Natural Language Processing with Deep Learning

CS224N/Ling284

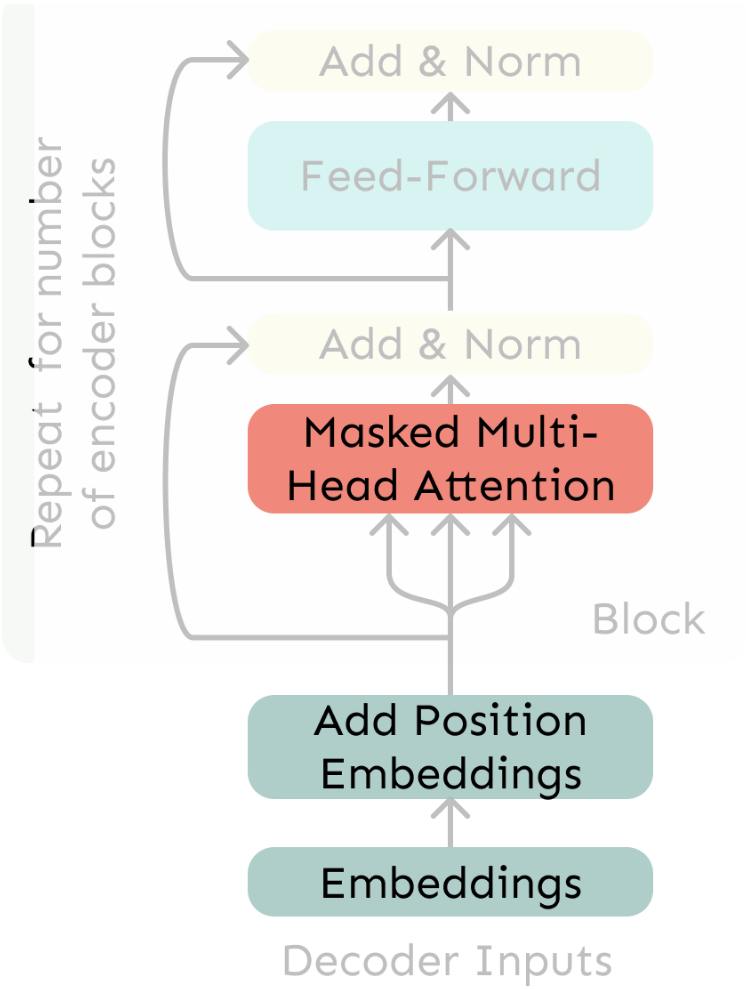
John Hewitt

Lecture 8: Self-Attention and Transformers

Adapted from slides by Anna Goldie, John Hewitt

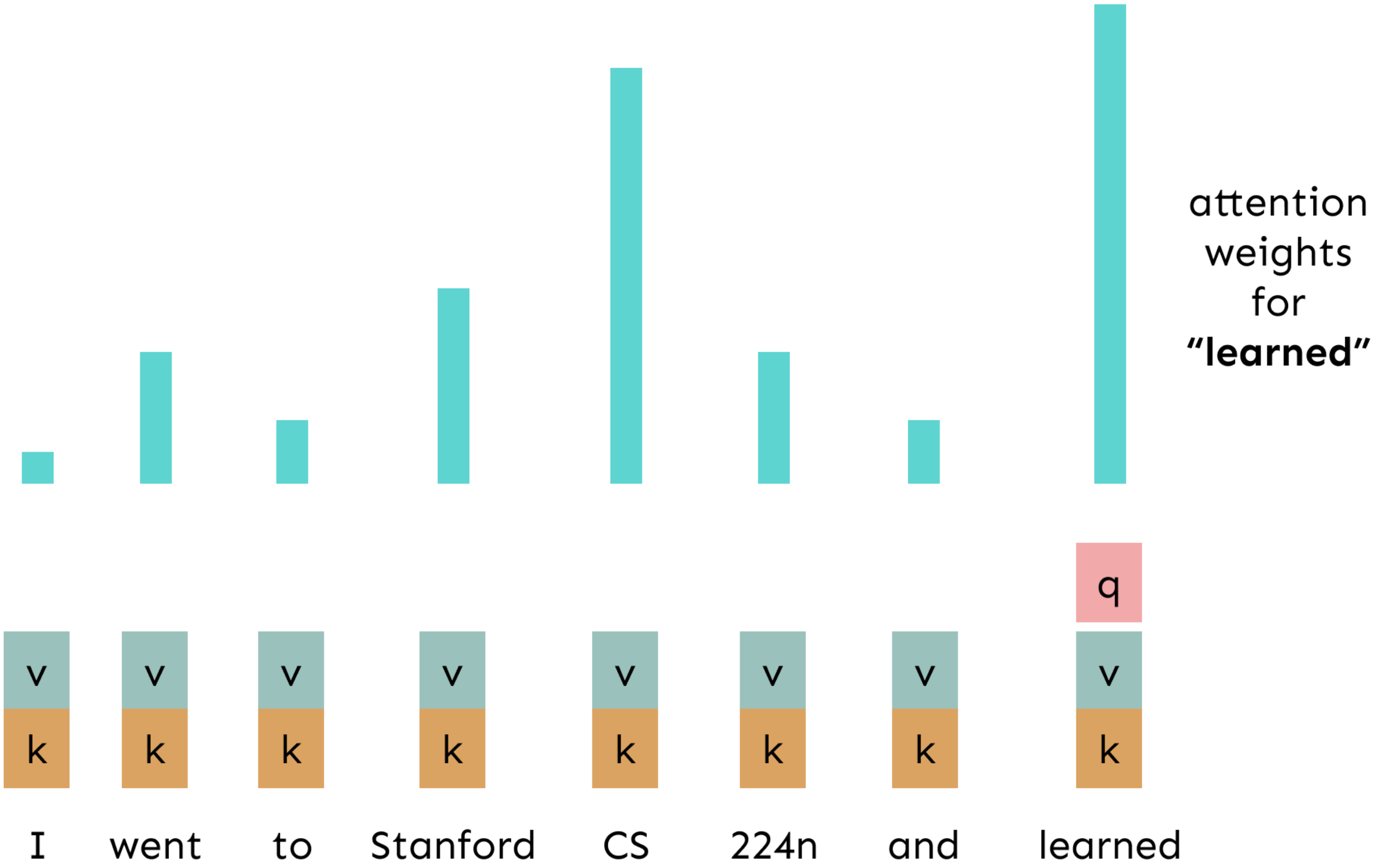
The Transformer Decoder

- A Transformer decoder is how we'll build systems like **language models**.
- It's a lot like our minimal self-attention architecture, but with a few more components.
- The embeddings and position embeddings are identical.
- We'll next replace our self-attention with **multi-head self-attention.**

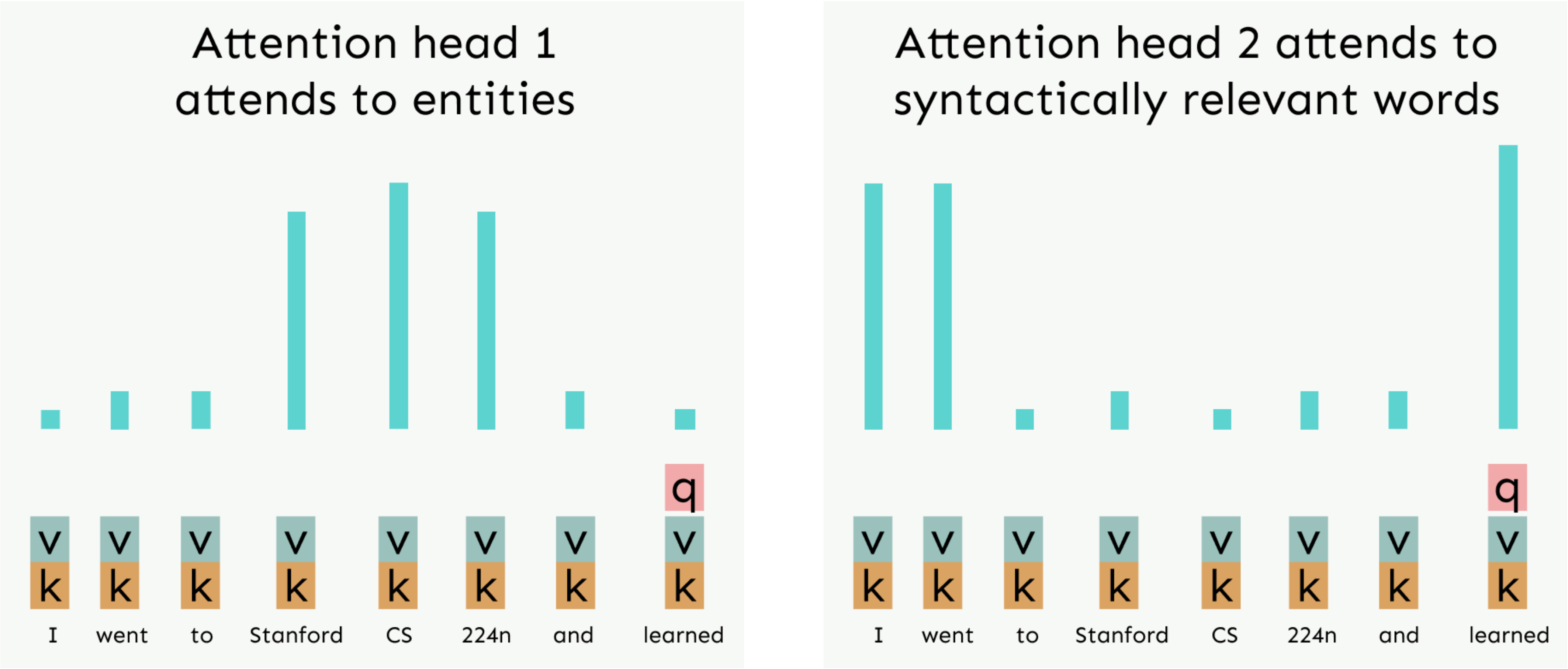


Transformer Decoder

Recall the Self-Attention Hypothetical Example



Hypothetical Example of Multi-Head Attention



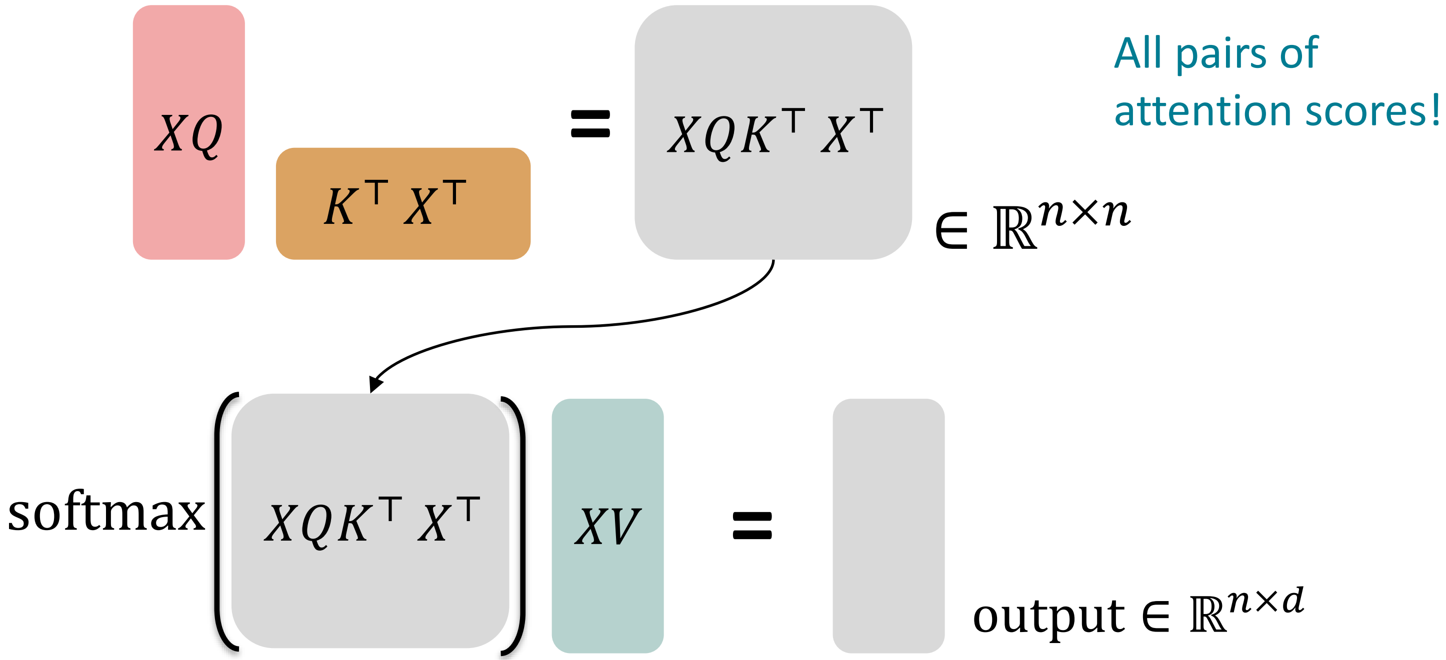
I went to Stanford CS 224n and learned

Sequence-Stacked form of Attention

- Let's look at how key-query-value attention is computed, in matrices.
  - Let $X = [x_1; \ldots; x_n] \in \mathbb{R}^{n \times d}$ be the concatenation of input vectors.
  - First, note that $XK \in \mathbb{R}^{n \times d}$, $XQ \in \mathbb{R}^{n \times d}$, $XV \in \mathbb{R}^{n \times d}$.
  - The output is defined as output $= \text{softmax}(XQ(XK)^\top)XV \in\in \mathbb{R}^{n \times d}$.

