# Natural Language Processing with Deep Learning CS224N/Ling284



John Hewitt

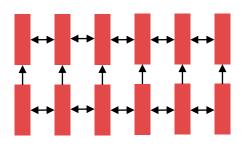
Lecture 9: Self-Attention and Transformers

#### **Lecture Plan**

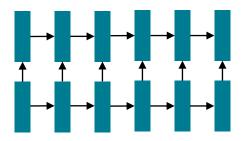
- 1. From recurrence (RNN) to attention-based NLP models
- 2. Introducing the Transformer model
- 3. Great results with Transformers
- 4. Drawbacks and variants of Transformers

## As of last week: recurrent models for (most) NLP!

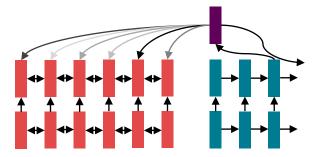
 Circa 2016, the de facto strategy in NLP is to encode sentences with a bidirectional LSTM: (for example, the source sentence in a translation)



 Define your output (parse, sentence, summary) as a sequence, and use an LSTM to generate it.

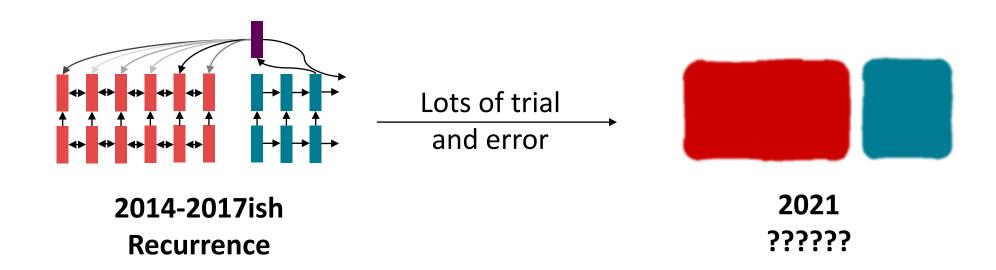


 Use attention to allow flexible access to memory



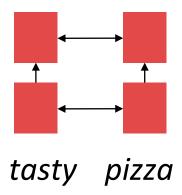
# Today: Same goals, different building blocks

- Last week, we learned about sequence-to-sequence problems and encoder-decoder models.
- Today, we're not trying to motivate entirely new ways of looking at problems (like Machine Translation)
- Instead, we're trying to find the best building blocks to plug into our models and enable broad progress.

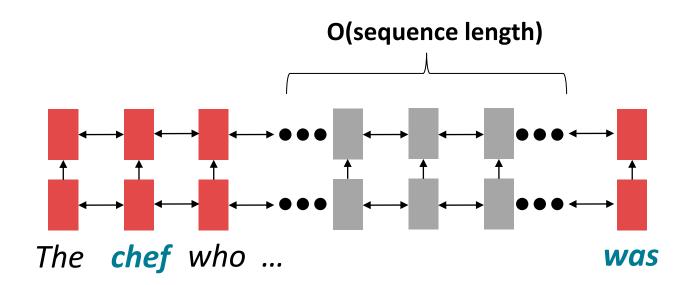


#### Issues with recurrent models: Linear interaction distance

- RNNs are unrolled "left-to-right".
- This encodes linear locality: a useful heuristic!
  - Nearby words often affect each other's meanings

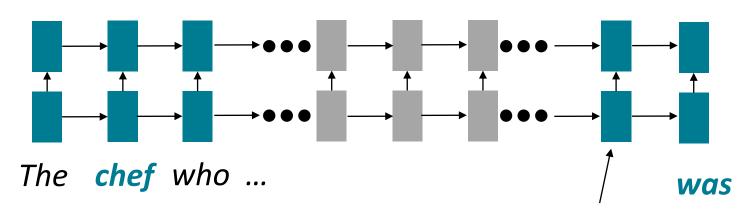


 Problem: RNNs take O(sequence length) steps for distant word pairs to interact.



#### Issues with recurrent models: Linear interaction distance

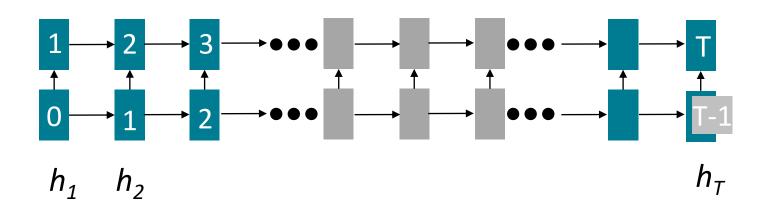
- O(sequence length) steps for distant word pairs to interact means:
  - Hard to learn long-distance dependencies (because gradient problems!)
  - Linear order of words is "baked in"; we already know linear order isn't the right way to think about sentences...



Info of *chef* has gone through O(sequence length) many layers!

## Issues with recurrent models: Lack of parallelizability

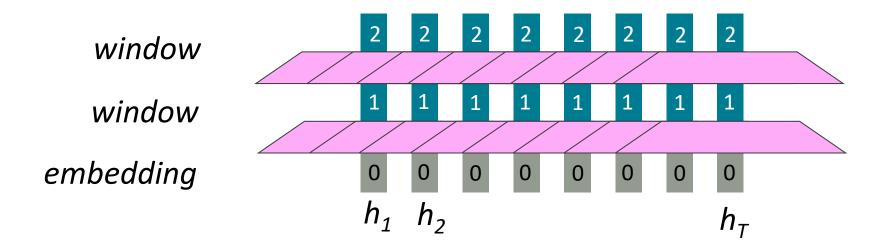
- Forward and backward passes have O(sequence length)
  unparallelizable operations
  - GPUs can perform a bunch of independent computations at once!
  - But future RNN hidden states can't be computed in full before past RNN hidden states have been computed
  - Inhibits training on very large datasets!



Numbers indicate min # of steps before a state can be computed

#### If not recurrence, then what? How about word windows?

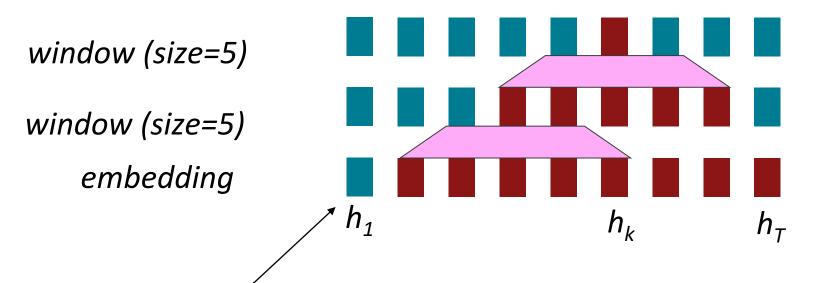
- Word window models aggregate local contexts
  - (Also known as 1D convolution; we'll go over this in depth later!)
  - Number of unparallelizable operations does not increase sequence length!



Numbers indicate min # of steps before a state can be computed

#### If not recurrence, then what? How about word windows?

- Word window models aggregate local contexts
- What about long-distance dependencies?
  - Stacking word window layers allows interaction between farther words
- Maximum Interaction distance = sequence length / window size
  - (But if your sequences are too long, you'll just ignore long-distance context)

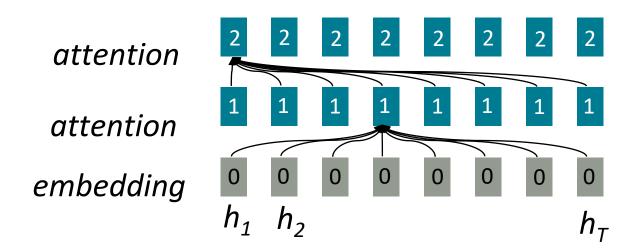


Red states indicate those "visible" to h<sub>k</sub>

Too far from h<sub>k</sub> to be considered

#### If not recurrence, then what? How about attention?

- Attention treats each word's representation as a query to access and incorporate information from a set of values.
  - We saw attention from the **decoder** to the **encoder**; today we'll think about attention **within a single sentence**.
- Number of unparallelizable operations does not increase sequence length.
- Maximum interaction distance: O(1), since all words interact at every layer!



All words attend to all words in previous layer; most arrows here are omitted

#### **Self-Attention**

- Recall: Attention operates on queries, keys, and values.
  - We have some queries  $q_1, q_2, ..., q_T$ . Each query is  $q_i \in \mathbb{R}^d$
  - We have some **keys**  $k_1, k_2, ..., k_T$ . Each key is  $k_i \in \mathbb{R}^d$
  - We have some **values**  $v_1, v_2, ..., v_T$ . Each value is  $v_i \in \mathbb{R}^d$

The number of queries can differ from the number of keys and values in practice.

- In **self-attention**, the queries, keys, and values are drawn from the same source.
  - For example, if the output of the previous layer is  $x_1, ..., x_T$ , (one vec per word) we could let  $v_i = k_i = q_i = x_i$  (that is, use the same vectors for all of them!)
- The (dot product) self-attention operation is as follows:

$$e_{ij} = q_i^{\mathsf{T}} k_j$$

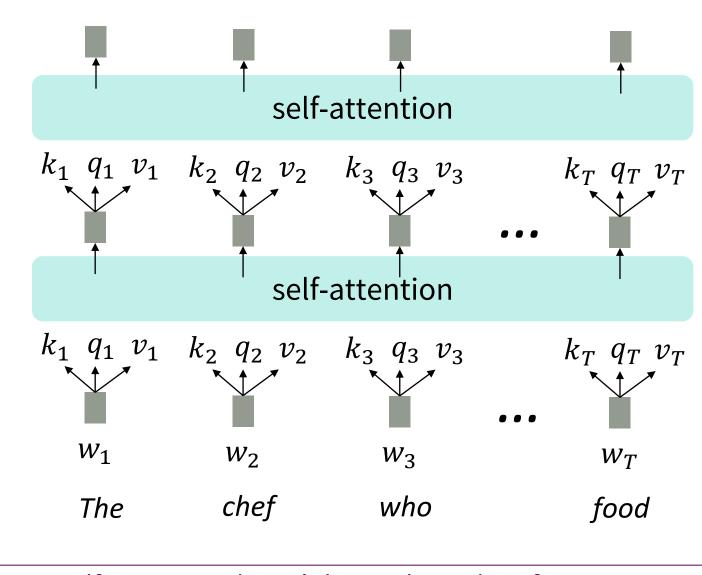
$$\alpha_{ij} = \frac{\exp(e_{ij})}{\sum_{j'} \exp(e_{ij'})}$$

$$output_i = \sum_j \alpha_{ij} v_j$$

Compute outputs as weighted sum of **values** 

# Self-attention as an NLP building block

- In the diagram at the right, we have stacked self-attention blocks, like we might stack LSTM layers.
- Can self-attention be a drop-in replacement for recurrence?
- No. It has a few issues, which we'll go through.
- First, self-attention is an operation on sets. It has no inherent notion of order.



Self-attention doesn't know the order of its inputs.

## Barriers and solutions for Self-Attention as a building block

#### **Barriers**

Solutions

 Doesn't have an inherent notion of order!

