Natural Language Processing with Deep Learning

CS224N/Ling284

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Lecture 9: Self-Attention and Transformers

Lecture Plan

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

Reminders:

Assignment 4 due on Thursday!

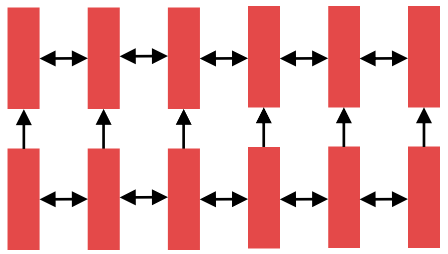
Mid-quarter feedback survey due Tuesday, Feb 16 at 11:59PM PST!

Final project proposal due Tuesday, Feb 16 at 4:30PM PST!

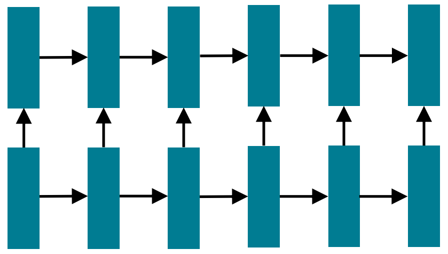
Please try to hand in the project proposal on time; we want to get you feedback quickly!

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

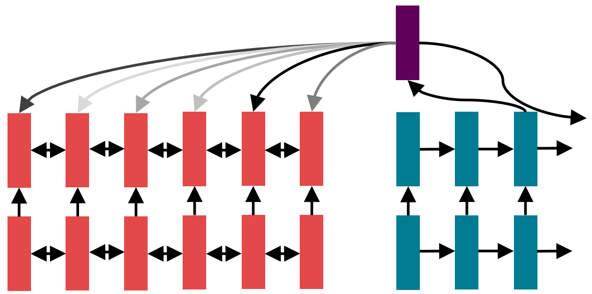
- Circa 2016, the de facto strategy in NLP is to **encode** sentences with a bidirectional LSTM: (for example, the source sentence in a translation)



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

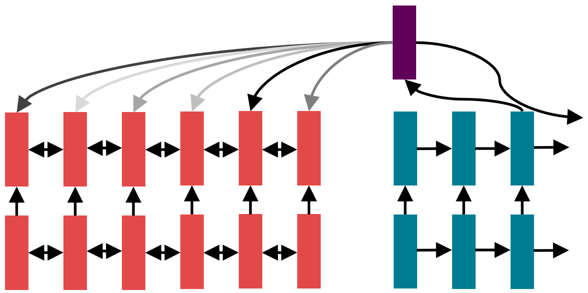


- Use attention to allow flexible access to memory



Today: Same goals, different building blocks

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



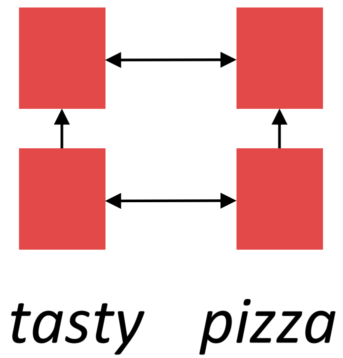
Lots of trial and error →

2014-2017ish
Recurrence

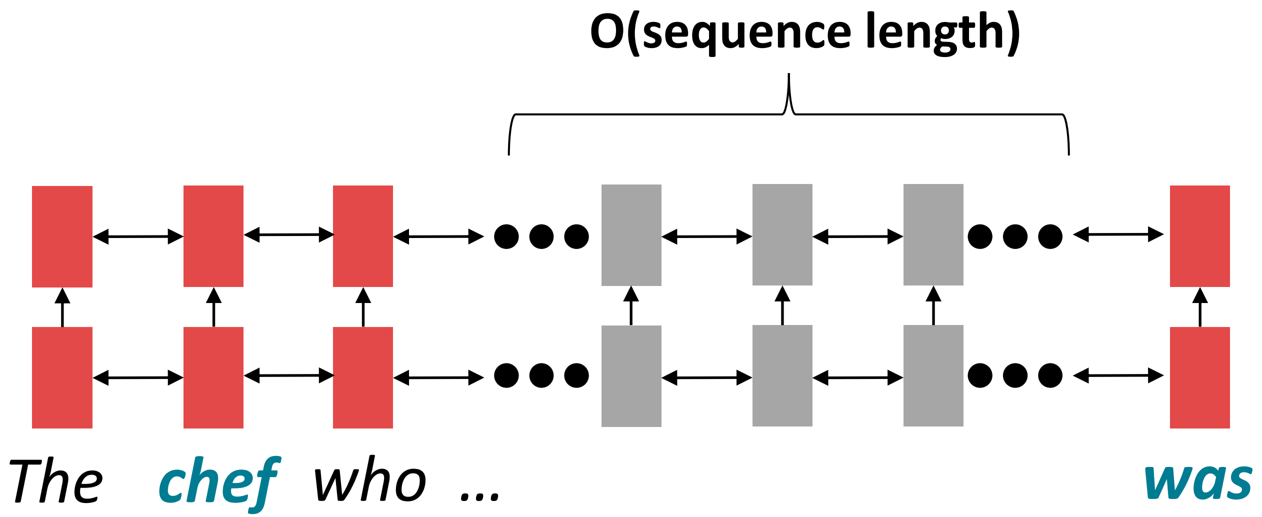
2021
??????

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

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

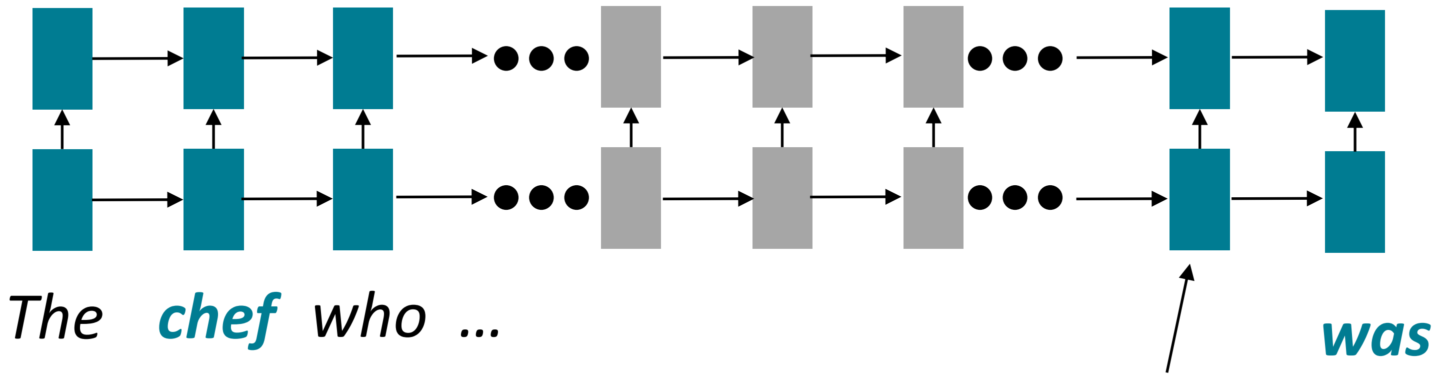


- **Problem:** RNNs take **O(sequence length)** steps for distant word pairs to interact.



