

10-423/10-623 Generative Al

Machine Learning Department School of Computer Science Carnegie Mellon University

# Encoder-only Transformers + Vision Transformers

Matt Gormley Lecture 5 Jan. 31, 2024

# Reminders

- Homework 1: Generative Models of Text
  - Out: Thu, Jan 25
  - Due: Wed, Feb 7 at 11:59pm
- Matt's office hours on GCal

#### Q&A

**Q:** Does pre-training always involve layer-by-layer unsupervised training?

- A: No! That's just where it started in 2006 for standard feed forward neural networks.
  - To pretrain a CNN or Vision Transformer, we typically train the entire model on a supervised classification problem (i.e. image classification)
  - To pretrain an LLM, we typically train the entire model on the likelihood of unlabeled sentences.

#### Course Staff



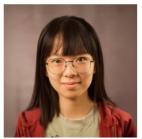
Meghana



Ifigeneia Apostolopoulou



Advaith Sridhar



Qin Han



Afreen Shaikh



Jing Gao





Ritu Gala







Yuanzhi Li





Asmita



Matt Gormley



Samuel Sokota



Haoyang He

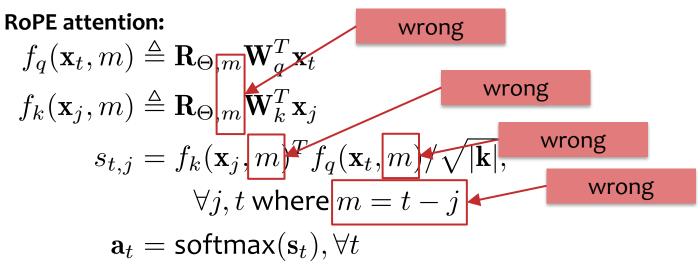
Tiancheng Zhao



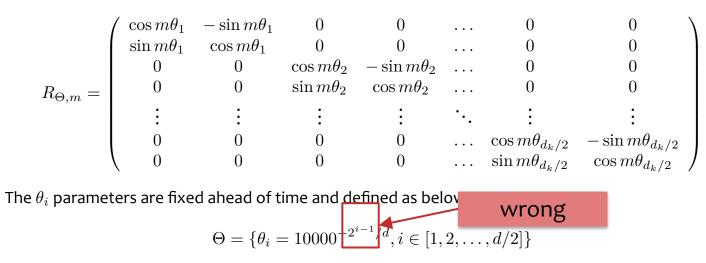
\*take two

# **ROTARY POSITION EMBEDDINGS (ROPE)**

- **Q:** Why does this slide have so many typos?
- A: I'm really not sure. I very meticulously type up the latex for my slides myself and think carefully about all the things I put in them.

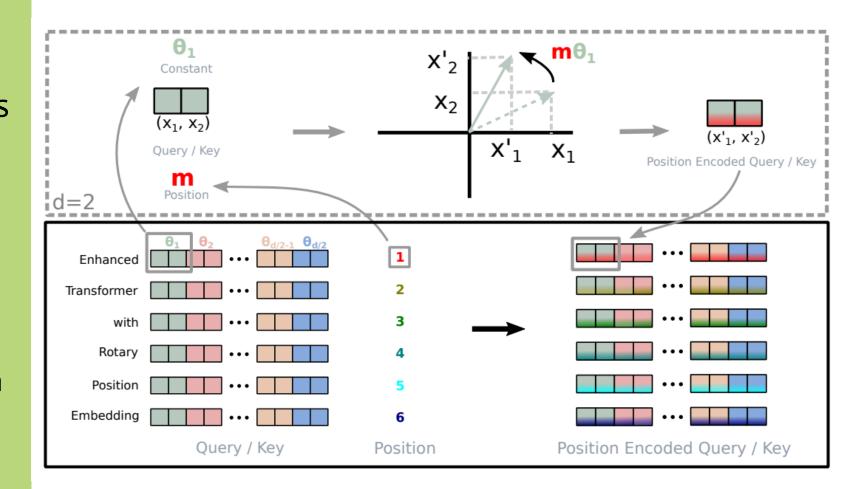


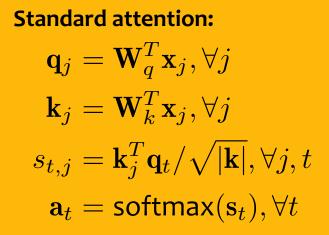
where  $\mathbf{W}_k, \mathbf{W}_q \in \mathbb{R}^{d_{model} \times d_k}$ , and the rotary matrix  $\mathbf{R}_{\Theta,m} \in \mathbb{R}^{d_k \times d_k}$  is given by:



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- A: I'm not really sure. I very meticulously type up the latex for my slides myself and think carefully about all the things I put in them.

- Rotary position embeddings are a kind of relative position embeddings
- Key idea:
  - break each ddimensional input vector into d/2 vectors of length 2
  - rotate each of the d/2 vectors by an amount scaled by m
  - m is the relative position between the query and key





**ROPE attention:**  

$$\mathbf{q}_j = \mathbf{W}_q^T \mathbf{x}_j, \forall j$$
  
 $\tilde{\mathbf{q}}_j = \mathbf{R}_{\Theta,j} \mathbf{q}_j$   
 $s_{t,j} = \tilde{\mathbf{k}}_j^T \tilde{\mathbf{q}}_t / \sqrt{d_k}, \forall j, t$   
 $\mathbf{a}_t = \operatorname{softmax}(\mathbf{s}_t), \forall t$  $\mathbf{k}_j = \mathbf{W}_k^T \mathbf{x}_j, \forall j$   
 $\tilde{\mathbf{k}}_j = \mathbf{R}_{\Theta,j} \mathbf{k}_j$ 

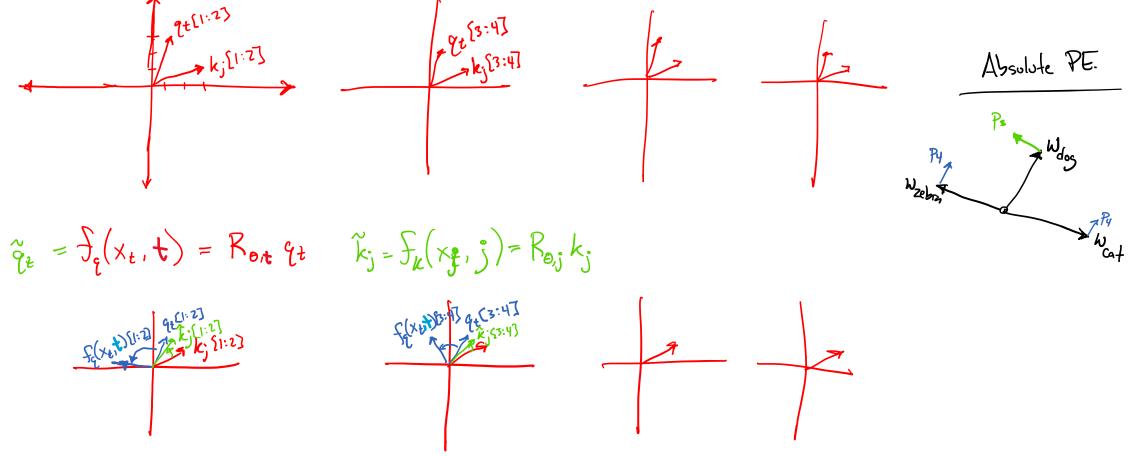
where  $d = d_k/2$ ,  $\mathbf{W}_k$ ,  $\mathbf{W}_q \in \mathbb{R}^{d_{model} \times d_k}$ . For some fixed absolute position m, the rotary matrix  $\mathbf{R}_{\Theta,m} \in \mathbb{R}^{d_k \times d_k}$  is given by:

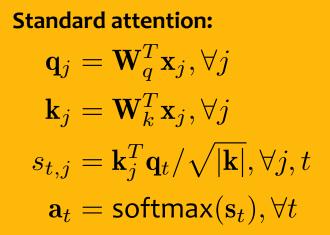
$$R_{\Theta,m} = \begin{pmatrix} \cos m\theta_1 & -\sin m\theta_1 & 0 & 0 & \dots & 0 & 0 \\ \sin m\theta_1 & \cos m\theta_1 & 0 & 0 & \dots & 0 & 0 \\ 0 & 0 & \cos m\theta_2 & -\sin m\theta_2 & \dots & 0 & 0 \\ 0 & 0 & \sin m\theta_2 & \cos m\theta_2 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \dots & \cos m\theta_{d_k/2} & -\sin m\theta_{d_k/2} \\ 0 & 0 & 0 & 0 & \dots & \sin m\theta_{d_k/2} & \cos m\theta_{d_k/2} \end{pmatrix}$$

The  $\theta_i$  parameters are fixed ahead of time and defined as below.

$$\Theta = \{\theta_i = 10000^{-2(i-1)/d}, i \in [1, 2, \dots, d/2]\}$$

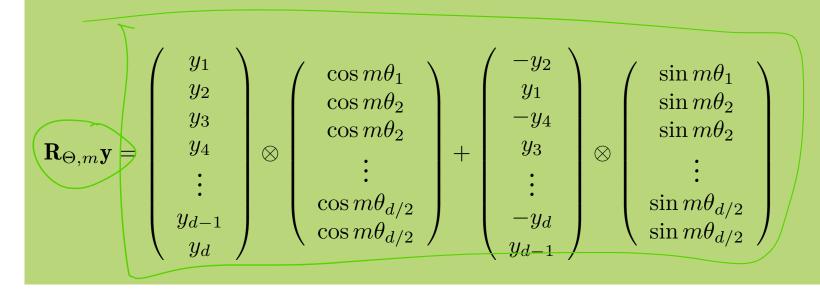
 $\begin{array}{l} Q_{t} = W_{q}^{T} \times_{t} = \begin{bmatrix} 1, 3, 1, 3, 1, 3, 1, 3 \\ 3 \end{bmatrix} \\ k_{j} = W_{k}^{T} \times_{j} = \begin{bmatrix} 3, 1, 3, 1, 3, 1, 3, 1 \\ 3 \end{bmatrix} \end{array}$ 





**RoPE attention:**<br/>  $\mathbf{q}_j = \mathbf{W}_q^T \mathbf{x}_j, \forall j$ <br/>  $\tilde{\mathbf{q}}_j = \mathbf{R}_{\Theta,j} \mathbf{q}_j$ <br/>  $s_{t,j} = \tilde{\mathbf{k}}_j^T \tilde{\mathbf{q}}_t / \sqrt{d_k}, \forall j, t$ <br/>  $\mathbf{a}_t = \operatorname{softmax}(\mathbf{s}_t), \forall t$  $\mathbf{k}_j = \mathbf{W}_k^T \mathbf{x}_j, \forall j$ <br/>  $\tilde{\mathbf{k}}_j = \mathbf{R}_{\Theta,j} \mathbf{k}_j$ 

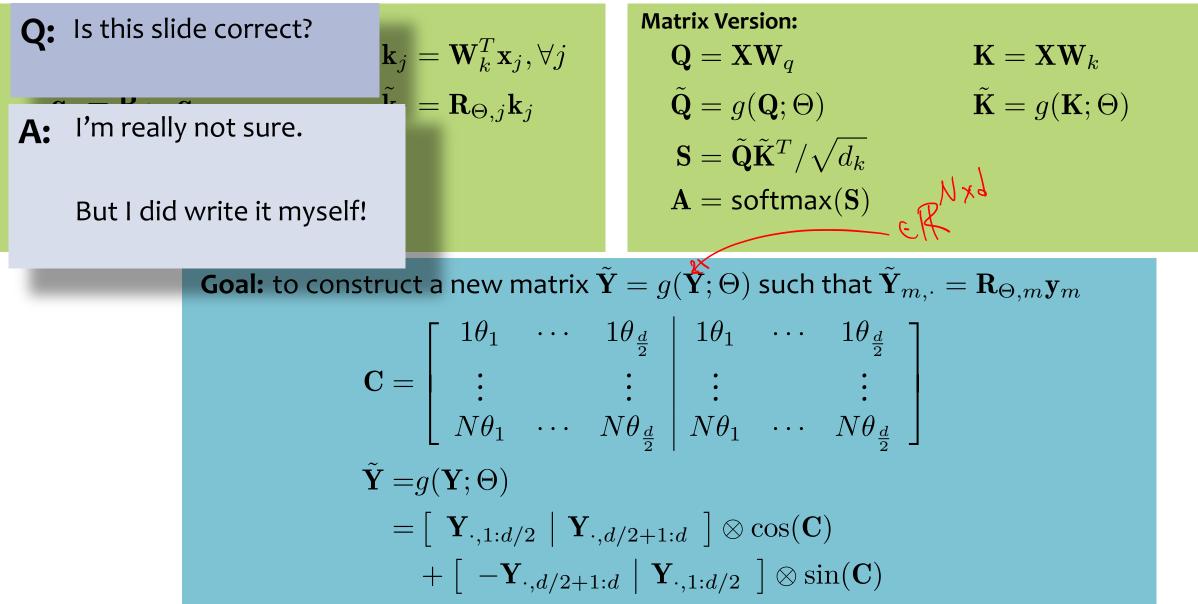
Because of the block sparse pattern in  $\mathbf{R}_{\theta,m}$ , we can efficiently compute the matrix-vector product of  $\mathbf{R}_{\theta,m}$  with some arbitrary vector  $\mathbf{y}$  in a more efficient manner:



### Matrix Version of RoPE

RoPE attention: $\mathbf{q}_j = \mathbf{W}_q^T \mathbf{x}_j, orall j$	$\mathbf{k}_j = \mathbf{W}_k^T \mathbf{x}_j, orall j$	Matrix Version: $\mathbf{Q} = \mathbf{X} \mathbf{W}_q$	$\mathbf{K} = \mathbf{X} \mathbf{W}_k$
$ ilde{\mathbf{q}}_j = \mathbf{R}_{\Theta,j} \mathbf{q}_j$	$\widetilde{\mathbf{k}}_j = \mathbf{R}_{\Theta,j} \mathbf{k}_j$	$ ilde{\mathbf{Q}} = g(\mathbf{Q}; \Theta)$	$ ilde{\mathbf{K}} = g(\mathbf{K}; \Theta)$
$s_{t,j} = \tilde{\mathbf{k}}_j^T \tilde{\mathbf{q}}_t / \sqrt{d_k}, \forall j, t$	<u>,</u>	$\mathbf{S} =  ilde{\mathbf{Q}}  ilde{\mathbf{K}}^T / \sqrt{d_k}$	
$\mathbf{a}_t = softmax(\mathbf{s}_t), \forall t$		$\mathbf{A} = softmax(\mathbf{S})$	
Goal: to	$\mathbf{C} = \begin{bmatrix} 1\theta_1 & \cdots & 1\\ \vdots & & \\ N\theta_1 & \cdots & N \end{bmatrix}$ $\tilde{\mathbf{Y}} = g(\mathbf{Y}; \Theta)$ $= \begin{bmatrix} \mathbf{Y}_{\cdot,1:d/2} &   \mathbf{Y}_{\cdot,d} \end{bmatrix}$	$ \begin{array}{c c} & = g(\mathbf{Y}; \boldsymbol{\Theta}) \text{ such that } \tilde{\mathbf{Y}}_{m, \cdot} \\ & & & \\ & & $	$= \mathbf{R}_{\Theta,m} \mathbf{y}_m$

### Matrix Version of RoPE

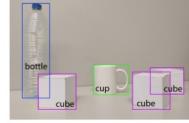


### **COMPUTER VISION**

# Common Tasks in Computer Vision

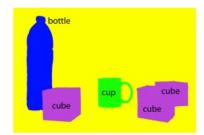
- 1. Image Classification
- 2. Image Classification + Localization
- 3. Human Pose Estimation
- 4. Semantic Segmentation
- 5. Object Detection
- 6. Instance Segmentation
- 7. Image Captioning
- 8. Image Generation



