

Transformers and Self-Attention

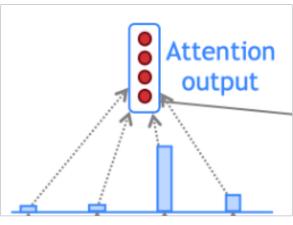
Spring 2024 2024-02-12

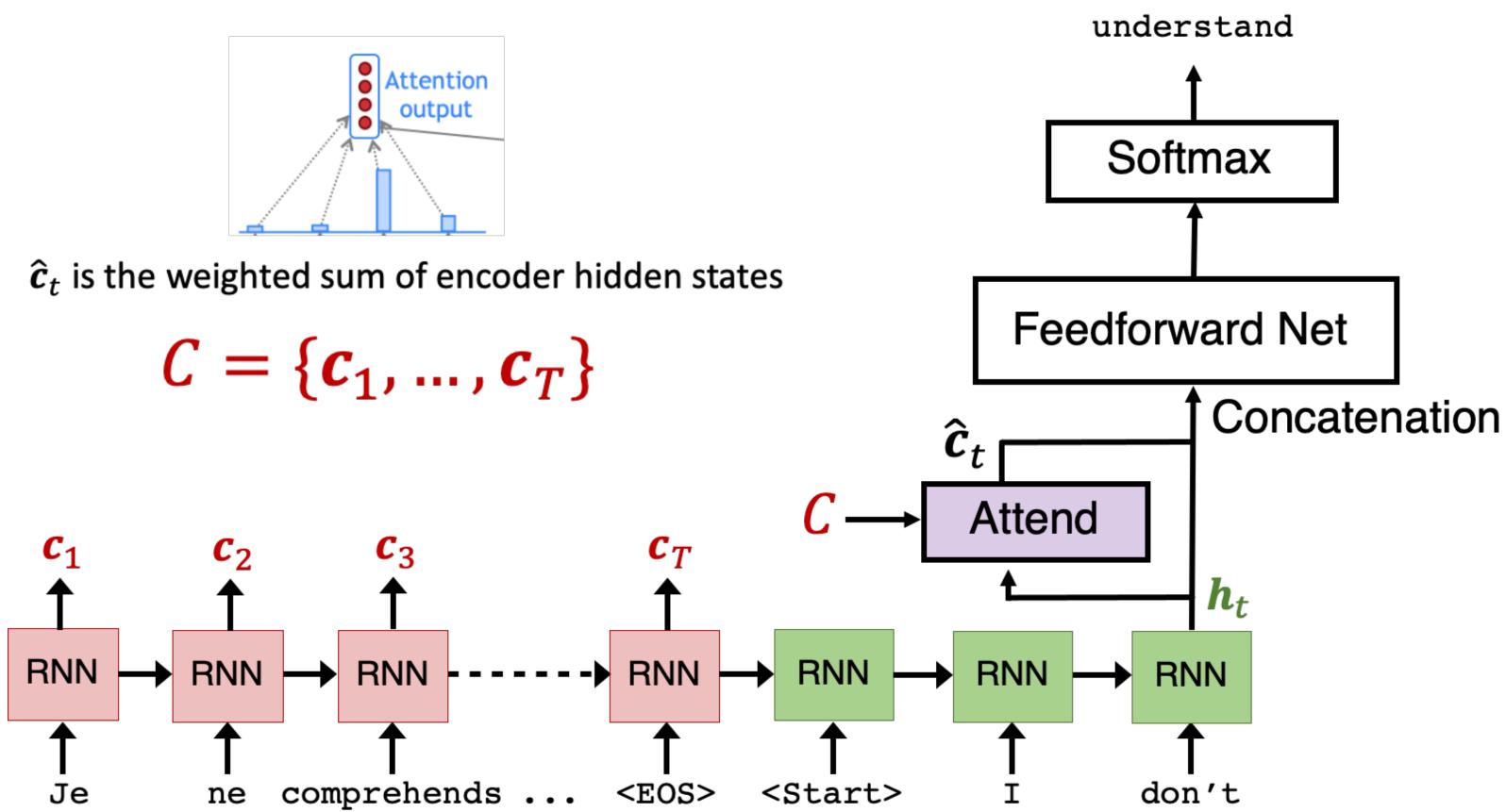
Adapted from slides from Dangi Chen and Karthik Narasimhan (with some content from slides from Chris Manning and Abigail See)

CMPT 413/713: Natural Language Processing

Review of attention in sequence to sequence models

Attentive machine translation summary



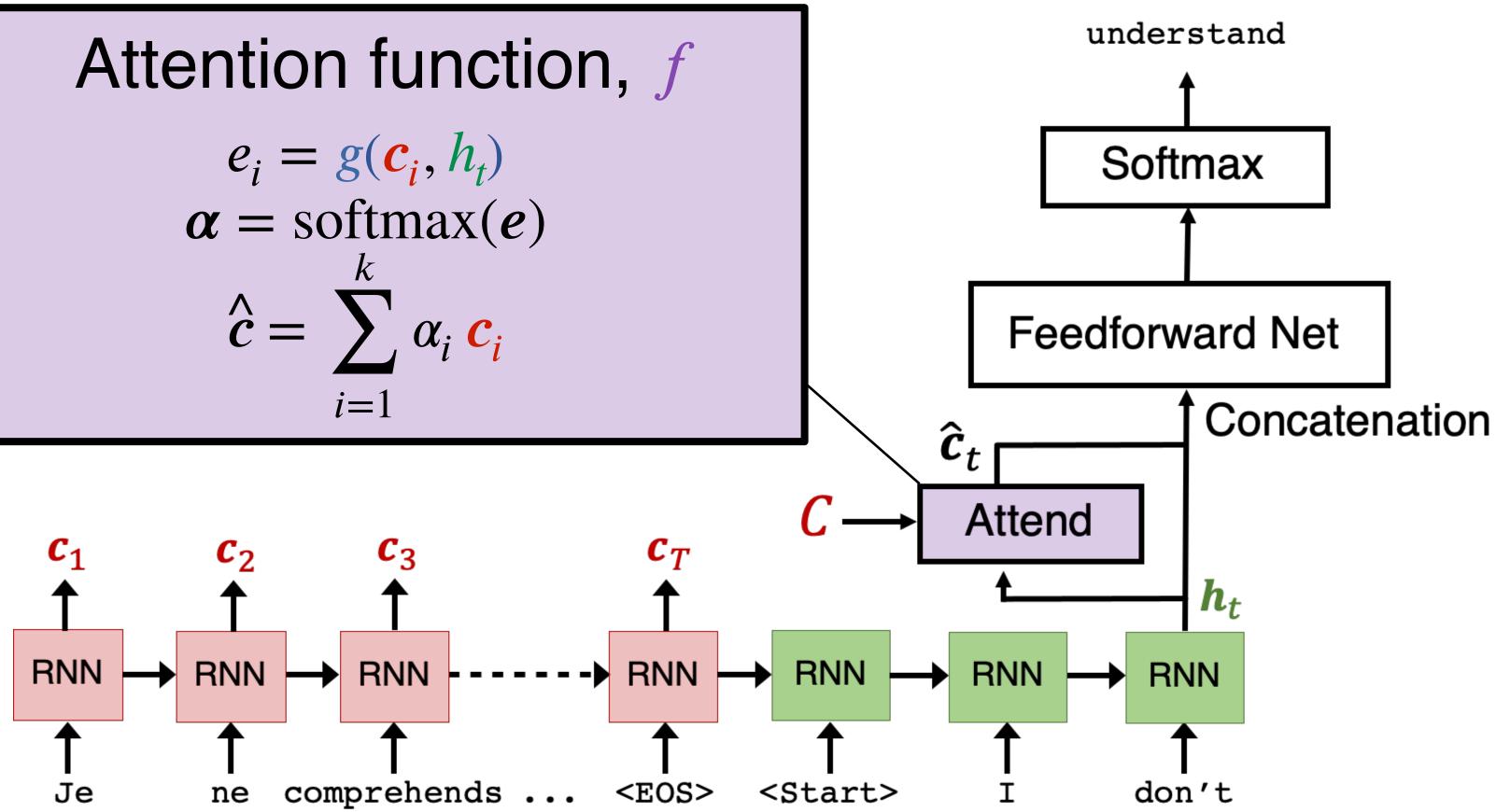


(slide credit: Peter Anderson)



Attentive machine translation summary

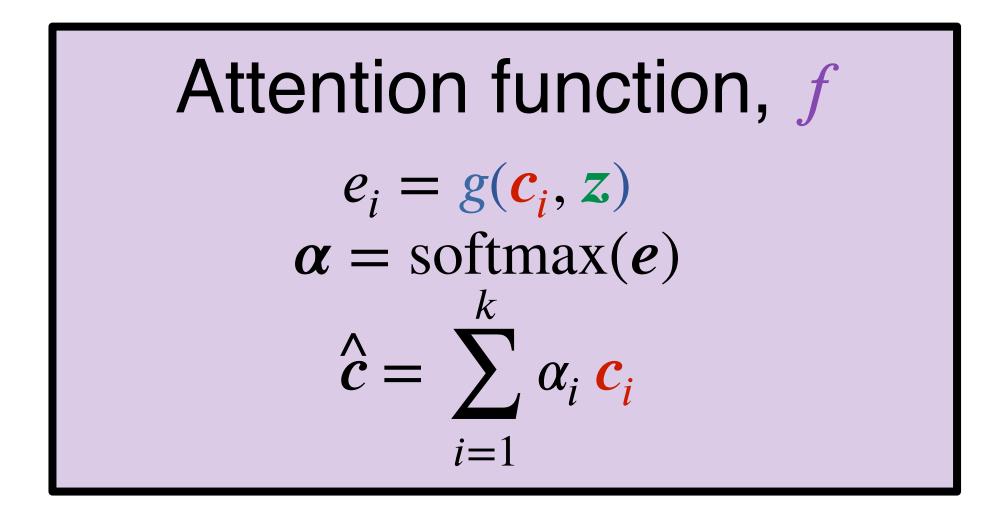
$e_i = g(\boldsymbol{c}_i, \boldsymbol{h}_t)$ $\alpha = \operatorname{softmax}(e)$ $\hat{c} = \sum \alpha_i c_i$ i=1



(slide credit: Peter Anderson)



Summary of attention

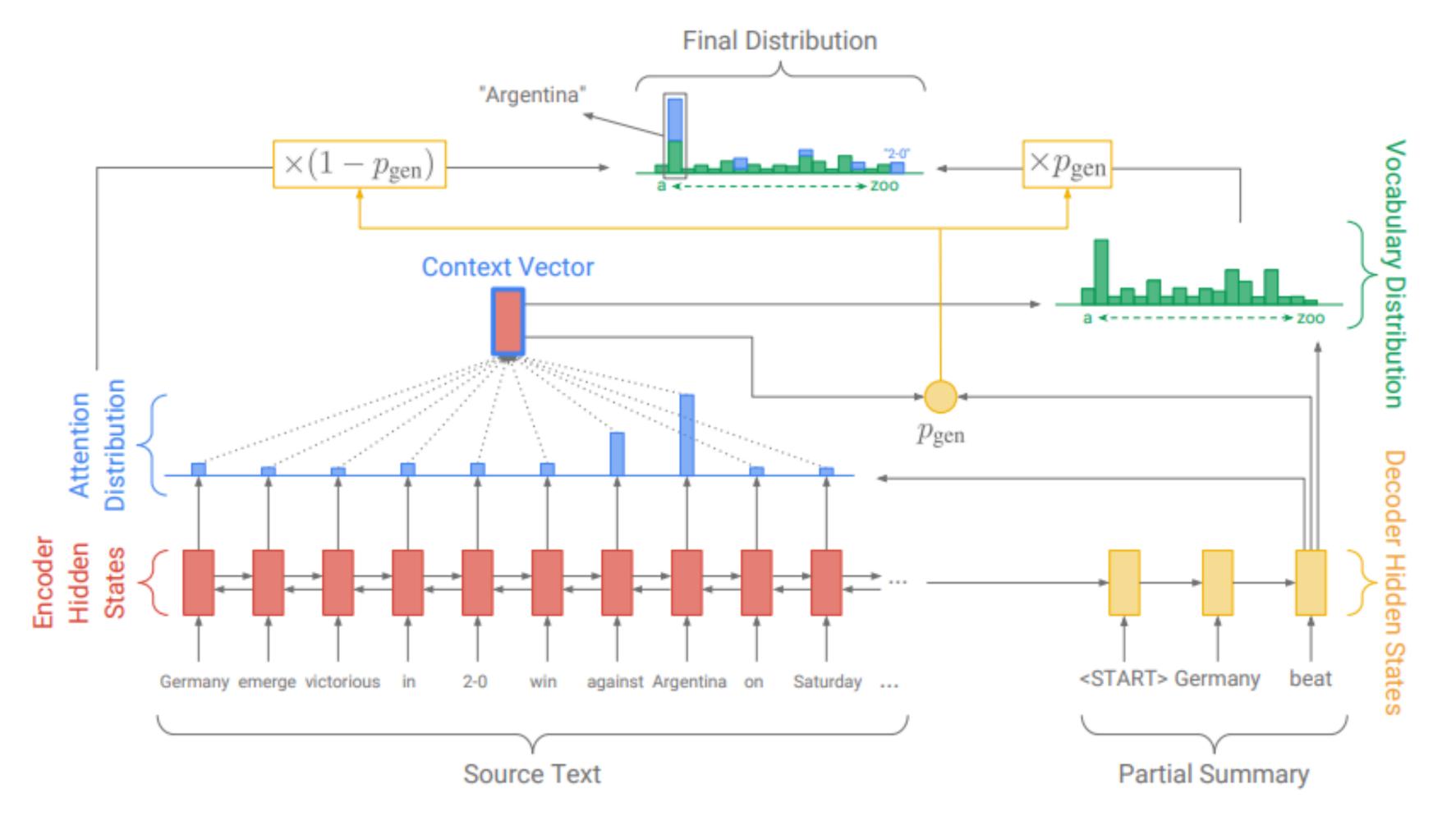


Attention score $e_i = g(c_i, z)$ how well does the attention candidate c_i match the query z

- Attention scores: *e* (unnormalized)
- Attention weights: α (normalized)
- Final attention output
 - Weighted sum of context features (or values)
- Dot-product attention: $g(c_i, z) = z \, \, ^{\mid} c_i$
- Neural network $g(\boldsymbol{c_i}, z) = v^{\top} \tanh\left(W_1\boldsymbol{c_i} + W_2z\right)$



Attention can be used to copy from input



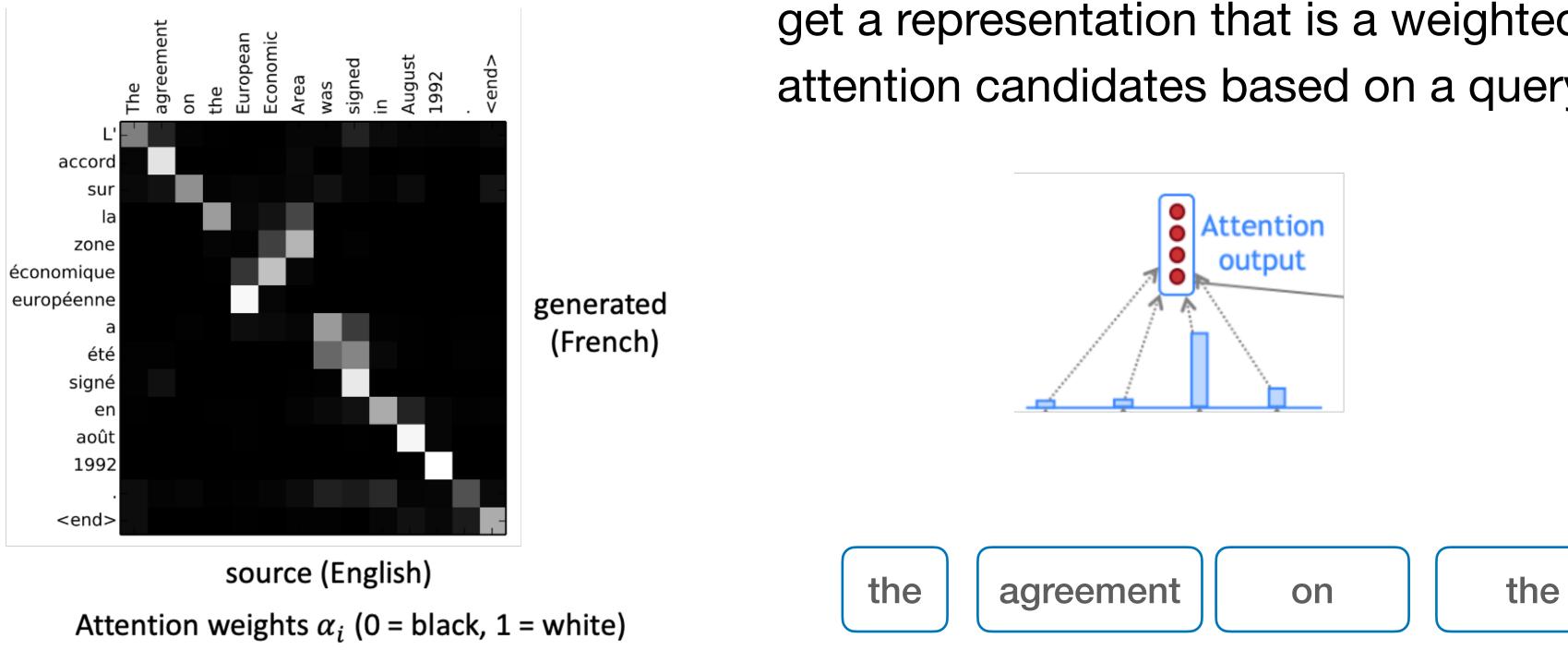
- Probability of copying specific word (similar to attention)

Probability of generating from vocabulary or copying from input



Motivation of attention

- How much does this attention candidate match the query vector?
- Motivated by biological attention and alignment in machine translation



get a representation that is a weighted sum over the attention candidates based on a query vector