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

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



Multi-headed attention

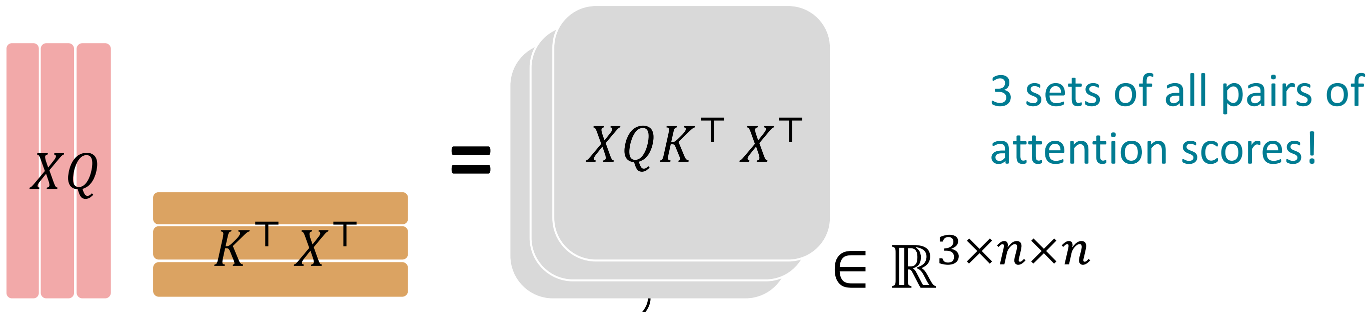
- What if we want to look in multiple places in the sentence at once?
  - For word i, self-attention "looks" where $x_i^\top Q^\top K x_j$ is high, but maybe we want to focus on different j for different reasons?
- We'll define **multiple attention "heads"** through multiple Q,K,V matrices
- Let, $Q_\ell, K_\ell, V_\ell \in \mathbb{R}^{d \times \frac{d}{h}}$, where h is the number of attention heads, and ℓ ranges from 1 to h.
- Each attention head performs attention independently:
  - $\text{output}_\ell = \text{softmax}\left(X Q_\ell K_\ell^\top X^\top\right) * X V_\ell$, where $\text{output}_\ell \in \mathbb{R}^{d/h}$
- Then the outputs of all the heads are combined!
  - $\text{output} = [\text{output}_1; \ldots; \text{output}_h] Y$, where $Y \in \mathbb{R}^{d \times d}$

- Each head gets to "look" at different things, and construct value vectors differently.

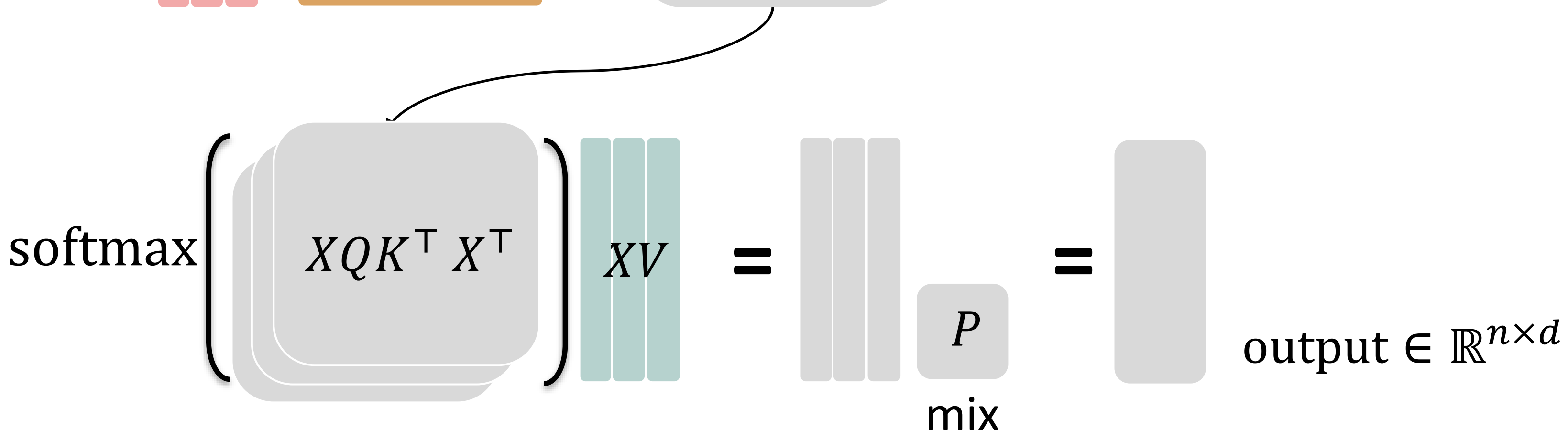
Multi-head self-attention is computationally efficient

- Even though we compute h many attention heads, it's not really more costly.
  - We compute $XQ \in \mathbb{R}^{n\times d}$, and then reshape to $\mathbb{R}^{n\times h\times d/h}$. (Likewise for XK, XV.)
  - Then we transpose to $\mathbb{R}^{h\times n\times d/h}$; now the head axis is like a batch axis.
  - Almost everything else is identical, and the **matrices are the same sizes.**

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



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



Scaled Dot Product [Vaswani et al., 2017]

- **"Scaled Dot Product"** attention aids in 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:

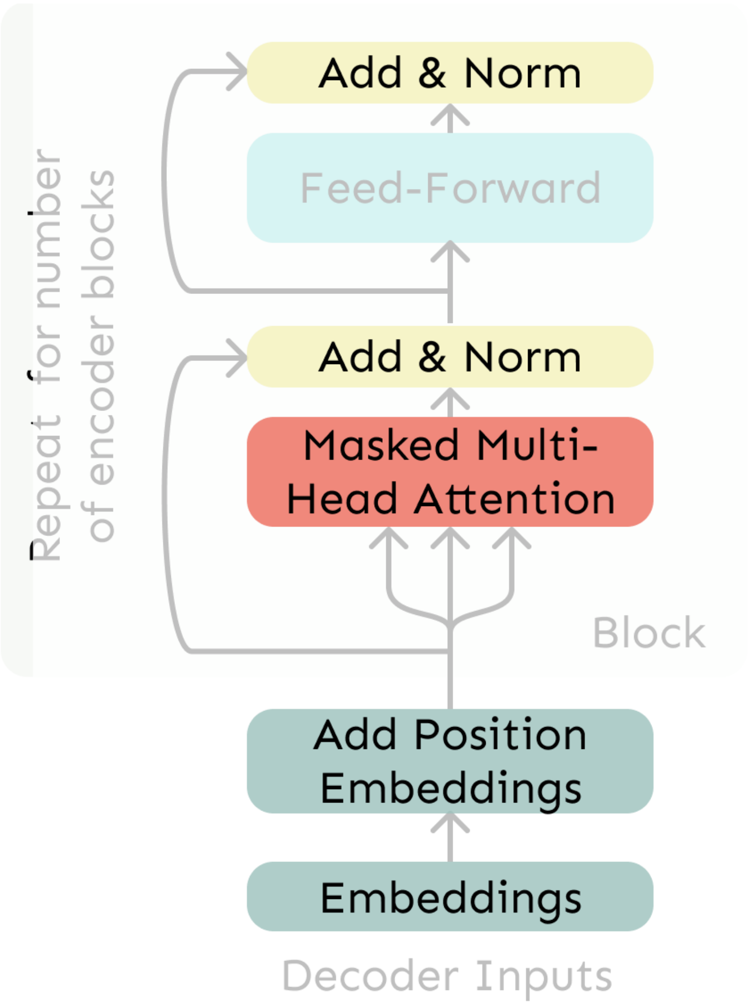
$$\mathrm{output}_\ell = \mathrm{softmax}\left(XQ_\ell K_\ell^\top X^\top\right) * XV_\ell$$

- 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.)

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

The Transformer Decoder

- Now that we've replaced self-attention with multi-head self-attention, we'll go through two **optimization tricks** that end up being :
  - **Residual Connections**
  - **Layer Normalization**
- In most Transformer diagrams, these are often written together as "Add & Norm"

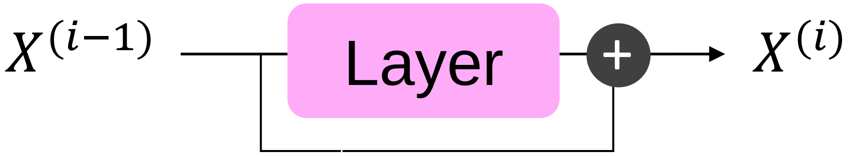


Transformer Decoder

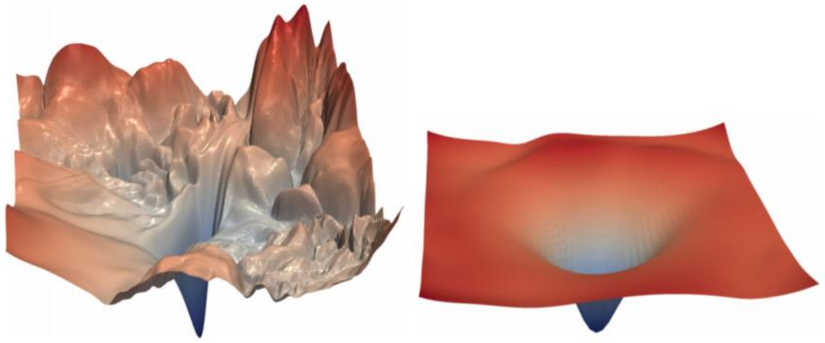
The Transformer Encoder: **Residual connections** [He et al., 2016]

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

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



  - Gradient is **great** through the residual connection; it's 1!
  - Bias towards the identity function!



[no residuals] [residuals]

[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 $\mu = \sum_{j=1}^{d} x_j$; this is the mean; $\mu \in \mathbb{R}$.
- Let $\sigma = \sqrt{\frac{1}{d} \sum_{j=1}^{d} \left(x_j - \mu\right)^2}$; 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:

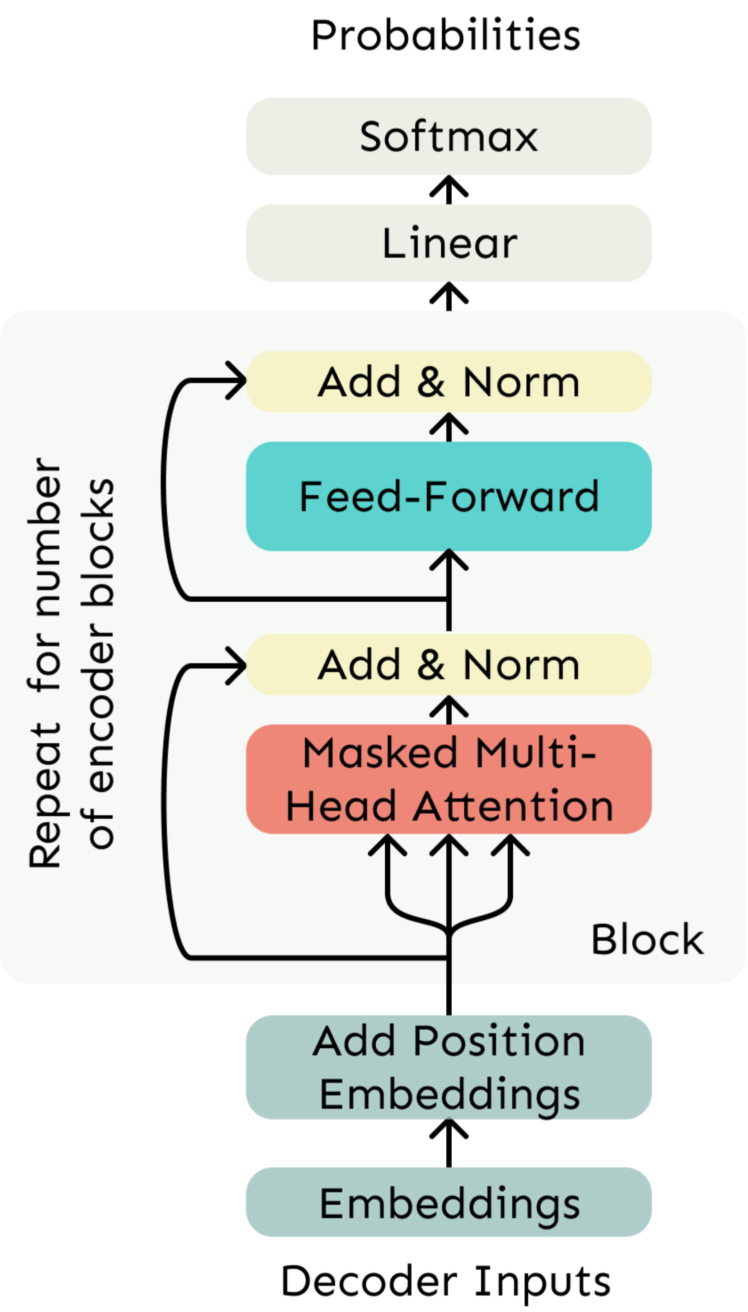
$$\text{output} = \frac{x - \mu}{\sqrt{\sigma} + \epsilon} * \gamma + \beta$$

