JOHNS HOPKINS
WHITING SCHOOL of ENGINEERING

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

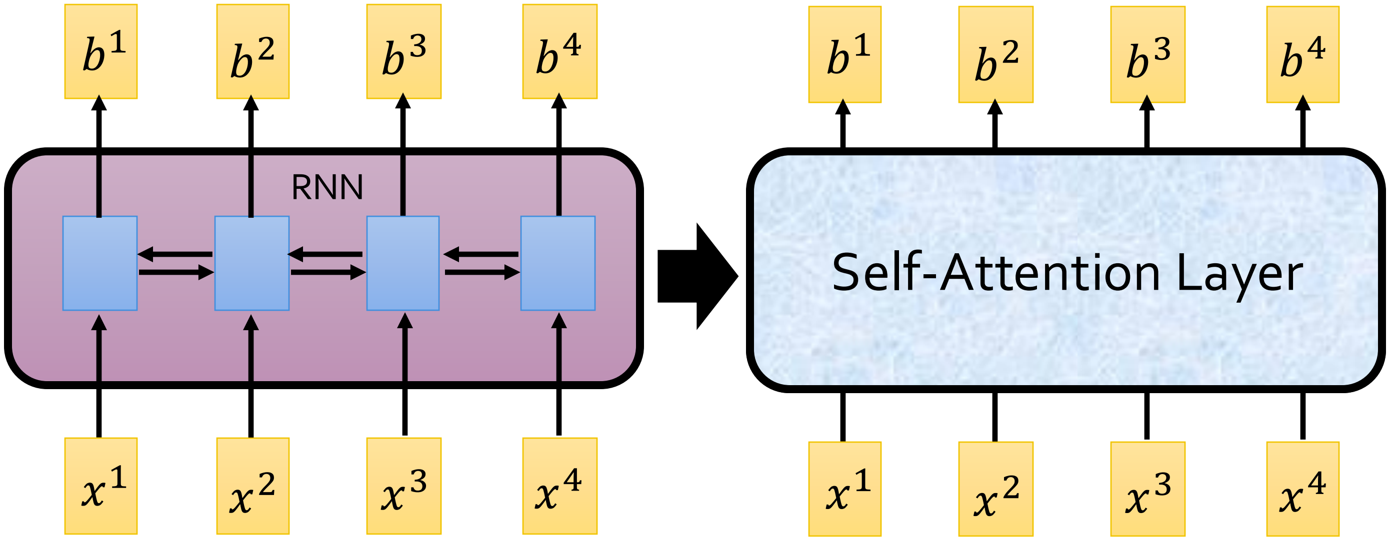
1. Self-Attention module
2. Transformer architecture
3. Computation/space cost
4. Thinking about Transformer implementation

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

Self-Attention Module

Self-Attention

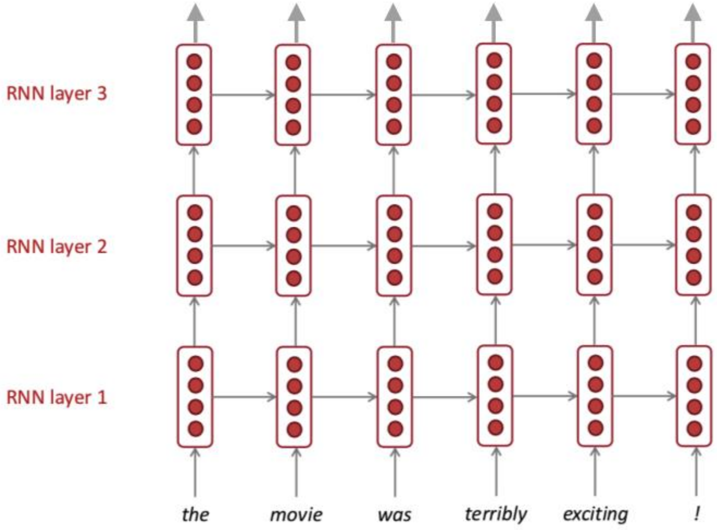
- b^i is obtained based on the whole input sequence.
- can be parallelly computed.

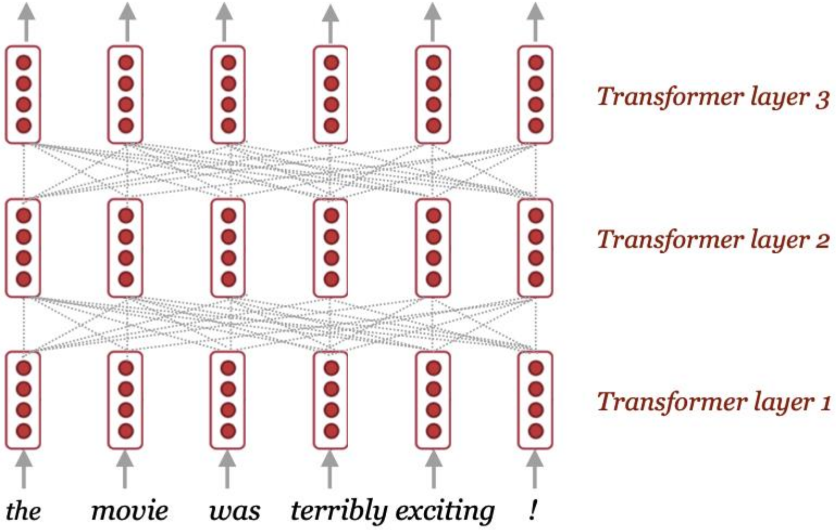


Idea: replace any thing done by RNN with self-attention.

"Neural machine translation by jointly learning to align and translate" Bahdanau etl. 2014;
"Attention is All You Need" Vaswani et al. 2017

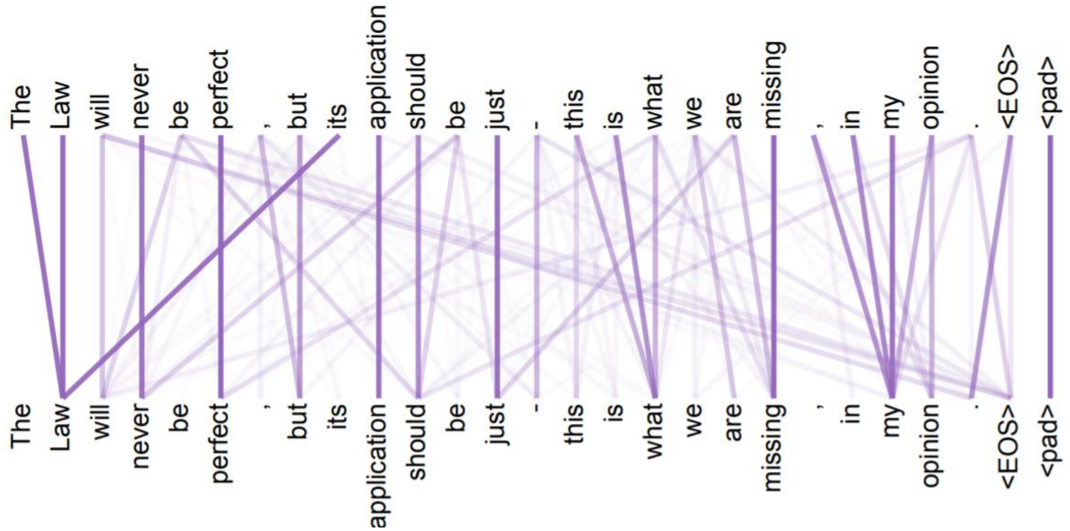
RNN vs Transformer





Attention

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



[Attention Is All You Need, Vaswani et al. 2017]

Defining Self-Attention

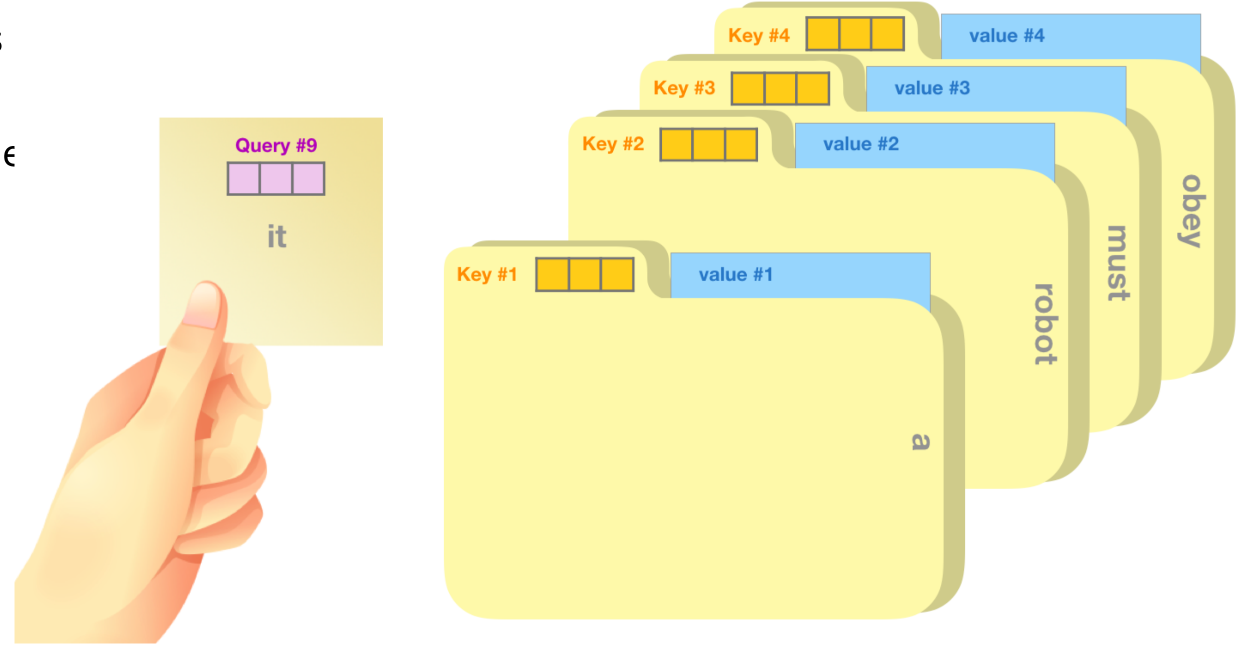
- Terminology:
  - Query: to match others
  - Key: to be matched
  - Value: information to be extracted

[Vaswani et al. 2017: https://arxiv.org/abs/1706.03762]

Defining Self-Attention

An analogy ....

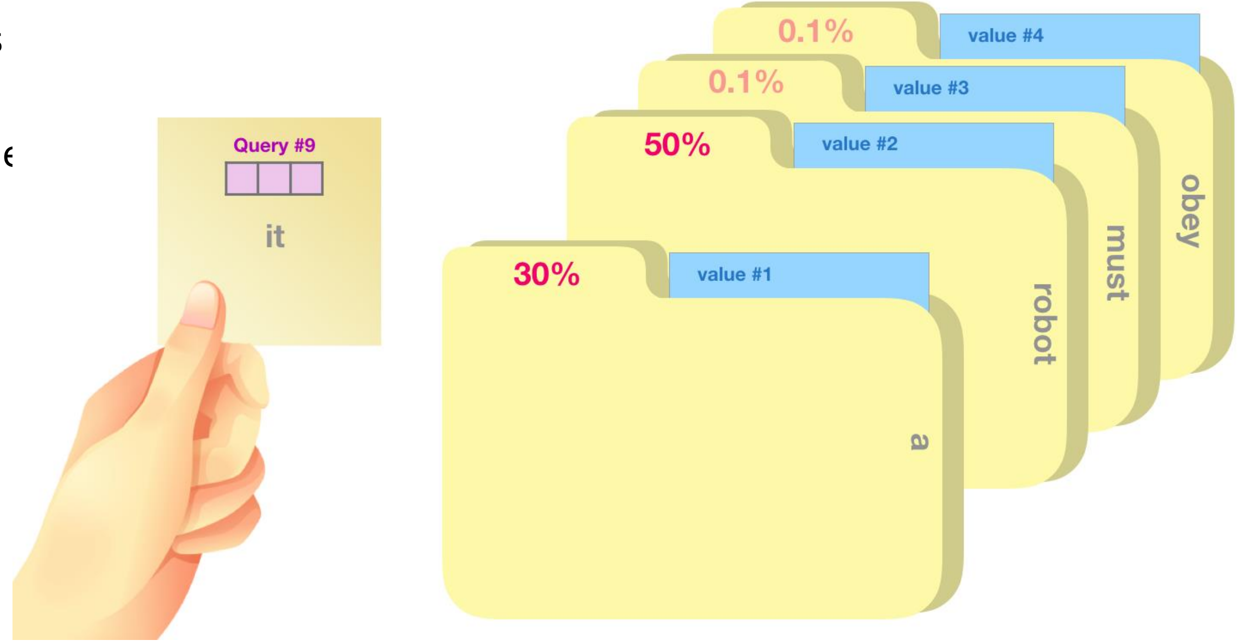
- Terminology:
  - Query: to match others
  - Key: to be matched
  - Value: information to be



[Vaswani et al. 2017: https://arxiv.org/abs/1706.03762]

Defining Self-Attention

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



[Vaswani et al. 2017: https://arxiv.org/abs/1706.03762]

q: query (to match others)

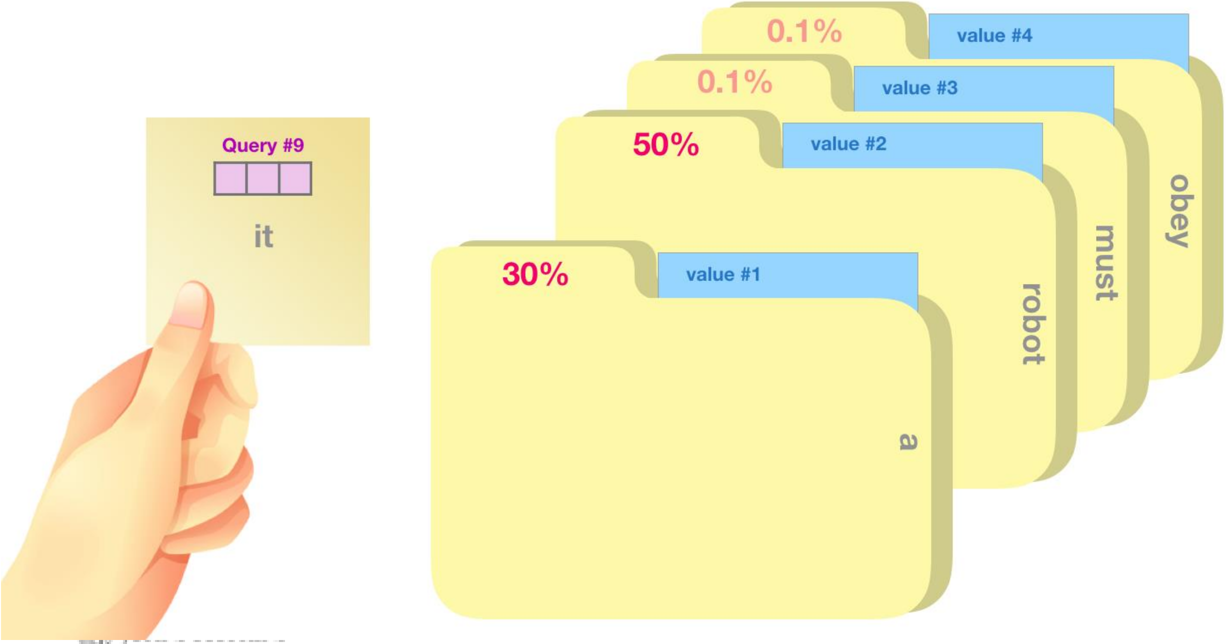
$$q_i = W^q x_i$$

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)

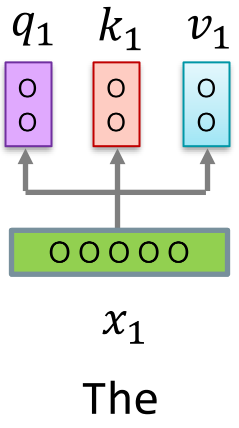
$$q_i = W^q x_i$$

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)

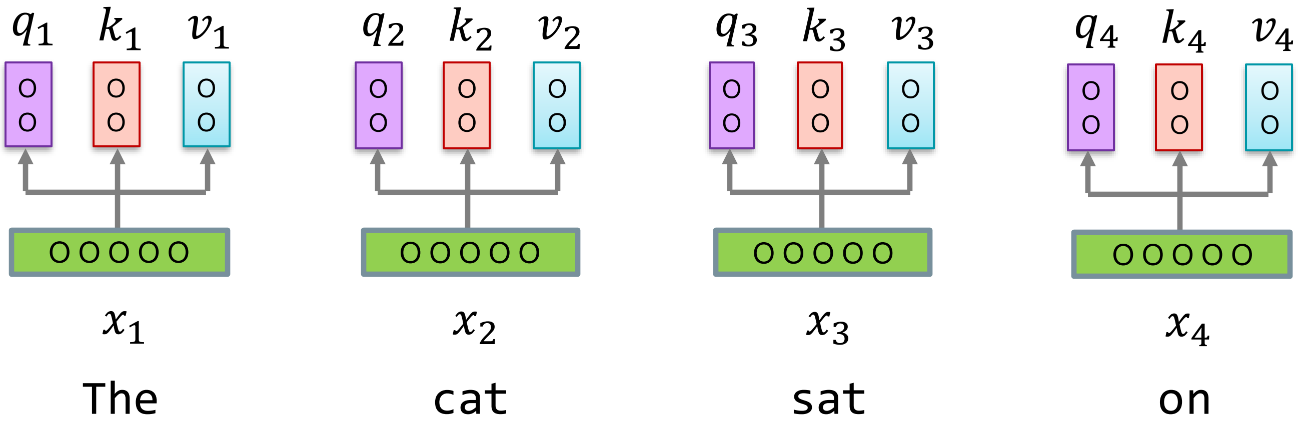
$$q_i = W^q x_i$$

k: key (to be matched)

$$k_i = W^k x_i$$

v: value (information to be extracted)

$$v_i = W^v x_i$$



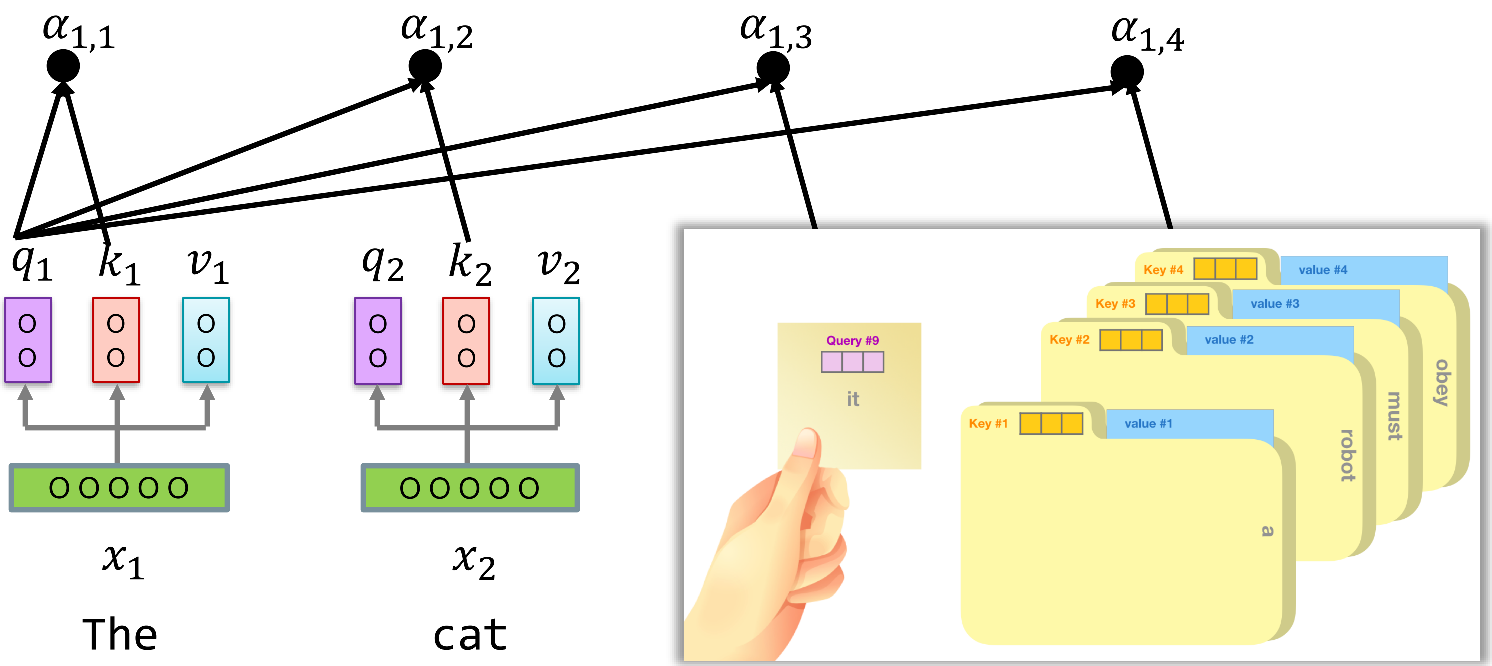
$$\underbrace{\alpha_{1,i} = q^1 \cdot k^i \big/ \sqrt{d}}_{\text{Scaled dot product}}$$

q: query (to match others)

k: key (to be matched)

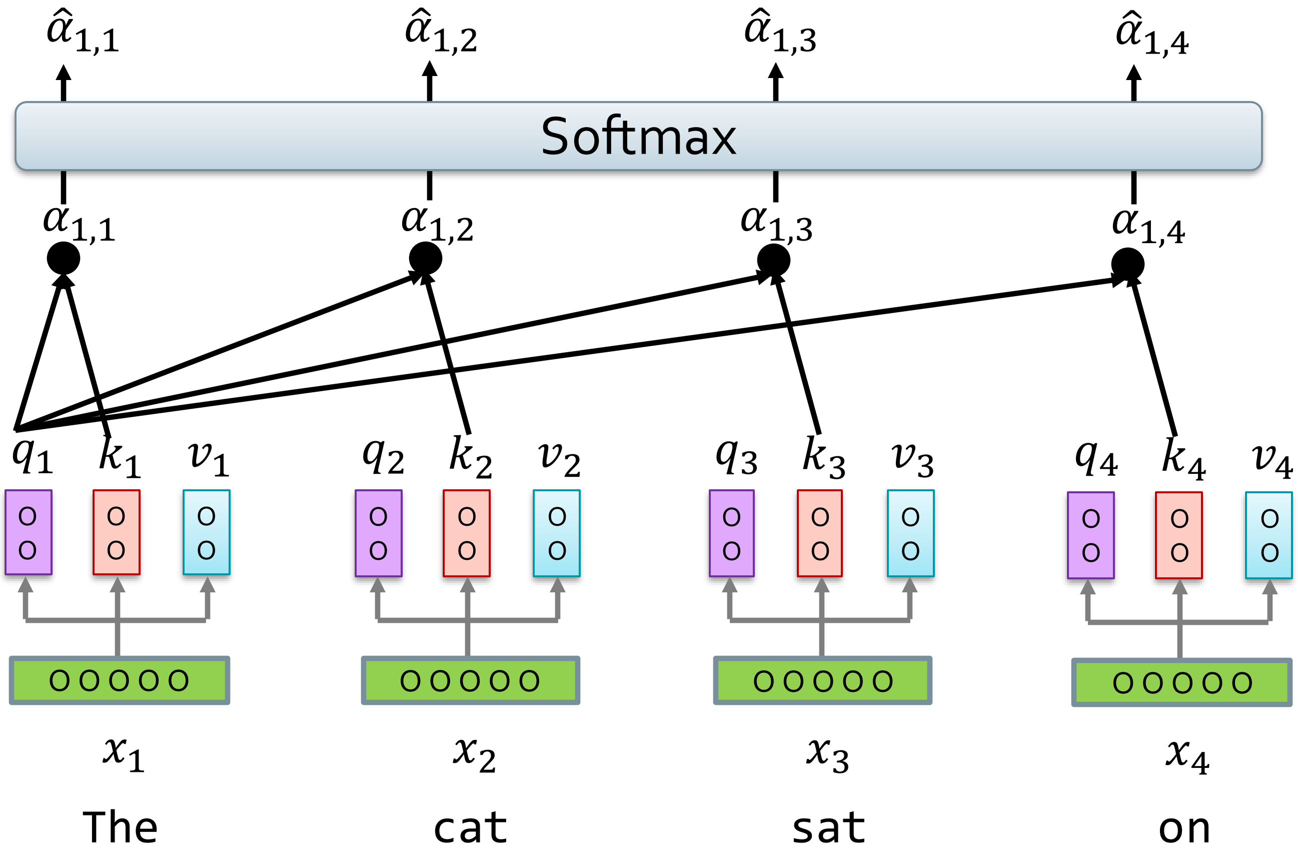
v: value (information to be extracted)

How much should "The" attend to other positions?



