Transformer and Applications

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Summary

- We have shown:
  - CNN Architectures: LeNet5, Alexnet, VGG, GoogleNet, Resnet
  - Recurrent Neural Networks and LSTM (GRU)
  - Attention and Transformer
- Today:
  - **Applications of Transformer**
    - **BERT, GPT, and ViT**
- Reference:
  - Feifei Li, Stanford cs231n
  - Chris Manning, Stanford cs224n

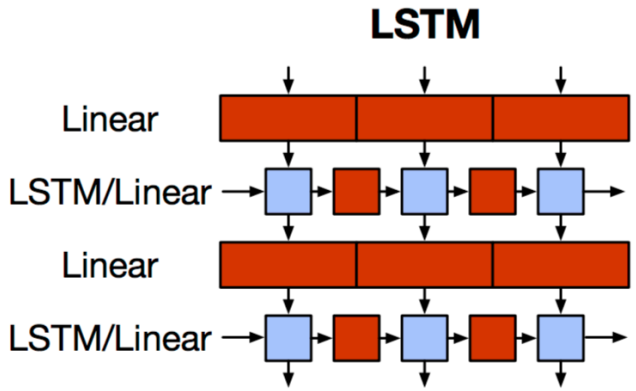
A Brief History in NLP

- In 2013-2015, LSTMs started achieving state-of-the-art results
  - Successful tasks include: handwriting recognition, speech
  - recognition, machine translation, parsing, image captioning
  - LSTM became the dominant approach
- Now (2019), other approaches (e.g. Transformers) have become more dominant for Machine Translation.
  - For example in **WMT** (a MT conference + competition):
  - In WMT 2016, the summary report contains "RNN" 44 times
  - In WMT 2018, the report contains "RNN" 9 times and "Transformer" 63 times

  - **Source:** "Findings of the 2016 Conference on Machine Translation (WMT16)", Bojar et al. 2016, http://www.statmt.org/wmt16/pdf/W16-2301.pdf
  - **Source:** "Findings of the 2018 Conference on Machine Translation (WMT18)", Bojar et al. 2018, http://www.statmt.org/wmt18/pdf/WMT028.pdf

Motivation of Transformer

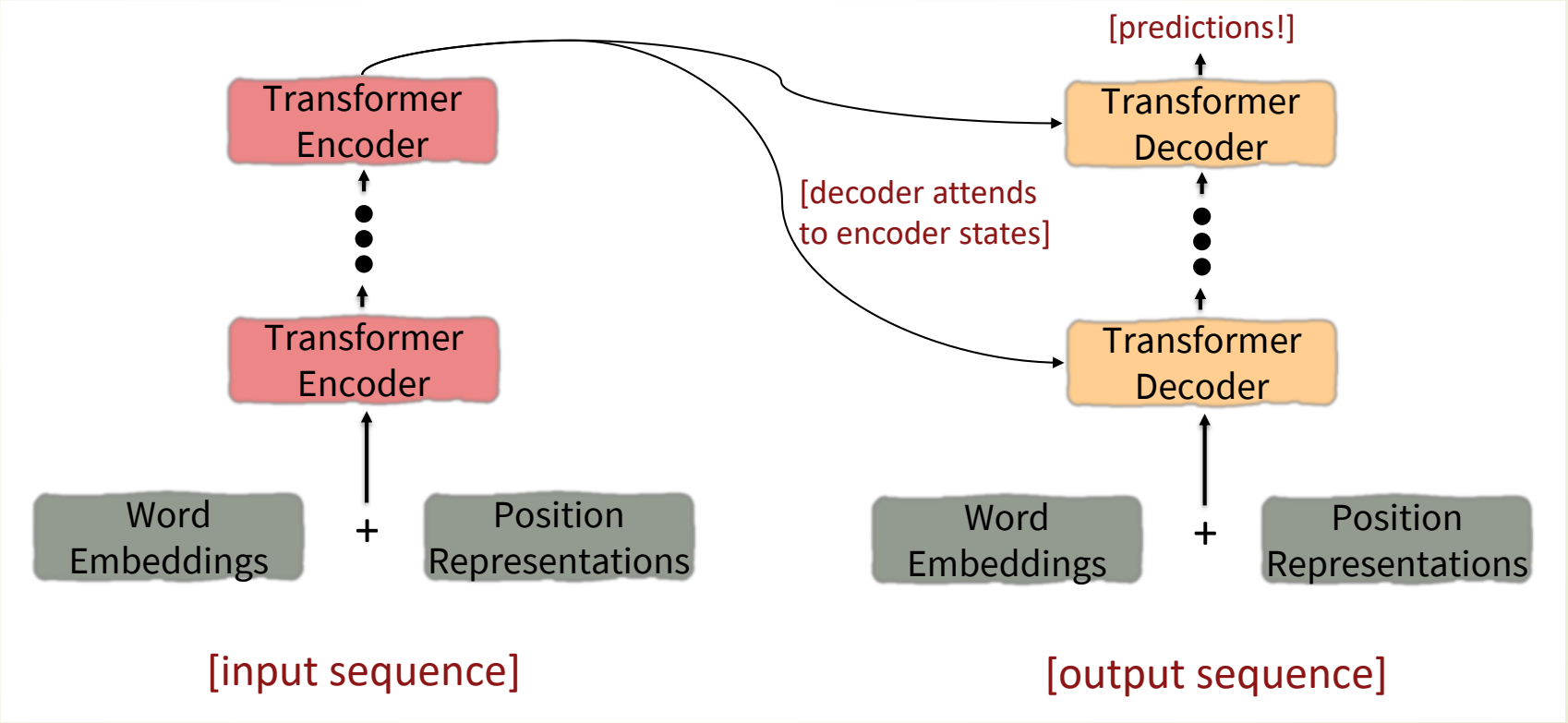
- We want **parallelization** but RNNs are inherently sequential



- Despite LSTMs, RNNs generally need attention mechanism to deal with long range dependencies – **path length** between states grows with distance otherwise
- But if **attention** gives us access to any state… maybe we can just use attention and don't need the RNN? 🤔
- And then NLP can have deep models … and solve our vision envy

The Transformer Encoder-Decoder [Vaswani et al. 2017]

- Looking back at the whole model



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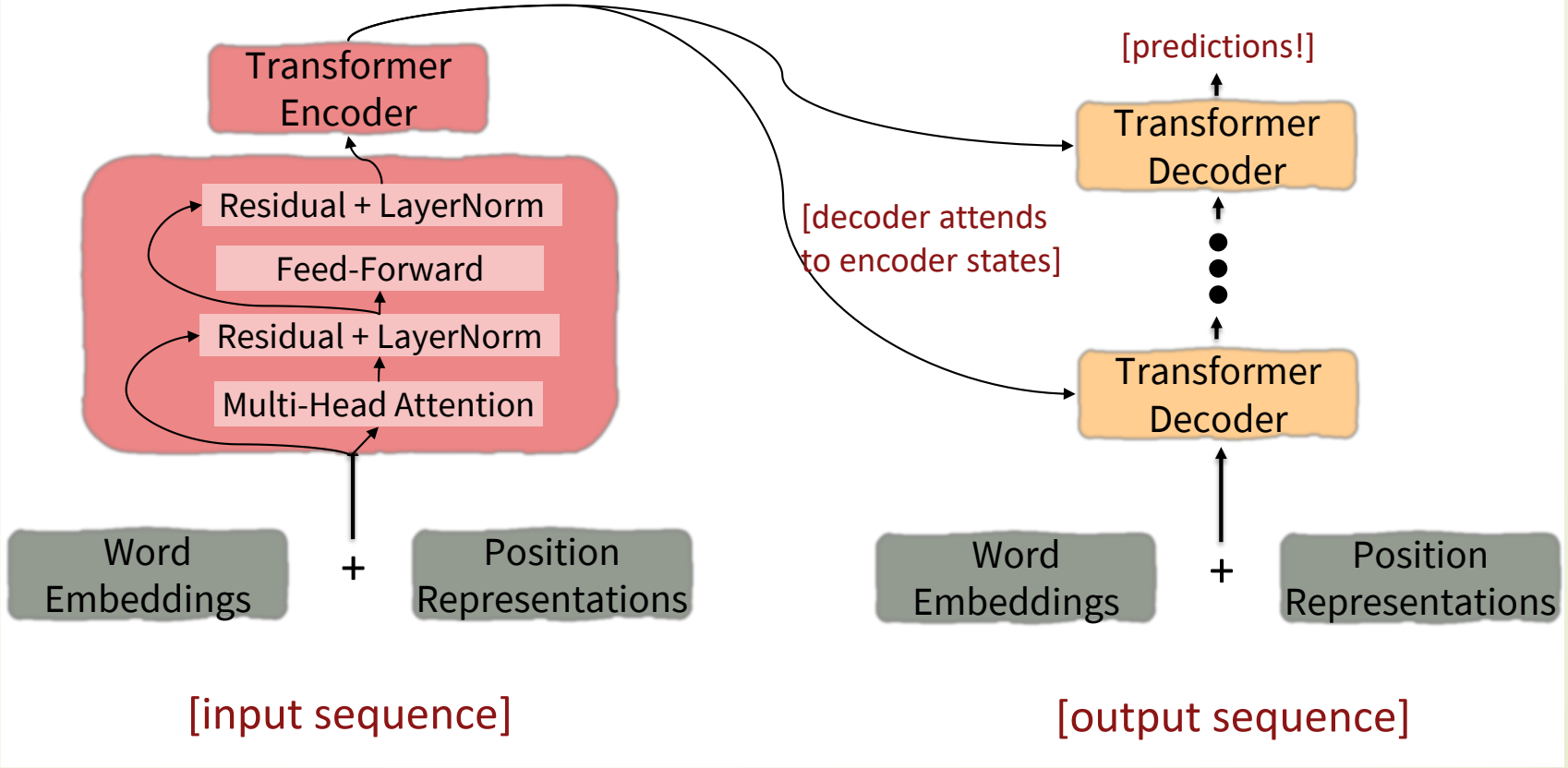

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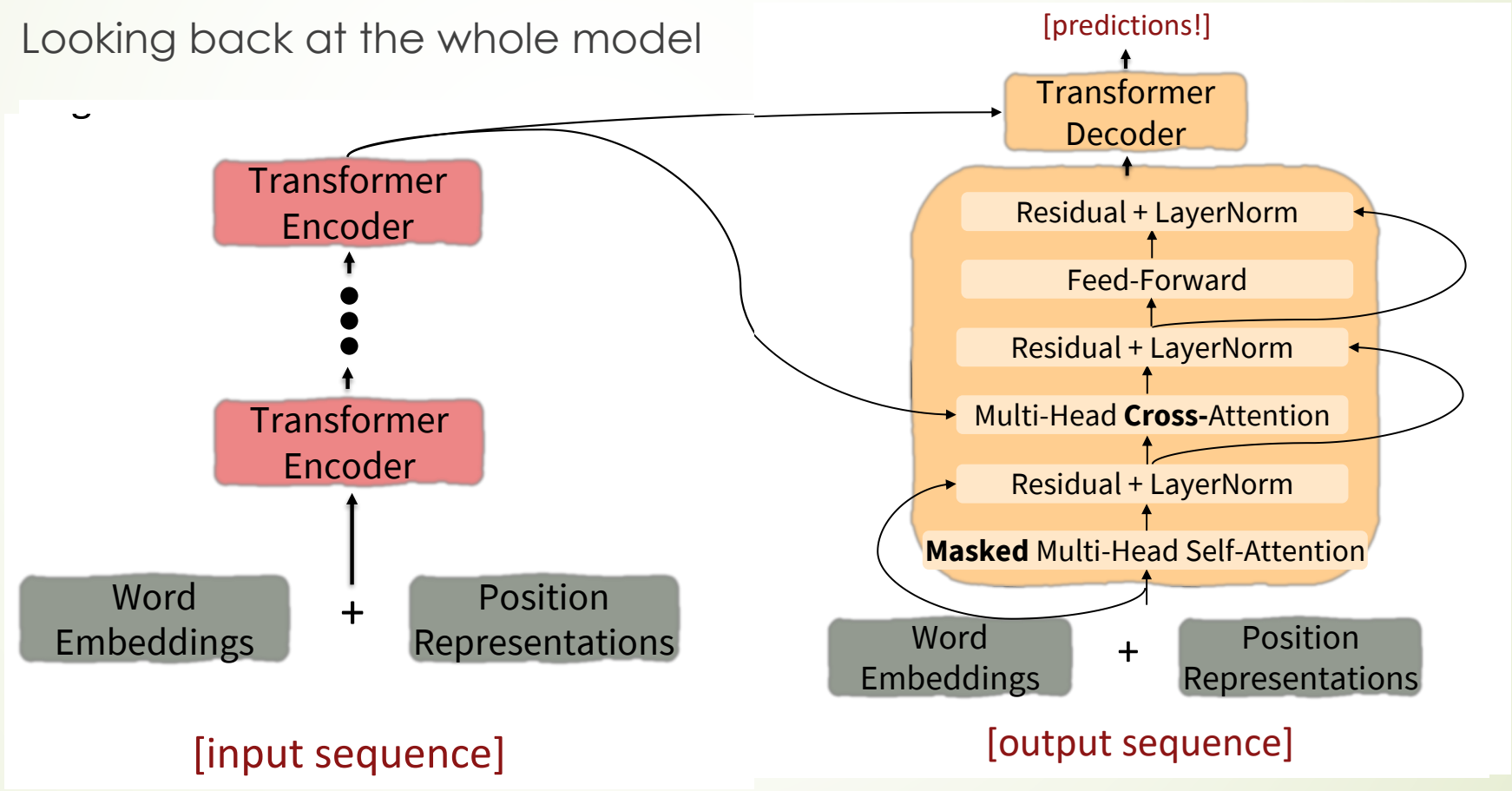


Table 2.1: In our network configurations, *Sublayer* refers to either a feed-forward neural network (FFN) or a self-attention module within a Transformer layer. The symbol d represents the size of the hidden states in the network. The position embedding at a specific position i is denoted by pi. In the attention mechanism, A_{ij} signifies the attention score computed between a given query and its corresponding key. The difference in positions between the query and the key is represented by r_{i-j}, a learnable scalar value. Finally, the term $R_{\theta,t}$ refers to a rotary matrix, which rotates by an angle determined by multiplying t by θ.

