Attention & Transformers

Ivo Verhoeven | Advanced Topics in Computational Semantics

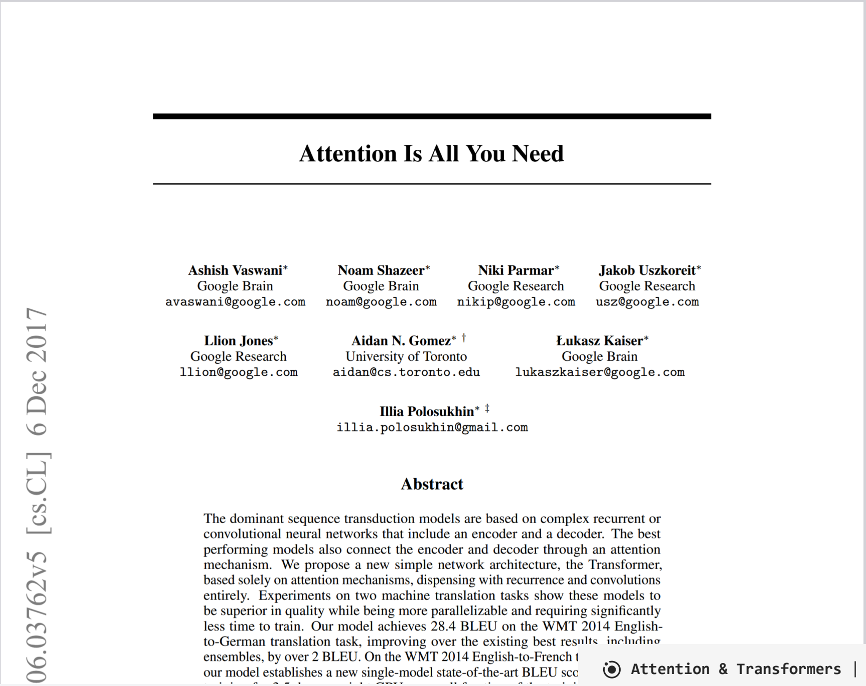
About Me

- 2017 - 2020: BSc. Liberal Arts & Sciences
- 2020 – 2022: MSc. AI at University of Amsterdam
  - Thesis on meta-learning, morphology and translation
  - Took ATCS in 2021
- 2022 - ???: PhD at ILLC
  - Misinformation detection and generalisation with Katia Shutova

Vaswani et al.: Attention is All You Need

- Introduces the Transformer architecture in late 2017
  - Google Brain/Google Research collab

`Vaswani et al. (2017). Attention is all you need. Advances in neural information processing systems, 30.`



06.03762v5 [cs.CL] 6 Dec 2017

Attention Is All You Need

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Abstract

The dominant sequence transduction models are based on complex recurrent or convolutional neural networks that include an encoder and a decoder. The best performing models also connect the encoder and decoder through an attention mechanism. We propose a new simple network architecture, the Transformer, based solely on attention mechanisms, dispensing with recurrence and convolutions entirely. Experiments on two machine translation tasks show these models to be superior in quality while being more parallelizable and requiring significantly less time to train. Our model achieves 28.4 BLEU on the WMT 2014 English-to-German translation task, improving over the existing best results, including ensembles, by over 2 BLEU. On the WMT 2014 English-to-French t our model establishes a new single-model state-of-the-art BLEU sco

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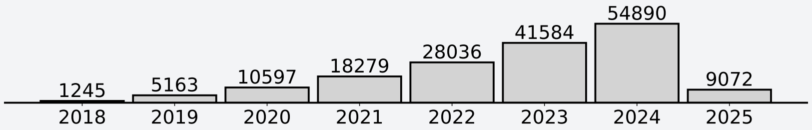

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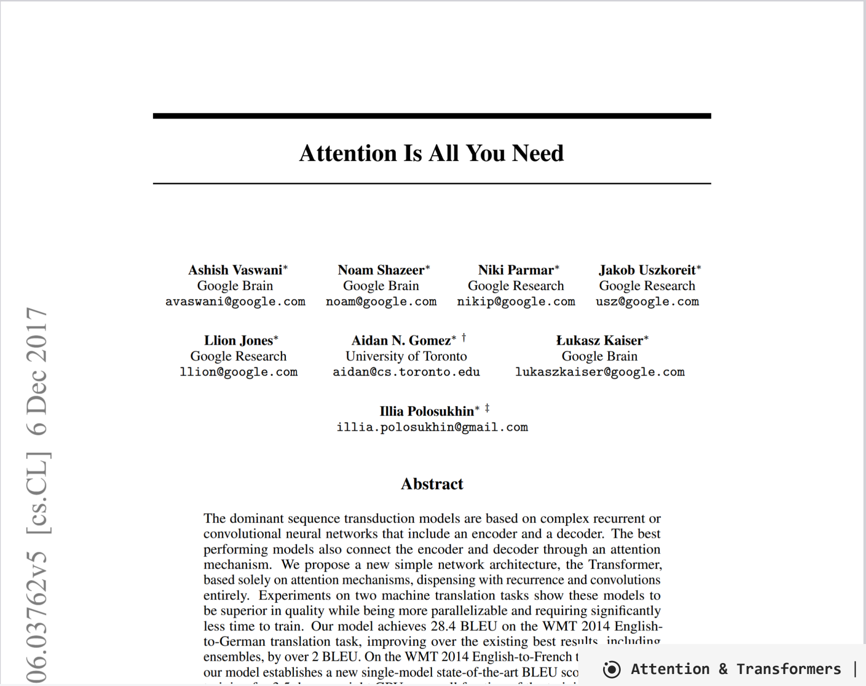

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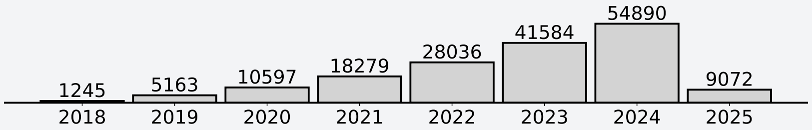

- Most cited paper ever has **233 829** citations

Lowry et al. (1951) Protein measurement with the folin phenol reagent.

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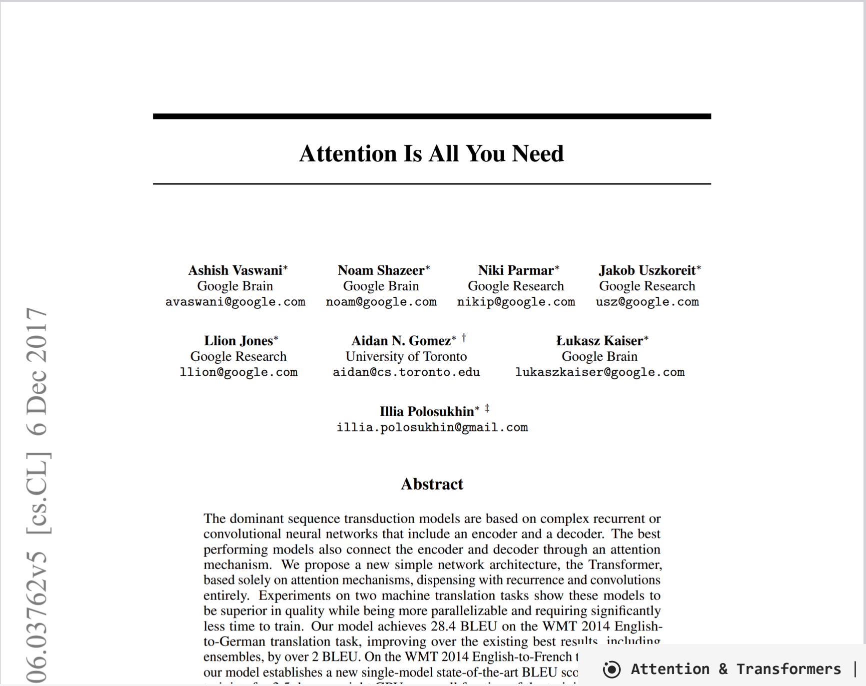

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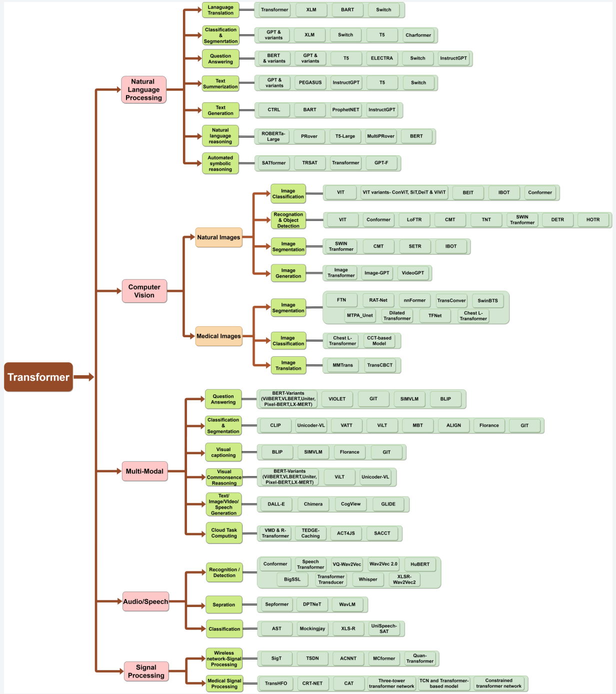

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    - Classification: encoder-only transformers
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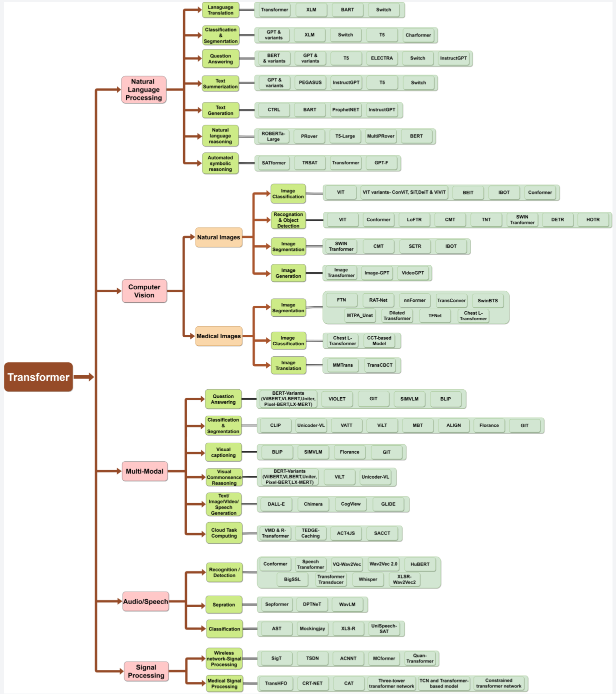