Attention is a general deep learning technique

- Given a set of value vectors and a query vector, attention is a way to compute a weighted sum of the values dependent on the query.
 - The query determines what values to focus on,
 - We say: the query "attends" to the values
 - In NMT, each decoder hidden state (query) attends to all the encoder hidden state (values)
- A more general form: use a set of keys and values
 - The keys are used to compute the attention scores
 - The values are used to compute the output vector

Attention is always computed the same way

- $\mathbf{v}_1, \ldots, \mathbf{v}_n \in \mathbb{R}^{d_v}$, and a query vector $\mathbf{q} \in \mathbb{R}^{d_q}$
- Computing attention consists of the following steps:
 - Compute the attention scores
 - Take softmax to get the attention distribution
 - Use attention distribution to take weighted sum of values

$$\hat{\mathbf{c}} = \sum_{i=1}^{n} =$$

• Assume that we have a set of key-value pairs $\mathbf{k}_1, \dots, \mathbf{k}_n \in \mathbb{R}^{d_k}$,

s:
$$e_i = g(\mathbf{k}_i, \mathbf{q}), \mathbf{e} \in \mathbb{R}^n$$

 $\alpha = \operatorname{softmax}(\mathbf{e}) \in \mathbb{R}^n$

$$\alpha_i \mathbf{v}_i \in \mathbb{R}^{d_v}$$

Query-Value-Key view of attention

Attention function, f $e_i = g(c_i, z)$ $\alpha = \operatorname{softmax}(e)$ $\hat{c} = \sum_{i=1}^k \alpha_i c_i$

Projected query,key,value

Attention function,
$$f$$

 $e_i = g(k_i, q)$
 $\alpha = \operatorname{softmax}(e)$
 $\hat{c} = \sum_{i=1}^k \alpha_i v_i$

$$q = W_Q z \qquad Matrix form
q = W_Q z \qquad q = W_Q z
k_i = W_K c_i \longrightarrow K = W_K C^T
v_i = W_V c_i \qquad V = W_V C^T$$



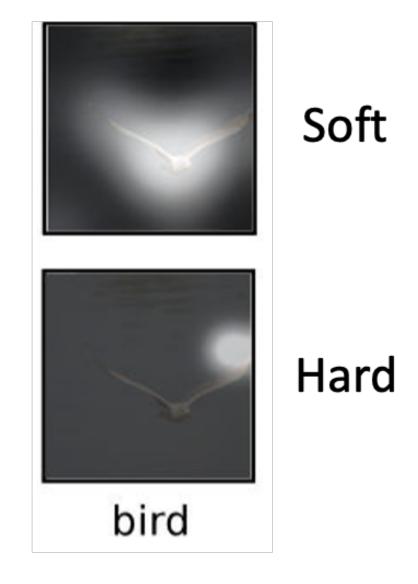
General form of attention: key-value-query

- Attention is a way to compute a weighted sum of the values dependent on the query and the corresponding keys.
 - All of these (key value query) are represented using vectors
 - The query and key are used for addressing (contains partial information).
 While the values provide more complete information
 - The weighted sum is a **selective summary** of the information found in the values.
 - It is a way to obtain a **fixed-sized representation** of an arbitrary set of representations (values) based on some other representation (the query)

Different types of attention

Soft vs Hard Attention

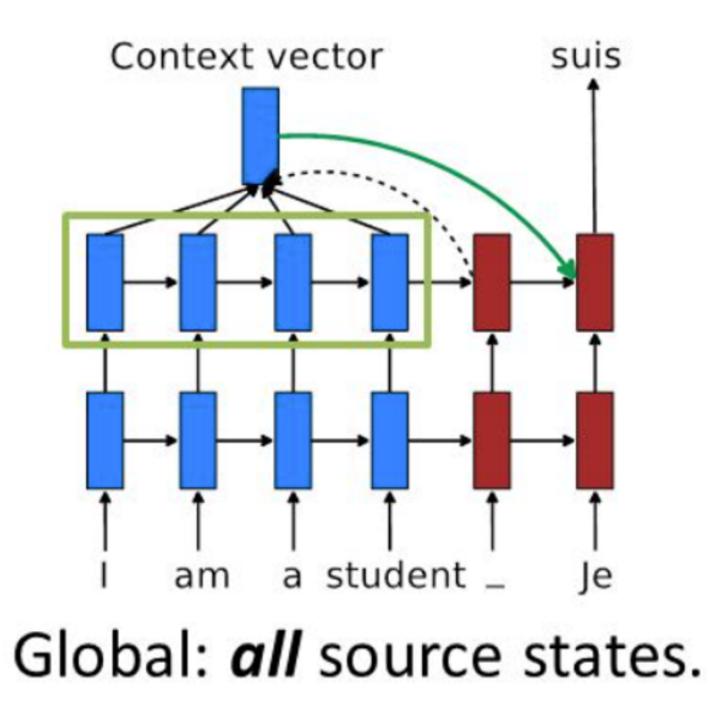
- Soft: Each attention candidate is weighted by α_i $\widehat{\boldsymbol{v}} = \sum_{i=1}^{k} \alpha_i \, \boldsymbol{v}_i$
 - Easy to train (smooth and differentiable) • But can be expensive over large input
- Hard: Use α_i as a sample probability to pick one attention candidate as input to subsequent layers Trainable with REINFORCE approaches (Xu et al. ICML) 2015), or Gumbel-Softmax (Jang et al. ICLR 2017)



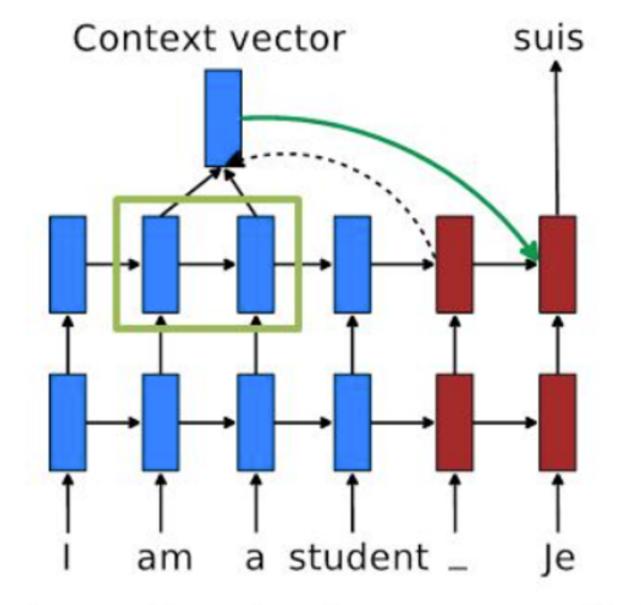
Xu et al. ICML 2015

Global vs Local Attention

- Global: attention over the entire input
- Local: attention over a window (or subset) of the input



e input (or subset) of the input

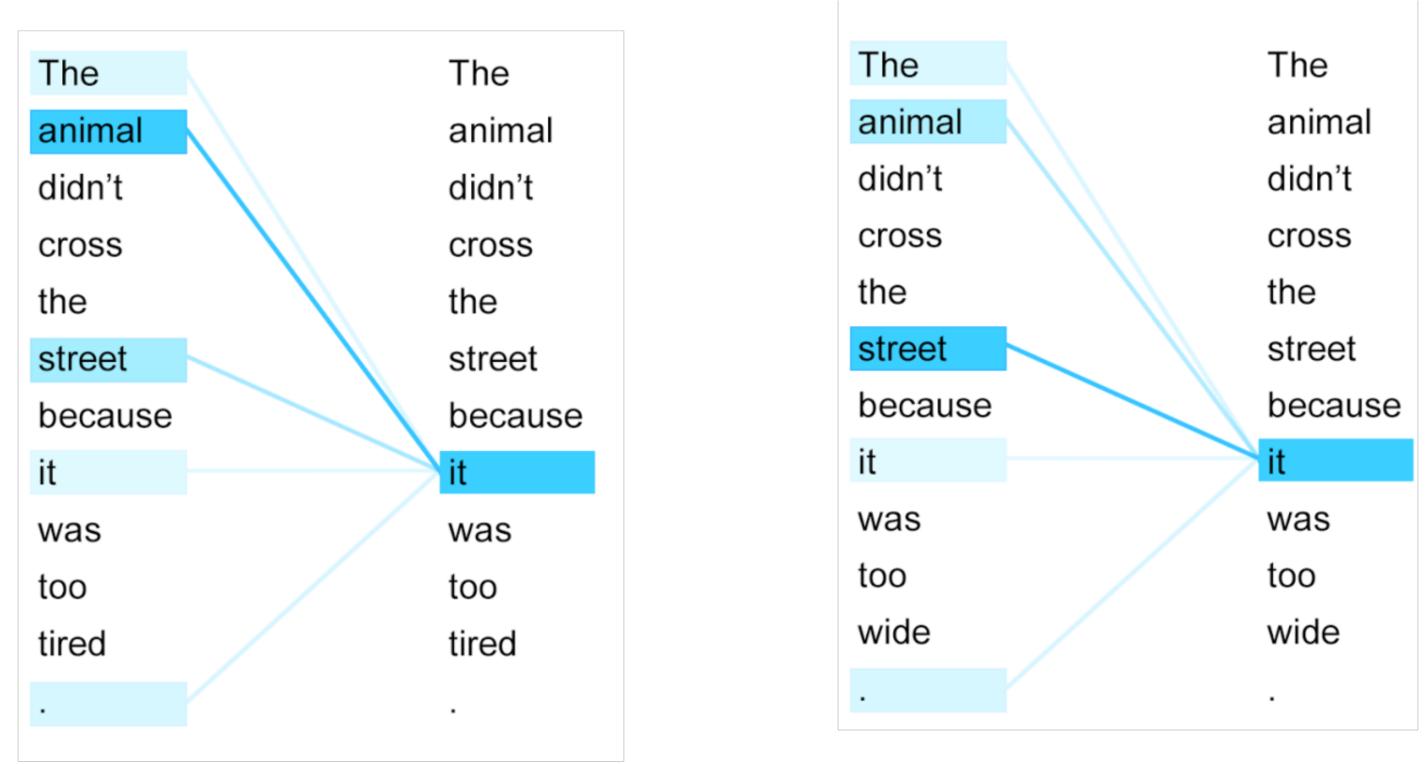


Local: subset of source states.

Luong et al, 2015

Self-Attention

• Attention (correlation) with different parts of itself

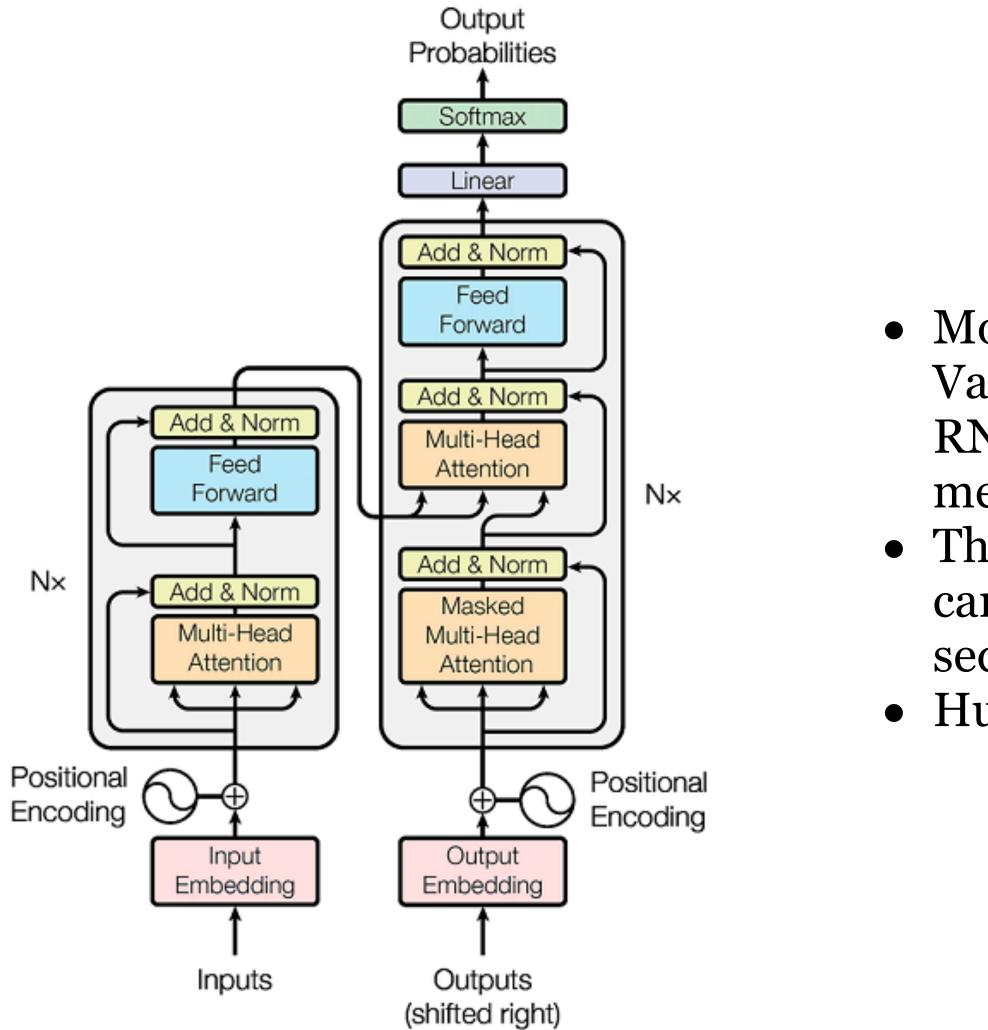


https://ai.googleblog.com/2017/08/transformer-novel-neural-network.html

Transformers: modules with scaled dot-product self-attention



Transformers: self-attention

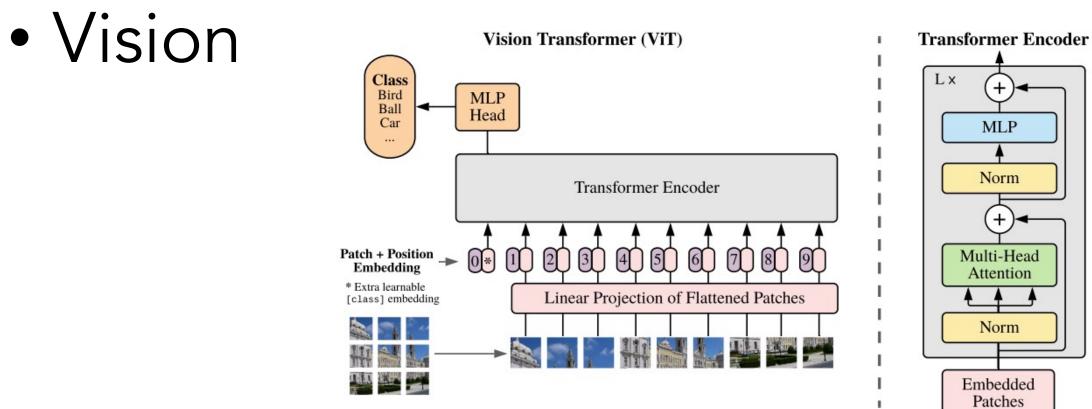


• More recent models (e.g. Transformer,

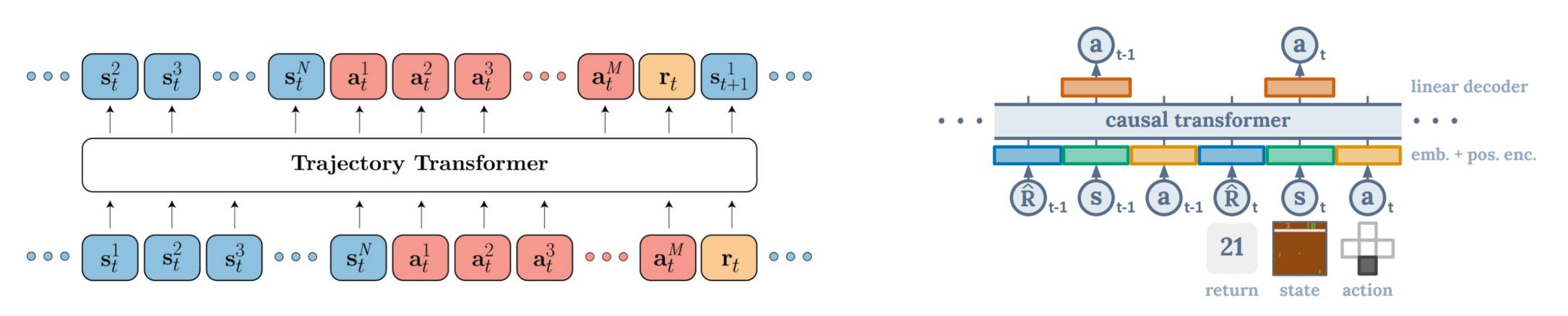
- Vaswani et al., 2017) have replaced
- RNNs entirely with attention
- mechanisms
- Theoretically limiting (since recurrence
 - can help handle arbitrarily long
 - sequences)
- Huge gains in practical performance

Transformers

Transformers are everywhere!