Issues with recurrent models: Linear interaction distance

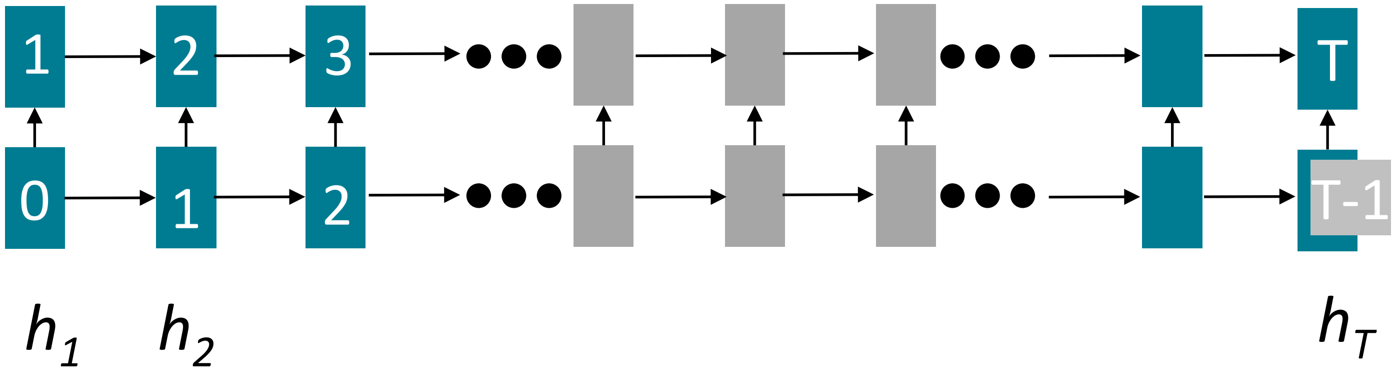
- **O(sequence length)** steps for distant word pairs to interact means:
  - Hard to learn long-distance dependencies (because gradient problems!)
  - Linear order of words is “baked in”; we already know linear order isn’t the right way to think about sentences…



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

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

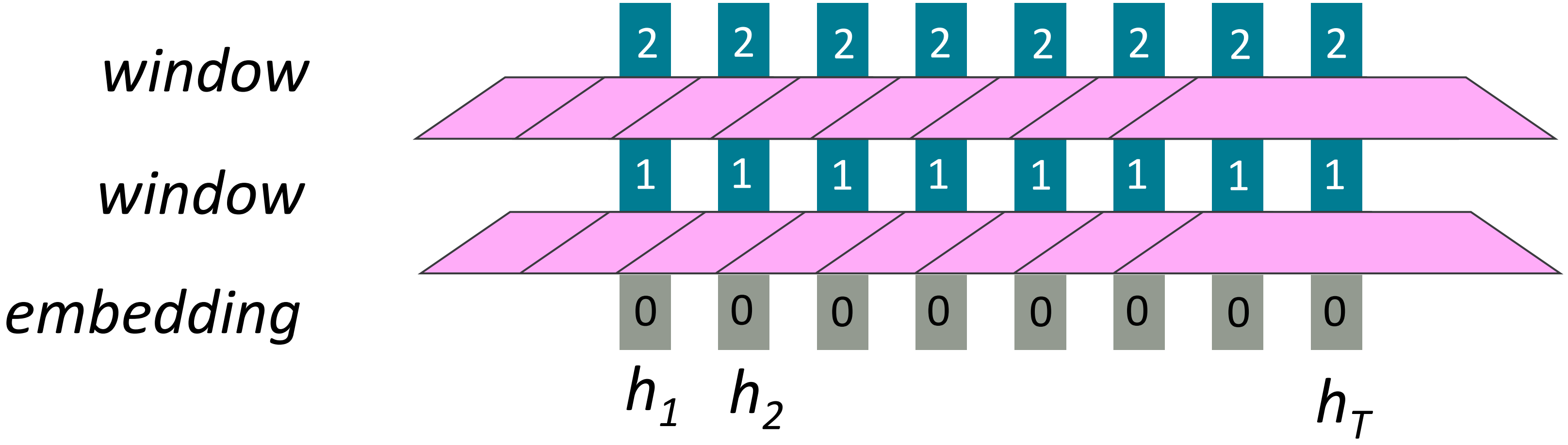
- Forward and backward passes have **O(sequence length)** unparallelizable operations
  - GPUs can perform a bunch of independent computations at once!
  - But future RNN hidden states can't be computed in full before past RNN hidden states have been computed
  - Inhibits training on very large datasets!



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

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

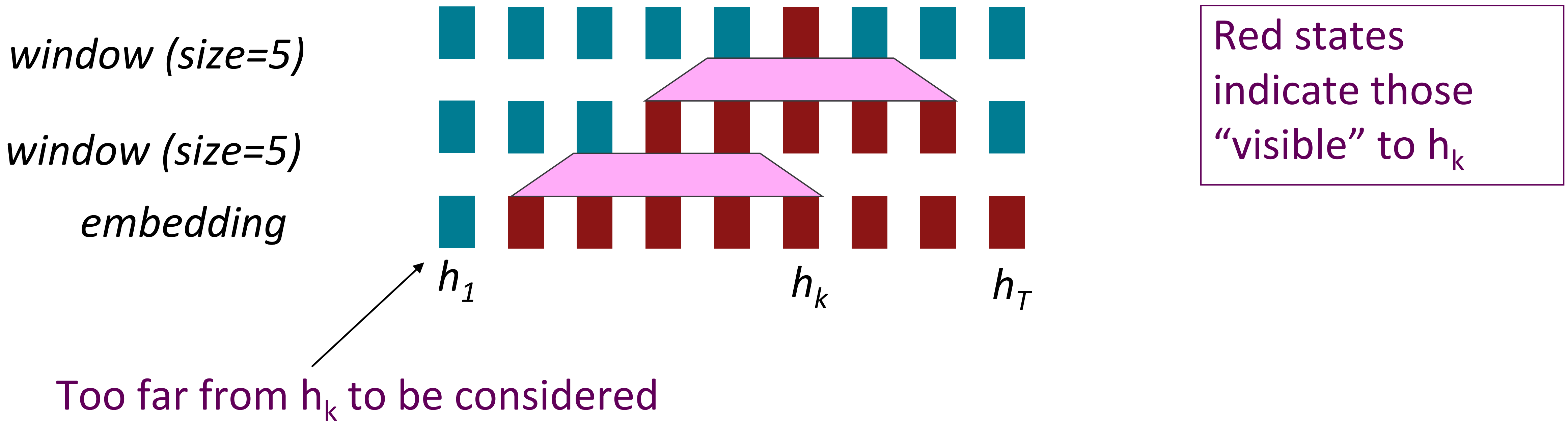
- **Word window models aggregate local contexts**
  - (Also known as 1D convolution; we'll go over this in depth later!)
  - Number of unparallelizable operations does not increase sequence length!



