



Transformer Architecture

CSCI 601-471/671 (NLP: Self-Supervised Models)

<https://self-supervised.cs.jhu.edu/sp2025/>

RNNs, Back to the Cons

- While RNNs in theory can represent long sequences, they quickly **forget** portions of the input.
- Vanishing/exploding gradients
- Difficult to parallelize
- The alternative solution we will see: Transformers!



Language Models: History Recap

- Probabilistic n-gram models of text generation [Jelinek+ 1980's, ...]
 - Applications: Speech Recognition, Machine Translation
- Statistical or shallow neural LMs (late 90's – mid 00's) [Bengio+ 2001, ...]
- Recurrent neural nets (2010s)
- Pre-training deep neural language models (2017's onward):
 - Many models based on: **Self-Attention**

Chapter Plan

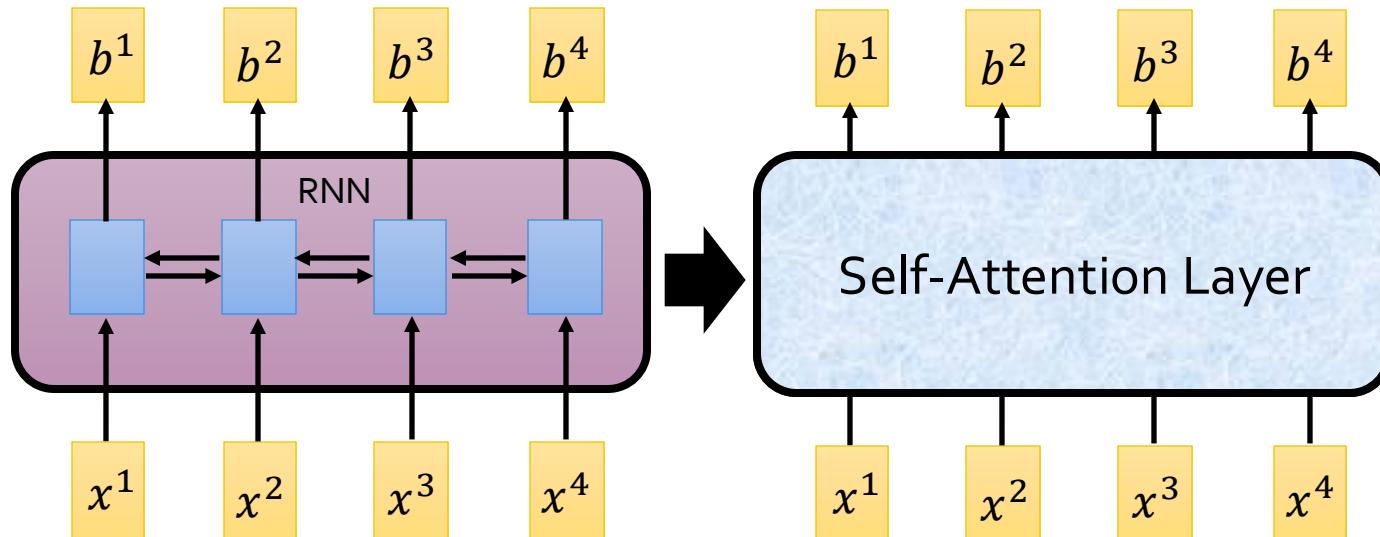
1. Self-Attention module
2. Transformer architecture
3. Computation/space cost
4. Thinking about Transformer implementation

Chapter goal — getting very comfortable with nuances involved in Transformers.

Self-Attention Module

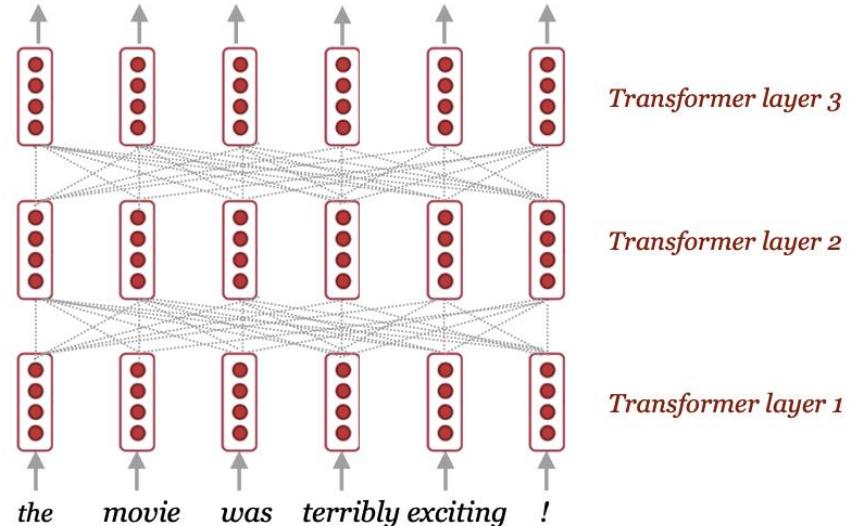
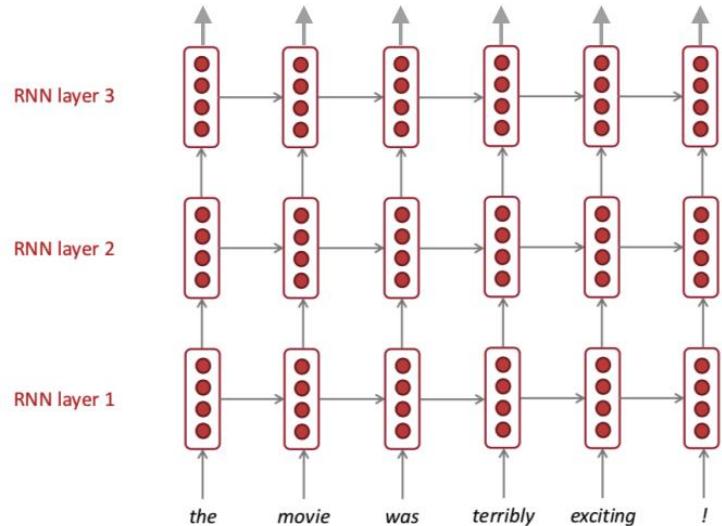
Self-Attention

- b^i is obtained based on the whole input sequence.
- can be parallelly computed.



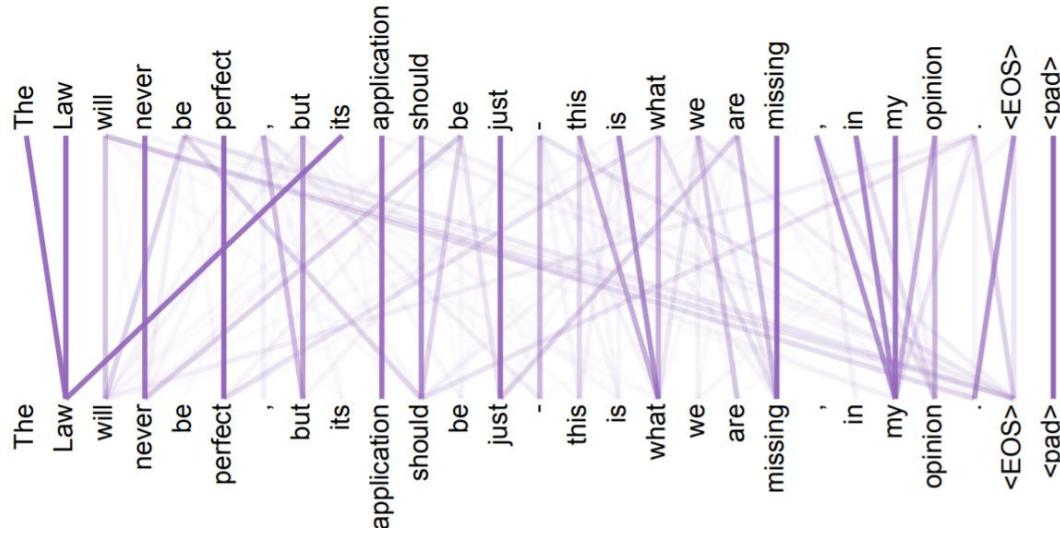
Idea: replace any thing done by RNN with **self-attention**.

RNN vs Transformer



Attention

- Core idea: build a mechanism to focus ("attend") on a particular part of the context.



Defining Self-Attention

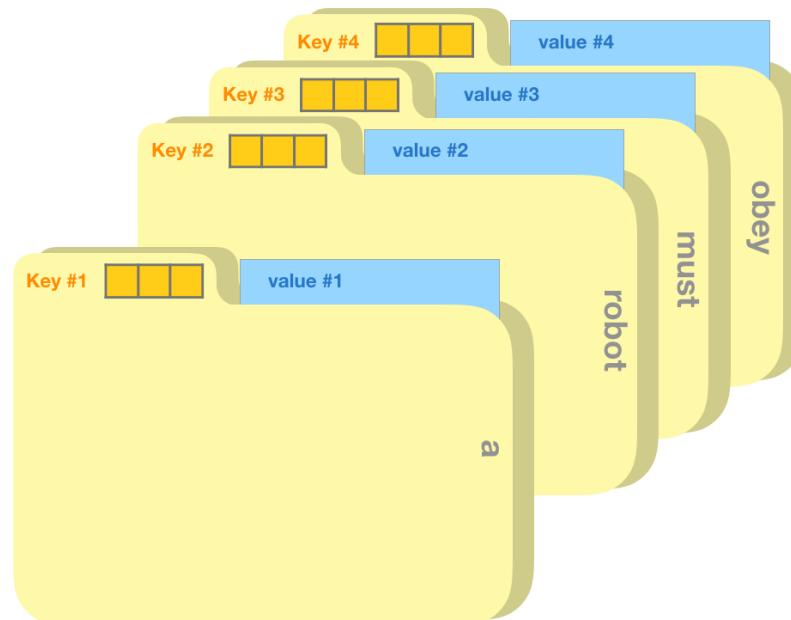
- Terminology:
 - **Query**: to match others
 - **Key**: to be matched
 - **Value**: information to be extracted

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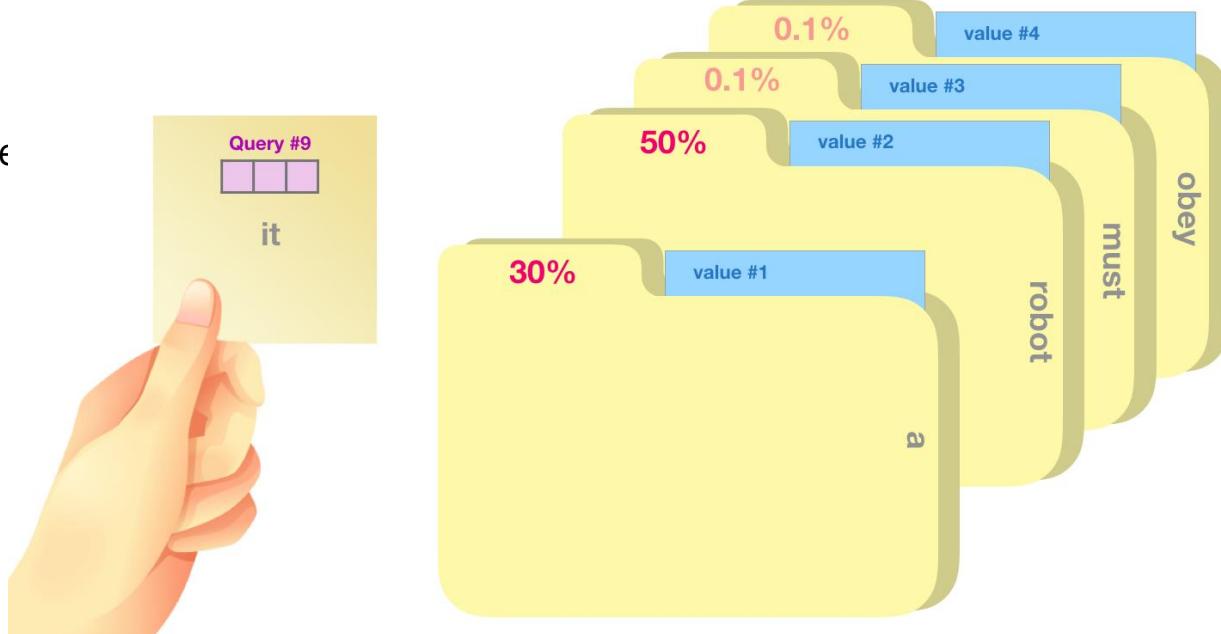


An analogy



Defining Self-Attention

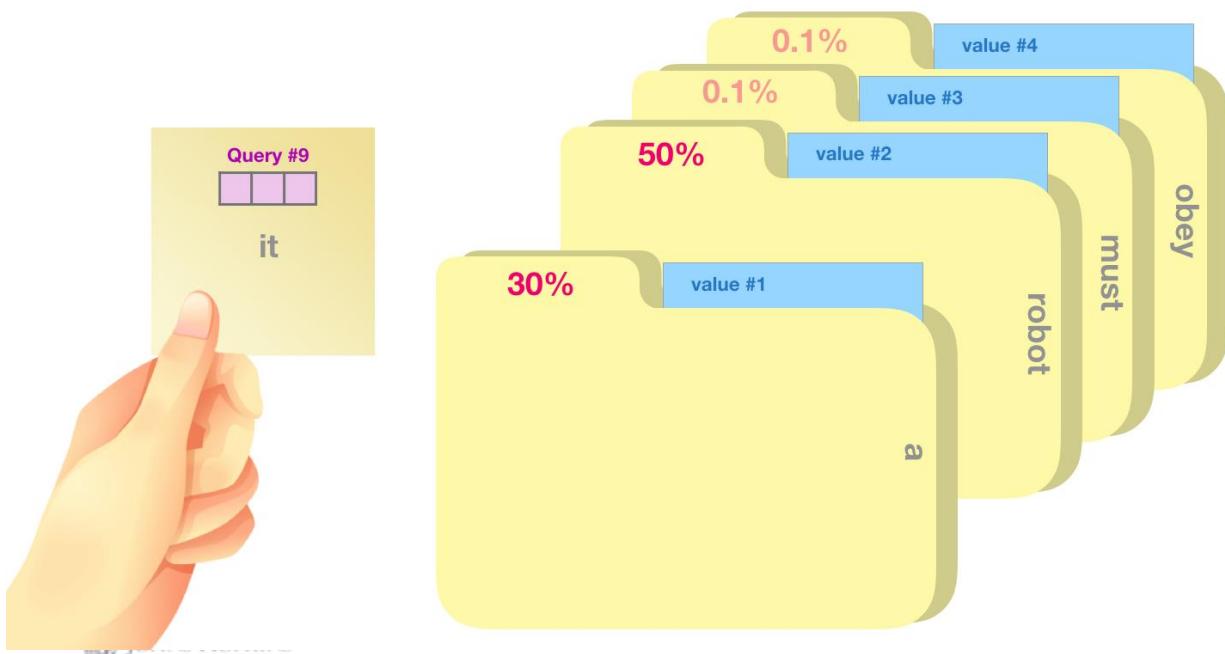
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q : query (to match others)
 $q_i = W^q x_i$

k : key (to be matched)
 $k_i = W^k x_i$

v : value (information to be extracted)
 $v_i = W^v x_i$



q : query (to match others)

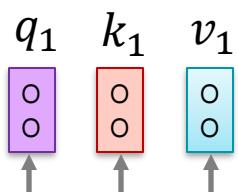
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$$v_i = W^v x_i$$



x_1

The

q: query (to match others)

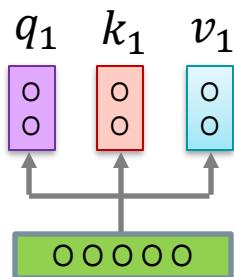
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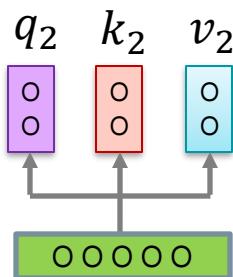
v: value (information to be extracted)

$$v_i = W^v x_i$$



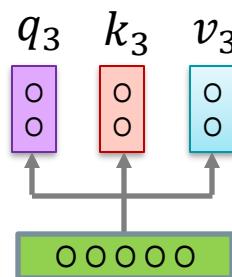
x_1

The



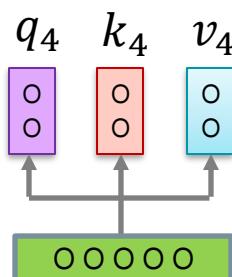
x_2

cat



x_3

sat



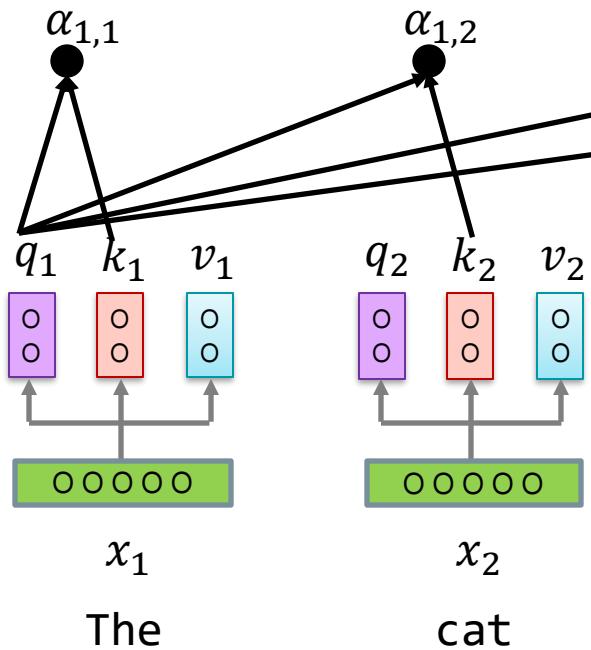
x_4

on

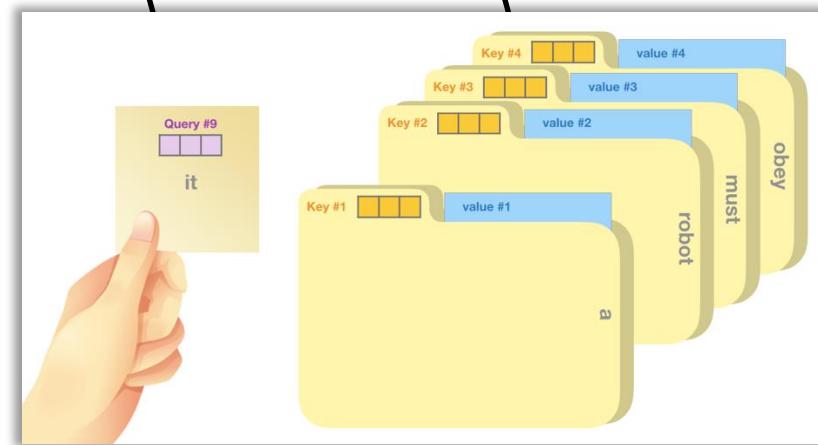
$$\alpha_{1,i} = \frac{q^1 \cdot k^i}{\sqrt{d}}$$

Scaled dot product

How much
should "The"
attend to other
positions?

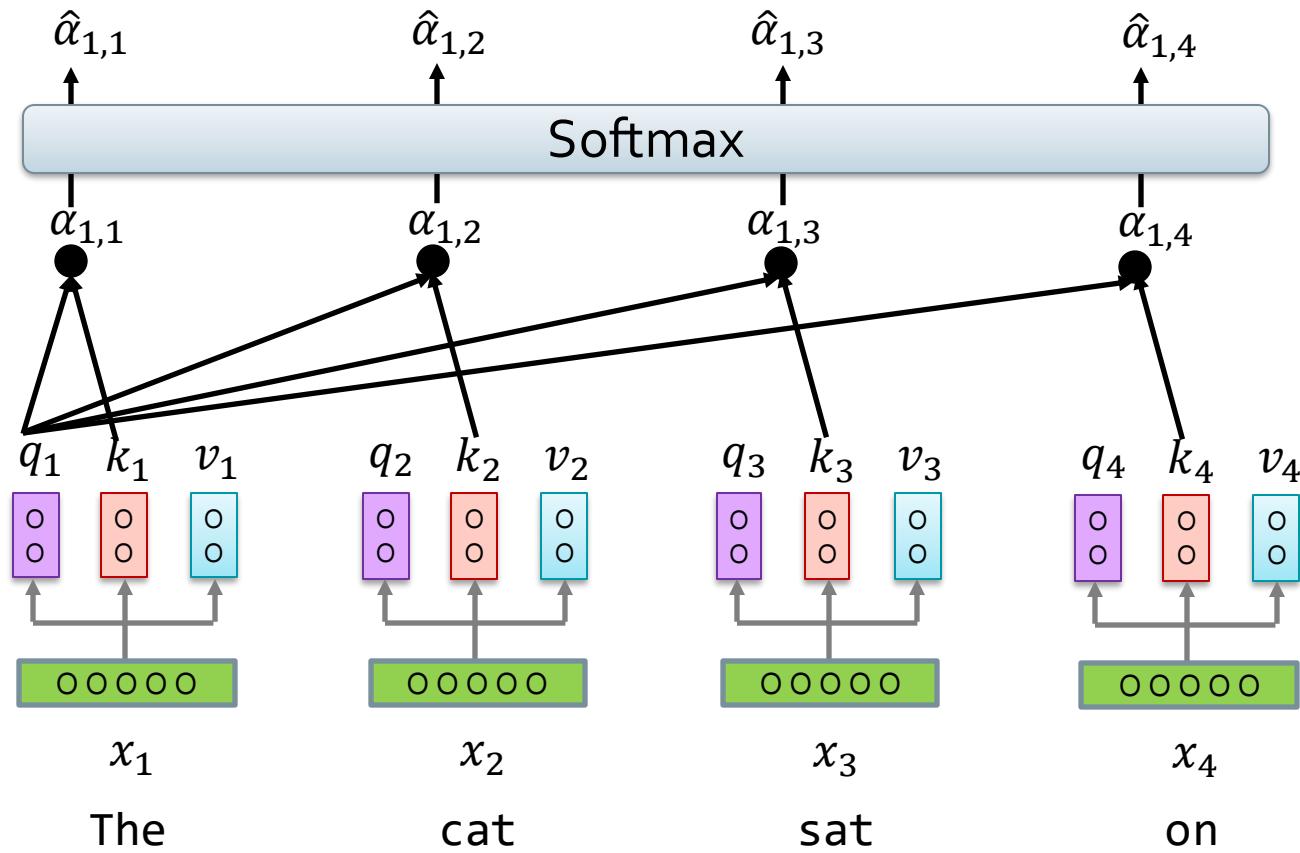


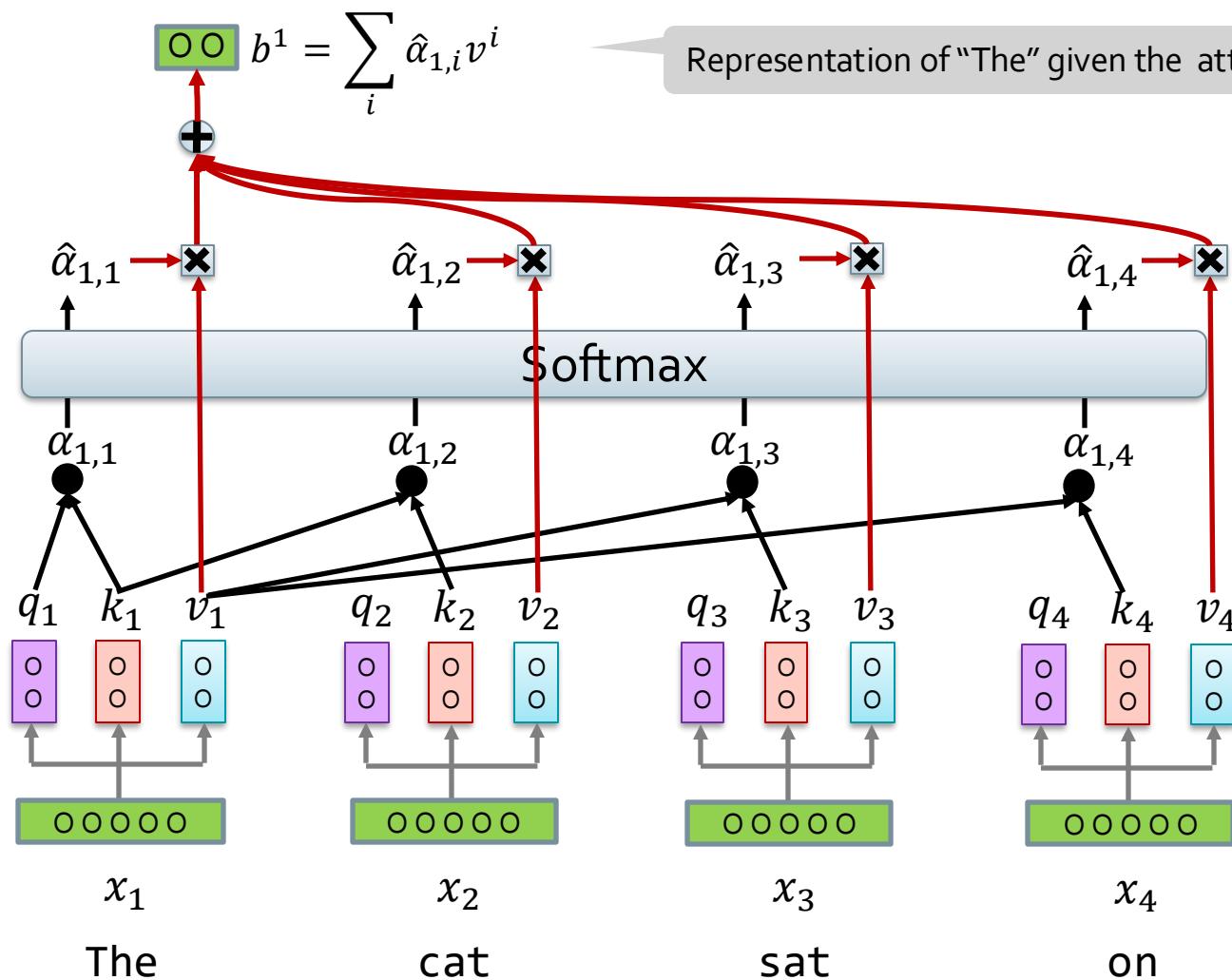
q: query (to match others)
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v: value (information to be extracted)



$$\sigma(z)_i = \frac{\exp(z_i)}{\sum_j \exp(z_j)}$$

How much
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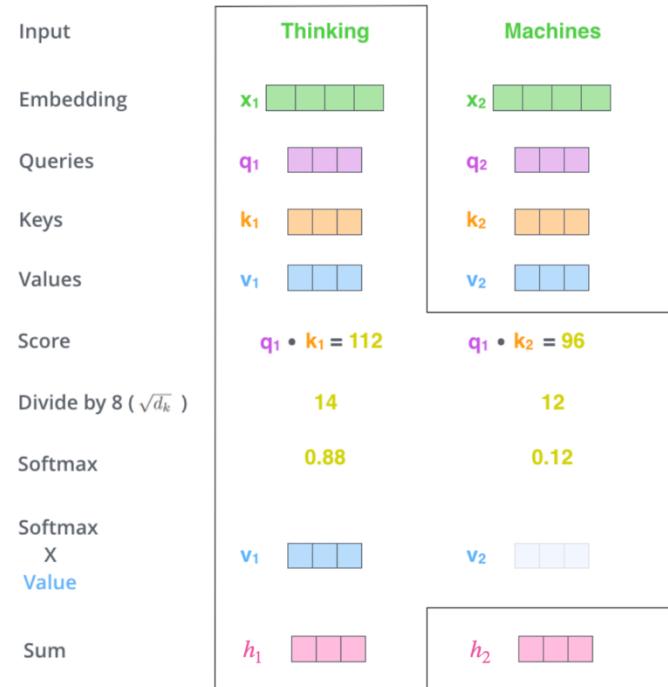




Question

- What would be the output vector for the word “Thinking”?