Reinforcement Learning



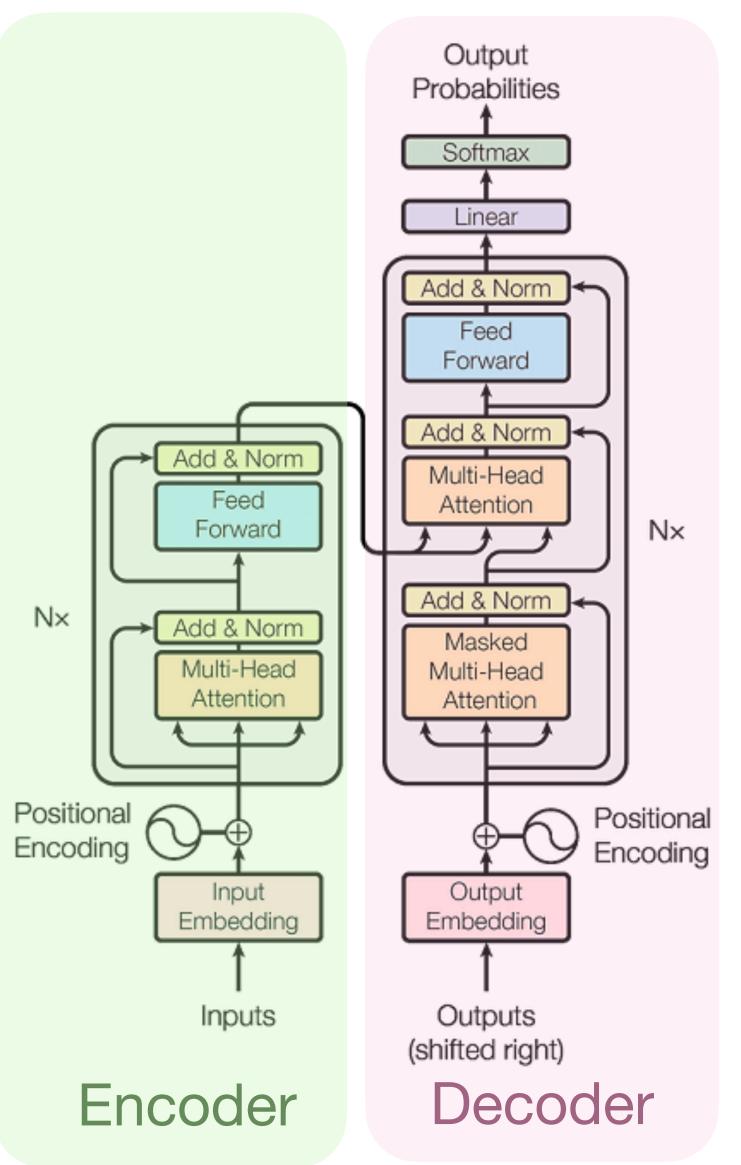
Trajectory Transformer [Janner et al, 2021]

An Image is Worth 16x16 Words: Transformers for Image Recognition at Scale, Dosovitskiy et al, ICLR 2021

Decision Transformer [Chen et al, 2021]

Transformers

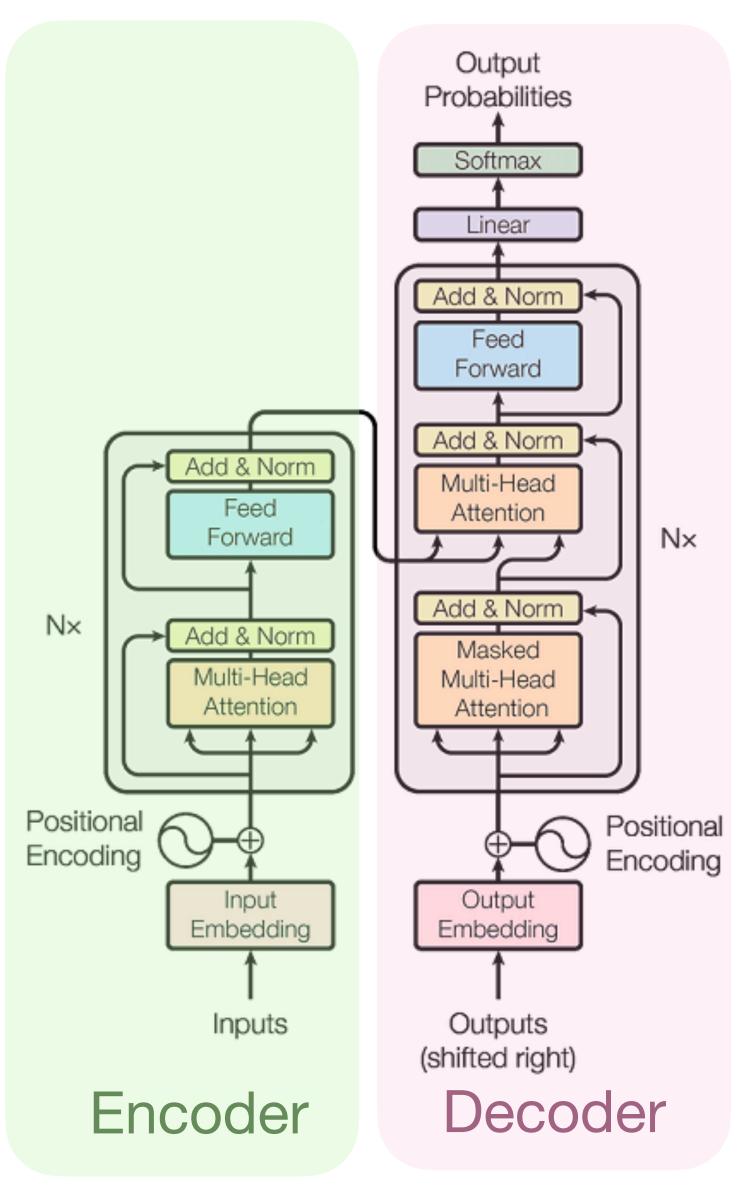
- NIPS'17: Attention is All You Need
- Originally proposed for NMT (encoderdecoder framework)
- Used in most LLMs!
- Key idea: Multi-head self-attention
- No recurrence structure any more so it trains much faster



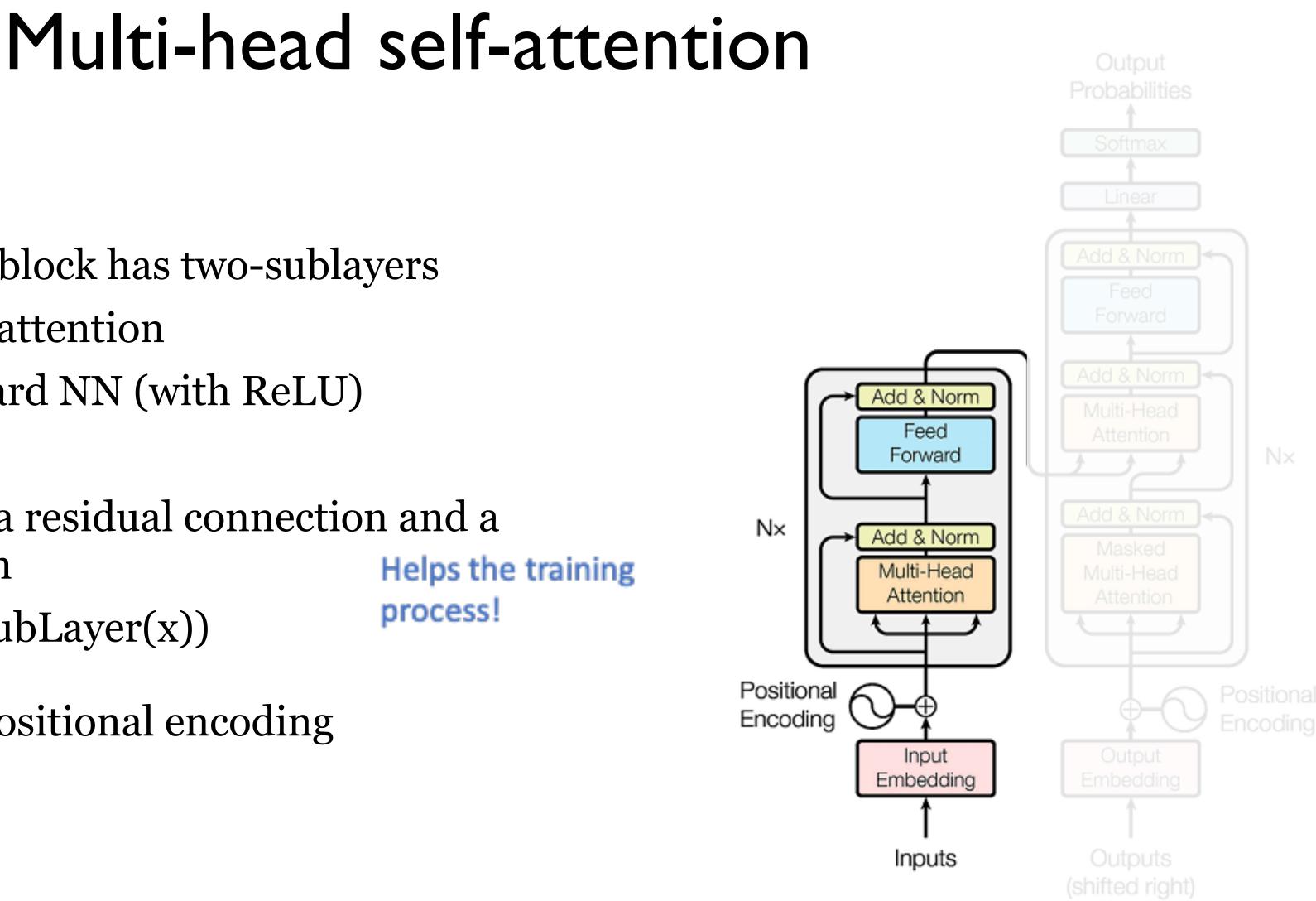
Understanding transformers

- From attention to self-attention
- From self-attention to multi-headed self-attention
- Transformer encoder
- Transformer decoder
- Putting the pieces together

ion -headed

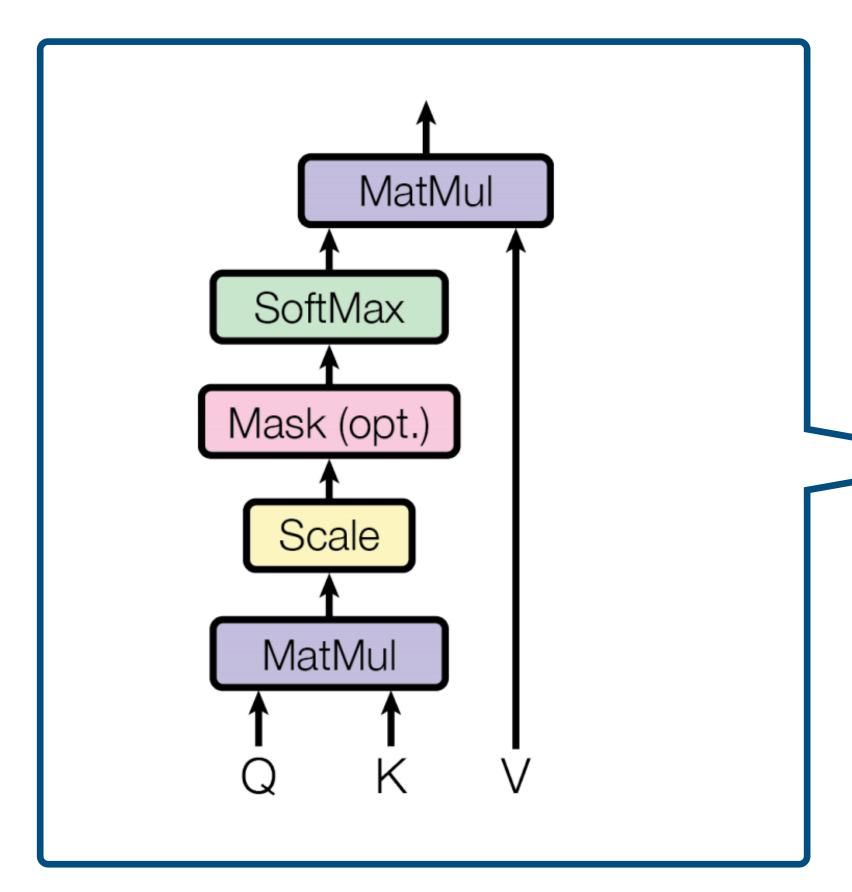


- Each Transformer block has two-sublayers
 - Multi-Head self-attention
 - 2 layer feedforward NN (with ReLU)
- Each sublayer has a residual connection and a layer normalization
 - LayerNorm(x+SubLayer(x))
- Input layer has a positional encoding



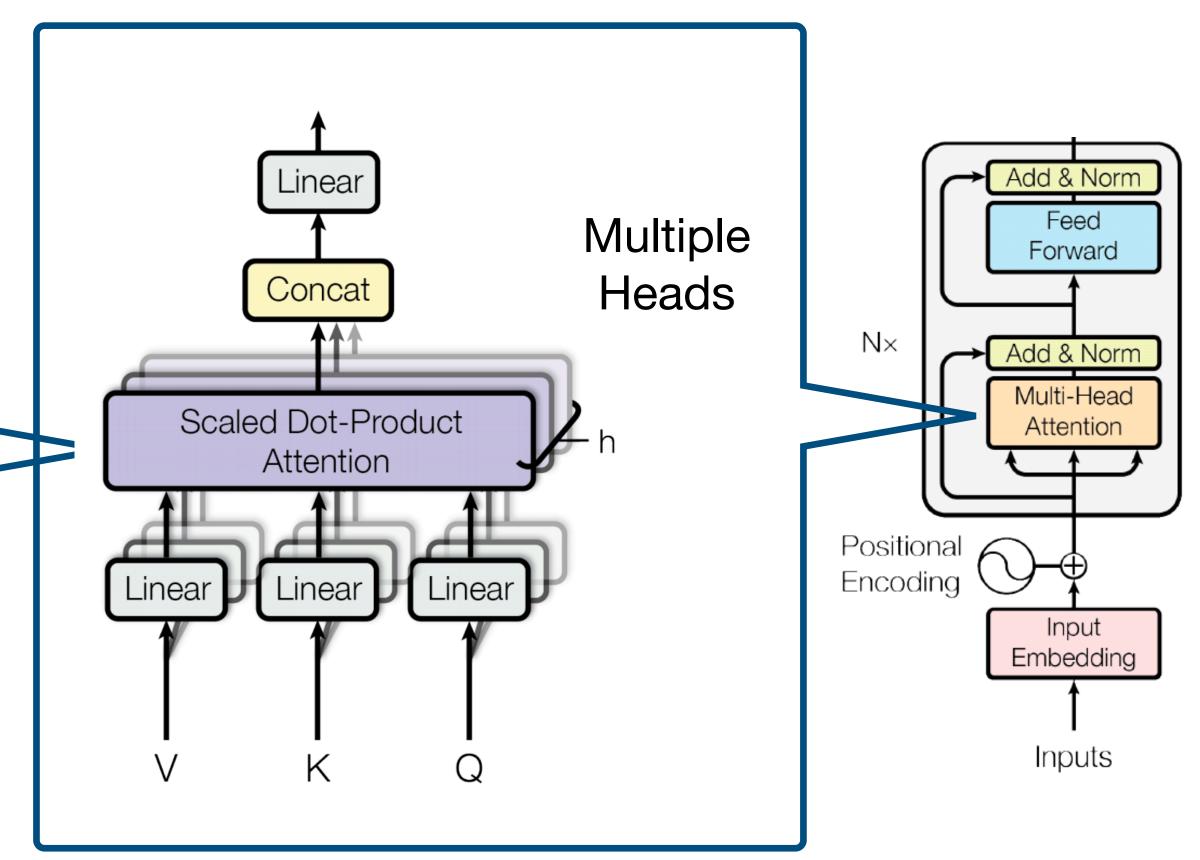
Multi-head self-attention

Scaled Dot-Product Attention



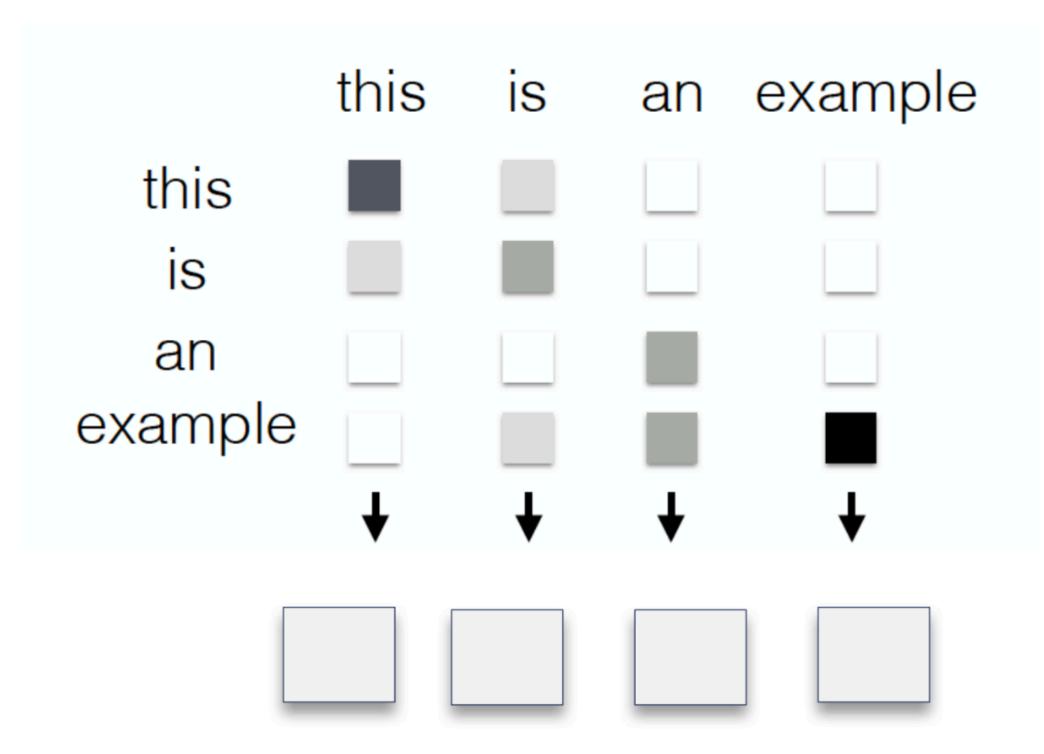
Attention Is All You Need https://arxiv.org/pdf/1706.03762.pdf

self-attention

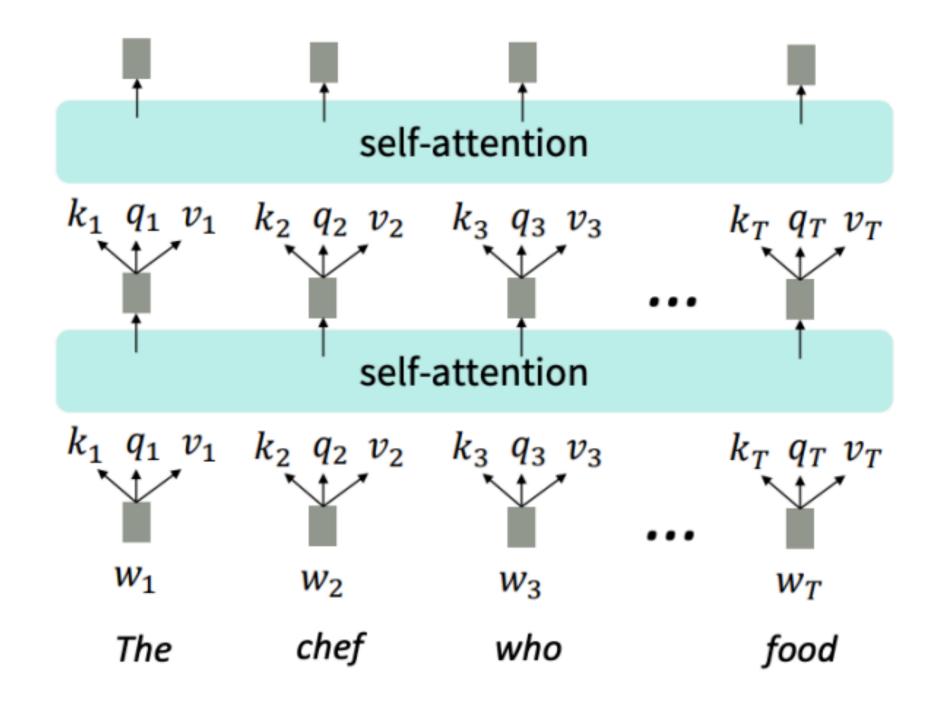


Self Attention

- **Self-attention**: let's use each word as query and compute the attention with all the other words (other words are the keys and values)
 - = the word vectors themselves select each other

