WEB INTELLIGENCE

Lecture 9: Transformers

Russa Biswas

November 11, 2025

AALBORG UNIVERSITY

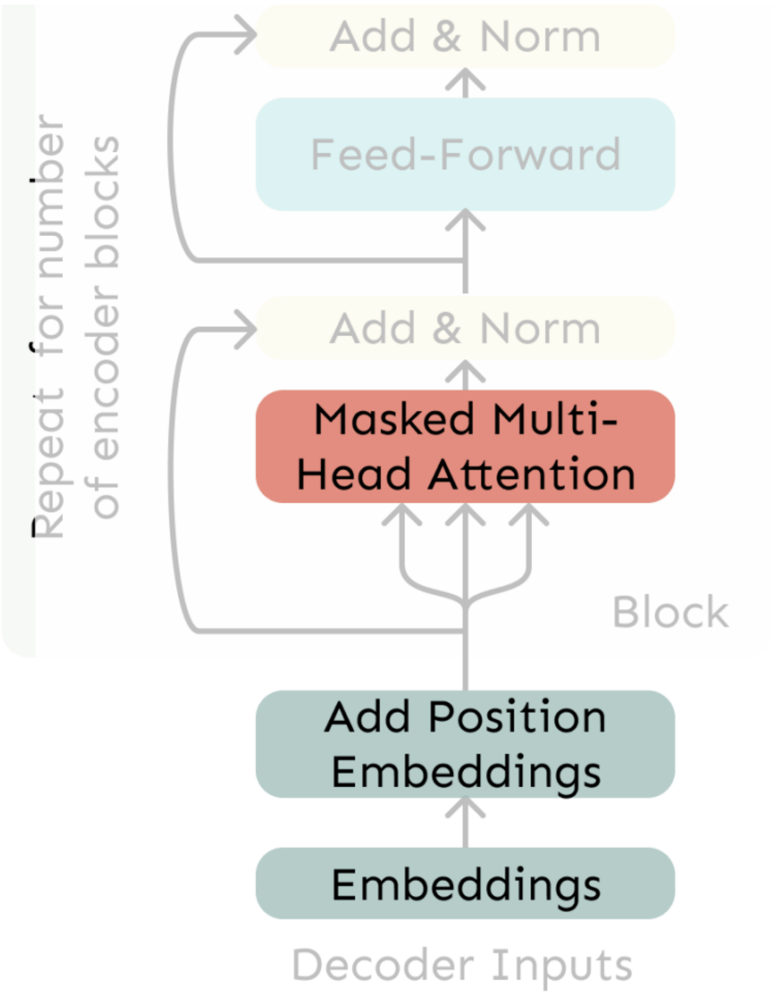
Based on Slides by Anna Goldie, John Hewitt, Stanford CS