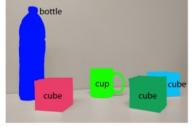


(a) Image classification

(b) Object localization



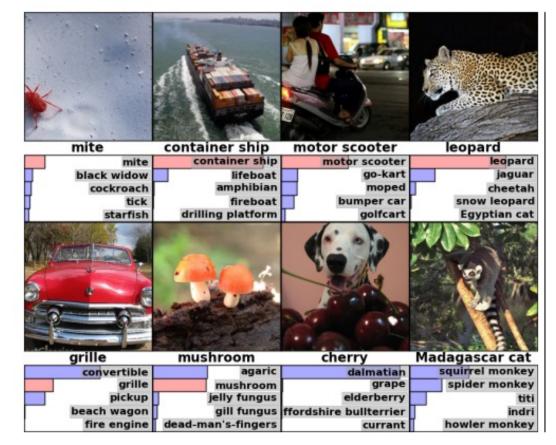
(c) Semantic segmentation



(d) Instance segmentation

# Image Classification

- Given an image, predict a single label
- A multi-class classification problem



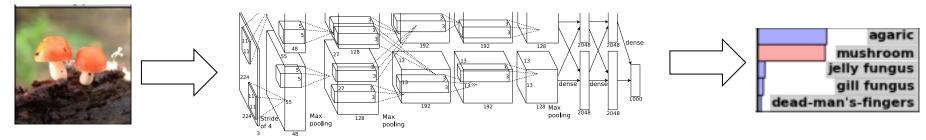
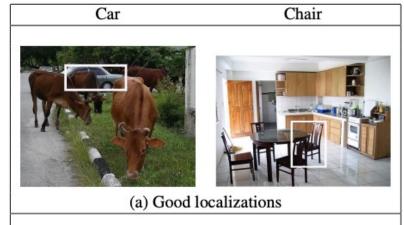


Figure from https://proceedings.neurips.cc/paper/2012/file/c399862d3b9d6b76c8436e924a68c45b-Paper.pdf

# Image Classification + Localization

- Given an image, predict a single label and a bounding box for the object
- Bounding box is represented as (x, y, h, w), position (x,y) and height/width (h,w)





(b) Strong false positive



(c) Missed objects

### Human Pose Estimation



- Given an image of a human, predict the position of several keypoints (left hand, right hand, left elbow, ..., right foot)
- This is a multiple regression problem, where each keypoint has a corresponding position (x<sub>i</sub>,y<sub>i</sub>)

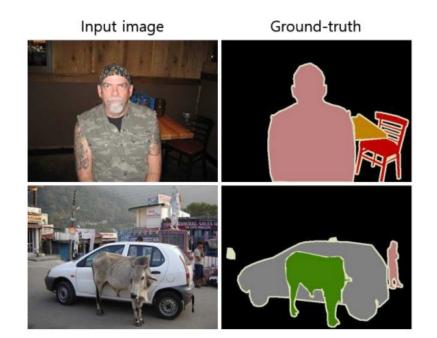


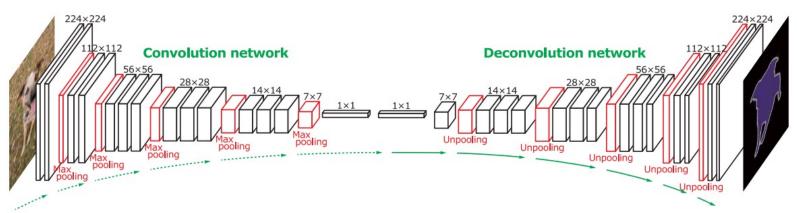
#### Figure from

https://openaccess.thecvf.com/content\_cvpr\_2014/papers/Toshev\_DeepPose\_Human\_Pose\_2014\_CVPR\_paper.pdf

# Semantic Segmentation

- Given an image, predict a label for every pixel in the image
- Not merely a classification problem, because there are strong correlations between pixel-specific labels

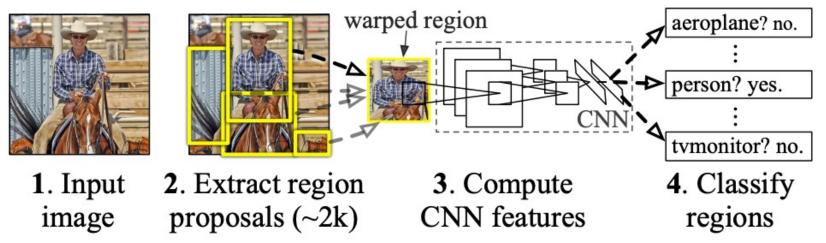




### **Object Detection**

- Given an image, for each object predict a bounding box and a label (x,y,w,h,l)
- Example: R-CNN
  - (x=110, y=13, w=50, h=72, l=person)
  - (x=90, y=55, w=81, h=87, l=horse)
  - (x=421, y=533, w=24, h=30, l=chair)
  - (x=2, y=25, w=51, h=121, l=gate)

#### **R-CNN:** Regions with CNN features



#### Figure from

https://openaccess.thecvf.com/content\_cvpr\_2014/papers/Girshick\_Rich\_Feature\_Hierarchies\_2014\_CVPR\_paper.pdf

## Instance Segmentation

- Predict per-pixel labels as in semantic segmentation, but differentiate between different instances of the same label
- Example: if there are two people in the image, one person should be labeled **person-1** and one should be labeled **person-2**

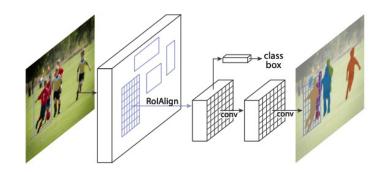


Figure 1. The Mask R-CNN framework for instance segmentation.

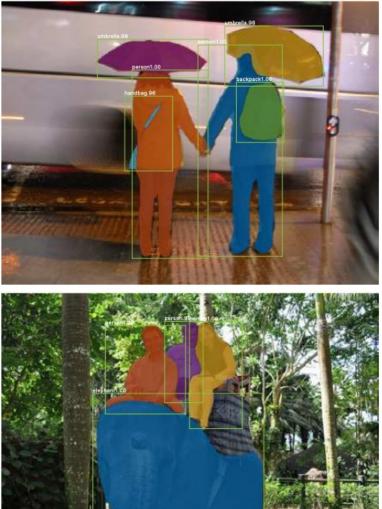


Figure from https://openaccess.thecvf.com/content\_ICCV\_2017/papers/He\_Mask\_R-CNN\_ICCV\_2017\_paper.pdf

# Image Captioning



**Ground Truth Caption:** A little boy runs away from the approaching waves of the ocean.

Generated Caption: A young boy is running on the beach.



Ground Truth Caption: A brunette girl wearing sunglass	es
and a yellow shirt.	

Generated Caption: A woman in a black shirt and sunglasses smiles.

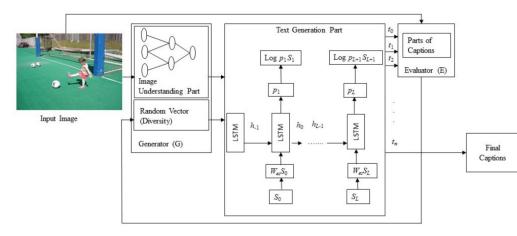


Fig. 3. A block diagram of other deep-learning-based captioning.