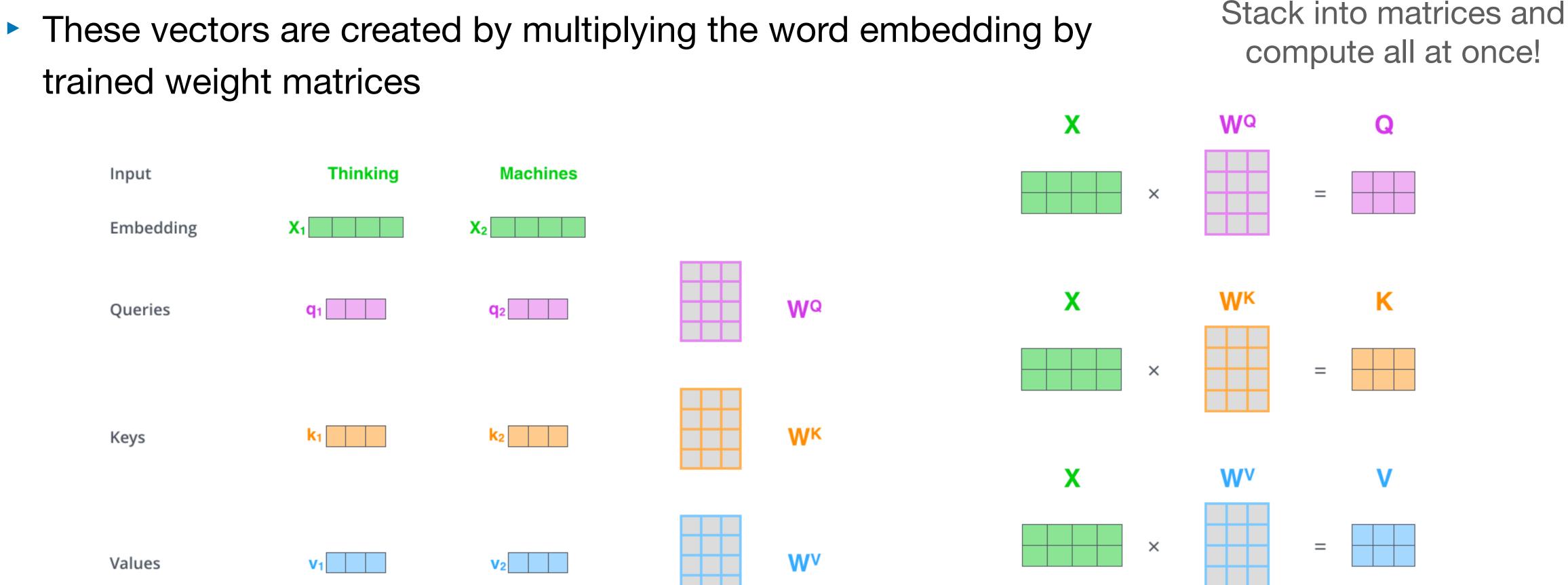


(also referred to as Intra-Attention)



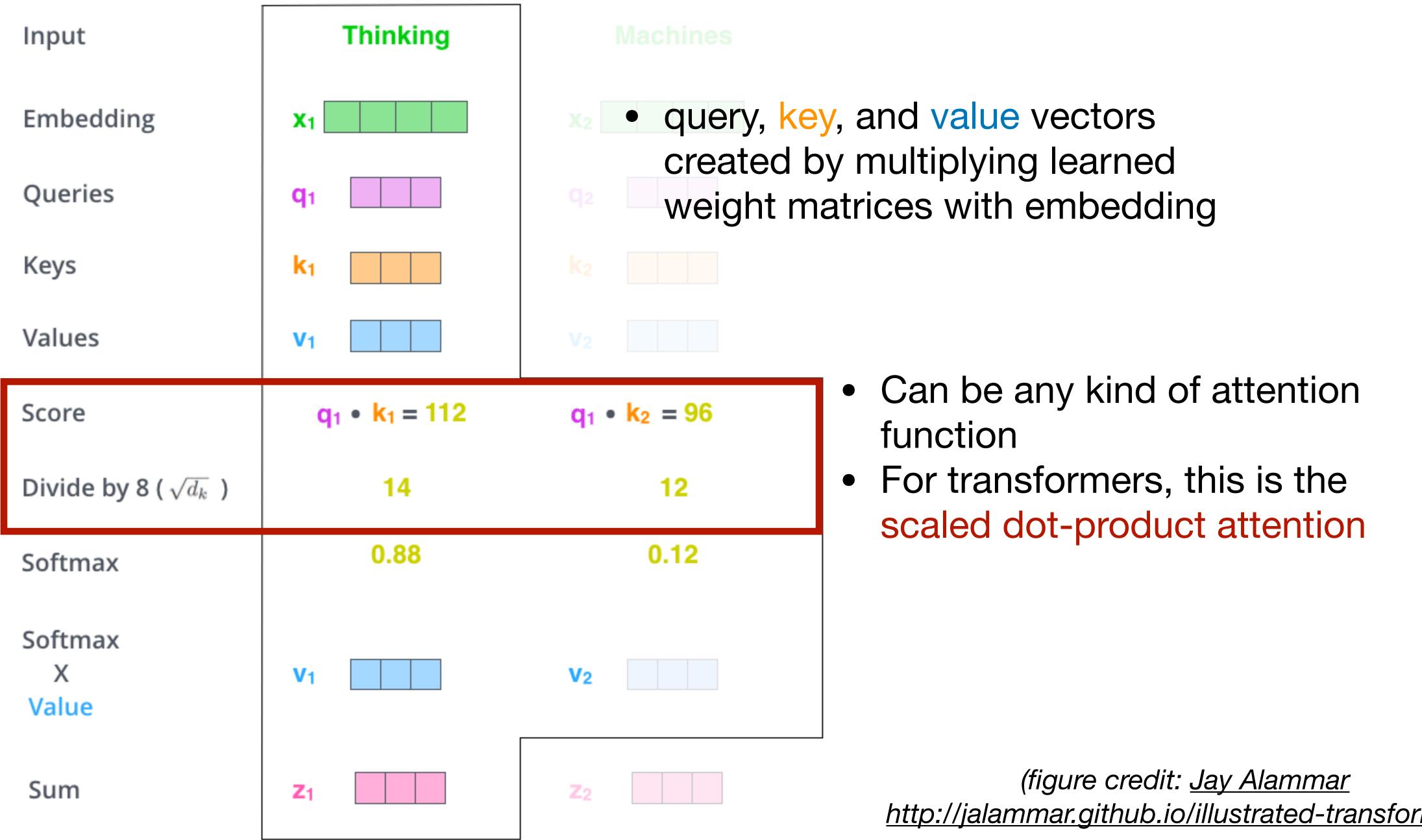
How to get key-value-query for each word?

- For each word, we have vectors for the key-value-query
- trained weight matrices



Inguie vieur. <u>Jay marinai</u> http://jalammar.github.io/illustrated-transformer/)





http://jalammar.github.io/illustrated-transformer/)



Recall: types of attention

- Assume keys $\mathbf{k}_1, \mathbf{k}_2, \ldots, \mathbf{k}_n$ and query \mathbf{q}
- **Dot-product attention** (assumes equal dimensions for \mathbf{k}_i and \mathbf{q}): 1. Simplest (no extra parameters) $g(\mathbf{k}_i, \mathbf{q}) = \mathbf{q}^T \mathbf{k}_i \in \mathbb{R}$ more efficient Does not work well for large dimensions (matrix multiplication) 2. Bilinear / multiplicative attention: More flexible $g(\mathbf{k}_i, \mathbf{q}) = \mathbf{k}^T \mathbf{W} \mathbf{k}_i \in \mathbb{R}$, where W is a weight matrix than dot-product (W is trainable)
 - Additive attention (essentially MLP): 3. $g(\mathbf{k}_i, \mathbf{q}) = \mathbf{w}^T \tanh(\mathbf{W}_1 \mathbf{k}_i + \mathbf{W}_2 \mathbf{q}) \in \mathbb{R}$ Perform better for larger dimensions where $\mathbf{W}_1, \mathbf{W}_2$ are weight matrices and \mathbf{w} is a weight vector







Scaled dot-product attention

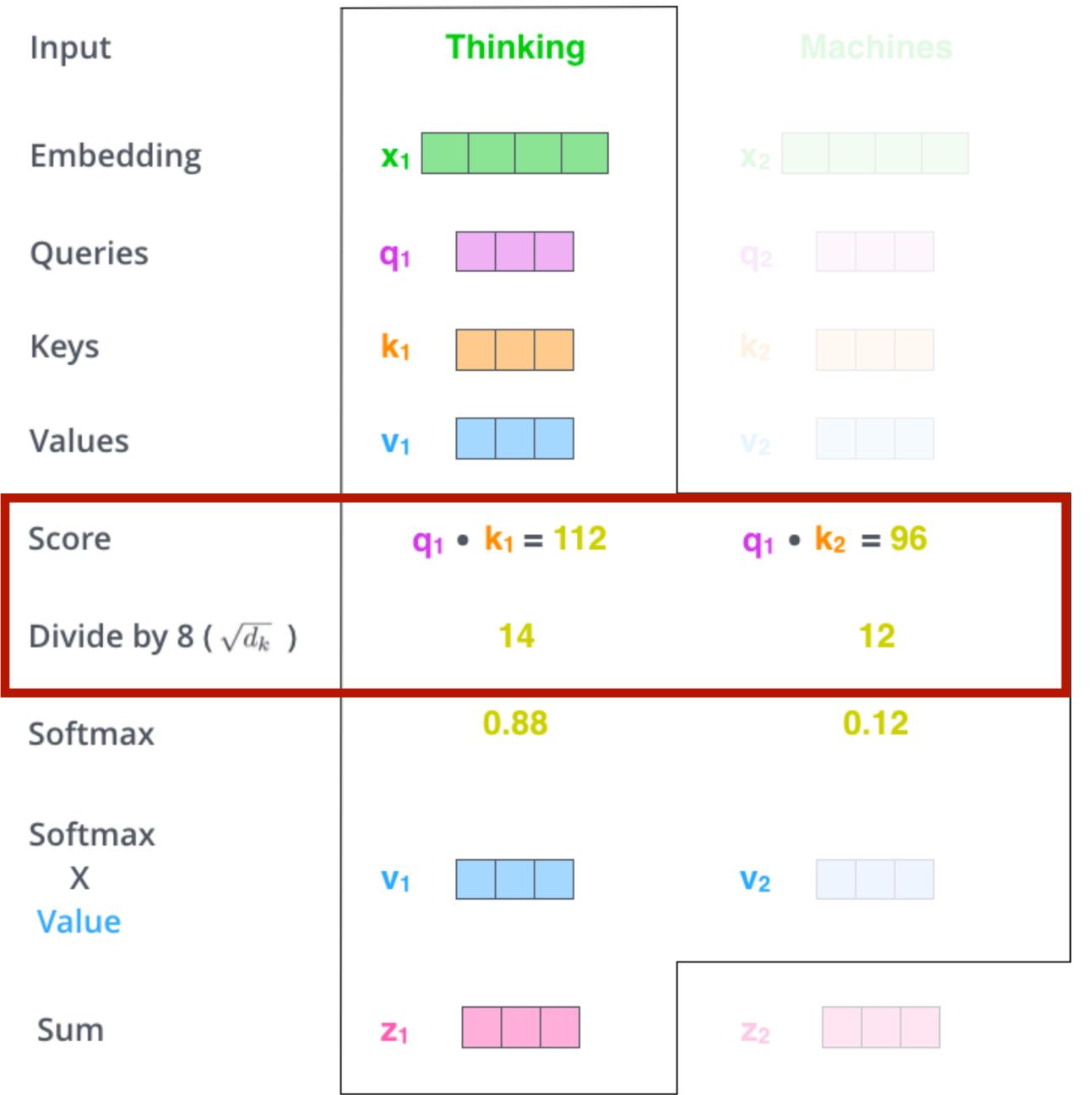
- Assume keys $\mathbf{k}_1, \mathbf{k}_2, \ldots, \mathbf{k}_n$ and query \mathbf{q}
- 1. $g(\mathbf{k}_i, \mathbf{q}) = \mathbf{q}^T \mathbf{k}_i \in \mathbb{R}$
- **Scaled dot-product attention:** 2. $g(\mathbf{k}_i, \mathbf{q}) = \frac{\mathbf{q}^T \mathbf{k}_i}{\sqrt{d}} \in \mathbb{R}$

Scaling factor: d = dimension of hidden state

Dot-product attention (assumes equal dimensions for \mathbf{k}_i and \mathbf{q}):

Scale of dot product increases as dimension gets larger Perform poorly for large d Softmax has small gradient

Scaled dot product will perform well for larger dimensions



- Can be any kind of attention function
- For transformers, this is the scaled dot-product attention
- z_1 is the final vector of attended values for "Thinking" as the query

(figure credit: <u>Jay Alammar</u> http://jalammar.github.io/illustrated-transformer/)



Self-attention in equations

- sequence of n vectors: $\mathbf{y}_1, \dots, \mathbf{y}_n \in \mathbb{R}^{d_2}$
 - $\mathbf{q}_{i} = W^{Q} \mathbf{x}_{i}, W^{Q} \in \mathbb{R}^{d_{q} \times d_{1}}$ $\mathbf{k}_{i} = W^{K} \mathbf{x}_{i}, W^{K} \in \mathbb{R}^{d_{k} \times d_{1}}$
- Note: this is similar as an RNN layer and can be used to replace an RNN layer $\begin{array}{l} \text{attention distribution} \\ \alpha_{i,j} = \operatorname{softmax} \left(\frac{\mathbf{q}_i \cdot \mathbf{k}_j}{\sqrt{d_k}} \right) \\ \text{Scaled dot-product} \\ \text{so } d_k = d_q \end{array}$
- First, construct a set of queries, keys, and values: • Second, for each \mathbf{q}_i , compute attentions scores and $\mathbf{v}_i = W^V \mathbf{x}_i, W^V \in \mathbb{R}^{d_v \times d_1}$

• Finally, compute the weighted sum:

• A self-attention layer maps a sequence of input vectors $\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathbb{R}^{d_1}$ to a

n $\mathbf{y}_i = \sum \alpha_{i,j} \mathbf{v}_j \in \mathbb{R}^{d_v}$ $d_{v} = d_{2}$ *j*=1

