Introduction to NLP

CSE5321/CSEG321

Lecture 10. Transformers

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Materials are referenced from Stanford CS224n

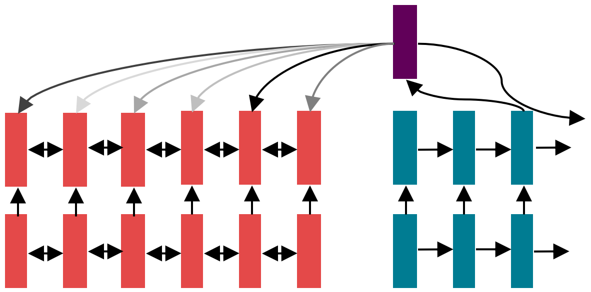
Lecture Plan

Lecture 11: Transformers

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

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!



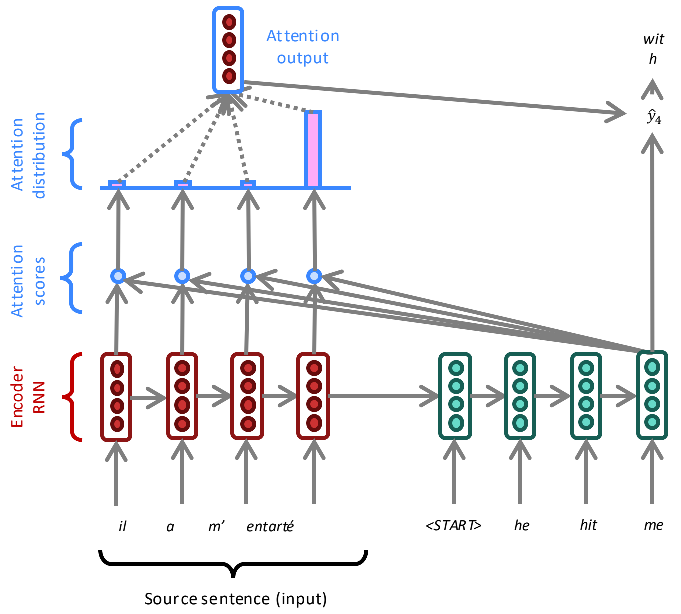
Lots of trial and error

2014-2017ish
Recurrence

2021
??????

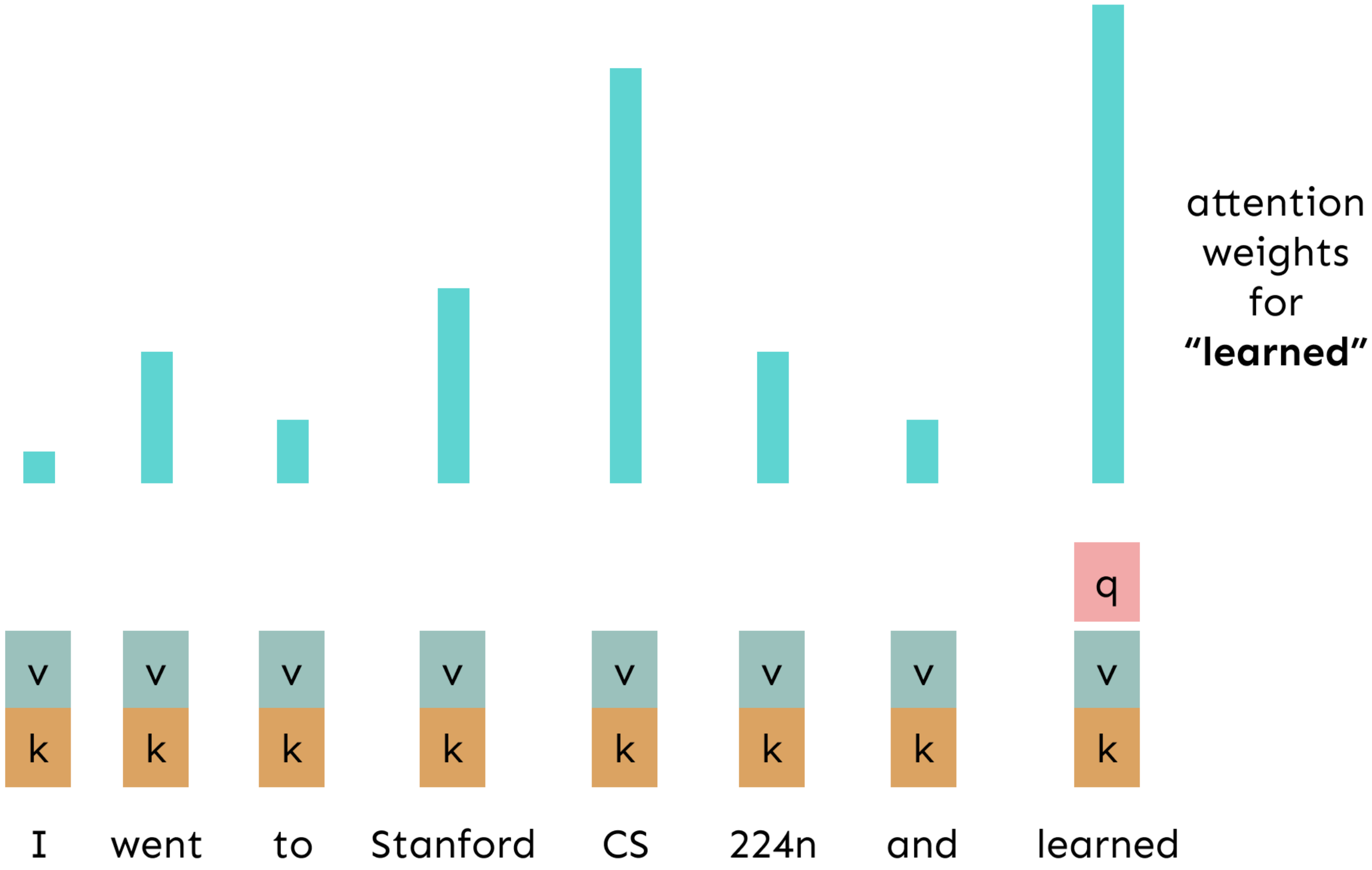
The building block we need: *self* attention

- 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 $y_{<t}$

Self-Attention Hypothetical Example



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 $\boldsymbol{x}_i = E\boldsymbol{w}_{\boldsymbol{i}}$, 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 $\mathbb{R}^{d\times d}$

$$\boldsymbol{q}_i = Q\boldsymbol{x}_{\boldsymbol{i}} \text{ (queries)} \qquad \boldsymbol{k}_i = K\boldsymbol{x}_{\boldsymbol{i}} \text{ (keys)} \qquad \boldsymbol{v}_i = V\boldsymbol{x}_{\boldsymbol{i}} \text{ (values)}$$

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

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

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

$$\boldsymbol{o}_i = \sum_{\boldsymbol{j}} \boldsymbol{\alpha}_{ij}\,\boldsymbol{v}_i$$

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**

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

- 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:

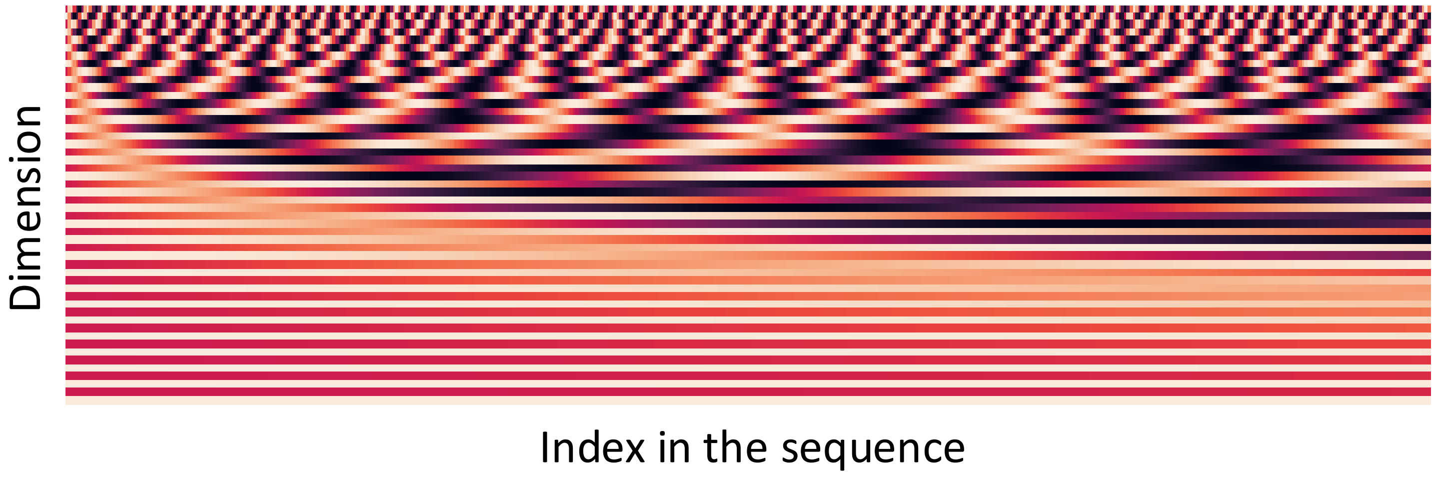
$$\tilde{\boldsymbol{x}}_i = \boldsymbol{x}_i + \boldsymbol{p}_i$$

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

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/

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]

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

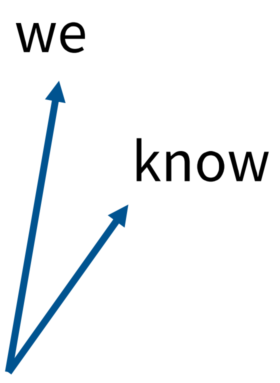
- **Absolute:**

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

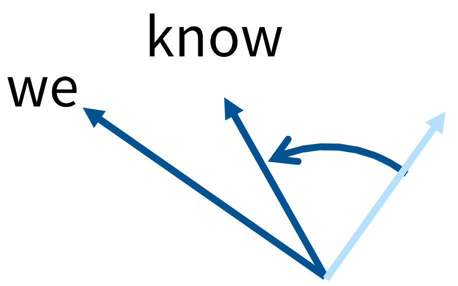
RoPE – Embedding via rotation

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.

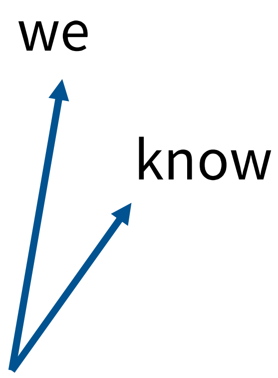


Position independent embedding



Embedding
“of course we know”

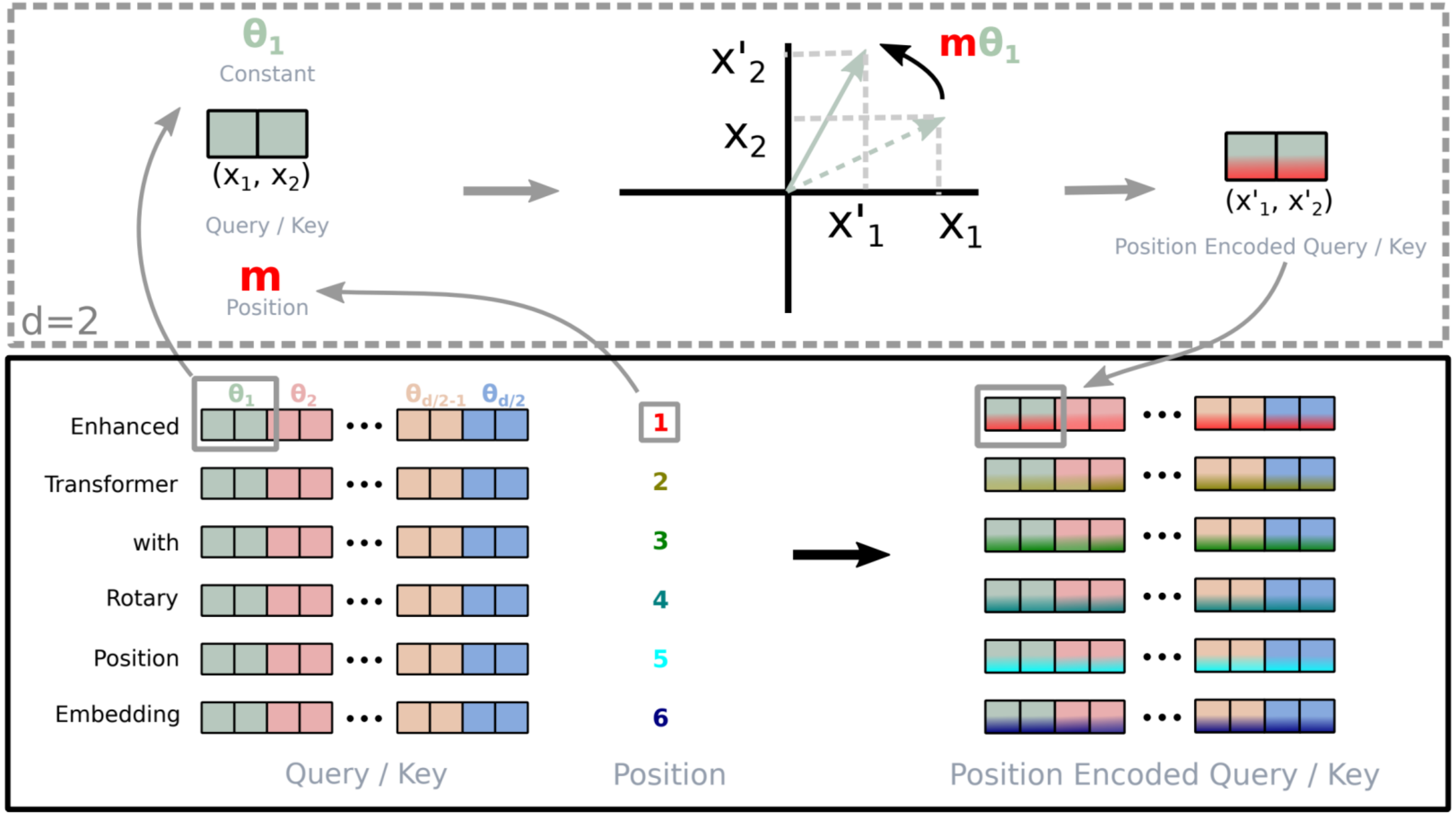
Rotate by ‘2 positions’



