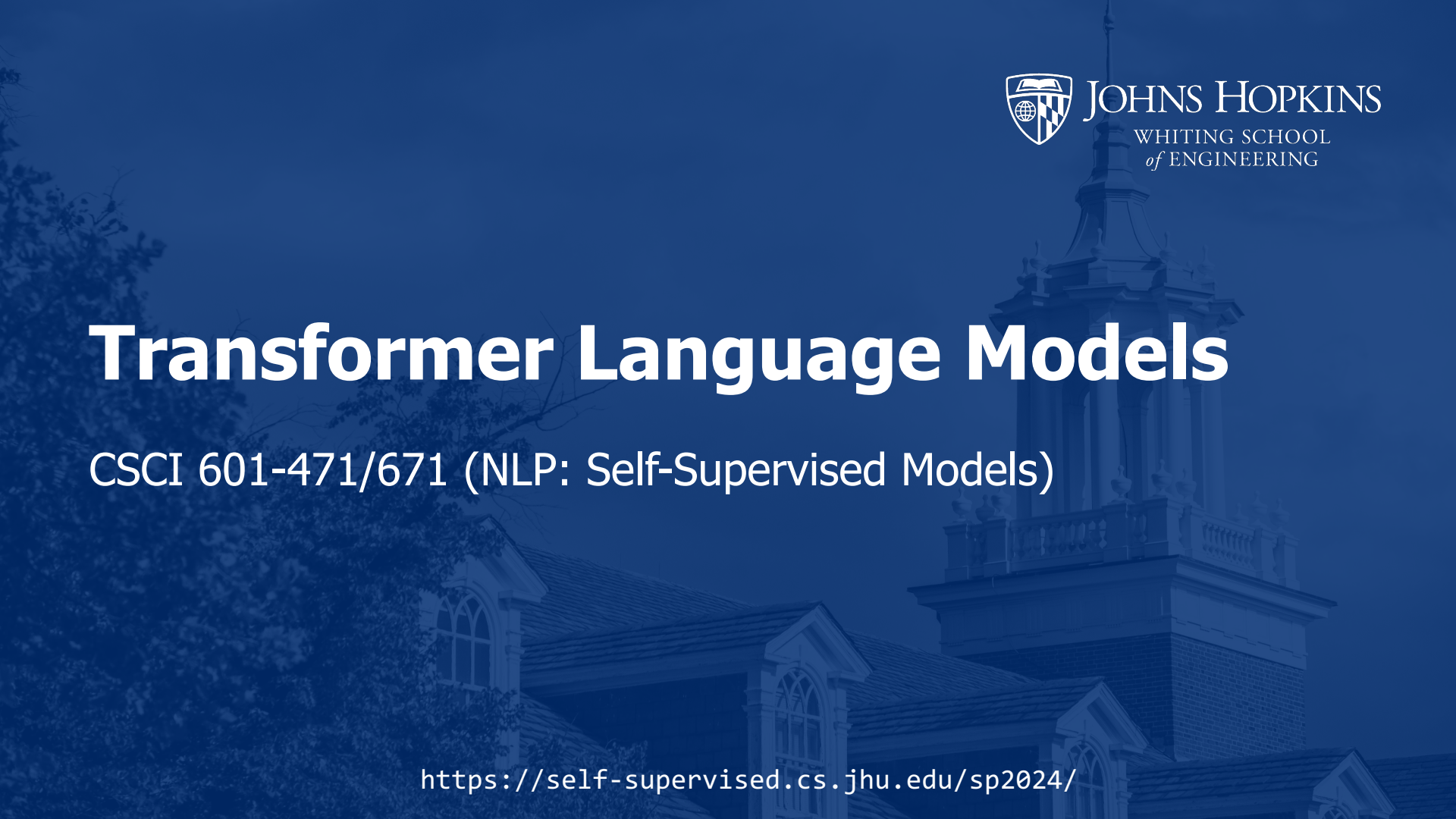


Transformer Language Models

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

https://self-supervised.cs.jhu.edu/sp2024/

Language Models: A History

- Probabilistic n-gram models of text generation [Jelinek+ 1980's, …]
  - Applications: Speech Recognition, Machine Translation
- Word representation learning [Brown 1992, …]
  - Brown, LSA, Word2Vec, Glove …
- Statistical or shallow neural LMs (late 90's – mid 00's) [Bengio+ 2001, …]
- Pre-training deep neural language models (2017's onward):
  - Many models based on: Self-Attention

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!

Chapter Plan

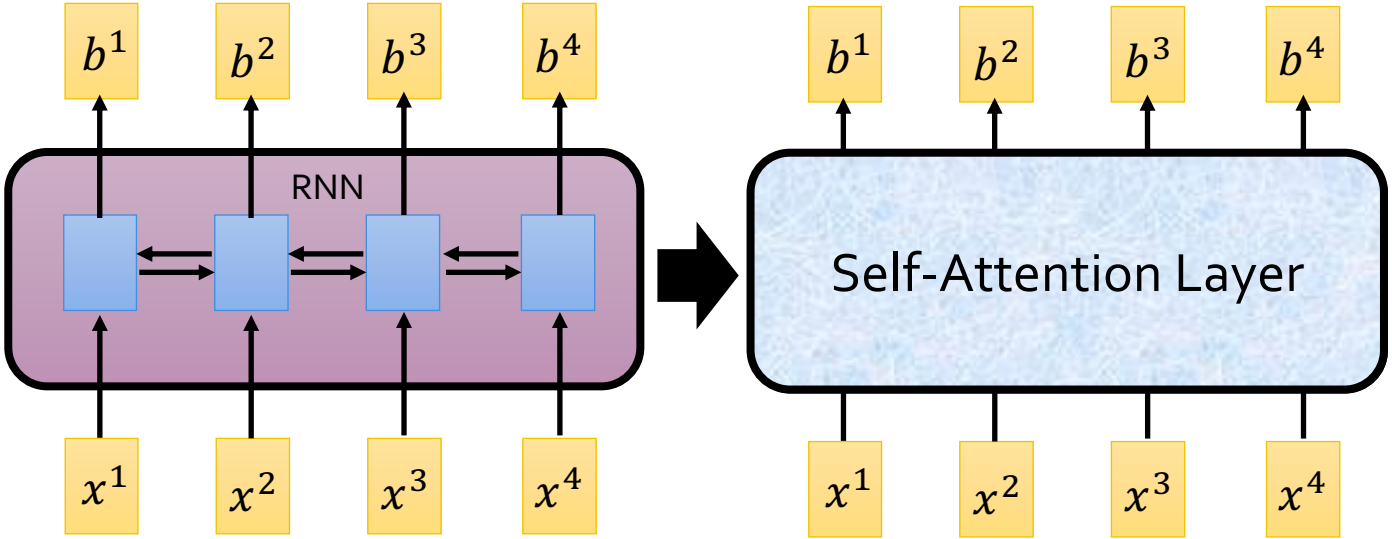
1. Self-Attention: how it works
2. Transformer architecture
3. Transformer-based families of Language Models
4. Practical hacks and variants
5. Various objective functions

Chapter goal----

Self-Attention

Self-Attention

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



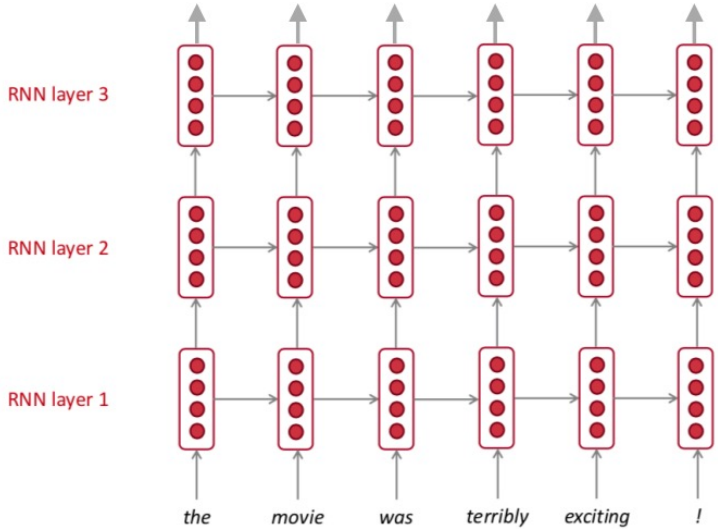
Idea: replace any thing done by RNN with self-attention.

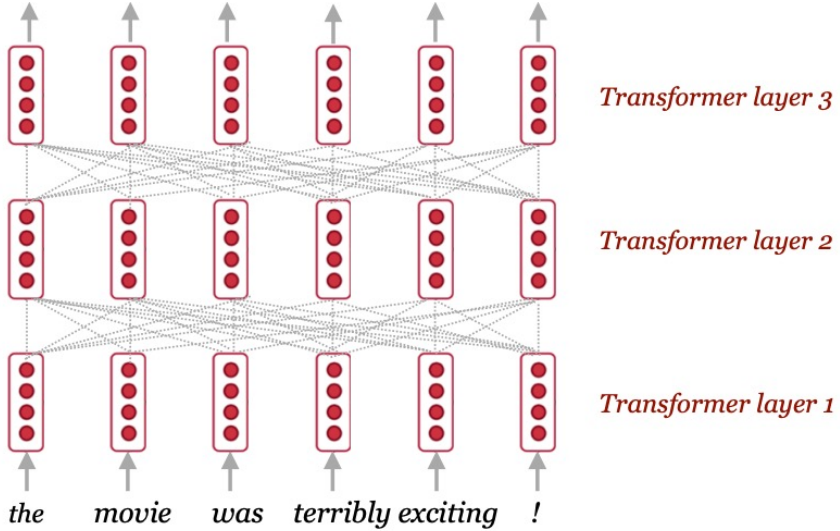
"Neural machine translation by jointly learning to align and translate" Bahdanau etl. 2014;
"Attention is All You Need" Vaswani et al. 2017

[adopted from Hung-yi Lee]

6

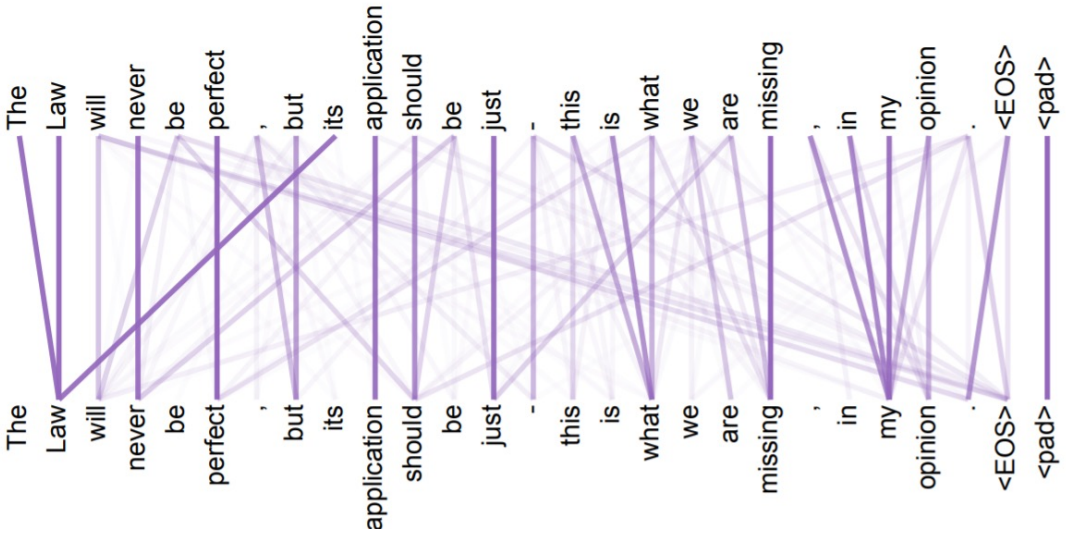
RNN vs Transformer





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

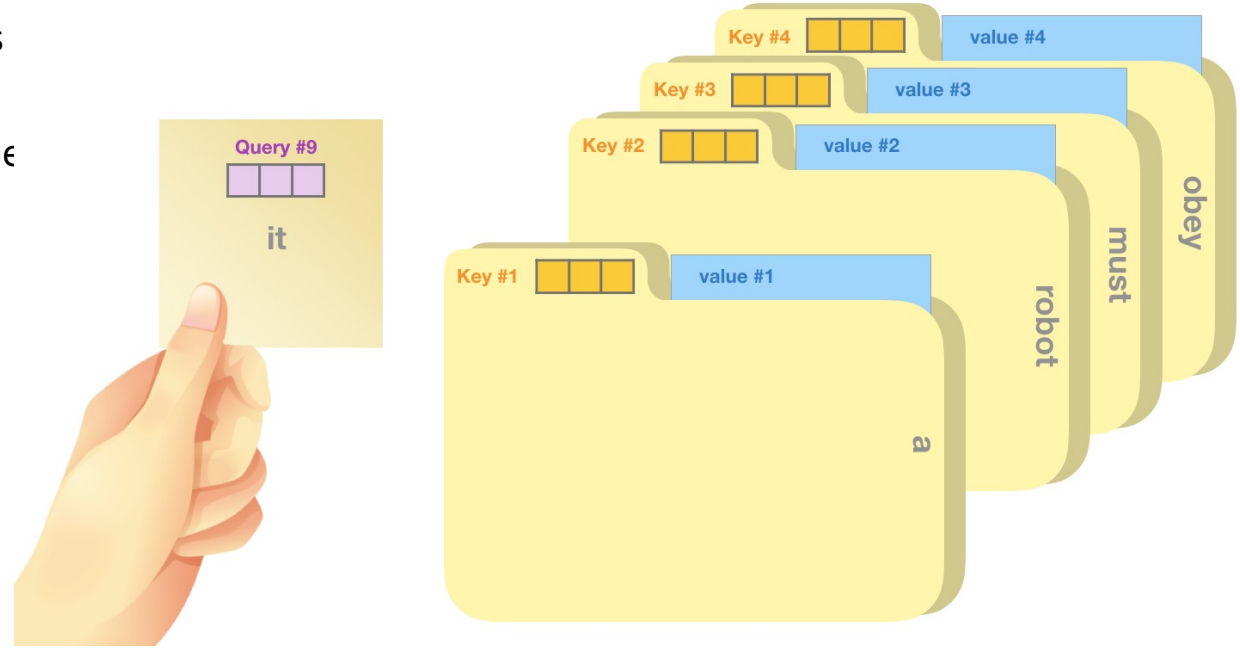
- Terminology:
  - Query: to match others
  - Key: to be matched
  - Value: information to be extracted

[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

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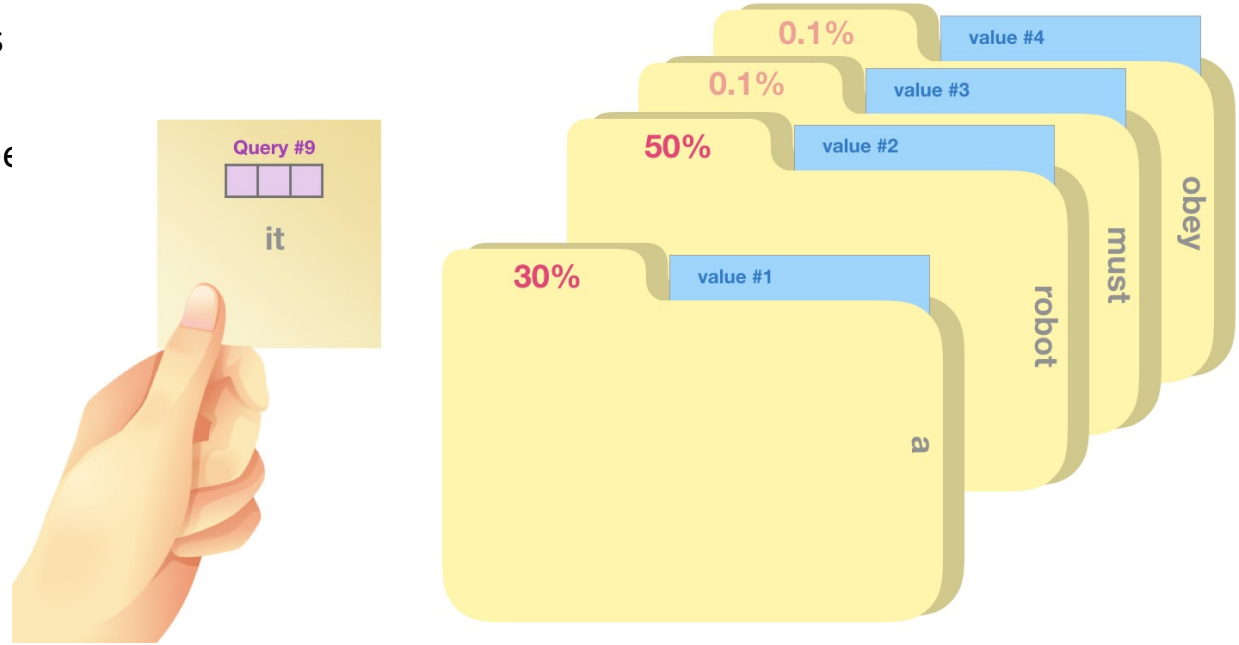


[Vaswani et al. 2017: https://arxiv.org/abs/1706.03762]

q: query (to match others)

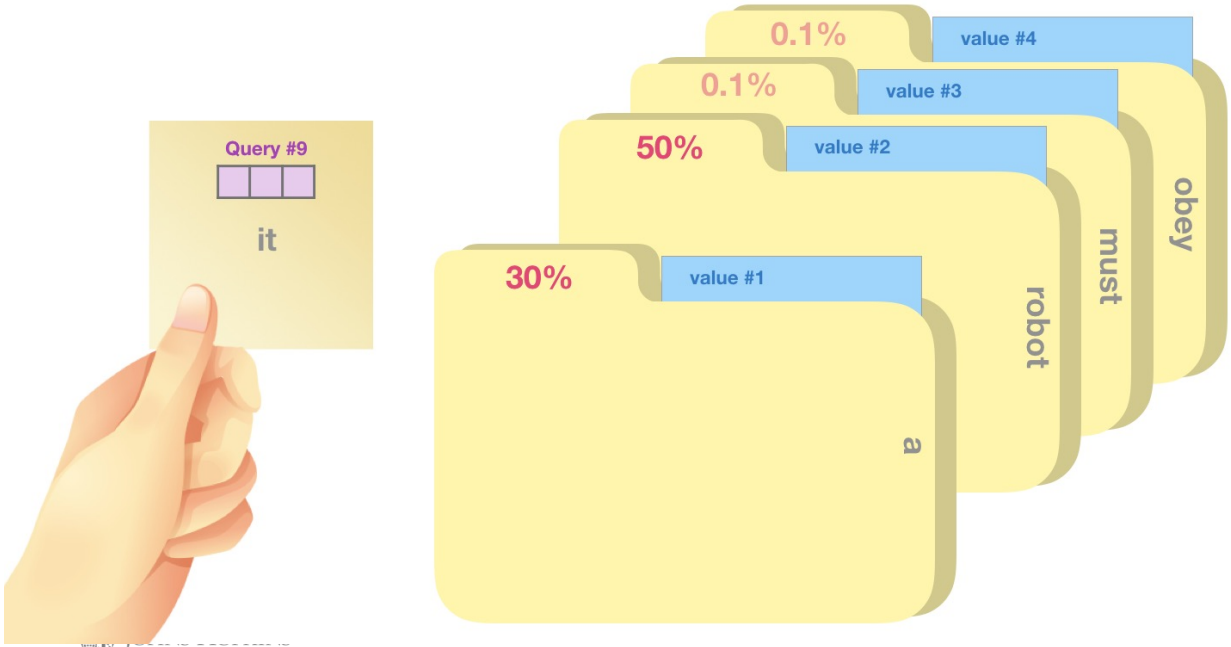
$$q_i = W^q x_i$$

k: key (to be matched)

$$k_i = W^k x_i$$

v: value (information to be extracted)

$$v_i = W^v x_i$$



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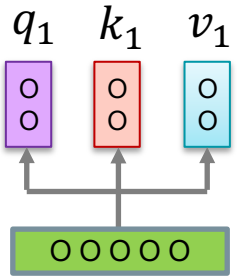


The

q: query (to match others)

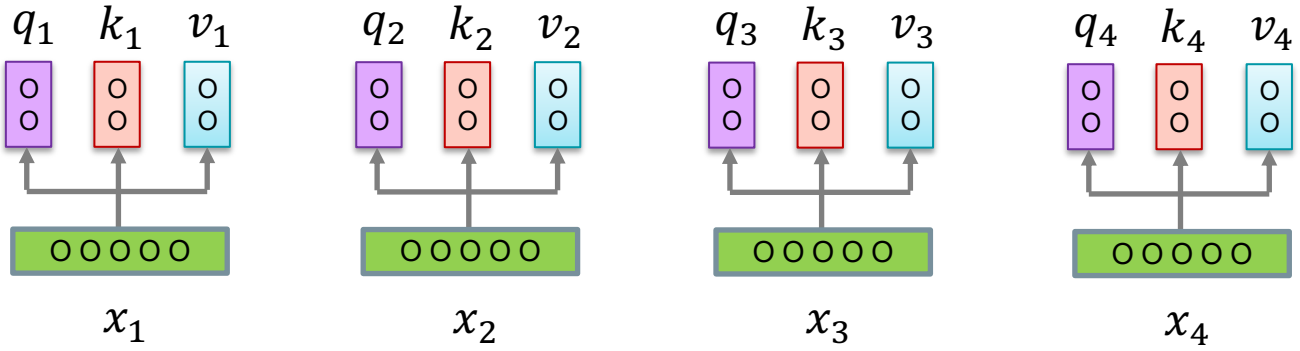
$$q_i = W^q x_i$$

k: key (to be matched)

$$k_i = W^k x_i$$

v: value (information to be extracted)

$$v_i = W^v x_i$$



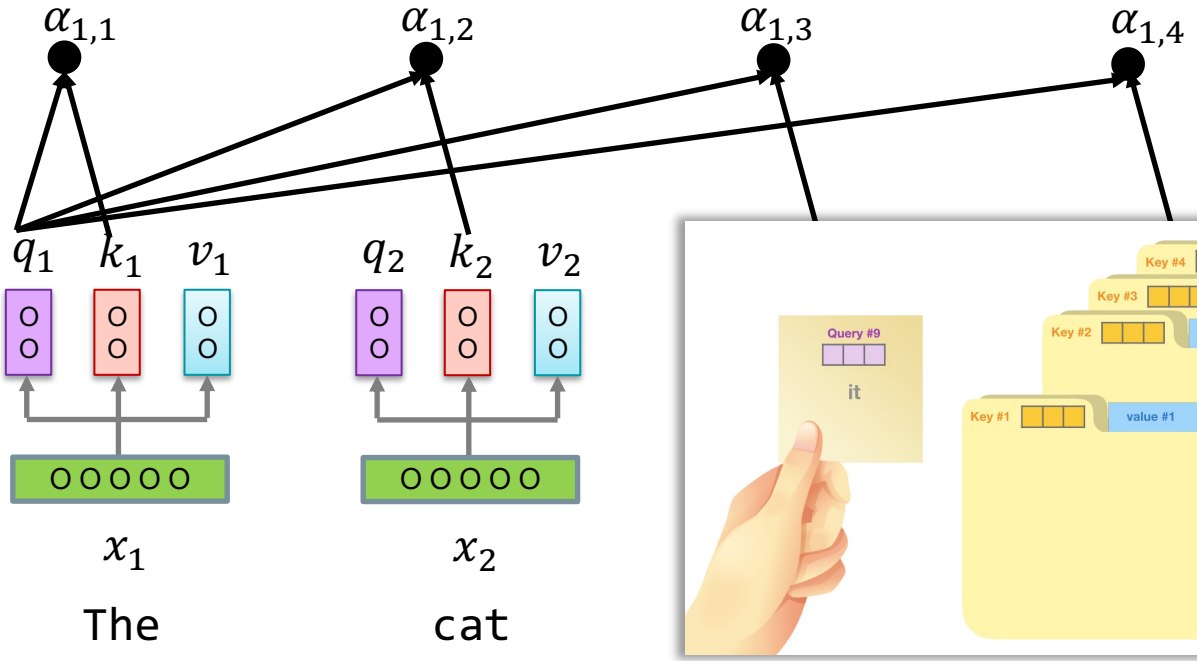
$$\alpha_{1,i} = \underbrace{q^1 \cdot k^i / \sqrt{d}}_{\text{Scaled dot product}}$$

q: query (to match others)

k: key (to be matched)

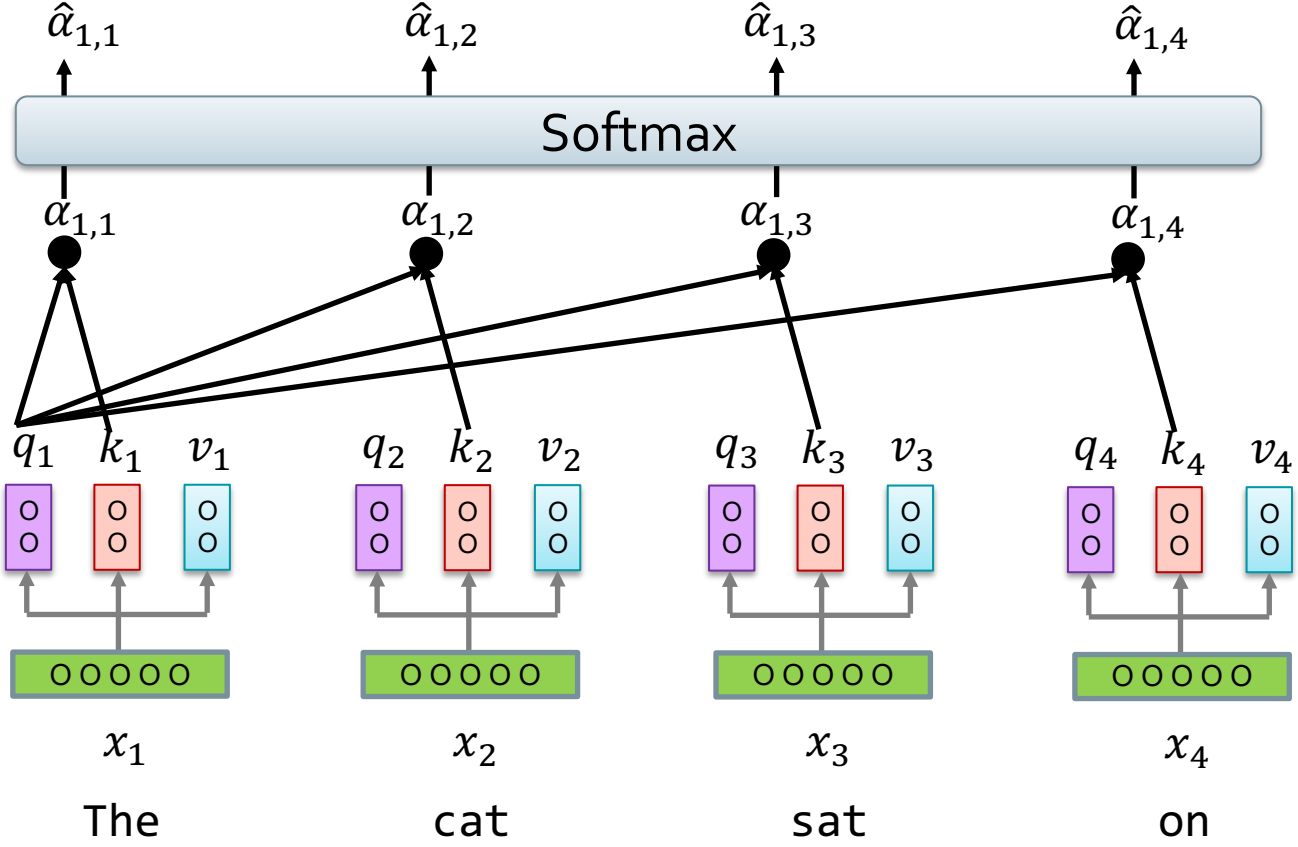
v: value (information to be extracted)

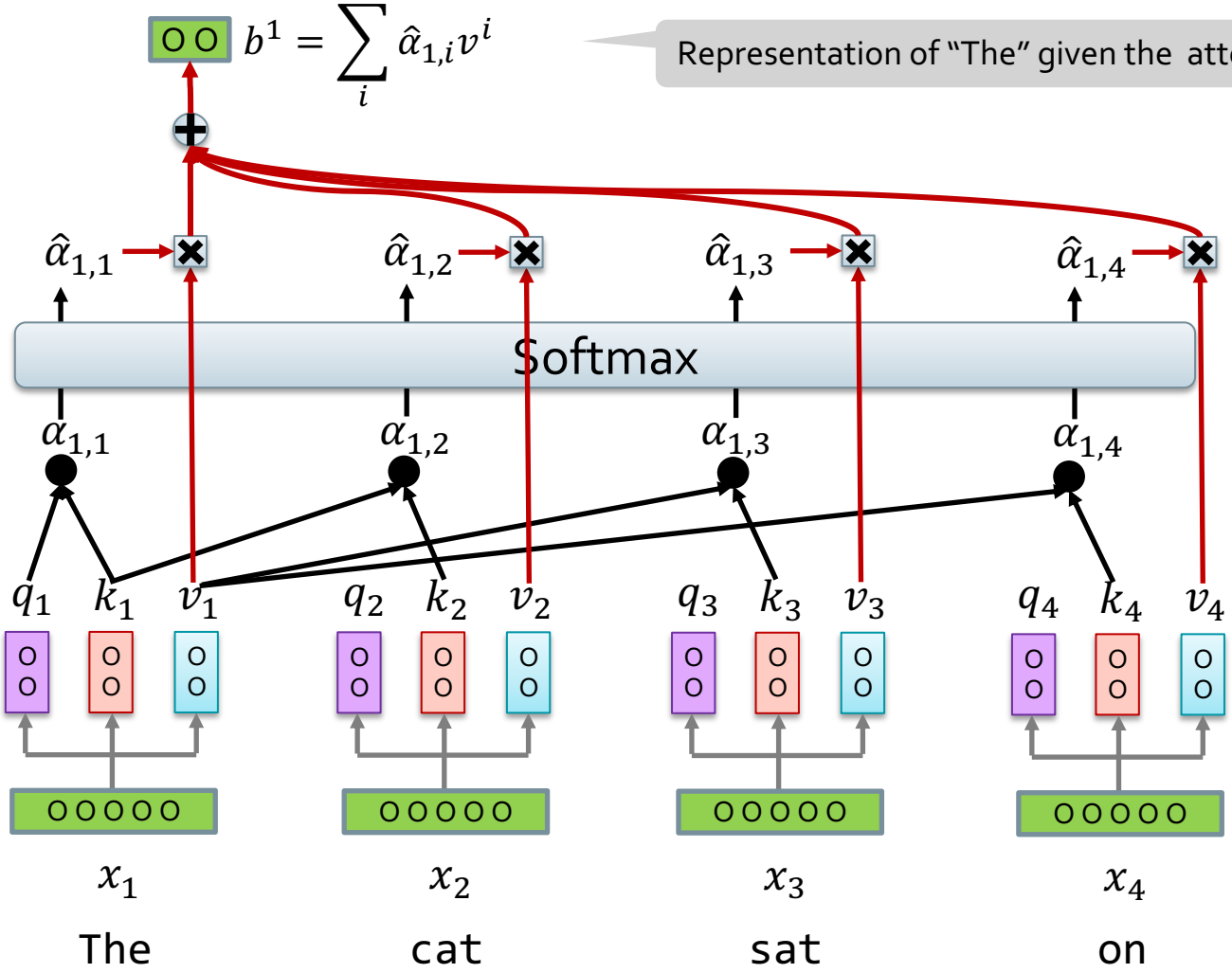
How much should "The" attend to other positions?



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

How much should "The" attend to other positions?



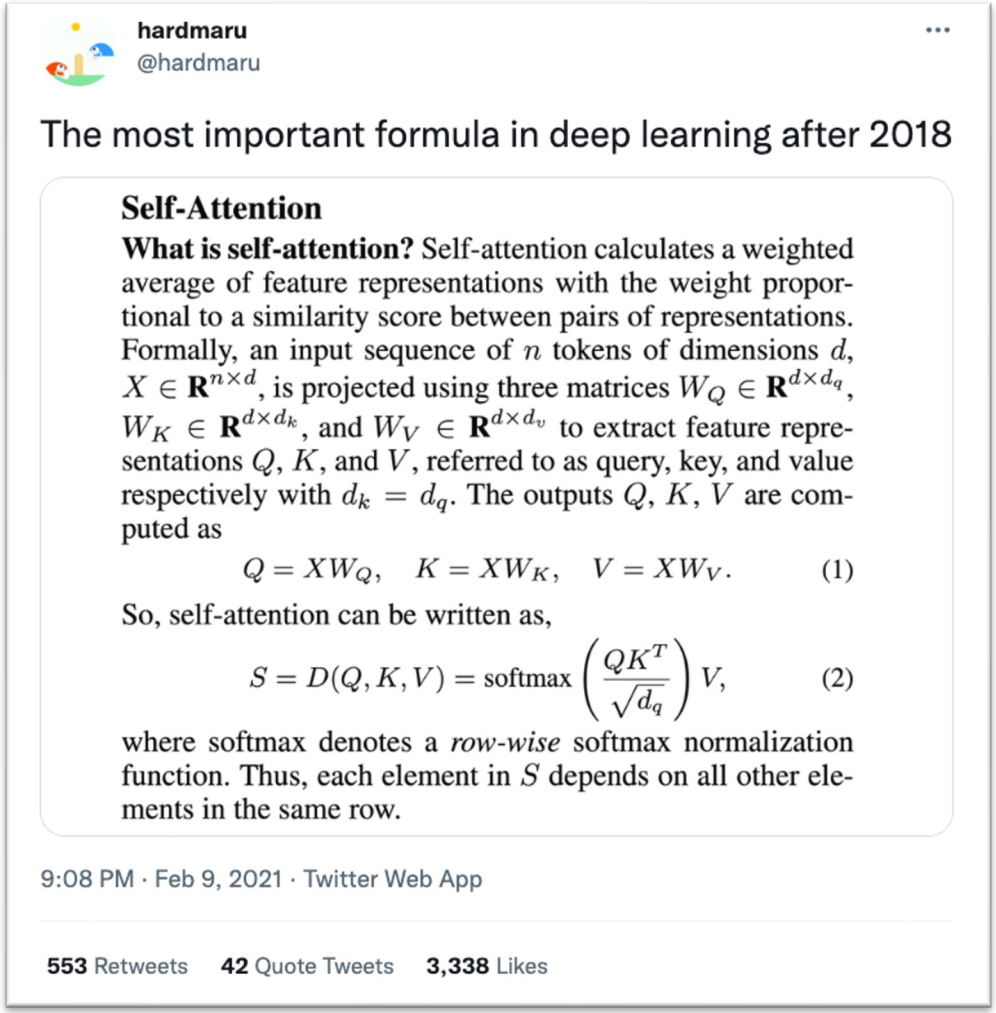

$b^1 = \sum_i \hat{\alpha}_{1,i} v^i$
Representation of "The" given the attention weights
$\hat{\alpha}_{1,1}$
$\hat{\alpha}_{1,2}$
$\hat{\alpha}_{1,3}$
$\hat{\alpha}_{1,4}$
Softmax
$\alpha_{1,1}$
$\alpha_{1,2}$
$\alpha_{1,3}$
$\alpha_{1,4}$
q_1 k_1 v_1
q_2 k_2 v_2
q_3 k_3 v_3
q_4 k_4 v_4
x_1 x_2 x_3 x_4
The cat sat on

Self-Attention

- Can write it in matrix form:
- Given input $\mathbf{x}$:

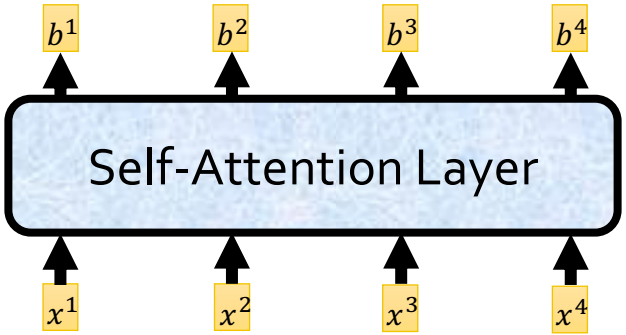
$$Q = \mathbf{W}^q \mathbf{x}$$
$$K = \mathbf{W}^k \mathbf{x}$$
$$V = \mathbf{W}^v \mathbf{x}$$

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



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]

19

Properties of Self-Attention

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

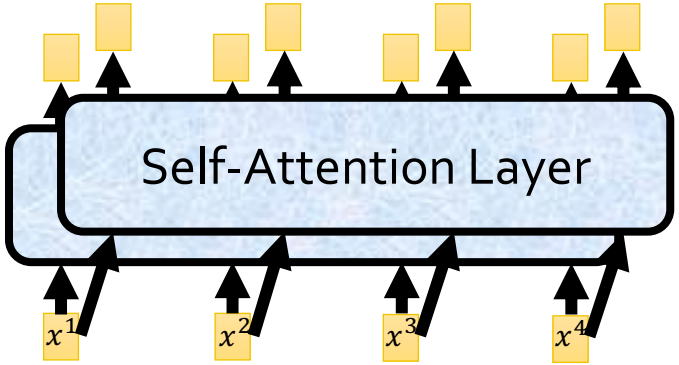
- n = sequence length, d = hidden dimension
- Quadratic complexity, but:
  - O(1) sequential operations (not linear like in RNN)

- Efficient implementations

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

Multi-Headed Self-Attention

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



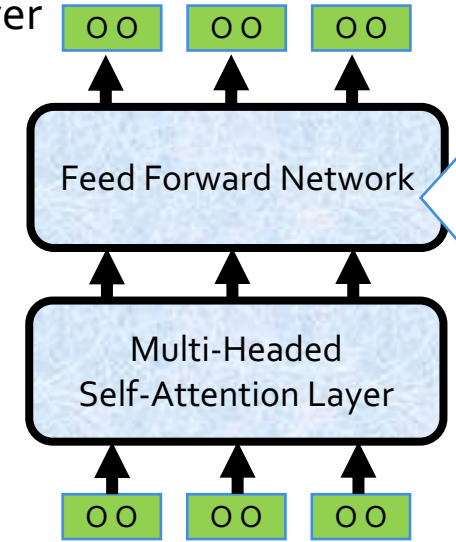
[Attention Is All You Need, Vaswani et al. 2017]

24

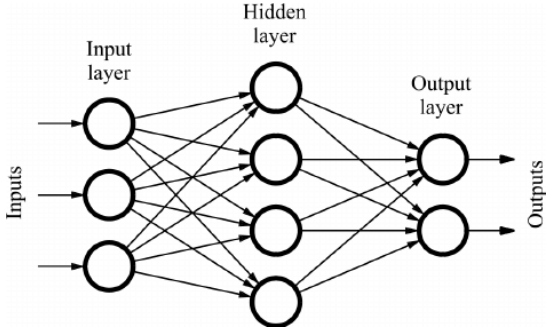
Combine with FFN

- 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.