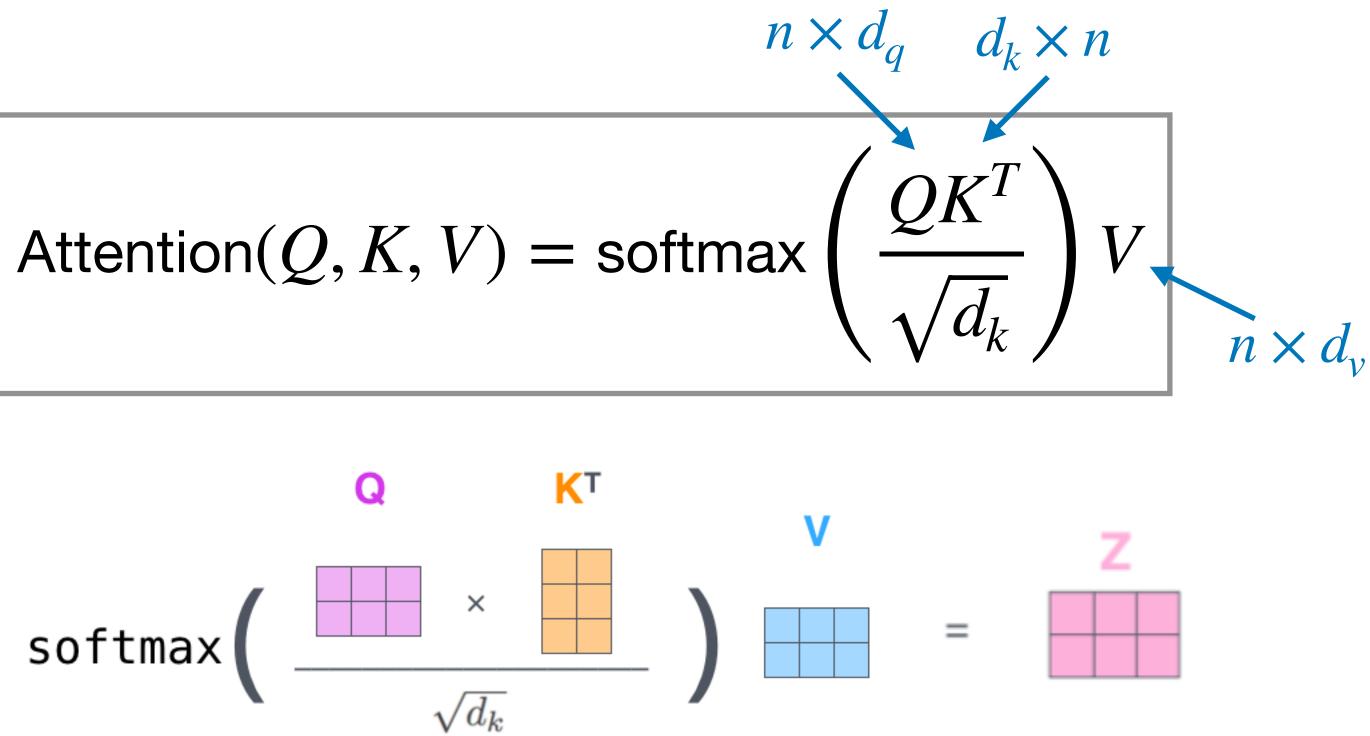
Self-attention: matrix notation

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

Note: the notation on this slide are following the original paper (= the transpose of the matrices in the previous slide)

Be careful to make sure the softmax is over the correct dimension

softmax



(figure credit: <u>Jay Alammar</u> http://jalammar.github.io/illustrated-transformer/)



Scaled Dot Product Attention Efficient, stable training vectors to attend to Scaled Dot-Product Attention attend over MatMul SoftMax Mask (opt.) Scale

Attention Is All You Need <u>https://arxiv.org/pdf/1706.03762.pdf</u>

K V

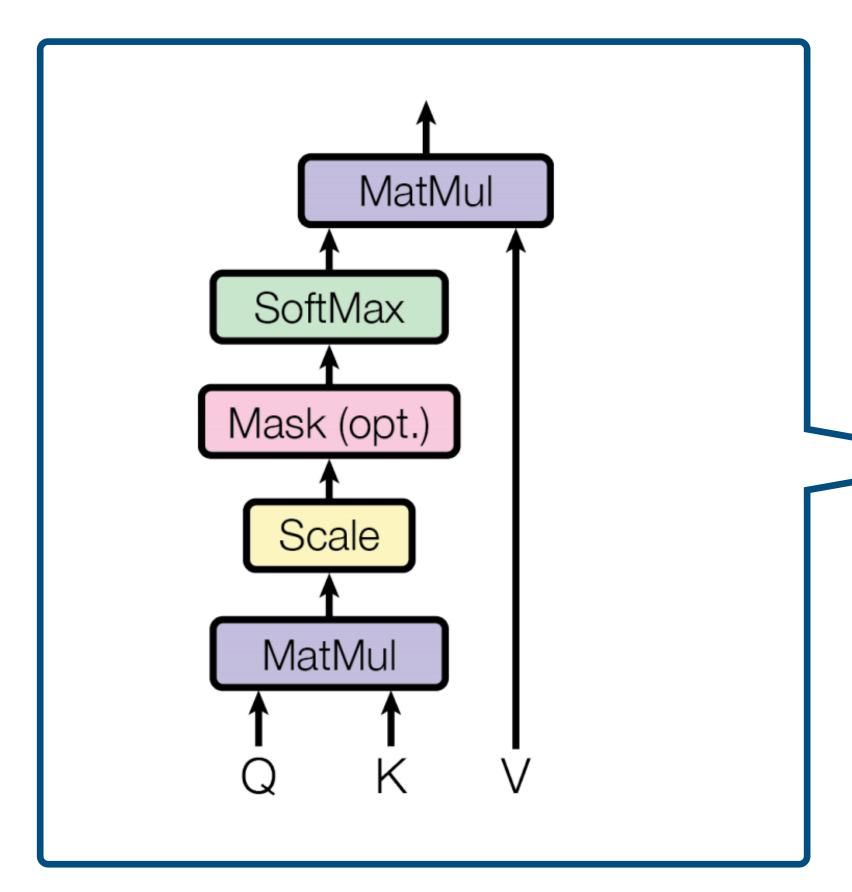
MatMul

- Let $Z \in \mathbb{R}^{M \times d_z}$ be a matrix of task context
- Let $C \in \mathbb{R}^{N \times d_C}$ be a matrix of input vectors to
- **SDPAttention**(**Z**, **C**):
- $Q = W_Q Z^T \qquad W_Q \in \mathbb{R}^{d_q \times d_Z} \qquad d_q = d_k$ $K = W_K C^T \qquad W_K \in \mathbb{R}^{d_k \times d_C}$ $V = W_V C^T \qquad W_V \in \mathbb{R}^{d_v \times d_C}$ Return $\hat{V} = softmax \left(\frac{Q^T K}{\sqrt{d_k}}\right) V$ $\hat{V} \in \mathbb{R}^{M \times d_{v}}$ be a matrix of attended values



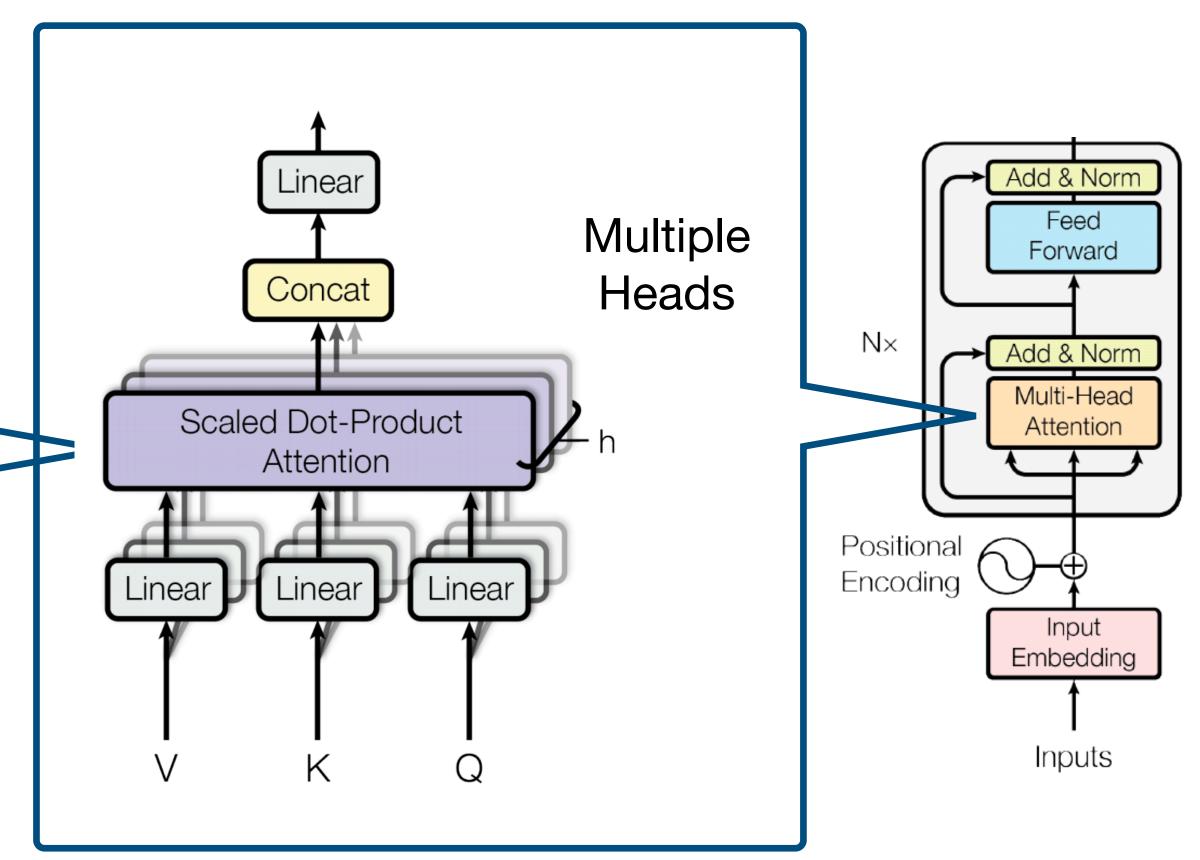
Multi-head self-attention

Scaled Dot-Product Attention



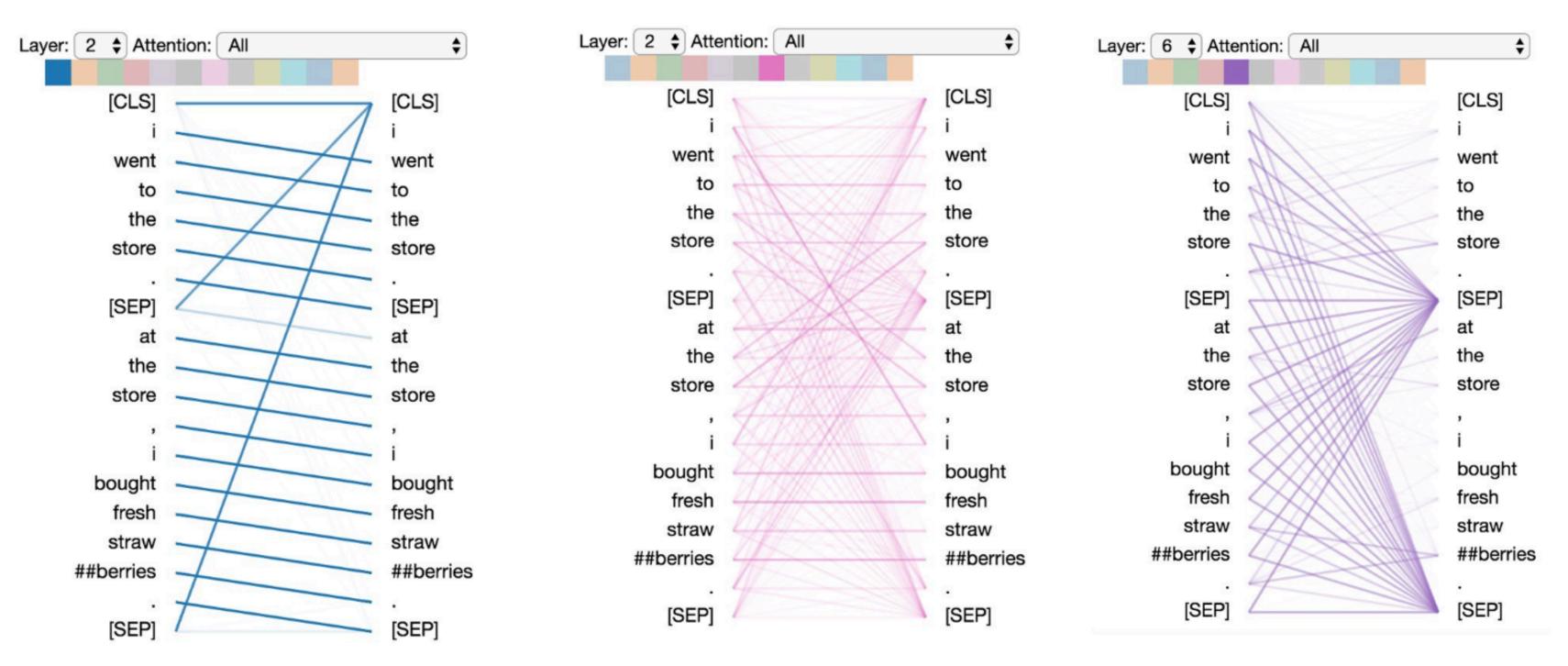
Attention Is All You Need https://arxiv.org/pdf/1706.03762.pdf

self-attention



Multi-head self-attention

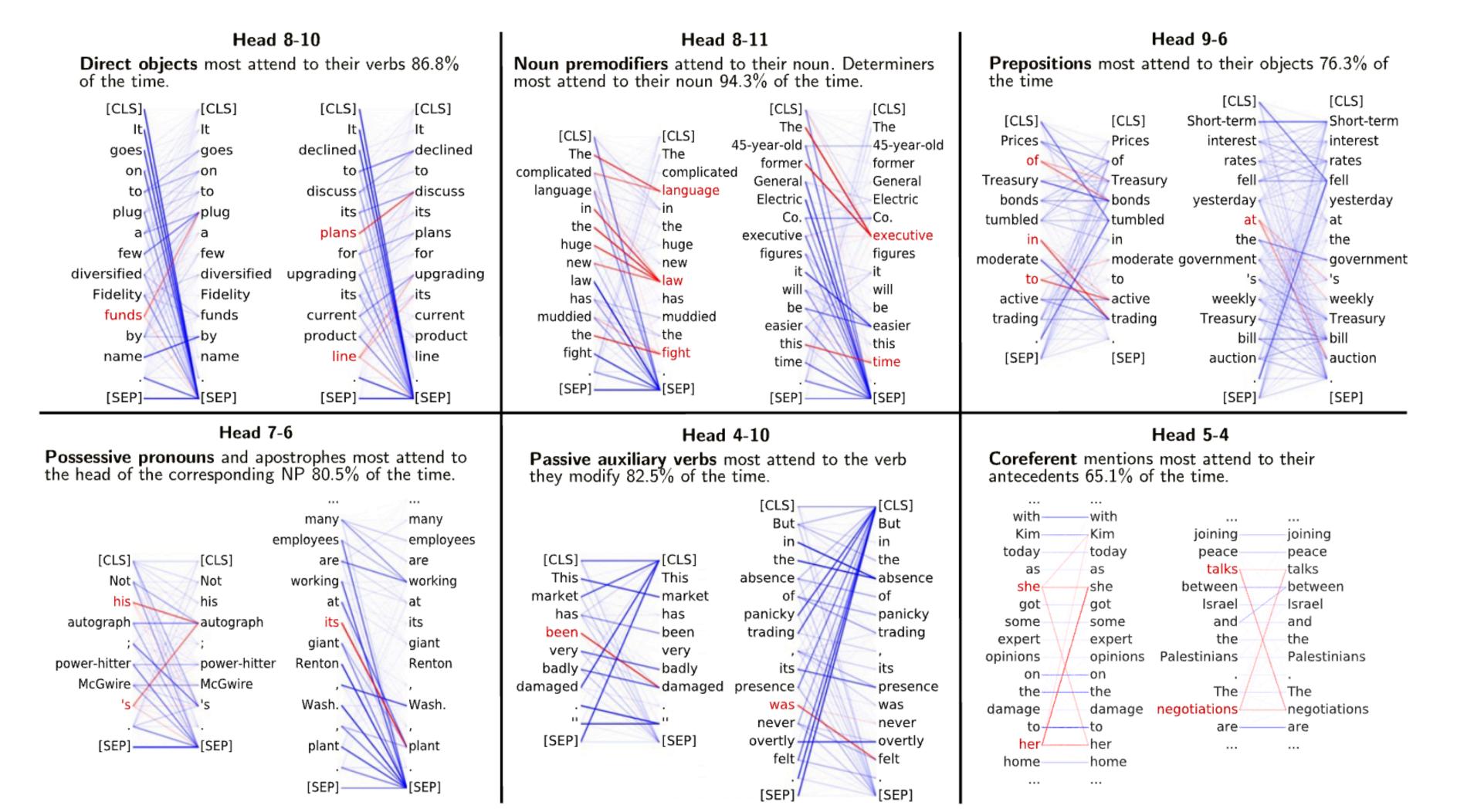
One head is not expressive enough. Let's have multiple heads! Multihead(Q, K, V) = Concat(head₁, ..., head_h) W^O In practice, h = 8, $d = d_{out}/h, W^O \in \mathbb{R}^{d_{out} \times d_{out}}$ head_i = $A(XW_i^Q, XW_i^K, XW_i^V)$



https://github.com/jessevig/bertviz

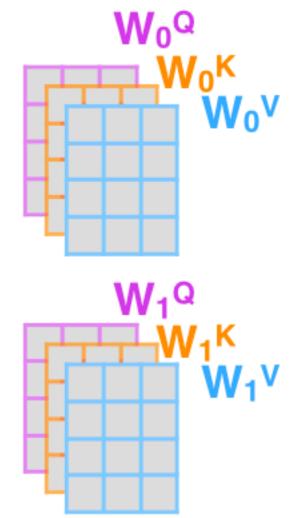
Why different heads?