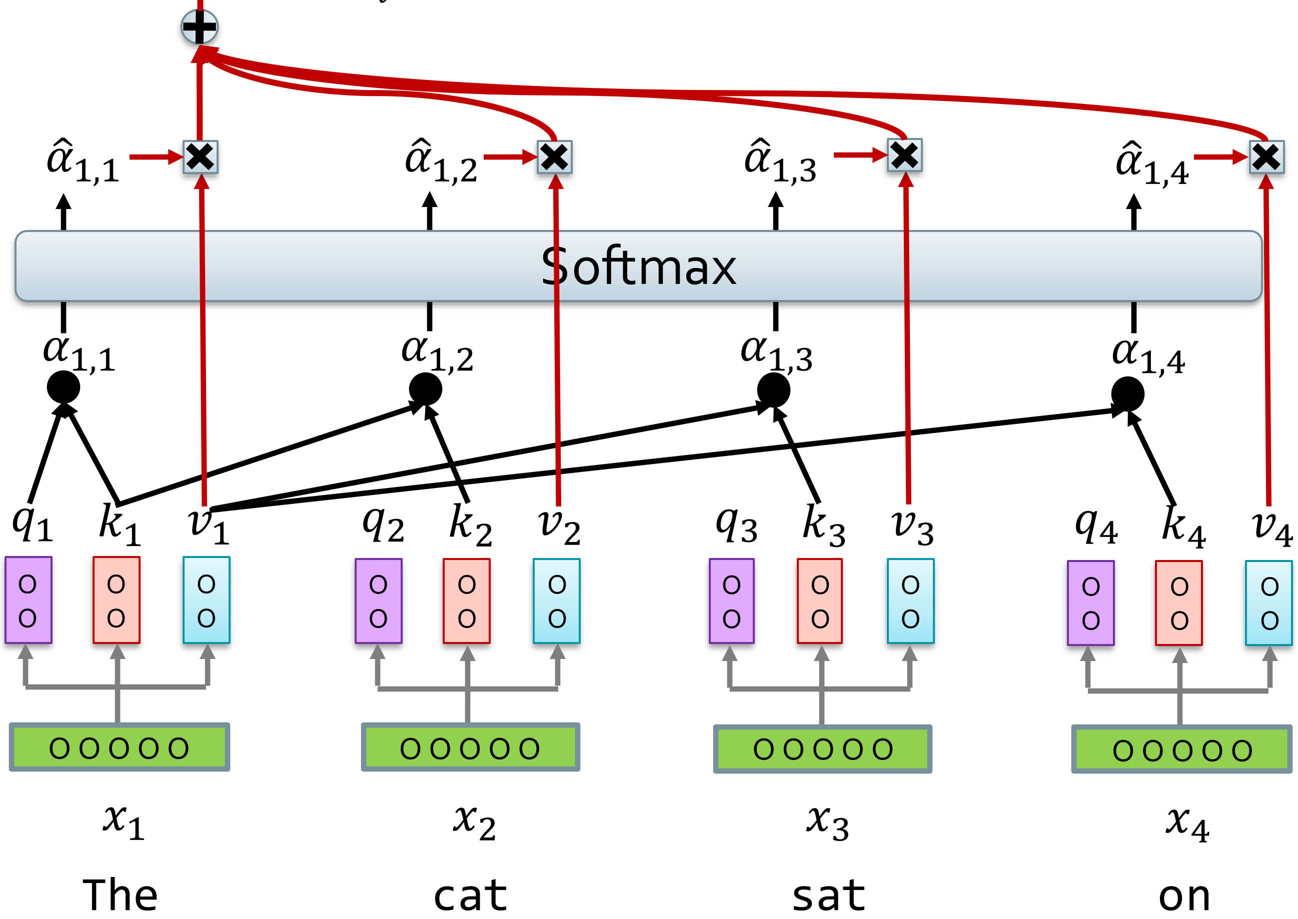
$$\sigma(z)_i = \frac{\exp(z_i)}{\sum_j \exp(z_j)}$$

How much should "The" attend to other positions?



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

Representation of "The" given the attention weights



Question

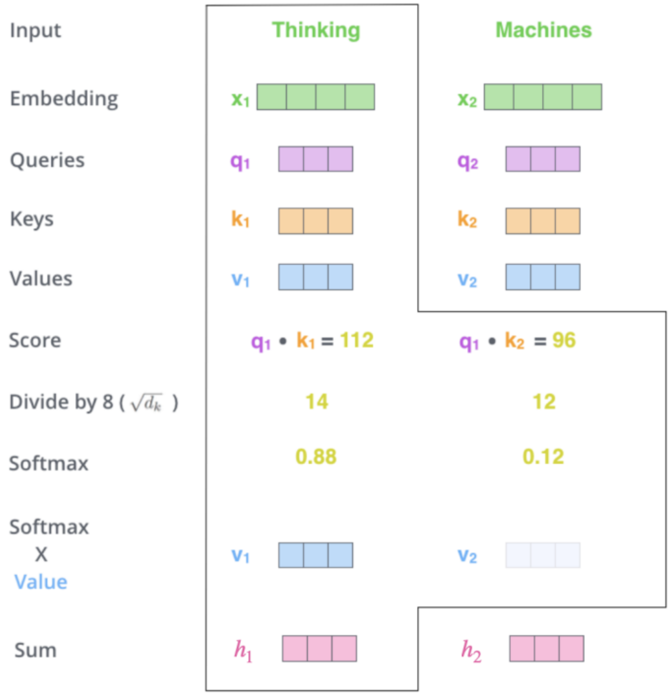
- What would be the output vector for the word "Thinking"?

(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) $0.12\mathbf{v}_1 + 0.88\mathbf{v}_2$



[Slide credit: Danqi Chen]

Self-Attention: Matrix Notation

$X \in \mathbb{R}^{n \times d_1}$ (n = input length)

$Q = XW^Q \quad K = XW^K \quad V = XW^V$

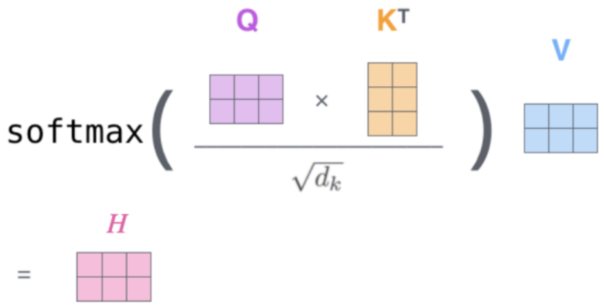
$W^Q \in \mathbb{R}^{d_1 \times d_q}, W^K \in \mathbb{R}^{d_1 \times d_k}, W^V \in \mathbb{R}^{d_1 \times d_v}$

$n \times d_q$ $\quad$ $d_k \times n$

$$\boxed{\text{Attention}(Q, K, V) = \text{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right)V}$$

n :

Q: What is this softmax operation?



[Slide credit: Danqi Chen]

Self-Attention

- Can write it in matrix form:

- Given input $\mathbf{x}$:

$$Q = \mathbf{W}^q \mathbf{x}$$
$$K = \mathbf{W}^k \mathbf{x}$$
$$V = \mathbf{W}^v \mathbf{x}$$

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

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, $X \in \mathbf{R}^{n\times d}$, is projected using three matrices $W_Q \in \mathbf{R}^{d\times d_q}$, $W_K \in \mathbf{R}^{d\times d_k}$, and $W_V \in \mathbf{R}^{d\times d_v}$ 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

$$Q = XW_Q, \quad K = XW_K, \quad V = XW_V. \tag{1}$$

So, self-attention can be written as,

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

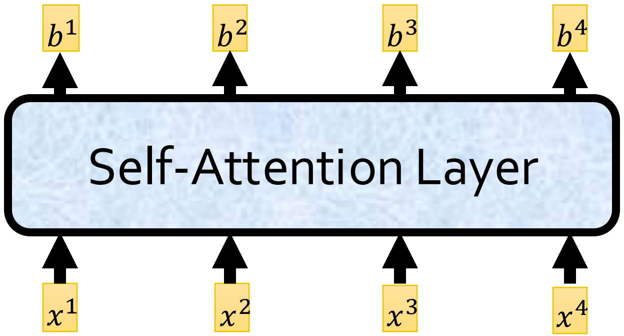
where softmax denotes a *row-wise* softmax normalization function. Thus, each element in S depends on all other elements in the same row.

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

553 Retweets 42 Quote Tweets 3,338 Likes

Self-Attention: 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.

[Attention Is All You Need, Vaswani et al. 2017]

Computational and Space Complexity

- The attention function:

$$\text{Attention}(Q, K, V) = \text{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right)V$$

- $\dim(QK^T) = N^2 \rightarrow O(N^2 d_k)$ time complexity to calculate QK.
- Attention matrix $\dim\left(\text{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right)\right) = N \times N$
  - Storing the attention matrix for each head $\rightarrow O(N^2 h)$.
- If $N \gg d_k, h$, the time and space complexity is $O(N^2)$.
  - Scalability, resource consumption, adoption, etc.

Computational and Space Complexity (2)

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

- *n* = sequence length, *d* = hidden dimension
- Quadratic complexity, but:
  - O(1) sequential operations (not linear like in RNN)

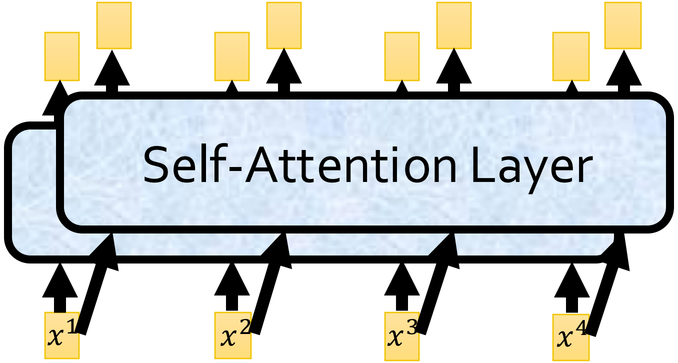
- Can be efficiently parallelized

[Attention Is All You Need, Vaswani et al. 2017]

Multi-Headed Self-Attention

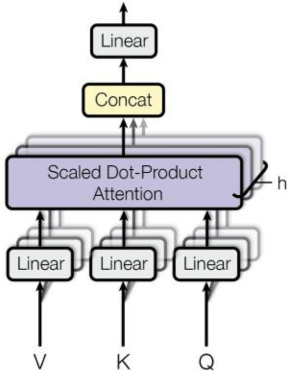
- Multiple parallel attention layers.
  - Each attention layer has its own parameters.
  - Concatenate the results and run them through a linear projection.

- Main idea: Allows model to jointly attend to information from different representation subspaces (like ensembling)



[Attention Is All You Need, Vaswani et al. 2017]

Multi-Headed Self-Attention



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

$$\mathrm{head}_i = \mathrm{Attention}\left(\mathbf{W}_i^q \mathbf{x}, \mathbf{W}_i^k \mathbf{x}, \mathbf{W}_i^v \mathbf{x}\right)$$
$$\mathrm{MultiHead}(Q, K, V) = \mathrm{Concat}(\mathrm{head}_1, \dots, \mathrm{head}_h) W^O$$

- In practice, we use a reduced dimension for each head.
  - Denote: $d = \text{hidden dimension, m} = \text{number of heads}$

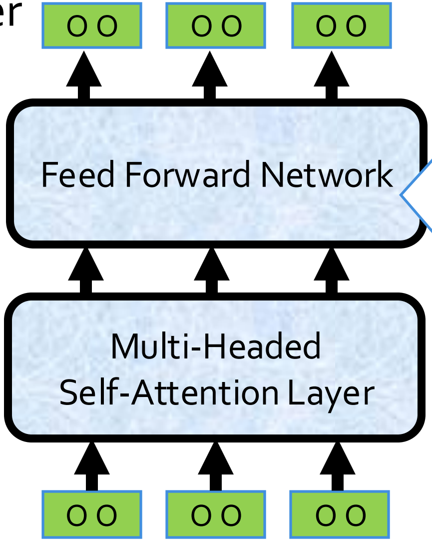
    $\mathbf{W}_i^q \in \mathbb{R}^{d \times \frac{d}{m}}$, $\mathbf{W}_i^k \in \mathbb{R}^{d \times \frac{d}{m}}$, $\mathbf{W}_i^v \in \mathbb{R}^{d \times \frac{d}{m}}$, $W^O \in \mathbb{R}^{d \times d}$

- The total computational cost is similar to that of single-hear attention with full dimensionality.

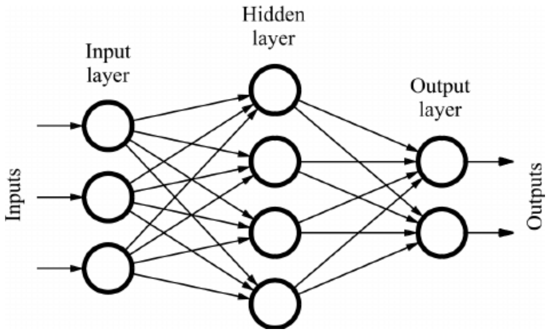
Combine with FFN

- 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.

$$\mathrm{FFN}(\mathbf{x}) = f(cW_1 + b_1)W_2 + b_2$$



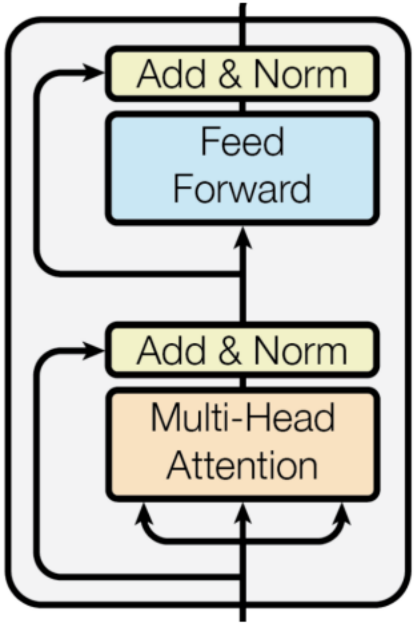
Feedforward Net: Refresher



A fully-connected network of nodes and weights.

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

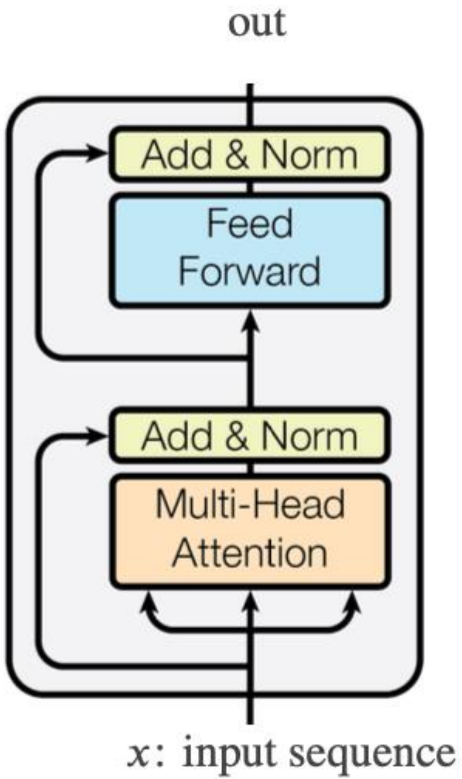


Putting it Together: Self-Attention Block

Given input $\mathbf{x}$:

$$\text{out} = LN(\tilde{\boldsymbol{c}} + \boldsymbol{c}')$$
$$\tilde{\boldsymbol{c}} = \text{FFN}(\boldsymbol{c}') = f(\boldsymbol{c}' W_1 + b_1) W_2 + b_2$$

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



Summary: Self-Attention Block

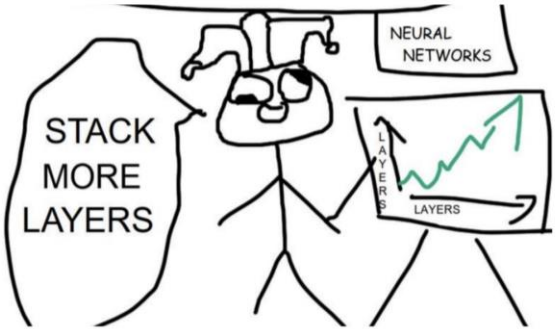
- **Self-Attention:** A critical building block of modern language models.
  - The idea is to compose meanings of words weighted according some similarity notion.

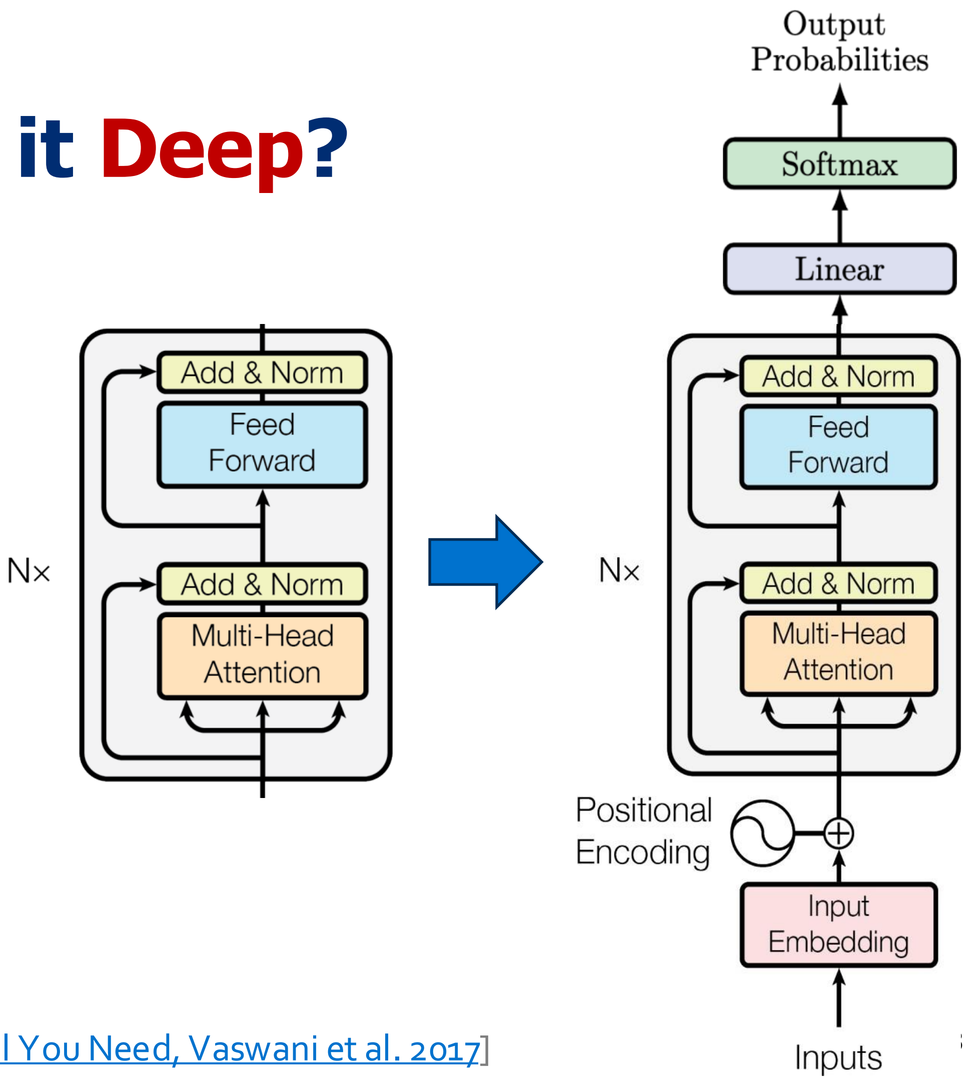
- **Next:** We will combine self-attention blocks to build various architectures known as Transformer.

Transformer

How Do We Make it Deep?

- Stack more layers!