Recap Self Attention

- https://www.menti.com/alxvwmmu2vhd

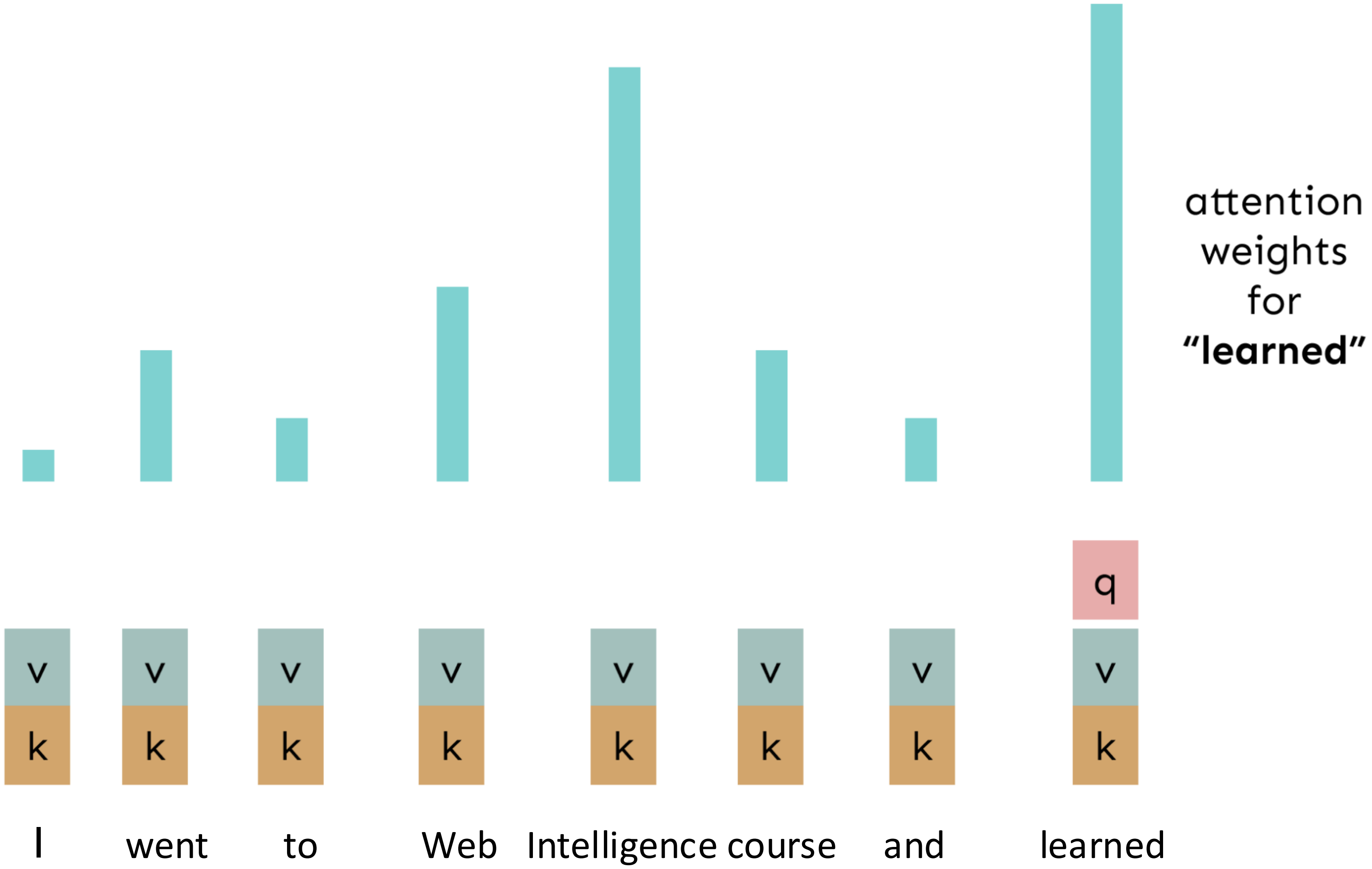
The Transformer Decoder

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



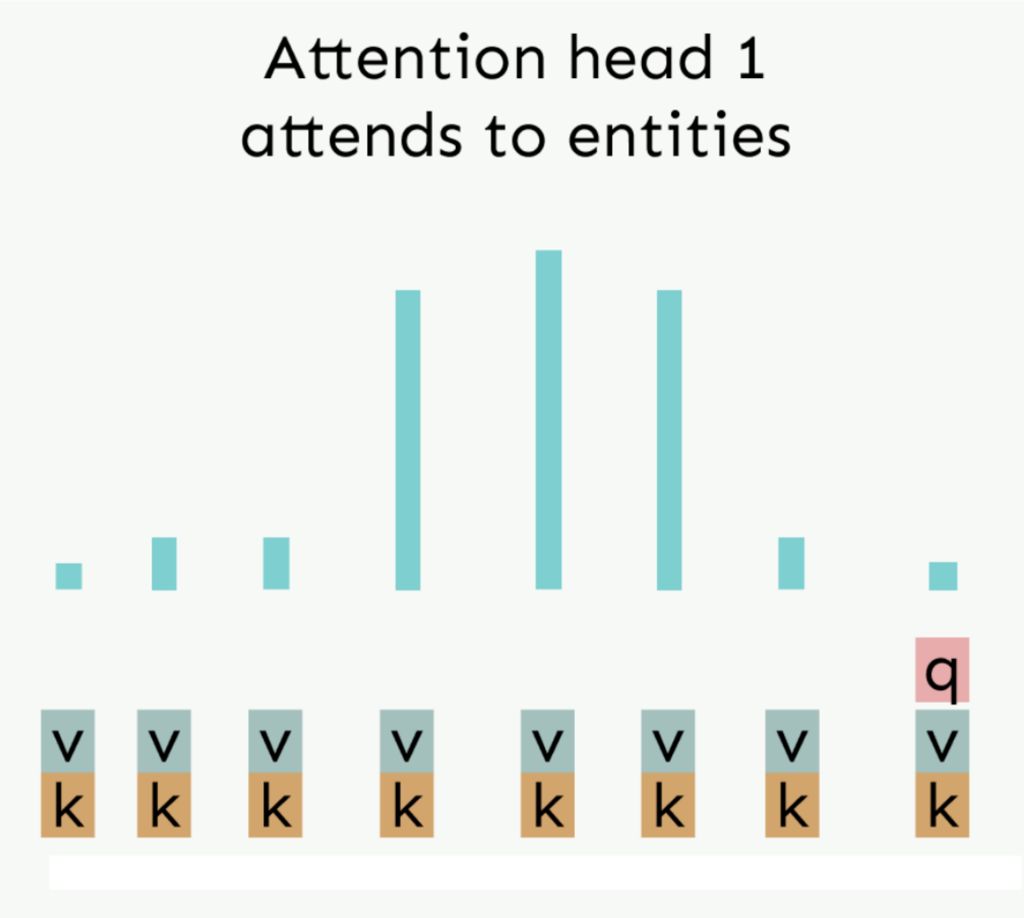
Transformer Decoder

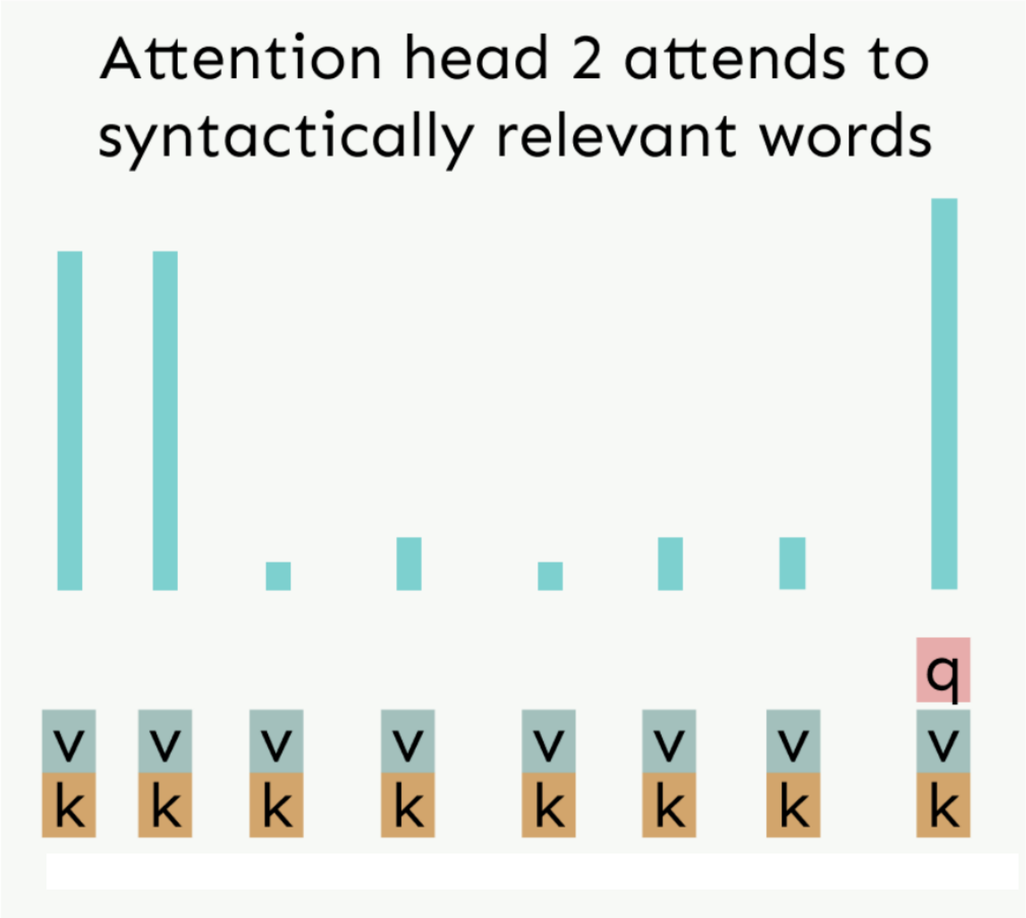
Example



attention weights for **“learned”**
q
v v v v v v v v
k k k k k k k k
I went to Web Intelligence course and learned

Example





I went to Web Intelligence course and learned

Scaled Dot Product

- **"Scaled Dot Product"** attention aids in training.
- When dimensionality d becomes large, dot products between vectors tend to become large.
  - Because of this, inputs to the softmax function can be large, making the gradients small.
- Instead of the self-attention function we've seen:

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

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

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

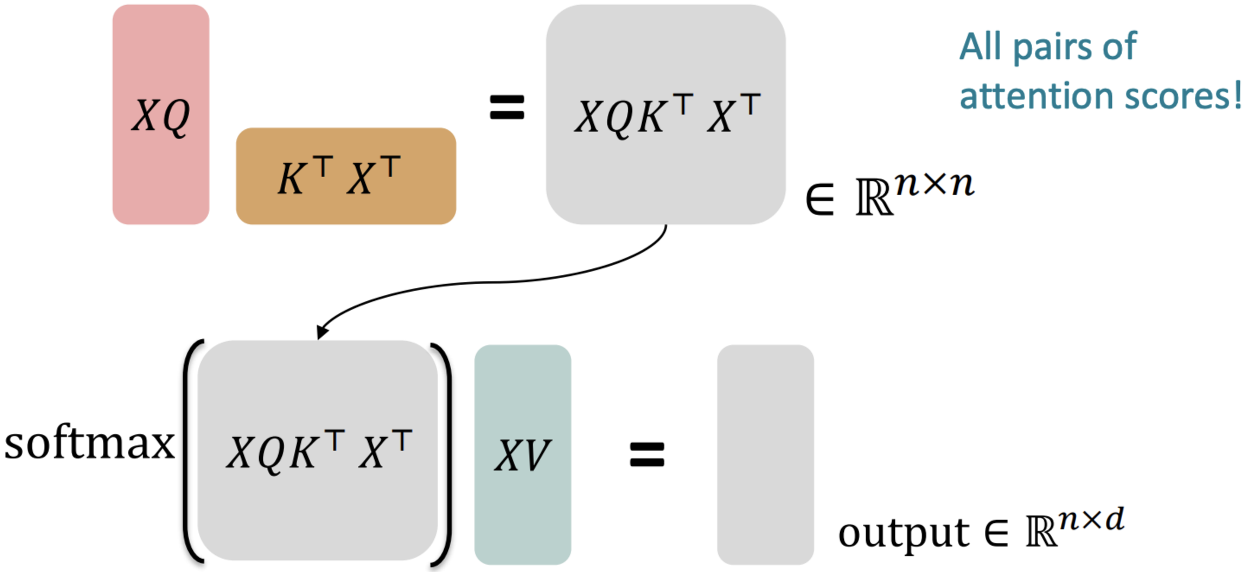
https://arxiv.org/abs/1706.03762

Sequence stacked form of Attention

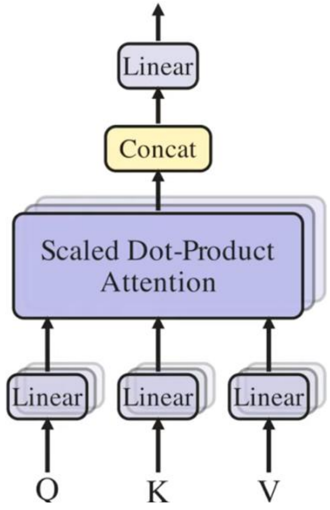
- Let's look at how key-query-value attention is computed, in matrices.
  - Let $X = [x_1; \ldots ; x_n] \in \mathbb{R}^{n \times d}$ be the concatenation of input vectors.
  - First, note that $XK \in \mathbb{R}^{n \times d}$, $XQ \in \mathbb{R}^{n \times d}$, $XV \in \mathbb{R}^{n \times d}$.
  - The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

