

04. Transformers

Transformers may not fix all your NLP problems.

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But they are worth some attention.



CS 2731 / ISSP 2230

Introduction to Natural Language Processing

Session 13: Transformers part 1, beam search

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February 21, 2024

Course logistics

- Proposal and literature review is **due tomorrow, Thu Feb 22**
 - Instructions are on the [project webpage](#)
 - Submit on Canvas
 - One submission per group
 - Organize at least 4 papers into themes of approaches, datasets, findings
- Late work and resubmission policy clarifications on the syllabus
 - The latest you can submit homework is 2 weeks after the deadline (2.5% penalty/day)
 - If you are unsatisfied with your homework grade, resubmissions are generally possible

Course logistics

- Discussion post instead of reading quiz for Monday
- Homework 3 is out (most of it)
 - **Due Thu Mar 7**

Midterm OMET survey results (~20% response rate)

- What helps learning
 - Reading before class to make lectures easy to digest
 - Interactive lectures
- What could be improved
 - Activities can slow pace of the lecture
 - Reading
 - Remove reading quizzes
 - If I read the whole thing, hard to pay attention in class
 - Homework
 - Less homework (not enough time)
 - Alignment between lectures and homework
 - Suggest additional reading materials for SOTA work
- What I will change
 - Work to integrate activities in lecture more cleanly
 - Consider lightening homework, aligning it better with lectures

Lecture overview: Transformers part 1, beam search

- Self-attention
- Multi-headed attention
- Residual connections and layer normalization
- Transformer blocks
- Beam search
- GPT preview



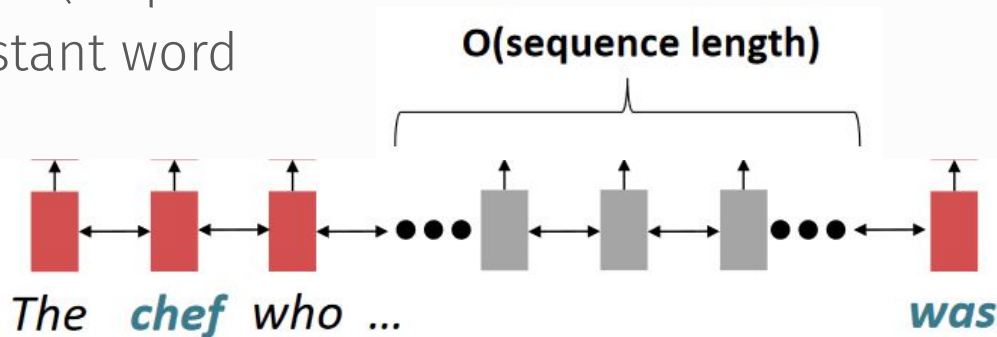
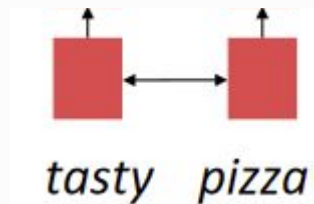
From recurrence to self-attention

Transformers improved on RNNs and CNNs

- Google introduced Transformers in 2017 [Vaswani et al. 2017, “Attention is all you need”]
- At that time, most neural NLP models were based on
 - RNNs
 - CNNs
- These were good
- For many tasks, Transformers were better
- Has become the most successful NN architecture in NLP
- Adopted by famous pretrained LLMs (BERT, GPT)

Issues with recurrent models: Linear interaction distance

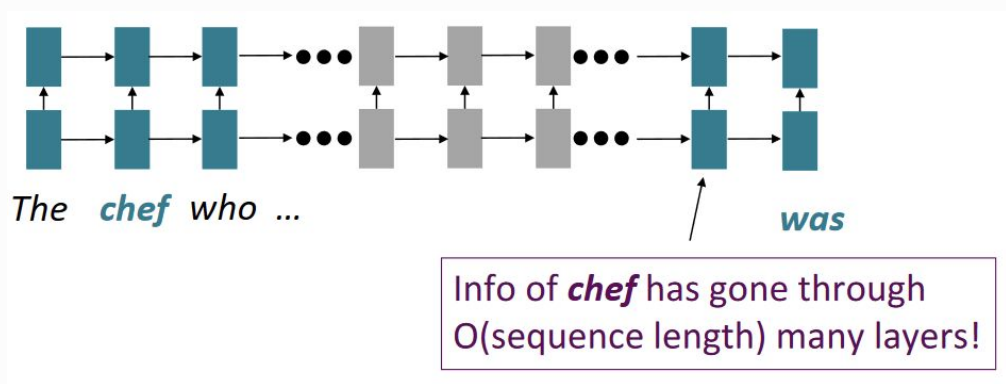
- RNNs are unrolled “left-to-right”.
 - This encodes linear locality: a useful heuristic!
 - Nearby words often affect each other’s meanings
- **Problem:** RNNs take $O(\text{sequence length})$ steps for distant word pairs to interact



Issues with recurrent models: Linear interaction distance

$O(\text{sequence length})$ 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...