- Take an image as input, and generate a sentence describing it as output (i.e. the caption)
- Typical methods include a deep CNN/transformer and a RNN-like language model
- (The task of Dense Captioning is to generate one caption per bounding box)

## Image Captioning

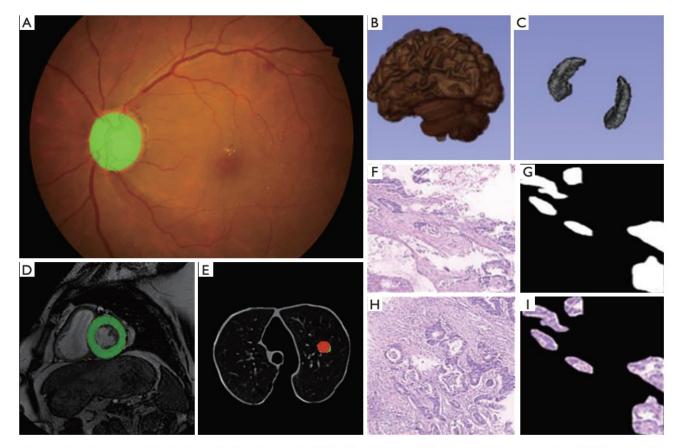
Table 1. An Overview of the Deep-Learning-Based Approaches for Image Captioning

Reference	Image Encoder	Language Model	Category
Kiros et al. 2014 [69]	AlexNet	LBL	MS, SL, WS, EDA
Kiros et al. 2014 [70]	AlexNet, VGGNet	1. LSTM 2. SC-NLM	MS, SL, WS, EDA
Mao et al. 2014 [95]	AlexNet	RNN	MS, SL, WS
Karpathy et al. 2014 [66]	AlexNet	DTR	MS, SL, WS, EDA
Mao et al. 2015 [94]	AlexNet, VGGNet	RNN	MS, SL, WS
Chen et al. 2015 [23]	VGGNet	RNN	VS, SL, WS, EDA
Fang et al. 2015 [33]	AlexNet, VGGNet	MELM	VS, SL, WS, CA
Jia et al. 2015 [59]	VGGNet	LSTM	VS, SL, WS, EDA
Karpathy et al. 2015 [65]	VGGNet	RNN	MS, SL, WS, EDA
Vinyals et al. 2015 [142]	GoogLeNet	LSTM	VS, SL, WS, EDA
Xu et al. 2015 [152]	AlexNet	LSTM	VS, SL, WS, EDA, AB
Jin et al. 2015 [61]	VGGNet	LSTM	VS, SL, WS, EDA, AB
Wu et al. 2016 [151]	VGGNet	LSTM	VS, SL, WS, EDA, AB
Sugano et at. 2016 [129]	VGGNet	LSTM	VS, SL, WS, EDA, AB
Mathews et al. 2016 [97]	GoogLeNet	LSTM	VS, SL, WS, EDA, SC
Wang et al. 2016 [144]	AlexNet, VGGNet	LSTM	VS, SL, WS, EDA
Johnson et al. 2016 [62]	VGGNet	LSTM	VS, SL, DC, EDA
Mao et al. 2016 [92]	VGGNet	LSTM	VS, SL, WS, EDA
Wang et al. 2016 [146]	VGGNet	LSTM	VS, SL, WS, CA
Tran et al. 2016 [135]	ResNet	MELM	VS, SL, WS, CA
Ma et al. 2016 [90]	AlexNet	LSTM	VS, SL, WS, CA
You et al. 2016 [156]	GoogLeNet	RNN	VS, SL, WS, EDA, SCI
Yang et al. 2016 [153]	VGGNet	LSTM	VS, SL, DC, EDA
Anne et al. 2016 [6]	VGGNet	LSTM	VS, SL, WS, CA, NOB
Yao et al. 2017 [155]	GoogLeNet	LSTM	VS, SL, WS, EDA, SCI
Lu et al. 2017 [88]	ResNet	LSTM	VS, SL, WS, EDA, AB
Chen et al. 2017 [21]	VGGNet, ResNet	LSTM	VS, SL, WS, EDA, AB
Gan et al. 2017 [41]	ResNet	LSTM	VS, SL, WS, CA, SCB
Pedersoli et al. 2017 [112]		RNN	VS, SL, WS, EDA, AB
Ren et al. 2017 [119]	VGGNet	LSTM	VS, ODL, WS, EDA
Park et al. 2017 [111]	ResNet	LSTM	VS, SL, WS, EDA, AB
Wang et al. 2017 [148]	ResNet	LSTM	VS, SL, WS, EDA
Tavakoli et al. 2017 [134]	VGGNet	LSTM	VS, SL, WS, EDA, AB
Liu et al. 2017 [84]	VGGNet	LSTM	VS, SL, WS, EDA, AB
Gan et al. 2017 [39]	ResNet	LSTM	VS, SL, WS, EDA, SC
Dai et al. 2017 [26]	VGGNet	LSTM	VS, ODL, WS, EDA
Shetty et al. 2017 [126]	GoogLeNet	LSTM	VS, ODL, WS, EDA
Liu et al. 2017 [85]	Inception-V3	LSTM	VS, ODL, WS, EDA
Gu et al. 2017 [51]	VGGNet	<ol> <li>Language CNN</li> <li>LSTM</li> </ol>	VS, SL, WS, EDA
Yao et al. 2017 [154]	VGGNet	LSTM	VS, SL, WS, CA, NOB

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- (The task of Dense Captioning is to generate one caption per bounding box)

# Medical Image Analysis

Notice that **most** of these tasks are structured prediction problems, not merely classification



**Figure 2** Deep learning application in medical image analysis. (A) Fundus detection; (B,C) hippocampus segmentation; (D) left ventricular segmentation; (E) pulmonary nodule classification; (F,G,H,I) gastric cancer pathology segmentation. The staining method is H&E, and the magnification is ×40.

(aka. BERT-style models)

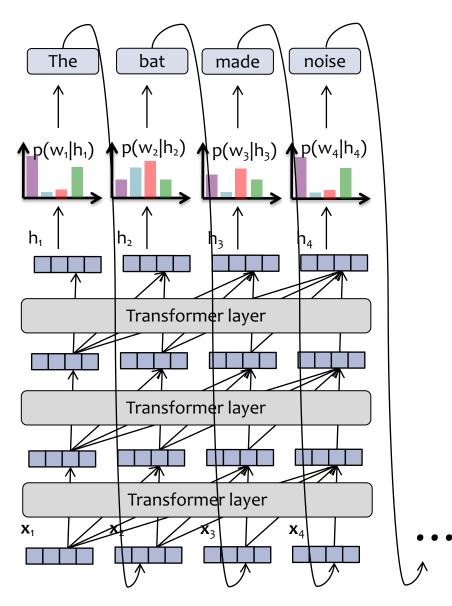
# TRANSFORMER (ENCODER ONLY VERSION)

#### Autoregressive Language Model

**Definition:** An *autoregressive language model* defines a probability distribution over sequences  $\mathbf{x}_{1:T}$  of the form:

$$p(\mathbf{x}_{1:T}) = \prod_{t=1}^{T} p(x_t \mid x_1, \dots, x_{t-1})$$

Also called a Transformer language model



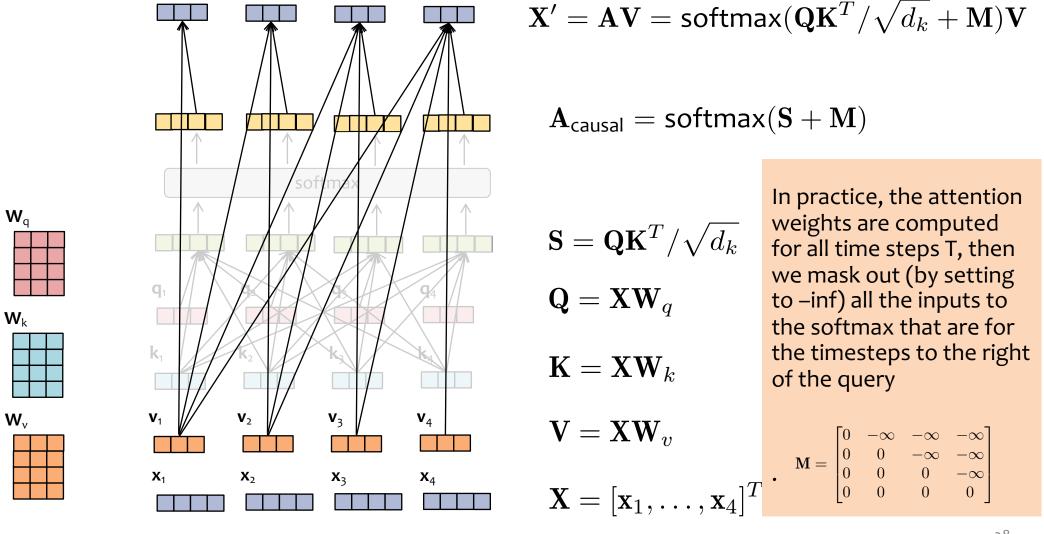
**Each layer** of a Transformer LM consists of several **sublayers**:

- 1. causal attention
- 2. feed-forward neural network
- 3. layer normalization
- 4. residual connections

Each hidden vector looks back at the hidden vectors of the **current and previous timesteps in the previous layer.** 

The language model part is just like an RNN-LM.