Configuration	**Method**	**Equation**
Normalization position	Post Norm [1]	$\text{Norm}(\mathbf{x} + \text{Sublayer}(\mathbf{x}))$
	Pre Norm [2]	$\mathbf{x} + \text{Sublayer}(\text{Norm}(\mathbf{x}))$
	Sandwich Norm [3]	$\mathbf{x} + \text{Norm}(\text{Sublayer}(\text{Norm}(\mathbf{x})))$
Normalization method	LayerNorm [4]	$\frac{\mathbf{x}-\mu}{\sqrt{\sigma}} \cdot \gamma + \beta, \mu = \frac{1}{d}\sum_{i=1}^{d}\mathbf{x}_i, \sigma = \sqrt{\frac{1}{d}\sum_{i=1}^{d}(\mathbf{x}_i - \mu)^2}$
	RMSNorm [5]	$\frac{x}{\text{RMS}(\mathbf{x})} \cdot \gamma, \text{RMS}(\mathbf{x}) = \sqrt{\frac{1}{d}\sum_{i=1}^{d}\mathbf{x}_i^2}$
	DeepNorm [6]	$\text{LayerNorm}(\alpha \cdot \mathbf{x} + \text{Sublayer}(\mathbf{x}))$
Activation function	ReLU [7]	$\text{ReLU}(\mathbf{x}) = \max(0, \mathbf{x})$
	GeLU [8]	$\text{GeLU}(\mathbf{x}) = 0.5\mathbf{x} \bigotimes \left(1 + \tanh\left(\sqrt{\frac{2}{\pi}}\left(x + 0.044715x^3\right)\right)\right)$
	Swish [9]	$f(x) = x \cdot \frac{1}{1+e^{-x}}$
	SwiGLU [10]	$f(x) = x \odot \sigma(Wx + b)$
	GeGLU [10]	Similar to SwiGLU with GeLU
Positional embeddings	Absolute [1]	$x_i = x_i + p_i$
	Relative [11]	$A_{ij} = W_q x_i x_j^T W_k + r_{i-j}$
	RoPE [12]	$A_{ij} = W_q x_i R_{\theta,i-j} x_j^T W_k$
	Alibi [13]	$A_{ij} = W_q x_i x_j^T W_k - m(i-j)$

Key: [1] (Vaswani et al., 2017), [2] (Radford et al., 2019), [3] (Ding et al., 2021), [4] (Ba et al., 2016), [5] (Zhang and Sennrich, 2019), [6] (Wang et al., 2022), [7] (Nair and Hinton, 2010), [8] (Wang et al., 2019), [9] (Ramachandran et al., 2017), [10] (Shazeer, 2020), [11] (Raffel et al., 2020), [12] (Su et al., 2021), [13] (Press et al., 2021)

Mixture of Experts (MoE)

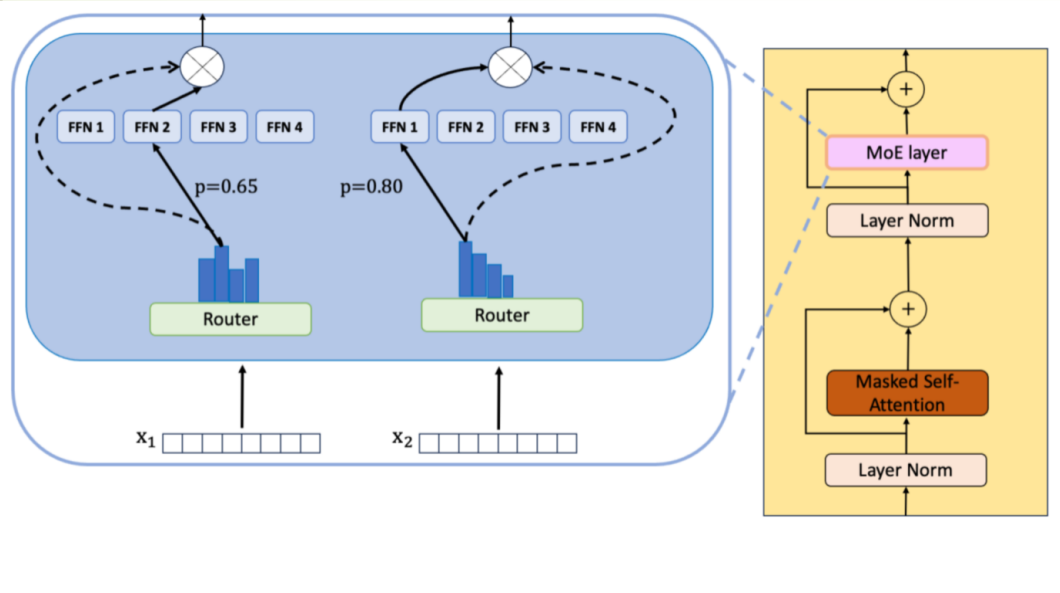


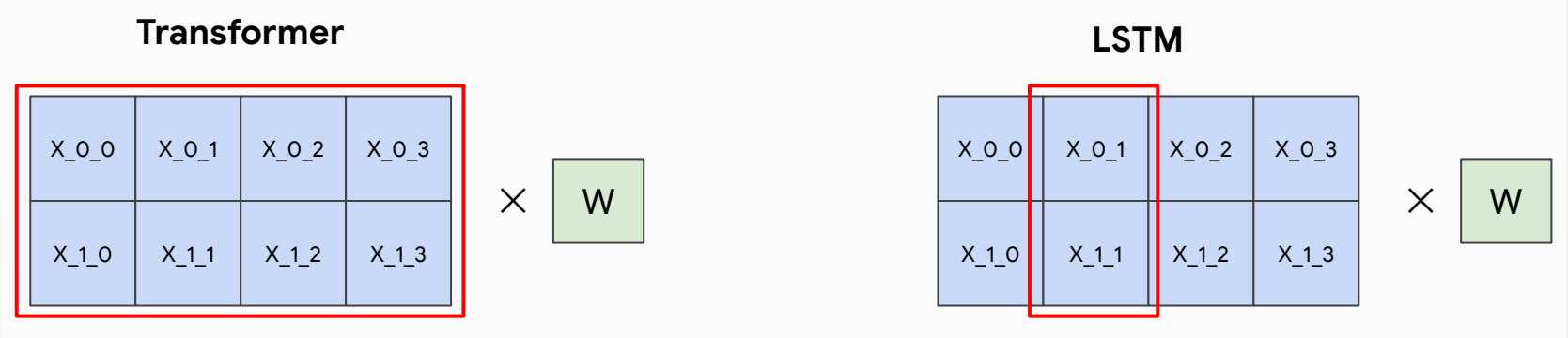
Fig. 2.9: Mixture-of-experts variant of the Transformer architecture.

- MoE layer replaces the standard feed-forward blocks by multiple parallel `experts' as feed-forward blocks weighted by probability gates.
- MoE architecture simultaneously activates only a few experts. This sparse activation allows the architecture to support larger model sizes without a proportional increase in computational demand, maintaining efficient performance.

Shazeer, Noam; Mirhoseini, Azalia; Maziarz, Krzysztof; Davis, Andy; Le, Quoc; Hinton, Geoffrey; Dean, Jeff (2017). "Outrageously Large Neural Networks: The Sparsely-Gated Mixture-of-Experts Layer". arXiv:1701.06538

Empirical advantages of Transformer vs. LSTM

- 1. Self-attention == no locality bias
  - Long-distance context has “equal opportunity”
- 2. Single multiplication per layer == efficiency on TPU



Major disadvantage of Transformer

- **Quadratic compute in self-attention (today)**:
  - Computing all pairs of interactions means our computation grows **quadratically** with the sequence length!
  - For recurrent models, it only grew linearly!

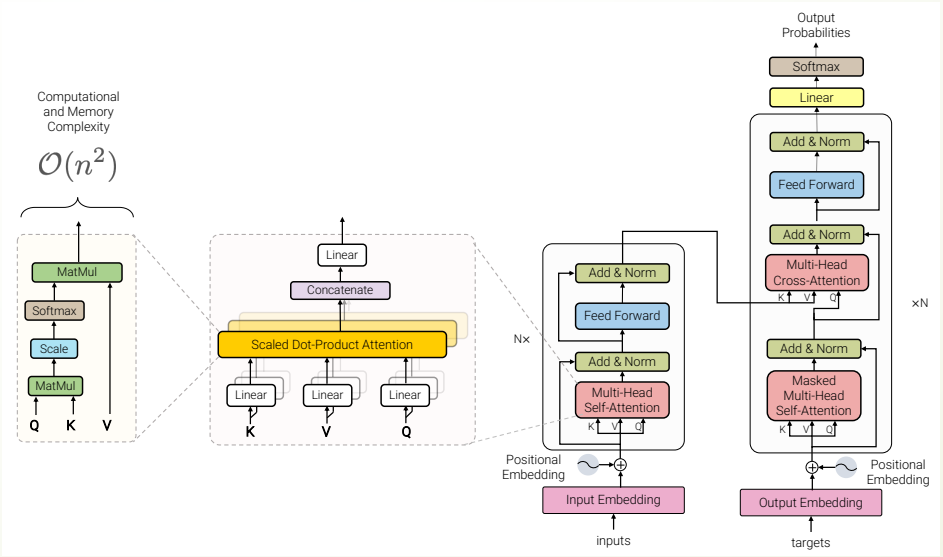


Figure 1: Architecture of the standard Transformer (Vaswani et al., 2017)

Quadratic computation as a function of sequence length

- One of the benefits of self-attention over recurrence was that it's highly parallelizable.
- However, its total number of operations grows as $O(\ n^2\ d\ )$, where n is the sequence length, and d is the dimensionality.
- Think of d as around $\mathbf{1{,}000}$ (though for large language models it's much larger!).
  - So, for a single (shortish) sentence, $n \leq 30$; $n^2 \leq \mathbf{900}$.
  - In practice, we set a bound like $n = 512$.
  - **But what if we'd like $n \geq \mathbf{50{,}000}$?** For example, to work on long documents?

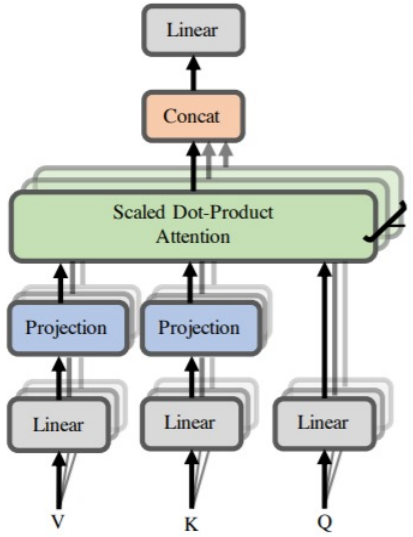
$$XQ \quad K^\top X^\top \quad = \quad XQK^\top X^\top \in \mathbb{R}^{n \times n}$$

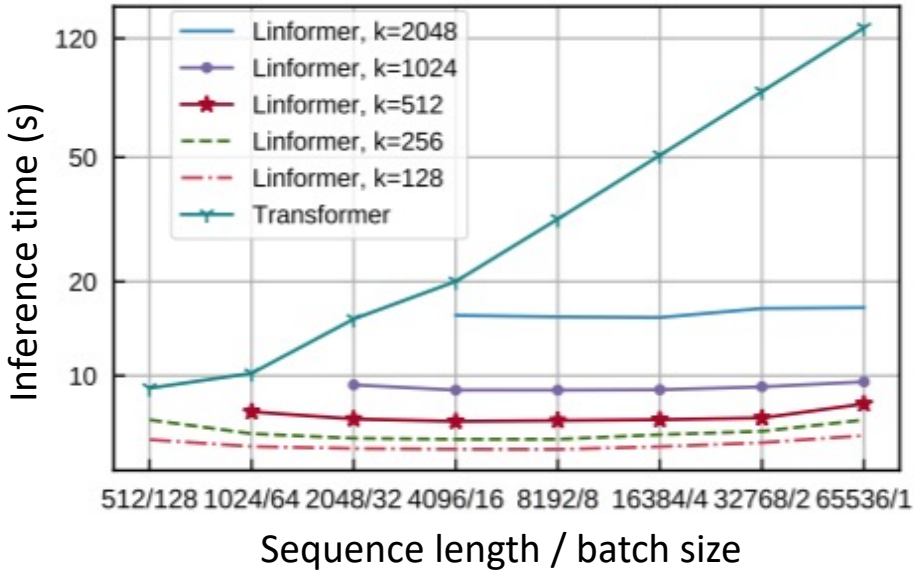
Need to compute all pairs of interactions!
$O(n^2 d)$

Improving quadratic self-attention cost

- Considerable recent work has gone into the question, *Can we build models like Transformers without paying the all-pairs self-attention cost?*
- For example, **Linformer** [Wang et al., 2020, **Linformer: Self-Attention with Linear Complexity**, arXiv:2006.04768]

Key idea: map the sequence length dimension to a lower-dimensional space for values, keys





Efficient Transformers

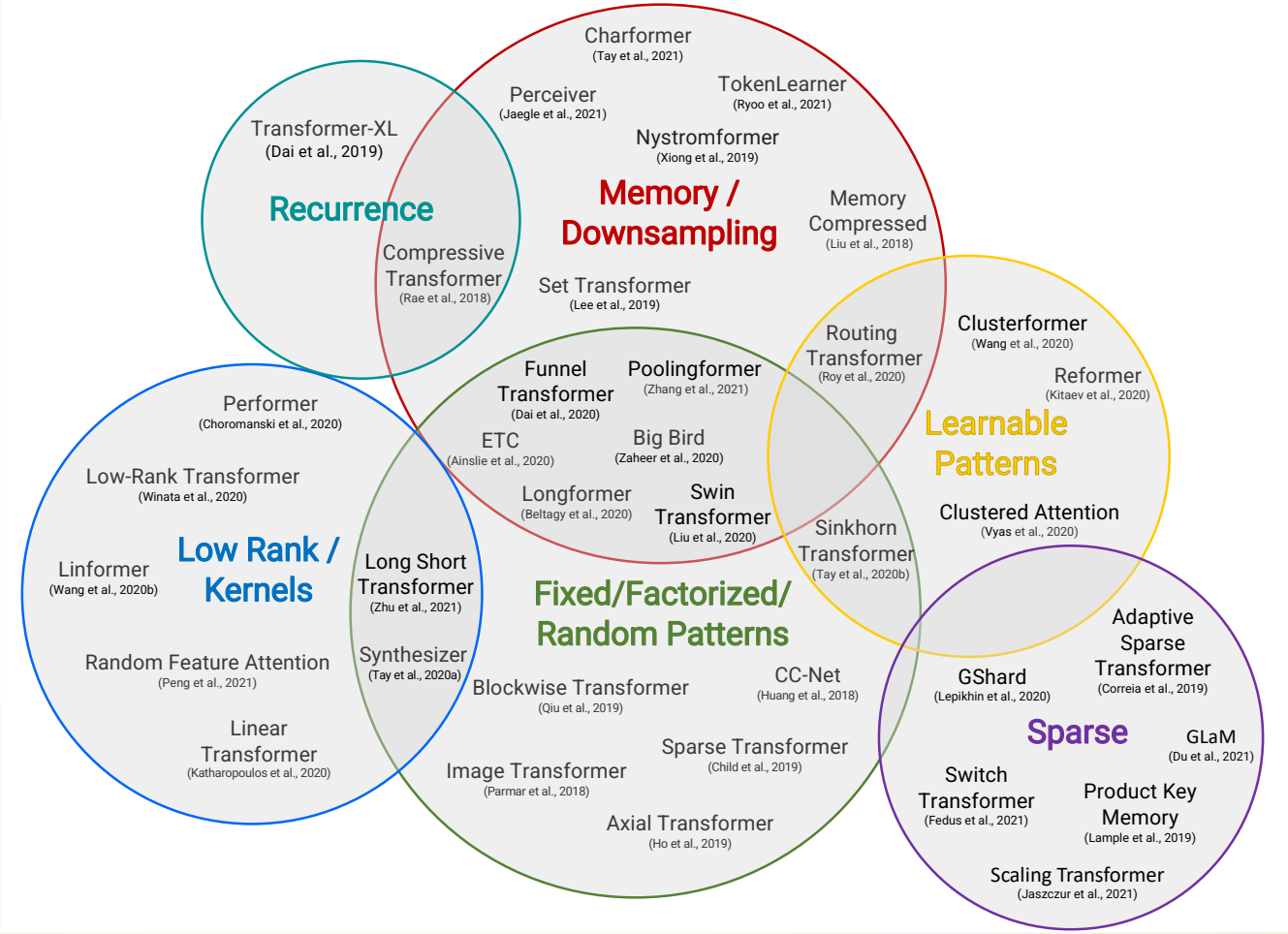
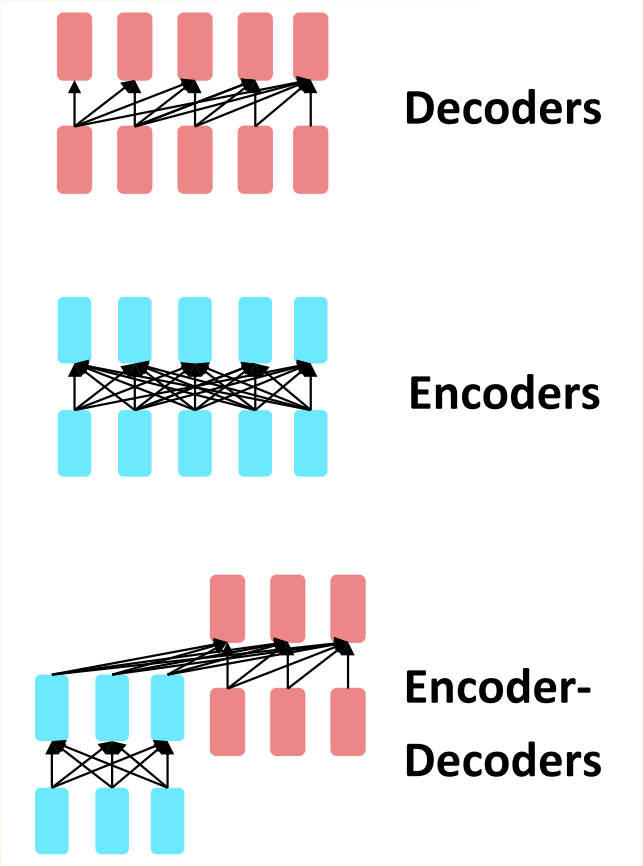


Figure 2: Taxonomy of Efficient Transformer Architectures.

