# Natural Language Processing with Deep Learning CS224N/Ling284

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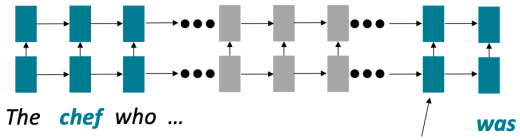
Lecture 8: Self-Attention and Transformers

## 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...

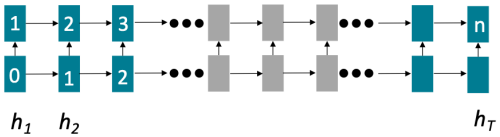



Info of ***chef*** has gone through O(sequence length) many layers!



## 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



## Attention

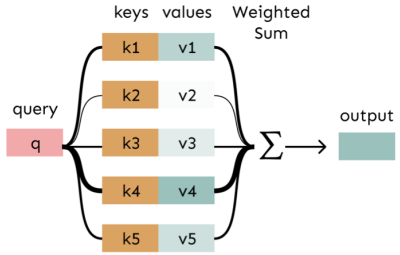
- **Attention** provides a solution to the bottleneck problem.
- **Core idea**: on each step of the decoder, use *direct connection to the encoder* to *focus on a particular part* of the source sequence

- First, we will show via diagram (no equations), then we will show with equations

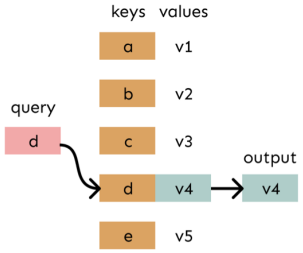
## Attention is *weighted* averaging, which lets you do lookups!

Attention is just a **weighted** average – this is very powerful if the weights are learned!

In **attention**, the query matches all keys *softly*, to a weight between 0 and 1. The keys' values are multiplied by the weights and summed.



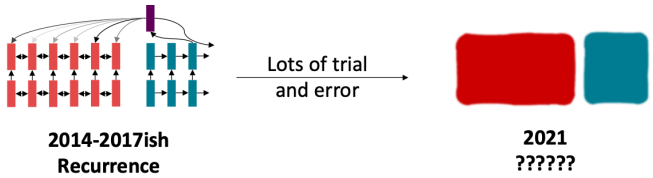

In a **lookup table**, we have a table of keys that map to values. The query matches one of the keys, returning its value.






## Do we even need recurrence at all?

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



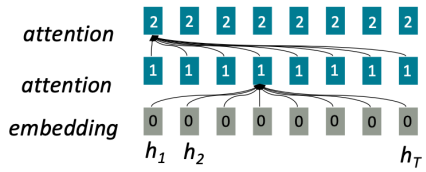

**2014-2017ish Recurrence**

**2021 ??????**



## Attention is parallelizable, and solves bottleneck issues.

- **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 with sequence length.
- Maximum interaction distance: O(1), since all words interact at every layer!

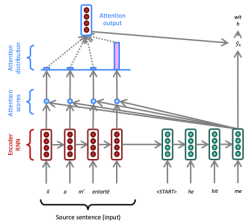



All words attend to all words in previous layer; most arrows here are omitted



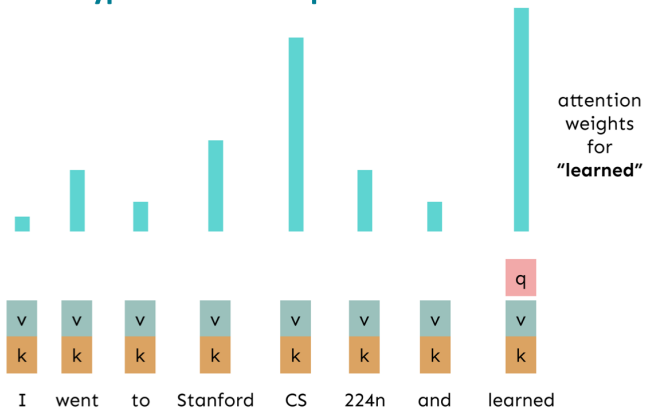
## The building block we need: *self* attention

