EE-608: Deep Learning For Natural Language Processing: Transformers

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DLNLP, Lecture 2

Outline

Attention instead of Recurrence

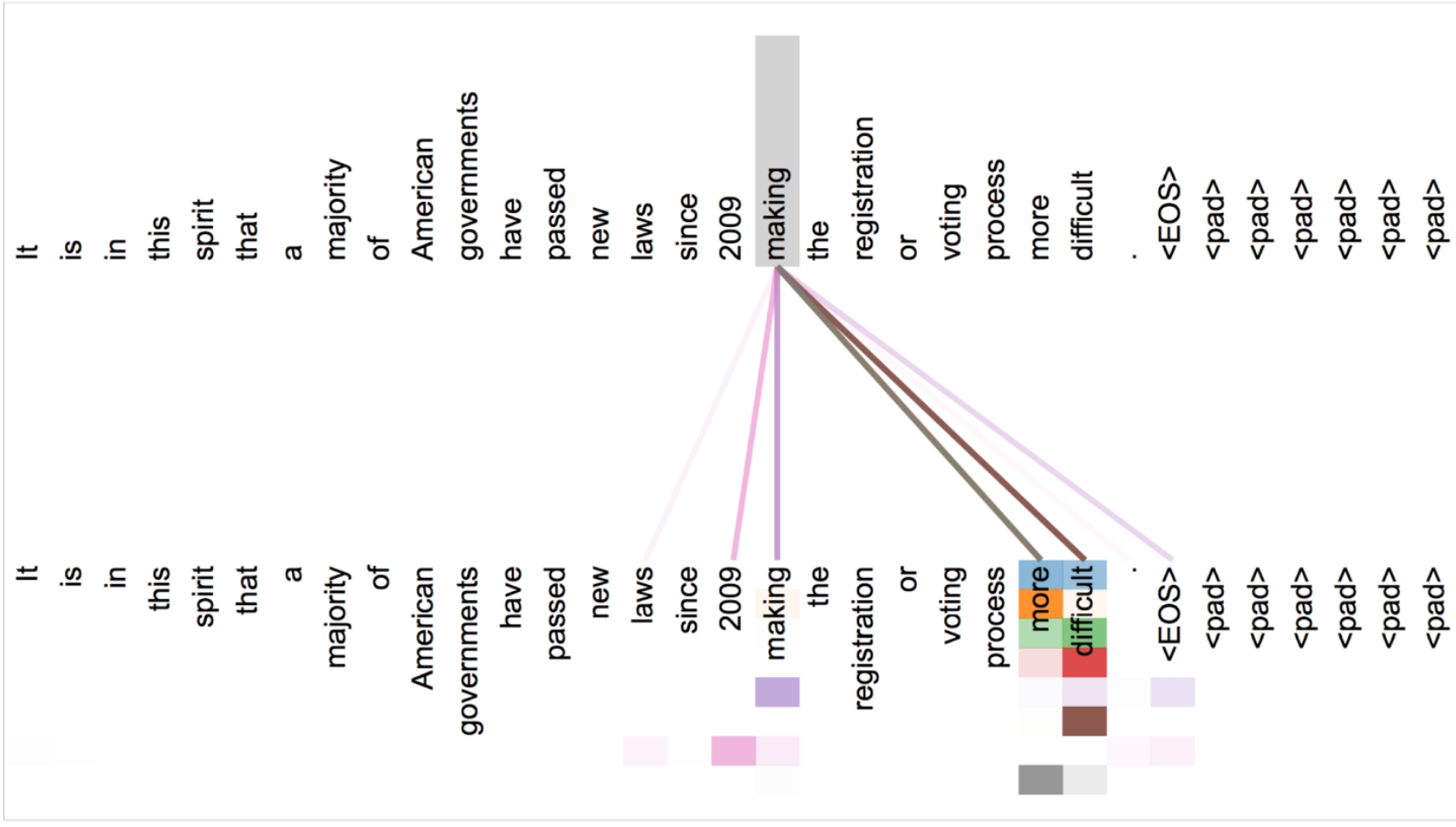
Transformer Architecture

Transformer Results

Transformer Variants

Pretrained Transformers (preview)

Overview of Transformers

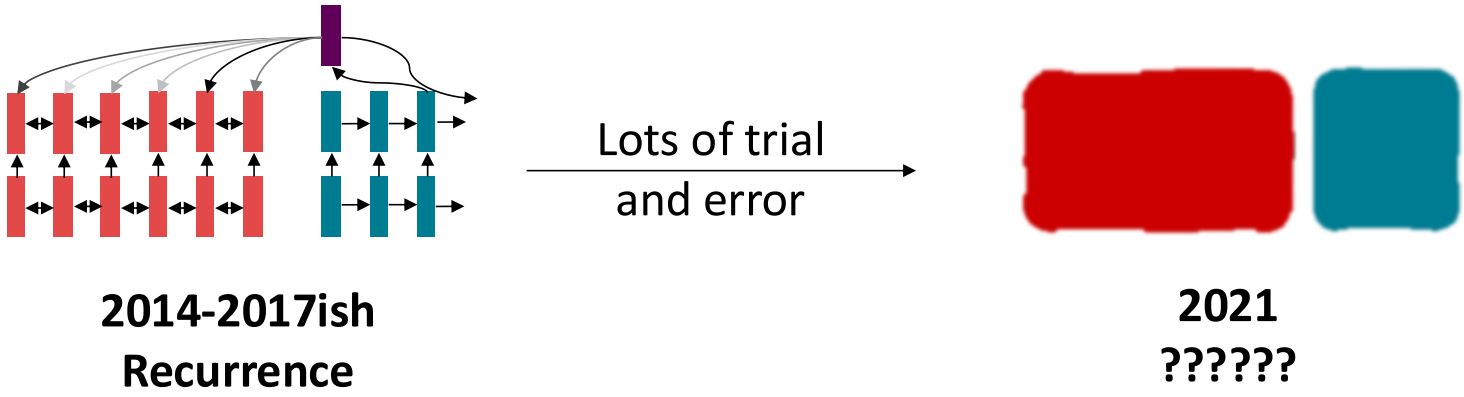


- Multiple layers, each outputting one vector per token
- Self-attention between layers (often bidirectional, depicted)
- All positions share the same parameters

Outline

Do we even need recurrence at all?

- Abstractly: Attention is a way to pass information from a sequence (x) to a neural network input. (h_t)
  - This is also *exactly* what RNNs are used for – to pass information!
  - **Can we just get rid of the RNN entirely?** Maybe attention is just a better way to pass information!



2014-2017ish Recurrence

2021 ??????

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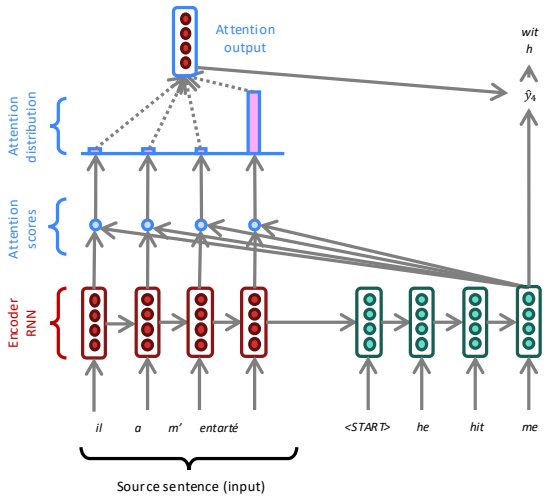
The building block we need: *self* attention

- What we talked about – **Cross** attention: paying attention to the input x to generate y_t



- What we need – **Self** attention: to generate y_t, we need to pay attention to $y_{<t}$

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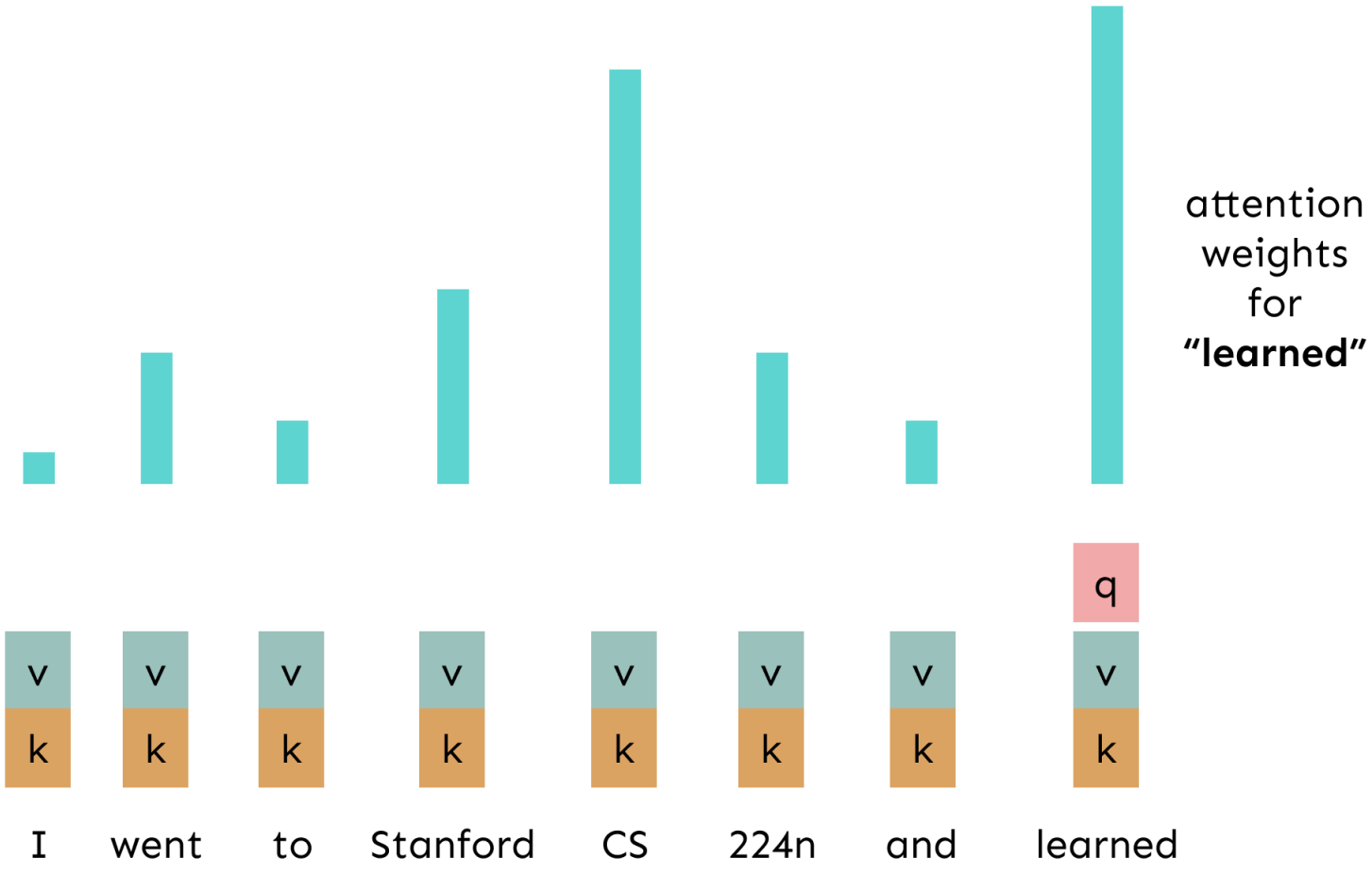
Self-Attention Hypothetical Example



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Self-Attention: keys, queries, values from the same sequence

Let $\boldsymbol{w}_{1:n}$ be a sequence of words in vocabulary V, like *Zuko made his uncle tea*.