Yi Tay, Mostafa Dehghani, Dara Bahri, Donald Metzler (2020), Efficient Transformers: A Survey, arXiv:2009.06732v3

Pretraining for three types of architectures in Transformers

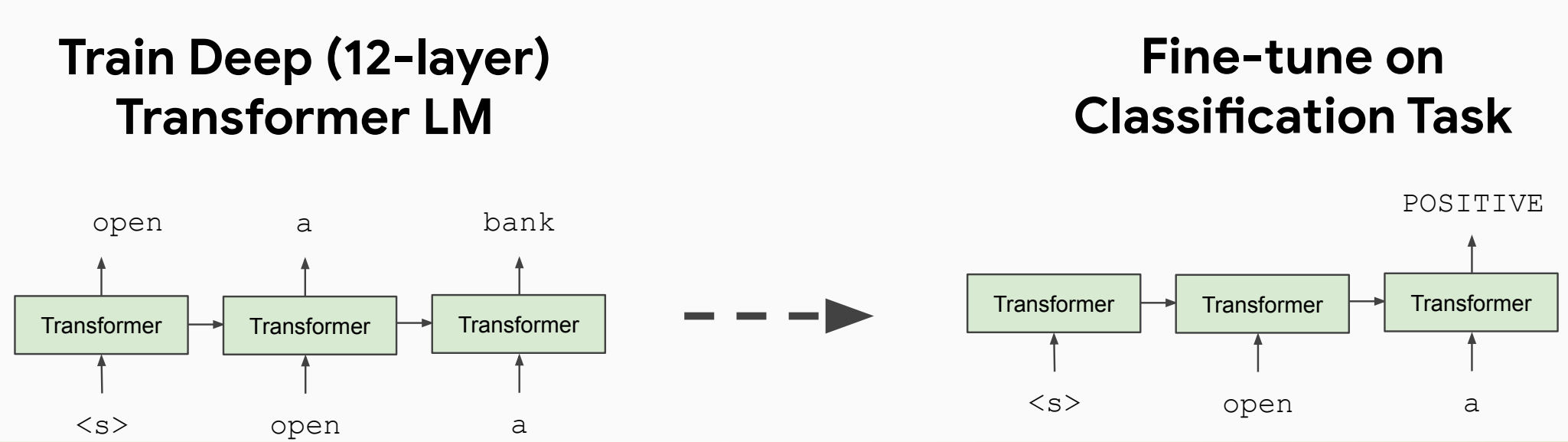
The transformer architecture influences the type of pretraining:



- Decoders:
  - **Unidirectional** Language models! What we've seen so far.
  - Nice to generate from; can't condition on future words: **GPT**
- Encoders:
  - Gets **bidirectional** context – can condition on future!
  - Wait, how do we pretrain them? -- **BERT**
- Encoder-Decoders:
  - Good parts of decoders and encoders?
  - What's the best way to pretrain them? --**T5**

GPT (Generative Pre-Training): uni-directional transformer decoder

- *Improving Language Understanding by Generative Pre-Training*, OpenAI, 2018



Pretraining decoders

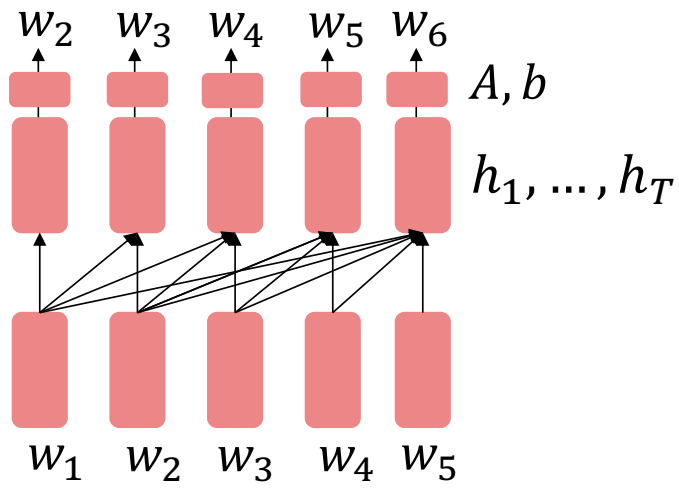
It's natural to pretrain decoders as language models and then use them as generators, finetuning their $p_\theta(w_t|w_{1:t-1})$!

This is helpful in tasks **where the output is a sequence** with a vocabulary like that at pretraining time!

- Dialogue (context=dialogue history)
- Summarization (context=document)

$$h_1, \dots, h_T = \text{Decoder}(w_1, \dots, w_T)$$
$$w_t \sim Ah_{t-1} + b$$

Where A, b were pretrained in the language model!



[Note how the linear layer has been pretrained.]

Finetuning decoders

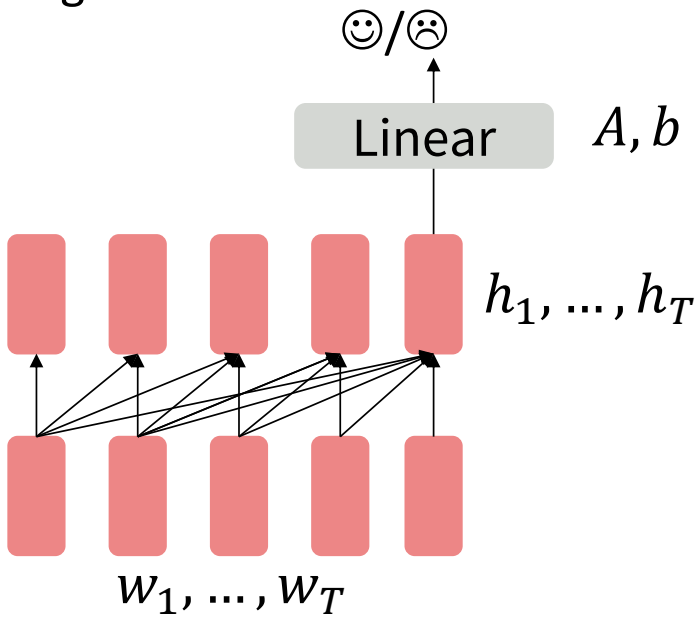
When using language model pretrained decoders, we can ignore that they were trained to model $p(w_t|w_{1:t-1})$.

We can finetune them by training a classifier on the last word's hidden state.

$$h_1, \dots, h_T = \text{Decoder}(w_1, \dots, w_T)$$
$$y \sim Ah_T + b$$

Where A and b are randomly initialized and specified by the downstream task.

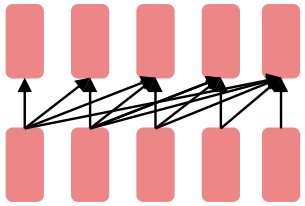
Gradients backpropagate through the whole network.



[Note how the linear layer hasn't been pretrained and must be learned from scratch.]

GPT (Generative Pre-Trained Transformer): uni-directional transformer-decoder

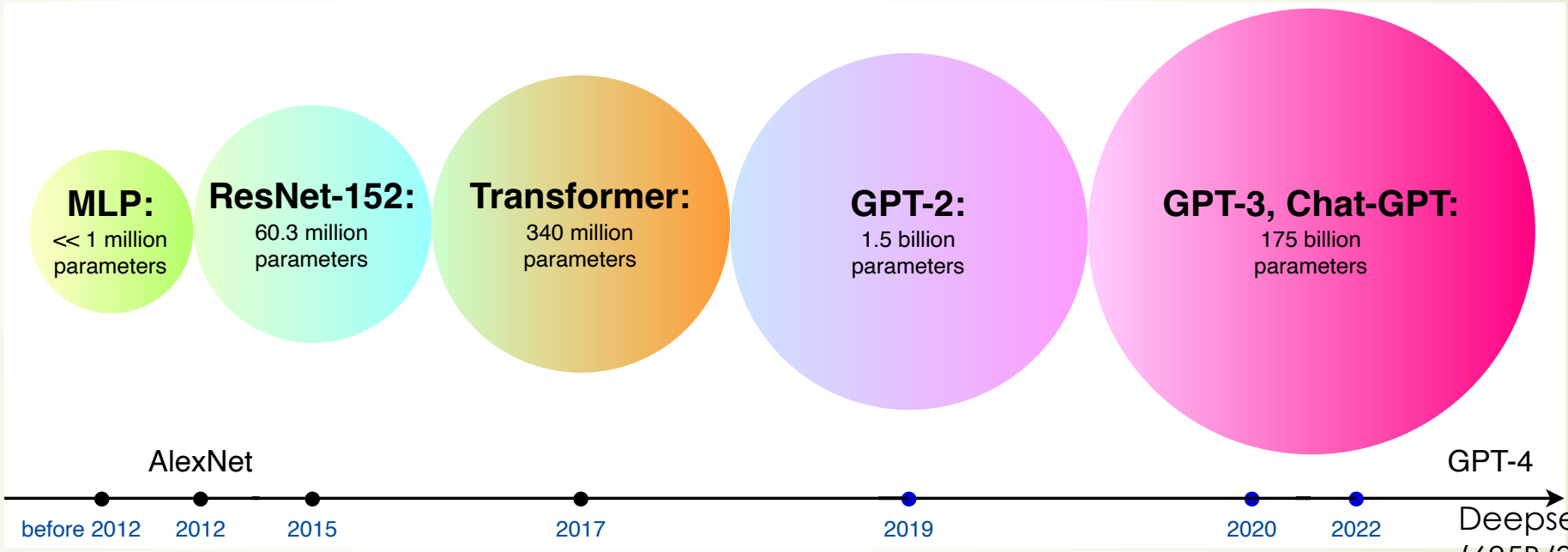
- 2018's GPT was a big success in pretraining a decoder!
  - Transformer decoder with 12 layers.
  - 768-dimensional hidden states, 3072-dimensional feed-forward hidden layers.
  - Byte-pair encoding with 40,000 merges
  - Trained on BooksCorpus: over 7000 unique books.
    - Contains long spans of contiguous text, for learning long-distance dependencies.
- GPT-3 (2020) and GPT-3.5 (ChatGPT 2022) has 175 billion parameters or more
- Llama3.1: > 400 billion parameters
- Deepseek-v3: > 600 billion parameters



Decoders

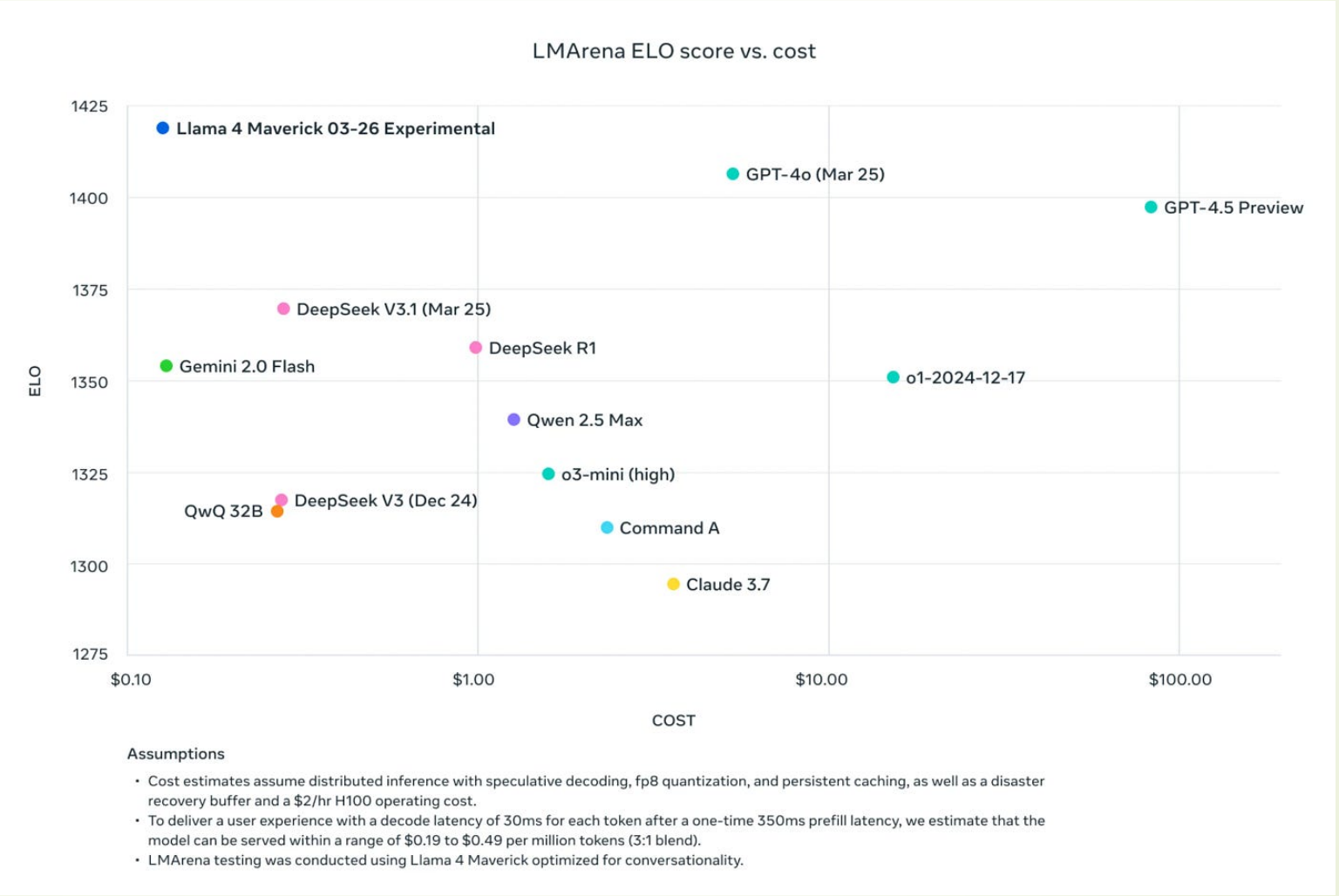
- Language models! What we've seen so far.
- Nice to generate from; can't condition on future words