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

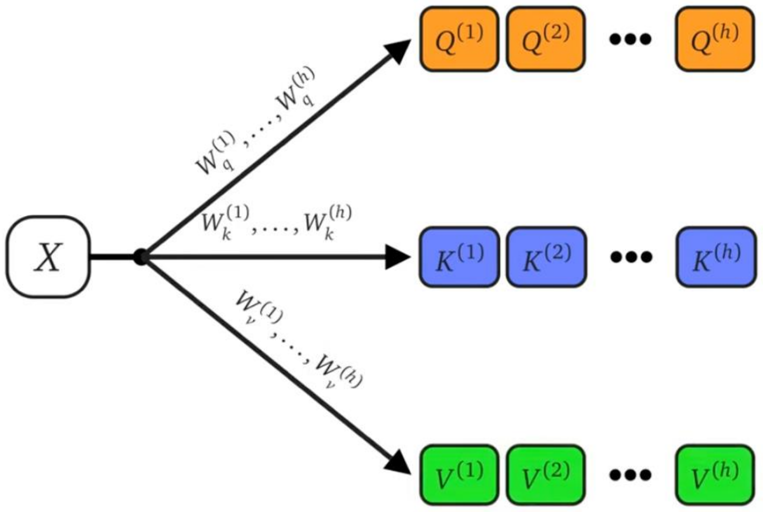
Next, softmax, and compute the weighted average with another matrix multiplication.

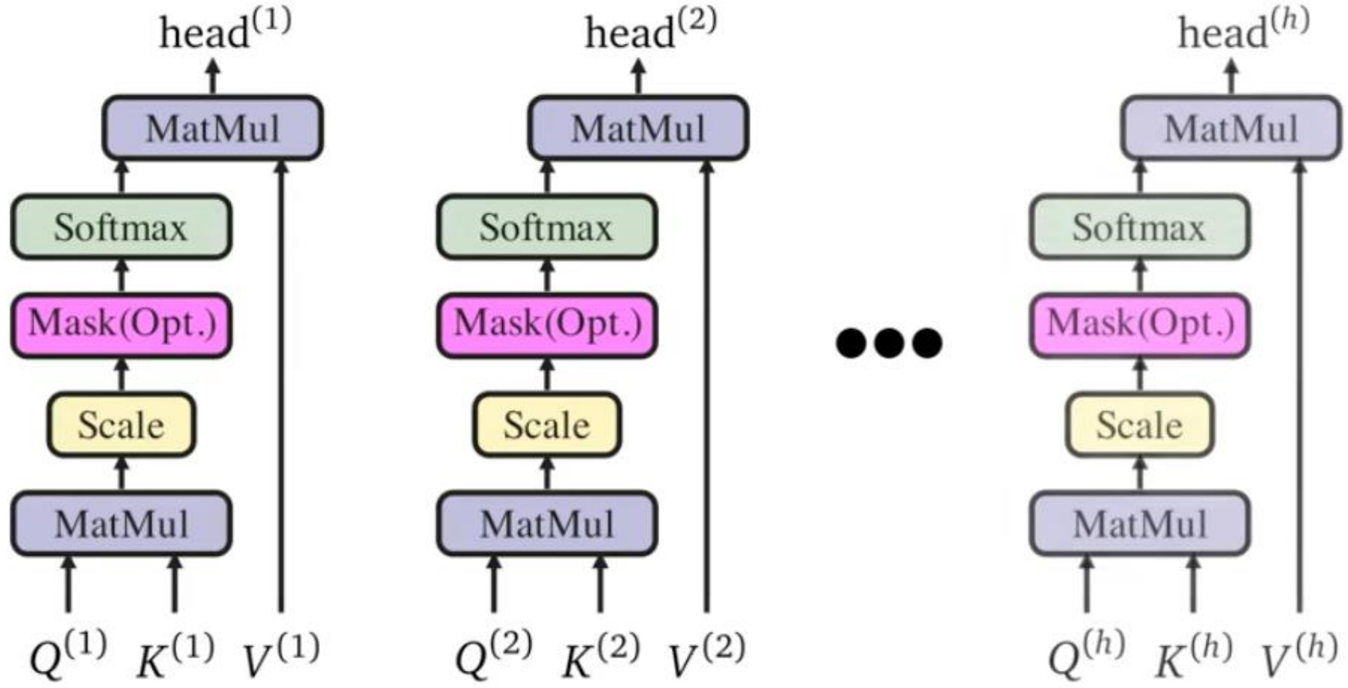


Multi-head Attention



h: number of heads





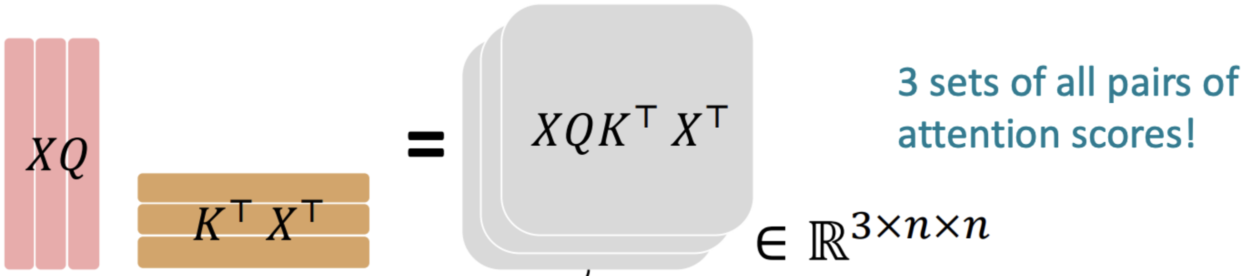
Multi-headed Attention

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

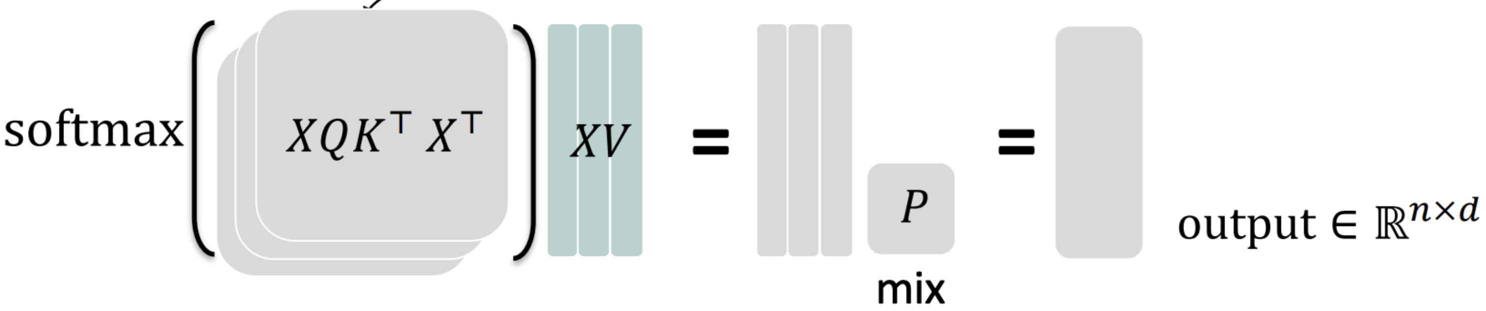
Multi-headed Self Attention

- Even though we compute h many attention heads, it's not really more costly.
  - We compute $XQ \in \mathbb{R}^{n \times d}$, and then reshape to $\mathbb{R}^{n \times h \times d/h}$. (Likewise for XK, XV.)
  - Then we transpose to $\mathbb{R}^{h \times n \times d/h}$; now the head axis is like a batch axis.
  - Almost everything else is identical, and the **matrices are the same sizes.**