- (a) $0.5\mathbf{v}_1 + 0.5\mathbf{v}_2$
- (b) $0.54\mathbf{v}_1 + 0.46\mathbf{v}_2$
- (c) $0.88\mathbf{v}_1 + 0.12\mathbf{v}_2$
- (d) $0.12\mathbf{v}_1 + 0.88\mathbf{v}_2$



Self-Attention: Matrix Notation

- Input sequence: $\mathbf{x} = [x_1, x_2, \dots, x_n] \in \mathbb{R}^{n \times d}$

- Calculate:

$$\mathbf{Q} = \mathbf{x}\mathbf{W}^q \in \mathbb{R}^{n \times h}$$

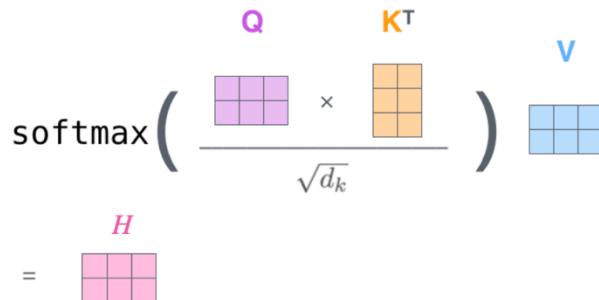
$$\mathbf{K} = \mathbf{x}\mathbf{W}^k \in \mathbb{R}^{n \times h}$$

$$\mathbf{V} = \mathbf{x}\mathbf{W}^v \in \mathbb{R}^{n \times h}$$

- Pairwise similarity matrix between queries and keys: $\mathbf{Q}\mathbf{K}^T \in \mathbb{R}^{n \times n}$
- Attention output:

$$\text{Attention}(\mathbf{x}) = \text{softmax}\left(\frac{\mathbf{Q}\mathbf{K}^T}{\sqrt{d}}\right)\mathbf{V} \in \mathbb{R}^{n \times d}$$

Attention raw scores												
0	-0.08	1.24	0.69	-0.98	1.43	-0.6	0.7	0.16	0.93	1.28	-1.61	-1.1
1	-0.09	-0.0	-0.7	0.06	0.25	0.23	0.26	0.18	0.78	-0.21	-1.01	1.01
2	0.86	1.19	1.59	0.86	-0.13	-0.15	-2.13	-0.98	-0.87	-1.72	1.87	-0.72
3	0.12	-0.03	-0.02	0.88	-0.46	-0.7	0.54	-0.42	-1.89	-0.38	0.04	-0.84
4	0.51	0.17	0.13	-1.64	0.24	-0.02	1.68	-0.36	0.64	0.36	0.27	0.66
5	0.24	-1.44	0.43	0.74	0.96	-1.21	-0.31	1.54	1.66	1.14	0.58	-1.44
6	0.26	-0.1	0.93	0.72	-0.38	1.65	0.47	-0.96	-0.17	-0.9	-1.57	0.22
7	-0.55	0.81	0.71	1.7	-0.8	-1.14	-0.32	1.78	-0.7	-0.04	1.54	0.81
8	0.74	-0.76	-0.44	-0.08	-1.38	-0.13	1.25	-1.37	1.84	0.3	0.57	0.74
9	-0.97	-0.91	0.15	0.35	-0.81	0.11	1.14	-1.52	1.06	1.87	0.5	-0.3
10	1.56	0.9	0.39	1.46	1.44	-1.05	0.9	-0.73	0.36	-0.67	-0.62	-0.43
11	0.32	0.74	0.44	-0.1	1.19	0.83	0.29	2.06	0.51	-0.26	1.51	0.11



Self-Attention: Matrix Notation

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- Calculate:

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- Pairwise similarity matrix between queries and keys: $\mathbf{Q}\mathbf{K}^T \in \mathbb{R}^{n \times n}$
- Attention output:

$$\text{Attention}(\mathbf{x}) = \text{softmax}\left(\frac{\mathbf{Q}\mathbf{K}^T}{\sqrt{d}}\right)\mathbf{V} \in \mathbb{R}^{n \times d}$$

hardmaru
@hardmaru

The most important formula in deep learning after 2018

Self-Attention

What is self-attention? Self-attention calculates a weighted average of feature representations with the weight proportional to a similarity score between pairs of representations. Formally, an input sequence of n tokens of dimensions d , $X \in \mathbb{R}^{n \times d}$, is projected using three matrices $W_Q \in \mathbb{R}^{d \times d_q}$, $W_K \in \mathbb{R}^{d \times d_k}$, and $W_V \in \mathbb{R}^{d \times d_v}$ to extract feature representations Q , K , and V , referred to as query, key, and value respectively with $d_k = d_q$. The outputs Q , K , V are computed as

$$Q = XW_Q, \quad K = XW_K, \quad V = XW_V. \quad (1)$$

So, self-attention can be written as,

$$S = D(Q, K, V) = \text{softmax}\left(\frac{QK^T}{\sqrt{d_q}}\right)V, \quad (2)$$

where softmax denotes a *row-wise* softmax normalization function. Thus, each element in S depends on all other elements in the same row.

9:08 PM - Feb 9, 2021 - Twitter Web App

553 Retweets 42 Quote Tweets 3,338 Likes

Self-Attention: Thinking about batching

- Suppose our data comes in batches of size b , i.e., $\mathbf{x} \in \mathbb{R}^{b \times n \times d}$
- Self-attention's matrix form extends to this batched data. Let's verify:
- Calculate the keys, queries and values, per-batch:

$$\mathbf{Q} = \mathbf{x} \mathbf{W}^q \in \mathbb{R}^{b \times n \times h}$$

$$\mathbf{K} = \mathbf{x} \mathbf{W}^k \in \mathbb{R}^{b \times n \times h}$$

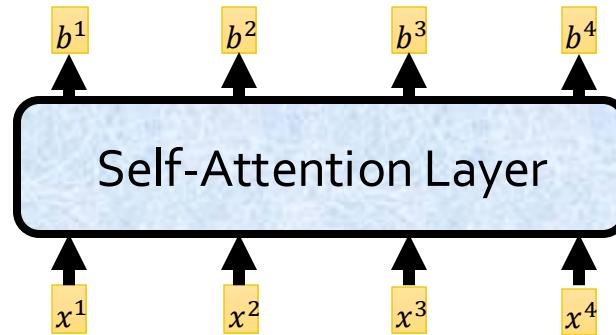
$$\mathbf{V} = \mathbf{x} \mathbf{W}^v \in \mathbb{R}^{b \times n \times h}$$

- Pairwise similarity matrix between queries and keys, per batch: $\mathbf{Q} \mathbf{K}^T \in \mathbb{R}^{b \times n \times n}$
- Attention output for the whole batched data:

$$\text{Attention}(\mathbf{x}) = \text{softmax}\left(\frac{\mathbf{Q} \mathbf{K}^T}{\sqrt{d}}\right) \mathbf{V} \in \mathbb{R}^{b \times n \times d}$$

Self-Attention: Back to Big Picture

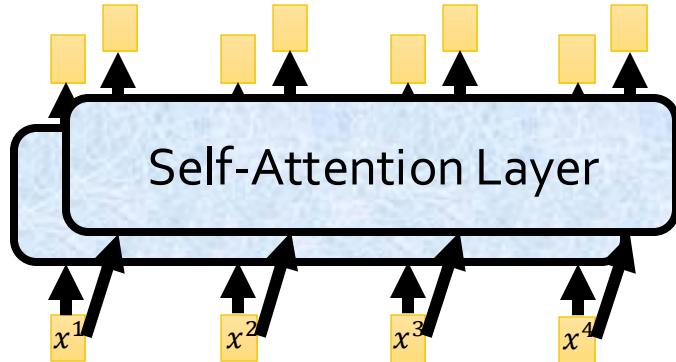
- **Attention** is a powerful mechanism to create context-aware representations
- A way to focus on select parts of the input



- Better at maintaining **long-distance dependencies** in the context.

Multi-Headed Self-Attention

- Multiple parallel attention layers.
 - Each attention layer has its own parameters.
 - Concatenate the results and run them through a linear projection.
- **Main idea:** Allows model to jointly attend to information from different representation subspaces (like ensembling).

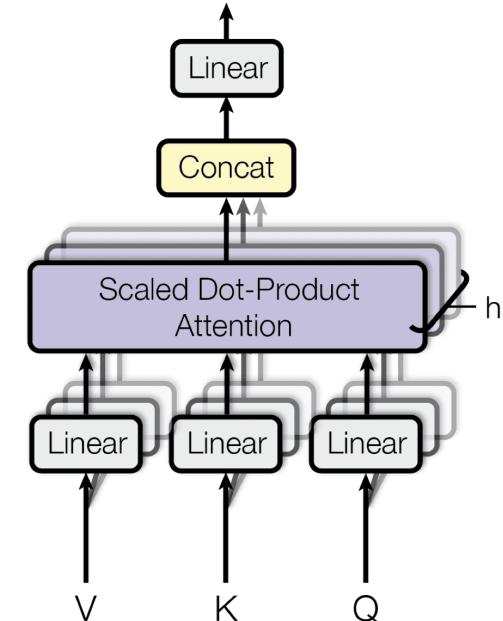


Multi-Headed Self-Attention

- Just concatenate all the heads and apply an output projection.

$$\text{head}_i = \text{Attention}(\mathbf{x}W_i^q, \mathbf{x}W_i^k, \mathbf{x}W_i^v)$$
$$\text{MultiHeadedAttention}(\mathbf{x}) = \text{Concat}(\text{head}_1, \dots, \text{head}_h)W^o$$

- Previously, we used the following dimensions for **single**-head SA:
 $\mathbf{W}_i^q \in \mathbb{R}^{d \times d}, \quad \mathbf{W}_i^k \in \mathbb{R}^{d \times d}, \quad \mathbf{W}_i^v \in \mathbb{R}^{d \times d},$
- In practice, we use a reduced dimension for each head.
 $\mathbf{W}_i^q \in \mathbb{R}^{d \times \frac{d}{m}}, \quad \mathbf{W}_i^k \in \mathbb{R}^{d \times \frac{d}{m}}, \quad \mathbf{W}_i^v \in \mathbb{R}^{d \times \frac{d}{m}}, \quad \mathbf{W}^o \in \mathbb{R}^{d \times d}$
- The total computational cost is similar to that of single-head attention with full dimensionality.

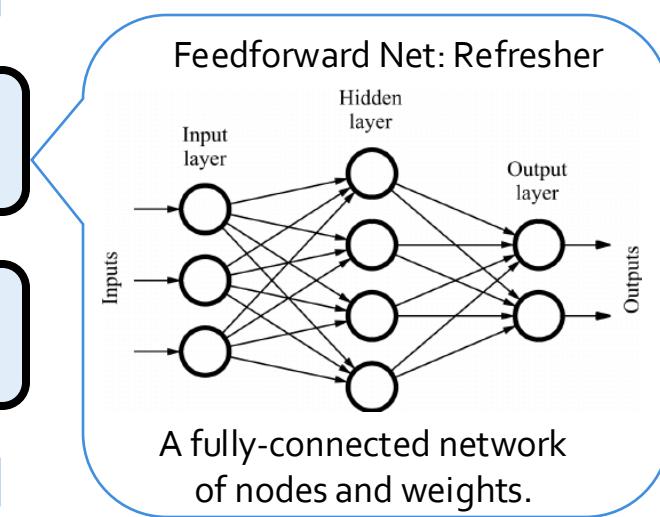
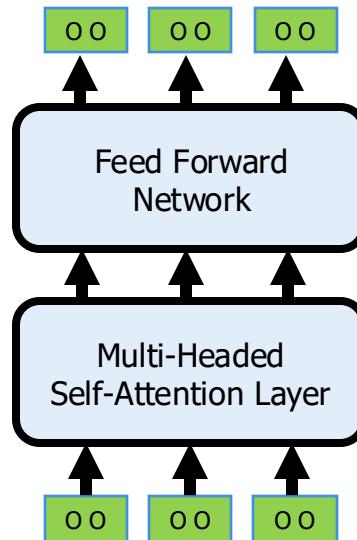


m : number of heads
 d : feature dimension in output of SA

Combine with FFN

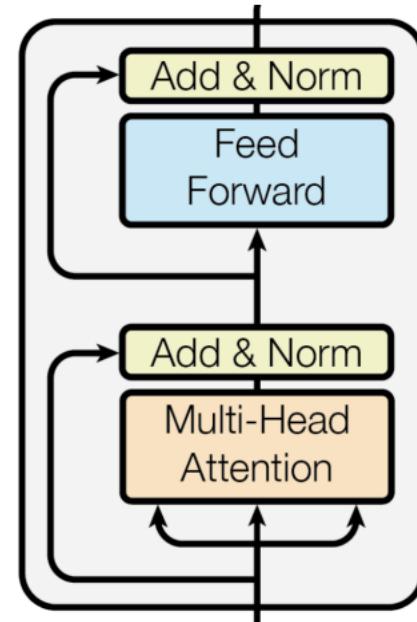
- Add a **feed-forward network** on top it to add more expressivity.
 - This allows the model to apply another transformation to the contextual representations (or “post-process” them).
 - Usually, the dimensionality of the hidden feedforward layer is 2-8 times larger than the input dimension.

$$\text{FFN}(\mathbf{x}) = f(c\mathbf{W}_1 + \mathbf{b}_1)\mathbf{W}_2 + \mathbf{b}_2$$
$$\mathbf{W}_1 \in \mathbb{R}^{d \times d_{ff}}$$
$$\mathbf{W}_2 \in \mathbb{R}^{d_{ff} \times d}$$



How Do We Prevent Vanishing Gradients?

- Residual connections let the model “skip” layers
 - These connections are particularly useful for training deep networks
- Use layer normalization to stabilize the network and allow for proper gradient flow

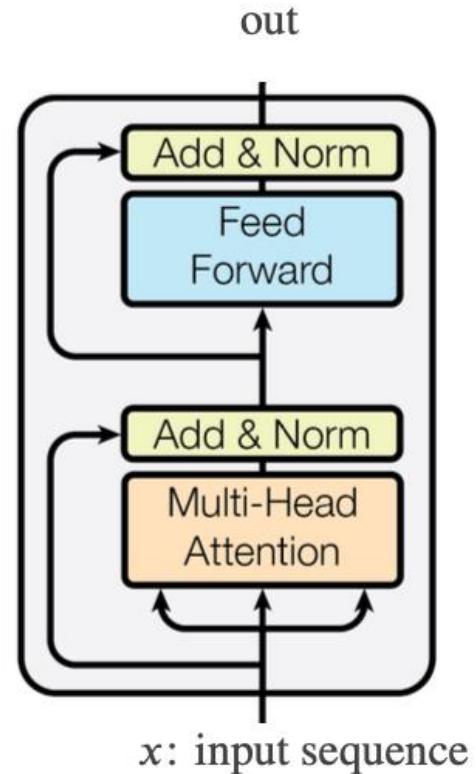


Putting it Together: Self-Attention Block

Given input \mathbf{x} :

$$\begin{aligned}\text{out} &= LN(\tilde{\mathbf{c}} + \mathbf{c}') \\ \tilde{\mathbf{c}} &= \text{FFN}(\mathbf{c}') = f(\mathbf{c}'W_1 + b_1)W_2 + b_2\end{aligned}$$

$$\begin{aligned}\mathbf{c}' &= LN(\mathbf{c} + \mathbf{x}) \\ \mathbf{c} &= \text{MultiHeadedAttention}(\mathbf{x}; \mathbf{W}^q, \mathbf{W}^k, \mathbf{W}^v)\end{aligned}$$



Summary: Self-Attention Block

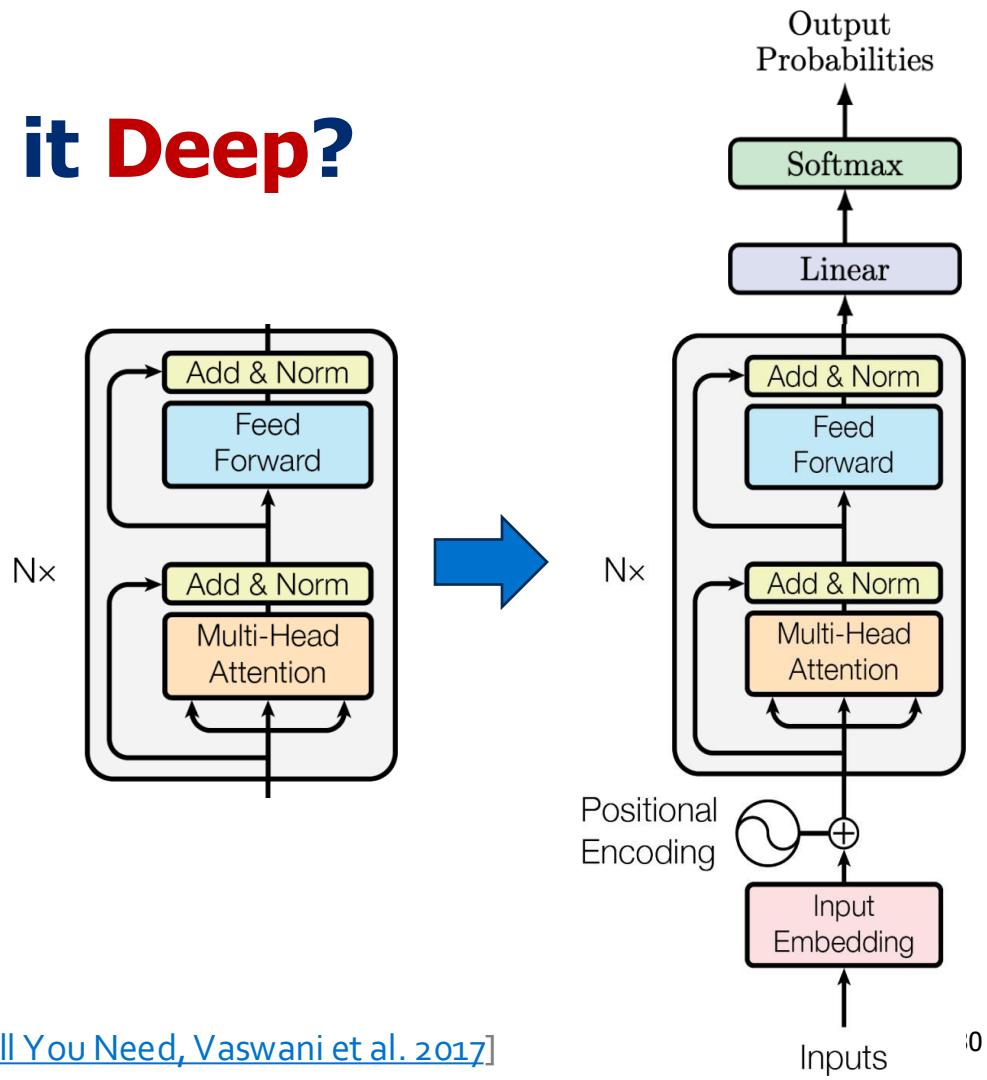
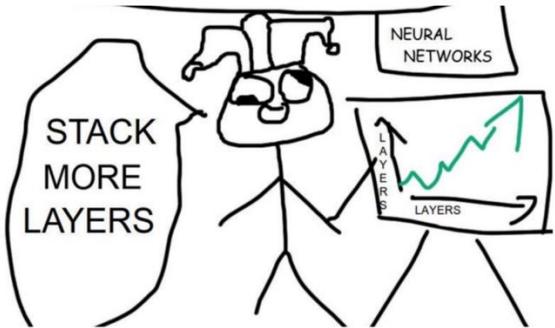
- **Self-Attention:** A critical building block of modern language models.
 - The idea is to compose meanings of words weighted according some similarity notion.
- **Next:** We will combine self-attention blocks to build various architectures known as Transformer.



A Decoder-Only Transformer

How Do We Make it Deep?

- Stack more layers!