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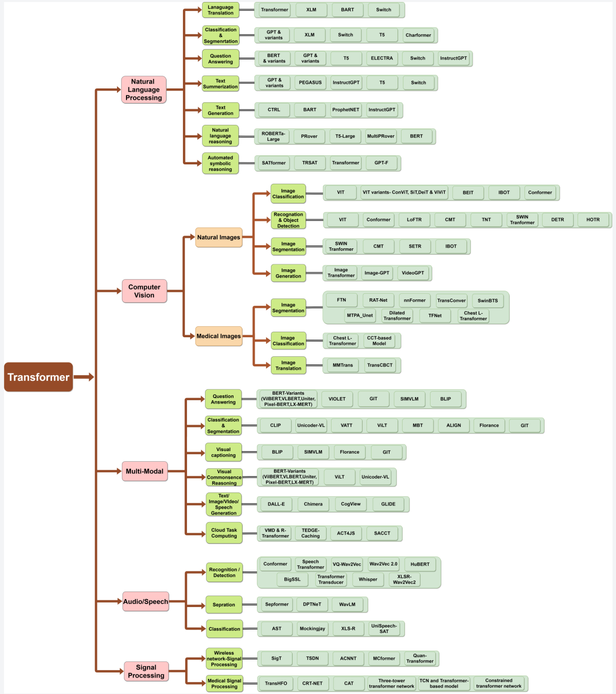
  - **CV:** ViT > CNN
  - **Multi-modal:** Transformer > different architectures
  - **Speech:** Transformer > CNN
  - **Graphs:** Transformer/Attention > GCN



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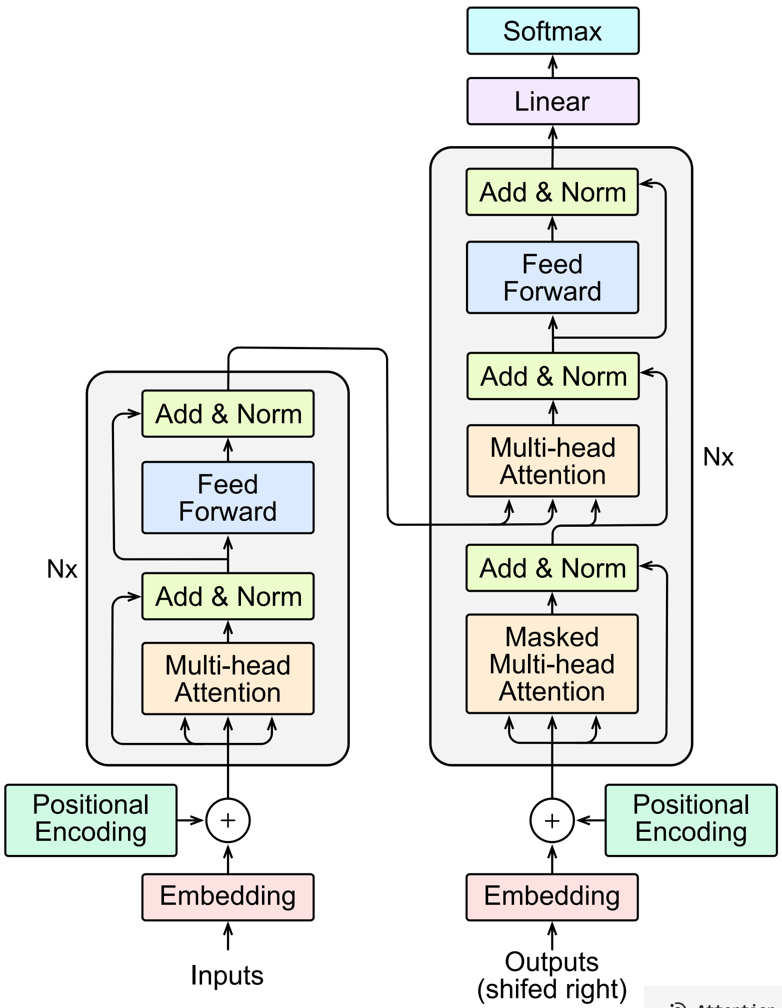
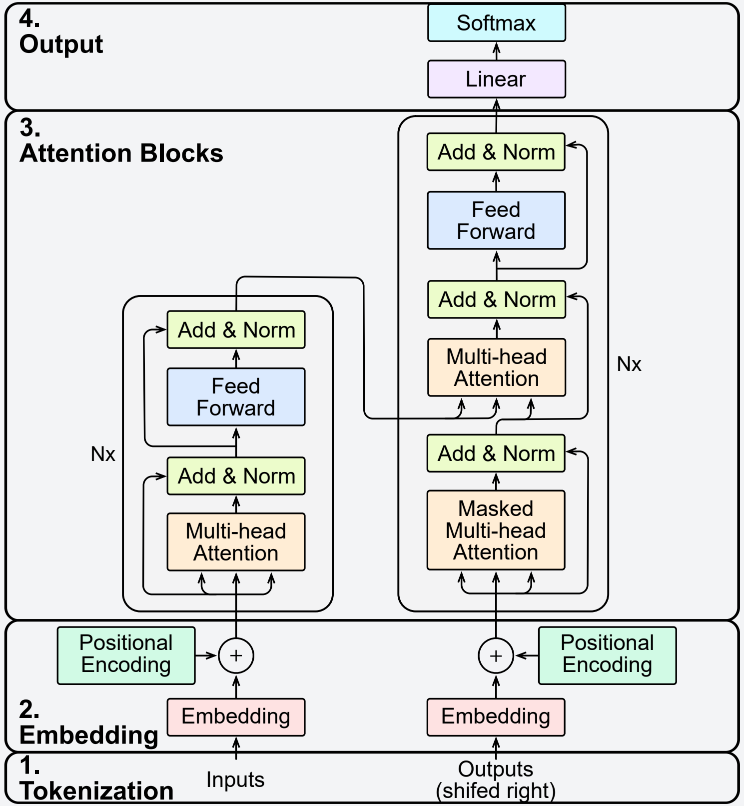
The Transformer



Breaking the Transformer into modules



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    - Softmax
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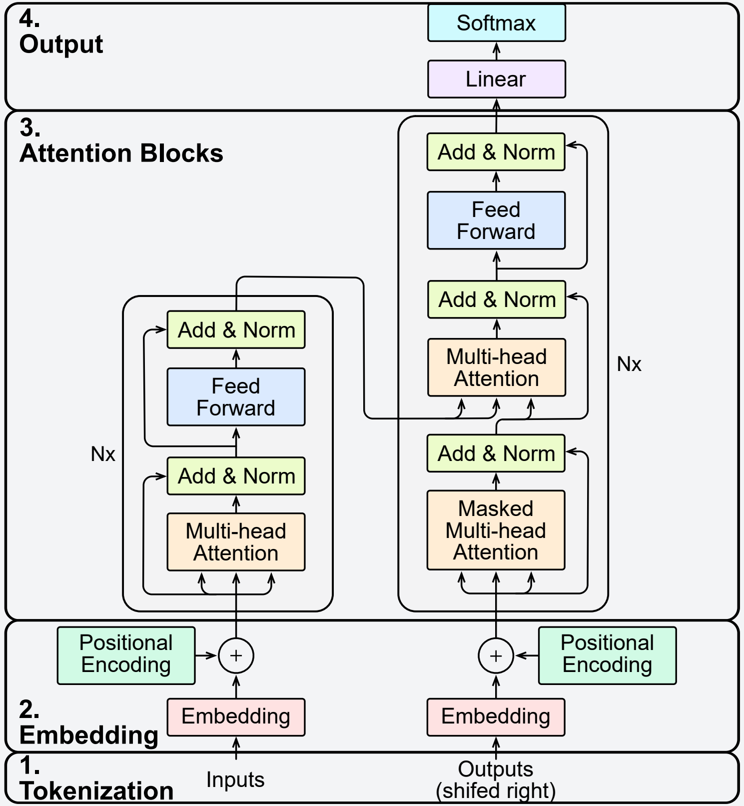

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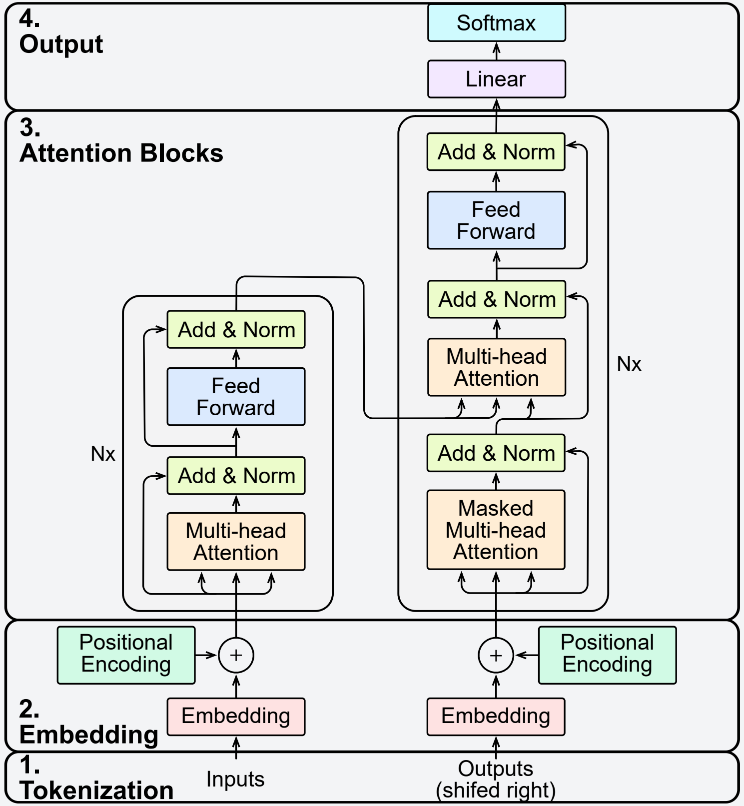
   - Multi-head Attention
   - Add & Norm
   - Feed Forward