For each $\boldsymbol{w}_i$, let $\boldsymbol{x}_i = E\boldsymbol{w}_i$, where $E \in \mathbb{R}^{d \times |V|}$ is an embedding matrix.

1. Transform each word embedding with weight matrices $\mathrm{Q}, \mathrm{K}, \mathrm{V}$, each in $\mathbb{R}^{d \times d}$

$\boldsymbol{q}_i = Q\boldsymbol{x}_i$ (queries) $\quad$ $\boldsymbol{k}_i = K\boldsymbol{x}_i$ (keys) $\quad$ $\boldsymbol{v}_i = V\boldsymbol{x}_i$ (values)

2. Compute pairwise similarities between keys and queries; normalize with softmax

$$\boldsymbol{e}_{ij} = \boldsymbol{q}_i^\top \boldsymbol{k}_j \qquad \boldsymbol{\alpha}_{ij} = \frac{\exp(\boldsymbol{e}_{ij})}{\sum_{j'} \exp(\boldsymbol{e}_{ij'})}$$

3. Compute output for each word as weighted sum of values

$$\boldsymbol{o}_i = \sum_j \boldsymbol{\alpha}_{ij} \boldsymbol{v}_i$$

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Barriers and solutions for Self-Attention as a building block

Barriers

- Doesn't have an inherent notion of order!

Solutions

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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**

$$\boldsymbol{p}_i \in \mathbb{R}^d, \text{ for } i \in \{1,2,\ldots,n\} \text{ are position vectors}$$

- 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 $\boldsymbol{p}_i$ to our inputs!
- Recall that $\boldsymbol{x}_i$ is the embedding of the word at index i. The positioned embedding is:

$$\tilde{\boldsymbol{x}}_i = \boldsymbol{x}_i + \boldsymbol{p}_i$$

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

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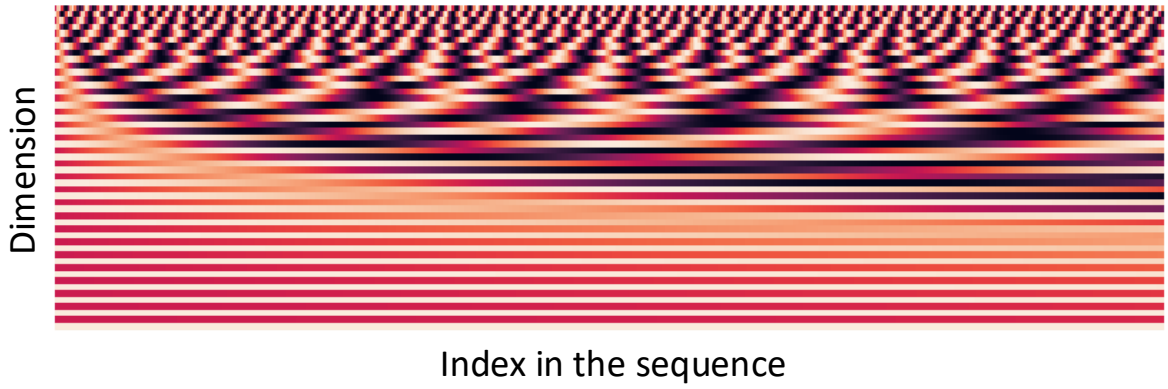
Position representation vectors through sinusoids

- **Sinusoidal position representations:** concatenate sinusoidal functions of varying periods:

$$\boldsymbol{p}_i = \begin{pmatrix} \sin(i/10000^{2*1/d}) \\ \cos(i/10000^{2*1/d}) \\ \vdots \\ \sin(i/10000^{2*\frac{d}{2}/d}) \\ \cos(i/10000^{2*\frac{d}{2}/d}) \end{pmatrix}$$



- 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!

Image: https://timodenk.com/blog/linear-relationships-in-the-transformers-positional-encoding

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Position representation vectors learned from scratch

- **Learned absolute position representations:** Let all p_i be learnable parameters!
  Learn a matrix $\boldsymbol{p} \in \mathbb{R}^{d \times n}$, *and let each* $\boldsymbol{p}_i$ *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 $1, \ldots, n$.
- 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]

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Common, modern position embeddings - RoPE

High level thought process: a *relative* position embedding should be some $f(x, i)$ s.t.

$$\langle f(x,i), f(y,j) \rangle = g(x, y, i-j)$$

That is, the attention function *only* gets to depend on the relative position (i-j). How do existing embeddings not fulfill this goal?

•**Sine:** Has various cross-terms that are not relative

- **Absolute:**

$$e_{ij} = \frac{x_i W^Q (x_j W^K + a_{ij}^K)^T}{\sqrt{d_z}}$$ is not an inner product

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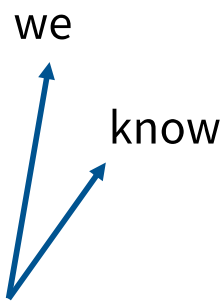
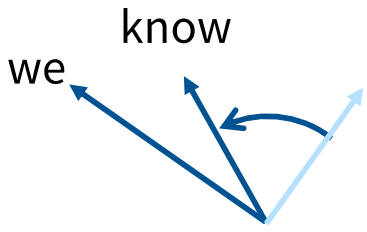
RoPE – Embedding via rotation

How can we solve this problem?

- We want our embeddings to be invariant to absolute position
- We know that inner products are invariant to arbitrary rotation.

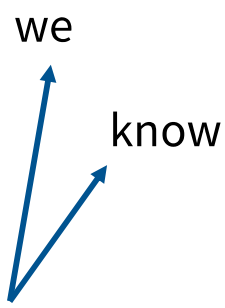


Position independent embedding



Embedding
“of course we know”

Rotate by ‘2 positions’



Embedding
“we know that”

Rotate by ‘0 positions’

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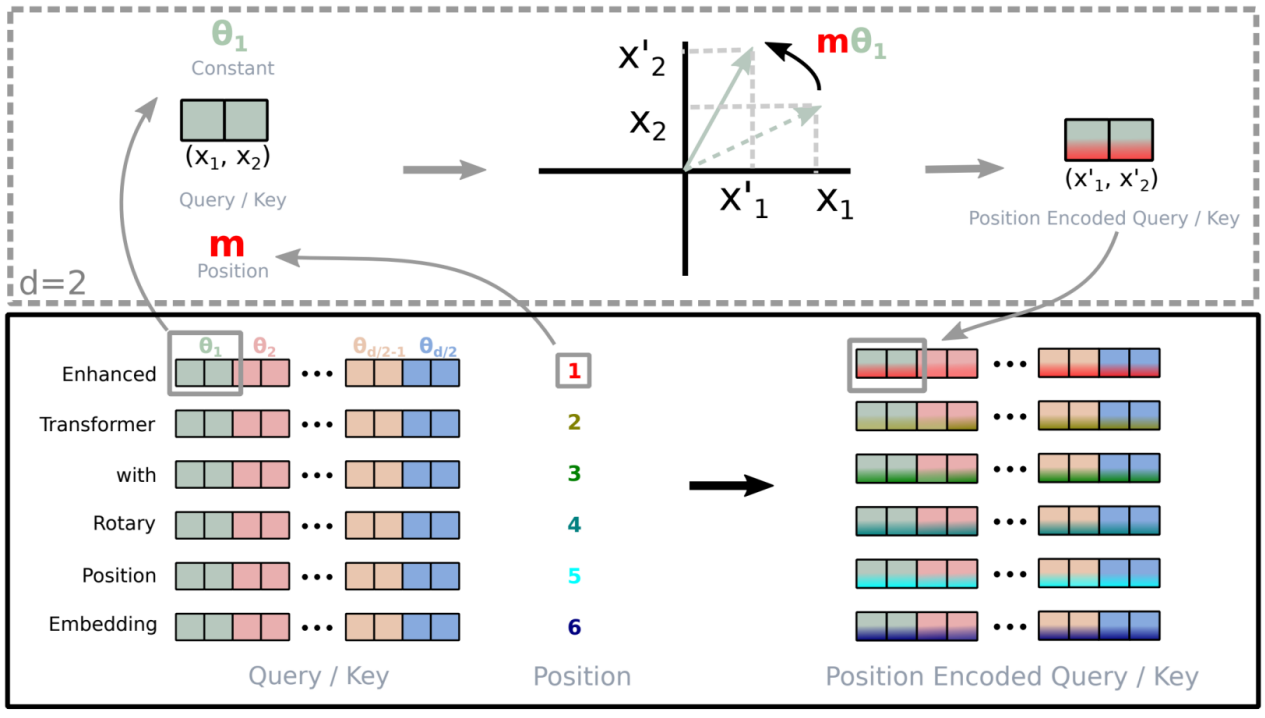
RoPE – From 2 to many dimensions



[Su et al 2021]

Just pair up the coordinates and rotate them in 2d (motivation: complex numbers)

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Barriers and solutions for Self-Attention as a building block

Barriers	Solutions
• Doesn't have an inherent notion of order!	• Add position representations to the inputs
• No nonlinearities for deep learning! It's all just weighted averages	