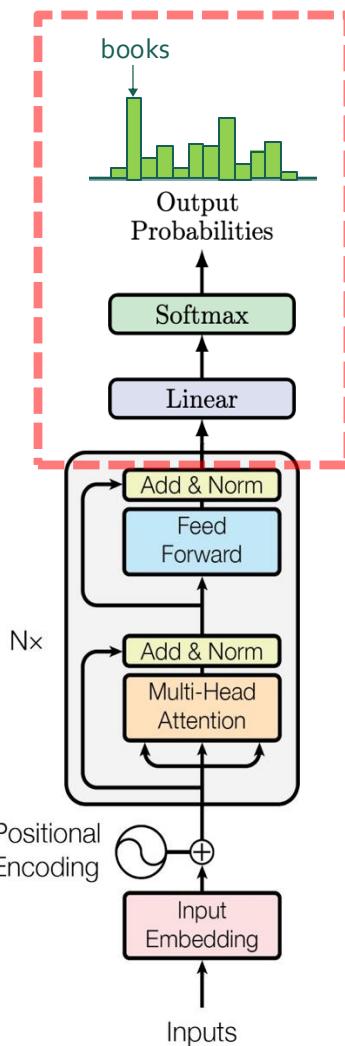
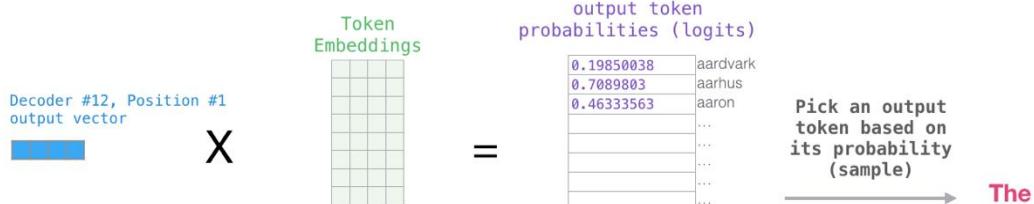
From Representations to Prediction

- To perform prediction, add a classification head on top of the final layer of the transformer.
- This can be per token (Language modeling)
- Or can be for the entire sequence (only one token)

$\text{out} \in \mathbb{R}^{S \times d}$ (S : Sequence length)

$\text{logits} = \text{Linear}_{(d, V)}(\text{out}) = f(\text{out} \cdot W_V) \in \mathbb{R}^{S \times V}$

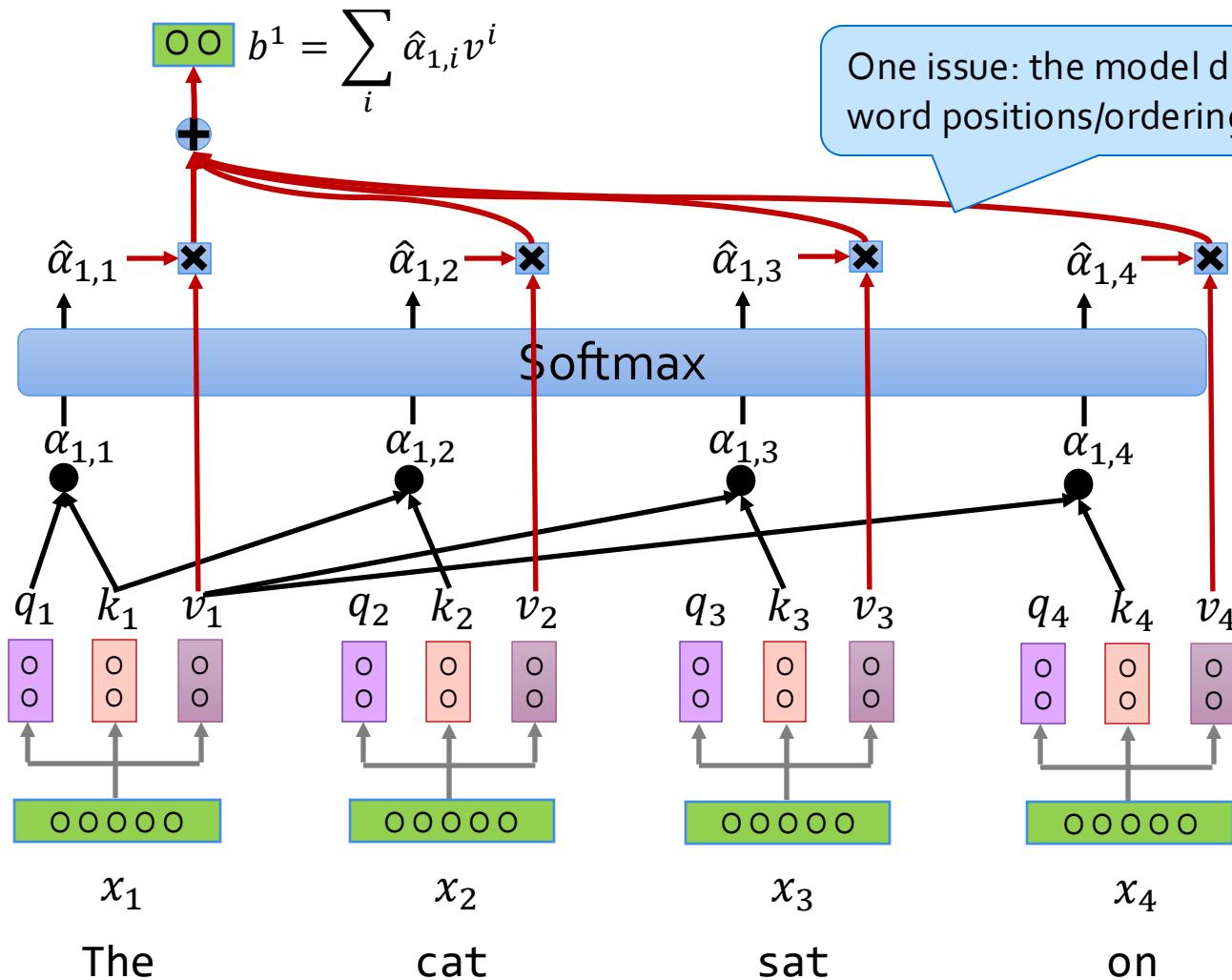
$\text{probabilities} = \text{softmax}(\text{logits}) \in \mathbb{R}^{S \times V}$





One last wrinkle though ...

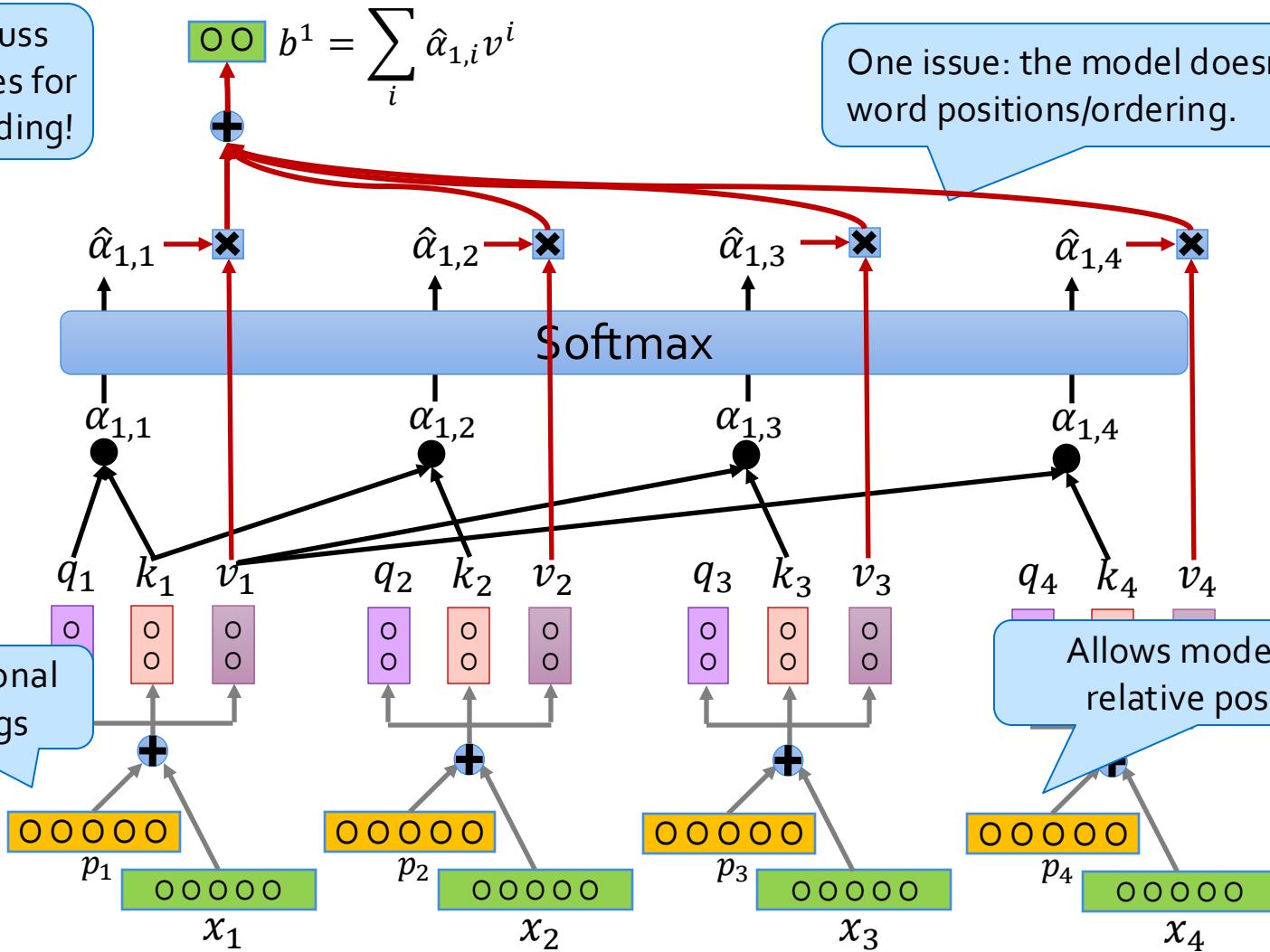




We will discuss various choices for these embedding!

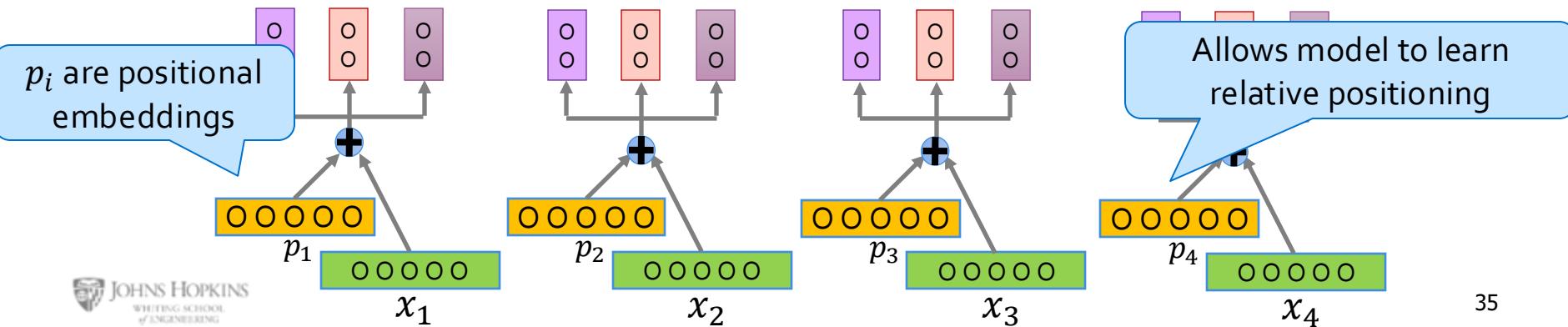
$$OO = b^1 + \sum_i \hat{\alpha}_{1,i} v^i$$

One issue: the model doesn't know word positions/ordering.



Absolute Positional Embeddings

- Why “add”? Why not, say, “concatenate and then project”?
 - “concatenate and then project” would be a more general approach with more trainable parameters.
 - In practice, “sum” works fine that
 - The intuition here is that “summing” forms point clouds of word embedding information around position embeddings unique to each position.



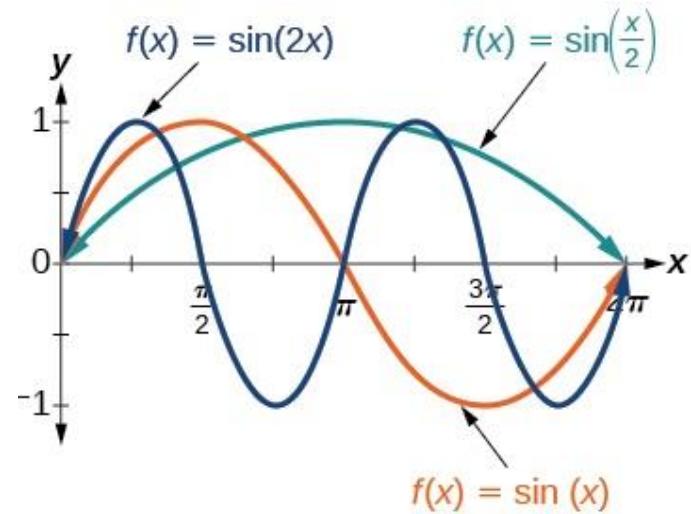
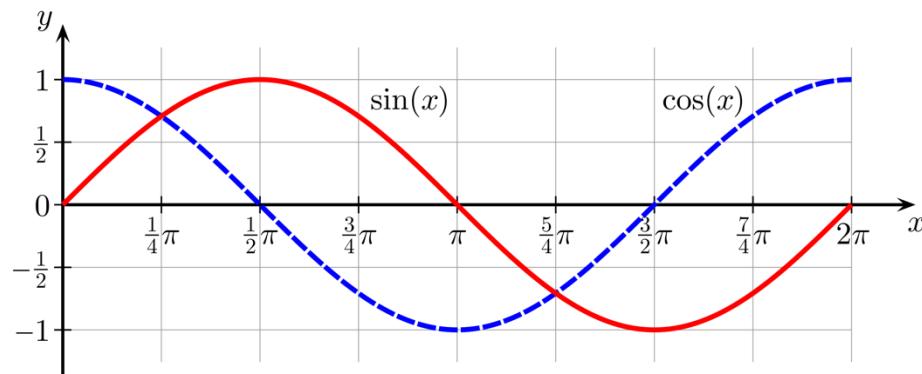
Absolute Positional Embeddings

- The idea is to create vectors that uniquely encoder each position.
- For example, consider vectors of binary values.
 - Example below shows 4-dimensional position encodings for 16 positions.

0 :	0	0	0	0	8 :	1	0	0	0
1 :	0	0	0	1	9 :	1	0	0	1
2 :	0	0	1	0	10 :	1	0	1	0
3 :	0	0	1	1	11 :	1	0	1	1
4 :	0	1	0	0	12 :	1	1	0	0
5 :	0	1	0	1	13 :	1	1	0	1
6 :	0	1	1	0	14 :	1	1	1	0
7 :	0	1	1	1	15 :	1	1	1	1

The issue with binary encoding is that the positional information is localized around a few bits.

Math Recap: Sine and Cosine Functions



Absolute Positional Embeddings

- Let t be a desired position. Then the i -th element of the positional vector is:

$$\vec{p}_t^{(i)} = f(t)^{(i)} := \begin{cases} \sin(\omega_k \cdot t), & \text{if } i = 2k \\ \cos(\omega_k \cdot t), & \text{if } i = 2k + 1 \end{cases} \quad \omega_k = \frac{1}{10000^{2k/d}}$$

- Here d is the maximum dimension.
- This provides unique vectors for each position.

Quiz

- Let t be a desired position:

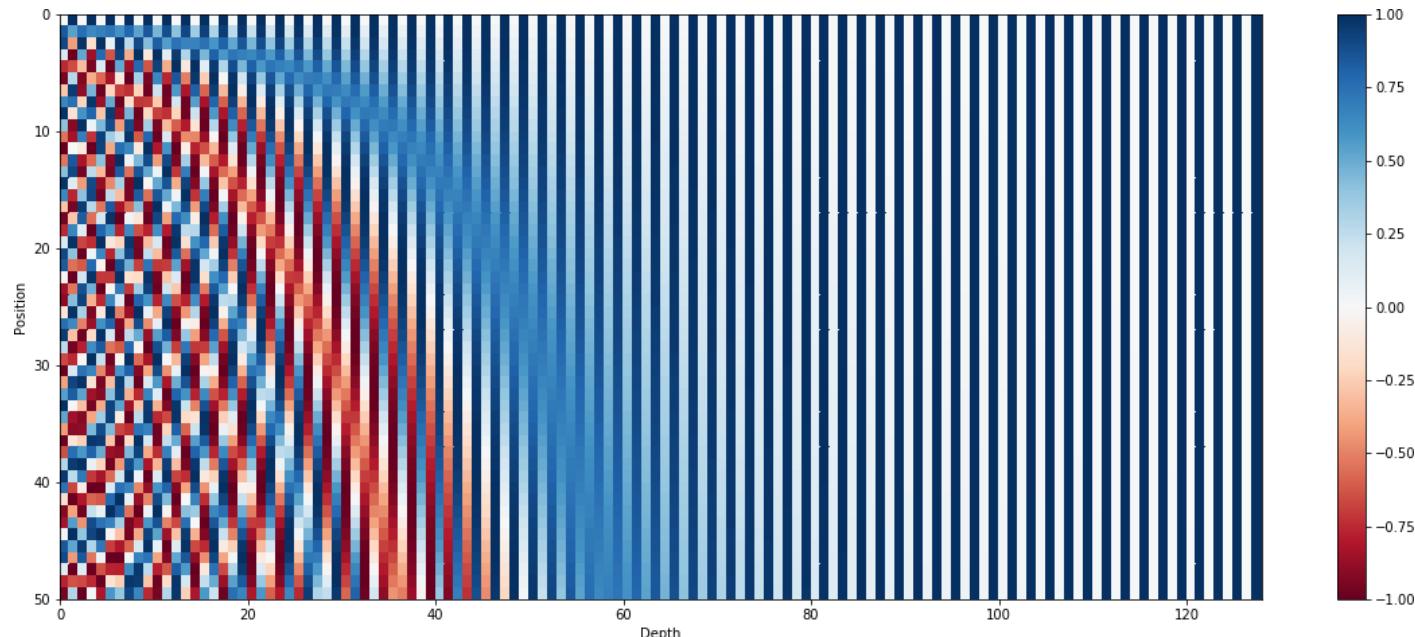
$$\vec{p}_t^{(i)} = f(t)^{(i)} := \begin{cases} \sin(\omega_k \cdot t), & \text{if } i = 2k \\ \cos(\omega_k \cdot t), & \text{if } i = 2k + 1 \end{cases}$$

$$\omega_k = \frac{1}{10000^{2k/d}}$$

- Q:** Are the frequencies increasing with dimension i ?
- Answer:** The frequencies are decreasing along the vector dimension.

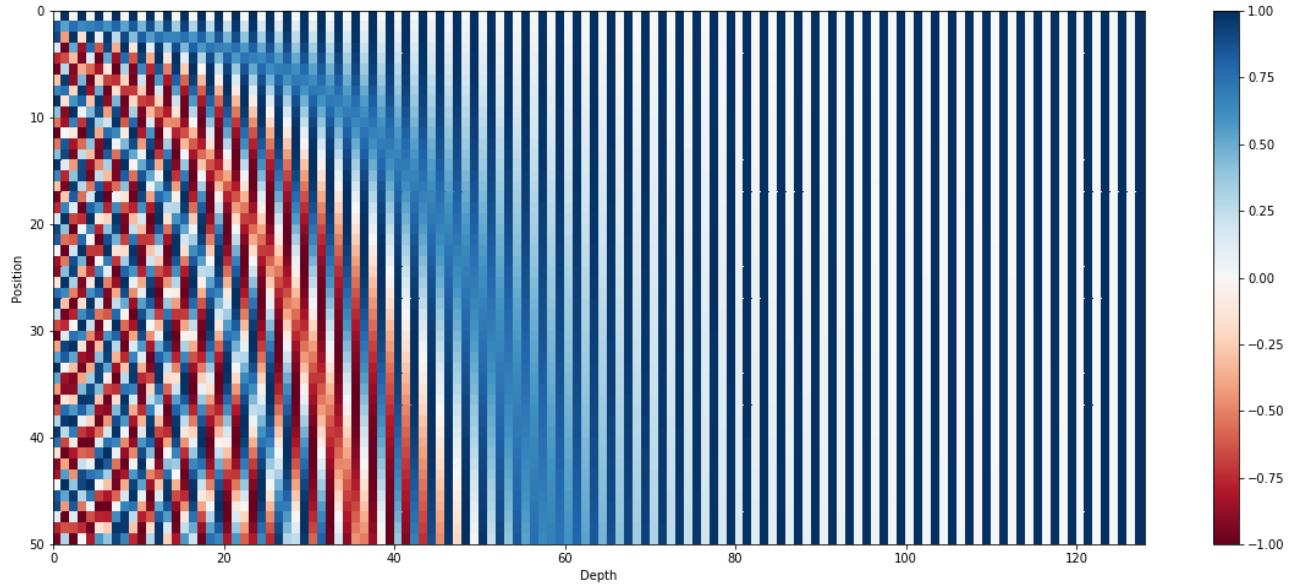
Visualizing Absolute Positional Embeddings

- Here positions range from 0-50, for an embedding dimension of 130.

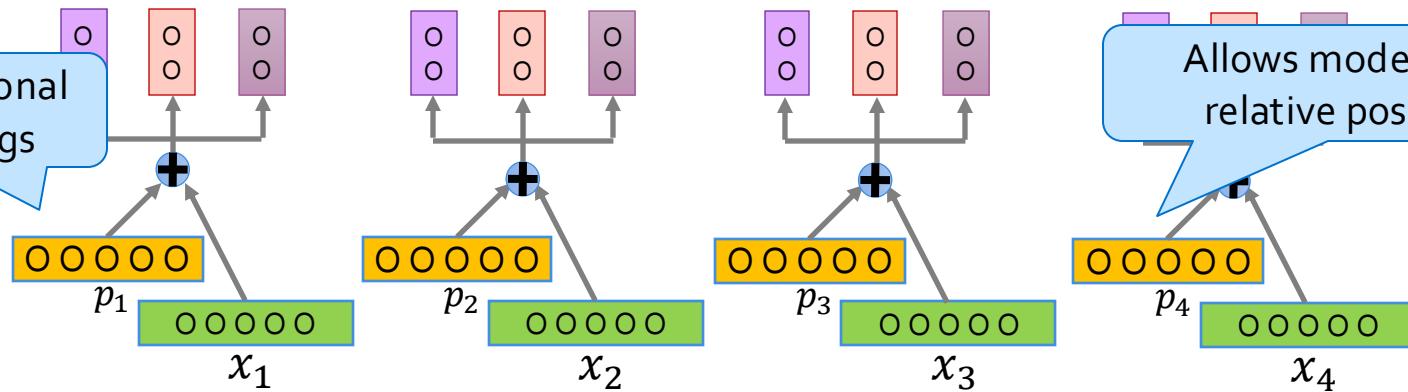


An approach:
Sine/Cosine encoding

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



p_i are positional embeddings



Recap—positional encoding

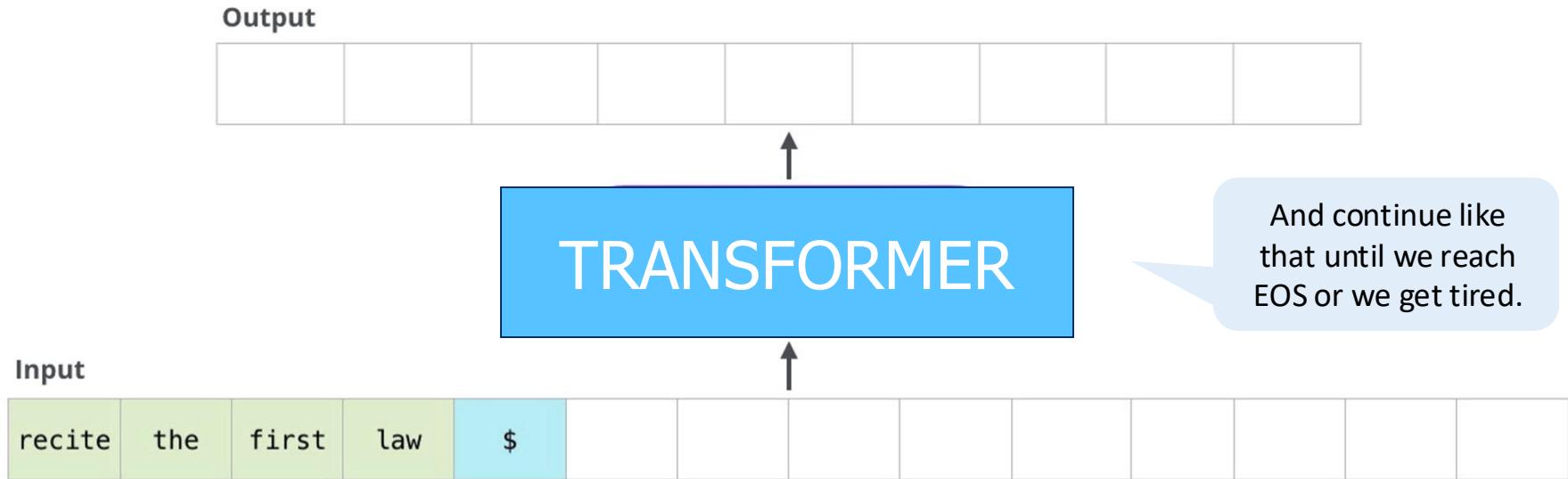
- TODO



How does inference work?



Transformer-based Language Modeling





How does training work?



Quiz

- What do we optimize in the attention layer during training?
 1. X and q
 2. W_k and W_V
 3. Softmax function
 4. Sine/cos positional encodings
 5. The embedding matrix

Answer: 2 and 5.

Training a Transformer Language Model

- **Goal:** Train a Transformer for language modeling (i.e., predicting the next word).
- **Approach:** Train it so that each position is predictor of the next (right) token.
 - We just shift the input to right by one, and use as labels

(gold output) $Y = \text{cat sat on the mat } </s>$

EOS special token



TRANSFORMER

$X = \text{the cat sat on the mat}$

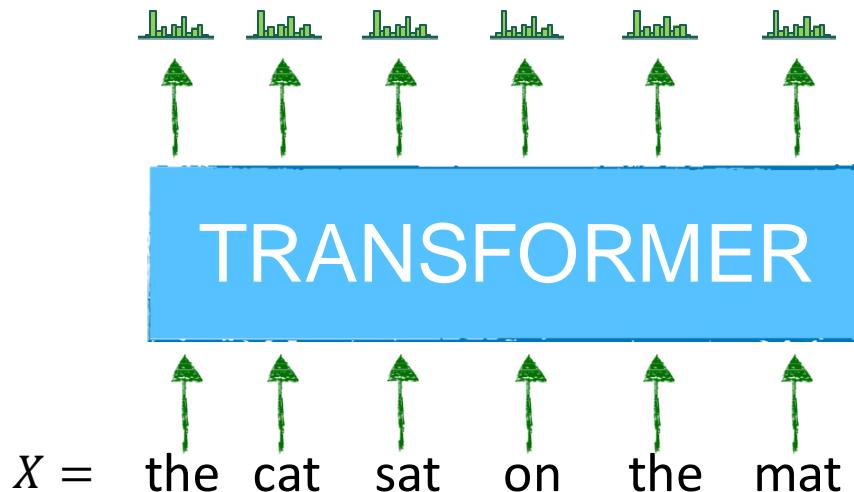
```
X = text[:, :-1]  
Y = text[:, 1:]
```

[Slide credit: Arman Cohan]

Training a Transformer Language Model

- For each position, compute their corresponding **distribution** over the whole vocab.

