Advanced Deep Learning Architectures
COMP 5214 & ELEC 5680

Instructor: Dr. Qifeng Chen

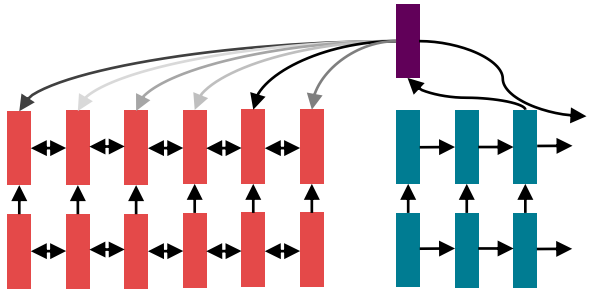
https://cqf.io

Credit: CS224N@Stanford

Transformer

Today: Same goals, different building blocks

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



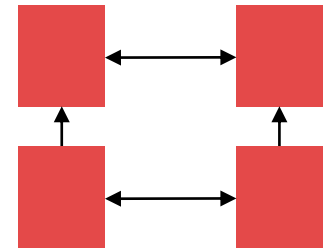
2014-2017ish
Recurrence

Lots of trial
and error

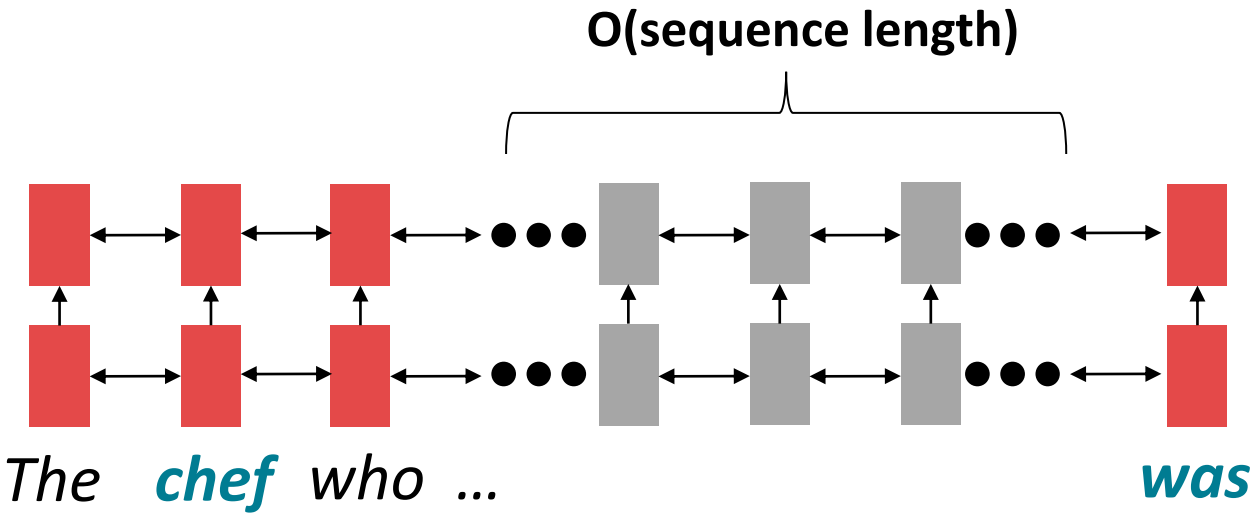
2021
??????

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

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

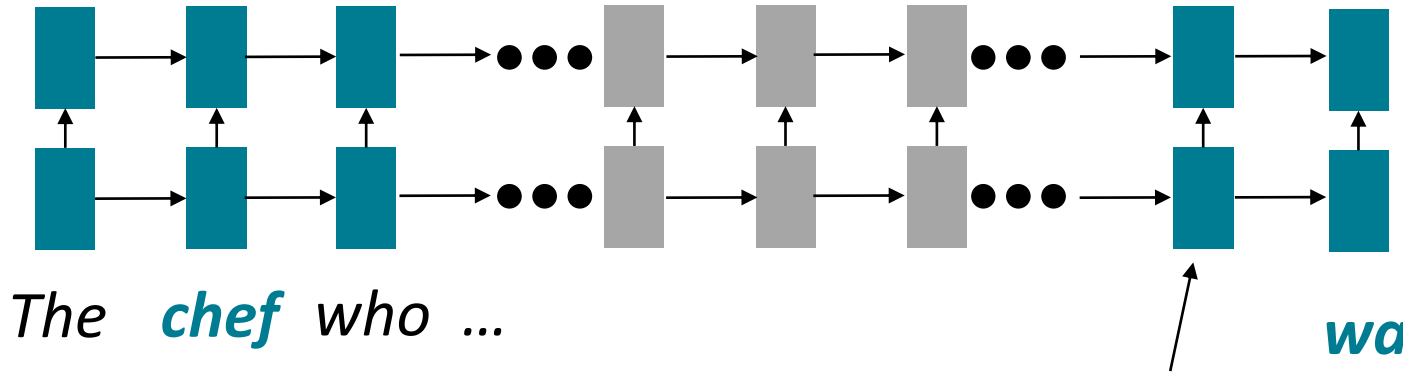


- **Problem:** RNNs take **O(sequence length)** steps for distant word pairs to interact.



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

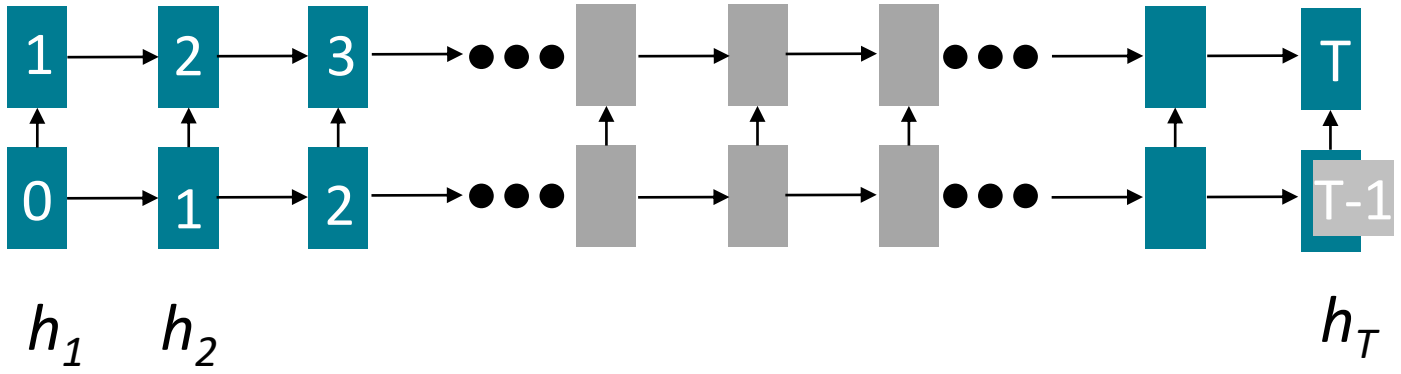
- **O(sequence length)** steps for distant word pairs to interact means:
  - Hard to learn long-distance dependencies (because gradient problems!)
  - Linear order of words is "baked in"; we already know linear order isn't the right way to think about sentences…



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

Issues with recurrent models: **Lack of parallelizability**

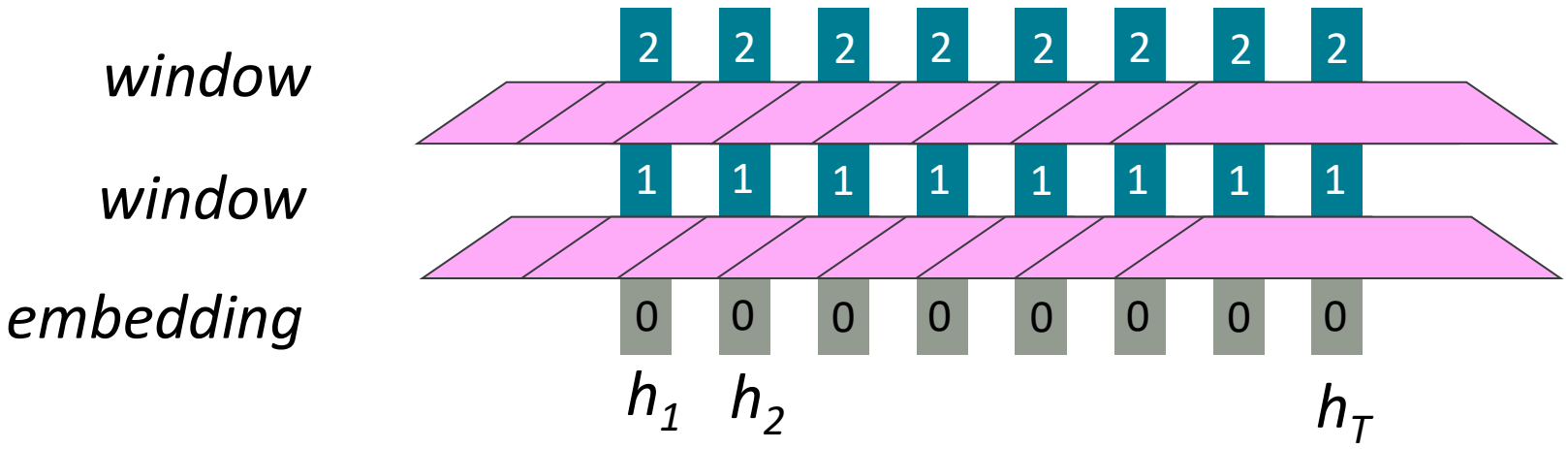
- Forward and backward passes have **O(sequence length)** unparallelizable operations
  - GPUs can perform a bunch of independent computations at once!
  - But future RNN hidden states can't be computed in full before past RNN hidden states have been computed
  - Inhibits training on very large datasets!



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

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

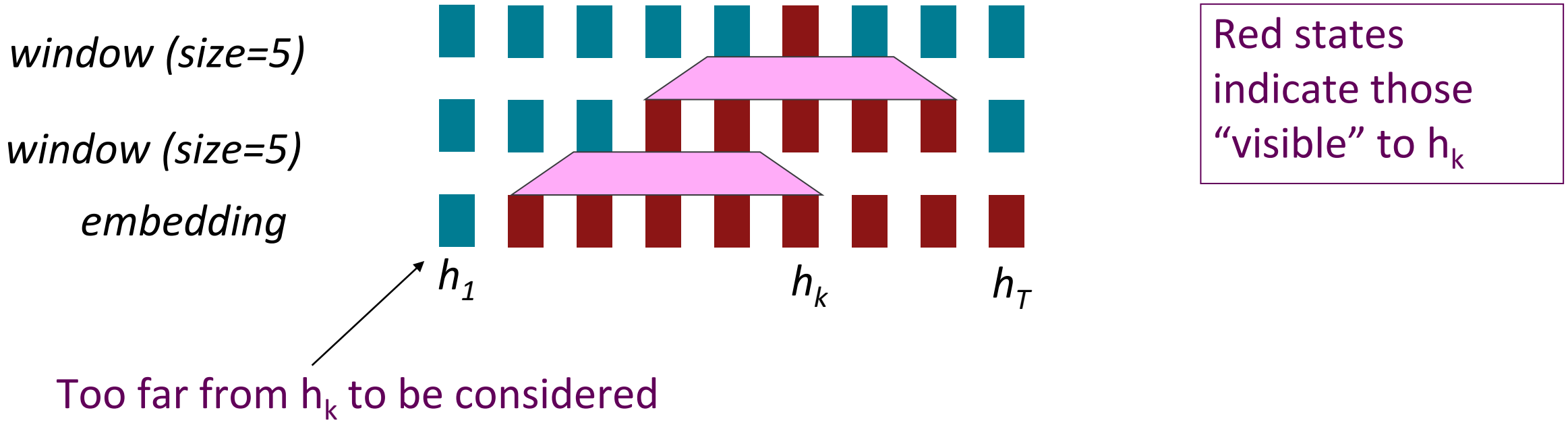
- **Word window models aggregate local contexts**
  - (Also known as 1D convolution; we'll go over this in depth later!)
  - Number of unparallelizable operations does not increase sequence length!



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

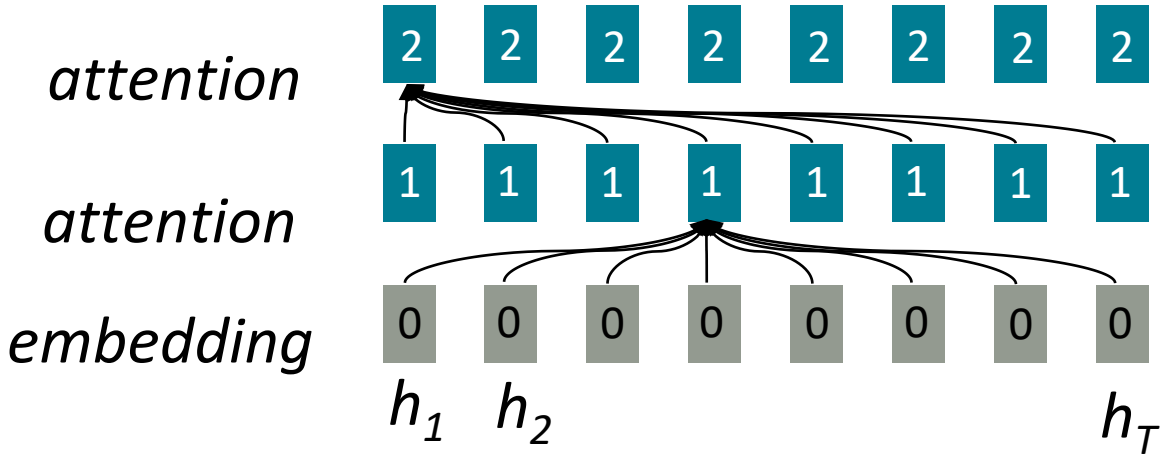
If not recurrence, then what? **How about word windows?**