Normalize by scalar mean and variance

Modulate by learned elementwise gain and bias

The Transformer Decoder

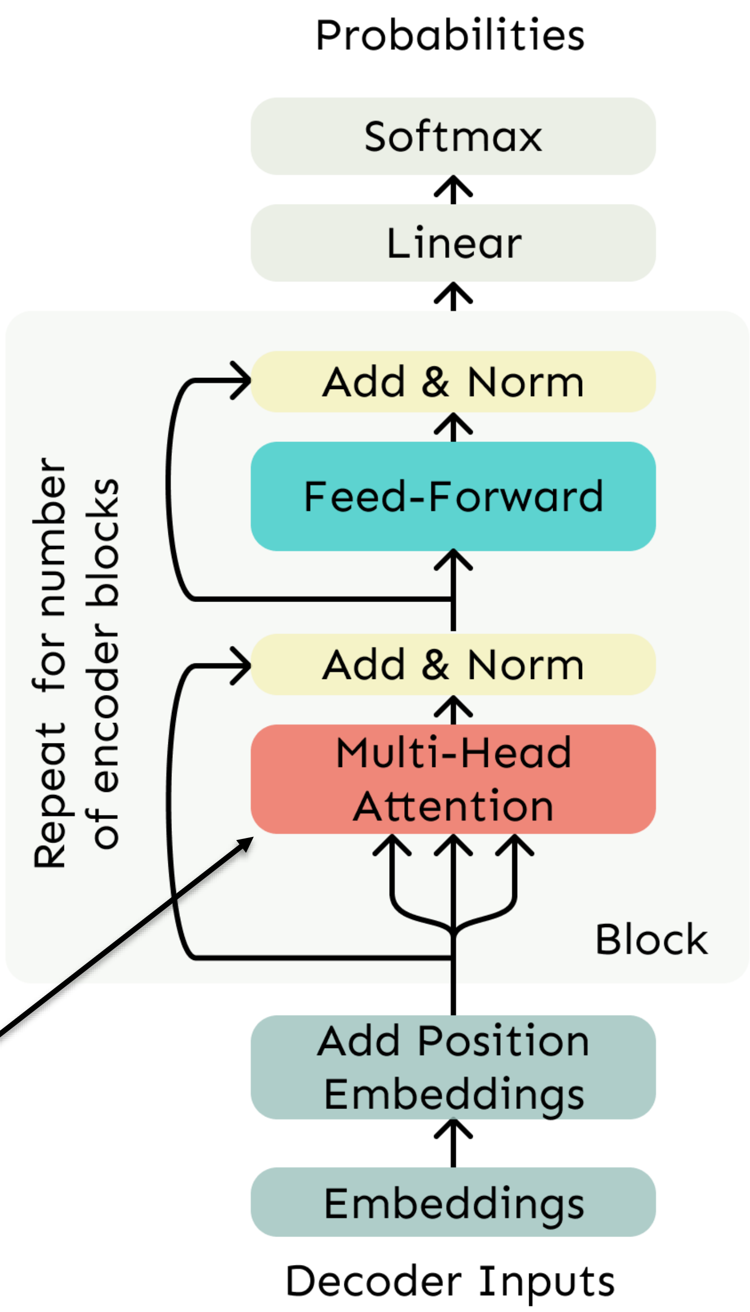
- The Transformer Decoder is a stack of Transformer Decoder **Blocks**.
- Each Block consists of:
  - Self-attention
  - Add & Norm
  - Feed-Forward
  - Add & Norm
- That's it! We've gone through the Transformer Decoder.



The Transformer Encoder

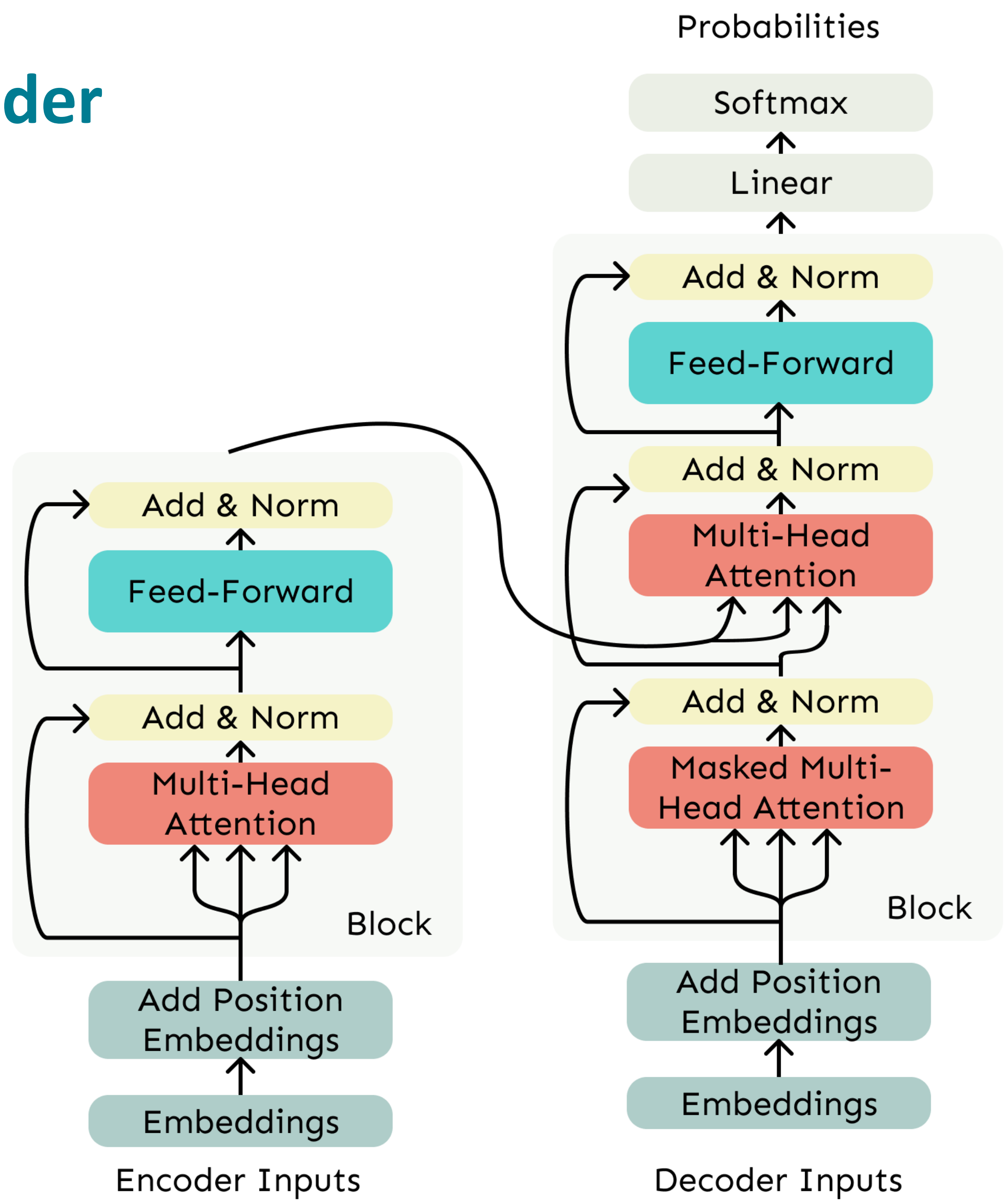
- The Transformer Decoder constrains to **unidirectional context**, as for **language models.**
- What if we want **bidirectional context**, like in a bidirectional RNN?
- This is the Transformer Encoder. The only difference is that we **remove the masking** in the self-attention.

No Masking!



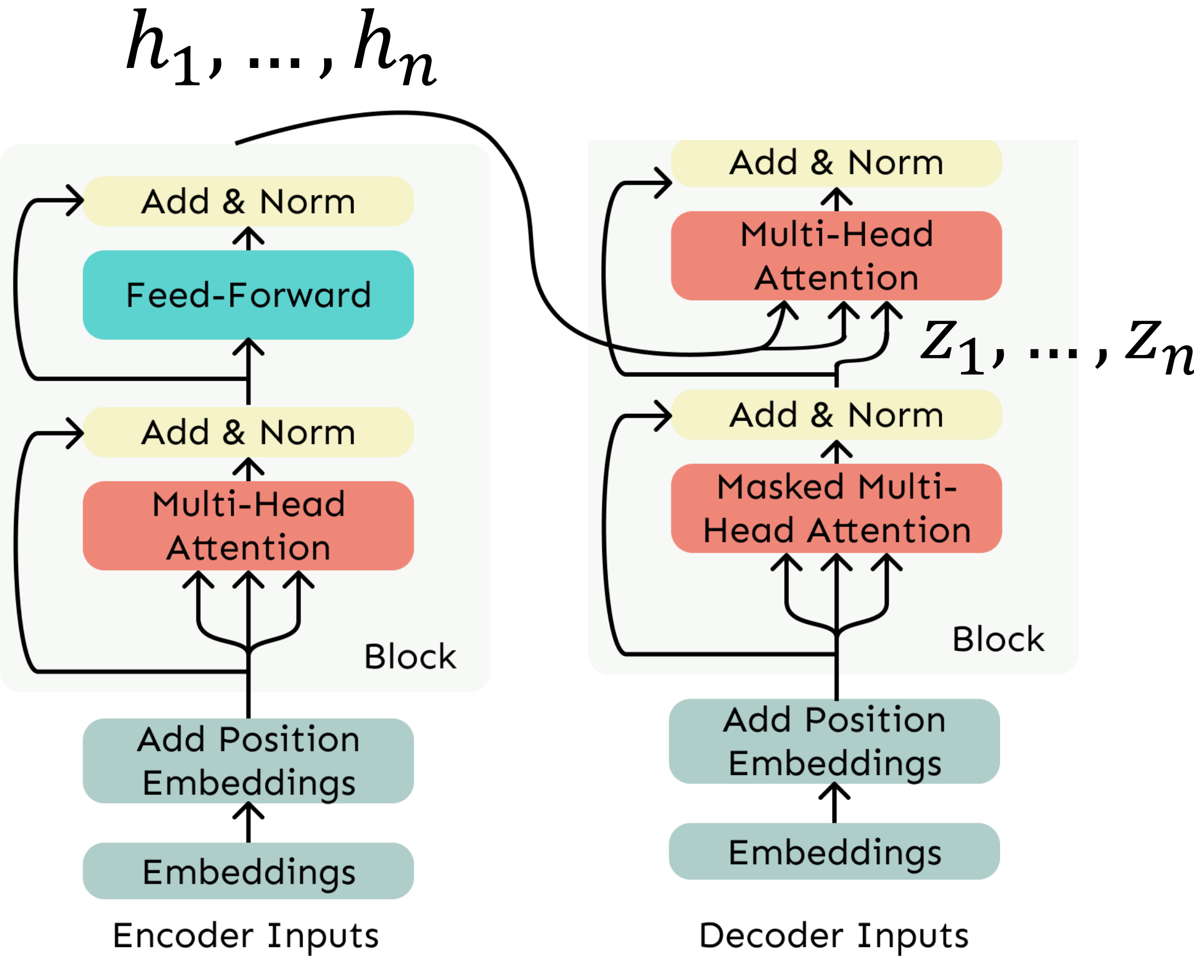
The Transformer Encoder-Decoder

- Recall that in machine translation, we processed the source sentence with a **bidirectional** model and generated the target with a **unidirectional model**.
- For this kind of seq2seq format, we often use a Transformer Encoder-Decoder.
- We use a normal Transformer Encoder.
- Our Transformer Decoder is modified to perform **cross-attention** to the output of the Encoder.



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 $h_1, \dots, h_n$ be **output** vectors **from** the Transformer **encoder**; $x_i \in \mathbb{R}^d$
- Let $z_1, \dots, z_n$ 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**, $q_i = Qz_i$.



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)	
	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**	$7.7 \cdot 10^{19}$	$1.2 \cdot 10^{21}$

 [Test sets: WMT 2014 English-German and English-French]

[Vaswani et al., 2017]

Great Results with Transformers

Next, document generation!

Model	Test perplexity	ROUGE-L
seq2seq-attention, $L = 500$	5.04952	12.7
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

The old standard

Transformers all the way down.

[Liu et al., 2018]; WikiSum dataset

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:

GLUE

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		90.6
+	4	PING-AN Omni-Sinitic	ALBERT + DAAF + NAS		90.6
	5	ERNIE Team - Baidu	ERNIE		90.4
	6	T5 Team - Google	T5		90.3

More results Thursday when we discuss pretraining.

[Liu et al., 2018]

Outline

1. From recurrence (RNN) to attention-based NLP models
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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 $O(n^2 d)$, where n is the sequence length, and d is the dimensionality.