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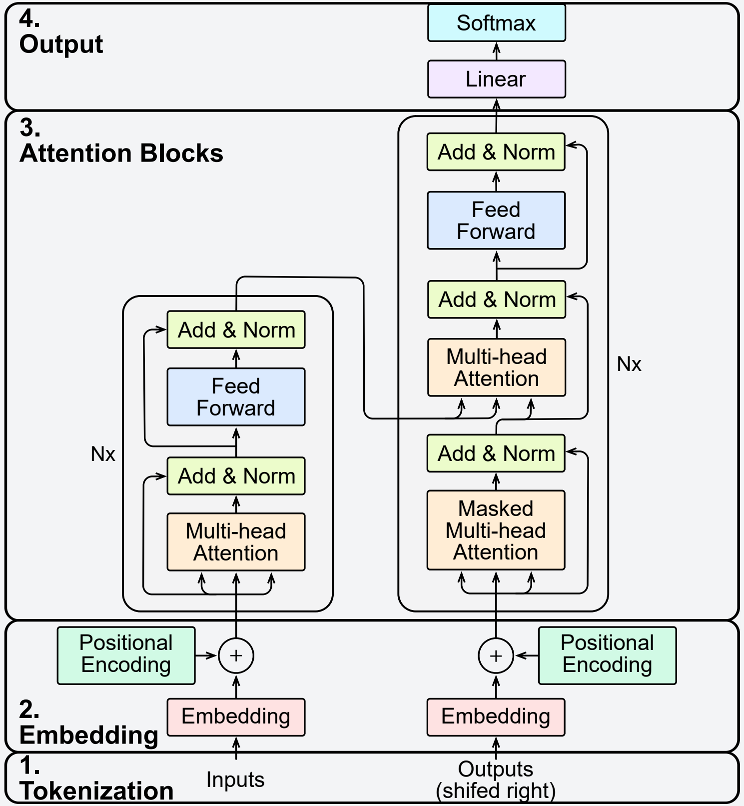

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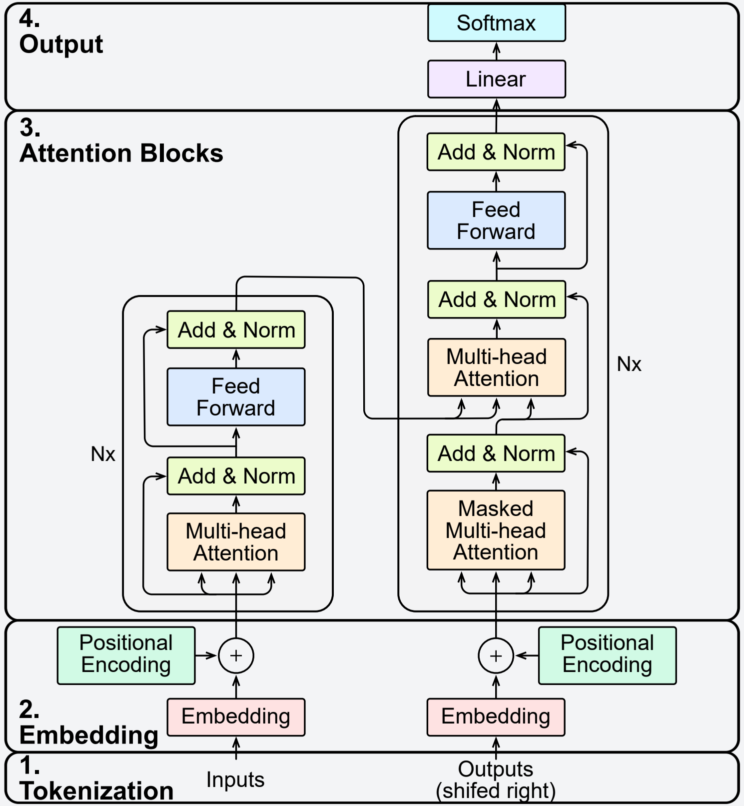

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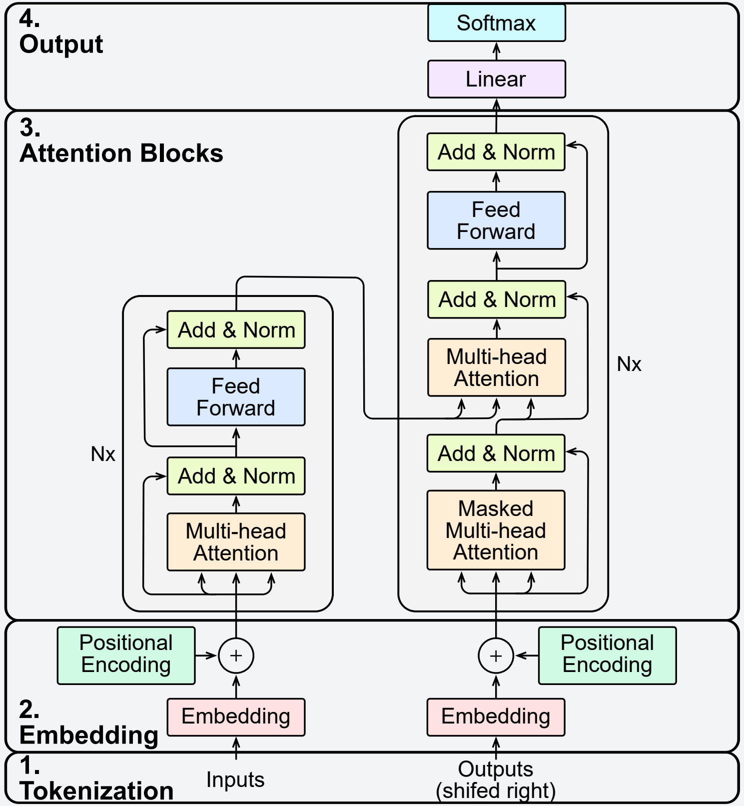

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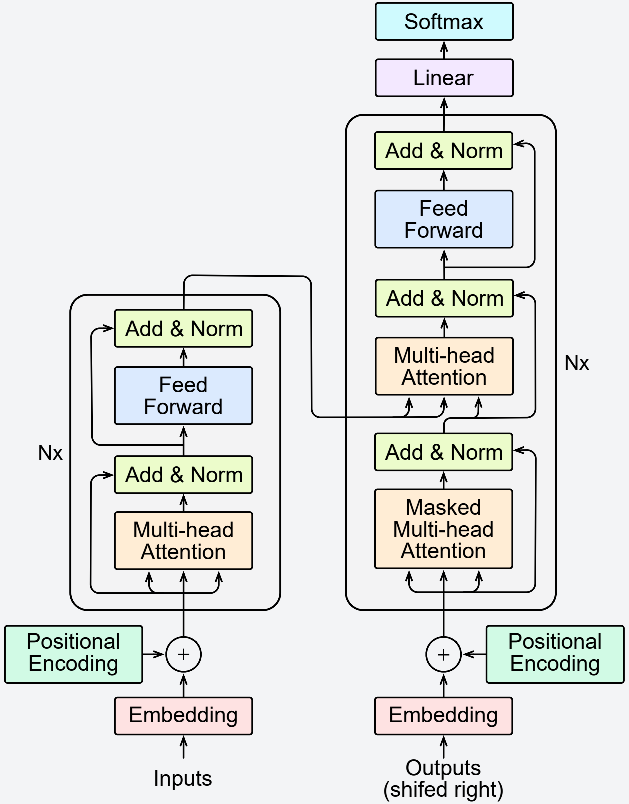


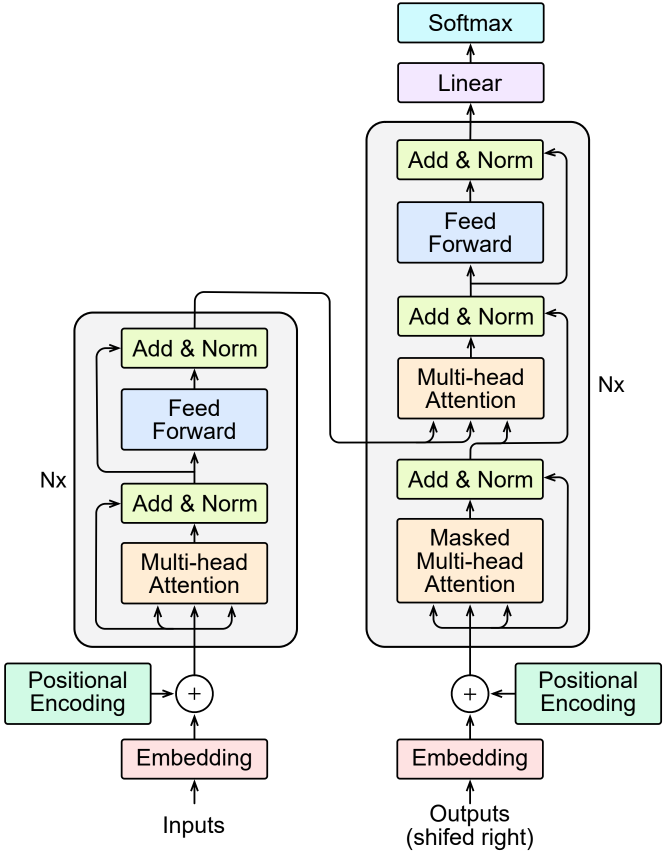
Encoders & Decoders

Text comes in, text goes out

Attention Blocks

What makes the Transformer what it is — and where it came from

Multi-head Attention



Definition & Properties

Multi-head Attention

- Let $\mathbf{V}$ be a matrix of (word) vectors
  - It has a sequence length of t_V
  - It has a dimensionality of d_V

$$\texttt{Attention}(?, ?, \mathbf{V}) = \mathbf{A}\mathbf{V}$$

$$\mathbf{A} \in (0,1)^{[t_V \times t_V]}$$

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- $\texttt{Attention}$ is just a matrix product of $\mathbf{V}$ with an attention matrix $\mathbf{A}$
  - $\mathbf{A}$ is a square matrix of size $t_V \times t_V$
  - It's elements are all between $(0, 1)$
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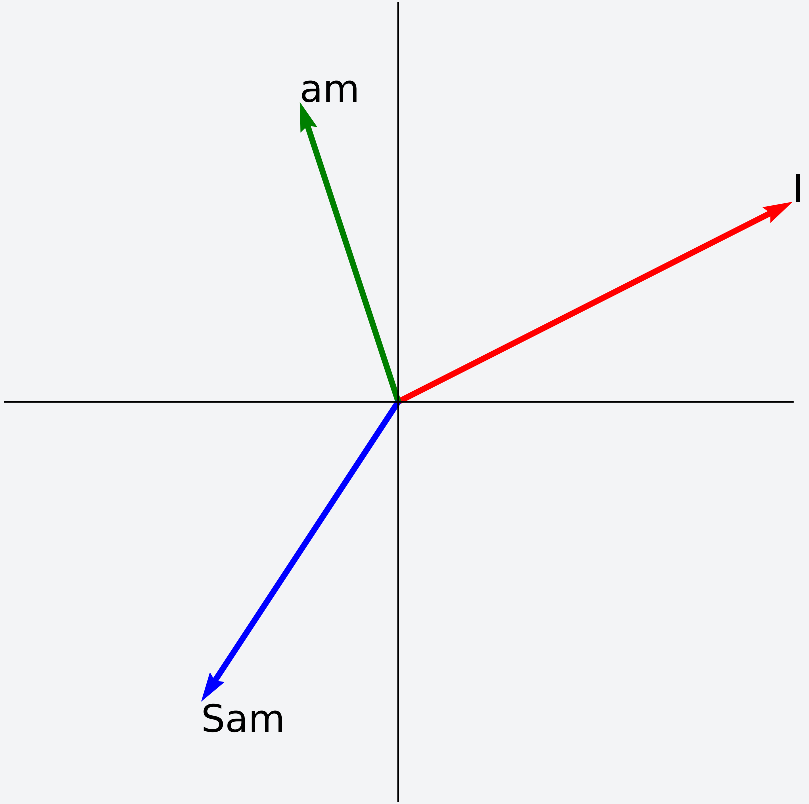
- The result of **`Attention`** is just a convex combination of $\mathbf{V}$

$$\begin{array}{cc} \mathbf{A} & \mathbf{V} \\ \begin{bmatrix} 0.6 & 0.1 & 0.3 \\ 0.3 & 0.5 & 0.2 \\ 0.2 & 0.1 & 0.7 \end{bmatrix} & \begin{bmatrix} 2.0 & 1.0 \\ -0.5 & 2.0 \\ -1.0 & -0.5 \end{bmatrix} \begin{array}{l} \color{red}{\mathrm{I}} \\ \color{green}{\mathrm{am}} \\ \color{blue}{\mathrm{Sam}} \end{array} \end{array}$$