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



Feedforward Net: Refresher

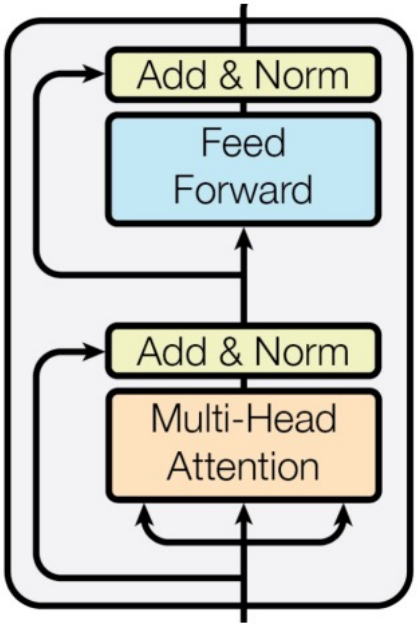


A fully-connected network of nodes and weights.

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



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

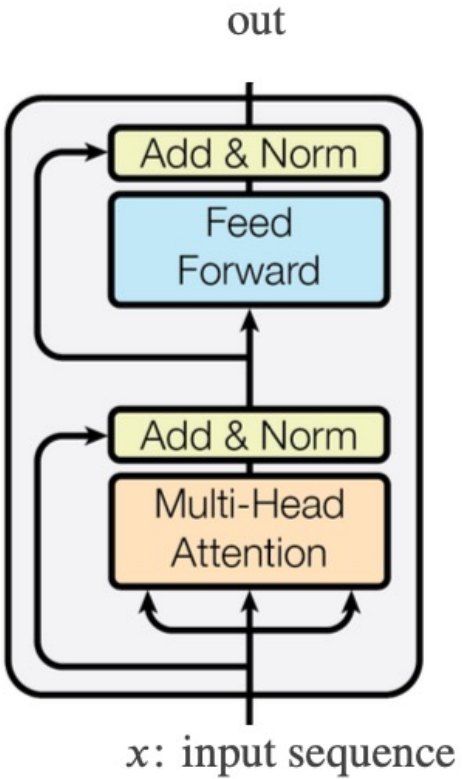
26

Putting it Together: Self-Attention Block

Given input $\mathbf{x}$:

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

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



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

Summary: Self-Attention Block

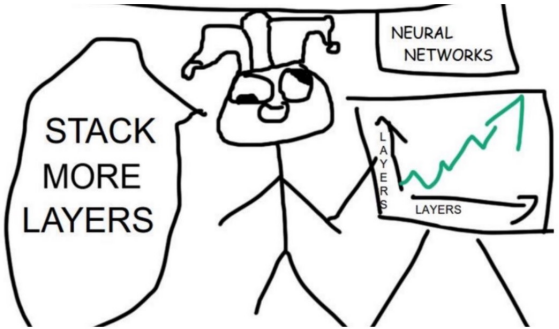
- **Self-Attention:** A critical building block of modern language models.
  - The idea is to compose meanings of words weighted according some similarity notion.

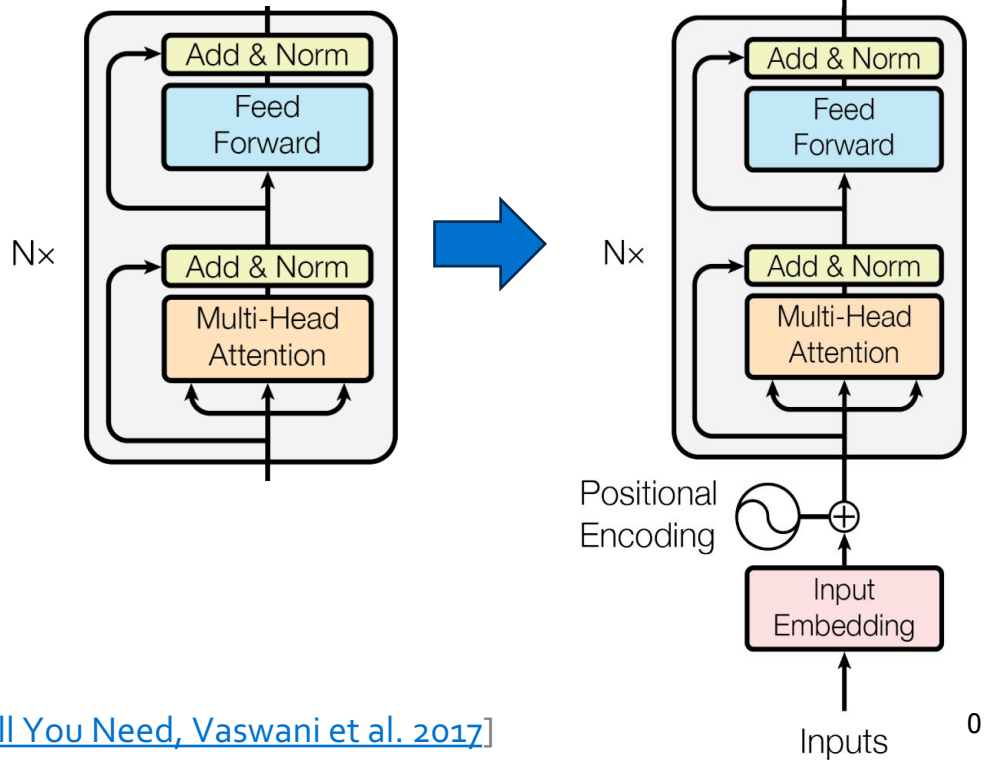
- **Next:** We will combine self-attention blocks to build various architectures known as Transformer.

Transformer

How Do We Make it Deep?

- Stack more layers!





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

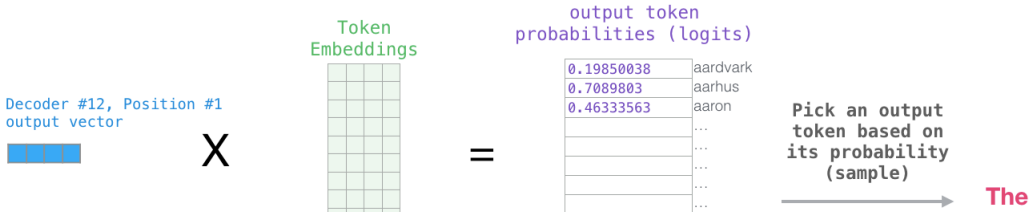
From Representations to Prediction

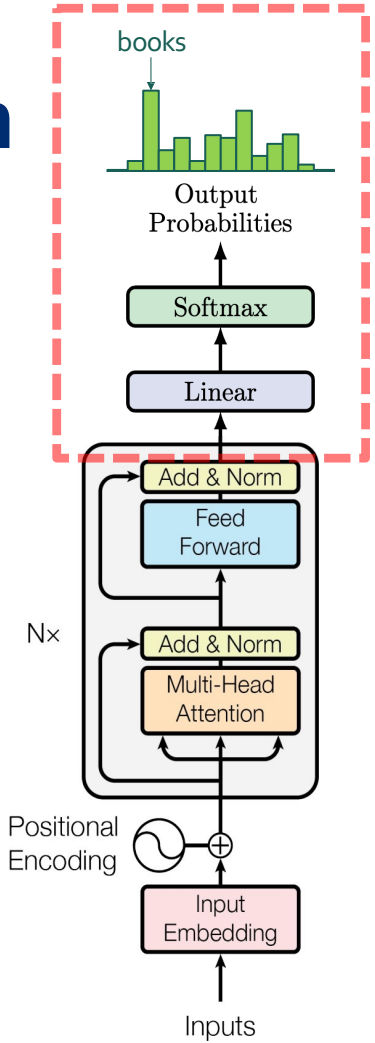
- To perform prediction, add a classification head on top of the final layer of the transformer.
- This can be per token (Language modeling)
- Or can be for the entire sequence (only one token)

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

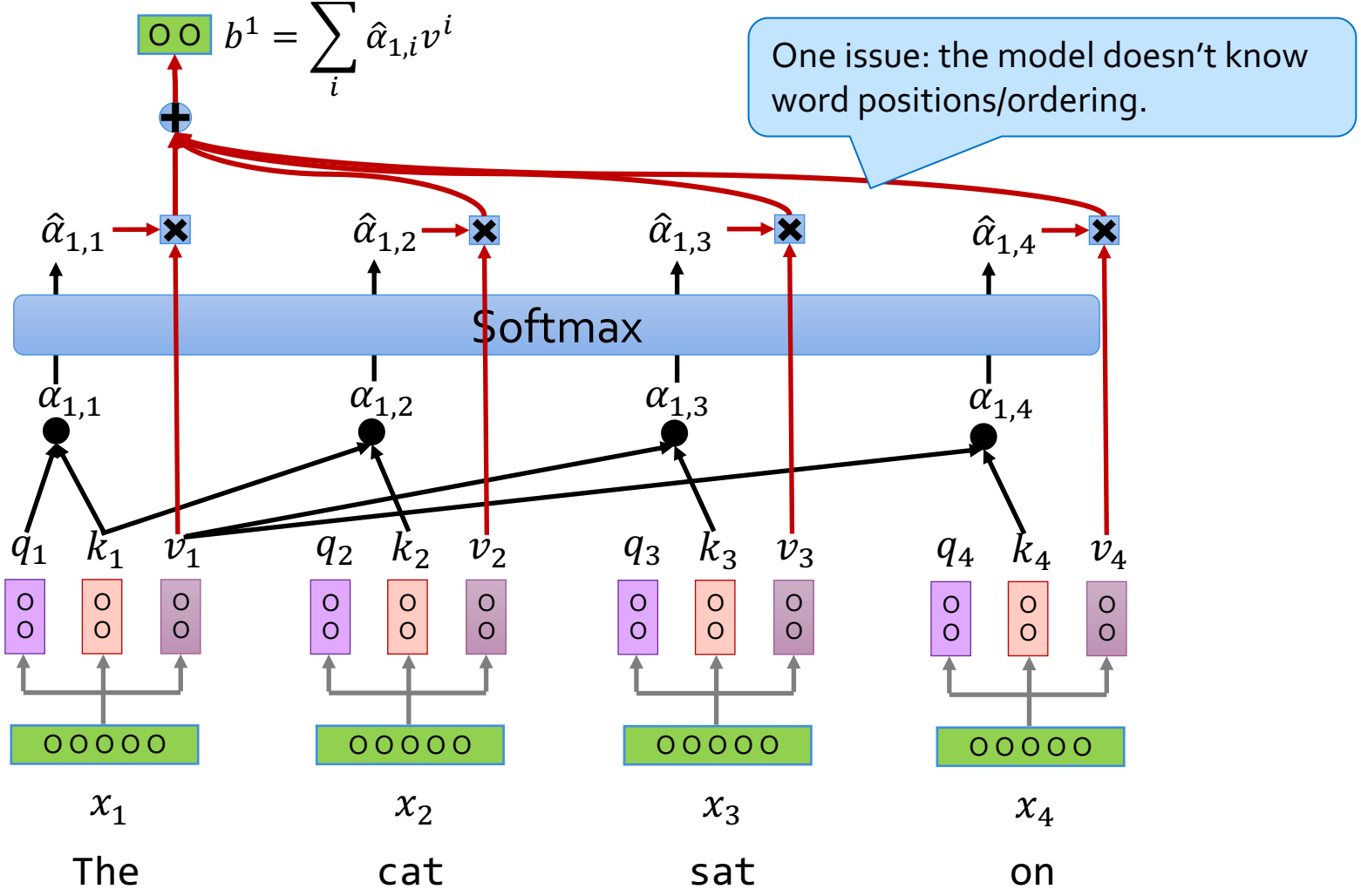
$$\text{logits} = \text{Linear}_{(\text{d, V})}(out) = f\left(out \,.\, W_V\right) \in \mathbb{R}^{S \times V}$$

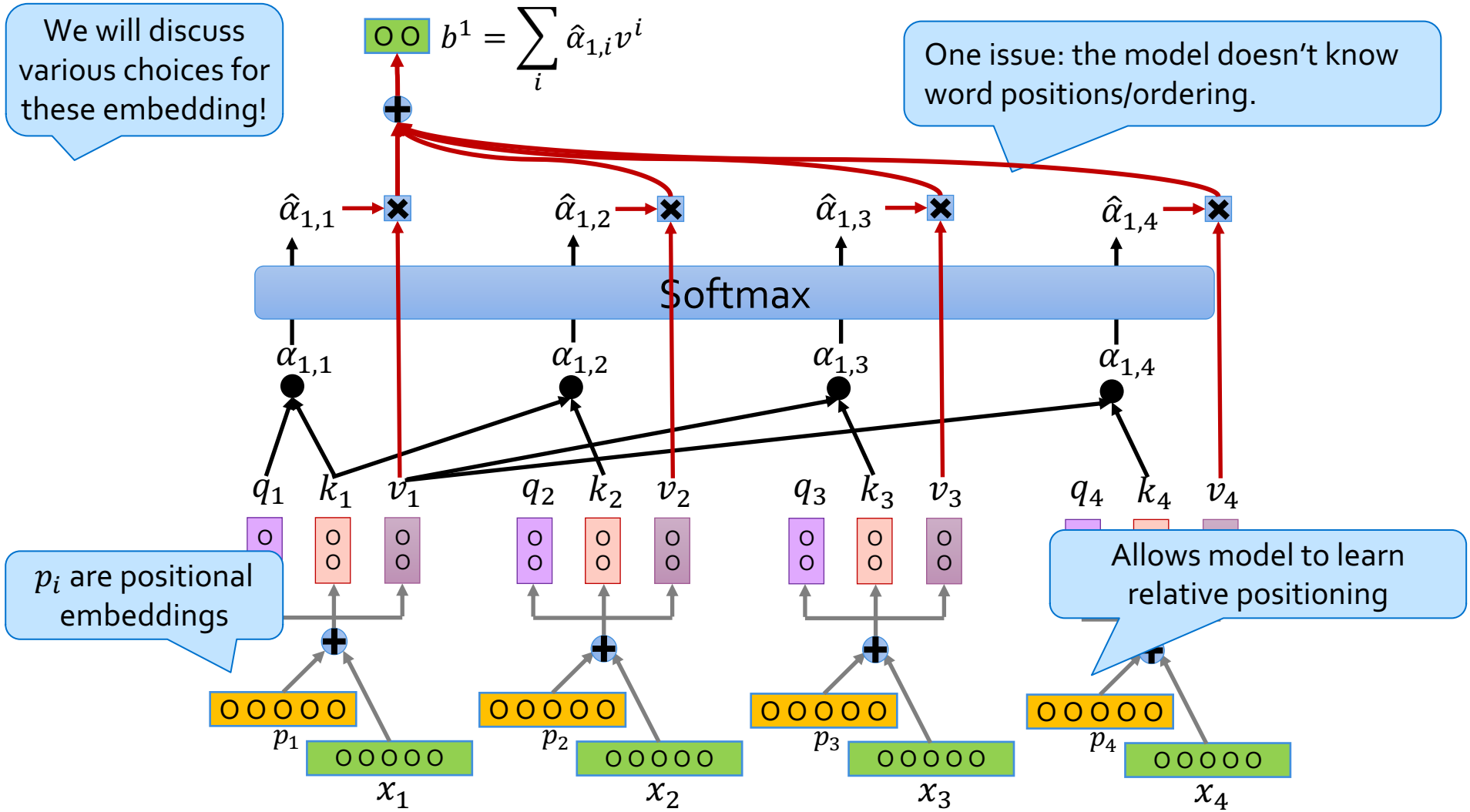
$$\text{probabilies} = \text{softmax}(\text{logits}) \in \mathbb{R}^{S \times V}$$





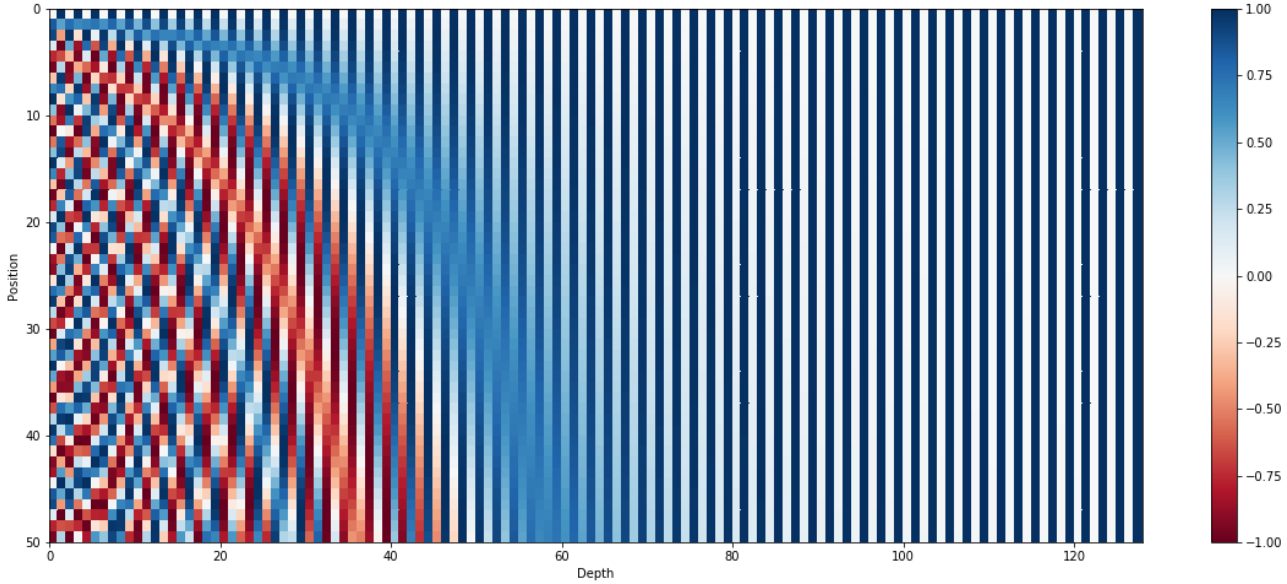
One last wrinkle though …

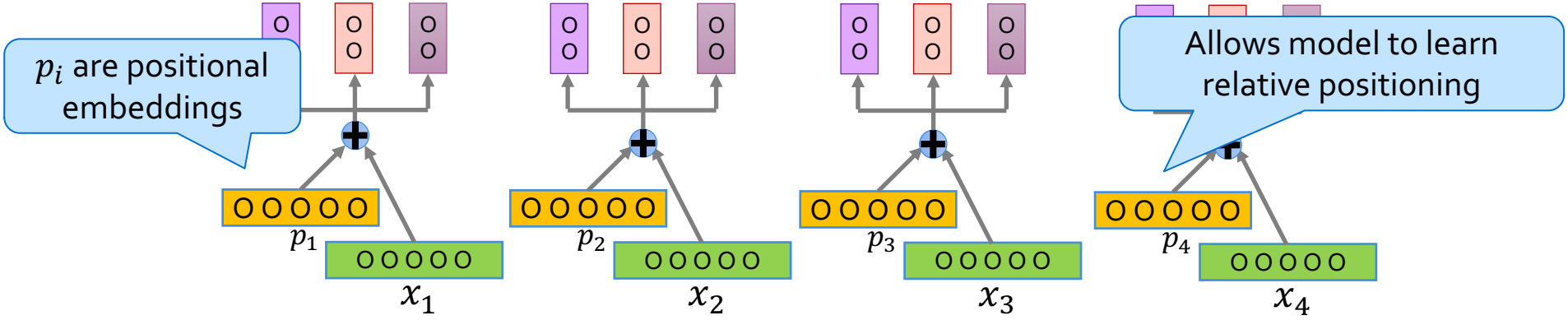

$b^1 = \sum_i \hat{\alpha}_{1,i} v^i$
One issue: the model doesn't know word positions/ordering.
$\hat{\alpha}_{1,1}$
$\hat{\alpha}_{1,2}$
$\hat{\alpha}_{1,3}$
$\hat{\alpha}_{1,4}$
Softmax
$\alpha_{1,1}$
$\alpha_{1,2}$
$\alpha_{1,3}$
$\alpha_{1,4}$
q_1 k_1 v_1
q_2 k_2 v_2
q_3 k_3 v_3
q_4 k_4 v_4
x_1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

An approach:

Sine/Cosine encoding



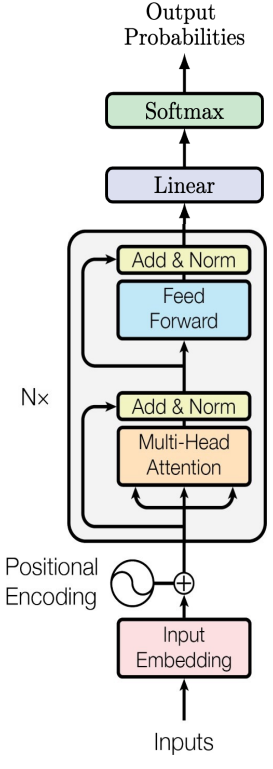


The Transformer Stack in PyTorch

```python
class Block(nn.Module):
    def __init__(self, config):
        super().__init__()
        self.ln_1 = LayerNorm(config.n_embd, bias=config.bias)
        self.attn = CausalSelfAttention(config)
        self.ln_2 = LayerNorm(config.n_embd, bias=config.bias)
        self.mlp = MLP(config)

    def forward(self, x):
        x = x + self.attn(self.ln_1(x))
        x = x + self.mlp(self.ln_2(x))
        return x
```

```python
self.transformer = nn.ModuleDict(
    dict(
        wte=nn.Embedding(config.vocab_size, config.n_embd),
        wpe=nn.Embedding(config.block_size, config.n_embd),
        drop=nn.Dropout(config.dropout),
        h=nn.ModuleList([Block(config) for _ in range(config.n_layer)]),
        ln_f=LayerNorm(config.n_embd, bias=config.bias),
    )
)
self.lm_head = nn.Linear(config.n_embd, config.vocab_size, bias=False)
```



Transformer-based Language Modeling

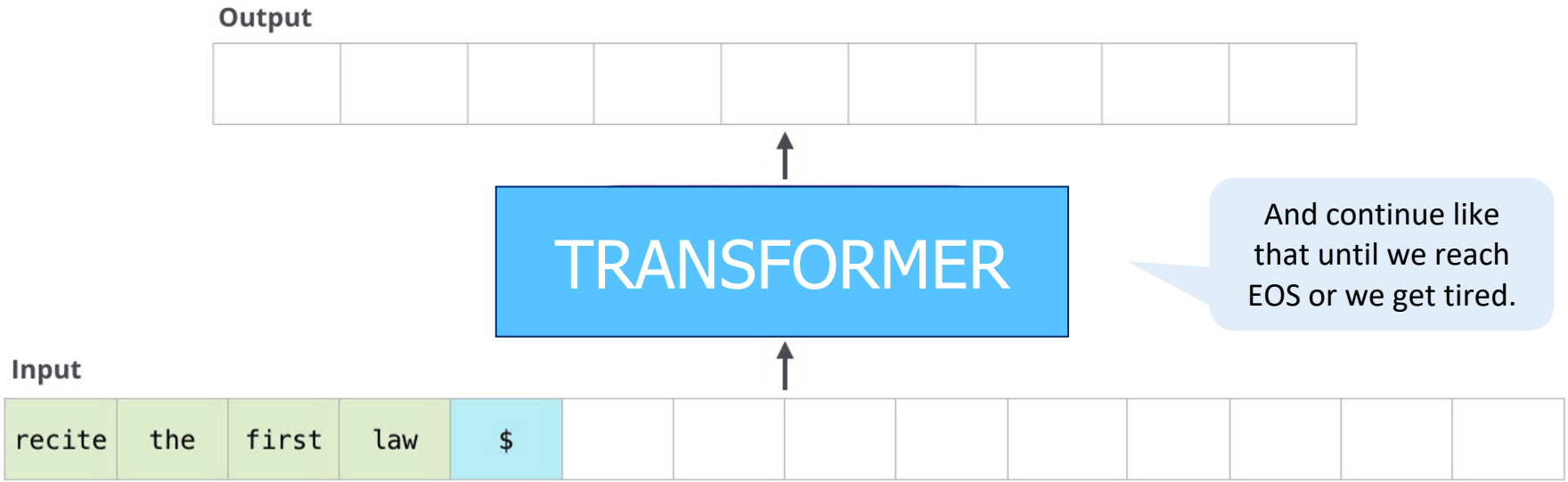
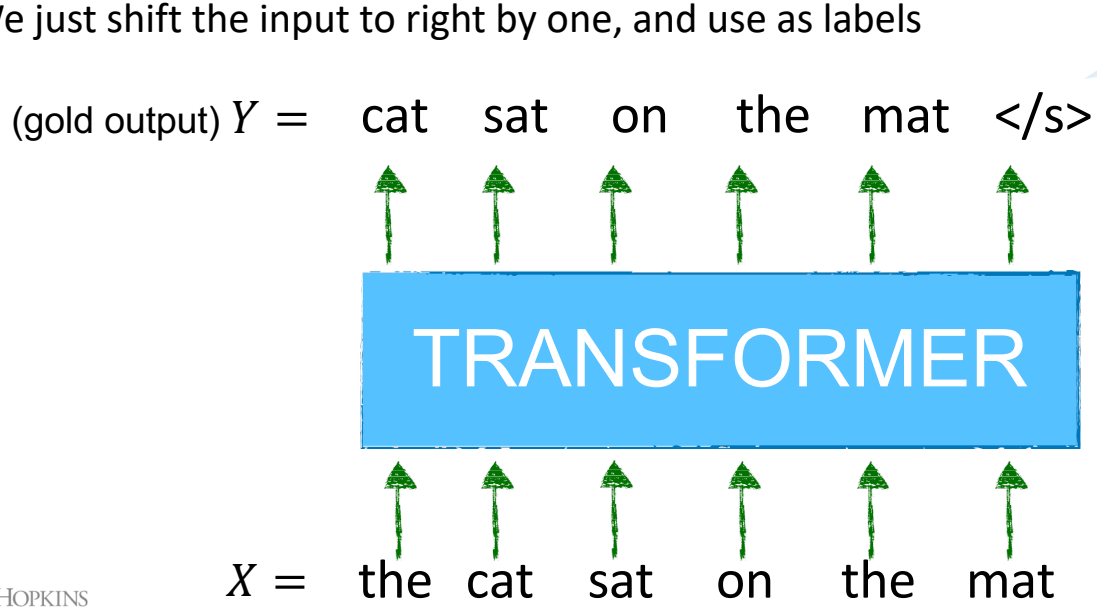


Image by http://jalammar.github.io/illustrated-gpt2/

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



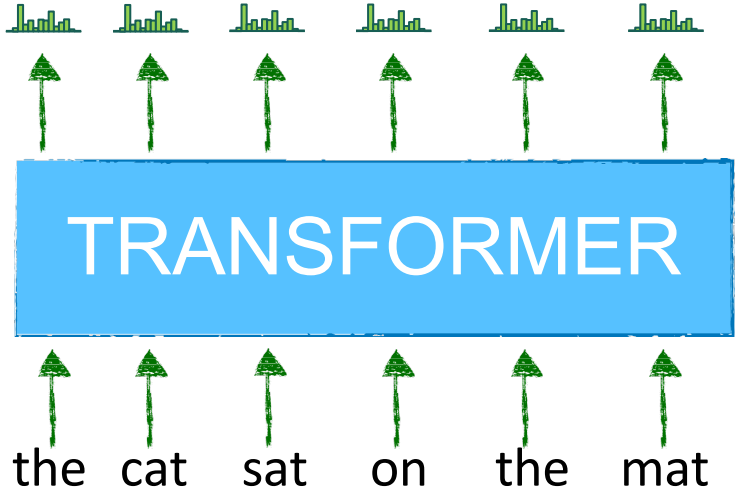

```
X = text[:, :-1]
Y = text[:, 1:]
```

[Slide credit: Arman Cohan]

Training a Transformer Language Model

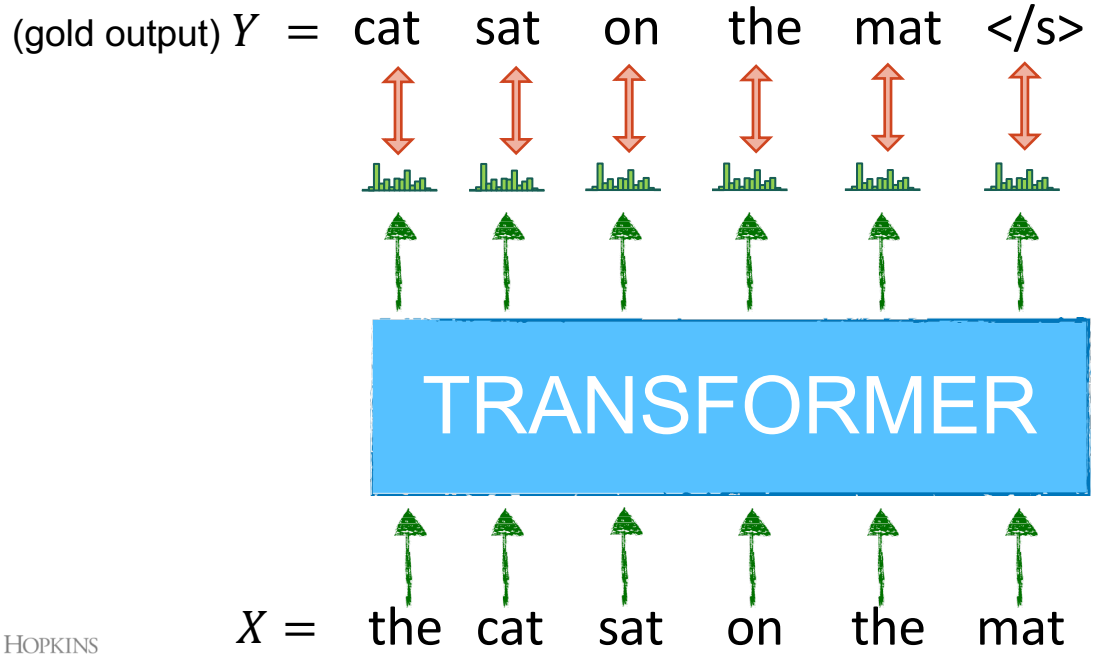
- For each position, compute their corresponding **distribution** over the whole vocab.