[Attention Is All You Need, Vaswani et al. 2017]

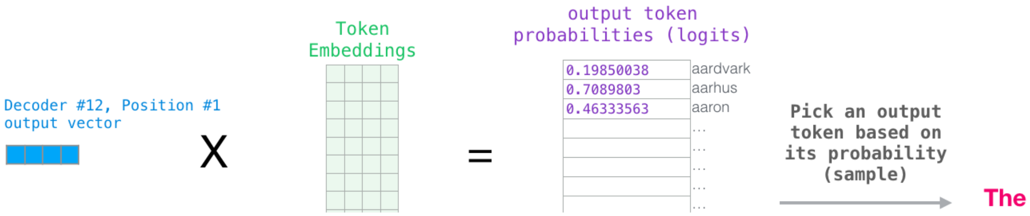
From Representations to Prediction

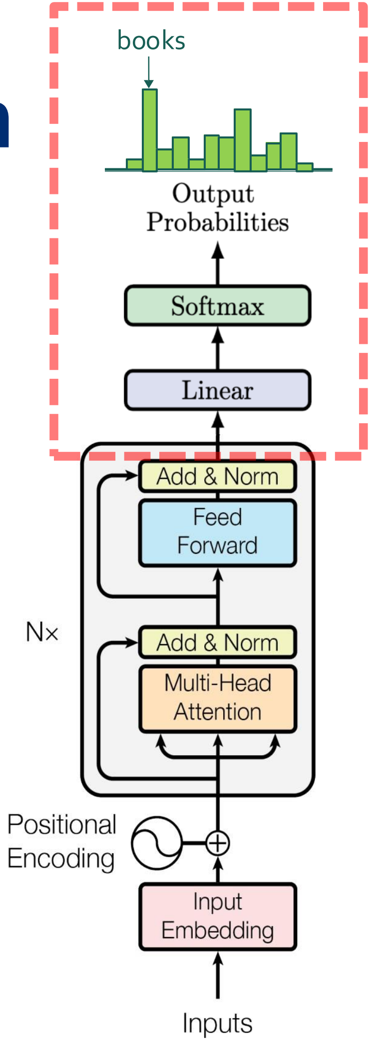
- To perform prediction, add a classification head on top of the final layer of the transformer.
- This can be per token (Language modeling)
- Or can be for the entire sequence (only one token)

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

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

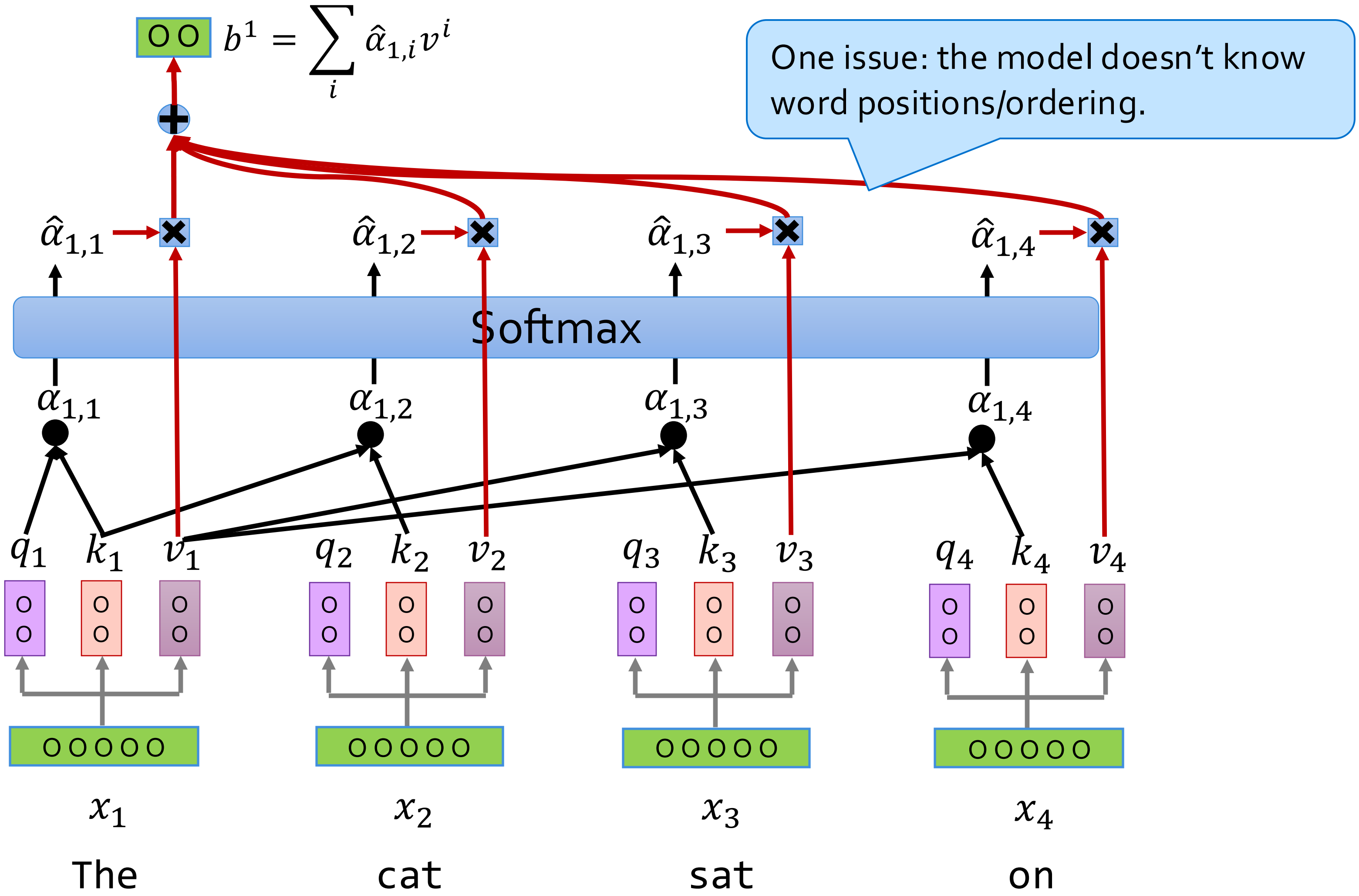
$$\text{probabilies} = \text{softmax}(\text{logits}) \in \mathbb{R}^{S \times V}$$



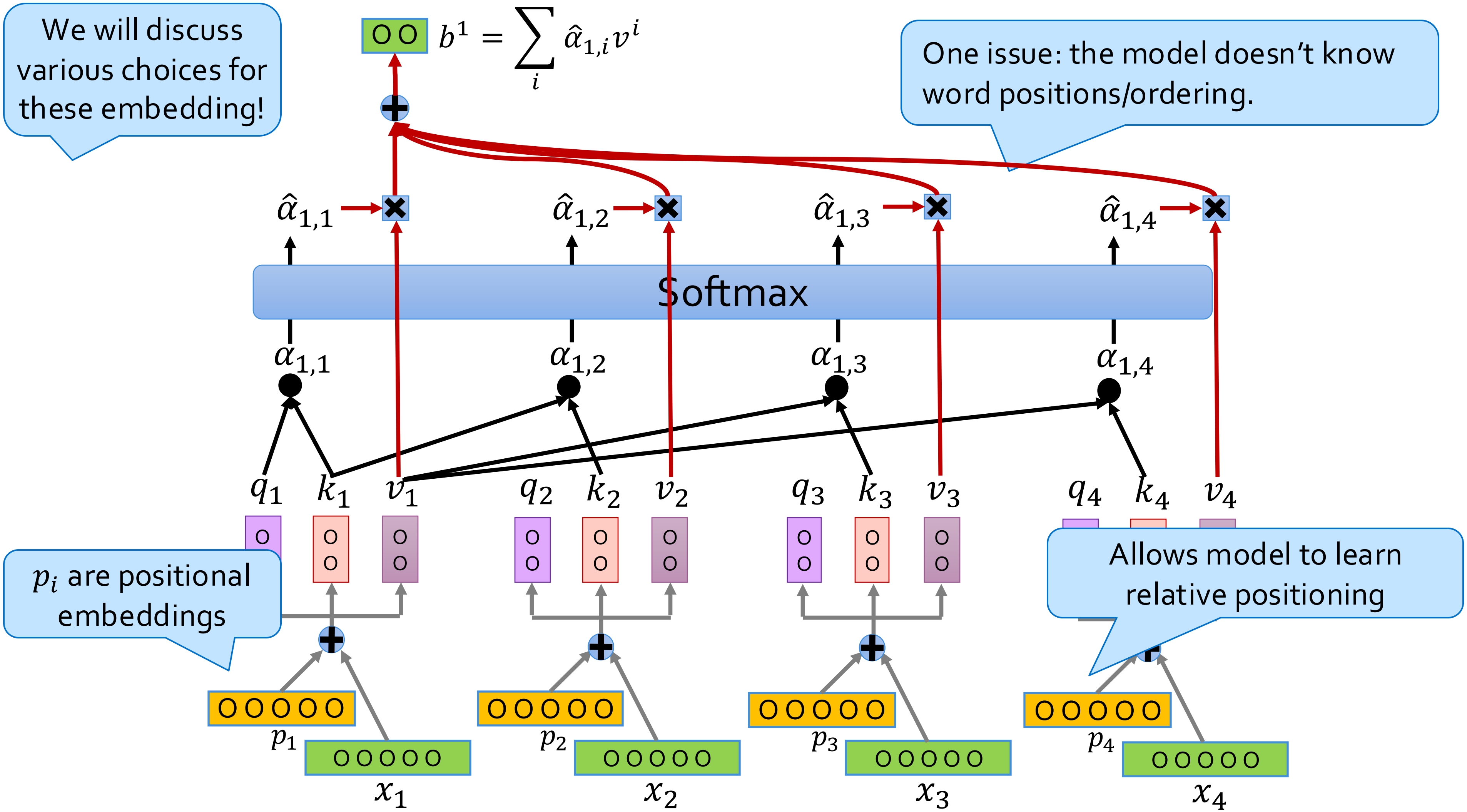


Johns Hopkins Whiting School of Engineering

One last wrinkle though …



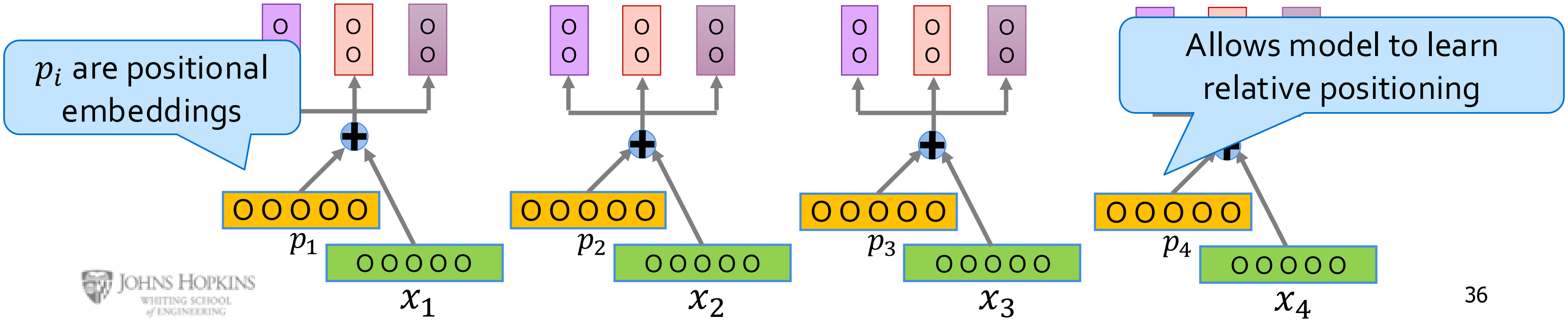
$b^1 = \sum_i \hat{\alpha}_{1,i} v^i$
One issue: the model doesn't know word positions/ordering.
$\hat{\alpha}_{1,1}$
$\hat{\alpha}_{1,2}$
$\hat{\alpha}_{1,3}$
$\hat{\alpha}_{1,4}$
Softmax
$\alpha_{1,1}$
$\alpha_{1,2}$
$\alpha_{1,3}$
$\alpha_{1,4}$
q_1 k_1 v_1
q_2 k_2 v_2
q_3 k_3 v_3
q_4 k_4 v_4
x_1
x_2
x_3
x_4
The
cat
sat
on



We will discuss various choices for these embedding!
$b^1 = \sum_i \hat{\alpha}_{1,i} v^i$
One issue: the model doesn't know word positions/ordering.
$\hat{\alpha}_{1,1}$ $\hat{\alpha}_{1,2}$ $\hat{\alpha}_{1,3}$ $\hat{\alpha}_{1,4}$
Softmax
$\alpha_{1,1}$ $\alpha_{1,2}$ $\alpha_{1,3}$ $\alpha_{1,4}$
q_1 k_1 v_1 q_2 k_2 v_2 q_3 k_3 v_3 q_4 k_4 v_4
p_i are positional embeddings
Allows model to learn relative positioning
p_1 p_2 p_3 p_4
x_1 x_2 x_3 x_4

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.



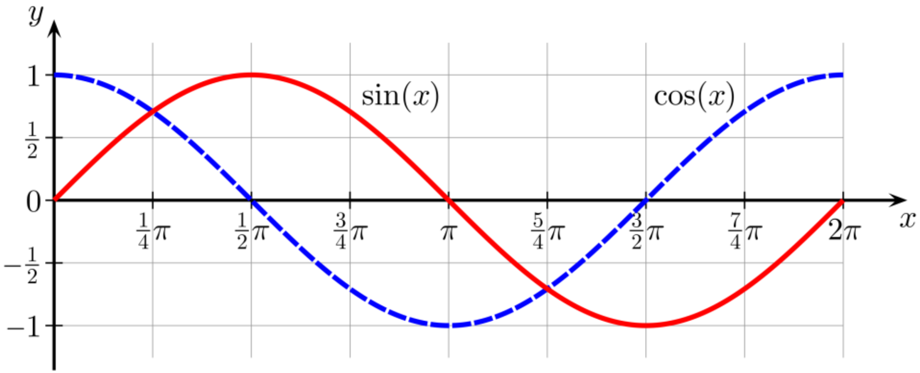
Absolute Positional Embeddings

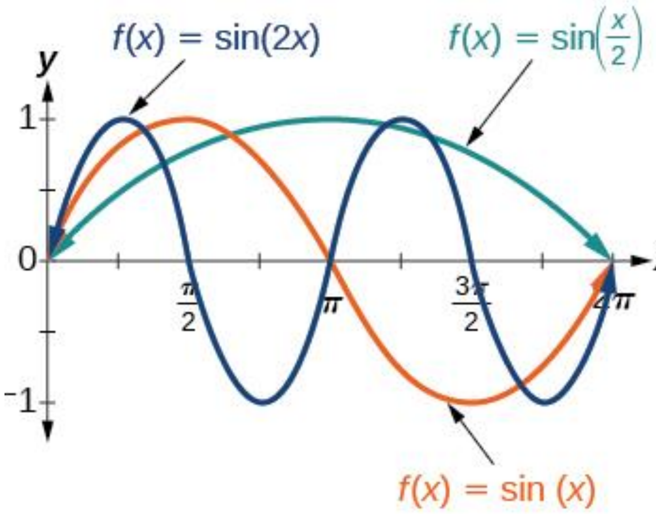
- The idea is to create vectors that uniquely encoder each position.
- For example, consider vectors of binary values.
  - Example below shows 4-dimensional position encodings for 16 positions.

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:

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

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

Quiz

- Let t be a desired position:

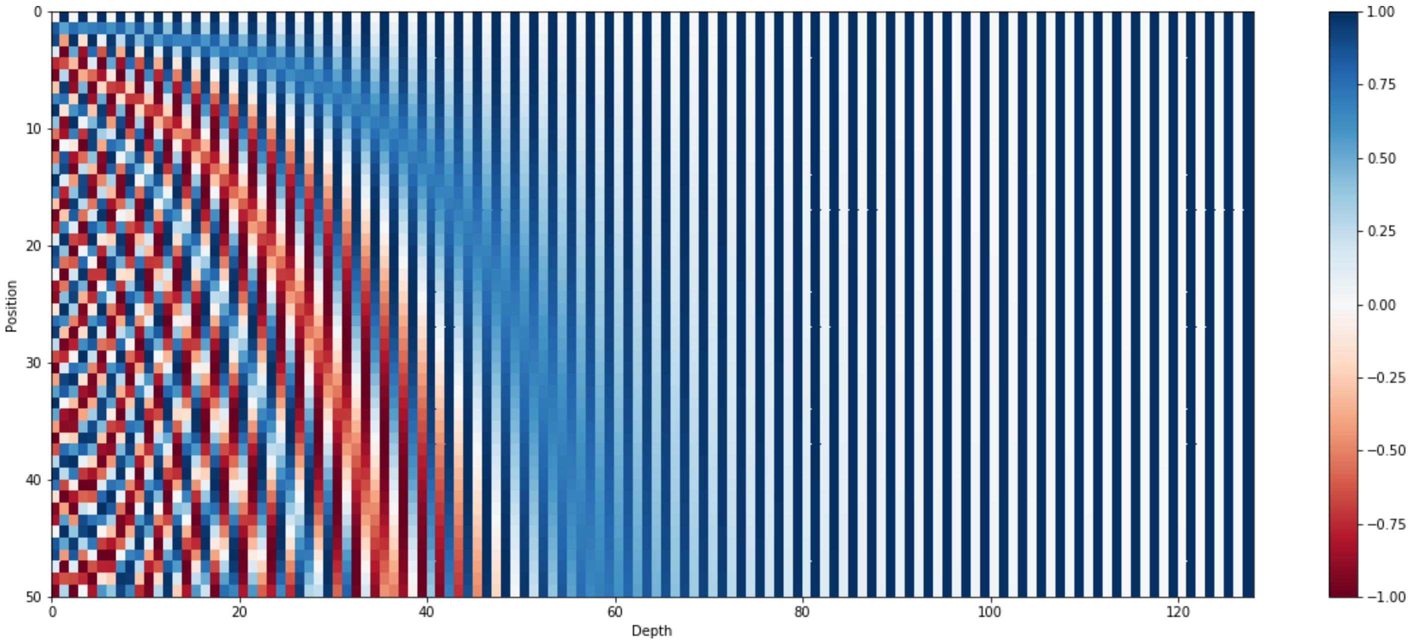
$$\vec{p_t}^{(i)} = f(t)^{(i)} := \begin{cases} \sin(\omega_k . t), & \text{if } i = 2k \\ \cos(\omega_k . t), & \text{if } i = 2k+1 \end{cases} \qquad \omega_k = \frac{1}{10000^{2k/d}}$$

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

https://kazemnejad.com/blog/transformer_architecture_positional_encoding/

Visualizing Absolute Positional Embeddings

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

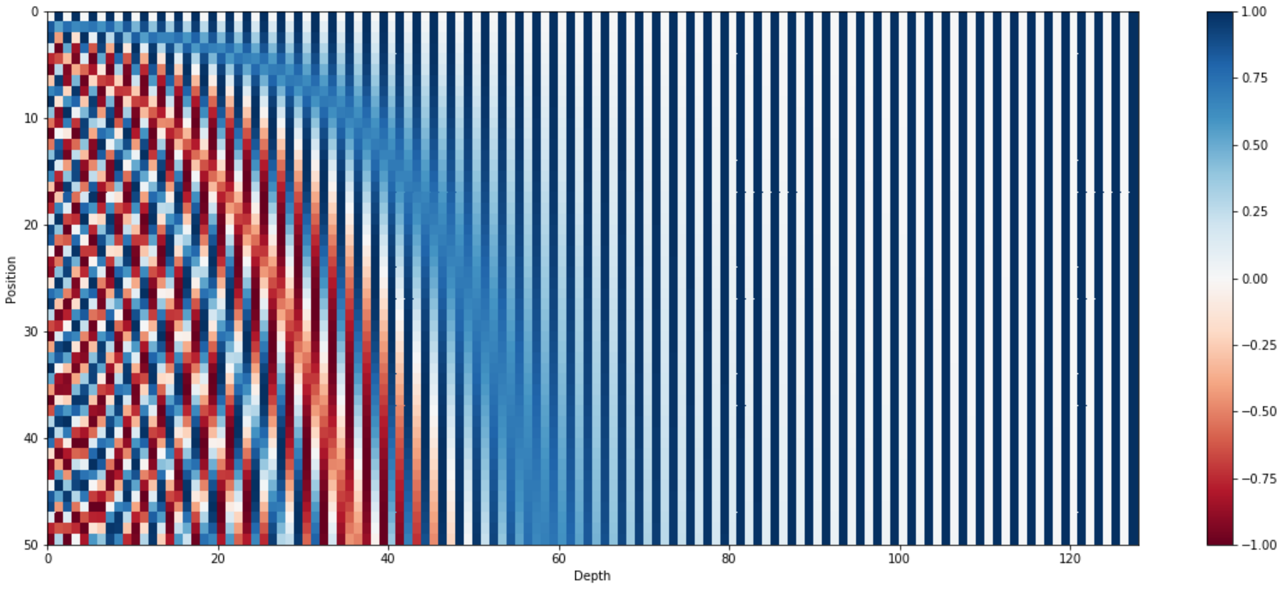


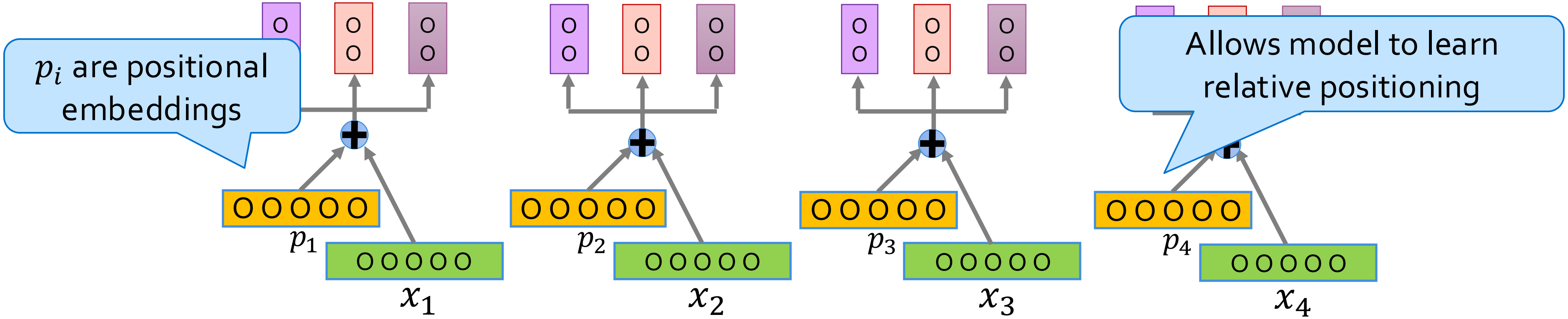
JOHNS HOPKINS
WHITING SCHOOL of ENGINEERING

An approach:

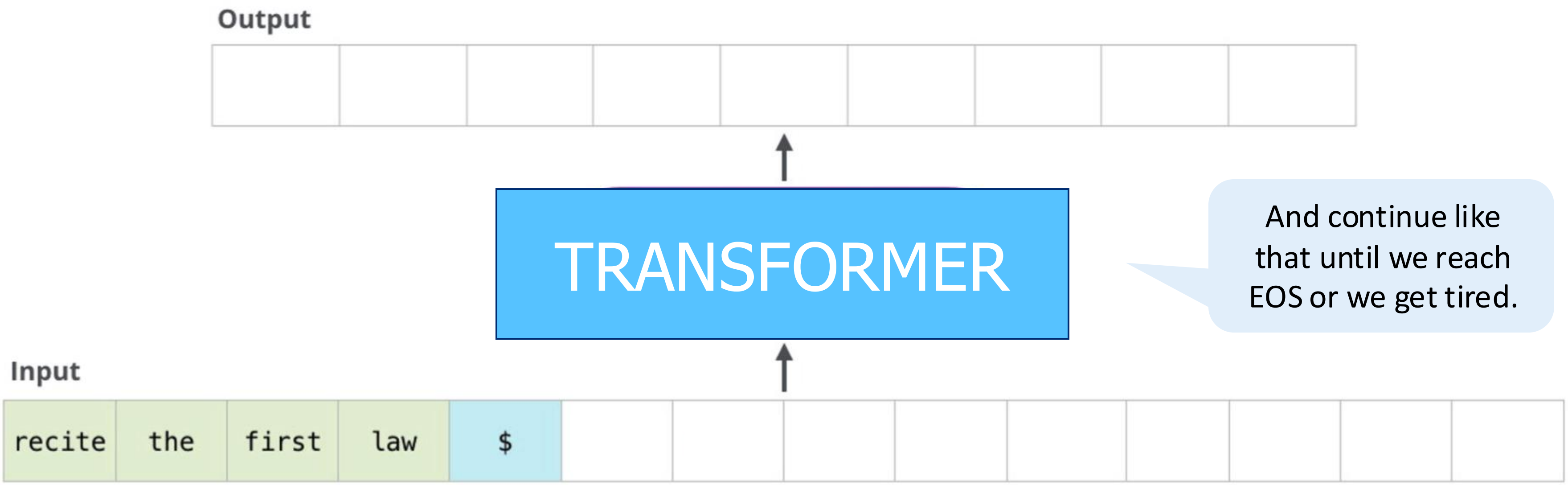
Sine/Cosine encoding

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





Transformer-based Language Modeling

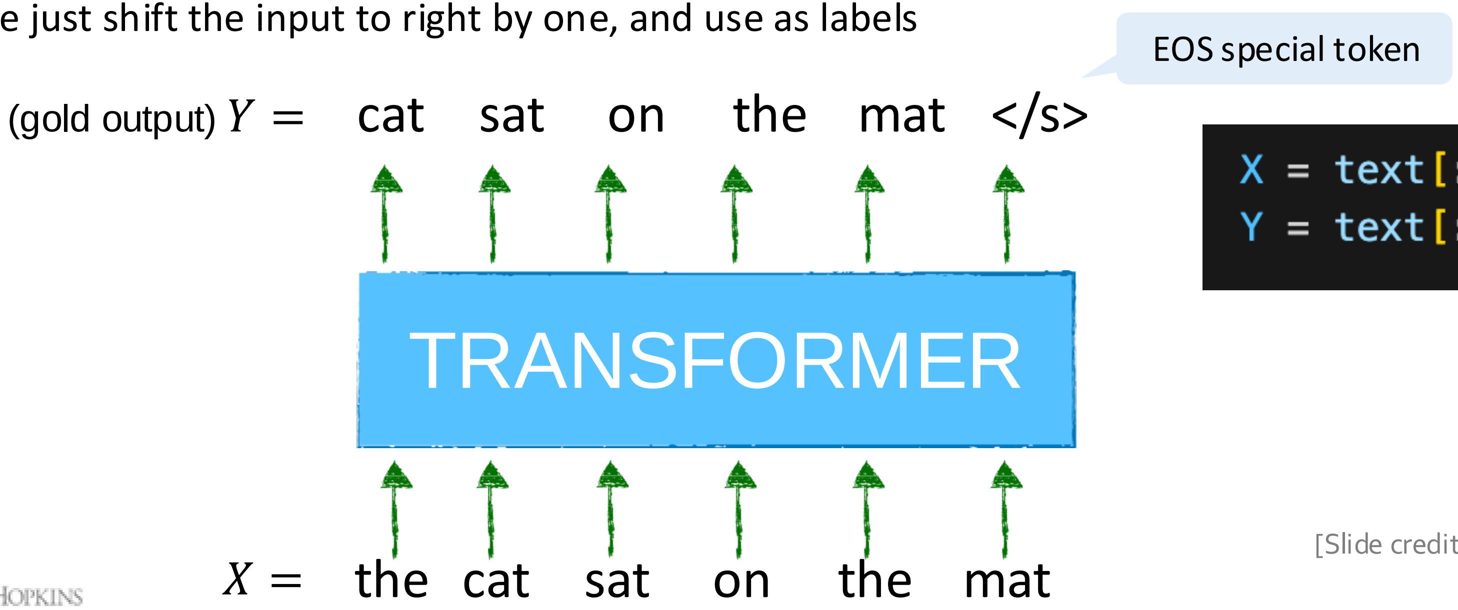


And continue like that until we reach EOS or we get tired.

Image by http://jalammar.github.io/illustrated-gpt2/

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



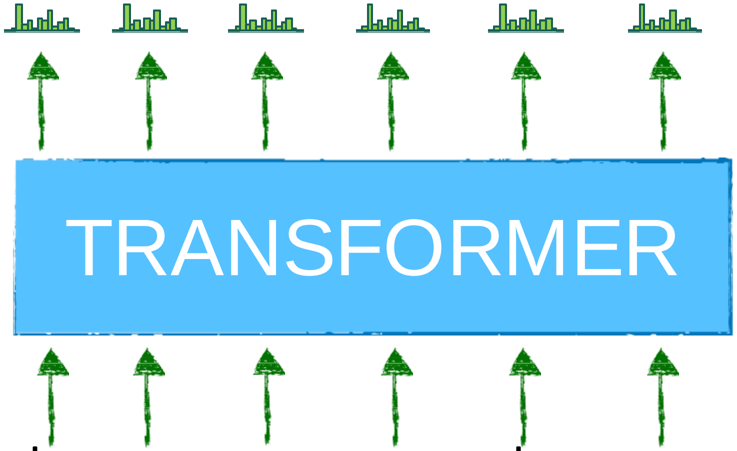

```
X = text[:, :-1]
Y = text[:, 1:]
```

[Slide credit: Arman Cohan]

Training a Transformer Language Model

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

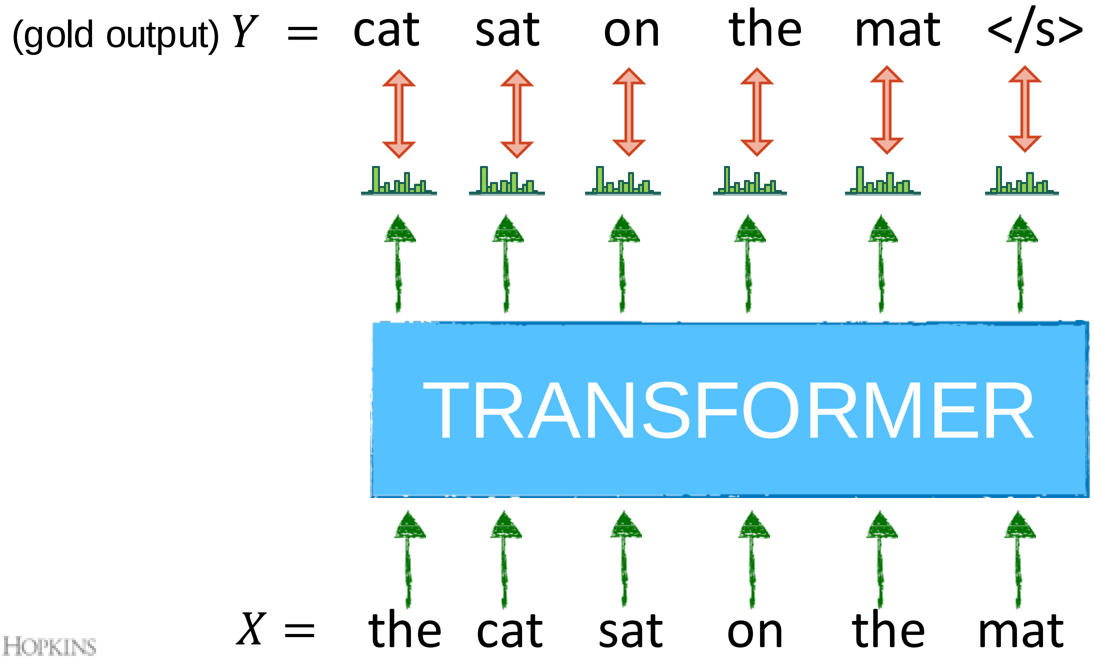
(gold output) Y = cat sat on the mat </s>



X = the cat sat on the mat

Training a Transformer Language Model

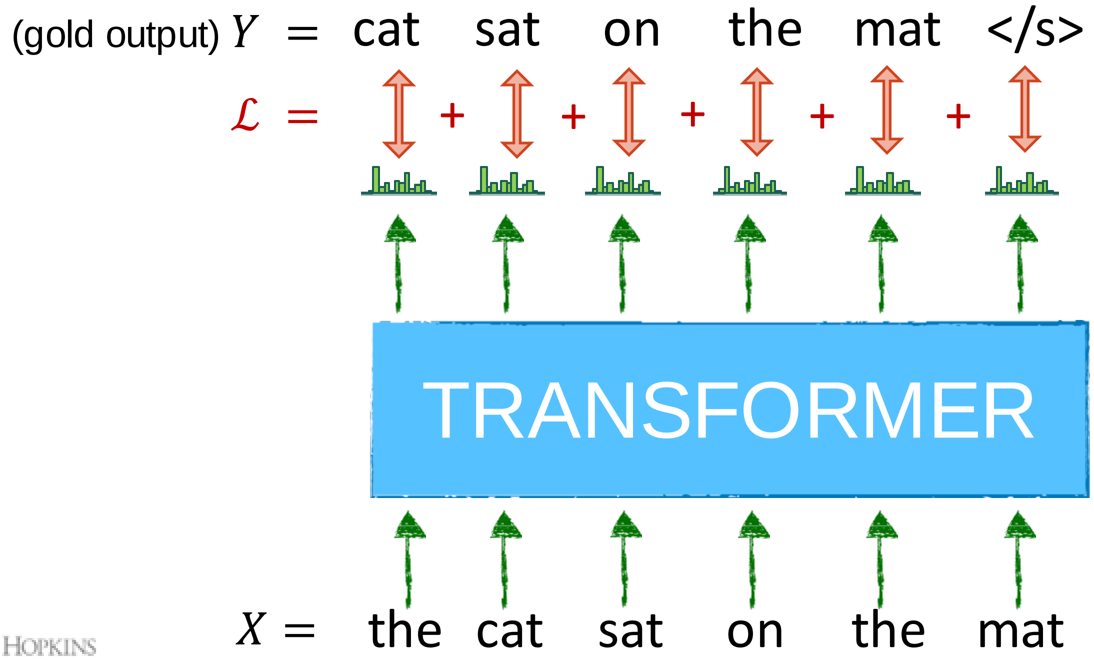
- For each position, compute the **loss** between the distribution and the gold output label.



JOHNS HOPKINS WHITING SCHOOL of ENGINEERING

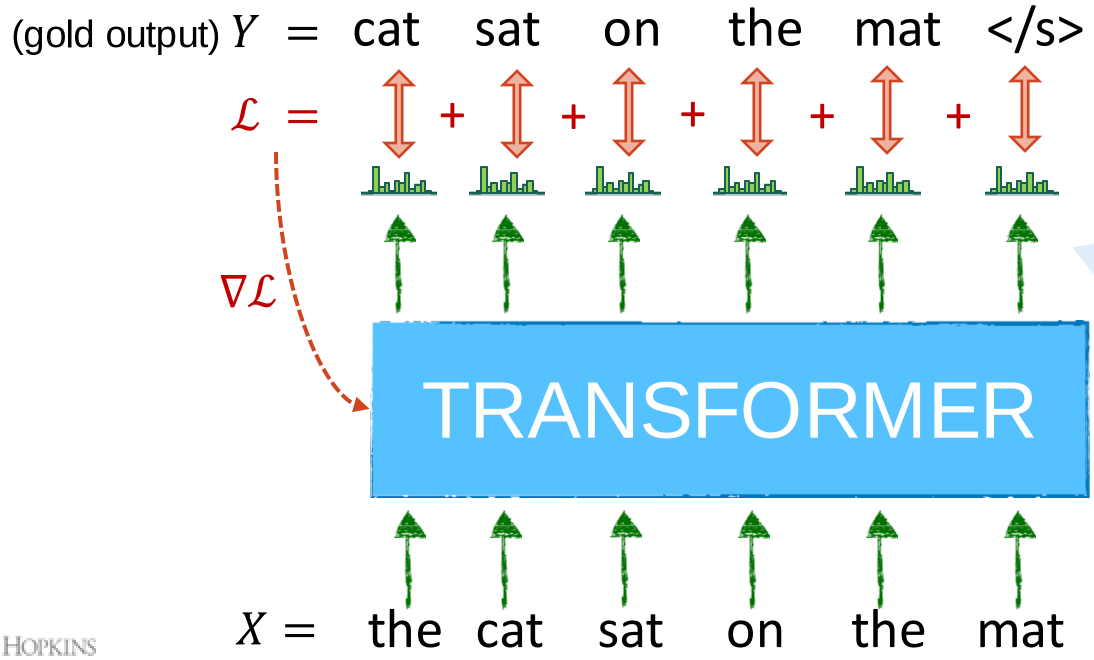
Training a Transformer Language Model

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



Training a Transformer Language Model

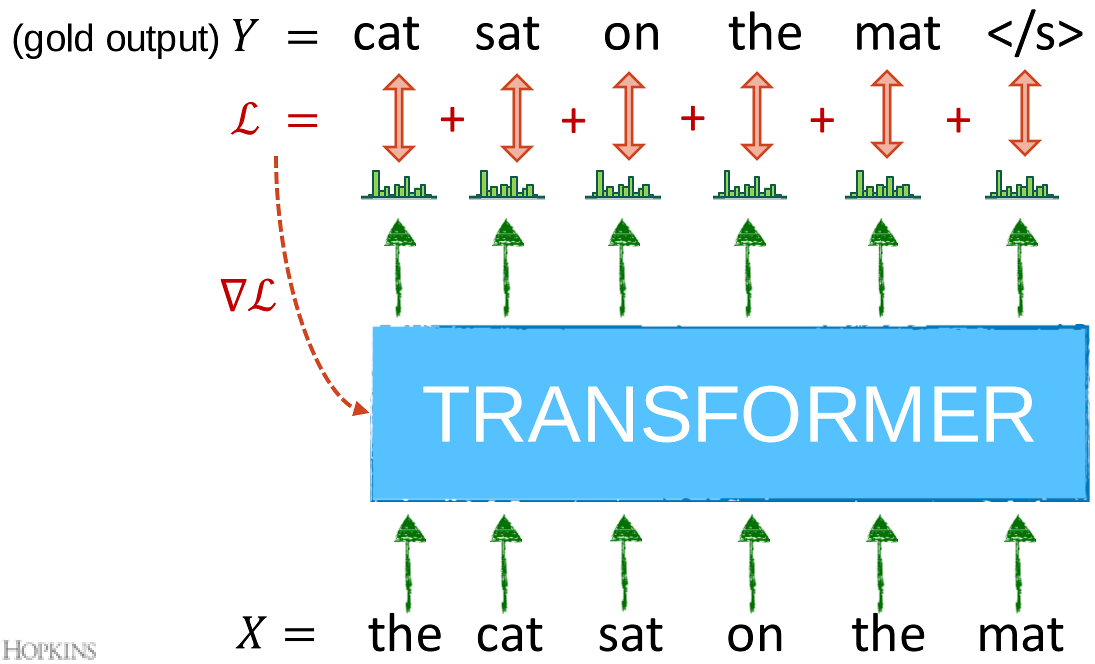
- Using this loss, do **Backprop** and **update** the Transformer parameters.



Well, this is not quite right 🤡
…
what is the problem with this?

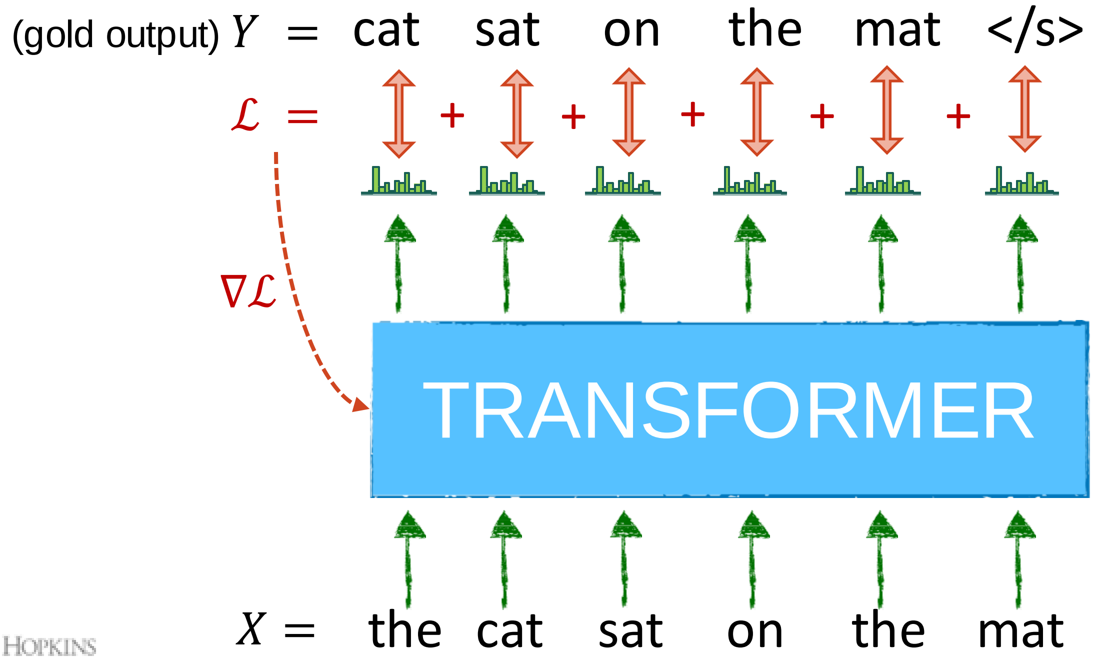
Training a Transformer Language Model

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



Training a Transformer Language Model

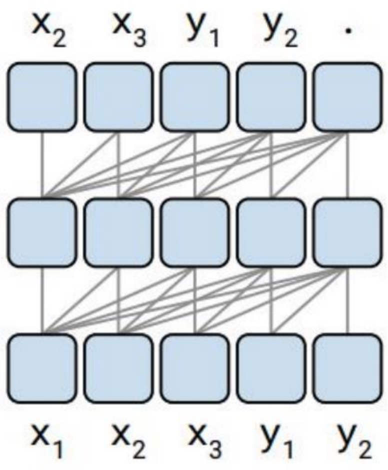
- We need to **prevent information leakage** from future tokens! How?



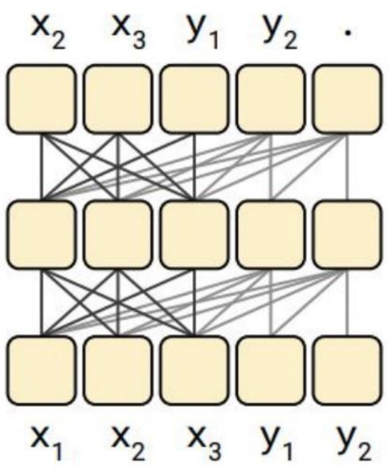
Attention mask

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

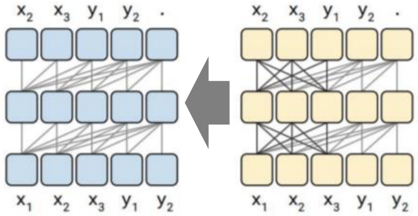


What we want



What we have

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

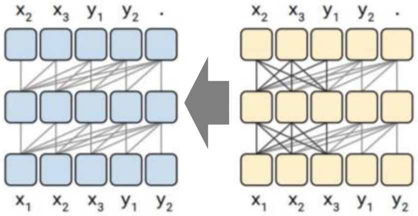
	0	1	2	3								
0	1.0	-inf	-inf	-inf	-inf	-inf	-inf	-inf	-inf	-inf	-inf	-inf
1	1.0	1.0	-inf	-inf	-inf	-inf	-inf	-inf	-inf	-inf	-inf	-inf
2	1.0	1.0	1.0	-inf	-inf	-inf	-inf	-inf	-inf	-inf	-inf	-inf
3	1.0	1.0	1.0	1.0	-inf	-inf	-inf	-inf	-inf	-inf	-inf	-inf
4	1.0	1.0	1.0	1.0	1.0	-inf	-inf	-inf	-inf	-inf	-inf	-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	-in
10	1.0	1.0	1.0	1.0								
11	1.0	1.0	1.0	1.0								

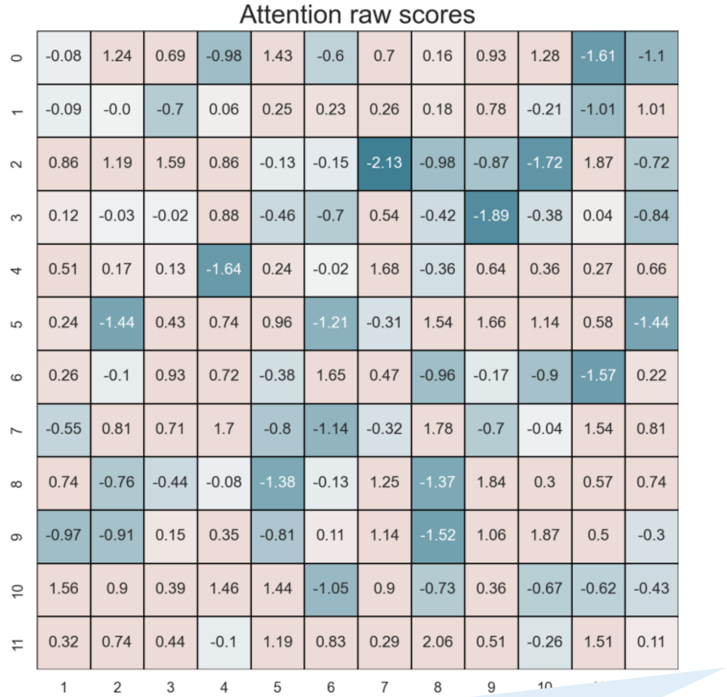
0.30 0.25 0.20 0.15 0.10 0.05 0.00

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

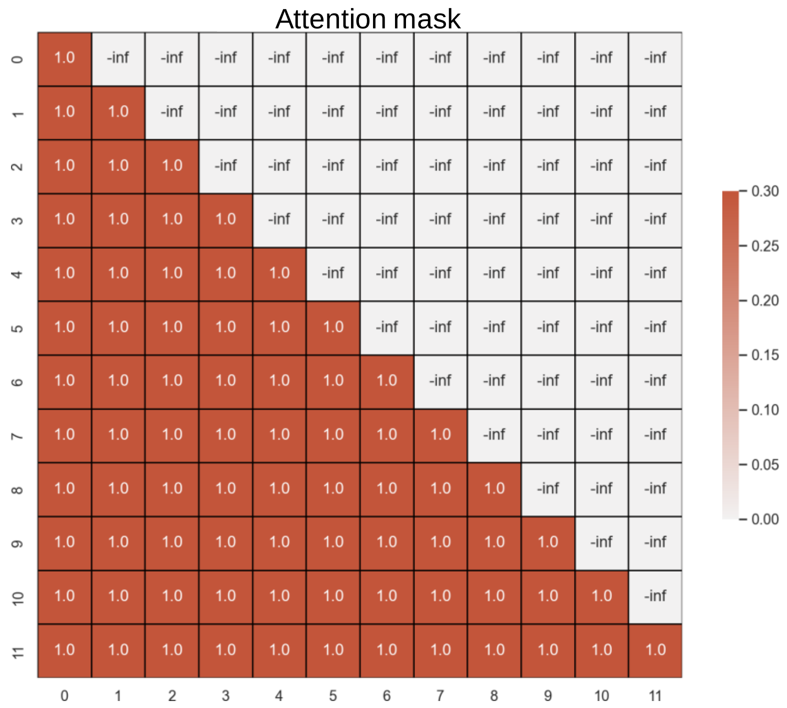
Slide credit: Arman Cohan

Attention mask





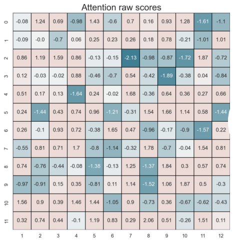
X



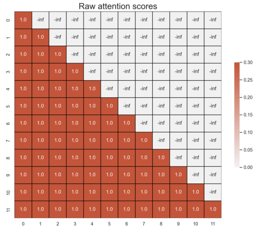
Note matrix multiplication is quite fast in GPUs.