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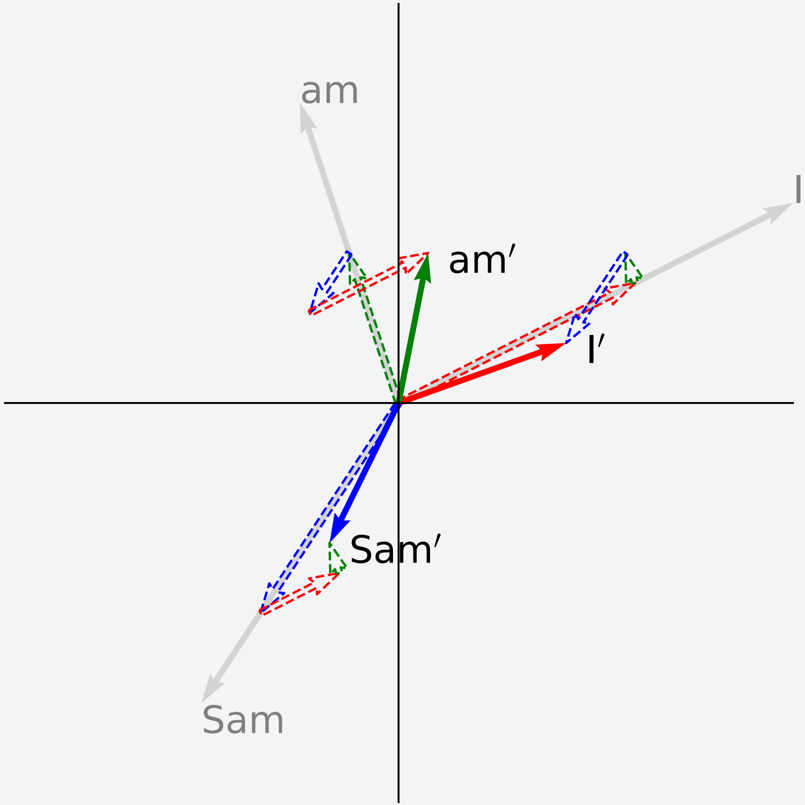
$$= \begin{bmatrix} 0.6 * \color{red}{\mathrm{I}} + 0.1 * \color{green}{\mathrm{am}} + 0.3 * \color{blue}{\mathrm{Sam}} \\ 0.3 * \color{red}{\mathrm{I}} + 0.5 * \color{green}{\mathrm{am}} + 0.2 * \color{blue}{\mathrm{Sam}} \\ 0.2 * \color{red}{\mathrm{I}} + 0.1 * \color{green}{\mathrm{am}} + 0.7 * \color{blue}{\mathrm{Sam}} \end{bmatrix}$$



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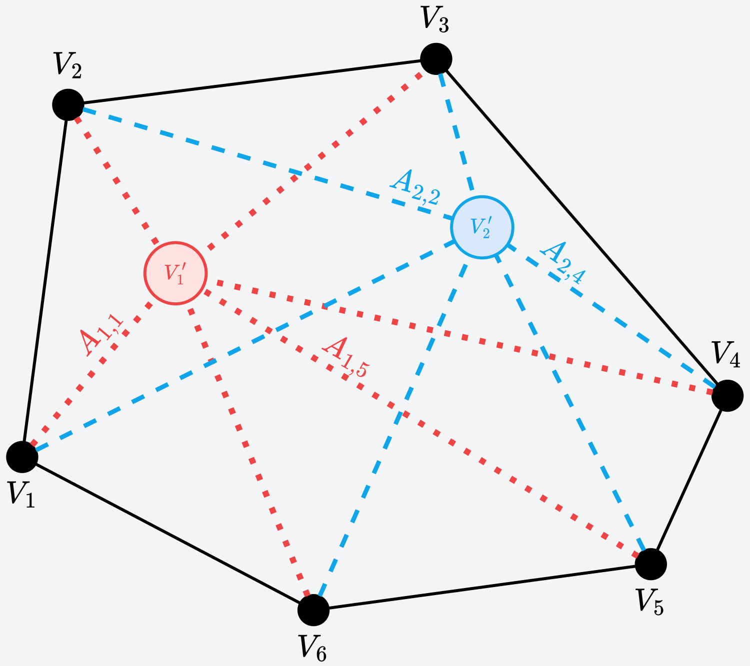
Convex Combination

The elements of V' will lie inside the convex hull of all of the elements in V



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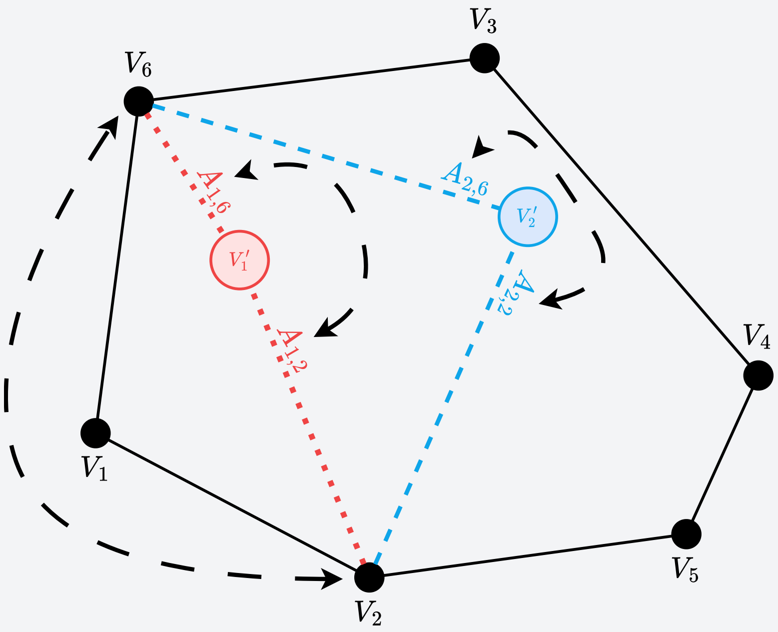
Permutation Equivariance

The elements of $\mathbf{V}'$ are *equivariant* to a change in the order of the columns of $\mathbf{A}$ and the rows of $\mathbf{V}$

- Attention does not care about word order
  - 'I am Sam' ~ 'Sam I am'



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So is `Attention` just a linear map?

- Not quite

Linear maps are:

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- Parameter inefficient
- Invariant to the input content

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- Let $\mathbf{K}$ be a matrix of **key** vectors
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- Let $\mathbf{Q}$ be a matrix of **query** vectors
  - It has a sequence length of t_Q
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$$\mathtt{Attention}(\mathbf{Q}, \mathbf{K}, \mathbf{V}) = \underbrace{\mathtt{softmax}\left(f\left(\mathbf{Q}, \mathbf{K}\right)\right)}_{\mathbf{A}}\mathbf{V}$$

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Non-Transformer Examples

Multi-head Attention

- $\mathbf{V}$ contains information
- $\mathbf{K}$ contains information about information (i.e, metadata)
- $\mathbf{Q}$ contains metadata about what we want from $\mathbf{V}$
- $f(\mathbf{Q}, \mathbf{K})$ is high when $\mathbf{Q}$ is similar to $\mathbf{K}$

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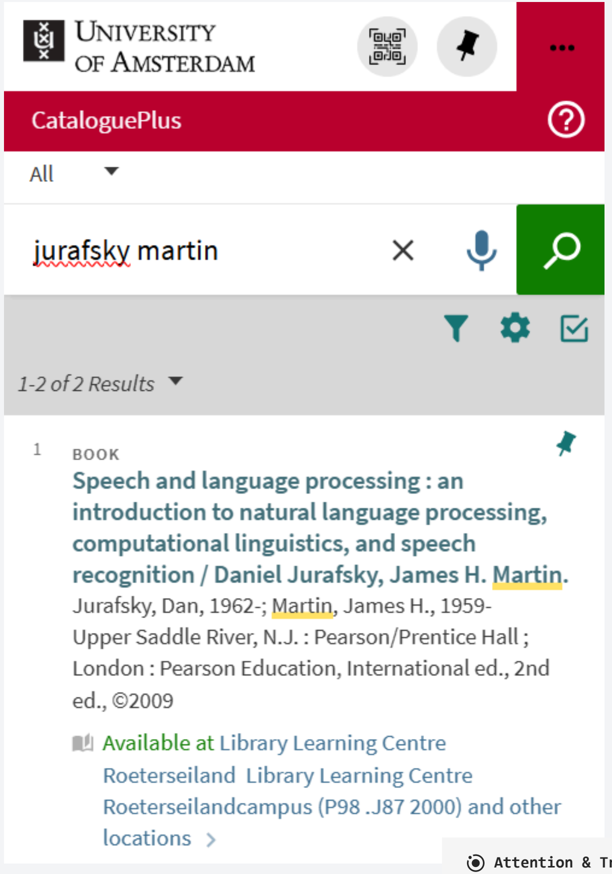
> **E Soft lookup**
>
> We want to find a textbook about NLP in the library ($\mathbf{V}$). We search for titles ($\mathbf{K}$) with "jurafsky" and "martin" as authors ($\mathbf{Q}$). The computer returns books with similar titles (f)



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- $f(\mathbf{Q}, \mathbf{K})$ is high when $\mathbf{Q}$ is similar to $\mathbf{K}$
- The output of f must a matrix of size $\mathbf{A} \in (0,1)^{[T_Q \times T_V]}$