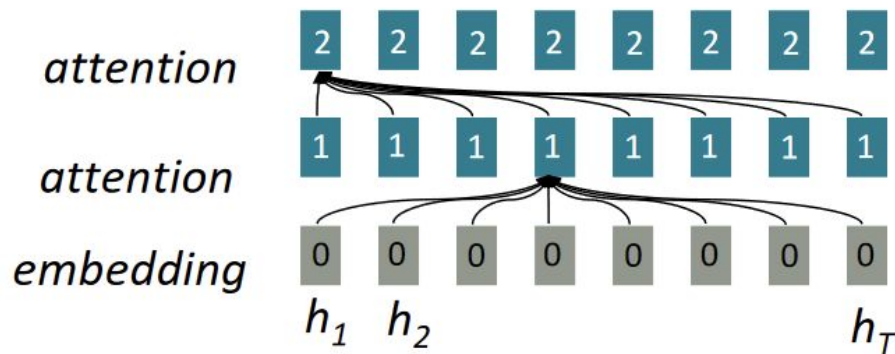
Issues with recurrent models: Lack of parallelizability

Forward and backward passes have $O(\text{sequence length})$ 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!

If not recurrence, then what? How about attention?

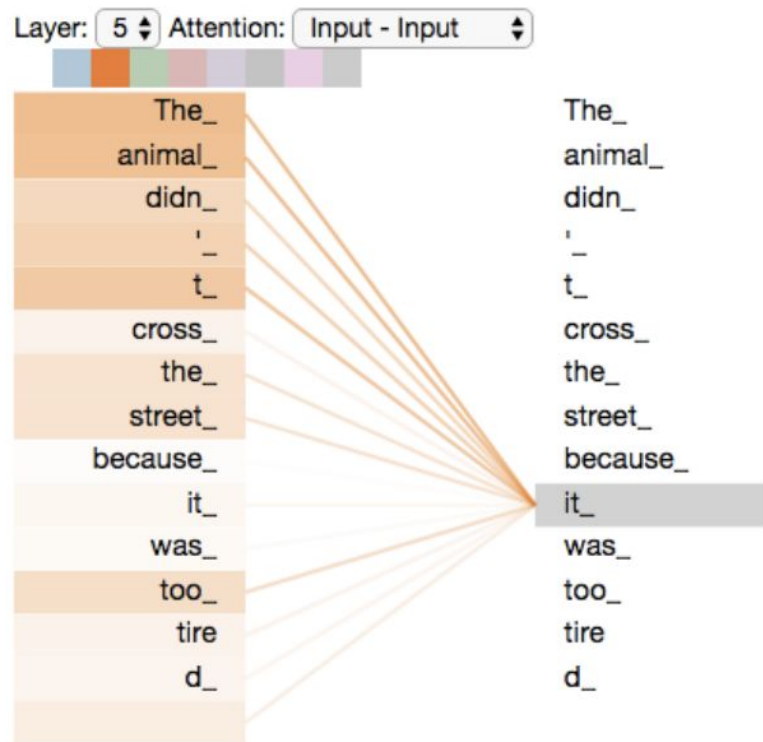
- Attention treats each word's representation as a query to access and incorporate information from a set of values.
- We saw attention from the decoder to the encoder; today we'll think about attention within a single sentence (self-attention)
- Number of unparallelizable operations does not increase 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

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

Self-attention: all you need



Take the sentence: “The animal didn’t cross the street because it was too tired”. What is the antecedent of *it*?

Self-attention allows the model to “attend” to all of the other positions and to process each position (including *the* and *animal*) to help it better encode the pronoun *it*.