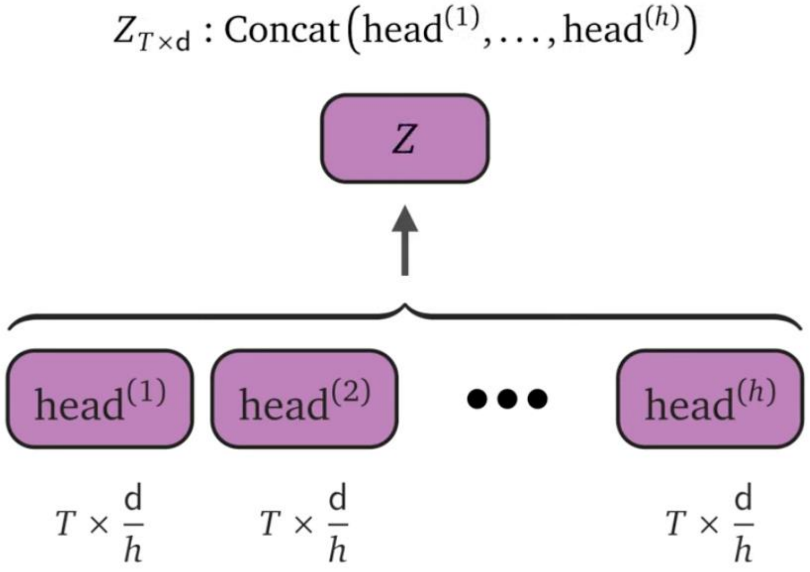
First, take the query-key dot products in one matrix multiplication: $XQ(XK)^{\top}$



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



Multihead Attention



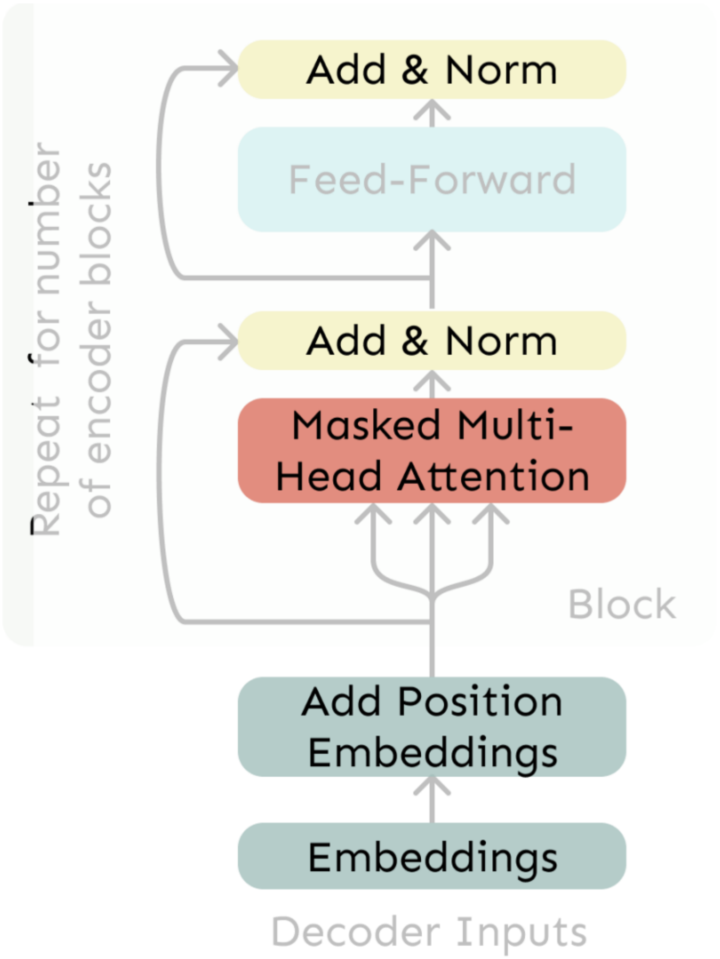
$$\text{MultiHead}(Q, K, V) = Z \times W^O$$

$$Z_{T \times \mathrm{d}} : \text{Concat}\left(\text{head}^{(1)}, \ldots, \text{head}^{(h)}\right)$$

$$W^O{}_{\mathrm{d} \times \mathrm{d}_{\text{model}}} : \text{Learnable weights}$$

Transformer Decoder

- Now that we've replaced self-attention with multi-head self-attention, we'll go through two **optimization tricks** that end up being :
  - **Residual Connections**
  - **Layer Normalization**
- In most Transformer diagrams, these are often written together as "Add & Norm"



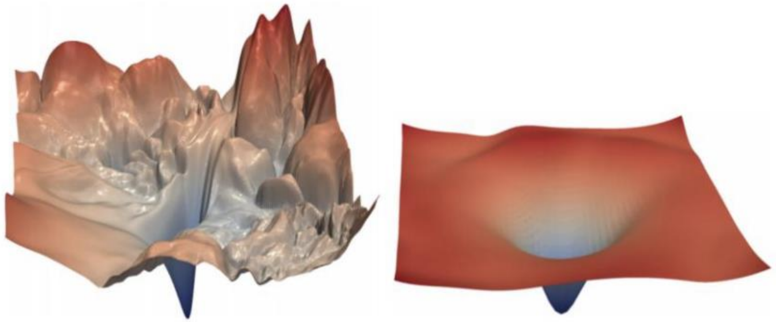
Transformer Decoder

Residual Connections – Transformer Encoder

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

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

  - Gradient is **great** through the residual connection; it's 1!
  - Bias towards the identity function!



[no residuals] [residuals]

[Loss landscape visualization, Li et al., 2018, on a ResNet]

Layer Normalisation – Transformer Encoder

- **Layer normalization** is a trick to help models train faster.
- Idea: cut down on uninformative variation in hidden vector values by normalizing to unit mean and standard deviation **within each layer**.
  - LayerNorm's success may be due to its normalizing gradients
- Let $x \in \mathbb{R}^d$ be an individual (word) vector in the model.
- Let $\mu = \sum_{j=1}^{d} x_j$; this is the mean; $\mu \in \mathbb{R}$.
- Let $\sigma = \sqrt{\frac{1}{d} \sum_{j=1}^{d} \left(x_j - \mu\right)^2}$; this is the standard deviation; $\sigma \in \mathbb{R}$.
- Let $\gamma \in \mathbb{R}^d$ and $\beta \in \mathbb{R}^d$ be learned "gain" and "bias" parameters. (Can omit!)
- Then layer normalization computes:

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

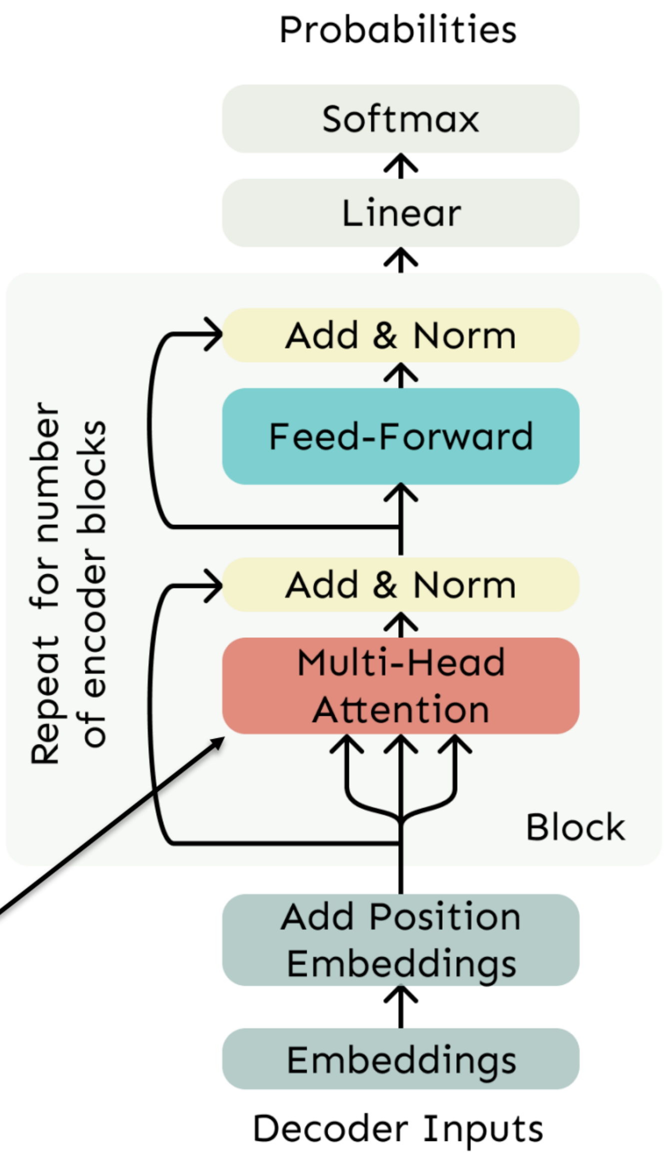
Normalize by scalar mean and variance

Modulate by learned elementwise gain and bias

Transformer Encoder

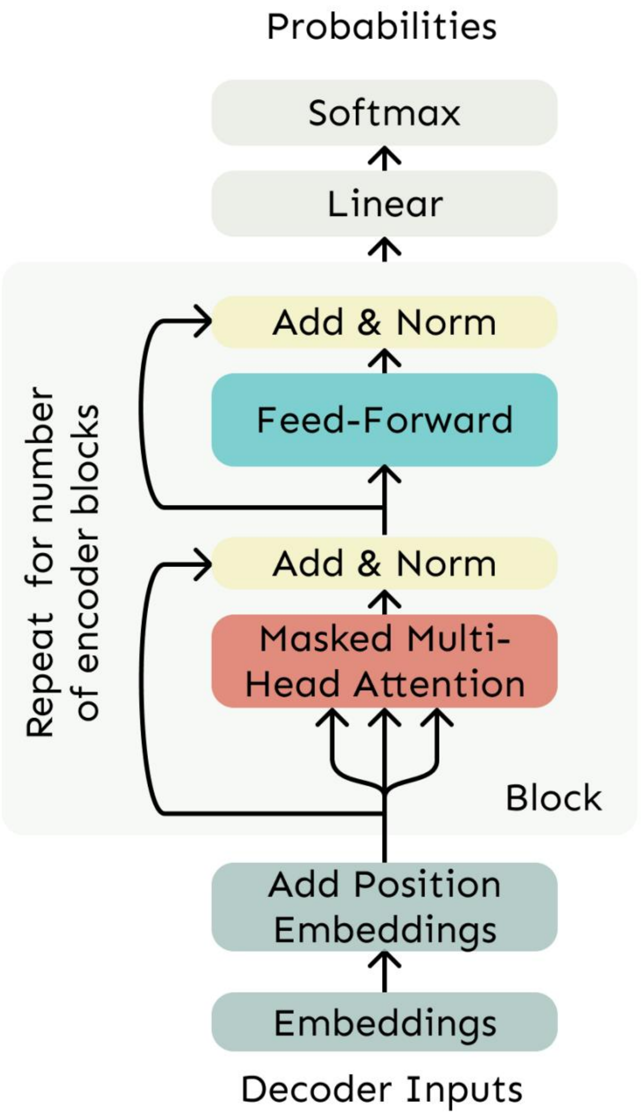
- The Transformer Decoder constrains to **unidirectional context**, as for **language models.**
- What if we want **bidirectional context**, like in a bidirectional RNN?
- This is the Transformer Encoder. The only difference is that we **remove the masking** in the self-attention.

No Masking!



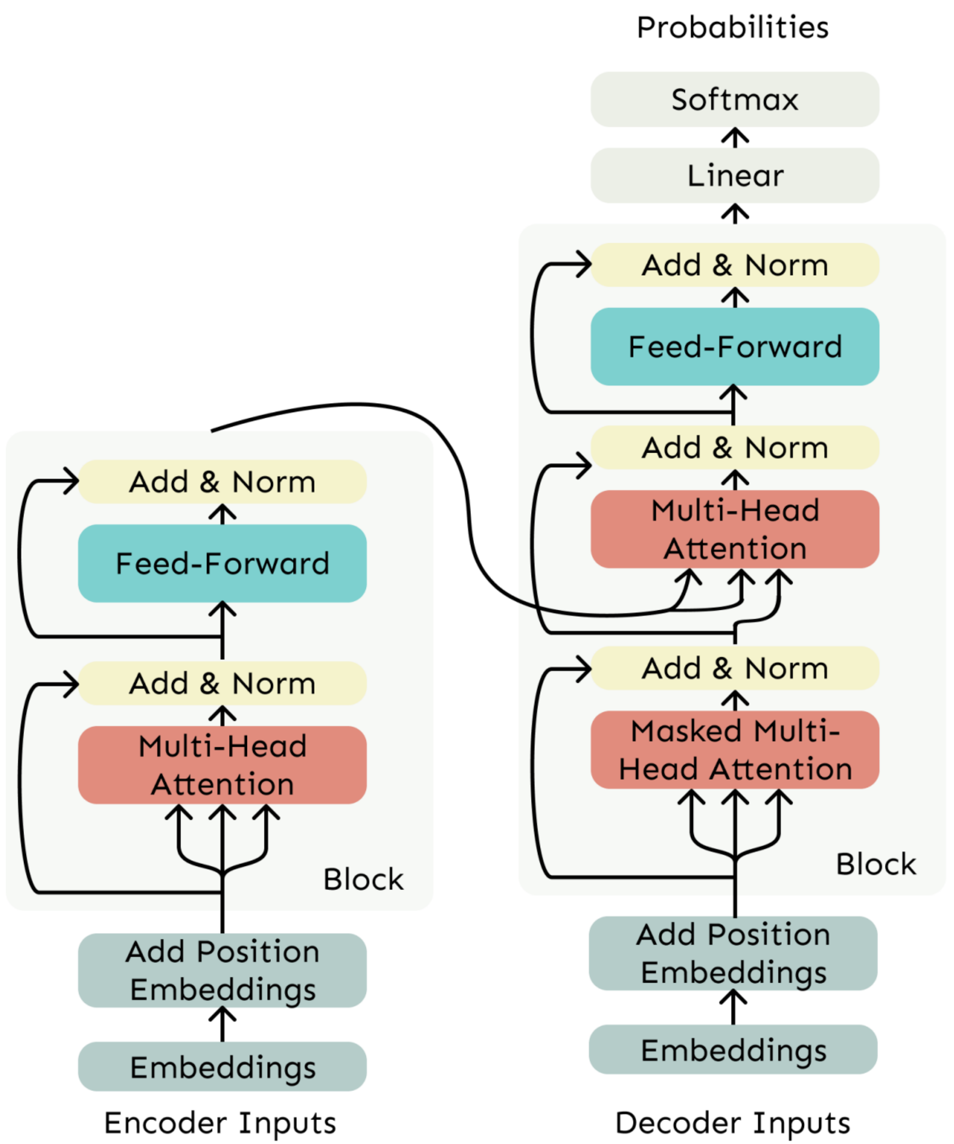
Transformer Decoder

- The Transformer Decoder is a stack of Transformer Decoder **Blocks**.
- Each Block consists of:
  - Self-attention
  - Add & Norm
  - Feed-Forward
  - Add & Norm
- That's it! We've gone through the Transformer Decoder.