Model size increases

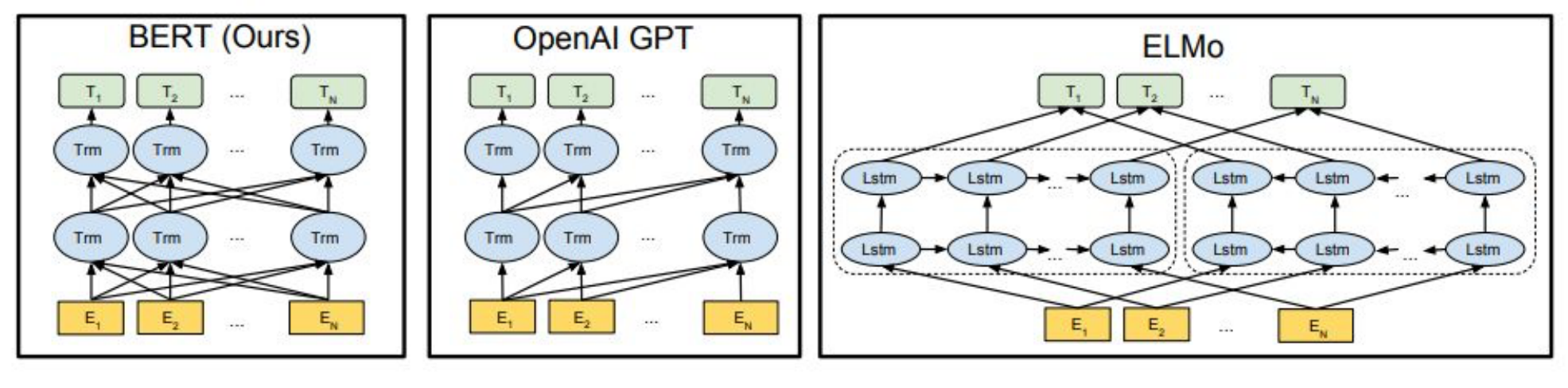


Deepseek-v3 (685B/37B)
Llamma 4 (Maverick 400B/17B)

LMArena score vs. Cost

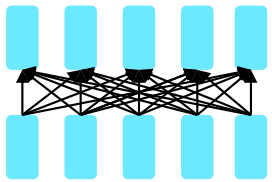


How about bi-directional transformers? – BERT



BERT: Devlin, Chang, Lee, Toutanova (2018)

- BERT (**Bidirectional Encoder Representations from Transformers**):
- Pre-training of Deep Bidirectional Transformers for Language Understanding, which is then fine-tuned for a task
- Want: truly bidirectional information flow without leakage in a deep model



Encoders

- Gets bidirectional context – can condition on future!
- Wait, how do we pretrain them?

Masked Language Model

- **Problem**: How the words see each other in bi-directions?
- **Solution**: Mask out *k*% of the input words, and then predict the masked words
  - We always use *k* = 15%

- Too little masking: Too expensive to train
- Too much masking: Not enough context

Masked LM

- **Problem**: Masked token never seen at fine-tuning
- **Solution**: 15% of the words to predict, but don't replace with [MASK] 100% of the time. Instead:
- 80% of the time, replace with [MASK]
  - went to the store → went to the [MASK]
- 10% of the time, replace random word
  - went to the store → went to the running
- 10% of the time, keep same
  - went to the store → went to the store

Next Sentence Prediction

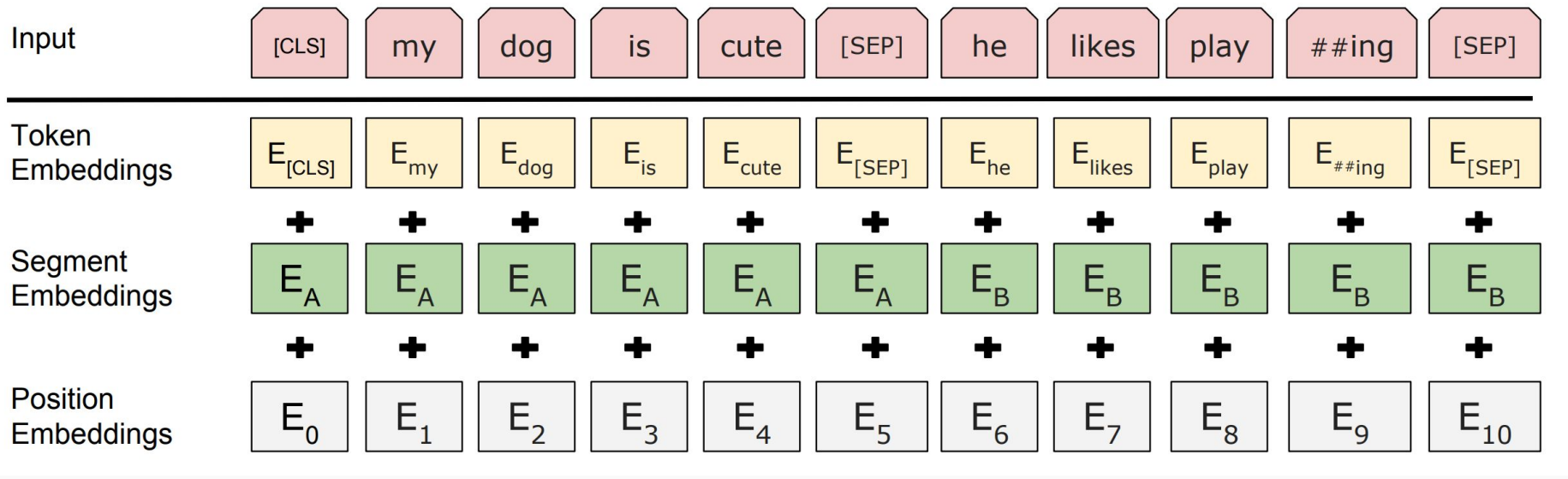
- To learn *relationships* between sentences, predict whether Sentence B is actual sentence that proceeds Sentence A, or a random sentence

Sentence A = `The man went to the store.`
Sentence B = `He bought a gallon of milk.`
Label = `IsNextSentence`

Sentence A = `The man went to the store.`
Sentence B = `Penguins are flightless.`
Label = `NotNextSentence`

BERT sentence pair encoding

- Token embeddings are word pieces (30k)
- Learned segmented embedding represents each sentence
- Positional embedding is as for other Transformer architectures

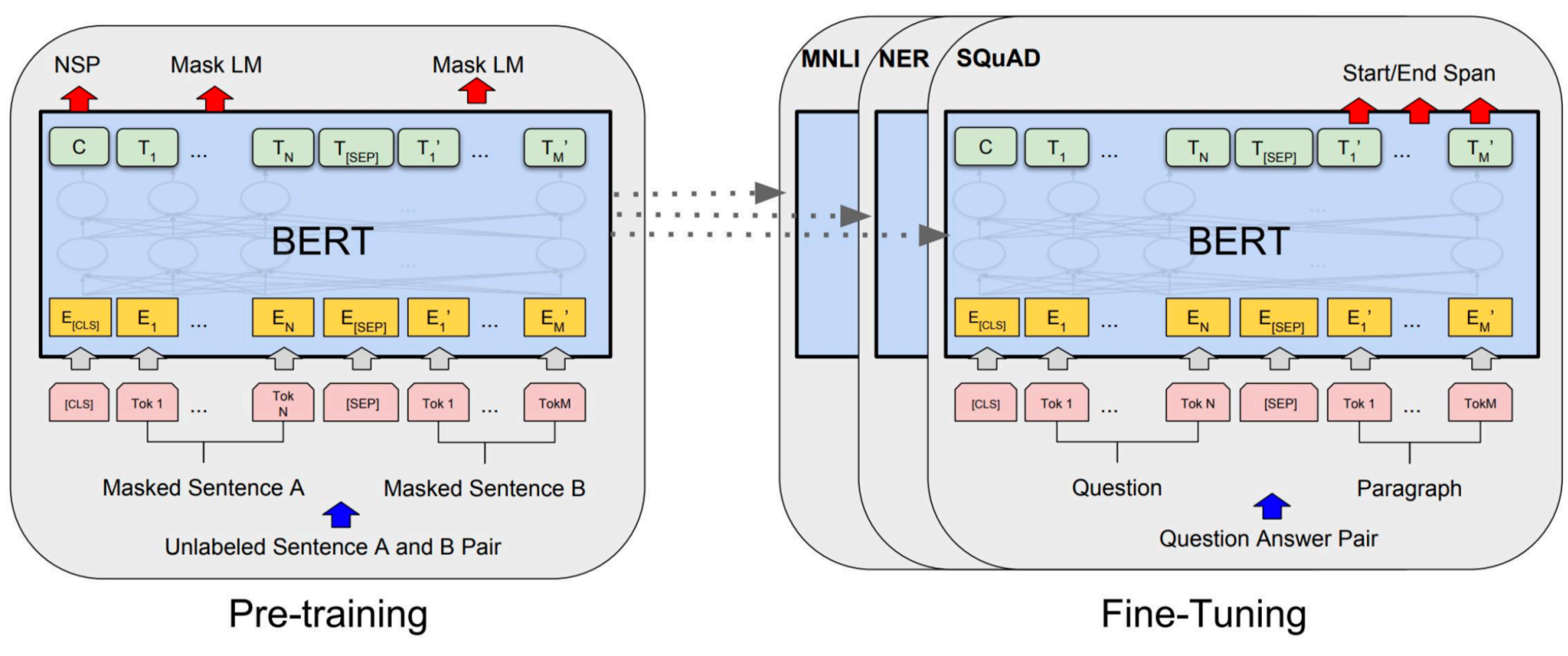


PreTraining

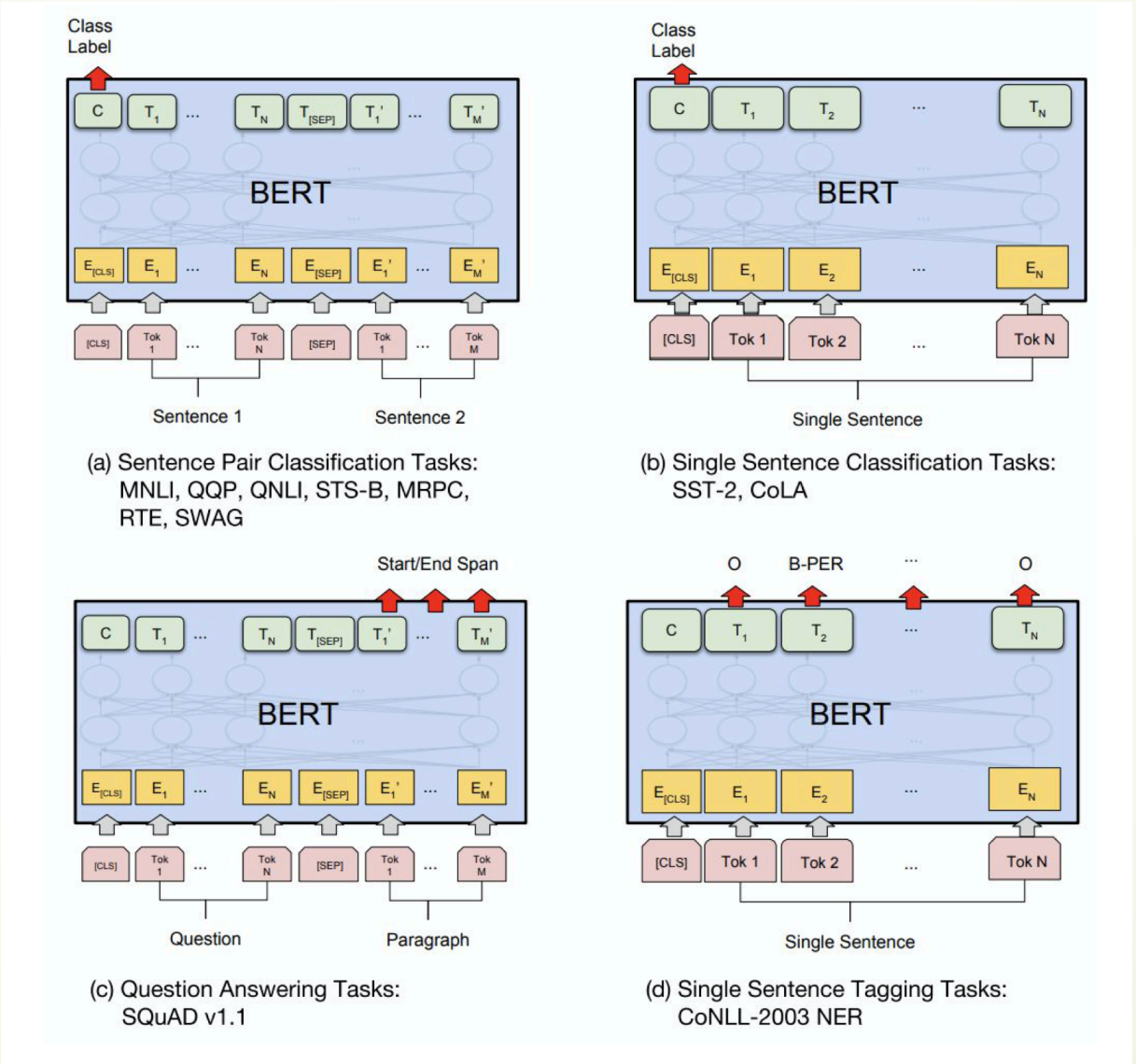
- 2 model released:
  - BERT-Base: 12-layer, 768-hidden, 12-head, 110 million params.
  - BERT-Large: 24-layer, 1024-hidden, 16-head, 340 million params.
- Training Data:
  - BookCorpus (800M words)
  - English Wikipedia (2.5B words)
- Batch Size: 131,072 words
  - (1024 sequences * 128 length or 256 sequences * 512 length)
- Training Time: 1M steps (~40 epochs)
- Optimizer: AdamW, 1e-4 learning rate, linear decay
- Trained on 4x4 or 8x8 TPU slice for 4 days
- Pretraining is expensive and impractical on a single GPU; Finetuning is practical and common on a single GPU