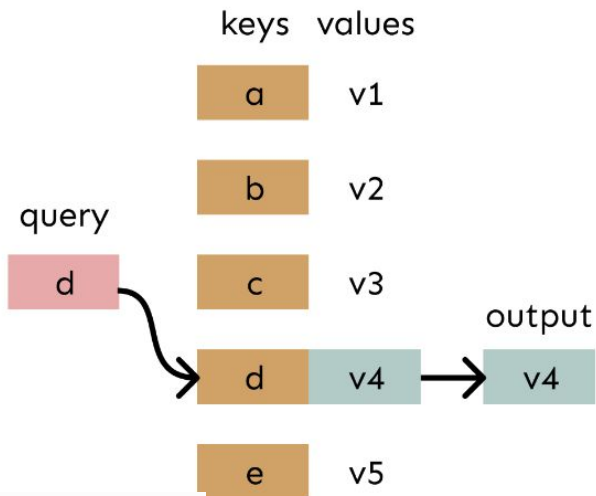
You can compare this to the hidden state in an RNN—it conveys information about other words in the sequence to the position one is currently processing.

Transformers rely on self-attention.

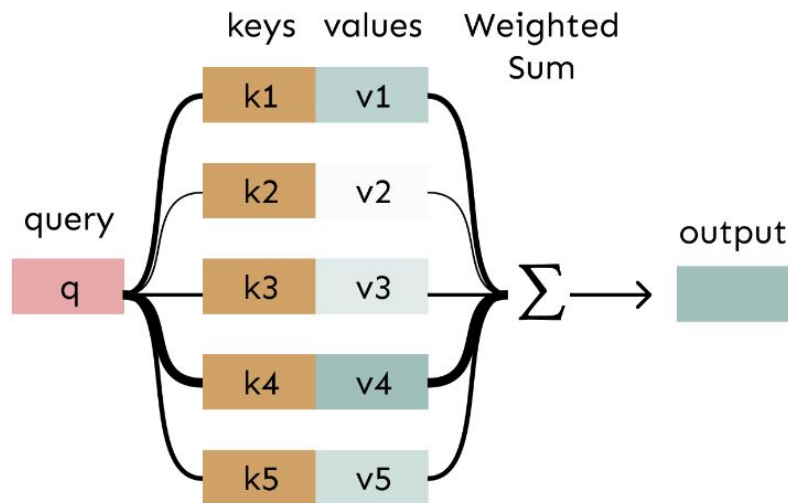
Attention as a soft, averaging lookup table

We can think of **attention** as performing fuzzy lookup in a key-value store.

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



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.

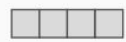


Computing Self-Attention, Step One: Compute Key, Query, and Value Vectors

d_x -dimensional
embeddings

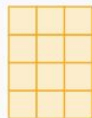
$d_k \times d_x$ -dimensional
Weight Matrices

d_k -dimensional vectors



x_1

\times



W^Q

$=$



q_1

queries



x_1

\times



W^K

$=$



k_1

keys



x_1

\times



W^V

$=$



v_1

values

Computing Self-Attention, Step Two: Weighted Sum of Value Vectors

We wash our cats
 x_1 x_2 x_3 x_4
query-key dot product $q_1 \cdot k_1 = 13$ $q_1 \cdot k_2 = 24$ $q_1 \cdot k_3 = 20$ $q_1 \cdot k_4 = 12$

divide by $\sqrt{d_k}$ $\frac{13}{\sqrt{64}} = 1.63$ $\frac{24}{\sqrt{64}} = 3.0$ $\frac{20}{\sqrt{64}} = 2.5$ $\frac{12}{\sqrt{64}} = 1.5$

softmax

0.12	0.48	0.29	0.10
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\times value

$0.12 \times v_1$ $0.48 \times v_2$ $0.29 \times v_3$ $0.10 \times v_4$

sum



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

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

- Don't worry about what the \mathbf{p}_i are made of yet!
- Easy to incorporate this info into our self-attention block: just add the \mathbf{p}_i to our inputs!
- Recall that \mathbf{x}_i is the embedding of the word at index i . The positioned embedding is:

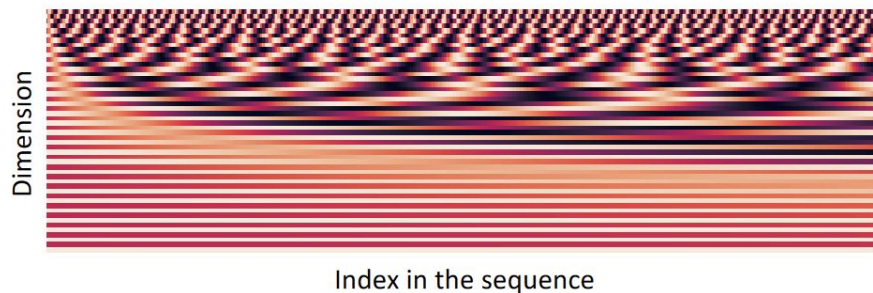
$$\tilde{\mathbf{x}}_i = \mathbf{x}_i + \mathbf{p}_i$$

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

Position embeddings through sinusoids

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

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



- 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!