# Fixing the first self-attention problem: sequence order

- Since self-attention doesn't build in order information, we need to encode the order of the sentence in our keys, queries, and values.
- Consider representing each sequence index as a vector

$$p_i \in \mathbb{R}^d$$
, for  $i \in \{1,2,...,T\}$  are position vectors

- Don't worry about what the  $p_i$  are made of yet!
- Easy to incorporate this info into our self-attention block: just add the  $p_i$  to our inputs!
- Let  $\tilde{v}_i$   $\tilde{k}_i$ ,  $\tilde{q}_i$  be our old values, keys, and queries.

$$v_i = \tilde{v}_i + p_i$$

$$q_i = \tilde{q}_i + p_i$$

$$k_i = \tilde{k}_i + p_i$$

In deep self-attention networks, we do this at the first layer! You could concatenate them as well, but people mostly just add...

# Position representation vectors through sinusoids

• Sinusoidal position representations: concatenate sinusoidal functions of varying periods:

$$p_i = \begin{pmatrix} \sin(i/10000^{2*1/d}) \\ \cos(i/10000^{2*1/d}) \\ \vdots \\ \sin(i/10000^{2*\frac{d}{2}/d}) \\ \cos(i/10000^{2*\frac{d}{2}/d}) \end{pmatrix}$$
 Index in the sequence

- Pros:
  - Periodicity indicates that maybe "absolute position" isn't as important
  - Maybe can extrapolate to longer sequences as periods restart!
- Cons:
  - Not learnable; also the extrapolation doesn't really work!

## Position representation vectors learned from scratch

• Learned absolute position representations: Let all  $p_i$  be learnable parameters! Learn a matrix  $p \in \mathbb{R}^{d \times T}$ , and let each  $p_i$  be a column of that matrix!

- Pros:
  - Flexibility: each position gets to be learned to fit the data
- Cons:
  - Definitely can't extrapolate to indices outside 1, ..., T.
- Most systems use this!
- Sometimes people try more flexible representations of position:
  - Relative linear position attention [Shaw et al., 2018]
  - Dependency syntax-based position [Wang et al., 2019]

# Barriers and solutions for Self-Attention as a building block

#### **Barriers**

- Doesn't have an inherent notion of order!

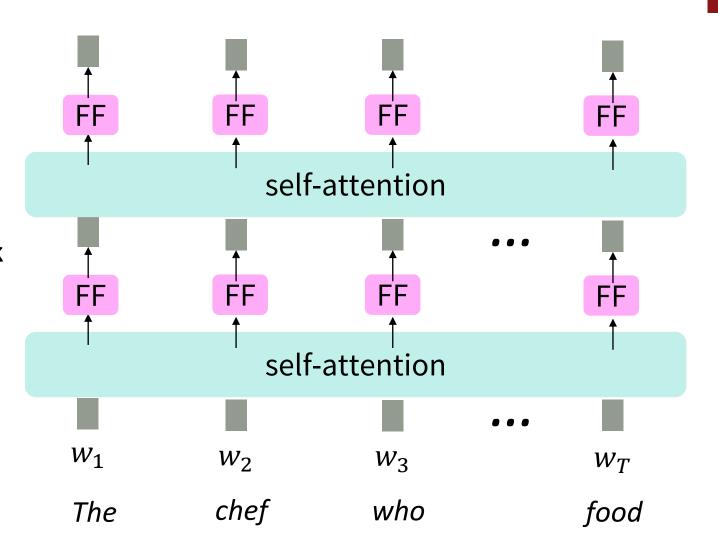
#### **Solutions**

 Add position representations to the inputs

# Adding nonlinearities in self-attention

- Note that there are no elementwise nonlinearities in self-attention; stacking more self-attention layers just re-averages value vectors
- Easy fix: add a feed-forward network to post-process each output vector.

$$m_i = MLP(\text{output}_i)$$
  
=  $W_2 * \text{ReLU}(W_1 \times \text{output}_i + b_1) + b_2$ 



Intuition: the FF network processes the result of attention

## Barriers and solutions for Self-Attention as a building block

#### **Barriers**

- Doesn't have an inherent notion of order!
- No nonlinearities for deep learning magic! It's all just weighted averages
- Need to ensure we don't "look at the future" when predicting a sequence
  - Like in machine translation
  - Or language modeling

#### **Solutions**

- Add position representations to the inputs
- Easy fix: apply the same feedforward network to each selfattention output.

# Masking the future in self-attention

 To use self-attention in decoders, we need to ensure we can't peek at the future.

 At every timestep, we could change the set of keys and queries to include only past words. (Inefficient!)

 To enable parallelization, we mask out attention to future words by setting attention scores to -∞. We can look at these (not greyed out) words

[START]

The chef who

[START]

For encoding these words

$$e_{ij} = \begin{cases} q_i^{\mathsf{T}} k_j, j < i \\ -\infty, j \ge i \end{cases}$$

[The matrix of  $e_{ij}$  values]

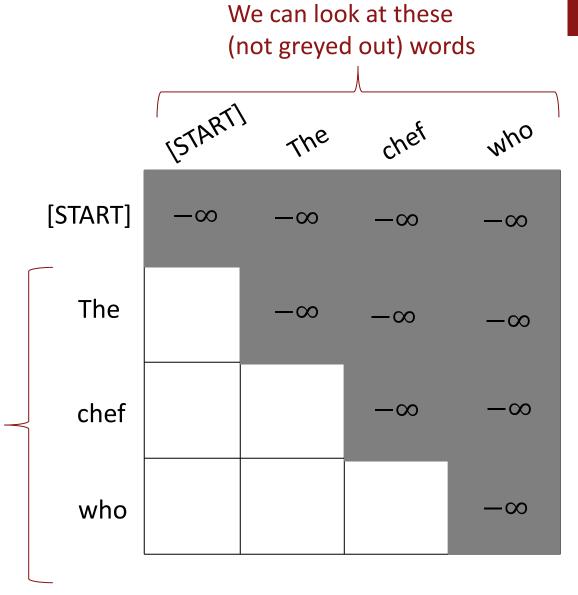
# Masking the future in self-attention

 To use self-attention in decoders, we need to ensure we can't peek at the future.

 At every timestep, we could change the set of keys and queries to include only past words. (Inefficient!)

 To enable parallelization, we mask out attention to future words by setting attention scores to -∞.

For encoding these words  $e_{ij} = \begin{cases} q_i^{\mathsf{T}} k_j, j < i \\ -\infty, j > i \end{cases}$ 



## Barriers and solutions for Self-Attention as a building block

#### **Barriers**

- Doesn't have an inherent notion of order!
- No nonlinearities for deep learning magic! It's all just weighted averages
- Need to ensure we don't "look at the future" when predicting a sequence
  - Like in machine translation
  - Or language modeling

#### **Solutions**

- Add position representations to the inputs
- Easy fix: apply the same feedforward network to each selfattention output.
- Mask out the future by artificially setting attention weights to 0!

#### Necessities for a self-attention building block:

#### Self-attention:

• the basis of the method.

#### Position representations:

• Specify the sequence order, since self-attention is an unordered function of its inputs.

#### Nonlinearities:

- At the output of the self-attention block
- Frequently implemented as a simple feed-forward network.

#### Masking:

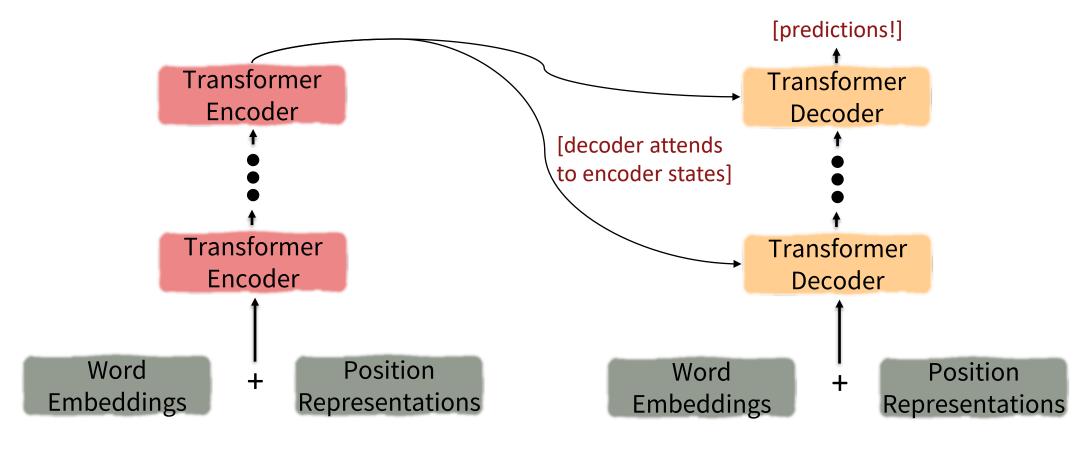
- In order to parallelize operations while not looking at the future.
- Keeps information about the future from "leaking" to the past.
- That's it! But this is not the Transformer model we've been hearing about.

#### **Outline**

- 1. From recurrence (RNN) to attention-based NLP models
- 2. Introducing the Transformer model
- 3. Great results with Transformers
- 4. Drawbacks and variants of Transformers

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

First, let's look at the Transformer Encoder and Decoder Blocks at a high level



[input sequence]

[output sequence]

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

Next, let's look at the Transformer Encoder and Decoder Blocks

What's left in a Transformer Encoder Block that we haven't covered?

- **1. Key-query-value attention:** How do we get the k, q, v vectors from a single word embedding?
- 2. Multi-headed attention: Attend to multiple places in a single layer!
- 3. Tricks to help with training!
  - 1. Residual connections
  - 2. Layer normalization
  - 3. Scaling the dot product
  - 4. These tricks **don't improve** what the model is able to do; they help improve the training process. Both of these types of modeling improvements are very important!

# The Transformer Encoder: Key-Query-Value Attention

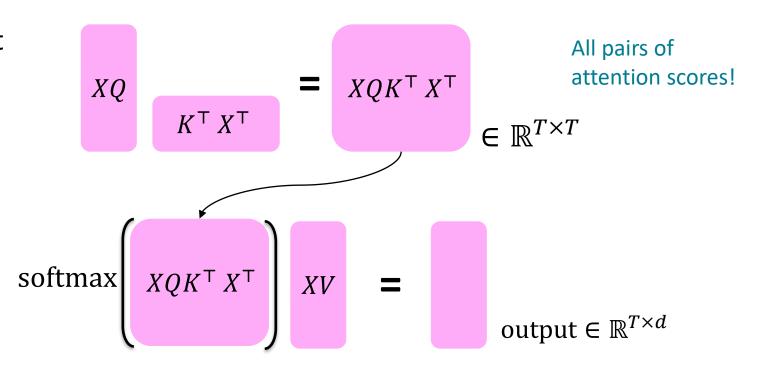
- We saw that self-attention is when keys, queries, and values come from the same source. The Transformer does this in a particular way:
  - Let  $x_1, ..., x_T$  be input vectors to the Transformer encoder;  $x_i \in \mathbb{R}^d$
- Then keys, queries, values are:
  - $k_i = Kx_i$ , where  $K \in \mathbb{R}^{d \times d}$  is the key matrix.
  - $q_i = Qx_i$ , where  $Q \in \mathbb{R}^{d \times d}$  is the query matrix.
  - $v_i = Vx_i$ , where  $V \in \mathbb{R}^{d \times d}$  is the value matrix.
- These matrices allow *different aspects* of the *x* vectors to be used/emphasized in each of the three roles.