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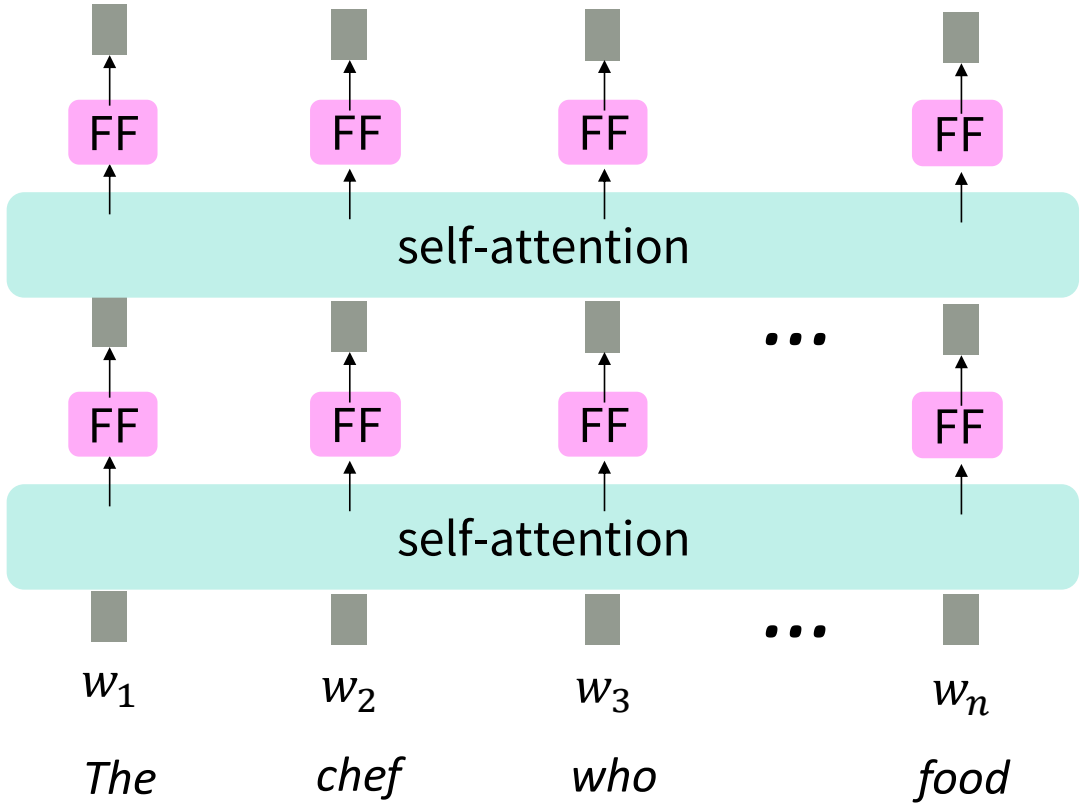
Adding nonlinearities in self-attention

- Note that there are no elementwise nonlinearities in self-attention; stacking more self-attention layers just re-averages **value** vectors (Why? Look at the notes!)

- Easy fix: add a **feed-forward network** to post-process each output vector.

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



Intuition: the FF network processes the result of attention

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Barriers and solutions for Self-Attention as a building block

Barriers	Solutions
• Doesn't have an inherent notion of order!	• Add position representations to the inputs
• No nonlinearities for deep learning magic! It's all just weighted averages	• Easy fix: apply the same feedforward network to each self-attention output.

• Need to ensure we don't "look at the future" when predicting a sequence
  • Like in machine translation
  • Or language modeling	

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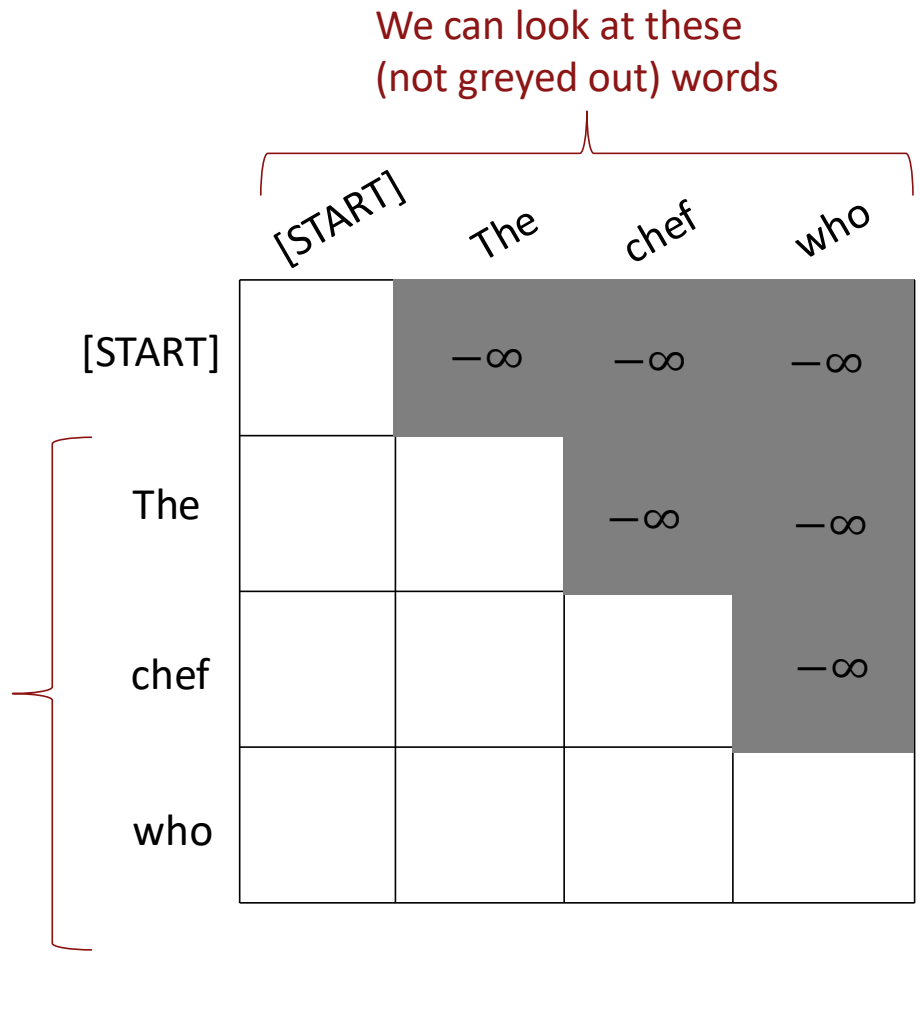
Masking the future in self-attention

- 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 $-\infty$.

$$e_{ij} = \begin{cases} q_i^\top k_j, j \leq i \\ -\infty, j > i \end{cases}$$



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Barriers and solutions for Self-Attention as a building block

Barriers	Solutions
• Doesn't have an inherent notion of order!	• Add position representations to the inputs
• No nonlinearities for deep learning magic! It's all just weighted averages	• Easy fix: apply the same feedforward network to each self-attention output.

• Need to ensure we don't "look at the future" when predicting a sequence
  • Like in machine translation
  • Or language modeling
	• Mask out the future by artificially setting attention weights to 0!

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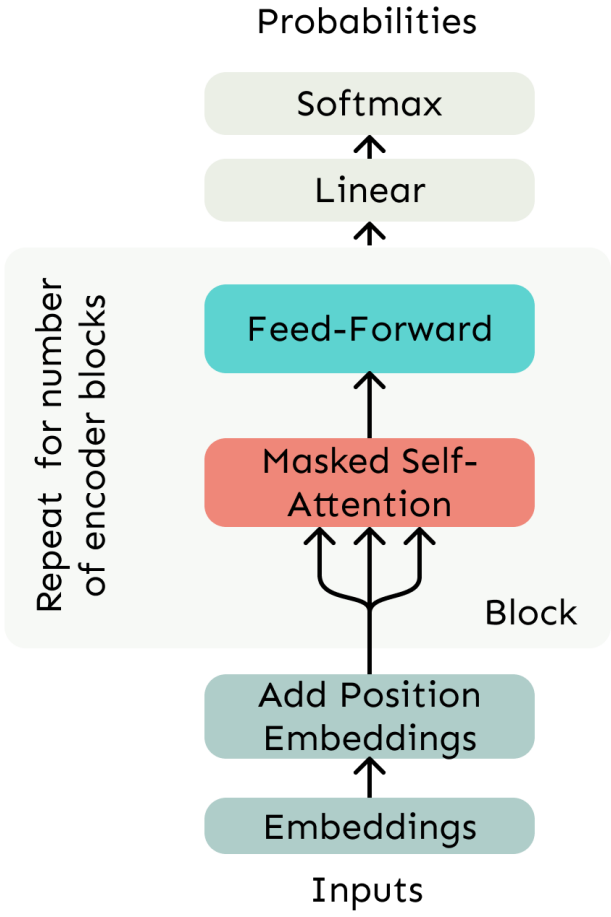
Necessities for a self-attention building block:

- **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.



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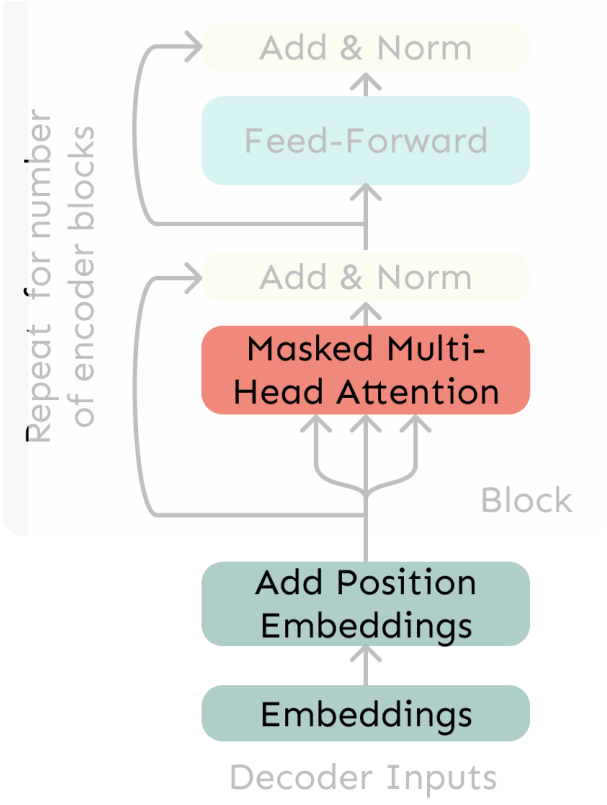
Summary of Attention instead of Recurrence

- Attention is all you need
- Plus a represention of sequence order, with absolute (or relative) positions
- Plus layers of nonlinearity, for a fixed number of layers
- Plus causal masking, to similate running multiple models on the same computation graph