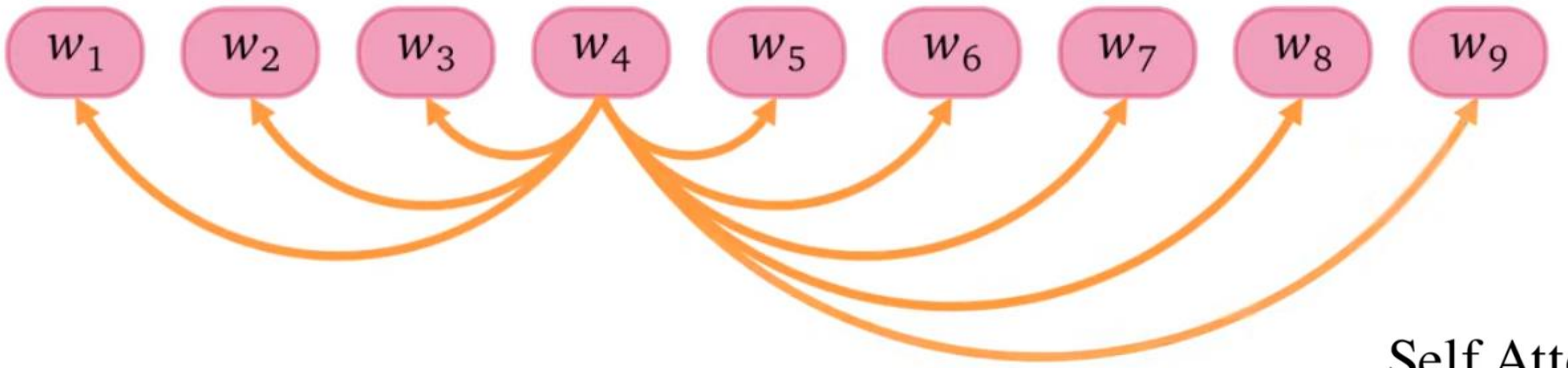


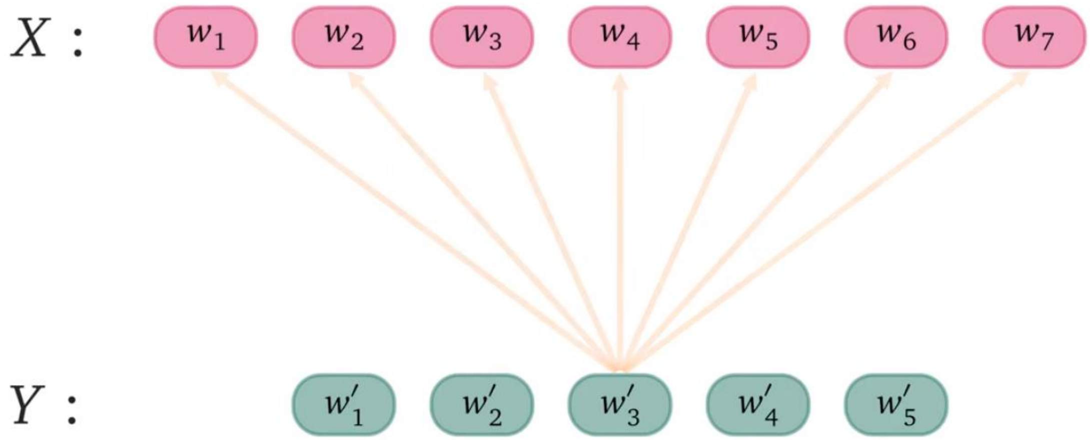
Transformer Encoder - Decoder

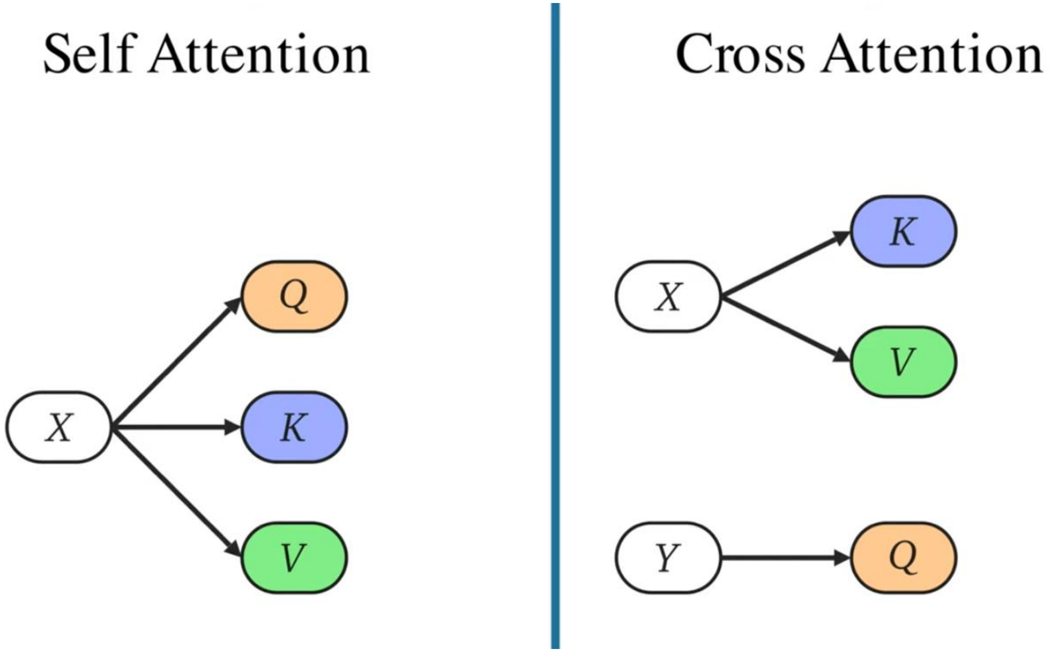
- Recall that in machine translation, we processed the source sentence with a **bidirectional** model and generated the target with a **unidirectional model**.
- For this kind of seq2seq format, we often use a Transformer Encoder-Decoder.
- We use a normal Transformer Encoder.
- Our Transformer Decoder is modified to perform **cross-attention** to the output of the Encoder.