BERT model fine tuning

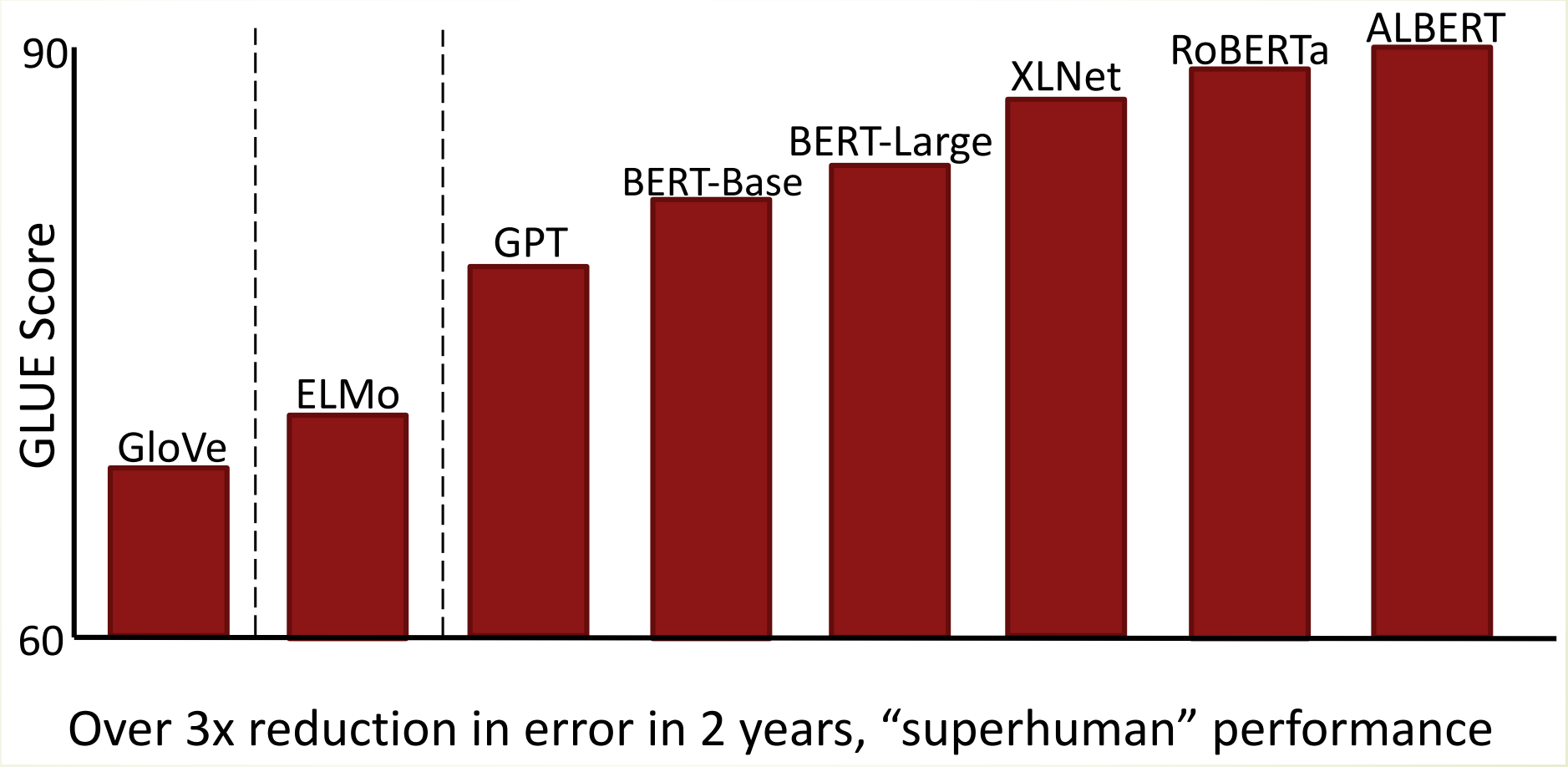
- Simply learn a classifier built on the top layer for each task that you fine tune for



BERT model fine tuning

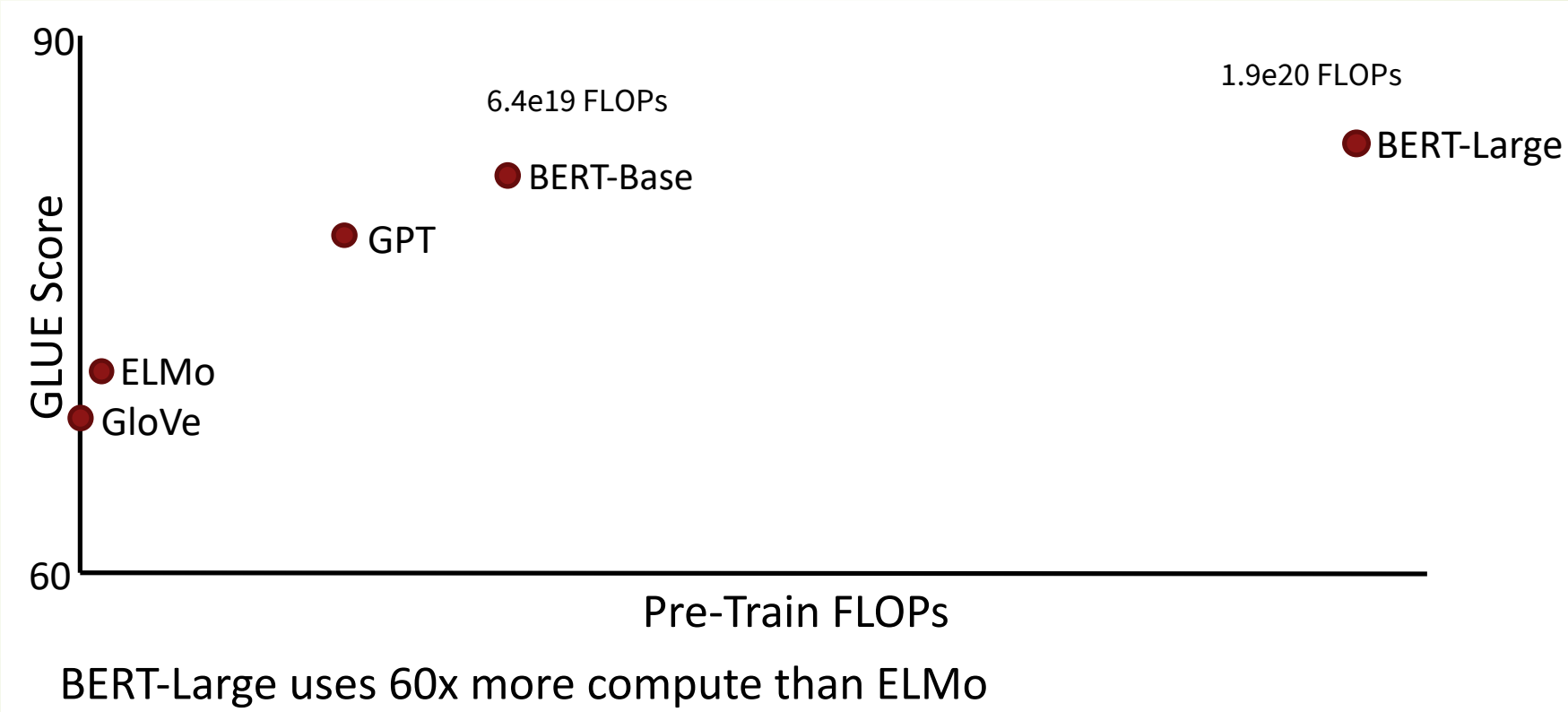


Rapid Progress for Pre-training (GLUE Benchmark)



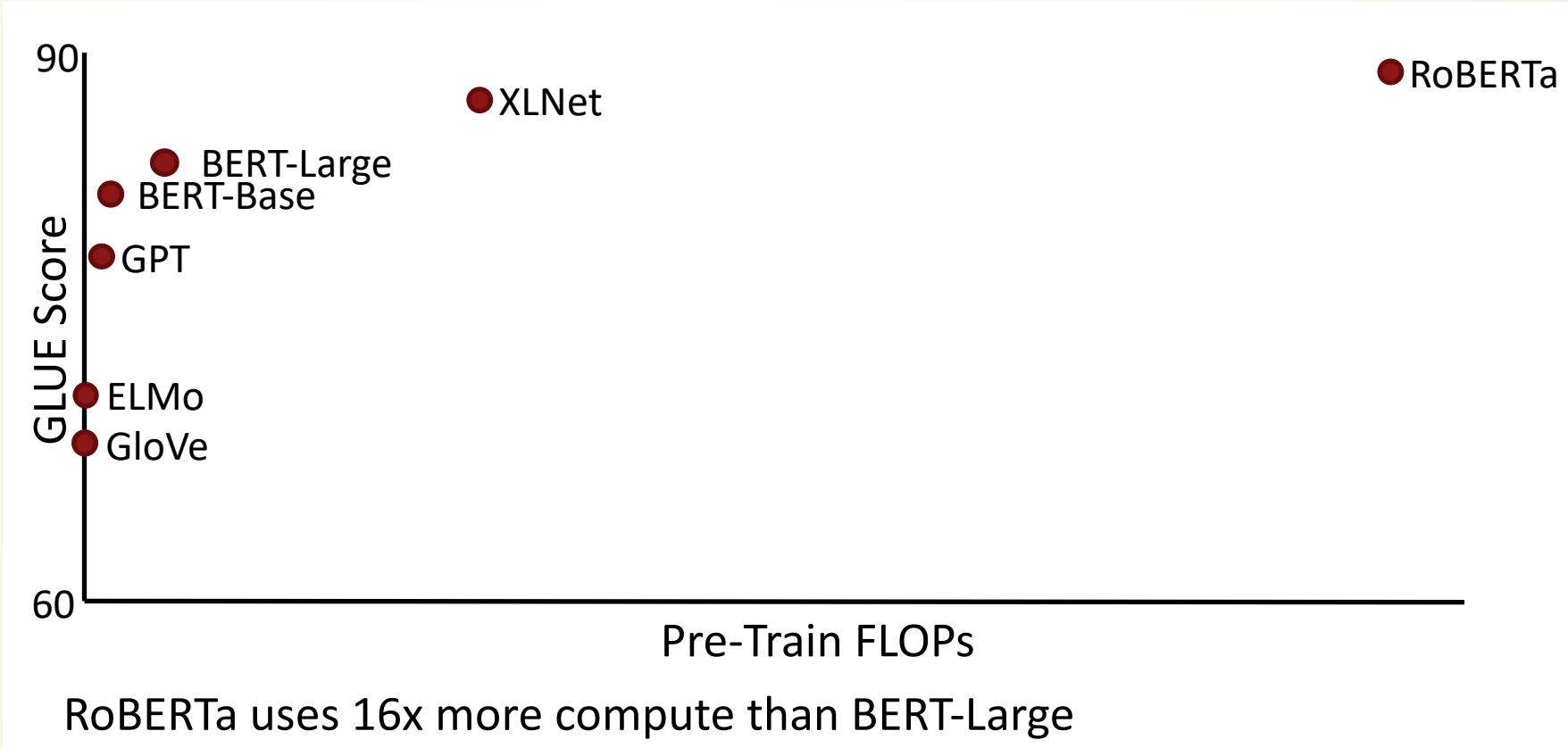
Over 3x reduction in error in 2 years, “superhuman” performance

But let's change the x-axis to computational cost…



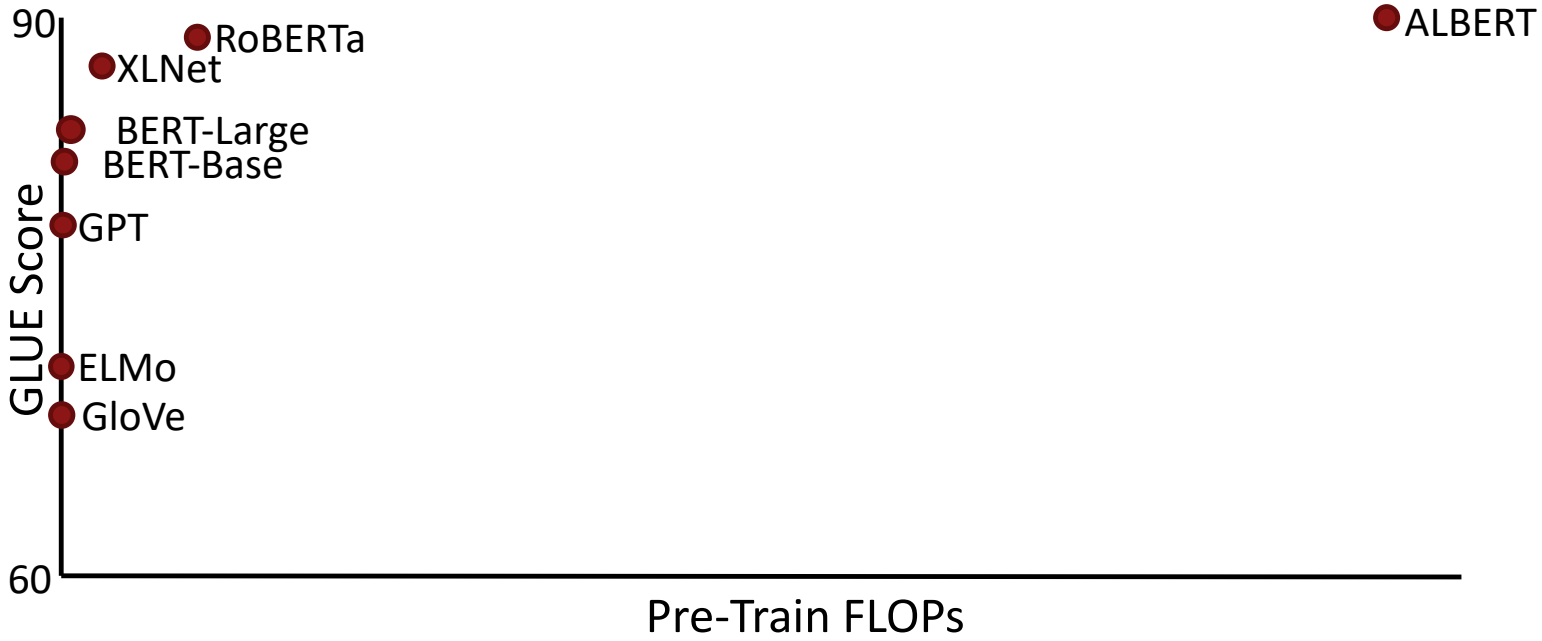
BERT-Large uses 60x more compute than ELMo

But let's change the x-axis to computational cost…



RoBERTa uses 16x more compute than BERT-Large

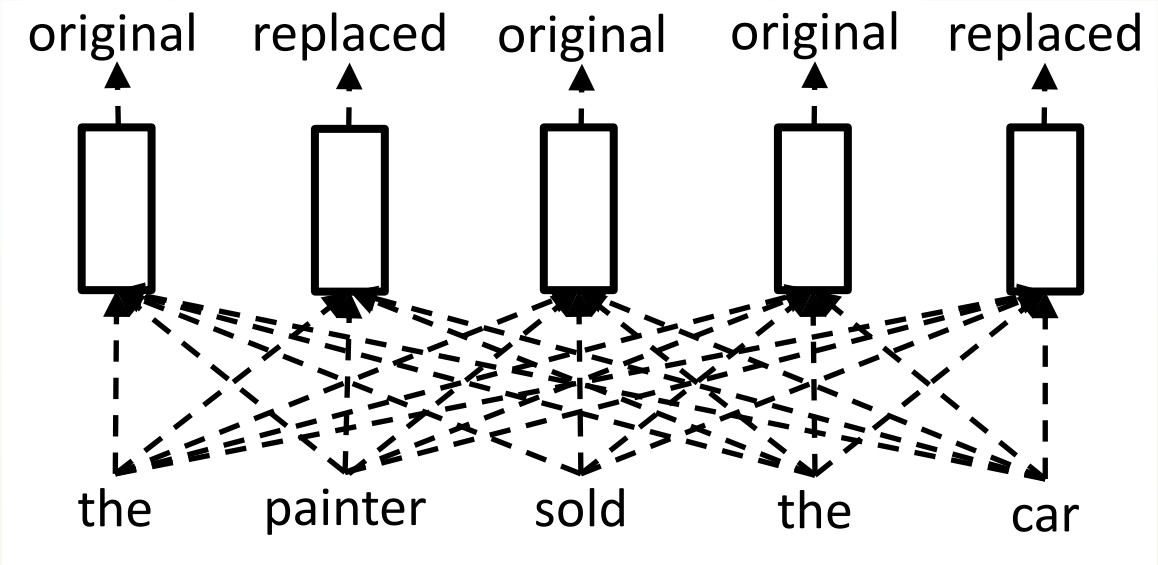
More compute, more better?



