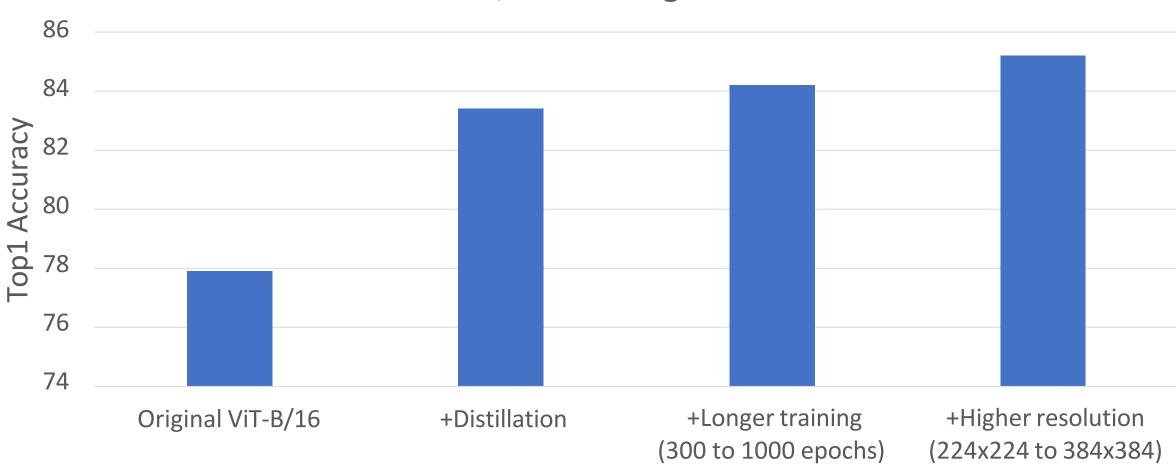
$$P(dog) = 0.8$$

$$P(cat) = 0.2$$



Improving ViT: Distillation





Touvrom et al, "Training data-efficient image transformers & distillation through attention", ICML 2021

ViT vs CNN

Stage 3: 256 x 14 x 14

Stage 2:

3x3 conv, 128

Stage 1: 64 x 56 x 56

Input: 3 x 224 x 224

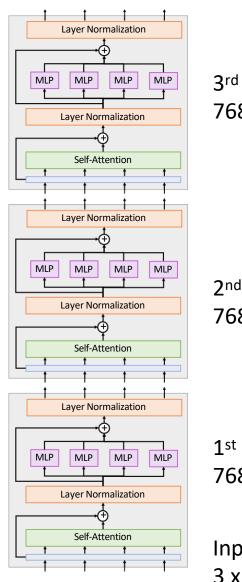
3x3 conv. 512 3x3 conv, 512 3x3 conv, 512 3x3 conv, 512 3x3 conv. 512. /2 3x3 conv, 64 3x3 conv, 64 3x3 conv, 64 3x3 conv, 64 3x3 conv, 64

Input

In most CNNs (including ResNets), decrease resolution and increase channels as you go deeper in the network (Hierarchical architecture)

Useful since objects in images can occur at various scales

In a ViT, all blocks have same resolution and number of channels (Isotropic architecture)



3rd block: 768 x 14 x 14

2nd block: 768 x 14 x 14

1st block: 768 x 14 x 14

Input: 3 x 224 x 224

ViT vs CNN

3x3 conv, 512 3x3 conv, 512

3x3 conv, 512

3x3 conv, 512

3x3 conv. 512. /2

3x3 conv, 64

Input

Stage 3: 256 x 14 x 14

Stage 2: 3x3 conv, 128

Stage 1: 64 x 56 x 56

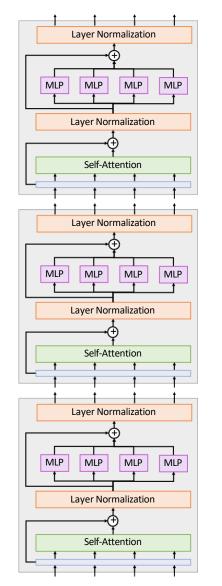
Input: 3 x 224 x 224

In most CNNs (including ResNets), decrease resolution and increase channels as you go deeper in the network (Hierarchical architecture)

Useful since objects in images can occur at various scales

In a ViT, all blocks have same resolution and number of channels (Isotropic architecture)

Can we build a hierarchical ViT model?