Position embeddings learned from scratch

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

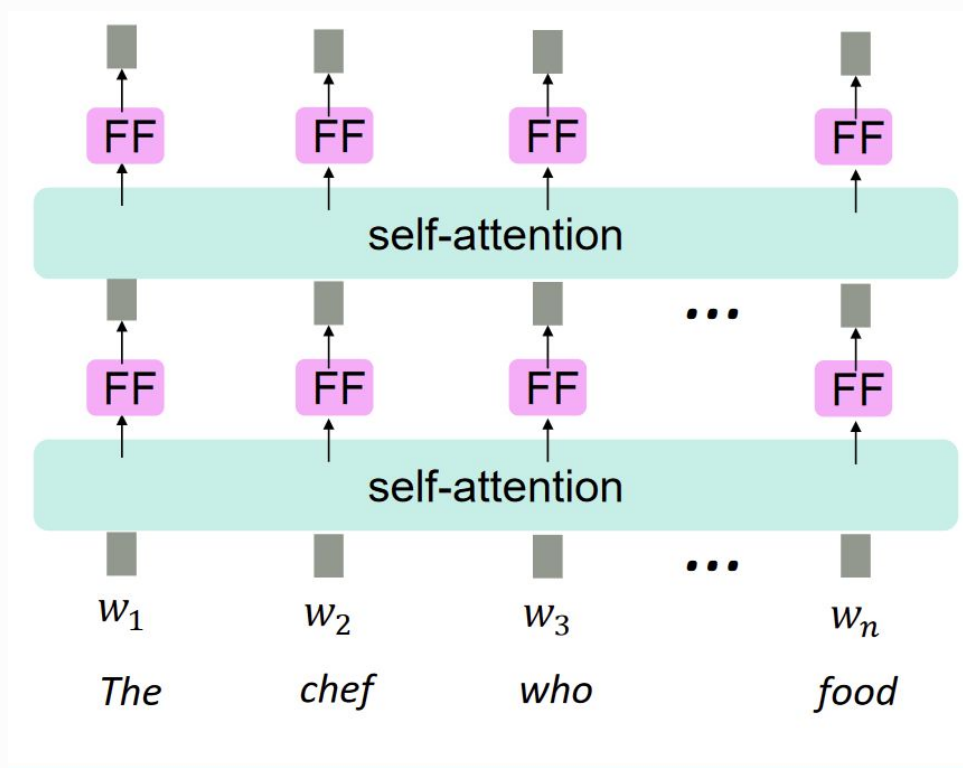
- Doesn't have an inherent notion of order!
- No nonlinearities for deep learning! It's all just weighted averages



Solutions

- Add position representations to the inputs

Solution: add some feedforward NNs!