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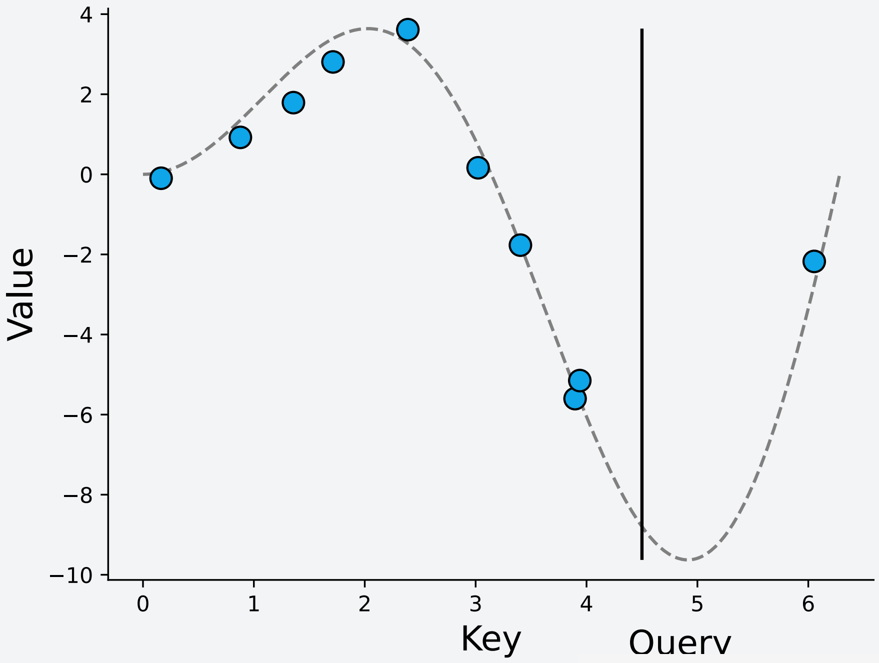
E Nadaraya-Watson Kernel Regression

We have some sequence of values $\mathcal{D} = [(1.36, 1.79), (3.40, -1.77)\ldots, (6.05, -2.17)]$

We want to predict a new sample at $x = 4.25$

We compute the negative Euclidean distance of our new sample with all training samples (f). We normalize the outputs to lie between $(0,1)$

We compute our predicted value as the mean of the seen values, weighted by the computed similarities



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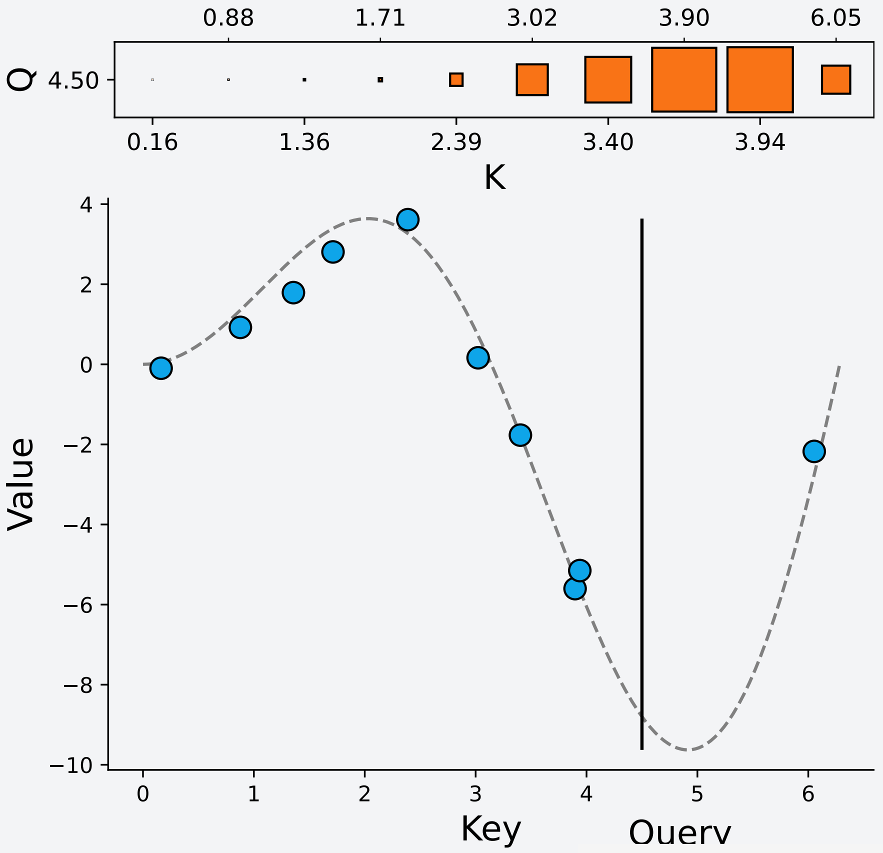

Non-Transformer Examples

Multi-head Attention

- $f(\mathbf{Q}, \mathbf{K})$ is high when $\mathbf{Q}$ is similar to $\mathbf{K}$
- The output of f must a matrix of size $\mathbf{A} \in (0,1)^{[T_Q \times T_V]}$

E **Nadaraya-Watson Kernel Regression**

We have some sequence of values $\mathcal{D} = [(1.36, 1.79), (3.40, -1.77) \ldots, (6.05, -2.17)]$

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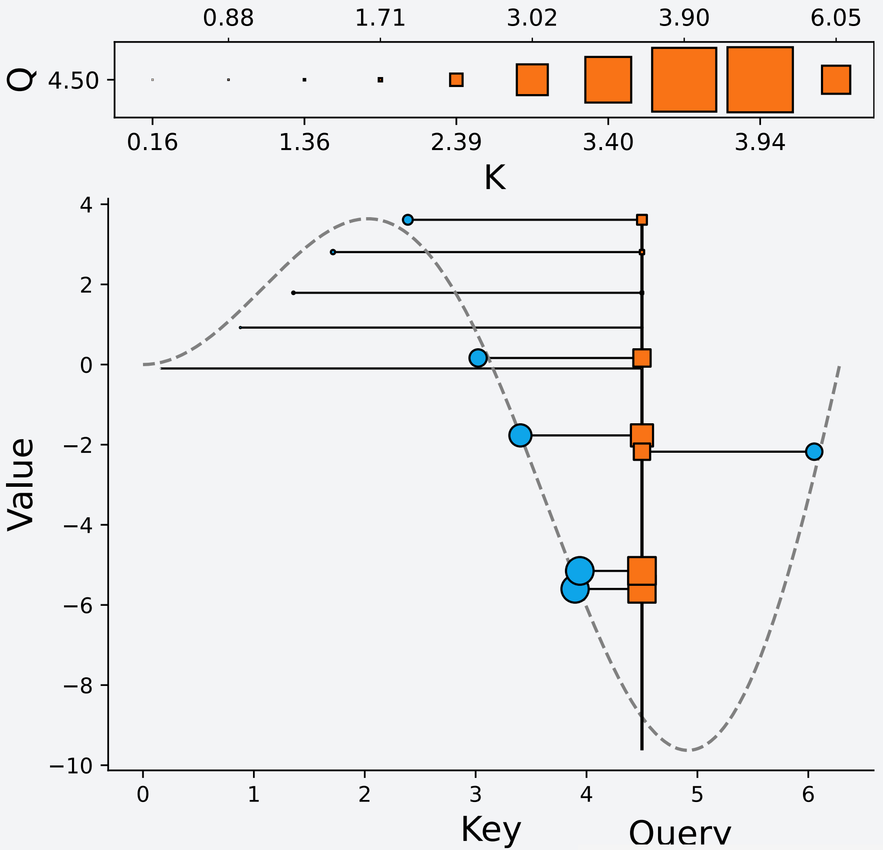

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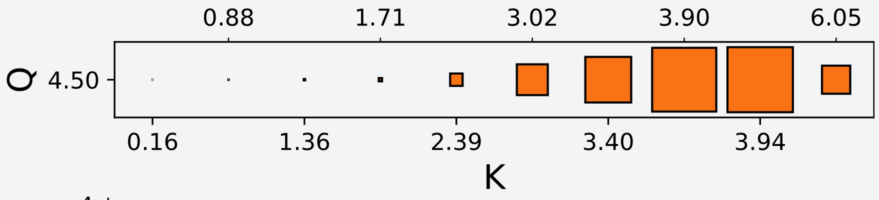

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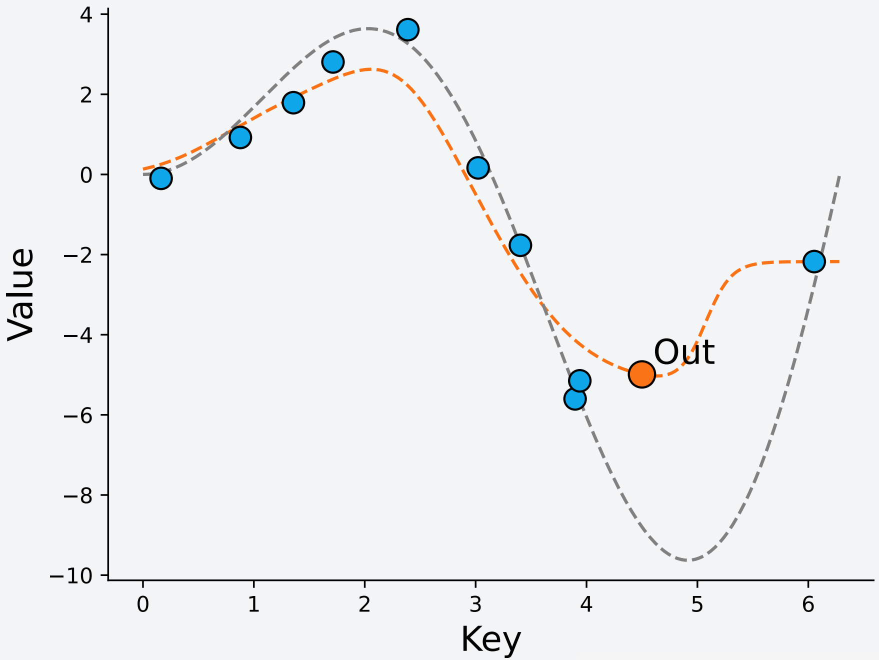

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Multi-head Attention

- The $\mathbf{Q}$ and $\mathbf{V}$ do not need to have the same sequence length
- Attention output will always have sequence length T_Q