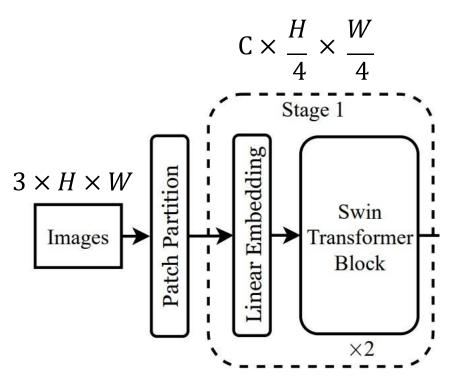


3rd block: 768 x 14 x 14

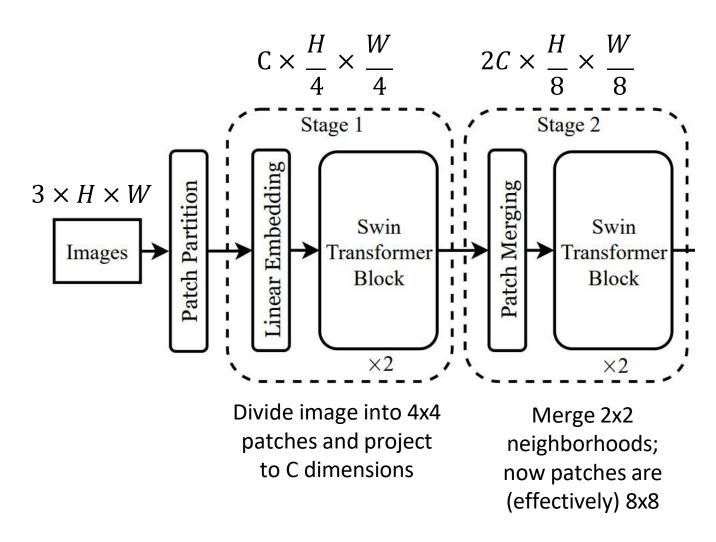
2nd block: 768 x 14 x 14

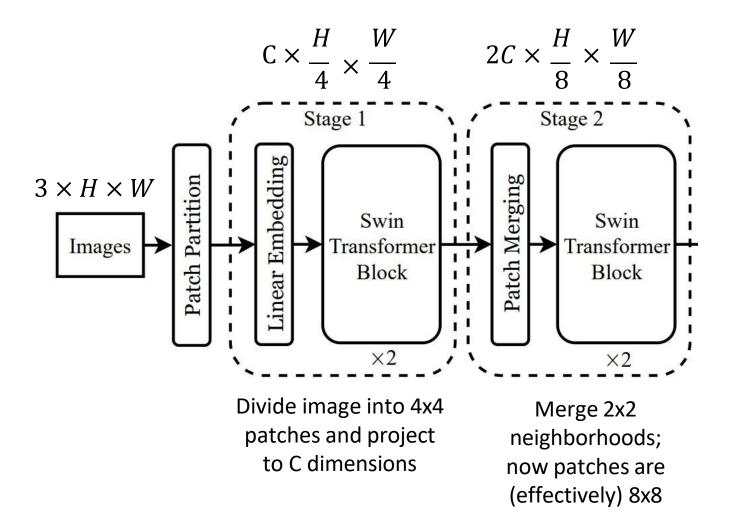
1st block: 768 x 14 x 14

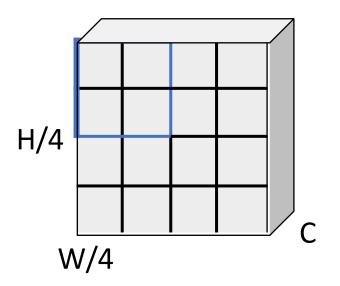
Input: 3 x 224 x 224

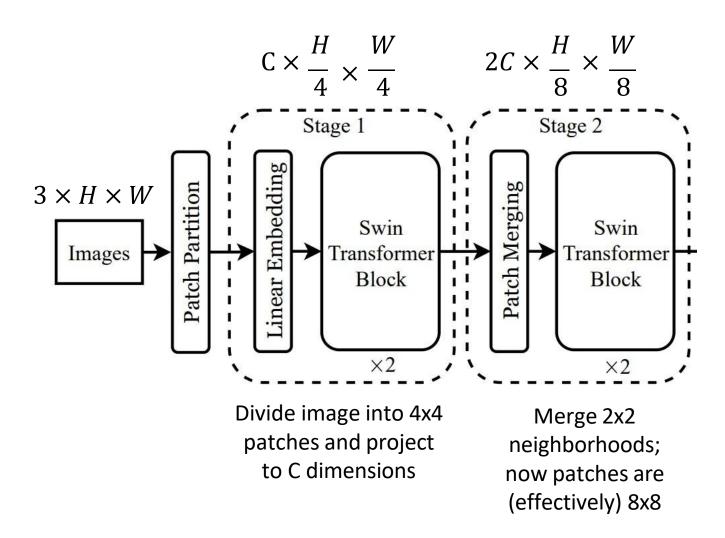


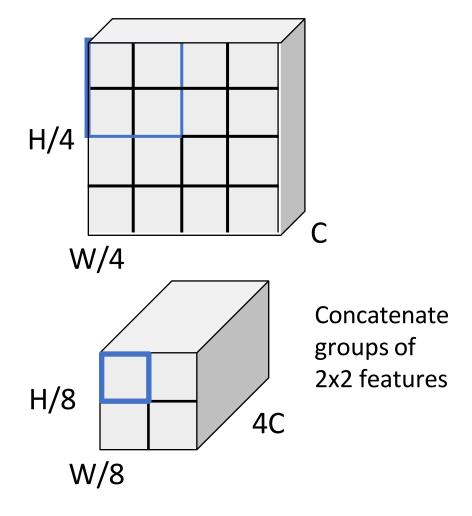
Divide image into 4x4 patches and project to C dimensions