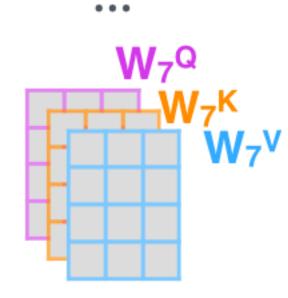
• Different heads learn to attend to different things



Emergent linguistic structure in artificial neural networks trained by self-supervision, Manning et al, PNAS 2019

- Multiple (different) representations for each query, key, and values
- Different weight matrices —> different vectors
- Different ways for the words to interact with each other

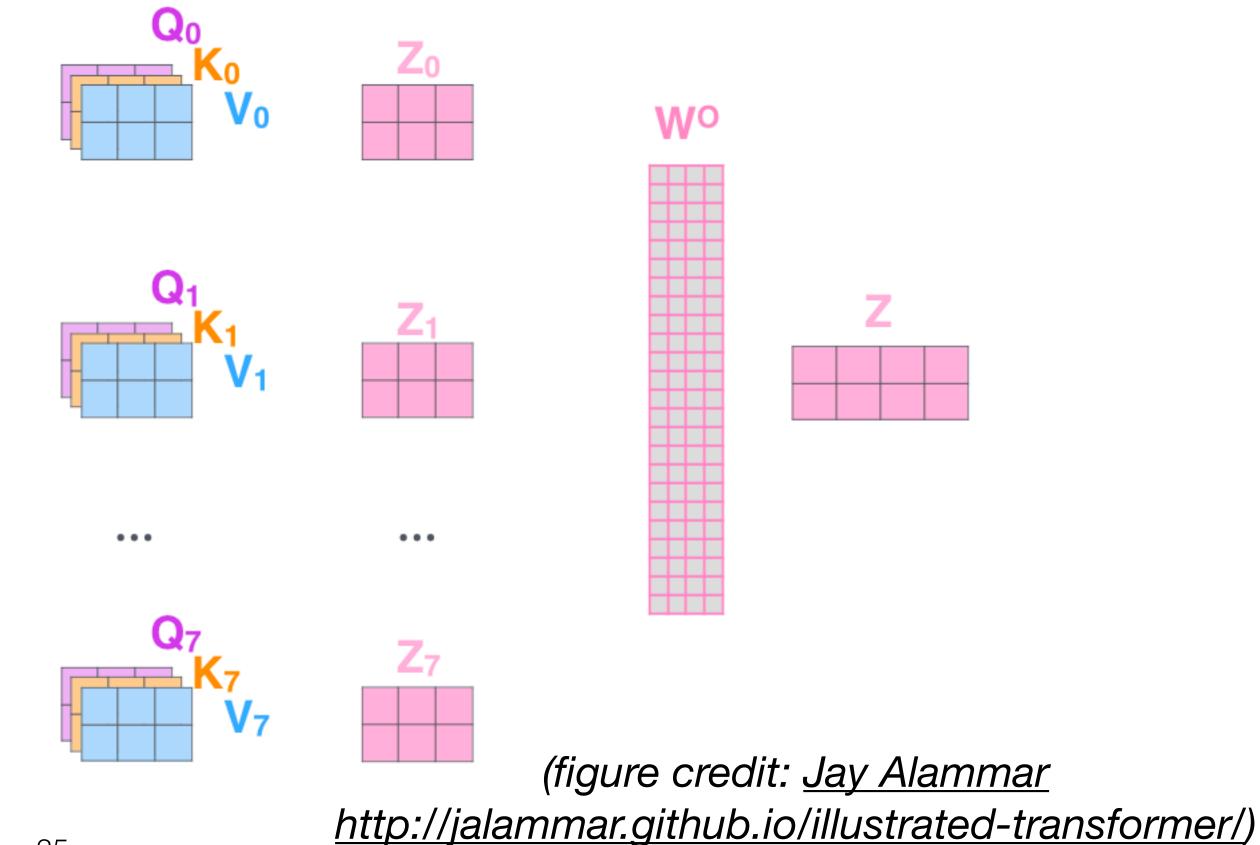




Multiple heads

4) Calculate attention using the resulting Q/K/V matrices

5) Concatenate the resulting Z matrices, then multiply with weight matrix W^o to produce the output of the layer





Multi-head attention

Multihead(Q, K, V)

In practice, we use a reduced dimension for each head.

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

$$d_q = d_k = d_v = d/h$$
 $d = hidden size, h = # of heads$

$$W^{O} \in \mathbb{R}^{d \times d_{2}}$$

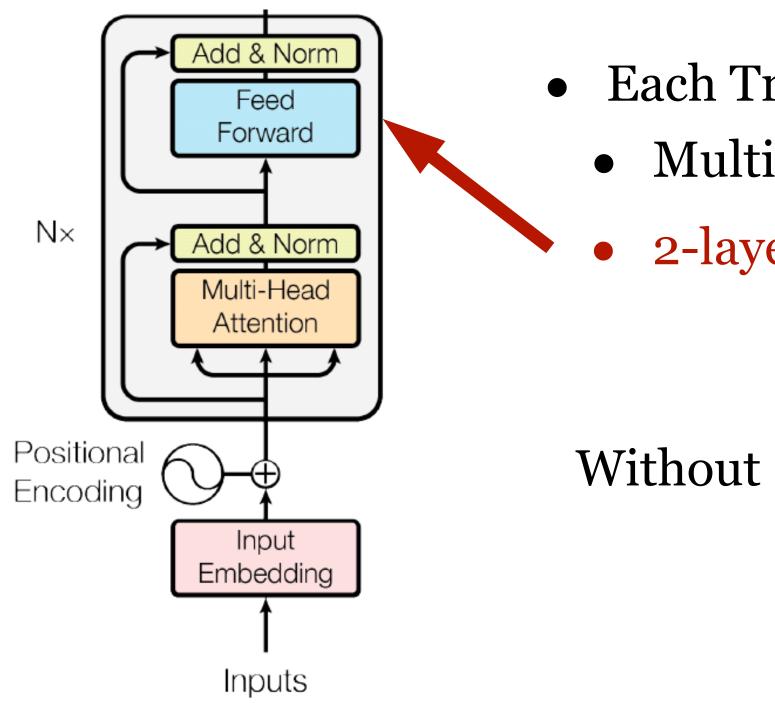
head attention with full dimensionality

= Concat(head₁, ..., head_h)
$$W^O$$

head_i = $A(XW_i^Q, XW_i^K, XW_i^V)$

If we stack multiple layers, usually $d_1 = d_2 = d$ The total computational cost is similar to that of single-

Transformer Encoder



Each Transformer block has two sub-layers
Multi-head attention

2-layer feedforward NN (with ReLU)

Without FFNN: No non-linearity!

Adding nonlinearities

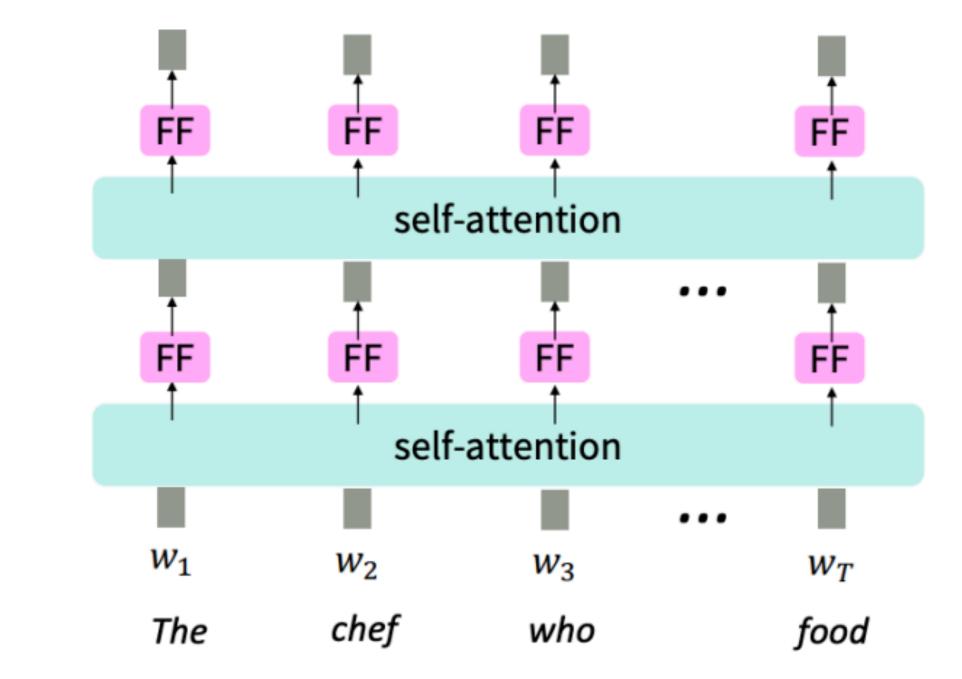
- There is no elementwise nonlinearities in selfattention; stacking more self-attention layers just reaverages value vectors
- Simple fix: add a feed-forward network to post-process each output vector

$$FFN(\mathbf{x}_i) = W_2 ReLU(W_1 \mathbf{x}_i + \mathbf{b}_1) + \mathbf{b}_2$$

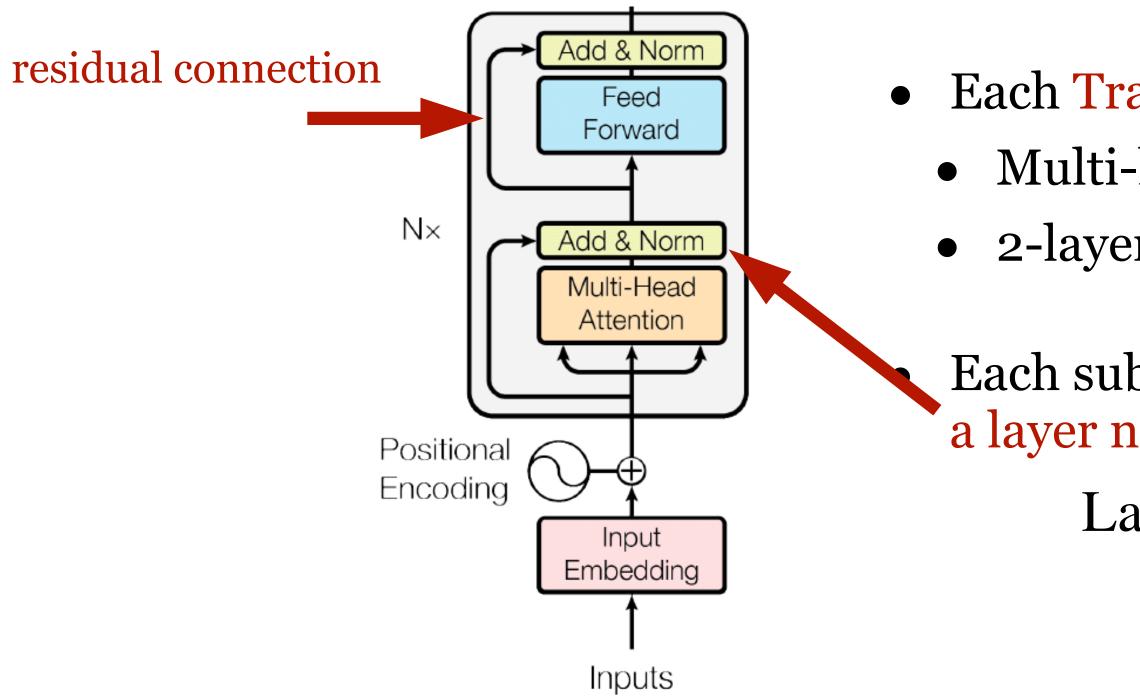
 $W_1 \in \mathbb{R}^{d_{ff} \times d}, \mathbf{b}_1 \in \mathbb{R}^{d_{ff}}$

$$W_2 \in \mathbb{R}^{d \times d_{ff}}, \mathbf{b}_2 \in \mathbb{R}^d$$

In practice, they use $d_{ff} = 4d$



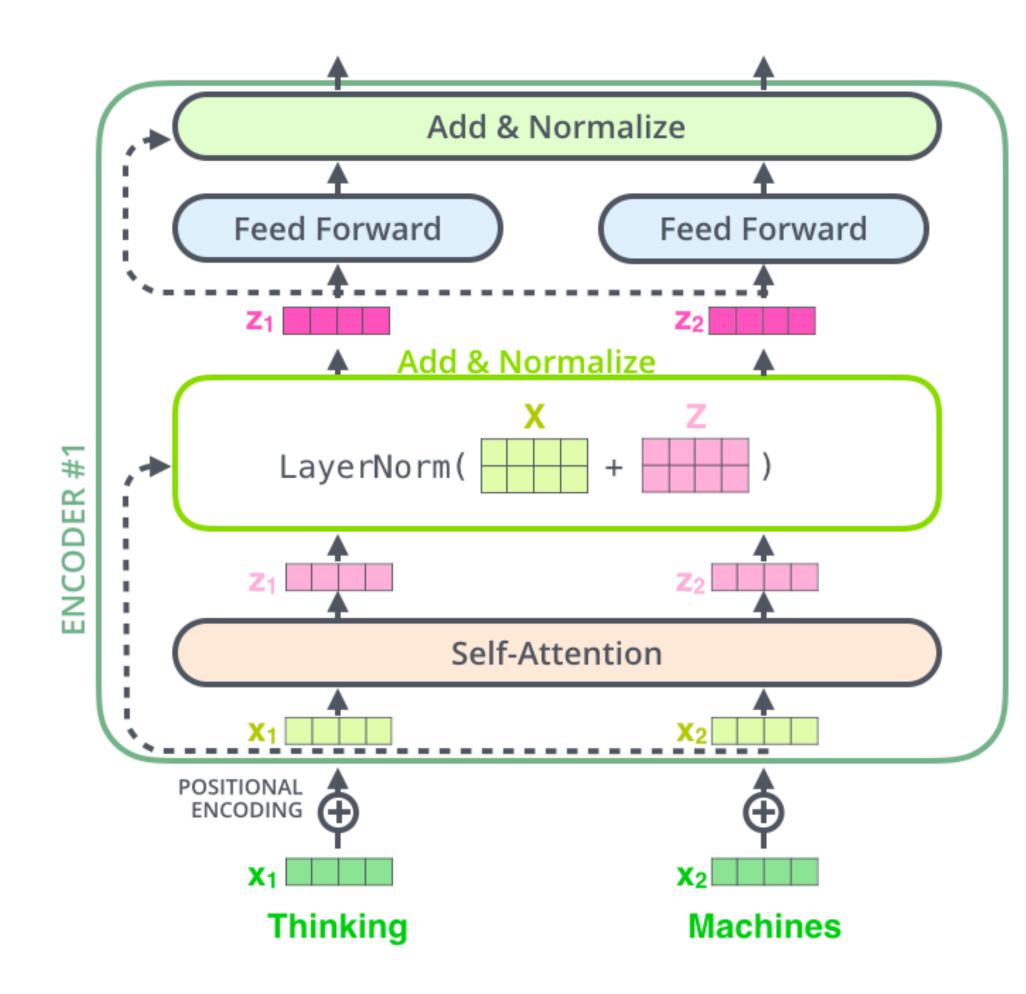
Transformer Encoder



(He et al, 2016): Residual connections

- Each Transformer block has two sub-layers
- Multi-head attention
- 2-layer feedforward NN (with ReLU)
- Each sublayer has a residual connection and a layer normalization
 - LayerNorm(x + SubLayer(x))

Residual connections and Layer Normalization



(figure credit: <u>Jay Alammar</u> http://jalammar.github.io/illustrated-transformer/)40

LayerNorm

- changes input features to have mean 0 and variance 1 per layer.
- Adds two more parameters

$$u^{l} = rac{1}{H} \sum_{i=1}^{H} a_{i}^{l} \qquad \sigma^{l} = \sqrt{rac{1}{H} \sum_{i=1}^{H} (a_{i}^{l} - \mu^{l})^{2}}$$

$$h_i = \frac{g_i}{\sigma_i} \left(a_i - \mu_i \right) + b_i$$

• For more stable and efficient training

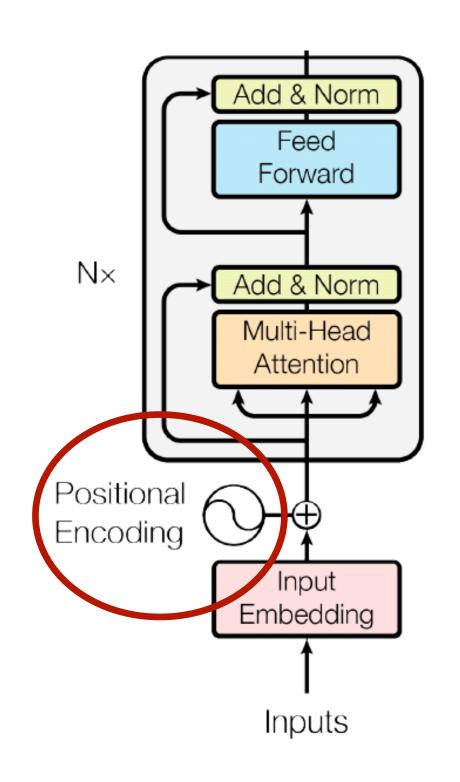
(Ba et al, 2016): Layer Normalization





Transformer Encoder

- Each Transformer block has two sub-layers
 - Multi-head attention
 - 2-layer feedforward NN (with ReLU)
- Each sublayer has a residual connection and a layer normalization
- Input layer has a positional encoding