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

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

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

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

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

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

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

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



## Barriers and solutions for Self-Attention as a building block

| Barriers | Solutions |
|---|---|
| • Doesn't have an inherent notion of order! | → |

## 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**

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

- 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:

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

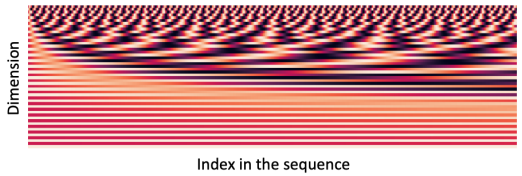
In deep self-attention networks, we do this at the first layer! You could concatenate them as well, but people mostly just add…



## 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 $1, \dots, n$.
- 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]



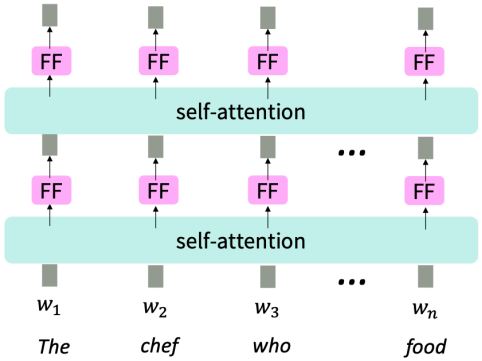
## Barriers and solutions for Self-Attention as a building block

| 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 (Why? Look at the notes!)
- Easy fix: add a **feed-forward network** to post-process each output vector.

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




Intuition: the FF network processes the result of attention



## Barriers and solutions for Self-Attention as a building block

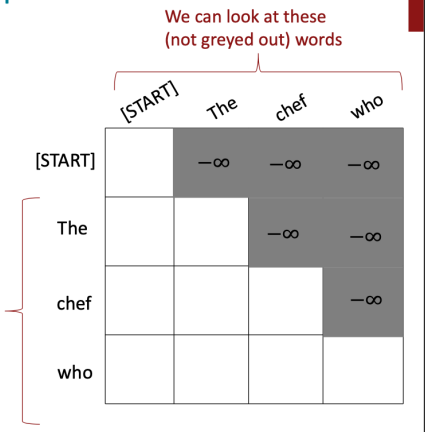
| Barriers | Solutions |
|---|---|
| • Doesn't have an inherent notion of order! | • Add position representations to the inputs |
| • No nonlinearities for deep learning magic! It's all just weighted averages | • Easy fix: apply the same feedforward network to each self-attention output. |
| • Need to ensure we don't "look at the future" when predicting a sequence<br>  • Like in machine translation<br>  • 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 $-\infty$.

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



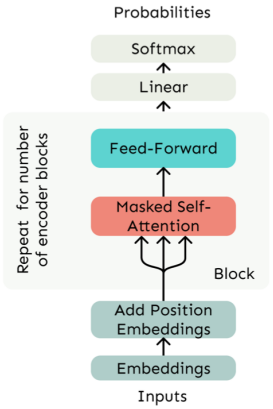



## Barriers and solutions for Self-Attention as a building block

| 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<br>  • Like in machine translation<br>  • 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.





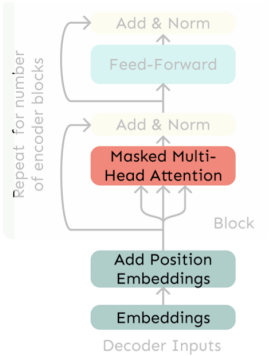

## Outline

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



## The Transformer Decoder

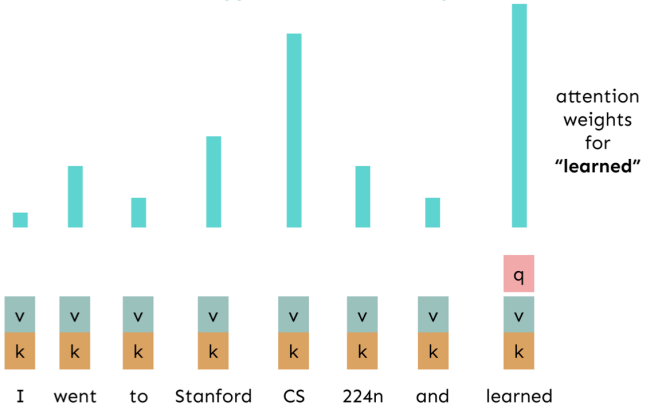
- A Transformer decoder is how we'll build systems like **language models**.
- It's a lot like our minimal self-attention architecture, but with a few more components.
- The embeddings and position embeddings are identical.
- We'll next replace our self-attention with **multi-head self-attention.**