Slide credit: Arman Cohan

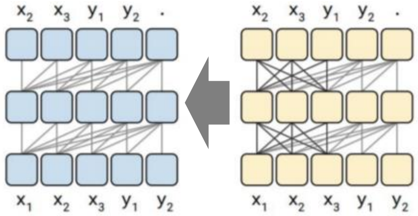
Attention mask



X



=



Masked attention raw scores

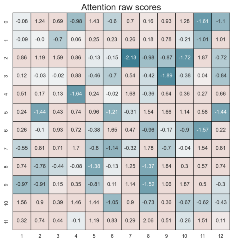
	1	2	3	4	5	6	7	8	9	10	11	12
0	-0.08	-inf	-inf	-inf	-inf	-inf	-inf	-inf	-inf	-inf	-inf	-inf
1	-0.09	-0.0	-inf	-inf	-inf	-inf	-inf	-inf	-inf	-inf	-inf	-inf
2	0.86	1.19	1.59	-inf	-inf	-inf	-inf	-inf	-inf	-inf	-inf	-inf
3	0.12	-0.03	-0.02	0.88	-inf	-inf	-inf	-inf	-inf	-inf	-inf	-inf
4	0.51	0.17	0.13	-1.64	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

Johns Hopkins Whiting School of Engineering

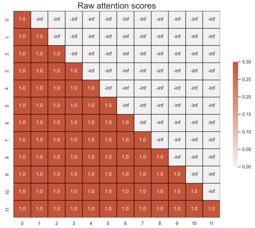
Slide credit: Arman Cohan

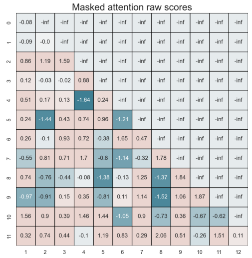
Attention mask

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

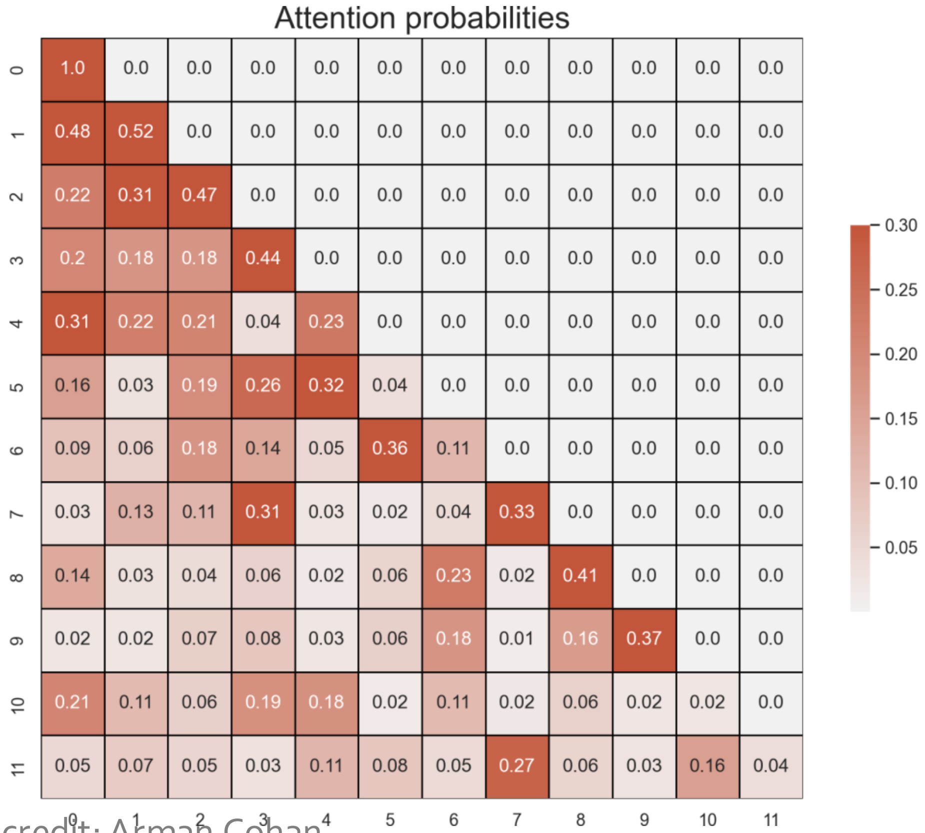


X





softmax

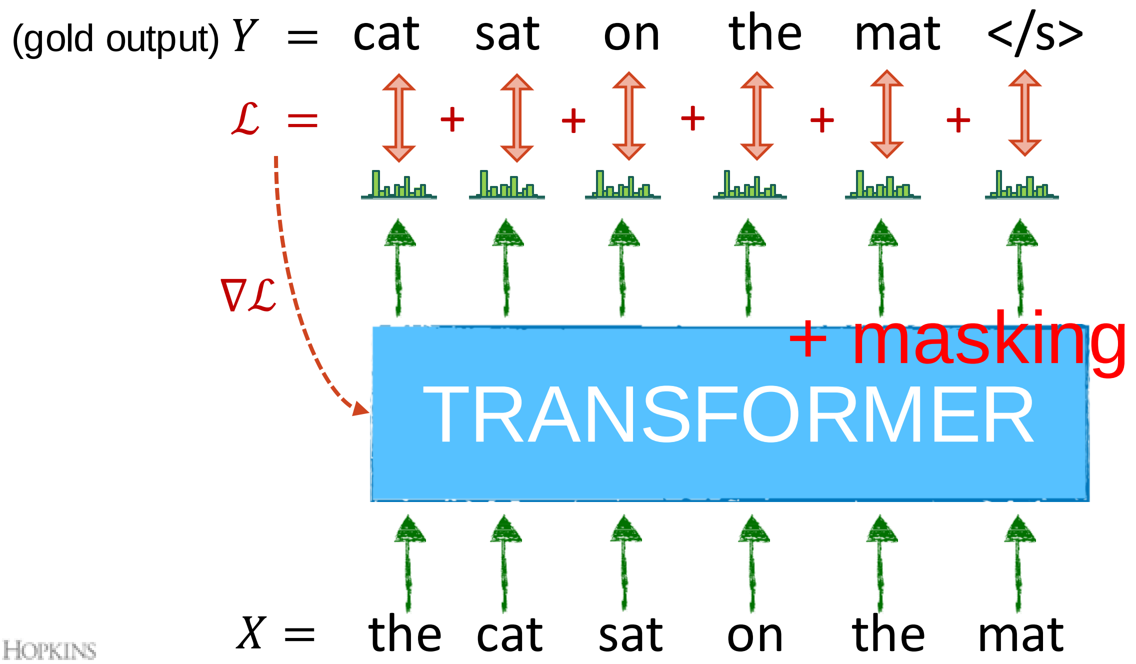


Slide credit: Arman Cohan

JOHNS HOPKINS WHITING SCHOOL of ENGINEERING

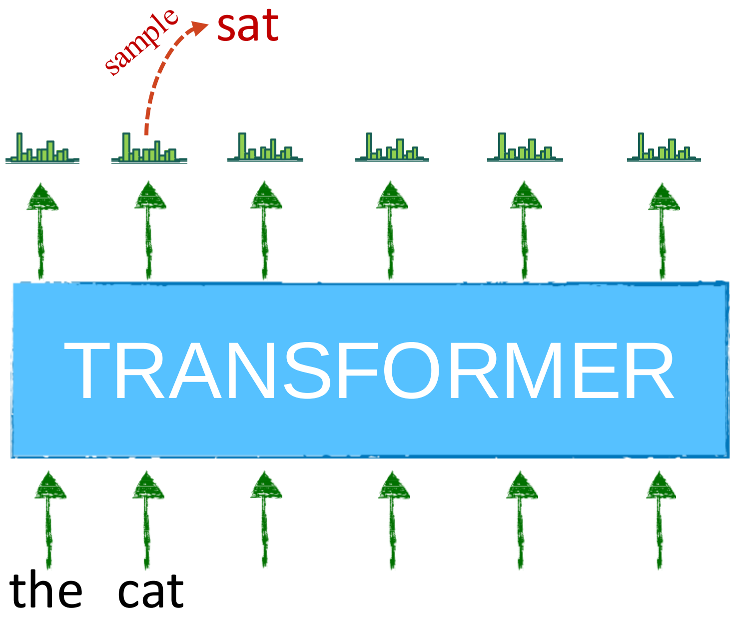
Training a Transformer Language Model

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



How to use the model to generate text?

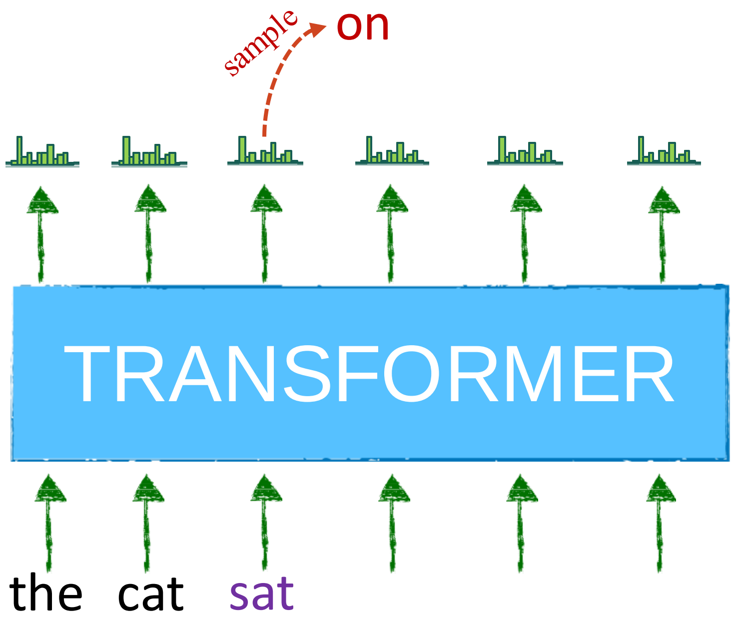
- Use the output of previous step as input to the next step repeatedly



How to use the model to generate text?

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

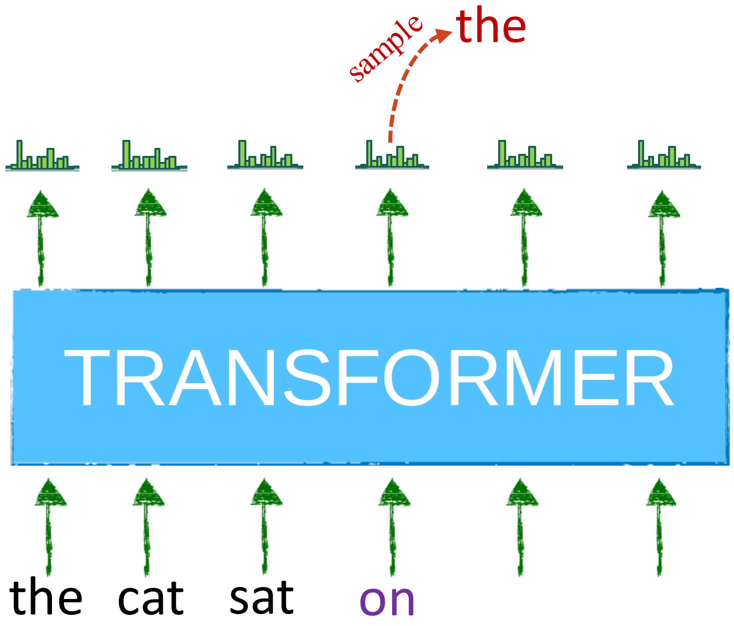
The probabilities get revised upon adding a new token to the input.



How to use the model to generate text?

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

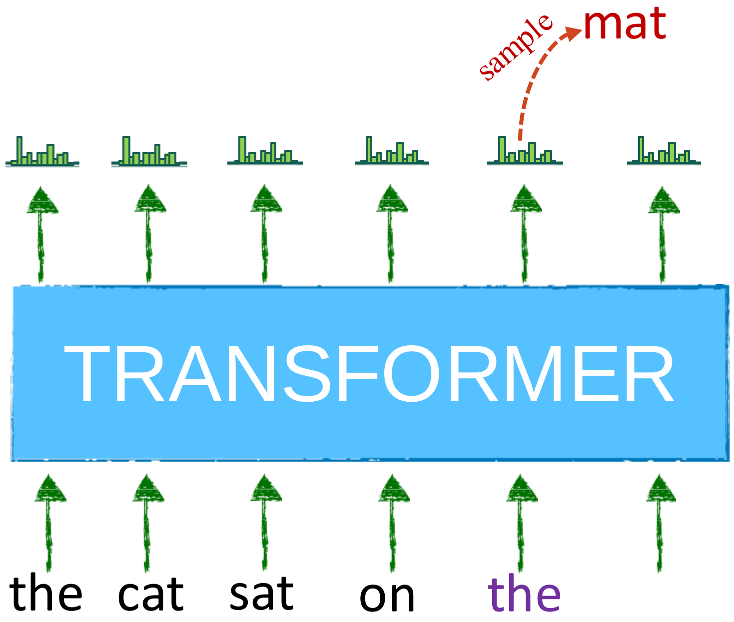
The probabilities get revised upon adding a new token to the input.



How to use the model to generate text?

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

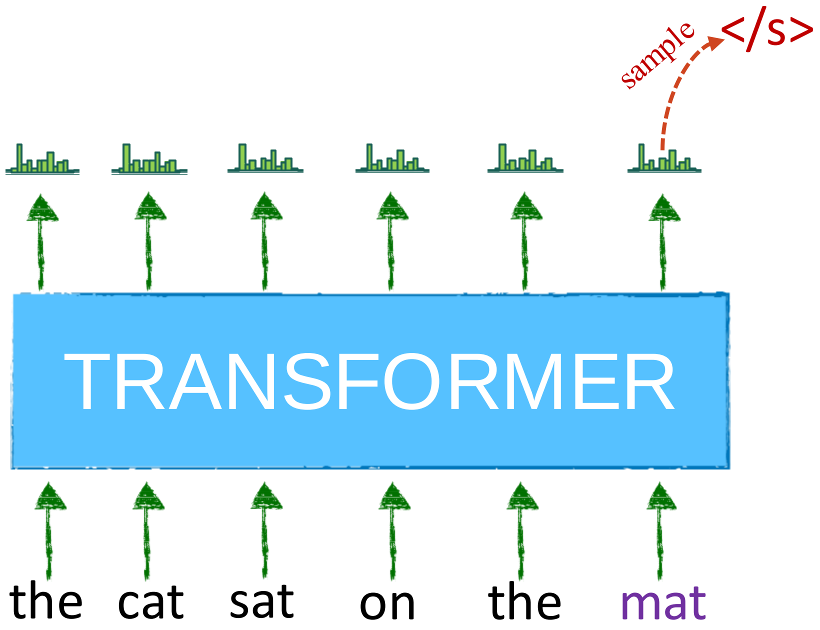
The probabilities get revised upon adding a new token to the input.



How to use the model to generate text?

- 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.



Summary

- This is a very generic Transformer!
- We will implement this in HW5 to build a simple Transformer Language Model!!

- **Next:**
  - Architectural variants

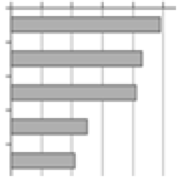
Transformer Architectural Variants

Encoder-Decoder Architectures

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

“The cat sat on the [MASK]”

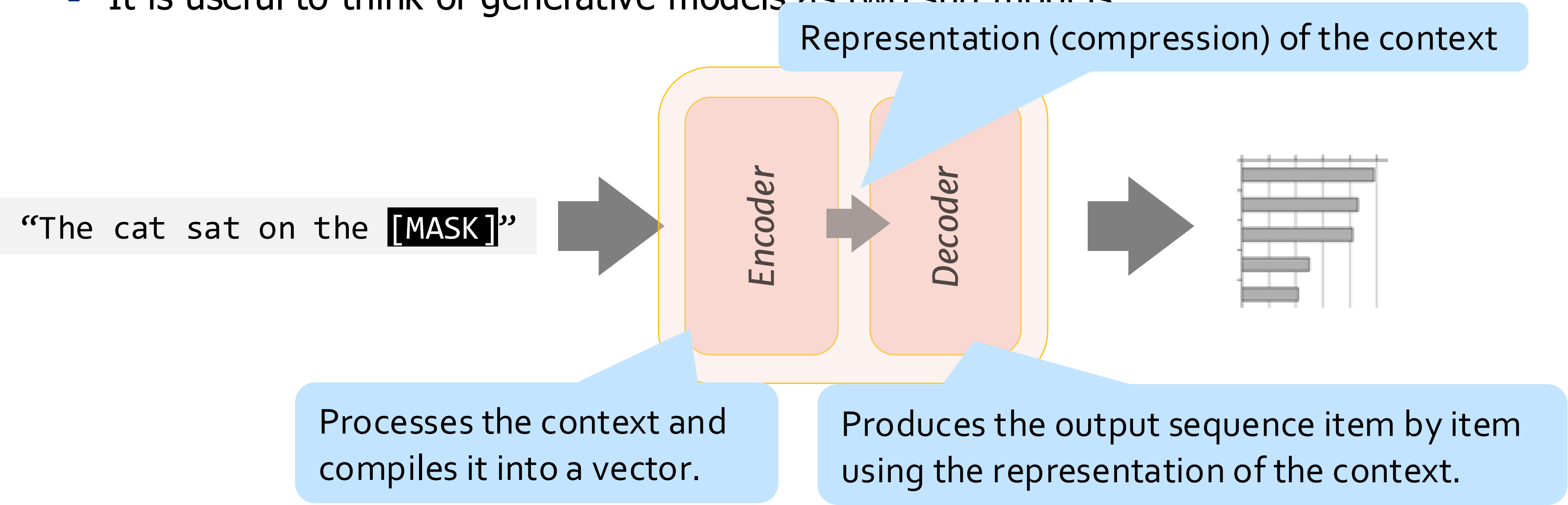
Some model



64

Encoder-Decoder Architectures

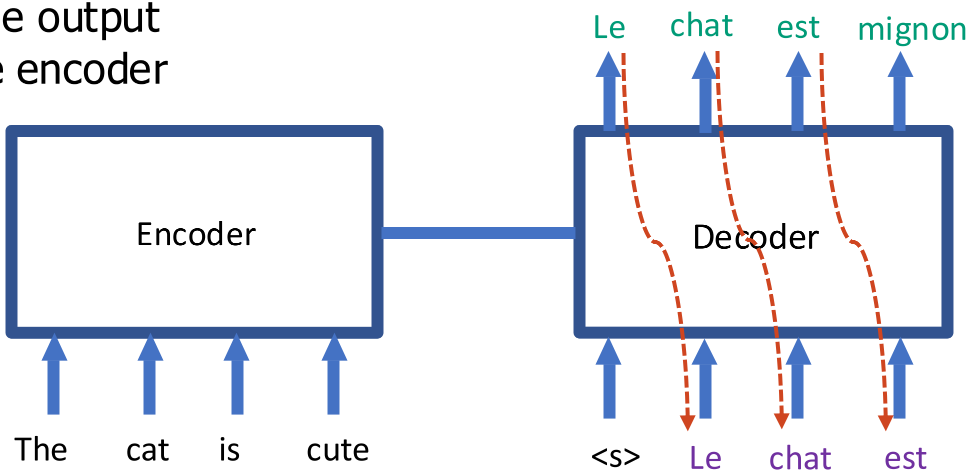
- It is useful to think of generative models as two sub-models