Self vs Cross Attention

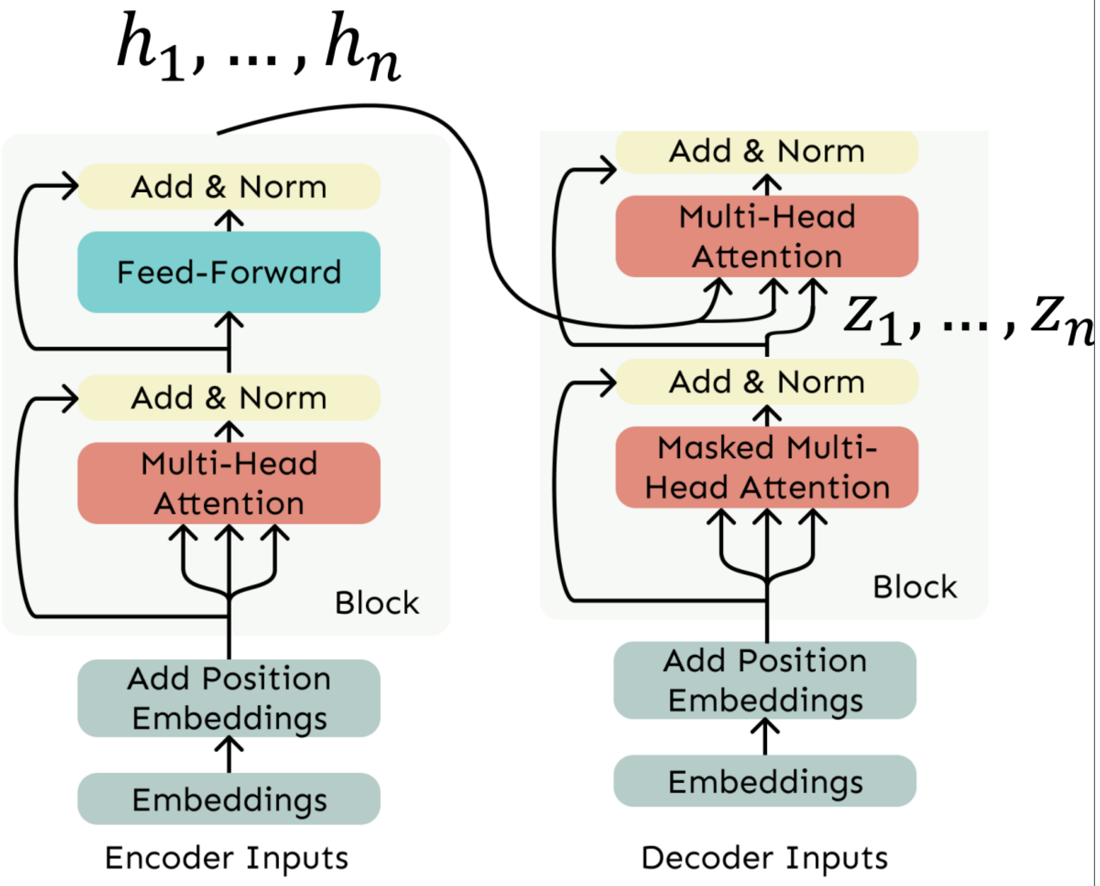






Cross Attention

- We saw that self-attention is when keys, queries, and values come from the same source.
- In the decoder, we have attention that looks more like what we saw last week.
- Let $h_1, \ldots, h_n$ be **output** vectors **from** the Transformer **encoder**; $x_i \in \mathbb{R}^d$
- Let $z_1, \ldots, z_n$ be input vectors from the Transformer **decoder**, $z_i \in \mathbb{R}^d$
- Then keys and values are drawn from the **encoder** (like a memory):
  - $k_i = K h_i, v_i = V h_i$.
- And the queries are drawn from the **decoder**, $q_i = Q z_i$.



Drawbacks

Quadratic computation as a function of sequence length

- One of the benefits of self-attention over recurrence was that it's highly parallelizable.
- However, its total number of operations grows as $O(n^2 d)$, where n is the sequence length, and d is the dimensionality.

$$XQ \; K^\top X^\top = XQK^\top X^\top \in \mathbb{R}^{n \times n}$$

Need to compute all pairs of interactions! $O(n^2 d)$

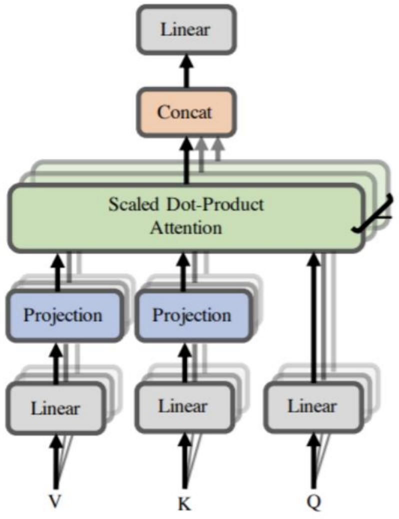
- Think of d as around $\mathbf{1,000}$ (though for large language models it's much larger!).
  - So, for a single (shortish) sentence, $n \leq 30$; $n^2 \leq \mathbf{900}$**.**
  - In practice, we set a bound like $n = 512$.
  - **But what if we'd like $\boldsymbol{n} \geq \mathbf{50,000}$?** For example, to work on long documents?

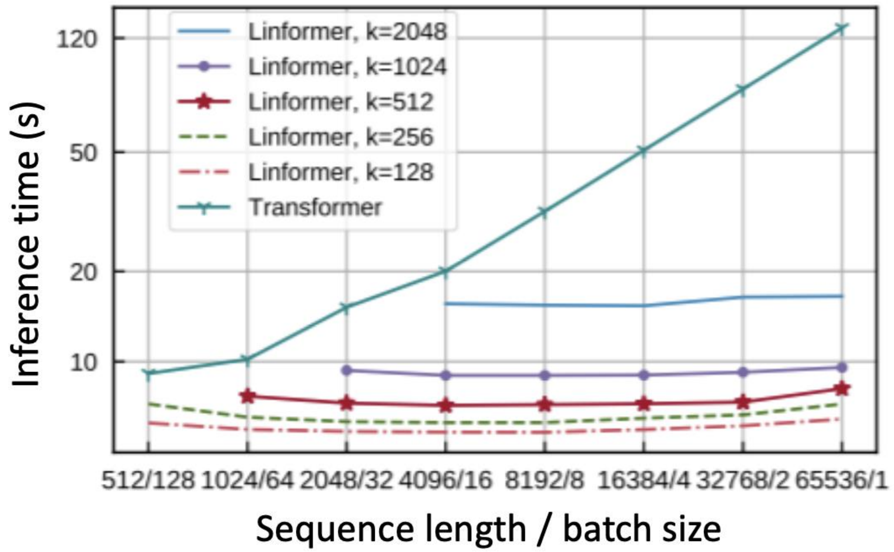
Drawbacks

Work on improving on quadratic self-attention cost

- Considerable recent work has gone into the question, *Can we build models like Transformers without paying the $O(T^2)$ all-pairs self-attention cost?*
- For example, **Linformer** [Wang et al., 2020]

Key idea: map the sequence length dimension to a lower-dimensional space for values, keys





Drawbacks

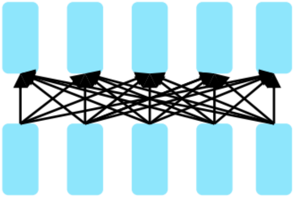
Do we even need to remove the quadratic cost of attention?

- As Transformers grow larger, a larger and larger percent of compute is **outside** the self-attention portion, despit the quadratic cost.
- In practice, **almost no large Transformer language models use anything but the quadratic cost attention we've presented here.**
  - The cheaper methods tend not to work as well at scale.
- So, is there no point in trying to design cheaper alternatives to self-attention?
- Or would we unlock much better models with much longer contexts (>100k tokens?) if we were to do it right?

Pretraining Models

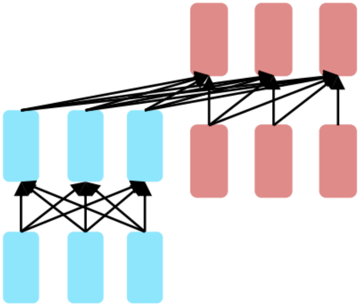
Pretraining for three types of architectures

The neural architecture influences the type of pretraining, and natural use cases.



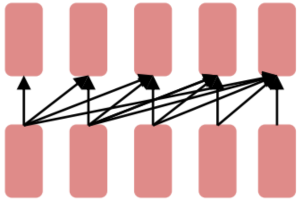
Encoders

- Gets bidirectional context – can condition on future!
- How do we train them to build strong representations?



Encoder-Decoders

- Good parts of decoders and encoders?
- What's the best way to pretrain them?



Decoders

- Language models! What we've seen so far.
- Nice to generate from; can't condition on future words

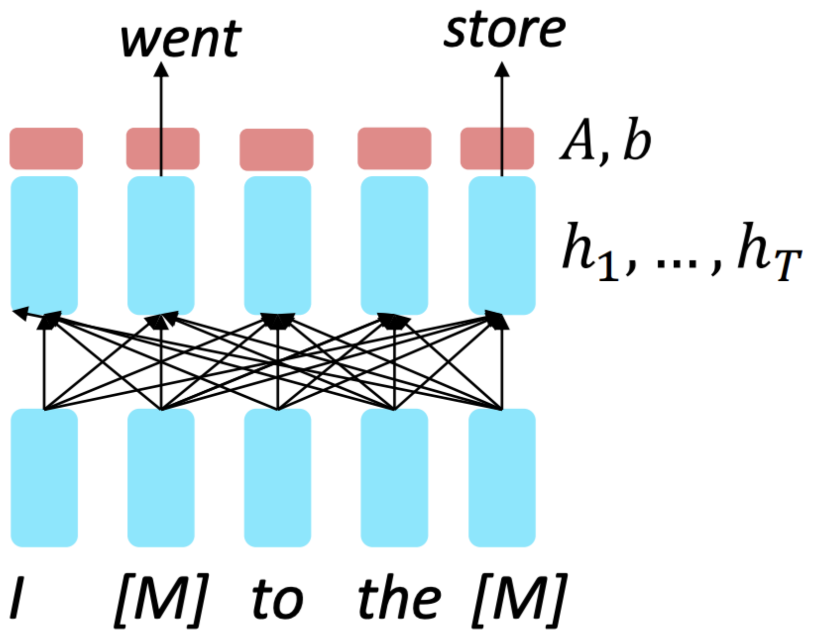
Pretraining Encoders

So far, we've looked at language model pretraining. But **encoders get bidirectional context,** so we can't do language modeling!