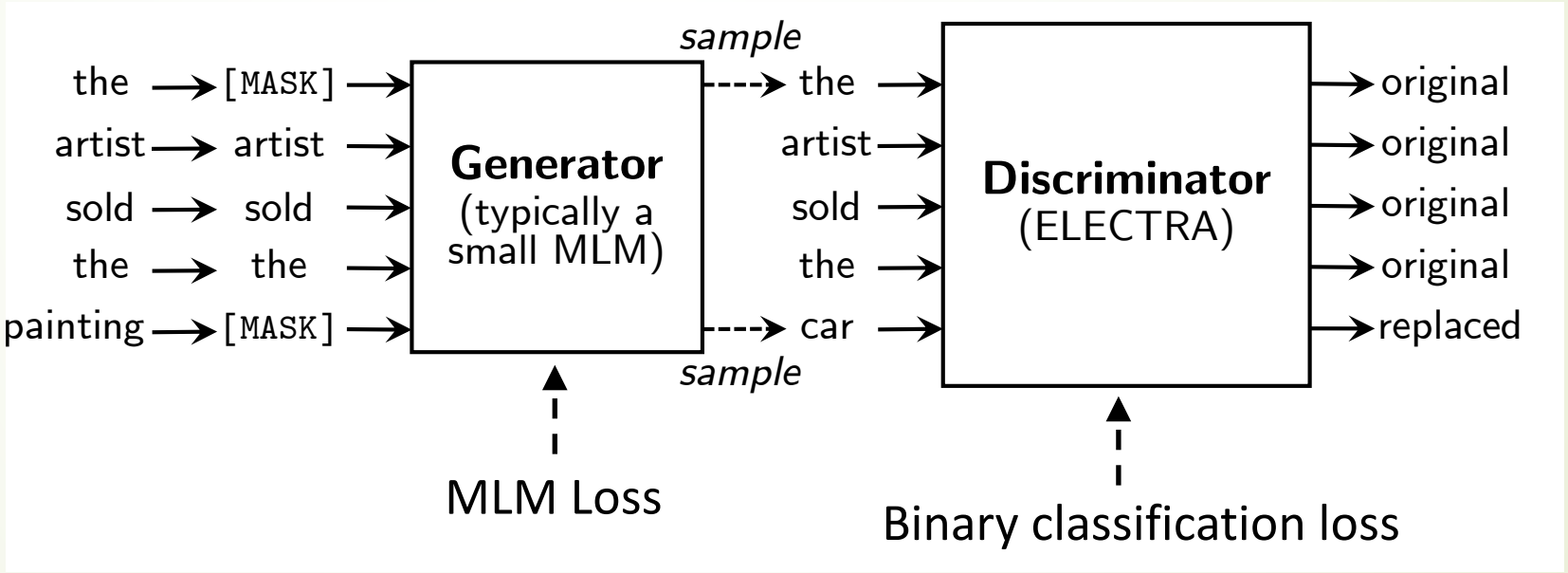
ALBERT uses 10x more compute than RoBERTa

ELECTRA: "Efficiently Learning an Encoder to Classify Token Replacements Accurately"

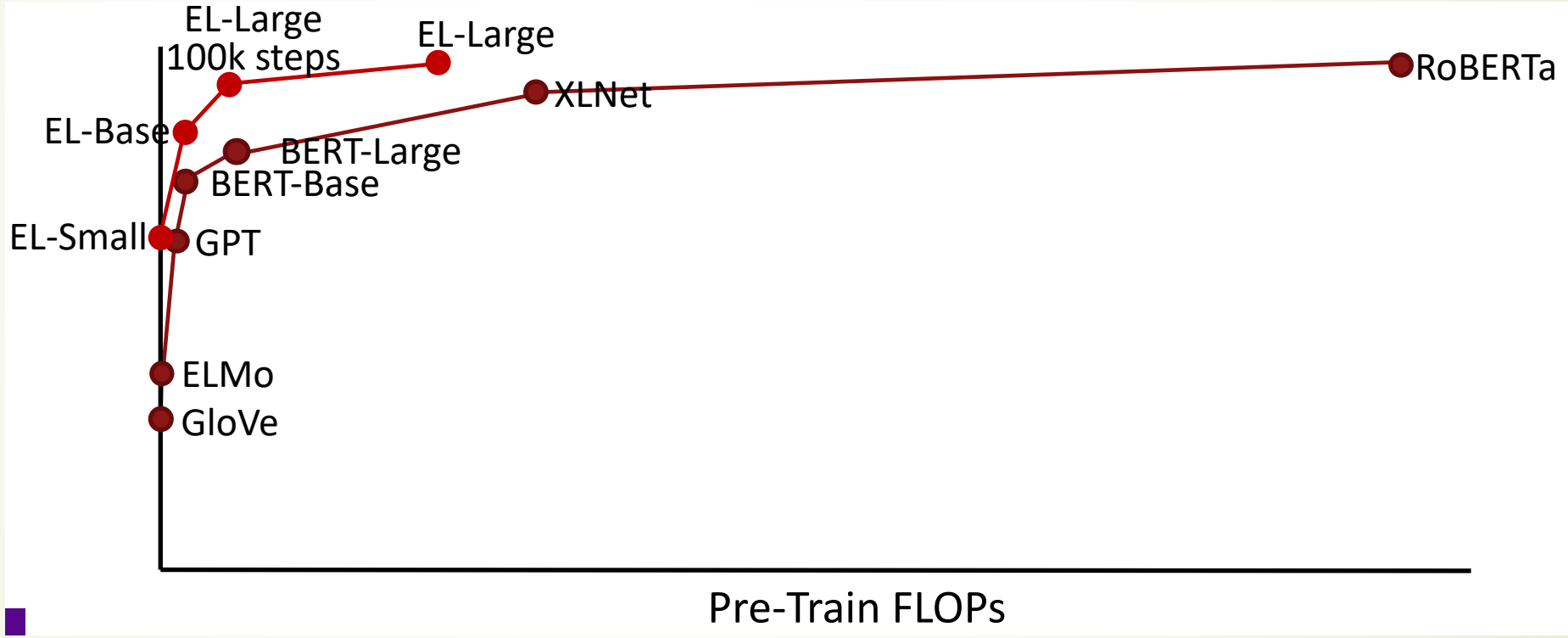
- Clark, Luong, Le, and Manning, ICLR 2020. https://openreview.net/pdf?id=r1xMH1BtvB
- Bidirectional model but learn from all tokens



Generating Replacements

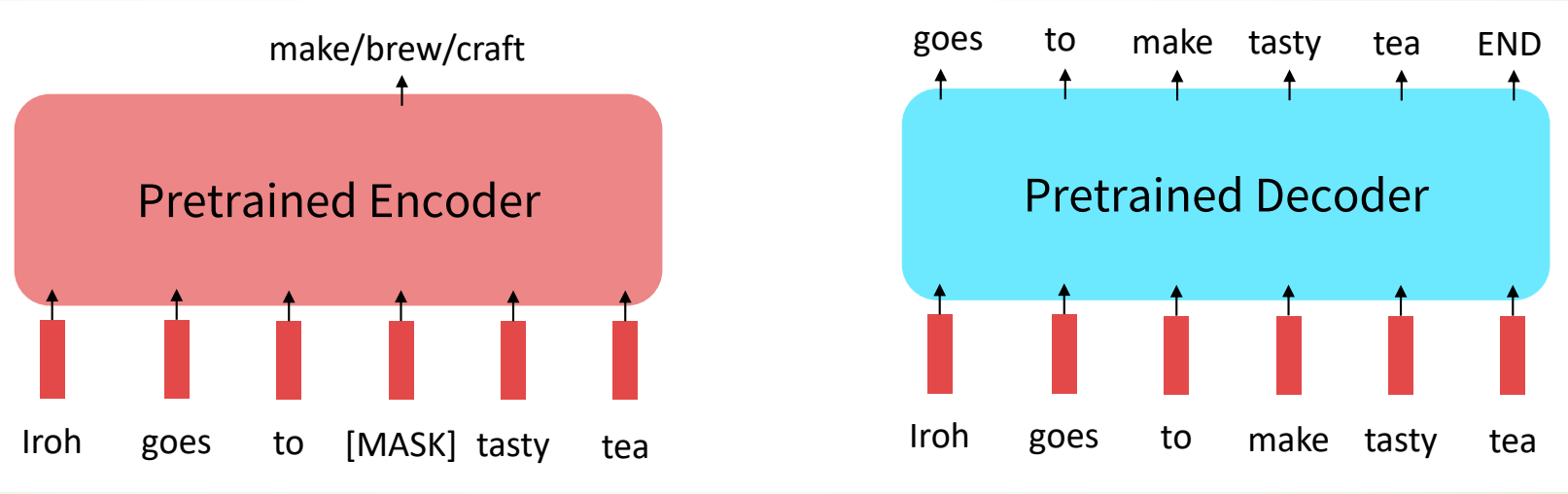


Results: GLUE Score vs Compute



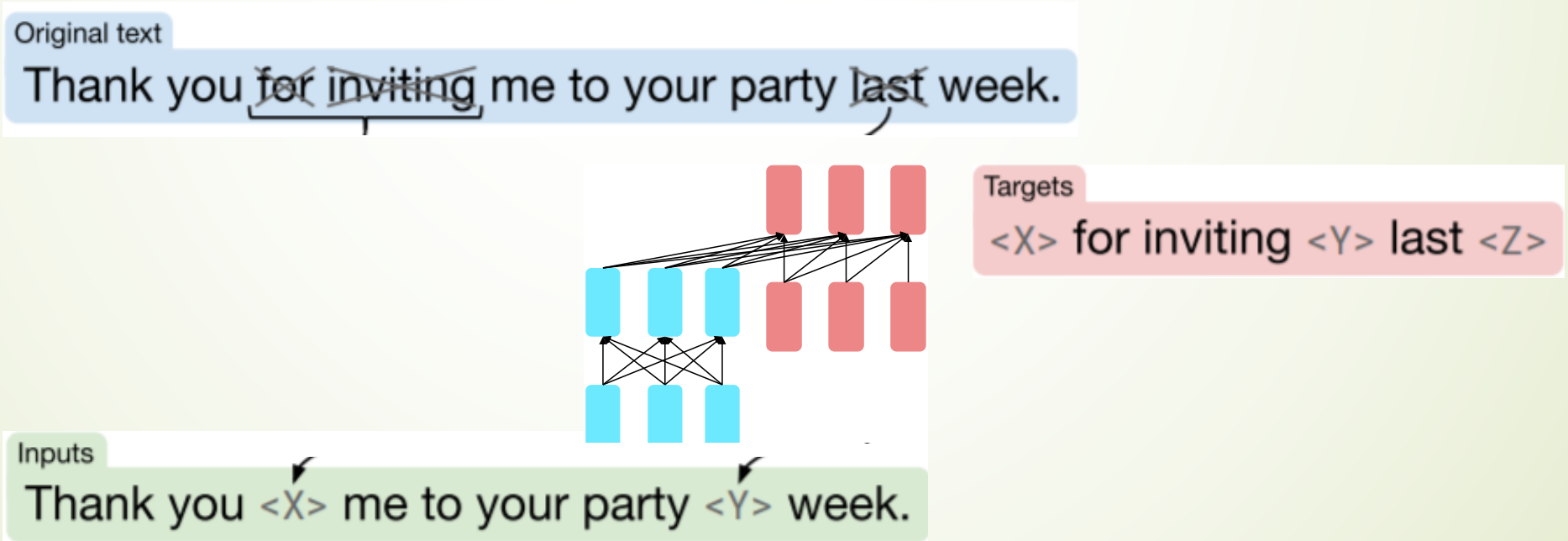
Limitations of Pretrained Encoders vs. Decoders

- BERT and other pretrained **encoders** are good for classifications, but don't naturally lead to nice autoregressive (1-word-at-a-time) generative methods.
- **Decoders** like GPT are good at generating sequences in autoregressive way.



Pretraining encoders-decoders: T5

- Pretraining encoder-decoders: what pretraining objective to use?
- What Raffel et al., 2018 found to work best was **span corruption**: **T5**.
- Replace different-length spans from the input with unique placeholders; decode out the spans that were removed!
- The largest T5 model had 11 billion parameters.