Embedding
“we know that”

Rotate by ‘0 positions’

RoPE – From 2 to many dimensions



[Su et al 2021]

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

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

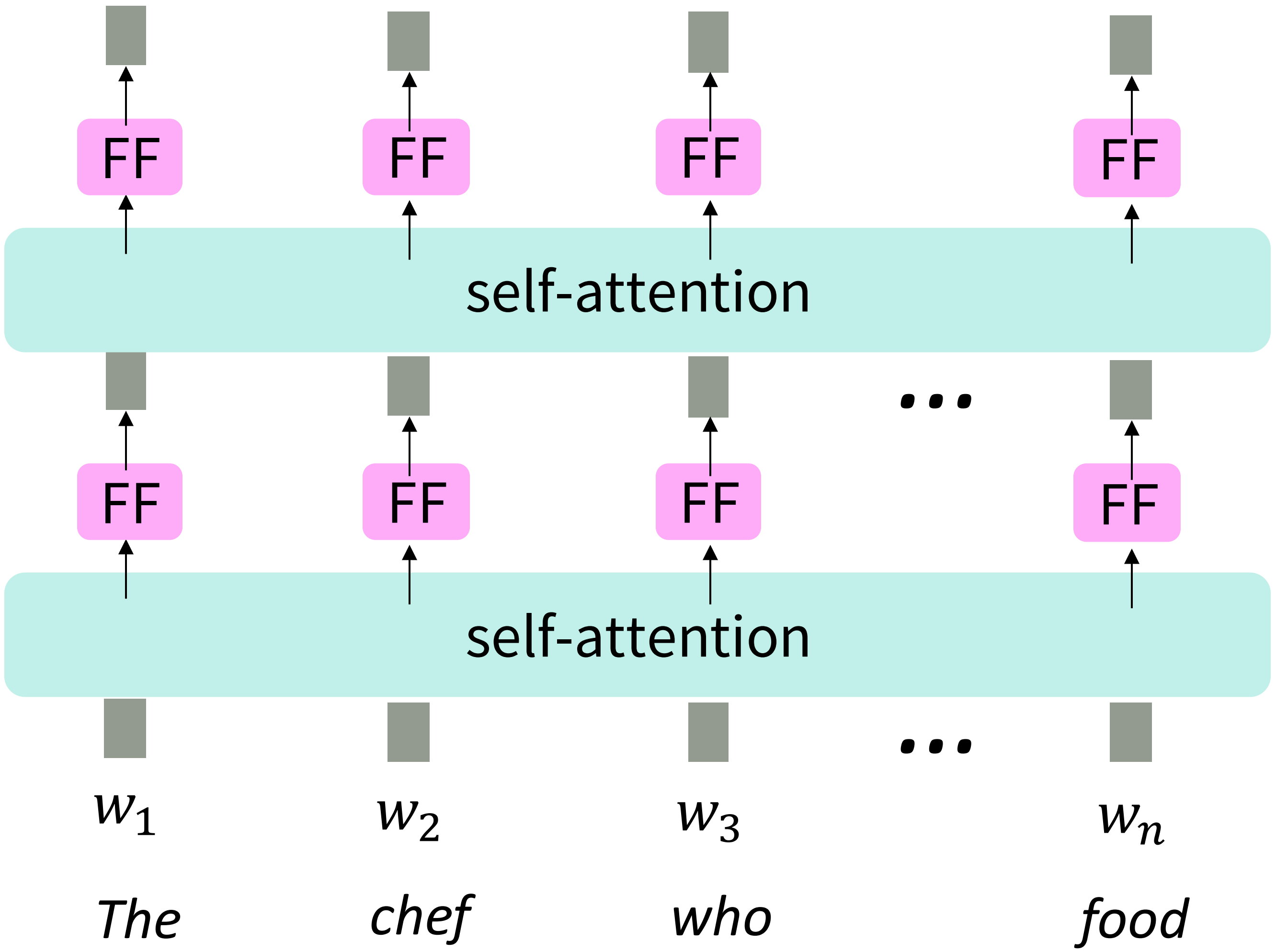
- Add position representations to the inputs

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 (Why? Look at the notes!)

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

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



Intuition: the FF network processes the result of attention

Barriers and solutions for Self-Attention as a building block

Barriers

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

Solutions

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

Masking the future in self-attention

- To use self-attention in **decoders**, we need to ensure we can't peek at the future.
- At every timestep, we could change the set of **keys and queries** to include only past words. (Inefficient!)
- To enable parallelization, we **mask out attention** to future words by setting attention scores to $-\infty$.

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

We can look at these (not greyed out) words

For encoding these words

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

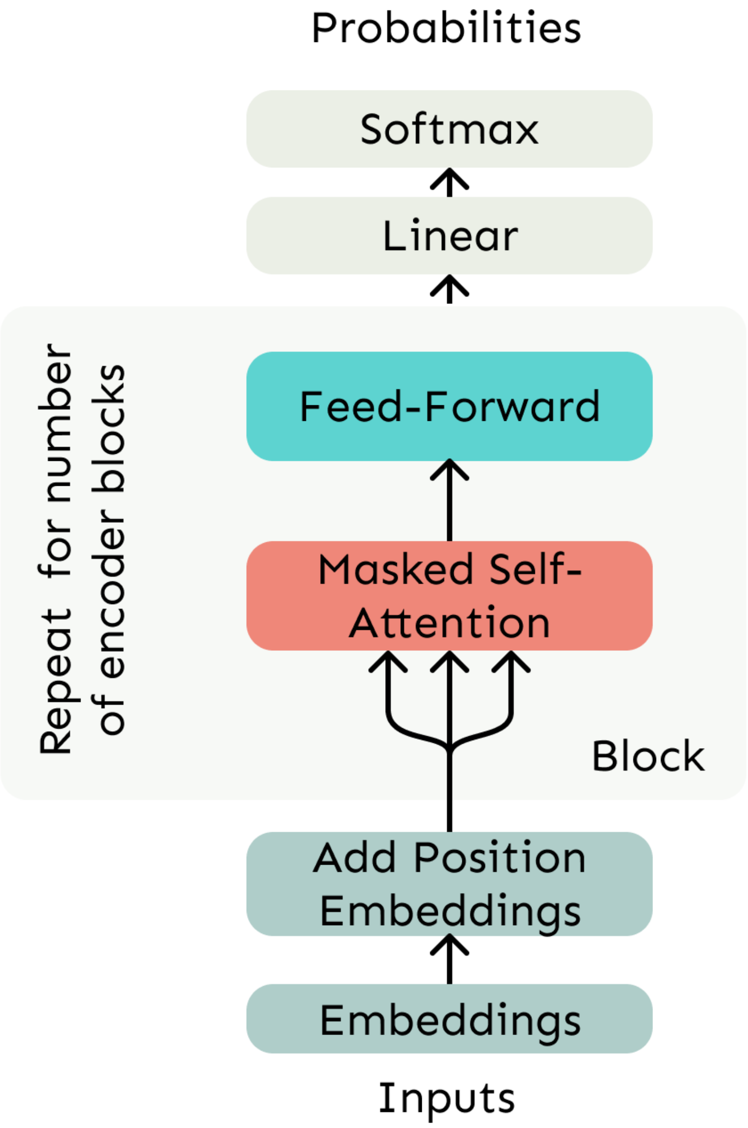
Barriers and solutions for Self-Attention as a building block