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



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

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



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

Self-Attention

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

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

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

$$e_{ij} = q_i^\top k_j$$

Compute **key-query** affinities

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

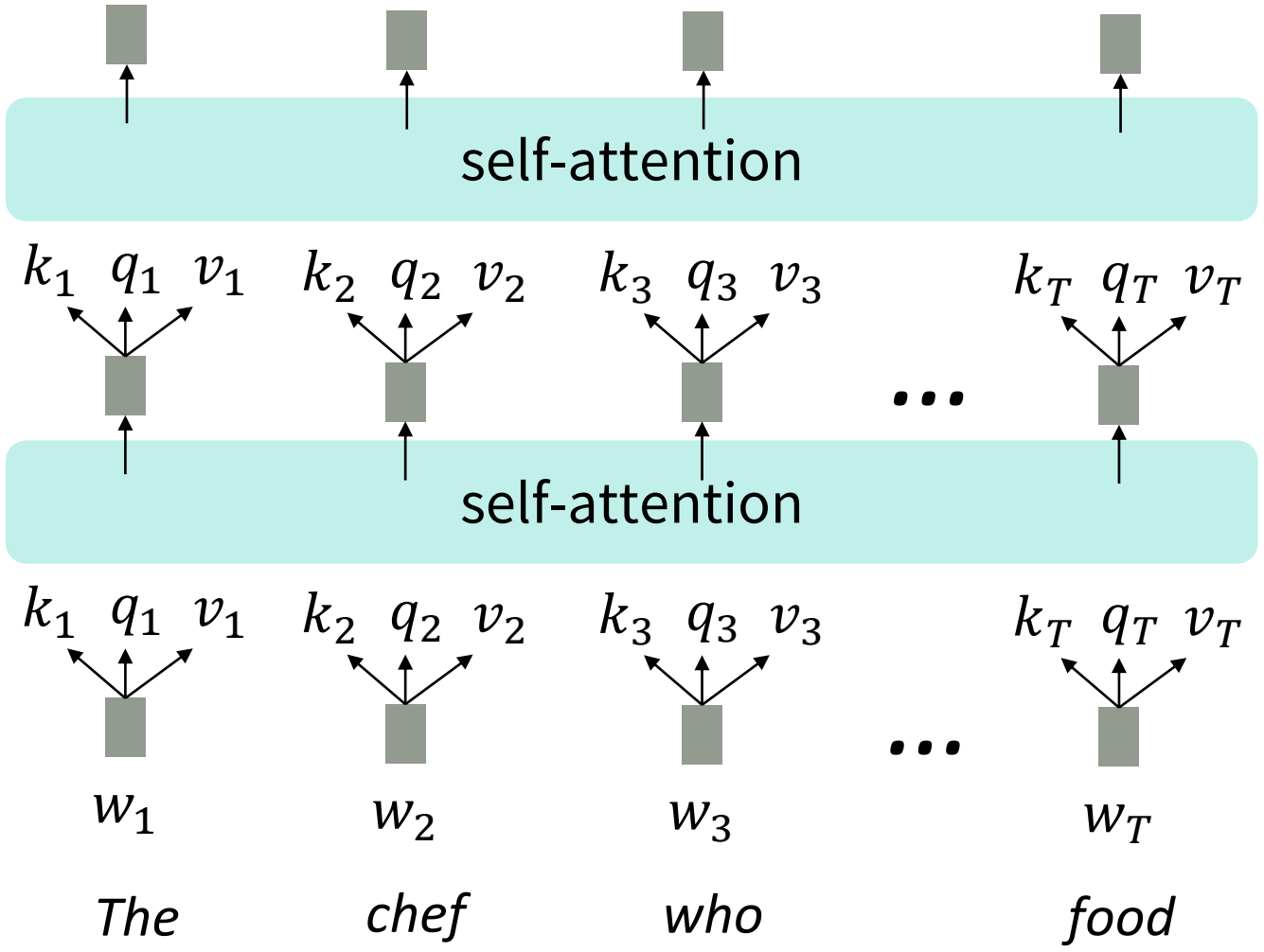
Compute attention weights from affinities (softmax)

$$\text{output}_i = \sum_j \alpha_{ij} v_j$$

Compute outputs as weighted sum of **values**

Self-attention as an NLP building block

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



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

Barriers and solutions for Self-Attention as a building block

Barriers

- Doesn't have an inherent notion of order!

Solutions

Fixing the first self-attention problem: **sequence order**

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

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

- 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 p_i to our inputs!
- Let $\tilde{v}_i\ \tilde{k}_i, \tilde{q}_i$ be our old values, keys, and queries.

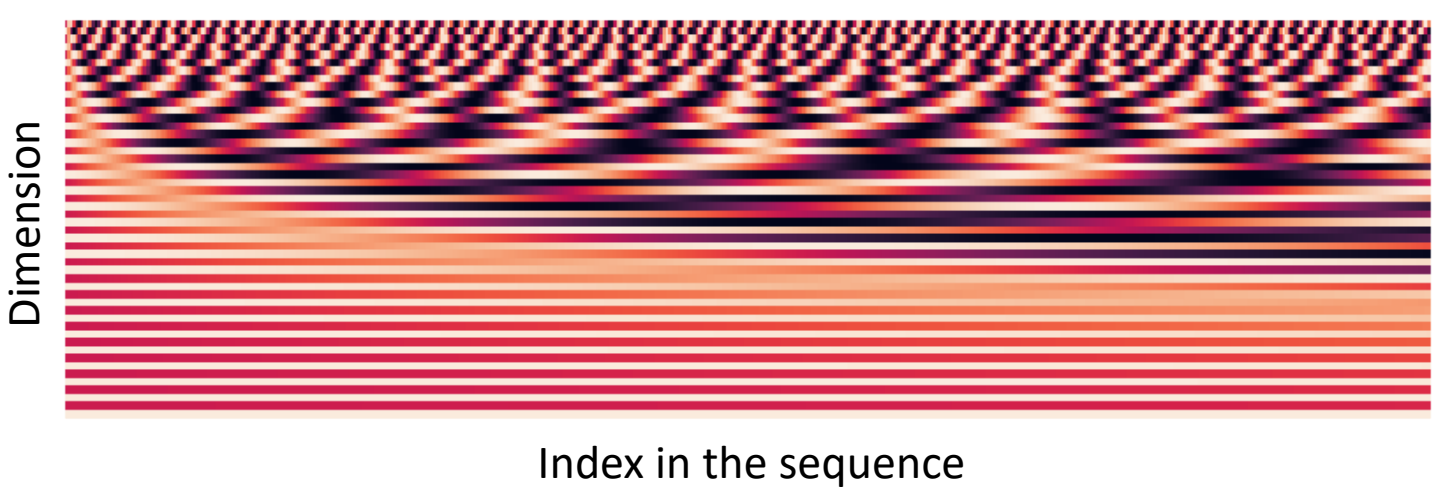
$$v_i = \tilde{v}_i + p_i$$
$$q_i = \tilde{q}_i + p_i$$
$$k_i = \tilde{k}_i + p_i$$

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

Position representation vectors through sinusoids

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

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



- 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/

Position representation vectors learned from scratch

- **Learned absolute position representations:** Let all p_i be learnable parameters!

  Learn a matrix $p \in \mathbb{R}^{d \times T}$, *and let each* p_i *be a column of that matrix!*

- Pros:
  - Flexibility: each position gets to be learned to fit the data
- Cons:
  - Definitely can't extrapolate to indices outside $1, \ldots, T$.
- Most systems use this!

- Sometimes people try more flexible representations of position:
  - Relative linear position attention [Shaw et al., 2018]
  - Dependency syntax-based position [Wang et al., 2019]

Barriers and solutions for Self-Attention as a building block

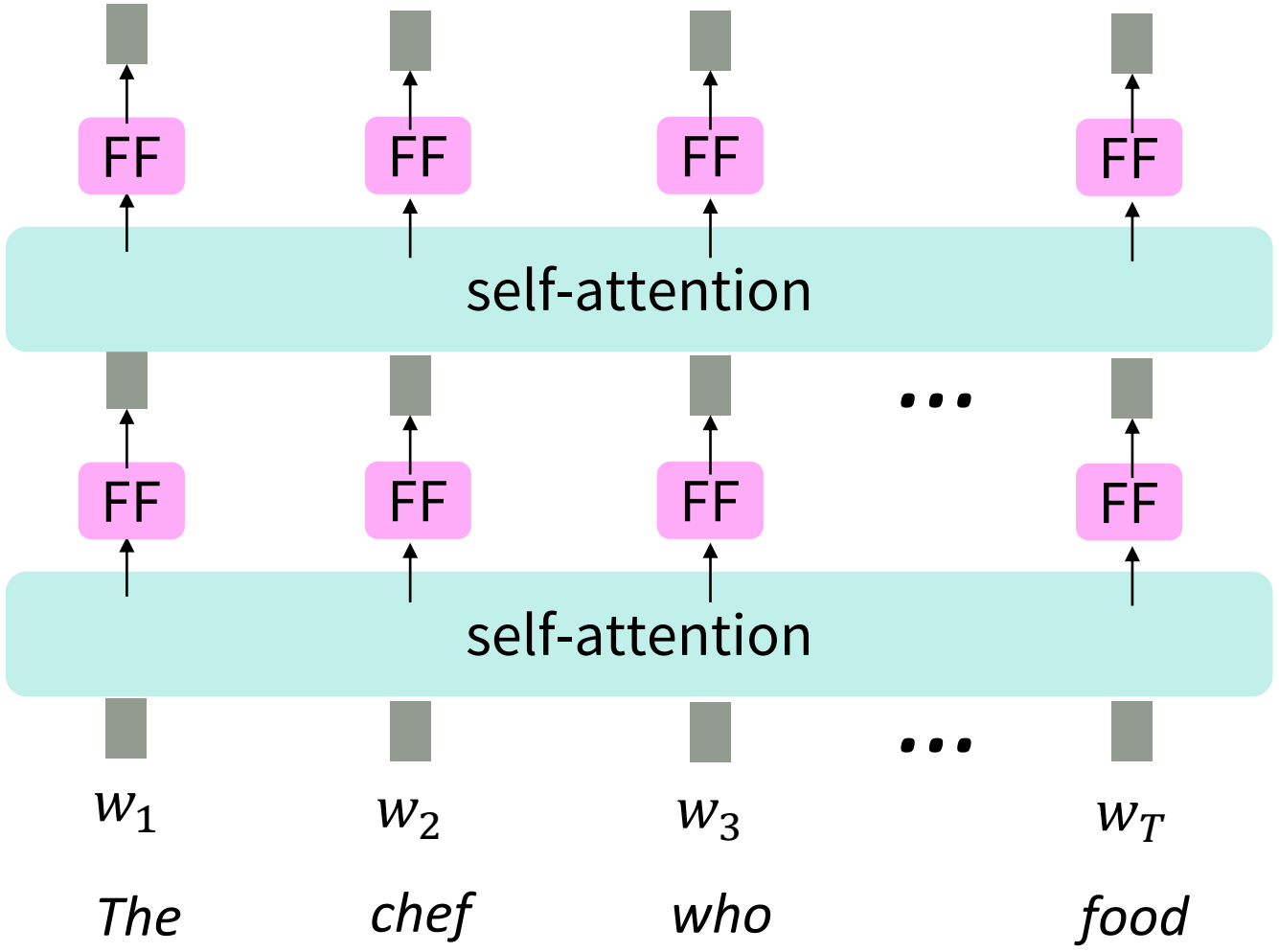
Barriers	Solutions
• Doesn't have an inherent notion of order!	• Add position representations to the inputs
• No nonlinearities for deep learning! It's all just weighted averages	

Adding nonlinearities in self-attention

- Note that there are no elementwise nonlinearities in self-attention; stacking more self-attention layers just re-averages **value** vectors

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

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



Intuition: the FF network processes the result of attention

Barriers and solutions for Self-Attention as a building block

Barriers	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	

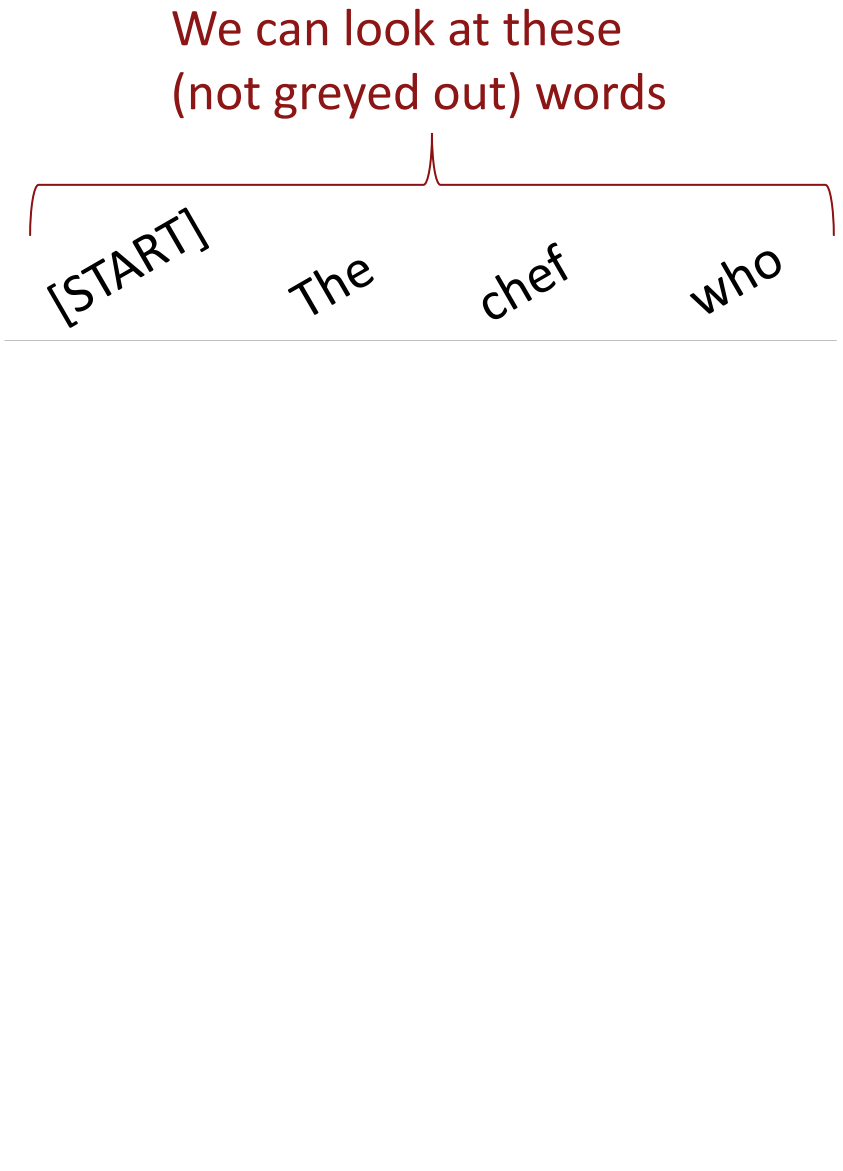
Masking the future in self-attention

- 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 $-\infty$.