## The Transformer Encoder: Key-Query-Value Attention

- Let's look at how key-query-value attention is computed, in matrices.
  - Let  $X = [x_1; ...; x_T] \in \mathbb{R}^{T \times d}$  be the concatenation of input vectors.
  - First, note that  $XK \in \mathbb{R}^{T \times d}$ ,  $XQ \in \mathbb{R}^{T \times d}$ ,  $XV \in \mathbb{R}^{T \times d}$ .
  - The output is defined as output =  $\operatorname{softmax}(XQ(XK)^{\mathsf{T}}) \times XV$ .

First, take the query-key dot products in one matrix multiplication:  $XQ(XK)^{T}$ 

Next, softmax, and compute the weighted average with another matrix multiplication.

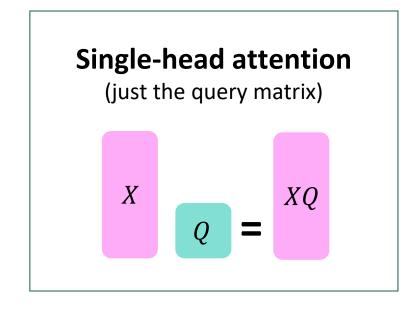


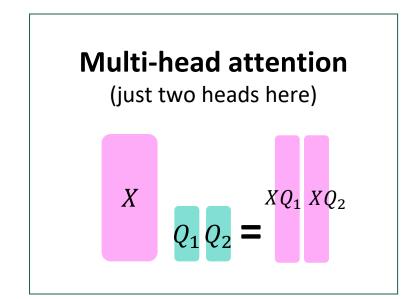
#### The Transformer Encoder: Multi-headed attention

- What if we want to look in multiple places in the sentence at once?
  - For word i, self-attention "looks" where  $x_i^T Q^T K x_j$  is high, but maybe we want to focus on different j for different reasons?
- We'll define multiple attention "heads" through multiple Q,K,V matrices
- Let,  $Q_{\ell}, K_{\ell}, V_{\ell} \in \mathbb{R}^{d \times \frac{d}{h}}$ , where h is the number of attention heads, and  $\ell$  ranges from 1 to h.
- Each attention head performs attention independently:
  - output<sub>\ell</sub> = softmax $(XQ_{\ell}K_{\ell}^{\top}X^{\top}) * XV_{\ell}$ , where output<sub>\ell</sub>  $\in \mathbb{R}^{d/h}$
- Then the outputs of all the heads are combined!
  - output =  $Y[\text{output}_1; ...; \text{output}_h]$ , where  $Y \in \mathbb{R}^{d \times d}$
- Each head gets to "look" at different things, and construct value vectors differently.

#### The Transformer Encoder: Multi-headed attention

- What if we want to look in multiple places in the sentence at once?
  - For word i, self-attention "looks" where  $x_i^T Q^T K x_j$  is high, but maybe we want to focus on different j for different reasons?
- We'll define multiple attention "heads" through multiple Q,K,V matrices
- Let,  $Q_{\ell}, K_{\ell}, V_{\ell} \in \mathbb{R}^{d \times \frac{d}{h}}$ , where h is the number of attention heads, and  $\ell$  ranges from 1 to h.





Same amount of computation as single-head self-attention!

#### The Transformer Encoder: Residual connections [He et al., 2016]

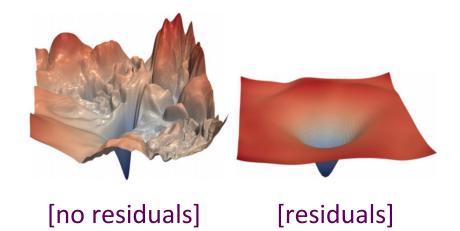
- Residual connections are a trick to help models train better.
  - Instead of  $X^{(i)} = \text{Layer}(X^{(i-1)})$  (where i represents the layer)

$$X^{(i-1)}$$
 Layer  $X^{(i)}$ 

• We let  $X^{(i)} = X^{(i-1)} + \text{Layer}(X^{(i-1)})$  (so we only have to learn "the residual" from the previous layer)

$$X^{(i-1)}$$
 Layer  $X^{(i)}$ 

 Residual connections are thought to make the loss landscape considerably smoother (thus easier training!)



[Loss landscape visualization, Li et al., 2018, on a ResNet]

# The Transformer Encoder: Layer normalization [Ba et al., 2016]

- Layer normalization is a trick to help models train faster.
- Idea: cut down on uninformative variation in hidden vector values by normalizing to unit mean and standard deviation within each layer.
  - LayerNorm's success may be due to its normalizing gradients [Xu et al., 2019]
- Let  $x \in \mathbb{R}^d$  be an individual (word) vector in the model.
- Let  $\mu = \sum_{i=1}^{d} x_i$ ; this is the mean;  $\mu \in \mathbb{R}$ .
- Let  $\sigma = \sqrt{\frac{1}{d} \sum_{j=1}^{d} (x_j \mu)^2}$ ; this is the standard deviation;  $\sigma \in \mathbb{R}$ .
- Let  $\gamma \in \mathbb{R}^d$  and  $\beta \in \mathbb{R}^d$  be learned "gain" and "bias" parameters. (Can omit!)
- Then layer normalization computes:

Normalize by scalar mean and variance 
$$\frac{x - \mu}{\sigma + \epsilon}$$

# The Transformer Encoder: Layer normalization [Ba et al., 2016]

- Layer normalization is a trick to help models train faster.
- Idea: cut down on uninformative variation in hidden vector values by normalizing to unit mean and standard deviation within each layer.
  - LayerNorm's success may be due to its normalizing gradients [Xu et al., 2019]
- Let  $x \in \mathbb{R}^d$  be an individual (word) vector in the model.
- Let  $\mu = \sum_{i=1}^{d} x_i$ ; this is the mean;  $\mu \in \mathbb{R}$ .
- Let  $\sigma = \sqrt{\frac{1}{d} \sum_{j=1}^{d} (x_j \mu)^2}$ ; this is the standard deviation;  $\sigma \in \mathbb{R}$ .
- Let  $\gamma \in \mathbb{R}^d$  and  $\beta \in \mathbb{R}^d$  be learned "gain" and "bias" parameters. (Can omit!)
- Then layer normalization computes:

$$\text{Output} = \frac{x - \mu}{\sigma + \epsilon} * \gamma + \beta$$
 Normalize by scalar mean and variance 
$$\text{Modulate by learned elementwise gain and bias}$$

#### The Transformer Encoder: Scaled Dot Product [Vaswani et al., 2017]

- "Scaled Dot Product" attention is a final variation to aid in Transformer training.
- When dimensionality d becomes large, dot products between vectors tend to become large.
  - Because of this, inputs to the softmax function can be large, making the gradients small.
- Instead of the self-attention function we've seen:

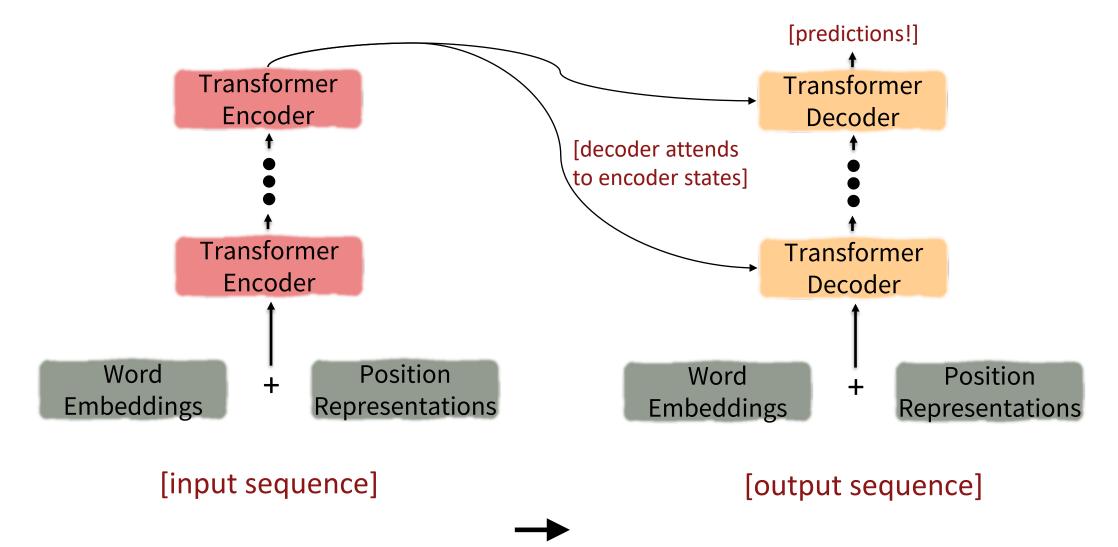
$$\operatorname{output}_{\ell} = \operatorname{softmax}(XQ_{\ell}K_{\ell}^{\mathsf{T}}X^{\mathsf{T}}) * XV_{\ell}$$

• We divide the attention scores by  $\sqrt{d/h}$ , to stop the scores from becoming large just as a function of d/h (The dimensionality divided by the number of heads.)

$$\operatorname{output}_{\ell} = \operatorname{softmax}\left(\frac{XQ_{\ell}K_{\ell}^{\mathsf{T}}X^{\mathsf{T}}}{\sqrt{d/h}}\right) * XV_{\ell}$$

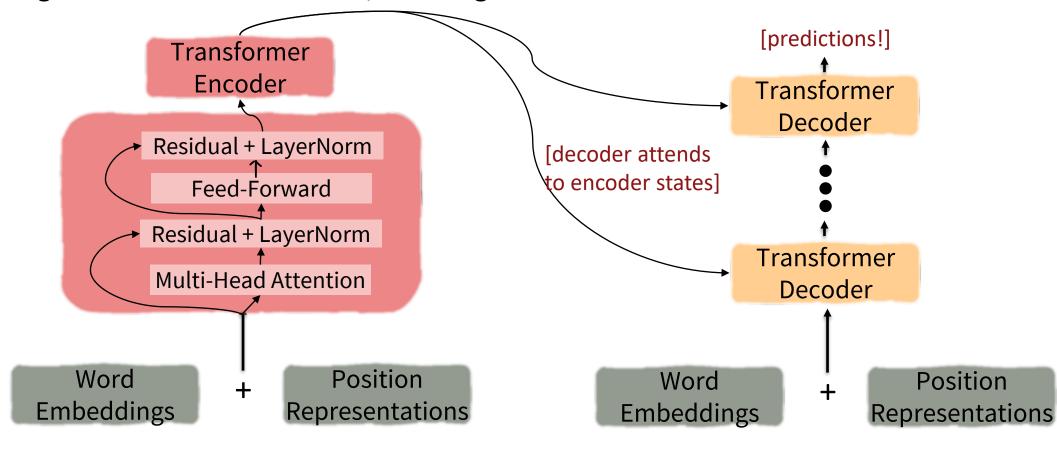
#### The Transformer Encoder-Decoder [Vaswani et al., 2017]

Looking back at the whole model, zooming in on an Encoder block:



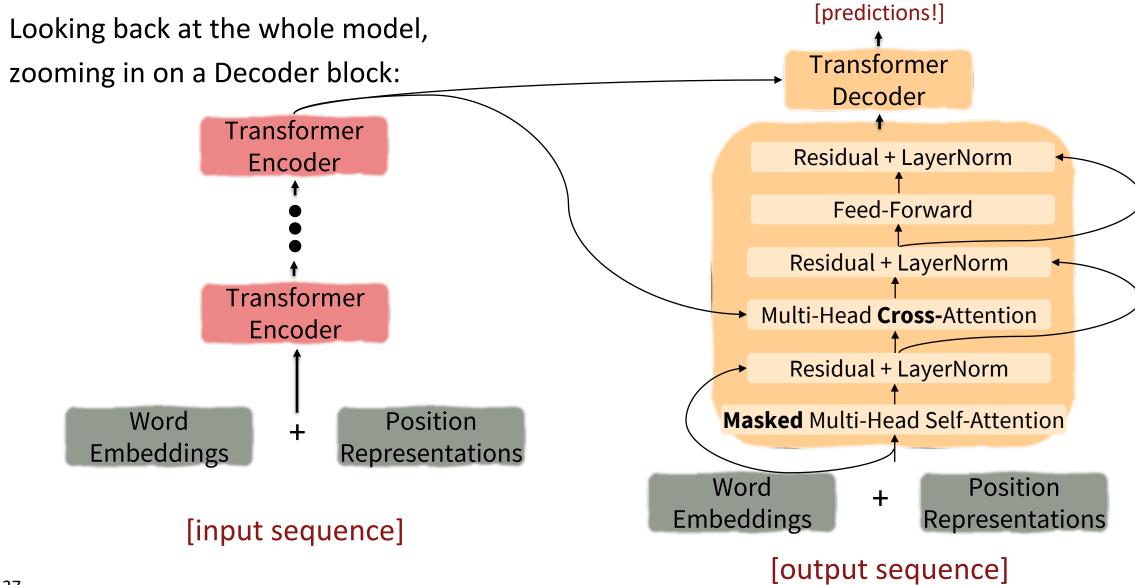
## The Transformer Encoder-Decoder [Vaswani et al., 2017]

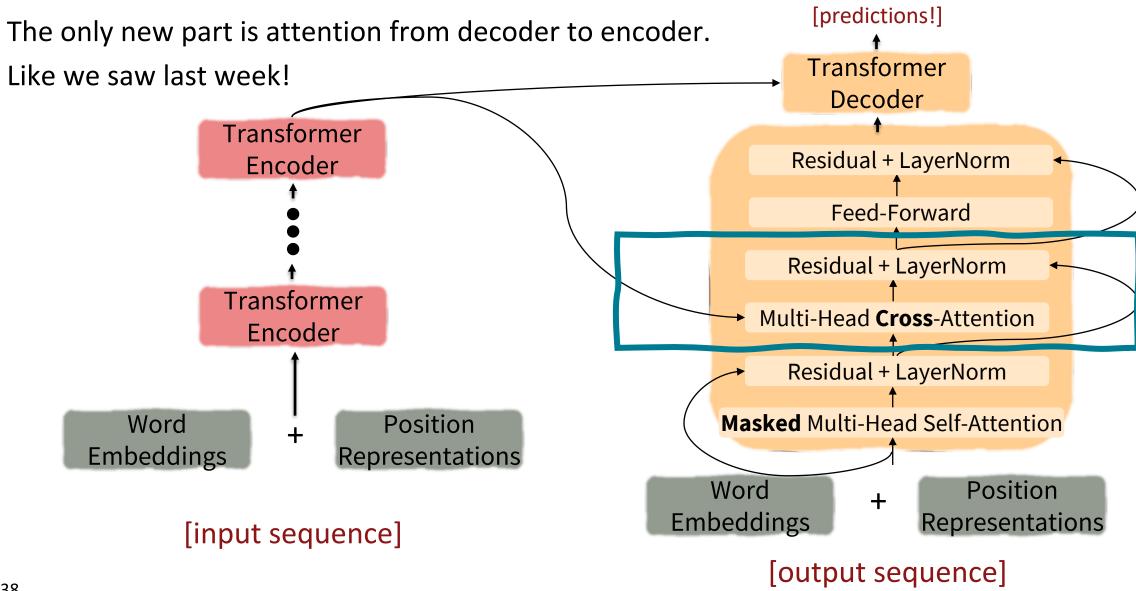
Looking back at the whole model, zooming in on an Encoder block:



[input sequence]

[output sequence]





# The Transformer Decoder: Cross-attention (details)

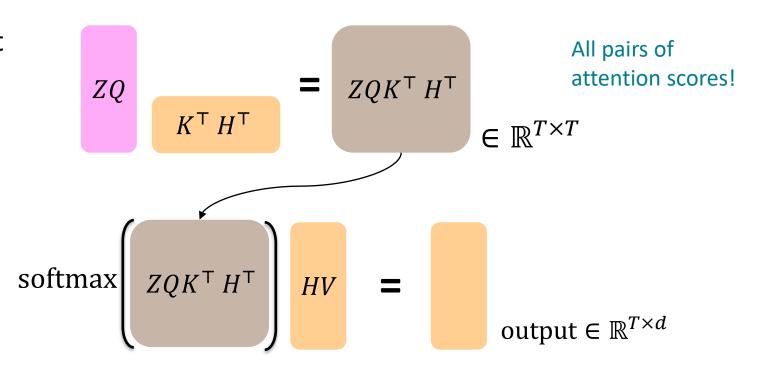
- We saw that self-attention is when keys, queries, and values come from the same source.
- In the decoder, we have attention that looks more like what we saw last week.
- Let  $h_1, ..., h_T$  be **output** vectors **from** the Transformer **encoder**;  $x_i \in \mathbb{R}^d$
- Let  $z_1, ..., z_T$  be input vectors from the Transformer **decoder**,  $z_i \in \mathbb{R}^d$
- Then keys and values are drawn from the encoder (like a memory):
  - $k_i = Kh_i$ ,  $v_i = Vh_i$ .
- And the queries are drawn from the **decoder**,  $q_i = Qz_i$ .

# The Transformer Encoder: Cross-attention (details)

- Let's look at how cross-attention is computed, in matrices.
  - Let  $H = [h_1; ...; h_T] \in \mathbb{R}^{T \times d}$  be the concatenation of encoder vectors.
  - Let  $Z = [z_1; ...; z_T] \in \mathbb{R}^{T \times d}$  be the concatenation of decoder vectors.
  - The output is defined as output =  $\operatorname{softmax}(ZQ(HK)^{\mathsf{T}}) \times HV$ .

First, take the query-key dot products in one matrix multiplication:  $ZQ(HK)^{T}$ 

Next, softmax, and compute the weighted average with another matrix multiplication.



## **Outline**

- 1. From recurrence (RNN) to attention-based NLP models
- 2. Introducing the Transformer model
- 3. Great results with Transformers
- 4. Drawbacks and variants of Transformers

## **Great Results with Transformers**

First, Machine Translation from the original Transformers paper!

Model	BLEU		Training Cost (FLOPs)	
Model	EN-DE	EN-FR	EN-DE	EN-FR
ByteNet [18]	23.75			
Deep-Att + PosUnk [39]		39.2		$1.0 \cdot 10^{20}$
GNMT + RL [38]	24.6	39.92	$2.3 \cdot 10^{19}$	$1.4 \cdot 10^{20}$
ConvS2S [9]	25.16	40.46	$9.6 \cdot 10^{18}$	$1.5 \cdot 10^{20}$
MoE [32]	26.03	40.56	$2.0 \cdot 10^{19}$	$1.2 \cdot 10^{20}$
Deep-Att + PosUnk Ensemble [39]		40.4		$8.0 \cdot 10^{20}$
GNMT + RL Ensemble [38]	26.30	41.16	$1.8 \cdot 10^{20}$	$1.1 \cdot 10^{21}$
ConvS2S Ensemble [9]	26.36	41.29	$7.7\cdot10^{19}$	$1.2 \cdot 10^{21}$

## **Great Results with Transformers**

Next, document generation!

	Model	Test perplexity	ROUGE-L	
	seq2seq-attention, $L = 500$	5.04952	12.7	
1	Transformer-ED, $L = 500$	2.46645	34.2	
	Transformer-D, $L = 4000$	2.22216	33.6	
	Transformer-DMCA, no MoE-layer, $L = 11000$	2.05159	36.2	
	Transformer-DMCA, MoE-128, $L = 11000$	1.92871	37.9	
	Transformer-DMCA, MoE-256, $L = 7500$	1.90325	38.8	
		<b>7</b>		

The old standard

Transformers all the way down.

## **Great Results with Transformers**

Before too long, most Transformers results also included **pretraining**, a method we'll go over on Thursday.

Transformers' parallelizability allows for efficient pretraining, and have made them the de-facto standard.

On this popular aggregate benchmark, for example:



All top models are Transformer (and pretraining)-based.

	Rank	Name	Model	URL	Score
	1	DeBERTa Team - Microsoft	DeBERTa / TuringNLRv4		90.8
	2	HFL iFLYTEK	MacALBERT + DKM		90.7
+	3	Alibaba DAMO NLP	StructBERT + TAPT	ď	90.6
+	4	PING-AN Omni-Sinitic	ALBERT + DAAF + NAS		90.6
	5	ERNIE Team - Baidu	ERNIE	Z'	90.4
	6	T5 Team - Google	T5	Z'	90.3

More results Thursday when we discuss pretraining.

## **Outline**

- 1. From recurrence (RNN) to attention-based NLP models
- 2. Introducing the Transformer model
- 3. Great results with Transformers
- 4. Drawbacks and variants of Transformers

## What would we like to fix about the 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!
- Position representations:
  - Are simple absolute indices the best we can do to represent position?
  - Relative linear position attention [Shaw et al., 2018]
  - Dependency syntax-based position [Wang et al., 2019]

# 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  $O(T^2d)$ , where T is the sequence length, and d is the dimensionality.

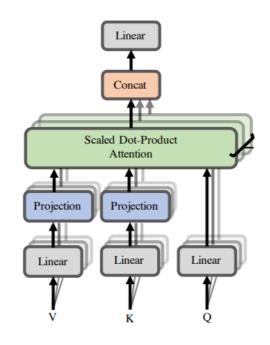
$$= \begin{array}{c} XQK^{\mathsf{T}}X^{\mathsf{T}} \\ K^{\mathsf{T}}X^{\mathsf{T}} \end{array} = \begin{bmatrix} XQK^{\mathsf{T}}X^{\mathsf{T}} \\ \in \mathbb{R}^{T \times T} \end{bmatrix} \begin{array}{c} \text{Need to compute all pairs of interactions!} \\ O(T^2d) \end{array}$$

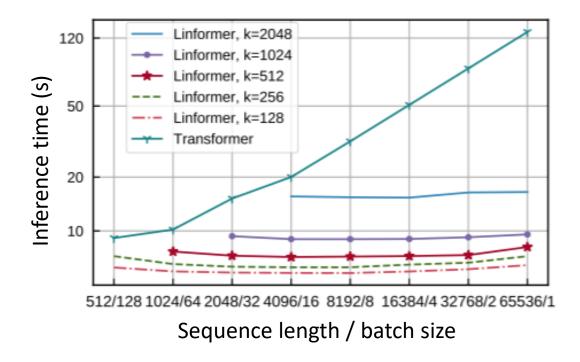
- Think of d as around  $\mathbf{1}$ ,  $\mathbf{000}$ .
  - So, for a single (shortish) sentence,  $T \le 30$ ;  $T^2 \le 900$ .
  - In practice, we set a bound like T=512.
  - But what if we'd like  $T \ge 10,000$ ? For example, to work on long documents?