### Single-Headed (Causal) Attention



# Single-Headed Attention

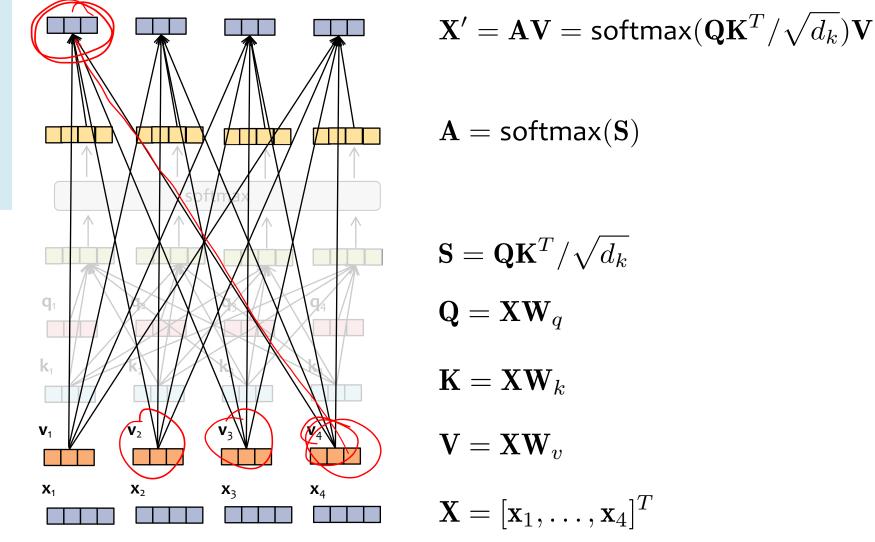
#### So what is this model?

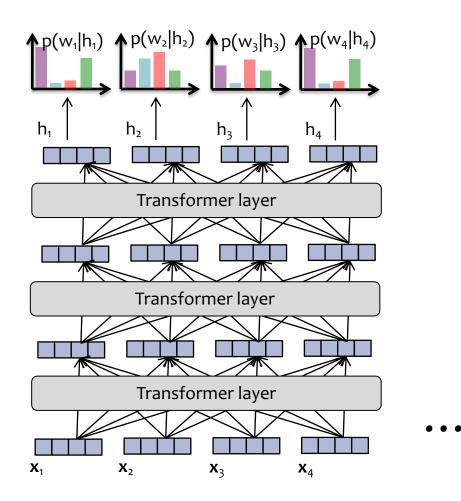
- Notice that each token can attend to all other tokens on the left and right
- It is **not** an autoregressive language model

 $W_q$ 

 $W_k$ 

 $W_{v}$ 





Each layer of an encoder-only Transformer consists of several sublayers:

- 1. non-causal attention
- 2. feed-forward neural network
- 3. layer normalization
- 4. residual connections

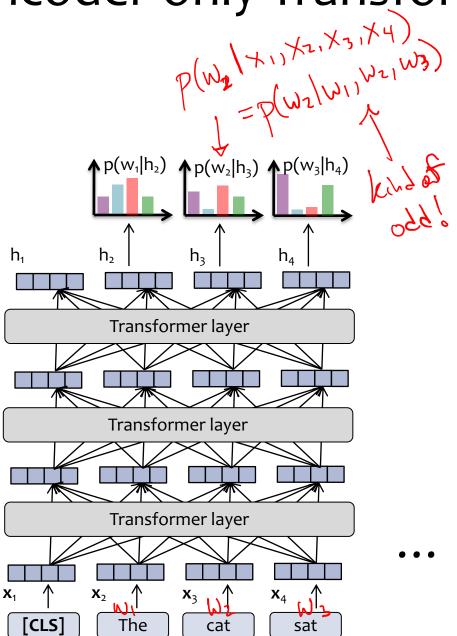
Each hidden vector looks at the the hidden vectors of **all timesteps in the previous layer.** 

**BERT** popularized this encoder-only Transformer architecture and style of pretraining

#### **MLM Pretraining:**

- Rather than trying to predict the next word from the previous ones...
- ... mask out a word

   (or a few words)
   and predict the
   missing words from
   the remaining ones



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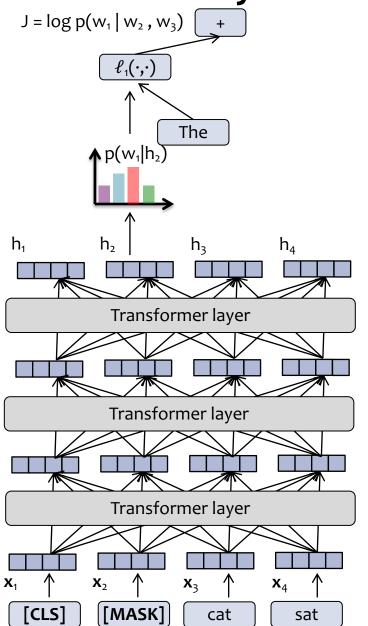
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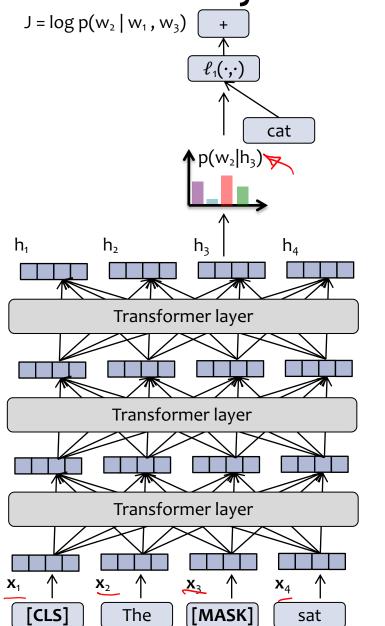
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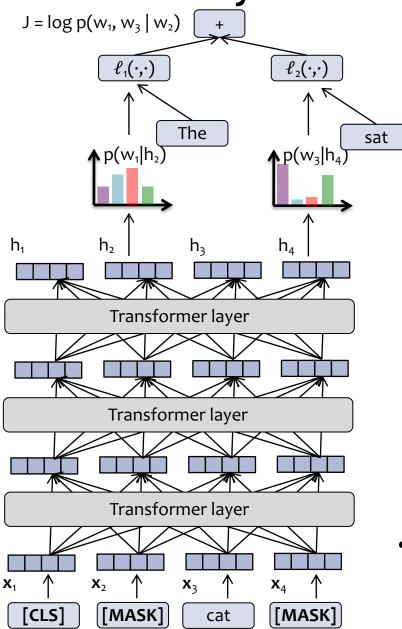
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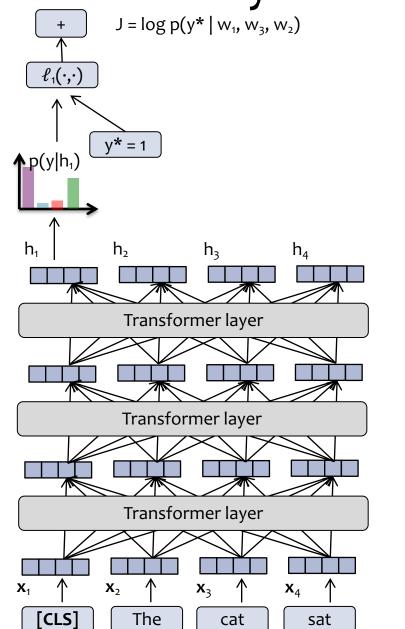
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#### **Supervised Fine-tuning:**

- How to fine-tune this model for a classification task?
- Predict the class label given the embedding for the special [CLS] token
- Fine-tune the model to be good at classification in this way

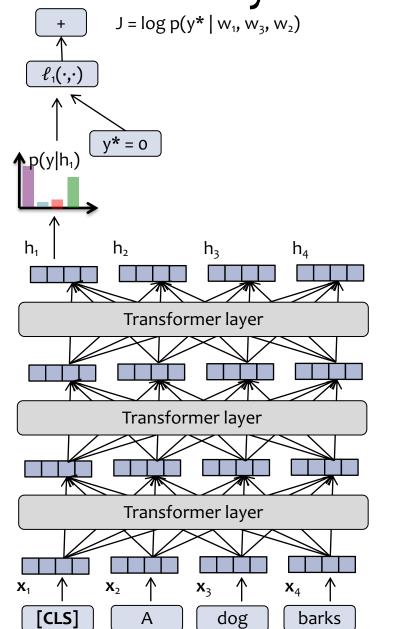
Although this is not a generative language model, it can be used very effectively as a discriminator