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

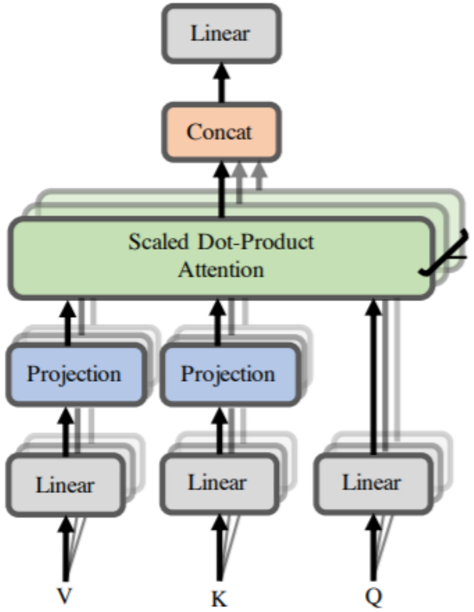
Need to compute all pairs of interactions! $O(n^2 d)$

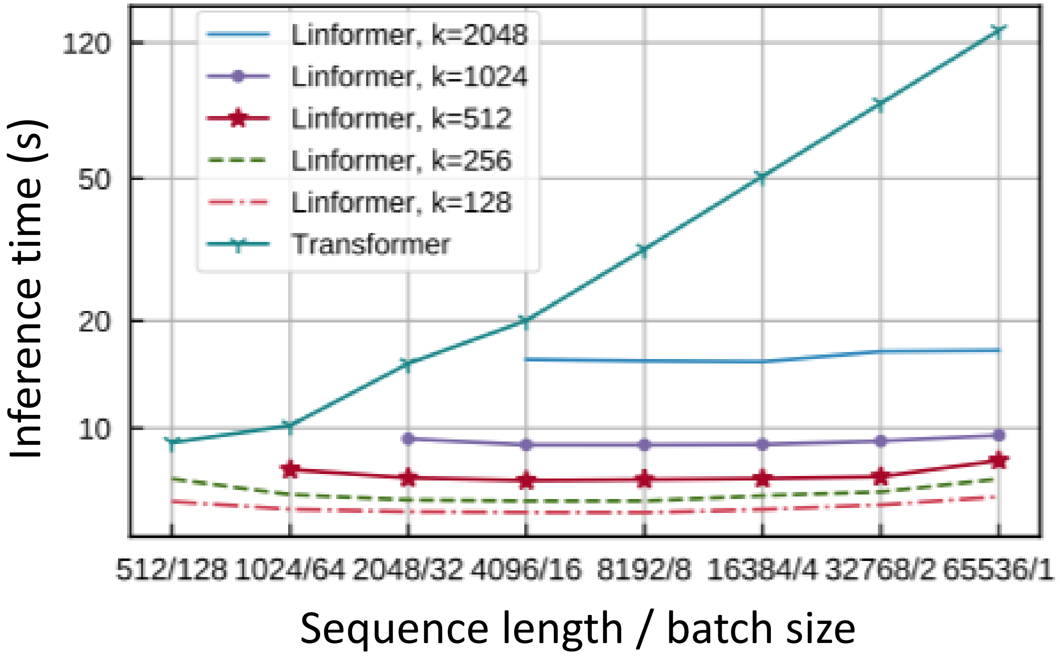
- Think of d as around $\mathbf{1,000}$ (though for large language models it's much larger!).
  - So, for a single (shortish) sentence, $n \leq 30; n^2 \leq \mathbf{900}$.
  - In practice, we set a bound like $n = 512$.
  - **But what if we'd like $\boldsymbol{n} \geq \mathbf{50,000}$?** For example, to work on long documents?

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





Do we even need to remove the quadratic cost of attention?

- As Transformers grow larger, a larger and larger percent of compute is **outside** the self-attention portion, despit the quadratic cost.
- In practice, **almost no large Transformer language models use anything but the quadratic cost attention we've presented here.**
  - The cheaper methods tend not to work as well at scale.
- So, is there no point in trying to design cheaper alternatives to self-attention?
- Or would we unlock much better models with much longer contexts (>100k tokens?) if we were to do it right?

Do Transformer Modifications Transfer?

- "Surprisingly, we find that most modifications do not meaningfully improve performance."

Model	Params	Ops	Step/s	Early loss	Final loss	SGLUE	XSum	WebQ	WMT EnDe
Vanilla Transformer	223M	11.1T	3.50	2.182 ± 0.005	1.838	71.66	17.78	23.02	26.62
GeLU	223M	11.1T	3.58	2.179 ± 0.003	1.838	**75.79**	**17.86**	**25.13**	26.47
Swish	223M	11.1T	3.62	2.186 ± 0.003	1.847	**73.77**	17.74	**24.34**	**26.75**
ELU	223M	11.1T	3.56	2.270 ± 0.007	1.932	67.83	16.73	23.02	26.08
GLU	223M	11.1T	3.59	2.174 ± 0.003	**1.814**	**74.20**	**17.42**	24.34	**27.12**
GeGLU	223M	11.1T	3.55	2.130 ± 0.006	**1.792**	**75.96**	**18.27**	**24.87**	**26.87**
ReGLU	223M	11.1T	3.57	2.145 ± 0.004	**1.803**	**76.17**	**18.36**	**24.87**	**27.02**
SeLU	223M	11.1T	3.55	2.315 ± 0.004	1.948	68.76	16.76	22.75	25.99
SwiGLU	223M	11.1T	3.53	2.127 ± 0.003	**1.789**	**76.00**	**18.20**	**24.34**	**27.02**
LiGLU	223M	11.1T	3.59	2.149 ± 0.005	**1.798**	**75.34**	**17.97**	**24.34**	26.53
Sigmoid	223M	11.1T	3.63	2.291 ± 0.019	1.867	**74.31**	17.51	23.02	26.30
Softplus	223M	11.1T	3.47	2.207 ± 0.011	1.850	**72.45**	17.65	**24.34**	**26.89**
RMS Norm	223M	11.1T	3.68	2.167 ± 0.008	**1.821**	**75.45**	**17.94**	**24.07**	**27.14**
Rezero	223M	11.1T	3.51	2.262 ± 0.003	1.939	61.69	15.64	20.90	26.37
Rezero + LayerNorm	223M	11.1T	3.26	2.223 ± 0.006	1.858	70.42	17.58	23.02	26.29
Rezero + RMS Norm	223M	11.1T	3.34	2.221 ± 0.009	1.875	70.33	17.32	23.02	26.19
Fixup	223M	11.1T	2.95	2.382 ± 0.012	2.067	58.56	14.42	23.02	26.31
24 layers, $d_{ff} = 1536$, $H = 6$	224M	11.1T	3.33	2.200 ± 0.007	1.843	**74.89**	17.75	**25.13**	**26.89**
18 layers, $d_{ff} = 2048$, $H = 8$	223M	11.1T	3.38	2.185 ± 0.005	**1.831**	**76.45**	16.83	**24.34**	**27.10**
8 layers, $d_{ff} = 4608$, $H = 18$	223M	11.1T	3.69	2.190 ± 0.005	1.847	**74.58**	17.69	**23.28**	**26.85**
6 layers, $d_{ff} = 6144$, $H = 24$	223M	11.1T	3.70	2.201 ± 0.010	1.857	**73.55**	17.59	**24.60**	**26.66**
Block sharing	65M	11.1T	3.91	2.497 ± 0.037	2.164	64.50	14.53	21.96	25.48
+ Factorized embeddings	45M	9.4T	4.21	2.631 ± 0.305	2.183	60.84	14.00	19.84	25.27
+ Factorized & shared embeddings	20M	9.1T	4.37	2.907 ± 0.313	2.385	53.95	11.37	19.84	25.19
Encoder only block sharing	170M	11.1T	3.68	2.298 ± 0.023	1.929	69.60	16.23	23.02	26.23
Decoder only block sharing	144M	11.1T	3.70	2.352 ± 0.029	2.082	67.93	16.13	**23.81**	26.08
Factorized Embedding	227M	9.4T	3.80	2.208 ± 0.006	1.855	70.41	15.92	22.75	26.50
Factorized & shared embeddings	202M	9.1T	3.92	2.320 ± 0.010	1.952	68.69	16.33	22.22	26.44
Tied encoder/decoder input embeddings	248M	11.1T	3.55	2.192 ± 0.002	1.840	**71.70**	17.72	**24.34**	26.49
Tied decoder input and output embeddings	248M	11.1T	3.57	2.187 ± 0.007	**1.827**	**74.86**	17.74	**24.87**	**26.67**
Untied embeddings	273M	11.1T	3.53	2.195 ± 0.005	**1.834**	**72.99**	17.58	**23.28**	26.48
Adaptive input embeddings	204M	9.2T	3.55	2.250 ± 0.002	1.899	66.57	16.21	**24.07**	**26.66**
Adaptive softmax	204M	9.2T	3.60	2.364 ± 0.005	1.982	**72.91**	16.67	21.16	25.56
Adaptive softmax without projection	223M	10.8T	3.43	2.229 ± 0.009	1.914	**71.82**	17.10	23.02	25.72
Mixture of softmaxes	232M	16.3T	2.24	2.227 ± 0.017	**1.821**	**76.77**	17.62	22.75	**26.82**
Transparent attention	223M	11.1T	3.33	2.181 ± 0.014	1.874	54.31	10.40	21.16	**26.80**
Dynamic convolution	257M	11.8T	2.65	2.403 ± 0.009	2.047	58.30	12.67	21.16	17.03
Lightweight convolution	224M	10.4T	4.07	2.370 ± 0.010	1.989	63.07	14.86	23.02	24.73
Evolved Transformer	217M	9.9T	3.09	2.220 ± 0.003	1.863	**73.67**	10.76	**24.07**	26.58
Synthesizer (dense)	224M	11.4T	3.47	2.334 ± 0.021	1.962	61.03	14.27	16.14	**26.63**
Synthesizer (dense plus)	243M	12.6T	3.22	2.191 ± 0.010	1.840	**73.98**	16.96	**23.81**	**26.71**
Synthesizer (dense plus alpha)	243M	12.6T	3.01	2.180 ± 0.007	**1.828**	**74.25**	17.02	**23.28**	26.61
Synthesizer (factorized)	207M	10.1T	3.94	2.341 ± 0.017	1.968	62.78	15.39	**23.55**	26.42
Synthesizer (random)	254M	10.1T	4.08	2.326 ± 0.012	2.009	54.27	10.35	19.56	26.44
Synthesizer (random plus)	292M	12.0T	3.63	2.189 ± 0.004	1.842	**73.32**	17.04	**24.87**	26.43
Synthesizer (random plus alpha)	292M	12.0T	3.42	2.186 ± 0.007	**1.828**	**75.24**	17.08	**24.08**	26.39
Universal Transformer	84M	40.0T	0.88	2.406 ± 0.036	2.053	70.13	14.09	19.05	23.91
Mixture of experts	648M	11.7T	3.20	2.148 ± 0.006	**1.785**	**74.55**	**18.13**	**24.08**	**26.94**
Switch Transformer	1100M	11.7T	3.18	2.135 ± 0.007	**1.758**	**75.38**	**18.02**	**26.19**	**26.81**
Funnel Transformer	223M	1.9T	4.30	2.288 ± 0.008	1.918	67.34	16.26	22.75	23.20
Weighted Transformer	280M	71.0T	0.59	2.378 ± 0.021	1.989	69.04	16.98	23.02	26.30
Product key memory	421M	386.6T	0.25	2.155 ± 0.003	**1.798**	**75.16**	17.04	**23.55**	**26.73**

Do Transformer Modifications Transfer Across Implementations and Applications?

Sharan Narang[*] Hyung Won Chung Yi Tay William Fedus
Thibault Fevry[†] Michael Matena[†] Karishma Malkan[†] Noah Fiedel
Noam Shazeer Zhenzhong Lan[†] Yanqi Zhou Wei Li
Nan Ding Jake Marcus Adam Roberts Colin Raffel[†]

Parting remarks

- Pretraining on Tuesday!
- Good luck on assignment 4!
- Remember to work on your project proposal!

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		vocab mapping	embedding
Common words	hat	→	pizza (index)	
	learn	→	tasty (index)	
Variations	taaaaasty	→	UNK (index)	
misspellings	laern	→	UNK (index)	
novel items	Transformerify	→	UNK (index)	

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.

Conjugation of -*ambia* [less ▲]

Non-finite forms		
Form	Positive	Negative
Infinitive	kuambia	kutoambia

Simple finite forms		
Positive form	Singular	Plural
Imperative	ambia	ambieni
Habitual	huambia	