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

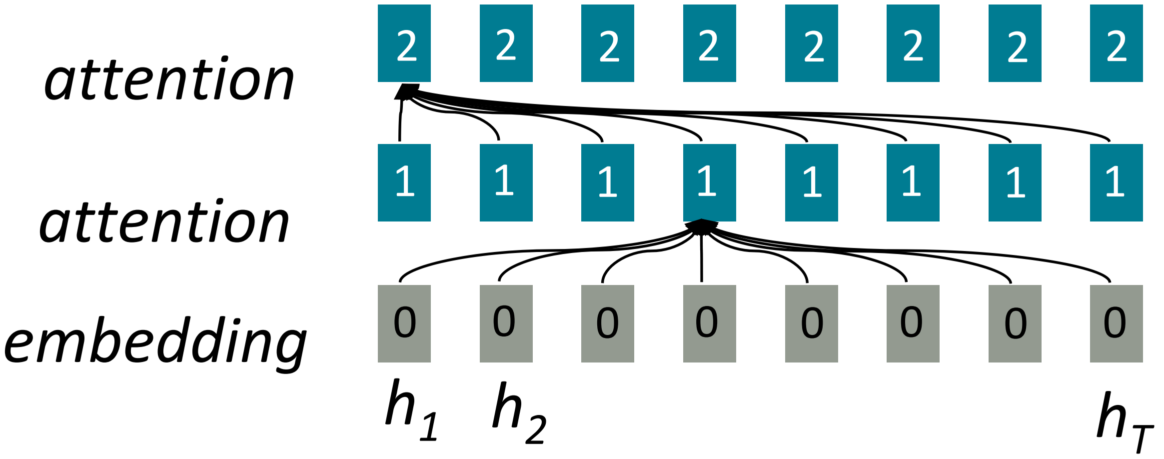
If not recurrence, then what? **How about word windows?**

- **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** $q_1, q_2, \ldots, q_T$. Each query is $q_i \in \mathbb{R}^d$
  - We have some **keys** $k_1, k_2, \ldots, k_T$. Each key is $k_i \in \mathbb{R}^d$
  - We have some **values** $v_1, v_2, \ldots, v_T$. Each value is $v_i \in \mathbb{R}^d$
- In **self-attention**, the queries, keys, and values are drawn from the same source.
  - For example, if the output of the previous layer is $x_1, \ldots, x_T$, (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:

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

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

Compute **key-query** affinities

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

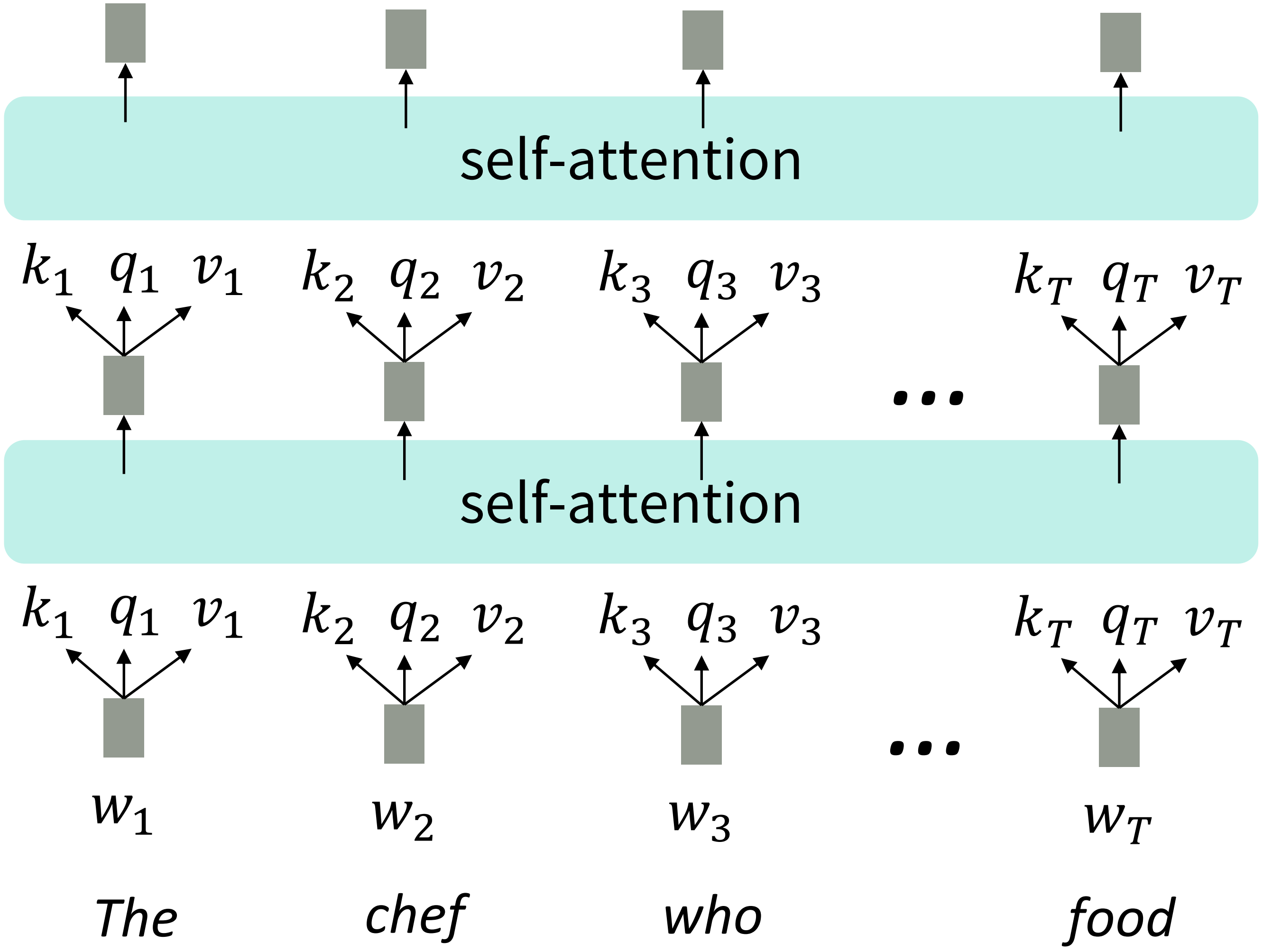
Compute attention weights from affinities (softmax)

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

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.
- 不速之客
- 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**

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

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

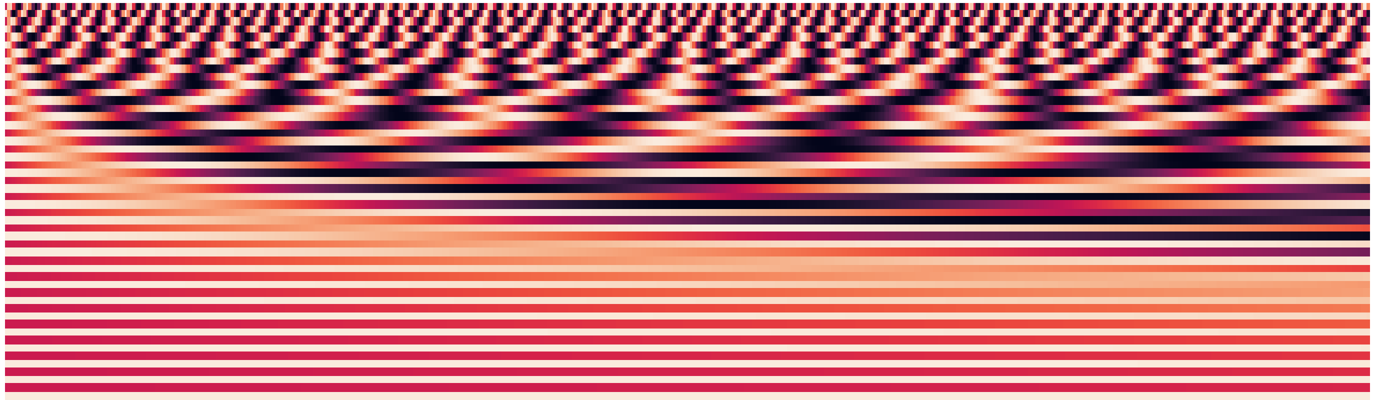
$$
\begin{aligned}
v_i &= \tilde{v}_i + p_i \\
q_i &= \tilde{q}_i + p_i \\
k_i &= \tilde{k}_i + p_i
\end{aligned}
$$

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:
  - 周期性
  - Periodicity indicates that maybe “absolute position” isn’t as important
  - Maybe can 外推 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 $1, \dots, T$.
- Most systems use this!