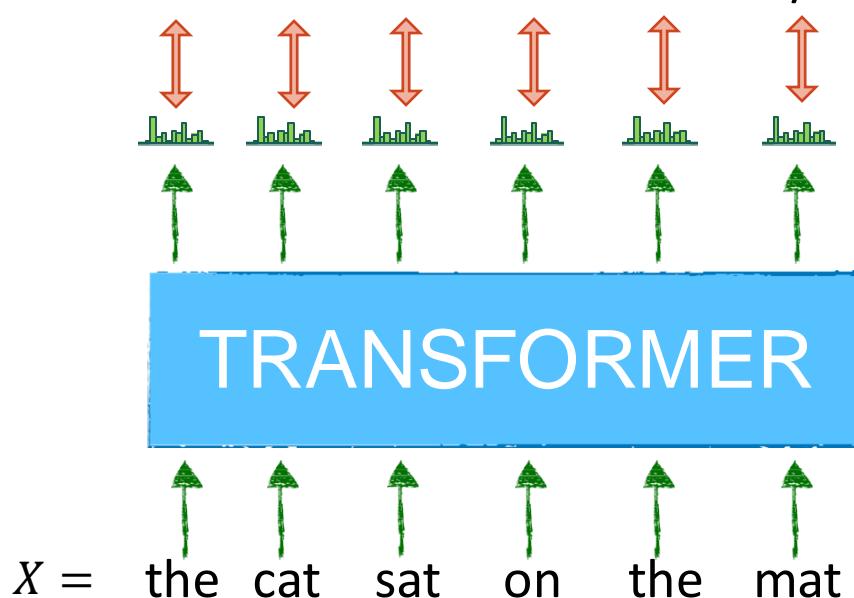
(gold output) $Y = \text{cat sat on the mat } </s>$



Training a Transformer Language Model

- For each position, compute the **loss** between the distribution and the gold output label.

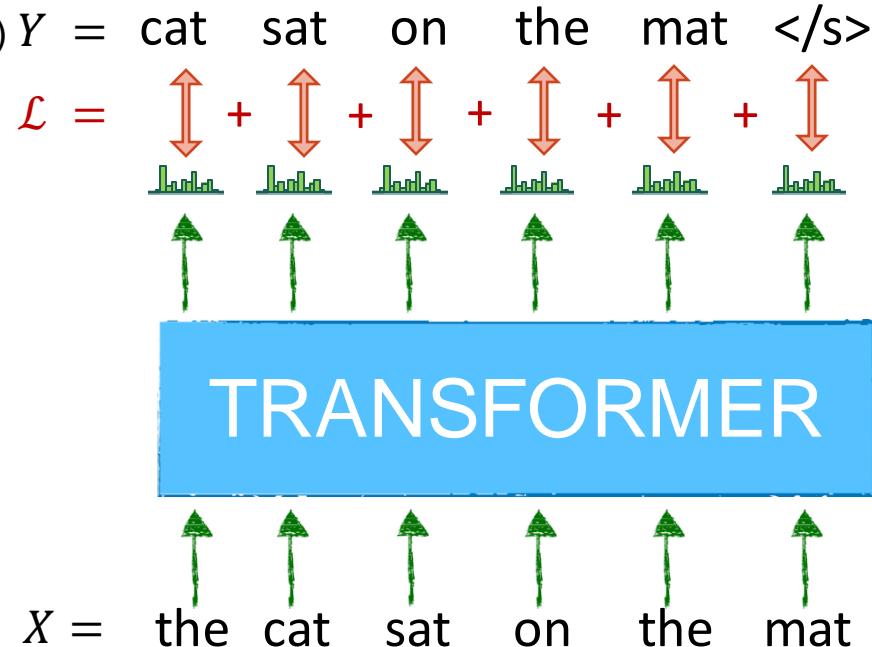
(gold output) $Y = \text{cat sat on the mat } </s>$



Training a Transformer Language Model

- Sum the position-wise loss values to obtain a **global loss**.

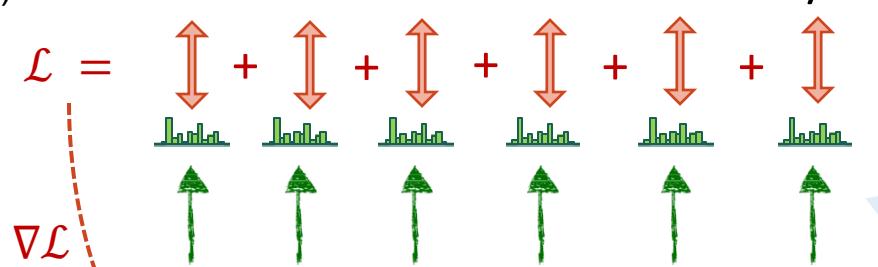
(gold output) $Y = \text{cat sat on the mat } </s>$



Training a Transformer Language Model

- Using this loss, do **Backprop** and **update** the Transformer parameters.

(gold output) $Y = \text{cat sat on the mat } </s>$

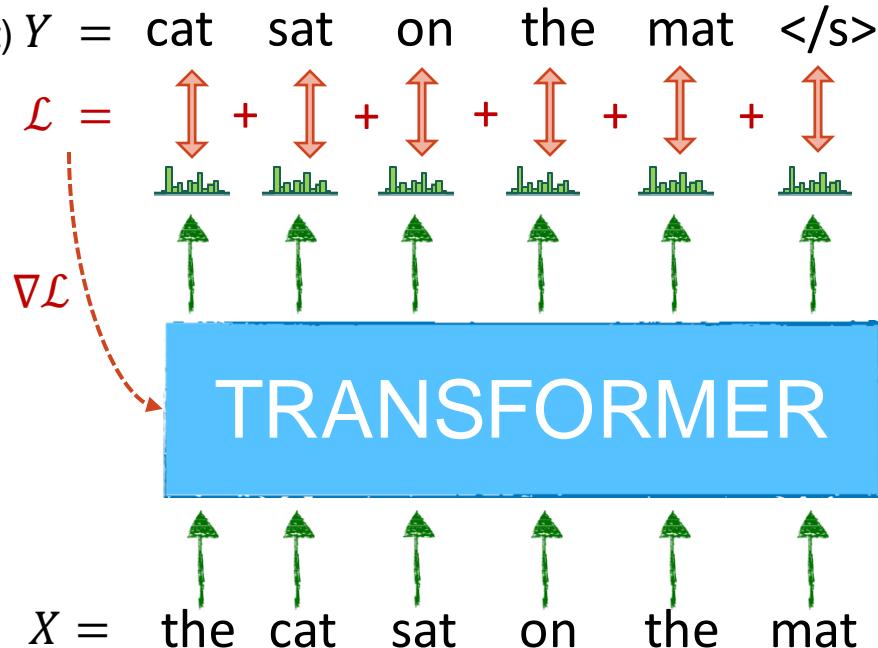


Well, this is not quite right 😊
...
what is the problem with this?

Training a Transformer Language Model

- The model would solve the task by **copying** the next token to output (data leakage).
 - Does **not** learn anything useful

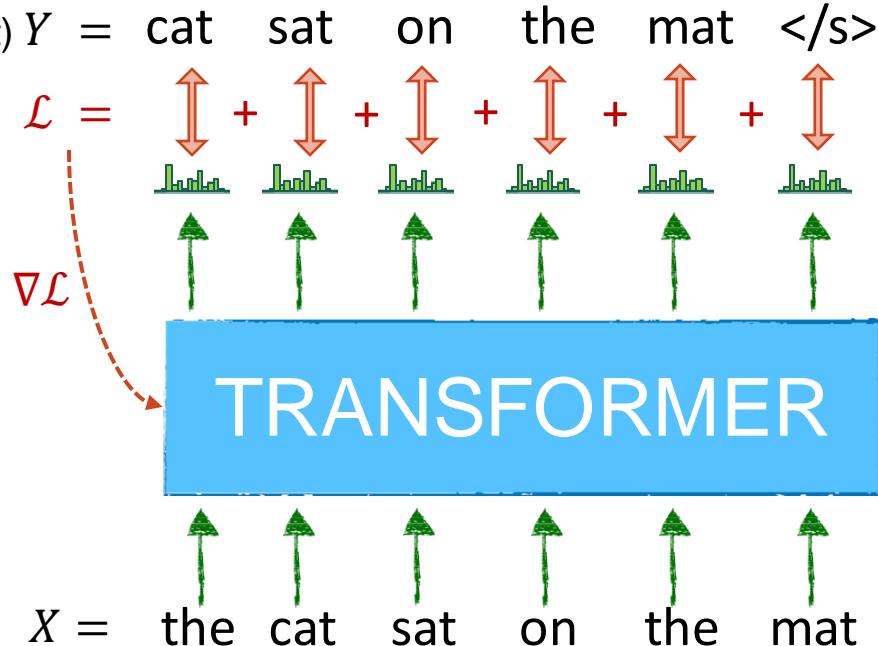
(gold output) $Y = \text{cat sat on the mat } </s>$



Training a Transformer Language Model

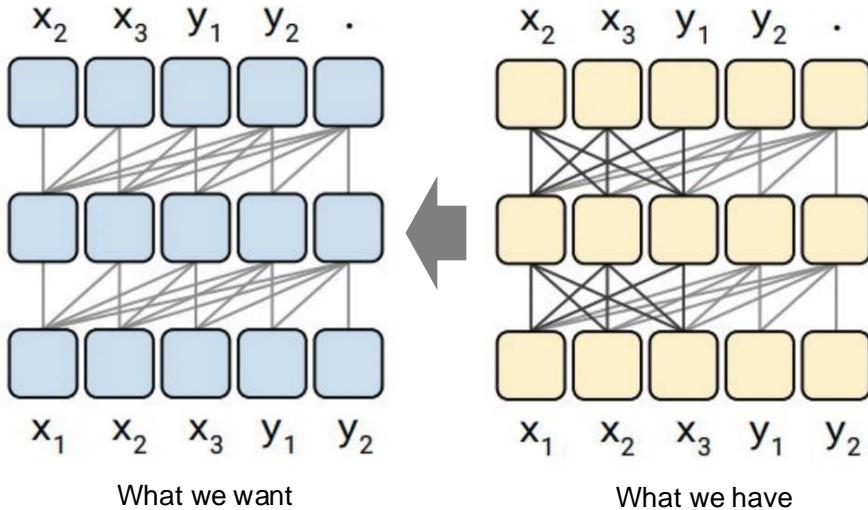
- We need to **prevent information leakage** from future tokens! How?

(gold output) $Y = \text{cat sat on the mat } </s>$

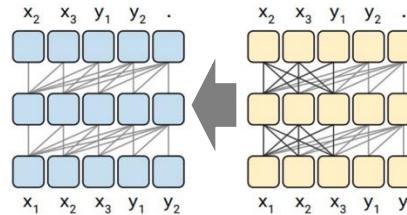


Attention mask

Attention raw scores												
0	-0.08	1.24	0.69	-0.98	1.43	-0.6	0.7	0.16	0.93	1.28	-1.61	-1.1
1	-0.09	-0.0	-0.7	0.06	0.25	0.23	0.26	0.18	0.78	-0.21	-1.01	1.01
2	0.86	1.19	1.59	0.86	-0.13	-0.15	-2.13	-0.98	-0.87	-1.72	1.87	-0.72
3	0.12	-0.03	-0.02	0.88	-0.46	-0.7	0.54	-0.42	-1.89	-0.38	0.04	-0.84
4	0.51	0.17	0.13	-1.64	0.24	-0.02	1.68	-0.36	0.64	0.36	0.27	0.66
5	0.24	-1.44	0.43	0.74	0.96	-1.21	-0.31	1.54	1.66	1.14	0.58	-1.44
6	0.26	-0.1	0.93	0.72	-0.38	1.65	0.47	-0.96	-0.17	-0.9	-1.57	0.22
7	-0.55	0.81	0.71	1.7	-0.8	-1.14	-0.32	1.78	-0.7	-0.04	1.54	0.81
8	0.74	-0.76	-0.44	-0.08	-1.38	-0.13	1.25	-1.37	1.84	0.3	0.57	0.74
9	-0.97	-0.91	0.15	0.35	-0.81	0.11	1.14	-1.52	1.06	1.87	0.5	-0.3
10	1.56	0.9	0.39	1.46	1.44	-1.05	0.9	-0.73	0.36	-0.67	-0.62	-0.43
11	0.32	0.74	0.44	-0.1	1.19	0.83	0.29	2.06	0.51	-0.26	1.51	0.11



Attention mask

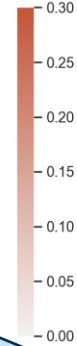


Attention raw scores

	1	2	3	4	5	6	7	8	9	10	11	12
0	-0.08	1.24	0.69	-0.98	1.43	-0.6	0.7	0.16	0.93	1.28	-1.61	-1.1
1	-0.09	-0.0	-0.7	0.06	0.25	0.23	0.26	0.18	0.78	-0.21	-1.01	1.01
2	0.86	1.19	1.59	0.86	-0.13	-0.15	-2.13	-0.98	-0.87	-1.72	1.87	-0.72
3	0.12	-0.03	-0.02	0.88	-0.46	-0.7	0.54	-0.42	-1.89	-0.38	0.04	-0.84
4	0.51	0.17	0.13	-1.64	0.24	-0.02	1.68	-0.36	0.64	0.36	0.27	0.66
5	0.24	-1.44	0.43	0.74	0.96	-1.21	-0.31	1.54	1.66	1.14	0.58	-1.44
6	0.26	-0.1	0.93	0.72	-0.38	1.65	0.47	-0.96	-0.17	-0.9	-1.57	0.22
7	-0.55	0.81	0.71	1.7	-0.8	-1.14	-0.32	1.78	-0.7	-0.04	1.54	0.81
8	0.74	-0.76	-0.44	-0.08	-1.38	-0.13	1.25	-1.37	1.84	0.3	0.57	0.74
9	-0.97	-0.91	0.15	0.35	-0.81	0.11	1.14	-1.52	1.06	1.87	0.5	-0.3
10	1.56	0.9	0.39	1.46	1.44	-1.05	0.9	-0.73	0.36	-0.67	-0.62	-0.43
11	0.32	0.74	0.44	-0.1	1.19	0.83	0.29	2.06	0.51	-0.26	1.51	0.11

Attention mask

	0	1	2	3	4	5	6	7	8	9	10	11
0	1.0	-inf										
1	1.0	1.0	-inf									
2	1.0	1.0	1.0	-inf								
3	1.0	1.0	1.0	1.0	-inf							
4	1.0	1.0	1.0	1.0	1.0	-inf						
5	1.0	1.0	1.0	1.0	1.0	1.0	-inf	-inf	-inf	-inf	-inf	-inf
6	1.0	1.0	1.0	1.0	1.0	1.0	1.0	-inf	-inf	-inf	-inf	-inf
7	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	-inf	-inf	-inf	-inf
8	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	-inf	-inf	-inf
9	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	-inf	-inf
10	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	-inf
11	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	-inf

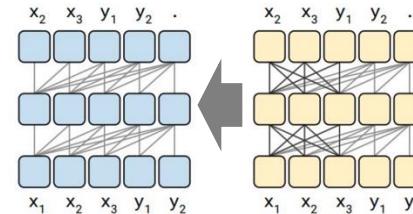


large negative numbers,
which leads to $\text{softmax}(-\infty) \approx 0$

Attention mask

Attention raw scores												
0	-0.08	1.24	0.69	-0.98	1.43	-0.6	0.7	0.16	0.93	1.28	-1.61	-1.1
1	-0.09	-0.0	-0.7	0.06	0.25	0.23	0.26	0.18	0.78	-0.21	-1.01	1.01
2	0.86	1.19	1.59	0.86	-0.13	-0.15	-2.13	-0.98	-0.87	-1.72	1.87	-0.72
3	0.12	-0.03	-0.02	0.88	-0.46	-0.7	0.54	-0.42	-1.89	-0.38	0.04	-0.84
4	0.51	0.17	0.13	-1.64	0.24	-0.02	1.68	-0.36	0.64	0.36	0.27	0.66
5	0.24	-1.44	0.43	0.74	0.96	-1.21	-0.31	1.54	1.66	1.14	0.58	-1.44
6	0.26	-0.1	0.93	0.72	-0.38	1.65	0.47	-0.96	-0.17	-0.9	-1.57	0.22
7	-0.55	0.81	0.71	1.7	-0.8	-1.14	-0.32	1.78	-0.7	-0.04	1.54	0.81
8	0.74	-0.76	-0.44	-0.08	-1.38	-0.13	1.25	-1.37	1.84	0.3	0.57	0.74
9	-0.97	-0.91	0.15	0.35	-0.81	0.11	1.14	-1.52	1.06	1.87	0.5	-0.3
10	1.56	0.9	0.39	1.46	1.44	-1.05	0.9	-0.73	0.36	-0.67	-0.62	-0.43
11	0.32	0.74	0.44	-0.1	1.19	0.83	0.29	2.06	0.51	-0.26	1.51	0.11

X



Attention mask

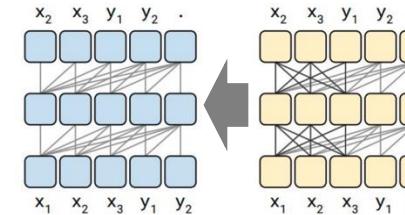
0	1	2	3	4	5	6	7	8	9	10	11
0	1.0	-inf									
1	1.0	1.0	-inf								
2	1.0	1.0	1.0	-inf							
3	1.0	1.0	1.0	1.0	-inf						
4	1.0	1.0	1.0	1.0	1.0	-inf	-inf	-inf	-inf	-inf	-inf
5	1.0	1.0	1.0	1.0	1.0	1.0	-inf	-inf	-inf	-inf	-inf
6	1.0	1.0	1.0	1.0	1.0	1.0	1.0	-inf	-inf	-inf	-inf
7	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	-inf	-inf	-inf
8	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	-inf	-inf
9	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	-inf
10	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	-inf
11	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0



Note matrix multiplication is quite fast in GPUs.

Arman Cohan

Attention mask



Attention raw scores												
0	0.09	1.34	0.69	0.98	3.43	-0.1	0.7	0.16	0.93	1.28	1.81	-1.13
1	-0.09	-0.7	0.06	0.25	0.26	0.18	0.78	-0.21	1.01	1.01	1.01	
2	-0.06	1.19	1.09	0.96	-0.15	0.15	-0.11	-0.06	-0.07	1.73	1.67	-0.72
3	0.12	-0.03	-0.02	0.88	-0.46	0.7	0.54	-0.42	1.86	-0.38	0.54	-0.84
4	0.51	0.17	0.51	0.34	0.24	-0.02	1.68	-0.36	0.84	0.36	0.27	0.66
5	0.24	-1.64	0.43	0.78	0.96	1.1	-0.31	1.54	1.86	1.14	0.58	-1.41
6	0.26	-0.1	0.63	0.72	-0.36	1.84	0.47	0.96	-0.17	-0.5	0.58	0.22
7	0.55	0.91	0.71	1.7	-0.8	1.16	-0.32	1.78	-0.7	-0.54	1.54	0.81
8	0.74	0.76	-0.48	-0.68	-0.38	0.13	0.13	1.25	1.37	1.84	0.3	0.57
9	0.87	0.91	0.15	0.36	-0.81	0.11	1.14	-1.51	1.08	1.87	0.5	-0.37
10	0.52	0.74	0.44	0.71	1.19	0.89	0.29	2.06	0.31	-0.28	1.51	0.11
11	1	2	3	4	5	6	7	8	9	10	11	12

X

=

Raw attention scores												
0	1.0	inf	inf	inf	inf							
1	-0.09	1.0	inf	inf	inf	inf	inf	inf	inf	inf	inf	
2	0.86	1.19	1.59	inf	inf	inf	inf	inf	inf	inf	inf	
3	0.12	-0.03	-0.02	0.88	inf	inf	inf	inf	inf	inf	inf	
4	0.51	0.17	0.13	-1.64	0.24	inf	inf	inf	inf	inf	inf	
5	0.24	-1.44	0.43	0.74	0.96	-1.21	inf	inf	inf	inf	inf	
6	0.26	-0.1	0.93	0.72	-0.38	1.65	0.47	inf	inf	inf	inf	
7	-0.55	0.81	0.71	1.7	-0.8	-1.14	-0.32	1.78	inf	inf	inf	
8	0.74	-0.76	-0.44	-0.08	-1.38	-0.13	1.25	-1.37	1.84	inf	inf	
9	-0.97	-0.91	0.15	0.35	-0.81	0.11	1.14	-1.52	1.06	1.87	inf	
10	1.56	0.9	0.39	1.46	1.44	-1.05	0.9	-0.73	0.36	-0.67	-0.62	
11	0.32	0.74	0.44	-0.1	1.19	0.83	0.29	2.06	0.51	-0.26	1.51	0.11
12	1	2	3	4	5	6	7	8	9	10	11	

Masked attention raw scores

0	-0.08	-inf	-inf	-inf	-inf	-inf						
1	-0.09	-0.0	-inf	-inf	-inf	-inf	-inf	-inf	-inf	-inf	-inf	-inf
2	0.86	1.19	1.59	-inf	-inf	-inf	-inf	-inf	-inf	-inf	-inf	-inf
3	0.12	-0.03	-0.02	0.88	-inf	-inf	-inf	-inf	-inf	-inf	-inf	-inf
4	0.51	0.17	0.13	-1.64	0.24	-inf	-inf	-inf	-inf	-inf	-inf	-inf
5	0.24	-1.44	0.43	0.74	0.96	-1.21	-inf	-inf	-inf	-inf	-inf	-inf
6	0.26	-0.1	0.93	0.72	-0.38	1.65	0.47	-inf	-inf	-inf	-inf	-inf
7	-0.55	0.81	0.71	1.7	-0.8	-1.14	-0.32	1.78	-inf	-inf	-inf	-inf
8	0.74	-0.76	-0.44	-0.08	-1.38	-0.13	1.25	-1.37	1.84	-inf	-inf	-inf
9	-0.97	-0.91	0.15	0.35	-0.81	0.11	1.14	-1.52	1.06	1.87	-inf	-inf
10	1.56	0.9	0.39	1.46	1.44	-1.05	0.9	-0.73	0.36	-0.67	-0.62	-inf
11	0.32	0.74	0.44	-0.1	1.19	0.83	0.29	2.06	0.51	-0.26	1.51	0.11
12	1	2	3	4	5	6	7	8	9	10	11	12

Slide credit: Arman Cohan

Attention mask

The effect is more than just pruning out some of the wirings in self-attention block.