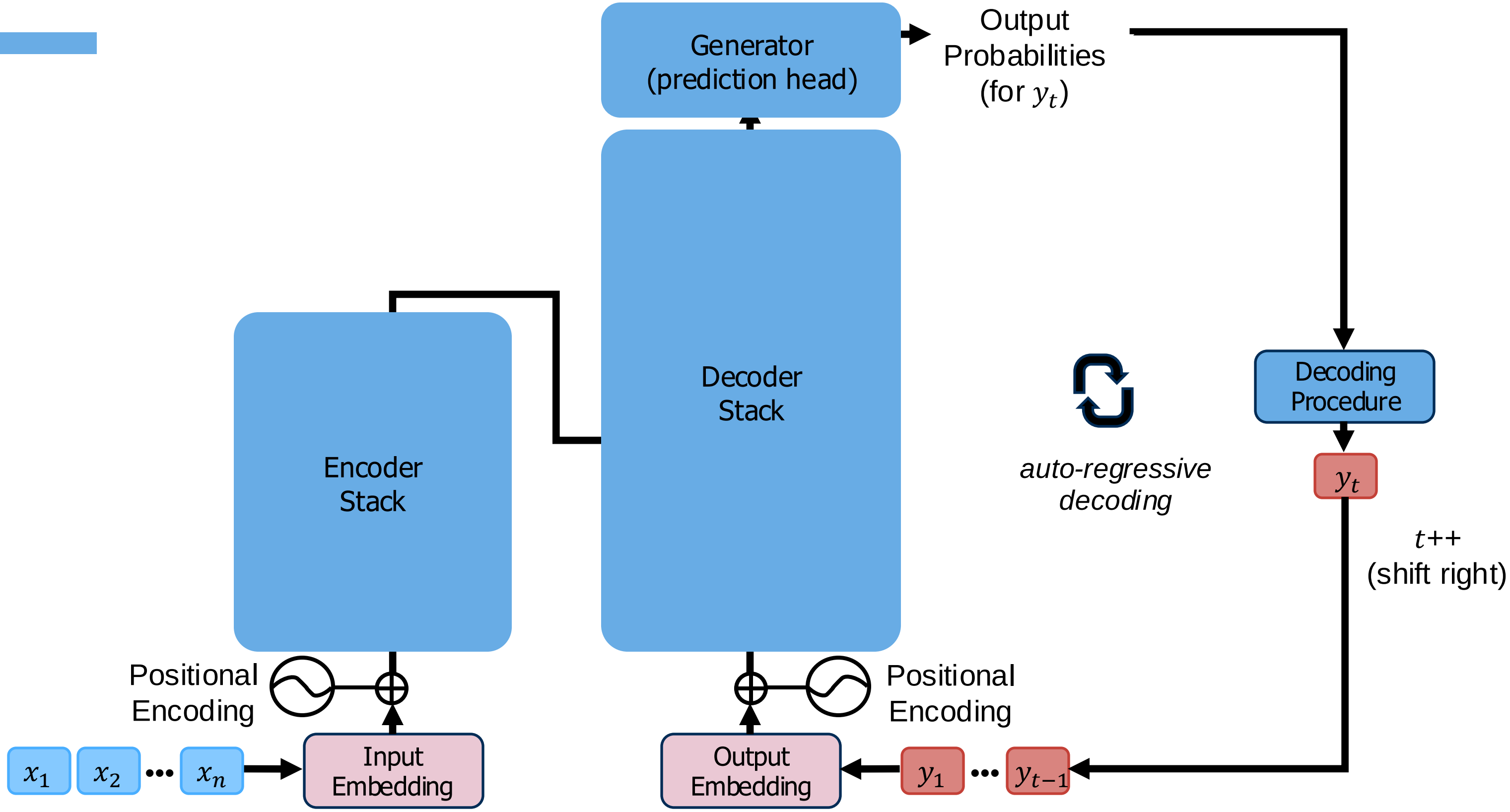
65

Encoder-decoder models

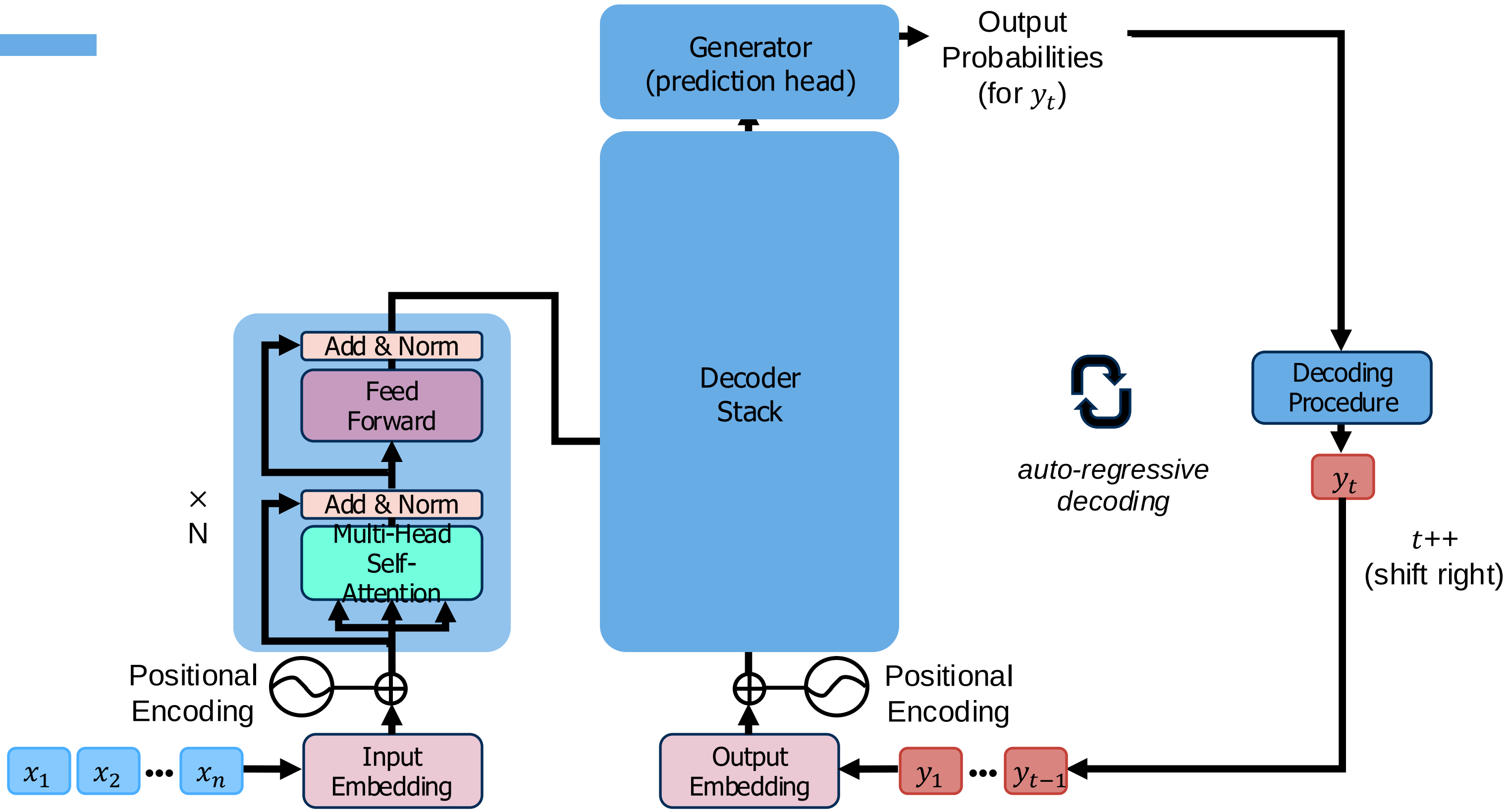
- Transformer is two blocks
- Encoder = read or encode the input,
  - Architecture is as we've seen
- Decoder = generate or decode the output
  - Architecture is identical to the encoder but we give it the ability to also attend to the input



Transformer [Vaswani et al. 2017]

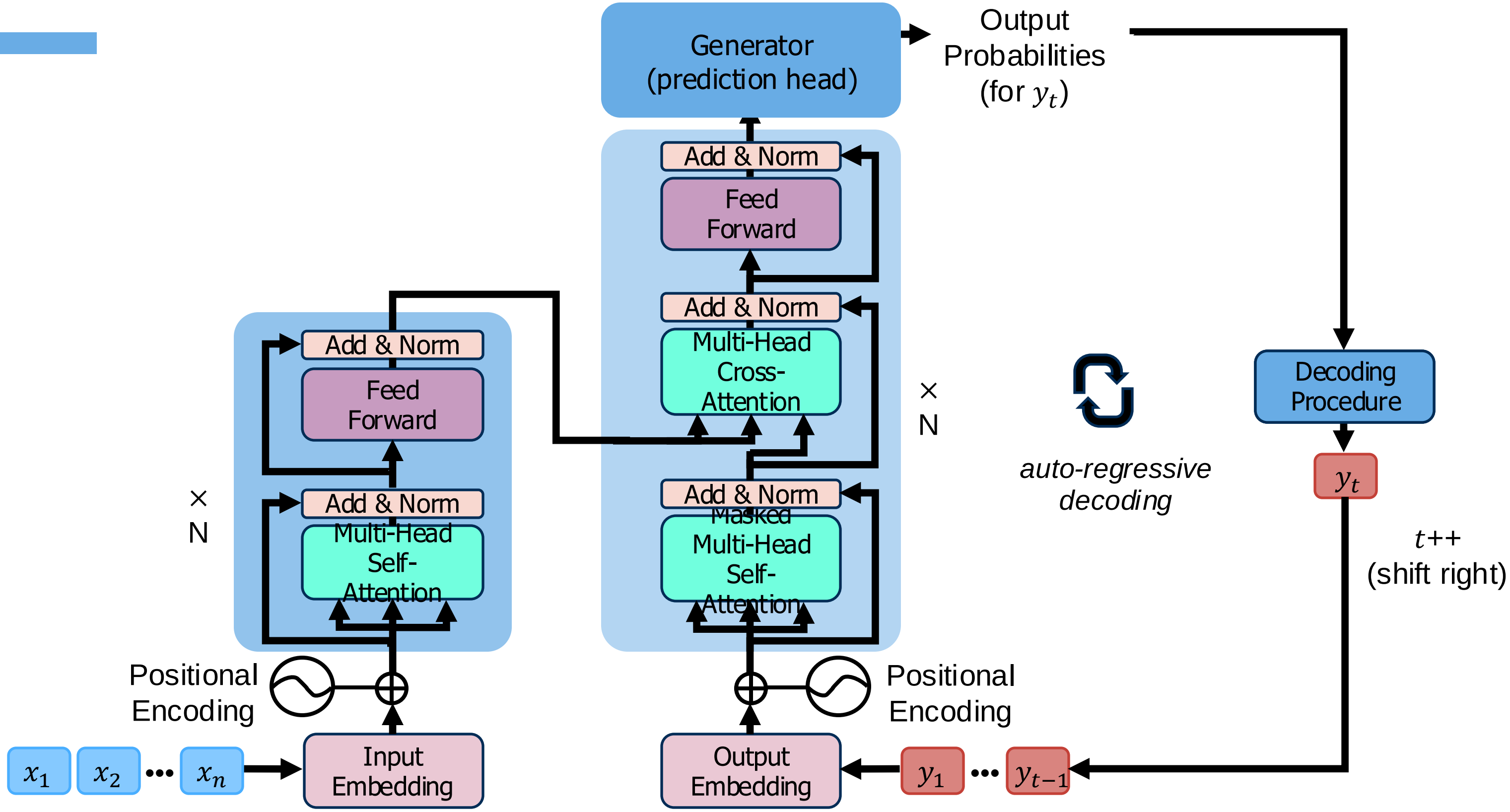


Transformer [Vaswani et al. 2017]



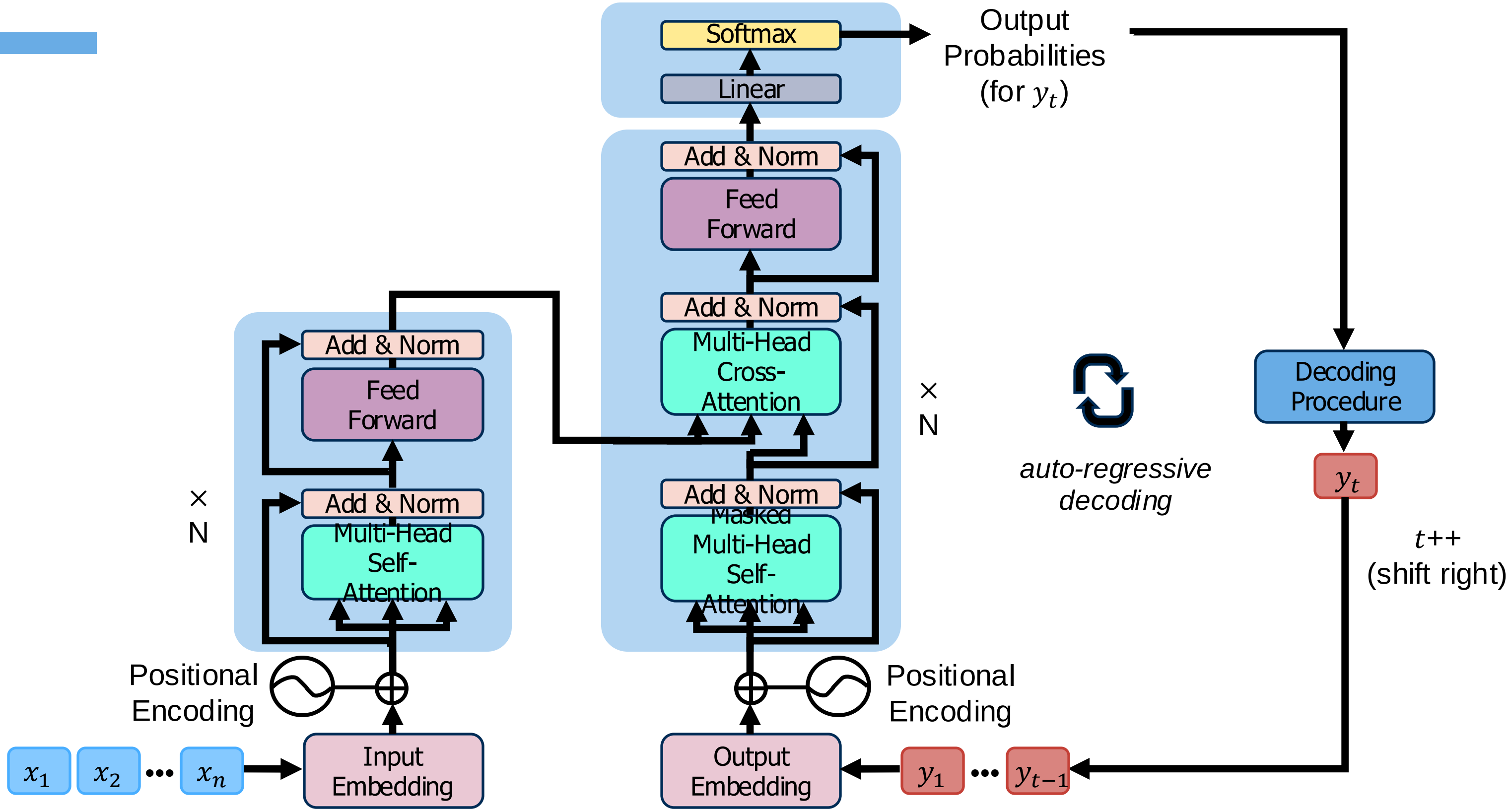
[Slide credit: CS886 at UWaterloo]

Transformer [Vaswani et al. 2017]



[Slide credit: CS886 at UWaterloo]

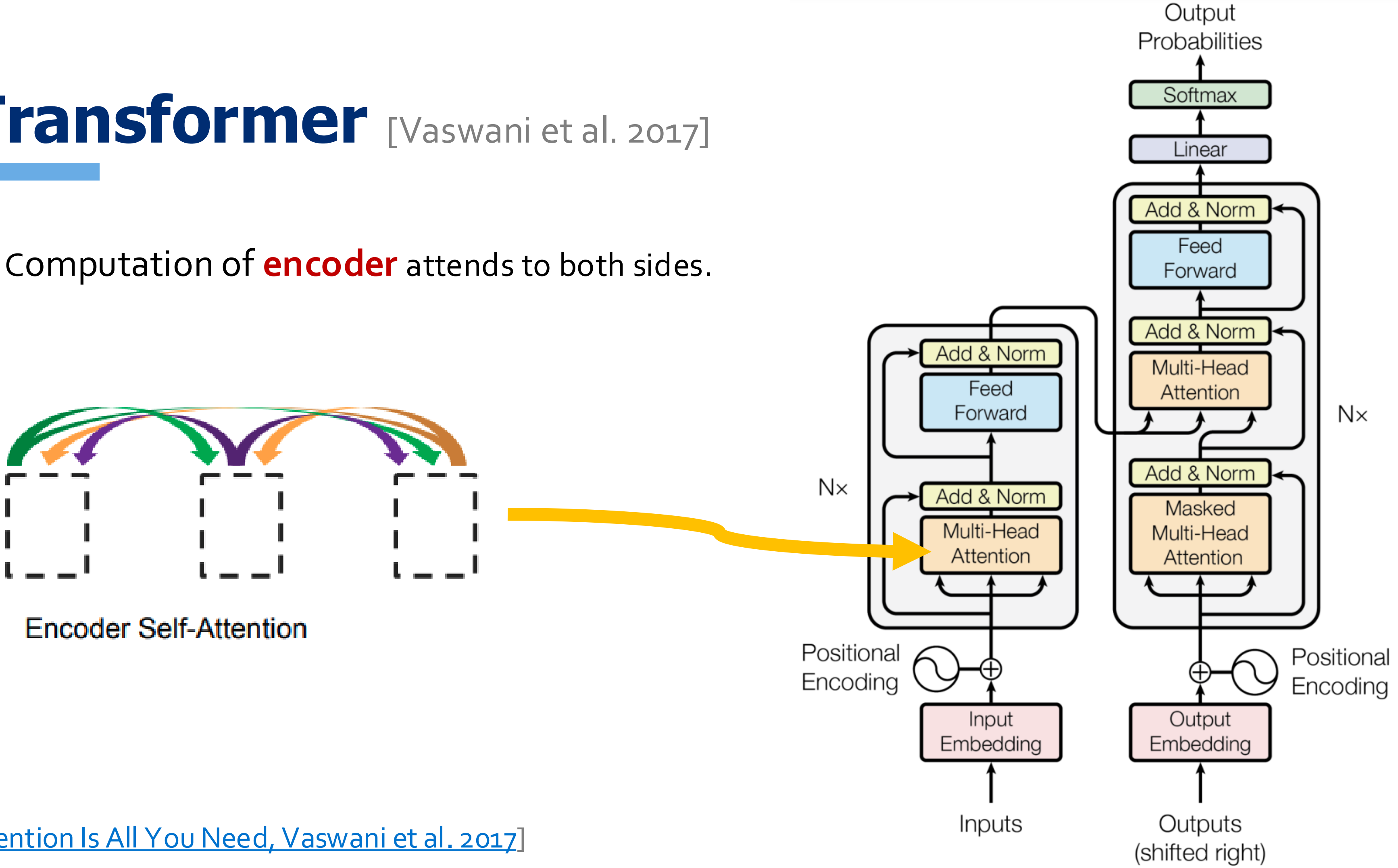
Transformer [Vaswani et al. 2017]



[Slide credit: CS886 at UWaterloo]

Transformer [Vaswani et al. 2017]

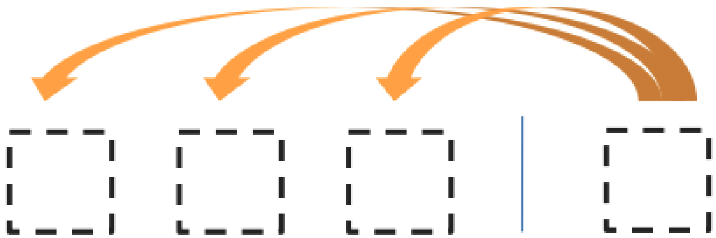
- Computation of **encoder** attends to both sides.



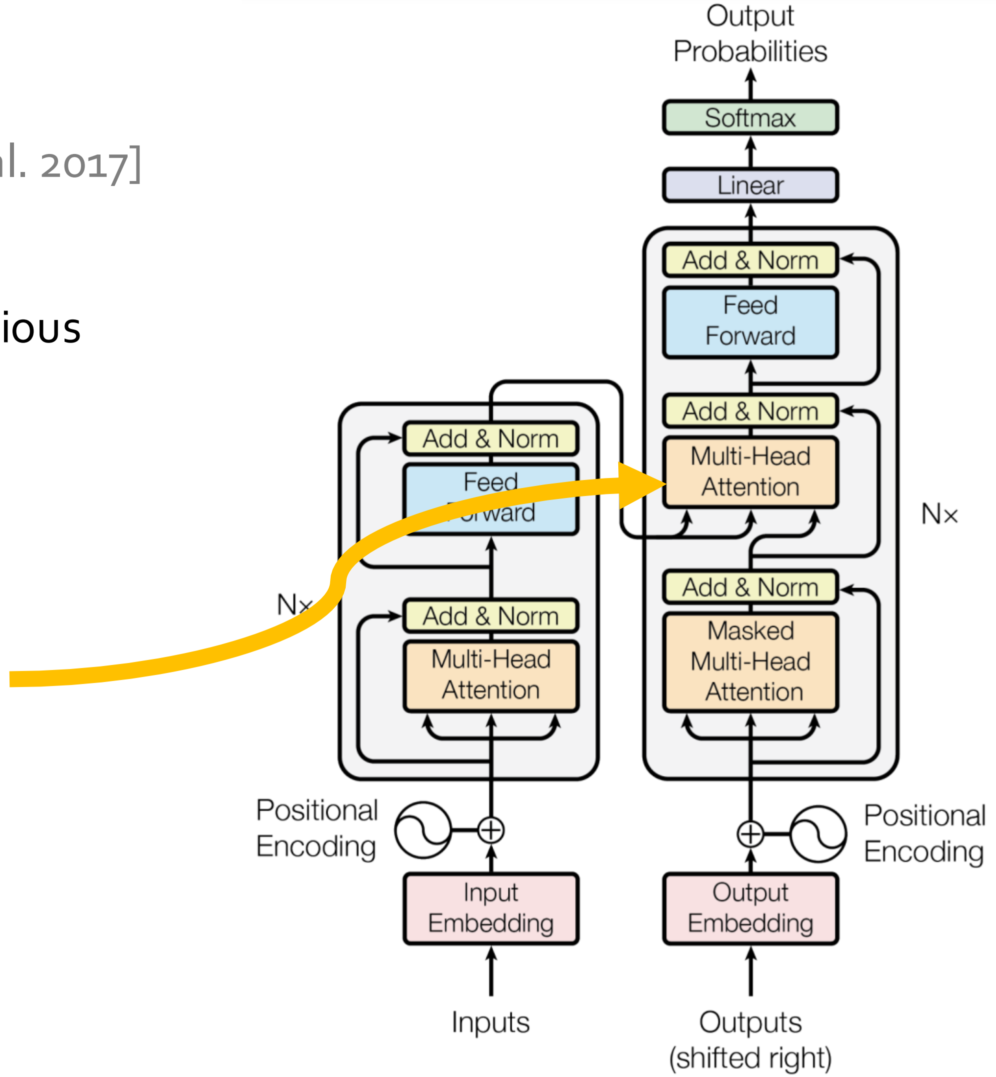
[Attention Is All You Need, Vaswani et al. 2017]

Transformer [Vaswani et al. 2017]

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



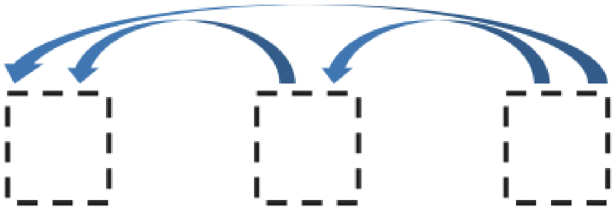
Encoder-Decoder Attention



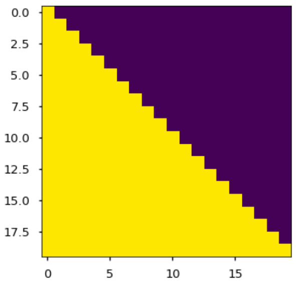
[Attention Is All You Need, Vaswani et al. 2017]