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



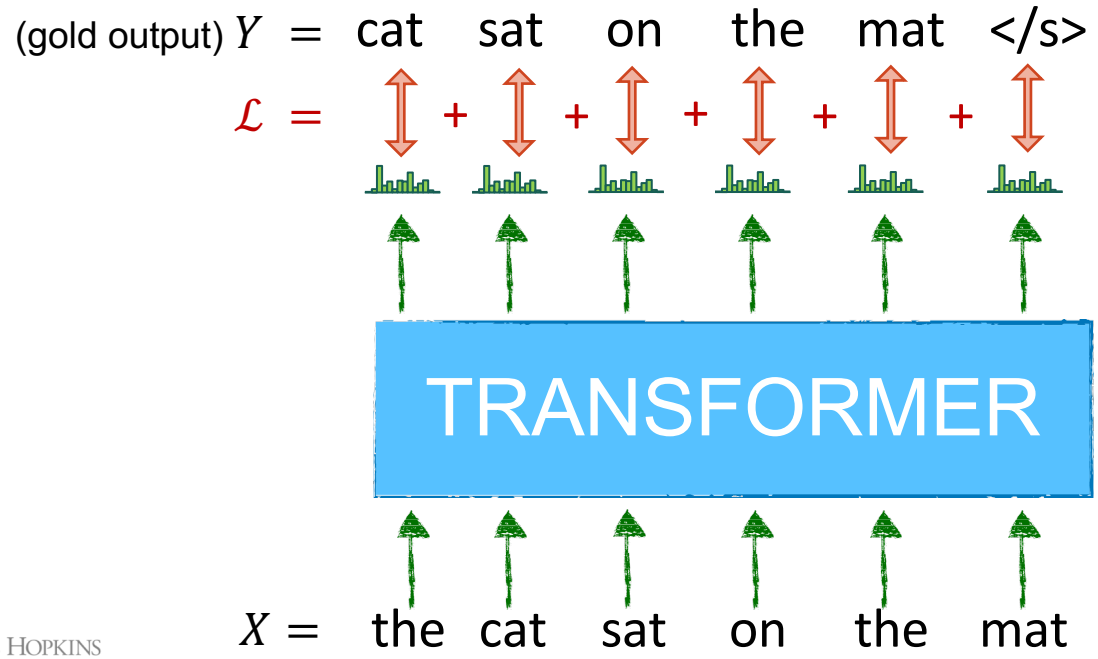
Training a Transformer Language Model

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



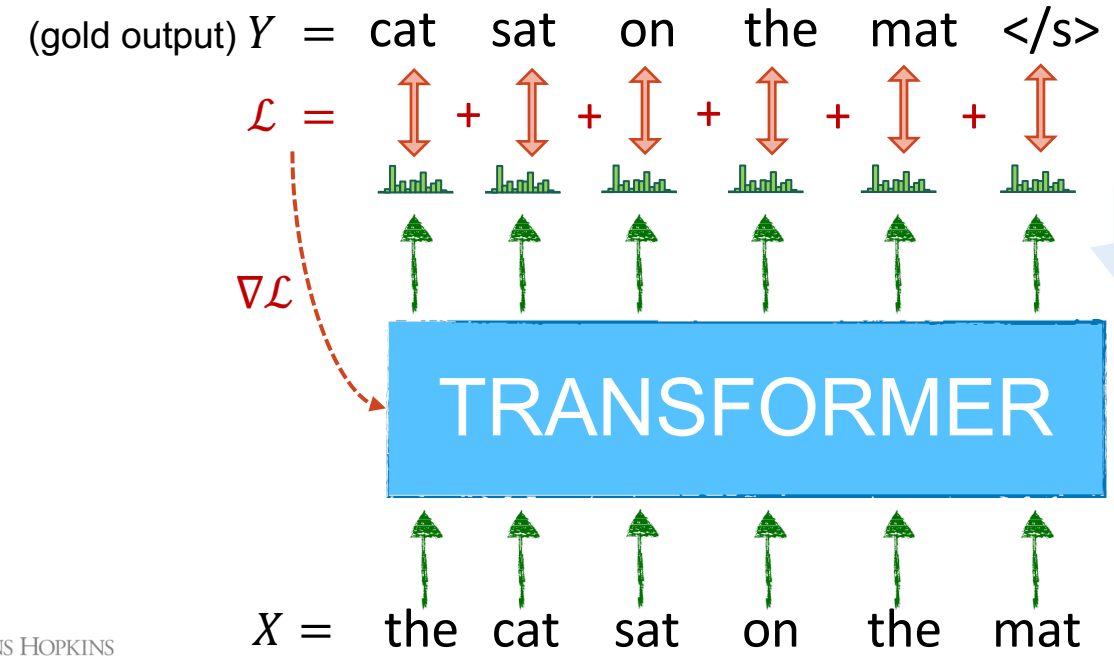
Training a Transformer Language Model

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



Training a Transformer Language Model

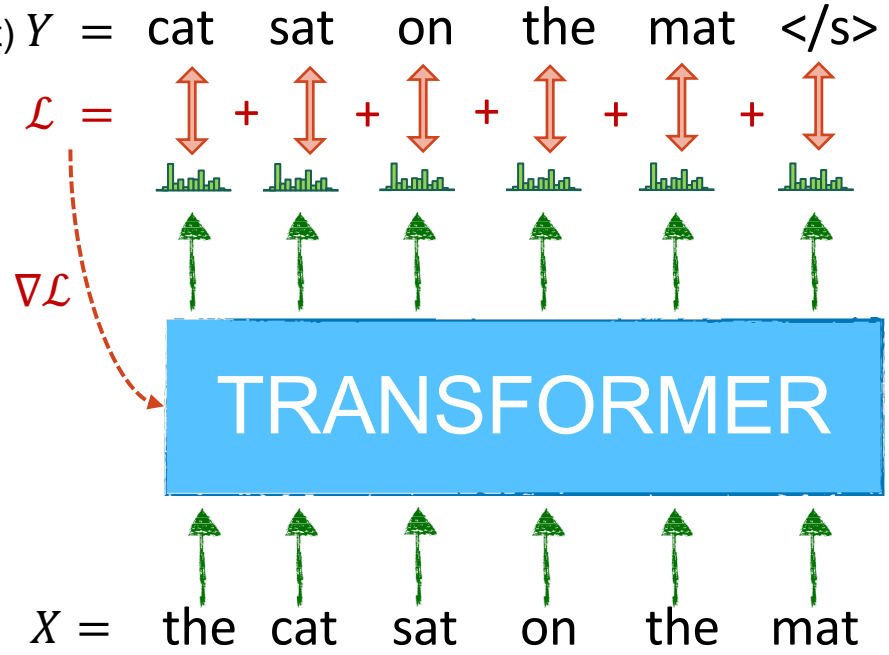
- Using this loss, do **Backprop** and **update** the Transformer parameters.



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

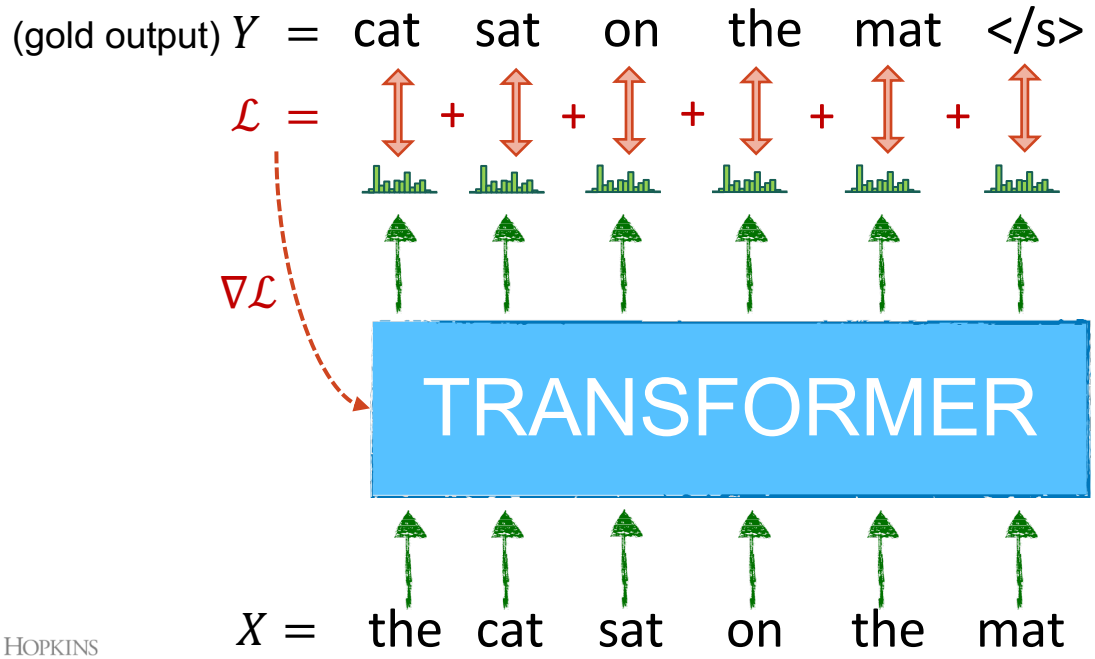
Training a Transformer Language Model

- 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

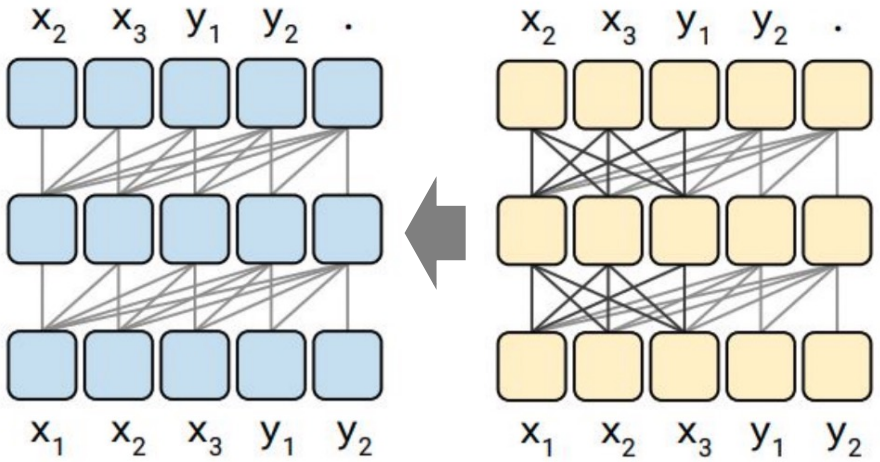
- We need to **prevent information leakage** from future tokens! How?



Attention mask

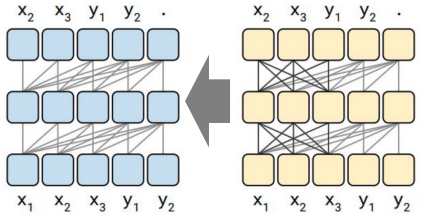
Attention raw scores

	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



Slide credit: Arman Cohan

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
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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
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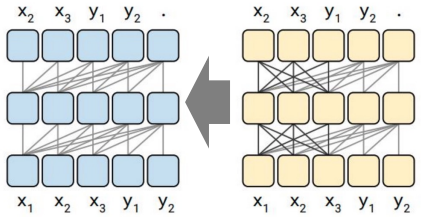
10	1.56	0.9	0.39	1.46	1.44	-1.05	0.9	-0.73	0.36	-0.67	-0.62	-0.43
11	0.32	0.74	0.44	-0.1	1.19	0.83	0.29	2.06	0.51	-0.26	1.51	0.11

Attention mask

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

Slide credit: Arman Cohan

Attention mask



Attention raw scores

	1	2	3	4	5	6	7	8	9	10	11
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
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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
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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

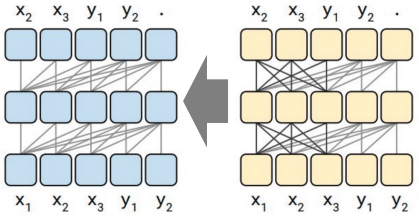
X

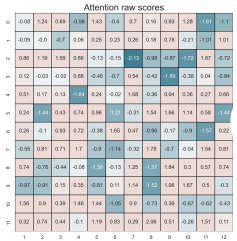
Attention mask

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

Note matrix multiplication is quite fast in GPUs.

Attention mask





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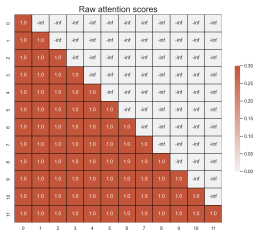


=

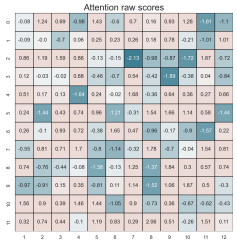
Masked attention raw scores

	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

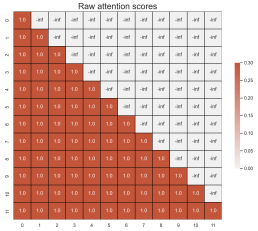
Slide credit: Arman Cohan

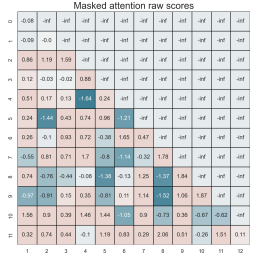
Attention mask

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

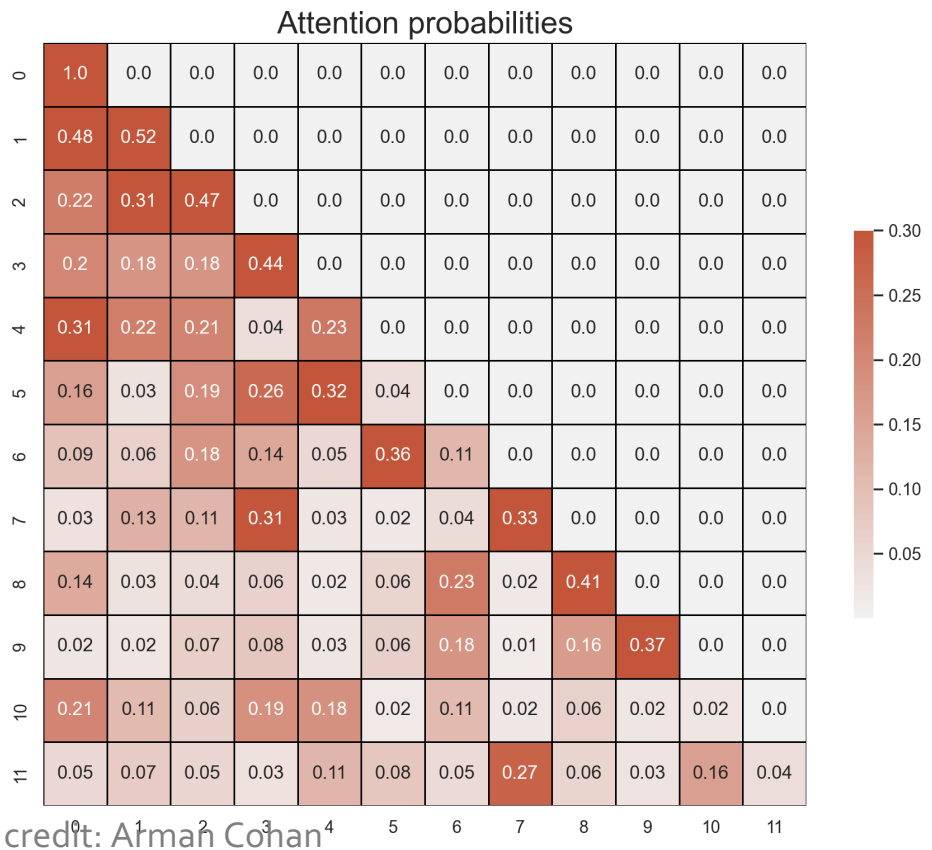


X





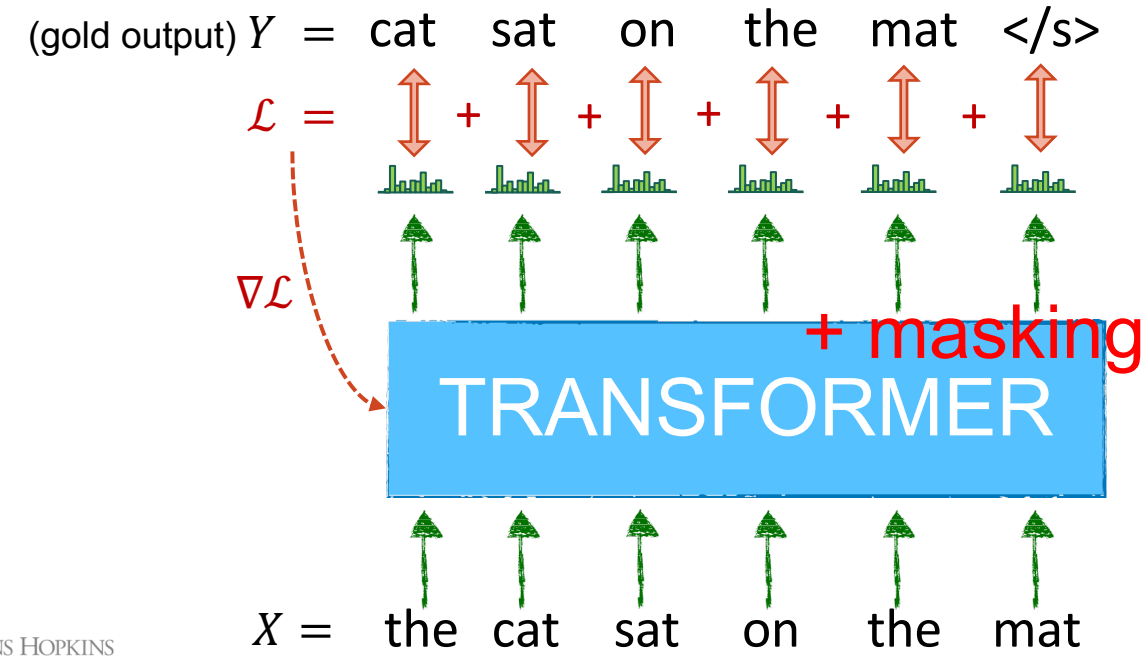
softmax



Slide credit: Arman Cohan

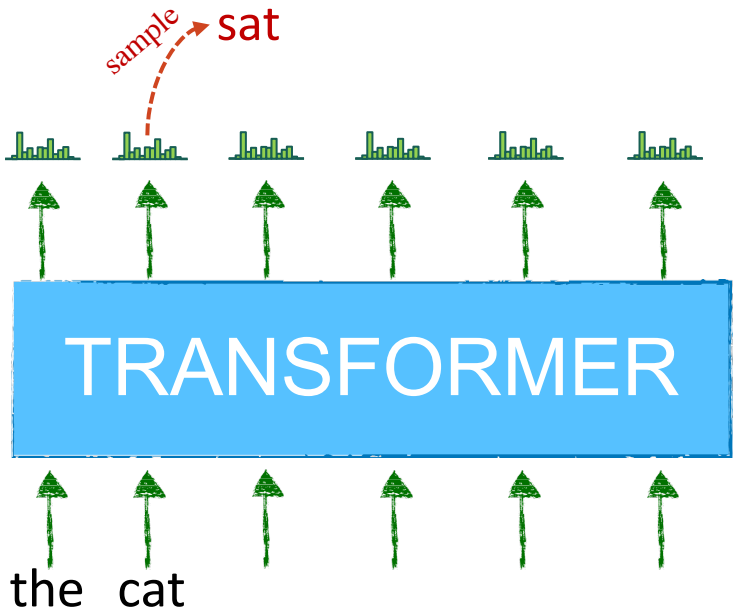
Training a Transformer Language Model

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



How to use the model to generate text?

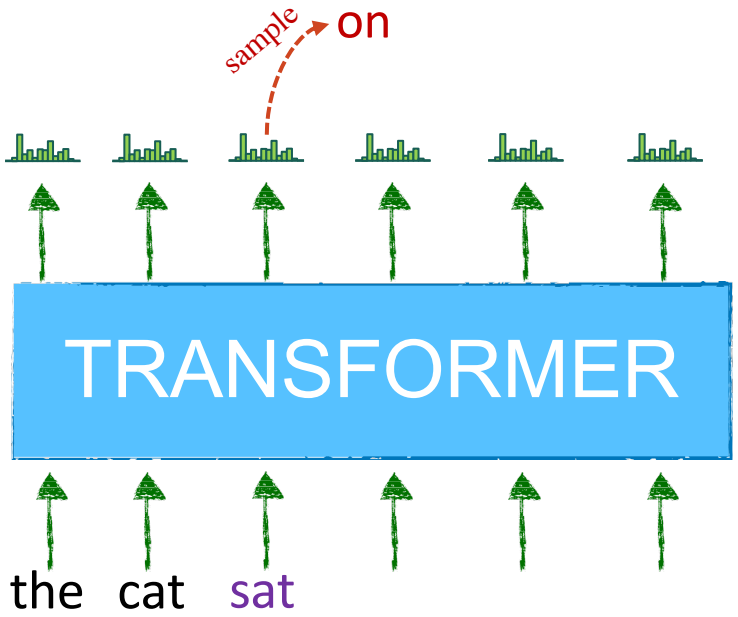
- Use the output of previous step as input to the next step repeatedly



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.



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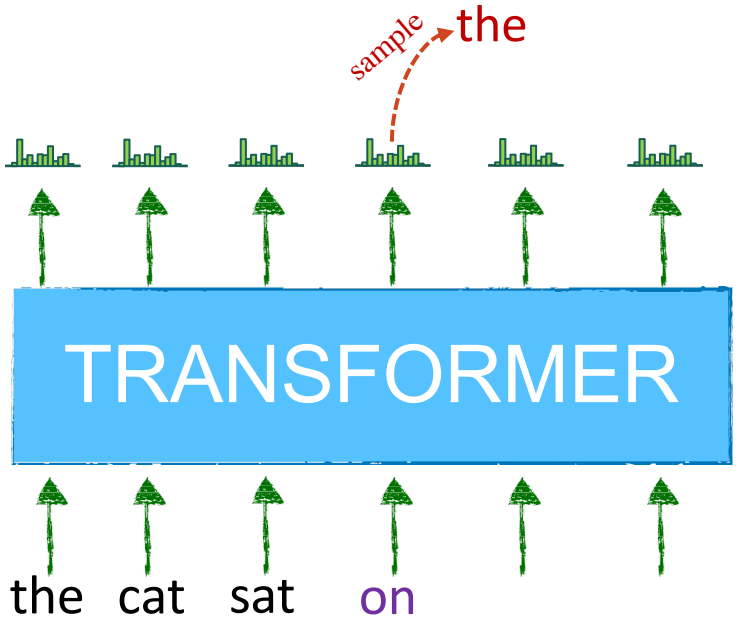

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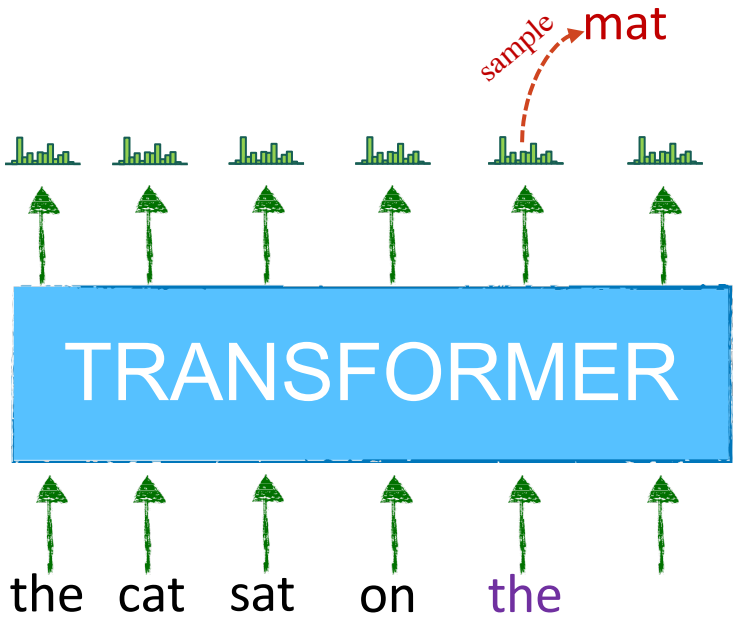

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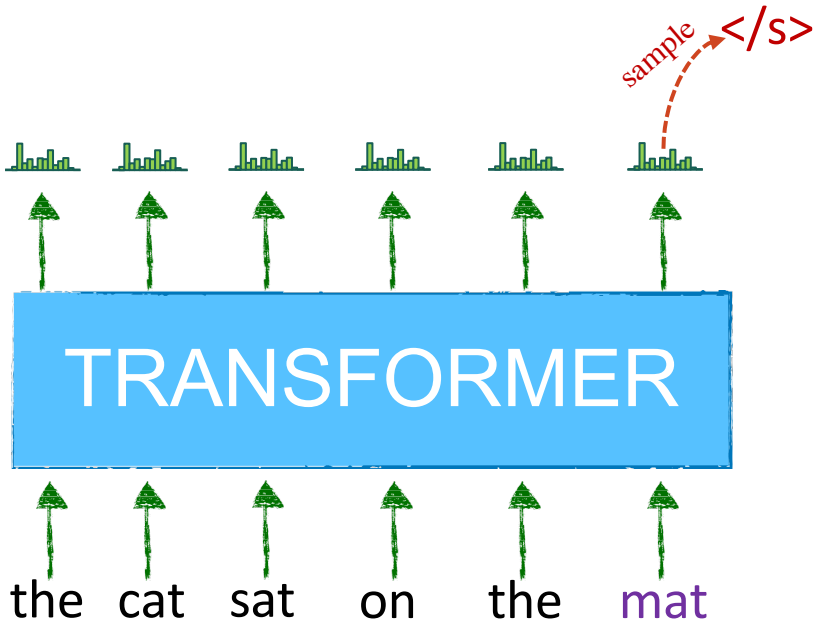
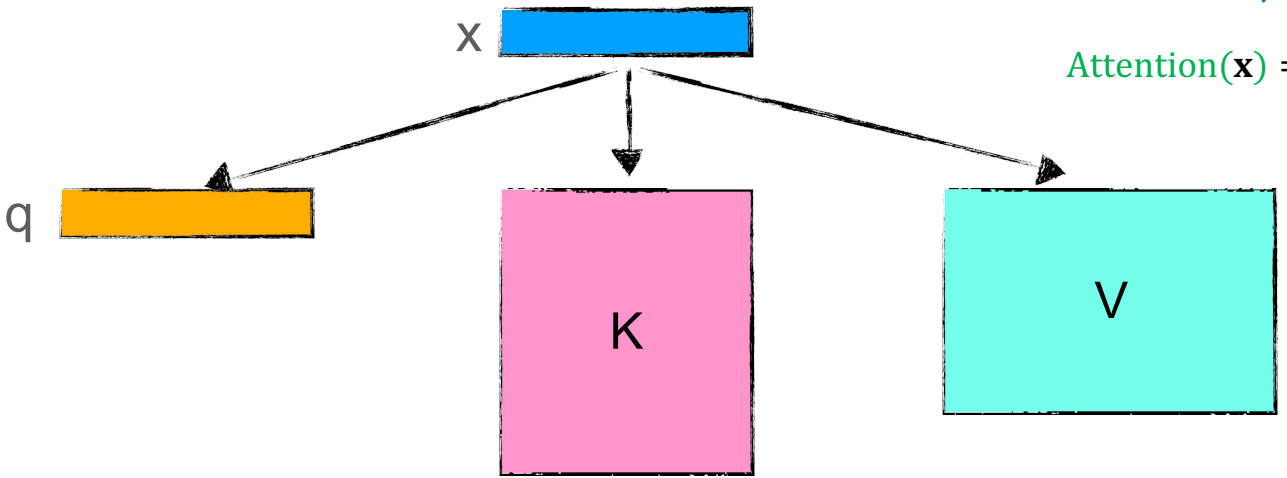


An important efficiency consideration about decoding!

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

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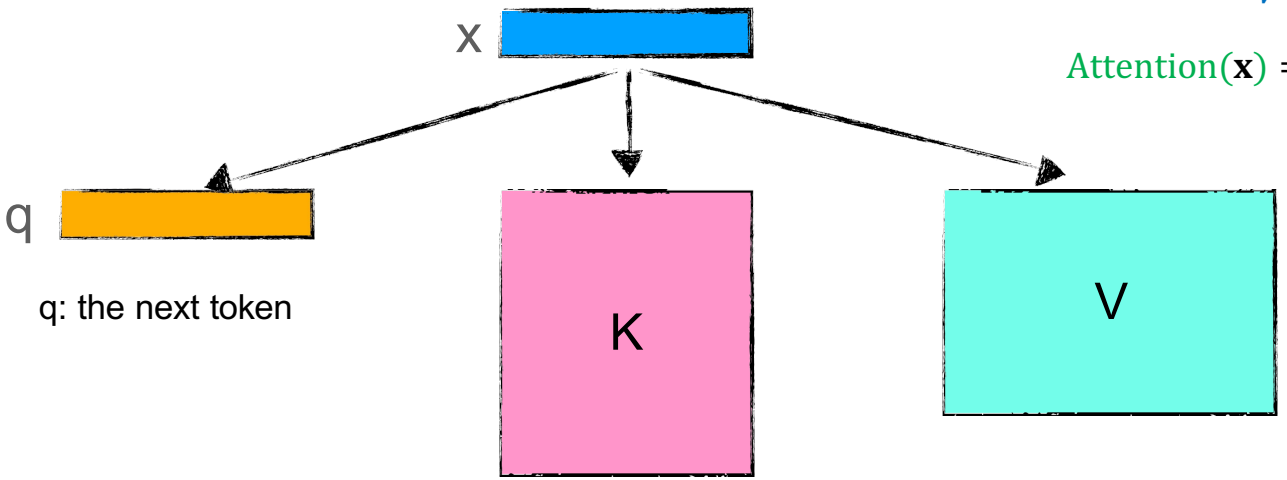

[Slide credit: Arman Cohan]

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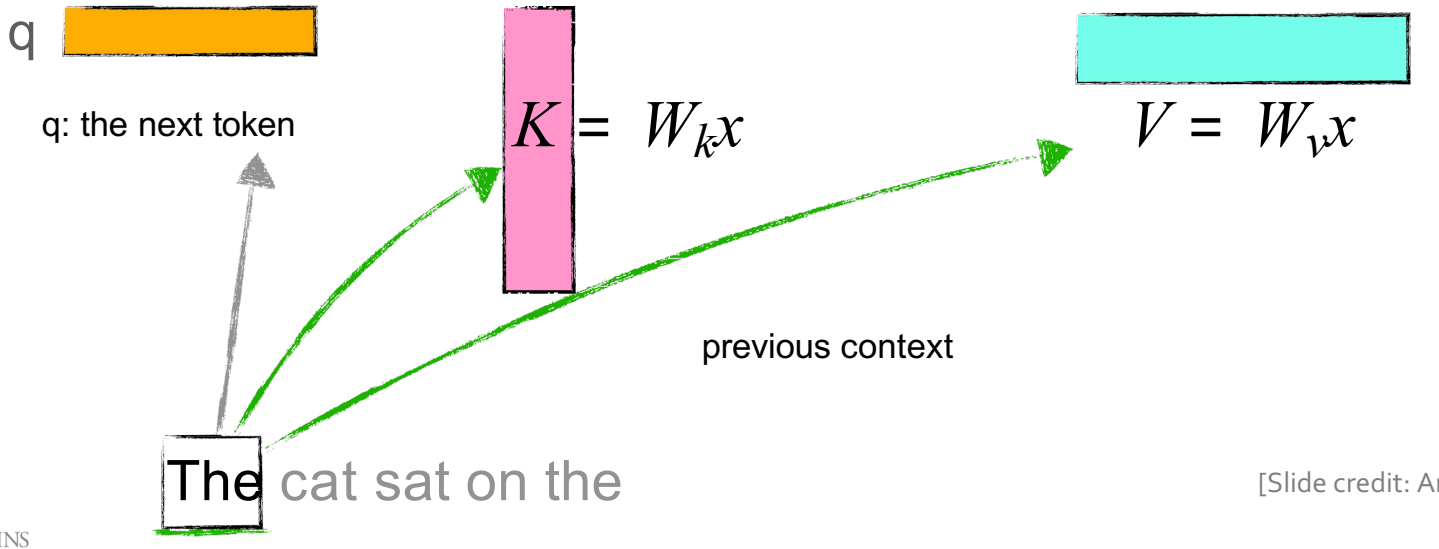
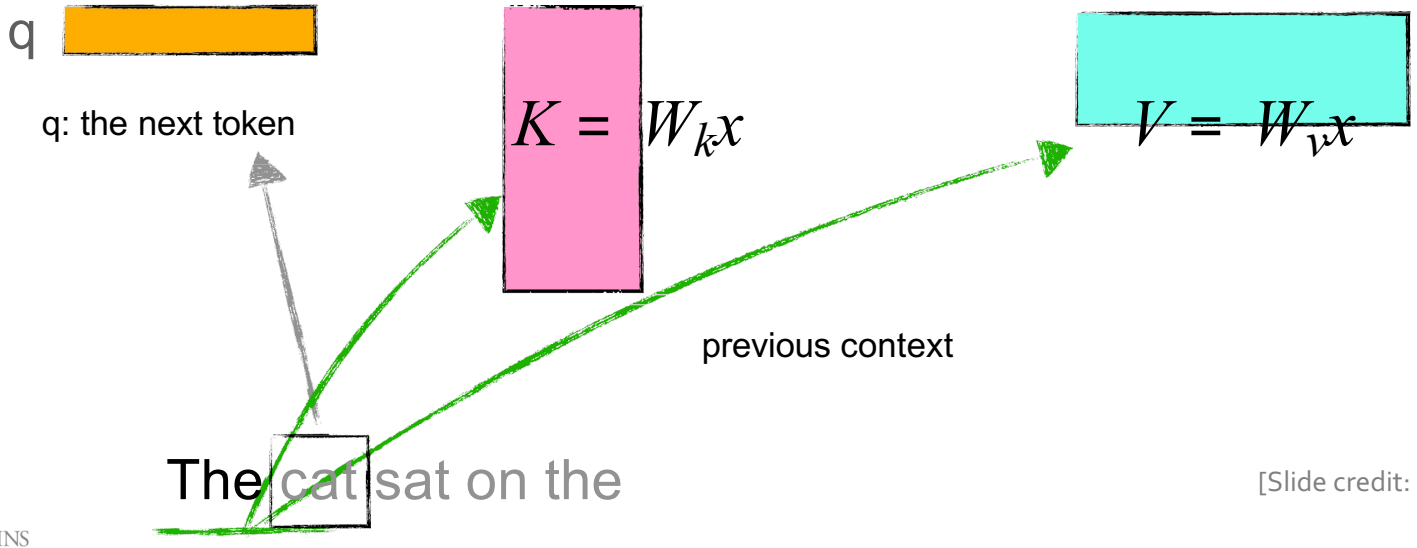
$$V = \mathbf{W}^v \mathbf{x}$$
$$\text{Attention}(\mathbf{x}) = \text{softmax}\left(\frac{QK^{\mathrm{T}}}{\sqrt{d}}\right)V$$



[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]

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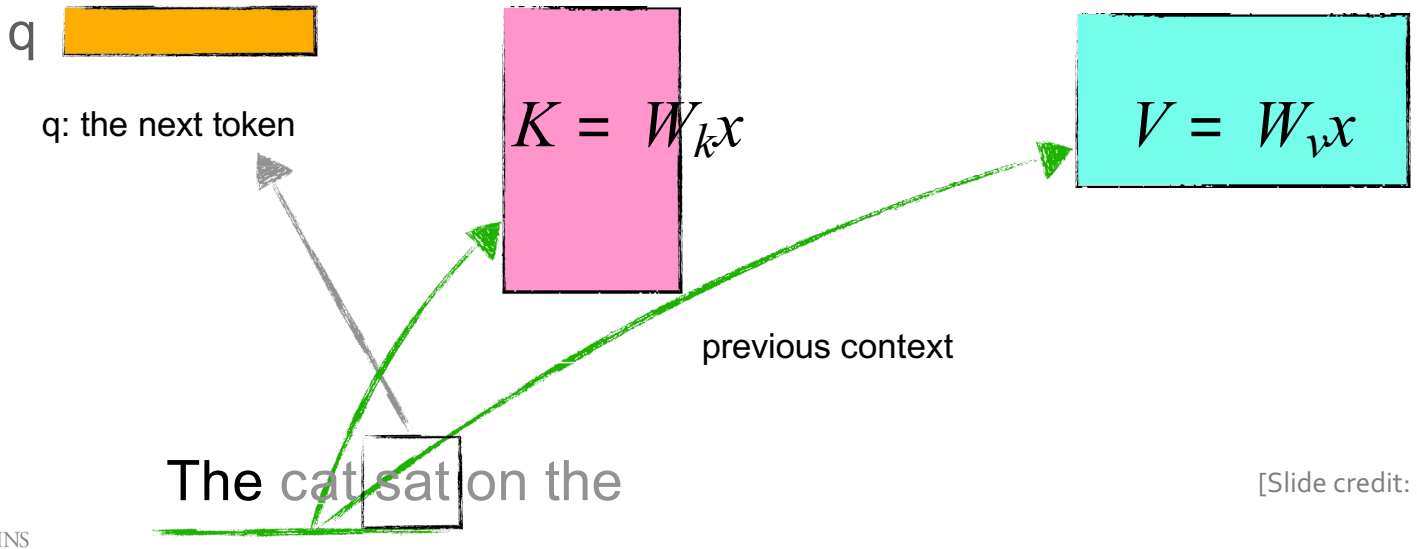

[Slide credit: Arman Cohan]