Outline

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

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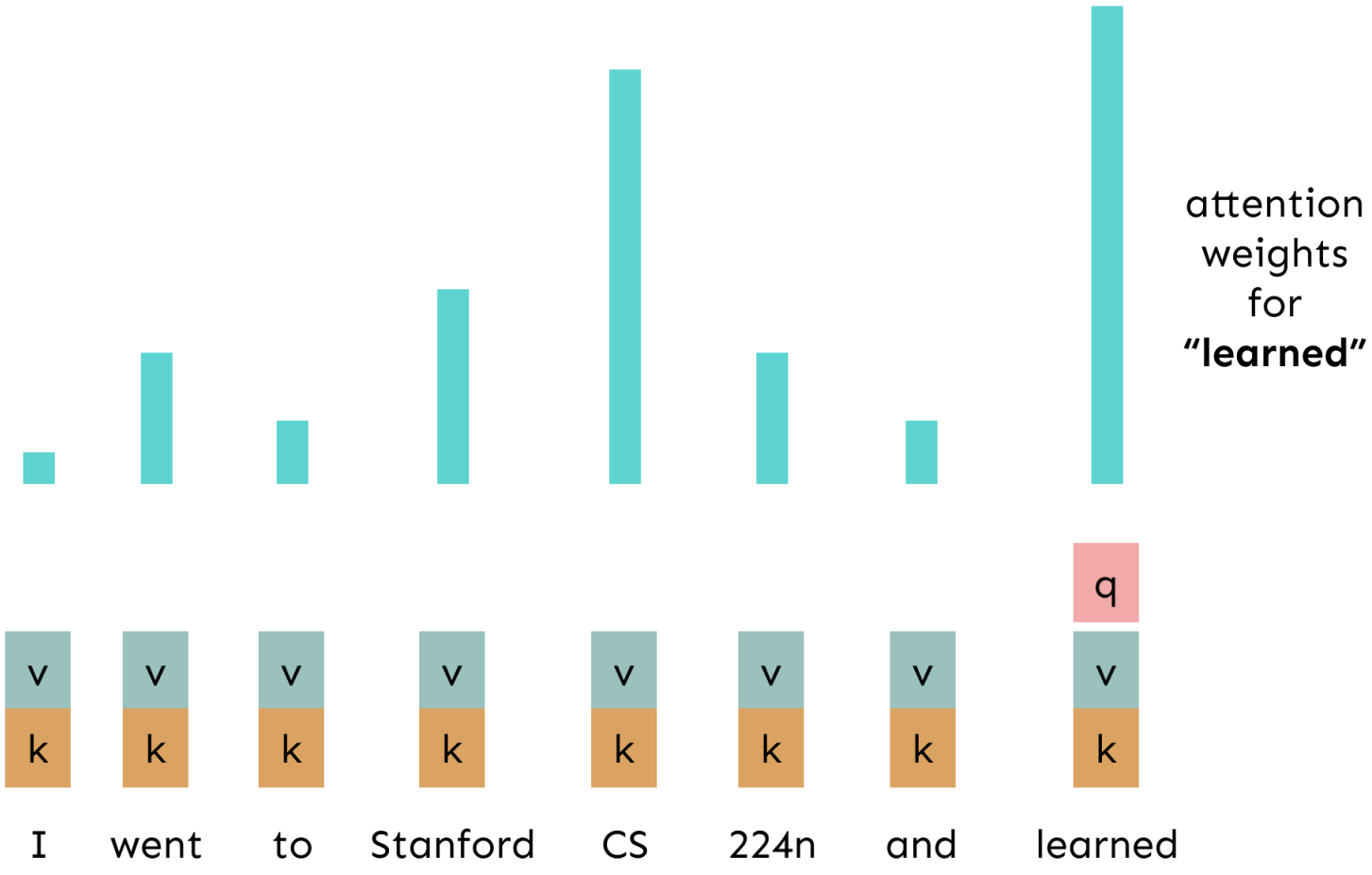
Recall the Self-Attention Hypothetical Example



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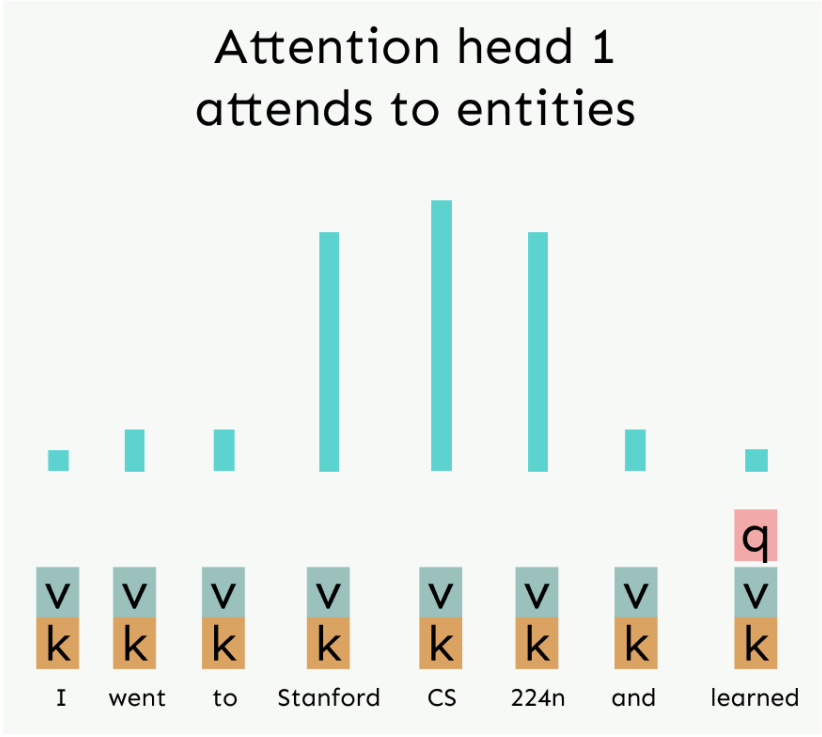
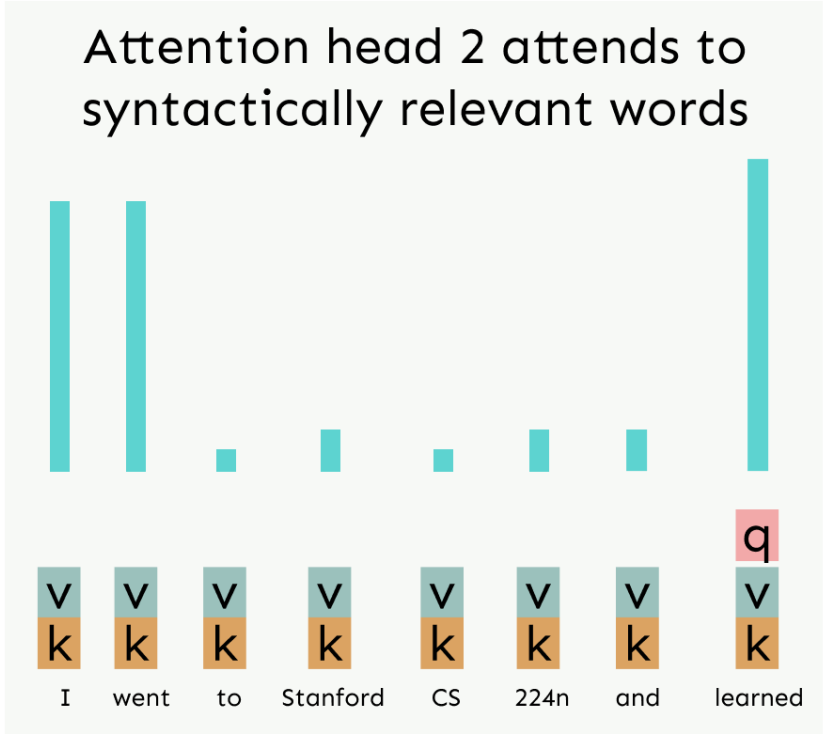
Hypothetical Example of Multi-Head Attention





I went to Stanford CS 224n and learned

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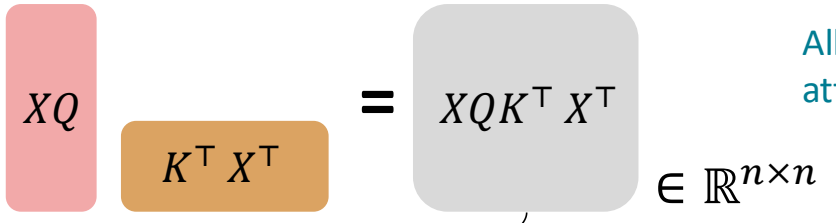
Sequence-Stacked form of Attention

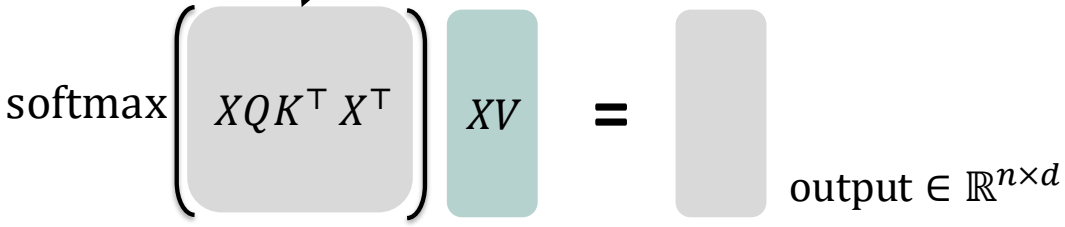
- Let's look at how key-query-value attention is computed, in matrices.
  - Let $X = [x_1; \ldots; x_n] \in \mathbb{R}^{n \times d}$ be the concatenation of input vectors.
  - First, note that $XK \in \mathbb{R}^{n \times d}$, $XQ \in \mathbb{R}^{n \times d}$, $XV \in \mathbb{R}^{n \times d}$.
  - The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



All pairs of attention scores!

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



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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:
  - $\text{output}_\ell = \text{softmax}\left(XQ_\ell K_\ell^\top X^\top\right) * XV_\ell$, 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.

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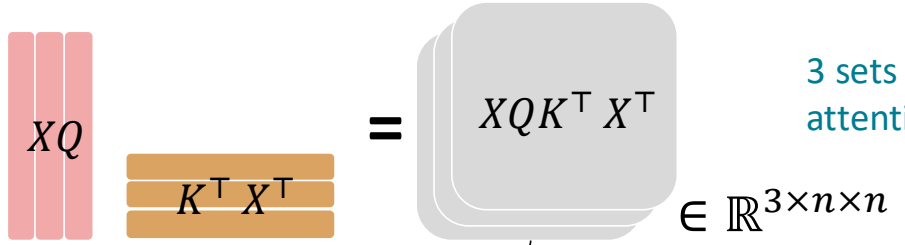
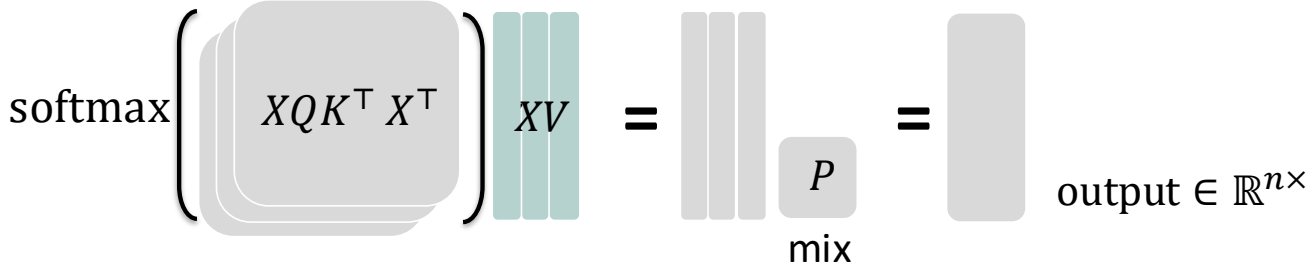
Multi-head self-attention is computationally efficient

- 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.



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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:

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

- 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.)