Idea: replace some fraction of words in the input with a special [MASK] token; predict these words.

$$h_1, \ldots, h_T = \text{Encoder}(w_1, \ldots, w_T)$$
$$y_i \sim Aw_i + b$$

Only add loss terms from words that are "masked out." If $\tilde{x}$ is the masked version of x, we're learning $p_\theta(x|\tilde{x})$. Called **Masked LM.**



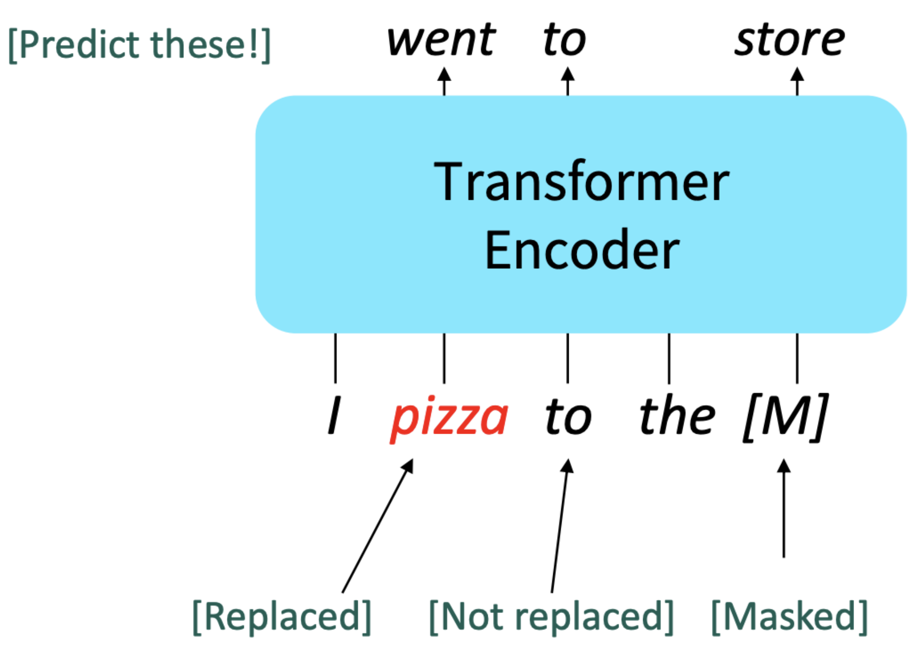
BERT

Bidirectional Encoder Representations from Transformers

Devlin et al., 2018 proposed the “Masked LM” objective and **released the weights of a pretrained Transformer**, a model they labeled BERT.

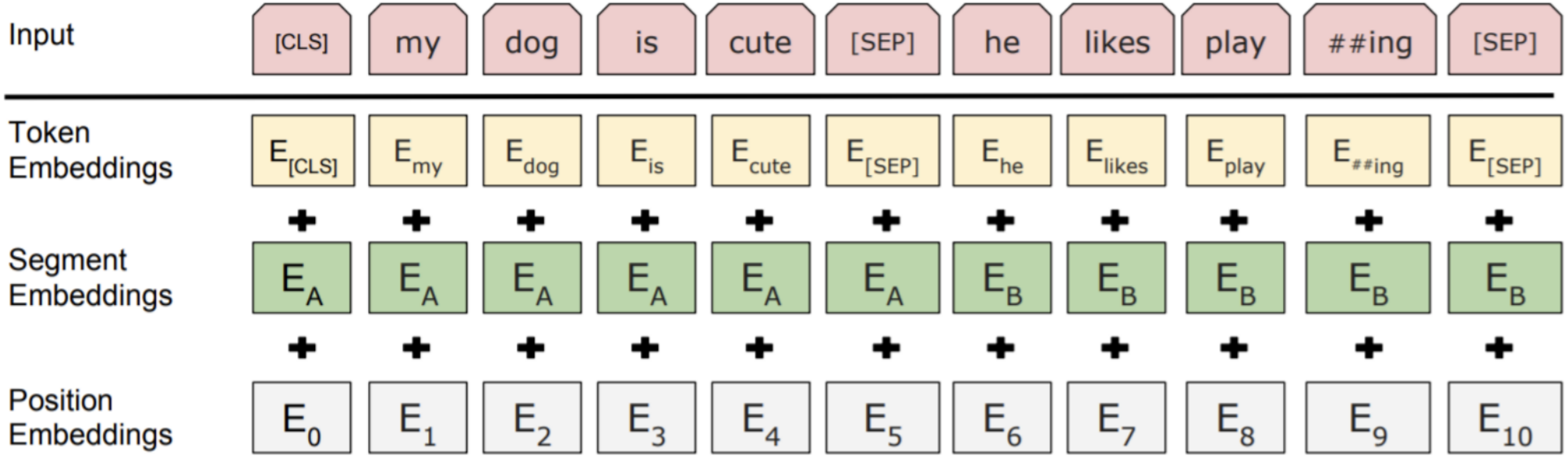
Some more details about Masked LM for BERT:

- Predict a random 15% of (sub)word tokens.
  - Replace input word with [MASK] 80% of the time
  - Replace input word with a random token 10% of the time
  - Leave input word unchanged 10% of the time (but still predict it!)
- Why? Doesn’t let the model get complacent and not build strong representations of non-masked words. (No masks are seen at fine-tuning time!)



BERT

- The pretraining input to BERT was two separate contiguous chunks of text:



- BERT was trained to predict whether one chunk follows the other or is randomly sampled.

BERT

Details about BERT

- Two models were released:
  - BERT-base: 12 layers, 768-dim hidden states, 12 attention heads, 110 million params.
  - BERT-large: 24 layers, 1024-dim hidden states, 16 attention heads, 340 million params.
- Trained on:
  - BooksCorpus (800 million words)
  - English Wikipedia (2,500 million words)
- Pretraining is expensive and impractical on a single GPU.
  - BERT was pretrained with 64 TPU chips for a total of 4 days.
  - (TPUs are special tensor operation acceleration hardware)
- Finetuning is practical and common on a single GPU
  - "Pretrain once, finetune many times."

BERT

BERT was massively popular and hugely versatile; finetuning BERT led to new state-of-the-art results on a broad range of tasks.

- **QQP:** Quora Question Pairs (detect paraphrase questions)
- **QNLI**: natural language inference over question answering data
- **SST-2**: sentiment analysis
- **CoLA**: corpus of linguistic acceptability (detect whether sentences are grammatical.)
- **STS-B**: semantic textual similarity
- **MRPC**: microsoft paraphrase corpus
- **RTE**: a small natural language inference corpus

System	MNLI-(m/mm)	QQP	QNLI	SST-2	CoLA	STS-B	MRPC	RTE	**Average**
	392k	363k	108k	67k	8.5k	5.7k	3.5k	2.5k	-
Pre-OpenAI SOTA	80.6/80.1	66.1	82.3	93.2	35.0	81.0	86.0	61.7	74.0
BiLSTM+ELMo+Attn	76.4/76.1	64.8	79.8	90.4	36.0	73.3	84.9	56.8	71.0
OpenAI GPT	82.1/81.4	70.3	87.4	91.3	45.4	80.0	82.3	56.0	75.1
$\text{BERT}_{\text{BASE}}$	84.6/83.4	71.2	90.5	93.5	52.1	85.8	88.9	66.4	79.6
$\text{BERT}_{\text{LARGE}}$	**86.7/85.9**	**72.1**	**92.7**	**94.9**	**60.5**	**86.5**	**89.3**	**70.1**	**82.1**

Literature

- https://web.stanford.edu/class/cs224n/readings/cs224n-self-attention-transformers-2023_draft.pdf
- https://arxiv.org/abs/1810.04805