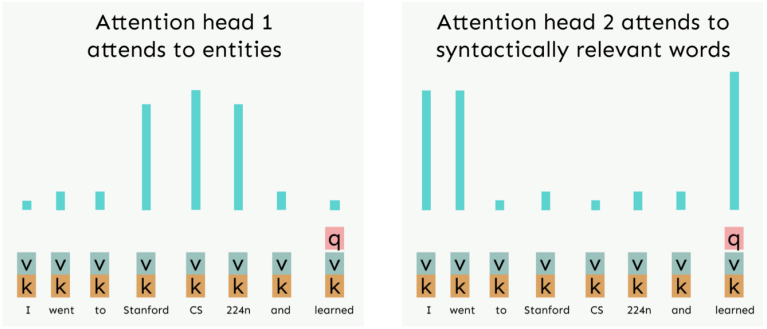

Transformer Decoder



## Recall the Self-Attention Hypothetical Example



## Hypothetical Example of Multi-Head Attention




I went to Stanford CS 224n and learned

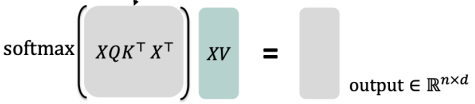


## Sequence-Stacked form of Attention

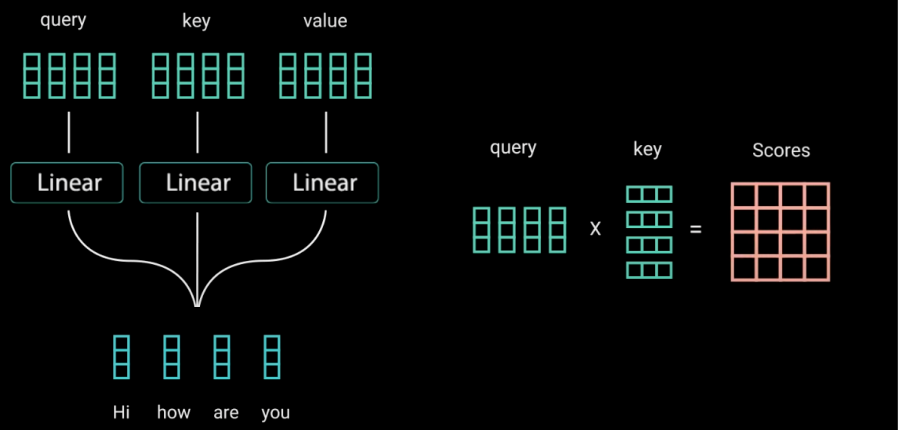
- Let's look at how key-query-value attention is computed, in matrices.
  - Let $X = [x_1; \ldots; x_n] \in \mathbb{R}^{n \times d}$ be the concatenation of input vectors.
  - First, note that $XK \in \mathbb{R}^{n \times d}$, $XQ \in \mathbb{R}^{n \times d}$, $XV \in \mathbb{R}^{n \times d}$.
  - The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

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

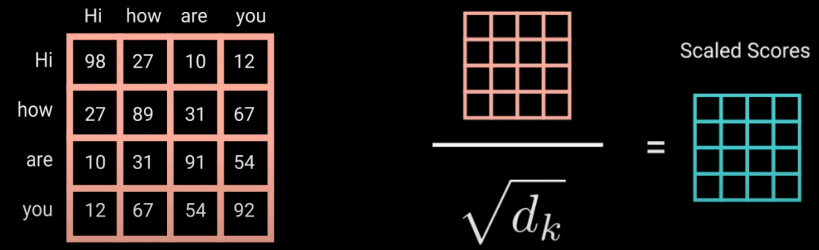

Next, softmax, and compute the weighted average with another matrix multiplication.