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



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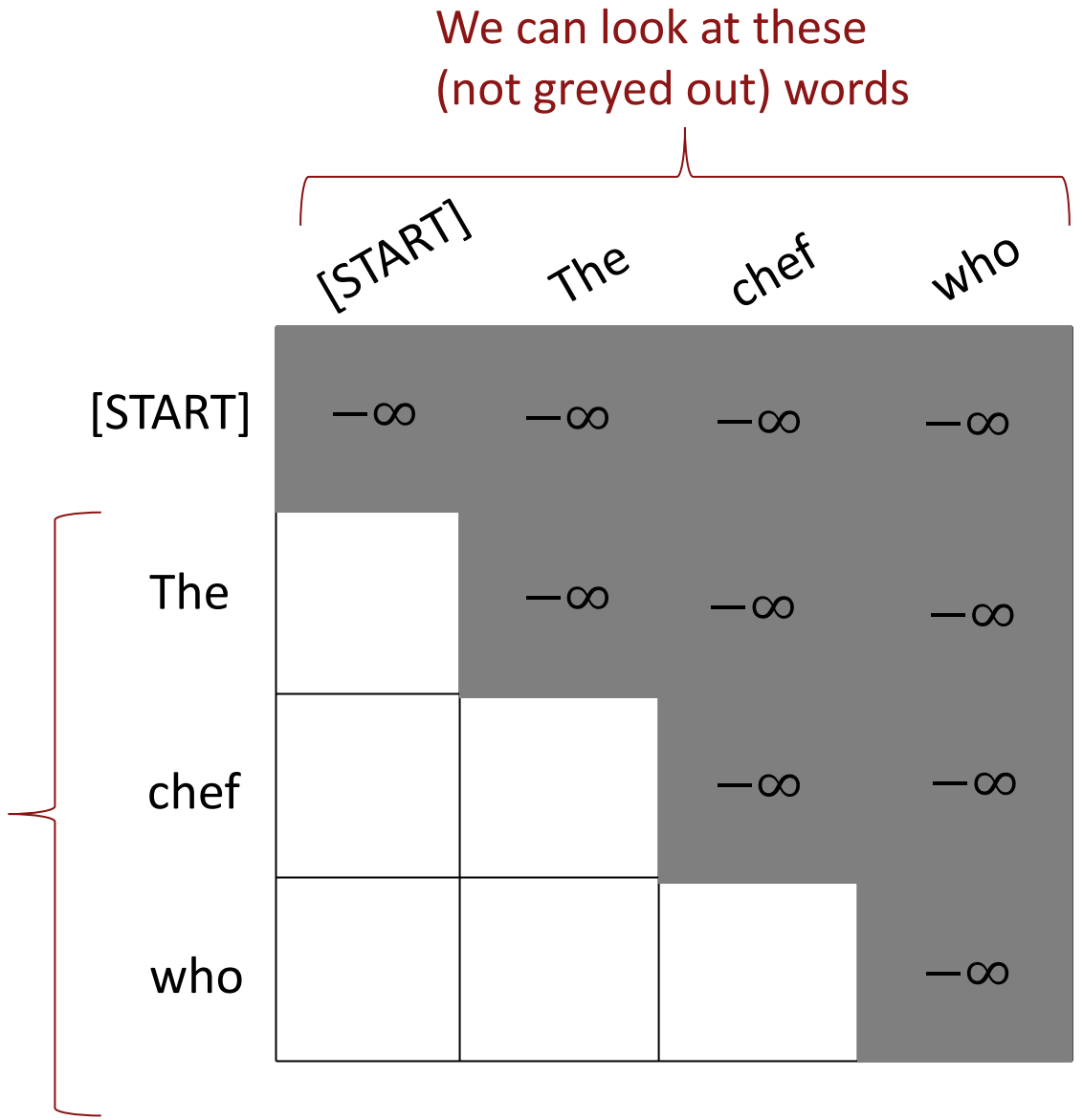


Barriers and solutions for Self-Attention as a building block

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!

Necessities for a self-attention building block:

- **Self-attention**:
  - the basis of the method.
- **Position representations**:
  - Specify the sequence order, since self-attention is an unordered function of its inputs.
- **Nonlinearities**:
  - At the output of the self-attention block
  - Frequently implemented as a simple feed-forward network.
- **Masking**:
  - In order to parallelize operations while not looking at the future.
  - Keeps information about the future from “leaking” to the past.

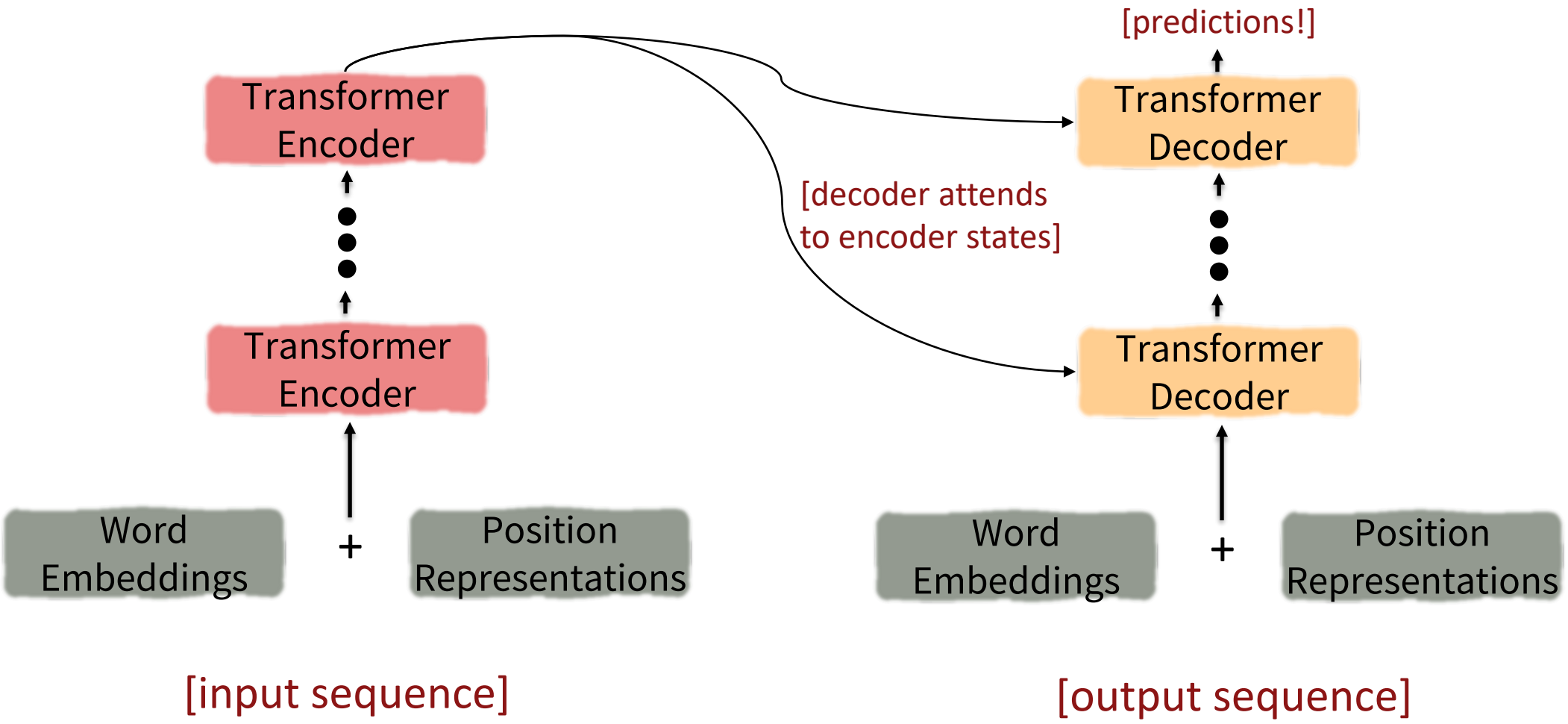
- That’s it! But this is not the **Transformer** model we’ve been hearing about.

Outline

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

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

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



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

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

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

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

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

- We saw that self-attention is when keys, queries, and values come from the same source. The Transformer does this in a particular way:
  - Let $x_1, \ldots, x_T$ be input vectors to the Transformer encoder; $x_i \in \mathbb{R}^d$

- Then keys, queries, values are:
  - $k_i = Kx_i$, where $K \in \mathbb{R}^{d \times d}$ is the key matrix.
  - $q_i = Qx_i$, where $\mathrm{Q} \in \mathbb{R}^{d \times d}$ is the query matrix.
  - $v_i = Vx_i$, where $\mathrm{V} \in \mathbb{R}^{d \times d}$ is the value matrix.

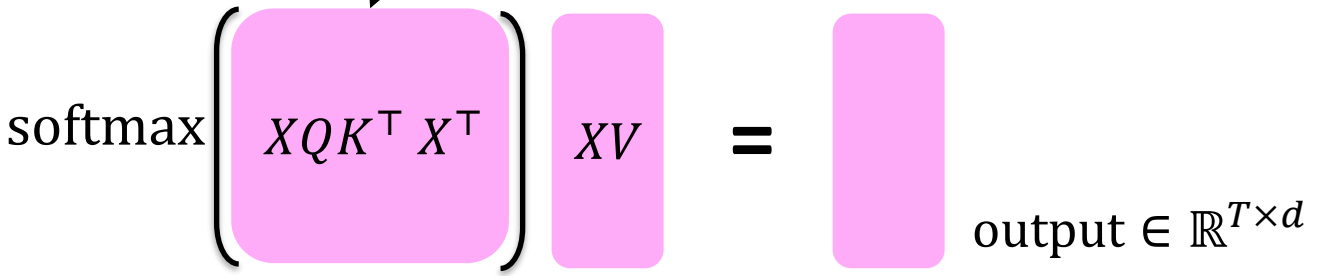
- These matrices allow *different aspects* of the x vectors to be used/emphasized in each of the three roles.

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

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

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.



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

- What if we want to look in multiple places in the sentence at once?
  - For word i, self-attention "looks" where $x_i^\top Q^\top K x_j$ 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!
  - $\text{output} = Y[\text{output}_1; \ldots; \text{output}_h]$, 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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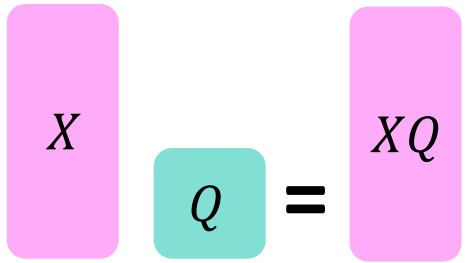
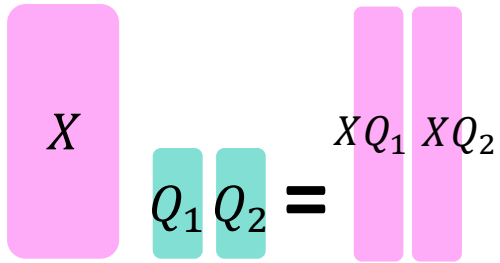
Single-head attention
(just the query matrix)



Multi-head attention
(just two heads here)

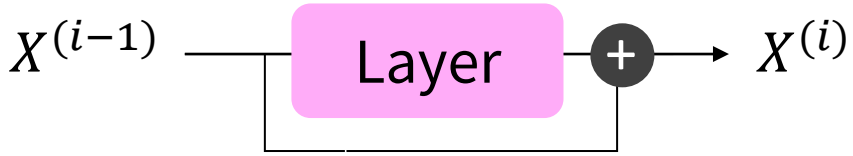


Same amount of computation as single-head self-attention!

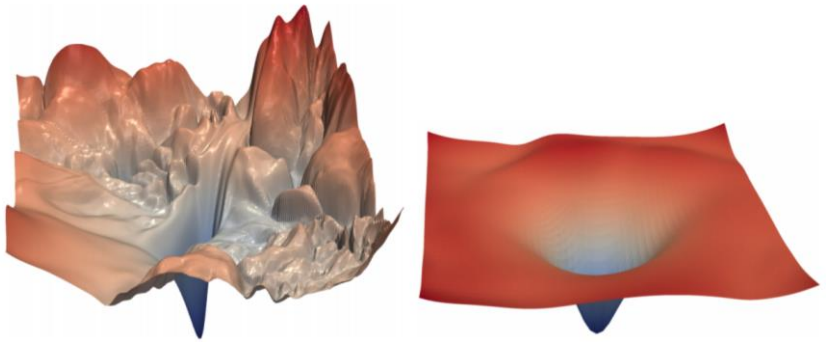
The Transformer Encoder: **Residual connections** [He et al., 2016]

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

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



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



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

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

Normalize by scalar mean and variance

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

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- 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 Encoder: **Scaled Dot Product** [Vaswani et al., 2017]

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

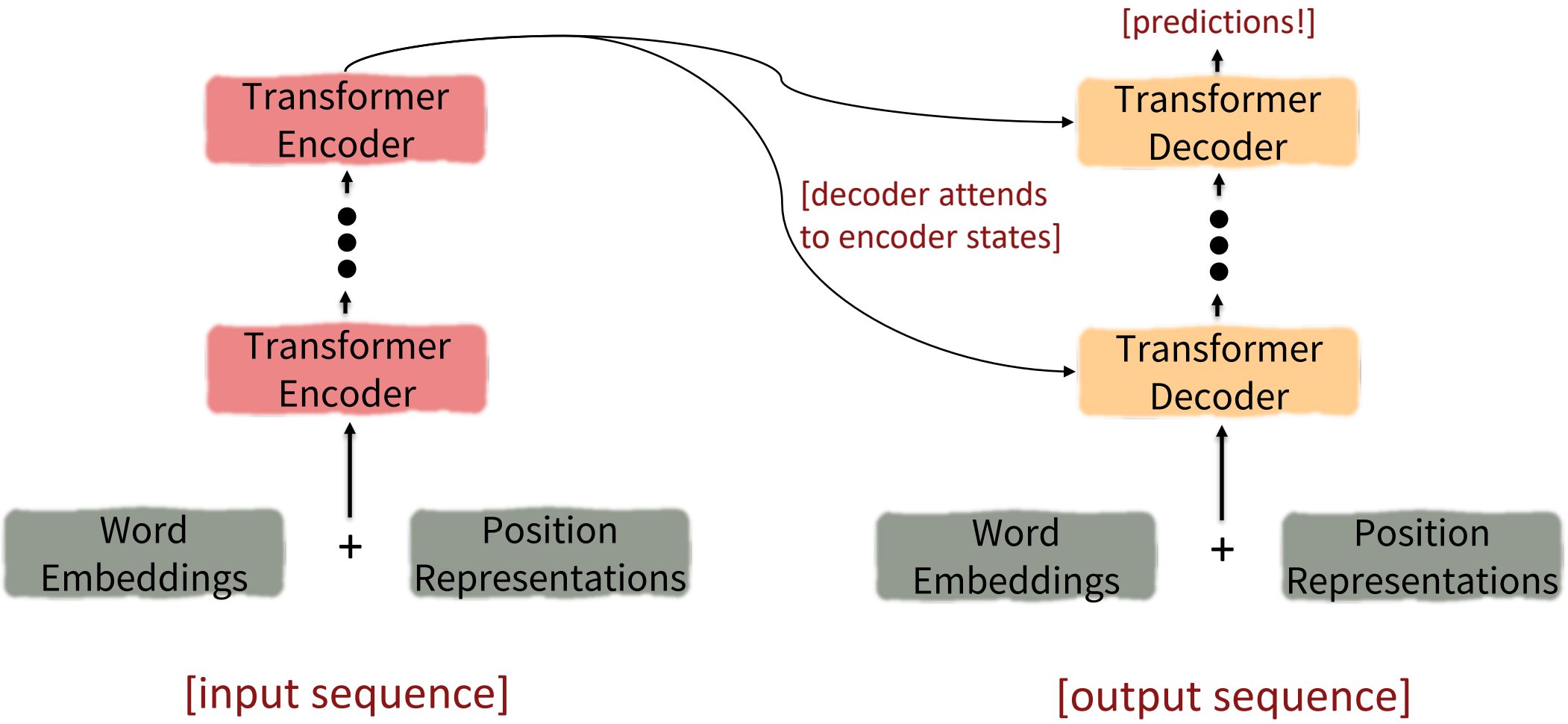
$$\text{output}_\ell = \text{softmax}\left(XQ_\ell K_\ell^\top X^\top\right) * XV_\ell$$

- 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.)