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

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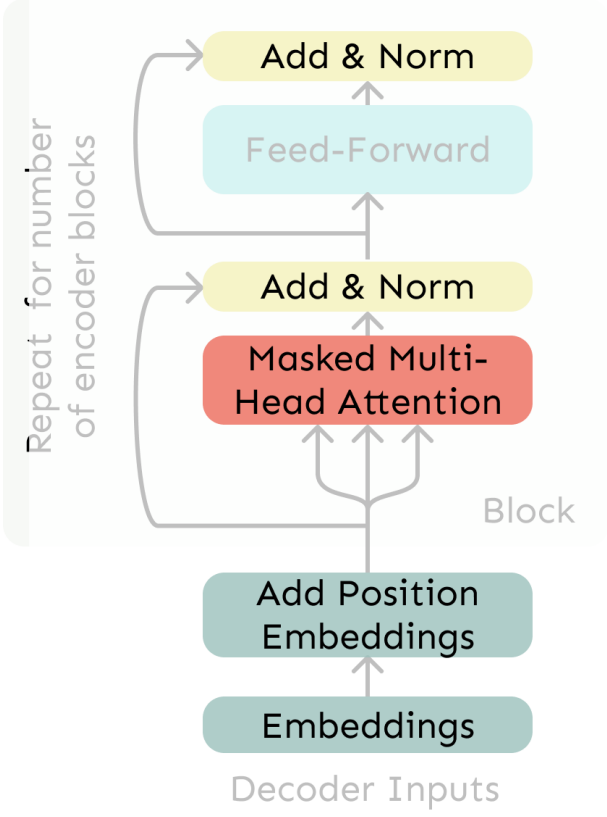
The Transformer Decoder

- 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"



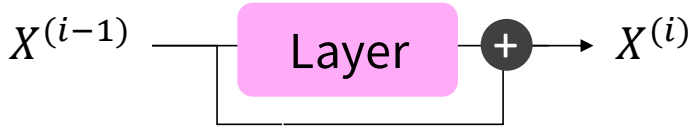
Transformer Decoder

Slide from Tatsunori Hashimoto

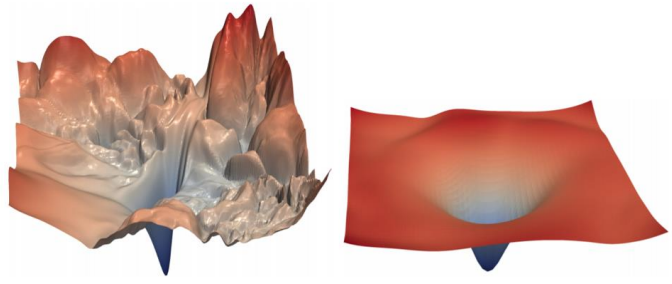
The Transformer Encoder: **Residual connections** [He et al., 2016]

- **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]

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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 $\sigma = \sqrt{\frac{1}{d}\sum_{j=1}^{d}(x_j - \mu)^2}$; 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:

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

Normalize by scalar mean and variance

Modulate by learned elementwise gain and bias

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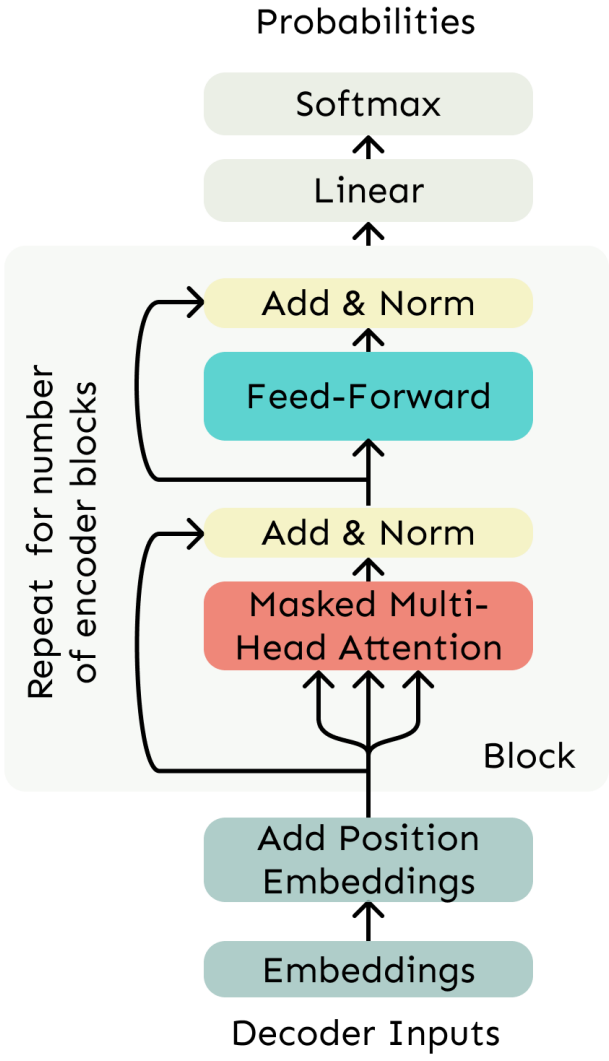
The Transformer Decoder

- 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.



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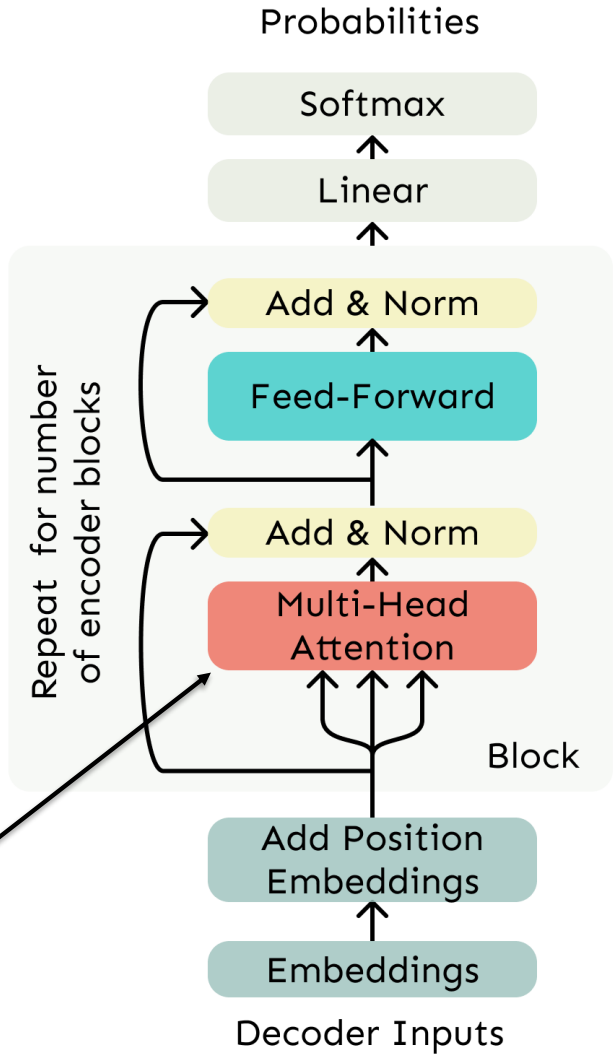
The Transformer Encoder

- 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.

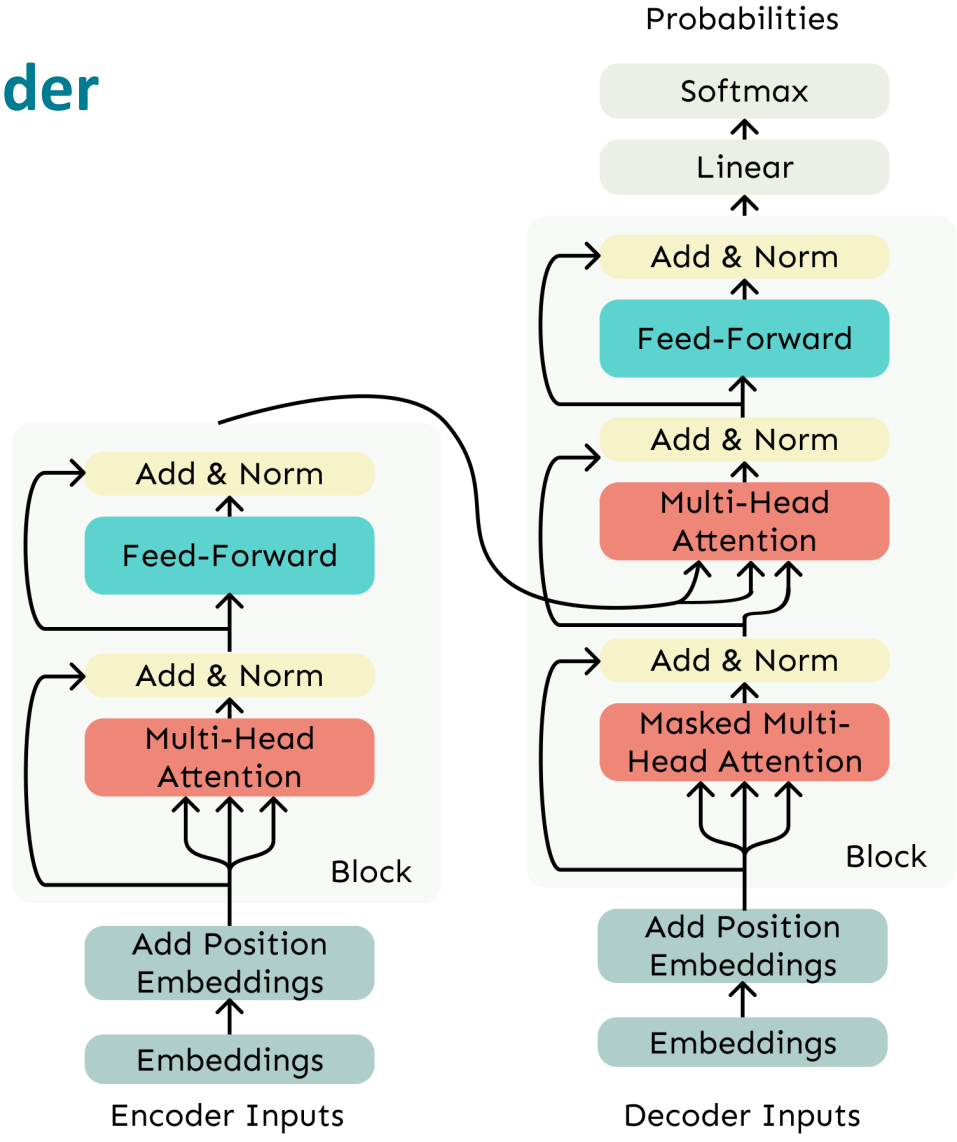


No Masking!