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



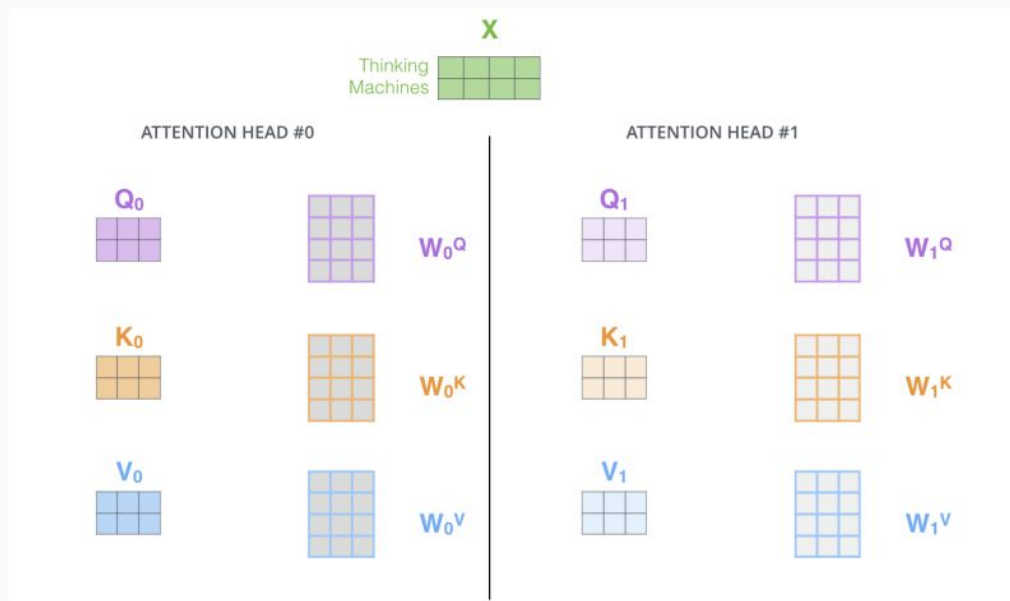
Solutions

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

Multi-headed attention

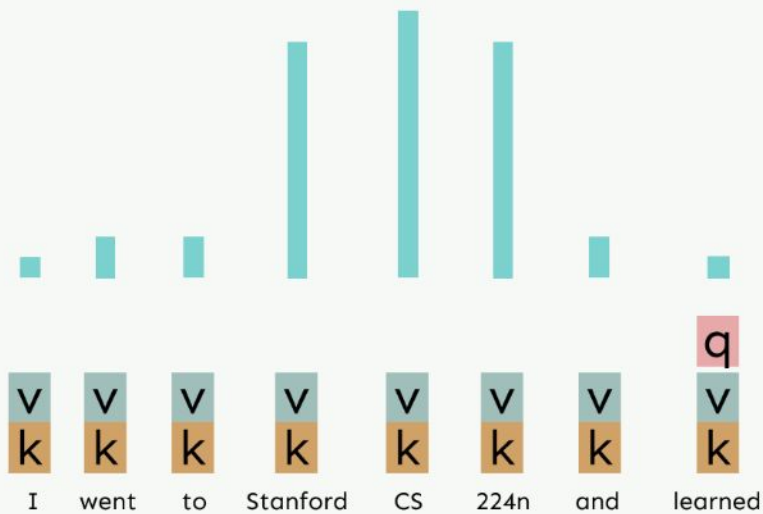
Multi-Headed Attention Expands Transformer Models' Ability to Focus on Different Positions

Maintain distinct weight matrices for each attention head—distinct representational subspaces:

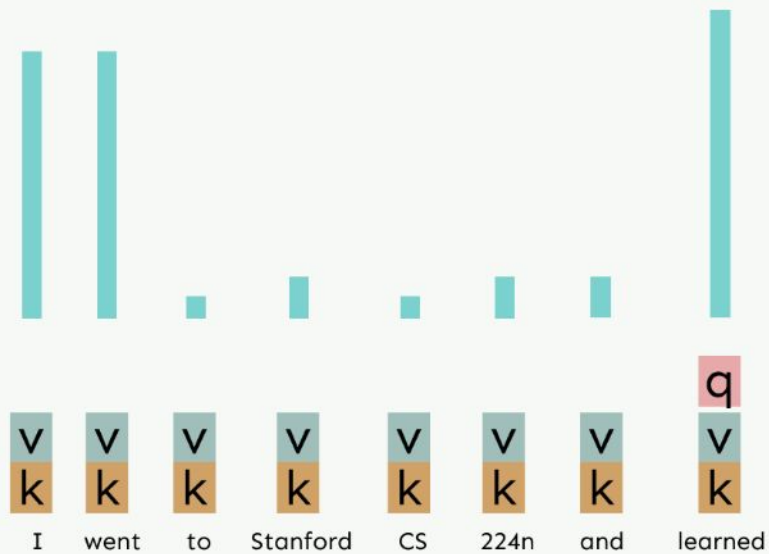


Hypothetical example of multi-headed attention

Attention head 1
attends to entities



Attention head 2 attends to
syntactically relevant words



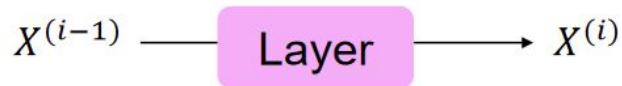
Multi-headed attention

- 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:
 - $\text{output}_\ell = \text{softmax}(X Q_\ell K_\ell^\top X^\top) * X V_\ell$, where $\text{output}_\ell \in \mathbb{R}^{d/h}$
- Then the outputs of all the heads are combined!
 - $\text{output} = [\text{output}_1; \dots; \text{output}_h] Y$, where $Y \in \mathbb{R}^{d \times d}$
- Each head gets to “look” at different things, and construct value vectors differently.