Making decoding more efficient

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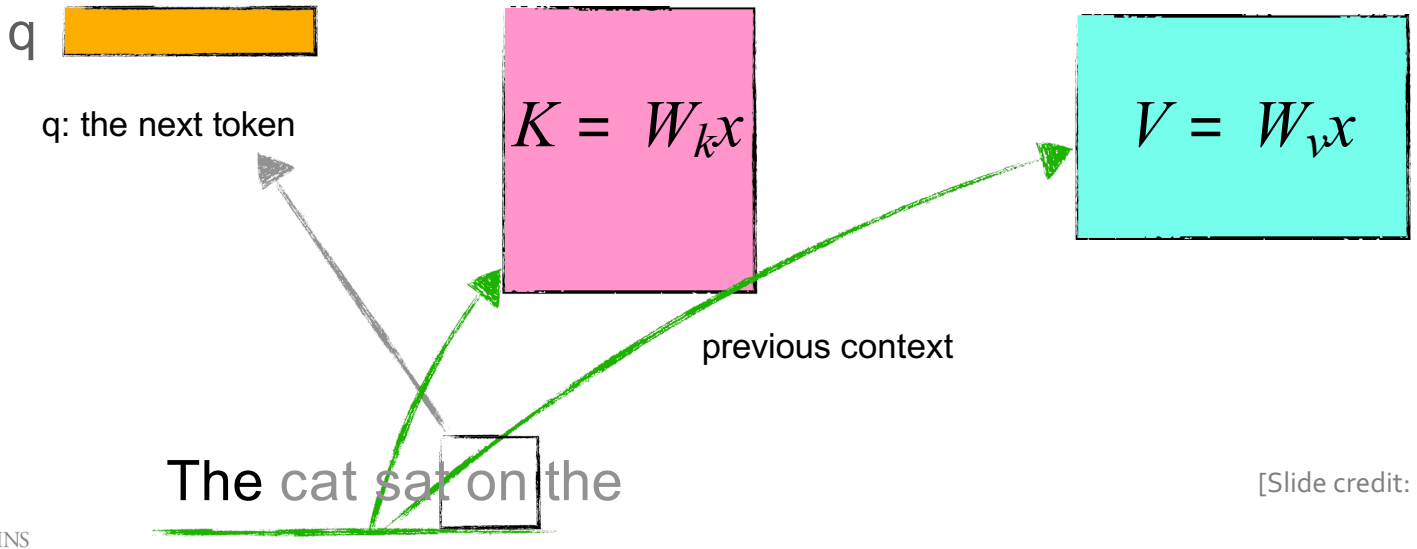

[Slide credit: Arman Cohan]

Making decoding more efficient

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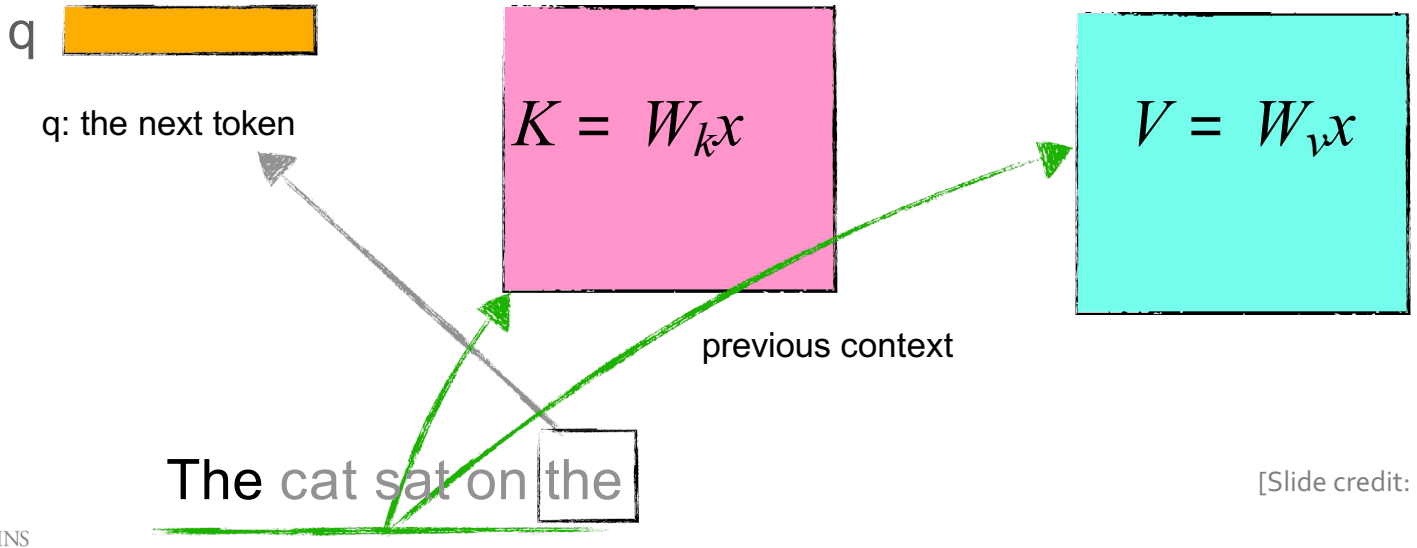


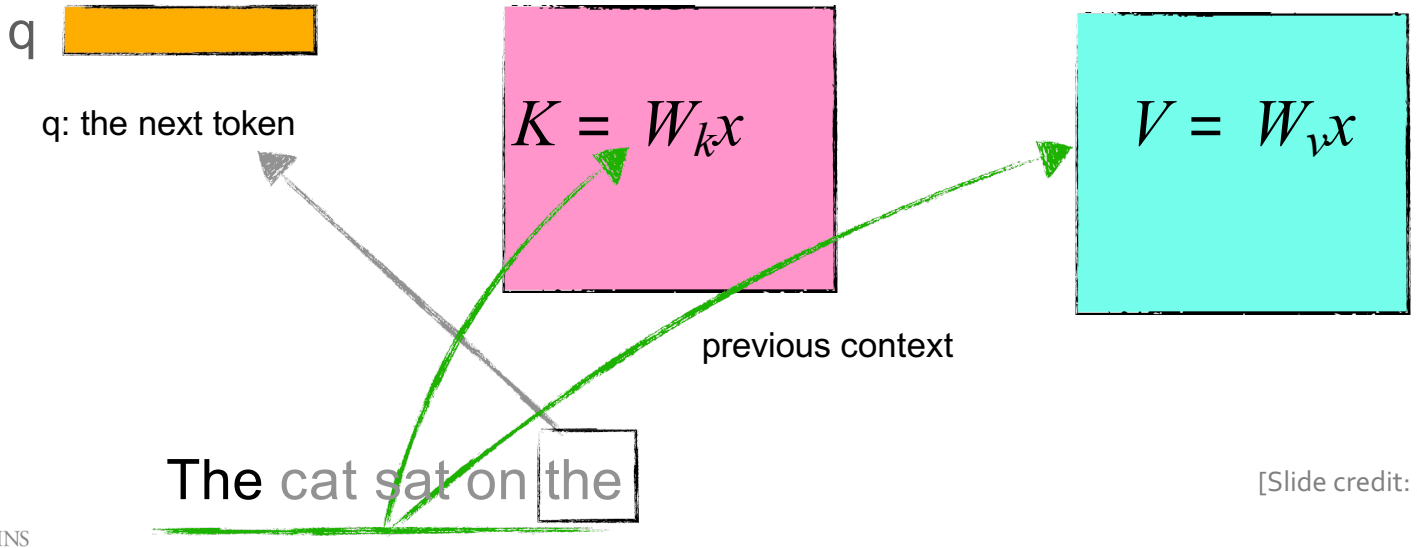
[Slide credit: Arman Cohan]

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

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

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

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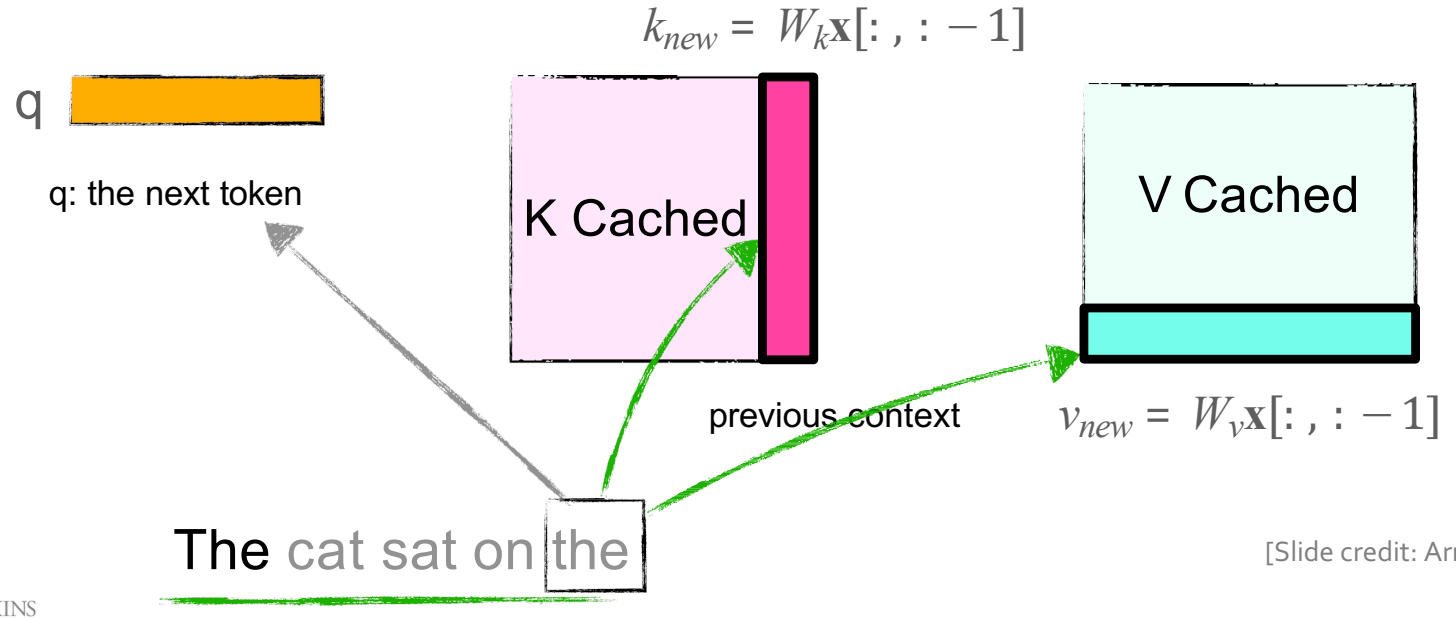
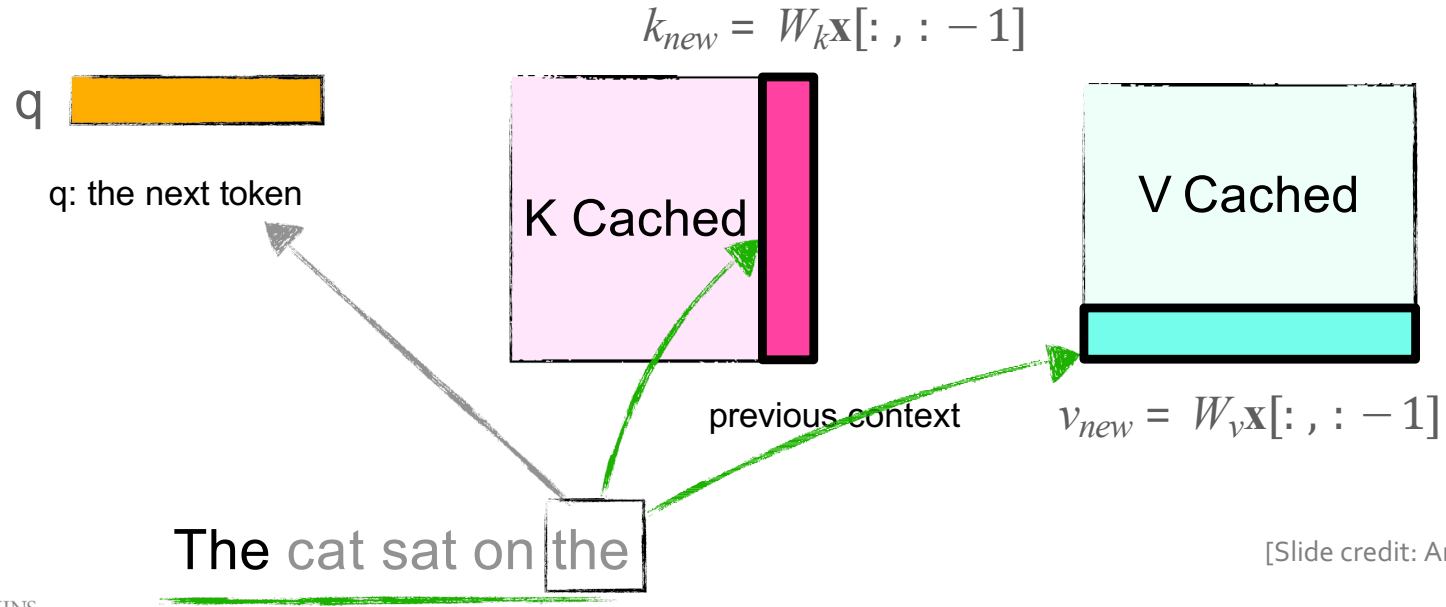


[Slide credit: Arman Cohan]

Making decoding more efficient

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

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



[Slide credit: Arman Cohan]

Summary

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

- **Next:**
  - Architectural variants
  - Efficiency issues.
  - …

Transformer Architectural Variants

Encoder-decoder

- It is possible to have two stacks of transformer layers
- The encoder is as we've seen
- We can also add a decoder layer that is identical to the encoder but we give it the ability to also attend to the input

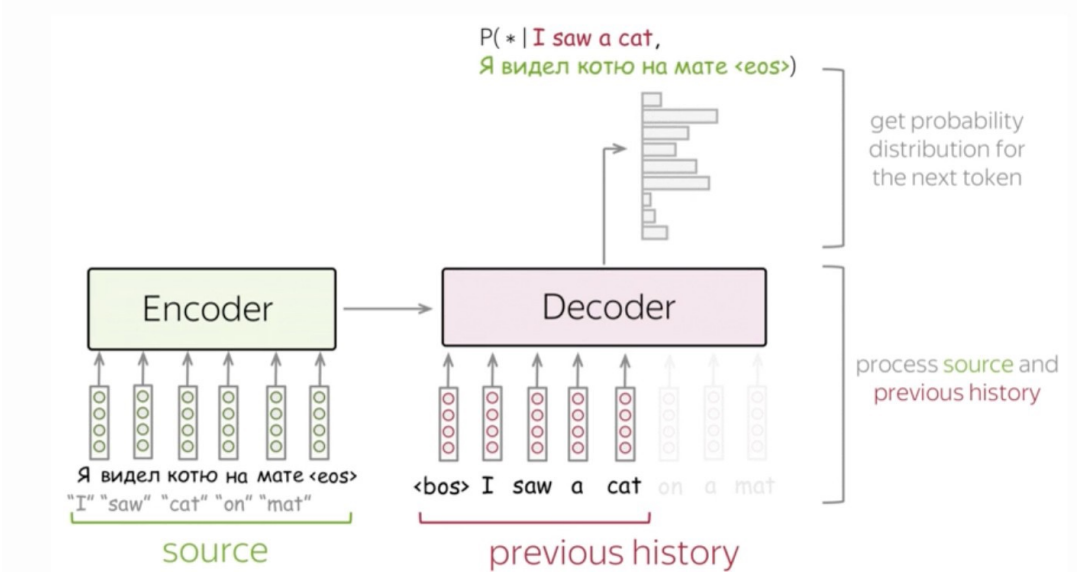
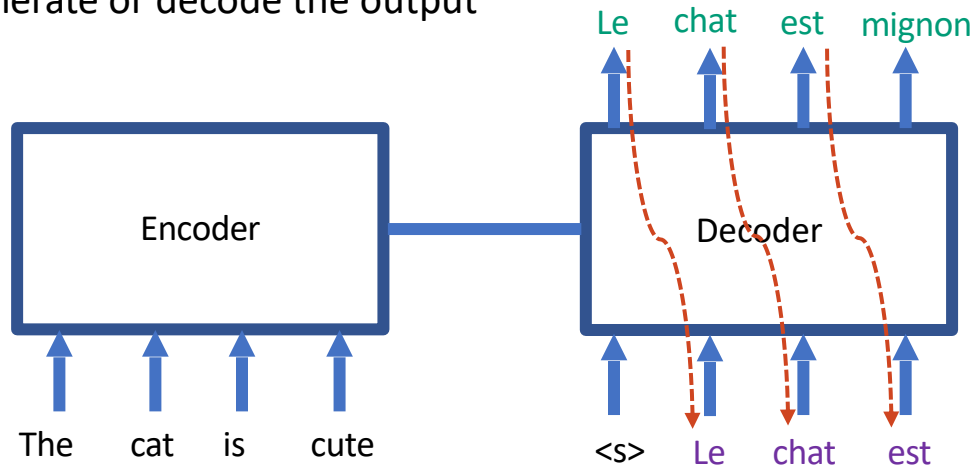


Fig from: https://lena-voita.github.io/nlp_course/seq2seq_and_attention.html

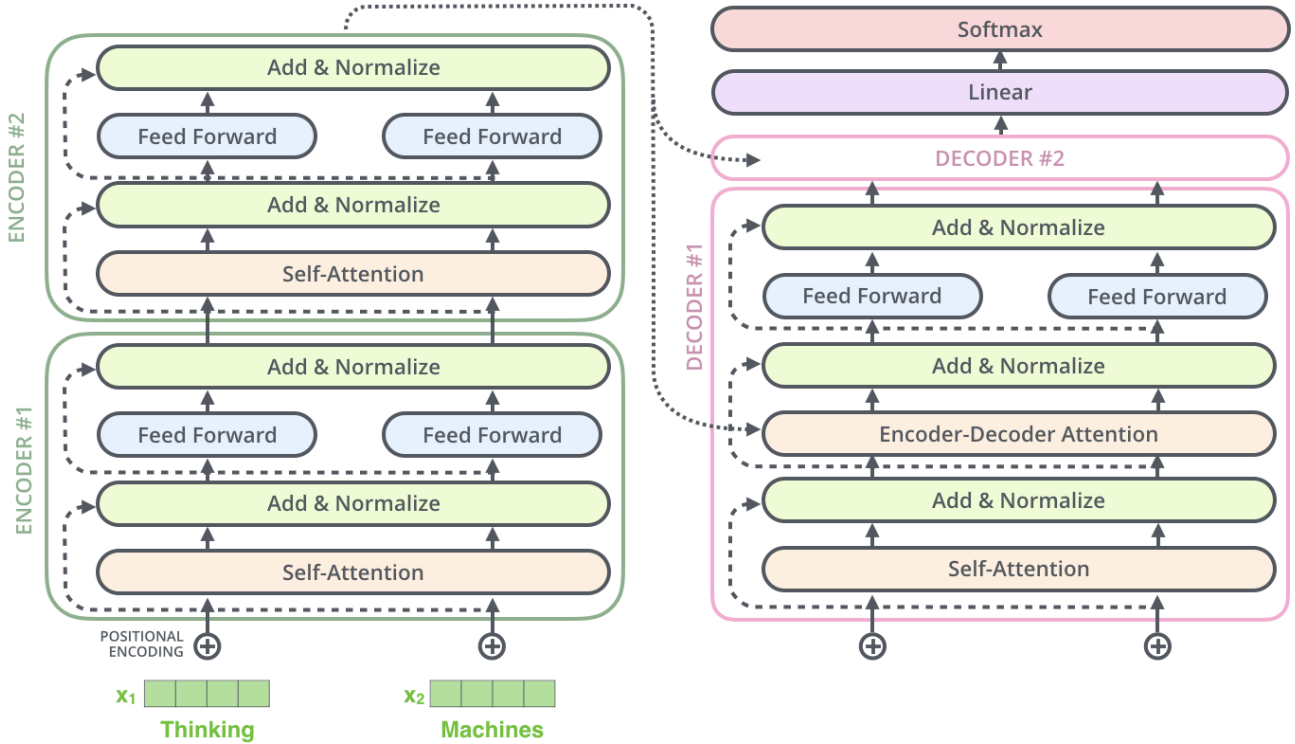
Encoder-decoder models

- Encoder = read or encode the input,
- Decoder = generate or decode the output



Transformer [Vaswani et al. 2017]

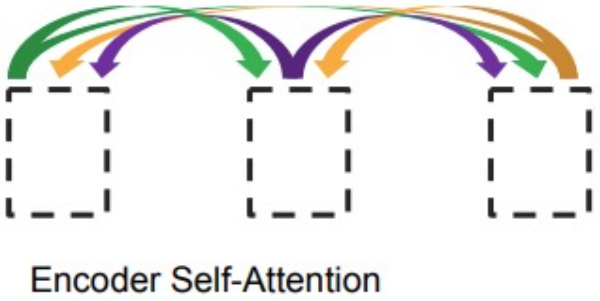
- An encoder-decoder architecture built with attention modules.

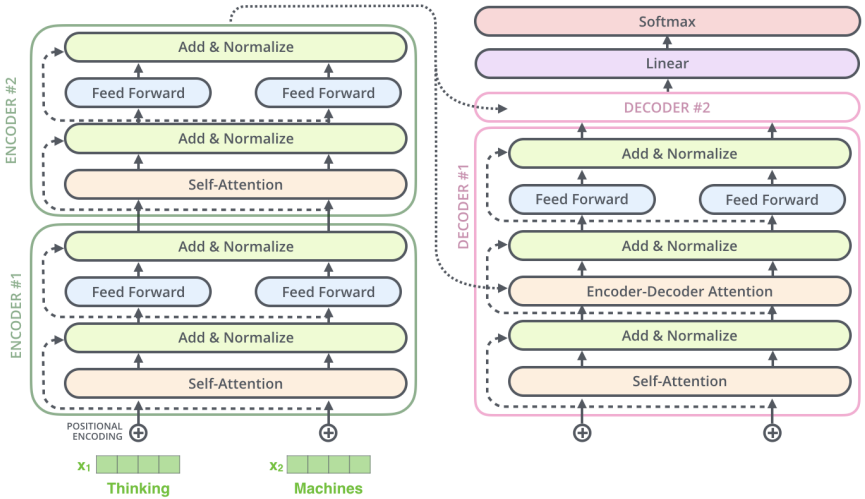


74

Transformer [Vaswani et al. 2017]

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



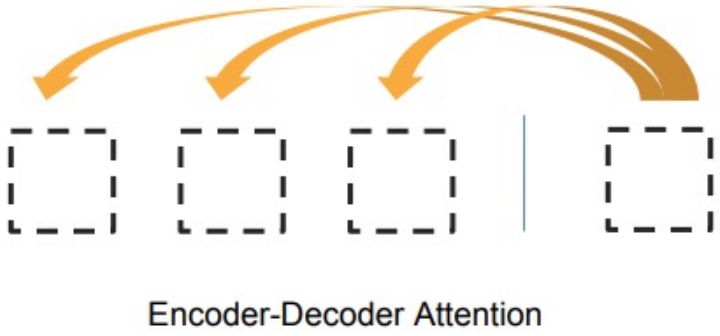


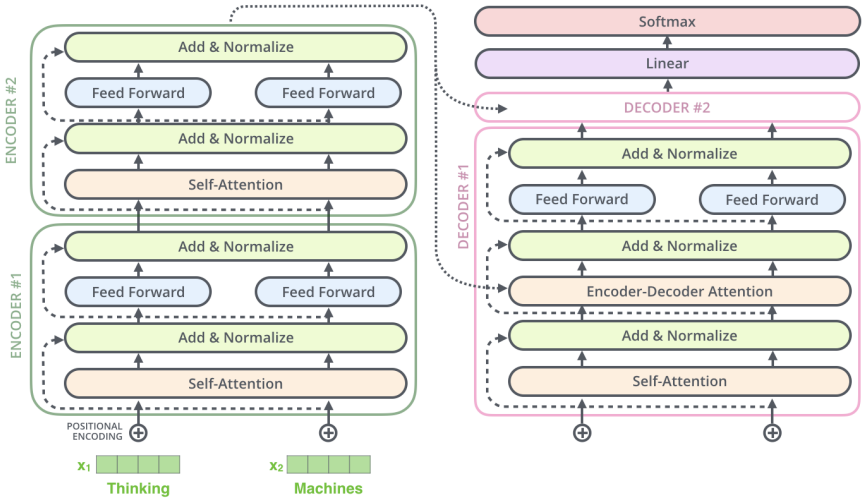
[Attention Is All You Need, Vaswani et al. 2017]

75

Transformer [Vaswani et al. 2017]

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



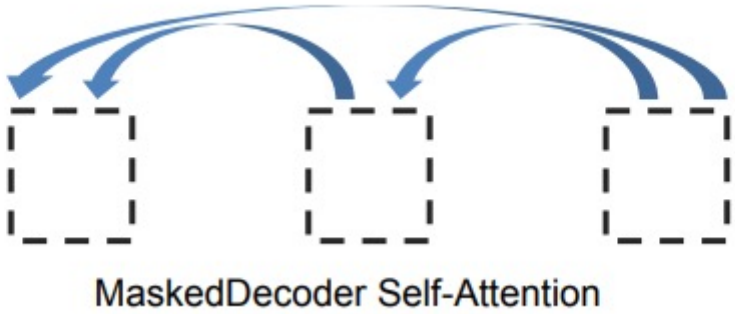


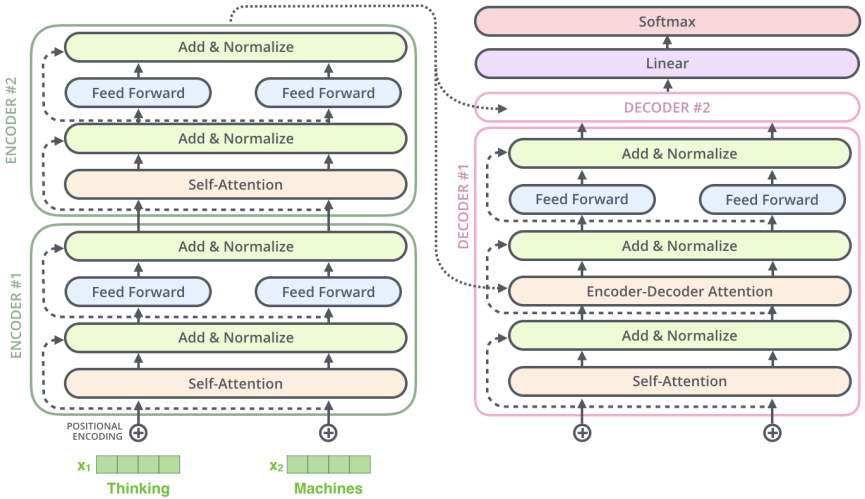
[Attention Is All You Need, Vaswani et al. 2017]

76

Transformer [Vaswani et al. 2017]

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





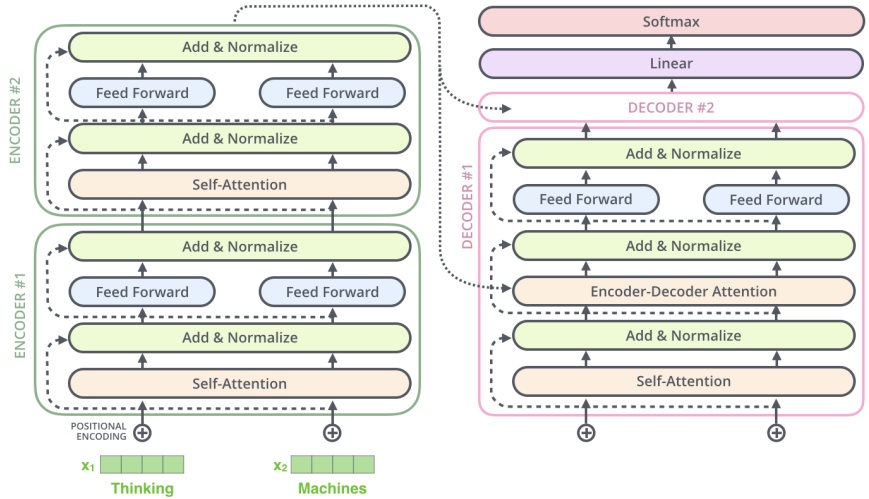
[Attention Is All You Need, Vaswani et al. 2017]

77

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.

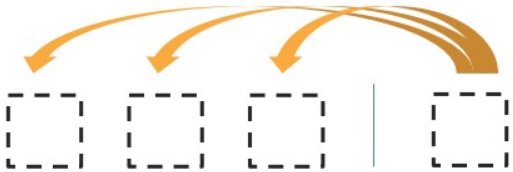


[Attention Is All You Need, Vaswani et al. 2017]

78

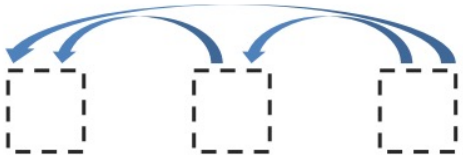
Recap: Transformer

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

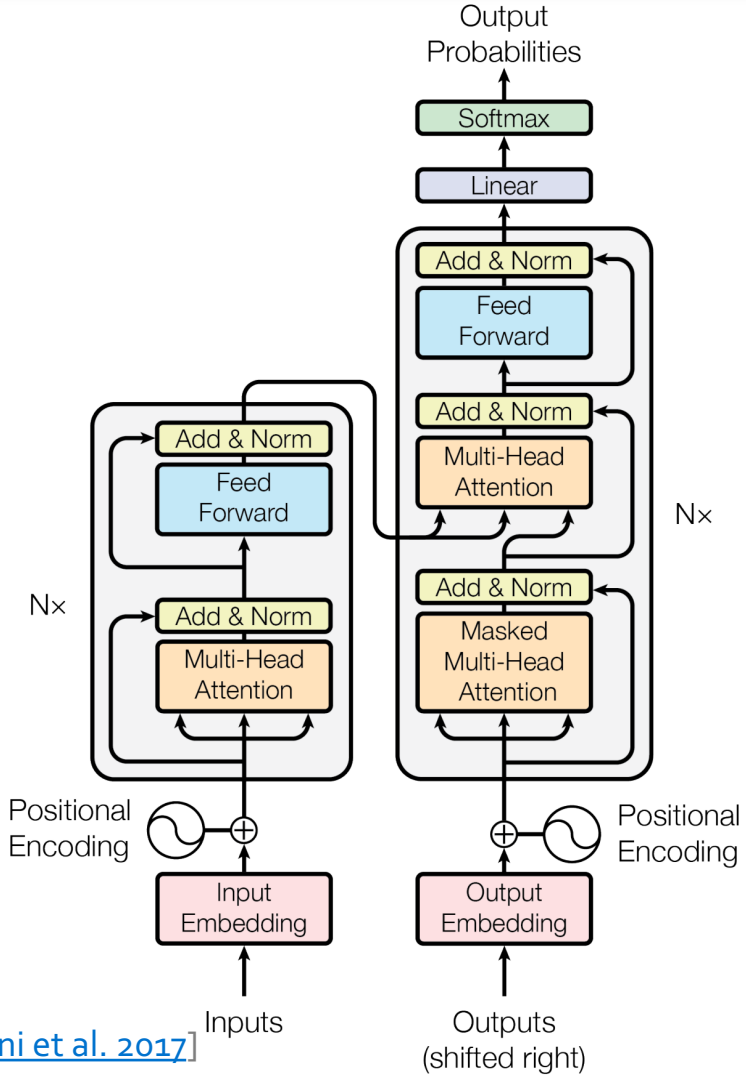


Encoder-Decoder Attention

Encoder Self-Attention

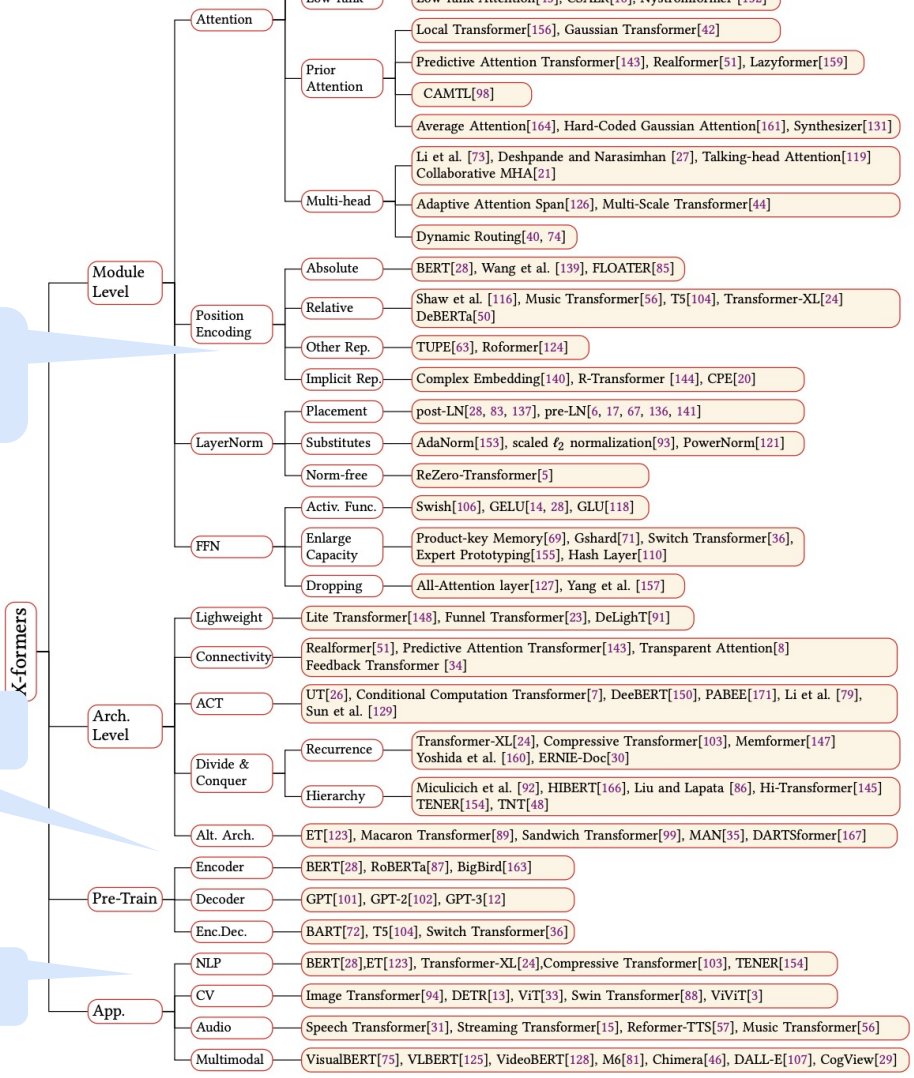


MaskedDecoder Self-Attention



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

After Transformer ...



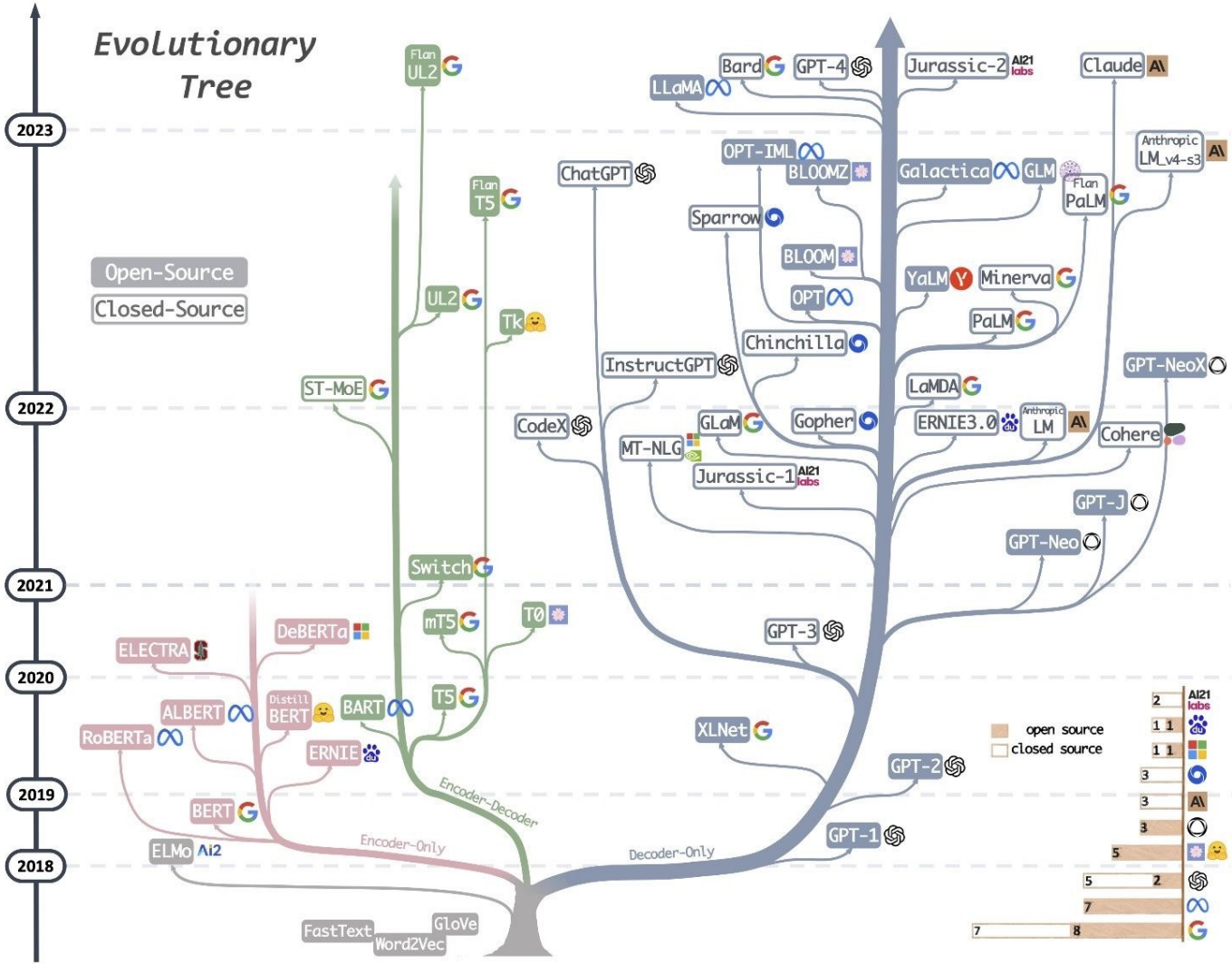
Variants of positional embeddings

Architectural choices

Multi-modal models

We will visit a few of these branches …

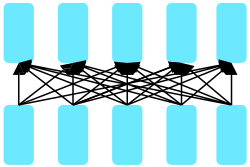
But there is a lot that we do **not** cover …



Yang et al. Harnessing the Power of LLMs in Practice: A Survey on ChatGPT and Beyond, 2023

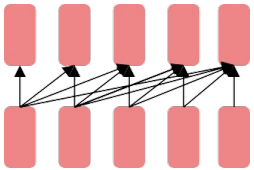
Impact of Transformers

- A building block for a variety of LMs



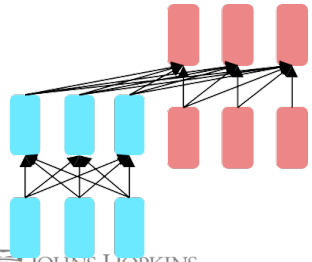
Encoders

- Examples: BERT, RoBERTa, SciBERT.
- Captures bidirectional context. Wait, how do we pretrain them?