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#### **VISION TRANSFORMER**

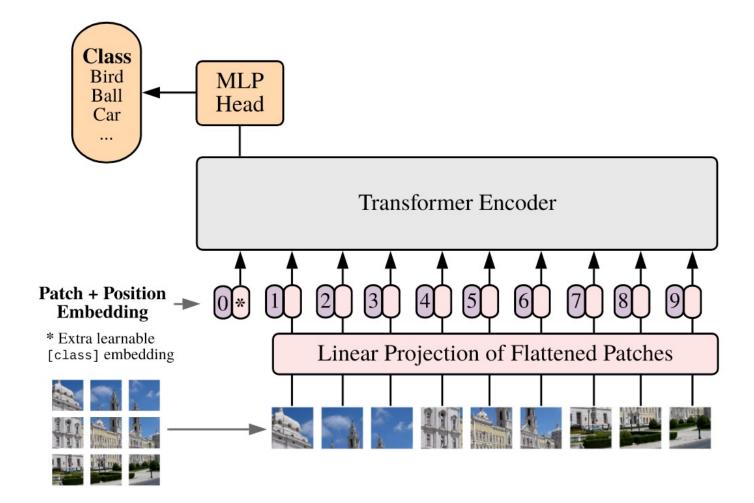
## Vision Transformer (ViT)

Model:

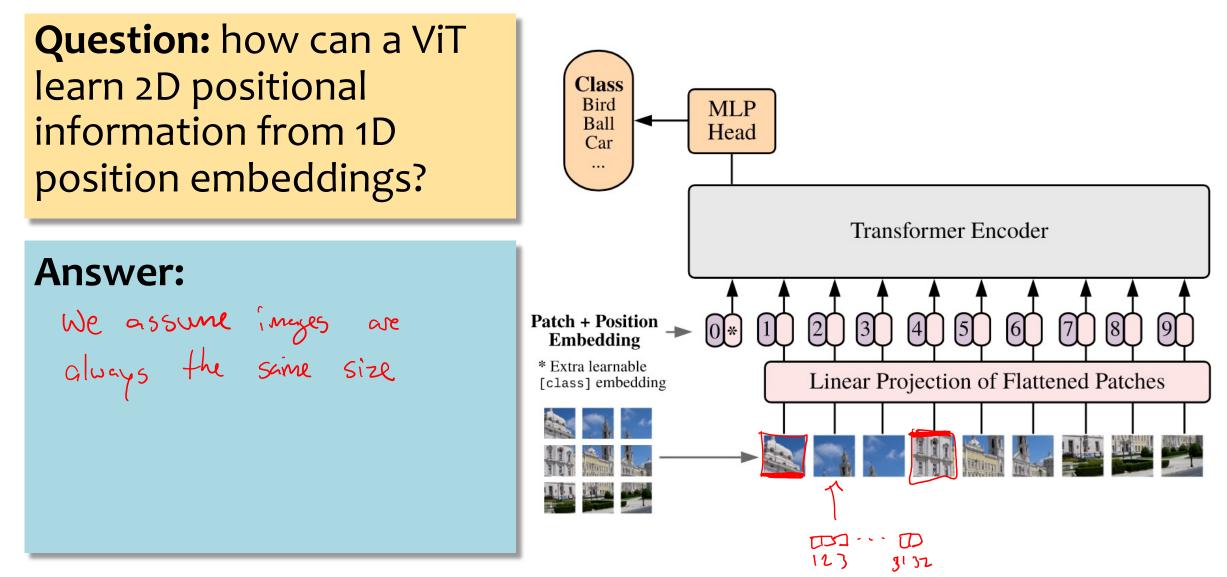
- model is almost identical to BERT
- instead of words as input the inputs are PxP pixel image patches, P ∈ {14, 16, 32} (no overlap)
- each patch is embedded linearly into a vector of size 1024
- 1D positional embeddings

Training:

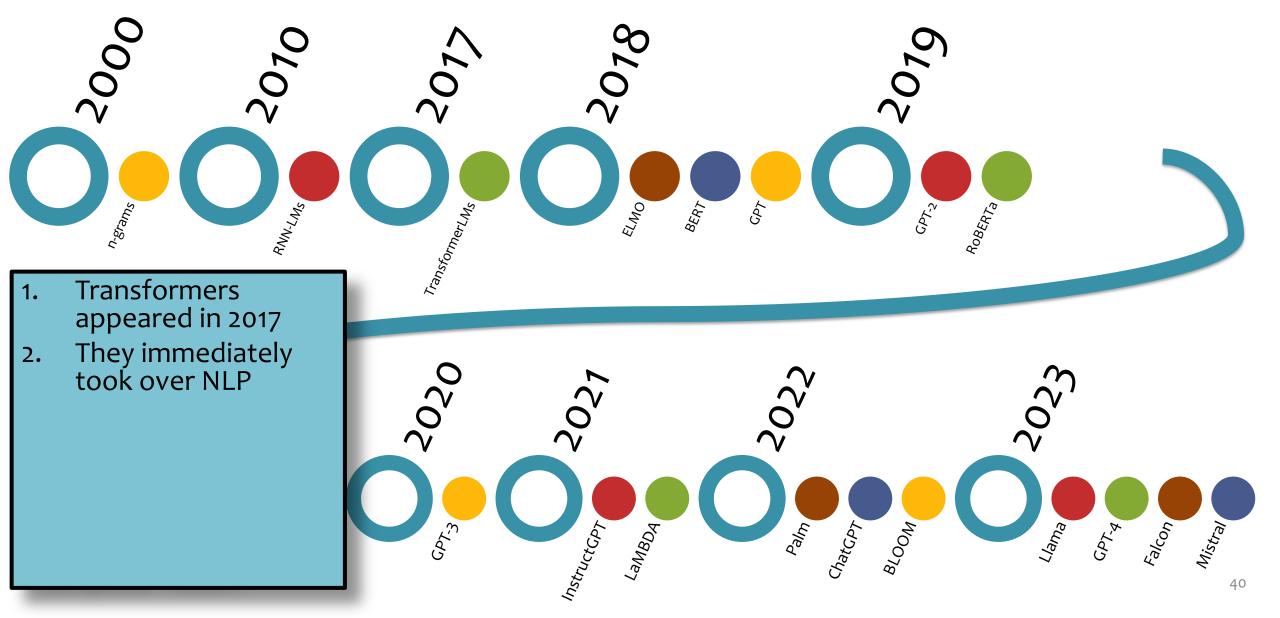
- for pre-training, optimize for image classification on large supervised dataset (e.g. ImageNet 21K, JFT-300M)—same setup as a CNN
- for fine-tuning, learn a new classification head on a small dataset (e.g. CIFAR-100)