Attention raw scores											
-0.09	1.24	0.69	0.38	3.43	-0.1	0.7	1.16	0.93	1.28	1.81	-1.13
-0.09	-0.0	-0.7	0.06	0.25	0.23	0.26	1.18	0.78	-0.21	1.01	1.01
-0.06	1.19	1.59	0.98	-0.15	0.15	1.11	-0.96	-0.97	1.22	1.67	-0.72
-0.12	-0.03	-0.42	0.88	-0.46	-0.1	0.54	-0.42	1.86	-0.38	0.94	-0.84
-0.51	0.17	0.55	0.34	0.24	0.02	1.68	-0.36	0.04	0.37	0.66	-0.27
-0.24	-1.64	0.43	0.78	0.96	1.2	-0.31	1.54	1.88	1.14	0.58	-1.44
-0.26	-0.1	0.63	0.72	0.36	1.84	0.47	1.96	-0.17	-0.5	0.67	0.22
-0.55	0.81	0.71	1.7	-0.18	0.32	1.78	-0.7	-0.94	1.54	0.81	-0.74
-0.74	-0.48	-0.48	0.88	-0.13	0.13	1.25	1.37	1.84	0.3	0.57	0.74
-0.87	0.91	0.15	0.36	0.81	0.11	1.14	-0.53	1.08	1.87	0.5	-0.37
-0.56	0.39	1.46	1.44	1.05	0.8	0.73	0.36	-0.67	0.62	-0.62	-0.43
-0.32	0.74	0.44	0.1	1.19	0.89	0.29	2.06	0.31	-0.28	1.51	0.11

X

Raw attention scores											
0	1.0	ad									
1	1.0	1.2	ad								
2	1.0	1.2	1.0	1.0	ad						
3	1.0	1.0	1.0	1.0	1.0	1.0	ad	ad	ad	ad	ad
4	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	ad	ad	ad
5	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	ad
6	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
7	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
8	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
9	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
10	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
11	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0

Masked attention raw scores											
-0.08	ad	ad	ad	ad	ad	ad	ad	ad	ad	ad	ad
-0.09	-0.0	ad	ad	ad	ad	ad	ad	ad	ad	ad	ad
-0.06	1.19	1.59	ad	ad	ad	ad	ad	ad	ad	ad	ad
-0.12	-0.03	0.88	ad	ad	ad	ad	ad	ad	ad	ad	ad
-0.51	0.17	0.33	-1.64	0.24	ad	ad	ad	ad	ad	ad	ad
-0.24	1.64	1.43	0.74	0.66	1.21	ad	ad	ad	ad	ad	ad
-0.26	-0.1	0.93	0.72	-0.38	1.65	0.67	ad	ad	ad	ad	ad
-0.56	0.81	0.71	1.7	-0.8	1.14	-0.22	1.78	ad	ad	ad	ad
-0.74	-0.76	-0.44	-0.36	-0.36	1.13	1.25	1.37	1.84	ad	ad	ad
-0.87	-0.91	0.15	0.35	-0.81	0.11	1.14	1.52	1.06	1.87	ad	ad
-1.56	0.8	0.39	1.46	1.44	1.05	0.8	-0.73	1.36	-0.67	0.62	ad
-0.32	0.74	0.44	-0.1	1.19	0.89	0.29	2.06	0.31	-0.28	1.51	0.11

softmax

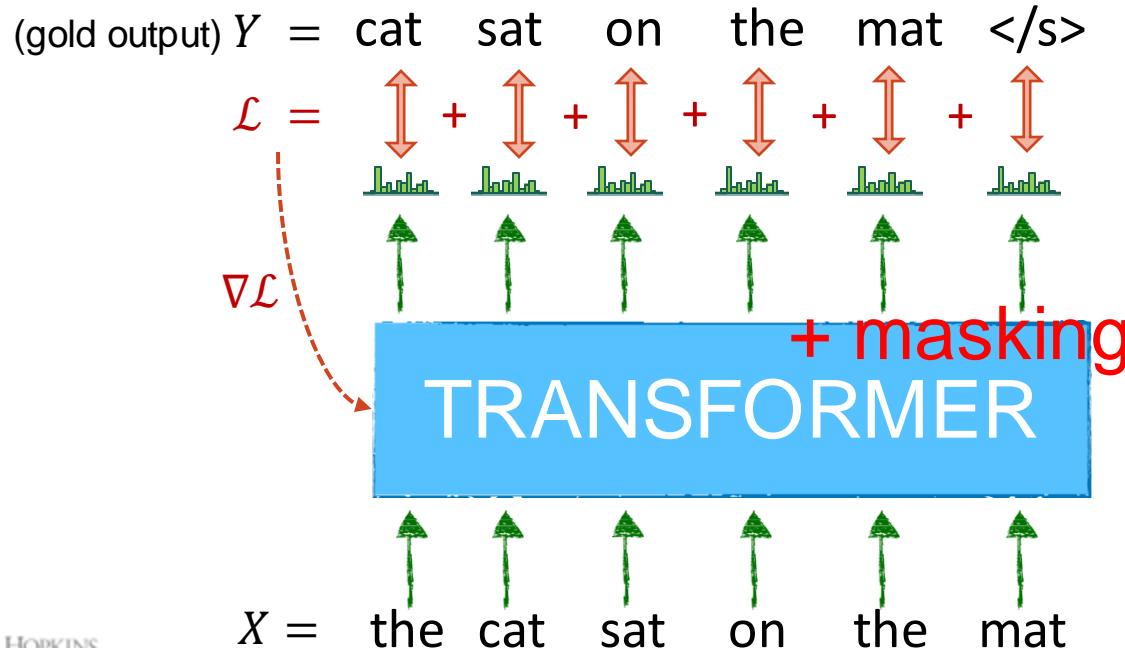


Slide credit: Alman Cohan



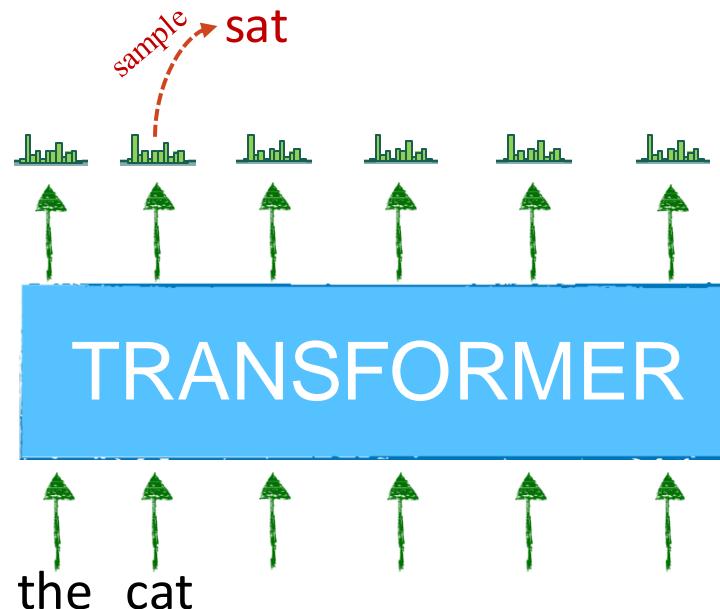
Training a Transformer Language Model

- We need to **prevent information leakage** from future tokens! How?



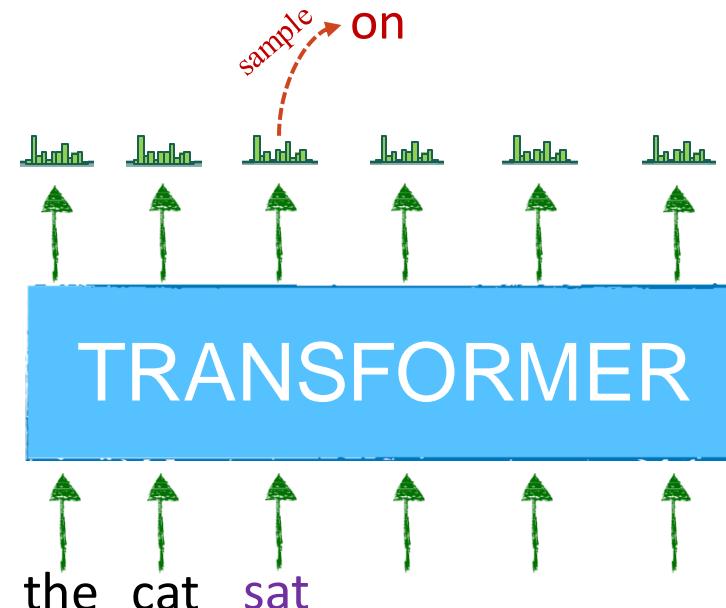
How to use the model to generate text?

- Use the output of previous step as input to the next step repeatedly



How to use the model to generate text?

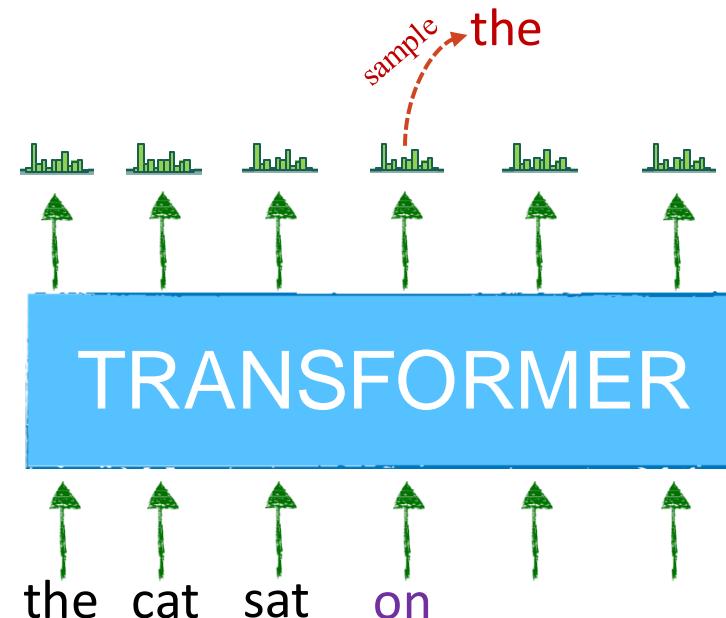
- Use the output of previous step as input to the next step repeatedly



The probabilities get revised upon adding a new token to the input.

How to use the model to generate text?

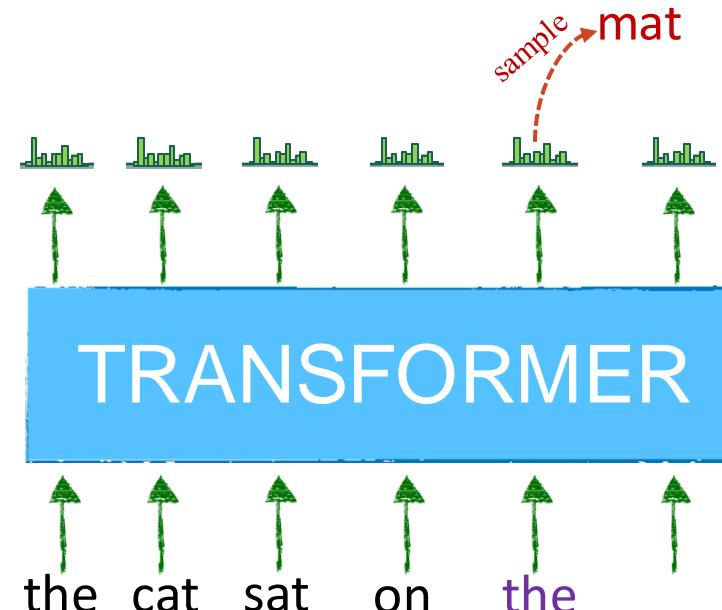
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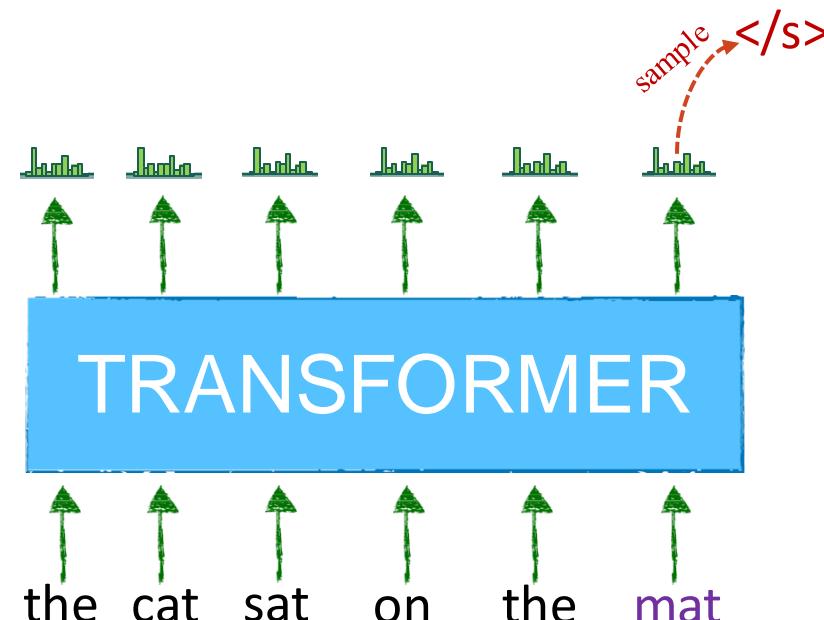
How to use the model to generate text?

- Use the output of previous step as input to the next step repeatedly



How to use the model to generate text?

- Use the output of previous step as input to the next step repeatedly



Quiz

- What's the point of attention masking during training?
 1. TODO

Answer: TODO

Summary: A Decoder-only Transformer

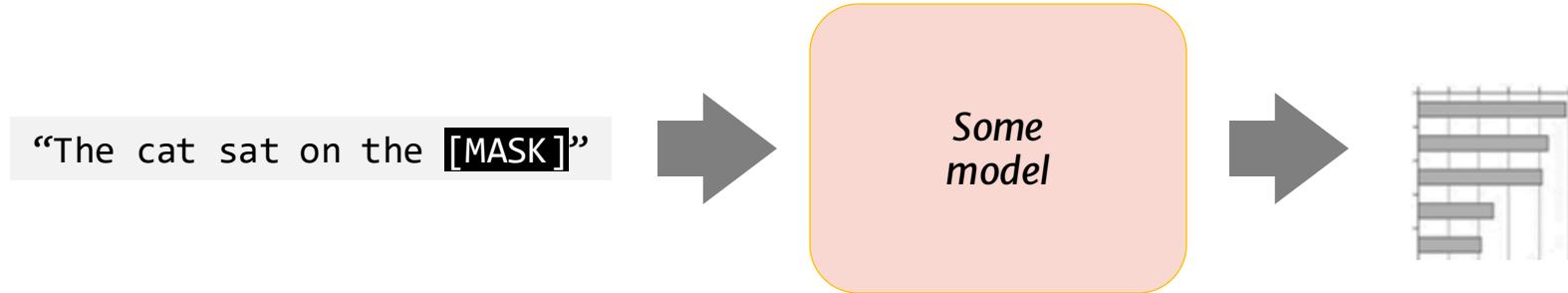
- This is a very generic Transformer!
 - We will implement this in HW5 to build a simple Transformer Language Model!!
-
- **Next:**
 - Architectural variants



Transformer Architectural Variants

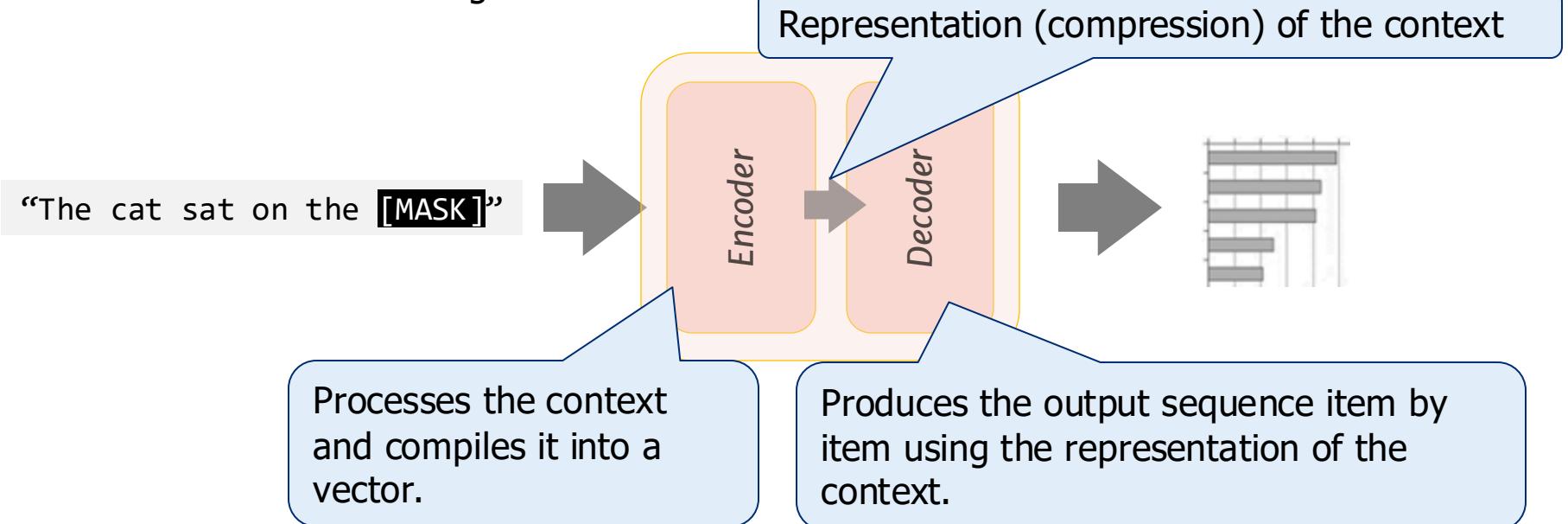
Encoder-Decoder Architectures

- It is useful to think of generative models as two sub-models.



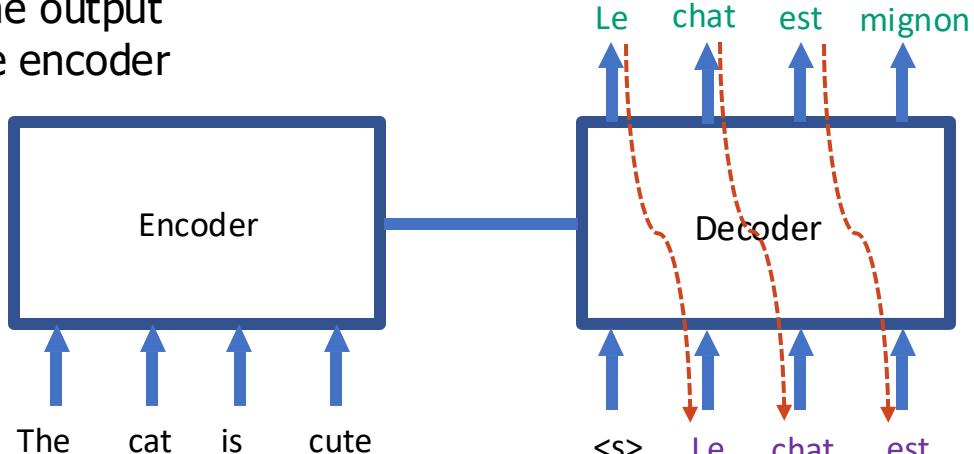
Encoder-Decoder Architectures

- It is useful to think of generative models as two sub-models



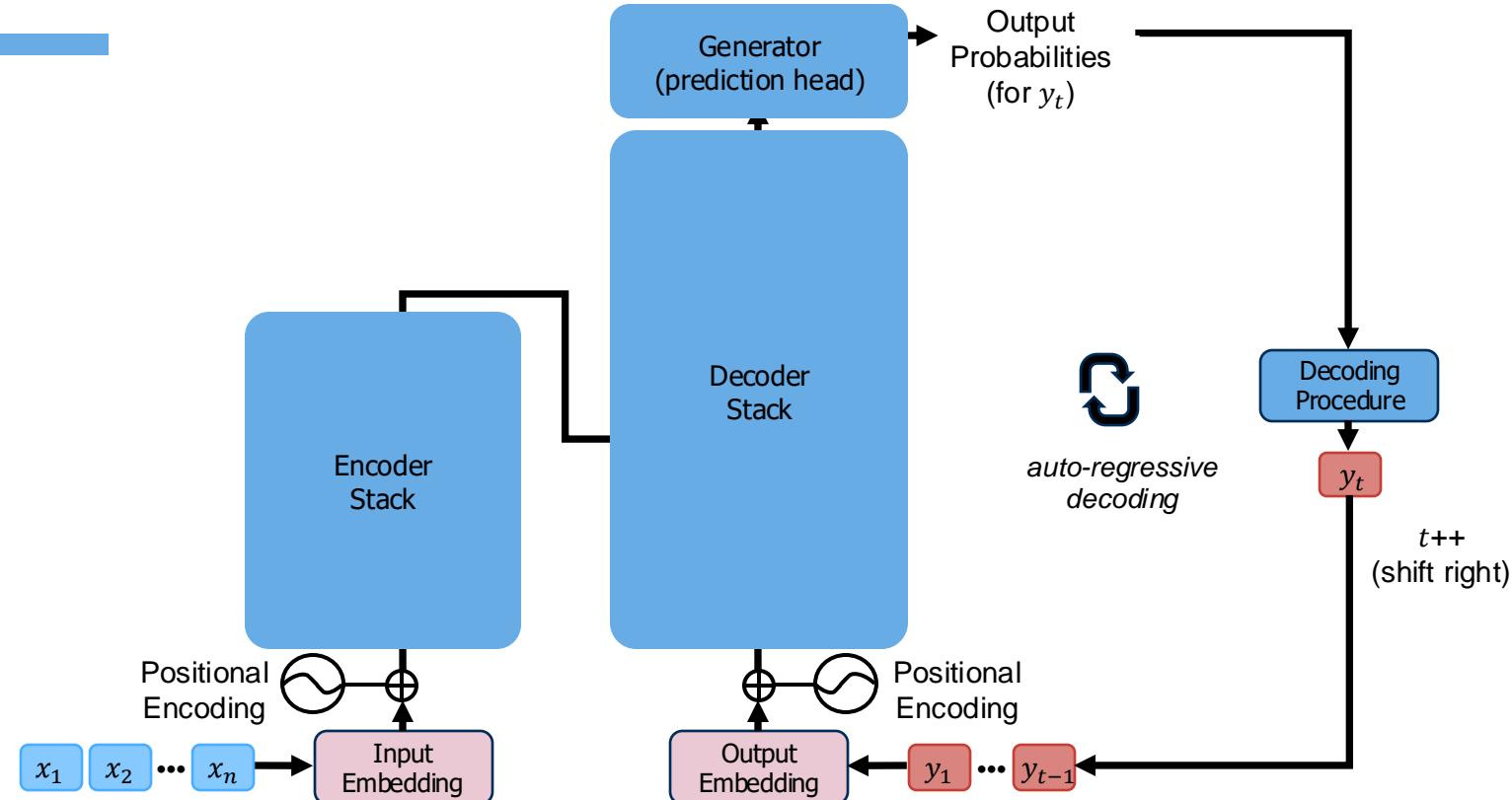
Encoder-decoder models

- Transformer is two blocks
- Encoder = read or encode the input,
 - Architecture is as we've seen
- Decoder = generate or decode the output
 - Architecture is identical to the encoder but we give it the ability to also attend to the input



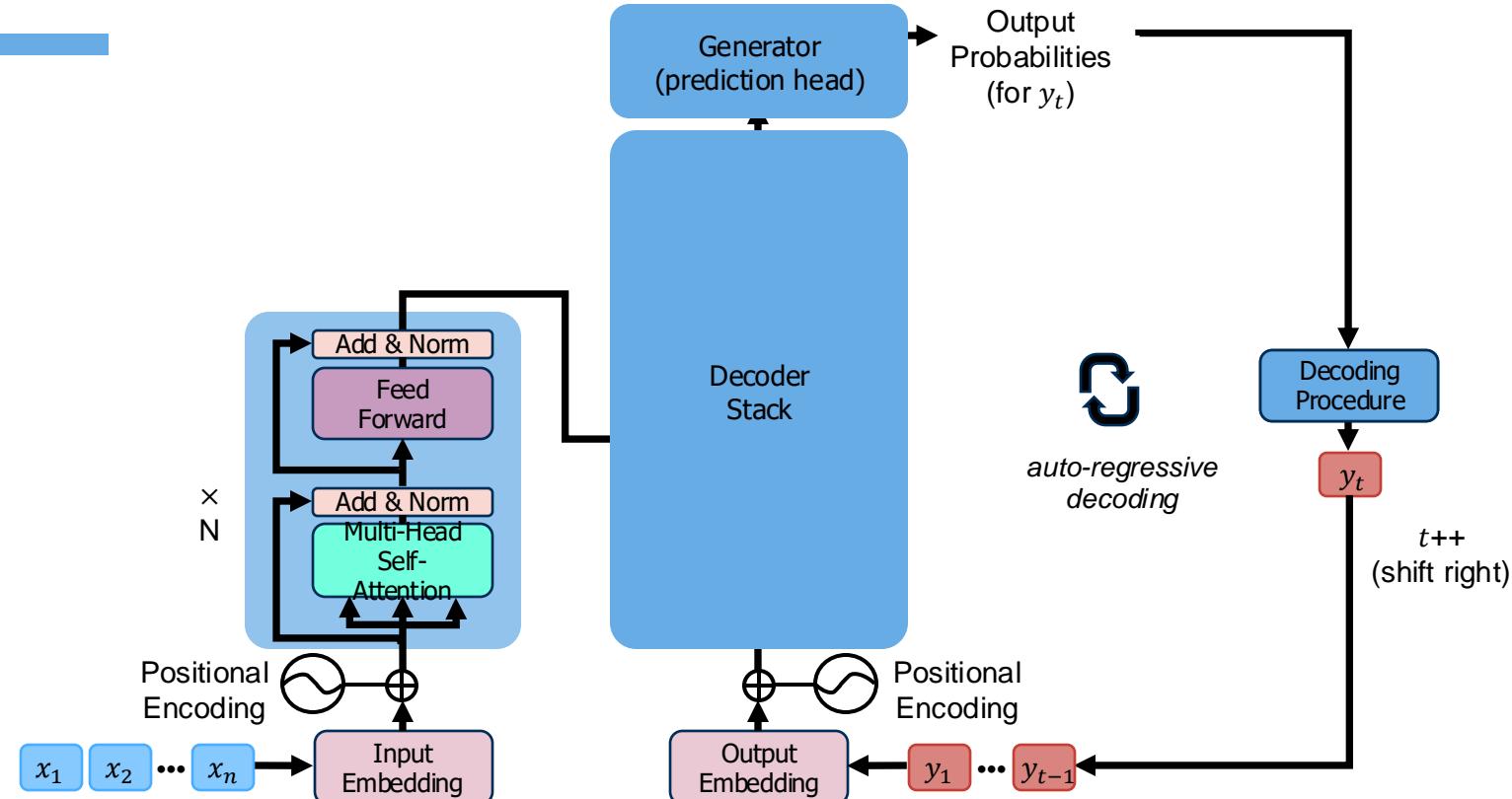
Transformer

[Vaswani et al. 2017]