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

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

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



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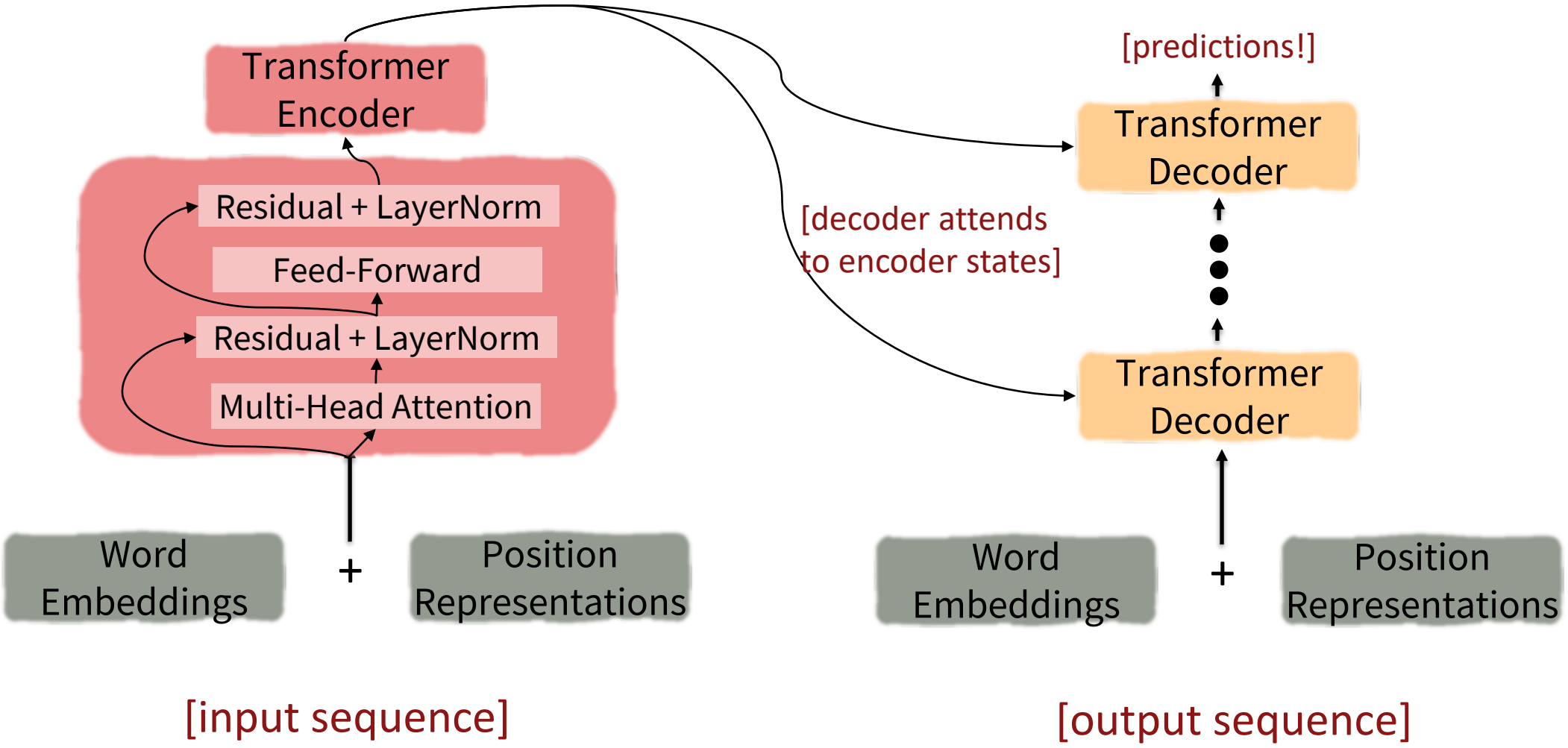

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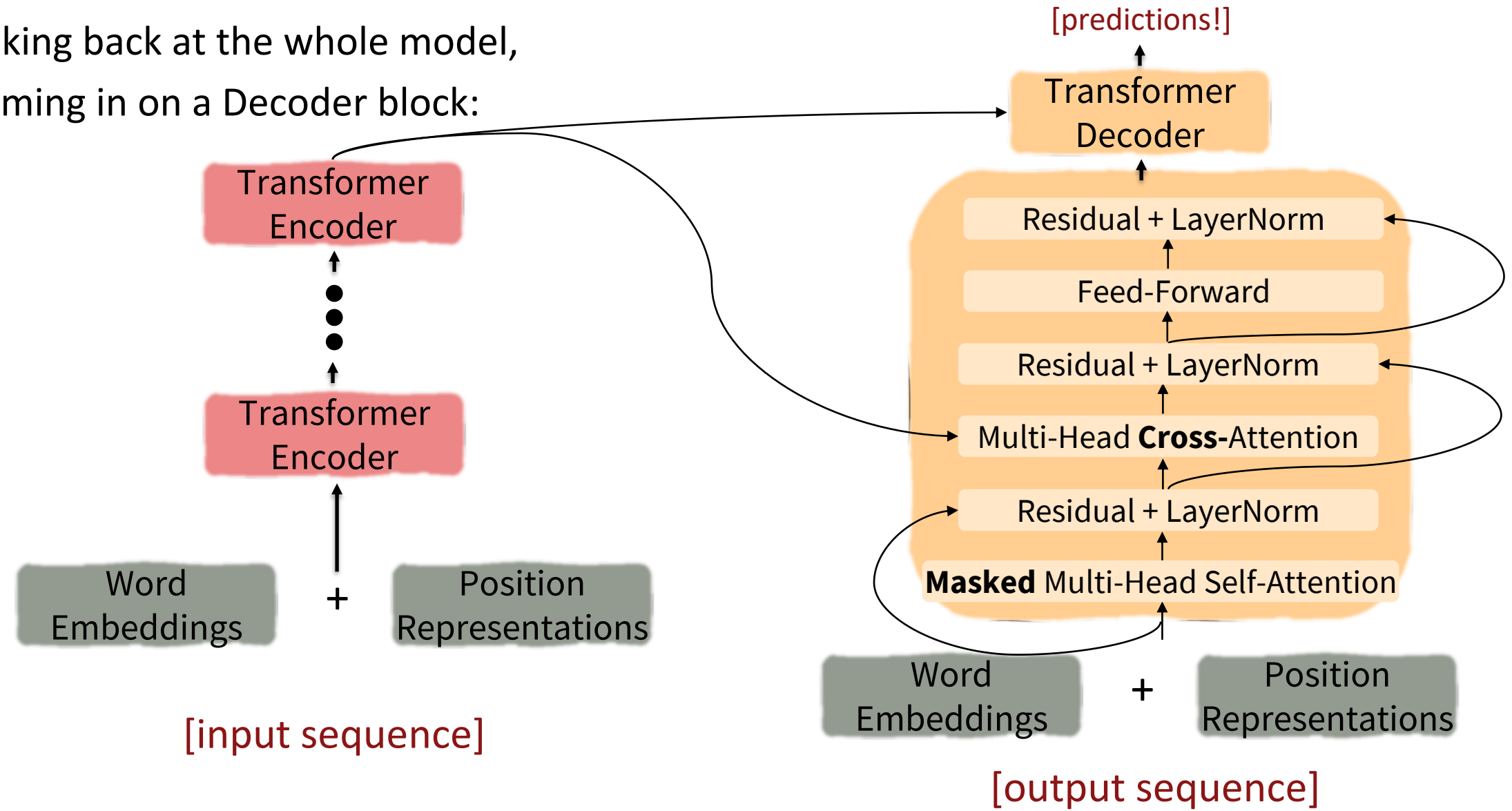
Looking back at the whole model,

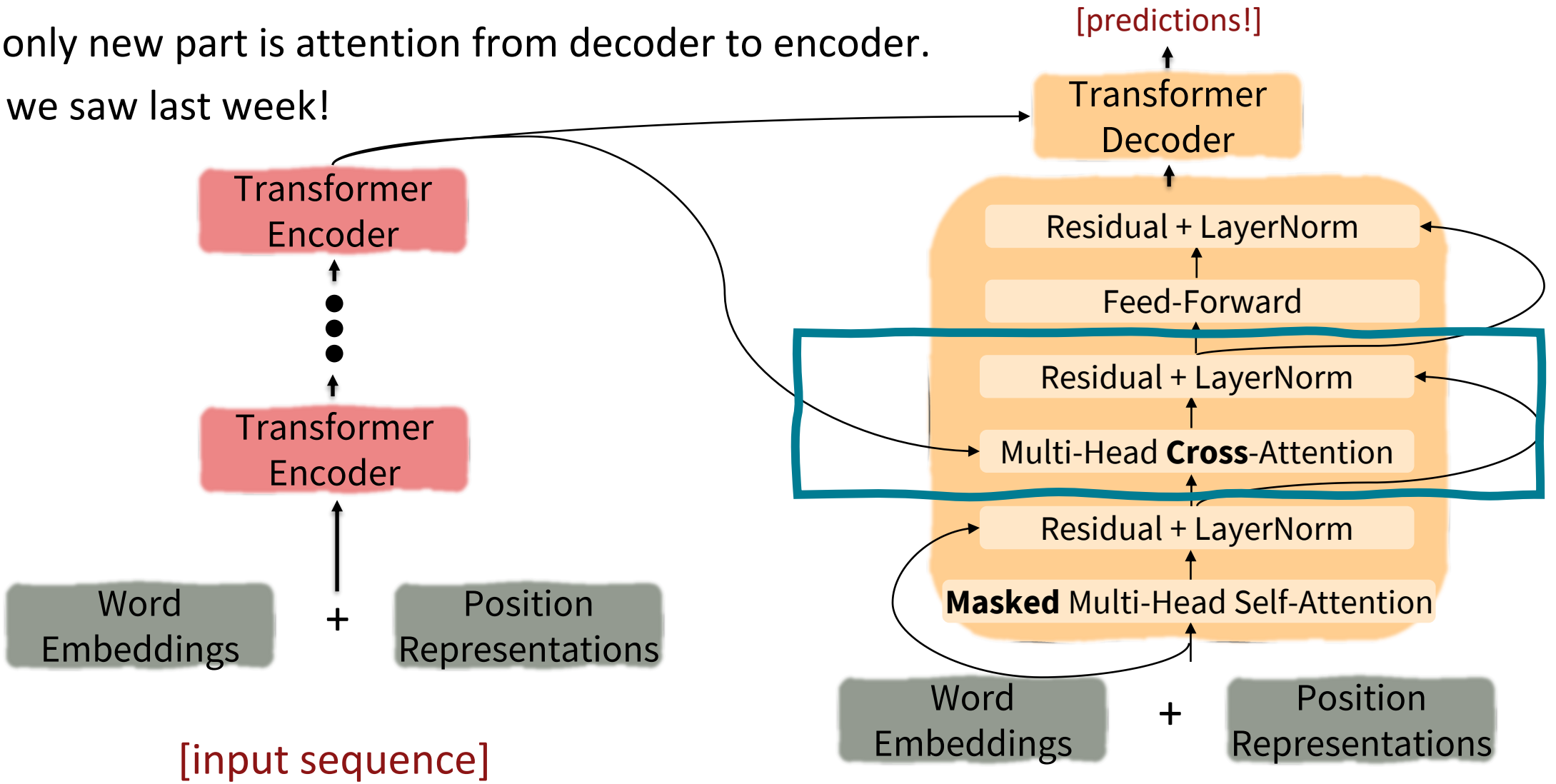
zooming in on a Decoder block:



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

The only new part is attention from decoder to encoder.

Like we saw last week!



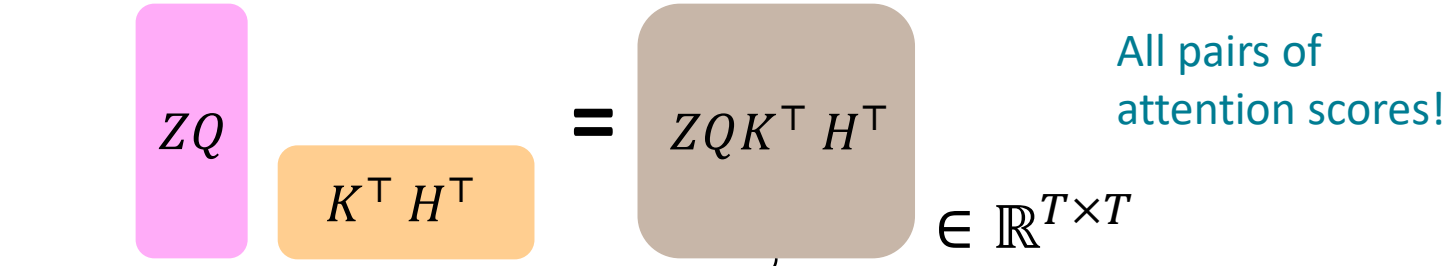
The Transformer Decoder: **Cross-attention (details)**

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

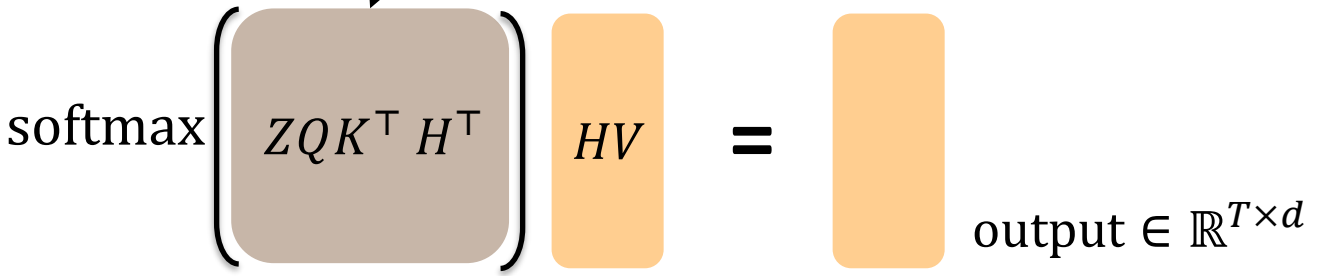
The Transformer Encoder: **Cross-attention (details)**

- Let's look at how cross-attention is computed, in matrices.
  - Let $\mathrm{H} = [h_1; \ldots; h_T] \in \mathbb{R}^{T \times d}$ 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: $ZQ(HK)^\top$



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



Outline

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

Great Results with Transformers

First, Machine Translation from the original Transformers paper!

Model	BLEU		Training Cost (FLOPs)	
	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:

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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What would we like to fix about the Transformer?

- **Quadratic compute in self-attention (today)**:
  - Computing all pairs of interactions means our computation grows **quadratically** with the sequence length!
  - For recurrent models, it only grew linearly!
- **Position representations**:
  - Are simple absolute indices the best we can do to represent position?
  - Relative linear position attention [Shaw et al., 2018]
  - Dependency syntax-based position [Wang et al., 2019]

Quadratic computation as a function of sequence length

- One of the benefits of self-attention over recurrence was that it's highly parallelizable.
- However, its total number of operations grows as $O(T^2 d)$, where T is the sequence length, and d is the dimensionality.