Slide from Tatsunori Hashimoto

The Transformer Encoder-Decoder

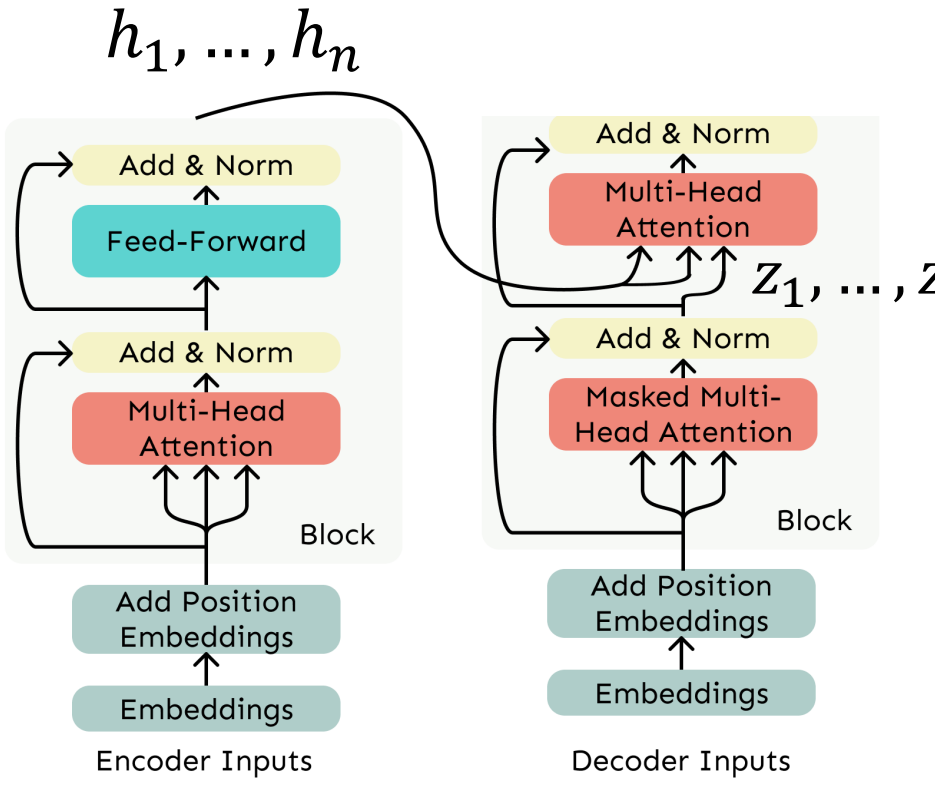
- Recall that in machine translation, we processed the source sentence with a **bidirectional** model and generated the target with a **unidirectional model**.
- For this kind of seq2seq format, we often use a Transformer Encoder-Decoder.
- We use a normal Transformer Encoder.
- Our Transformer Decoder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



Slide from Tatsunori Hashimoto

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

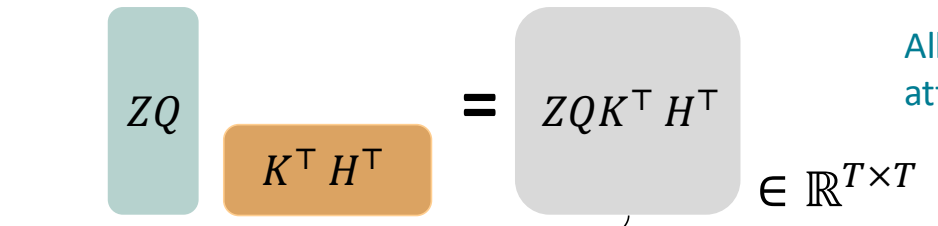


Slide from Tatsunori Hashimoto

Cross-attention (details)

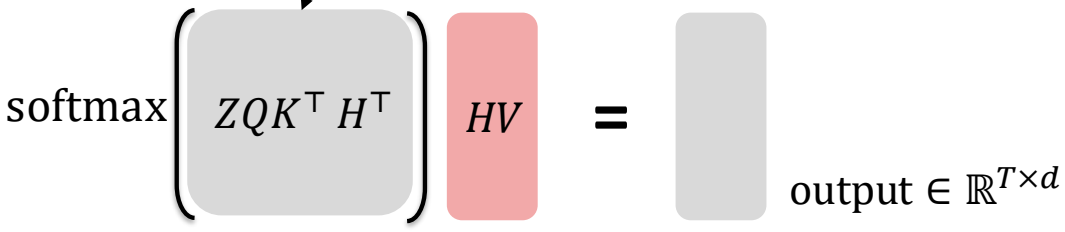
- Let's look at how cross-attention is computed, in matrices.
  - Let $\mathrm{H} = [h_1; \ldots; h_T] \in \mathbb{R}^{T \times d}$ be the concatenation of encoder vectors.
  - Let $\mathrm{Z} = [z_1; \ldots; z_T] \in \mathbb{R}^{T \times d}$ be the concatenation of decoder vectors.
  - The output is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

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



All pairs of attention scores!

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



Slide from Tatsunori Hashimoto

Outline

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]

Slide from Tatsunori Hashimoto

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

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Great Results with Transformers

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

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		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]

Slide from Tatsunori Hashimoto

Outline

What would we like to fix about the Transformer?

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

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Pre vs Post norm

The one thing *everyone* agrees on (in 2024)

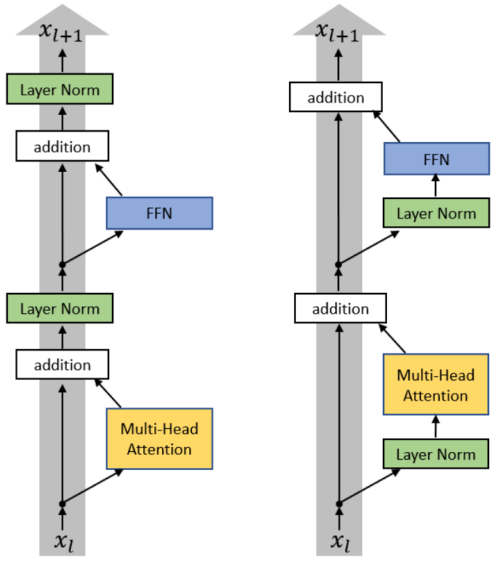


Figure from Xiong 2020

Post-LN Transformer	Pre-LN Transformer
$x_{l,i}^{post,1} = \text{MultiHeadAtt}(x_{l,i}^{post}, [x_{l,1}^{post}, \cdots, x_{l,n}^{post}])$	$x_{l,i}^{pre,1} = \text{LayerNorm}(x_{l,i}^{pre})$
$x_{l,i}^{post,2} = x_{l,i}^{post} + x_{l,i}^{post,1}$	$x_{l,i}^{pre,2} = \text{MultiHeadAtt}(x_{l,i}^{pre,1}, [x_{l,1}^{pre,1}, \cdots, x_{l,n}^{pre,1}])$
$x_{l,i}^{post,3} = \text{LayerNorm}(x_{l,i}^{post,2})$	$x_{l,i}^{pre,3} = x_{l,i}^{pre} + x_{l,i}^{pre,2}$
$x_{l,i}^{post,4} = \text{ReLU}(x_{l,i}^{post,3} W^{1,l} + b^{1,l}) W^{2,l} + b^{2,l}$	$x_{l,i}^{pre,4} = \text{LayerNorm}(x_{l,i}^{pre,3})$
$x_{l,i}^{post,5} = x_{l,i}^{post,3} + x_{l,i}^{post,4}$	$x_{l,i}^{pre,5} = \text{ReLU}(x_{l,i}^{pre,4} W^{1,l} + b^{1,l}) W^{2,l} + b^{2,l}$
$x_{l+1,i}^{post} = \text{LayerNorm}(x_{l,i}^{post,5})$	$x_{l+1,i}^{pre} = x_{l,i}^{pre,5} + x_{l,i}^{pre,3}$
	Final LayerNorm: $x_{Final,i}^{pre} \leftarrow \text{LayerNorm}(x_{L+1,i}^{pre})$

Set up LayerNorm so that it doesn't affect the main residual signal path (on the left)

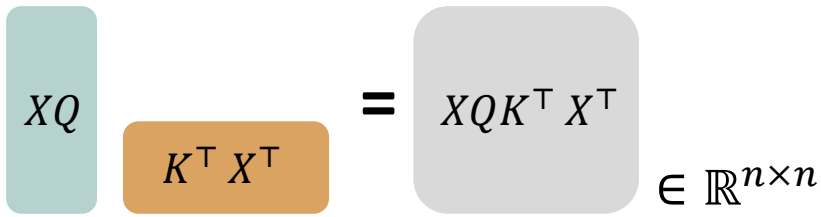
Almost all modern LMs use pre-norm (but BERT was post-norm)

(One somewhat funny exception – OPT350M. I don't know why this is post-norm)

Slide from Tatsunori Hashimoto

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.



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 $n \geq 50,000$?** For example, to work on long documents?

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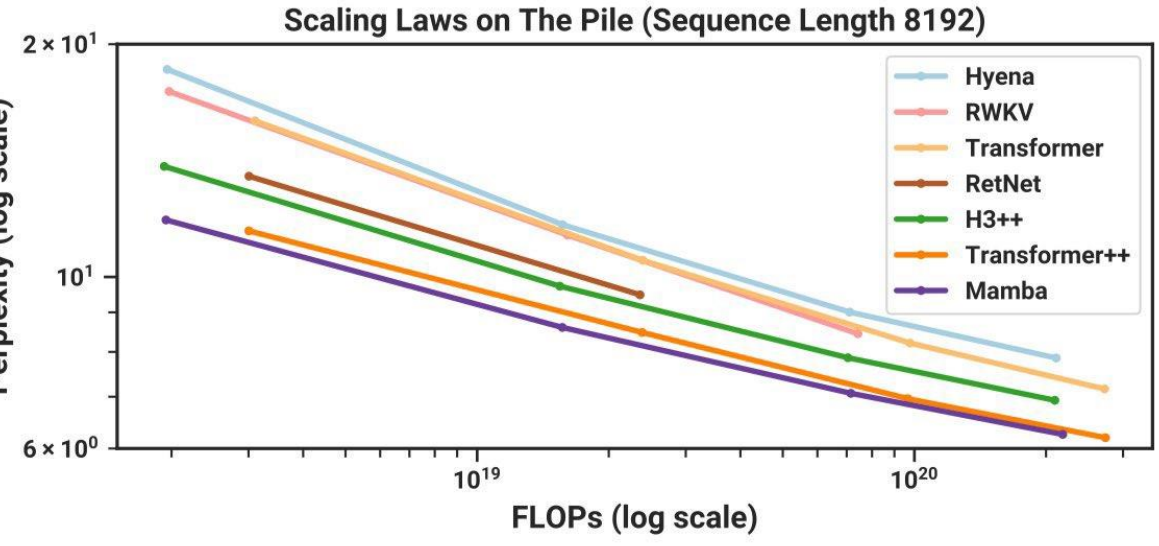
Back to the future – RNNs are back!