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E Bahdanau et al. Attention

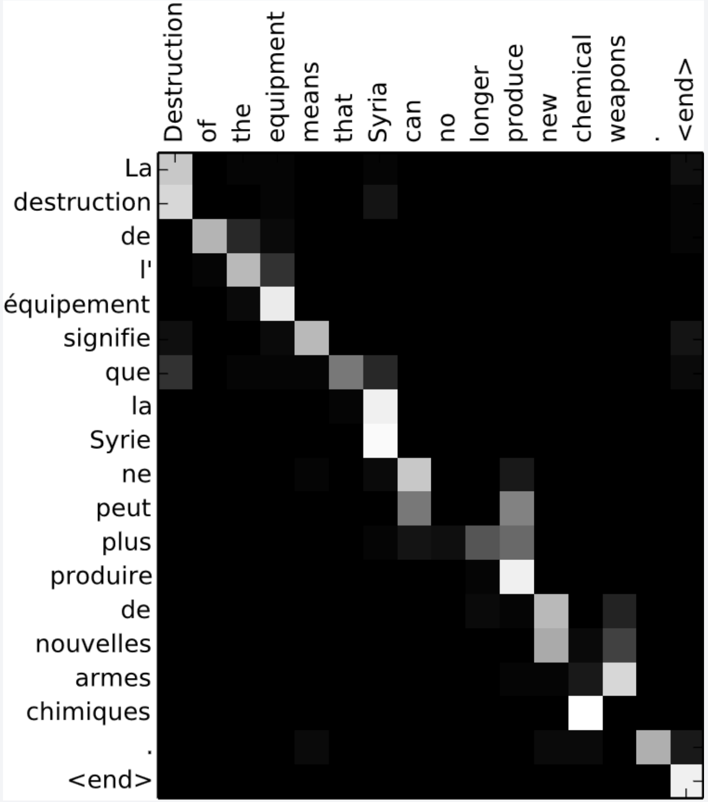
In Neural Machine Translation (NMT) the encoder generates a representation of the input language

The decoder needs to generate in a target language

Token in input language != token in output language

Solution: have each token in the target language ($\mathbf{Q}$) attend back to all input language tokens ($\mathbf{K}$, $\mathbf{V}$)

Bahdanau, Cho & Bengio (2014). Neural machine translation by jointly learning to align and translate.



Attention in Transformers

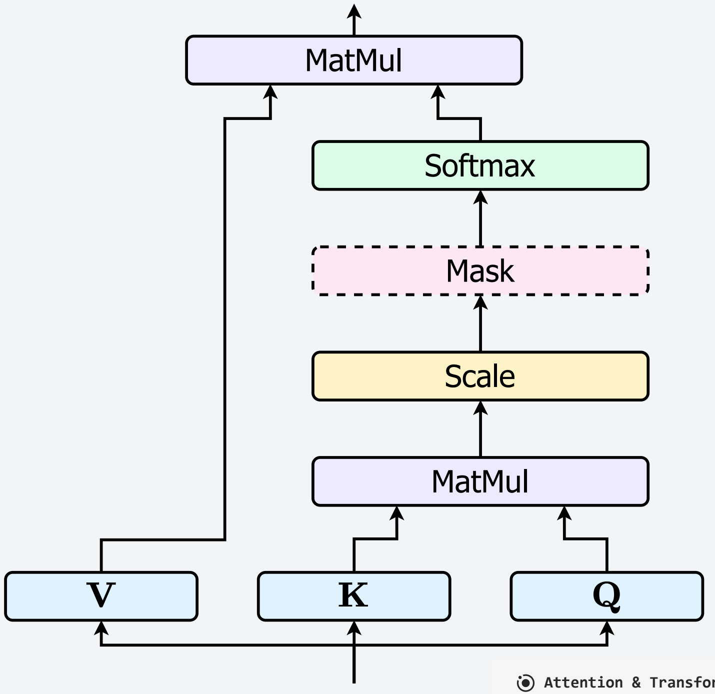
Multi-head Attention

- Transformer attention uses a scaled dot-product kernel function

$$f(\mathbf{Q}, \mathbf{K}) = \frac{\mathbf{Q}\mathbf{K}^\top}{\sqrt{d_k}}$$

- $\mathbf{Q}$ is of size $t_Q \times d_K$
- $\mathbf{K}$ is of size $t_V \times d_K$
- Attention matrix is thus of size $t_Q \times t_V$

$$\mathtt{attention}(\mathbf{Q}, \mathbf{K}, \mathbf{V}) = \mathtt{softmax}\left(f(\mathbf{Q}, \mathbf{K})\right)\mathbf{V}$$



Attention in Transformers

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- Transformer attention uses a scaled dot-product kernel function

$$f(\mathbf{Q}, \mathbf{K}) = \frac{\mathbf{Q}\mathbf{K}^\intercal}{\sqrt{d_k}}$$

- Why scale?
  - Assume the elements in $\mathbf{Q}$ and $\mathbf{K}$ come from *independent* normal distributions:

$$\mathbf{q}, \mathbf{k} \sim \mathcal{N}(0, 1)$$

  - The distribution of their dot-product is:

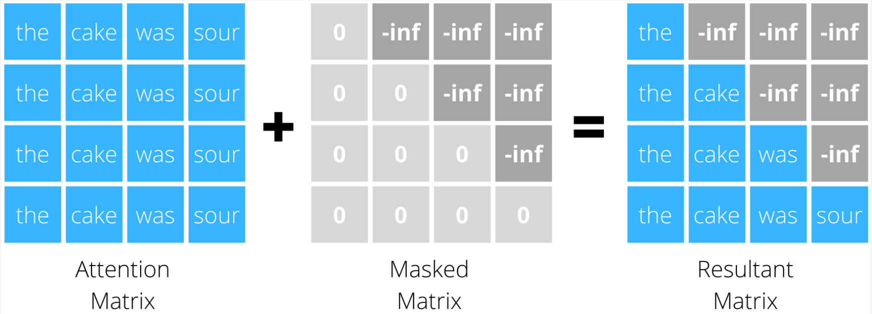
$$\mathbf{q}^\intercal\mathbf{k} \sim \mathcal{N}(0, \sqrt{d_k})$$

$$\begin{aligned}
\texttt{var}\left[\mathbf{q}^\intercal\mathbf{k}\right] &= \texttt{var}\left[\sum_i^{d_k} q_i k_i\right] \\
&= \sum_i^{d_k} \texttt{var}\left[q_i k_i\right] \\
&= \sum_i^{d_k} \texttt{var}\left[q_i\right] \texttt{var}\left[k_i\right] \\
&= \sum_i^{d_k} 1 \cdot 1 \\
&= d_k
\end{aligned}$$

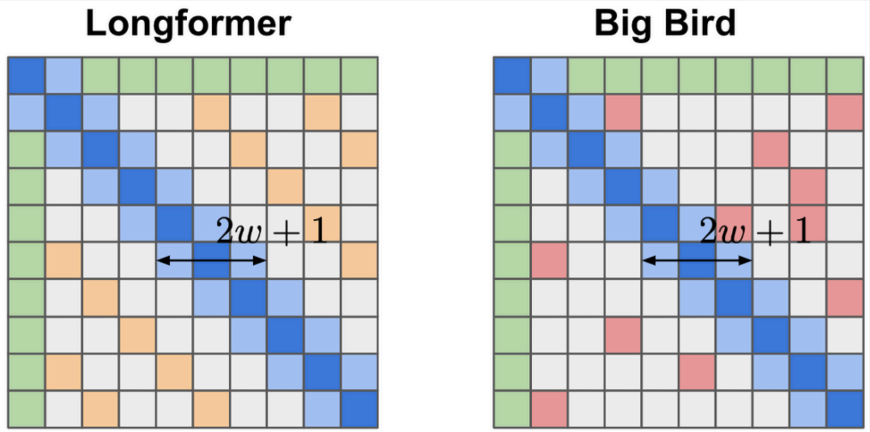
Attention in Transformers

Multi-head Attention

- Why mask?
  - Currently all tokens are treated equally
  - **Causal masking**: decoder tokens should never attend to future tokens, only to the past
  - **Local masking**: sometimes local attention is all you need



https://krypticmouse.hashnode.dev/attention-is-all-you-need

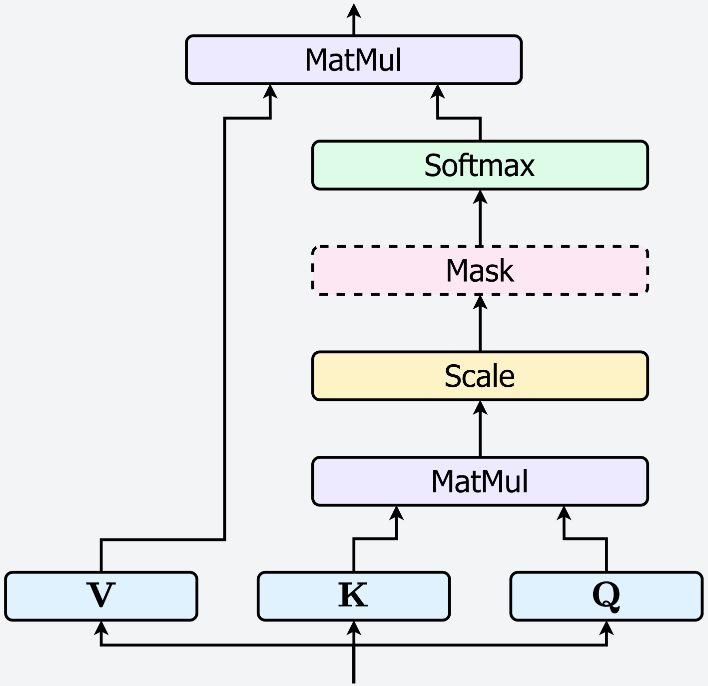


https://lilianweng.github.io/posts/2023-01-27-the-transformer-family-v2/

Attention in Transformers

Multi-head Attention

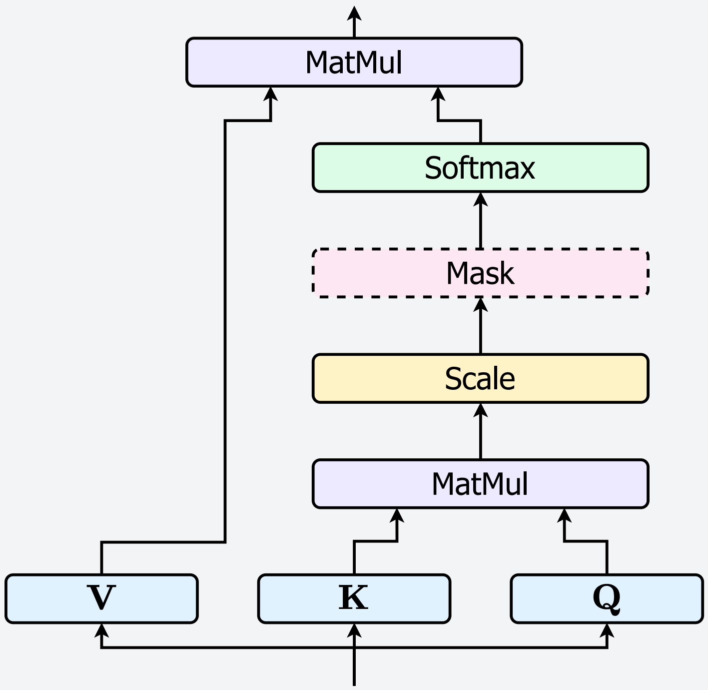
- Where do $\mathbf{V}$, $\mathbf{K}$, $\mathbf{Q}$ come from?