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:

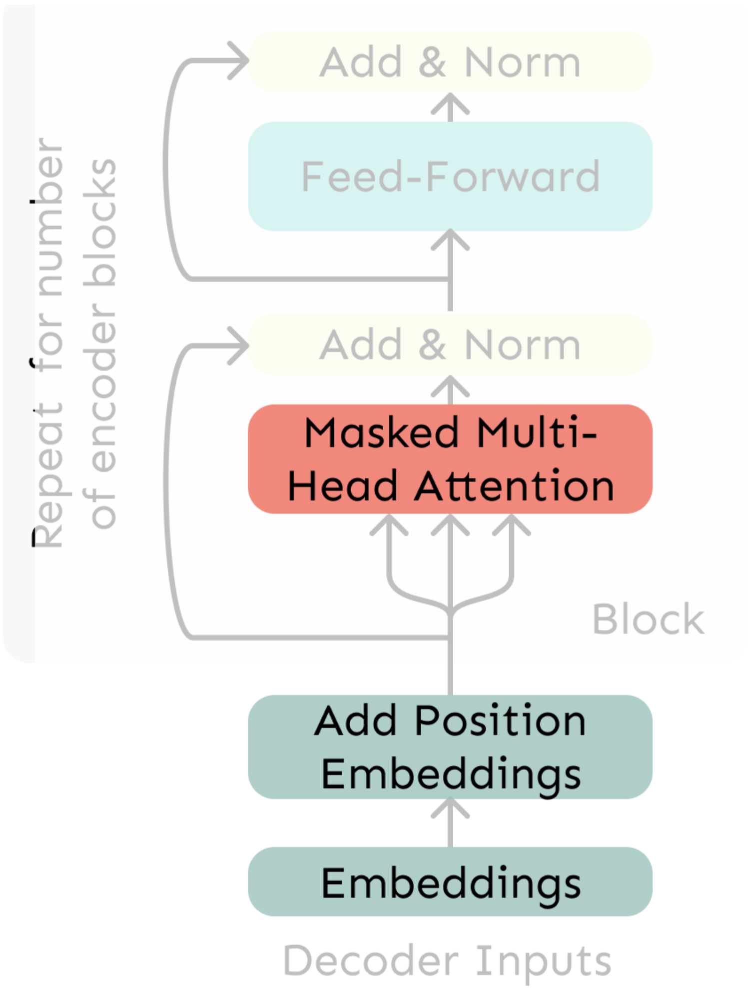
- **Self-attention**:
  - the basis of the method.
- **Position representations**:
  - Specify the sequence order, since self-attention is an unordered function of its inputs.
- **Nonlinearities**:
  - At the output of the self-attention block
  - Frequently implemented as a simple feed-forward network.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