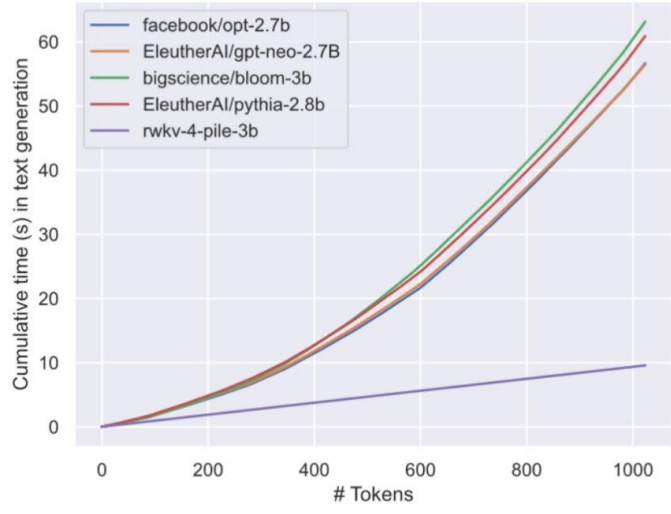


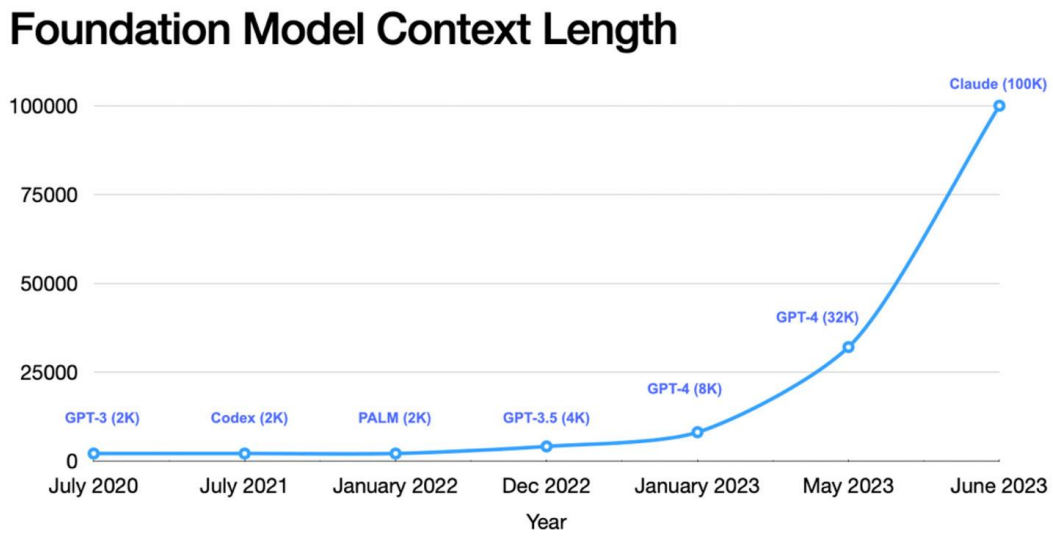
Figure 7: Cumulative time on text generation for LL
Unlike transformers, RWKV exhibits linear scaling

If you want *really* long context, RNNs provide this (linear complexity).
Modern RNNs (RWKV, Mamba, etc) are getting better!

Slide from Tatsunori Hashimoto

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, despite the quadratic cost.
- In practice, **production Transformer language models use quadratic cost attention**
  - The cheaper methods tend not to work as well at scale.
  - Systems optimizations work well (Flash attention – Jun 2022)



Slide from Tatsunori Hashimoto

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?

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Thibault Fevry† Michael Matena† Karishma Malkan† Noah Fiedel

Noam Shazeer Zhenzhong Lan† Yanqi Zhou Wei Li

Nan Ding Jake Marcus Adam Roberts Colin Raffel†

Slide from Tatsunori Hashimoto

Fixing sequence inputs: Graph-to-Graph Transformers

Instead of sequence-to-sequence Transformers, can we have graph-to-graph Transformers?
Yes! [Mohammadshahi and Henderson 2021, 2020]

- One "token" for each node of the graph
- Graph edges are properties of pairs of tokens

$\Rightarrow$ Input edge labels to the attention weight computation

- Given edge label embeddings $R \in \mathbb{R}^{n \times d_k}$, where R_{ij} is the embedding of length $j-i$,

$$E_{ij}(Q, K, R) = Q_i(K_j + R_{ij})^T$$

$$A(Q, K, V, R) = softmax\left(\frac{E(Q, K, R)}{\sqrt{d_k}}\right) V$$

with queries $Q \in \mathbb{R}^{n \times d_k}$, keys $K \in \mathbb{R}^{n \times d_k}$, values $V \in \mathbb{R}^{n \times d_v}$

Fixing unknown words: subword inputs

There are always new words you have never seen before. And for some languages words are not the natural way to segment the input.

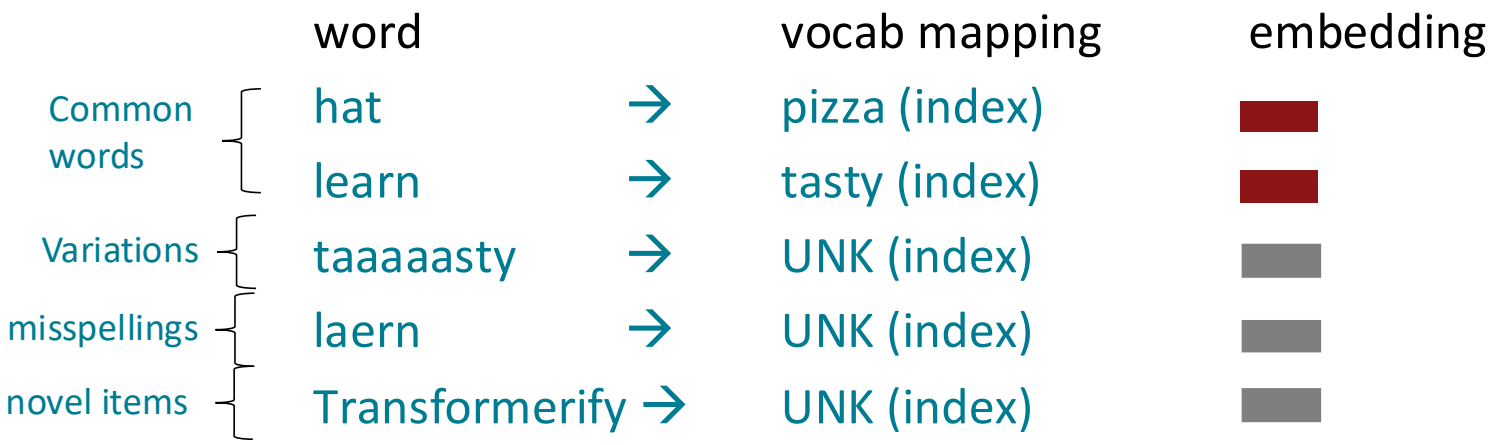
- input subwords rather than whole words
- choose the subword vocabulary based on frequency, so there are never any unknown subwords

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.



Slide from Tatsunori Hashimoto

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.

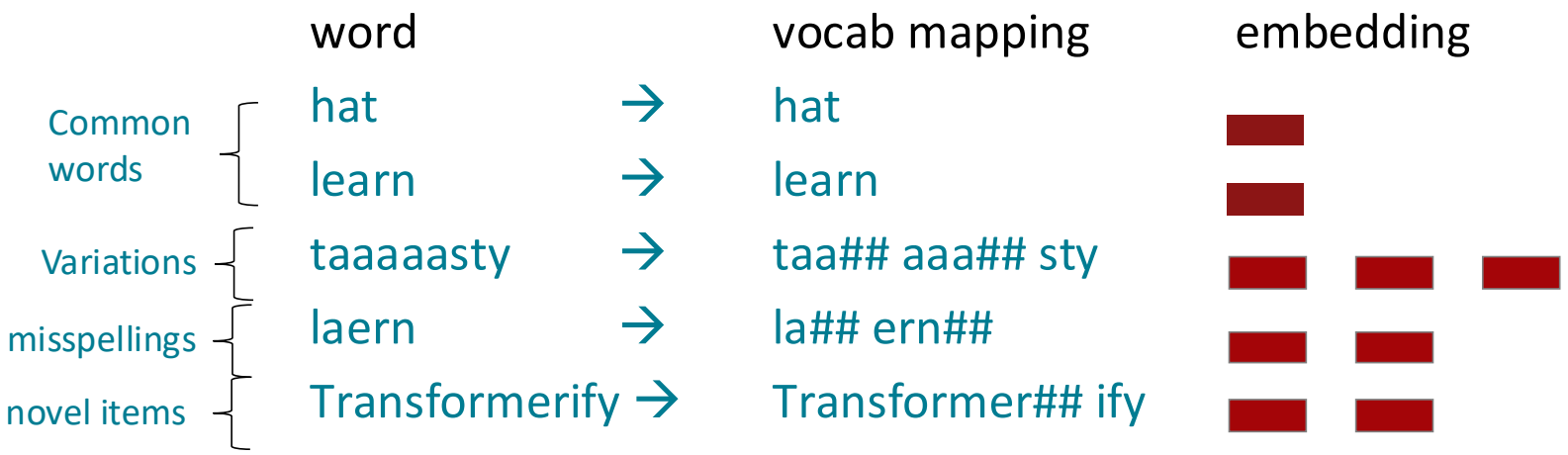
[Sennrich et al., 2016, Wu et al., 2016]

Slide from Tatsunori Hashimoto

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.



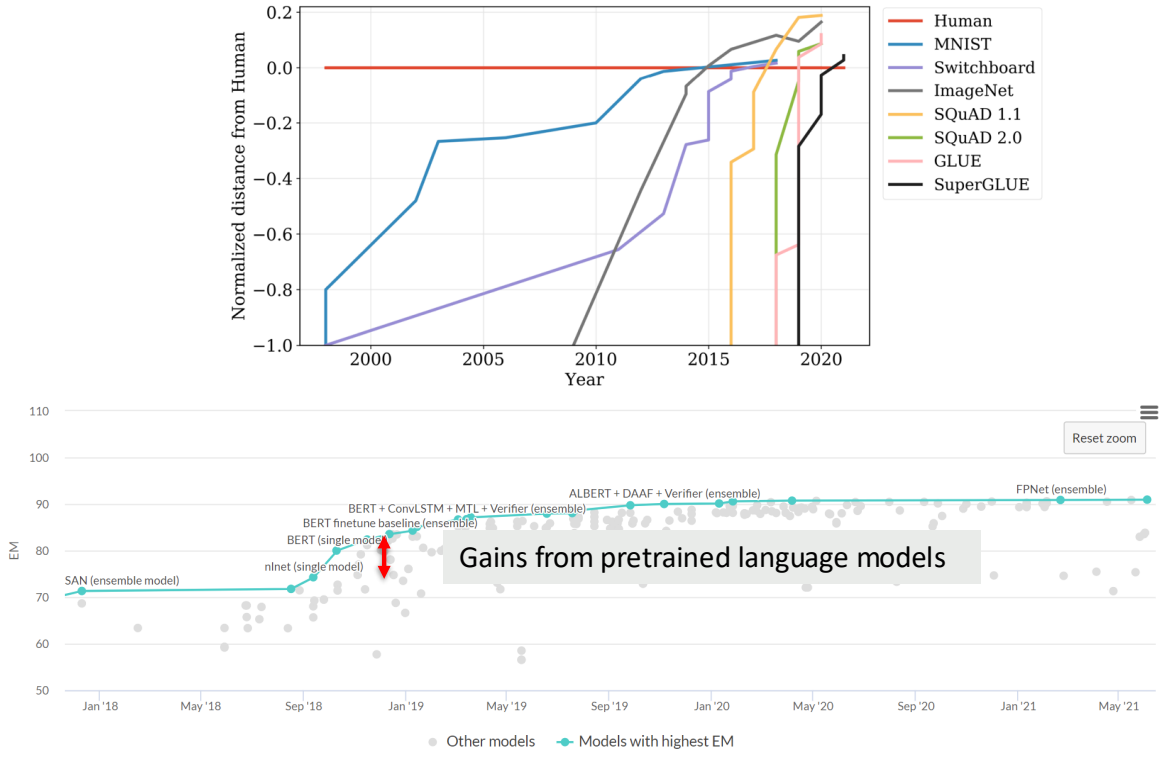
Slide from Tatsunori Hashimoto

Summary of Transformers

- Transformers are multi-layer attention-based sequence models
- Use causal/bidirectional self-attention: Each token at one layer uses attention over all tokens at the layer below
- Use multiple attention heads
- Use bag-of-vector representations, with sequential position encoded in the input vectors
- Decoder transformers are very good at generate text
- Transformers can be generalised to graphs