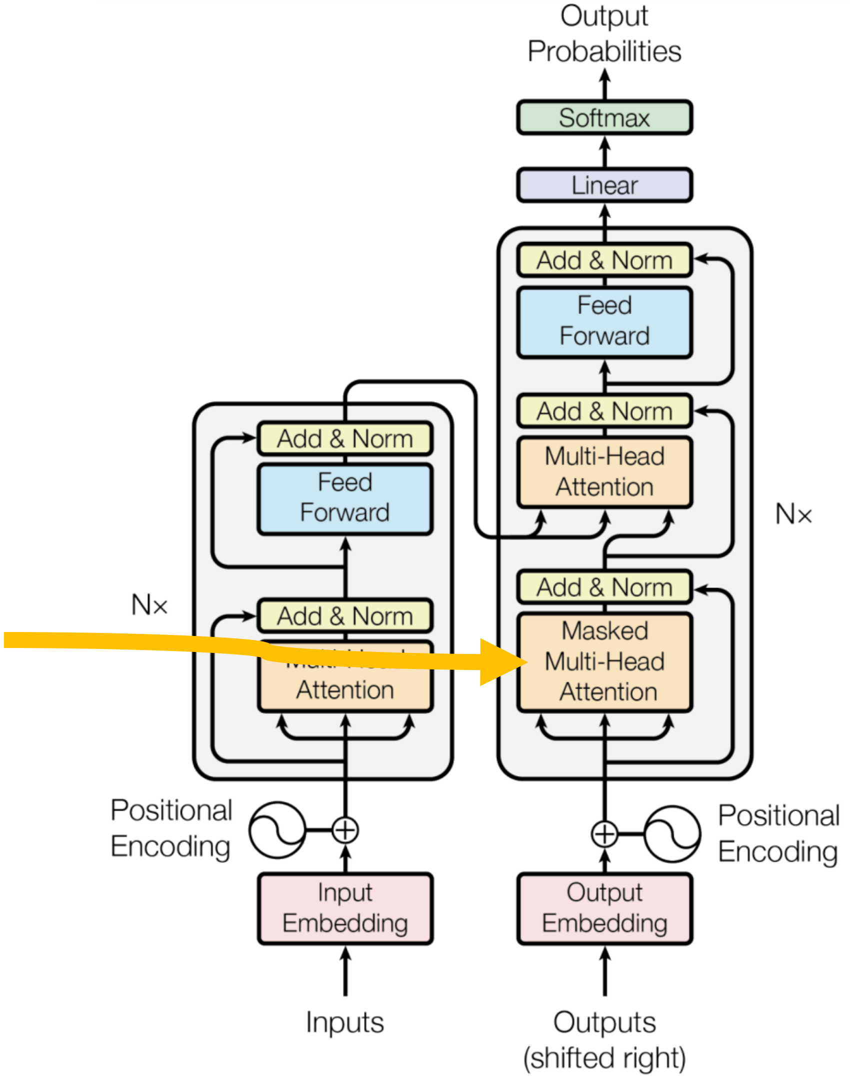
Transformer [Vaswani et al. 2017]

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



MaskedDecoder Self-Attention



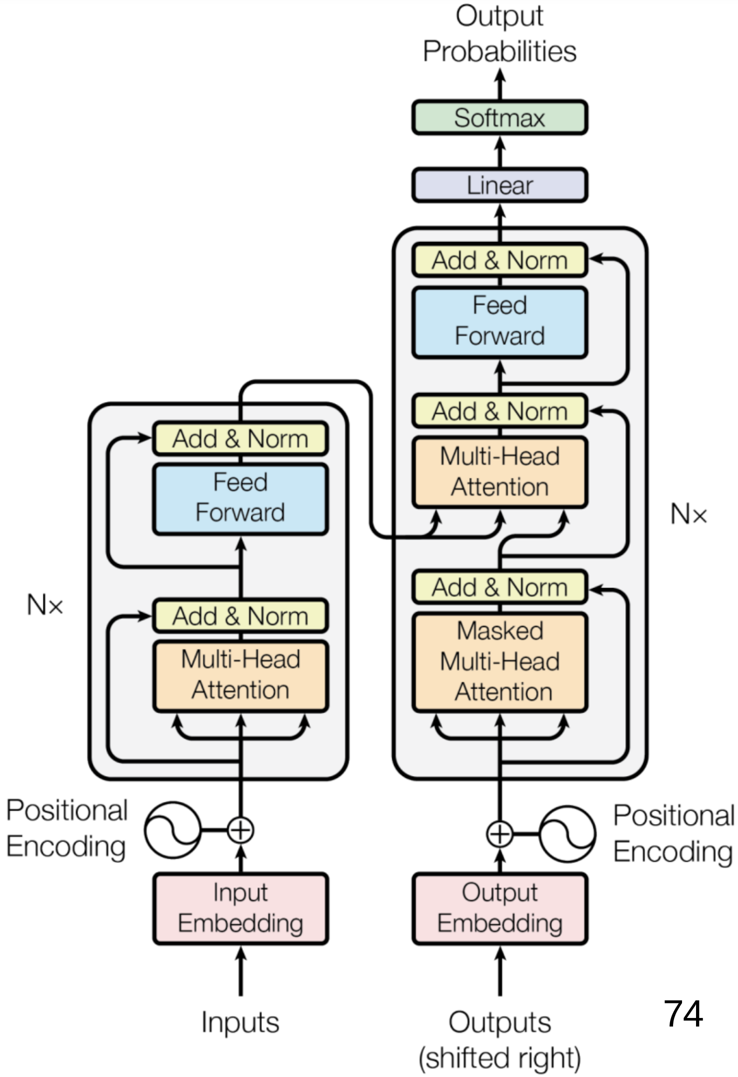


[Attention Is All You Need, Vaswani et al. 2017]

Transformer [Vaswani et al. 2017]

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

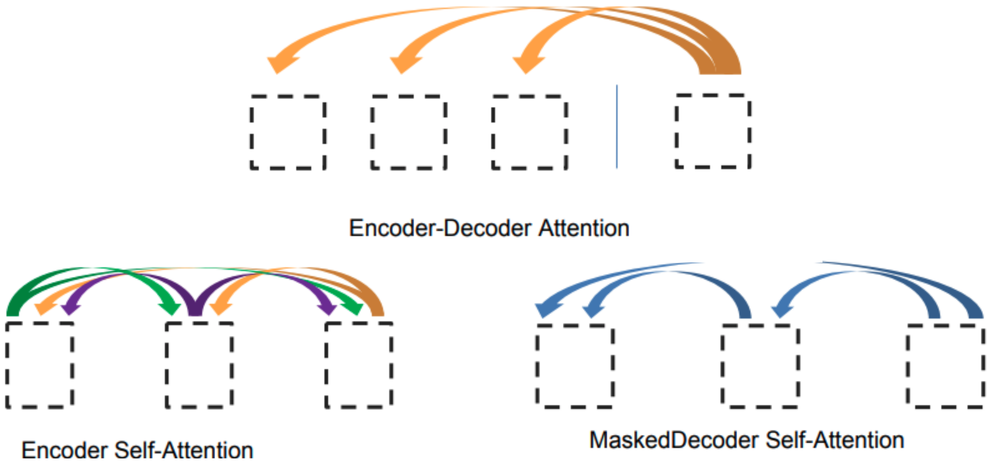
- At any step of decoder, **re-use** previous computation of encoder.
- Computation of decoder is **linear**, instead of quadratic.



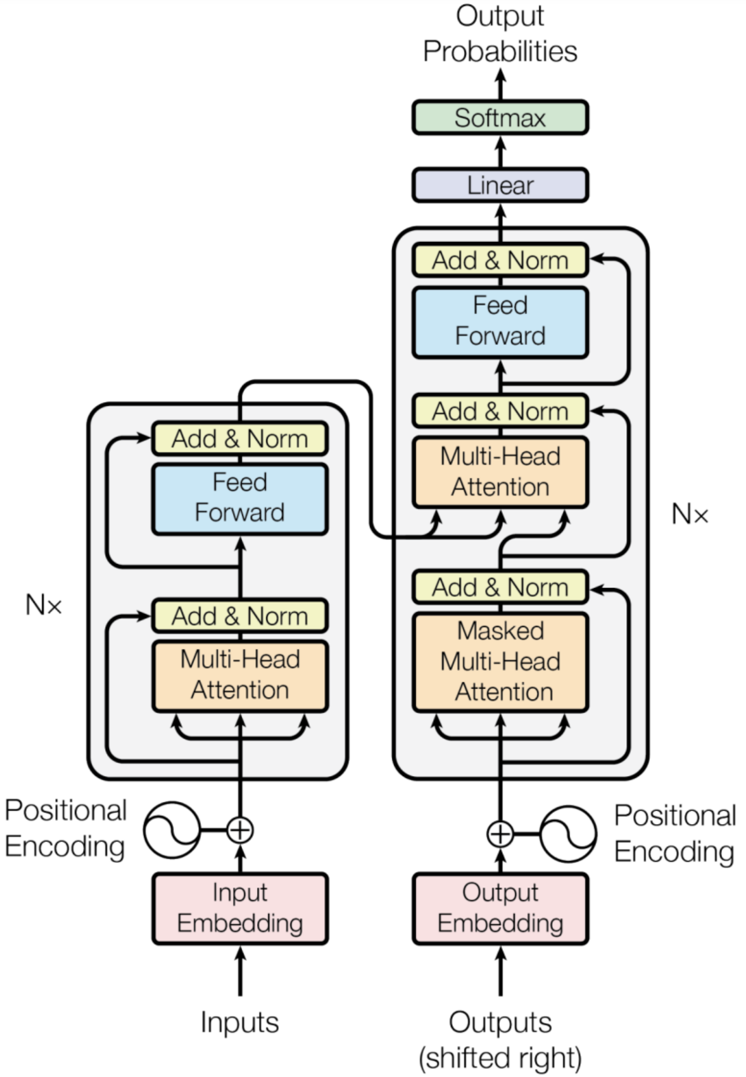
[Attention Is All You Need, Vaswani et al. 2017]

Recap: Transformer

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



[Attention Is All You Need, 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

- 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 in M and N.

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 in M and N.

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, cross attention is missing.

Quiz: Enc-Dec Cost

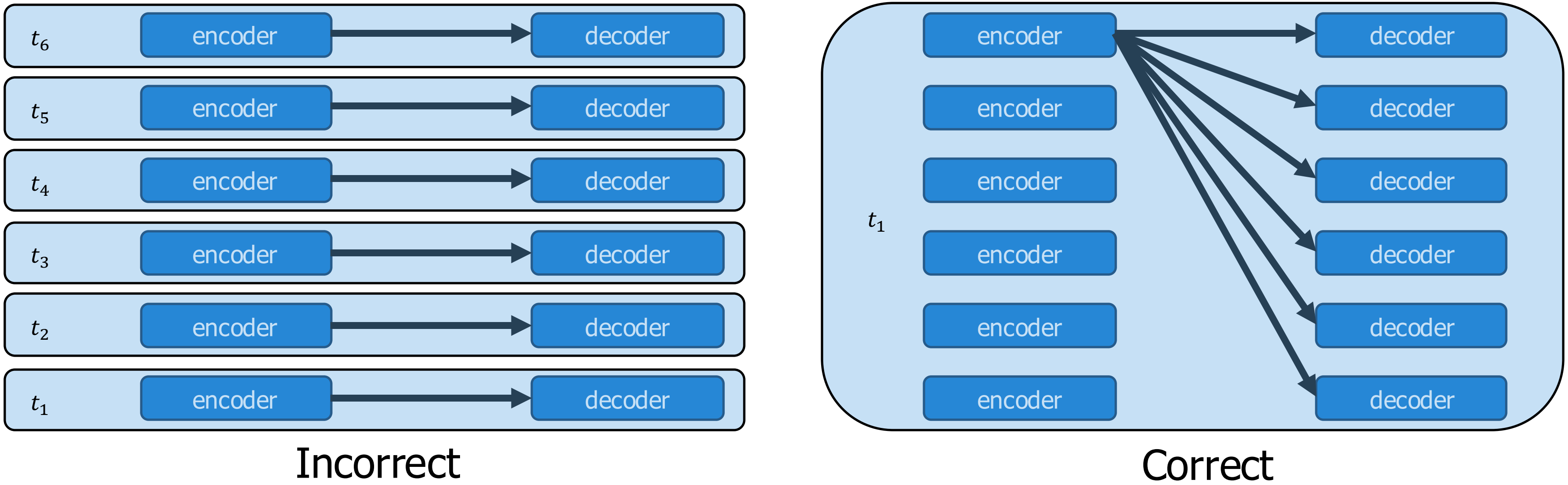
- Source data (large!):
  - The references for a Wikipedia article.
  - Web search using article section titles, ~ 10 web pages per query.

- For a passage of length N and a summary of length M, the complexity of the attention is:
  - $O(N) + O(M)$
  - $O(N) + O(M) + O(NM)$
  - $O(N^2) + O(M^2) + O(NM)$
  - $O(N^2) + O(M^2)$

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

Quiz: Enc-Dec Connections

- Which best represents encoder-decoder connections?



[Slide credit: CS886 at UWaterloo]

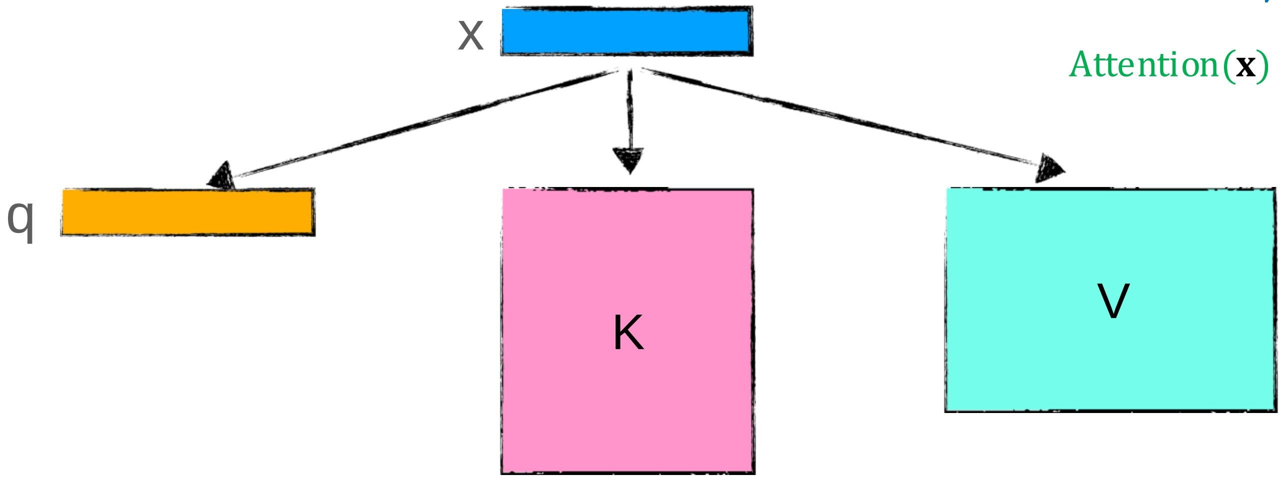
JOHNS HOPKINS
WHITING SCHOOL
of ENGINEERING

Considerations about computational cost in Transformers

Making decoding more efficient

$$Q = \mathbf{W}^q \mathbf{x}$$
$$K = \mathbf{W}^k \mathbf{x}$$
$$V = \mathbf{W}^v \mathbf{x}$$

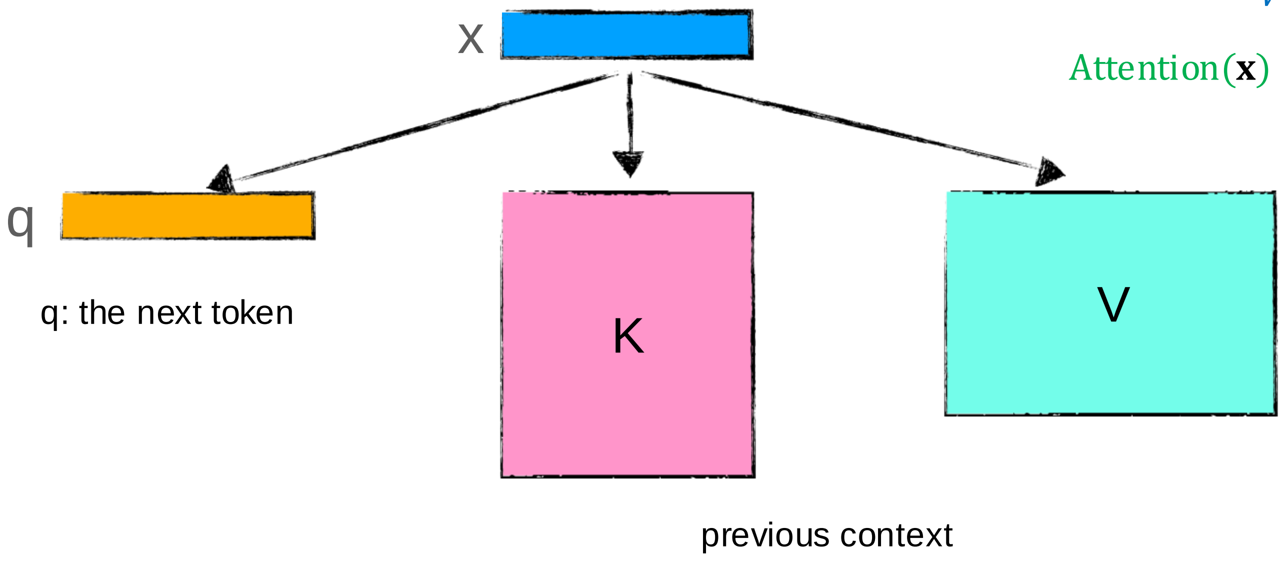
$$\text{Attention}(\mathbf{x}) = \text{softmax}\left(\frac{QK^{\mathrm{T}}}{\sqrt{d}}\right)V$$



[Slide credit: Arman Cohan]

Making decoding more efficient

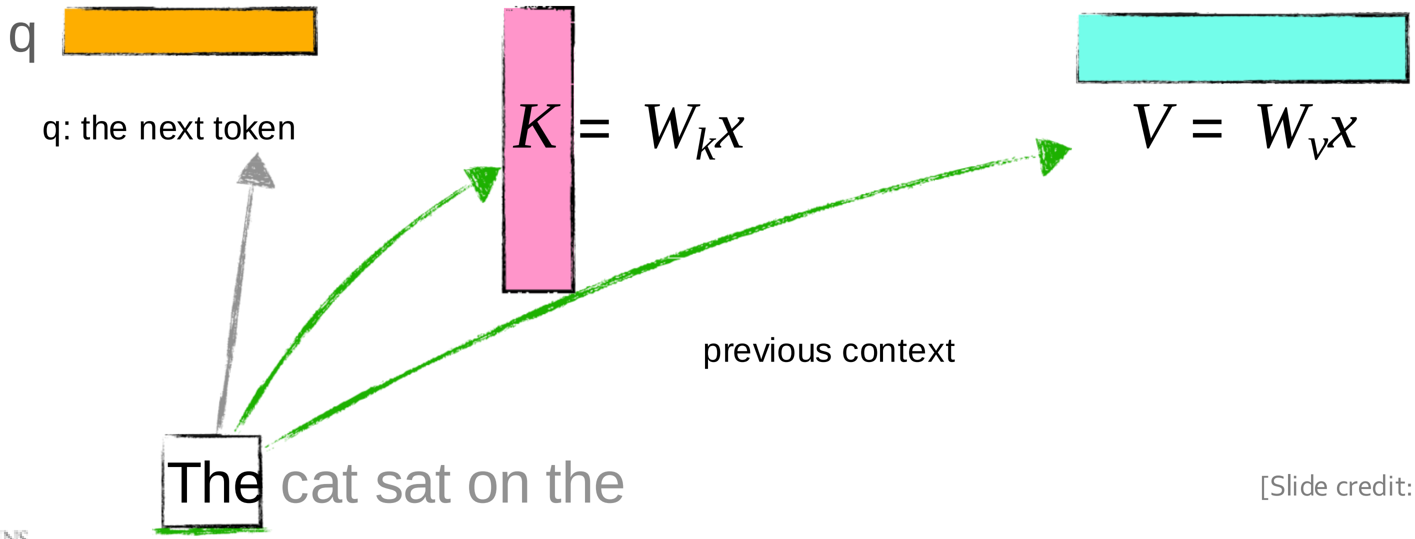
$$Q = \mathbf{W}^q \mathbf{x}$$
$$K = \mathbf{W}^k \mathbf{x}$$
$$V = \mathbf{W}^v \mathbf{x}$$
$$\text{Attention}(\mathbf{x}) = \text{softmax}\left(\frac{QK^{\mathrm{T}}}{\sqrt{d}}\right)V$$



[Slide credit: Arman Cohan]

Making decoding more efficient

$$Q = \mathbf{W}^q \mathbf{x}$$
$$K = \mathbf{W}^k \mathbf{x}$$
$$V = \mathbf{W}^v \mathbf{x}$$
$$\text{Attention}(\mathbf{x}) = \text{softmax}\left(\frac{QK^{\mathrm{T}}}{\sqrt{d}}\right)V$$

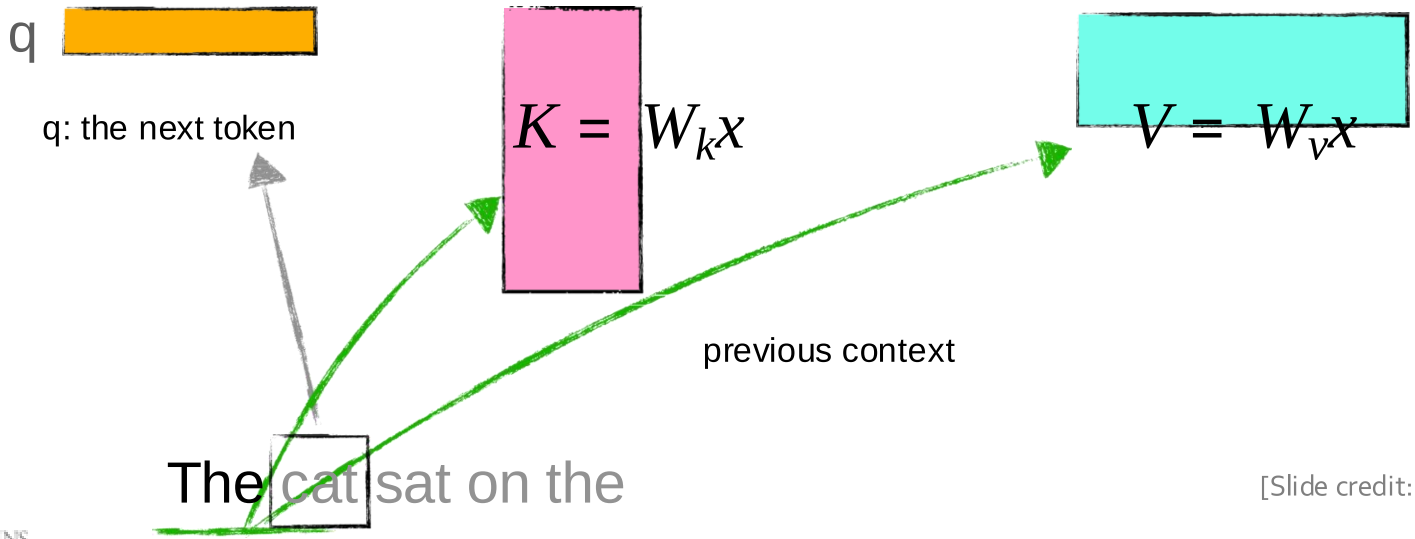


[Slide credit: Arman Cohan]