Outline

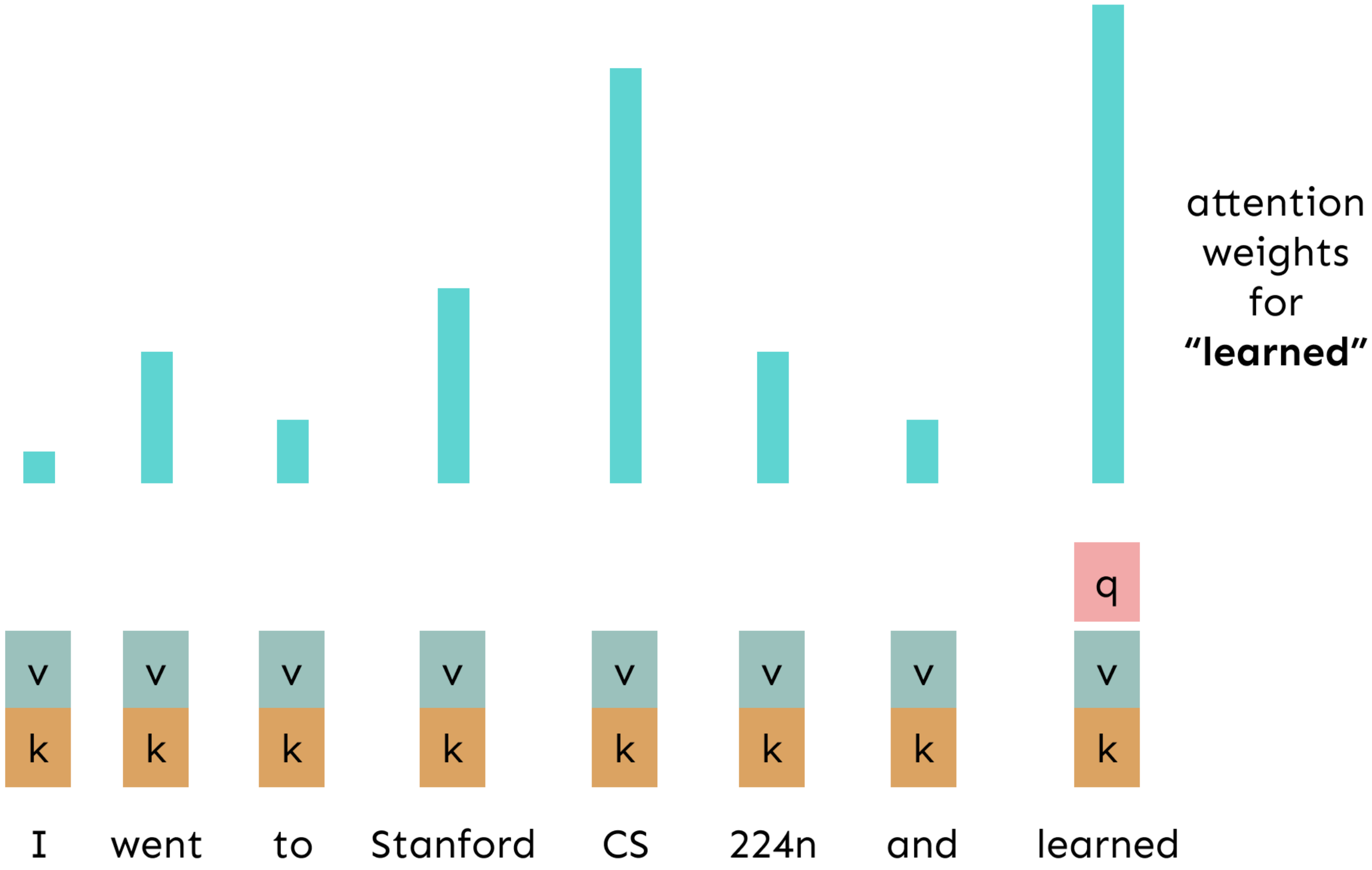
The Transformer Decoder

- 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.**

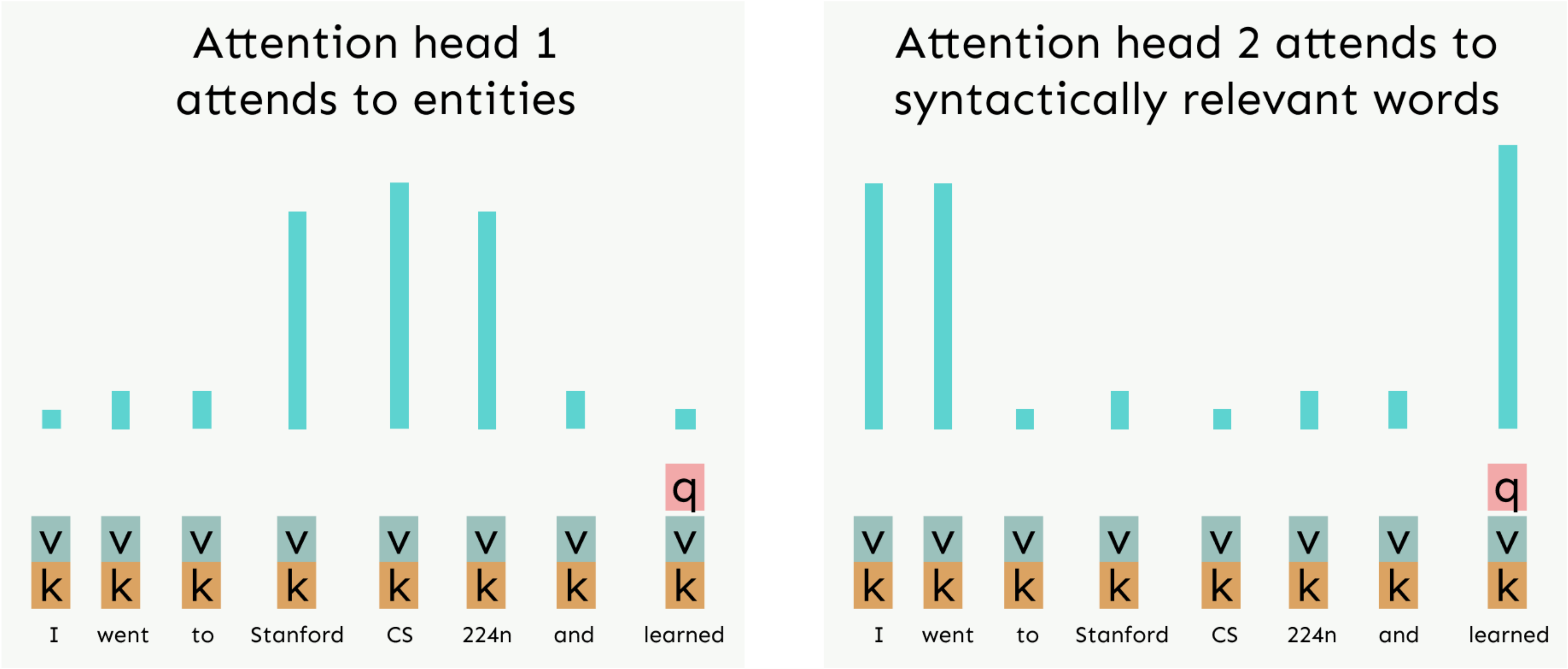


Transformer Decoder

Recall the Self-Attention Hypothetical Example



Hypothetical Example of Multi-Head Attention



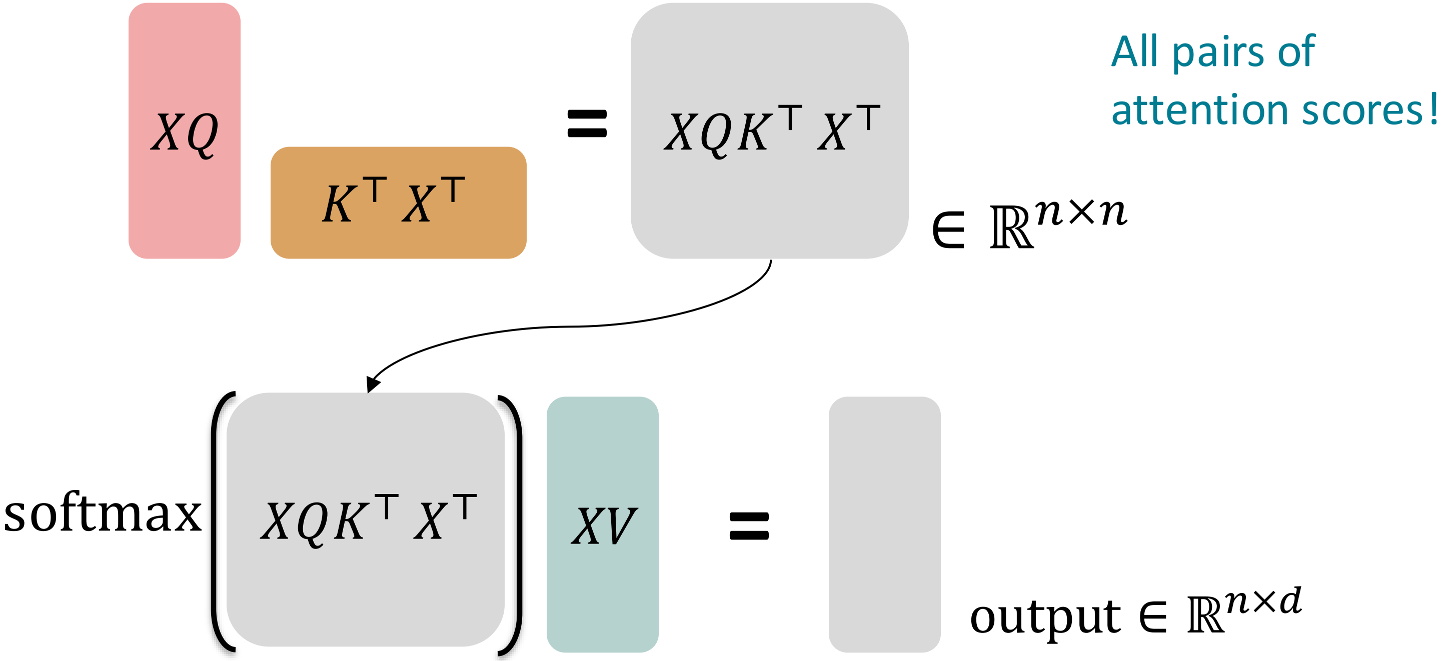
I went to Stanford CS 224n and learned

Sequence-Stacked form of Attention

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

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

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



Multi-headed attention

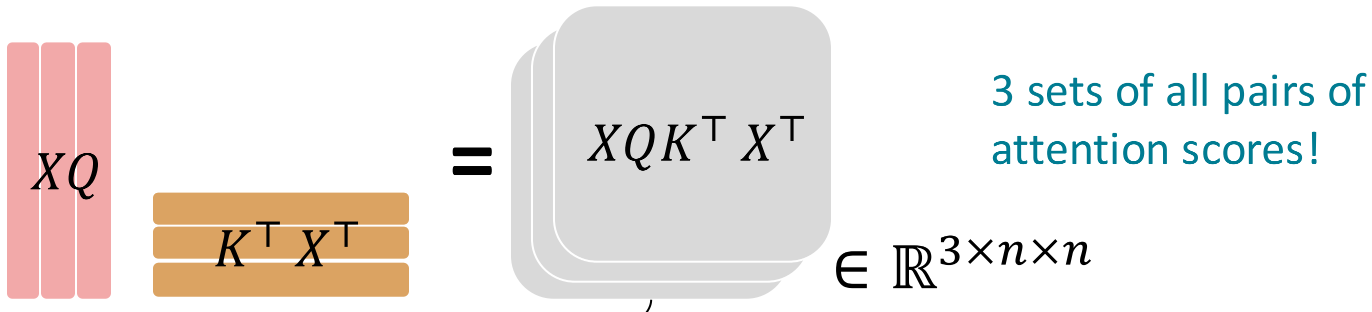
- What if we want to look in multiple places in the sentence at once?
  - For word i, self-attention “looks” where $x_i^\top Q^\top K x_j$ is high, but maybe we want to focus on different j for different reasons?
- We’ll define **multiple attention “heads”** through multiple Q,K,V matrices
- Let, $Q_\ell,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