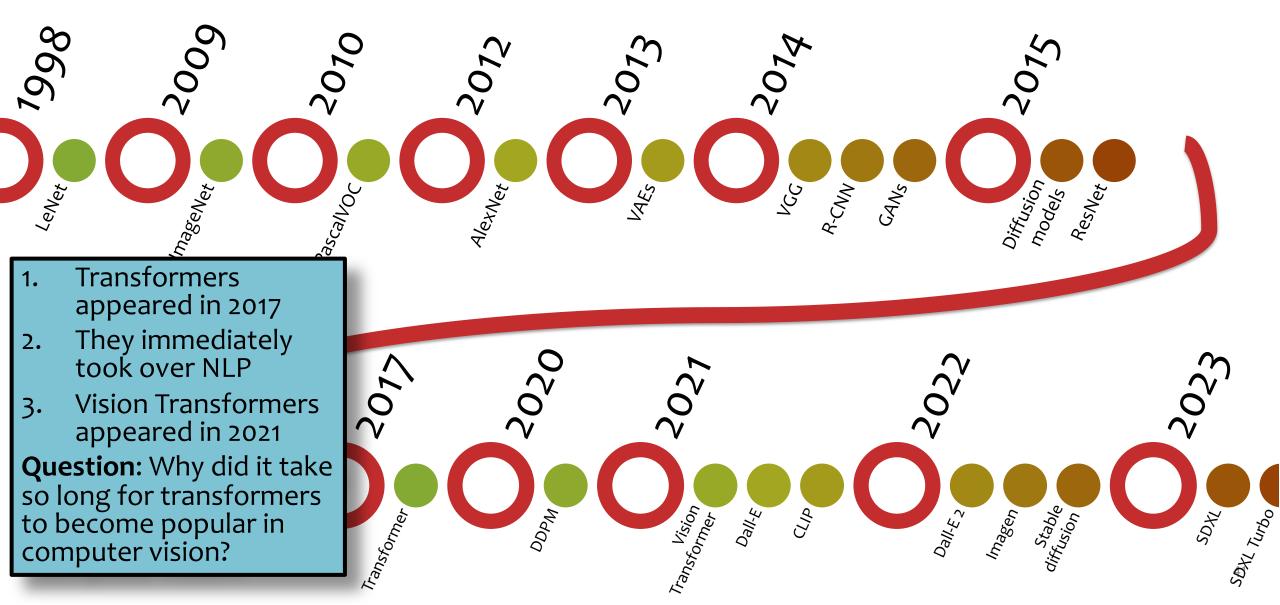
## Vision Transformer (ViT)



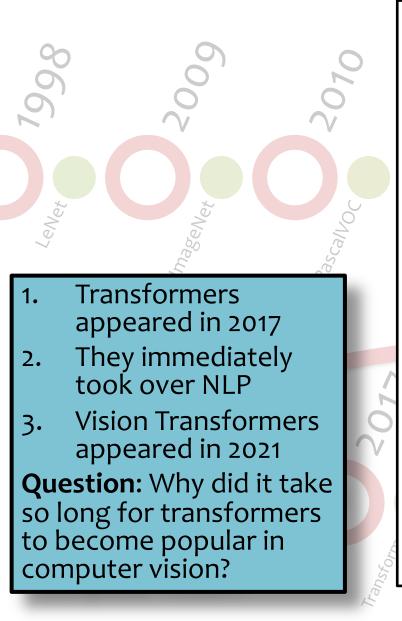
#### **Timeline: Language Modeling**



#### **Timeline: Image Generation**



### Timeline: Image Generation



#### 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>

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

When trained on mid-sized datasets such as ImageNet without strong regularization, these models yield modest accuracies of a few percentage points below ResNets of comparable size. This seemingly discouraging outcome may be expected: Transformers lack some of the inductive biases inherent to CNNs, such as translation equivariance and locality, and therefore do not generalize well when trained on insufficient amounts of data.

However, the picture changes if the models are trained on larger datasets (14M-300M images). We find that large scale training trumps inductive bias. Our Vision Transformer (ViT) attains excellent results when pre-trained at sufficient scale and transferred to tasks with fewer datapoints. When pre-trained on the public ImageNet-21k dataset or the in-house JFT-300M dataset, ViT approaches or beats state of the art on multiple image recognition benchmarks. In particular, the best model reaches the accuracy of 88.55% on ImageNet, 90.72% on ImageNet-ReaL, 94.55% on CIFAR-100, and 77.63% on the VTAB suite of 19 tasks.

SOA

## Timeline: Image Generation



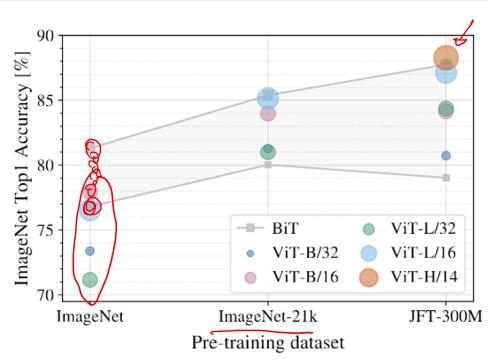


Figure 3: Transfer to ImageNet. While large ViT models perform worse than BiT ResNets (shaded area) when pre-trained on small datasets, they shine when pre-trained on larger datasets. Similarly, larger ViT variants overtake smaller ones as the dataset grows. Comparison of two model families:

- BiT large CNNs based on ResNet
- ViT vision transformers of various sizes



## Vision Transformer (ViT)

- The original Vision
   Transformer models
   were quite small
   compared to the Large
   Language Models
   (LLMs) of the time
- By 2023, ViT had been scaled to 22 billion parameters with good success

Model	Layers	Hidden size $D$	MLP size	Heads	Params
ViT-Base	12	768	3072	12	86M
ViT-Large	24	1024	4096	16	307M
ViT-Huge	32	1280	5120	16	632M

Table 1: Details of Vision Transformer model variants.

Table 1: ViT-22B model architecture details.

Name	Width	Depth	MLP	Heads	Params [M]
ViT-G	1664	48	8192	16	1843
ViT-e	1792	56	15360	16	3926
ViT-22B	6144	48	24576	48	21743

#### **TASK: IMAGE GENERATION**

## Image Generation

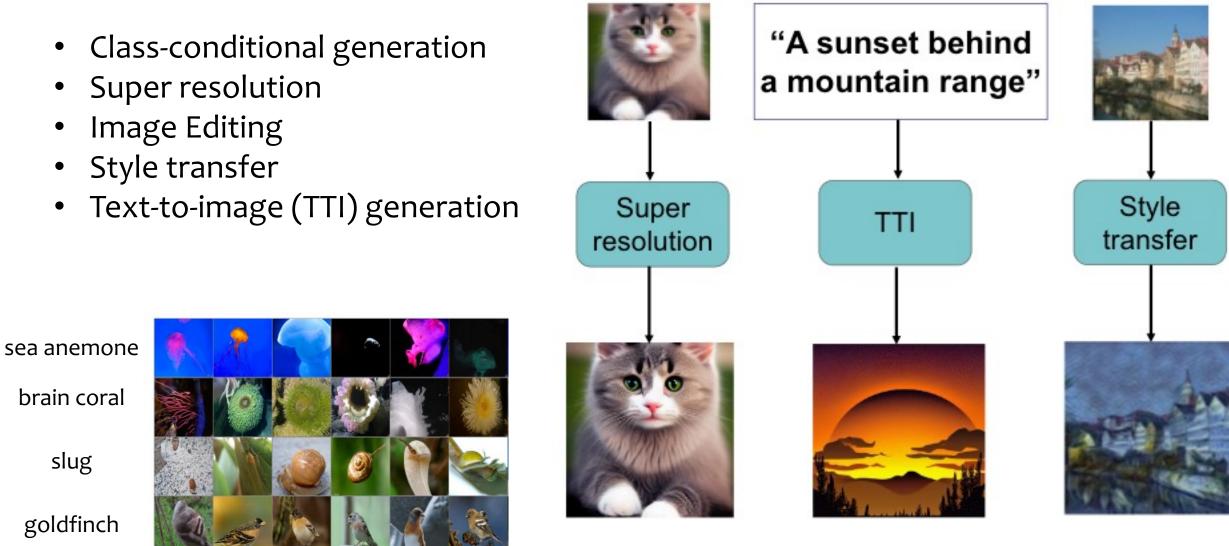
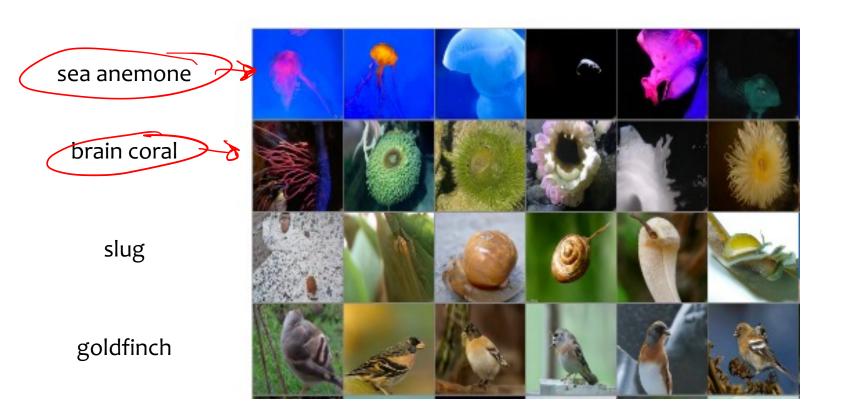