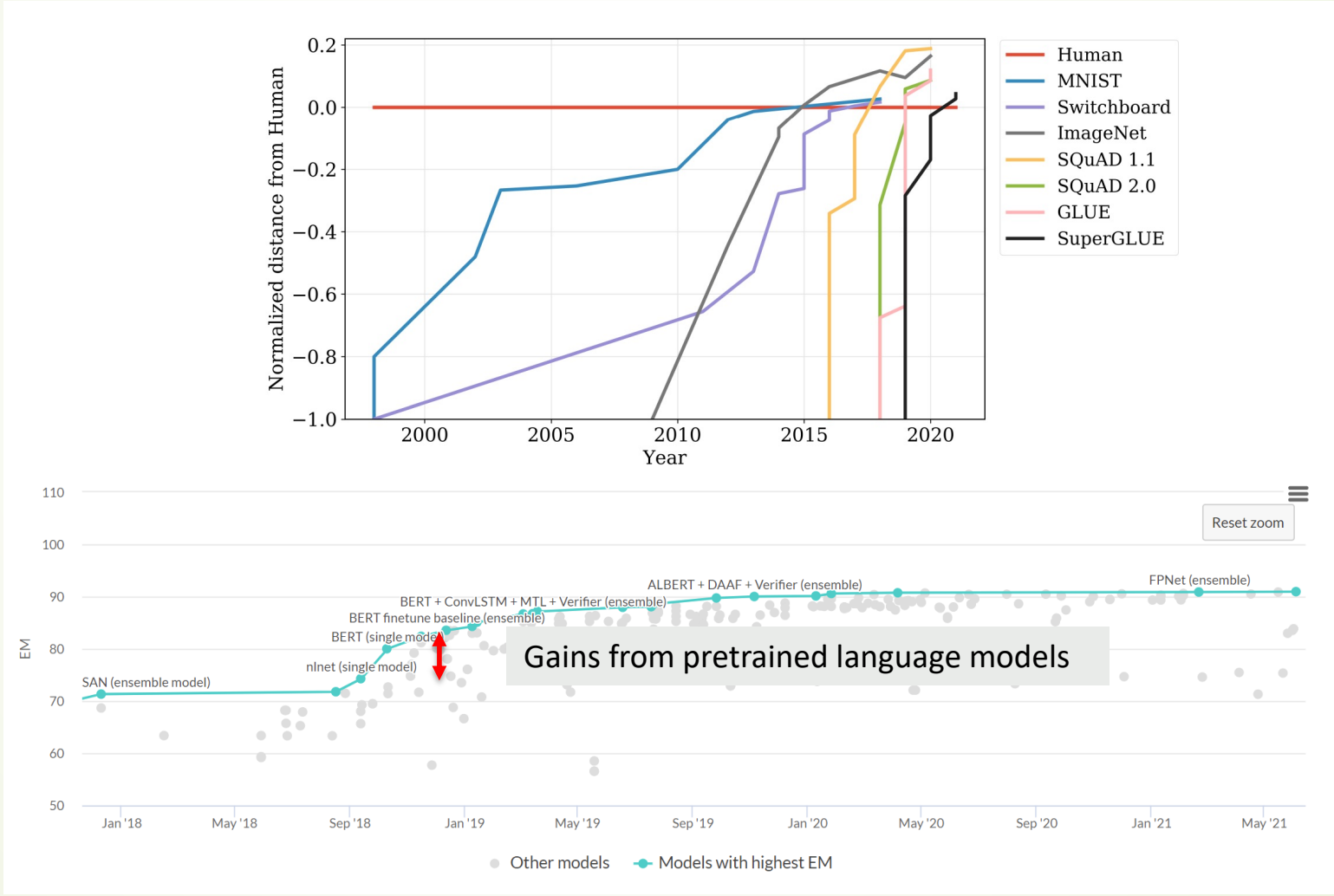


Transformers, In-context learning, and very large models

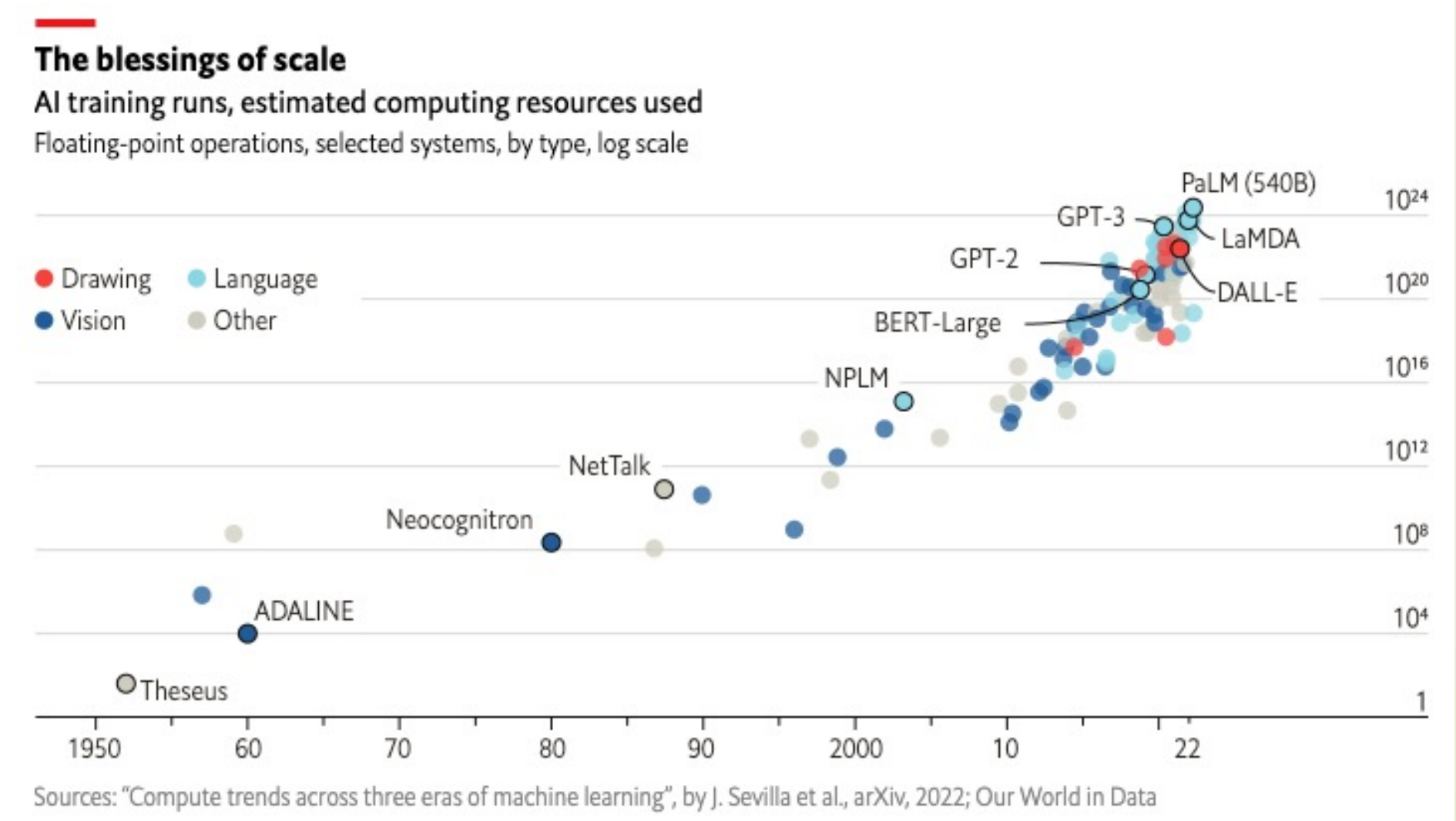
- So far, we've interacted with pretrained models in two ways:
  - Sample from the distributions they define (maybe providing a prompt)
  - Fine-tune them on a task we care about, and take their predictions.
- Very large language models seem to perform some kind of learning **without gradient steps** simply from examples you provide within their contexts.
- GPT-3 is the canonical example of this (Brown et al. NeurIPS 2020).
- Researchers try to interpret **in-context learning** of transformers as **nearest neighbor matching**.

Brown et al. Language models are few-shot learners. NeurIPS 2020.
Bai et al. Transformers as Statisticians. NeurIPS 2023.
Collins et al. In-Context Learning with Transformers: Softmax Attention Adapts to Function Lipschitzness. NeurIPS 2024.

Pretraining revolution



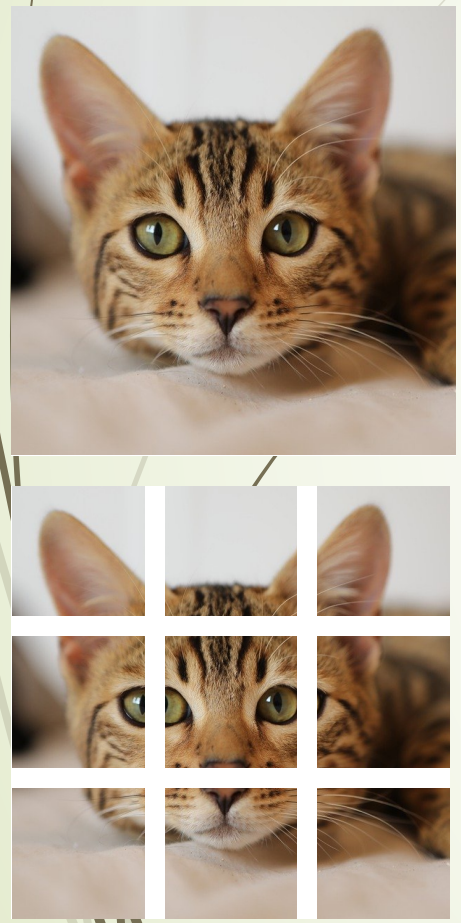
Exponential increase of computing



Vision Transformer

Transformer for images?

Vision Transformer (ViT)



Computer vision model with no convolutions!

Output vectors

Linear projection to C-dim vector of predicted class scores

Exact same as NLP Transformer!

Transformer

Add positional embedding: learned D-dim vector per position

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

Linear projection to D-dimensional vector

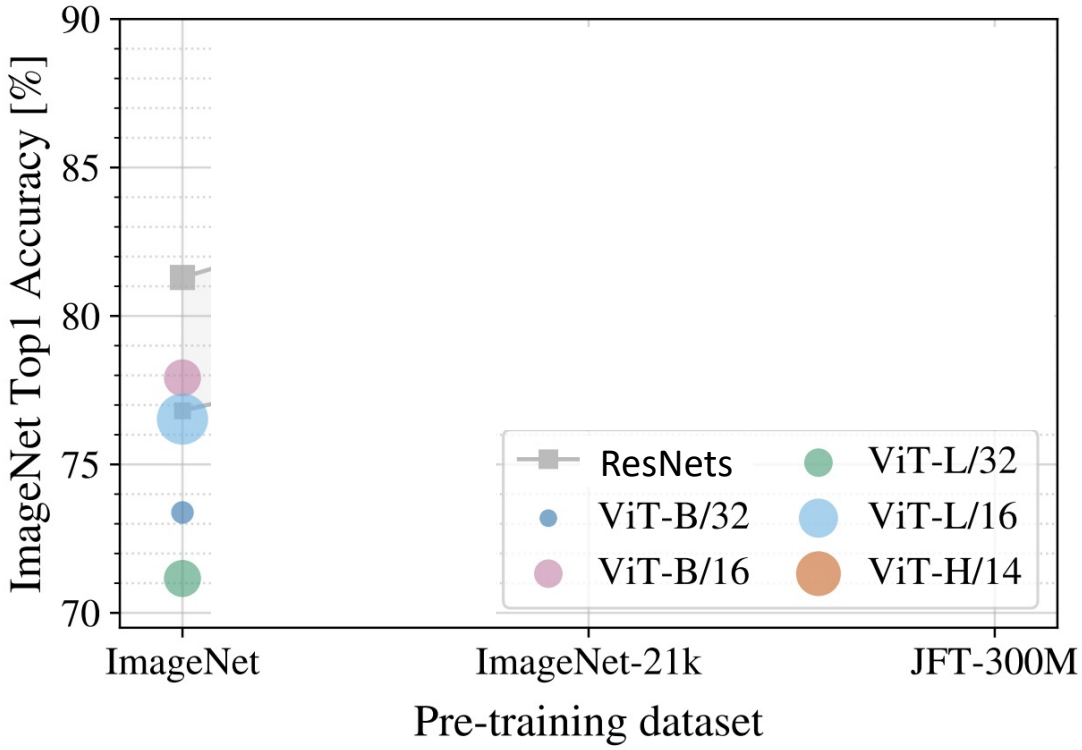
N input patches, each of shape 3x16x16

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

Vision Transformer (ViT) vs ResNets

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

When trained on ImageNet, ViT models perform worse than ResNets



B = Base
L = Large
H = Huge

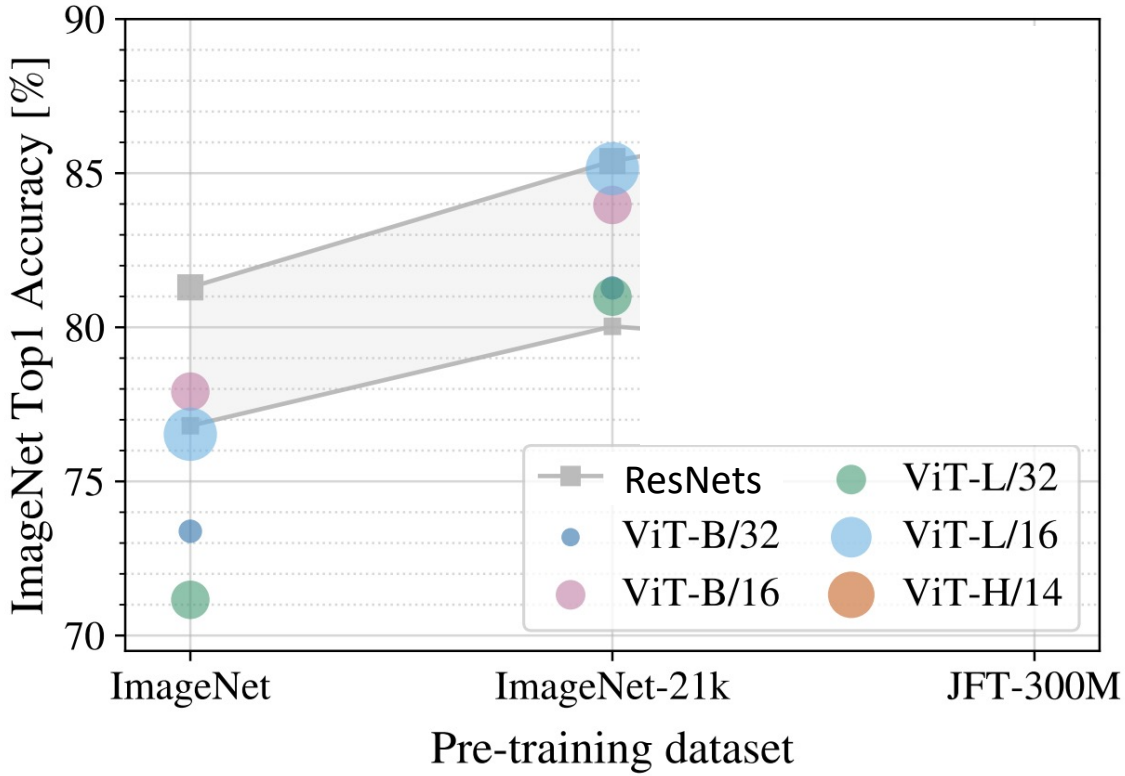
/32, /16, /14 is patch size; smaller patch size is a bigger model (more patches)

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

Vision Transformer (ViT) vs 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



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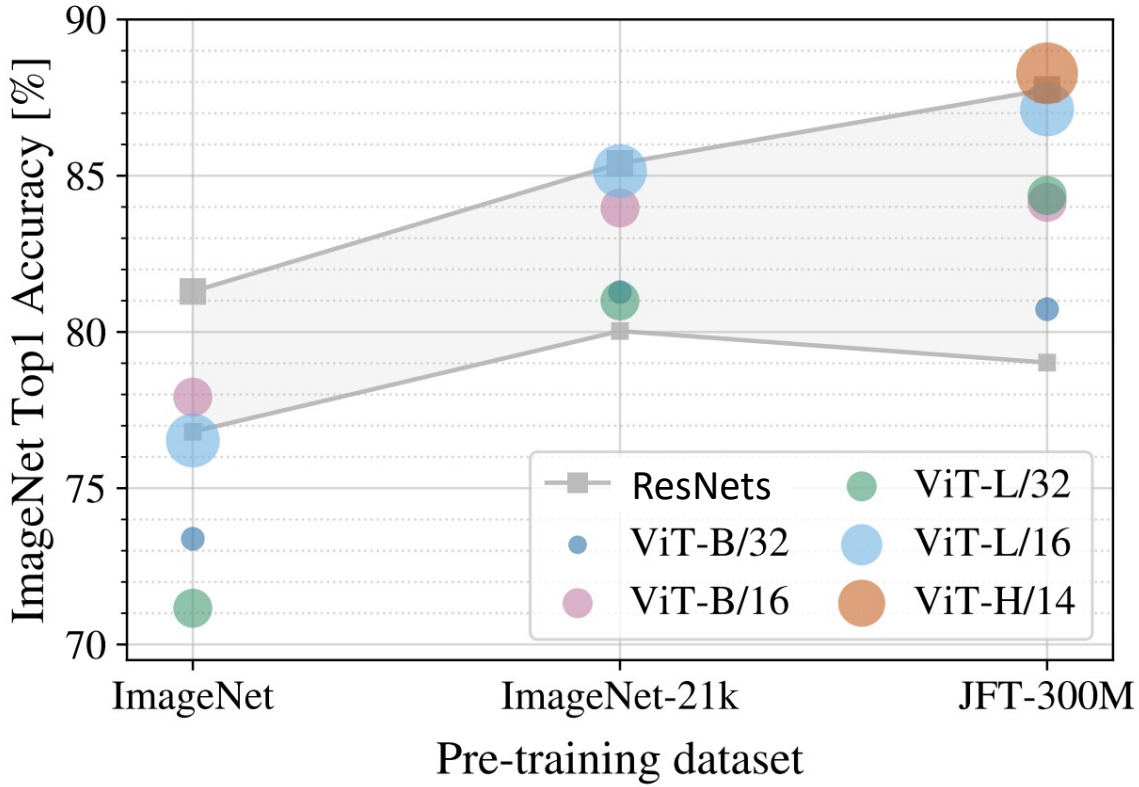
/32, /16, /14 is patch size; smaller patch size is a bigger model (more patches)