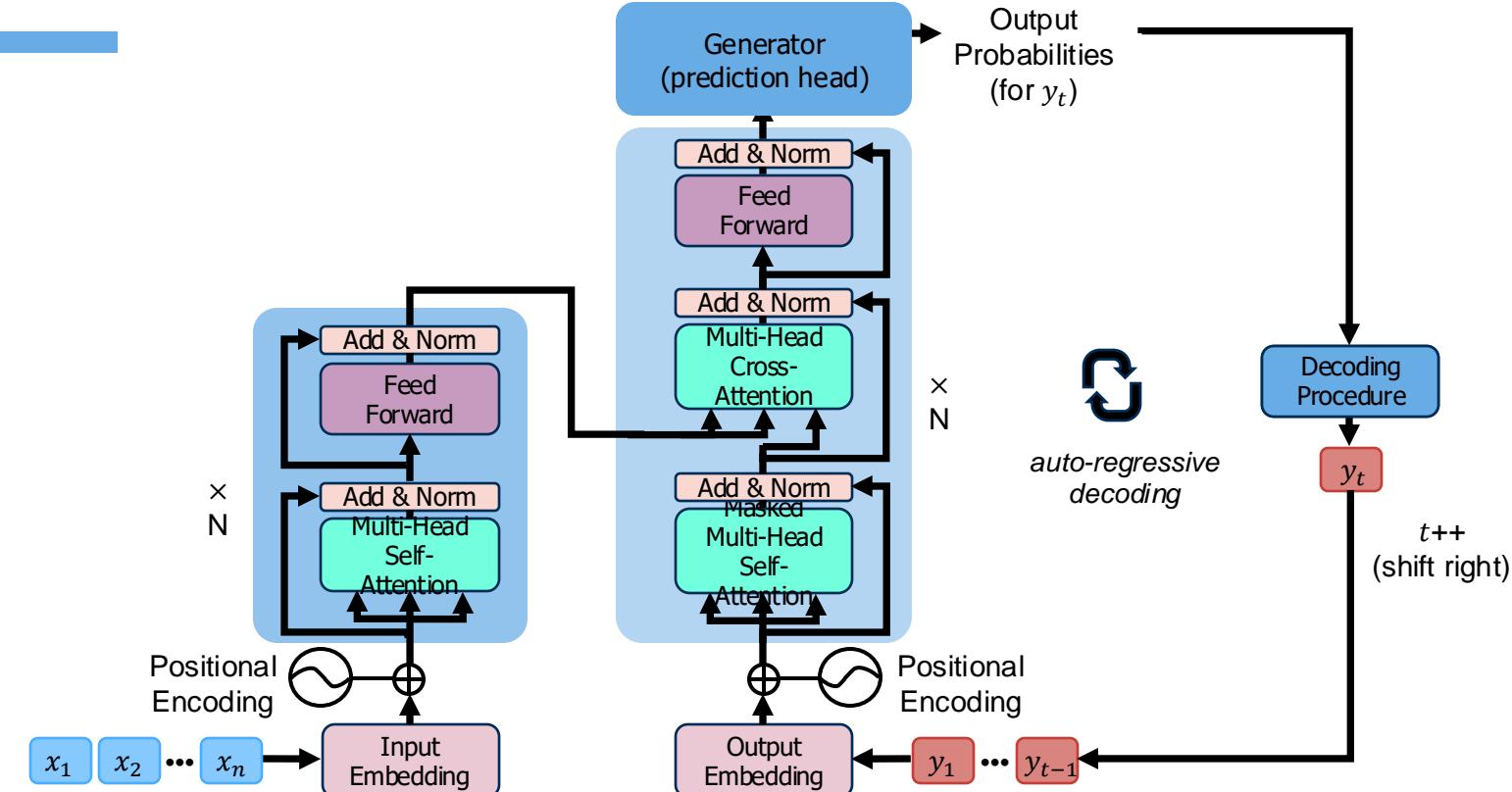
Transformer

[Vaswani et al. 2017]



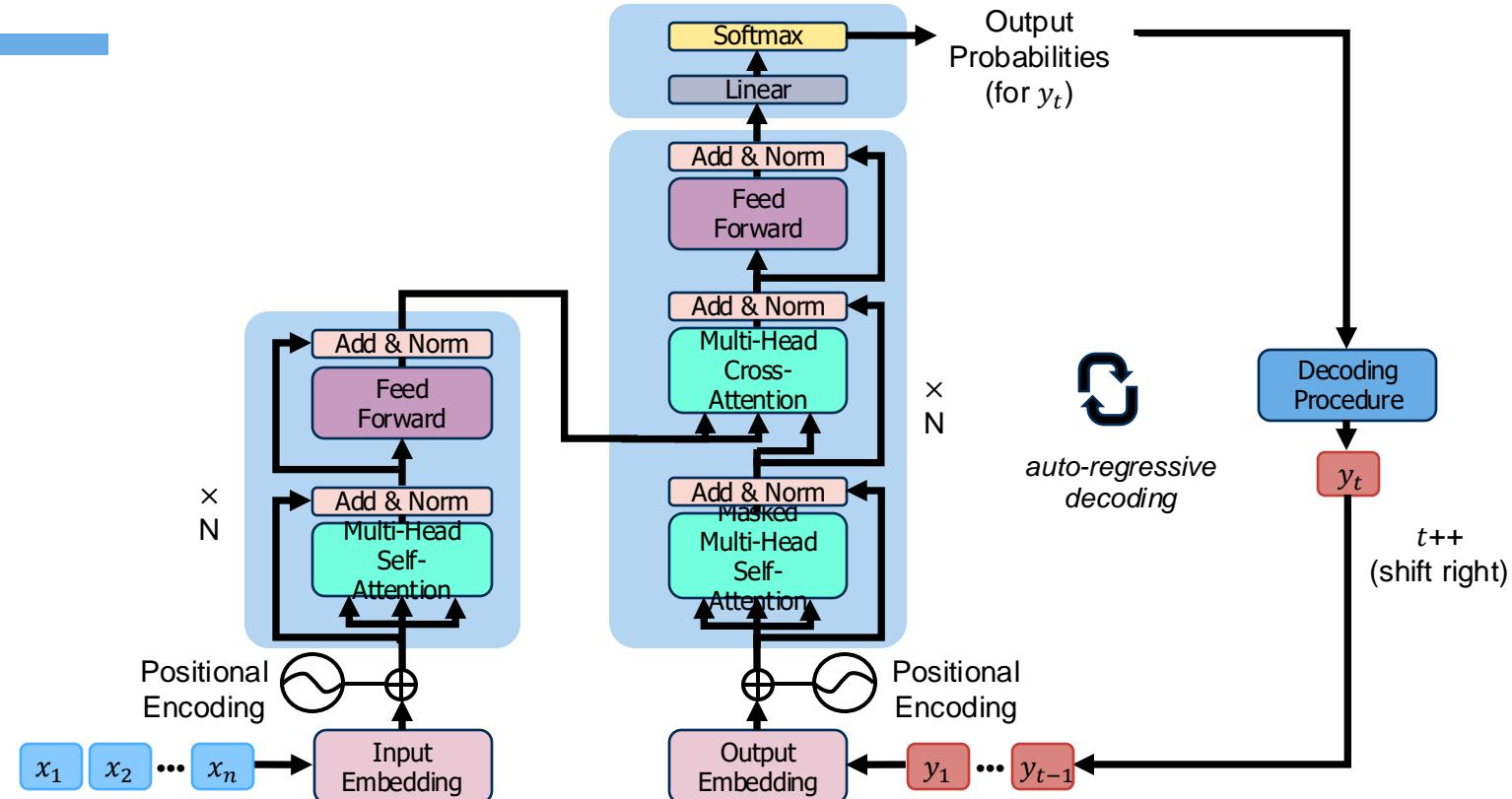
Transformer

[Vaswani et al. 2017]



Transformer

[Vaswani et al. 2017]



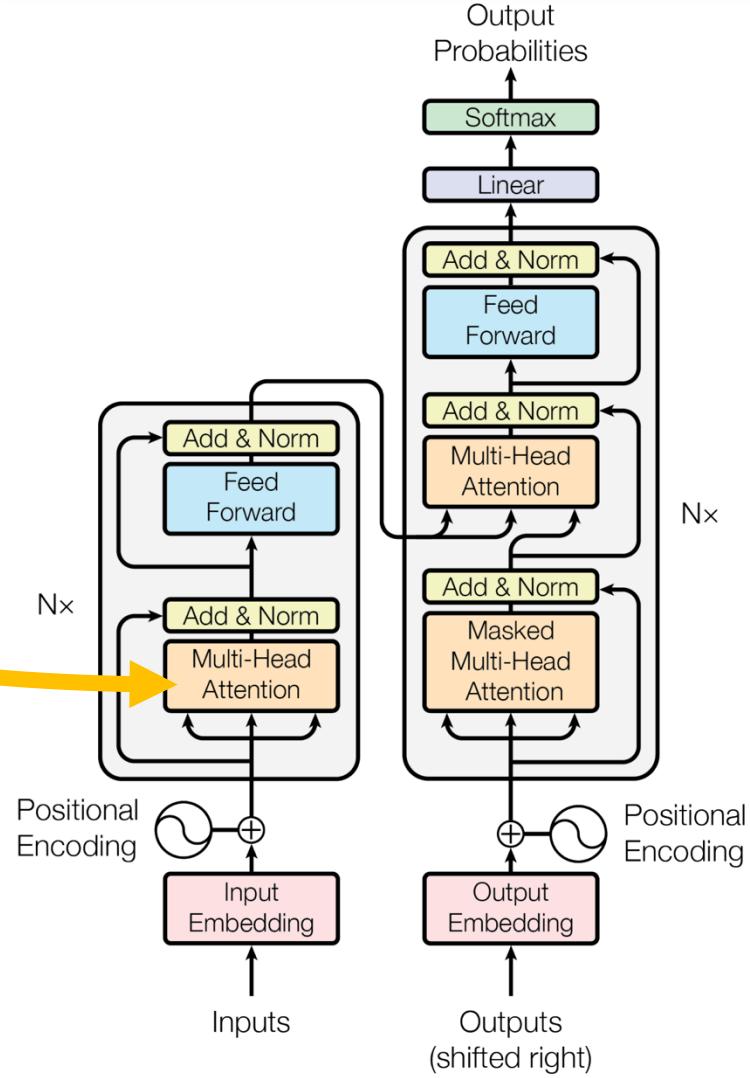
Transformer

[Vaswani et al. 2017]

- Computation of **encoder** attends to both sides.



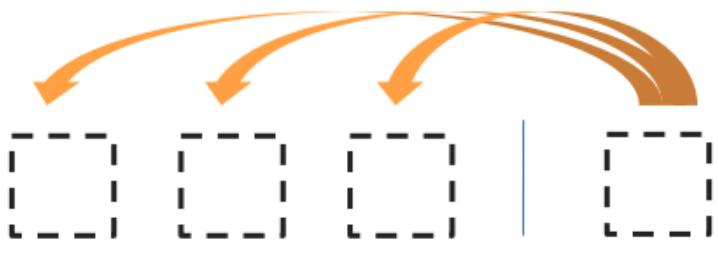
Encoder Self-Attention



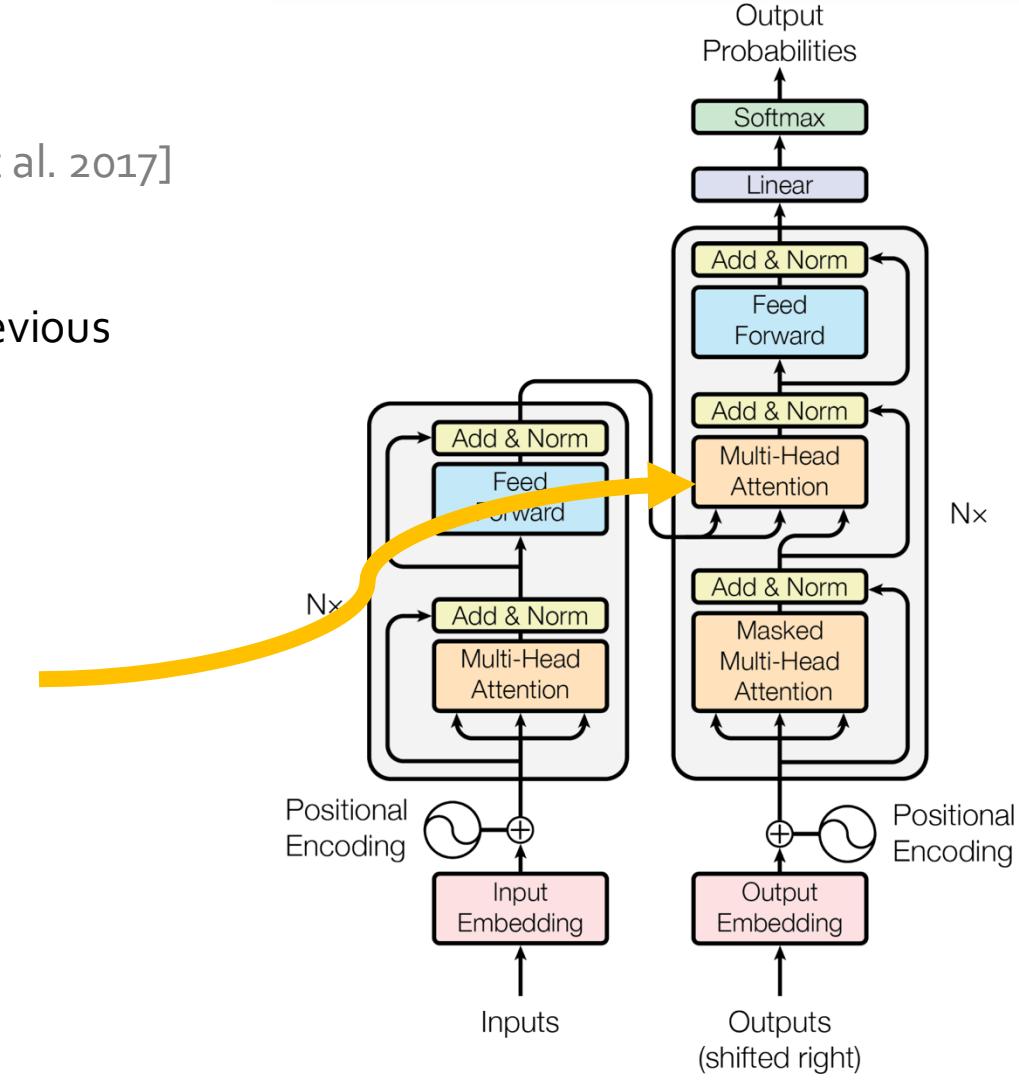
Transformer

[Vaswani et al. 2017]

- At any step of **decoder**, it attends to previous computation of **encoder**



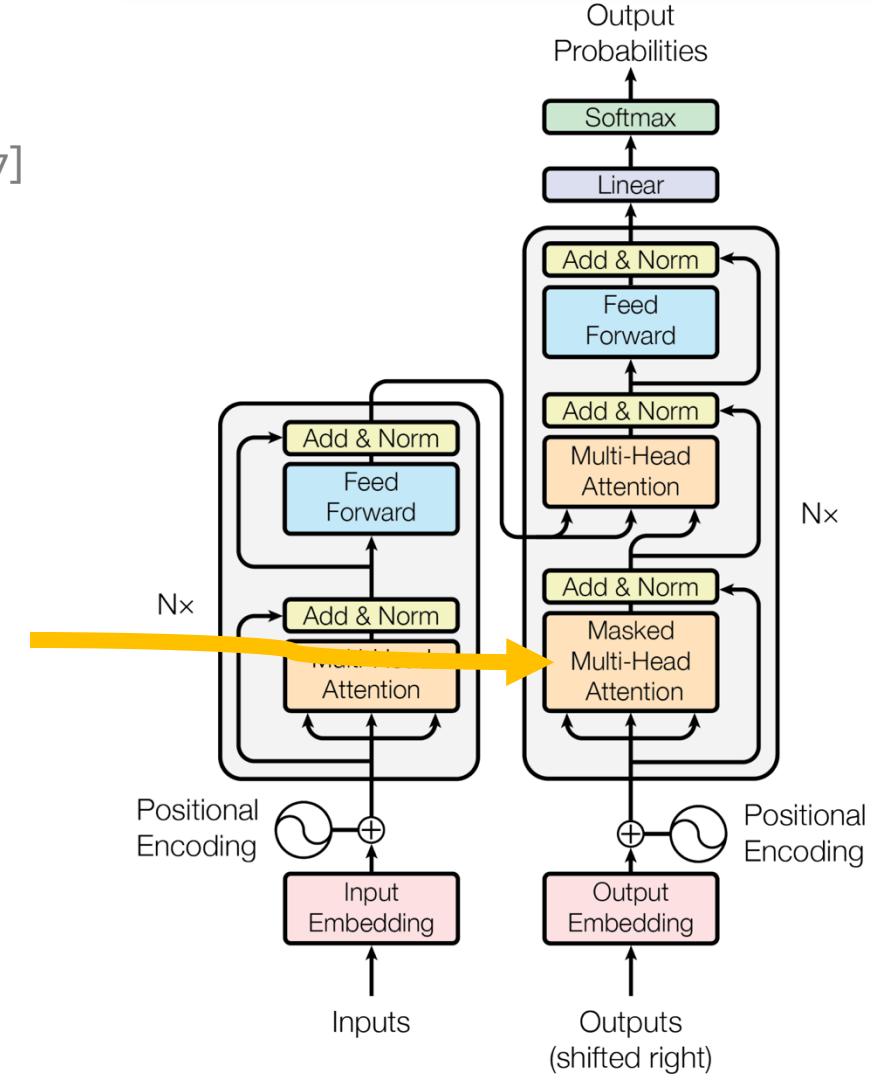
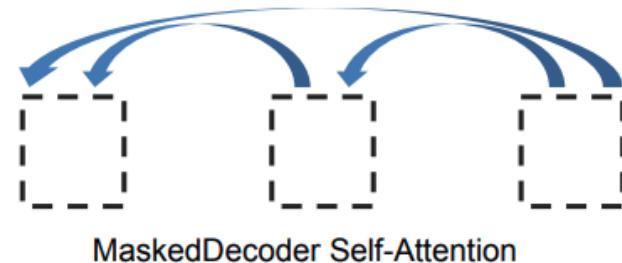
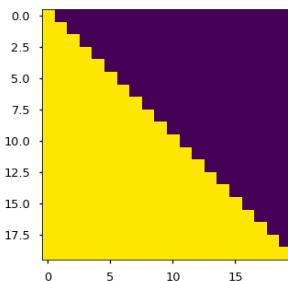
Encoder-Decoder Attention



Transformer

 [Vaswani et al. 2017]

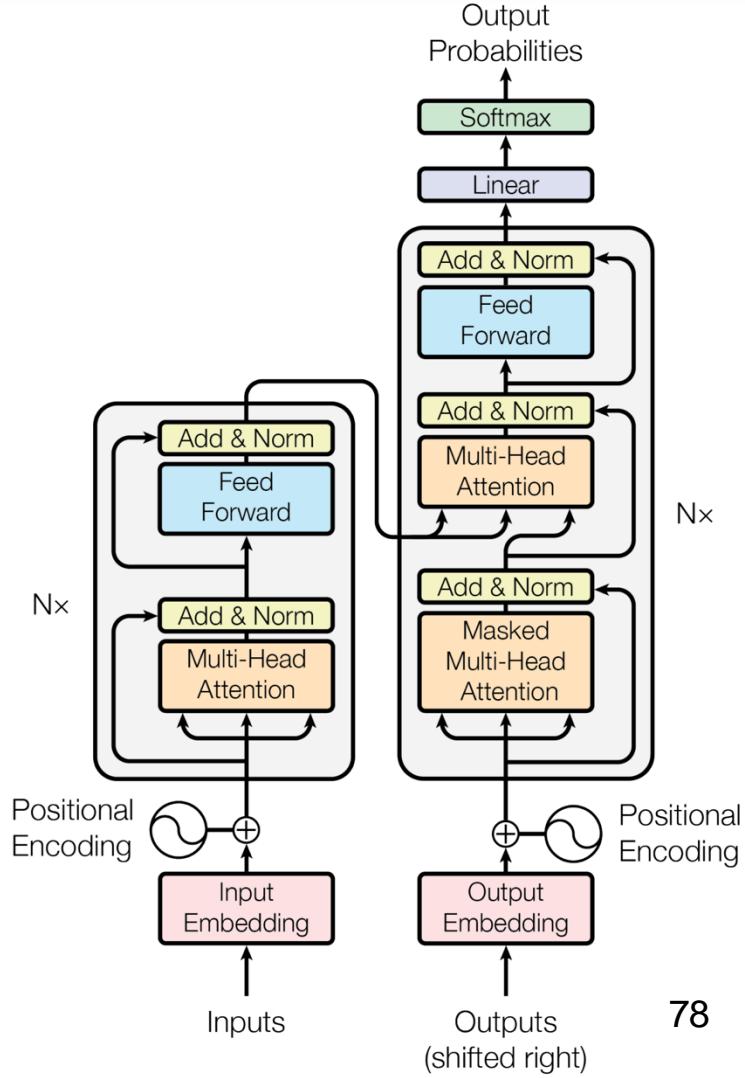
- At any step of **decoder**, it attends to previous computation of **encoder** as well as **decoder's** own generations



Transformer

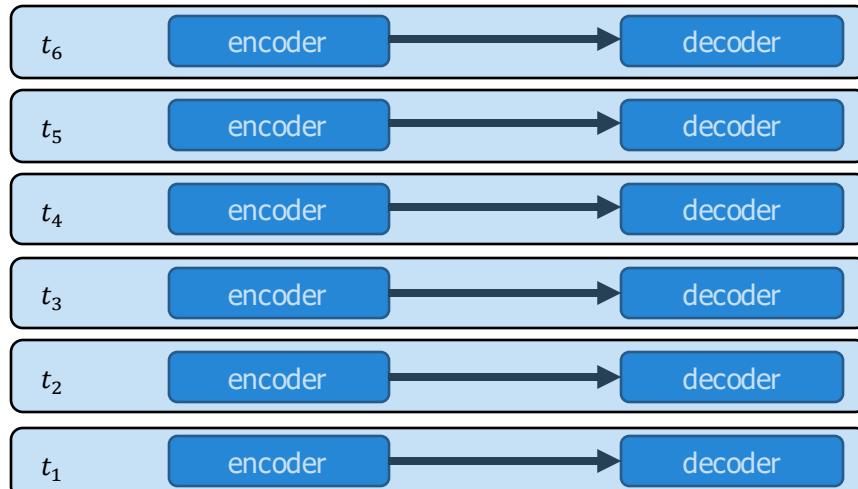
[Vaswani et al. 2017]

- At any step of **decoder**, it attends to previous computation of **encoder** as well as **decoder's** own generations
- At any step of **decoder**, **re-use** previous computation of **encoder**.
- Computation of **decoder** is **linear**, instead of quadratic.

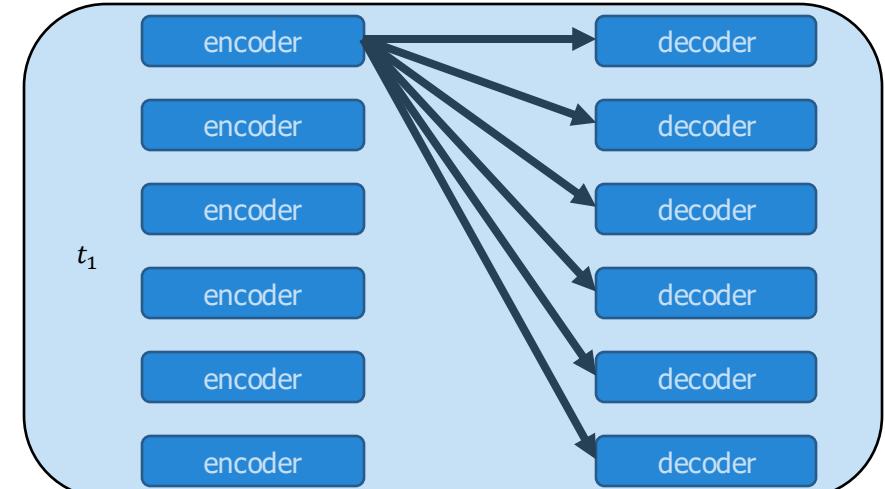


Quiz: Enc-Dec Connections

- Which best represents encoder-decoder connections?