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

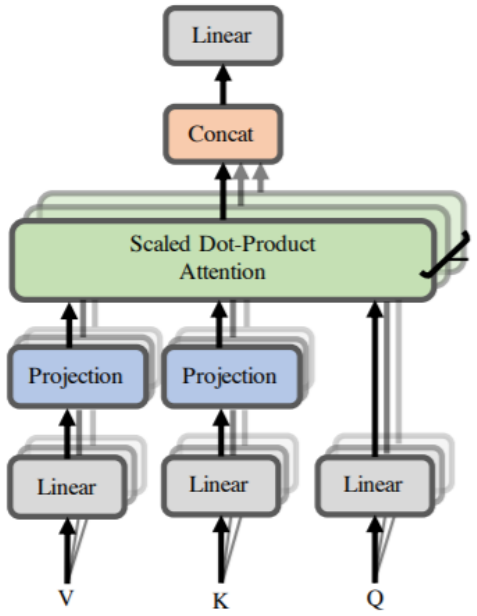
Need to compute all pairs of interactions!
$O(T^2 d)$

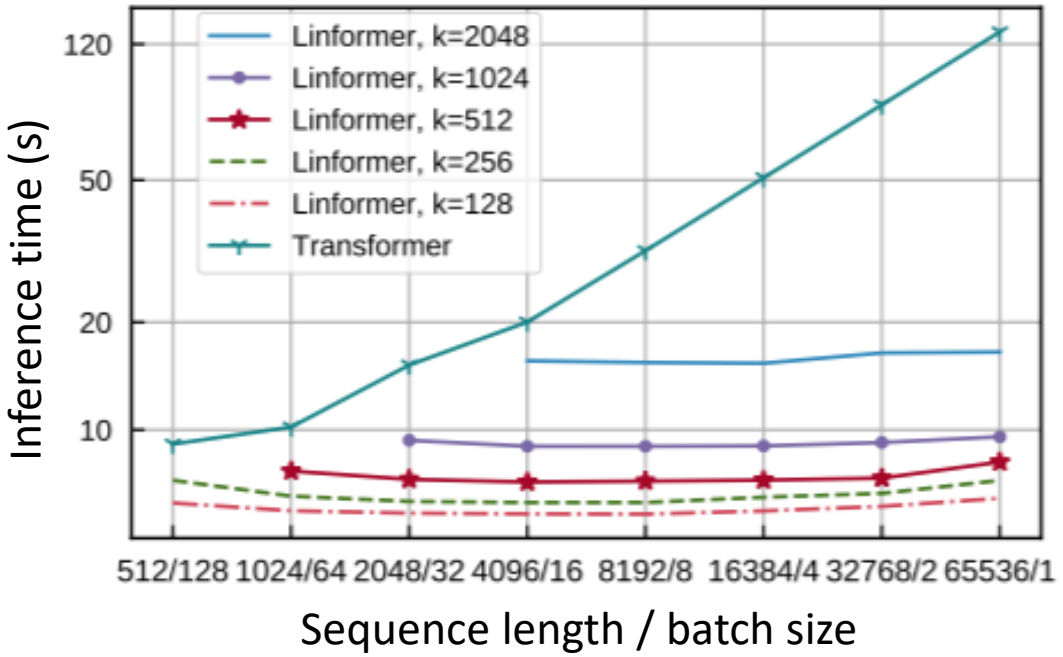
- Think of d as around $\mathbf{1,000}$.
  - So, for a single (shortish) sentence, $T \leq 30; T^2 \leq \mathbf{900}$.
  - In practice, we set a bound like $T = 512$.
  - **But what if we'd like $T \geq 10,000$?** For example, to work on long documents?

Recent work on improving on quadratic self-attention cost

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

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

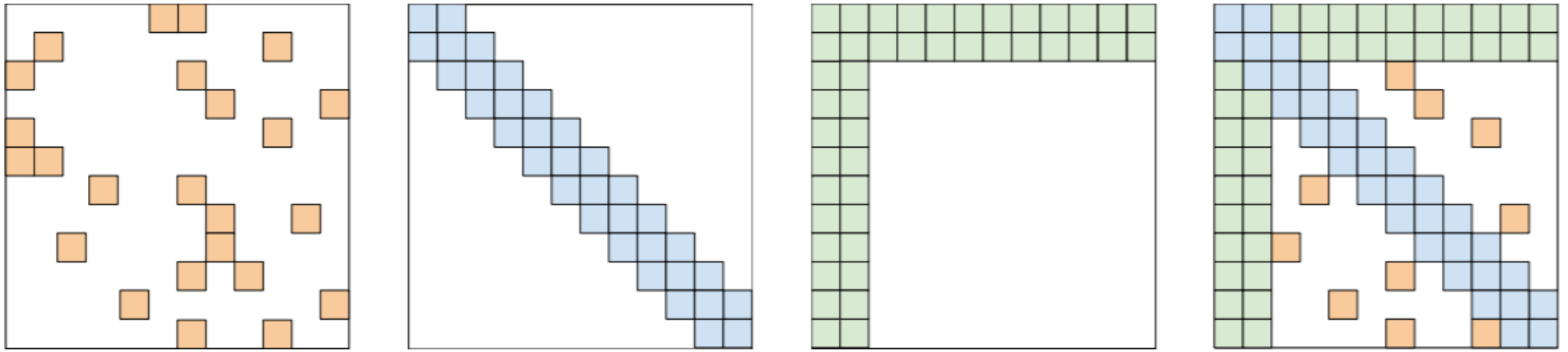




Recent work on improving on quadratic self-attention cost

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

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



(a) Random attention (b) Window attention (c) Global Attention (d) BIGBIRD

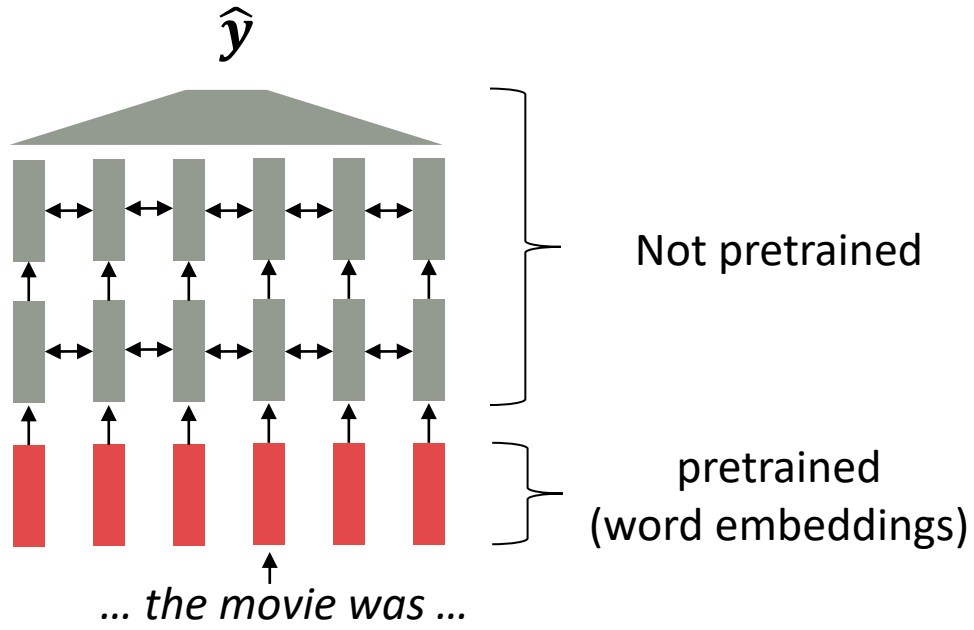
Where we were: **pretrained word embeddings**

Circa 2017:

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

Some issues to think about:

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



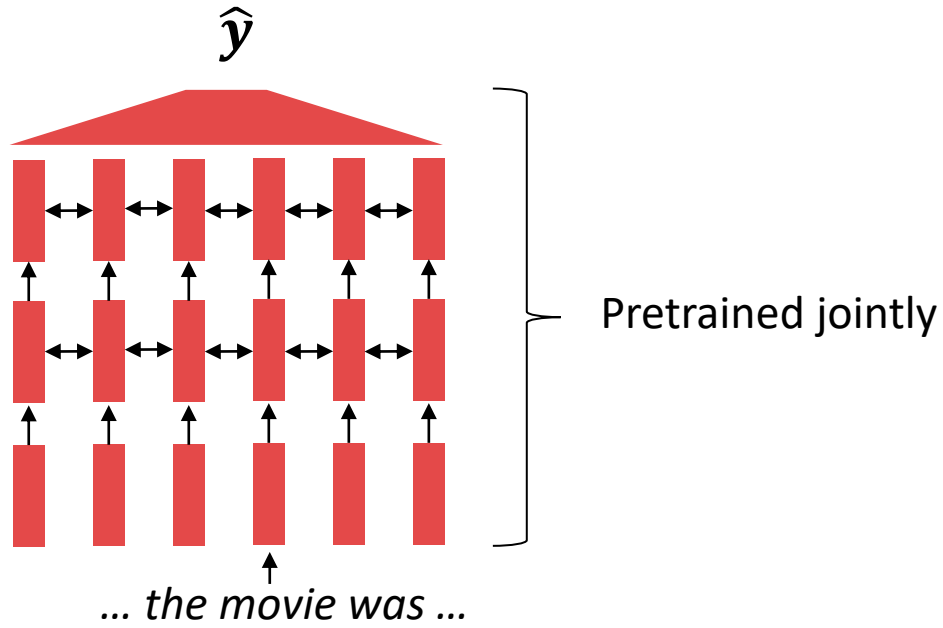
[Recall, *movie* gets the same word embedding, no matter what sentence it shows up in]

Where we're going: **pretraining whole models**

In modern NLP:

- All (or almost all) parameters in NLP networks are initialized via **pretraining**.
- Pretraining methods hide parts of the input from the model, and train the model to reconstruct those parts.

- This has been exceptionally effective at building strong:
  - **representations of language**
  - **parameter initializations** for strong NLP models.
  - **Probability distributions** over language that we can sample from



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

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 _____.

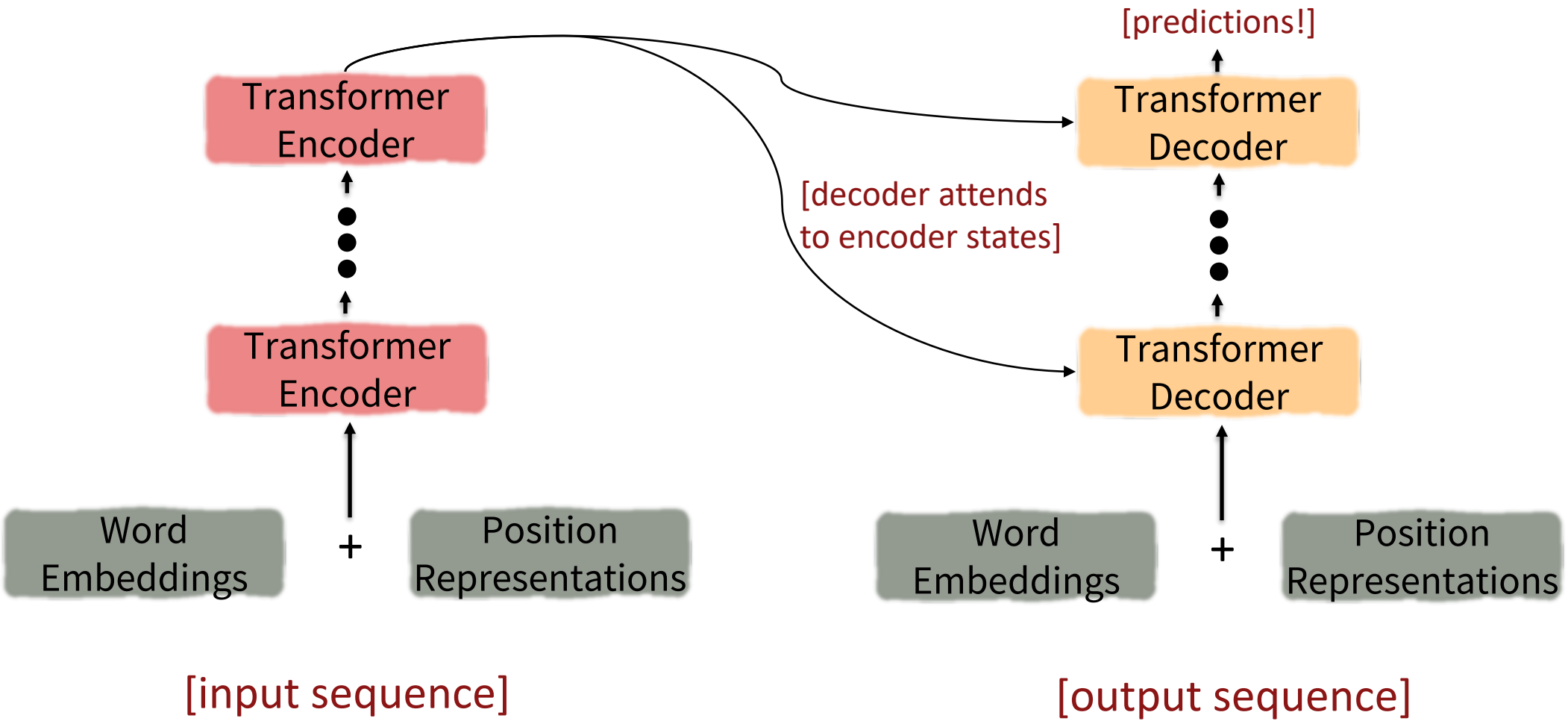
What can we learn from reconstructing the input?