Decoders

- Examples: GPT-2, GPT-3, LaMDA
- Other name: causal or auto-regressive language model
- Nice to generate from; can't condition on future words



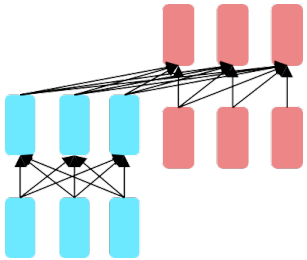
Encoder-Decoders

- Examples: Transformer, T5, Meena
- What's the best way to pretrain them?

86

Transformer Language Model Families

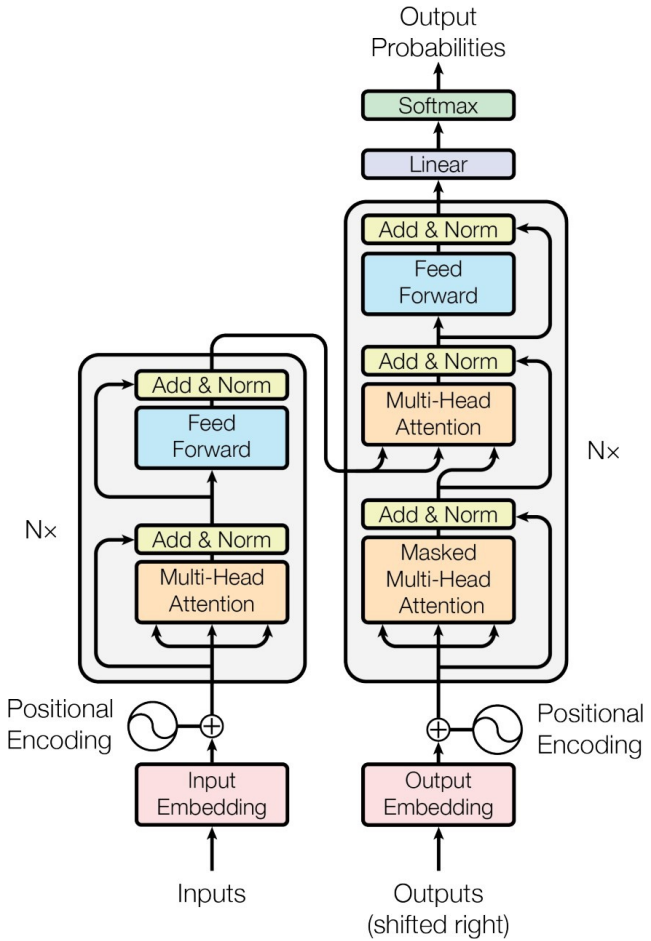
Encoder-Decoder Family of Transformers



Encoder-Decoders

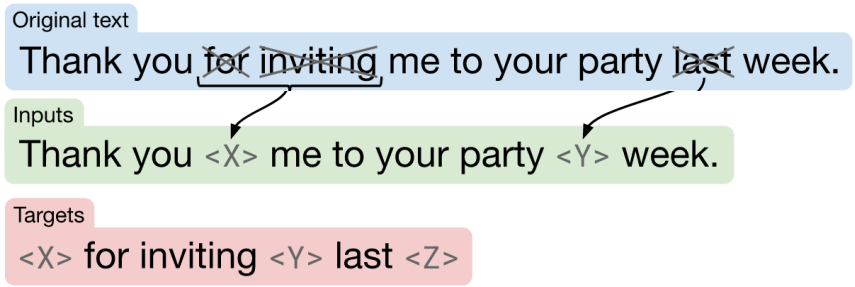
Encoder-decoder Models

- The original transformer architecture was encoder decoder
- Encoder-decoder models are flexible in both generation and classification tasks
- How can we pretrain an encoder-decoder model like BERT to be a good general language pretrained LM?



T5: Text-To-Text Transfer Transformer

- An encoder-decoder architecture
- Pre-training objective:
  corrupt and reconstruct objective



Model	Parameters	No. of layers	d_{model}	d_{ff}	d_{kv}	No. of heads
Small	60M	6	512	2048	64	8
Base	220M	12	768	3072	64	12
Large	770M	24	1024	4096	64	16
3B	3B	24	1024	16384	128	32
11B	11B	24	1024	65536	128	128

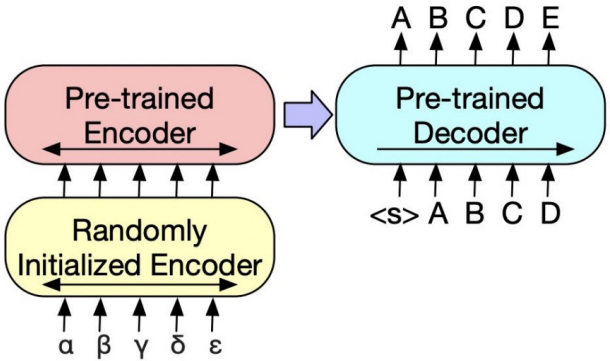
- The original paper is an excellent set of in-depth analysis of various parameters of model design. We discuss some of these results in other places.

`https://huggingface.co/t5-base`

Exploring the limits of transfer learning with text-to-text transfer transformers, 2020

BART (Lewis et al. 2020)

- Similar Architecture as T5.
  - Corrupt the input -> ask the model to reconstruct the original input
  - Outperformed existing methods on generative tasks (question answering, and summarization).



BART: Denoising Sequence-to-Sequence Pre-training for Natural Language Generation, Translation, and Comprehension

Mike Lewis*, Yinhan Liu*, Naman Goyal*, Marjan Ghazvininejad, Abdelrahman Mohamed, Omer Levy, Ves Stoyanov, Luke Zettlemoyer
Facebook AI
{mikelewis,yinhanliu,naman}@fb.com

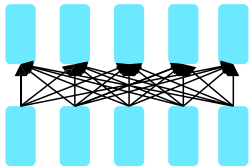
BART

The code might be outdated, but the logic is the same …

```
from transformers import BartTokenizer, BartForConditionalGeneration

tokenizer = BartTokenizer.from_pretrained("facebook/bart-large")
model = BartForConditionalGeneration.from_pretrained("facebook/bart-large")

TXT = "The sun is <mask> ."
input_ids = tokenizer([TXT], return_tensors="pt")["input_ids"]
logits = model(input_ids).logits

masked_index = (input_ids[0] == tokenizer.mask_token_id).nonzero().item()
probs = logits[0, masked_index].softmax(dim=0)
values, predictions = probs.topk(5)

tokenizer.decode(predictions).split()
```

Result: `['located', 'at', 'approximately', 'also', 'about']`

Encoder-only Family of Transformers



BERT

Bidirectional Encoder Representations from Transformers

BERT

Bidirectional Encoder Representations from Transformers

Like Bidirectional LSTMs (ELMo), let's look in **both** directions

BERT

Bidirectional Encoder Representations from Transformers

Let's only use Transformer Encoders, no Decoders

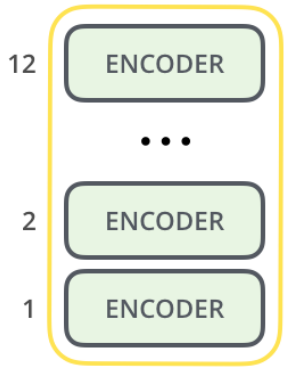
BERT

Bidirectional Encoder Representations from Transformers

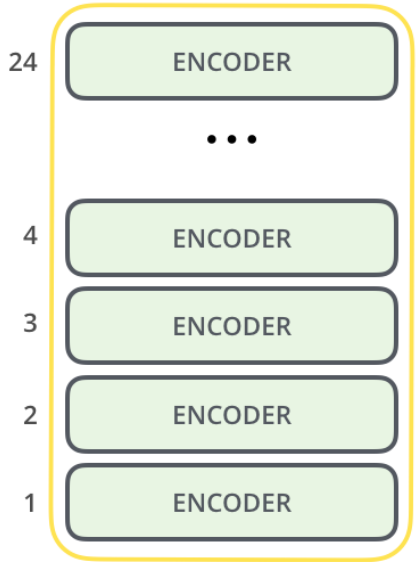
It's a language model that builds rich representations
via self-supervised learning (pre-training)

BERT: Architecture

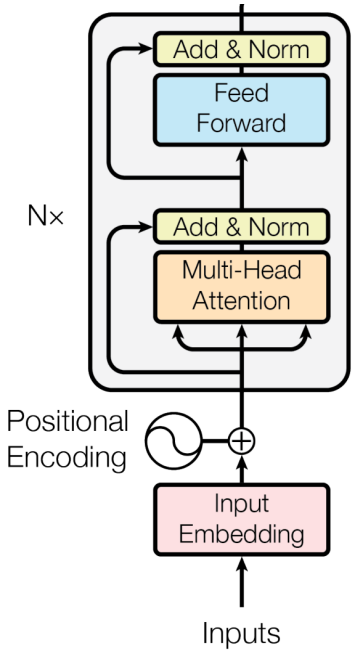
- Stacks of Transformer encoders



$BERT_{BASE}$



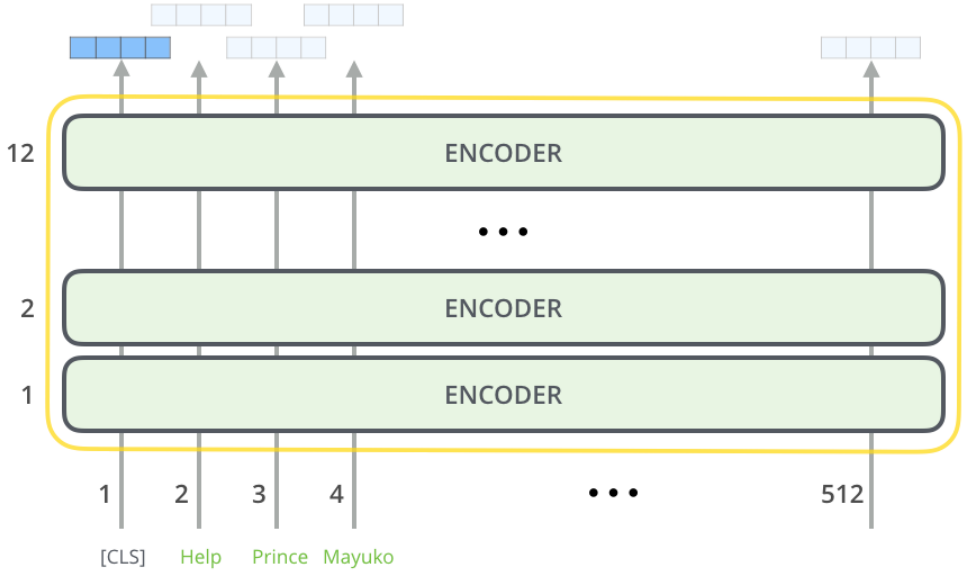
$BERT_{LARGE}$

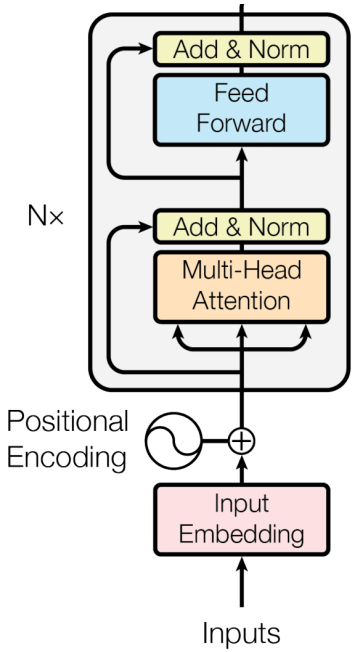


[BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding, Devlin et al. 2018]

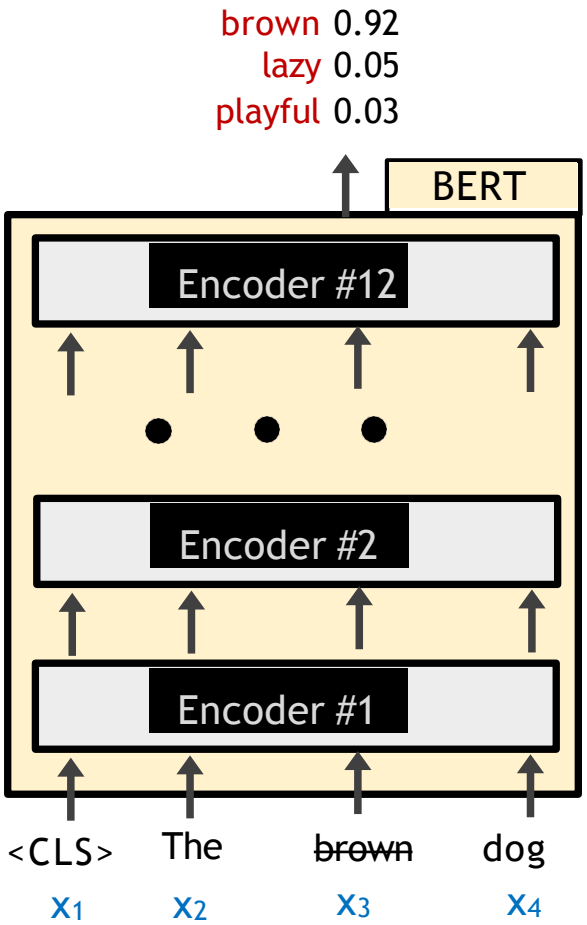
BERT: Architecture

- Model output dimension: 512





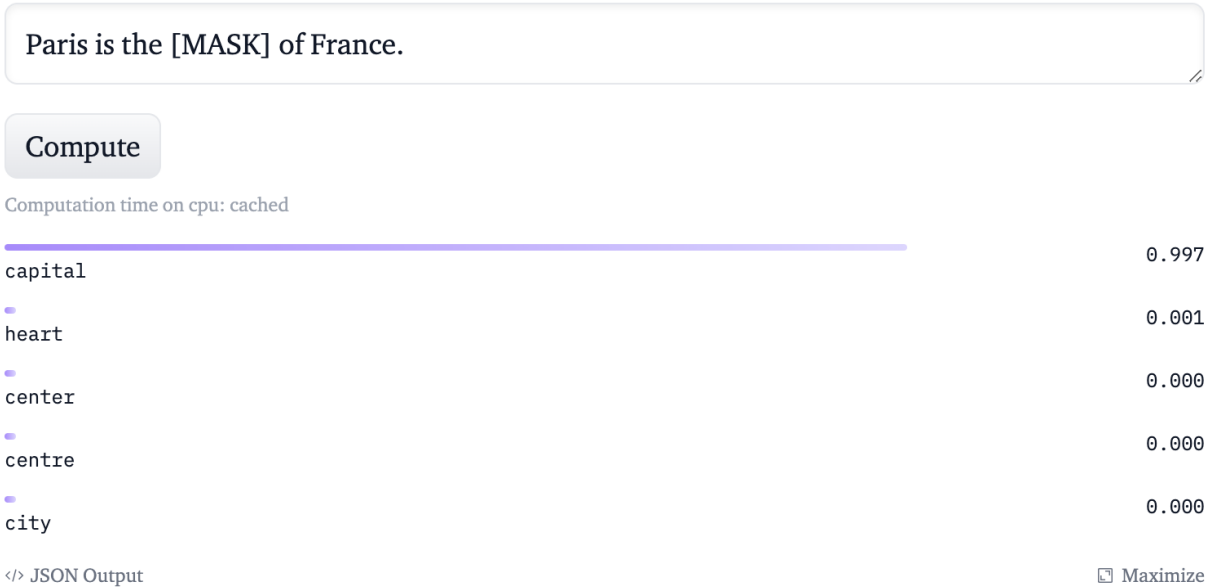
[BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding, Devlin et al. 2018]



BERT is trained to uncover masked tokens.

Probing BERT Masked LM

- Masking words forces BERT to use context in both directions to predict the masked word.

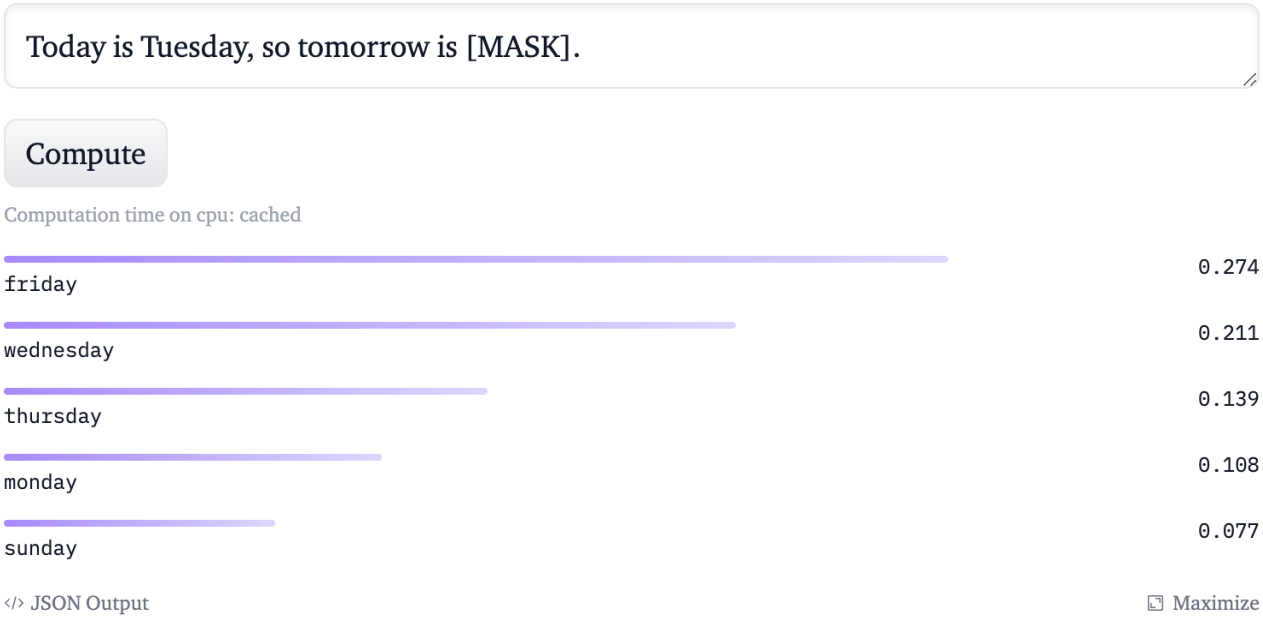


https://huggingface.co/bert-base-uncased

101

Probing BERT Masked LM

- Masking words forces BERT to use context in both directions to predict the masked word.

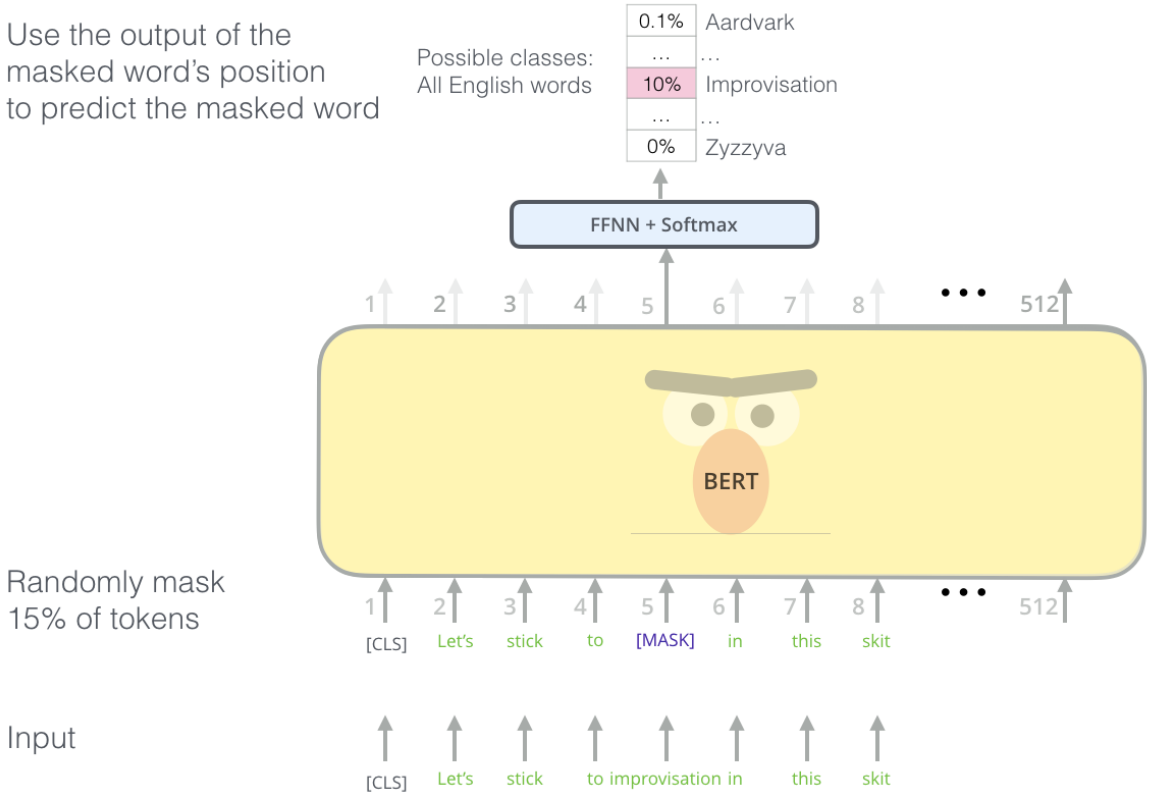


https://huggingface.co/bert-base-uncased

102

BERT: Pre-training Objective (1): Masked Tokens

- Randomly mask 15% of the tokens and train the model to predict them.



[BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding, Devlin et al. 2018]

BERT: Pre-training Objective (1): Masked Tokens

store

Galon

`the man went to the [MASK] to buy a [MASK] of milk`

- Too little masking: Too expensive to train
- Too much masking: Underdefined
  - (not enough info for the model to recover the masked tokens)

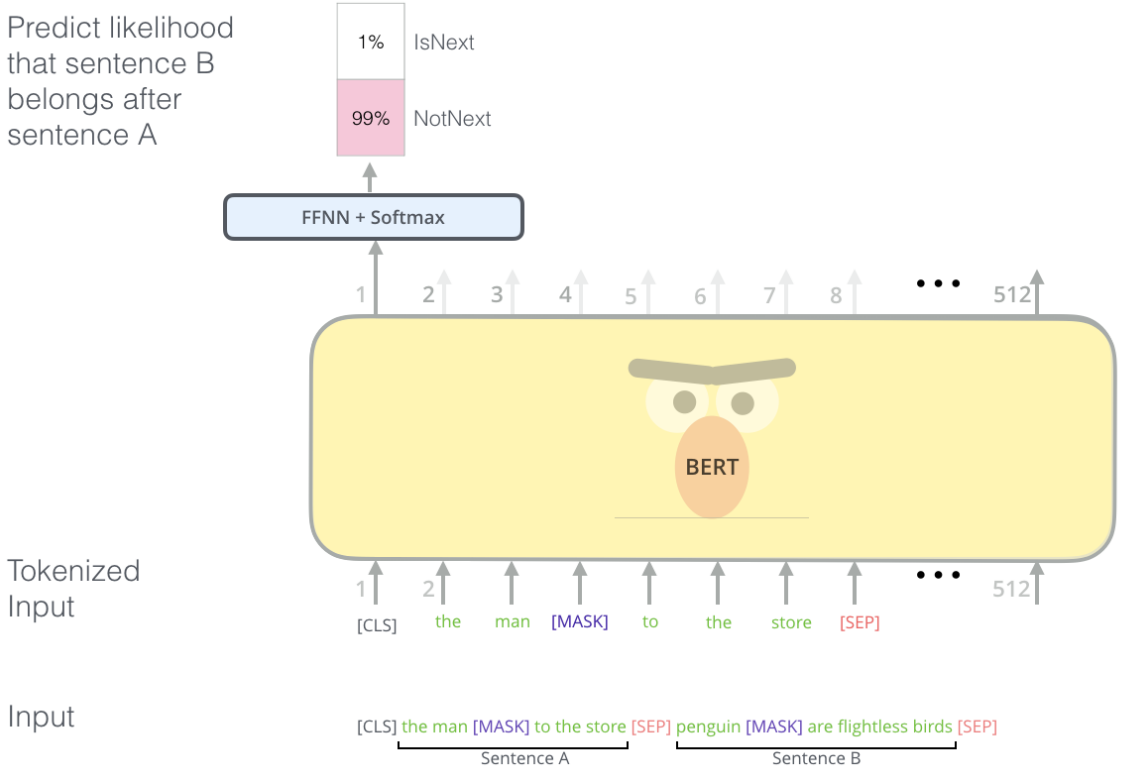
Later work shows that more principled masking (instead of uniformly random) could benefit downstream task performance and result in faster training.

PMI Masking (Levine et al., 2021) https://arxiv.org/pdf/2010.01825.pdf
SpanBERT (Joshi et al., 2020) https://arxiv.org/pdf/1907.10529.pdf

[BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding, Devlin et al. 2018]

BERT: Pre-training Objective (2): Sentence Ordering

- Predict sentence ordering
- 50% correct ordering, and 50% random incorrect ones



[BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding, Devlin et al. 2018]

BERT Pre-training Objective (2): Sentence Ordering

- Learn relationships between sentences, predict whether Sentence B is actual sentence that proceeds Sentence A, or a random sentence

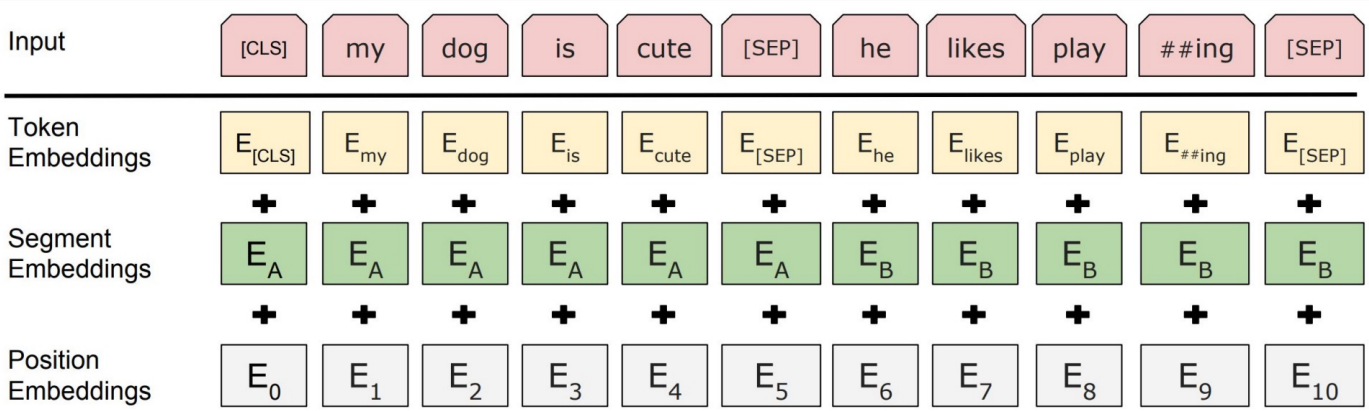
Sentence A = `The man went to the store.`
Sentence B = `He bought a gallon of milk.`
Label = `IsNextSentence`

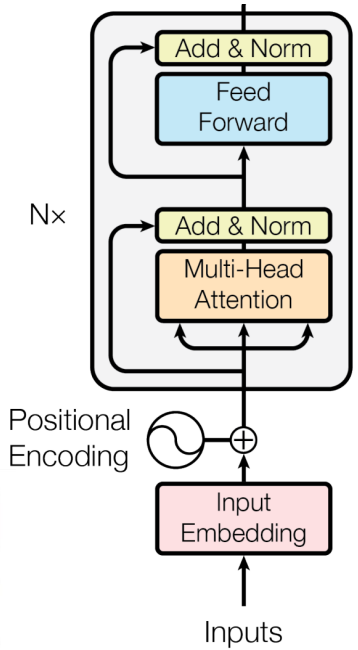
Sentence A = `The man went to the store.`
Sentence B = `Penguins are flightless.`
Label = `NotNextSentence`

[BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding, Devlin et al. 2018]

BERT: Input Representation

- Use 30,000 WordPiece vocabulary on input.
- Each token is sum of three embeddings
  - Addition to transformer encoder: sentence embedding





[BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding, Devlin et al. 2018]

Training

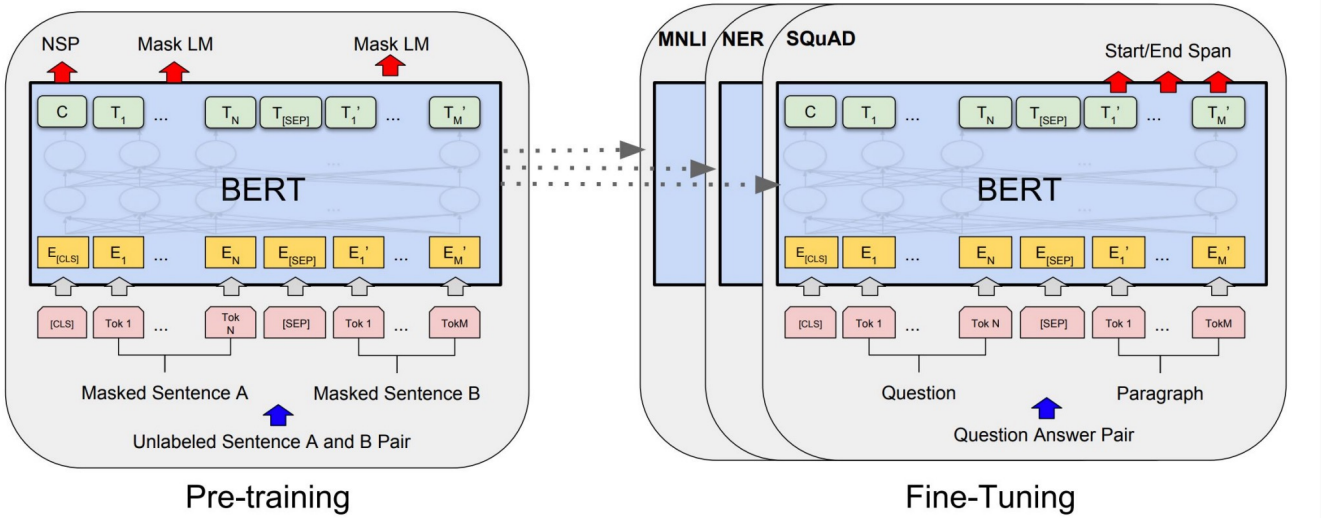
- Trains model on unlabeled data over different pre-training tasks (self-supervised learning)
- **Data:** Wikipedia (2.5B words) + BookCorpus (0.8B words)
- **Training Time:** 1M steps (~40 epochs)
- **Optimizer:** AdamW, 1e-4 learning rate, linear decay
- **BERT-Base:** 12-layer, 768-hidden, 12-head, sequence length of 512
- **BERT-Large:** 24-layer, 1024-hidden, 16-head, sequence length of 512
- Trained on 4x4 and 8x8 TPUs for 4 days (cost today using cloud TPU: $1.3K and $5K)

[BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding, Devlin et al. 2018]

Fine-tuning BERT

"Pretrain once, finetune many times."

- **Idea:** Make pre-trained model **usable** in **downstream tasks**
- Initialized with pre-trained model parameters
- Fine-tune model parameters using labeled data from downstream tasks



[BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding, Devlin et al. 2018]

An Example Result: SWAG

A girl is going across a set of monkey bars. She

(i) jumps up across the monkey bars.

(ii) struggles onto the bars to grab her head.

(iii) gets to the end and stands on a wooden plank.

(iv) jumps up and does a back flip.

Leaderboard

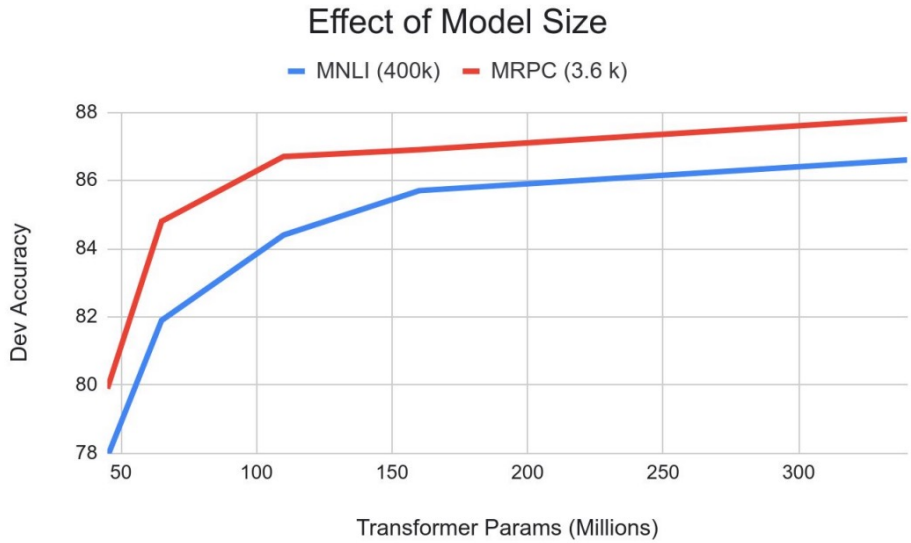
Human Performance (88.00%)
Running Best
Submissions

Rank	Model	Test Score
1	**BERT (Bidirectional Encoder Representations from Transfo...** *Jacob Devlin, Ming-Wei Chang, Kenton Lee, Kristina Toutanova* 10/11/2018	**86.28%**
2	**OpenAI Transformer Language Model** *Original work by Alec Radford, Karthik Narasimhan, Tim Salimans, ...* 10/11/2018	**77.97%**
3	**ESIM with ELMo** *Zellers, Rowan and Bisk, Yonatan and Schwartz, Roy and Choi, Yejin* 08/30/2018	**59.06%**
4	**ESIM with Glove** *Zellers, Rowan and Bisk, Yonatan and Schwartz, Roy and Choi, Yejin* 08/29/2018	**52.45%**

- Run each Premise + Ending through BERT.
- Produce logit for each pair on token 0 ([CLS])

[BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding, Devlin et al. 2018]

Effect of Model Size



- Big models help a lot
- Going from 110M -> 340M params helps even on datasets with 3,600 labeled examples
- Improvements have **not** plateaued!

[BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding, Devlin et al. 2018]

Impact of BERT

- In order to have state-of-the-art performance on different tasks, there is no need for coming up with a novel model architecture
  - End of task-specific model architecture engineering

- An early sign that larger scales and self-supervised learning (language modeling) are the key for future performance improvements

Why did no one think of this before?

- Why wasn't contextual pre-training popular before 2018 with ELMo?

- Good results on pre-training is >1,000x to 100,000 more expensive than supervised training.

What Happened After BERT?

- RoBERTa (Liu et al., 2019)
  - Exact same architecture as BERT
  - Drops the next sentence prediction loss!
  - Trained on 10x data (the original BERT was actually under-trained)
  - Much stronger performance than BERT (e.g., 94.6 vs 90.9 on SQuAD)

Model	data	bsz	steps	SQuAD (v1.1/2.0)	MNLI-m	SST-2
RoBERTa						
with BOOKS + WIKI	16GB	8K	100K	93.6/87.3	89.0	95.3
+ additional data (§3.2)	160GB	8K	100K	94.0/87.7	89.3	95.6
+ pretrain longer	160GB	8K	300K	94.4/88.7	90.0	96.1
+ pretrain even longer	160GB	8K	500K	**94.6/89.4**	**90.2**	**96.4**
$\text{BERT}_{\text{LARGE}}$						
with BOOKS + WIKI	13GB	256	1M	90.9/81.8	86.6	93.7

What Happened After BERT?

- RoBERTa (Liu et al., 2019)
  - Exact same architecture as BERT
  - Drops the next sentence prediction loss!
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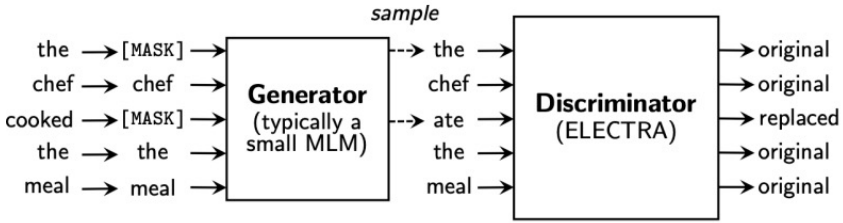
  - Much stronger performance than BERT (e.g., 94.6 vs 90.9 on SQuAD)

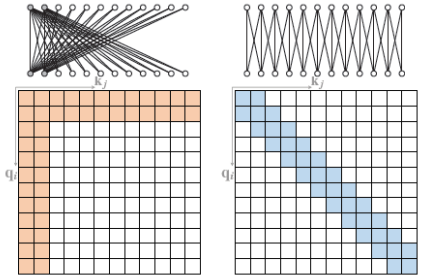
- ALBERT (Lan et al., 2020)
  - Increasing model sizes by sharing model parameters across layers
  - Less storage, much stronger performance but runs slower..

- ELECTRA (Clark et al., 2020)
  - Pre-training objective: replaced-token detection
  - Two models generator and discriminator (GAN-like)
  - It provides a more efficient training method

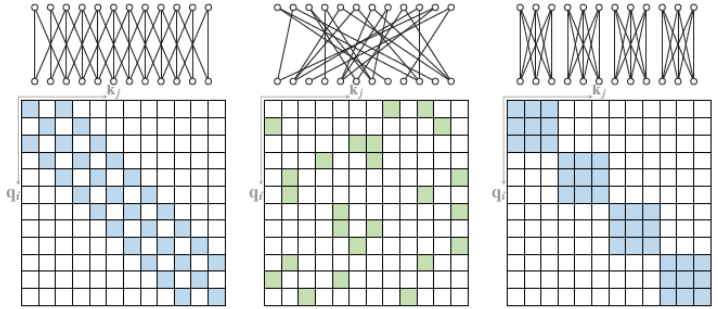


What Happened After BERT?

- Models that handle long contexts
  - Longformer, Big Bird, …
- Multilingual BERT
  - Trained single model on 104 languages from Wikipedia.
- BERT extended to different domains
  - SciBERT, BioBERT, FinBERT, ClinicalBERT, …
- Making BERT smaller to use
  - DistillBERT, TinyBERT, …



(a) global (b) band



(c) dilated (d) random (e) block local

Text generation using BERT

- Does not support generation or sequence-to-sequence tasks
  - Summarization, Translation, Text simplification, etc

BERT has a Mouth, and It Must Speak: BERT as a Markov Random Field Language Model

Alex Wang
New York University
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Kyunghyun Cho
New York University
Facebook AI Research
CIFAR Azrieli Global Scholar
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Mask-Predict: Parallel Decoding of Conditional Masked Language Models

Marjan Ghazvininejad* **Omer Levy*** **Yinhan Liu*** **Luke Zettlemoyer**
Facebook AI Research
Seattle, WA

Exposing the Implicit Energy Networks behind Masked Language Models via Metropolis--Hastings

Kartik Goyal, Chris Dyer, Taylor Berg-Kirkpatrick

Leveraging Pre-trained Checkpoints for Sequence Generation Tasks

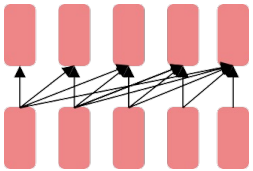
Sascha Rothe, Shashi Narayan, Aliaksei Severyn

src	Der Abzug der franzsischen Kampftruppen wurde am 20. November abgeschlossen .
$t = 0$	The departure of the French combat completed completed on 20 November .
$t = 1$	The departure of French combat troops was completed on 20 November .
$t = 2$	The withdrawal of French combat troops was completed on November 20th .

Summary Thus Far

- BERT and the family
- An encoder; Transformer-based networks trained on massive piles of data.
- Incredible for learning contextualized embeddings of words
- It's very useful to pre-train a large unsupervised/self-supervised LM then fine-tune on your particular task (replace the top layer, so that it can work)
- However, they were not designed to generate text.

Decoder-only Family of Transformers



Decoders

GPT

Generative Pre-trained Transformer

GPT-2: A Big Language Model (2019)

Language Models are Unsupervised Multitask Learners

Alec Radford [*1] Jeffrey Wu [*1] Rewon Child [1] David Luan [1] Dario Amodei [**1] Ilya Sutskever [**1]

GPT: An Auto-Regressive LM (2018)

Improving Language Understanding by Generative Pre-Training

Alec Radford OpenAI alec@openai.com
Karthik Narasimhan OpenAI karthikn@openai.com
Tim Salimans OpenAI tim@openai.com
Ilya Sutskever OpenAI ilyasu@openai.com

GPT-2

- GPT-2 uses only Transformer Decoders (no Encoders) to generate new sequences from scratch or from a starting sequence
- As it processes each subword, it masks the "future" words and conditions on and attends to the previous words

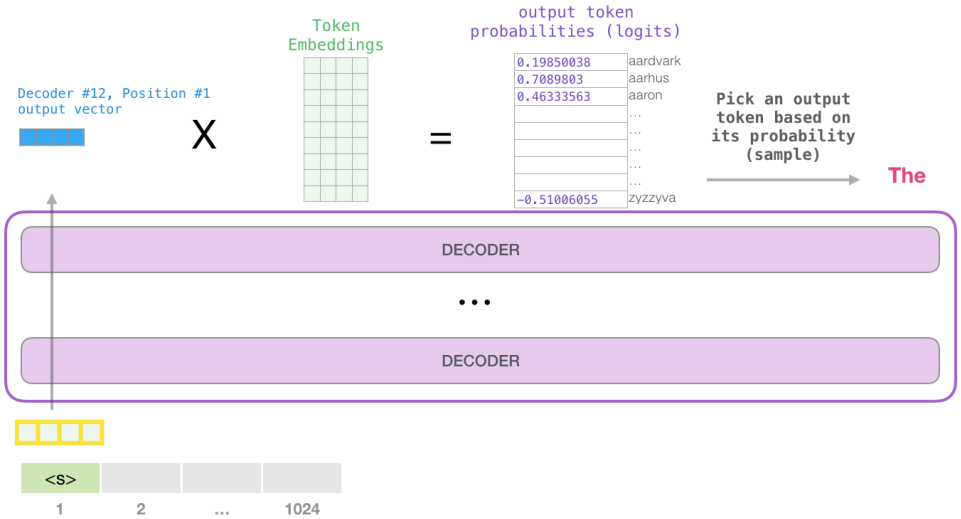
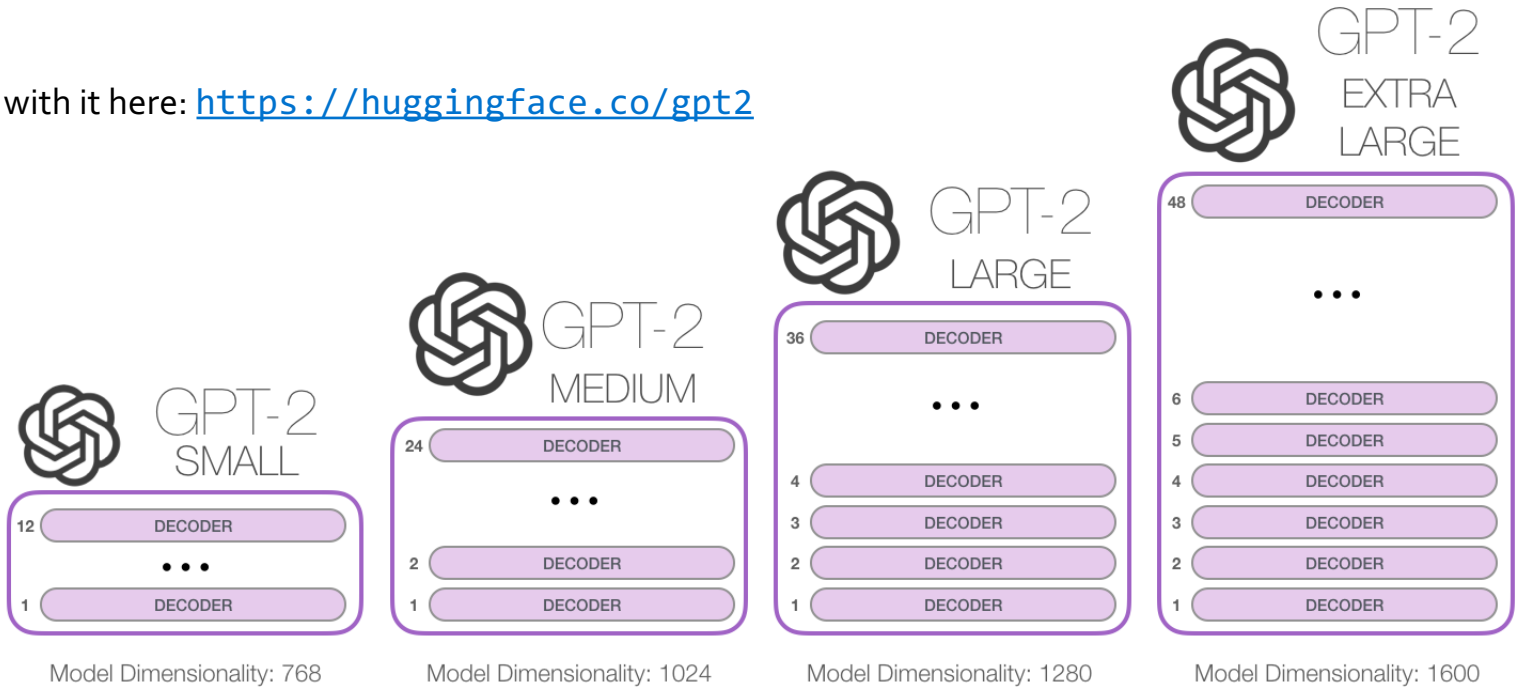


Image by http://jalammar.github.io/illustrated-gpt2/

GPT2: Model Sizes

Play with it here: https://huggingface.co/gpt2

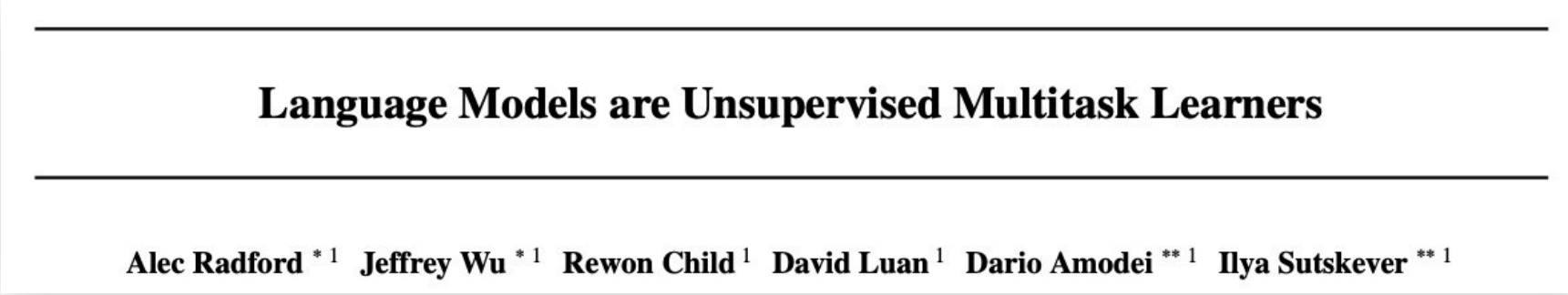


117M parameters 345M 762M 1542M

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

GPT-2 is identical to GPT-1, but:

- Has Layer normalization in between each sub-block (as we've already seen)
- Vocab extended to 50,257 tokens and context size increased from 512 to 1024
- Data: 8 million docs from the web (Common Crawl), minus Wikipedia



Language Models are Unsupervised Multitask Learners

Alec Radford [*1] **Jeffrey Wu** [*1] **Rewon Child** [1] **David Luan** [1] **Dario Amodei** [**1] **Ilya Sutskever** [**1]

GPT2: Some Results

Language Models are Unsupervised Multitask Learners

	LAMBADA (PPL)	LAMBADA (ACC)	CBT-CN (ACC)	CBT-NE (ACC)	WikiText2 (PPL)	PTB (PPL)	enwik8 (BPB)	text8 (BPC)	WikiText103 (PPL)	1BW (PPL)
SOTA	99.8	56.25	85.7	82.3	39.14	46.54	0.99	1.08	18.3	**21.8**
117M	**35.13**	45.99	**87.65**	**83.4**	**29.41**	65.85	1.16	1.17	37.50	75.20
345M	**15.60**	55.48	**92.35**	**87.1**	**22.76**	47.33	1.01	**1.06**	26.37	55.72
762M	**10.87**	**60.12**	**93.45**	**88.0**	**19.93**	**40.31**	**0.97**	**1.02**	22.05	44.575
1542M	**8.63**	**63.24**	**93.30**	**89.05**	**18.34**	**35.76**	**0.93**	**0.98**	**17.48**	42.16

Table 3. Zero-shot results on many datasets. No training or fine-tuning was performed for any of these results. PTB and WikiText-2 results are from (Gong et al., 2018). Other language model results are from (Dai et al., 2019).

Article: Prehistoric man sketched an incredible array of prehistoric beasts on the rough limestone walls of a cave in modern day France 36,000 years ago.
Now, with the help of cutting-edge technology, those works of art in the Chauvet-Pont-d'Arc Cave have been reproduced to create the biggest replica cave in the world.
The manmade cavern named the Caverne du Pont-d'Arc has been built a few miles from the original site in Vallon-Pont-D'arc in Southern France and contains 1,000 painstakingly-reproduced drawings as well as around 450 bones and other features...
Cavemen and women sketched an incredible array of prehistoric beasts on the rough limestone walls of a cave 36,000 years ago and now a replica has been created (pictured)
...

GPT-2: The original site in Vallon-Pont-D'arc in Southern France is a Unesco World Heritage site and is the oldest known and the best preserved cave decorated by man. The replica cave was built a few miles from the original site in Vallon-Pont-D'Arc in Southern France. The cave contains images of 14 different species of animals including woolly rhinoceros, mammoths, and big cats.	**Reference:** Cave mimics famous Caverne du Pont-d'Arc in France, the oldest cave decorated by man and the best preserved. The replica contains all 1,000 paintings which include 425 such as a woolly rhinoceros and mammoths. Minute details were copied using 3D modelling and anamorphic techniques, often used to shoot widescreen images. The modern cave also includes replica paw prints of bears, bones and details preserved in the original cave.

Impact of GPT2

- Zero-shot learning (no use of task-specific supervision) increasingly become a reality.

NMT: "Translate to french," <English text>, <French text>.

QA: "Answer the question," <Document>, <Question>, <Answer>.

SUMM: <Document> "TL; DR:" <Summarization>

GPT-3: A Very Large Language Model (2020)

- More layers & parameters
- Bigger dataset
- Longer training
- Larger embedding/hidden dimension
- Larger context window

[Slide credit: Sbhya Chhabria & Michael Tang]

Size Comparisons

- BERT-Base model has 12 transformer blocks, 12 attention heads,
  - 110M parameters!
- BERT-Large model has 24 transformer blocks, 16 attention heads,
  - 340M parameters!
- GPT-2 is trained on 40GB of text data (8M webpages)!
  - 1.5B parameters!
- GPT-3 is an even bigger version of GPT-2, but isn't open-source
  - 175B parameters!

Impact of GPT3

- Moving away from the fine-tuning paradigm
  - Zero/Few-shot learning and in-context learning
- Massive LM scale makes high zero/few-shot performance possible
- Start of closed source models
  - Not too many details about their model
  - No released code / model checkpoint
- Also revitalized ppen source efforts:
  - OPT, LLaMA by Meta, BLOOM by Huggingface, etc.

GPT4

- Transformer-based
  - The rest is …. mystery! ☺

- Note, these language models involve more than just pre-training.
  - Pre-training provides the foundation based on which we build the model.
  - We will discuss the later stages (post hoc alignment) in a 2-3 weeks.

Accessing API Models

```
import openai
openai.api_key = ("sk-[redacted]")
my_prompt = '''The sun is [MASK].

    Replace [MASK] with the most probable 5 words to replace, and give me their probabilities.'''
# Here set parameters as you like
response = openai.Completion.create(
  engine="text-davinci-002",
  prompt=my_prompt,
  temperature=0,
  max_tokens=100,
)

print(response['choices'][0]['text'])
```

Try it yourself!

Ada	Babbage	Curie	Davinci
Fastest			Most powerful
$0.0004 / 1K tokens	$0.005 / 1K tokens	$0.0020 / 1K tokens	$0.0200 / 1K tokens

Fine-tuned models

Create your own custom models by fine-tuning our base models with your training data. Once you fine-tune a model, you'll be billed only for the tokens you use in requests to that model.

Learn more about fine-tuning ↗

Model	Training	Usage
Ada	$0.0004 / 1K tokens	$0.0016 / 1K tokens
Babbage	$0.0006 / 1K tokens	$0.0024 / 1K tokens
Curie	$0.0030 / 1K tokens	$0.0120 / 1K tokens
Davinci	$0.0300 / 1K tokens	$0.1200 / 1K tokens

Other Available [Decoder] LMs

EleutherAI: GPT-Neo (6.7B), GPT-J (6B), GPT-NeoX (20B)
https://huggingface.co/EleutherAI
https://6b.eleuther.ai/

LLaMA, 65B: https://github.com/facebookresearch/llama

Revisiting Encoding Positional Information

- Toward Length Extrapolatable Transformers -- Ta-Chung Chi (CMU) – YouTube

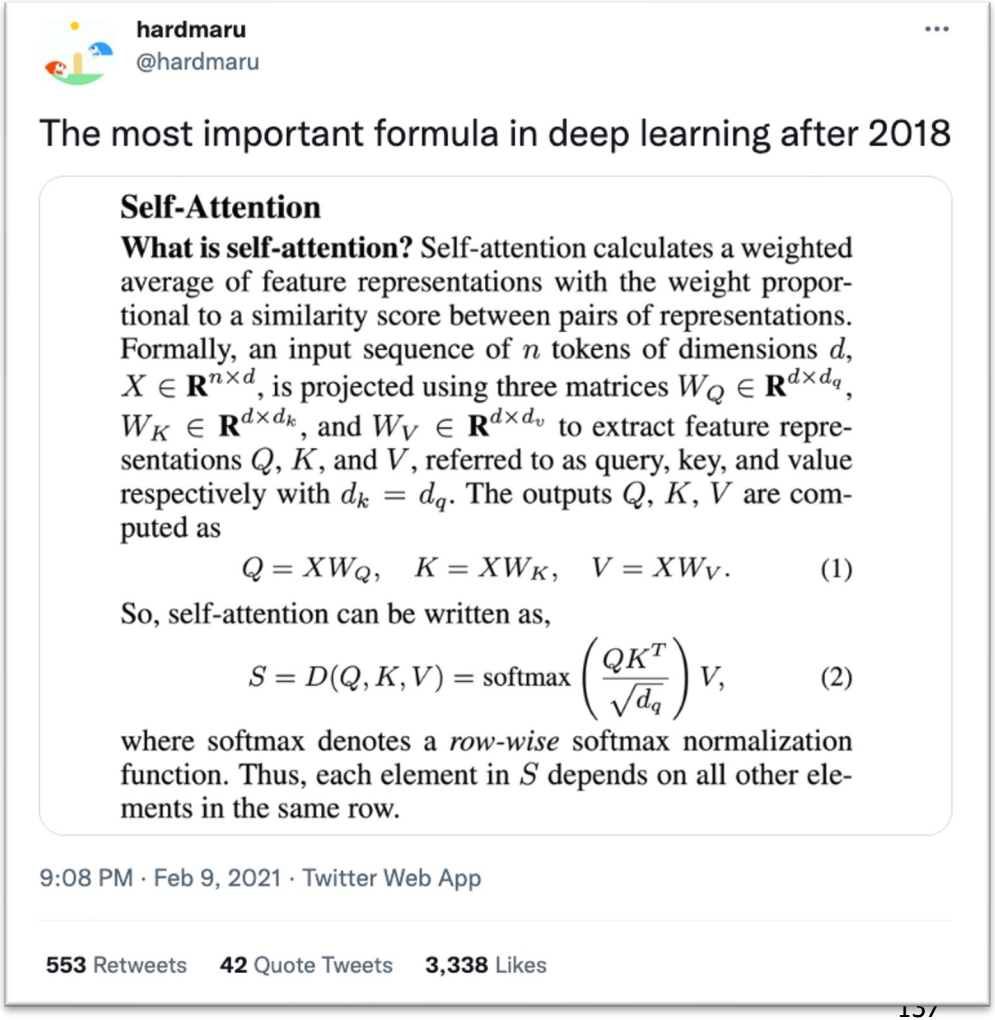
Self-Attention

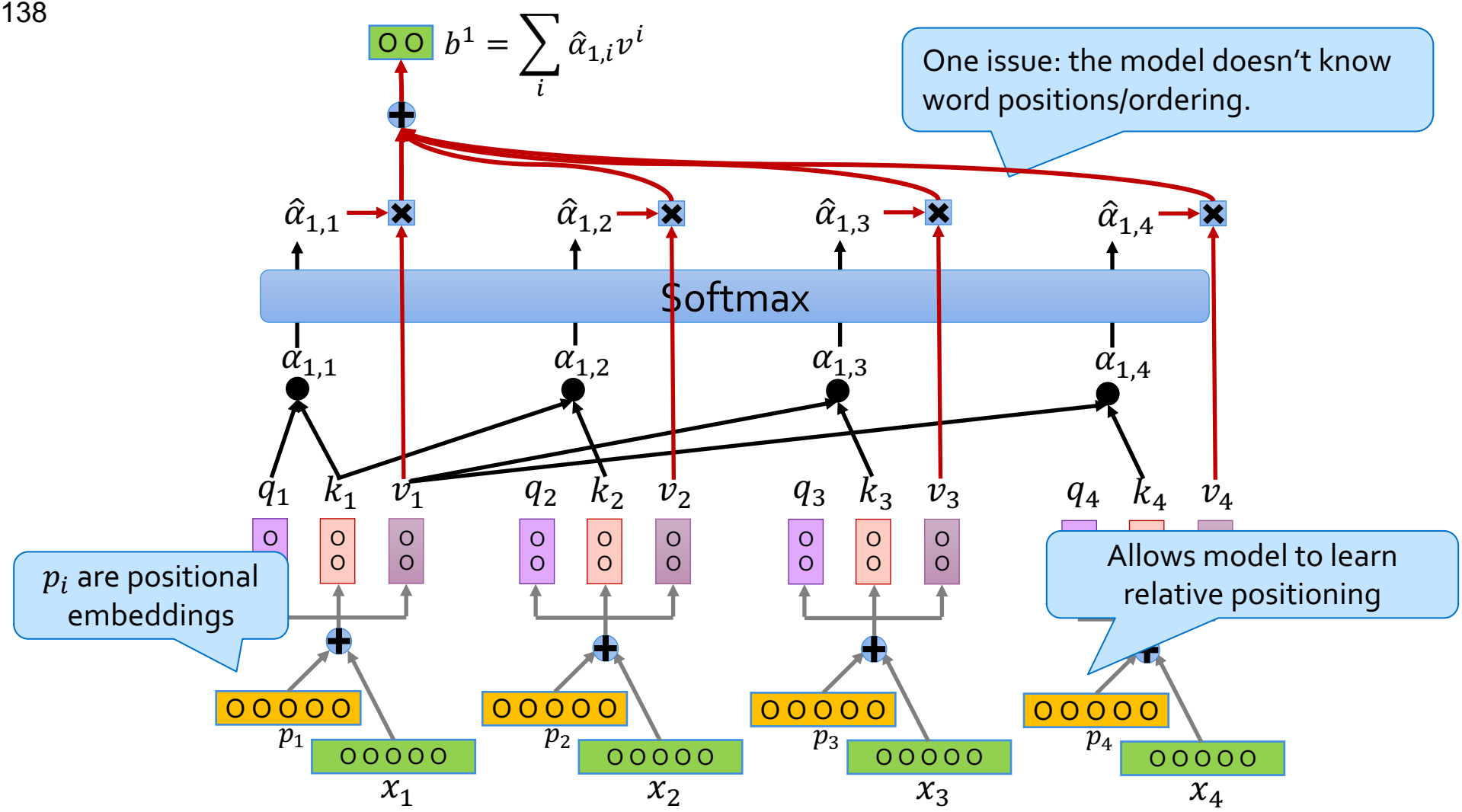
- Can write it in matrix form:

- Given input $\mathbf{x}$:

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

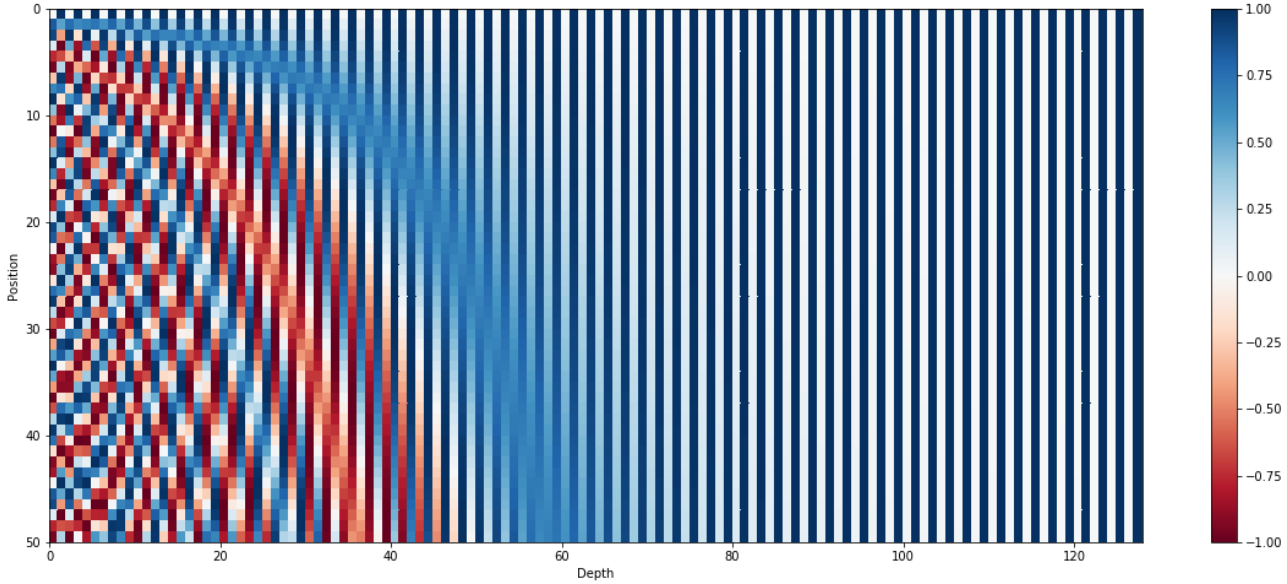
$$\text{Attention}(\mathbf{x}) = \text{softmax}\left(\frac{QK^{\mathrm{T}}}{\alpha}\right)V$$

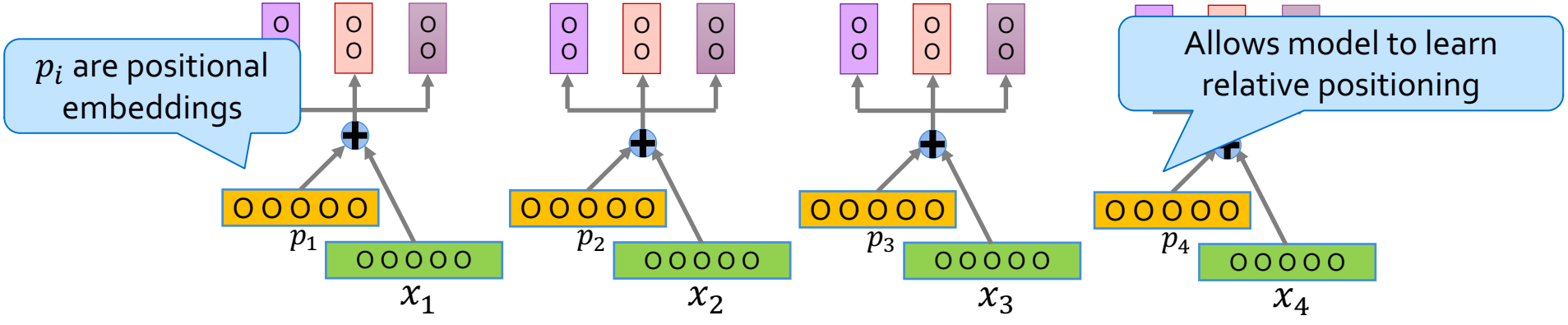



$b^1 = \sum_i \hat{\alpha}_{1,i} v^i$
One issue: the model doesn't know word positions/ordering.
$\hat{\alpha}_{1,1}$
$\hat{\alpha}_{1,2}$
$\hat{\alpha}_{1,3}$
$\hat{\alpha}_{1,4}$
Softmax
$\alpha_{1,1}$
$\alpha_{1,2}$
$\alpha_{1,3}$
$\alpha_{1,4}$
q_1 k_1 v_1
q_2 k_2 v_2
q_3 k_3 v_3
q_4 k_4 v_4
p_i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

An approach:

Sine/Cosine encoding





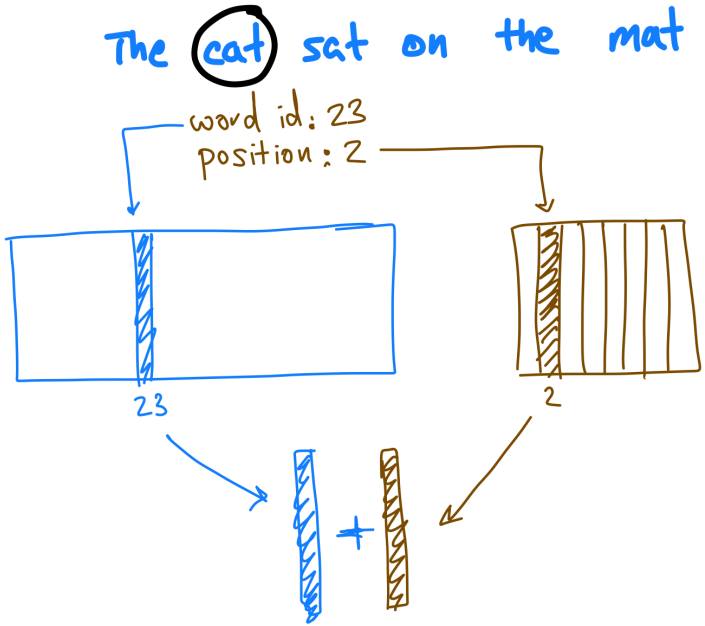
How to encode position information?

- Multi-head attention doesn't have a way to know whether an input token comes before or after another
  - Position is important in sequence modeling in NLP
- One way to introduce position information is add individual position encodings to the input for each position in the sequence

$$x_j = x_j + pos_j$$

- Where pos_j is a position vector

How to encode position information?