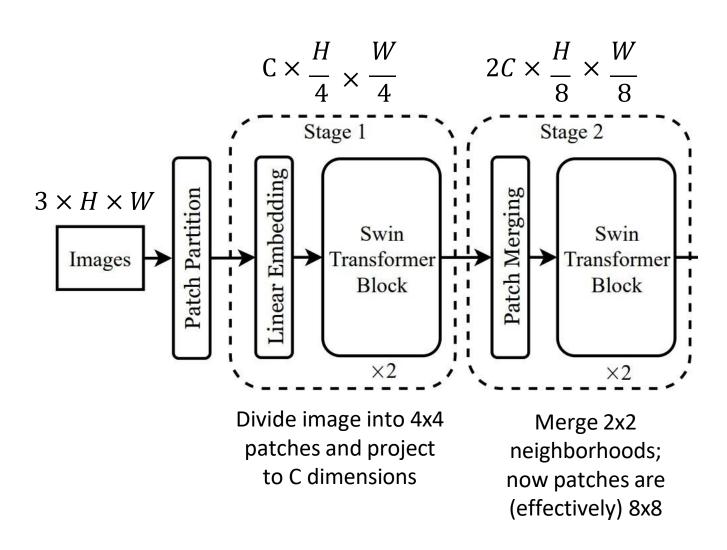


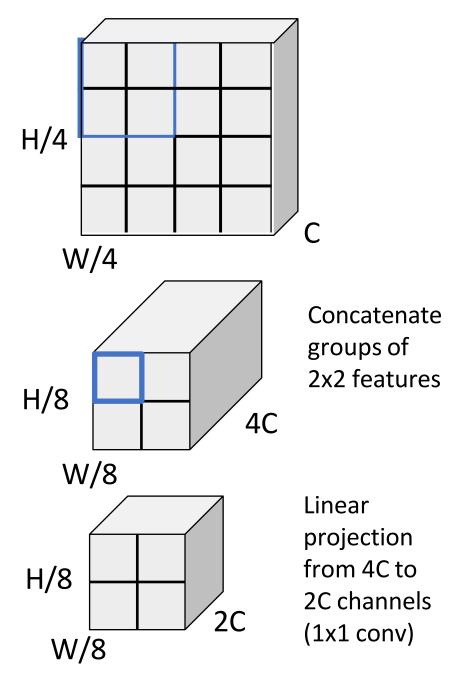


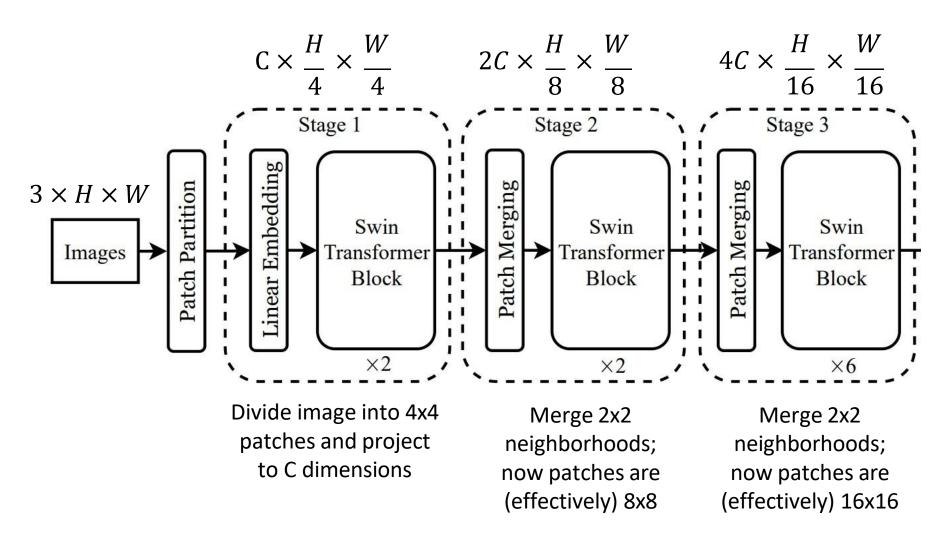


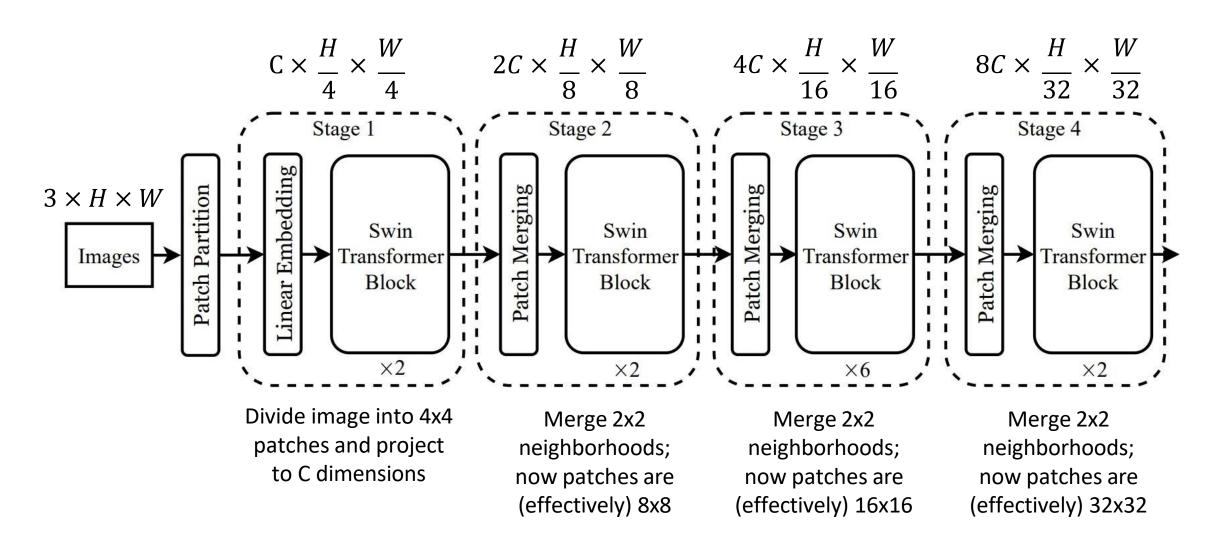










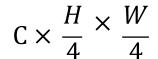


Problem: 224x224 image

with 56x56 grid of 4x4

patches: attention matrix

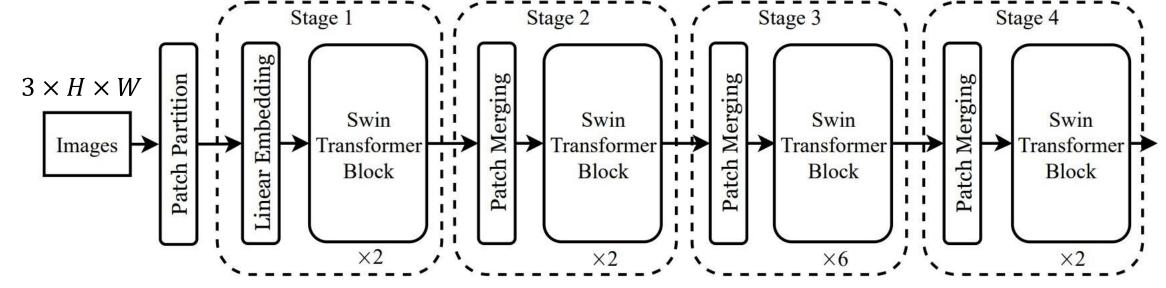
has $56^4 = 9.8M$ entries



$$2C \times \frac{H}{8} \times \frac{W}{8}$$

$$4C \times \frac{H}{16} \times \frac{W}{16}$$
 $8C \times \frac{H}{32} \times \frac{W}{32}$

$$8C \times \frac{H}{32} \times \frac{W}{32}$$



Divide image into 4x4 patches and project to C dimensions

Merge 2x2 neighborhoods; now patches are (effectively) 8x8

Merge 2x2 neighborhoods; now patches are (effectively) 16x16

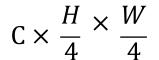
Merge 2x2 neighborhoods; now patches are (effectively) 32x32