(He et al, 2016): Residual connections

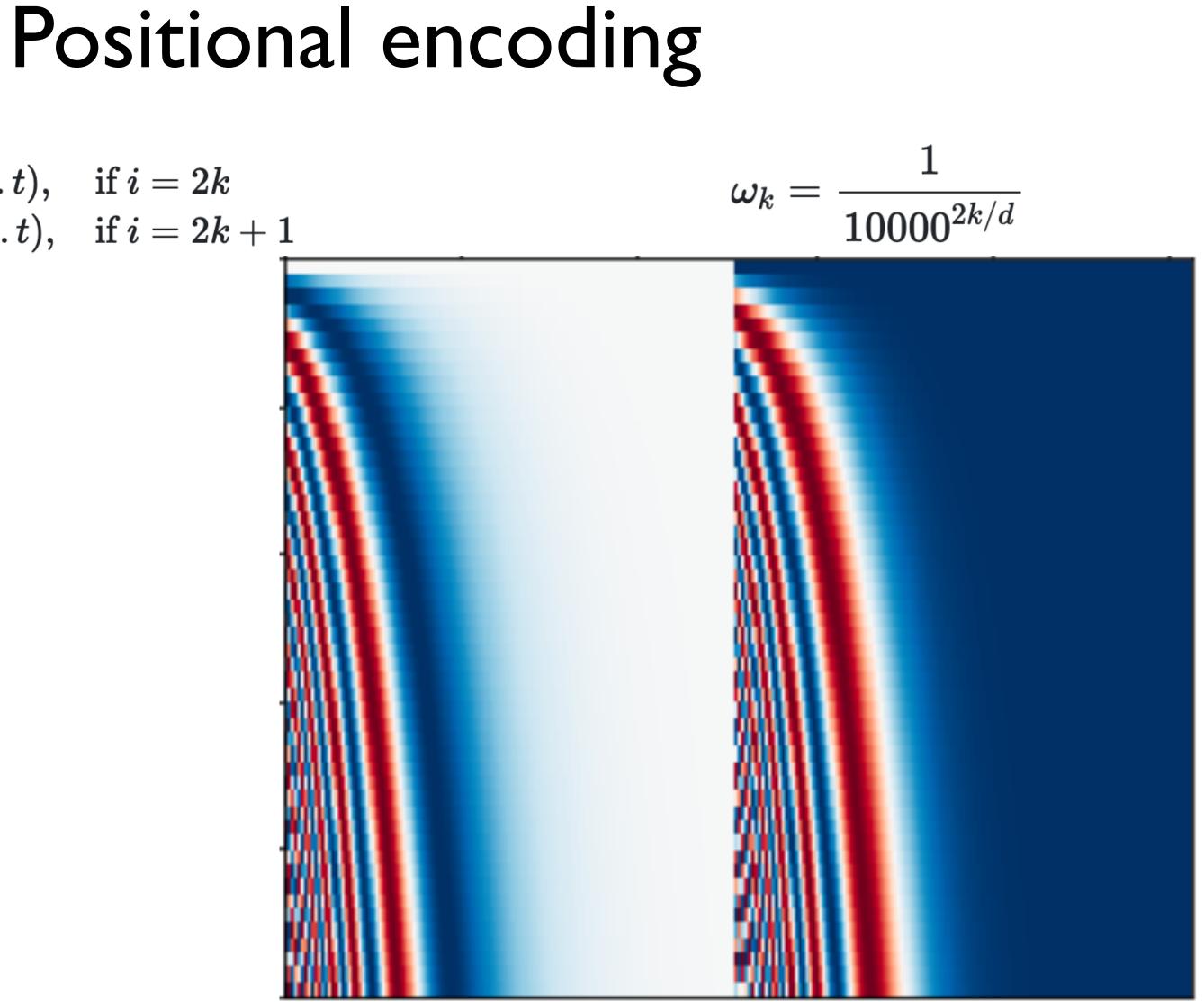
LayerNorm(x + SubLayer(x))

Necessary for the model to know the position of the token

(Ba et al, 2016): Layer Normalization

$$\overrightarrow{p_t}^{(i)} = f(t)^{(i)} := egin{cases} \sin(\omega_k.t), & ext{if } i = 2k \ \cos(\omega_k.t), & ext{if } i = 2k+1 \ \cos(\omega_1.t) \ \sin(\omega_2.t) \ \cos(\omega_2.t) \ dots \ \sin(\omega_{d/2}.t) \ \cos(\omega_{d/2}.t) \ \cos(\omega_{d/2}.t) \end{bmatrix}_{d imes 1}$$

t = position d = embedding dimension i = embedding index (0 to d-1)



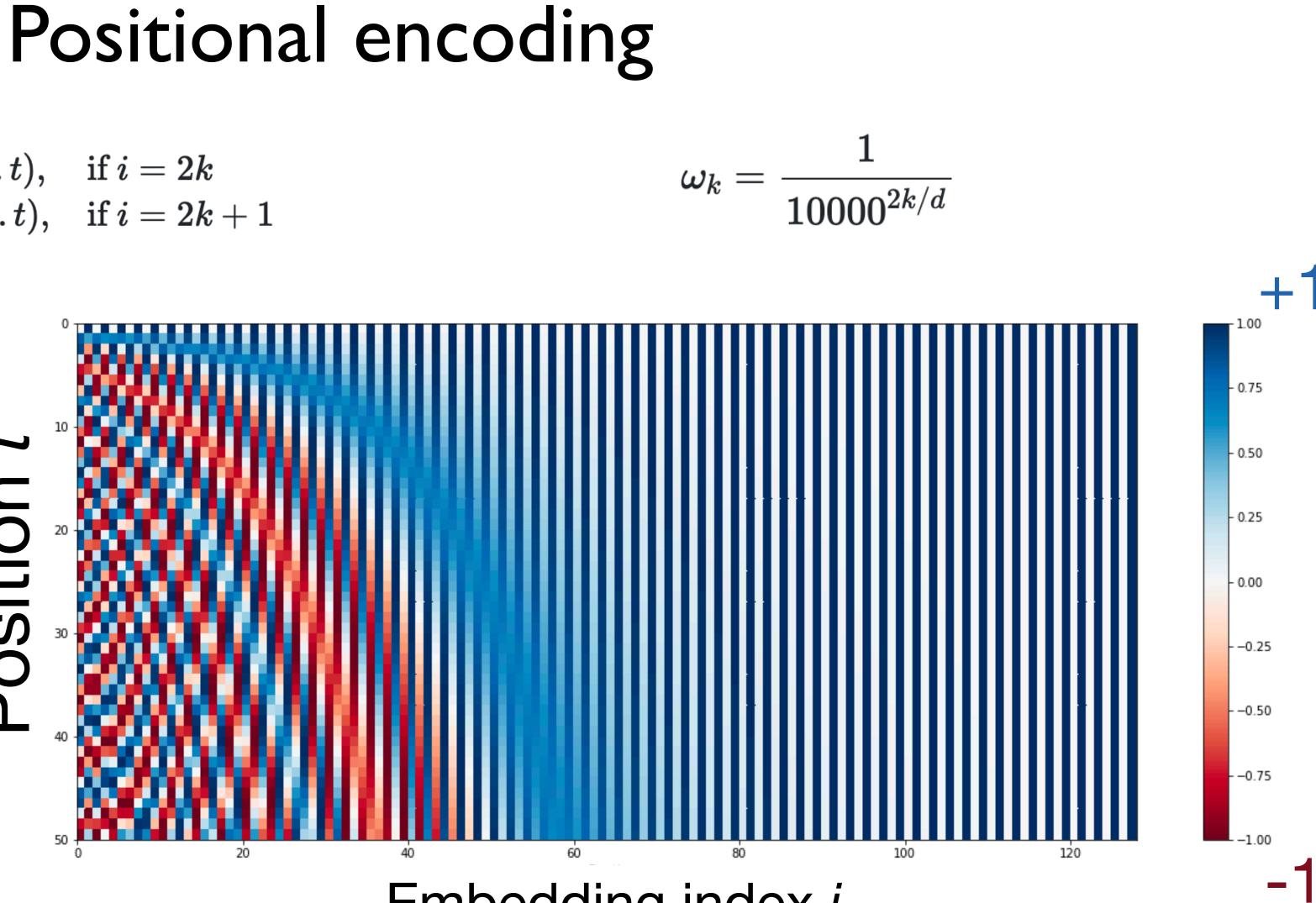
Sine

Cosine

$$\overrightarrow{p_t}^{(i)} = f(t)^{(i)} := egin{cases} \sin(\omega_k,t), & ext{if } i = 2k \ \cos(\omega_k,t), & ext{if } i = 2k+1 \end{cases}$$

$$\vec{p}_{t} = \begin{bmatrix} \sin(\omega_{1}, t) \\ \cos(\omega_{1}, t) \\ \sin(\omega_{2}, t) \\ \cos(\omega_{2}, t) \\ \vdots \\ \sin(\omega_{d/2}, t) \\ \cos(\omega_{d/2}, t) \end{bmatrix}_{d \times 1}$$

t = position d = embedding dimension i = embedding index (0 to d-1)



Embedding index *i*



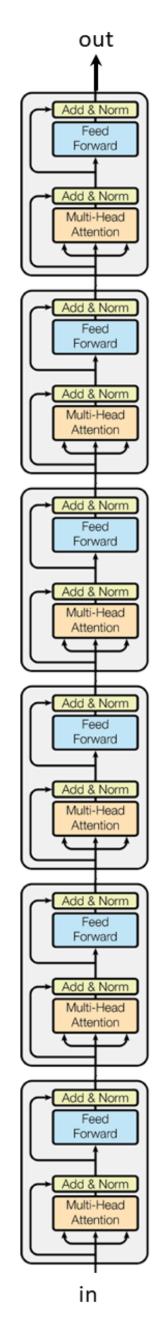
4

Transformer Non-recurrent, deep model with attention

Add & Norm Feed Forward N× Add & Norm Multi-Head Attention Positional Encoding Input Embedding Inputs

- BERT_base: 12 layers, 12 heads, hidden size = 768, 110M parameters
- BERT_large: 24 layers, 16 heads, hidden size = 1024, 340M parameters

(He et al, 2016): Residual connections



Transformer encoder

- Each Transformer block has two sub-layers
- Multi-head attention
 - 2-layer feedforward NN (with ReLU)
- Each sublayer has a residual connection and a layer normalization
 - LayerNorm(x + SubLayer(x))
- Input layer has a positional encoding
 - Input embedding is byte pair encoding (BPE)

Encoder Layer 2

original

Encoder Layer 6

Encoder Layer 5

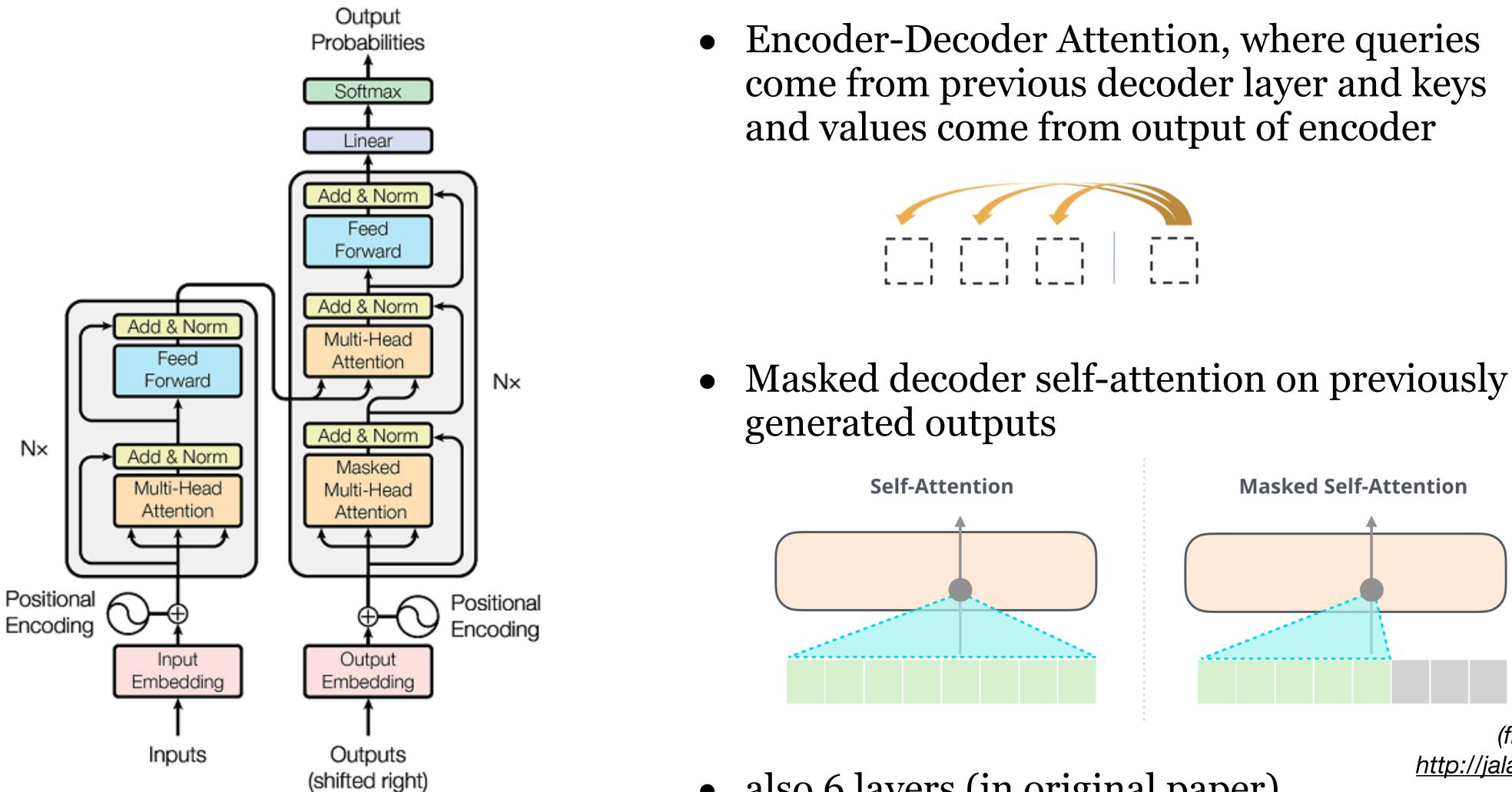
Encoder Layer 4

Encoder Layer 3

Encoder Layer 1

(Ba et al, 2016): Layer Normalization

Transformer decoder

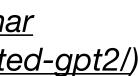




(figure credit: <u>Jay Alammar</u> http://jalammar.github.io/illustrated-gpt2/)

• also 6 layers (in original paper)

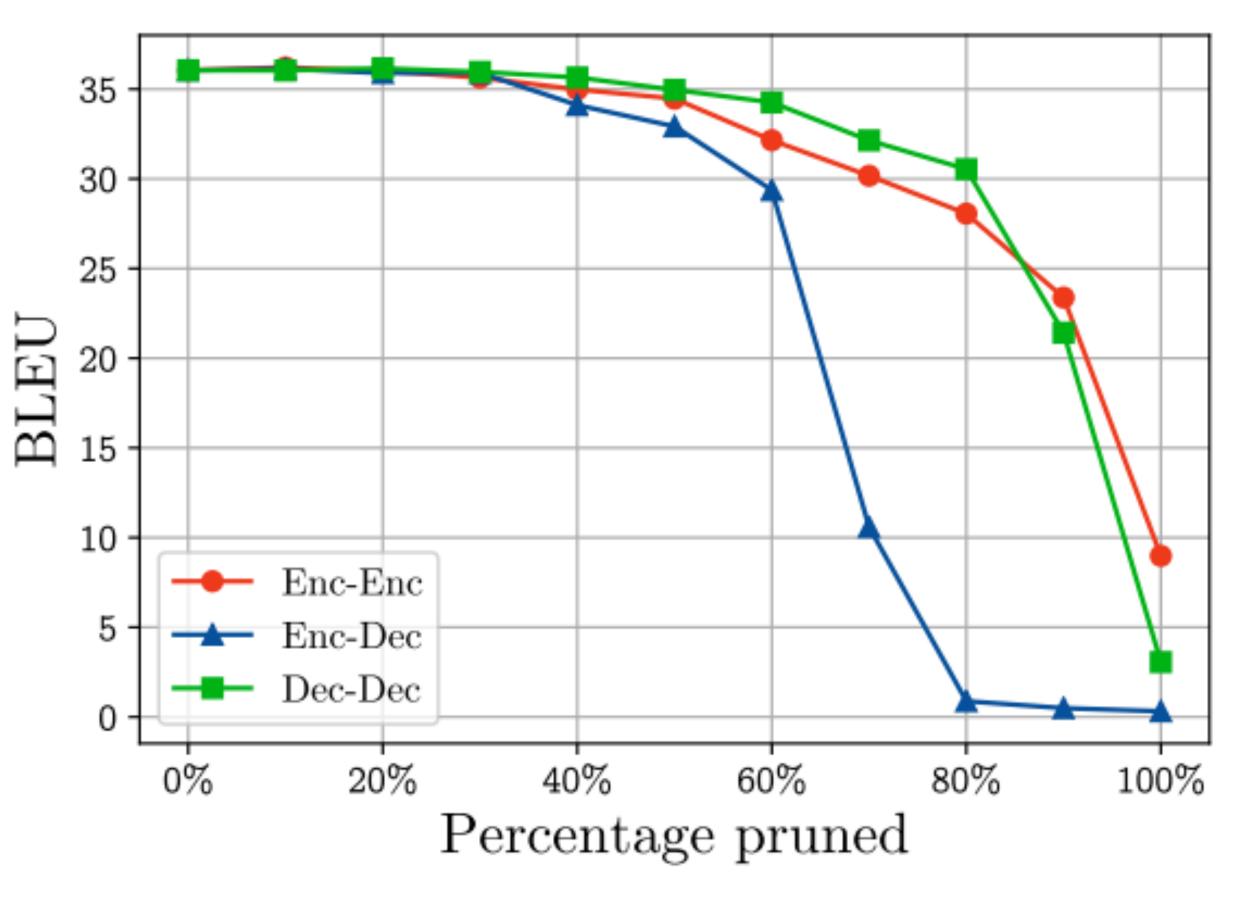
45



Do we need all these heads?