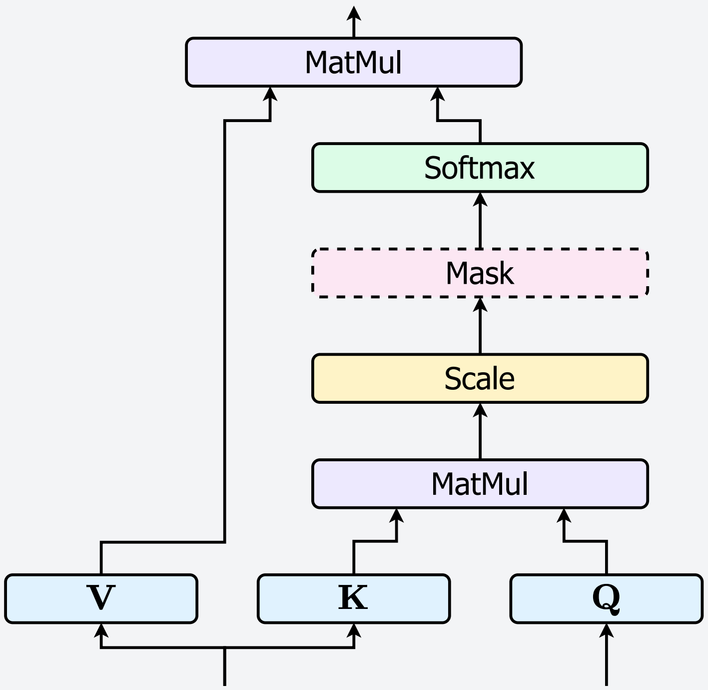
Attention in Transformers

Multi-head Attention

Self-attention



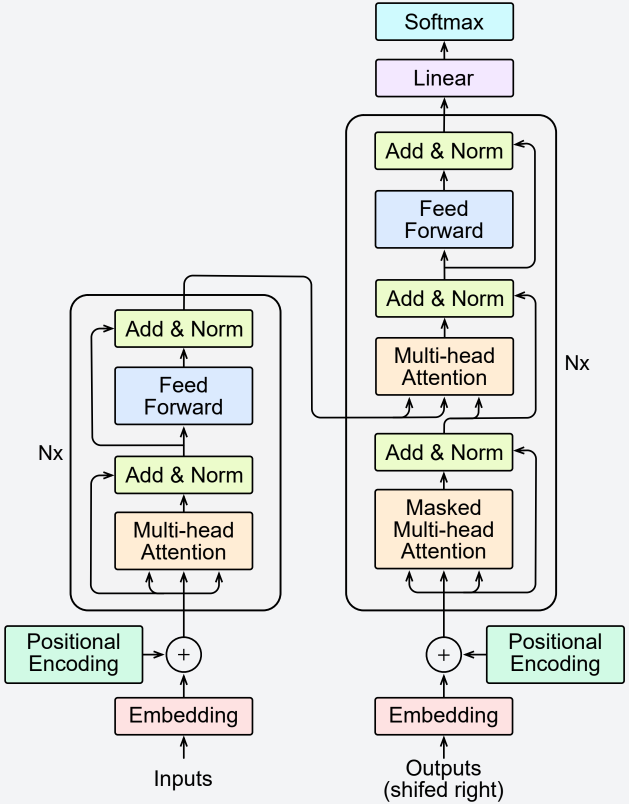
Cross-attention



Attention in Transformers

Multi-head Attention

- Where do $\mathbf{V}$, $\mathbf{K}$, $\mathbf{Q}$ come from?
  - **Self-attention**: everything comes from the same sequence
  - **Cross-attention**: $\mathbf{V}$, $\mathbf{K}$ come from source sequence, $\mathbf{Q}$ comes from target sequence
  - All components constructed from a projection of the token embeddings
    1. $\mathbf{V} = \mathbf{X}\mathbf{W}_V$
    2. $\mathbf{K} = \mathbf{X}\mathbf{W}_K$
    3. $\underbrace{\mathbf{Q} = \mathbf{X}\mathbf{W}_Q}_{\text{Self-attention}}$ or $\underbrace{\mathbf{Q} = \mathbf{Y}\mathbf{W}_Q}_{\text{Cross-attention}}$



Attention in Transformers

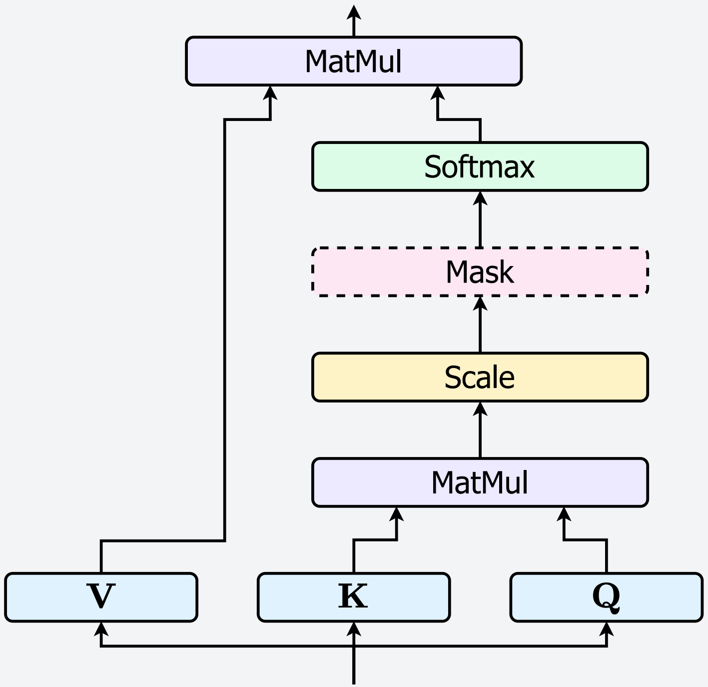
Multi-head Attention

- Even in self-attention, attention matrix is **not** symmetric

$$\frac{\mathbf{Q}\mathbf{K}^\intercal}{\sqrt{d_k}} = \frac{\mathbf{X}\mathbf{W}_Q(\mathbf{X}\mathbf{W}_K)^\intercal}{\sqrt{d_k}} = \frac{\mathbf{X}\mathbf{W}_Q\mathbf{W}_K^\intercal\mathbf{X}^\intercal}{\sqrt{d_k}}$$

Asymmetry

The contribution of token $\mathbf{x}_i$ to $\mathbf{x}_j$, is **not** the same as the contribution of tokn $\mathbf{x}_j$ to $\mathbf{x}_i$



Attention in Transformers

Multi-head Attention

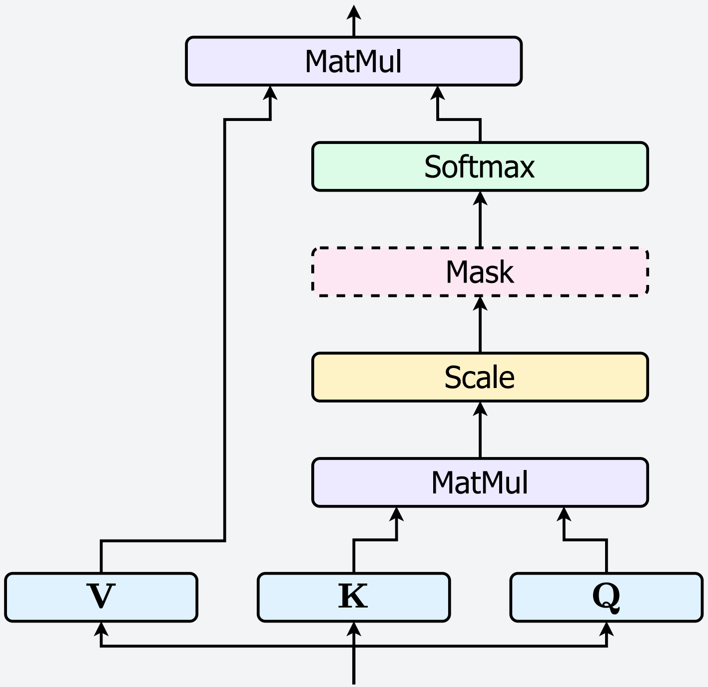
- Transformer attention between two sequences, $\mathbf{X}$ and $\mathbf{Y}$ has a computational cost of (excluding projections):

$$\mathcal{O}\left(\underbrace{t_x \cdot t_y \cdot d_k}_{\text{MatMul 1}} + \underbrace{t_x \cdot t_y \cdot d_v}_{\text{MatMul 2}}\right)$$

- But RNNs have linear time complexity...

$$\mathcal{O}\left(t_x \cdot d_k^2 + t_x \cdot d_q^2\right)$$

- RNNs are serial, Attention is parallel
  - GPUs *looove* parallelism



Jakob Uszkoreit (August 31, 2017). Transformer: A Novel Neural Network Architecture for Language Understanding. https://research.google/blog/transformer-a-novel-neural-network-architecture-for-language-understanding/

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- Currently we use 1 set of attention weights
  - Can only process 1 query type

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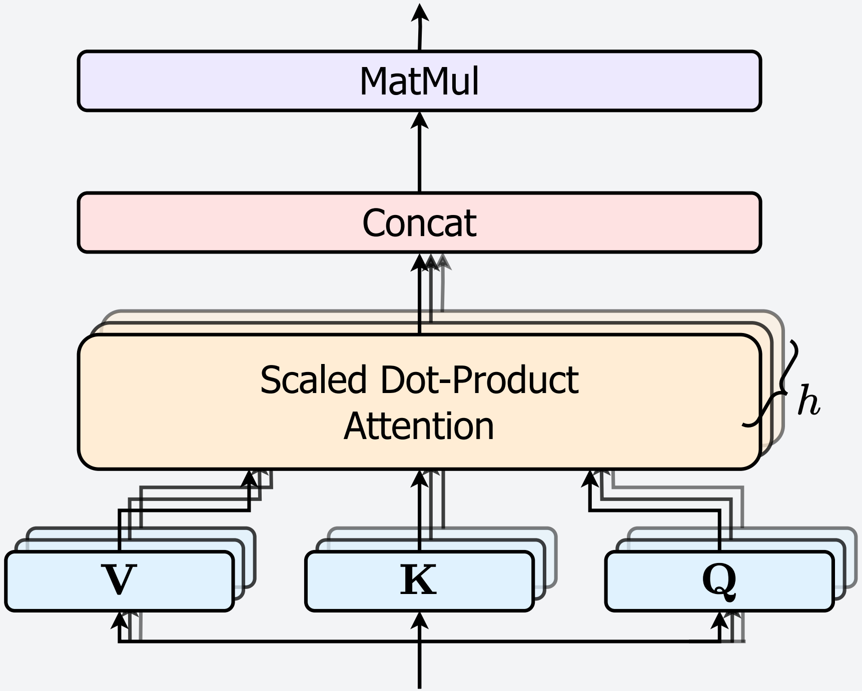
- With h attention heads, we learn h concepts
  - To reduce cost, reduce dimensionality $d_{K,V}/h$