Problem: 224x224 image

with 56x56 grid of 4x4

patches: attention matrix

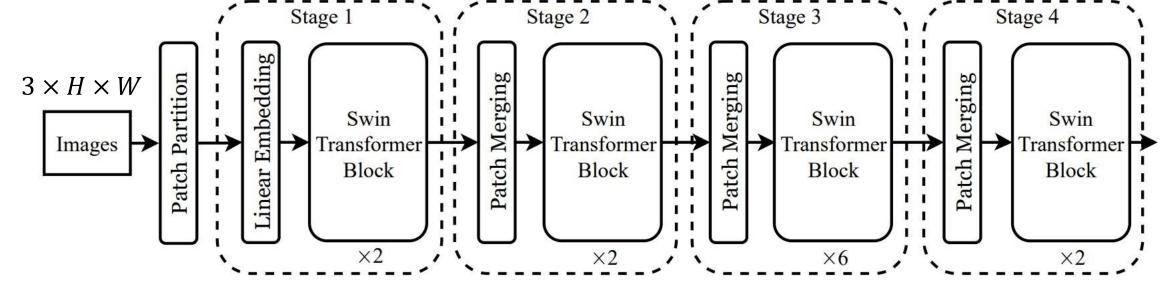
has $56^4 = 9.8M$ entries



$$2C \times \frac{H}{8} \times \frac{W}{8}$$

$$4C \times \frac{H}{16} \times \frac{W}{16}$$
 $8C \times \frac{H}{32} \times \frac{W}{32}$

$$8C \times \frac{H}{32} \times \frac{W}{32}$$



Solution: don't use full attention, instead use attention over patches Divide image into 4x4 patches and project to C dimensions

Merge 2x2 neighborhoods; now patches are (effectively) 8x8

Merge 2x2 neighborhoods; now patches are (effectively) 16x16

Merge 2x2 neighborhoods; now patches are (effectively) 32x32

Swin Transformer: Window Attention



With H x W grid of **tokens**, each attention matrix is H²W² – **quadratic** in image size

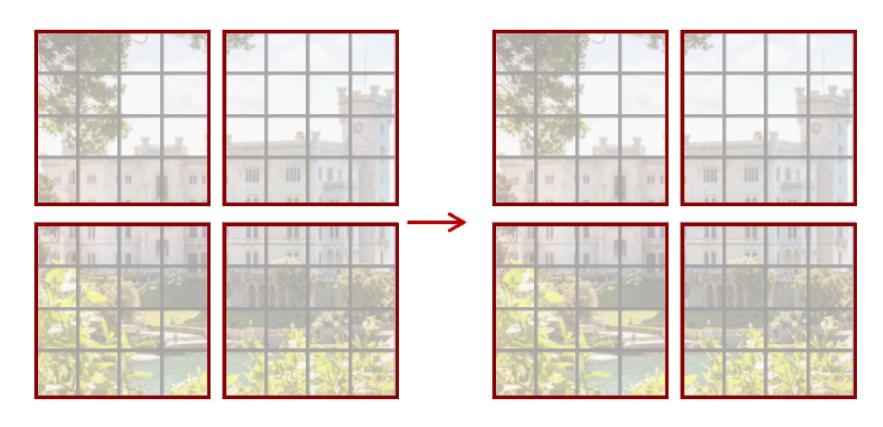
Rather than allowing each **token** to attend to all other tokens, instead divide into **windows** of M x M tokens (here M=4); only compute attention within each window

Total size of all attention matrices is now: $M^4(H/M)(W/M) = M^2HW$

Linear in image size for fixed M! Swin uses M=7 throughout the network

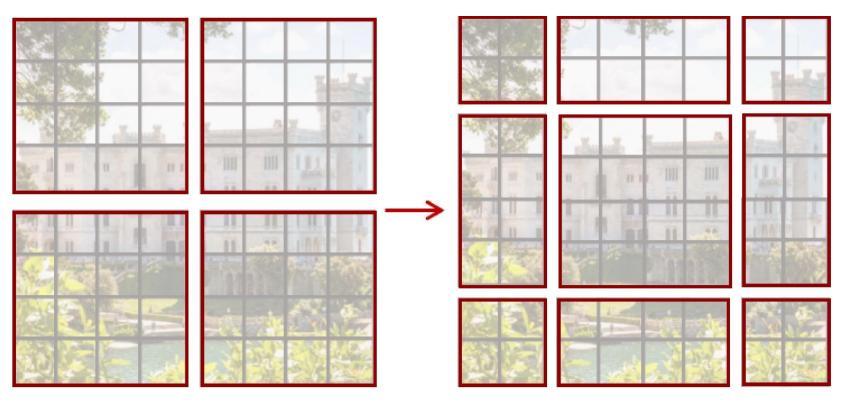
Swin Transformer: Window Attention

Problem: tokens only interact with other tokens within the same window; no communication across windows