https://www.youtube.com/watch?v=4Bdc55j80l8&t=2s

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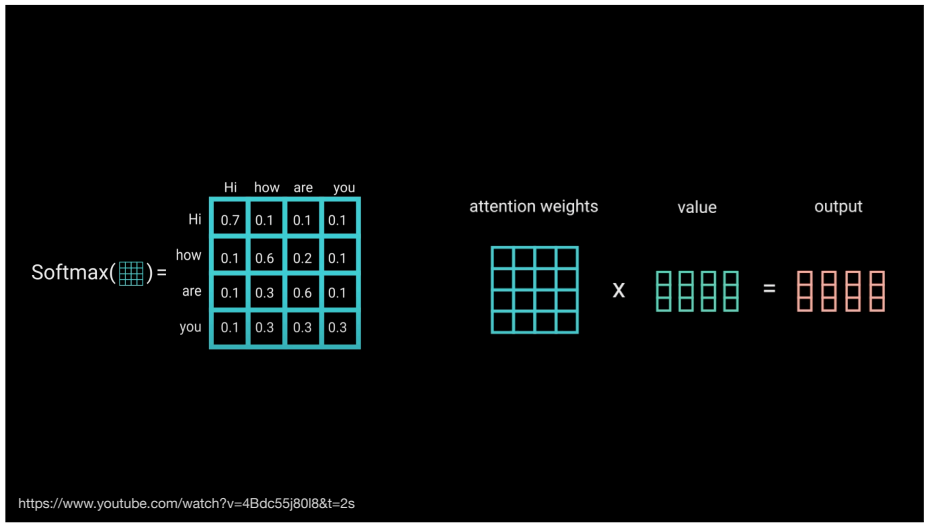
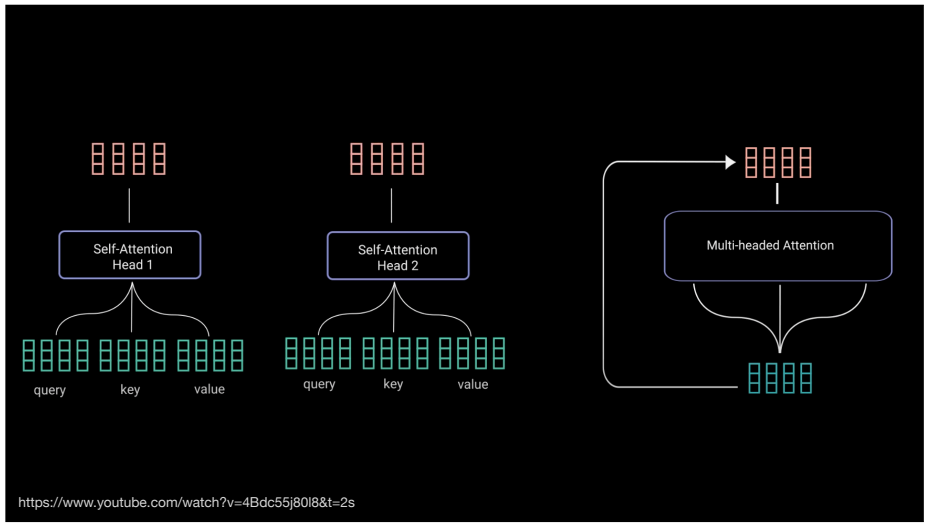



## Multi-headed attention

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



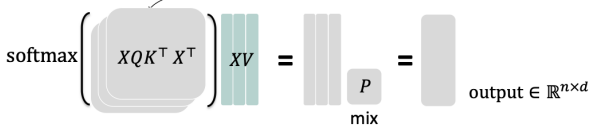



## Multi-head self-attention is computationally efficient

- 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:

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

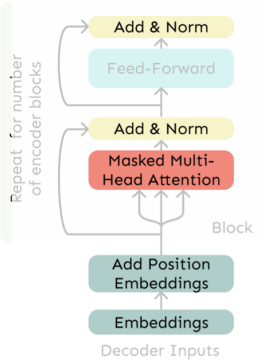
- We divide the attention scores by $\sqrt{d/h}$, to stop the scores from becoming large just as a function of $d/h$ (The dimensionality divided by the number of heads.)