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

Barriers and solutions for Self-Attention as a building block

Barriers

- Doesn't have an inherent notion of order!
- No nonlinearities for deep learning! It's all just weighted averages

Solutions

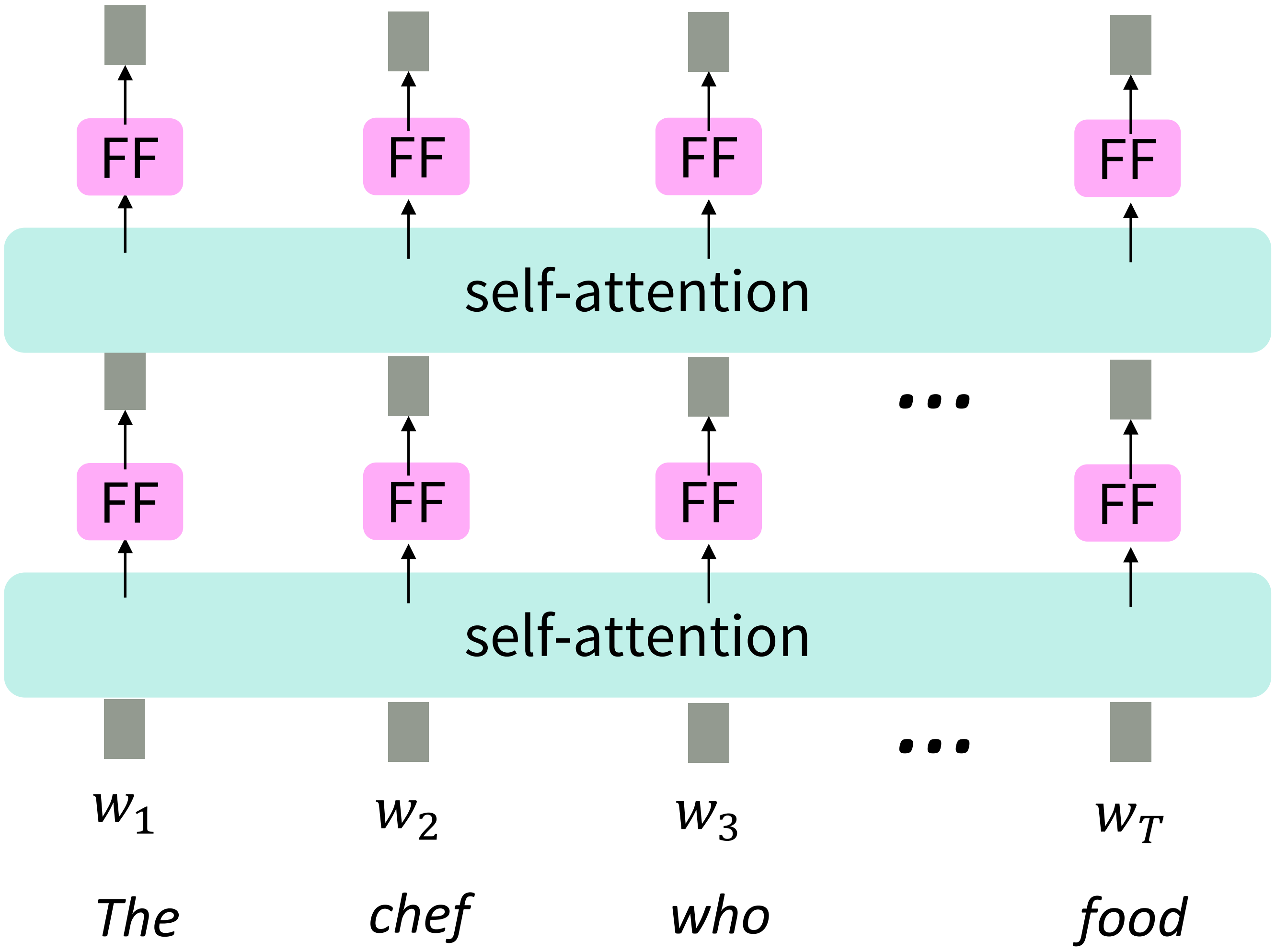
- Add position representations to the inputs

Adding nonlinearities in self-attention

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

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

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



Intuition: the FF network processes the result of attention

Barriers and solutions for Self-Attention as a building block

Barriers	**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 $-\infty$.

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

We can look at these (not greyed out) words

[START] The chef who

[START]

For encoding these words

[The matrix of e_{ij} values]

Masking the future in self-attention

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For encoding these words

	[START]	The	chef	who
[START]	$-\infty$	$-\infty$	$-\infty$	$-\infty$
The		$-\infty$	$-\infty$	$-\infty$
chef			$-\infty$	$-\infty$
who				$-\infty$

Barriers and solutions for Self-Attention as a building block

Barriers

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

Solutions

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

Necessities for a self-attention building block:

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

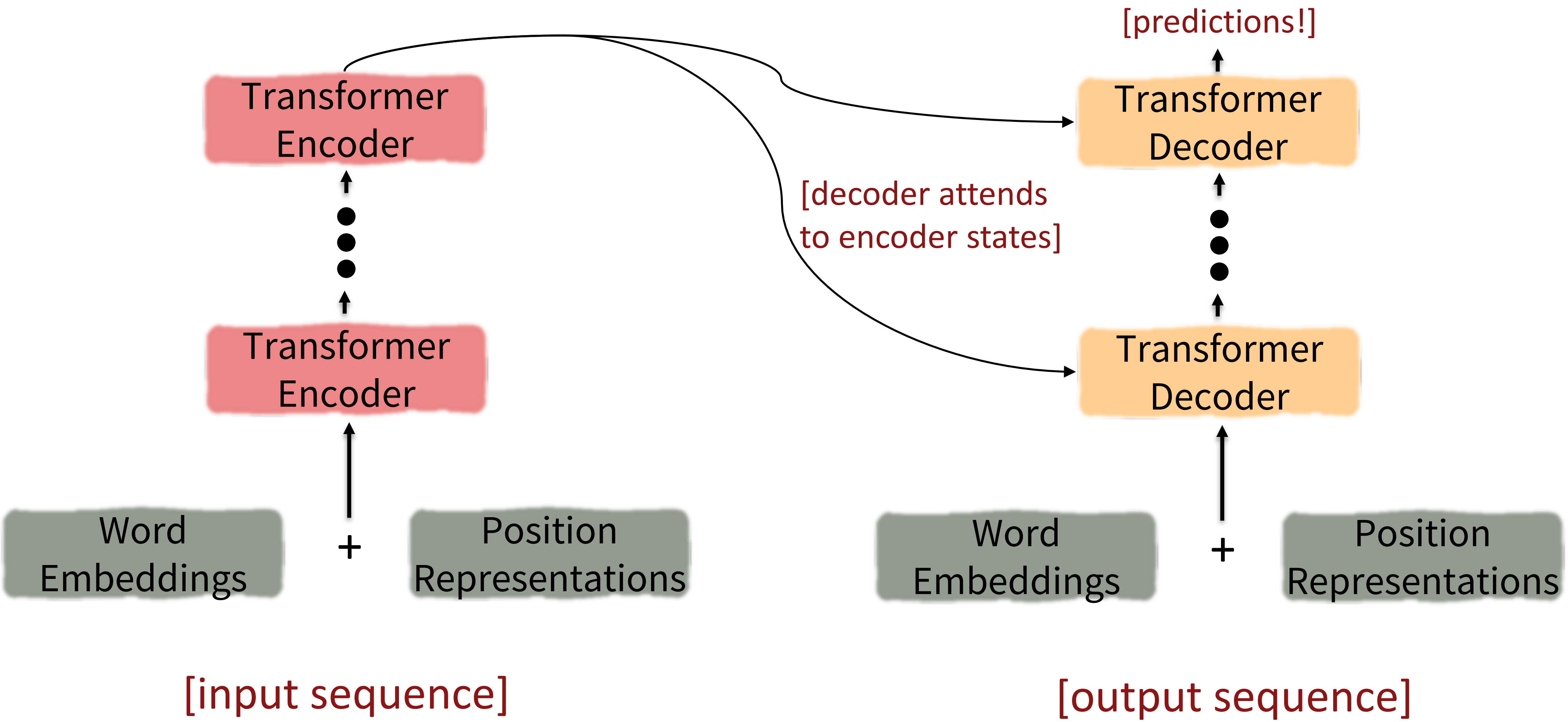
- That’s it! But this is not the **Transformer** model we’ve been hearing about.