Complex finite forms																		
Polarity	Persons				Persons / Classes		Classes											
	1st		2nd		3rd / M-wa		M-mi		Ma		Ki-vi		N		U	Ku	Pa	Mu
	Sg.	Pl.	Sg.	Pl.	Sg. / 1	Pl. / 2	3	4	5	6	7	8	9	10	11 / 14	15 / 17	16	18
Past [less ▲]																		
Positive	niliambia naliambia	tuliambia twaliambia	uliambia waliambia	mliambia mwaliambia	aliambia	waliambia	uliambia	iliambia	liliambia	yaliambia	kiliambia	viliambia	iliambia	ziliambia	uliambia	kuliambia	paliambia	muliambia
Negative	sikuambia	hatukuambia	hukuambia	hamkuambia	hakuambia	hawakuambia	haukuambia	haikuambia	halikuambia	hayakuambia	hakikuambia	havikuambia	haikuambia	hazikuambia	haukuambia	hakukuambia	hapakuambia	hamukuambia
Present [less ▲]																		
Positive	ninaambia naambia	tunaambia	unaambia	mnaambia	anaambia	wanaambia	unaambia	inaambia	linaambia	yanaambia	kinaambia	vinaambia	inaambia	zinaambia	unaambia	kunaambia	panaambia	munaambia
Negative	siambii	hatuambii	huambii	hamambii	haambii	hawaambii	hauambii	haiambii	haliambii	hayaambii	hakiambii	haviambii	haiambii	haziambii	hauambii	hakuambii	hapaambii	hamuambii
Future [less ▲]																		
Positive	nitaambia	tutaambia	utaambia	mtaambia	ataambia	wataambia	utaambia	itaambia	litaambia	yataambia	kitaambia	vitaambia	itaambia	zitaambia	utaambia	kutaambia	pataambia	mutaambia
Negative	sitaambia	hatutaambia	hutaambia	hamtaambia	hataambia	hawataambia	hautaambia	haitaambia	halitaambia	hayataambia	hakitaambia	havitaambia	haitaambia	hazitaambia	hautaambia	hakutaambia	hapataambia	hamutaambia
Subjunctive [less ▲]																		
Positive	niambie	tuambie	uambie	mambie	aambie	waambie	uambie	iambie	liambie	yaambie	kiambie	viambie	iambie	ziambie	uambie	kuambie	paambie	muambie
Negative	nisiambie	tusiambie	usiambie	msiambie	asiambie	wasiambie	usiambie	isiambie	lisiambie	yasiambie	kisiambie	visiambie	isiambie	zisiambie	usiambie	kusiambie	pasiambie	musiambie
Present Conditional [less ▲]																		
Positive	ningeambia	tungeambia	ungeambia	mngeambia	angeambia	wangeambia	ungeambia	ingeambia	lingeambia	yangeambia	kingeambia	vingeambia	ingeambia	zingeambia	ungeambia	kungeambia	pangeambia	mungeambia
Negative	nisingeambia singeambia	tusingeambia hatungeambia	usingeambia hungeambia	msingeambia hamngeambia	asingeambia hangeambia	wasingeambia hawangeambia	usingeambia haungeambia	isingeambia haingeambia	lisingeambia halingeambia	yasingeambia hayangeambia	kisingeambia hakingeambia	visingeambia havingeambia	isingeambia haingeambia	zisingeambia hazingeambia	usingeambia haungeambia	kusingeambia hakungeambia	pasingeambia hapangeambia	musingeambia hamungeambia
Past Conditional [less ▲]																		
Positive	ningaliambia	tungaliambia	ungaliambia	mngaliambia	angaliambia	wangaliambia	ungaliambia	ingaliambia	lingaliambia	yangaliambia	kingaliambia	vingaliambia	ingaliambia	zingaliambia	ungaliambia	kungaliambia	pangaliambia	mungaliambia
Negative	nisingaliambia singaliambia	tusingaliambia hatungaliambia	usingaliambia hungaliambia	msingaliambia hamngaliambia	asingaliambia hangaliambia	wasingaliambia hawangaliambia	usingaliambia haungaliambia	isingaliambia haingaliambia	lisingaliambia halingaliambia	yasingaliambia hayangaliambia	kisingaliambia hakingaliambia	visingaliambia havingaliambia	isingaliambia haingaliambia	zisingaliambia hazingaliambia	usingaliambia haungaliambia	kusingaliambia hakungaliambia	pasingaliambia hapangaliambia	musingaliambia hamungaliambia
Conditional Contrary to Fact [less ▲]																		
Positive	ningeliambia	tungeliambia	ungeliambia	mngeliambia	angeliambia	wangeliambia	ungeliambia	ingeliambia	lingeliambia	yangeliambia	kingeliambia	vingeliambia	ingeliambia	zingeliambia	ungeliambia	kungeliambia	pangeliambia	mungeliambia
Gnomic [less ▲]																		
Positive	naambia	twaambia	waambia	mwaambia	aambia	waambia	waambia	yaambia	laambia	yaambia	chaambia	vyaambia	yaambia	zaambia	waambia	kwaambia	paambia	mwaambia
Perfect [less ▲]																		

[Wiktionary]

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.

1. 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.

[Sennrich et al., 2016, Wu et al., 2016]

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.

	word		vocab mapping	embedding
Common words	hat	→	hat	
	learn	→	learn	
Variations	taaaaasty	→	taa## aaa## sty	
misspellings	laern	→	la## ern##	
novel items	Transformerify	→	Transformer## ify	

Outline

1. A brief note on subword modeling
2. Motivating model pretraining from word embeddings
3. Model pretraining three ways
    1. Encoders
    2. Encoder-Decoders
    3. Decoders
4. What do we think pretraining is teaching?

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)

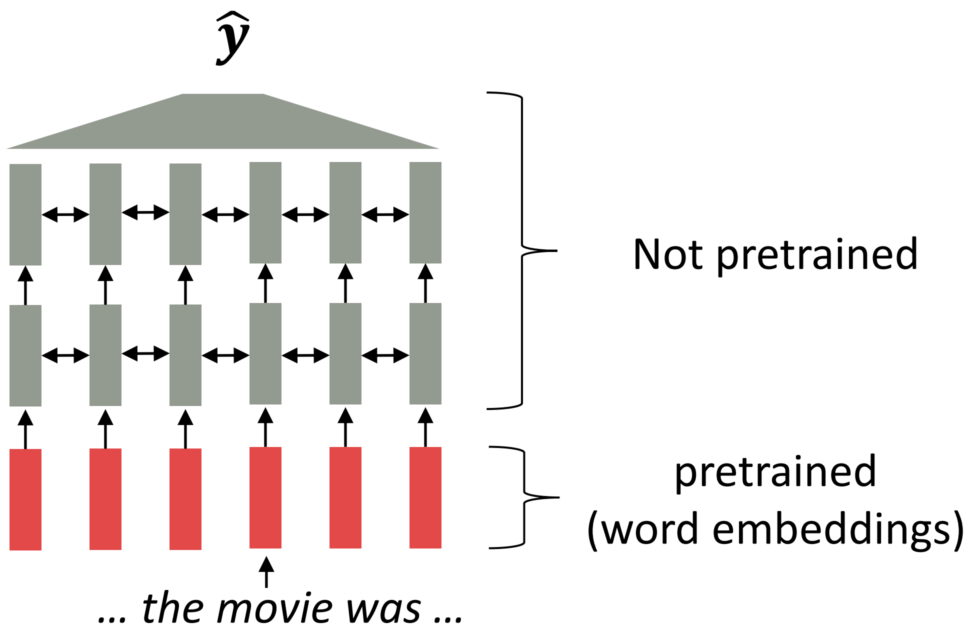
Consider *I **record** the **record***: the two instances of ***record*** mean different things.

[Thanks to Yoav Goldberg on Twitter for pointing out the 1935 Firth quote.]

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.



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

Some issues to think about:

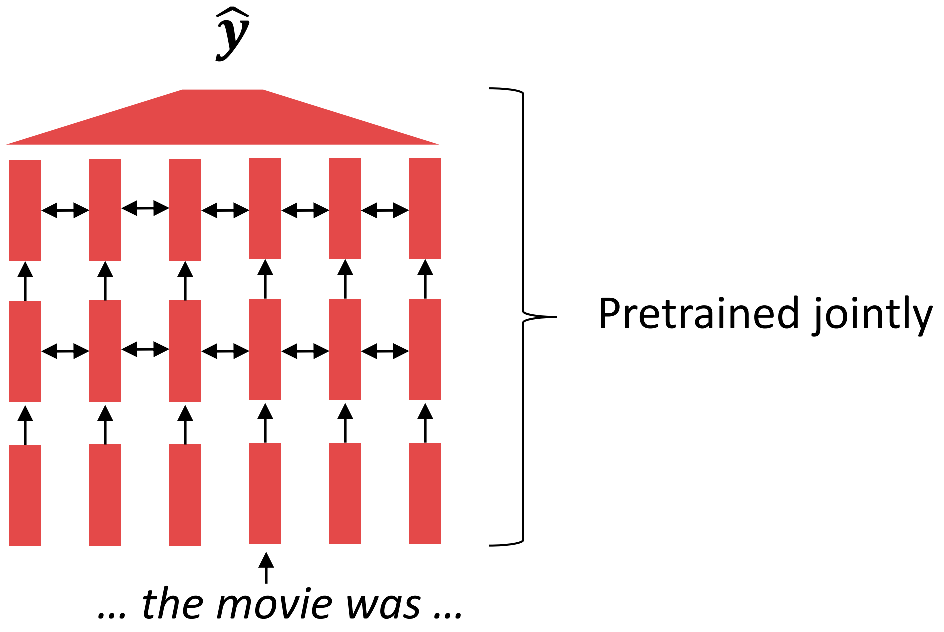
- The training data we have for our **downstream task** (like question answering) must be sufficient to teach all contextual aspects of language.
- Most of the parameters in our network are randomly initialized!

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]

What can we learn from reconstructing the input?

Stanford University is located in __________, California.

What can we learn from reconstructing the input?

I put ___ fork down on the table.

What can we learn from reconstructing the input?

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

What can we learn from reconstructing the input?

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

What can we learn from reconstructing the input?

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

What can we learn from reconstructing the input?

Iroh went into the kitchen to make some tea.

Standing next to Iroh, Zuko pondered his destiny.

Zuko left the _______.

What can we learn from reconstructing the input?

I was thinking about the sequence that goes

1, 1, 2, 3, 5, 8, 13, 21, ____

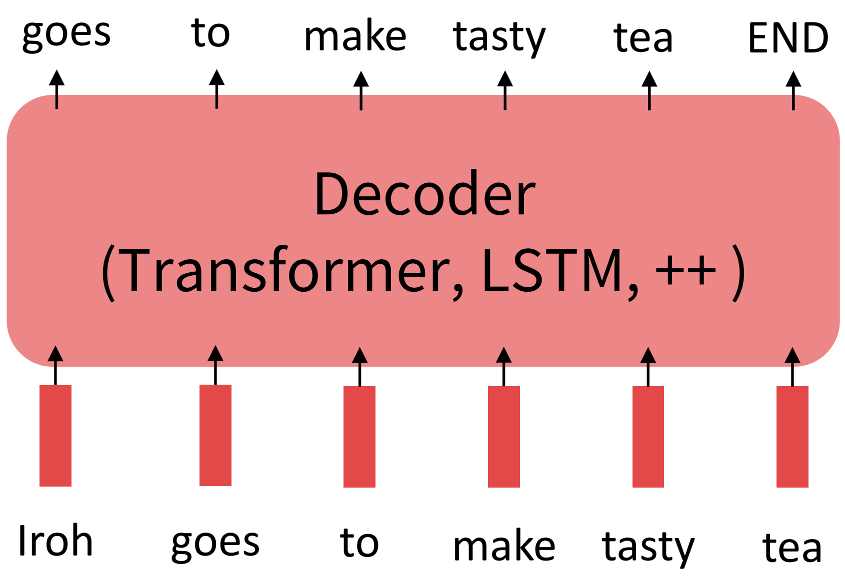
Pretraining through language modeling [Dai and Le, 2015]

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.

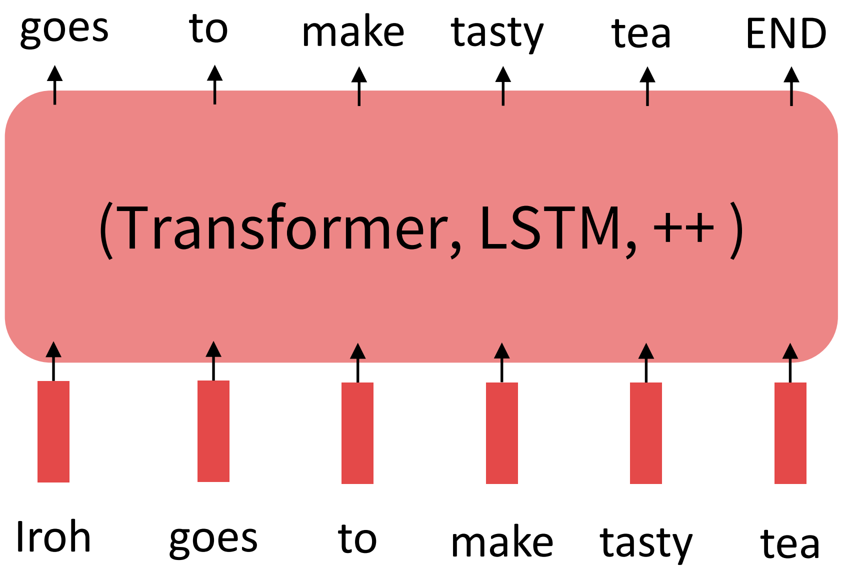


The Pretraining / Finetuning Paradigm

Pretraining can improve NLP applications by serving as parameter initialization.

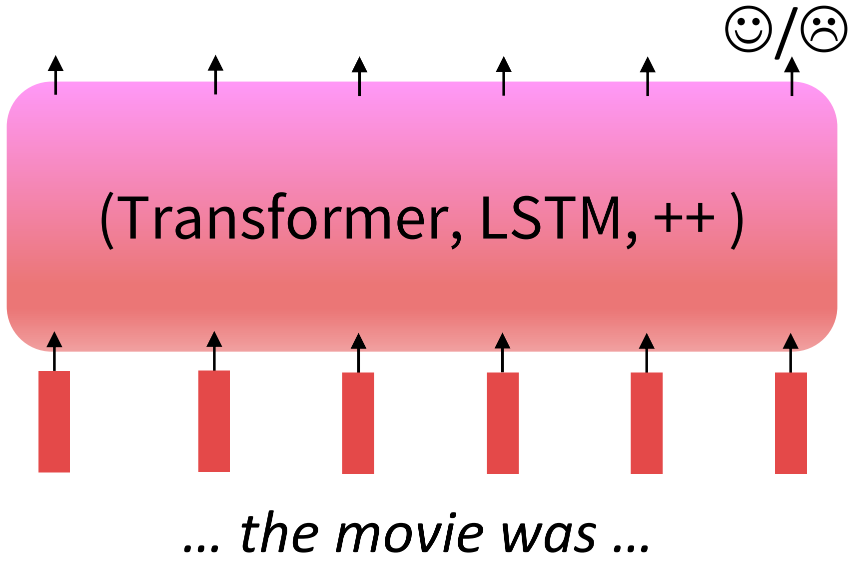
Step 1: Pretrain (on language modeling)

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

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   1. Encoders
   2. Encoder-Decoders
   3. Decoders
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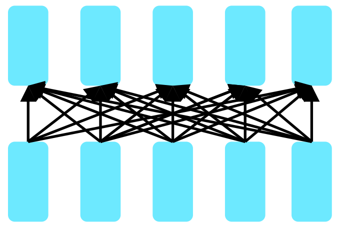
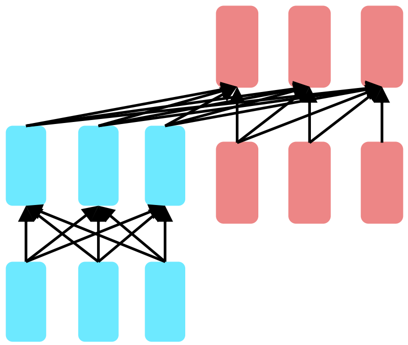
Pretraining for three types of architectures

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



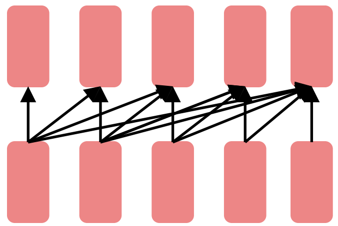
Encoders

- Gets bidirectional context – can condition on future!
- How do we train them to build strong representations?