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

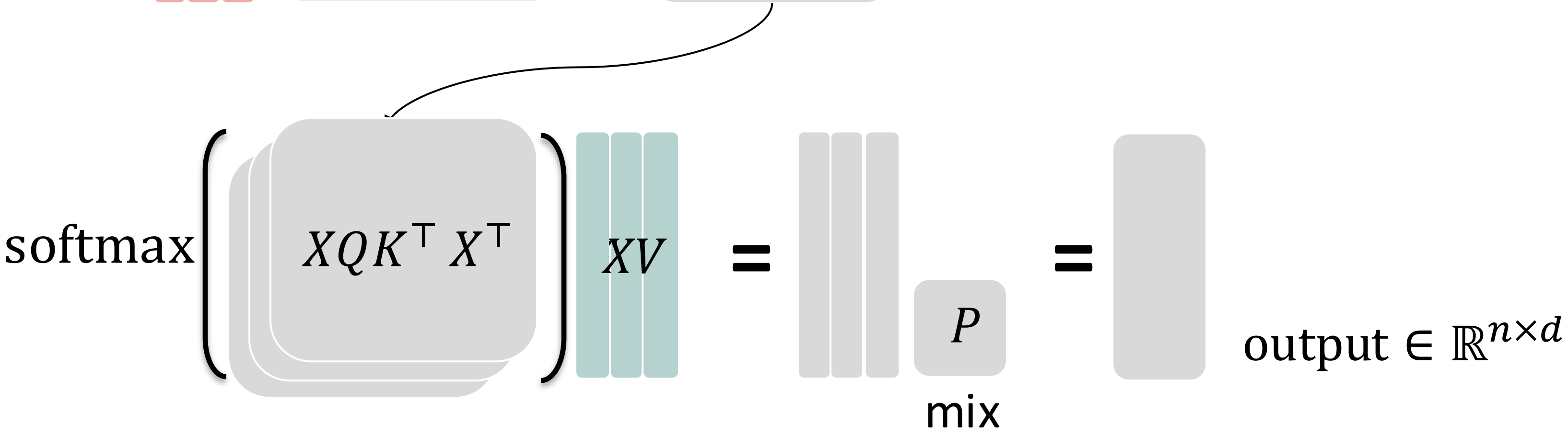
Multi-head self-attention is computationally efficient

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

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



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



Scaled Dot Product [Vaswani et al., 2017]

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

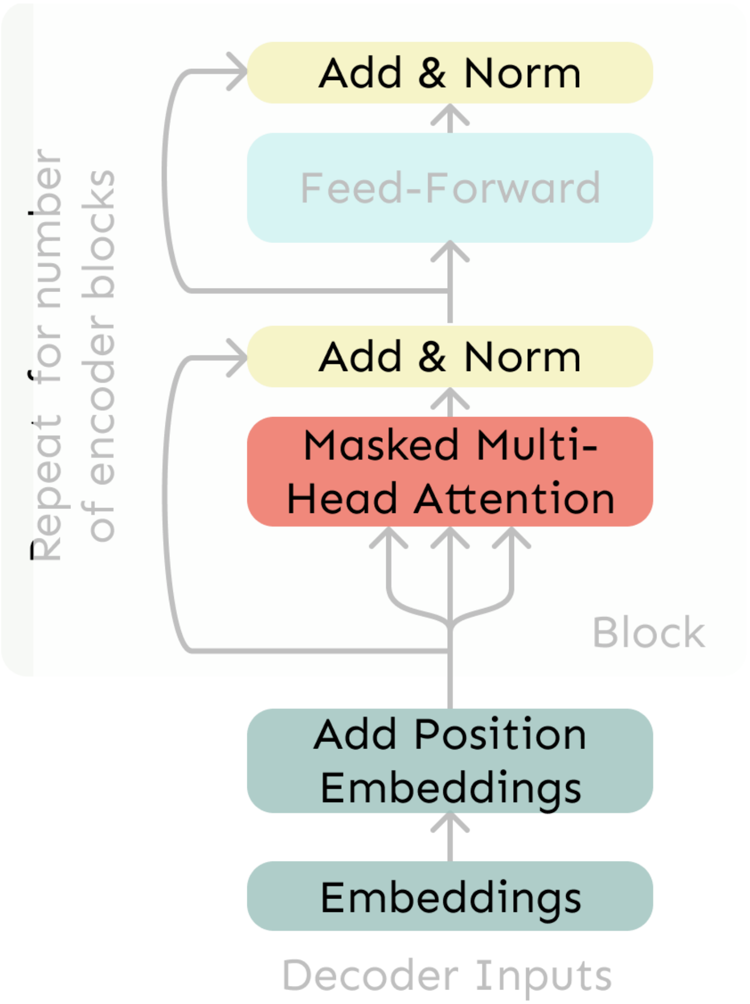
$$\text{output}_\ell = \text{softmax}\left(XQ_\ell K_\ell^\top X^\top\right) * XV_\ell$$

- 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 Decoder

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

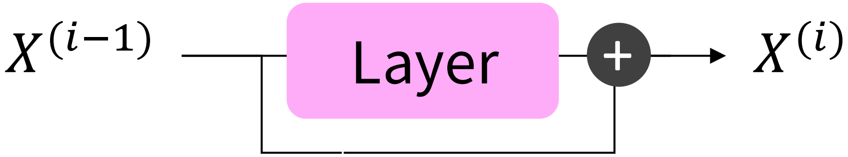


Transformer Decoder

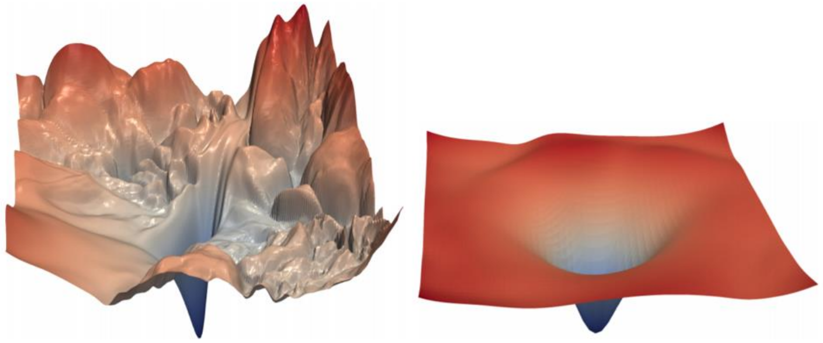
The Transformer Encoder: **Residual connections** [He et al., 2016]

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

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



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



[no residuals] [residuals]