Outline

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

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

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



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
      并不能改善模型的能力 但可以提高训练过程
   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.

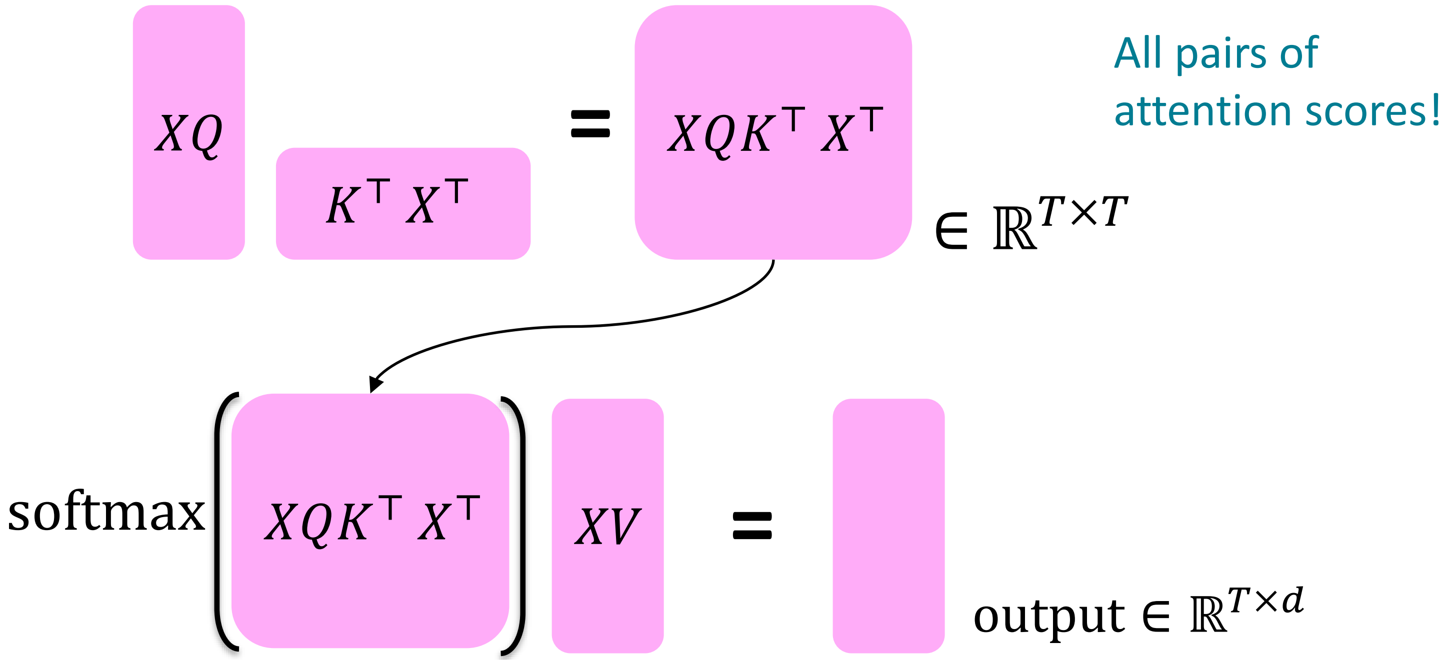
- These matrices allow *different aspects* of the x vectors to be used/emphasized in each of the three roles.

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

- Let's look at how key-query-value attention is computed, in matrices.
  - Let $X = [x_1; \dots; x_T] \in \mathbb{R}^{T\times d}$ 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 $\text{output} = \text{softmax}(XQ(XK)^\top) \times XV$.

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.

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

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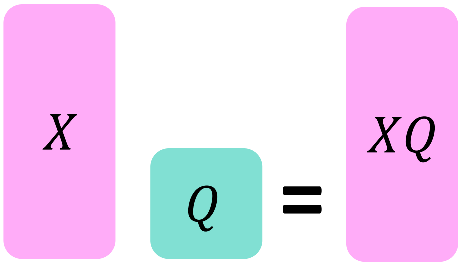
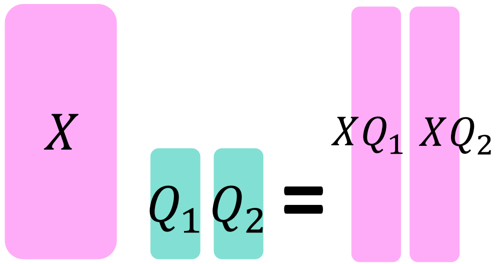
Single-head attention

(just the query matrix)



Multi-head attention

(just two heads here)

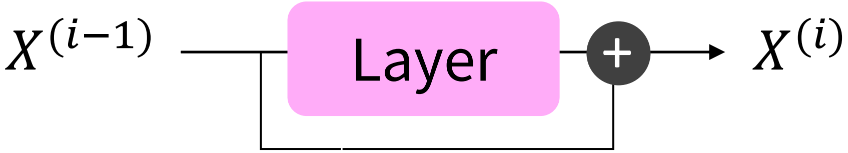


Same amount of computation as single-head self-attention!

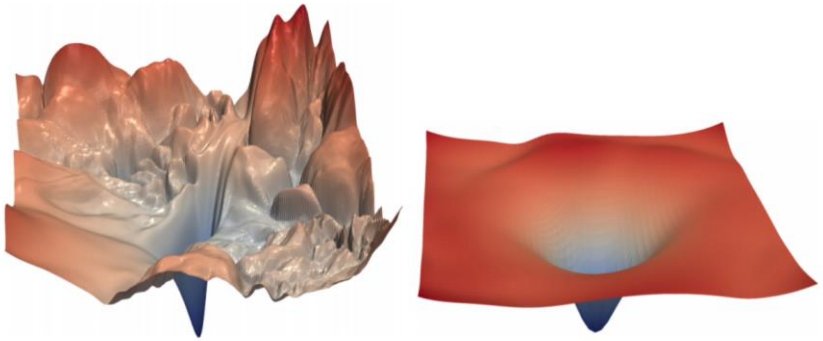
The Transformer Encoder: **Residual connections** [He et al., 2016]