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

Vision Transformer (ViT) vs 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



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

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

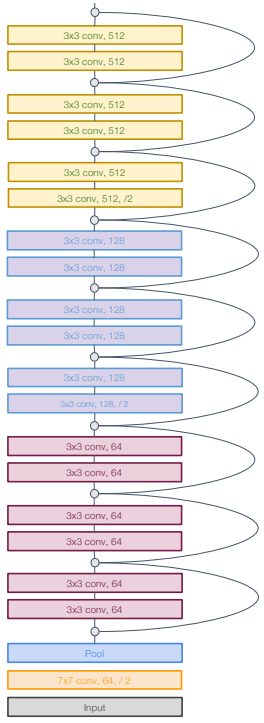
ViT vs CNN

Stage 3:
256 x 14 x 14

Stage 2:
128 x 28 x 28

Stage 1:
64 x 56 x 56

Input:
3 x 224 x 224

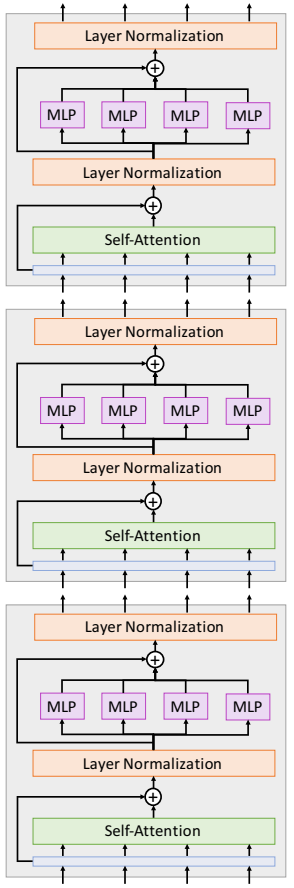


In most CNNs (including ResNets), **decrease** resolution and **increase** channels as you go deeper in the network (Hierarchical architecture)

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?



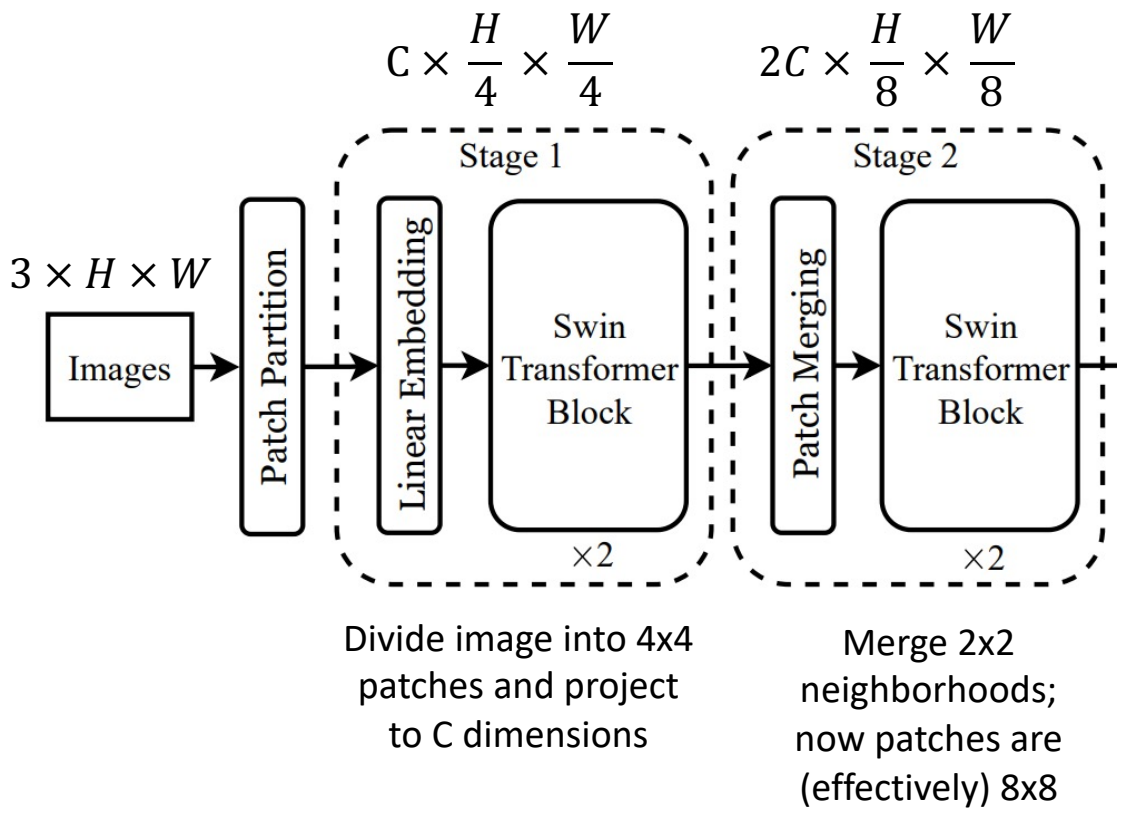
3rd block:
768 x 14 x 14

2nd block:
768 x 14 x 14

1st block:
768 x 14 x 14

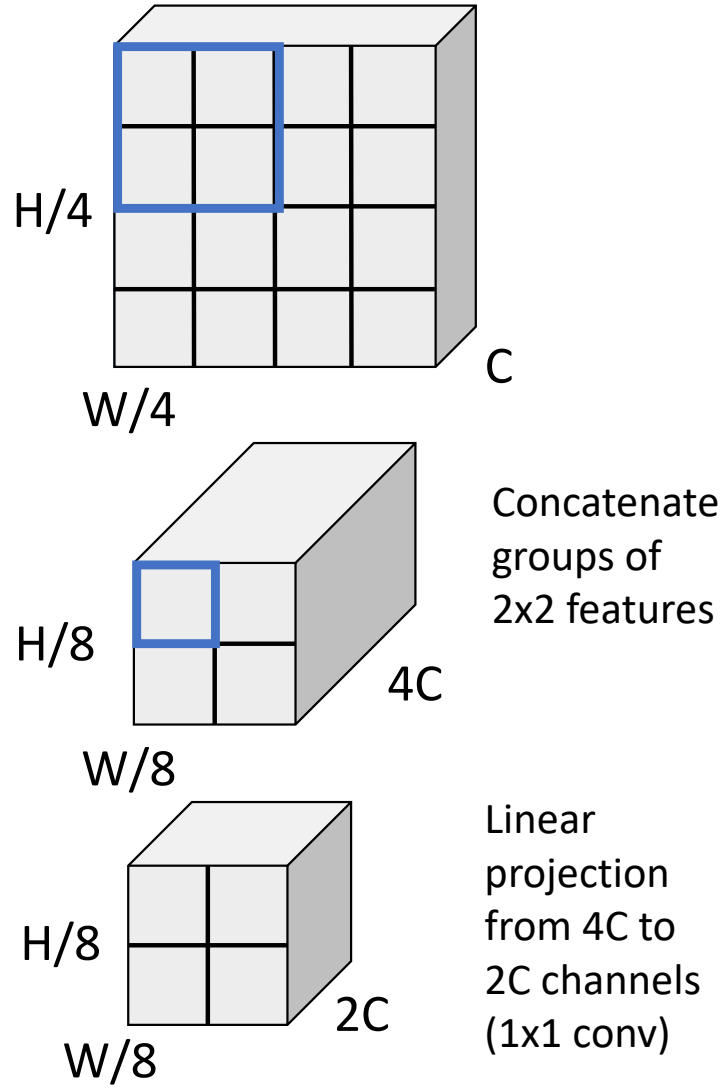
Input:
3 x 224 x 224

Hierarchical ViT: Swin Transformer



Divide image into 4x4 patches and project to C dimensions

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

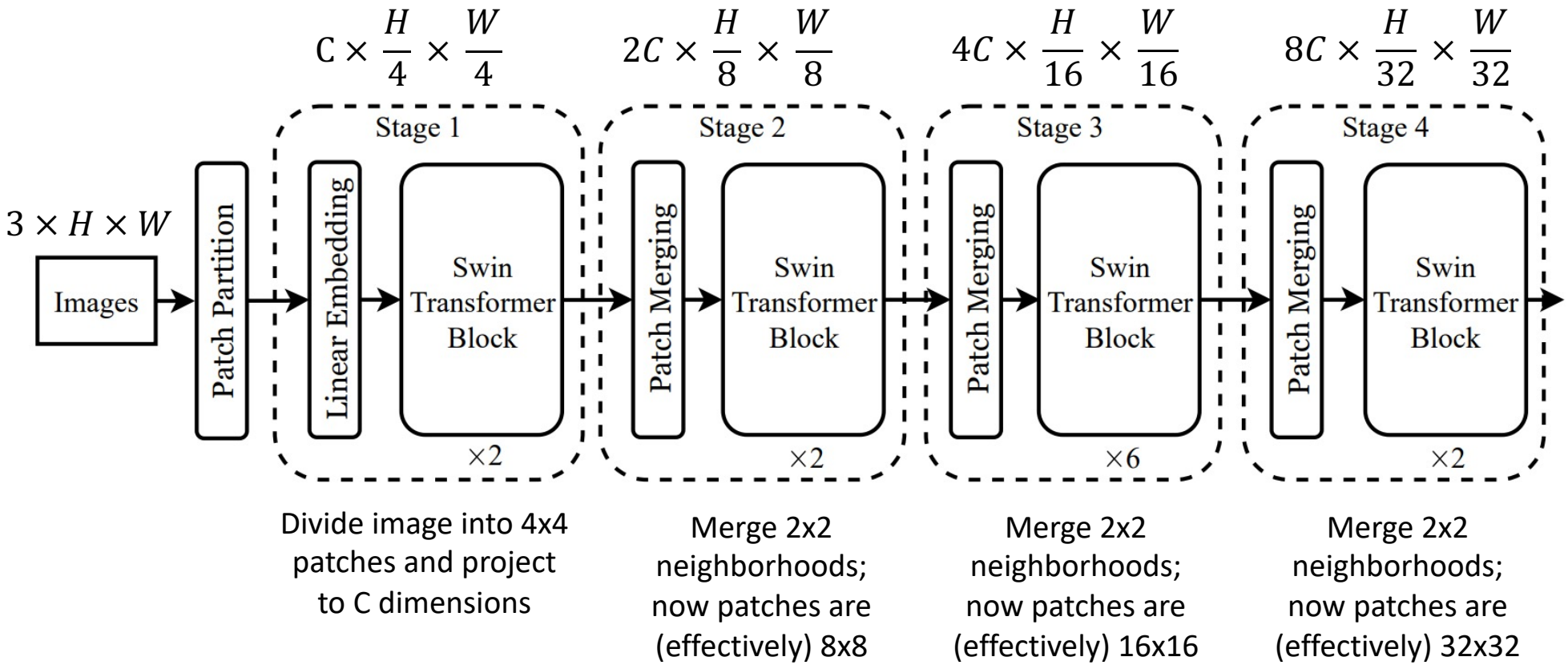


Concatenate groups of 2x2 features

Linear projection from 4C to 2C channels (1x1 conv)

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

Hierarchical ViT: Swin Transformer



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

Swin Transformer: Window Attention

With H x W grid of **tokens**, each attention matrix is H^2W^2 – **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

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

Swin Transformer: Window Attention

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

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

Swin Transformer: Shifted Window Attention

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

Block L: Normal windows

Block L+1: Shifted Windows

Detail: Relative Positional Bias

ViT adds positional embedding to input tokens, encodes *absolute position* of each token in the image

Swin does not use positional embeddings, instead encodes *relative position* between patches when computing attention:

Attention with relative bias:

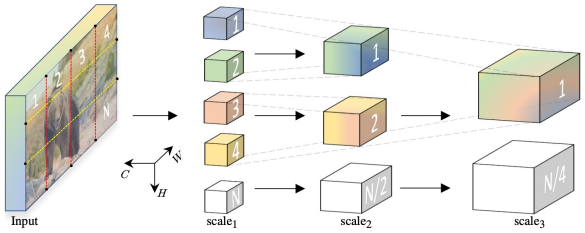
$$A = Softmax\left(\frac{QK^T}{\sqrt{D}} + B\right)V$$

$Q, K, V: M^2 \times D$ (Query, Key, Value)
$B: M^2 \times M^2$ (learned biases)

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

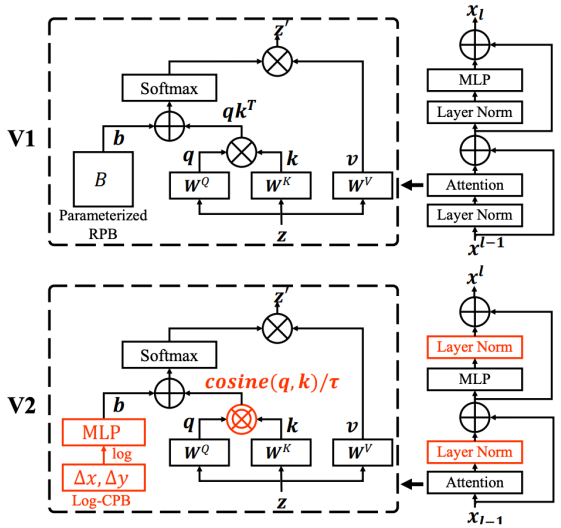
Other Hierarchical Vision Transformers

MViT



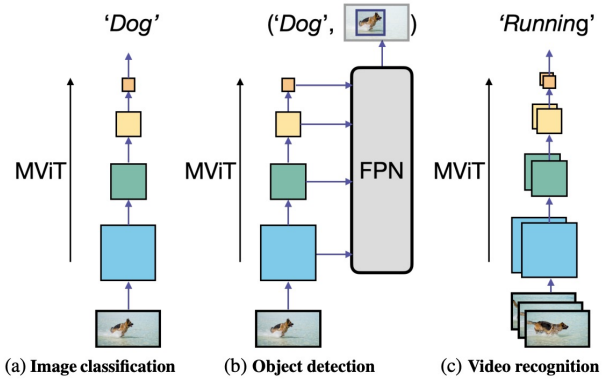
Fan et al, “Multiscale Vision Transformers”, ICCV 2021

Swin-V2



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

Thank you!