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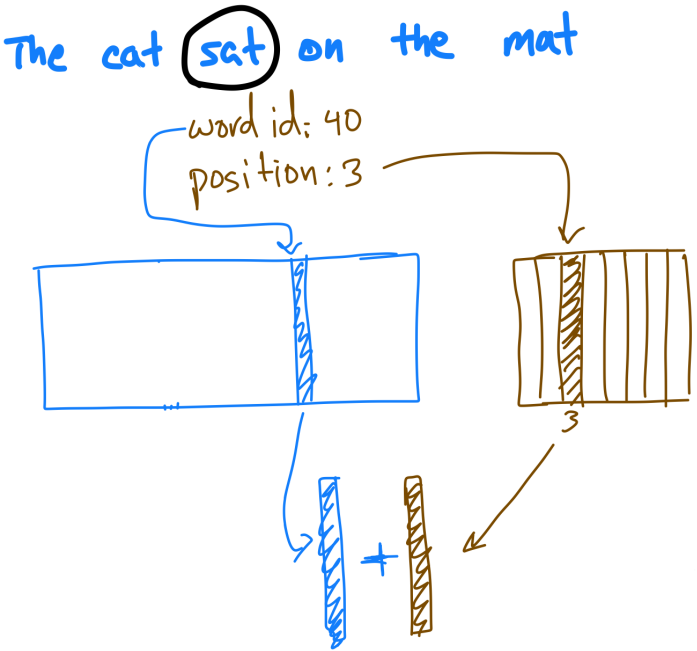

Absolute position embeddings

- Learned positions embeddings:
  - Maximum length that can be presented is limited

- Functional position embeddings (e.g., sinusoidal):

$$Embedding[i, 2k] = sin(position / (10000^{(2k / d\_model)}))$$

$$Embedding[i, 2k+1] = cos(position / (10000^{(2k / d\_model)}))$$

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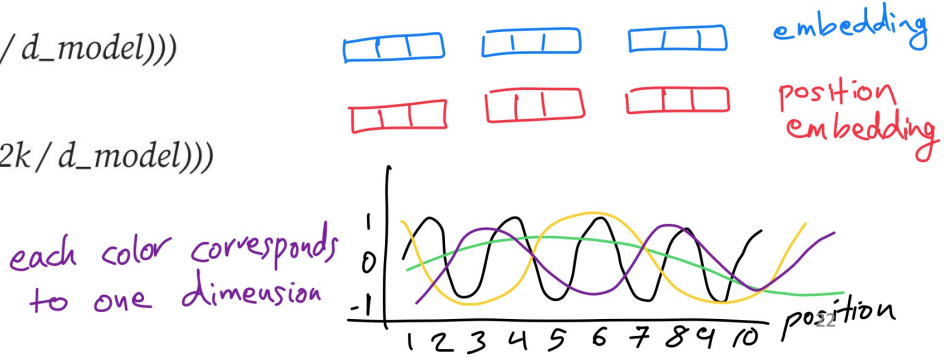

Limitations of learned positions embeddings

- Fixed length of the embedding matrix
- Do not directly model the distance between tokens
- Not always meaningful because of "packing" often used during pre- training
  - Pack multiple examples in a single context

cats sleep

The cat sat on the mat

Birds fly high

The sun rises daily

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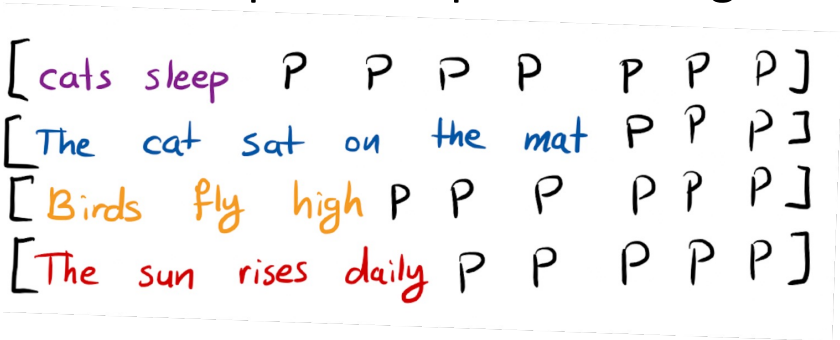

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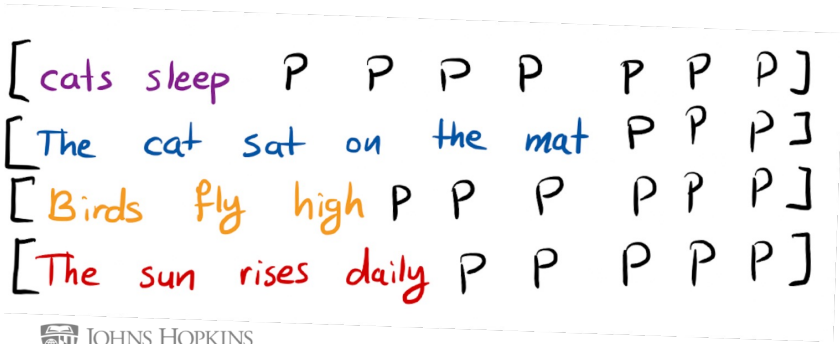

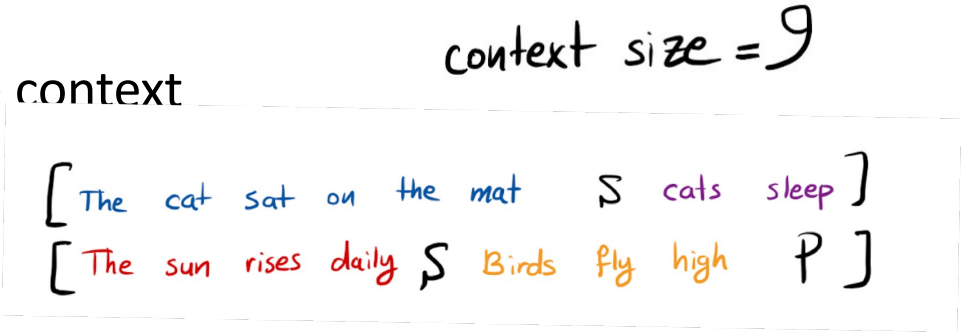

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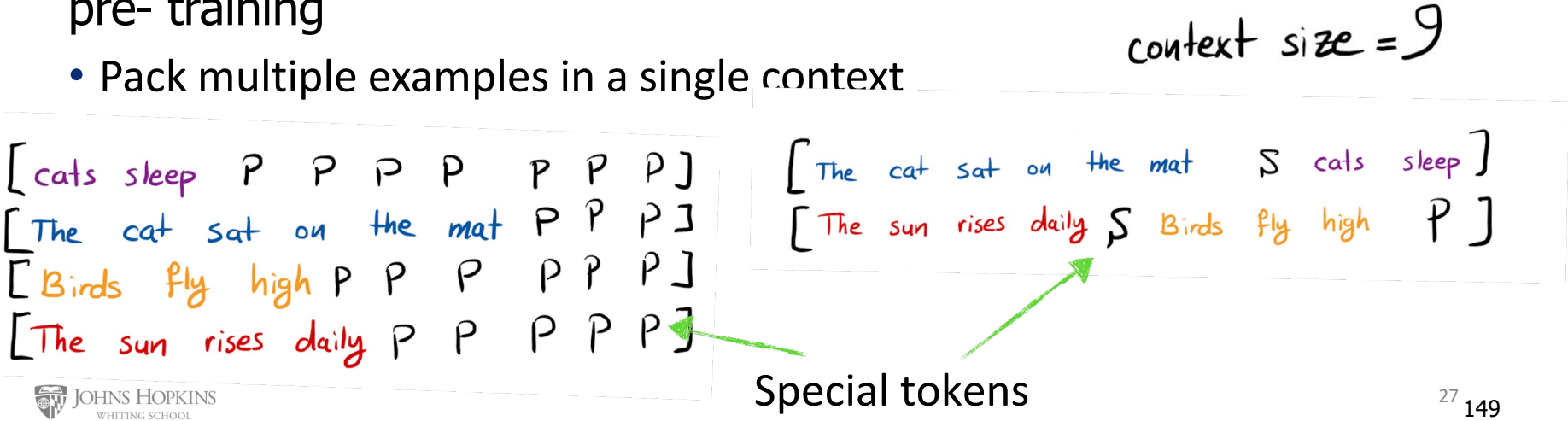
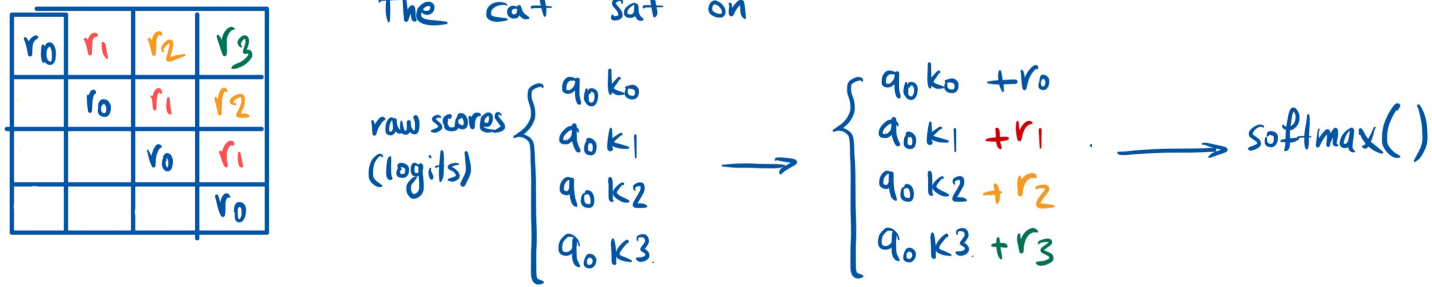


Relative position embedding

- Relative position embeddings produce different learned embedding according to the offset between query and key
- T5 (Raffel et al., 2019) uses a scalar that is added to the attention raw scores
- Each attention head uses a different position bias



Rotary position embeddings

- **Goal:** find a positional encoding function $f(\mathbf{x}, \ell)$ for an input and a position ℓ such that for two inputs $\mathbf{q}$ and $\mathbf{k}$ and positions m and n is only sensitive to values $\mathbf{q}$ and $\mathbf{k}$ and their relative position.
- Recall the geometric definition of the dot product between Euclidean vectors

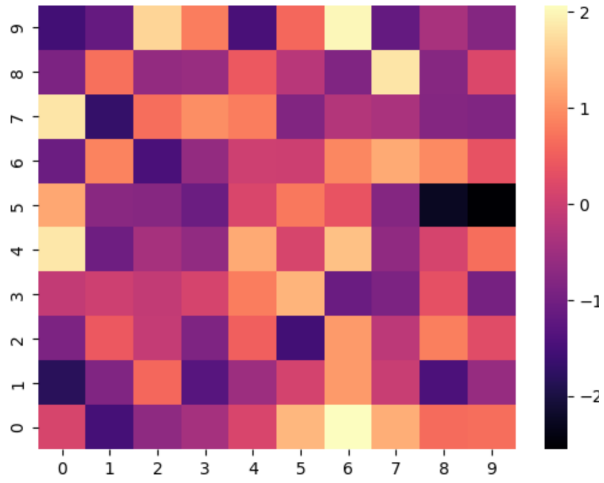
$$\mathbf{q} \cdot \mathbf{k} = \|\mathbf{q}\| \|\mathbf{k}\| \cos(\theta_{qk})$$

Rotary Positional Embeddings (ROPE)

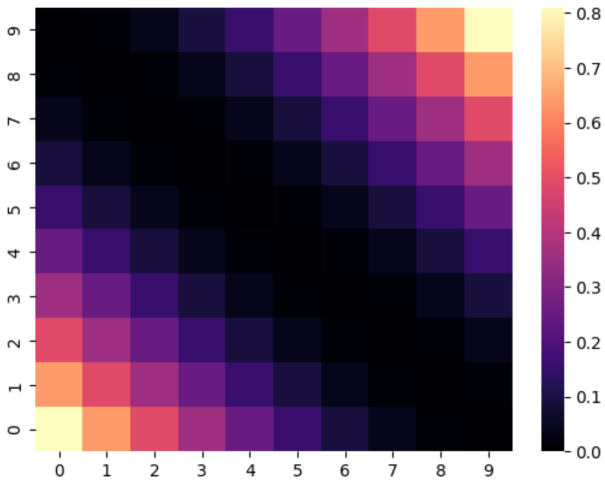
- The intuition behind RoPE is that we can represent the token embeddings as complex numbers and their positions as pure rotations that we apply to them.
- By exploiting the nature of rotations, the dot product used in self- attention will have the property we are looking for, preserving relative positional information while discarding absolute position.

Rotary Positional Embeddings (ROPE)

- Rotates the query and key vectors based on their positions in the sequence



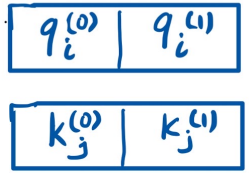
$\text{logits} = Q.K^T$

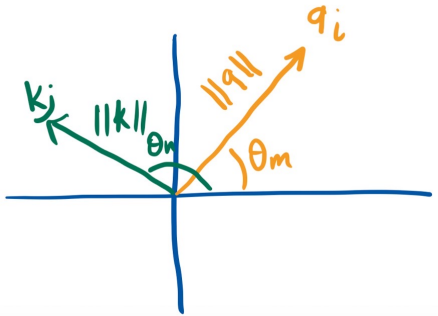


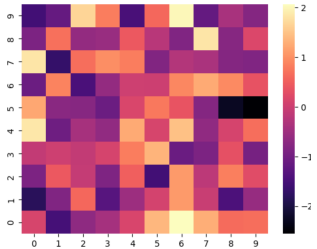
$\text{logits} = f(m-n)$

RoFormer: Enhanced Transformer with Rotary Position Embedding (2022)

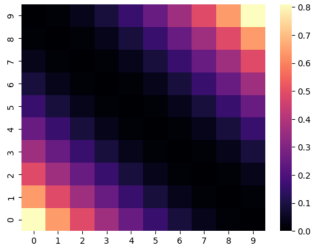
Rotary Positional Embeddings (ROPE)







$$a_{ij} = q_i \cdot k_j$$



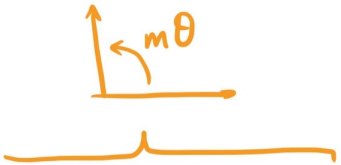
$$a_{ij} = \Theta(m - n)$$

Rotary Positional Embeddings (ROPE)

$$f_{\{q,k\}}(\boldsymbol{x}_m, m) = \begin{pmatrix} \cos m\theta & -\sin m\theta \\ \sin m\theta & \cos m\theta \end{pmatrix} \begin{pmatrix} W^{(11)}_{\{q,k\}} & W^{(12)}_{\{q,k\}} \\ W^{(21)}_{\{q,k\}} & W^{(22)}_{\{q,k\}} \end{pmatrix} \begin{pmatrix} x^{(1)}_m \\ x^{(2)}_m \end{pmatrix}$$

RoFormer: Enhanced Transformer with Rotary Position Embedding (2022)

Rotary Positional Embeddings (ROPE)



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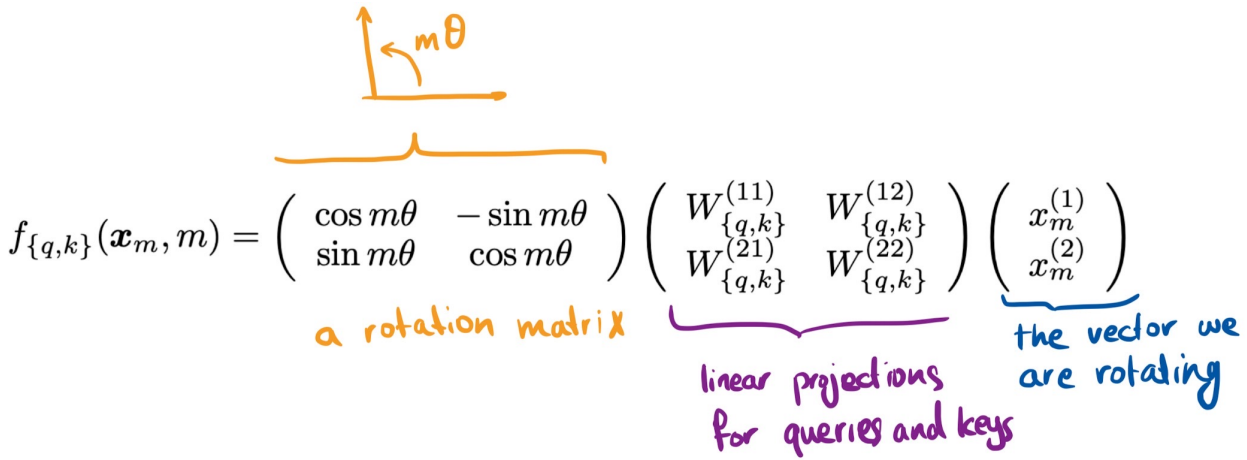
a rotation matrix

the vector we are rotating

Rotary Positional Embeddings (ROPE)



RoFormer: Enhanced Transformer with Rotary Position Embedding (2022)

Rotary Positional Embeddings (ROPE)

- General form

$$f_{\{q,k\}}(\boldsymbol{x}_m, m) = \boldsymbol{R}^d_{\Theta,m}\boldsymbol{W}_{\{q,k\}}\boldsymbol{x}_m$$

$$\boldsymbol{R}^d_{\Theta,m} = \begin{pmatrix} \cos m\theta_1 & -\sin m\theta_1 & 0 & 0 & \cdots & 0 & 0 \\ \sin m\theta_1 & \cos m\theta_1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & \cos m\theta_2 & -\sin m\theta_2 & \cdots & 0 & 0 \\ 0 & 0 & \sin m\theta_2 & \cos m\theta_2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & \cos m\theta_{d/2} & -\sin m\theta_{d/2} \\ 0 & 0 & 0 & 0 & \cdots & \sin m\theta_{d/2} & \cos m\theta_{d/2} \end{pmatrix}$$

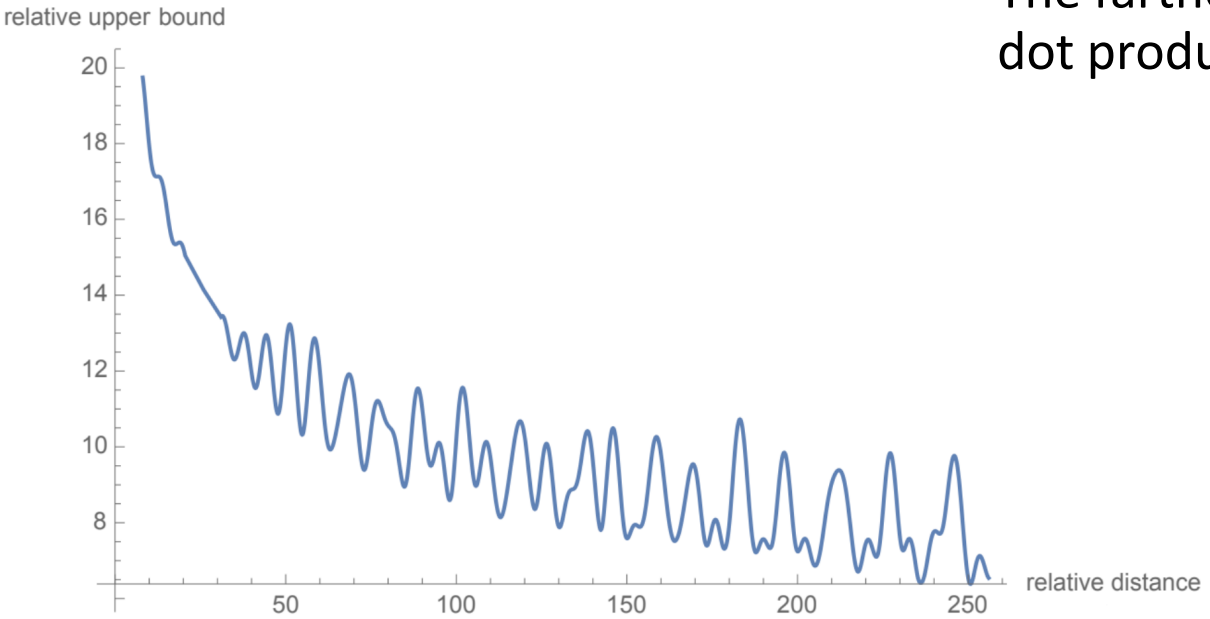
RoFormer: Enhanced Transformer with Rotary Position Embedding (2022)

Rotary Positional Embeddings (ROPE)

- The matrix multiplication is going to be very slow
- In practice we can use the following realization (taking advantage of the sparsity of R)

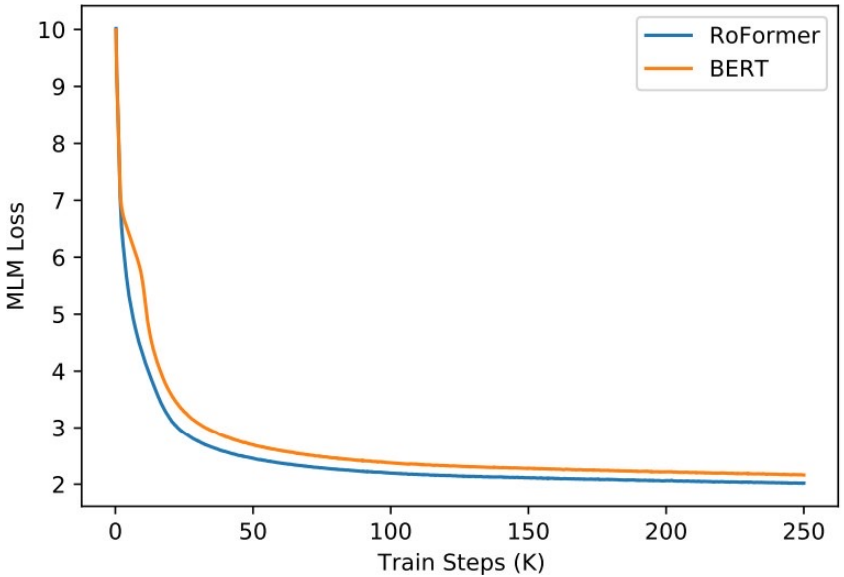
$$\boldsymbol{R}^d_{\Theta,m}\boldsymbol{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ \vdots \\ x_{d-1} \\ x_d \end{pmatrix} \otimes \begin{pmatrix} \cos m\theta_1 \\ \cos m\theta_1 \\ \cos m\theta_2 \\ \cos m\theta_2 \\ \vdots \\ \cos m\theta_{d/2} \\ \cos m\theta_{d/2} \end{pmatrix} + \begin{pmatrix} -x_2 \\ x_1 \\ -x_4 \\ x_3 \\ \vdots \\ -x_{d-1} \\ x_d \end{pmatrix} \otimes \begin{pmatrix} \sin m\theta_1 \\ \sin m\theta_1 \\ \sin m\theta_2 \\ \sin m\theta_2 \\ \vdots \\ \sin m\theta_{d/2} \\ \sin m\theta_{d/2} \end{pmatrix}$$

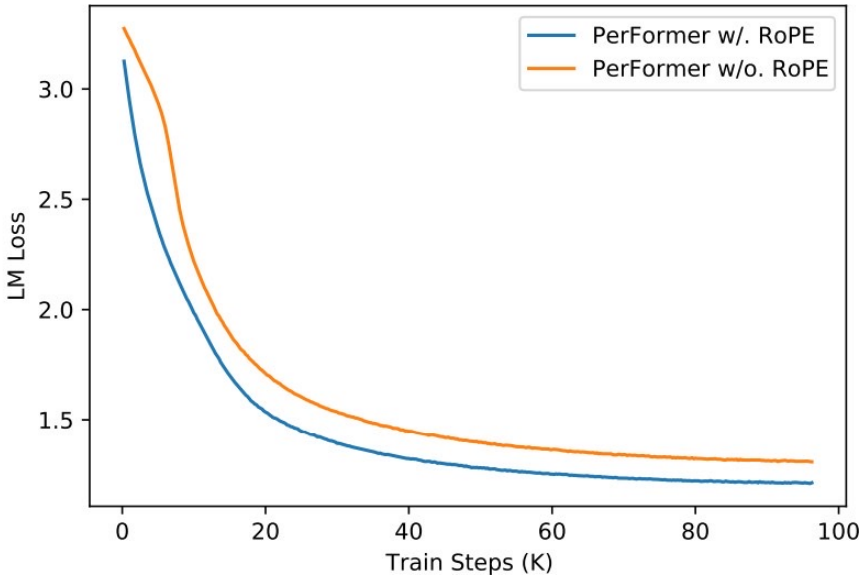
Rotary Positional Embeddings (ROPE)



The farther the tokens their dot product will be lower

RoFormer: Enhanced Transformer with Rotary Position Embedding (2022)


RoFormer
BERT
MLM Loss
Train Steps (K)
10
9
8
7
6
5
4
3
2
0
50
100
150
200
250


PerFormer w/. RoPE
PerFormer w/o. RoPE
LM Loss
Train Steps (K)
3.0
2.5
2.0
1.5
0
20
40
60
80
100

What is a good property of a positional encoding?

- Should extrapolate to longer inputs

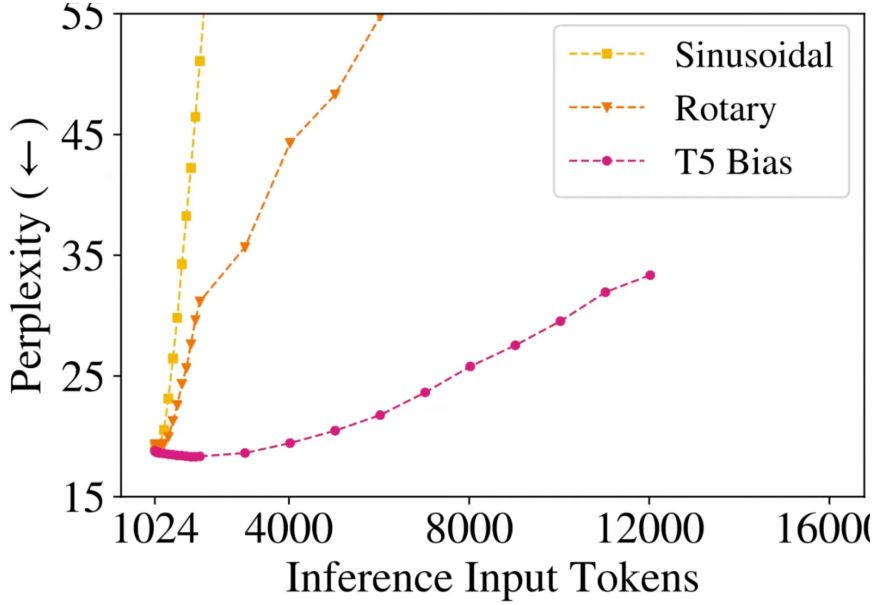
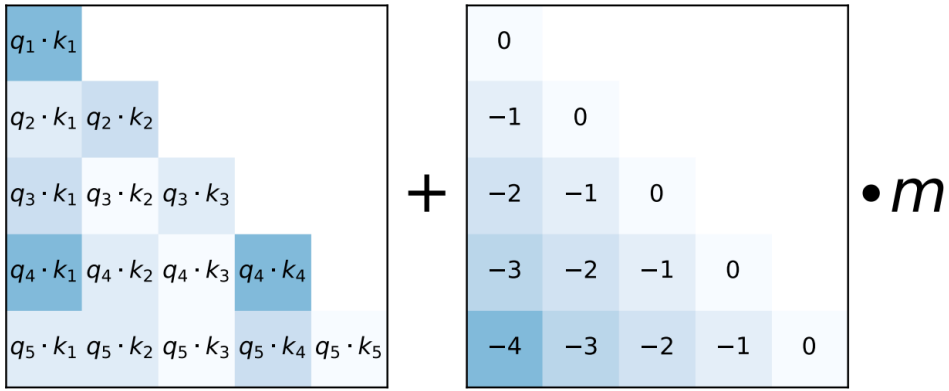


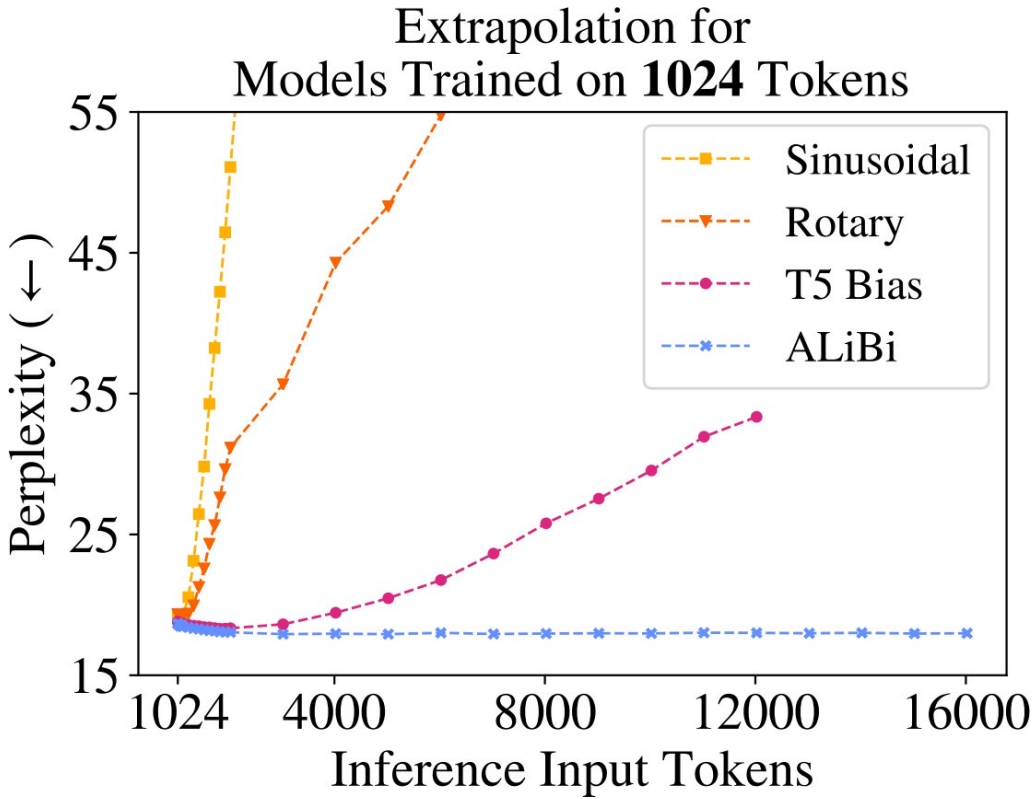
fig from Ofir Press (2023)

Attention with Linear Biases (ALiBi)

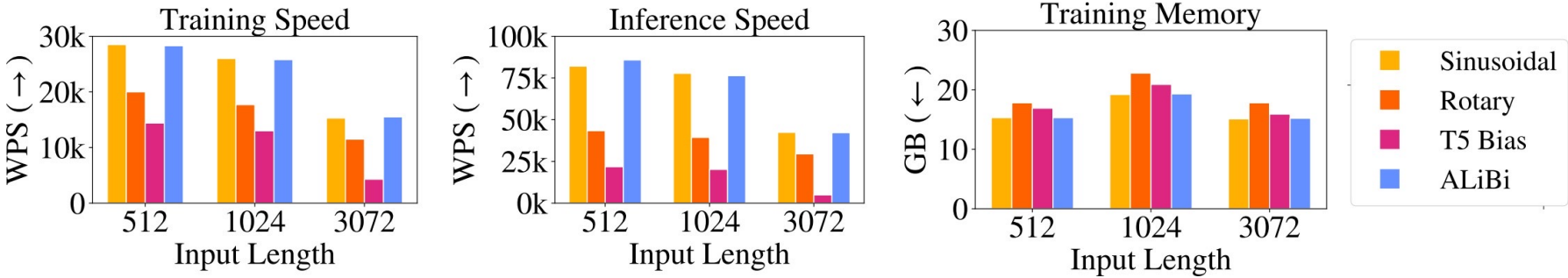
- Add a constant value to the attention logits
- Apply a head specific scalar **m**



Train Short, Test Long: Attention with Linear Biases Enables Input Length Extrapolation (2022)


Extrapolation for
Models Trained on 1024 Tokens
Perplexity (←)
55
45
35
25
15
1024
4000
8000
12000
16000
Inference Input Tokens
Sinusoidal
Rotary
T5 Bias
ALiBi

ALiBi


Training Speed
WPS (→)
30k
20k
10k
0
512
1024
3072
Input Length
Inference Speed
WPS (→)
100k
75k
50k
25k
0k
512
1024
3072
Input Length
Training Memory
GB (←)
30
20
10
0
512
1024
3072
Input Length
Sinusoidal
Rotary
T5 Bias
ALiBi

- TODO:
  - LMs might work without explicit positional encoding
  - Unifiying view of positional embeddings
  - Length generalization is different than keeping perplexity low.

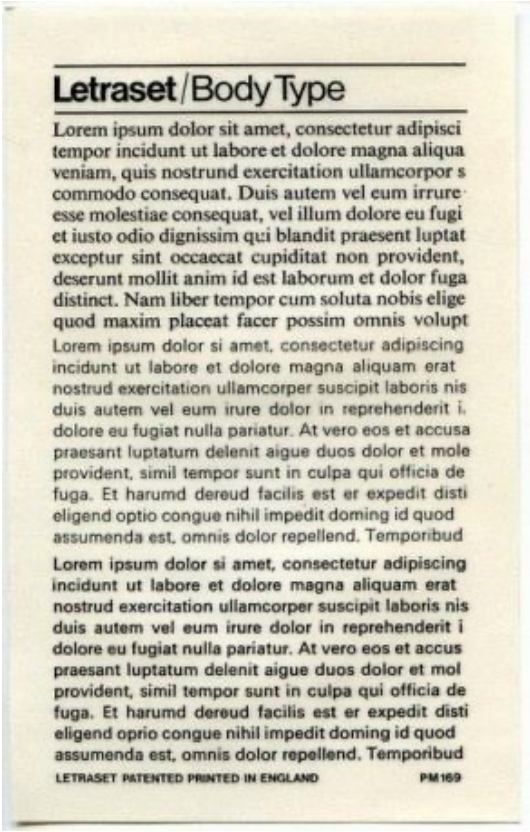
Summary

Pre-Training Data

- TODO:
  - data cleaning
  - Deduplicating
  - Shuffling
  - Nearest neighbor sorting
  -

C4: The Data

- C4: Colossal Clean Crawled Corpus
  - Web-extracted text
  - English language only (langdetect)
  - 750GB
- Retain:
  - Sentences with terminal punctuation marks
  - Pages with at least 5 sentences, sentences with at least 3 words
  - Deduplicate three sentence spans
- Remove:
  - References to Javascript
  - "Lorem ipsum" text — placeholder text commonly used to demonstrate the visual form of a document



Letraset/Body Type

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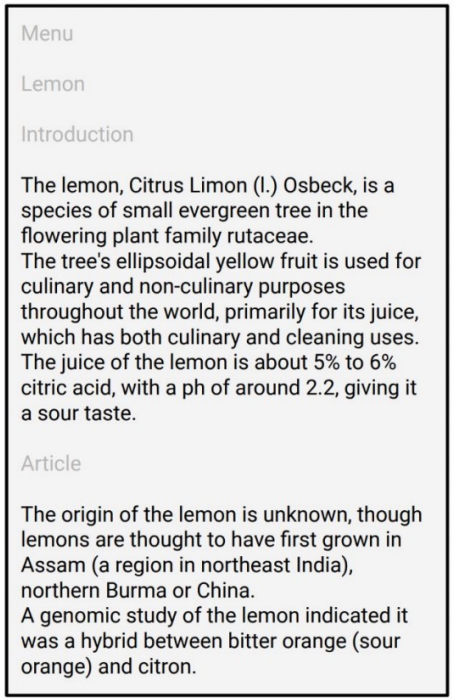
Lorem ipsum dolor si amet, consectetur adipiscing incidunt ut labore et dolore magna aliquam erat nostrud exercitation ullamcorper suscipit laboris nis duis autem vel eum irure dolor in reprehenderit i dolore eu fugiat nulla pariatur. At vero eos et accus praesant luptatum delenit aigue duos dolor et mol provident, simil tempor sunt in culpa qui officia de fuga. Et harumd dereud facilis est er expedit disti eligend oprio congue nihil impedit doming id quod assumenda est, omnis dolor repellend. Temporibud

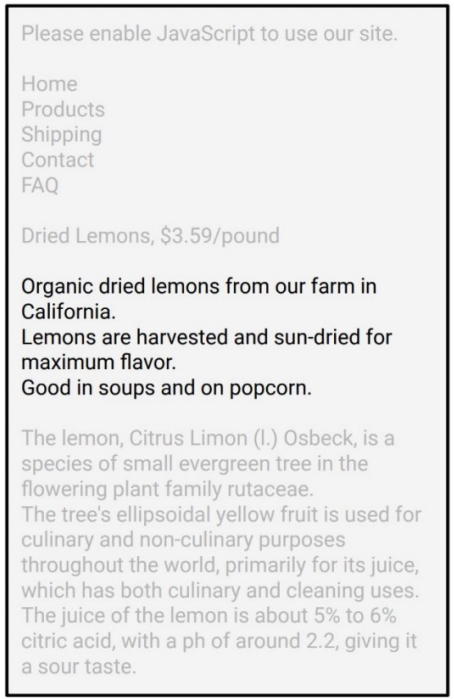
LETRASET PATENTED PRINTED IN ENGLAND PM169

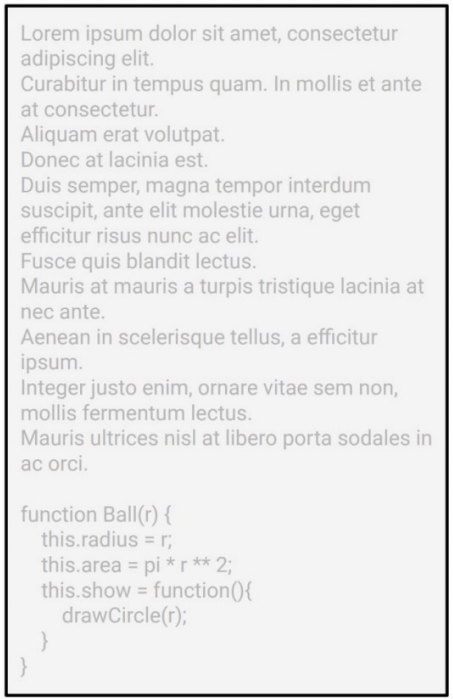
C4: The Data

Slide adapted from Colin Raffel

C4: The Data







Slide adapted from Colin Raffel

C4: The Data

- 750GB? What does that mean?