Encoder-Decoders

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



Decoders

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

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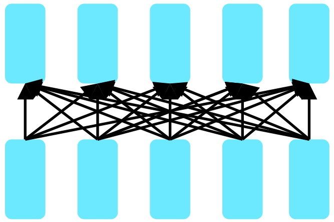

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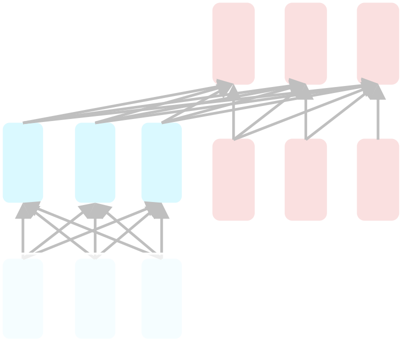

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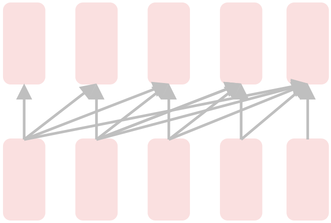

Decoders

- Language models! What we’ve seen so far.
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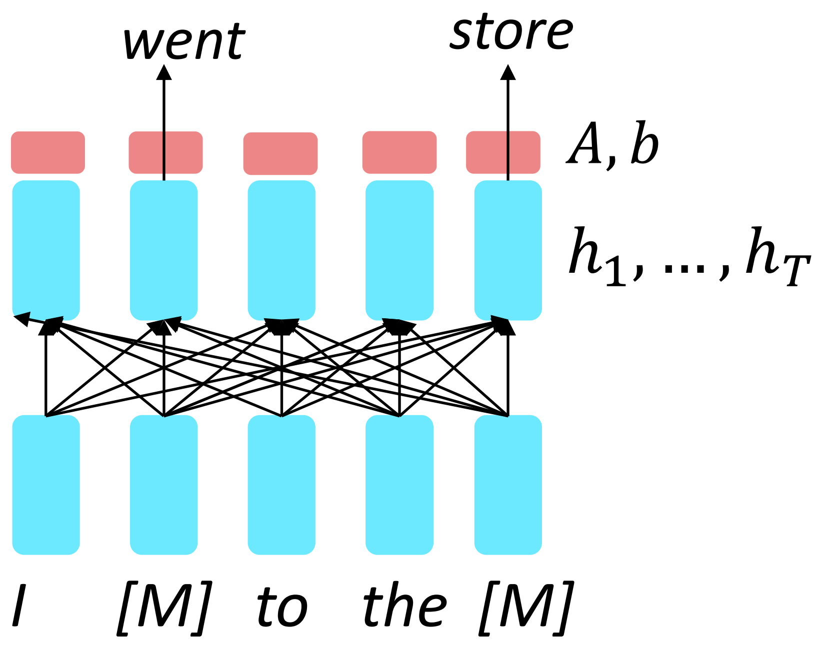
Pretraining encoders: what pretraining objective to use?

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**.

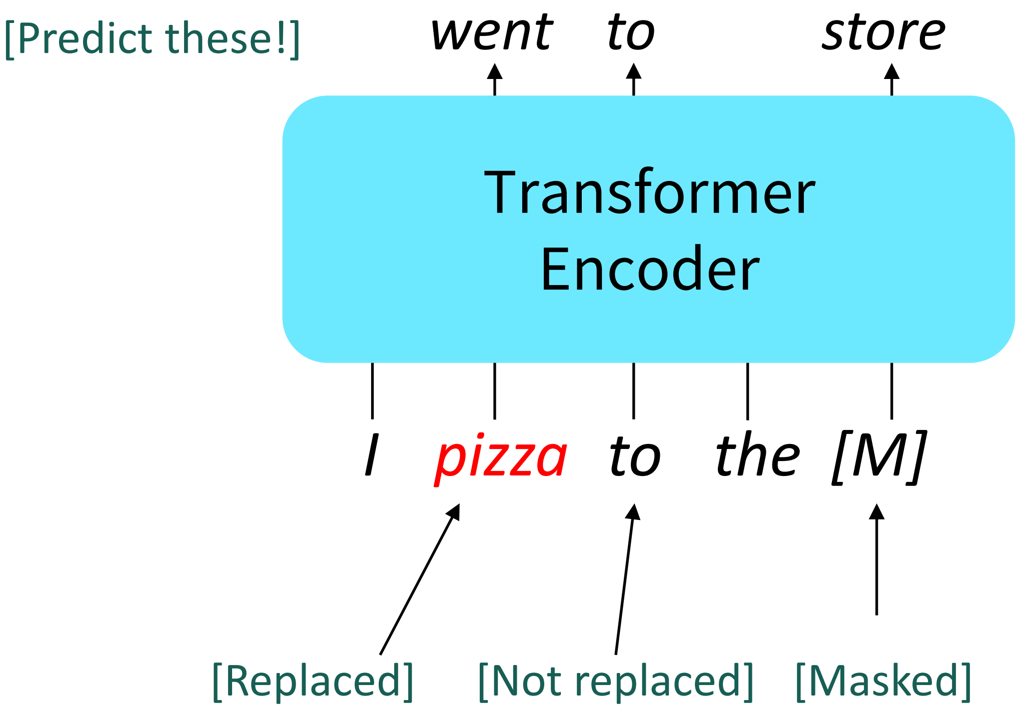
[Devlin et al., 2018]

BERT: Bidirectional Encoder Representations from Transformers

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:

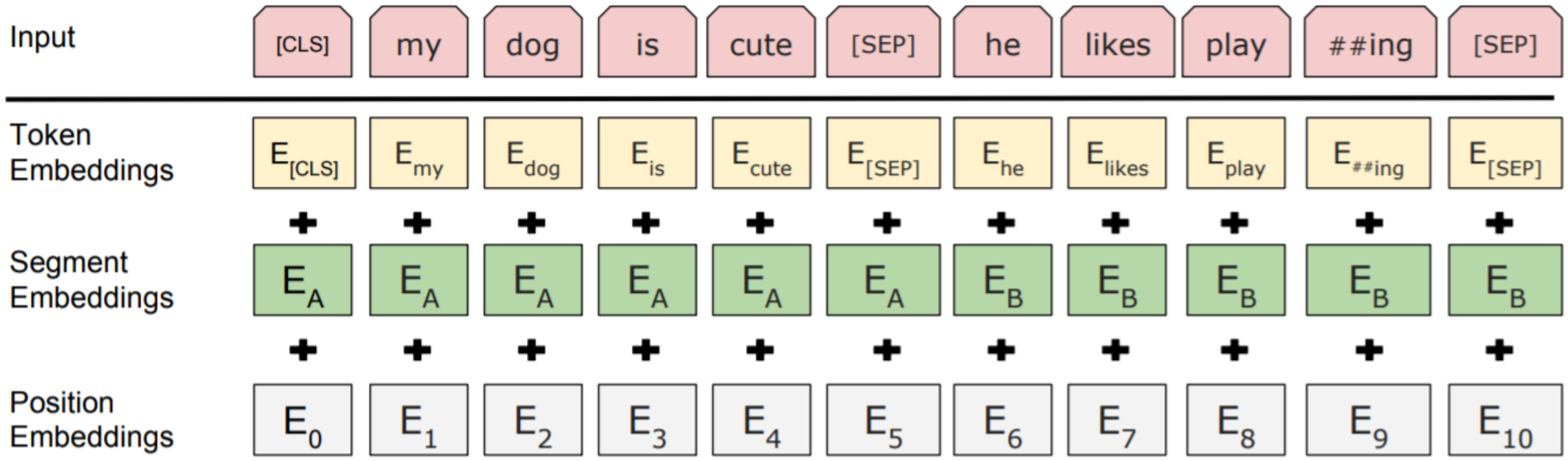
- Predict a random 15% of (sub)word tokens.
    - Replace input word with [MASK] 80% of the time
    - Replace input word with a random token 10% of the time
    - Leave input word unchanged 10% of the time (but still predict it!)
- Why? Doesn't let the model get complacent and not build strong representations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



[Devlin et al., 2018]

BERT: Bidirectional Encoder Representations from Transformers

- 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.

[Devlin et al., 2018, Liu et al., 2019]

BERT: Bidirectional Encoder Representations from Transformers

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."

[Devlin et al., 2018]

BERT: Bidirectional Encoder Representations from Transformers

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

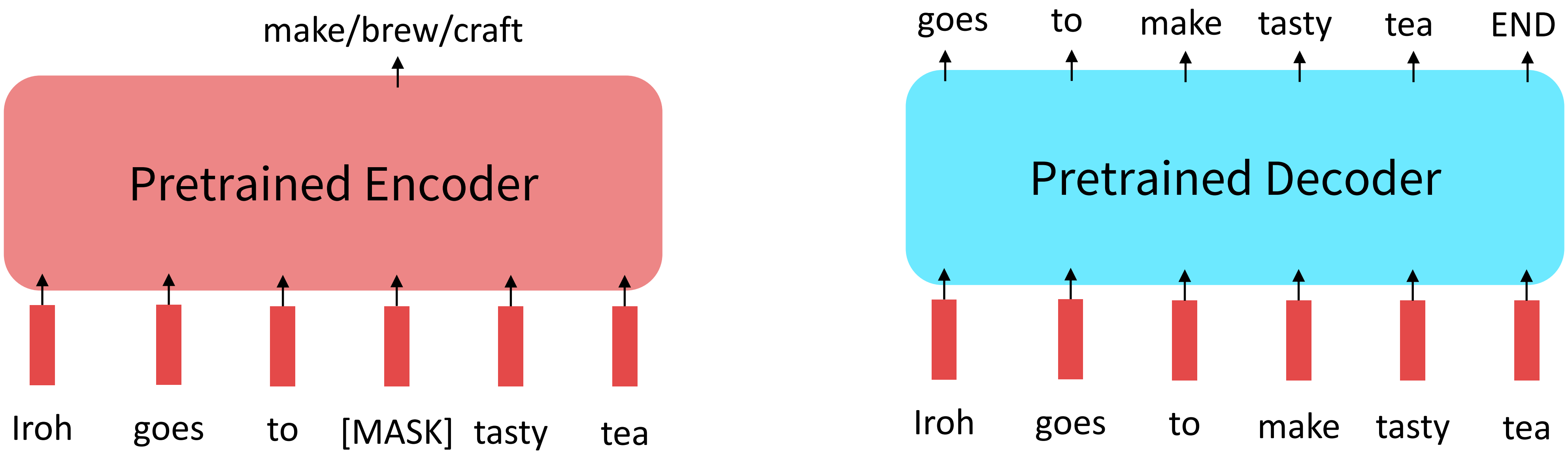
System	MNLI-(m/mm) 392k	QQP 363k	QNLI 108k	SST-2 67k	CoLA 8.5k	STS-B 5.7k	MRPC 3.5k	RTE 2.5k	**Average** -
Pre-OpenAI SOTA	80.6/80.1	66.1	82.3	93.2	35.0	81.0	86.0	61.7	74.0
BiLSTM+ELMo+Attn	76.4/76.1	64.8	79.8	90.4	36.0	73.3	84.9	56.8	71.0
OpenAI GPT	82.1/81.4	70.3	87.4	91.3	45.4	80.0	82.3	56.0	75.1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

[Devlin et al., 2018]

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.