# Recent work on improving on quadratic self-attention cost

- Considerable recent work has gone into the question, Can we build models like Transformers without paying the  $O(T^2)$  all-pairs self-attention cost?
- For example, Linformer [Wang et al., 2020]

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

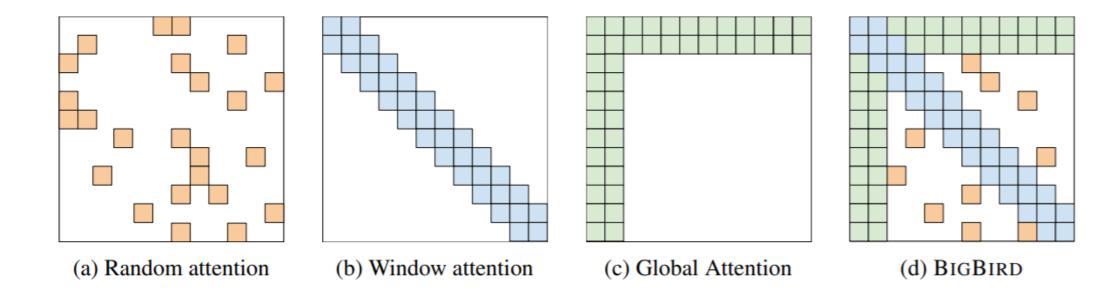




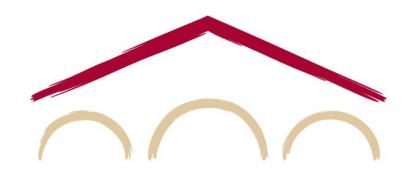
# Recent work on improving on quadratic self-attention cost

- Considerable recent work has gone into the question, Can we build models like Transformers without paying the  $O(T^2)$  all-pairs self-attention cost?
- For example, BigBird [Zaheer et al., 2021]

Key idea: replace all-pairs interactions with a family of other interactions, like local windows, looking at everything, and random interactions.



# Natural Language Processing with Deep Learning CS224N/Ling284



John Hewitt

Lecture 10: Pretraining

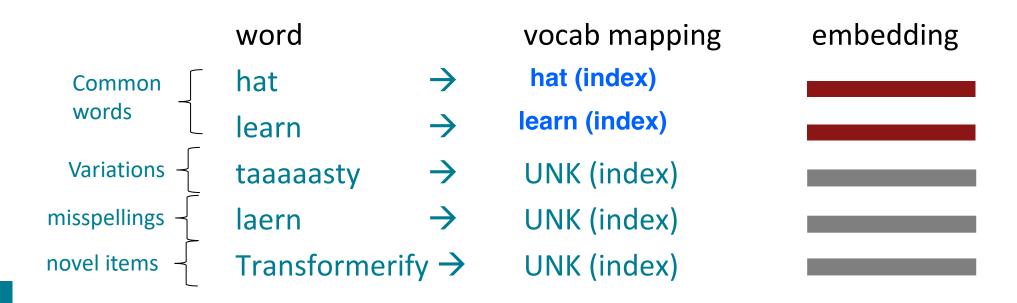
## **Lecture Plan**

- 1. A brief note on subword modeling
- 2. Motivating model pretraining from word embeddings
- 3. Model pretraining three ways
  - 1. Decoders
  - 2. Encoders
  - 3. Encoder-Decoders
- 4. Interlude: what do we think pretraining is teaching?
- 5. Very large models and in-context learning

## Word structure and subword models

Let's take a look at the assumptions we've made about a language's vocabulary.

We assume a fixed vocab of tens of thousands of words, built from the training set. All *novel* words seen at test time are mapped to a single UNK.



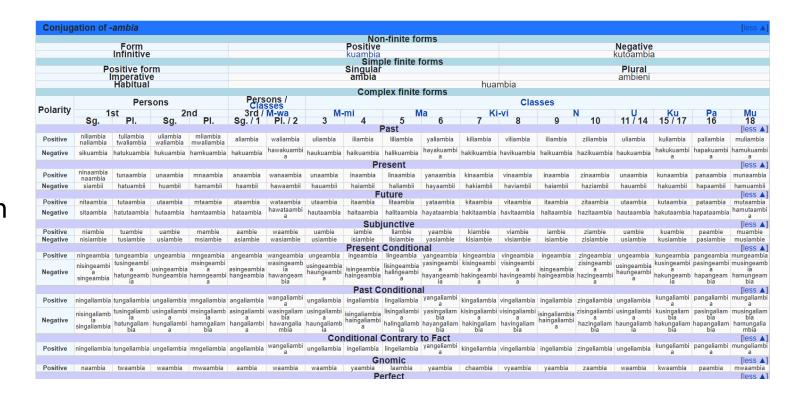
## Word structure and subword models

Finite vocabulary assumptions make even less sense in many languages.

- Many languages exhibit complex morphology, or word structure.
  - The effect is more word types, each occurring fewer times.

Example: Swahili verbs can have hundreds of conjugations, each encoding a wide variety of information. (Tense, mood, definiteness, negation, information about the object, ++)

Here's a small fraction of the conjugations for *ambia* – to tell.



## The byte-pair encoding algorithm

Subword modeling in NLP encompasses a wide range of methods for reasoning about structure below the word level. (Parts of words, characters, bytes.)

- The dominant modern paradigm is to learn a vocabulary of parts of words (subword tokens).
- At training and testing time, each word is split into a sequence of known subwords.

Byte-pair encoding is a simple, effective strategy for defining a subword vocabulary.

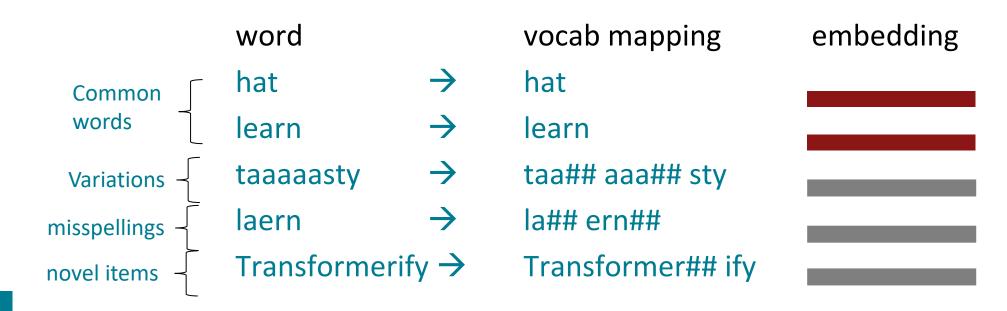
- Start with a vocabulary containing only characters and an "end-of-word" symbol.
- 2. Using a corpus of text, find the most common adjacent characters "a,b"; add "ab" as a subword.
- 3. Replace instances of the character pair with the new subword; repeat until desired vocab size.

Originally used in NLP for machine translation; now a similar method (WordPiece) is used in pretrained models.

## Word structure and subword models

Common words end up being a part of the subword vocabulary, while rarer words are split into (sometimes intuitive, sometimes not) components.

In the worst case, words are split into as many subwords as they have characters.



## **Outline**

- 1. A brief note on subword modeling
- 2. Motivating model pretraining from word embeddings
- 3. Model pretraining three ways
  - 1. Decoders
  - 2. Encoders
  - 3. Encoder-Decoders
- 4. Interlude: what do we think pretraining is teaching?
- 5. Very large models and in-context learning

## Motivating word meaning and context

Recall the adage we mentioned at the beginning of the course:

"You shall know a word by the company it keeps" (J. R. Firth 1957: 11)

This quote is a summary of distributional semantics, and motivated word2vec. But:

"... the complete meaning of a word is always contextual, and no study of meaning apart from a complete context can be taken seriously." (J. R. Firth 1935)

Consider I record the record: the two instances of record mean different things.

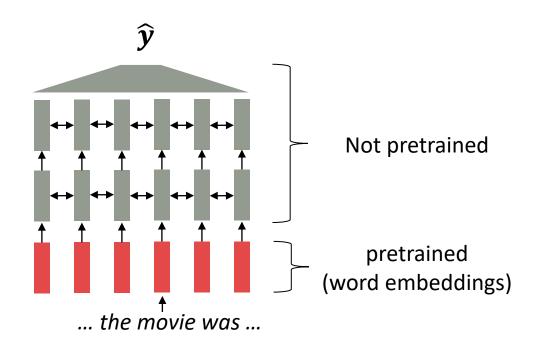
## Where we were: pretrained word embeddings

#### Circa 2017:

- Start with pretrained word embeddings (no context!)
- Learn how to incorporate context in an LSTM or Transformer while training on the task.

#### Some issues to think about:

- The training data we have for our downstream task (like question answering) must be sufficient to teach all contextual aspects of language.
- Most of the parameters in our network are randomly initialized!

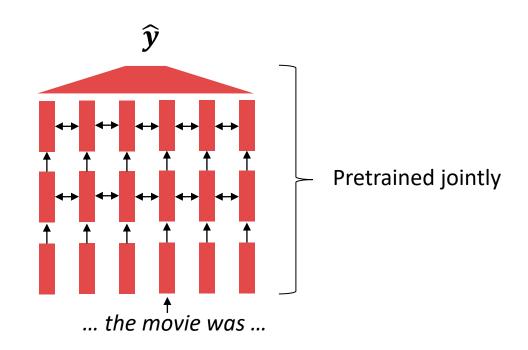


[Recall, *movie* gets the same word embedding, no matter what sentence it shows up in]

## Where we're going: pretraining whole models

#### In modern NLP:

- All (or almost all) parameters in NLP networks are initialized via pretraining.
- Pretraining methods hide parts of the input from the model, and train the model to reconstruct those parts.
- This has been exceptionally effective at building strong:
  - representations of language
  - parameter initializations for strong NLP models.
  - Probability distributions over language that we can sample from



[This model has learned how to represent entire sentences through pretraining]

Stanford University is located in \_\_\_\_\_\_, California.

I put \_\_\_\_ fork down on the table.

The woman walked across the street, checking for traffic over \_\_\_\_ shoulder.

I went to the ocean to see the fish, turtles, seals, and \_\_\_\_\_.

Overall, the value I got from the two hours watching it was the sum total of the popcorn and the drink.

The movie was .

Iroh went into the kitchen to make some tea.