- **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**.
  - 归一化梯度
  - LayerNorm's success may be due to its normalizing gradients [Xu et al., 2019]
- Let $x \in \mathbb{R}^d$ be an individual (word) vector in the model.
- Let $\mu = \sum_{j=1}^{d} x_j$; this is the mean; $\mu \in \mathbb{R}$.
- Let $\sigma = \sqrt{\frac{1}{d} \sum_{j=1}^{d} \left(x_j - \mu\right)^2}$; this is the standard deviation; $\sigma \in \mathbb{R}$.
- Let $\gamma \in \mathbb{R}^d$ and $\beta \in \mathbb{R}^d$ be learned "gain" and "bias" parameters. (Can omit!)
- Then layer normalization computes:

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

Normalize by scalar mean and variance

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

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

Normalize by scalar mean and variance

调整

Modulate by learned elementwise gain and bias

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

帮助

- **"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:

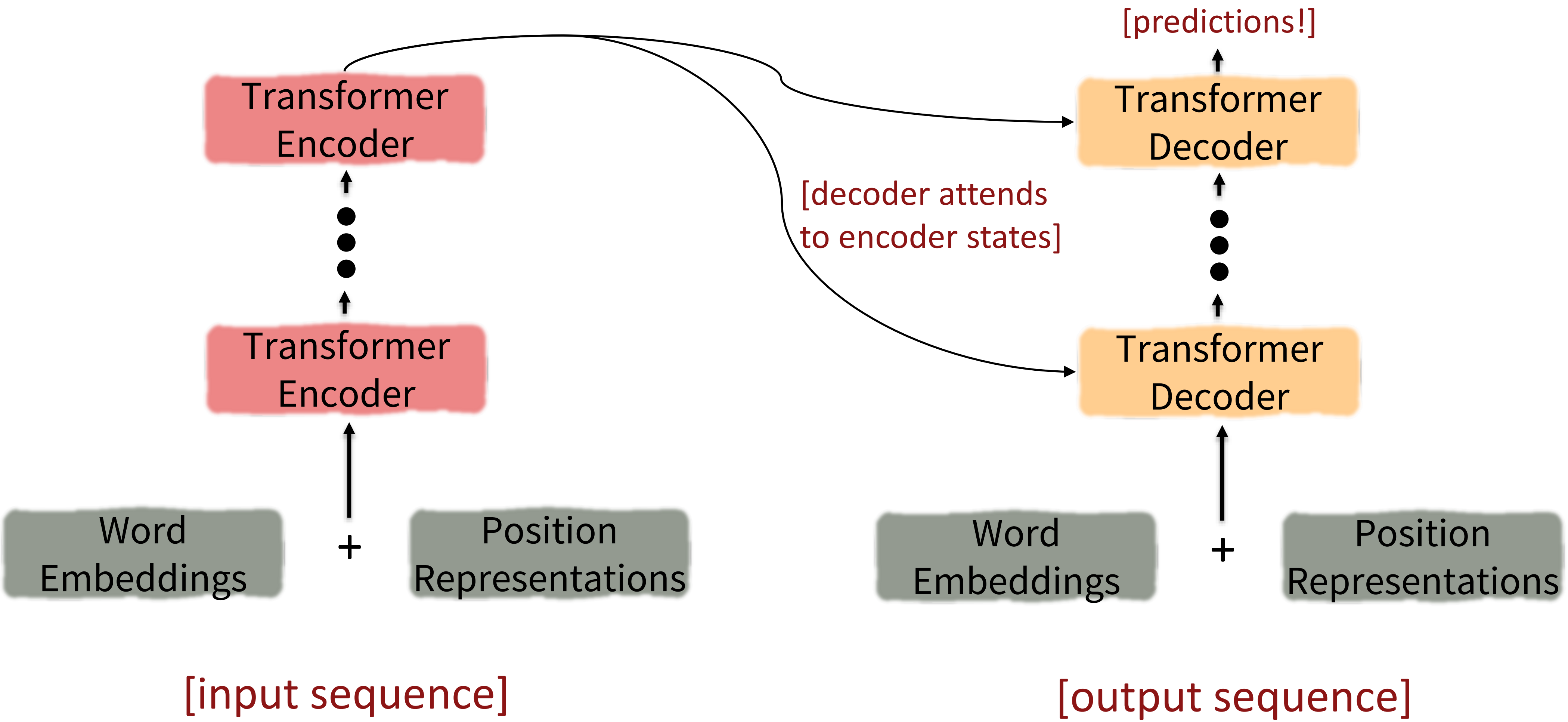
$$\mathrm{output}_\ell = \mathrm{softmax}\left(XQ_\ell K_\ell^\top X^\top\right) * XV_\ell$$