I was thinking about the sequence that goes

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

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

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



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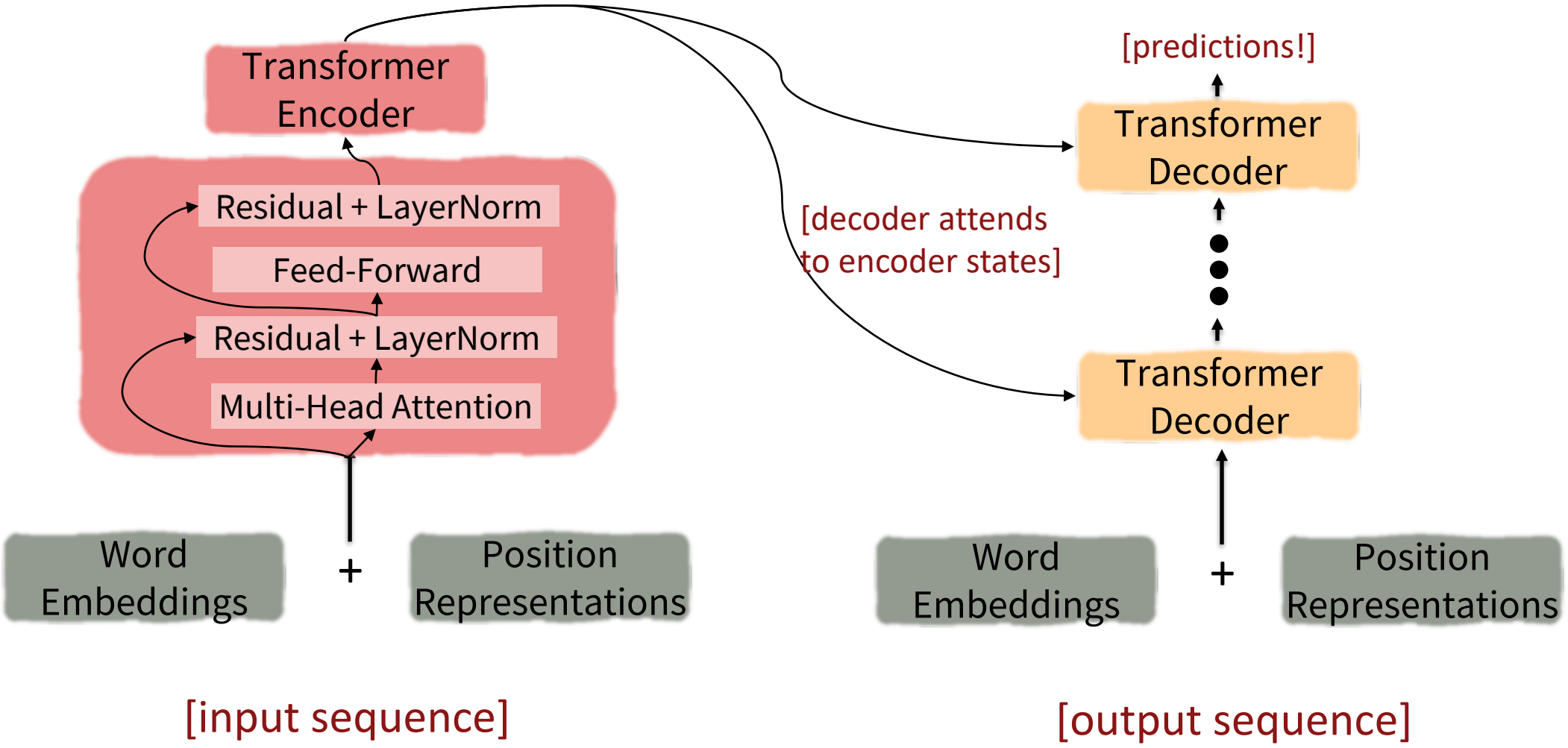

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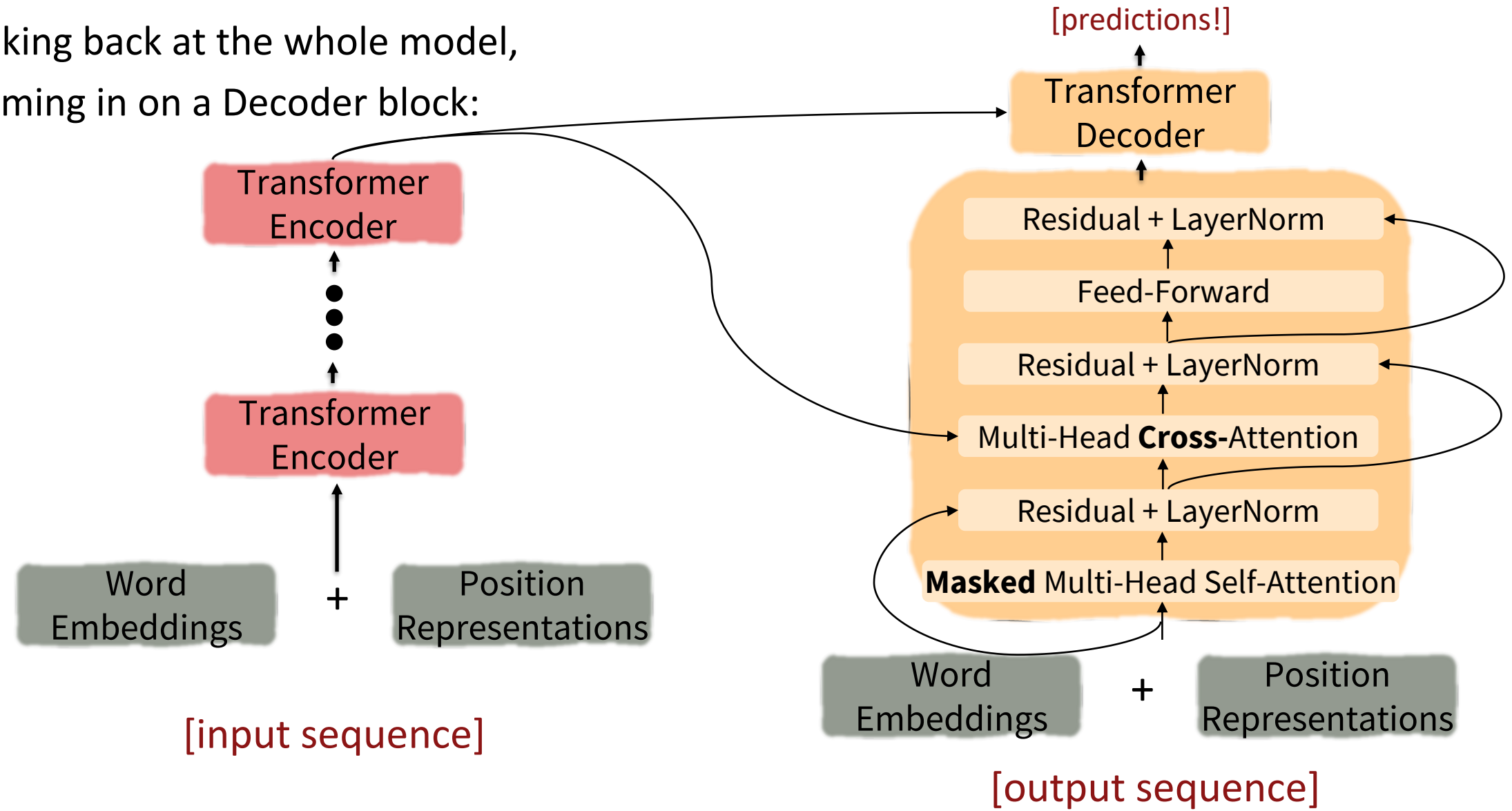

The Transformer Encoder-Decoder [Vaswani et al., 2017]

The only new part is attention from decoder to encoder.

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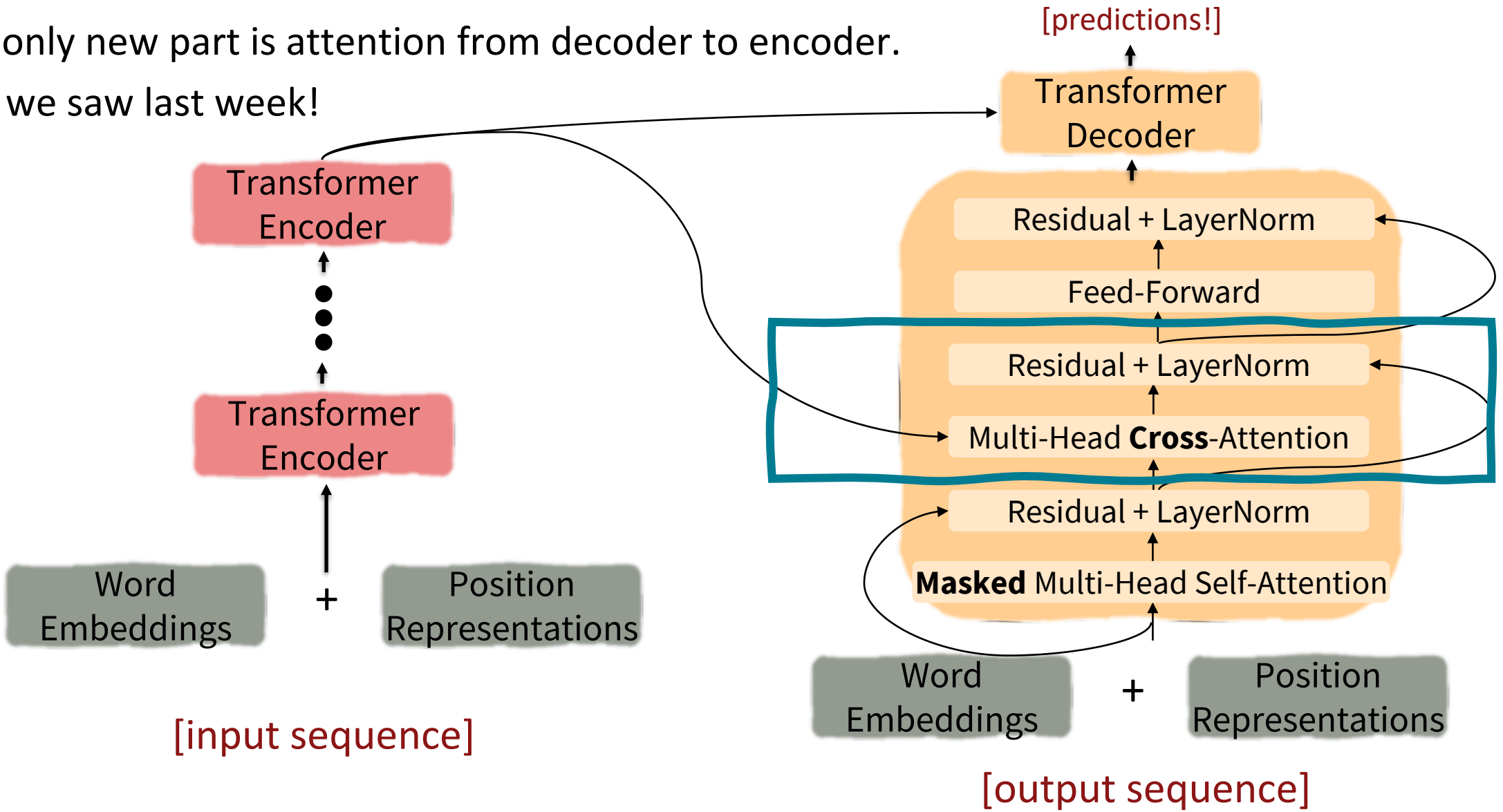


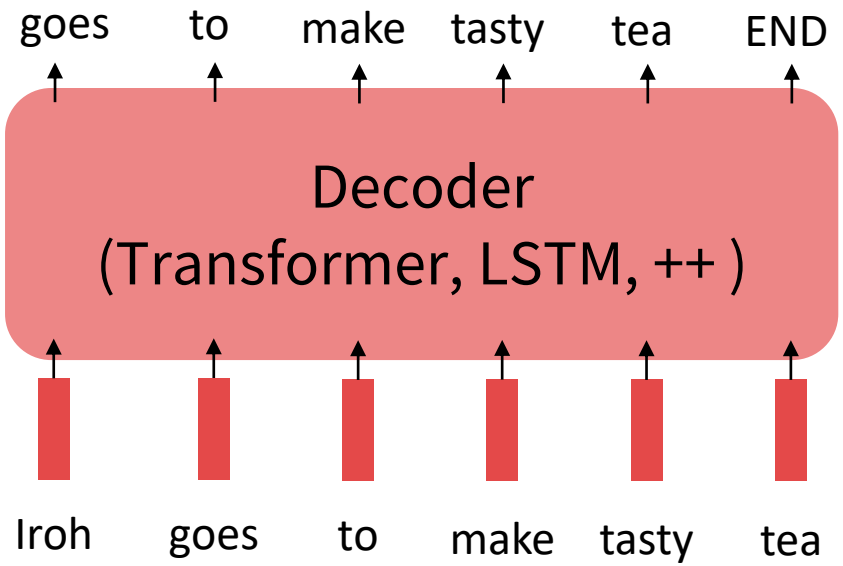
Pretraining through language modeling [Dai and Le, 2015]

Recall the **language modeling** task:

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

Pretraining through language modeling:

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

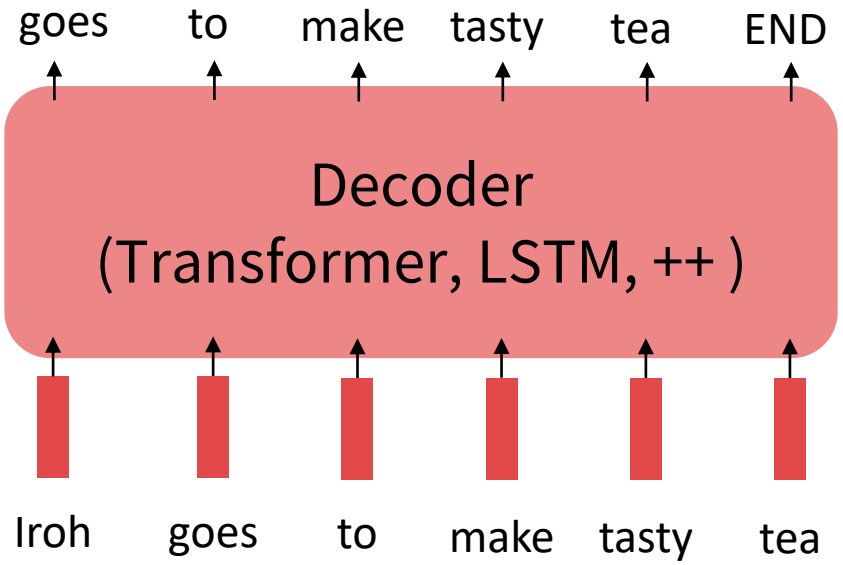


The Pretraining / Finetuning Paradigm

Pretraining can improve NLP applications by serving as parameter initialization.

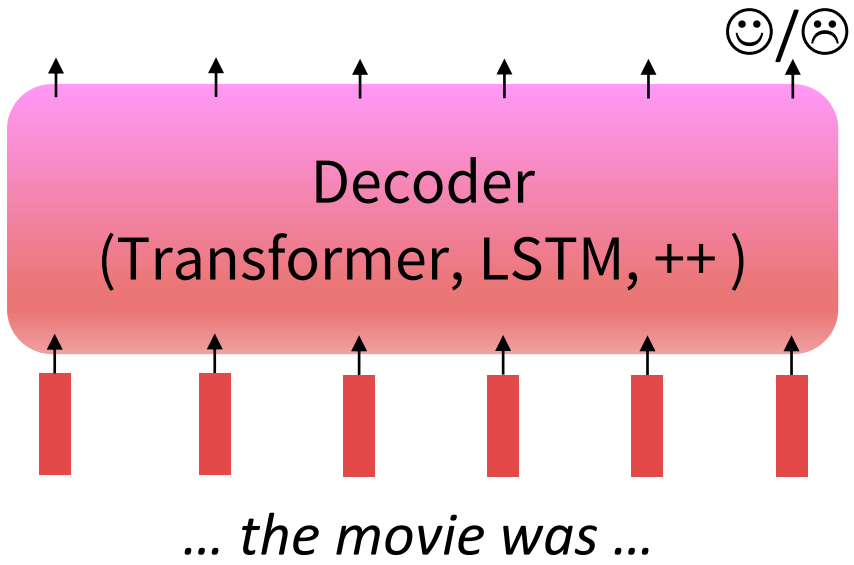
Step 1: Pretrain (on language modeling)

Lots of text; learn general things!



Step 2: Finetune (on your task)

Not many labels; adapt to the task!