Outline

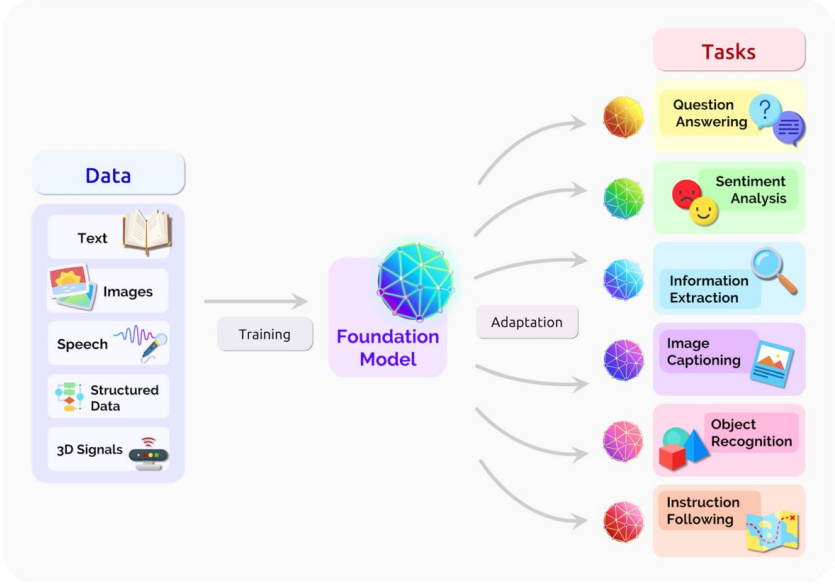
The pretraining revolution



Pretraining has had a major, tangible impact on how well NLP systems work

Slide from Tatsunori Hashimoto

Pretraining – scaling unsupervised learning on the internet



Key ideas in pretraining

- Make sure your model can process large-scale, diverse datasets
- Don’t use labeled data (otherwise you can’t scale!)
- Compute-aware scaling

Slide from Tatsunori Hashimoto

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.

Slide from Tatsunori Hashimoto

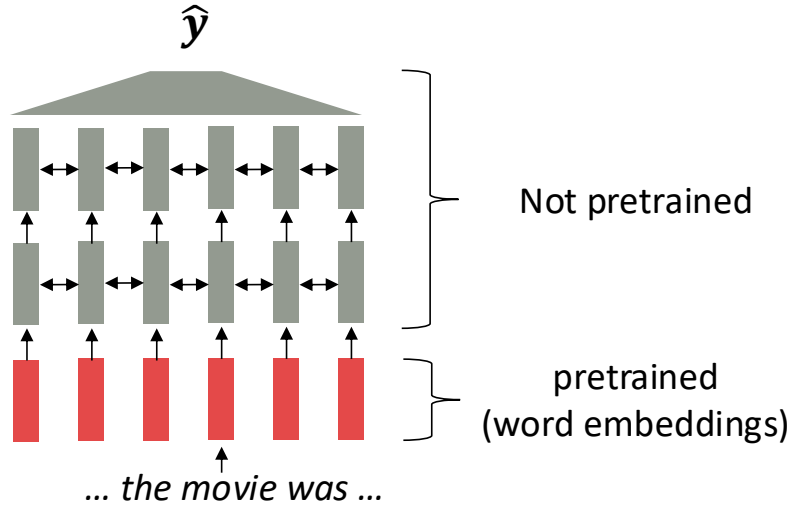
Where we were: **pretrained word embeddings**

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]

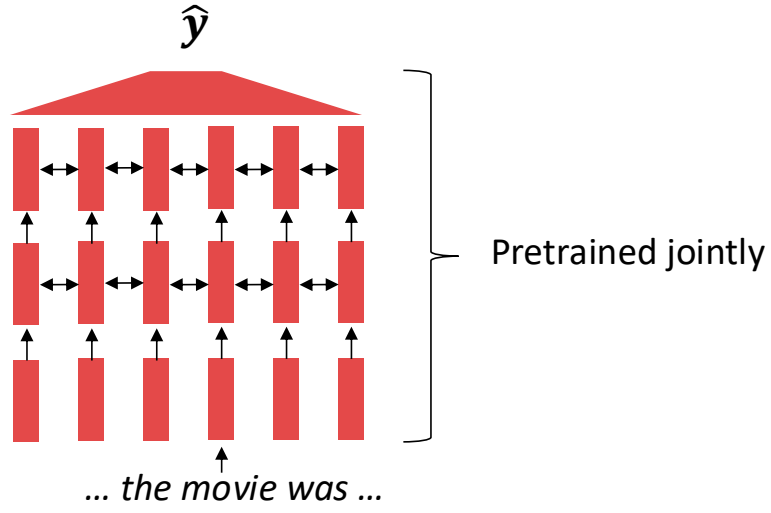
Slide from Tatsunori Hashimoto

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]

Slide from Tatsunori Hashimoto

What can we learn from reconstructing the input?

Stanford University is located in _____, California.

Slide from Tatsunori Hashimoto

What can we learn from reconstructing the input?

I put ___ fork down on the table.

Slide from Tatsunori Hashimoto

What can we learn from reconstructing the input?

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

Slide from Tatsunori Hashimoto

What can we learn from reconstructing the input?

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

Slide from Tatsunori Hashimoto

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 ___.

Slide from Tatsunori Hashimoto

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 _____.

Slide from Tatsunori Hashimoto

What can we learn from reconstructing the input?

I was thinking about the sequence that goes

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

Slide from Tatsunori Hashimoto

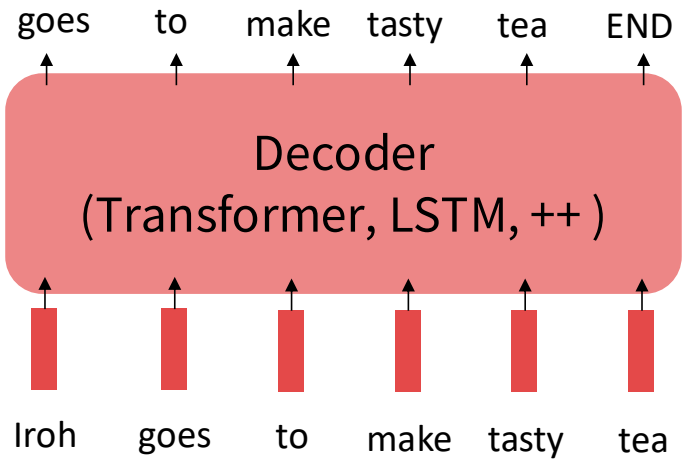
Pretraining through language modeling [Dai and Le, 2015]

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.



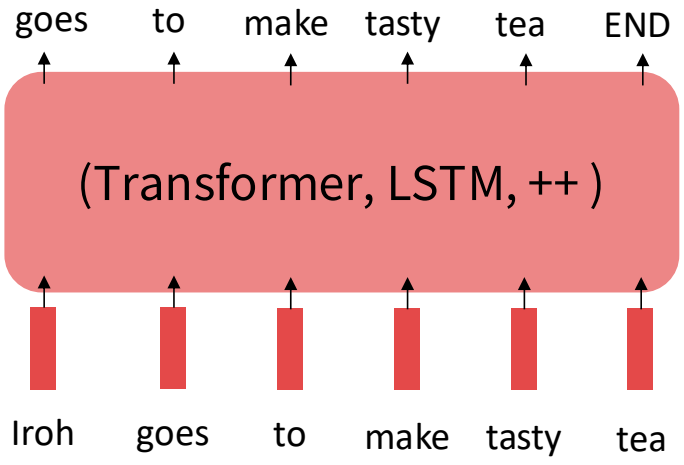
Slide from Tatsunori Hashimoto

The Pretraining / Finetuning Paradigm

Pretraining can improve NLP applications by serving as parameter initialization.

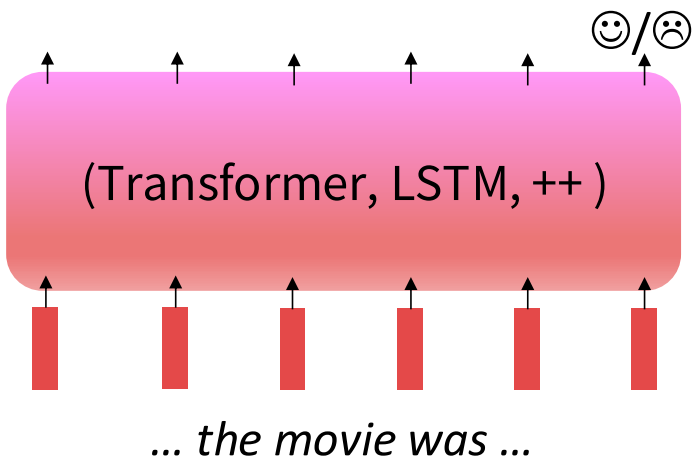
Step 1: Pretrain (on language modeling)

Lots of text; learn general things!



Step 2: Finetune (on your task)

Not many labels; adapt to the task!



Slide from Tatsunori Hashimoto

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!

Slide from Tatsunori Hashimoto

Summary of Pretraining Preview

Pretraining is hugely successful at improving the SOTA in many tasks, by inducing **transferable abstract representations**

- BERT models are Transformers pretrained on masked language modelling (and next sentence prediction)
- T5 are large Transformer encoder-decoder models trained on masked span prediction
- GPT (n) are very large Transformers trained on left-to-right language modelling
- GPT (n) have lots of information in the language model
- Finetuning changes or adds weights which specialise the model for the task on a dataset