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

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

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

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



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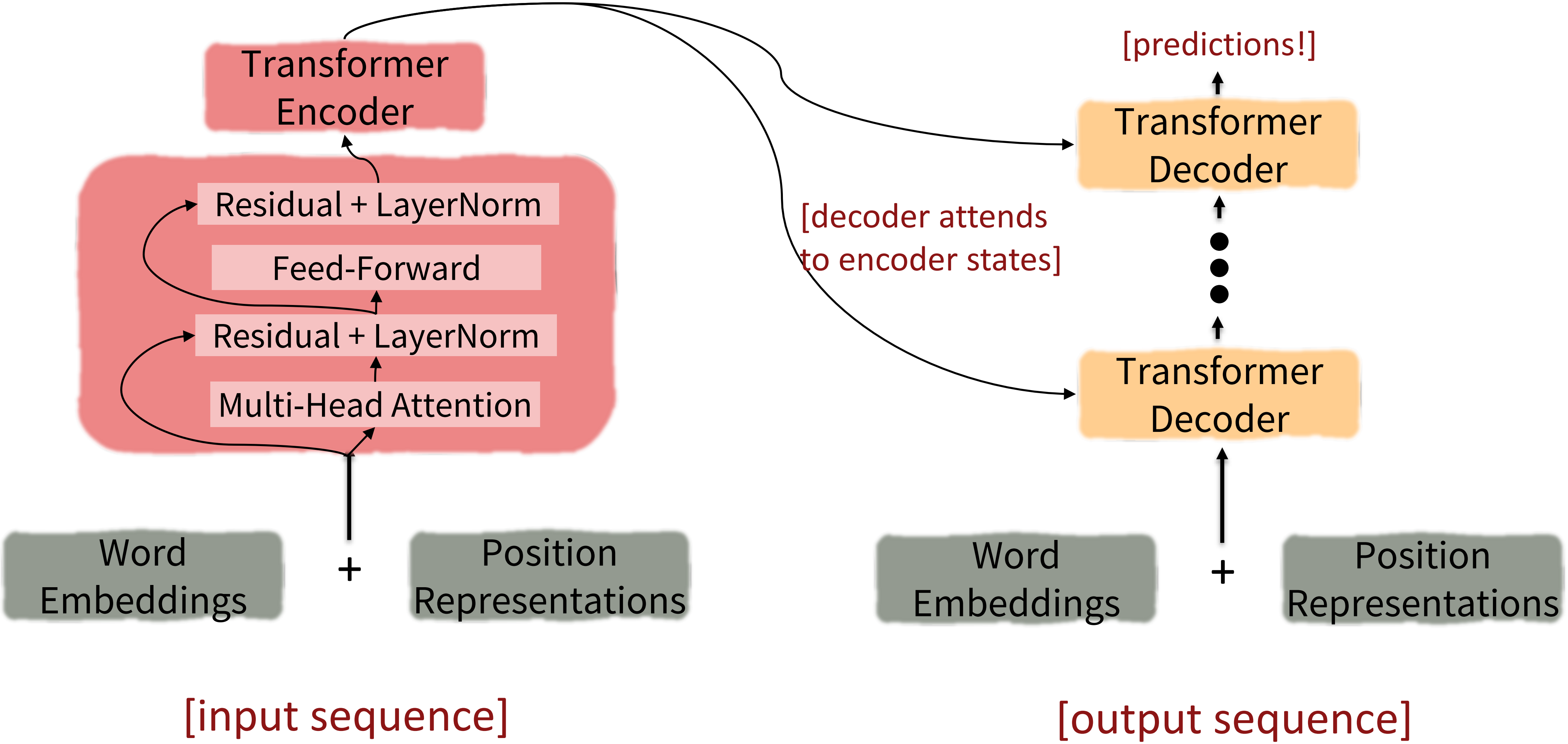
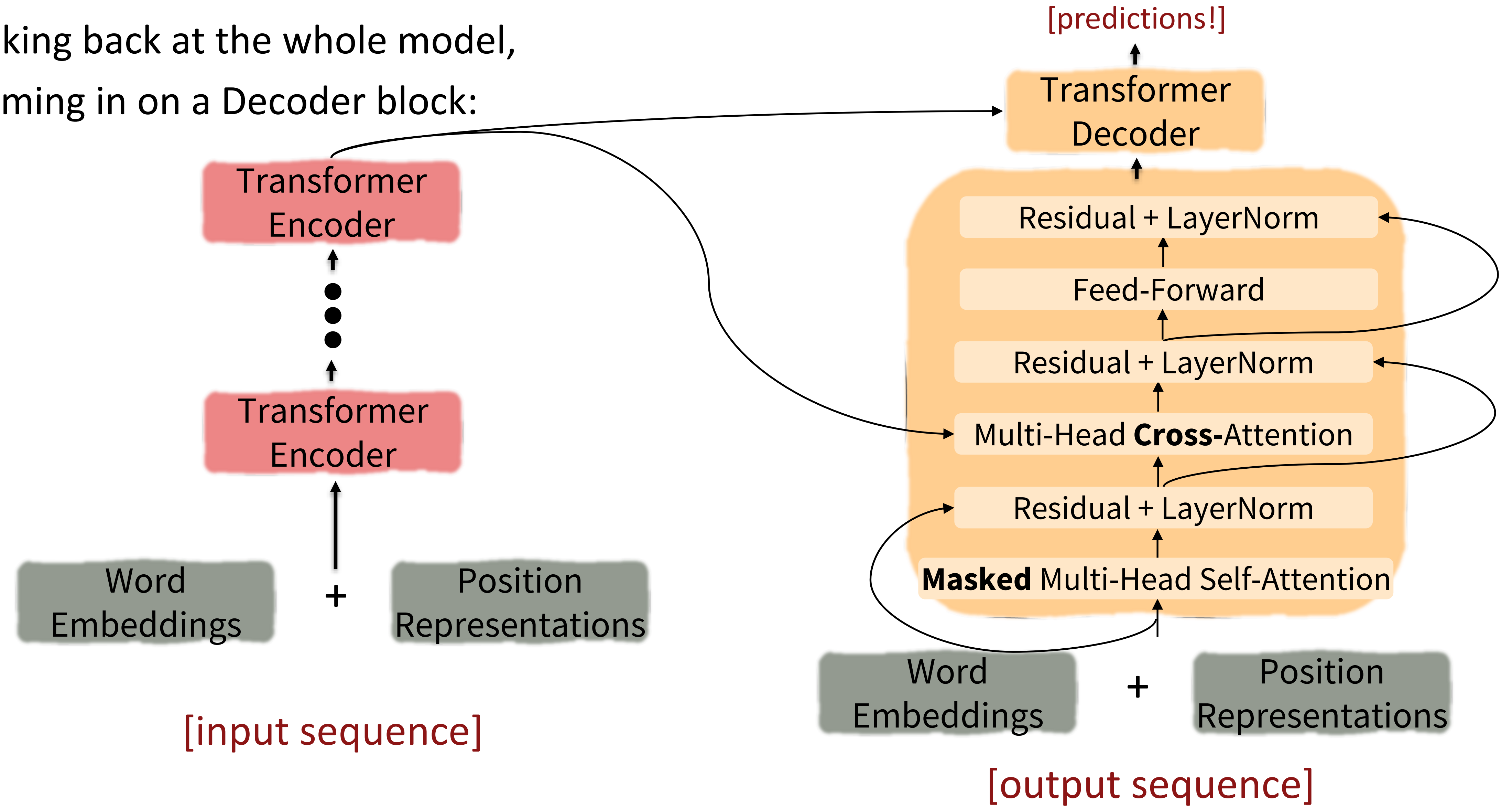


The Transformer Encoder-Decoder [Vaswani et al., 2017]

Looking back at the whole model,

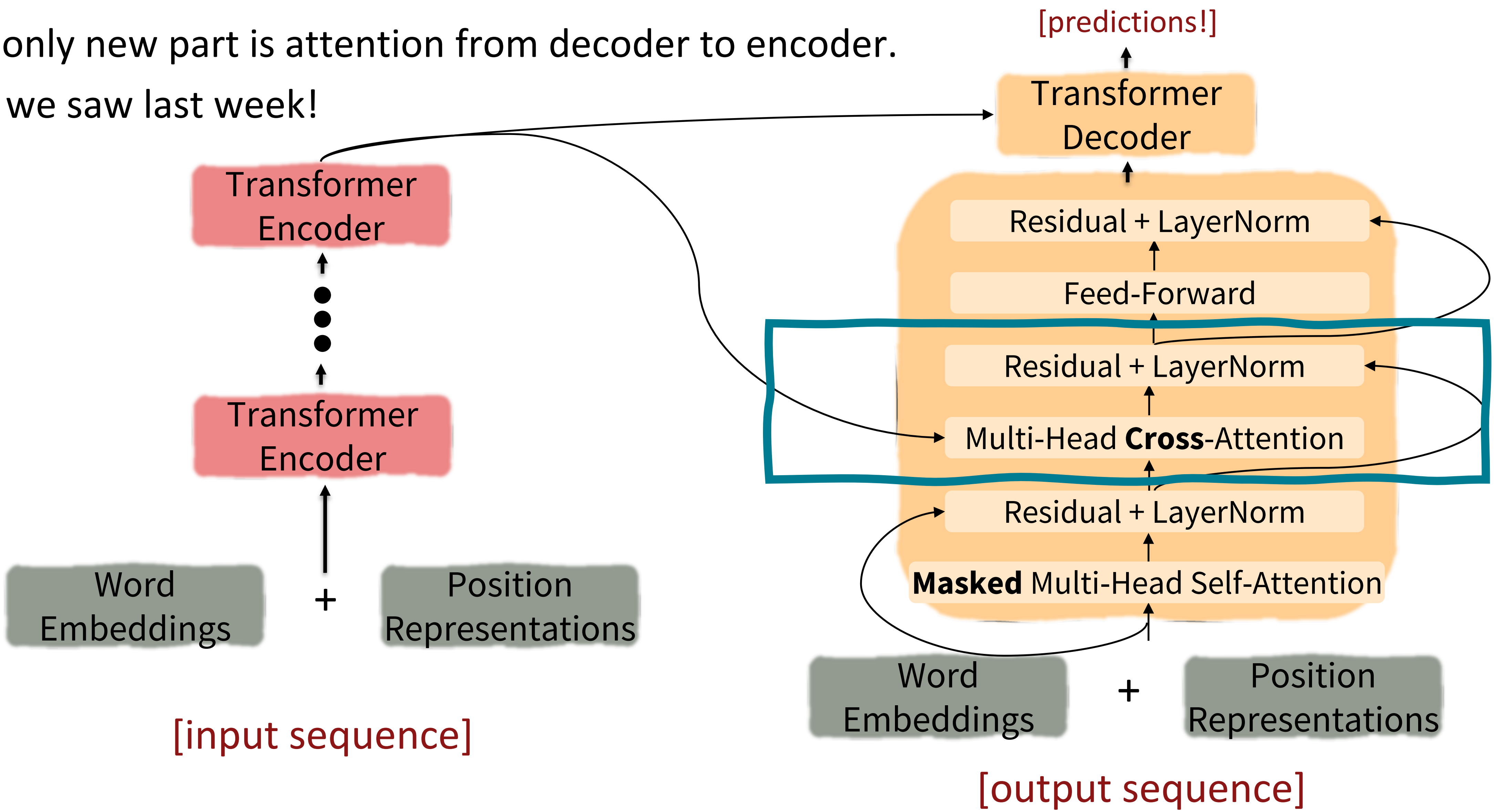
zooming in on a Decoder block:



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 output $=$ $\mathrm{softmax}(ZQ(HK)^\top) \times HV$.