Stochastic gradient descent and pretrain/finetune

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

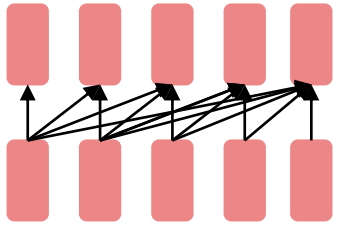
- Consider, provides parameters $\hat{\theta}$ by approximating $\min_{\theta} \mathcal{L}_{\text{pretrain}}(\theta)$.
  - (The pretraining loss.)
- Then, finetuning approximates $\min_{\theta} \mathcal{L}_{\text{finetune}}(\theta)$, starting at $\hat{\theta}$.
  - (The finetuning loss)
- The pretraining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

Lecture Plan

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

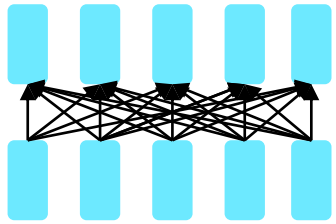
Pretraining for three types of architectures

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



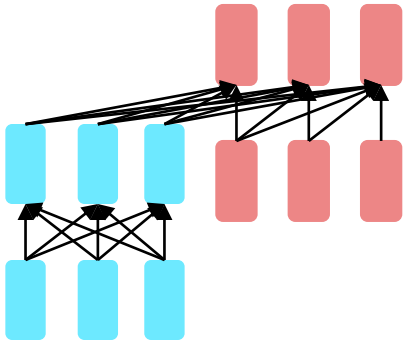
Decoders

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



Encoders

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



Encoder-Decoders

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

Pretraining for three types of architectures

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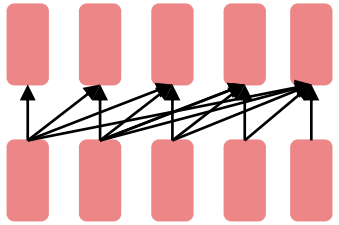

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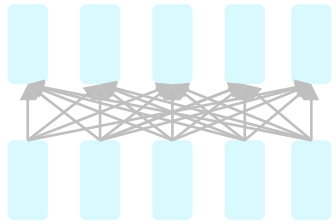

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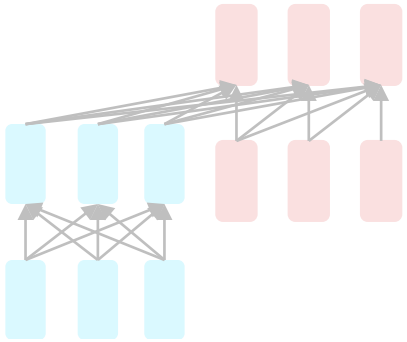

Encoder-Decoders

- Good parts of decoders and encoders?
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Pretraining decoders

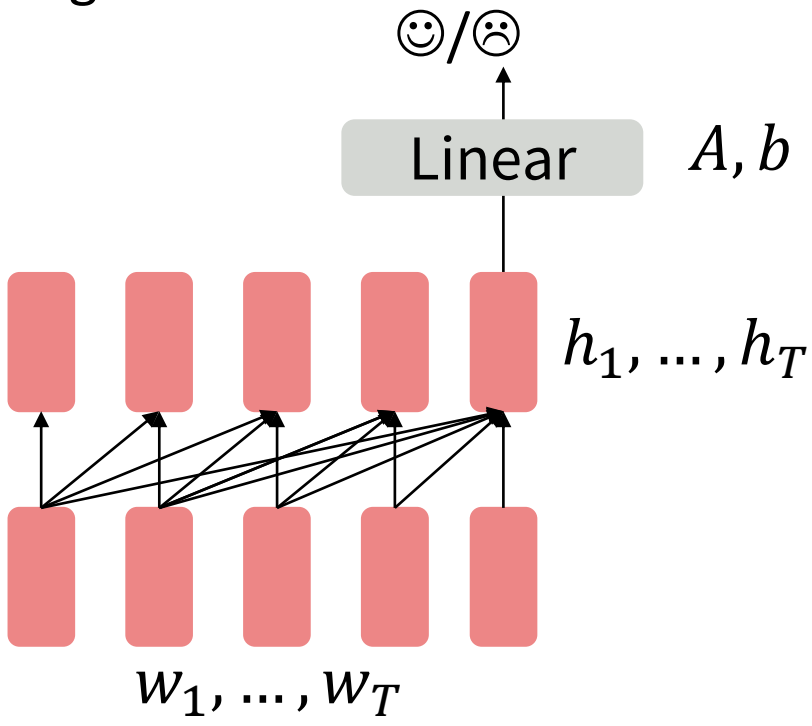
When using language model pretrained decoders, we can ignore that they were trained to model $p(w_t|w_{1:t-1})$.

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

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

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.]

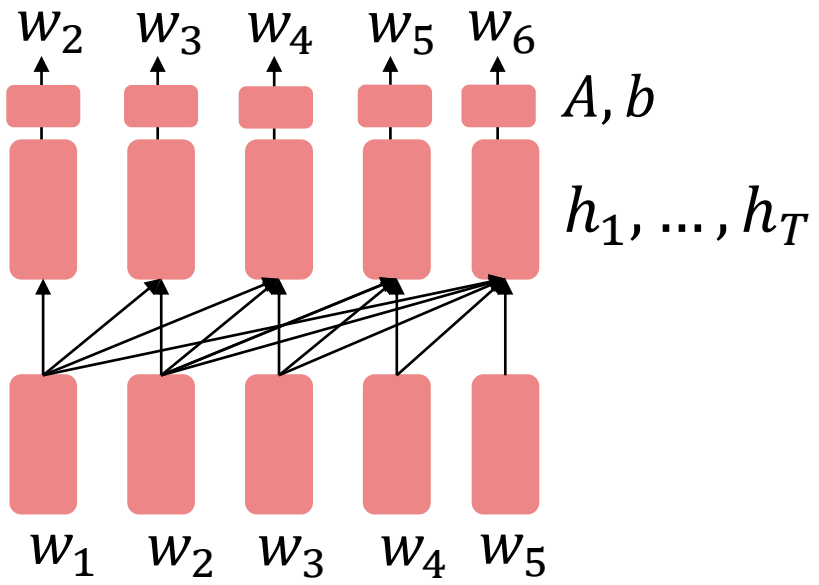
Pretraining decoders

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)

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



[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.
- 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 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.

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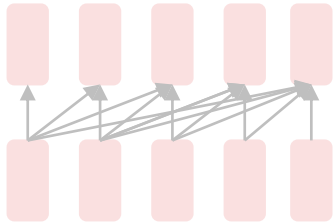

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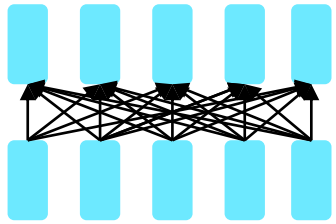

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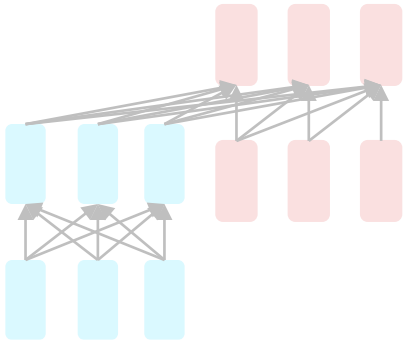

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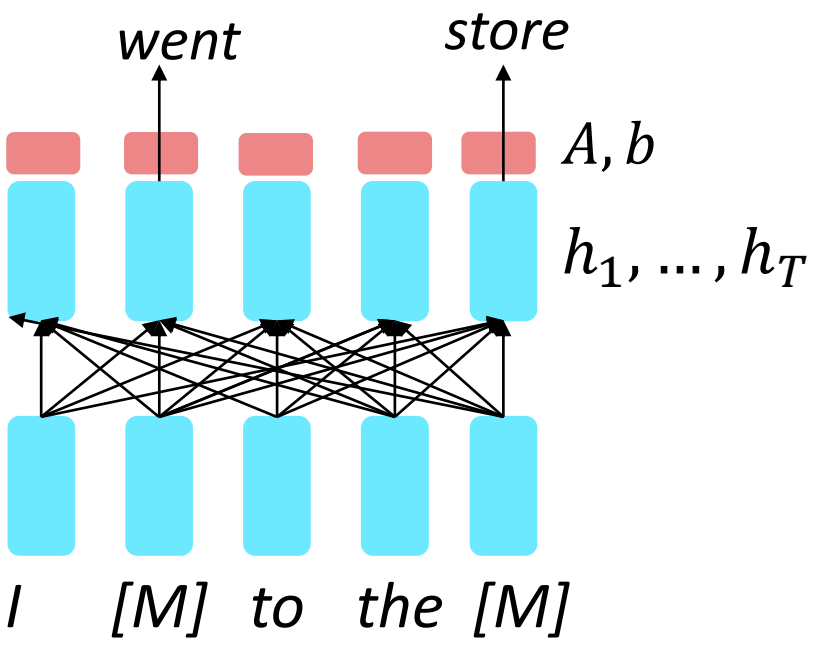
- Good parts of decoders and encoders?
- What's the best way to pretrain them?

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**.

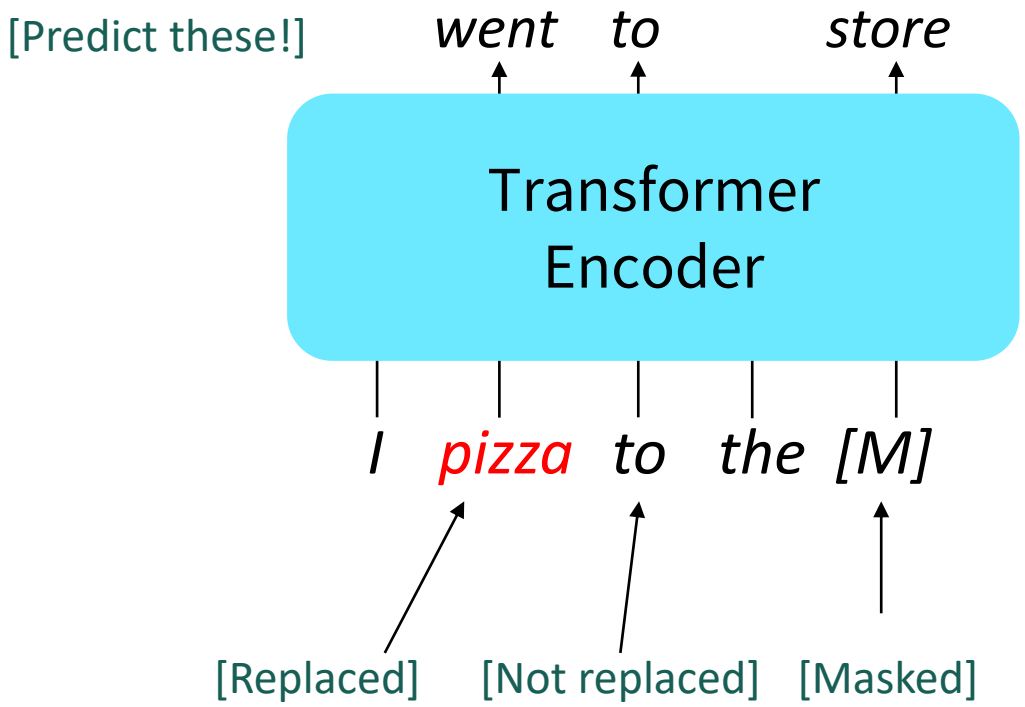
[Devlin et al., 2018]

BERT: Bidirectional Encoder Representations from Tranformers

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:

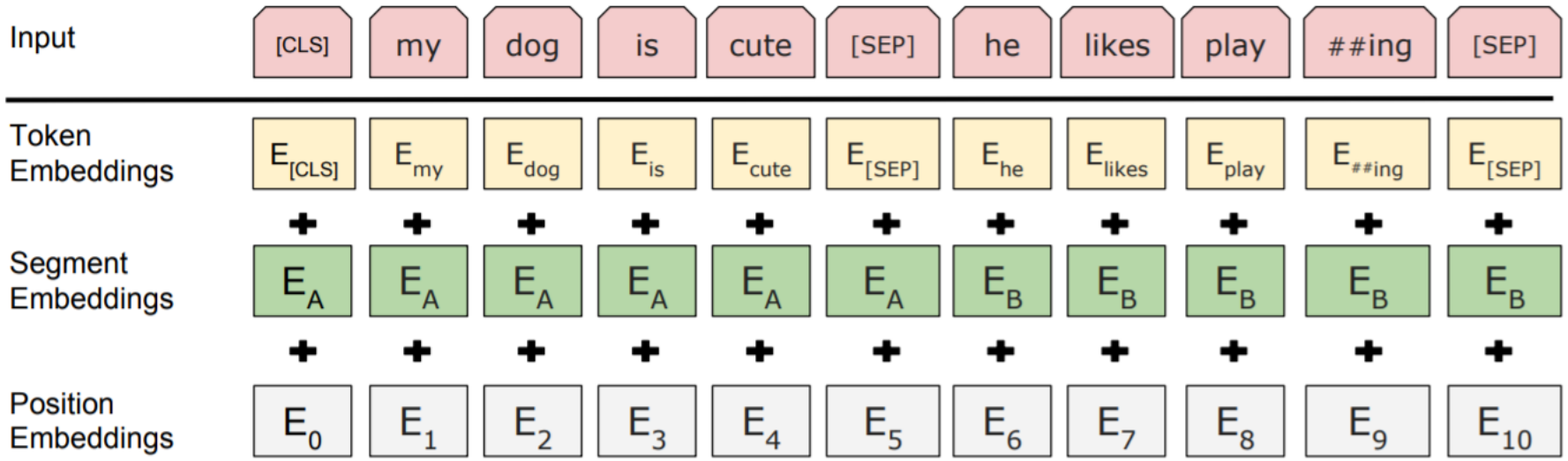
- Predict a random 15% of (sub)word tokens.
  - Replace input word with [MASK] 80% of the time
  - Replace input word with a random token 10% of the time
  - Leave input word unchanged 10% of the time (but still predict it!)
- Why? Doesn't let the model get complacent and not build strong representations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



[Devlin et al., 2018]

BERT: Bidirectional Encoder Representations from Tranformers

- 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 Tranformers

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 Tranformers

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

- **QQP:** Quora Question Pairs (detect paraphrase questions)
- **QNLI**: natural language inference over question answering data
- **SST-2**: sentiment analysis
- **CoLA**: corpus of linguistic acceptability (detect whether sentences are grammatical.)
- **STS-B**: semantic textual similarity
- **MRPC**: microsoft paraphrase corpus
- **RTE**: a small natural language inference corpus