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

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

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

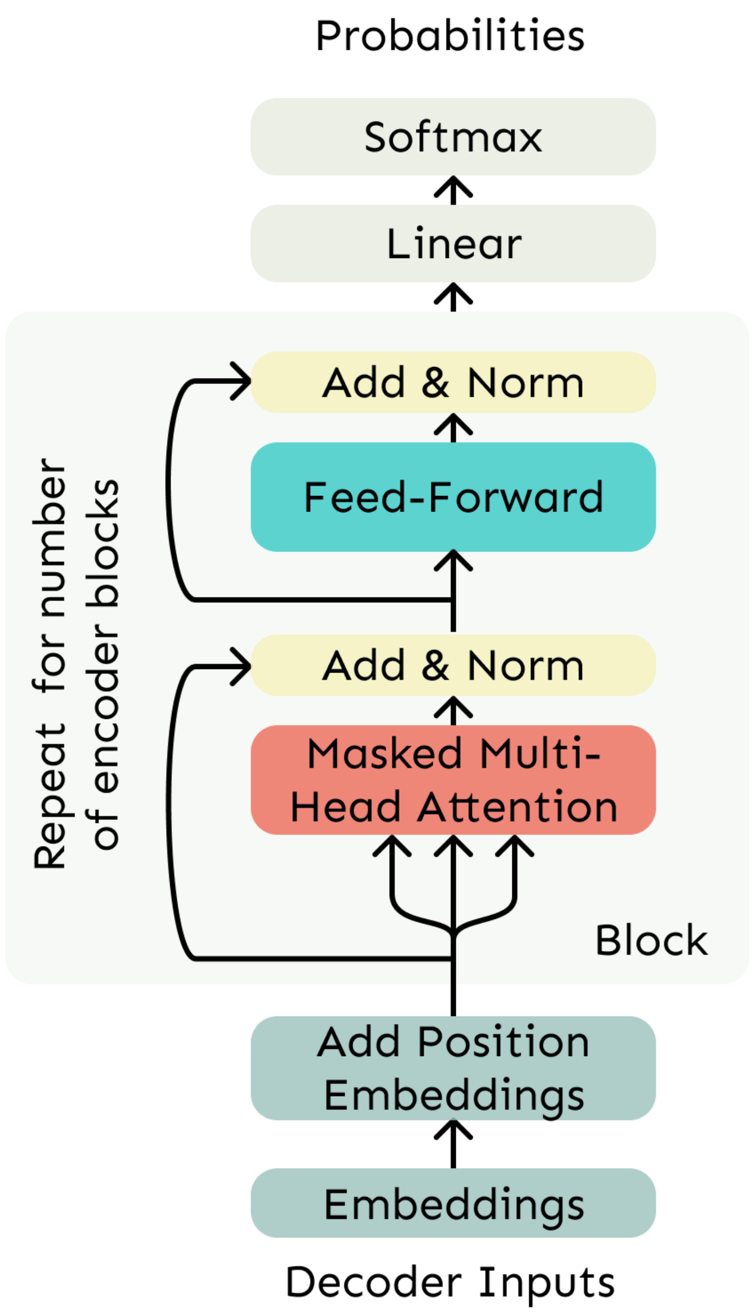
$$\text{output} = \frac{x - \mu}{\sqrt{\sigma} + \epsilon} * \gamma + \beta$$

Normalize by scalar mean and variance

Modulate by learned elementwise gain and bias

The Transformer Decoder

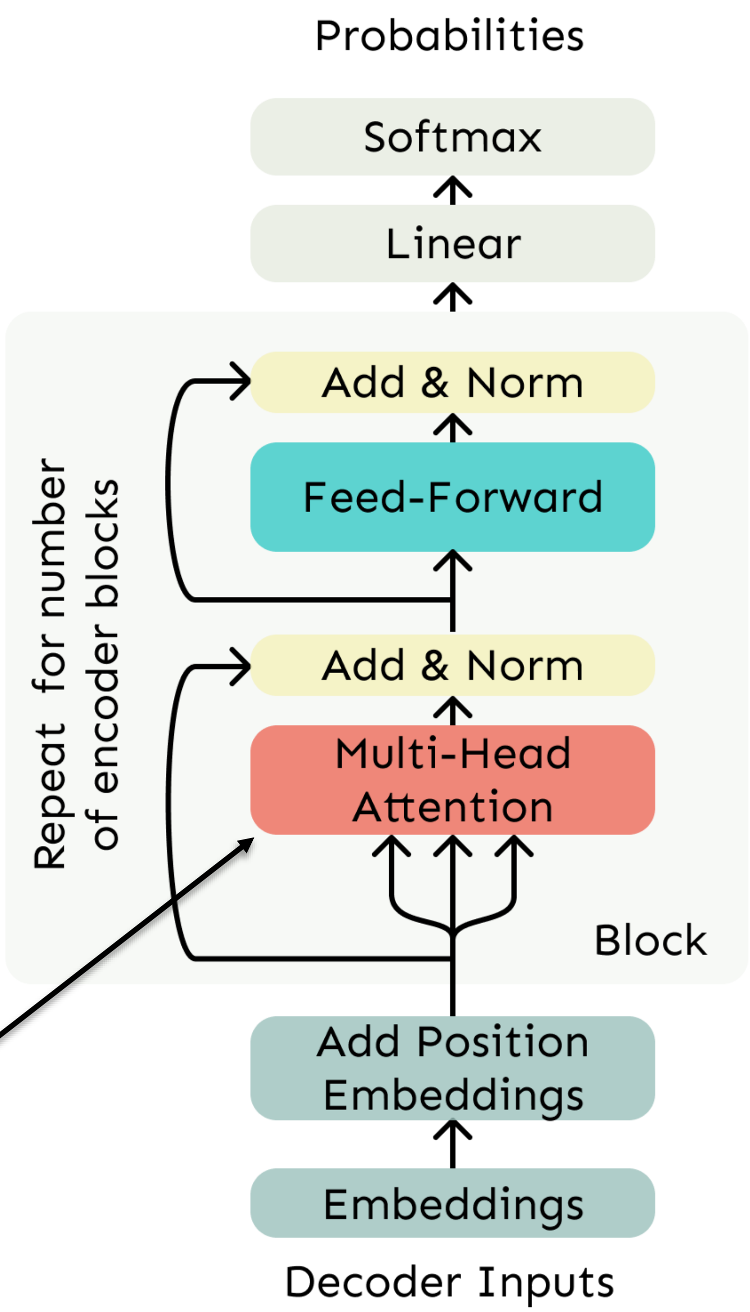
- The Transformer Decoder is a stack of Transformer Decoder **Blocks**.
- Each Block consists of:
  - Self-attention
  - Add & Norm
  - Feed-Forward
  - Add & Norm
- That's it! We've gone through the Transformer Decoder.