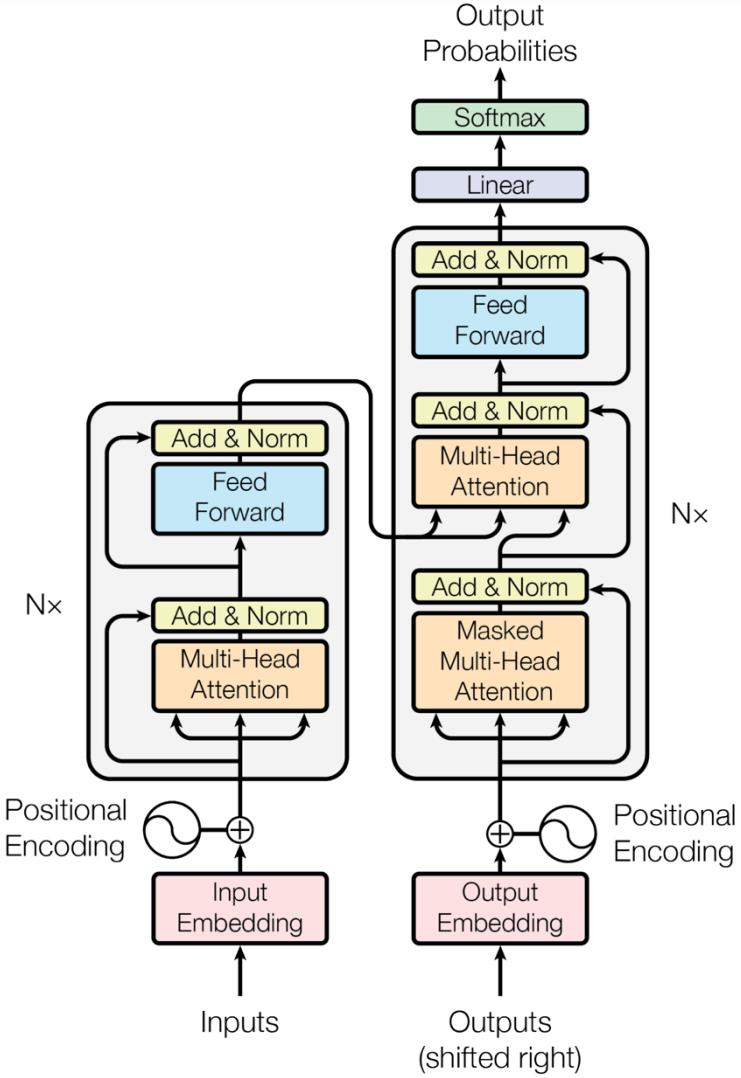
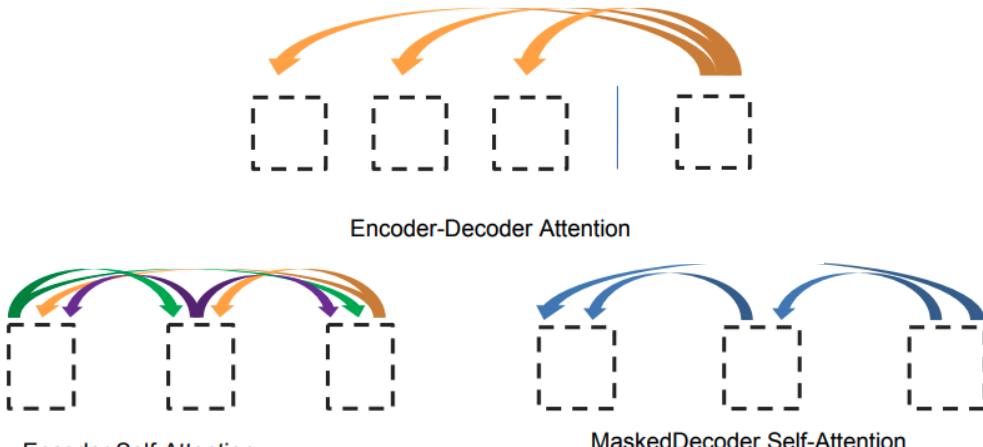
Incorrect



Correct

Recap: Transformer

- Yaaay we know Transformers now! 🎉
- An **encoder-decoder** architecture
- 3 forms of attention



Considerations about computational cost in Transformers

How many parameters does my Transformer have?

- Let's count the number of parameters:
- The self-attention block params:
 - $3 \times \left(d \times \frac{d}{m}\right) \times m + d^2 = 4d^2$
- The FFN block params:
 - $2 \times (d \times d_{\text{ff}})$
- So, in total: $4d^2 + 2dd_{\text{ff}}$
- The ratio of SA/FFN parameters is $2d/d_{\text{ff}}$. We will see how to see this.
- Notice that the num of params in independent of seq length (n) or batch size (b)!
 - So, in theory you should be able to run your SA on sequences of any length!
 - (but would it work on longer sequences? -- more on this later)

$$\mathbf{W}_i^q \in \mathbb{R}^{d \times \frac{d}{m}}, \mathbf{W}_i^k \in \mathbb{R}^{d \times \frac{d}{m}}, \mathbf{W}_i^v \in \mathbb{R}^{d \times \frac{d}{m}}, \mathbf{W}^o \in \mathbb{R}^{d \times d}$$
$$\text{head}_i \leftarrow \text{Attention}(\mathbf{x} \mathbf{W}_i^q, \mathbf{x} \mathbf{W}_i^k, \mathbf{x} \mathbf{W}_i^v)$$

$$\mathbf{x} \leftarrow \text{MHAttention}(\mathbf{x}) = \text{Concat}(\text{head}_1, \dots, \text{head}_h) \mathbf{W}^o$$

$$\mathbf{x} \leftarrow f(\mathbf{x} W_1 + b_1) W_2 + b_2$$
$$W_1 \in \mathbb{R}^{d \times d_{\text{ff}}}, W_2 \in \mathbb{R}^{d_{\text{ff}} \times d}$$

(note, not showing layer-norm and residuals)

m : number of heads

d : feature dimension in output of SA

Diversion: Floating-point Ops: FLOPS

- Floating point operations per second (FLOPS, flops or flop/s)
- Each FLOP can represent an addition, subtraction, multiplication, or division of floating-point numbers,
- The total FLOP of a model (e.g., Transformer) provides a basic approximation of computational costs associated with that model.

FLOPS of Matrix Multiplication

- Matrix-vector multiplication are common in Self-Attention (e.g., QKV projection)
 - Requires $2mn$ ($2 \times$ matrix size) operations for multiplying $A \in \mathbb{R}^{m \times n}$ and $b \in \mathbb{R}^n$
 - (2 because 1 for multiplication, 1 for addition)

$$\begin{bmatrix} A_{11} & A_{12} & \cdots & A_{1n} \\ A_{21} & A_{22} & \cdots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{m1} & A_{m2} & \cdots & A_{mn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} A_{11}x_1 + A_{12}x_2 + \cdots + A_{1n}x_n \\ A_{21}x_1 + A_{22}x_2 + \cdots + A_{2n}x_n \\ \vdots \\ A_{m1}x_1 + A_{m2}x_2 + \cdots + A_{mn}x_n \end{bmatrix}$$

Quiz: thinking about computations

- Consider the following matrix multiplication:

$$A \cdot B, \quad \text{where } A \in \mathbb{R}^{n \times m}, B \in \mathbb{R}^{m \times k}$$

- **Question 1:** Computing AB involves how many arithmetic operations?

- (also referred to as floating-point operations or FLOPs)

- **Answer:** It's $O(n \times m \times k)$.

- (to be a bit more precise, it's $\approx 2n \times m \times k$ since each element in $A \cdot B$ requires almost equal num of multiplications and summations.)

- **Question 2:** Computing AB involves how many memory/IO access?

- **Answer:** It's $n \times m$ (reading A) + $m \times k$ (reading B) + $n \times m$ (writing AB).

Computations in Self-Attention Block

- We are going to count computations and IO access in Transformer computations.
- Note we assume that the full input sequence is given at once (e.g., training time).
- Here is the first step. Given: $\mathbf{x} \in \mathbb{R}^{b \times n \times d}$, $\mathbf{W}_i^q \in \mathbb{R}^{d \times \frac{d}{m}}$
- Let's think about the following computation: $\mathbf{x}\mathbf{W}_i^q$
- **Q1:** What is the number of arithmetic operations? $O(b \times n \times d \times \frac{d}{m})$ for each head
- **Q2:** What about the number of IO? $O(b \times n \times d + d \times \frac{d}{m} + b \times n \times \frac{d}{m})$ for each head
- **Q3:** What are these quantities for all heads?
 - Number of arithmetic ops: $O(bnd^2)$
 - Number of IO ops: $O(2bnd + d^2)$

Computations in Self-Attention

b : batch size,
 n : sequence length,
 m : number of heads
 d : feature dimension in output of SA
 d/m : feature dimension inside each SA head
 $d_{\text{ff}} = 4d$: feature dimension inside FFN

Dimensions	Operation	Computations	IO
$\mathbf{x} \in \mathbb{R}^{b \times n \times d}, \mathbf{W}_i^q \in \mathbb{R}^{d \times \frac{d}{m}}$	$\mathbf{x}\mathbf{W}_i^q, \mathbf{x}\mathbf{W}_i^k, \mathbf{x}\mathbf{W}_i^v$ for m heads	$O(bnd^2)$	$O(d^2 + 2bnd)$
$\mathbf{Q}_i, \mathbf{K}_i \in \mathbb{R}^{b \times n \times \frac{d}{m}}$	$P_i \leftarrow \text{softmax}\left(\frac{\mathbf{Q}_i \mathbf{K}_i^T}{\sqrt{d/m}}\right)$ for m heads	$O(bn^2d)$	$O(2bnd + bmn^2)$
$\mathbf{V}_i \in \mathbb{R}^{b \times n \times \frac{d}{m}}, P_i \in \mathbb{R}^{b \times n \times n}$	$\text{head}_i \leftarrow P_i \mathbf{V}_i$ for m heads	$O(bn^2d)$	$O(2bnd + bmn^2)$
$\mathbf{W}^o \in \mathbb{R}^{d \times d}, \text{head}_i \in \mathbb{R}^{b \times n \times \frac{d}{m}}$	$Y = \text{Concat}(\text{head}_1, \dots, \text{head}_m) \mathbf{W}^o$	$O(bnd^2)$	$O(2bnd + d^2)$
$Y \in \mathbb{R}^{b \times n \times d}, \mathbf{W}_1 \in \mathbb{R}^{d \times d_{\text{ff}}}, \mathbf{W}_2 \in \mathbb{R}^{d_{\text{ff}} \times d}$	$Y = \text{ReLU}(Y \mathbf{W}_1) \mathbf{W}_2$	$O(16bnd^2)$	$O(2bnd + 8d^2)$
---	Total	$O(bnd^2 + bn^2d)$	$O(bnd + bmn^2 + d^2)$

Computations in Transformer – The bottlenecks

- So, in total, we have →
- The quadratic terms are based on n and d
- d is fixed (part of architecture) but n changes with input.
- **Bottlenecks #1:** If n (sequence length) $\gg d$ (feature dimension), the time and space complexity would be dominated by $O(n^2)$.
- **However,** these despite this quadratic dependence these are parallelizable operations which can be computed efficiently in GPUs.

- In comparison, RNNs perform less arithmetic ops but they're not all parallelizable.

- **Bottlenecks #2:** Another potential bottleneck is how fast we can run IO.
A good way to think about this is using "Arithmetic Intensity" (more on this later)

Computations	IO
$O(bnd^2 + bn^2d)$	$O(bnd + bmn^2 + d^2)$

Layer Type	Complexity per Layer	Sequential Operations
Self-Attention	$O(n^2 \cdot d)$	$O(1)$
Recurrent	$O(n \cdot d^2)$	$O(n)$

[Vaswani et al. 2017]

Quiz: Enc-Dec Cost

- Source data (large!):
 - The references for a Wikipedia article.
 - Web search using article section titles, ~ 10 web pages per query.
- For a passage of length N and a summary of length M , the complexity of the attention is:
 - $O(N) + O(M)$
 - $O(N) + O(M) + O(NM)$
 - $O(N^2) + O(M^2) + O(NM)$
 - $O(N^2) + O(M^2)$

No, self attention is all-to-all
and so quadratic.

Quiz: Enc-Dec Cost

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 - $O(N^2) + O(M^2)$

No, cross attention is missing.

Quiz: Enc-Dec Cost

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 - The references for a Wikipedia article.
 - Web search using article section titles, ~ 10 web pages per query.
- For a passage of length N and a summary of length M , the complexity of the attention is:
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 - $O(N) + O(M) + O(NM)$
 - $O(N^2) + O(M^2) + O(NM)$
 - $O(N^2) + O(M^2)$

Yes. The three terms are respectively the Encoder self-attention, Decoder self-attention, and Cross attention.

Recap

- Transformers computation of a full sequence is bounded by $O(bnd^2 + bn^2d)$.
 - Generally, the quadratic term that depends on seq len n is more concerning.
- We have not discussed yet how IO may impose other limits on this. (in a week)
- Also, the above calculations is for a given sentences.
- How bad is the computational complexity during the decoding time where we want to generate text one token at a time?

During decoding time, how slow
is attention computation?

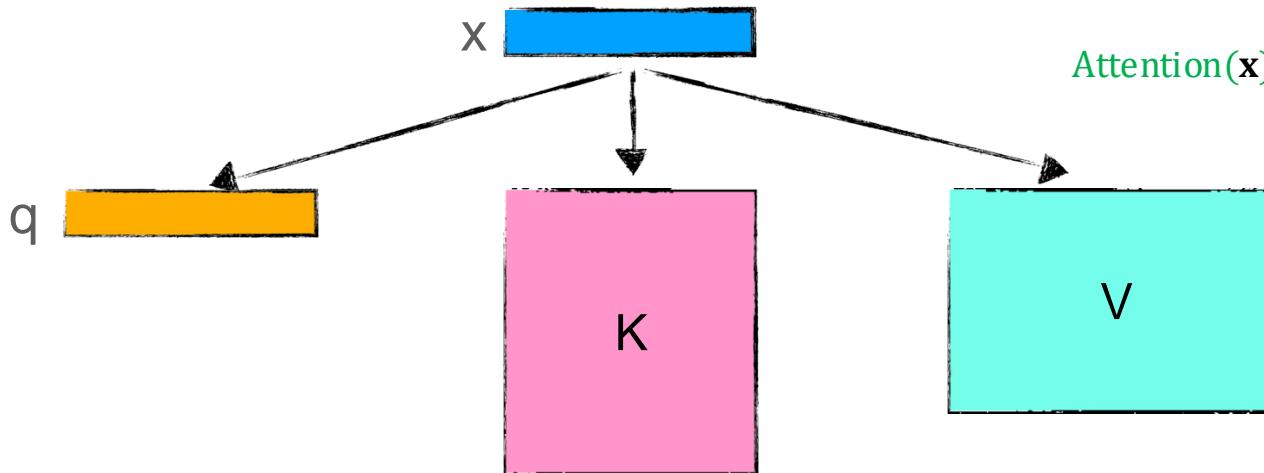
Self-Attention During Inference

$$Q = \mathbf{x}W^q$$

$$K = \mathbf{x}W^k$$

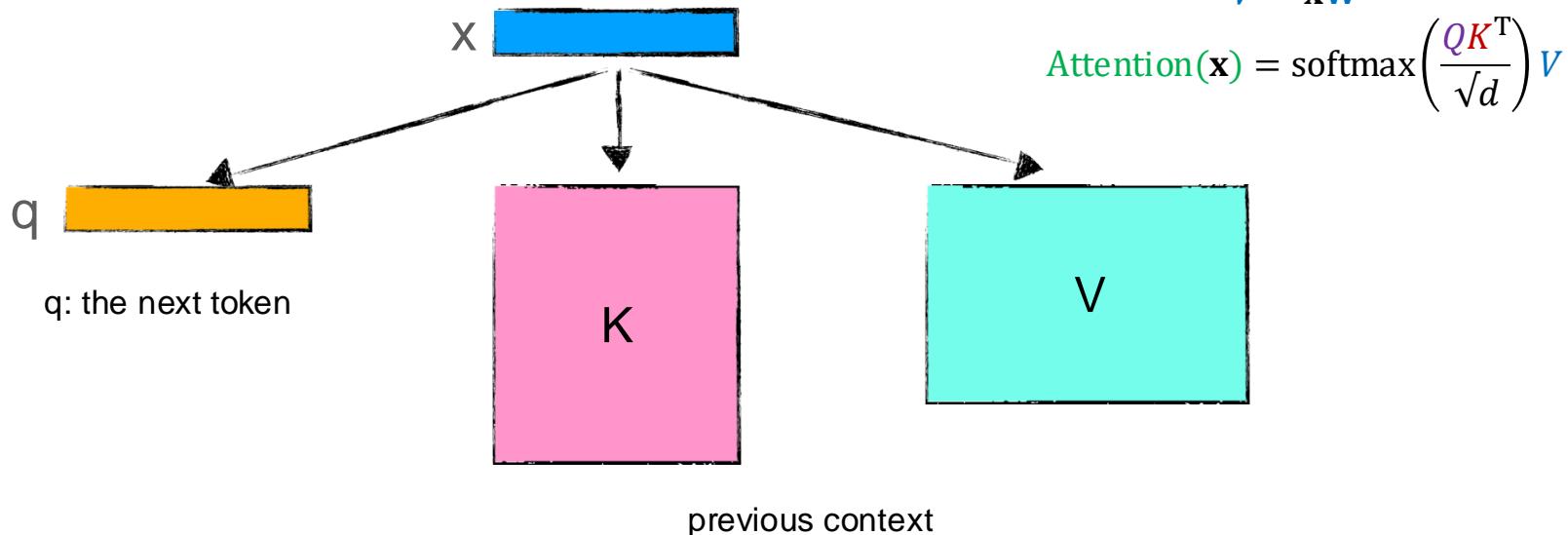
$$V = \mathbf{x}W^v$$

$$\text{Attention}(\mathbf{x}) = \text{softmax}\left(\frac{QK^T}{\sqrt{d}}\right)V$$



[Slide credit: Arman Cohan]

Self-Attention During Inference



[Slide credit: Arman Cohan]

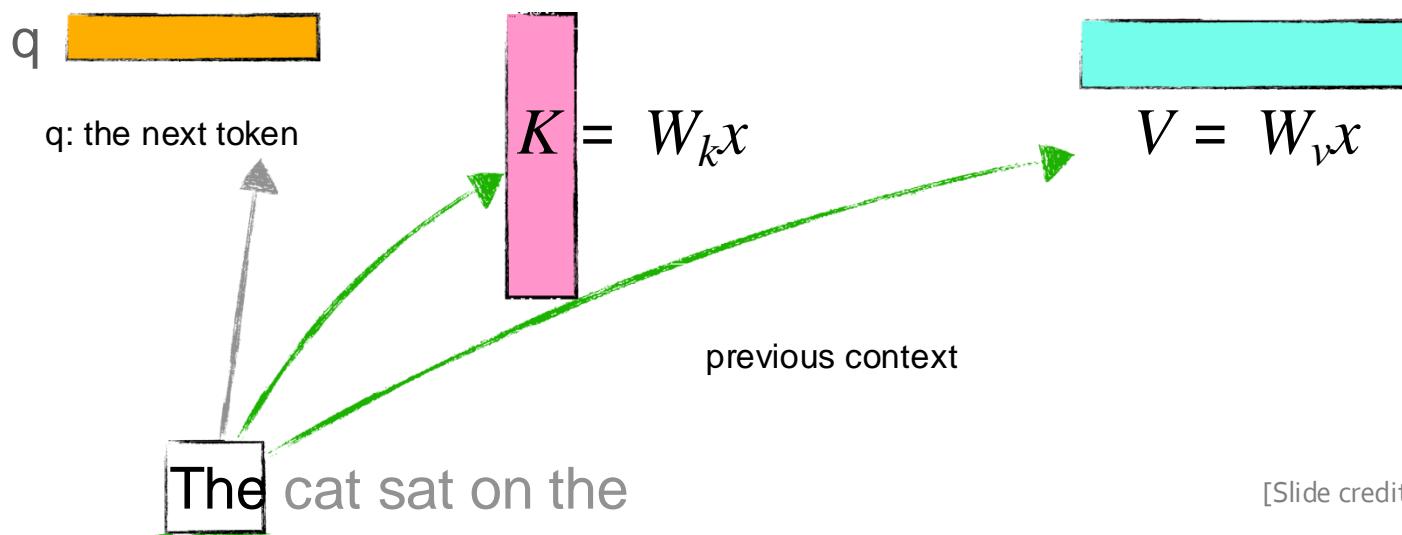
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[Slide credit: Arman Cohan]

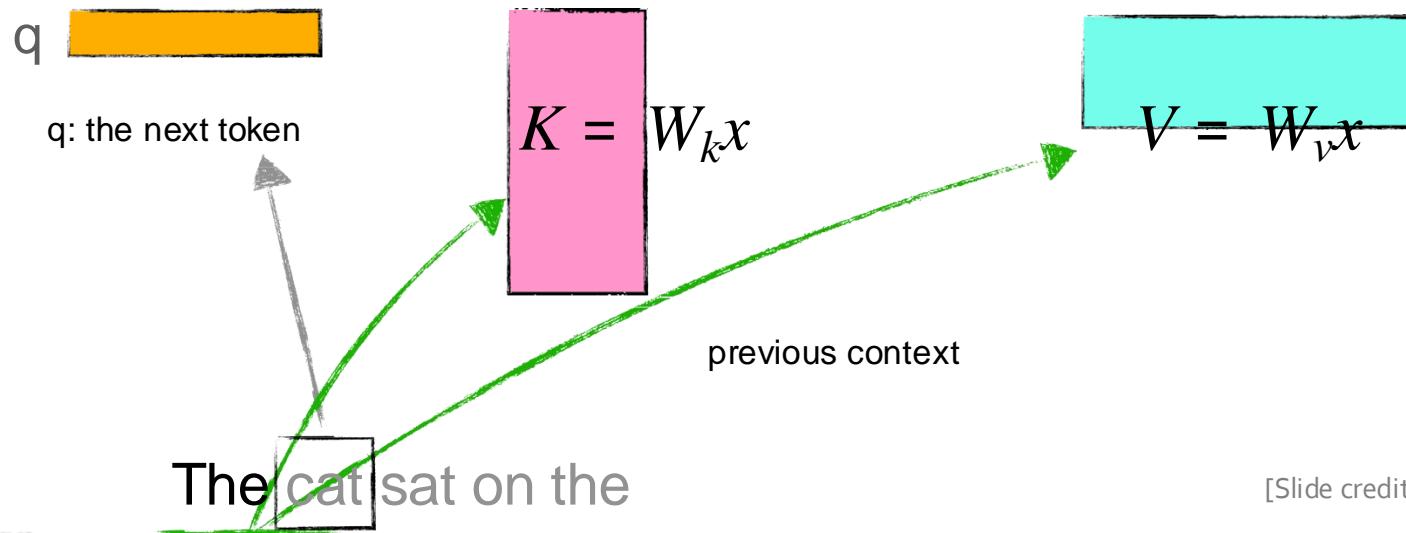
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[Slide credit: Arman Cohan]

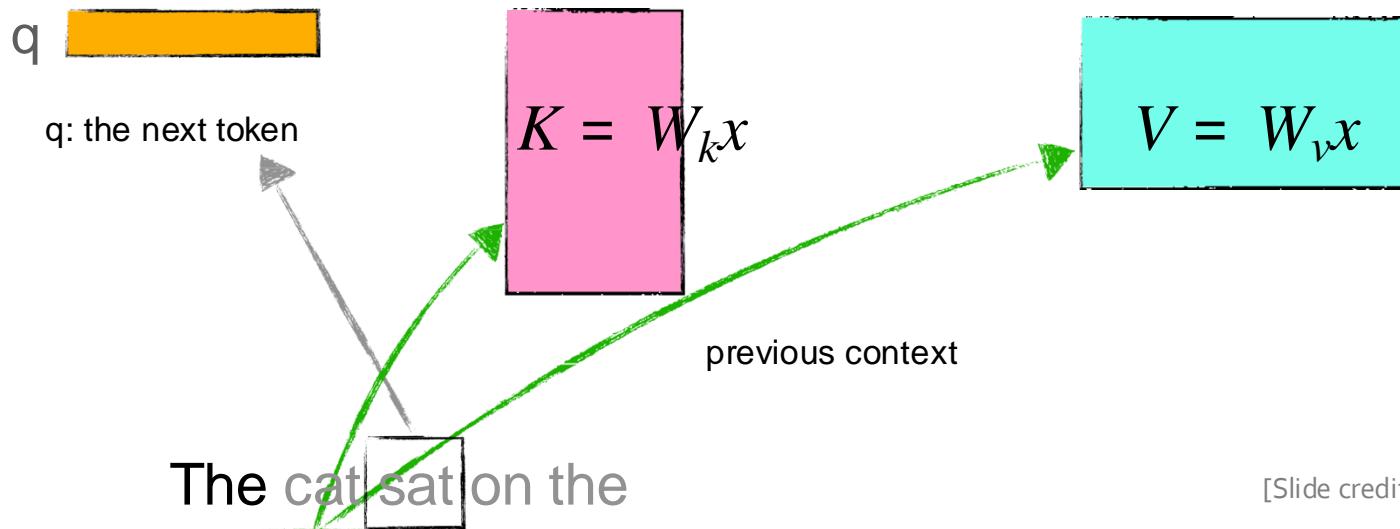
Self-Attention During Inference

$$Q = W^q \mathbf{x}$$

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[Slide credit: Arman Cohan]

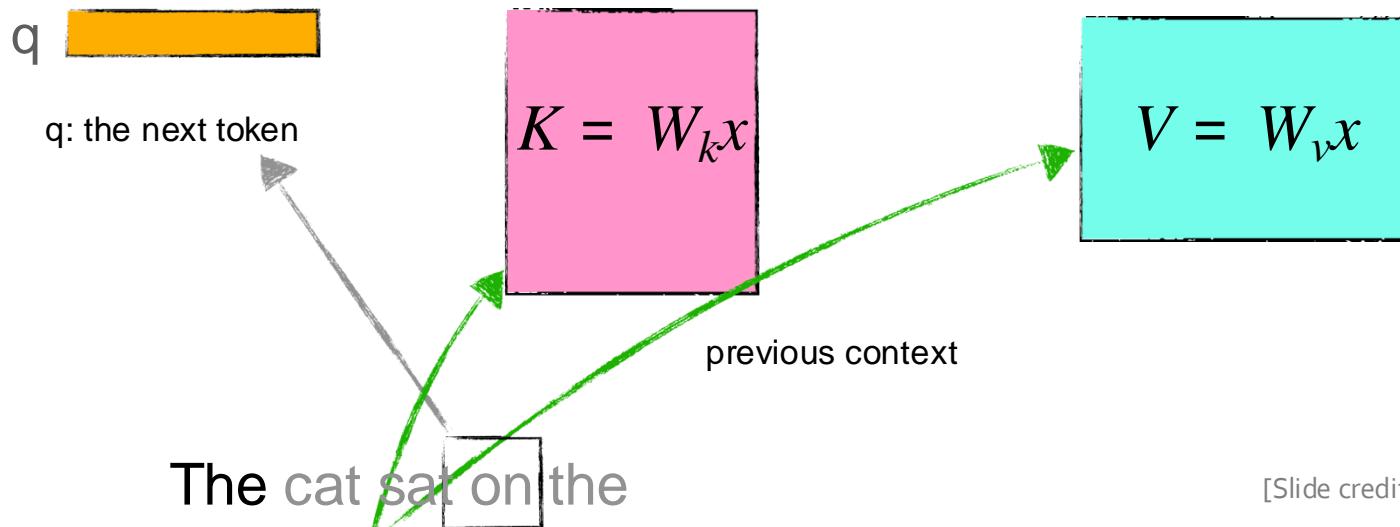
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[Slide credit: Arman Cohan]