Optimization tricks: residual connections and layer normalization

Residual connections [He et al. 2016]

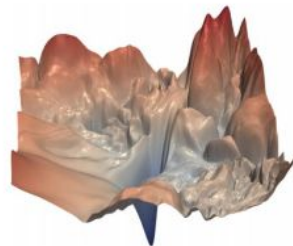
- **Residual connections** are a trick to help models train better.
 - Instead of $X^{(i)} = \text{Layer}(X^{(i-1)})$ (where i represents the layer)



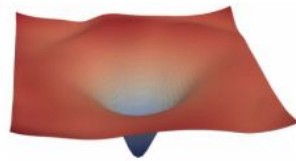
- We let $X^{(i)} = X^{(i-1)} + \text{Layer}(X^{(i-1)})$ (so we only have to learn “the residual” from the previous layer)



- 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]

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

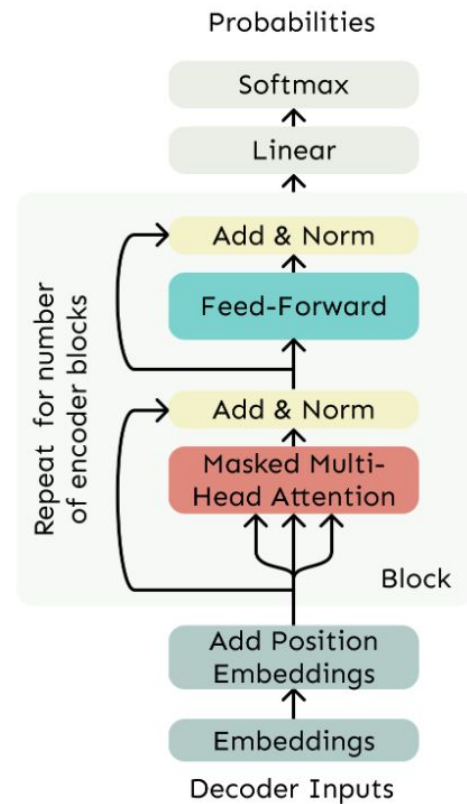
Modulate by learned elementwise gain and bias

Transformer blocks

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
- But for decoding (language modeling), we can't look into the future!



Decoding: apply a “causal mask” for self-attention

- To do auto-regressive LM, we need to apply a “causal” mask to self-attention, forbidding it from getting future context.
- At timestep t , we set $a_i = 0$ for $i > t$



For encoding
these words

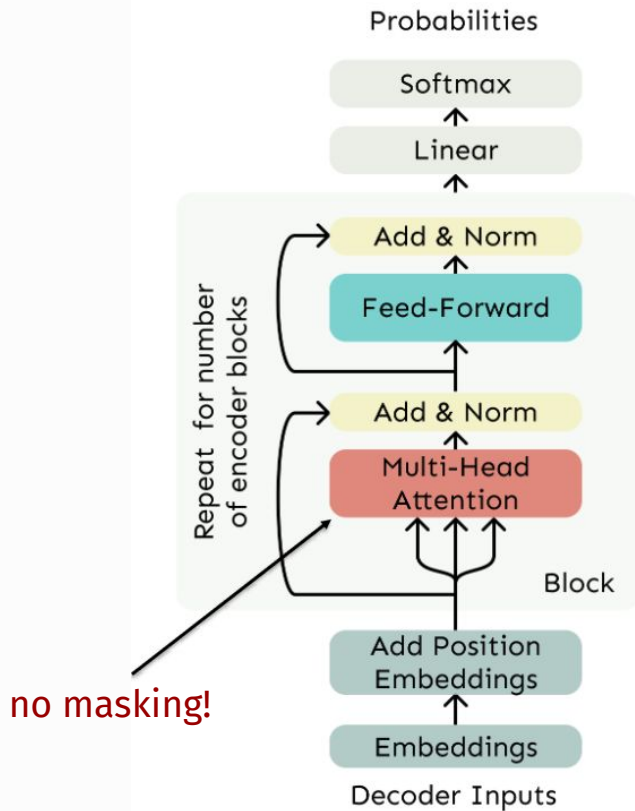
We can look at these
(not greyed out) words