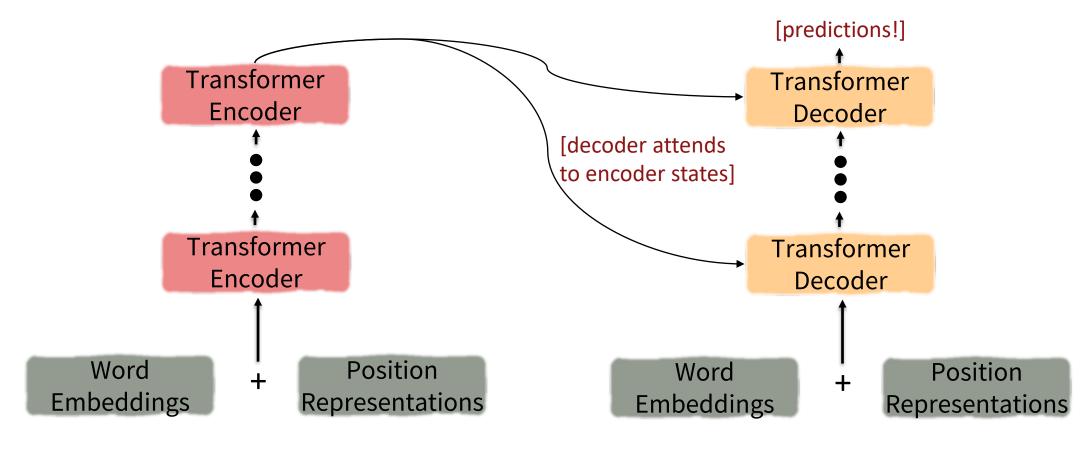
Standing next to Iroh, Zuko pondered his destiny.

Zuko left the \_\_\_\_\_.

I was thinking about the sequence that goes

1, 1, 2, 3, 5, 8, 13, 21, \_\_\_\_

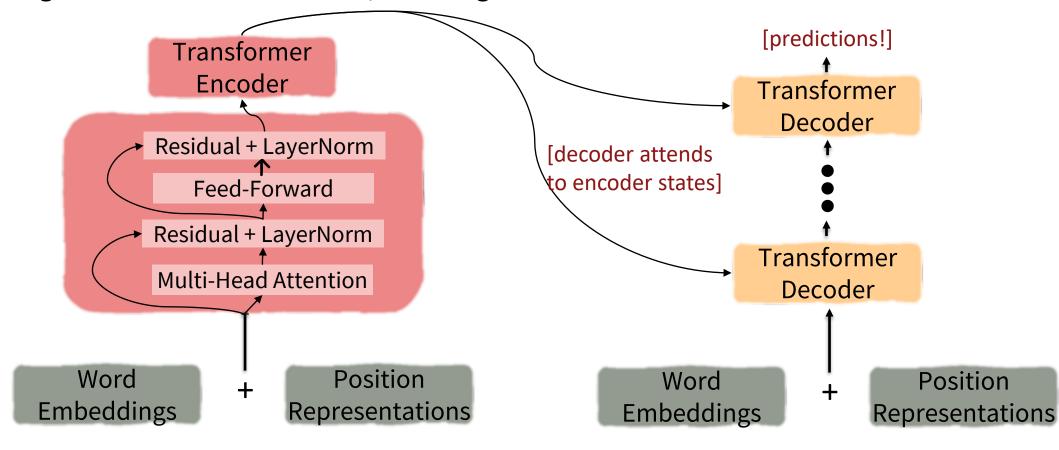
Looking back at the whole model, zooming in on an Encoder block:



[input sequence]

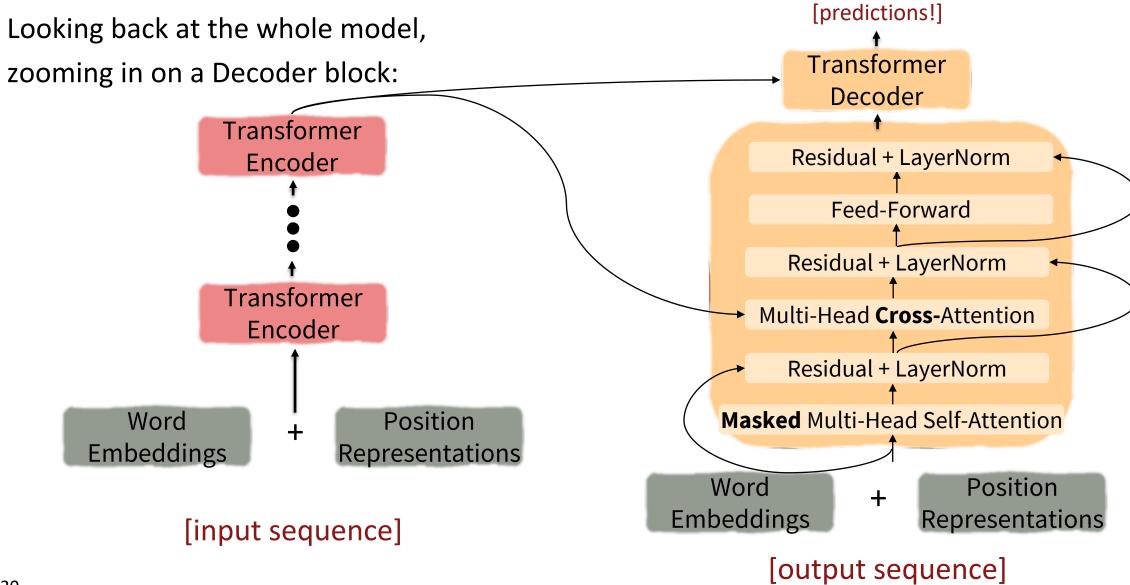
[output sequence]

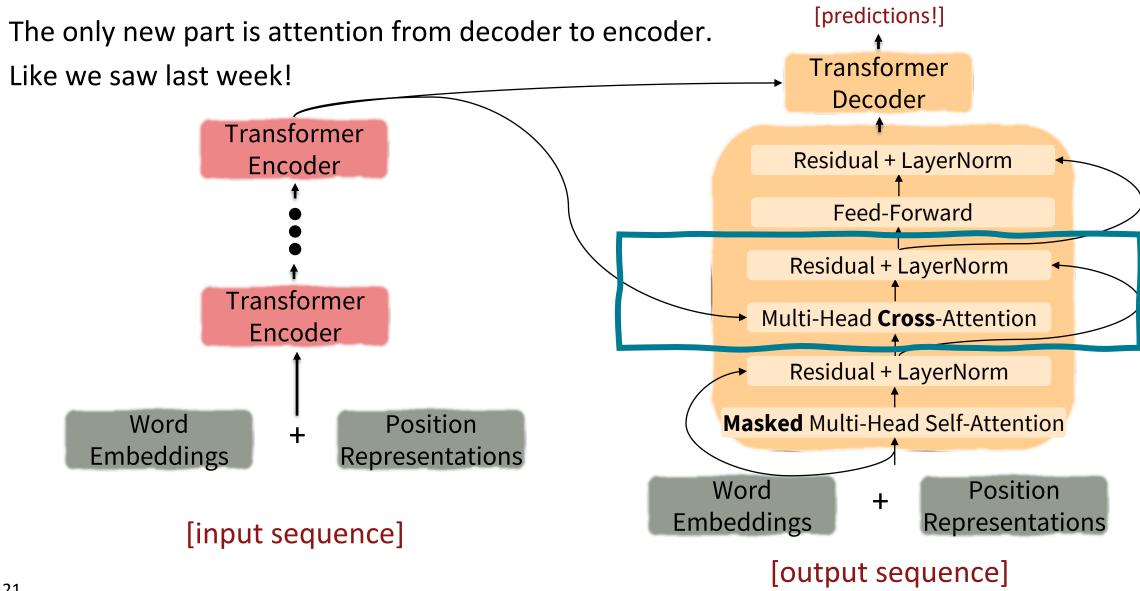
Looking back at the whole model, zooming in on an Encoder block:



[input sequence]

[output sequence]





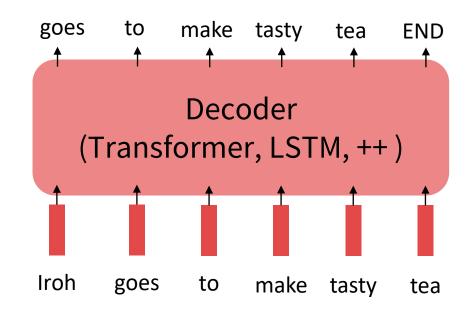
## Pretraining through language modeling [Dai and Le, 2015]

#### Recall the **language modeling** task:

- Model  $p_{\theta}(w_t|w_{1:t-1})$ , the probability distribution over words given their past contexts.
- There's lots of data for this! (In English.)

#### **Pretraining through language modeling:**

- Train a neural network to perform language modeling on a large amount of text.
- Save the network parameters.

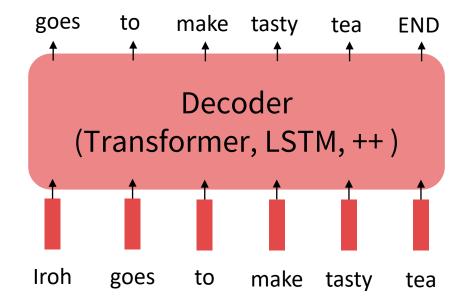


## The Pretraining / Finetuning Paradigm

Pretraining can improve NLP applications by serving as parameter initialization.

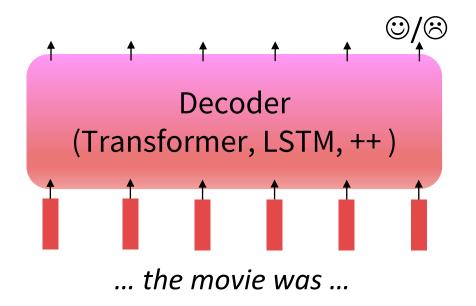
#### **Step 1: Pretrain (on language modeling)**

Lots of text; learn general things!



#### **Step 2: Finetune (on your task)**

Not many labels; adapt to the task!



## Stochastic gradient descent and pretrain/finetune

Why should pretraining and finetuning help, from a "training neural nets" perspective?

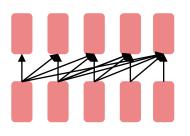
- Consider, provides parameters  $\hat{\theta}$  by approximating  $\min_{\theta} \mathcal{L}_{\text{pretrain}}(\theta)$ .
  - (The pretraining loss.)
- Then, finetuning approximates  $\min_{\theta} \mathcal{L}_{\text{finetune}}(\theta)$ , starting at  $\hat{\theta}$ .
  - (The finetuning loss)
- The pretraining may matter because stochastic gradient descent sticks (relatively) close to  $\hat{\theta}$  during finetuning.
  - So, maybe the finetuning local minima near  $\hat{\theta}$  tend to generalize well!
  - And/or, maybe the gradients of finetuning loss near  $\hat{\theta}$  propagate nicely!

#### **Lecture Plan**

- 1. A brief note on subword modeling
- 2. Motivating model pretraining from word embeddings
- 3. Model pretraining three ways
  - 1. Decoders
  - 2. Encoders
  - 3. Encoder-Decoders
- 4. Interlude: what do we think pretraining is teaching?
- 5. Very large models and in-context learning

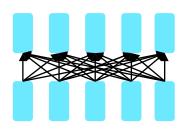
## Pretraining for three types of architectures

The neural architecture influences the type of pretraining, and natural use cases.



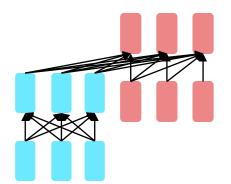
#### **Decoders**

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



#### **Encoders**

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

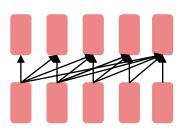


**Encoder- Decoders** 

- Good parts of decoders and encoders?
- What's the best way to pretrain them?