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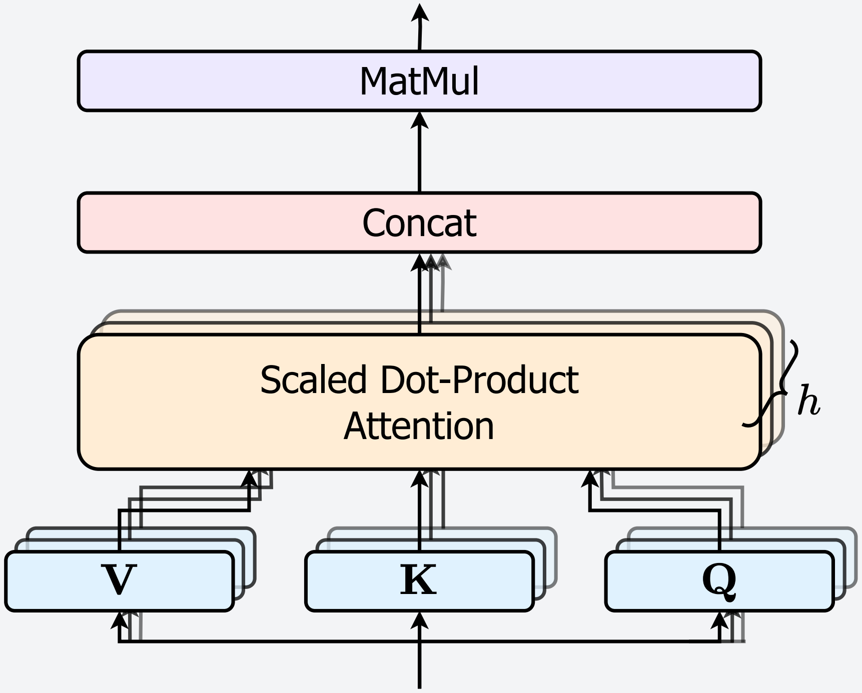
```
self.attention_heads = [
  AttentionHead(d=self.d // self.h) for i in range(self.h)
  ]

self.mha_proj = nn.Linear(self.d, self.d)

mha = torch.concat([
  attention_heads[i](x) for i in range(self.h)
  ])

out = self.mha_proj(mha)
```



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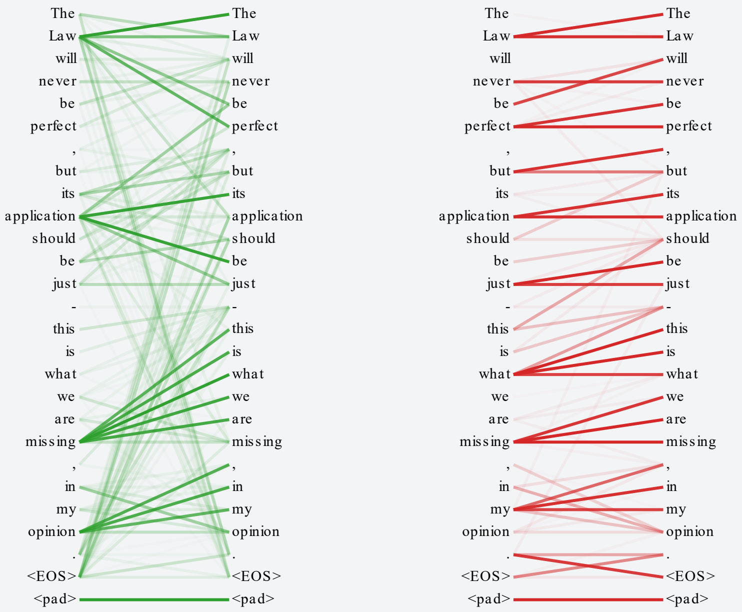
> Multi-head attention allows the model to jointly attend to information from different representation subspaces at different positions. [One] attention head, averaging inhibits this.

Vaswani et al. (2017). Attention is all you need. Advances in neural information processing systems, 30. (p. 5 & 15)



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Multiple heads, multiple different queries processed in parallel

- Positional heads
- Syntactic heads
- Rare words?

Voita et al. (2019). Analyzing Multi-Head Self-Attention: Specialized Heads Do the Heavy Lifting, the Rest Can Be Pruned. Association for Computational Linguistics.

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Do different heads attend to different concepts?

Multi-head Attention

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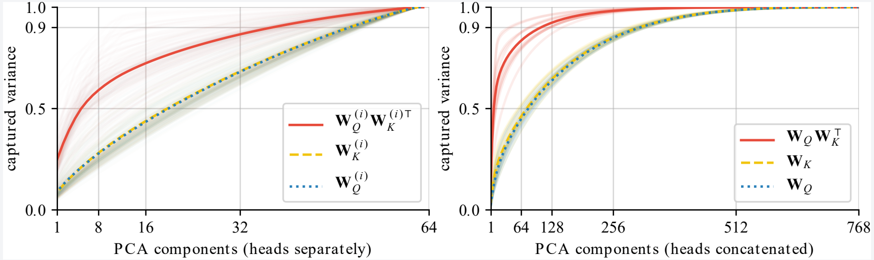
- Individual heads = high rank, concantenated heads = low rank

  Cordonnier, Loukas & Jaggi (2020). Multi-head attention: Collaborate instead of concatenate. arXiv:2006.16362.



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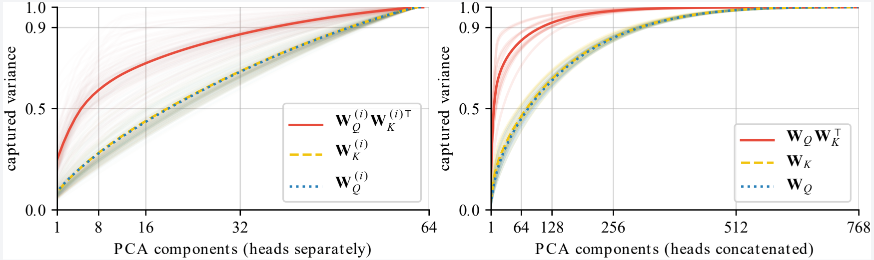

- Most heads can be pruned away
- Enc-Dec heads are more important than Enc-Enc heads

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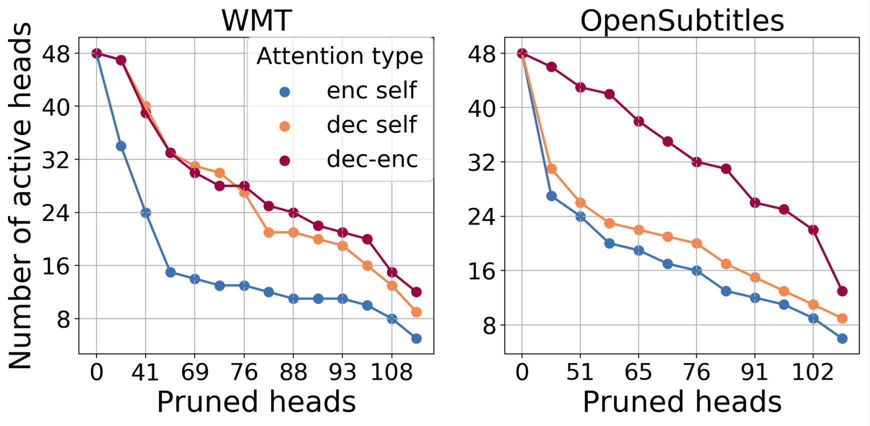
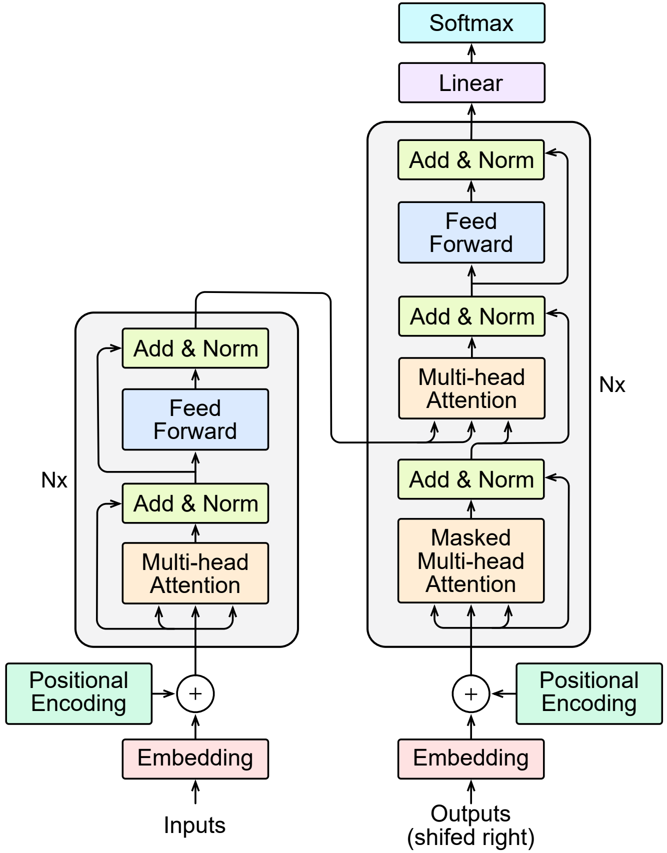


Add & Norm


Softmax
Linear
Add & Norm
Feed Forward
Add & Norm
Multi-head Attention
Nx
Add & Norm
Masked Multi-head Attention
Add & Norm
Feed Forward
Nx
Add & Norm
Multi-head Attention
Positional Encoding
Positional Encoding
Embedding
Embedding
Inputs
Outputs (shifed right)

Add & Norm

Residual Connections

Add & Norm

LayerNorm

Add & Norm

These are the equations

$$\mathbf{X}_l = \texttt{LayerNorm}\Big(\mathbf{X}_{l-1} + \texttt{SubLayer}\left(\mathbf{X}_{l-1}\right) \Big)$$

Feed Forward

Embedding

Position Encoding

Tokenization

Training Transformers

The End