Figure from Razavi et al. (2019)

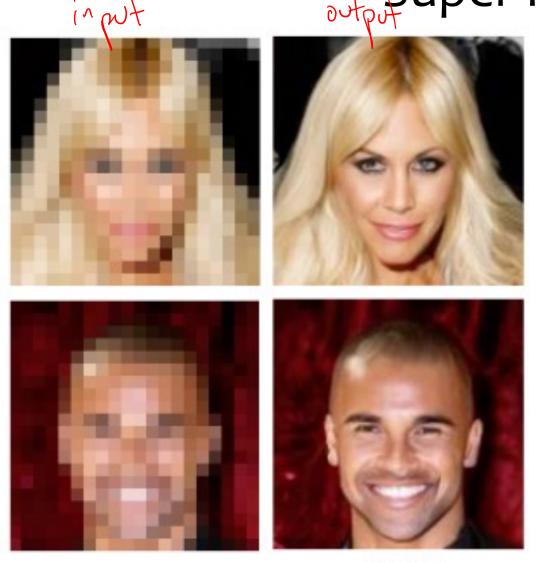
Figure from Bie et al. (2023)

#### **Class Conditional Generation**

- Task: Given a class label indicating the image type, sample a new image from the model with that type
- Image classification is the problem of taking in an image and predicting its label p(y|x)
- Class conditional generation is doing this in reverse p(x|y)



# Super Resolution



SRDiff

 Given a low resolution image, generate a high resolution reconstruction of the image

 Compelling on low resolution inputs (see example to the left) but also effective on high resolution inputs

Figure from Li et al. (2021)

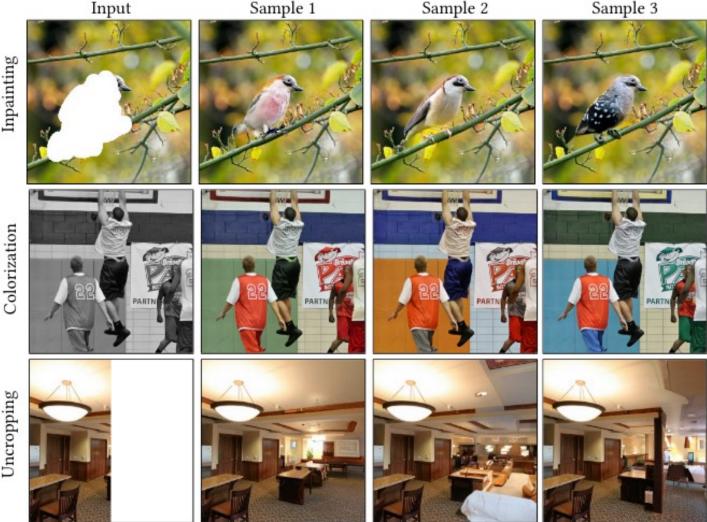
LR

## Image Editing

A variety of tasks involve automatic editing of an image:

- Inpainting fills in the (prespecified) missing pixels
- Colorization restores color to a greyscale image
- Uncropping creates a photo-realistic reconstruction of a missing side of an image





## Style Transfer

- The goal of style transfer is to blend two images
- Yet, the blend should retain the semantic content of the source image presented in the style of another image



Figure 3. Images that combine the content of a photograph with the style of several well-known artworks. The images were created by finding an image that simultaneously matches the content representation of the photograph and the style representation of the artwork. The original photograph depicting the Neckarfront in Tübingen, Germany, is shown in **A** (Photo: Andreas Praefcke). The painting that provided the style for the respective generated image is shown in the bottom left corner of each panel. **B** *The Shipwreck of the Minotaur* by J.M.W. Turner, 1805. **C** *The Starry Night* by Vincent van Gogh, 1889. **D** *Der Schrei* by Edvard Munch, 1893. **E** *Femme nue assise* by Pablo Picasso, 1910. **F** *Composition VII* by Wassily Kandinsky, 1913.



Figure from Gatys et al. (2016)

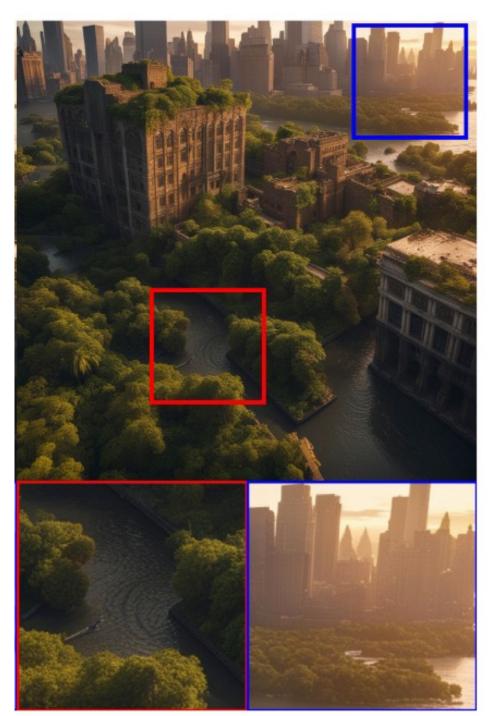
- Given a text description, sample an image that depicts the prompt
- The following images are samples from SDXL with refinement

*Prompt*: A propaganda poster depicting a cat dressed as french emperor napoleon holding a piece of cheese.



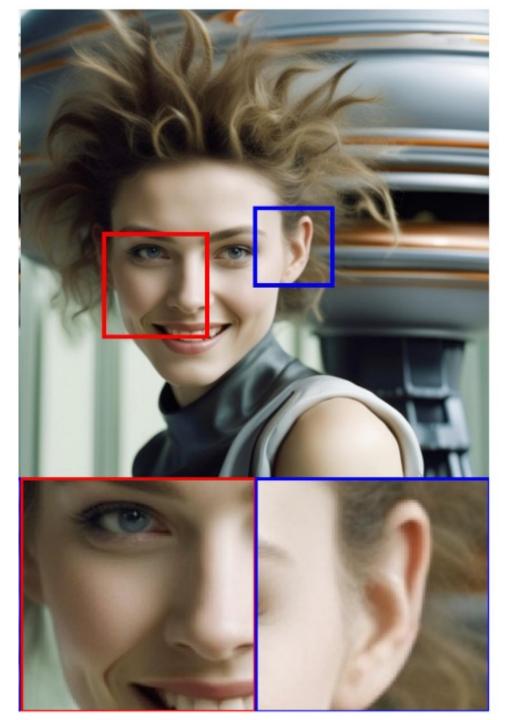
- Given a text description, sample an image that depicts the prompt
- The following images are samples from SDXL with refinement

Prompt: Epic long distance cityscape photo of New York City flooded by the ocean and overgrown buildings and jungle ruins in rainforest, at sunset, cinematic shot, highly detailed, 8k, golden light



- Given a text description, sample an image that depicts the prompt
- The following images are samples from SDXL with refinement

Prompt: close up headshot, futuristic young woman, wild hair sly smile in front of gigantic UFO, dslr, sharp focus, dynamic composition



- Given a text description, sample an image that depicts the prompt
- The following images are samples from SDXL with refinement

Prompt: close up headshot, futuristic **old man**, wild hair sly smile in front of gigantic UFO, dslr, sharp focus, dynamic composition, **rule of thirds** 



## In-Class Poll

#### **Question:**

What are the potential societal impacts of image generation?

Answer:

## Summary

- Computer Vision
- Task: Image Generation
- Model: Generative Adversarial Network (GAN)
- Learning for GANs
- Scaling Up the Model Size
- Societal Impacts of Image Generation

## MODEL: GENERATIVE ADVERSARIAL NETWORK (GAN)

## Stable Diffusion still can't explain GANs

Prompt: slide explaining Generative Adversarial Networks (GANs) for Intro to Machine Learning course, carefully designed, easy to follow

Negative Prompt: boring, unclear, nontechnical