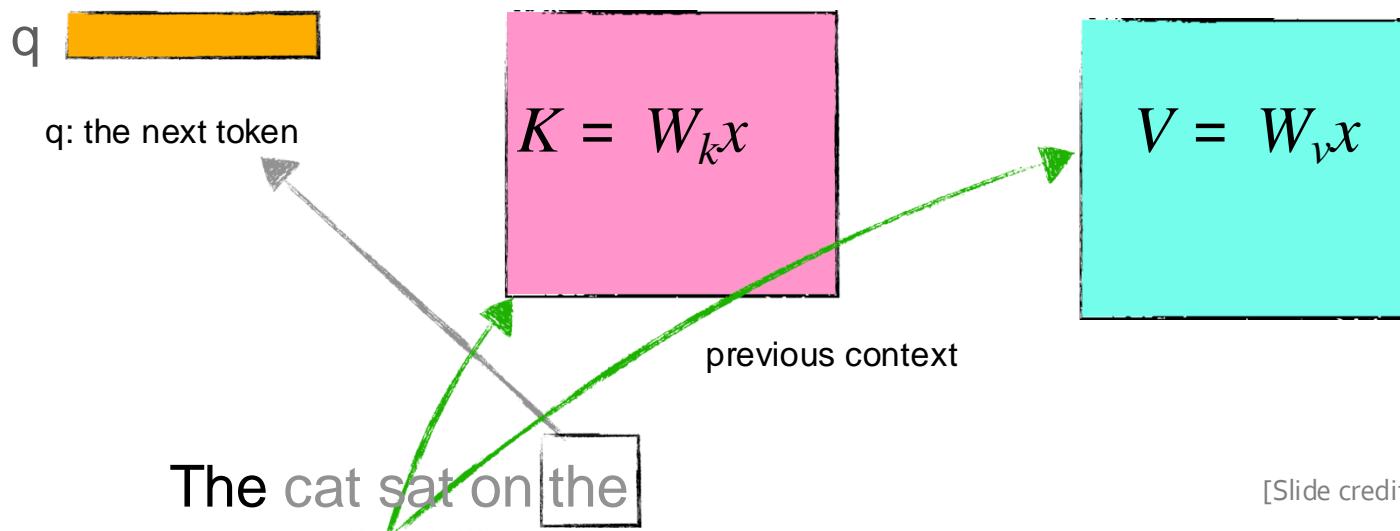
Self-Attention During Inference

$$Q = \mathbf{x}W^q$$

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[Slide credit: Arman Cohan]

Self-Attention During Inference

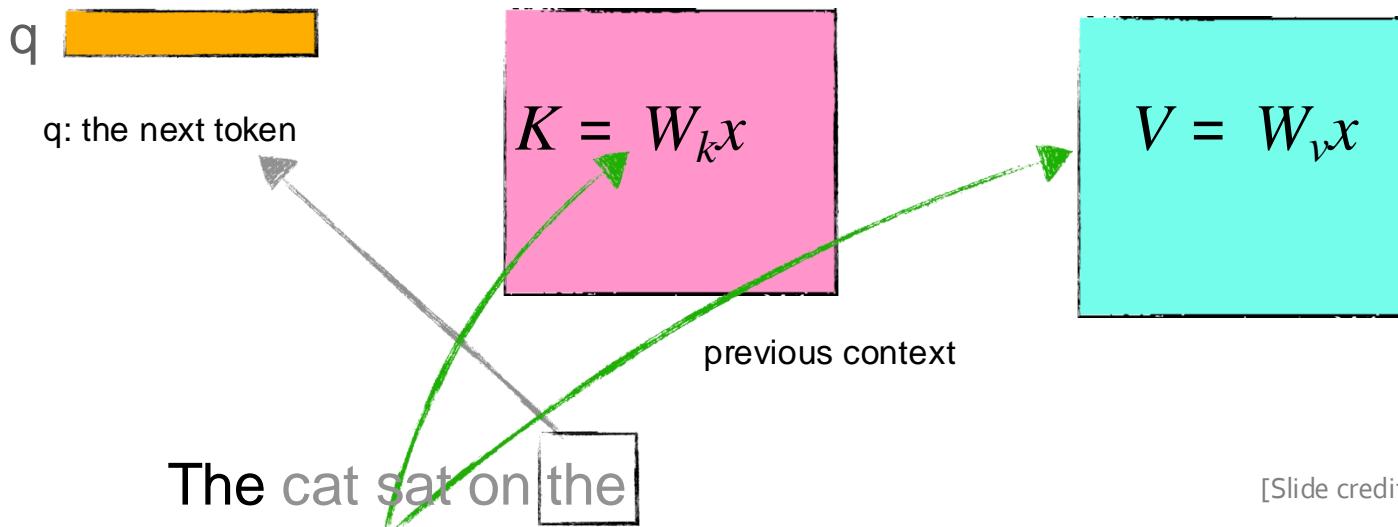
- We are computing the Keys and Values many times!
 - Let's reduce redundancy! 😊

$$Q = \mathbf{x}W^q$$

$$K = \mathbf{x}W^k$$

$$V = \mathbf{x}W^v$$

$$\text{Attention}(\mathbf{x}) = \text{softmax}\left(\frac{QK^T}{\sqrt{d}}\right)V$$



[Slide credit: Arman Cohan]

KV-Cache for reducing inference redundancy

- We are computing the Keys and Values many times!
 - Let's reduce redundancy! 😊

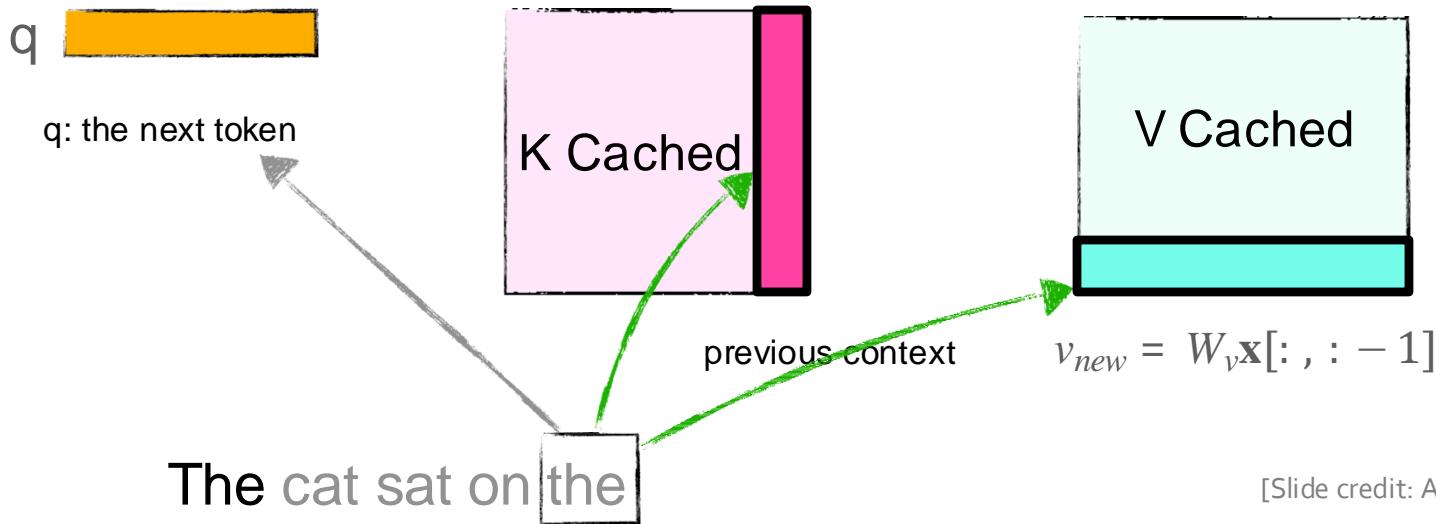
$$k_{new} = W_k \mathbf{x}[:, :, -1]$$

$$Q = \mathbf{x}W^q$$

$$K = \mathbf{x}W^k$$

$$V = \mathbf{x}W^v$$

$$\text{Attention}(\mathbf{x}) = \text{softmax}\left(\frac{QK^T}{\sqrt{d}}\right)V$$



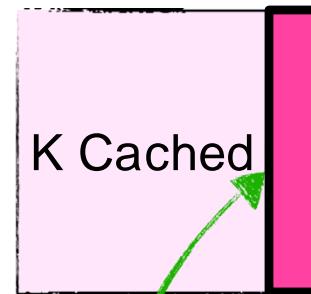
[Slide credit: Arman Cohan]

Quiz: KV-Cache

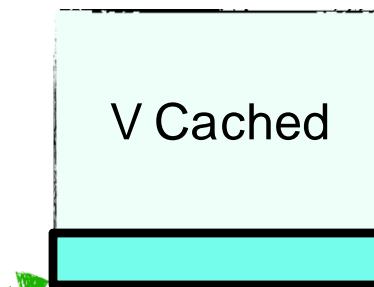
- Question: How much memory does this K, V cache require?

$$k_{new} = W_k \mathbf{x}[:, :, -1]$$

q
q: the next token



previous context



$$v_{new} = W_v \mathbf{x}[:, :, -1]$$

The cat sat on the

[Slide credit: Arman Cohan]

Recap

- To avoid redundant computations during decoding time, KV-cache is used to keep track of previous calculations of keys and values.
- But how exactly how costly are these computations?

Decoding Computations

Notice we're doing this computations for one token

Compared to the previous table (SA for a seq of length n), all the cells have one less dependence on n (e.g., $n^2 \rightarrow n$ or $n \rightarrow 1$).

Dimensions	Operation	Computations	IO
$\mathbf{x} \in \mathbb{R}^{b \times 1 \times d}, \mathbf{W}_i^q \in \mathbb{R}^{d \times \frac{d}{m}}$	Query/key computations get combined with KV-cache	$O(bd^2)$	$O(d^2 + 2bd)$
$\mathbf{Q}_i, \mathbf{K}_i \in \mathbb{R}^{b \times 1 \times \frac{d}{m}} + \text{KV-cache}$	$P_i \leftarrow \text{softmax}\left(\frac{\mathbf{Q}_i \mathbf{K}_i^T}{\sqrt{d/m}}\right)$ for m heads	$O(bnd)$	$O(bnm + bnd + bd)$
$\mathbf{V}_i \in \mathbb{R}^{b \times 1 \times \frac{d}{m}}, P_i \in \mathbb{R}^{b \times n \times 1}$	$\text{head}_i \leftarrow P_i \mathbf{V}_i$ for m heads	$O(bnd)$	$O(bnm + bnd + bd)$
$\mathbf{W}^o \in \mathbb{R}^{d \times d}, \text{head}_i \in \mathbb{R}^{b \times 1 \times \frac{d}{m}}$	$Y = \text{Concat}(\text{head}_1, \dots, \text{head}_m) \mathbf{W}^o$	$O(bd^2)$	$O(2bd + d^2)$
$Y \in \mathbb{R}^{b \times 1 \times d}, \mathbf{W}_1 \in \mathbb{R}^{d \times d_{ff}}, \mathbf{W}_2 \in \mathbb{R}^{d_{ff} \times d}$	$Y = \text{ReLU}(Y \mathbf{W}_1) \mathbf{W}_2$	$O(16bd^2)$	$O(2bd + 8d^2)$
---	Total	$O(bd^2 + bnd)$	$O(bmn + bnd + d^2)$

Now the computations (of next token) has linear dependence on seq length.

b : batch size,
 n : sequence length **thus far**,
 m : number of heads
 d : feature dimension in output of SA
 $d_{ff} = 4d$: feature dimension inside FFN

Summary: Computational Complexity of Transformers

- **Process a sequence at once:** Computation is bounded by $O(n^2)$.
- **Processing one token at a time during inference:**
 - **KV-Cache:** To avoid redundant computations during decoding time, KV-cache is used to keep track of previous calculations of keys and values.
 - The computation is bounded by $O(n)$.
- Though in all cases, the computations are penalizable (modulo Transformer layers).
- **IO bottlenecks:** we will get to this (next chapter).

Writing our own Transformer

Clone Helper Function

- Create N copies of pytorch nn.Module
- The Transformer's structure contains a lot of design repetition (like VGG)
- Remember these clones shouldn't share parameters (for the most part)

```
def clones(module, N):
    "Produce N identical layers."
    return nn.ModuleList([copy.deepcopy(module) for _ in range(N)])
```

Create Embedding

- Create vector representation of sequence vocabulary
- nn.Embedding creates a lookup table to map sequence vocabulary to unique vectors

```
class Embeddings(nn.Module):  
    def __init__(self, d_model, vocab):  
        super(Embeddings, self).__init__()  
        self.lut = nn.Embedding(vocab, d_model)  
        self.d_model = d_model  
  
    def forward(self, x):  
        return self.lut(x) * math.sqrt(self.d_model)
```

Positional Encoding

- Add information about an element's position in a sequence to its representation
- Element wise addition of sinusoidal encoding



```
class PositionalEncoding(nn.Module):
    "Implement the PE function."

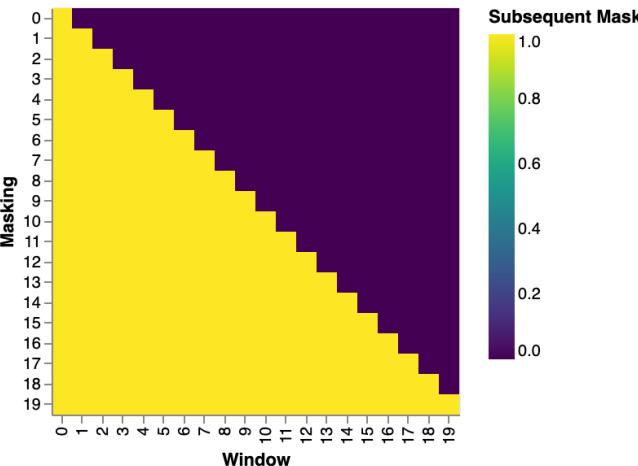
    def __init__(self, d_model, dropout, max_len=5000):
        super(PositionalEncoding, self).__init__()
        self.dropout = nn.Dropout(p=dropout)

        # Compute the positional encodings once in log space.
        pe = torch.zeros(max_len, d_model)
        position = torch.arange(0, max_len).unsqueeze(1)
        div_term = torch.exp(
            torch.arange(0, d_model, 2) * -(math.log(10000.0) / d_model))
        pe[:, 0::2] = torch.sin(position * div_term)
        pe[:, 1::2] = torch.cos(position * div_term)
        pe = pe.unsqueeze(0)
        self.register_buffer("pe", pe)

    def forward(self, x):
        x = x + self.pe[:, :, :x.size(1)].requires_grad_(False)
        return self.dropout(x)
```

Attention block

```
def attention(query, key, value, mask=None, dropout=None):
    "Compute 'Scaled Dot Product Attention'"
    d_k = query.size(-1)
    scores = torch.matmul(query, key.transpose(-2, -1)) / math.sqrt(d_k)
    if mask is not None:
        scores = scores.masked_fill(mask == 0, -1e9)
    p_attn = scores.softmax(dim=-1)
    if dropout is not None:
        p_attn = dropout(p_attn)
    return torch.matmul(p_attn, value), p_attn
```



$-1e9$ is a large negative number, which leads to $\text{softmax}(-1e9) \approx 0$

Multi-Head Attention

```
class MultiHeadedAttention(nn.Module):
    def __init__(self, h, d_model, dropout=0.1):
        "Take in model size and number of heads."
        super(MultiHeadedAttention, self).__init__()
        assert d_model % h == 0
        # We assume d_v always equals d_k
        self.d_k = d_model // h
        self.h = h
        self.linears = clones(nn.Linear(d_model, d_model), 4)
        self.attn = None
        self.dropout = nn.Dropout(p=dropout)
```

```
def forward(self, query, key, value, mask=None):
    "Implements Figure 2"
    if mask is not None:
        # Same mask applied to all h heads.
        mask = mask.unsqueeze(1)
    nbatches = query.size(0)

    # 1) Do all the linear projections in batch from d_model => h x d_k
    query, key, value = [
        lin(x).view(nbatches, -1, self.h, self.d_k).transpose(1, 2)
        for lin, x in zip(self.linears, (query, key, value))
    ]

    # 2) Apply attention on all the projected vectors in batch.
    x, self.attn = attention(
        query, key, value, mask=mask, dropout=self.dropout
    )

    # 3) "Concat" using a view and apply a final linear.
    x = (
        x.transpose(1, 2)
        .contiguous()
        .view(nbatches, -1, self.h * self.d_k)
    )
    del query
    del key
    del value
    return self.linears[-1](x)
```

[Slide credit: CS886 at Waterloo]

FeedForward Layer

```
class PositionwiseFeedForward(nn.Module):
    "Implements FFN equation.

    def __init__(self, d_model, d_ff, dropout=0.1):
        super(PositionwiseFeedForward, self).__init__()
        self.w_1 = nn.Linear(d_model, d_ff)
        self.w_2 = nn.Linear(d_ff, d_model)
        self.dropout = nn.Dropout(dropout)

    def forward(self, x):
        return self.w_2(self.dropout(self.w_1(x).relu()))
```

Sublayer Connections

```
class SublayerConnection(nn.Module):
    """
    A residual connection followed by a layer norm.
    Note for code simplicity the norm is first as opposed to last.
    """

    def __init__(self, size, dropout):
        super(SublayerConnection, self).__init__()
        self.norm = LayerNorm(size)
        self.dropout = nn.Dropout(dropout)

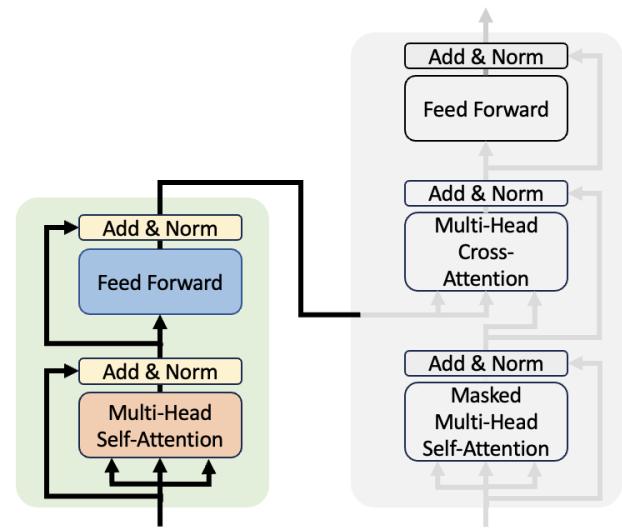
    def forward(self, x, sublayer):
        "Apply residual connection to any sublayer with the same size."
        return x + self.dropout(sublayer(self.norm(x)))
```

Encoder Layer

```
class EncoderLayer(nn.Module):
    "Encoder is made up of self-attn and feed forward (defined below)"

    def __init__(self, size, self_attn, feed_forward, dropout):
        super(EncoderLayer, self).__init__()
        self.self_attn = self_attn
        self.feed_forward = feed_forward
        self.sublayer = clones(SublayerConnection(size, dropout), 2)
        self.size = size

    def forward(self, x, mask):
        "Follow Figure 1 (left) for connections."
        x = self.sublayer[0](x, lambda x: self.self_attn(x, x, x, mask))
        return self.sublayer[1](x, self.feed_forward)
```



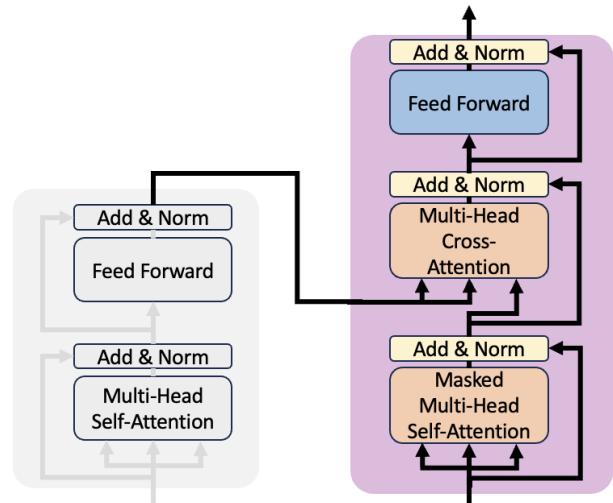
Decoder Layer

- Same as encoder layers other than:
 - the additional multi-head attention block to perform cross-attention with the output representation from the encoder

```
class DecoderLayer(nn.Module):
    "Decoder is made of self-attn, src-attn, and feed forward (defined below)"

    def __init__(self, size, self_attn, src_attn, feed_forward, dropout):
        super(DecoderLayer, self).__init__()
        self.size = size
        self.self_attn = self_attn
        self.src_attn = src_attn
        self.feed_forward = feed_forward
        self.sublayer = clones(SublayerConnection(size, dropout), 3)

    def forward(self, x, memory, src_mask, tgt_mask):
        "Follow Figure 1 (right) for connections."
        m = memory
        x = self.sublayer[0](x, lambda x: self.self_attn(x, x, x, tgt_mask))
        x = self.sublayer[1](x, lambda x: self.src_attn(x, m, m, src_mask))
        return self.sublayer[2](x, self.feed_forward)
```



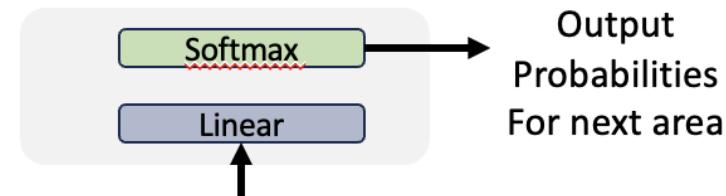
The Prediction Head

- A final linear mapping
- Apply softmax to convert logits to probabilities

```
class Generator(nn.Module):
    "Define standard linear + softmax generation step."

    def __init__(self, d_model, vocab):
        super(Generator, self).__init__()
        self.proj = nn.Linear(d_model, vocab)

    def forward(self, x):
        return log_softmax(self.proj(x), dim=-1)
```



Build each block

```
class Encoder(nn.Module):
    "Core encoder is a stack of N layers"

    def __init__(self, layer, N):
        super(Encoder, self).__init__()
        self.layers = clones(layer, N)
        self.norm = LayerNorm(layer.size)

    def forward(self, x, mask):
        "Pass the input (and mask) through each layer in turn."
        for layer in self.layers:
            x = layer(x, mask)
        return self.norm(x)
```

```
class Decoder(nn.Module):
    "Generic N layer decoder with masking."

    def __init__(self, layer, N):
        super(Decoder, self).__init__()
        self.layers = clones(layer, N)
        self.norm = LayerNorm(layer.size)

    def forward(self, x, memory, src_mask, tgt_mask):
        for layer in self.layers:
            x = layer(x, memory, src_mask, tgt_mask)
        return self.norm(x)
```

Putting it Together

```
class EncoderDecoder(nn.Module):
    """
    A standard Encoder-Decoder architecture. Base for this and many
    other models.
    """

    def __init__(self, encoder, decoder, src_embed, tgt_embed, generator):
        super(EncoderDecoder, self).__init__()
        self.encoder = encoder
        self.decoder = decoder
        self.src_embed = src_embed
        self.tgt_embed = tgt_embed
        self.generator = generator

    def forward(self, src, tgt, src_mask, tgt_mask):
        "Take in and process masked src and target sequences."
        return self.decode(self.encode(src, src_mask), src_mask, tgt, tgt_mask)

    def encode(self, src, src_mask):
        return self.encoder(self.src_embed(src), src_mask)

    def decode(self, memory, src_mask, tgt, tgt_mask):
        return self.decoder(self.tgt_embed(tgt), memory, src_mask, tgt_mask)
```

Initialize the model

```
def make_model(  
    src_vocab, tgt_vocab, N=6, d_model=512, d_ff=2048, h=8, dropout=0.1  
):  
    "Helper: Construct a model from hyperparameters."  
    c = copy.deepcopy  
    attn = MultiHeadedAttention(h, d_model)  
    ff = PositionwiseFeedForward(d_model, d_ff, dropout)  
    position = PositionalEncoding(d_model, dropout)  
    model = EncoderDecoder(  
        Encoder(EncoderLayer(d_model, c(attn), c(ff), dropout), N),  
        Decoder(DecoderLayer(d_model, c(attn), c(attn), c(ff), dropout), N),  
        nn.Sequential(Embeddings(d_model, src_vocab), c(position)),  
        nn.Sequential(Embeddings(d_model, tgt_vocab), c(position)),  
        Generator(d_model, tgt_vocab),  
    )  
  
    # This was important from their code.  
    # Initialize parameters with Glorot / fan_avg.  
    for p in model.parameters():  
        if p.dim() > 1:  
            nn.init.xavier_uniform_(p)  
    return model
```