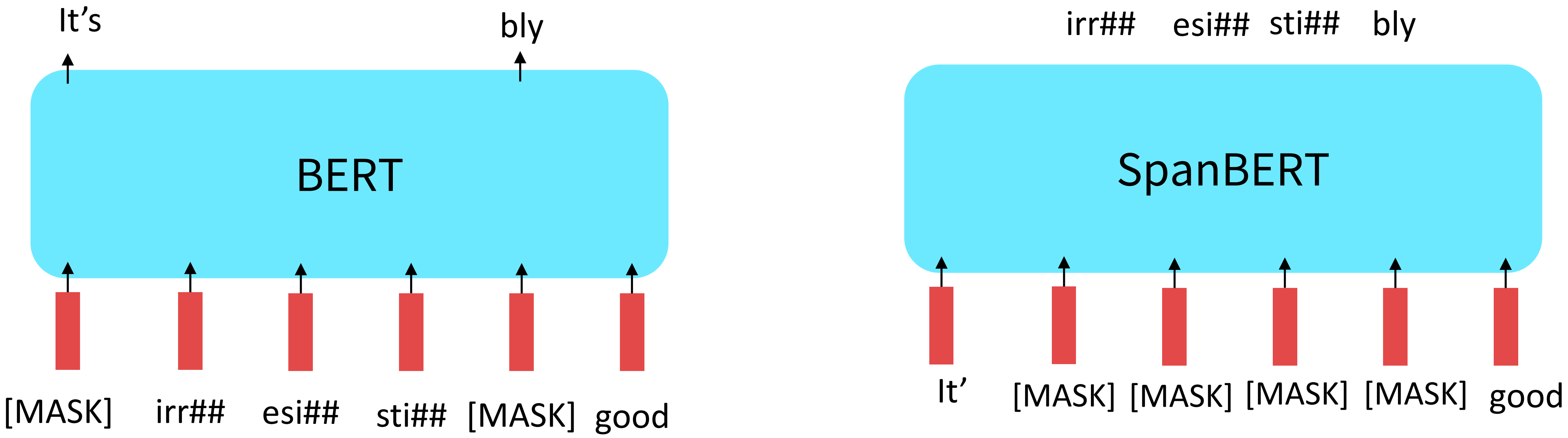


Extensions of BERT

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



[Liu et al., 2019; Joshi et al., 2020]

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	SQuAD (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**
$\text{BERT}_{\text{LARGE}}$						
with BOOKS + WIKI	13GB	256	1M	90.9/81.8	86.6	93.7

[Liu et al., 2019; Joshi et al., 2020]

Full Finetuning vs. Parameter-Efficient Finetuning

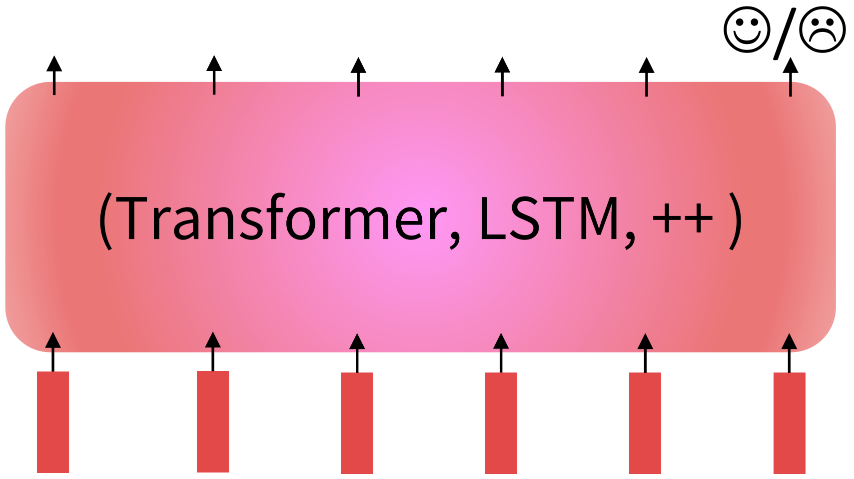
Finetuning every parameter in a pretrained model works well, but is memory-intensive.

But **lightweight** finetuning methods adapt pretrained models in a constrained way.

Leads to **less overfitting** and/or **more efficient finetuning and inference.**

Full Finetuning

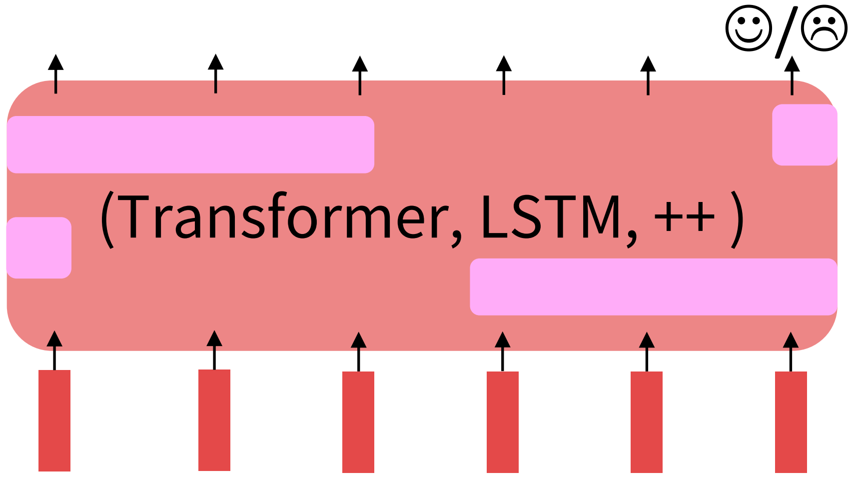
Adapt all parameters



… the movie was …

Lightweight Finetuning

Train a few existing or new parameters



… the movie was …

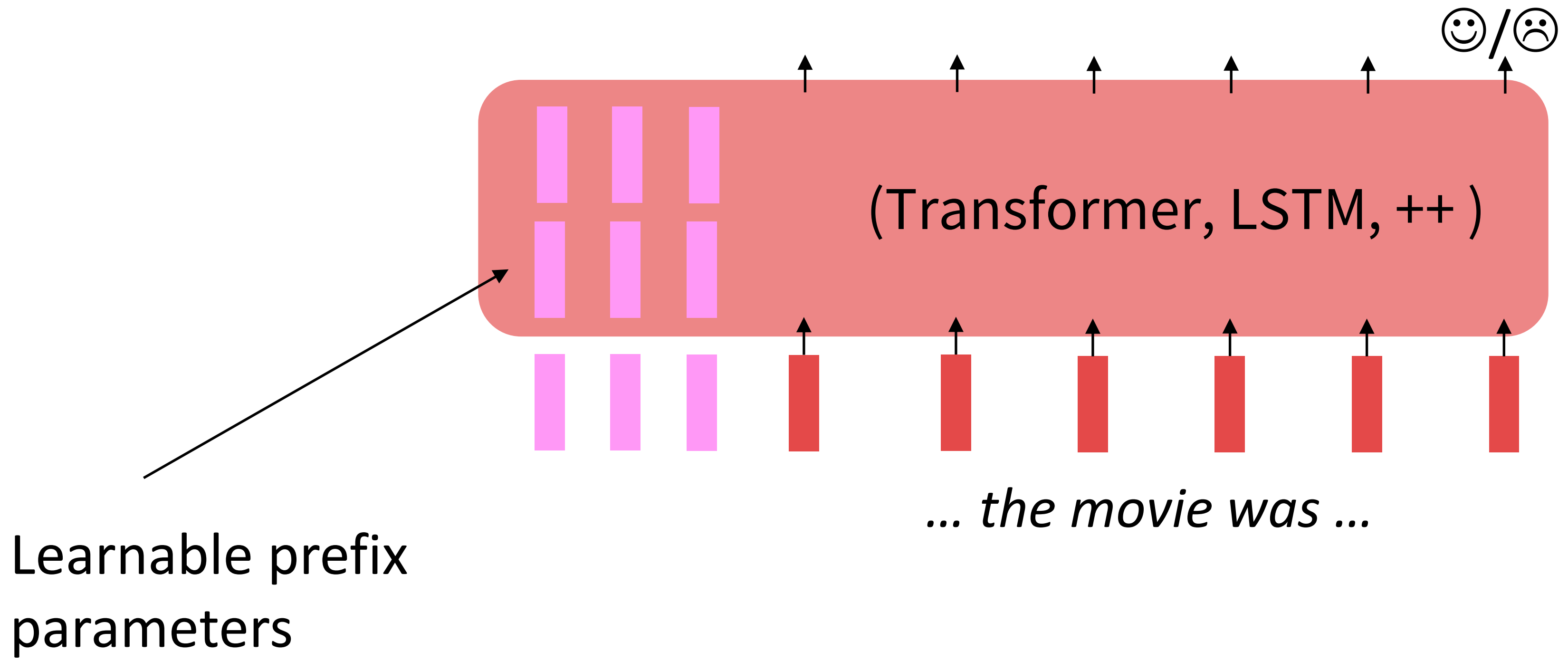
[Liu et al., 2019; Joshi et al., 2020]

Parameter-Efficient Finetuning: Prefix-Tuning, Prompt tuning

Prefix-Tuning adds a **prefix** of parameters, and **freezes all pretrained parameters.**

The prefix is processed by the model just like real words would be.

Advantage: each element of a batch at inference could run a different tuned model.

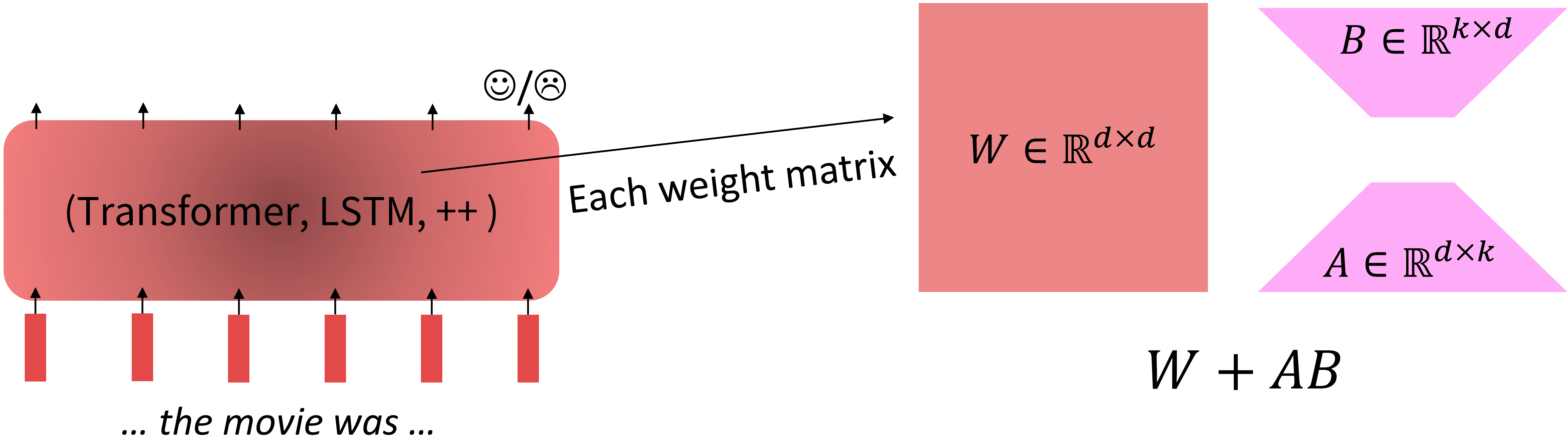


[Li and Liang, 2021; Lester et al., 2021]

Parameter-Efficient Finetuning: Low-Rank Adaptation

Low-Rank Adaptation Learns a low-rank "diff" between the pretrained and finetuned weight matrices.

Easier to learn than prefix-tuning.

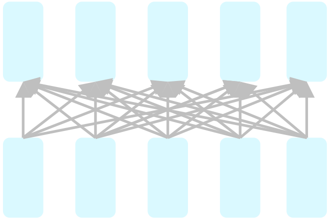


$$W + AB$$

[Hu et al., 2021]

Pretraining for three types of architectures

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



Encoders

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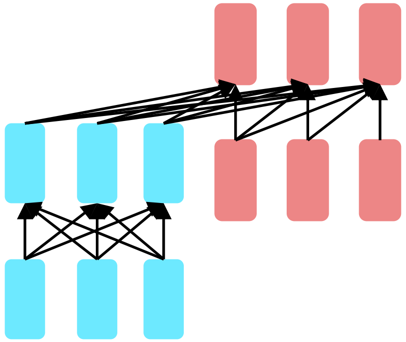
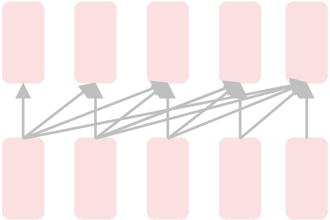


Encoder-Decoders

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



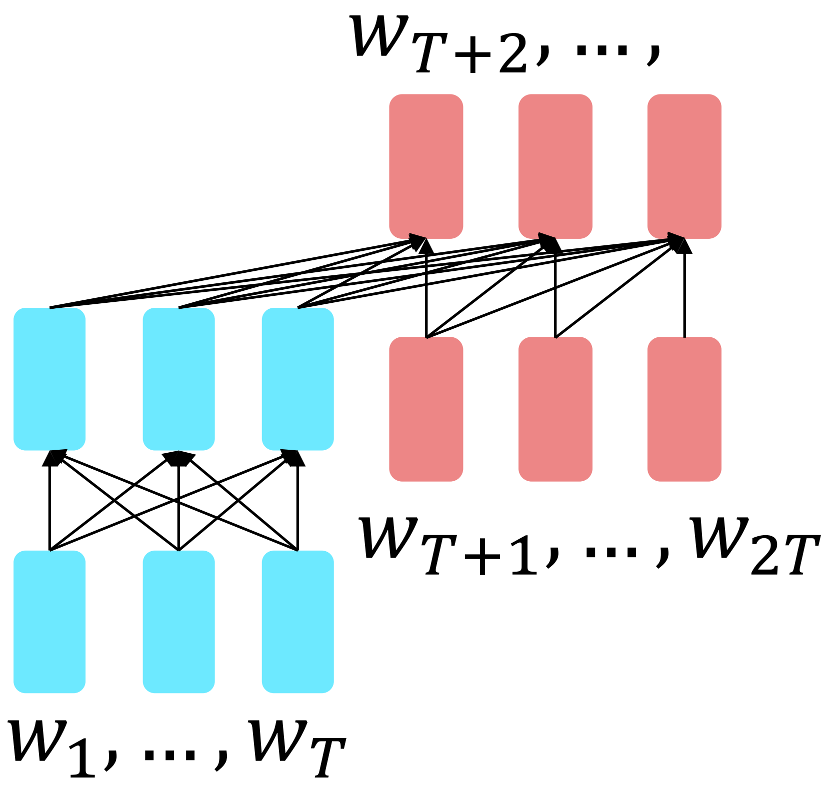
Decoders

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

Pretraining encoder-decoders: what pretraining objective to use?