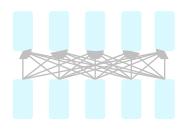
## Pretraining for three types of architectures

The neural architecture influences the type of pretraining, and natural use cases.



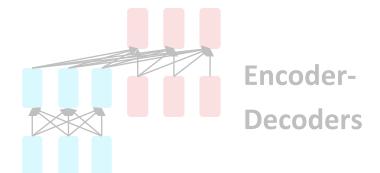
#### **Decoders**

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



#### **Encoders**

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



- Good parts of decoders and encoders?
- What's the best way to pretrain them?

#### Pretraining decoders

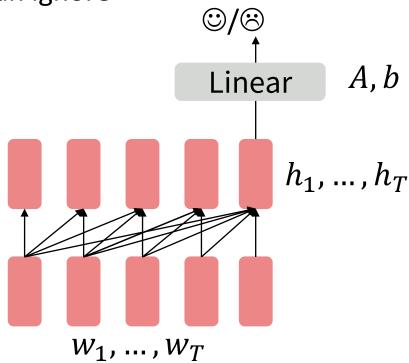
When using language model pretrained decoders, we can ignore that they were trained to model  $p(w_t|w_{1:t-1})$ .

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

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

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.]

#### Pretraining decoders

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

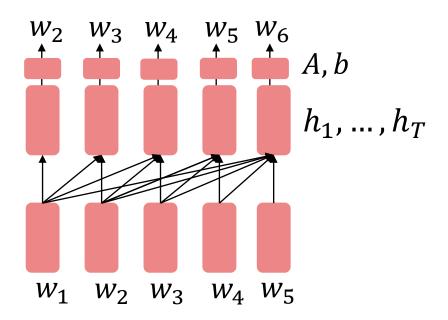
This is helpful in tasks where the output is a sequence with a vocabulary like that at pretraining time!

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

$$h_1, ..., h_T = \text{Decoder}(w_1, ..., w_T)$$

$$w_t \sim Ah_{t-1} + b$$

Where *A*, *b* were pretrained in the language model!



[Note how the linear layer has been pretrained.]

# Generative Pretrained Transformer (GPT) [Radford et al., 2018]

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.
- The acronym "GPT" never showed up in the original paper; it could stand for "Generative PreTraining" or "Generative Pretrained Transformer"

# Generative Pretrained Transformer (GPT) [Radford et al., 2018]

How do we format inputs to our decoder for **finetuning tasks?** 

**Natural Language Inference:** Label pairs of sentences as *entailing/contradictory/neutral* 

Premise: *The man is in the doorway*Hypothesis: *The person is near the door*entailment

Radford et al., 2018 evaluate on natural language inference.

Here's roughly how the input was formatted, as a sequence of tokens for the decoder.

[START] The man is in the doorway [DELIM] The person is near the door [EXTRACT]

The linear classifier is applied to the representation of the [EXTRACT] token.

## Generative Pretrained Transformer (GPT) [Radford et al., 2018]

GPT results on various natural language inference datasets.

Method	MNLI-m	MNLI-mm	SNLI	SciTail	QNLI	RTE
ESIM + ELMo [44] (5x)	-	-	89.3	-	-	-
CAFE [58] (5x)	80.2	79.0	89.3	-	-	-
Stochastic Answer Network [35] (3x)	80.6	80.1	-	-	-	-
CAFE [58]	78.7	77.9	88.5	83.3		
GenSen [64]	71.4	71.3	-	-	82.3	59.2
Multi-task BiLSTM + Attn [64]	72.2	72.1	-	-	82.1	61.7
Finetuned Transformer LM (ours)	82.1	81.4	89.9	88.3	88.1	56.0

# Increasingly convincing generations (GPT2) [Radford et al., 2018]

We mentioned how pretrained decoders can be used in their capacities as language models.

**GPT-2,** a larger version of GPT trained on more data, was shown to produce relatively convincing samples of natural language.

**Context (human-written):** In a shocking finding, scientist discovered a herd of unicorns living in a remote, previously unexplored valley, in the Andes Mountains. Even more surprising to the researchers was the fact that the unicorns spoke perfect English.

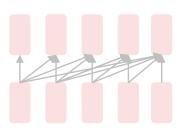
**GPT-2:** The scientist named the population, after their distinctive horn, Ovid's Unicorn. These four-horned, silver-white unicorns were previously unknown to science.

Now, after almost two centuries, the mystery of what sparked this odd phenomenon is finally solved.

Dr. Jorge Pérez, an evolutionary biologist from the University of La Paz, and several companions, were exploring the Andes Mountains when they found a small valley, with no other animals or humans. Pérez noticed that the valley had what appeared to be a natural fountain, surrounded by two peaks of rock and silver snow.

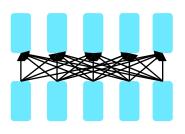
## Pretraining for three types of architectures

The neural architecture influences the type of pretraining, and natural use cases.



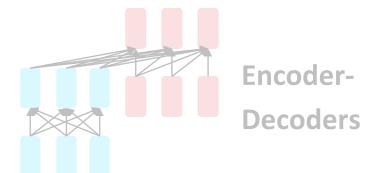
#### **Decoders**

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



#### **Encoders**

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



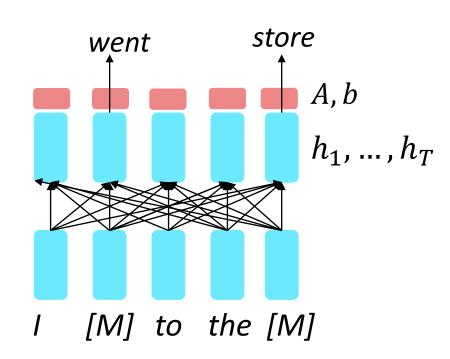
- Good parts of decoders and encoders?
- What's the best way to pretrain them?

So far, we've looked at language model pretraining. But **encoders get bidirectional context,** so we can't do language modeling!

Idea: replace some fraction of words in the input with a special [MASK] token; predict these words.

$$h_1, \dots, h_T = \text{Encoder}(w_1, \dots, w_T)$$
  
 $y_i \sim Aw_i + b$ 

Only add loss terms from words that are "masked out." If  $\tilde{x}$  is the masked version of x, we're learning  $p_{\theta}(x|\tilde{x})$ . Called **Masked LM**.

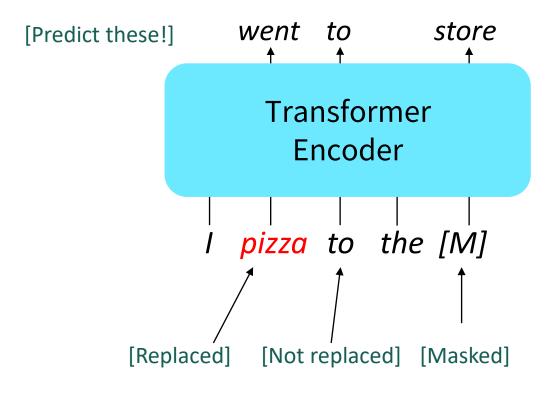


[Devlin et al., 2018]

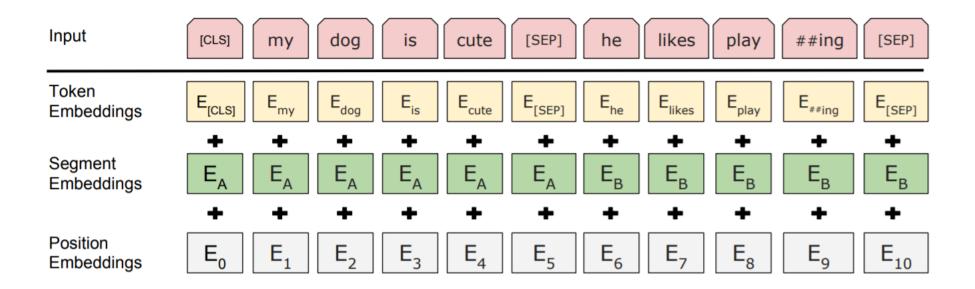
Devlin et al., 2018 proposed the "Masked LM" objective and released the weights of a pretrained Transformer, a model they labeled BERT.

Some more details about Masked LM for BERT:

- Predict a random 15% of (sub)word tokens.
  - Replace input word with [MASK] 80% of the time
  - Replace input word with a random token 10% of the time
  - Leave input word unchanged 10% of the time (but still predict it!)
- Why? Doesn't let the model get complacent and not build strong representations of non-masked words.
   (No masks are seen at fine-tuning time!)



The pretraining input to BERT was two separate contiguous chunks of text:



- BERT was trained to predict whether one chunk follows the other or is randomly sampled.
  - Later work has argued this "next sentence prediction" is not necessary.

#### **Details about BERT**

- Two models were released:
  - BERT-base: 12 layers, 768-dim hidden states, 12 attention heads, 110 million params.
  - BERT-large: 24 layers, 1024-dim hidden states, 16 attention heads, 340 million params.
- Trained on:
  - BooksCorpus (800 million words)
  - English Wikipedia (2,500 million words)
- Pretraining is expensive and impractical on a single GPU.
  - BERT was pretrained with 64 TPU chips for a total of 4 days.
  - (TPUs are special tensor operation acceleration hardware)
- Finetuning is practical and common on a single GPU
  - "Pretrain once, finetune many times."

BERT was massively popular and hugely versatile; finetuning BERT led to new state-of-the-art results on a broad range of tasks.

- QQP: Quora Question Pairs (detect paraphrase questions)
- QNLI: natural language inference over question answering data
- **SST-2**: sentiment analysis

**CoLA**: corpus of linguistic acceptability (detect whether sentences are grammatical.)

**STS-B**: semantic textual similarity

MRPC: microsoft paraphrase corpus

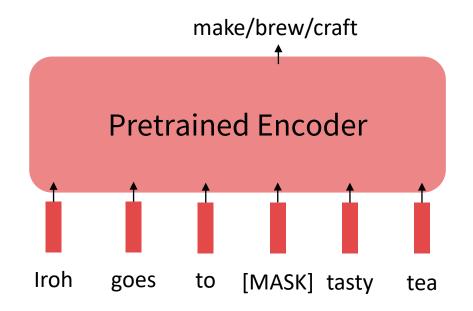
**RTE**: a small natural language inference corpus

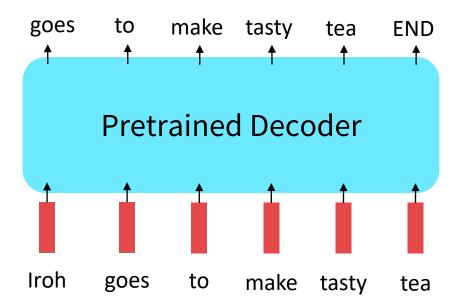
System	MNLI-(m/mm)	QQP	QNLI	SST-2	CoLA	STS-B	MRPC	RTE	Average
	392k	363k	108k	67k	8.5k	5.7k	3.5k	2.5k	-
Pre-OpenAI SOTA	80.6/80.1	66.1	82.3	93.2	35.0	81.0	86.0	61.7	74.0
BiLSTM+ELMo+Attn	76.4/76.1	64.8	79.8	90.4	36.0	73.3	84.9	56.8	71.0
OpenAI GPT	82.1/81.4	70.3	87.4	91.3	45.4	80.0	82.3	56.0	75.1
BERT <sub>BASE</sub>	84.6/83.4	71.2	90.5	93.5	52.1	85.8	88.9	66.4	79.6
$BERT_{LARGE}$	86.7/85.9	72.1	92.7	94.9	60.5	86.5	89.3	70.1	82.1

#### Limitations of pretrained encoders

Those results looked great! Why not used pretrained encoders for everything?