Making decoding more efficient

$$Q = \mathbf{W}^q \mathbf{x}$$
$$K = \mathbf{W}^k \mathbf{x}$$
$$V = \mathbf{W}^v \mathbf{x}$$

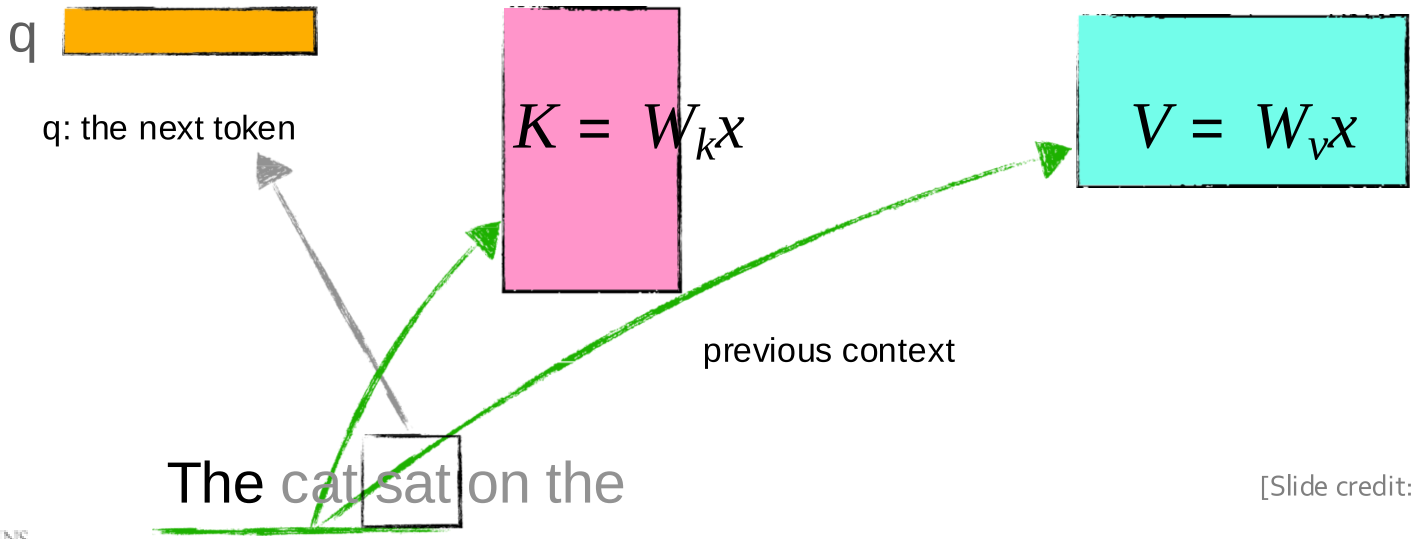
$$\text{Attention}(\mathbf{x}) = \text{softmax}\left(\frac{QK^\mathrm{T}}{\sqrt{d}}\right)V$$



[Slide credit: Arman Cohan]

Making decoding more efficient

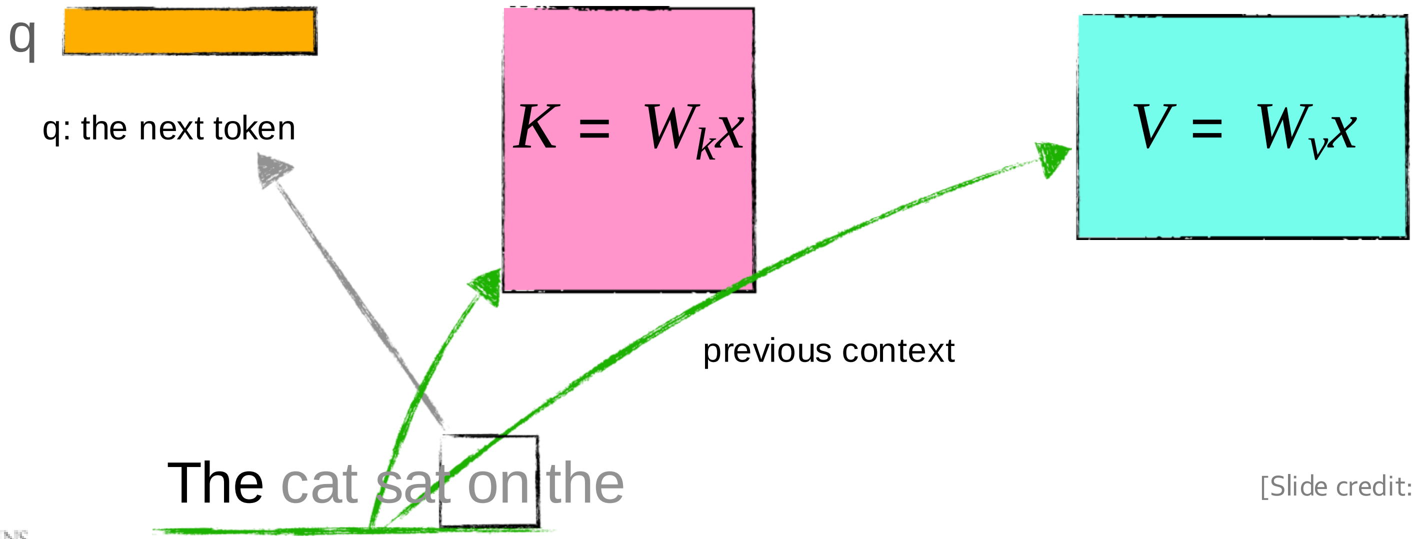
$$Q = \mathbf{W}^q \mathbf{x}$$
$$K = \mathbf{W}^k \mathbf{x}$$
$$V = \mathbf{W}^v \mathbf{x}$$
$$\text{Attention}(\mathbf{x}) = \text{softmax}\left(\frac{QK^{\mathrm{T}}}{\sqrt{d}}\right)V$$



[Slide credit: Arman Cohan]

Making decoding more efficient

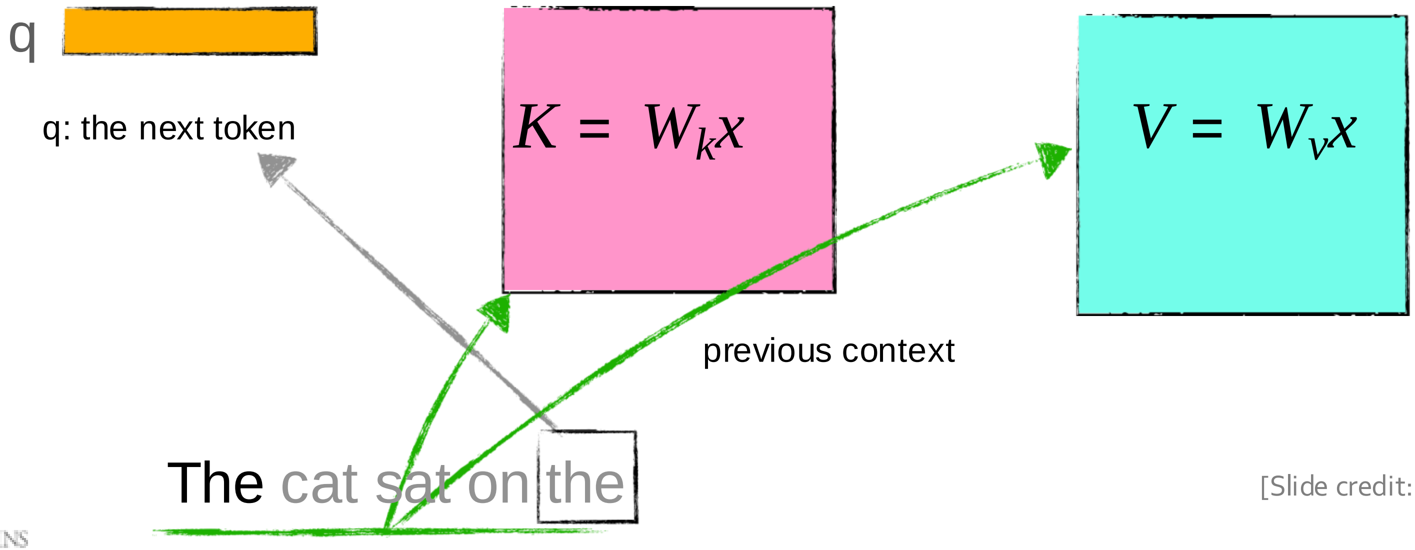
$$Q = \mathbf{W}^q \mathbf{x}$$
$$K = \mathbf{W}^k \mathbf{x}$$
$$V = \mathbf{W}^v \mathbf{x}$$
$$\text{Attention}(\mathbf{x}) = \text{softmax}\left(\frac{QK^{\mathrm{T}}}{\sqrt{d}}\right)V$$



[Slide credit: Arman Cohan]

Making decoding more efficient

$$Q = \mathbf{W}^q \mathbf{x}$$
$$K = \mathbf{W}^k \mathbf{x}$$
$$V = \mathbf{W}^v \mathbf{x}$$
$$\text{Attention}(\mathbf{x}) = \text{softmax}\left(\frac{QK^{\mathrm{T}}}{\sqrt{d}}\right)V$$

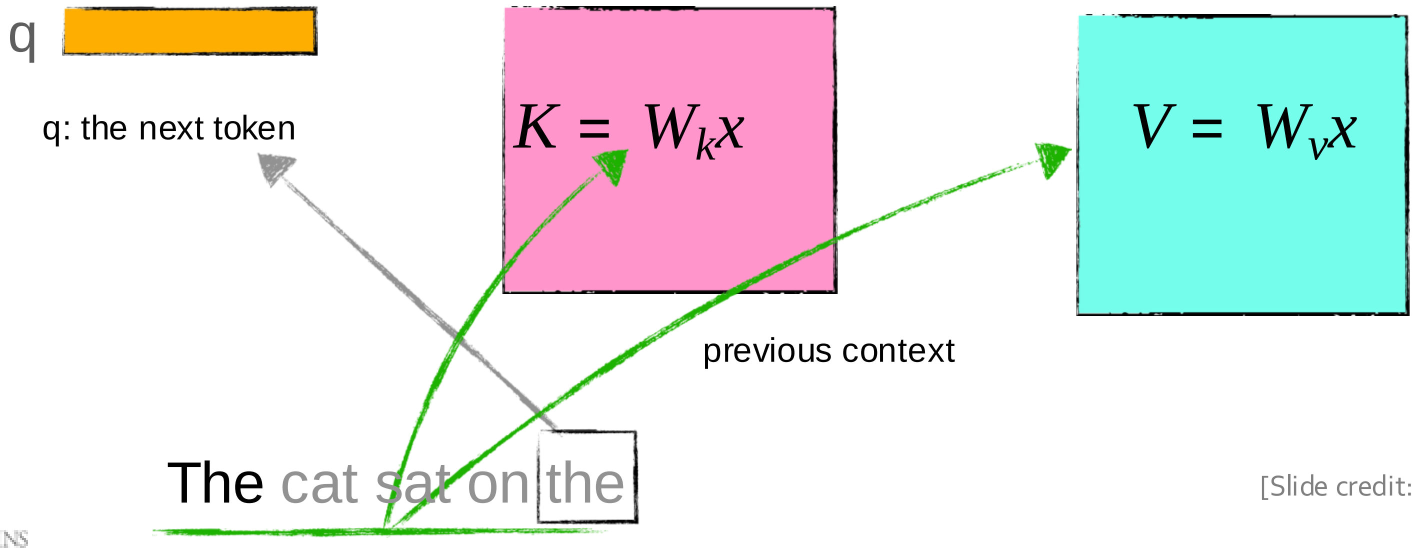


[Slide credit: Arman Cohan]

Making decoding more efficient

$$Q = \mathbf{W}^q \mathbf{x}$$
$$K = \mathbf{W}^k \mathbf{x}$$
$$V = \mathbf{W}^v \mathbf{x}$$
$$\text{Attention}(\mathbf{x}) = \text{softmax}\left(\frac{QK^{\mathrm{T}}}{\sqrt{d}}\right)V$$

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



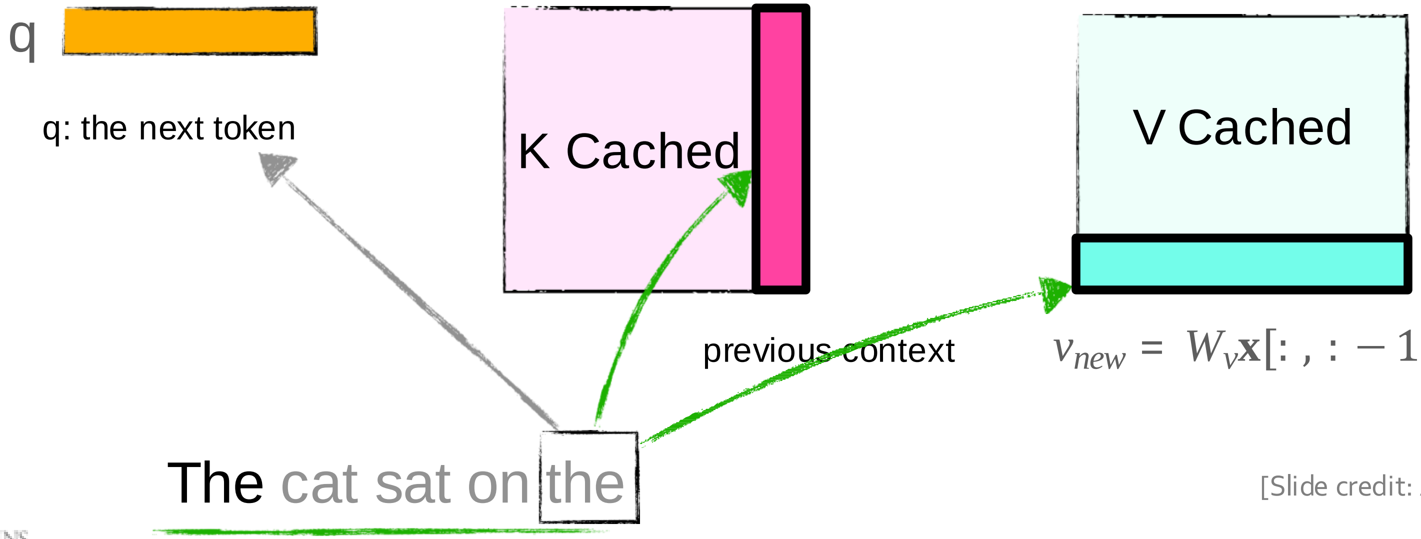
[Slide credit: Arman Cohan]

Making decoding more efficient

- We are computing the Keys and Values many times!
  - Let’s reduce redundancy! 😤

$$Q = \mathbf{W}^q \mathbf{x}$$
$$K = \mathbf{W}^k \mathbf{x}$$
$$V = \mathbf{W}^v \mathbf{x}$$
$$\text{Attention}(\mathbf{x}) = \text{softmax}\left(\frac{QK^{\mathrm{T}}}{\sqrt{d}}\right)V$$

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



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

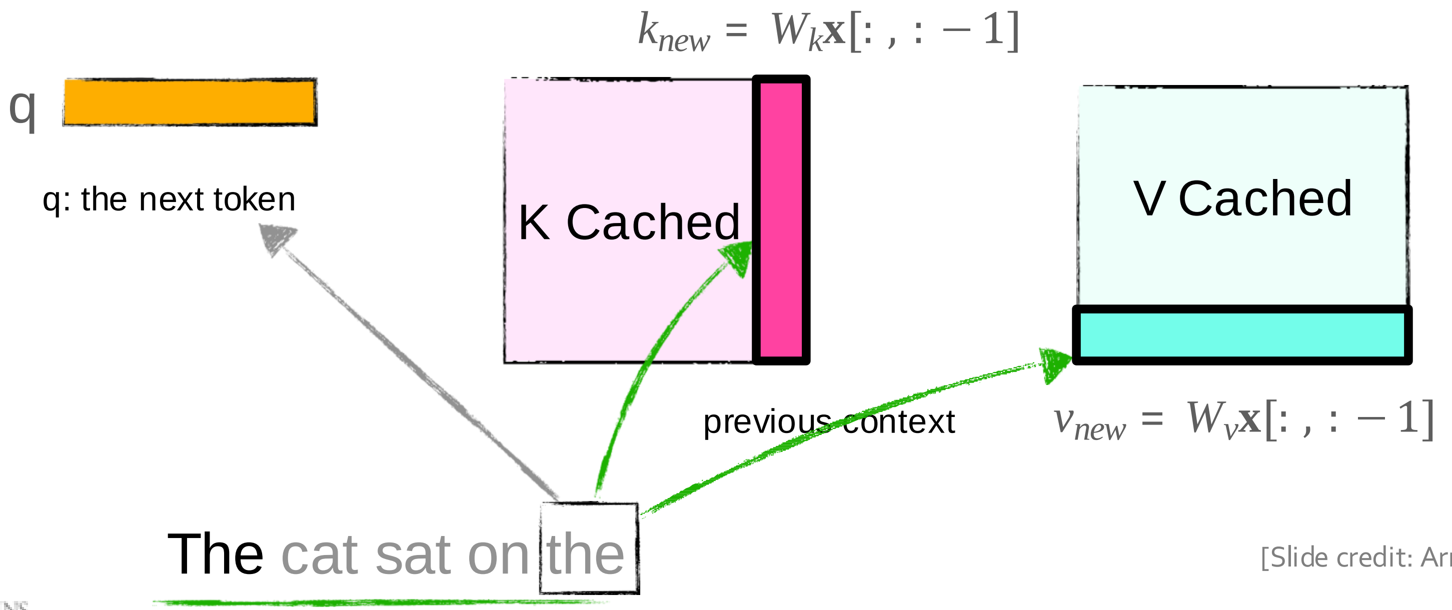
[Slide credit: Arman Cohan]

Making decoding more efficient

$$Q = \mathbf{W}^q \mathbf{x}$$
$$K = \mathbf{W}^k \mathbf{x}$$
$$V = \mathbf{W}^v \mathbf{x}$$

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

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



[Slide credit: Arman Cohan]

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

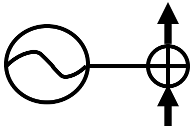
- Create vector representation of sequence vocabulary
- nn.Embedding creates a lookup table to map sequence vocabulary to unique vectors

```
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)
```


[Slide credit: CS886 at UWaterloo]

Positional Encoding

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

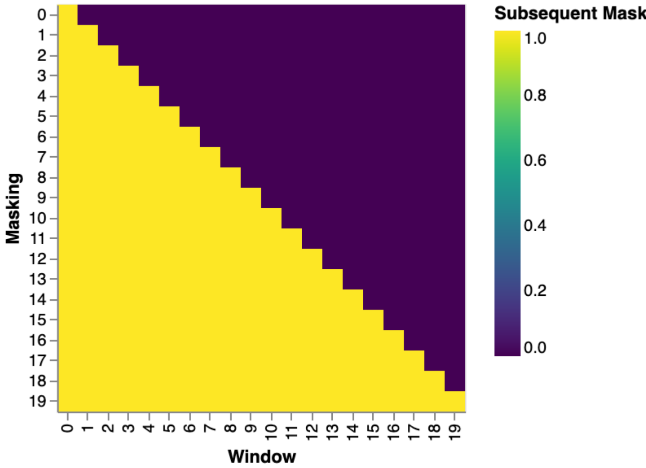



```python
class PositionalEncoding(nn.Module):
    "Implement the PE function."

    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)
```

JOHNS HOPKINS
WHITING SCHOOL of ENGINEERING

[Slide credit: CS886 at UWaterloo]

Attention block




```python
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 softmax(-1e9) ≈ 0

[Slide credit: CS886 at UWaterloo]

Multi-Head Attention

```python
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)
```

```python
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 UWaterloo]

FeedForward Layer

```python
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()))
```

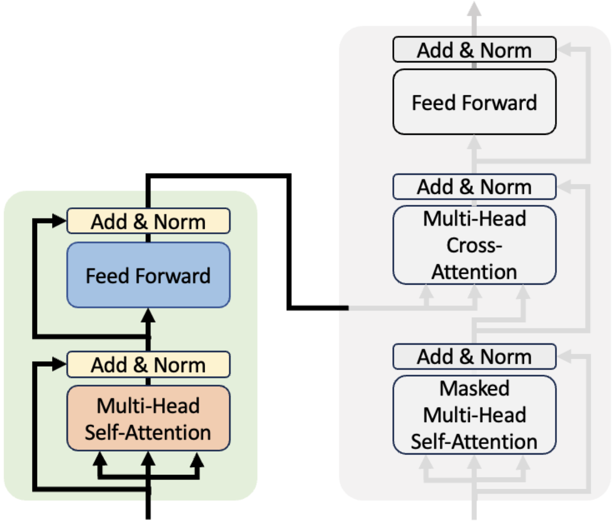
Sublayer Connections

```python
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)))
```


[Slide credit: CS886 at UWaterloo]

Encoder Layer

```python
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)
```

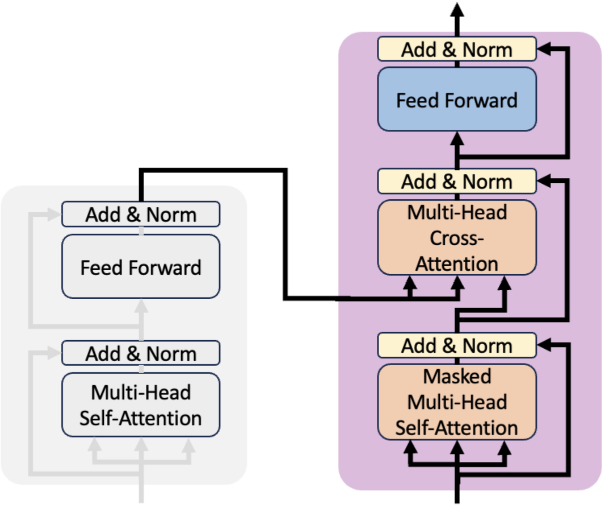


[Slide credit: CS886 at UWaterloo]

Decoder Layer

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

```python
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)
```

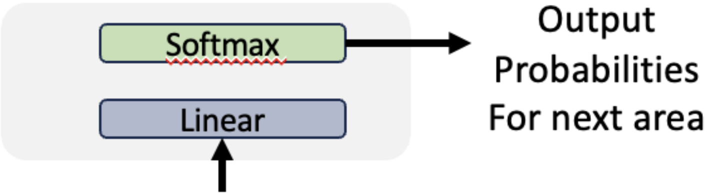


[Slide credit: CS886 at UWaterloo]

The Prediction Head

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

```python
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)
```



[Slide credit: CS886 at UWaterloo]

Build each block

```python
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)
```

```python
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)
```


[Slide credit: CS886 at UWaterloo]

Putting it Together

```python
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)
```

[Slide credit: CS886 at UWaterloo]

Initialize the model

```python
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
```


[Slide credit: CS886 at UWaterloo]