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

$$ZQ \quad K^\top H^\top = ZQK^\top H^\top \in \mathbb{R}^{T \times T}$$

All pairs of attention scores!

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

$$\mathrm{softmax}\left(ZQK^\top H^\top \right) HV = \quad \text{output} \in \mathbb{R}^{T \times d}$$

Outline

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

Great Results with Transformers

First, Machine Translation from the original Transformers paper!

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

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

[Vaswani et al., 2017]

Great Results with Transformers

Next, document generation!

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

The old standard

Transformers all the way down.

[Liu et al., 2018]; WikiSum dataset

Great Results with Transformers

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

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

On this popular aggregate benchmark, for example:

GLUE

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

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

More results Thursday when we discuss pretraining.

[Liu et al., 2018]

Outline

1. From recurrence (RNN) to attention-based NLP models
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What would we like to fix about the Transformer?

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

Quadratic computation as a function of sequence length

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

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

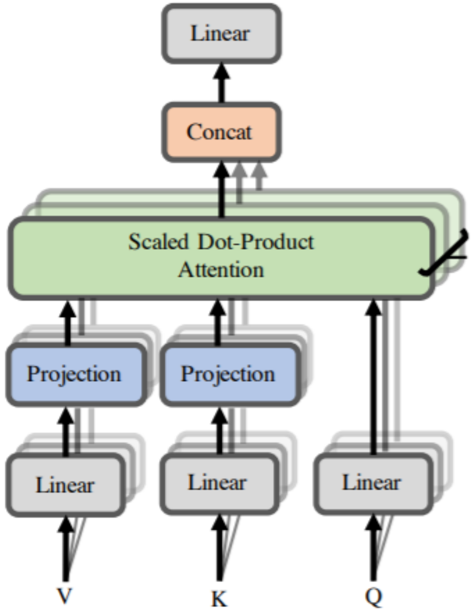
Need to compute all pairs of interactions! $O(T^2d)$

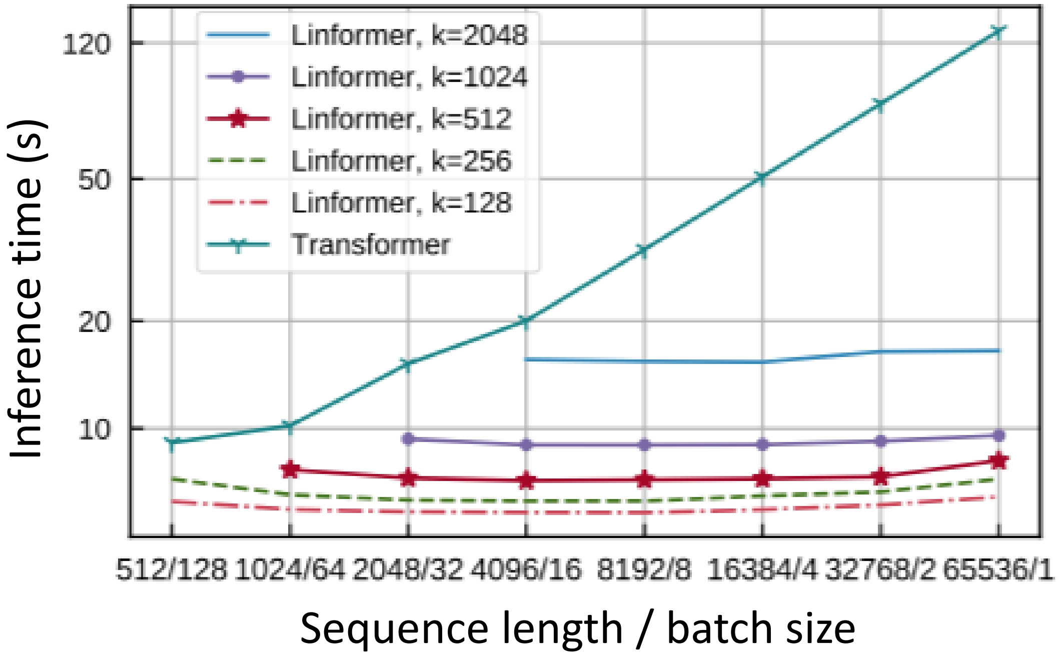
- Think of d as around $\mathbf{1,000}$.
  - So, for a single (shortish) sentence, $T \leq 30; T^2 \leq \mathbf{900}$.
  - In practice, we set a bound like $T = 512$.
  - **But what if we'd like $\boldsymbol{T} \geq \mathbf{10,000}$?** For example, to work on long documents?

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

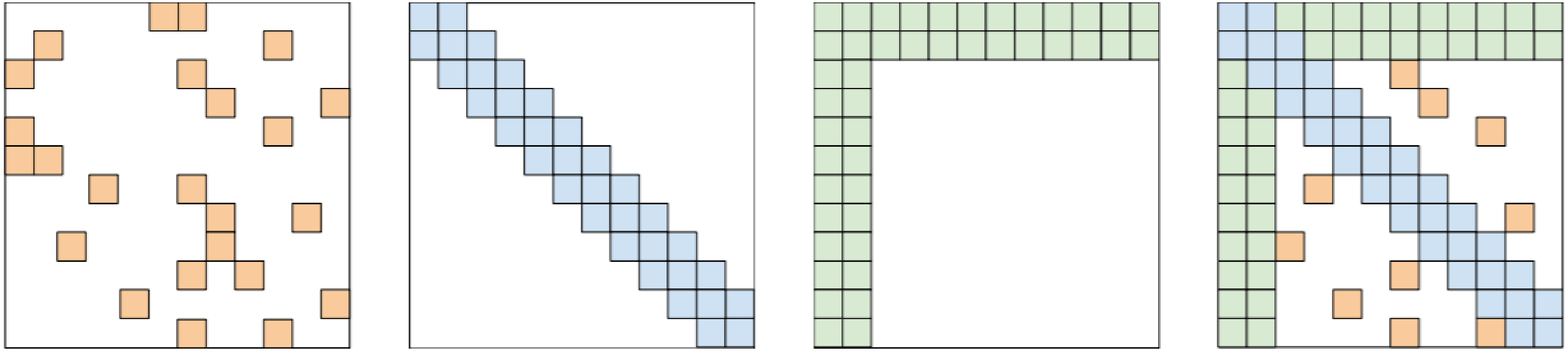




Recent work on improving on quadratic self-attention cost

- 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

Parting remarks

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