Swin Transformer: Shifted Window Attention

Solution: Alternate between normal windows and shifted windows in successive Transformer blocks

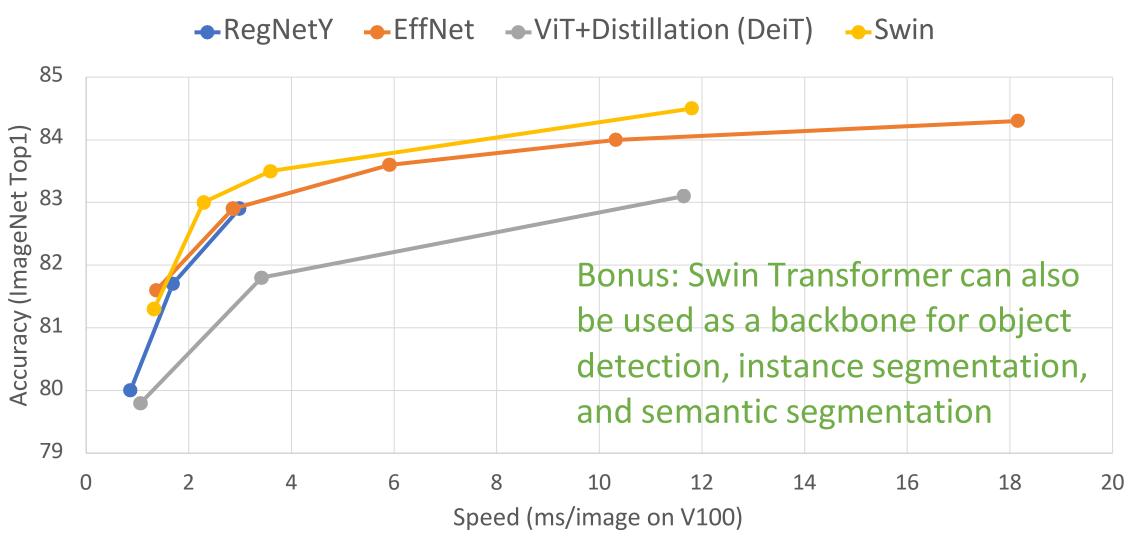


Ugly detail: Non-square windows at edges and corners

Block L: Normal windows

Block L+1: Shifted Windows

Swin Transformer: Speed vs Accuracy



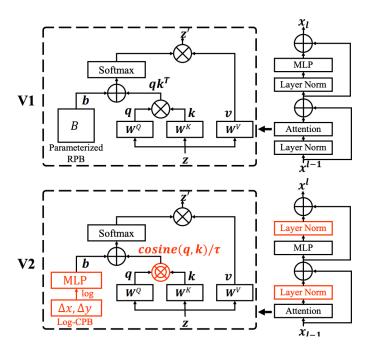
Liu et al, "Swin Transformer: Hierarchical Vision Transformer using Shifted Windows", CVPR 2021