The Transformer Encoder

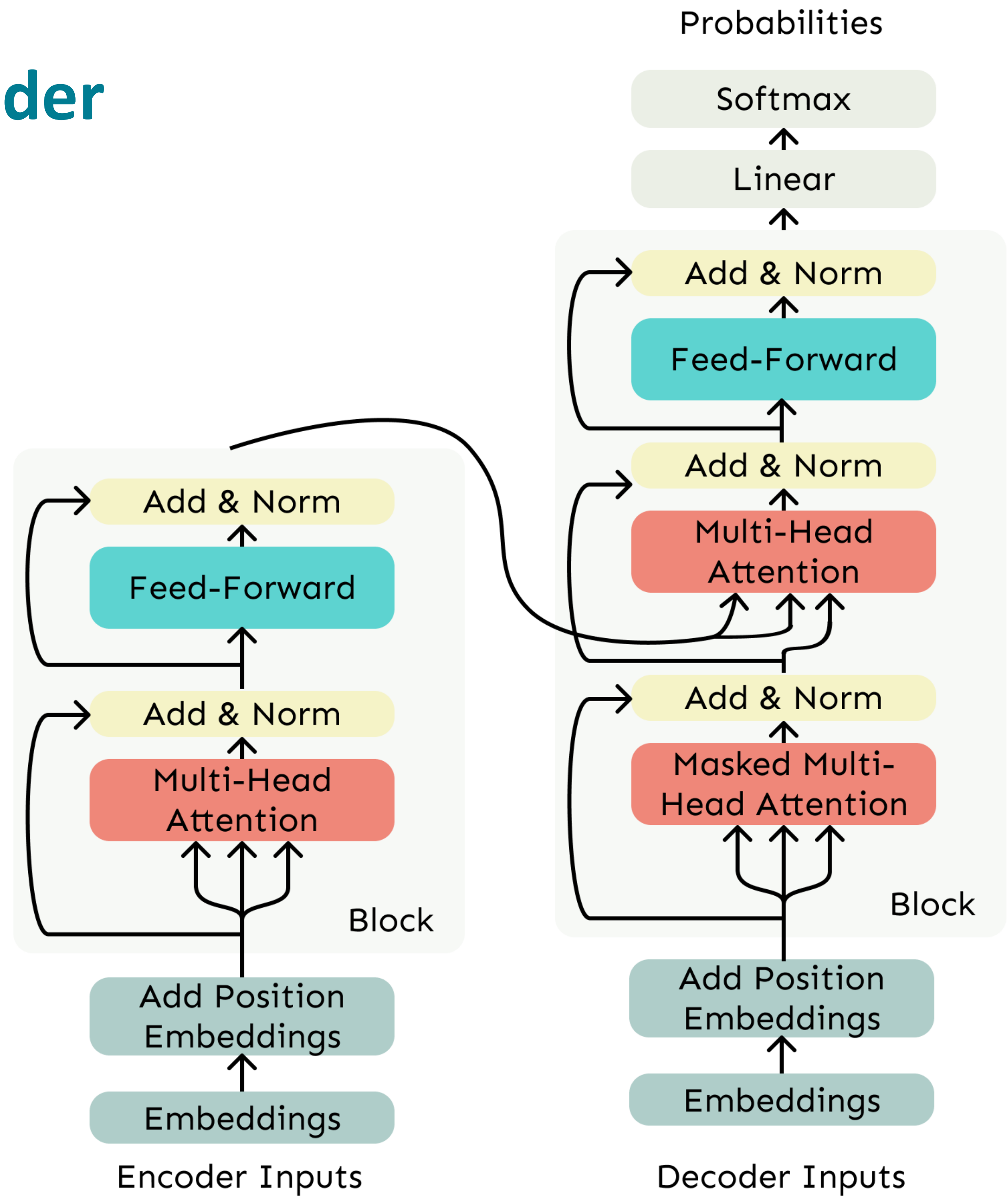
- The Transformer Decoder constrains to **unidirectional context**, as for **language models.**
- What if we want **bidirectional context**, like in a bidirectional RNN?
- This is the Transformer Encoder. The only difference is that we **remove the masking** in the self-attention.

No Masking!



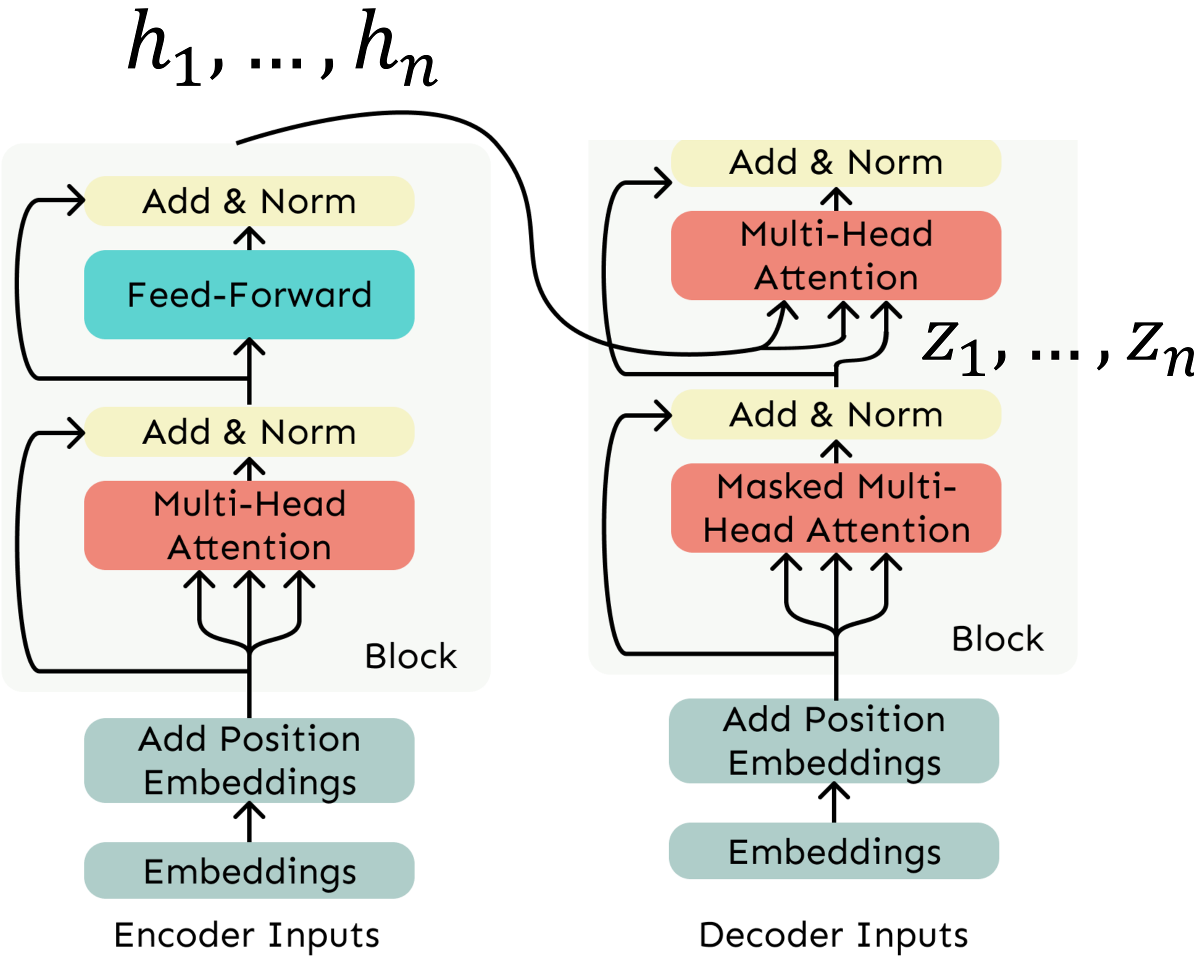
The Transformer Encoder-Decoder

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



Cross-attention (details)

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



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: $ZQ(HK)^\top$

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