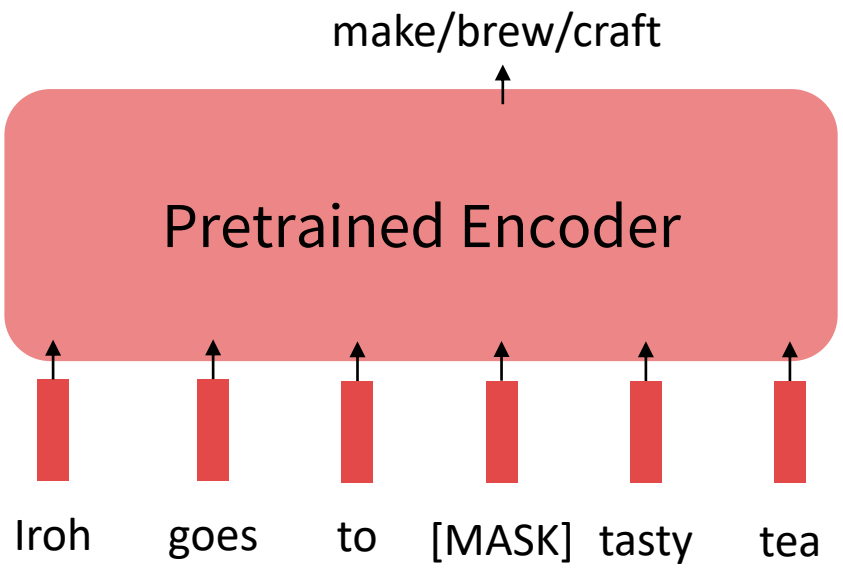
System	MNLI-(m/mm)	QQP	QNLI	SST-2	CoLA	STS-B	MRPC	RTE	**Average**
	392k	363k	108k	67k	8.5k	5.7k	3.5k	2.5k	-
Pre-OpenAI SOTA	80.6/80.1	66.1	82.3	93.2	35.0	81.0	86.0	61.7	74.0
BiLSTM+ELMo+Attn	76.4/76.1	64.8	79.8	90.4	36.0	73.3	84.9	56.8	71.0
OpenAI GPT	82.1/81.4	70.3	87.4	91.3	45.4	80.0	82.3	56.0	75.1
$\text{BERT}_{\text{BASE}}$	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**

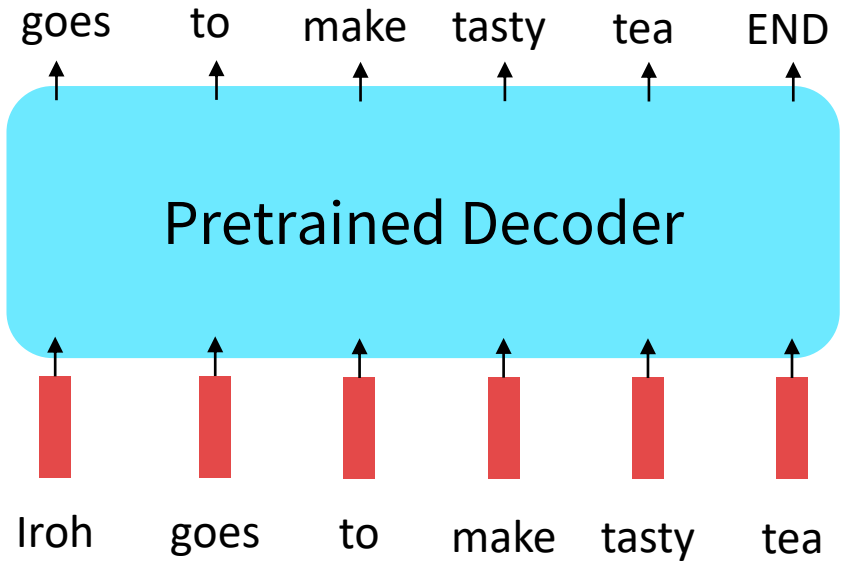
[Devlin et al., 2018]

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.



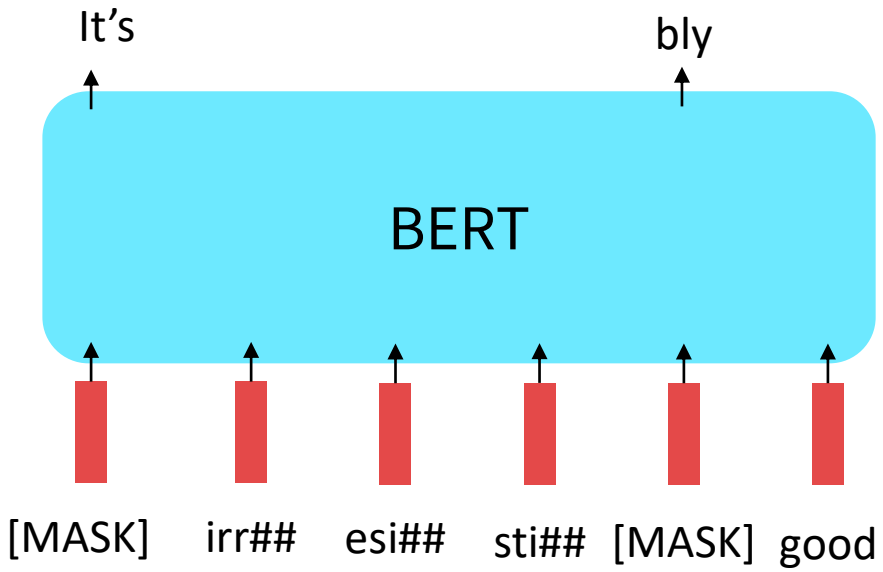


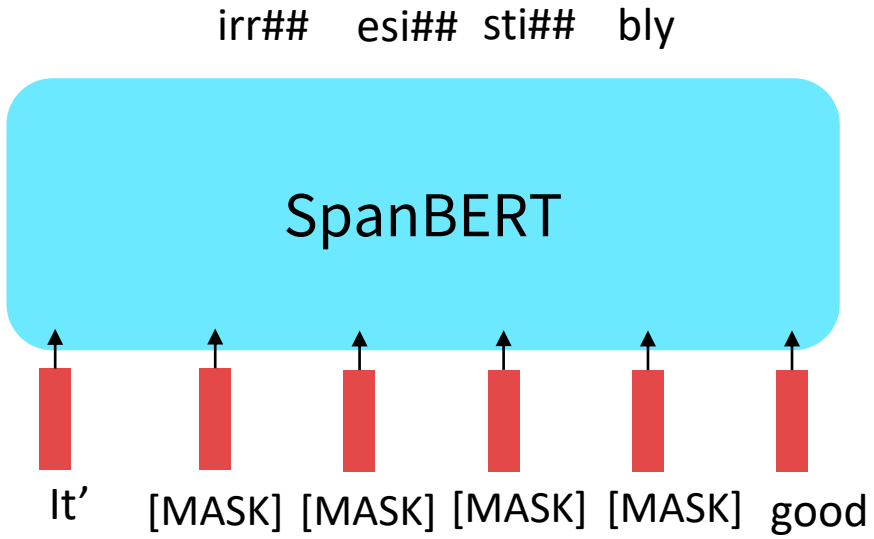
Extensions of BERT

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

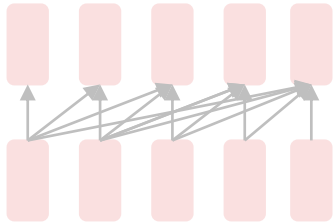
A takeaway from the RoBERTa paper: more compute, more data can improve pretraining even when not changing the underlying Transformer encoder.

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]

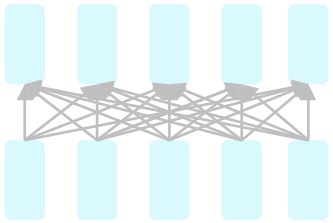
Pretraining for three types of architectures

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



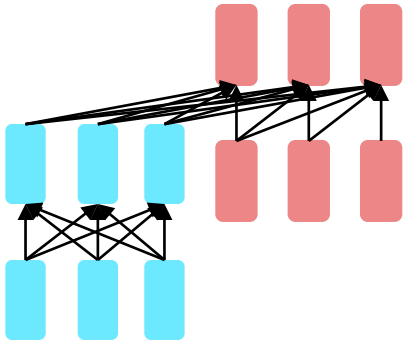
Decoders

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



Encoders

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



Encoder-Decoders

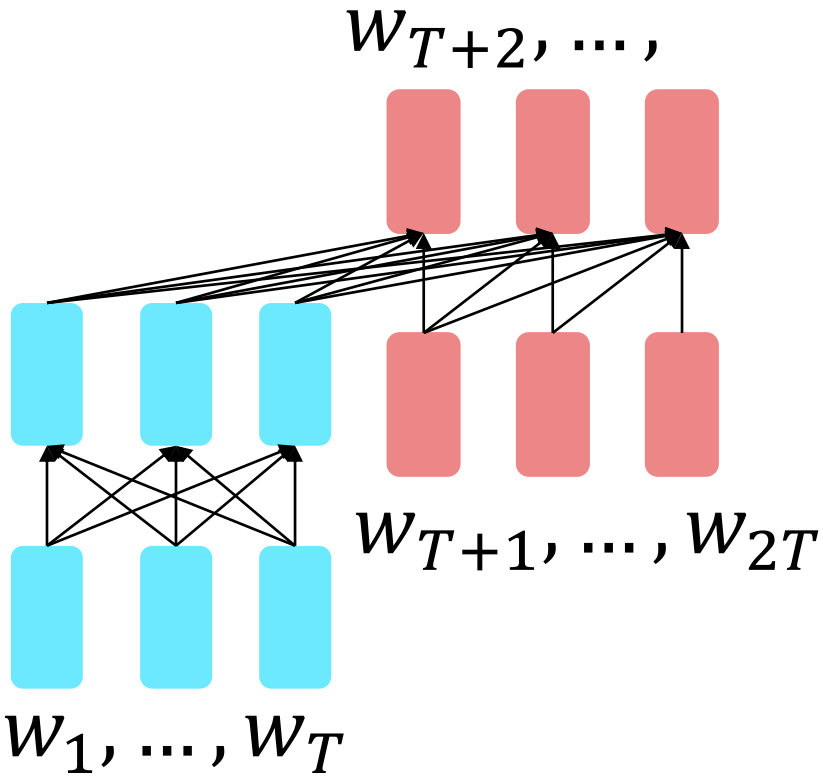
- Good parts of decoders and encoders?
- What's the best way to pretrain them?

Pretraining 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.

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

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



[Raffel et al., 2018]

Pretraining encoder-decoders: what pretraining objective to use?

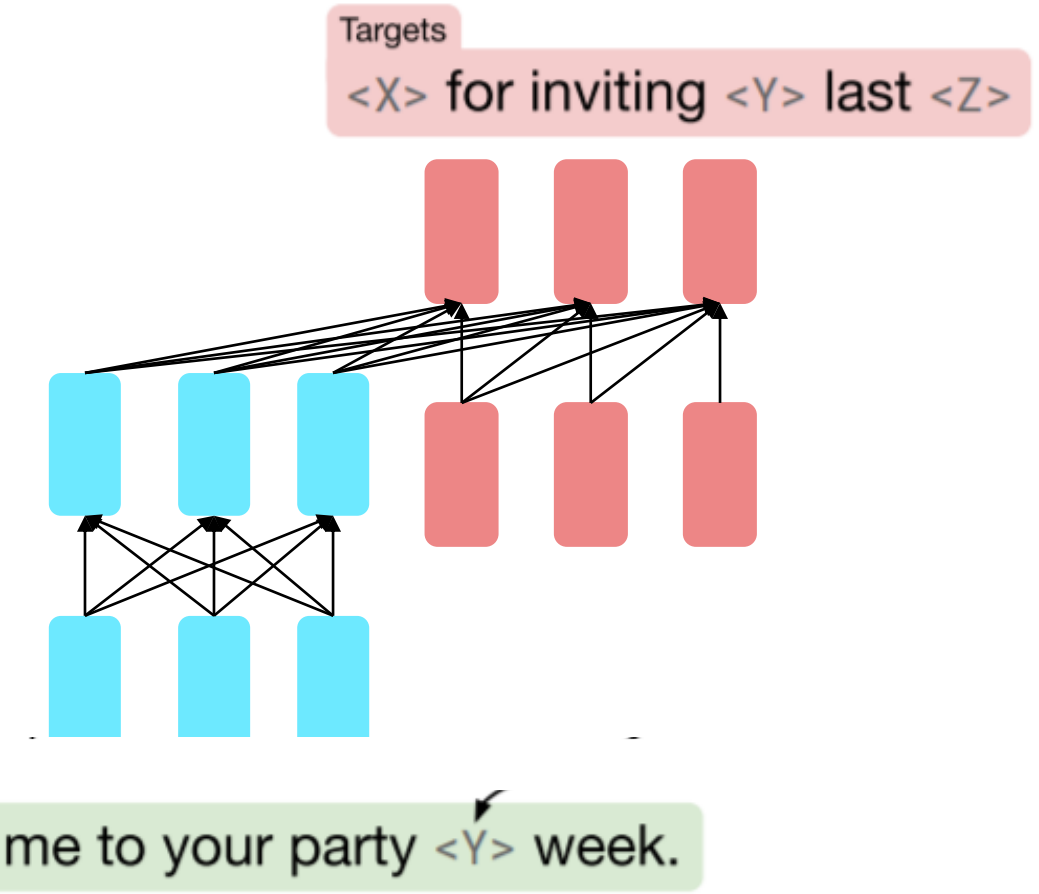
What Raffel et al., 2018 found to work best was **span corruption.** Their model: **T5**.

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

Original text

Thank you ~~for inviting~~ me to your party ~~last~~ week.

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



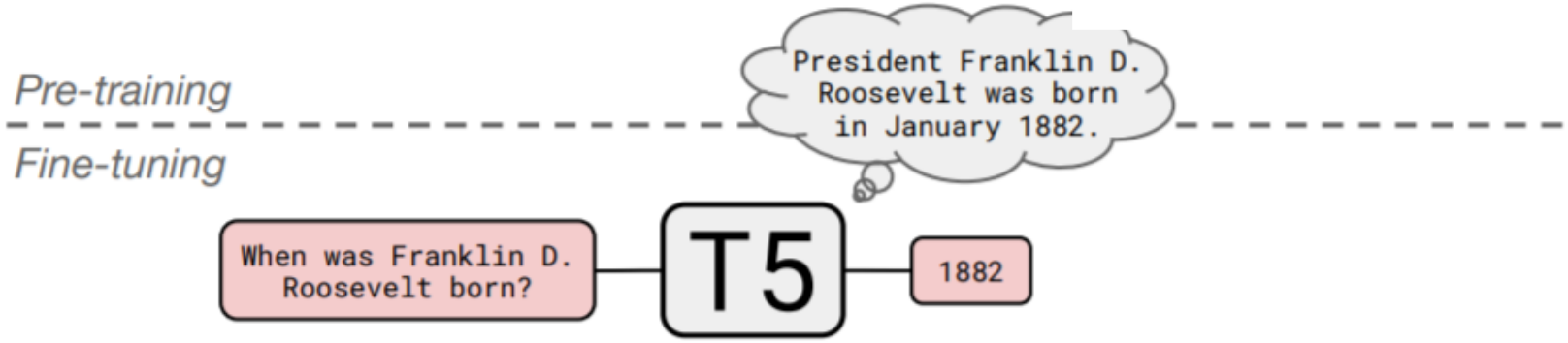
Pretraining encoder-decoders: what pretraining objective to use?

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]