Other Hierarchical Vision Transformers

MViT

1 N/4

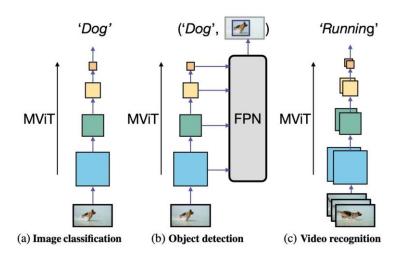
Swin-V2



Fan et al, "Multiscale Vision Transformers", ICCV 2021

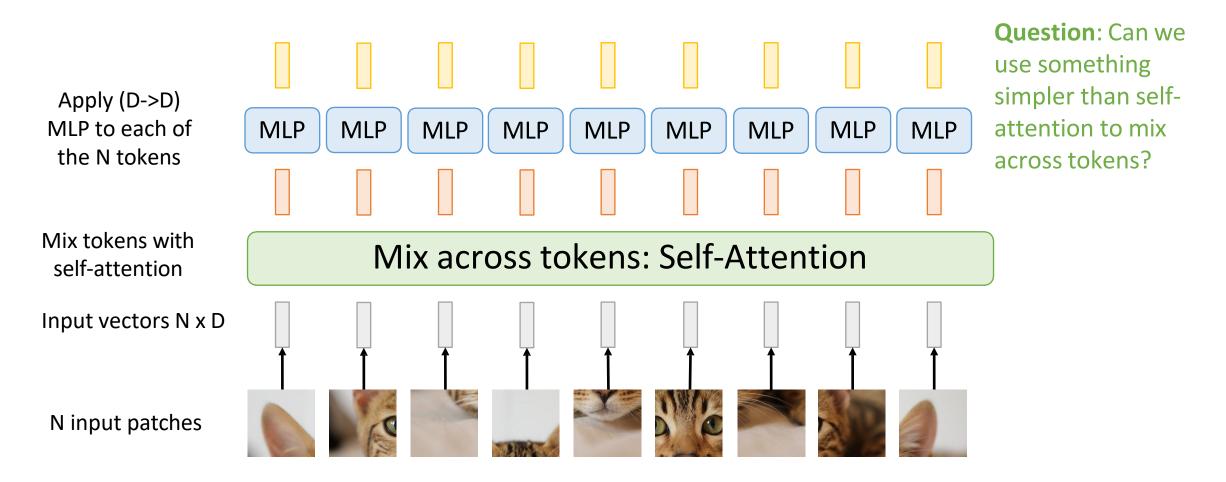
Liu et al, "Swin Transformer V2: Scaling up Capacity and Resolution", CVPR 2022

Improved MViT



Li et al, "Improved Multiscale Vision Transformers for Classification and Detection", arXiv 2021

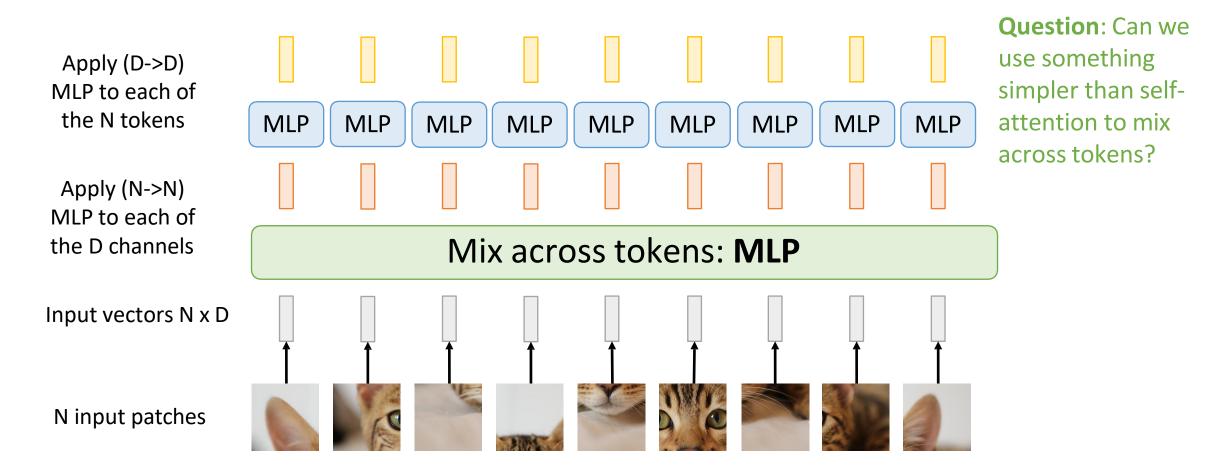
Vision Transformer: Another Look



Dosovitskiy et al, "An Image is Worth 16x16 Words: Transformers for Image Recognition at Scale", ICLR 2021

<u>Cat image</u> is free for commercial use under a Pixabay license

MLP-Mixer: An All-MLP Architecture



Tolstikhin et al, "MLP-Mixer: An all-MLP architecture for vision", NeurIPS 2021

MLP-Mixer: Many concurrent and followups

Touvron et al, "ResMLP: Feedforward Networks for Image Classification with Data-Efficient Training", arXiv 2021, https://arxiv.org/abs/2105.03404

Tolstikhin et al, "MLP-Mixer: An all-MLP architecture for vision", NeurIPS 2021, https://arxiv.org/abs/2105.01601

Liu et al, "Pay Attention to MLPs", NeurIPS 2021, https://arxiv.org/abs/2105.08050

Yu et al, "S2-MLP: Spatial-Shift MLP Architecture for Vision", WACV 2022, https://arxiv.org/abs/2106.07477