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

The transformer encoder

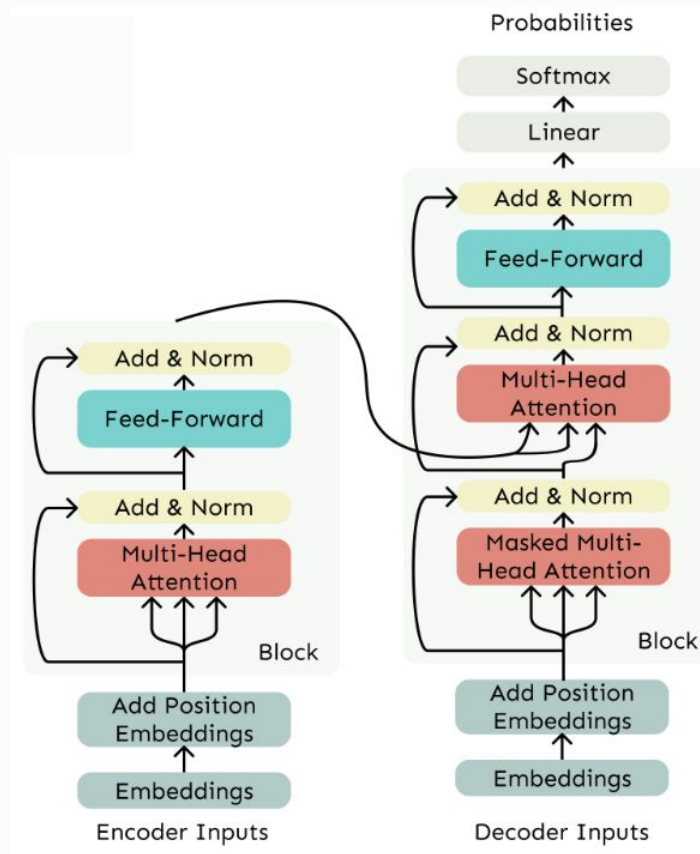
The Transformer Decoder constrains to unidirectional context, as for language models.

- What if we want bidirectional context, as for text classification?
- This is the Transformer Encoder. The only difference is that we remove the masking in the self-attention.



The transformer encoder-decoder

- Can use transformers for encoder-decoder (seq2seq) framework
- Transformer decoder modified to perform cross-attention to the output of the encoder

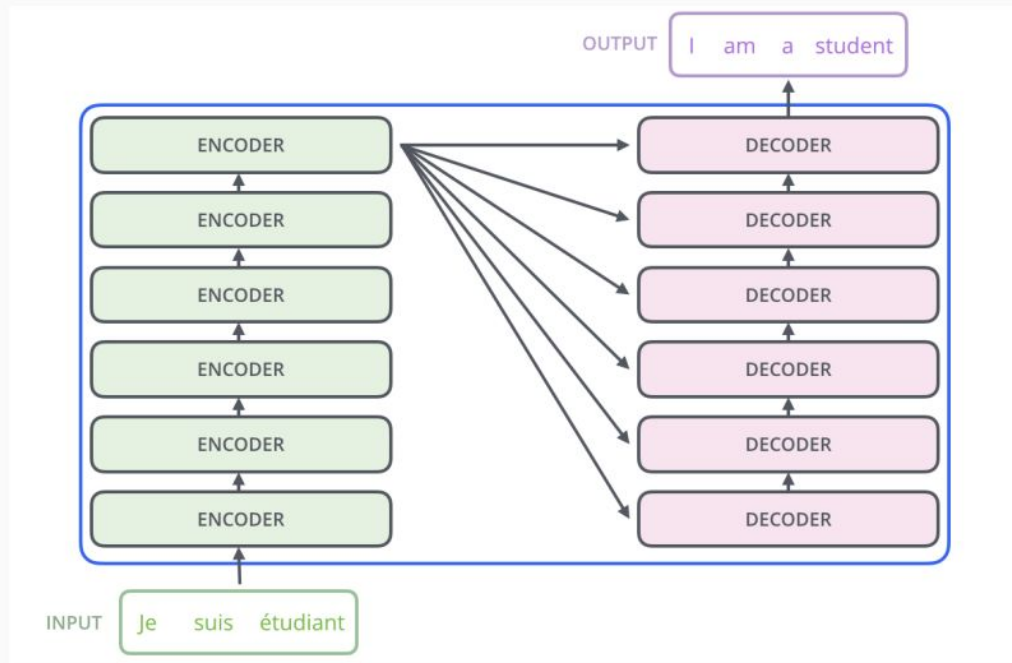


Transformers: Stacks of Encoders and Decoders

A transformer is a stack of ~ 6 encoders and decoders. The encoders are identical in structure but do not share weights.