Data set	Size
★ C4	745GB
C4, unfiltered	6.1TB
RealNews-like	35GB
WebText-like	17GB
Wikipedia	16GB
Wikipedia + TBC	20GB

Play with the data: https://c4-search.apps.allenai.org/

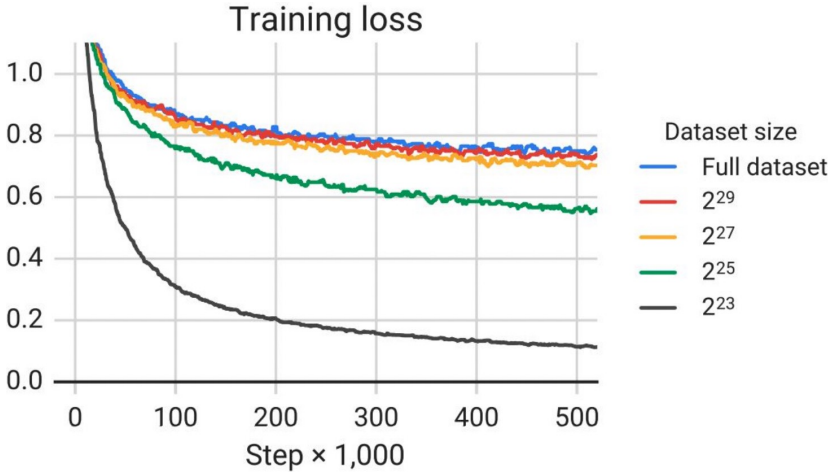
Pre-training Data: Experiment

- Takeaway:
  - Clean and compact data is better than large, but noisy data.
  - Pre-training on in-domain data helps.

Data set	Size	GLUE	CNNDM	SQuAD	SGLUE	EnDe	EnFr	EnRo
★ C4	745GB	83.28	**19.24**	80.88	71.36	**26.98**	**39.82**	**27.65**
C4, unfiltered	6.1TB	81.46	19.14	78.78	68.04	26.55	39.34	27.21
RealNews-like	35GB	**83.83**	**19.23**	80.39	72.38	**26.75**	**39.90**	**27.48**
WebText-like	17GB	**84.03**	**19.31**	**81.42**	71.40	**26.80**	**39.74**	**27.59**
Wikipedia	16GB	81.85	**19.31**	81.29	68.01	**26.94**	39.69	**27.67**
Wikipedia + TBC	20GB	83.65	**19.28**	**82.08**	**73.24**	**26.77**	39.63	**27.57**

Pre-training Data: Experiment

- Effect of data repetitions
- Takeaways:
  - (Table) Performance degrades as the information content shrinks.
  - (Figure) The model memorizes the pre-training data, with smaller/repeated datasets.



Number of tokens	Repeats	GLUE	CNNDM	SQuAD	SGLUE	EnDe	EnFr	EnRo
★ Full data set	0	**83.28**	**19.24**	**80.88**	**71.36**	**26.98**	**39.82**	**27.65**
2^{29}	64	**82.87**	**19.19**	**80.97**	**72.03**	**26.83**	**39.74**	**27.63**
2^{27}	256	82.62	**19.20**	79.78	69.97	**27.02**	**39.71**	27.33
2^{25}	1,024	79.55	18.57	76.27	64.76	26.38	39.56	26.80
2^{23}	4,096	76.34	18.33	70.92	59.29	26.37	38.84	25.81

LLM Name	Release Date	Pretraining		Checkpoints		Pretraining Dataset			Tokens (T)
		Code	Config	Model	Optim	Data Mix	Ordering	Available	
GPT-J [18]	May'21	✓	✓	✓	✓	✓	✓	✓	0.40
GPT-NeoX [19]	Apr'22	✓	✓	✓	✓	✓	✓	✓	0.40
OPT [20]	May'22	✓	✓	✓		✓			0.18
BLOOM [21]	Nov'22	✓	✓	✓	✓	✓	✓	✓	0.34
Pythia [16]	Feb'23	✓	✓	✓	✓	✓	✓	✓	0.30
LLaMA [3]	Feb'23		✓			✓			1.0
OpenLLaMA [11]	May'23	✓	✓	✓		✓		✓	1.0
INCITE [10]	May'23	✓	✓	✓		✓		✓	1.0
MPT [22]	May'23	✓	✓			✓			1.0
Falcon [23]	May'23		✓			✓			1.5
Llama 2 [4]	Jul'23		✓						2.0
Qwen [24]	Aug'23		✓						2.4
Mistral [6]	Sep'23								?
Yi [25]	Nov'23								?
AMBER	Dec'23	✓	✓	✓	*	✓	✓	✓	1.3
CRYSTALCODER	Dec'23	✓	✓	✓	✓	✓	✓	✓	1.4

Table 1: Summary of notable open-source LLMs. We note a trend of progressively less disclosure of important pretraining details over time: (1) availability of pretraining code, (2) disclosure of training configurations and hyperparameters, (3) intermediate checkpoints of model weights, (4) intermediate checkpoints of optimizer states, (5) disclosure of data mixture and sources, (6) reproducibility of pretraining data sequence, and (7) availability (or reconstruction scripts) of the pretraining data.
* *Amber optimizer states are lost due to errors in early implementation.*

https://www.llm360.ai/paper.pdf

- On data: https://huyenchip.com/2023/05/02/rlhf.html

Practical Considerations

Other Training Considerations

- Training objectives
- Learning rates
- Training divergence

Pre-training objectives

Objectives

- Prefix language modeling
  - **Input:** Thank you for inviting
  - **Output:** me to your party last week
- BERT-style denoising
  - **Input:** Thank you <M> <M> me to your party apple week
  - **Output:** Thank you for inviting me to your party last week
- Deshuffling
  - **Input:** party me for your to. last fun you inviting week Thanks.
  - **Output:** Thank you for inviting me to your party last week

- IID noise, replace spans
  - **Input:** Thank you <X> me to your party <X> week
  - **Output:** <X> for inviting <Y> last <Z>
- IID noise, drop tokens
  - **Input:** Thank you me to your party week .
  - **Output:** for inviting last

Objectives: Experiments

- All the variants perform similarly
- "Replace corrupted spans" and "Drop corrupted tokens" are more appealing because target sequences are shorter, speeding up training.

Objective	GLUE	CNNDM	SQuAD	SGLUE	EnDe	EnFr	EnRo
Prefix language modeling	80.69	18.94	77.99	65.27	**26.86**	39.73	**27.49**
Deshuffling	73.17	18.59	67.61	58.47	26.11	39.30	25.62
BERT-style (Devlin et al., 2018)	82.96	19.17	**80.65**	69.85	26.78	**40.03**	27.41
★ Replace corrupted spans	83.28	**19.24**	**80.88**	**71.36**	**26.98**	39.82	**27.65**
Drop corrupted tokens	**84.44**	**19.31**	**80.52**	68.67	**27.07**	39.76	**27.82**

Objectives: Experiments

- Performance of the i.i.d. corruption objective with different corruption rates

- Takeaway:
  - Little corruption rate may prevent effective learning.
  - Larger corruption rate leads to downstream performance degradation.
  - Larger corruption rate also leads to longer targets, slowing down training.

Corruption rate	GLUE	CNNDM	SQuAD	SGLUE	EnDe	EnFr	EnRo
10%	**82.82**	19.00	**80.38**	69.55	**26.87**	39.28	**27.44**
★ 15%	**83.28**	19.24	**80.88**	**71.36**	**26.98**	**39.82**	**27.65**
25%	**83.00**	**19.54**	**80.96**	70.48	**27.04**	**39.83**	**27.47**
50%	81.27	19.32	79.80	70.33	**27.01**	**39.90**	**27.49**

On Pre-training Objectives

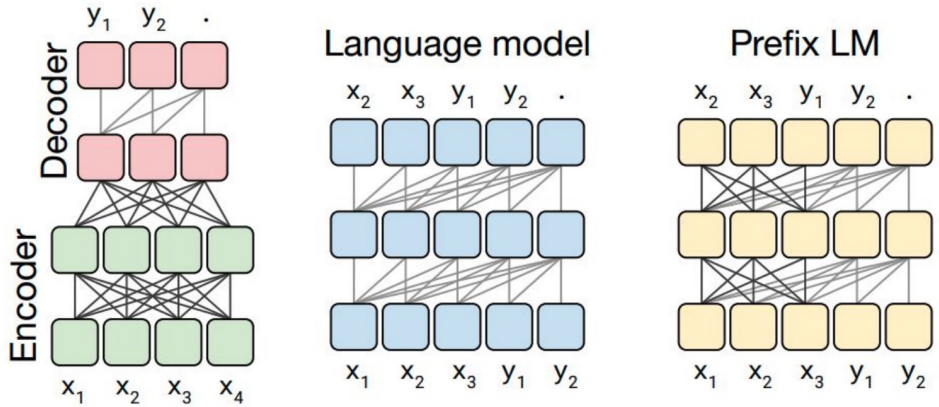
- TBD

- There is work on unifying various pre-training objectives.
  - Intuitively, different downstream tasks benefit from different objectives.

UL2: Unifying Language Learning Paradigms, Tay et al., (2022)

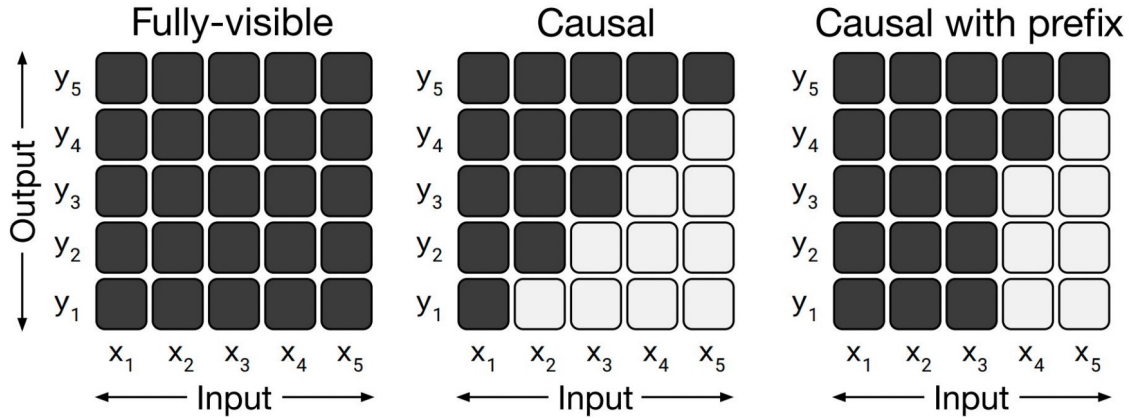
Architectural choices

Architectures: Different Choices



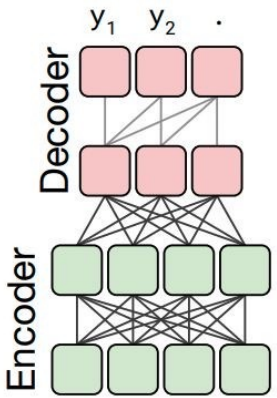
Architectures: Different Attention Masks

- **Fully visible** mask allows the self attention mechanism to attend to the full input.
- A **causal mask** doesn't allow output elements to look into the future.
- **Causal mask** with prefix allows to fully-visible masking on a portion of input.



Architectural Variants: Experiments

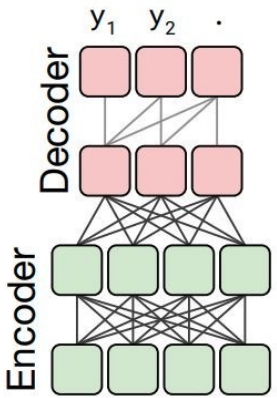
Architecture	Objective	Params	Cost	GLUE	CNNDM	SQuAD	SGLUE	EnDe	EnFr	EnRo
★ Encoder-decoder	Denoising	$2P$	M	**83.28**	**19.24**	**80.88**	**71.36**	**26.98**	**39.82**	**27.65**



Architectural Variants: Experiments

Architecture	Objective	Params	Cost	GLUE	CNNDM	SQuAD	SGLUE	EnDe	EnFr	EnRo
★ Encoder-decoder	Denoising	$2P$	M	**83.28**	**19.24**	**80.88**	**71.36**	**26.98**	**39.82**	**27.65**

Input: Thank you for <X> me to your party <Y>. Target: <X> inviting <Y> last week.



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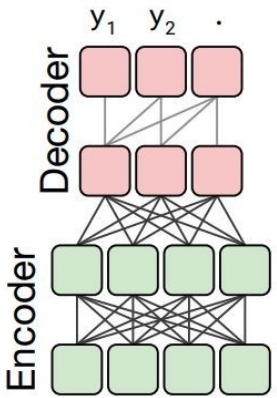
★ Encoder-decoder	Denoising	$2P$	M	**83.28**	**19.24**	**80.88**	**71.36**	**26.98**	**39.82**	**27.65**

Number of parameters



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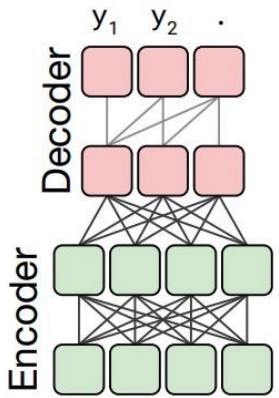
Number of FLOPS



Architectural Variants: Experiments

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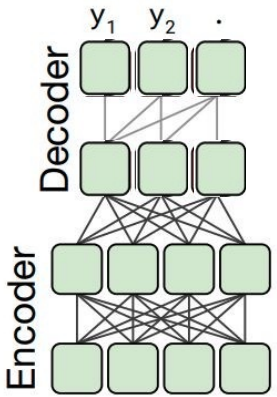
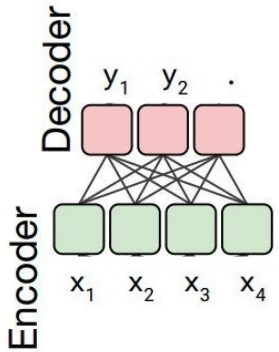
★ Encoder-decoder	Denoising	$2P$	M	**83.28**	**19.24**	**80.88**	**71.36**	**26.98**	**39.82**	**27.65**
Enc-dec, shared	Denoising	P	M	82.81	18.78	**80.63**	**70.73**	26.72	39.03	**27.46**



Architectural Variants: Experiments

Architecture	Objective	Params	Cost	GLUE	CNNDM	SQuAD	SGLUE	EnDe	EnFr	EnRo
★ Encoder-decoder	Denoising	$2P$	M	**83.28**	**19.24**	**80.88**	**71.36**	**26.98**	**39.82**	**27.65**
Enc-dec, shared	Denoising	P	M	82.81	18.78	**80.63**	**70.73**	26.72	39.03	**27.46**
Enc-dec, 6 layers	Denoising	P	$M/2$	80.88	18.97	77.59	68.42	26.38	38.40	26.95



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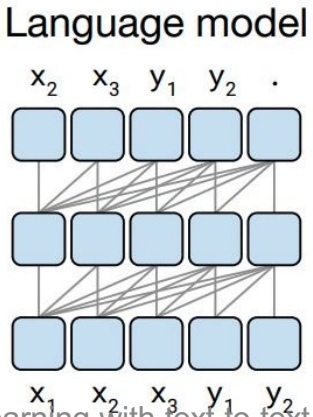
Language model	Denoising	P	M	74.70	17.93	61.14	55.02	25.09	35.28	25.86



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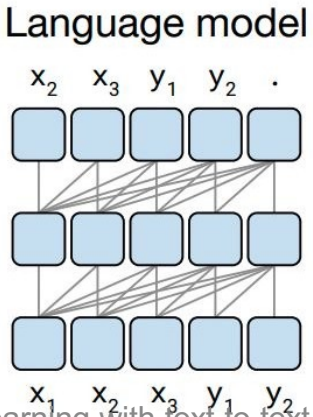
Language model is decoder-only



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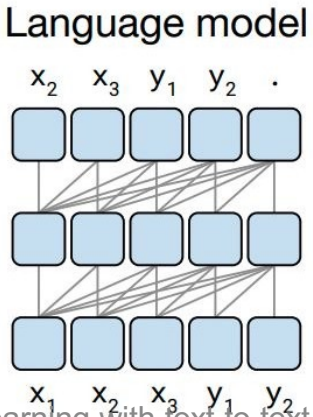
LM looks at both input and target, while encoder only looks at input sequence and decoder looks at output sequence.



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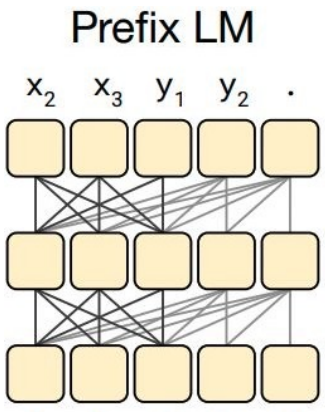

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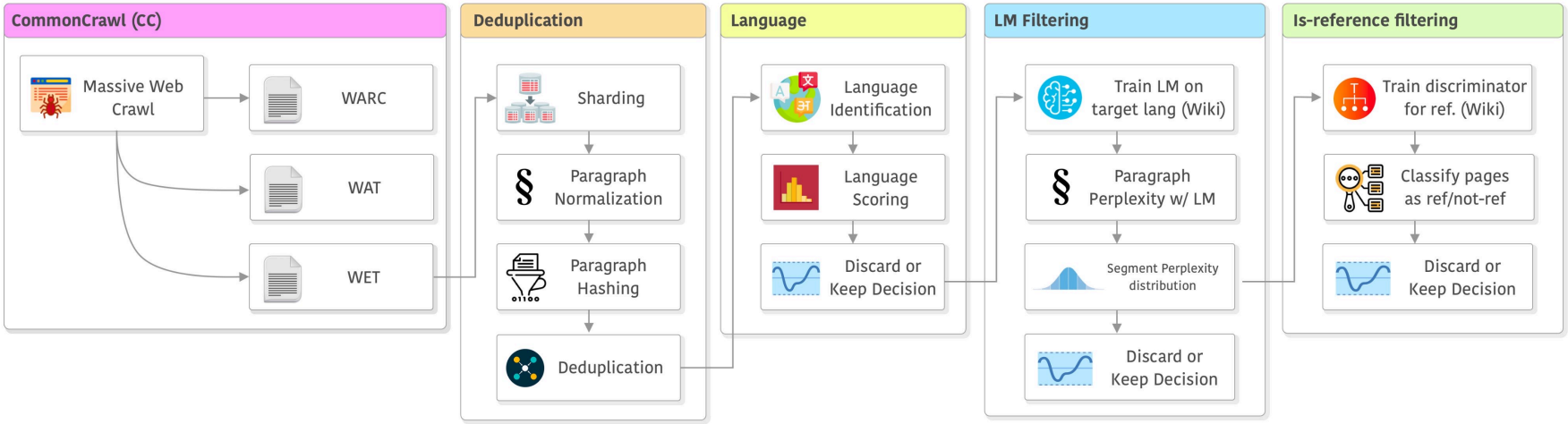
- Takeaways:
  - Halving the number of layers in encoder and decoder hurts the performance.
  - Performance of Encoder and Decoder with shared parameters is better than decoder only LM and prefix LM.

TODO: Elaborate the pipeline for dev of LMs

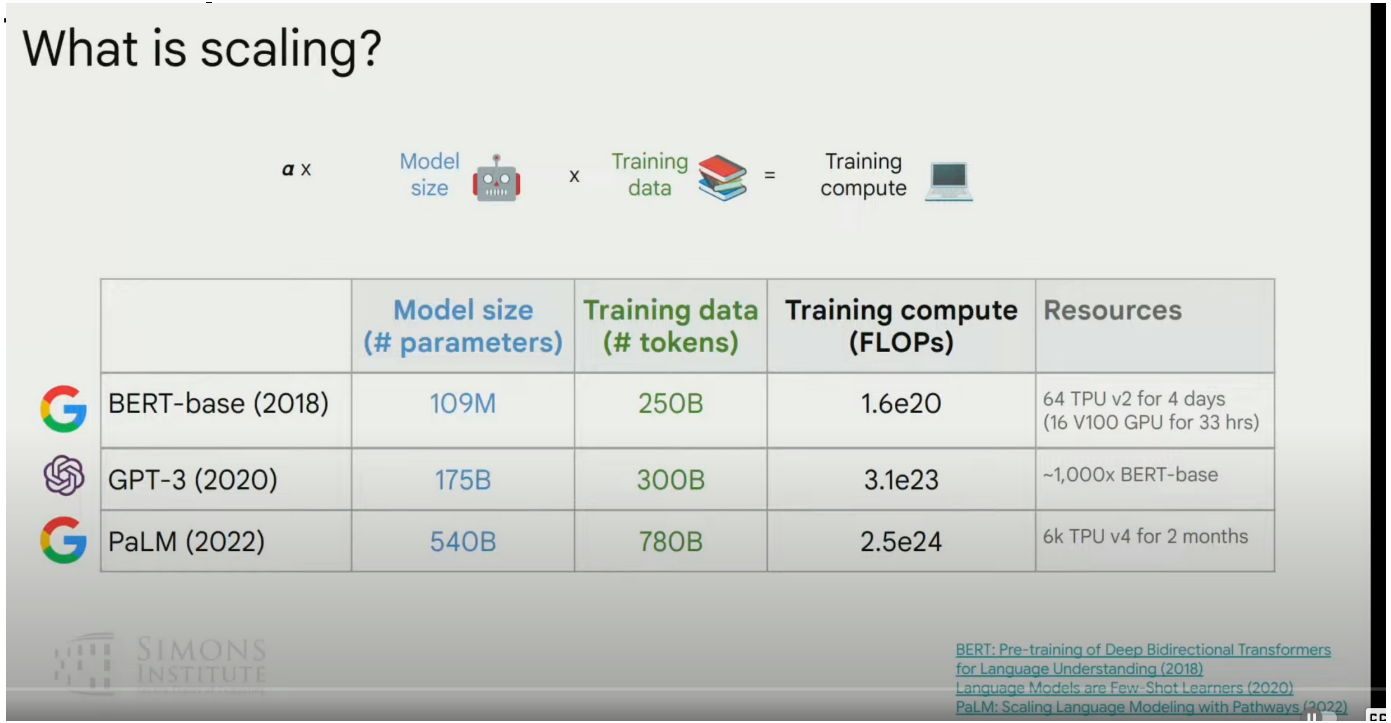


https://twitter.com/tarantulae/status/1650170087708454913?t=ncWWY0FI0tYC_dYLs76r5g&s=19

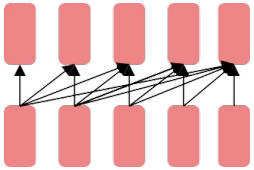
- Use the figures here to show the students how parameters are occupied in GPU memory during inference: https://arxiv.org/pdf/2309.06180.pdf

- Also discuss, how to select the batch size in GPUs.

Move i

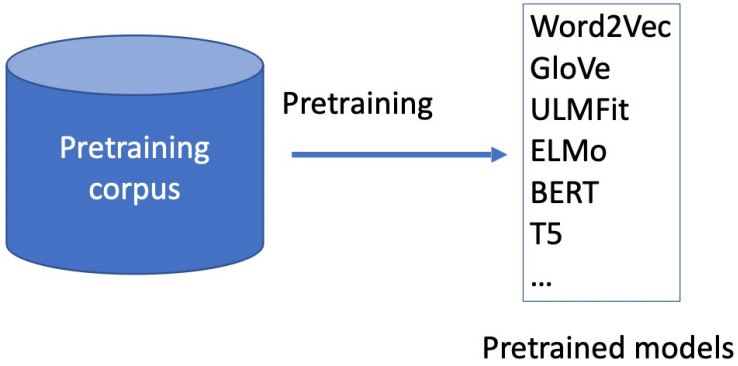


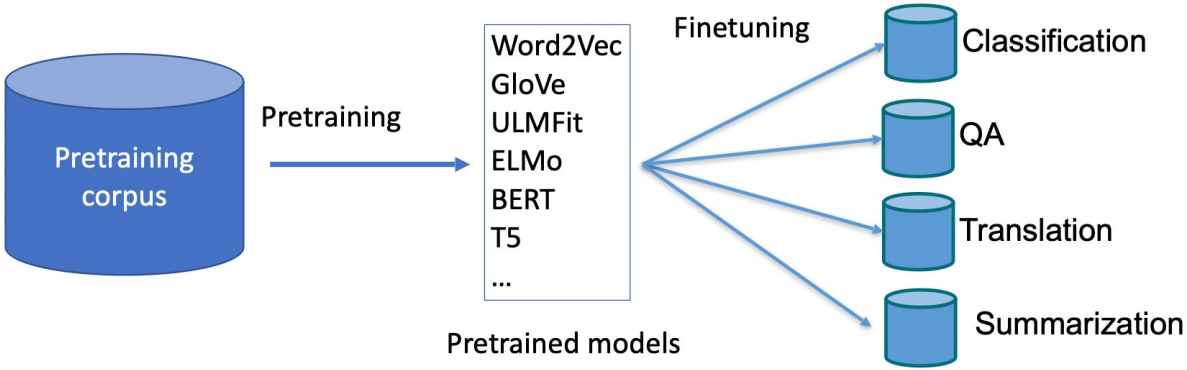
https://www.youtube.com/watch?v=Kp5R6GZh8O0&ab_channel=SimonsInstitute



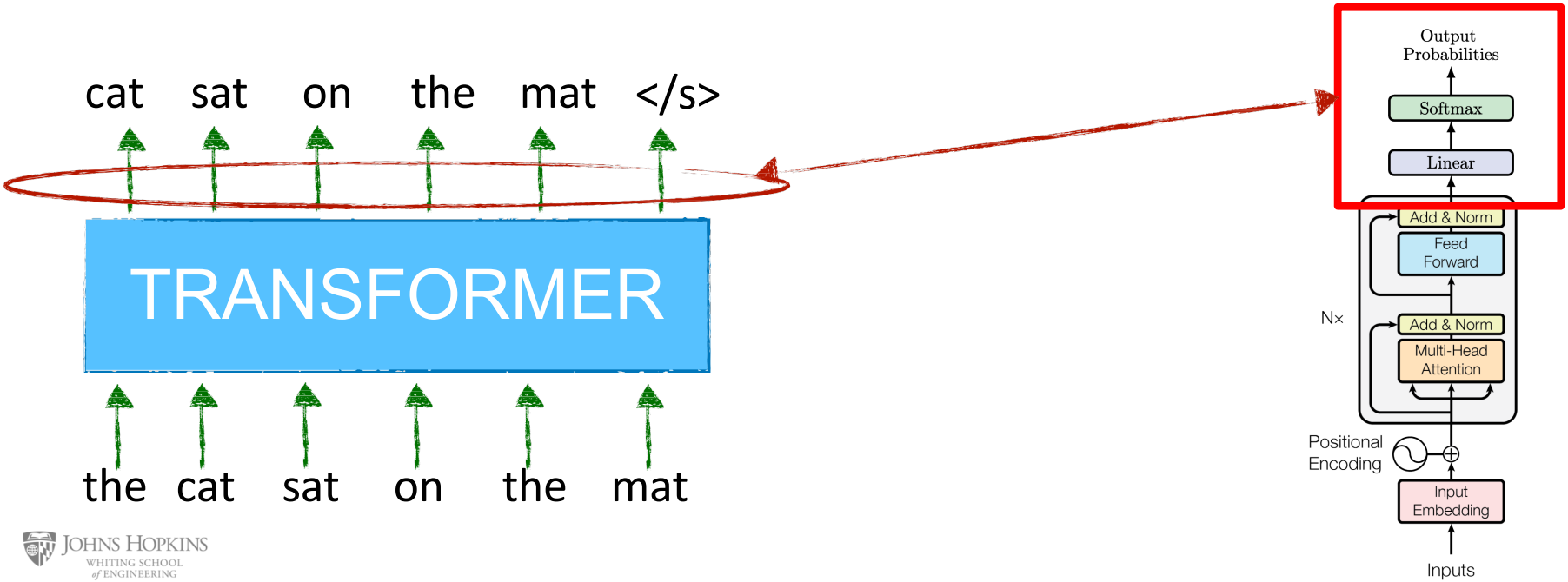
Decoders

Adapting LLMs


Pretraining corpus
Pretraining
Word2Vec
GloVe
ULMFit
ELMo
BERT
T5
...
Pretrained models


Pretraining corpus
Pretraining
Word2Vec
GloVe
ULMFit
ELMo
BERT
T5
...
Pretrained models
Finetuning
Classification
QA
Translation
Summarization

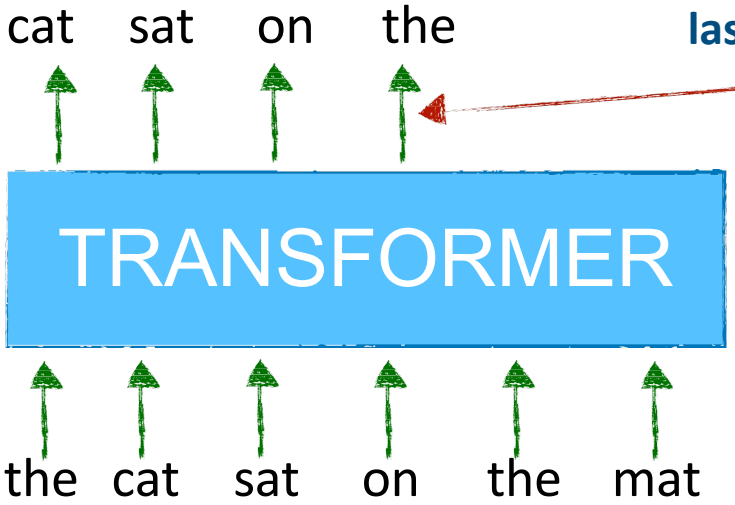
How to train models on language modeling?

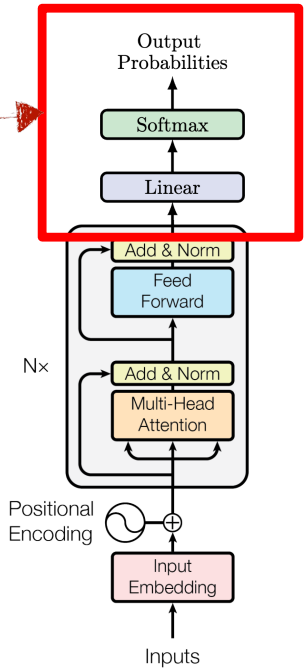


How to train models on language modeling?

One mini optimization

Instead of passing all outputs to the final linear layer, just pass the last word





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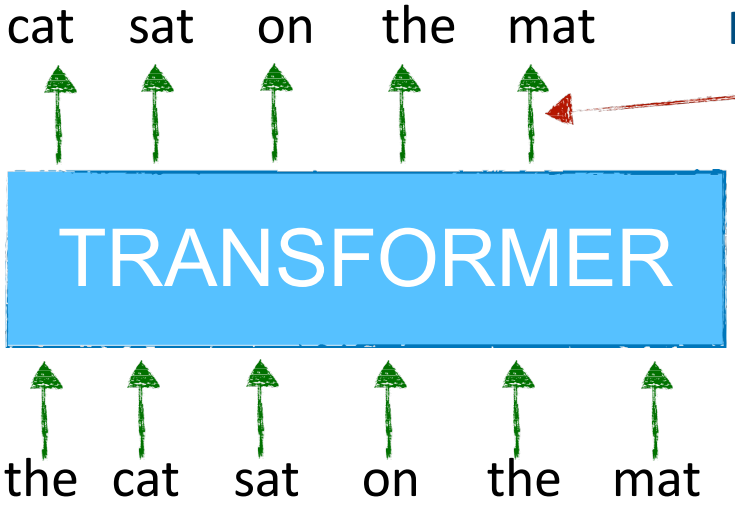
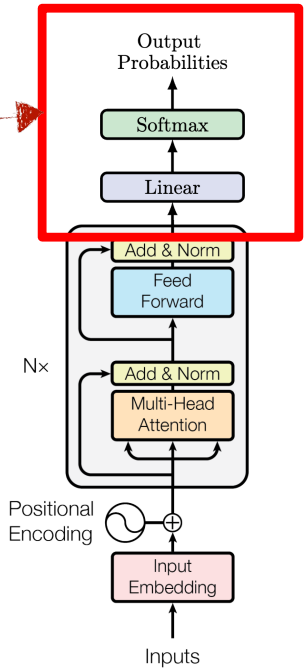
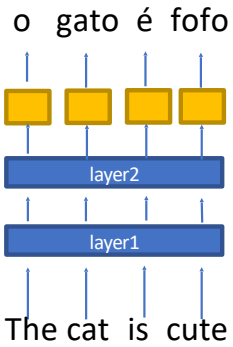


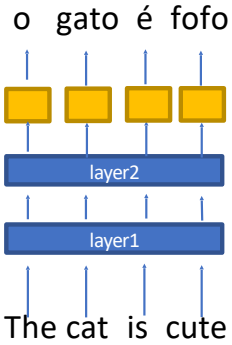


How to use a transformer for NLP tasks

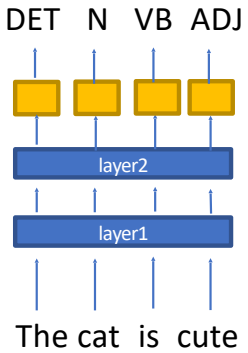


Translation

How to use a transformer for NLP tasks

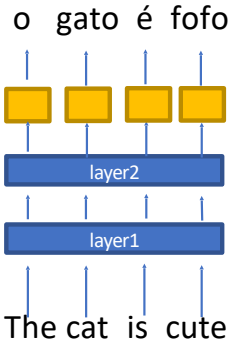


Translation

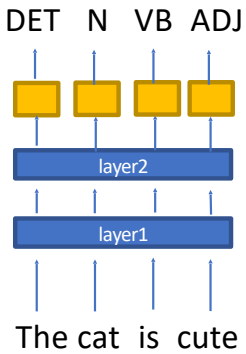


POS Tagging

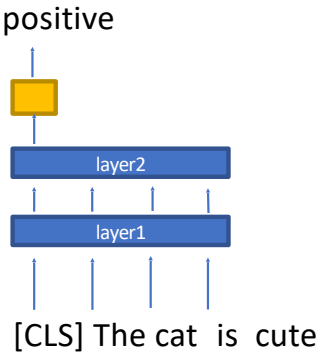
How to use a transformer for NLP tasks



Translation

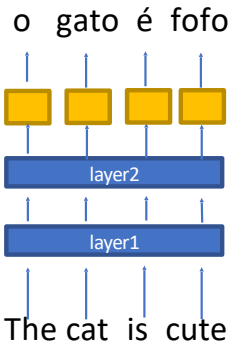


POS Tagging

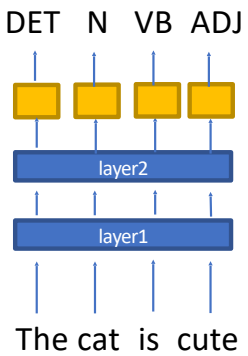


Text classification

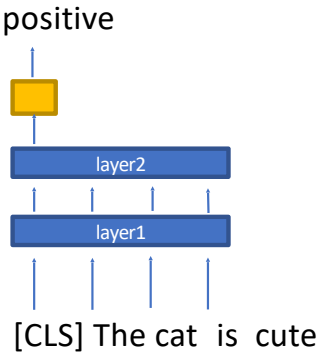
How to use a transformer for NLP tasks



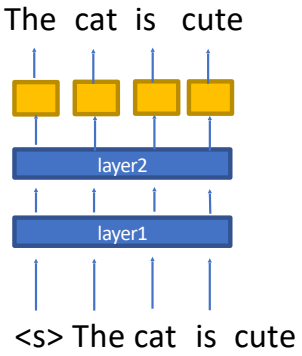
Translation



POS Tagging



Text classification



Language modeling

TODO

- Worth adding a short chapter on: how models resolve conflicts between their parameters and context?
  - 2310.15910.pdf (arxiv.org)
  - Orion has a paper
  - Eunsol has multiple papers too

- On Transformers: [lec15 (princeton-nlp.github.io)]