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



## 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"

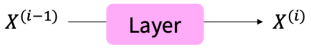



Transformer Decoder

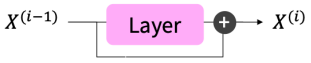


## The Transformer Encoder: **Residual connections** [He et al., 2016]

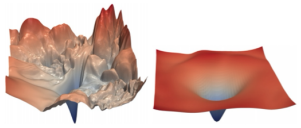
- **Residual connections** are a trick to help models train better.
  - Instead of $X^{(i)} = \text{Layer}(X^{(i-1)})$ (where $i$ represents the layer)




  - 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 $\sigma = \sqrt{\frac{1}{d}\sum_{j=1}^{d}(x_j - \mu)^2}$; this is the standard deviation; $\sigma \in \mathbb{R}$.
- Let $\gamma \in \mathbb{R}^d$ and $\beta \in \mathbb{R}^d$ be learned "gain" and "bias" parameters. (Can omit!)
- Then layer normalization computes:

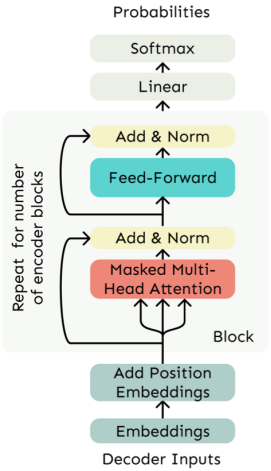
$$\text{output} = \frac{x - \mu}{\sqrt{\sigma + \epsilon}} * \gamma + \beta$$

Normalize by scalar mean and variance

Modulate by learned elementwise gain and bias

## 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.

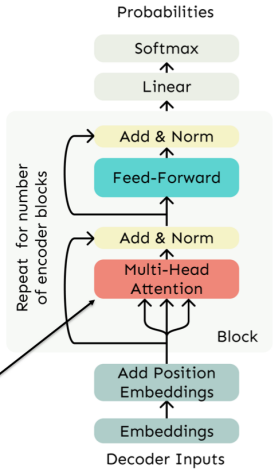





## The Transformer Encoder

- 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.

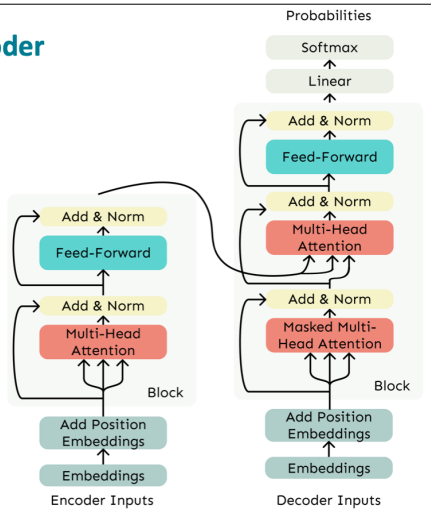
**No Masking!**






## The Transformer Encoder-Decoder

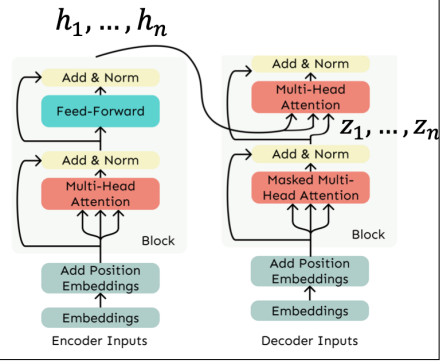
- Recall that in machine translation, we processed the source sentence with a **bidirectional** model and generated the target with a **unidirectional model**.
- For this kind of seq2seq format, we often use a Transformer Encoder-Decoder.
- We use a normal Transformer Encoder.
- Our Transformer Decoder 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 $h_1, \ldots, h_n$ be **output** vectors **from** the Transformer **encoder**; $x_i \in \mathbb{R}^d$
- Let $z_1, \ldots, z_n$ be input vectors from the Transformer **decoder**, $z_i \in \mathbb{R}^d$
- Then keys and values are drawn from the **encoder** (like a memory):
  - $k_i = Kh_i, v_i = Vh_i$.
- And the queries are drawn from the **decoder**, $q_i = Qz_i$.



## 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

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]

## 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]