Chen et al, "CycleMLP: A MLP-like Architecture for Dense Prediction", ICLR 2022, https://arxiv.org/abs/2107.10224

Data Modalities

- ✓ Language
- √ Vision
- Audio
- ... and many other modalities (e.g., biological/physiological signals, etc.)
- Multimodal (>2 data modalities)

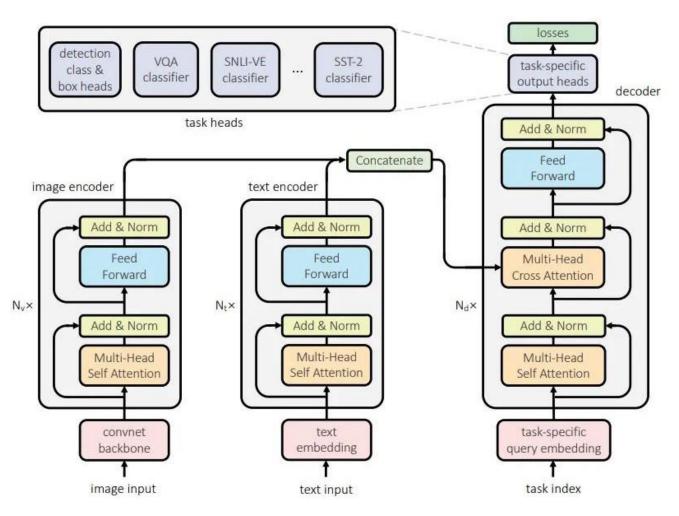
Audio

- Similar to the computer vision but with spectrograms instead of images.
- Exists as encoder-decoder variants or as an encoder-only variant with CTC loss.
- Could be augmented with the CNN.

Conformer: Convolution-augmented Transformer for Speech Recognition

AST: Audio Spectrogram Transformer

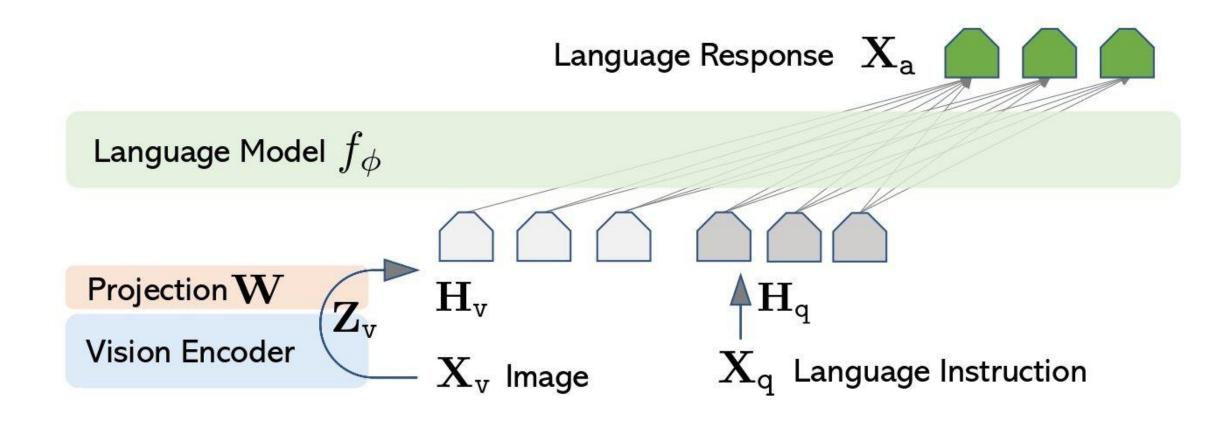
Multimodal Transformer - UniT



- UniT handles 7 tasks ranging from object detection to vision-and language reasoning and natural language understanding.
- 2. Components:
 - An image encoder to encode the visual inputs.
 - A text encoder to encode the language inputs.
 - A joint decoder with per-task query embedding.
 - Task-specific heads to make the final outputs for each task.

UniT: Multimodal Multitask Learning with a Unified Transformer

Multimodal Transformer - LLaVA



Multimodal Transformer - LLaVA

Start a new conversation, and the history is cleared.





Do you know who drew this painting?



The painting depicts a dog in a humorous situation, where it appears to be wearing a woman's dress and standing in front of a landscape. Although the artist of the painting is not explicitly identified, it could be a reference to the famous artist Da Vinci, known for his artistic works, including the Mona Lisa. The painting is likely a creative and comical take on the traditional portrait style, replacing a human figure with a dog dressed in a woman's clothing, making it an interesting and amusing visual piece.