If your task involves generating sequences, consider using a pretrained decoder; BERT and other pretrained encoders don't naturally lead to nice autoregressive (1-word-at-a-time) generation methods.



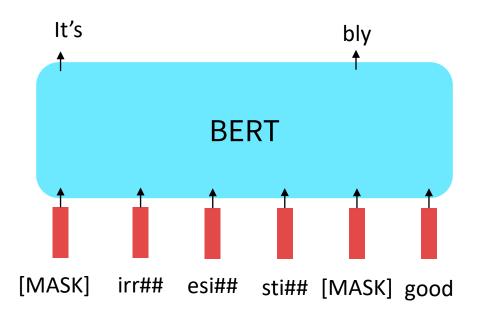


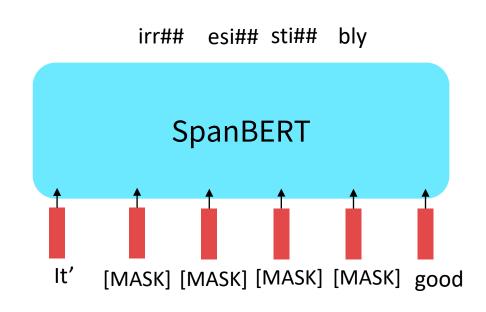
#### **Extensions of BERT**

You'll see a lot of BERT variants like RoBERTa, SpanBERT, +++

Some generally accepted improvements to the BERT pretraining formula:

- RoBERTa: mainly just train BERT for longer and remove next sentence prediction!
- SpanBERT: masking contiguous spans of words makes a harder, more useful pretraining task





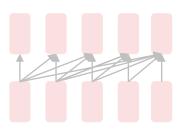
#### **Extensions of BERT**

A takeaway from the RoBERTa paper: more compute, more data can improve pretraining even when not changing the underlying Transformer encoder.

Model	data	bsz	steps	<b>SQuAD</b> (v1.1/2.0)	MNLI-m	SST-2
RoBERTa						
with BOOKS + WIKI	16GB	8K	100K	93.6/87.3	89.0	95.3
+ additional data (§3.2)	160GB	8K	100K	94.0/87.7	89.3	95.6
+ pretrain longer	160GB	8K	300K	94.4/88.7	90.0	96.1
+ pretrain even longer	160GB	8K	500K	94.6/89.4	90.2	96.4
BERT <sub>LARGE</sub>						
with BOOKS + WIKI	13GB	256	1M	90.9/81.8	86.6	93.7

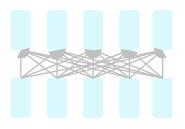
## Pretraining for three types of architectures

The neural architecture influences the type of pretraining, and natural use cases.



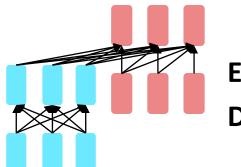
#### **Decoders**

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



#### **Encoders**

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



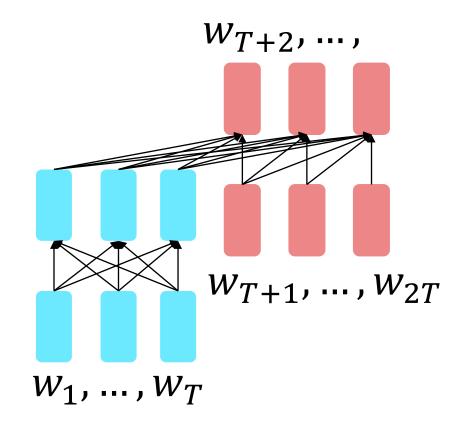
**Encoder- Decoders** 

- Good parts of decoders and encoders?
- What's the best way to pretrain them?

For **encoder-decoders**, we could do something like **language modeling**, but where a prefix of every input is provided to the encoder and is not predicted.

$$h_1,...,h_T = \text{Encoder}(w_1,...,w_T)$$
  
 $h_{T+1},...,h_{2T} = Decoder(w_1,...,w_T,h_1,...,h_T)$   
 $y_i \sim Aw_i + b, i > T$ 

The **encoder** portion benefits from bidirectional context; the **decoder** portion is used to train the whole model through language modeling.



[Raffel et al., 2018]

What Raffel et al., 2018 found to work best was span corruption. Their model: T5.

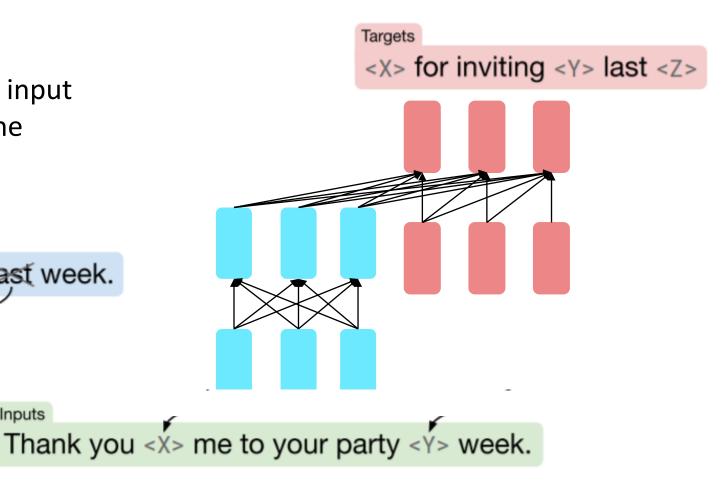
Inputs

Replace different-length spans from the input with unique placeholders; decode out the spans that were removed!

Original text

Thank you for inviting me to your party last week.

This is implemented in text preprocessing: it's still an objective that looks like **language modeling** at the decoder side.



Raffel et al., 2018 found encoder-decoders to work better than decoders for their tasks, and span corruption (denoising) to work better than language modeling.

Architecture	Objective	Params	Cost	GLUE	CNNDM	SQuAD	SGLUE	EnDe	EnFr	EnRo
★ Encoder-decoder	Denoising	2P	M	83.28	19.24	80.88	71.36	26.98	39.82	27.65
Enc-dec, shared	Denoising	P	M	82.81	18.78	80.63	70.73	26.72	39.03	27.46
Enc-dec, 6 layers	Denoising	P	M/2	80.88	18.97	77.59	68.42	26.38	38.40	26.95
Language model	Denoising	P	$\dot{M}$	74.70	17.93	61.14	55.02	25.09	35.28	25.86
Prefix LM	Denoising	P	M	81.82	18.61	78.94	68.11	26.43	37.98	27.39
Encoder-decoder	LM	2P	M	79.56	18.59	76.02	64.29	26.27	39.17	26.86
Enc-dec, shared	$_{ m LM}$	P	M	79.60	18.13	76.35	63.50	26.62	39.17	27.05
Enc-dec, 6 layers	$_{ m LM}$	P	M/2	78.67	18.26	75.32	64.06	26.13	38.42	26.89
Language model	$_{ m LM}$	P	$\dot{M}$	73.78	17.54	53.81	56.51	25.23	34.31	25.38
Prefix LM	$_{ m LM}$	P	M	79.68	17.84	76.87	64.86	26.28	37.51	26.76

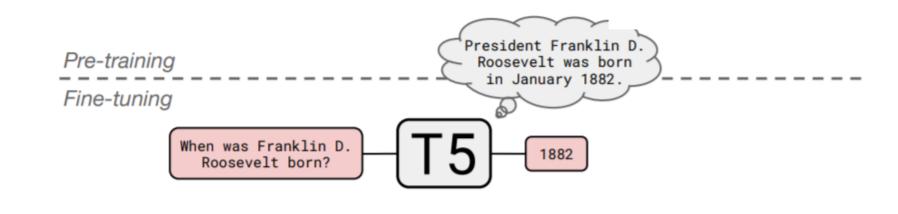
A fascinating property of T5: it can be finetuned to answer a wide range of questions, retrieving knowledge from its parameters.

NQ: Natural Questions

WQ: WebQuestions

TQA: Trivia QA

All "open-domain" versions



	NQ	WQ	TQA		
			dev	test	
Karpukhin et al. (2020)	41.5	42.4	<b>57.9</b>	_	-
T5.1.1-Base	25.7	28.2	24.2	30.6	220 million params
T5.1.1-Large	27.3	29.5	28.5	37.2	770 million params
T5.1.1-XL	29.5	32.4	36.0	45.1	3 billion params
T5.1.1-XXL	32.8	35.6	42.9	52.5	11 billion params
T5.1.1-XXL + SSM	35.2	42.8	51.9	61.6	

#### **Outline**

- 1. A brief note on subword modeling
- 2. Motivating model pretraining from word embeddings
- 3. Model pretraining three ways
  - 1. Decoders
  - 2. Encoders
  - 3. Encoder-Decoders
- 4. Interlude: what do we think pretraining is teaching?
- 5. Very large models and in-context learning

## What kinds of things does pretraining learn?

There's increasing evidence that pretrained models learn a wide variety of things about the statistical properties of language. Taking our examples from the start of class:

- Stanford University is located in \_\_\_\_\_\_, California. [Trivia]
- I put \_\_\_\_ fork down on the table. [syntax]
- The woman walked across the street, checking for traffic over \_\_\_\_ shoulder. [coreference]
- I went to the ocean to see the fish, turtles, seals, and \_\_\_\_\_. [lexical semantics/topic]
- Overall, the value I got from the two hours watching it was the sum total of the popcorn and the drink. The movie was \_\_\_\_. [sentiment]
- Iroh went into the kitchen to make some tea. Standing next to Iroh, Zuko pondered his destiny. Zuko left the \_\_\_\_\_. [some reasoning this is harder]
- I was thinking about the sequence that goes 1, 1, 2, 3, 5, 8, 13, 21, \_\_\_\_ [some basic arithmetic; they don't learn the Fibonnaci sequence]
- Models also learn and can exacerbate racism, sexism, all manner of bad biases.
- More on all this in the interpretability lecture!

#### **Outline**

- 1. A brief note on subword modeling
- 2. Motivating model pretraining from word embeddings
- 3. Model pretraining three ways
  - 1. Decoders
  - 2. Encoders
  - 3. Encoder-Decoders
- 4. Interlude: what do we think pretraining is teaching?
- 5. Very large models and in-context learning

## GPT-3, 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. The largest T5 model had 11 billion parameters. **GPT-3 has 175 billion parameters.** 

## GPT-3, In-context learning, and very large models

Very large language models seem to perform some kind of learning without gradient steps simply from examples you provide within their contexts.

The in-context examples seem to specify the task to be performed, and the conditional distribution mocks performing the task to a certain extent.

#### Input (prefix within a single Transformer decoder context):

```
" thanks -> merci
hello -> bonjour
mint -> menthe
otter -> "
```

#### **Output (conditional generations):**

loutre..."

## GPT-3, In-context learning, and very large models

Very large language models seem to perform some kind of learning without gradient steps simply from examples you provide within their contexts.