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.

$$h_1, \dots, h_T = \text{Encoder}(w_1, \dots, w_T)$$
$$h_{T+1}, \dots, h_2 = Decoder(w_1, \dots, w_T, h_1, \dots, h_T)$$
$$y_i \sim Ah_i + b, i > T$$



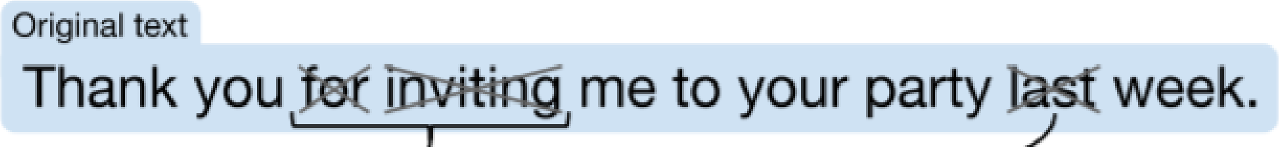
The **encoder** portion benefits from bidirectional context; the **decoder** portion is used to train the whole model through language modeling.

[Raffel et al., 2018]

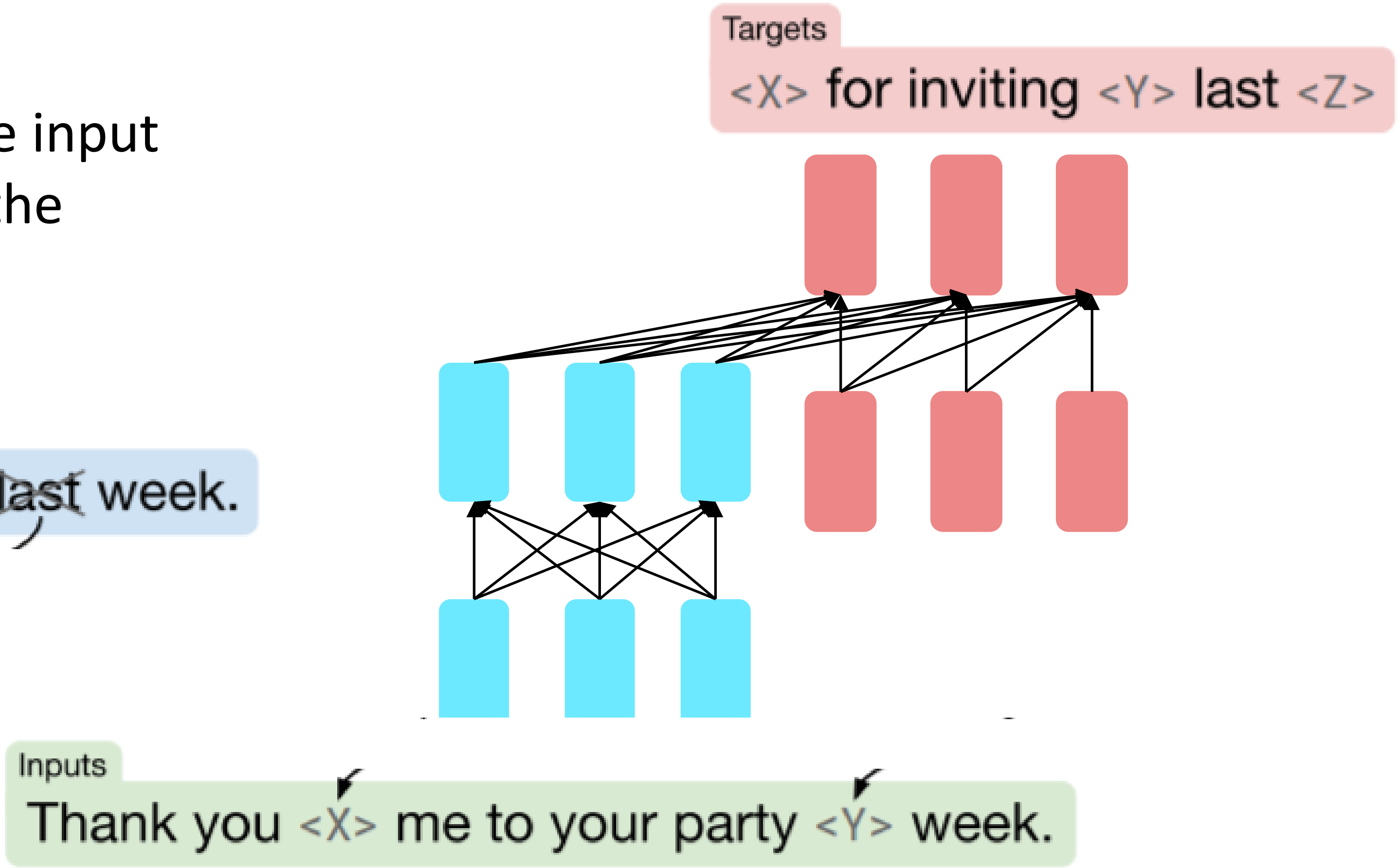
Pretraining encoder-decoders: what pretraining objective to use?

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

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



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



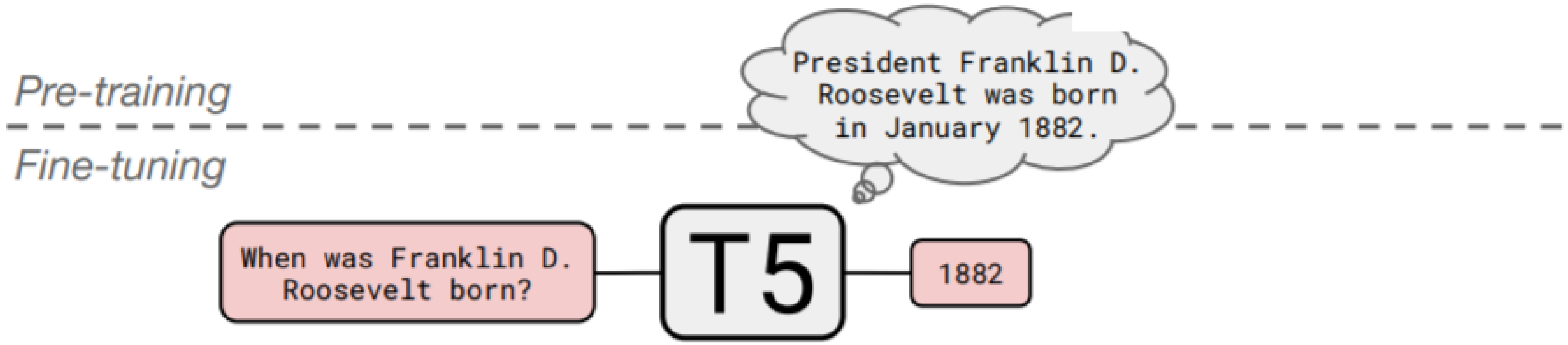
Pretraining encoder-decoders: what pretraining objective to use?

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	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	LM	P	M	79.60	18.13	76.35	63.50	26.62	39.17	27.05
Enc-dec, 6 layers	LM	P	$M/2$	78.67	18.26	75.32	64.06	26.13	38.42	26.89
Language model	LM	P	M	73.78	17.54	53.81	56.51	25.23	34.31	25.38
Prefix LM	LM	P	M	79.68	17.84	76.87	64.86	26.28	37.51	26.76

Pretraining encoder-decoders: what pretraining objective to use?

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

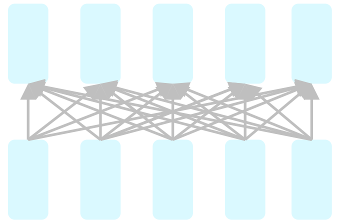
All "open-domain" versions

	NQ	WQ	TQA dev	TQA test	
Karpukhin et al. (2020)	**41.5**	42.4	**57.9**	–	
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**	

[Raffel et al., 2018]

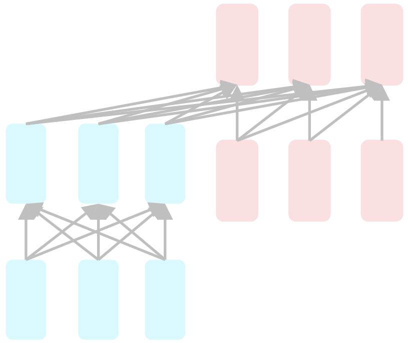
Pretraining for three types of architectures

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



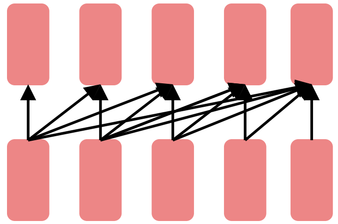
Encoders

- Gets bidirectional context – can condition on future!
- How do we train them to build strong representations?



Encoder-Decoders

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



Decoders

- Language models! What we've seen so far.
- Nice to generate from; can't condition on future words
- All the biggest pretrained models are Decoders.

Pretraining decoders

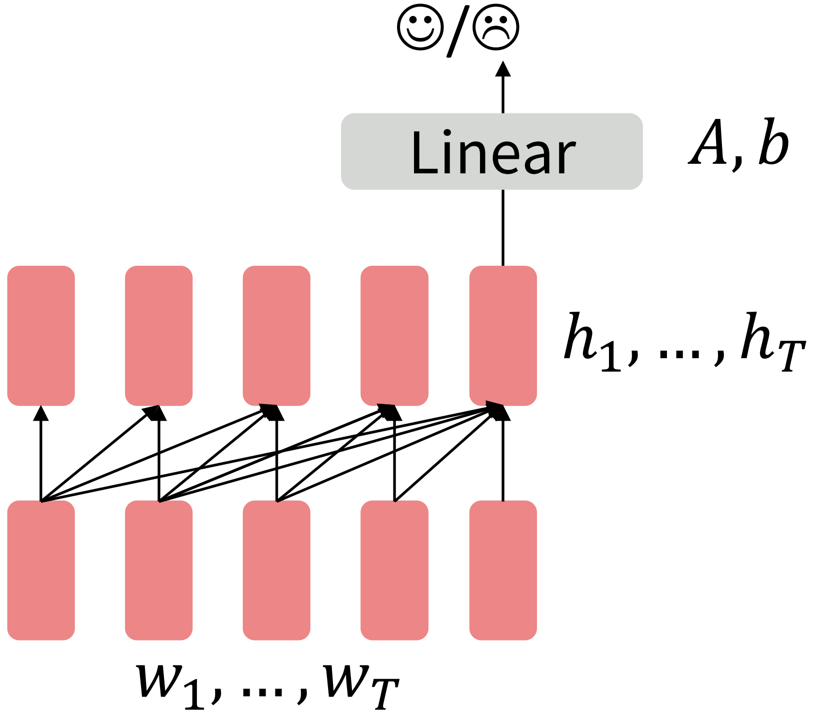
When using language model pretrained decoders, we can ignore that they were trained to model $p(w_t|w_{1:t-1})$.

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

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

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.]

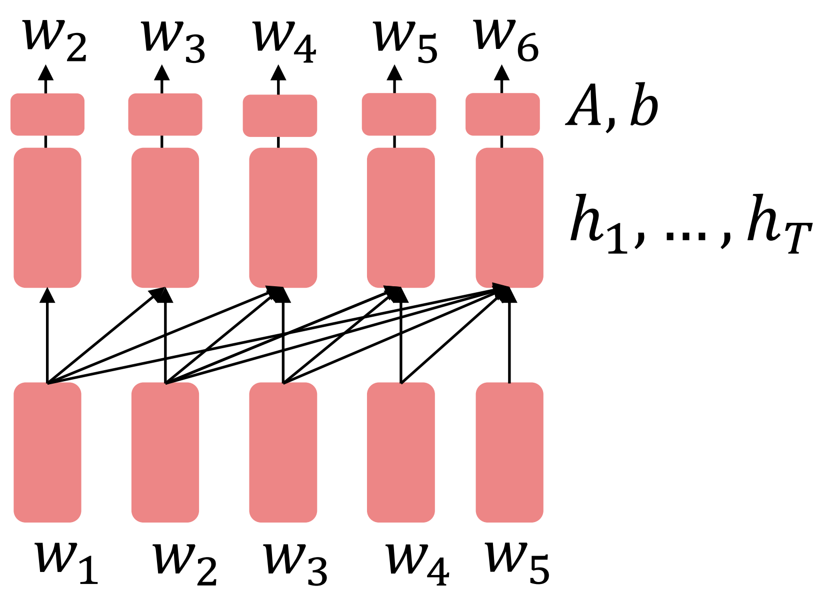
Pretraining decoders

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)

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



[Note how the linear layer has been pretrained.]

Where A, b were pretrained in the language model!

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

2018's GPT was a big success in pretraining a decoder!

- Transformer decoder with 12 layers, 117M parameters.
- 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"

[Devlin et al., 2018]

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 (1.5B) 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.