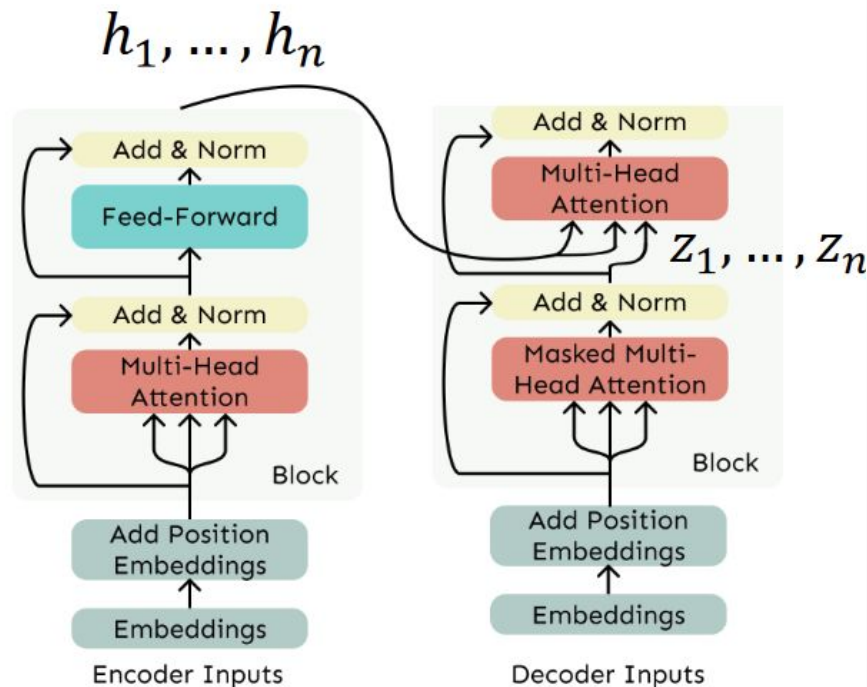
Encoders encode entire input sentences, so can look at future words

Decoders generate output text a step at a time, so can **not** look at future words (language modeling)



Cross-attention

- 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):
 - $k_i = Kh_i, v_i = Vh_i$.
- And the queries are drawn from the **decoder**, $q_i = Qz_i$.



Drawbacks of transformers

- 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!
- Can't easily handle long sequences; usually set a bound of 512 tokens
- 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]

Beam search

Beam search improves on greedy decoding

- Traditional encoder-decoder framework involves generating highest probability word (argmax) at each timestep in the decoding
- But this greedy approach suffers from issues if choosing early high-probability tokens leads to low-probability sequences!
- **Solution:** Don't commit to just the 1 highest probability word, but keep multiple options in a “beam”
- Prune to k highest-probability sequences after each timestep

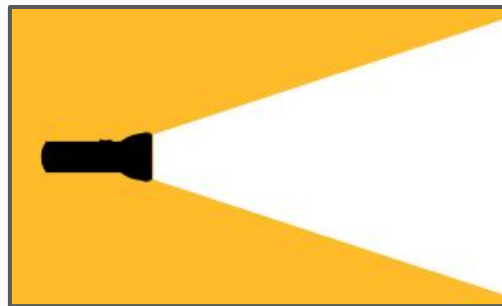


Image: iStock

log P ("the green witch arrived"|x)
 $= \log P(\text{the}|x) + \log P(\text{green}|\text{the},x) + \log P(\text{witch} | \text{the, green},x) + \log P(\text{arrived}|\text{the,green,witch},x) + \log P(\text{END}|\text{the,green,witch,arrived},x)$
 $= -2.7$

start

log P($y_1|x$) y_1

log P($y_2|y_1,x$) y_2

log P($y_3|y_2,y_1,x$) y_3

log P($y_4|y_3,y_2,y_1,x$) y_4

log P($y_5|y_4,y_3,y_2,y_1,x$) y_5

Wrapping up

- Transformers are a high-performing NLP architecture based on self-attention
- Transformers can be used for language modeling
- Beam search is used to find higher probability sequences than greedy approaches find in decoding

Questions?