3 types of attention: Enc-Enc, Enc-Dec, Dec-Dec 6 layers, 16 heads each layer for each type

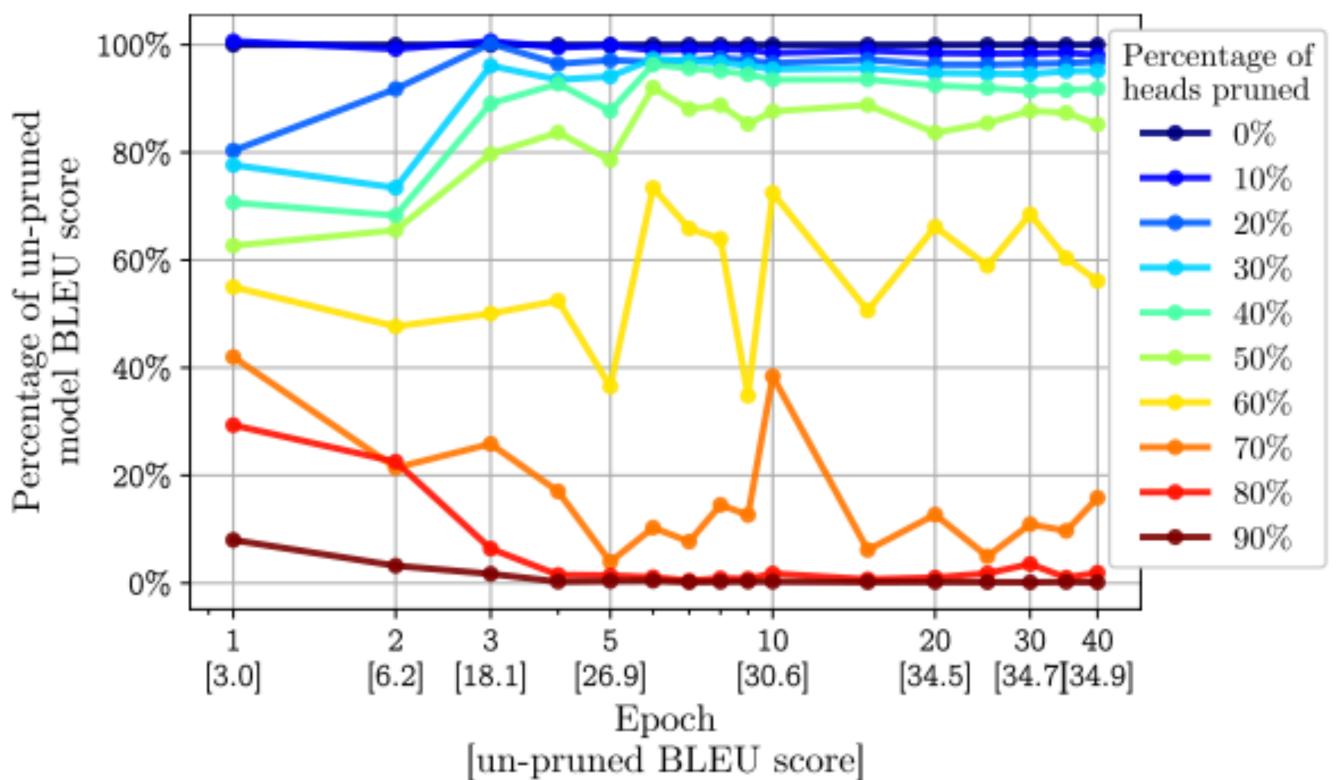
• Can we prune away some of the heads of a trained model during test time?



Are Sixteen Heads Really Better than One? Michel, Levy, and Neubig, NeurIPS 2019

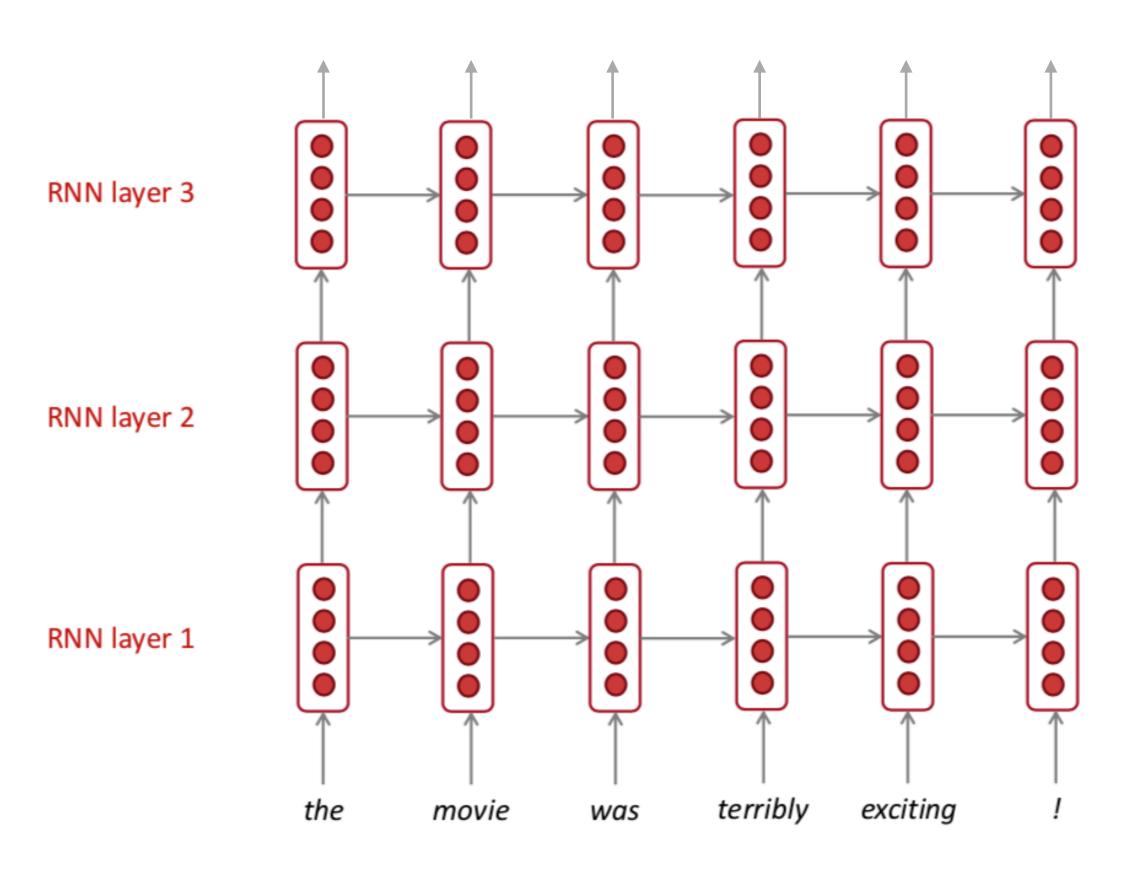
Do we need all these heads?

3 types of attention: Enc-Enc, Enc-Dec, Dec-Dec 6 layers, 16 heads each layer for each type



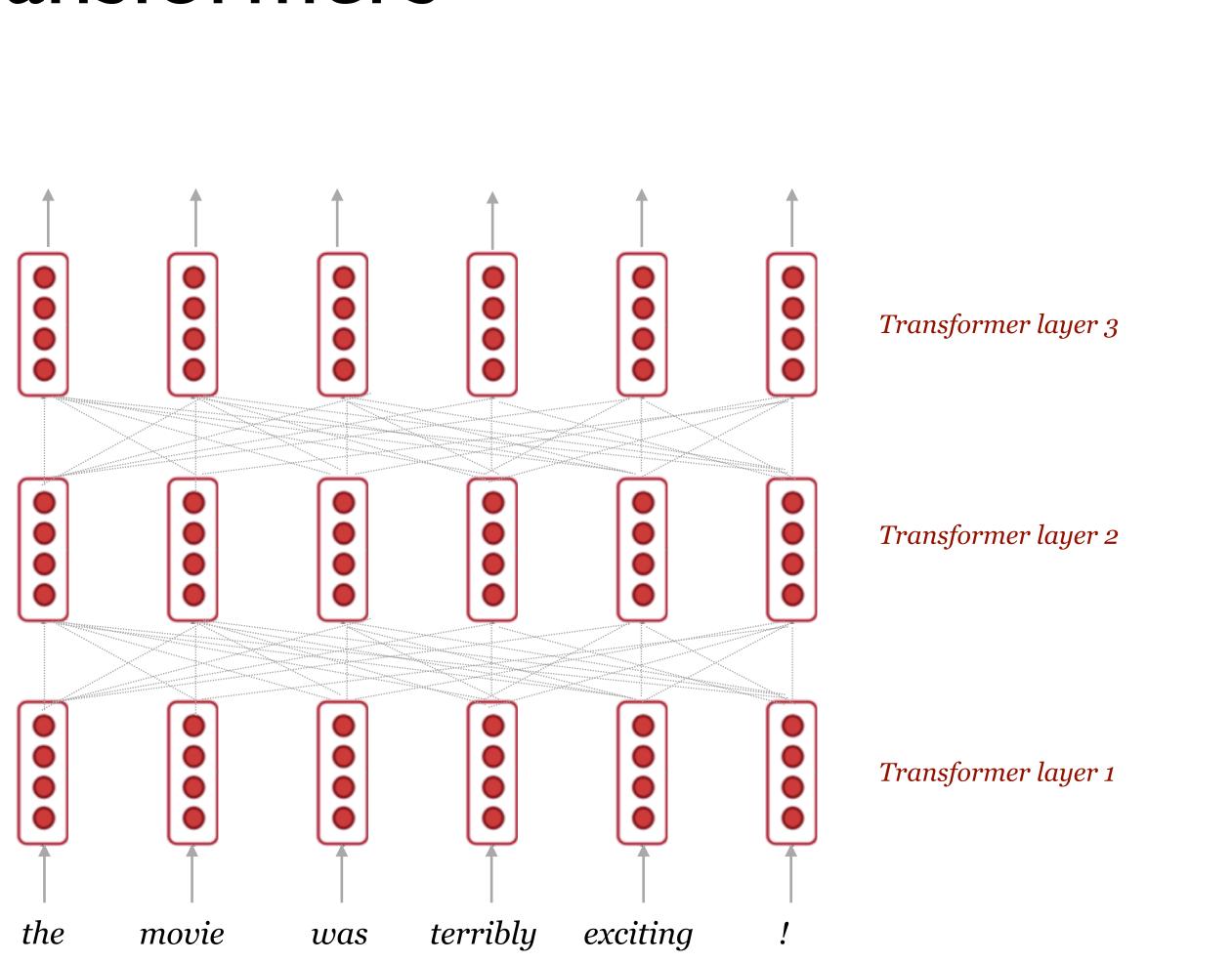
• Can we train a good MT model with less heads?

Are Sixteen Heads Really Better than One? Michel, Levy, and Neubig, NeurIPS 2019



RNN

RNNs vs Transformers



Transformer

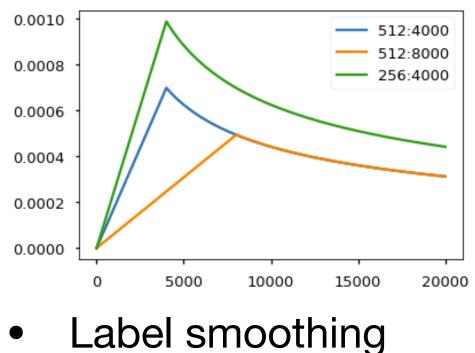
Pytorch (<u>https://pytorch.org/docs/stable/nn.html#transformer-layers</u>) nn.Transformer:

```
>>> transformer_model = nn.Transformer(nhead=16, num_encoder_layers=12)
>>> src = torch.rand((10, 32, 512))
>>> tgt = torch.rand((20, 32, 512))
>>> out = transformer_model(src, tgt)
```

nn.TransformerEncoder:

```
Other details
```

Learning rate with warmup and decay



>>> src = torch.rand(10, 32, 512) >>> out = transformer_encoder(src)

The Annotated Transformer: http://nlp.seas.harvard.edu/2018/04/03/attention.html A Jupyter notebook which explains how Transformer works line by line in PyTorch!

Useful Resources



https://github.com/ huggingface/transformers

>>> encoder_layer = nn.TransformerEncoderLayer(d_model=512, nhead=8) >>> transformer_encoder = nn.TransformerEncoder(encoder_layer, num_layers=6)



Model	BLEU		Training Cost (FLOPs)	
	EN-DE	EN-FR	EN-DE	EN-FR
ByteNet [18]	23.75			
Deep-Att + PosUnk [39]		39.2		$1.0 \cdot 10^{20}$
GNMT + RL [38]	24.6	39.92	$2.3\cdot10^{19}$	$1.4 \cdot 10^{20}$
ConvS2S [9]	25.16	40.46	$9.6 \cdot 10^{18}$	$1.5 \cdot 10^{20}$
MoE [32]	26.03	40.56	$2.0\cdot10^{19}$	$1.2\cdot 10^{20}$
Deep-Att + PosUnk Ensemble [39]		40.4		$8.0 \cdot 10^{20}$
GNMT + RL Ensemble [38]	26.30	41.16	$1.8 \cdot 10^{20}$	$1.1 \cdot 10^{21}$
ConvS2S Ensemble [9]	26.36	41.29	$7.7 \cdot 10^{19}$	$1.2\cdot10^{21}$
Transformer (base model)	27.3	38.1	$3.3 \cdot 10^{18}$	
Transformer (big)	28.4	41.8	$2.3\cdot 10^{19}$	

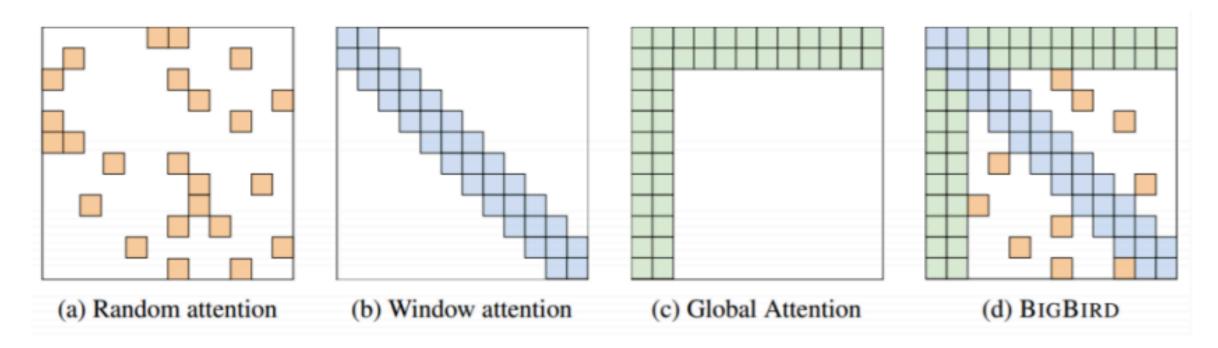
Attention is all you need Vaswani et al, NeurIPS 2017

Perfomance on machine translation

Transformer Pros and Cons

- Pros

 - Easier to parallelize (matrix operations)
- Cons
 - Quadratic computation in self-attention
 - Can become very slow when the sequence length is large



• Are these positional representations enough to capture positional information?

• Easier to capture dependencies: we draw attention between every pair of words $Q = XW^Q, W^Q \in \mathbb{R}^{d_1 \times d_q}$

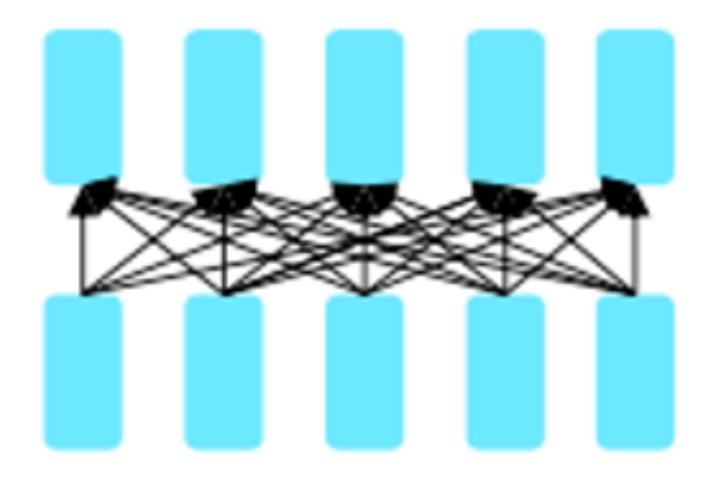
$$K = XW^K, W^K \in \mathbb{R}^{d_1 \times d_k}$$

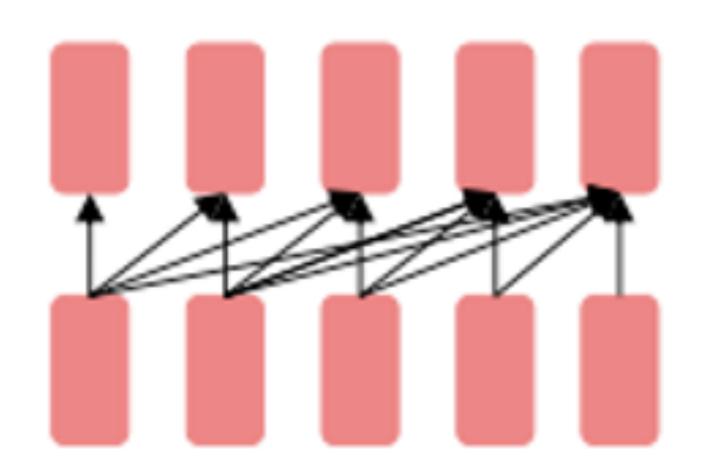
$$V = XW^V, W^V \in \mathbb{R}^{d_1 \times d_v}$$

Transformers for pretraining

- Trained on large text corpus with self-supervised objectives and then transferred.

Encoder only





- Masked language models
- Bidirectional context
- BERT + variants (e.g. RoBERTa)
- Language models

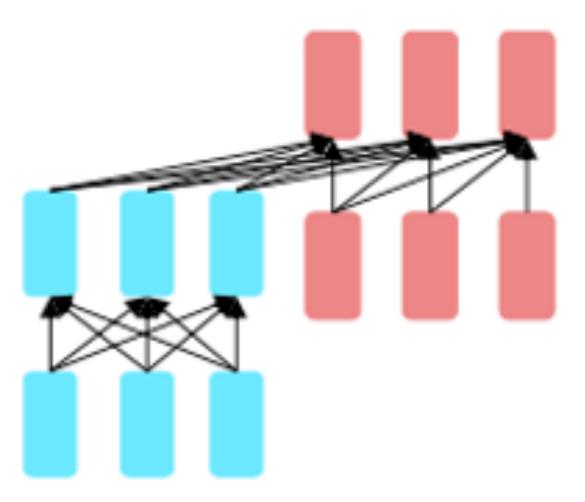
Slide adapted from: Stanford CS224n, John Hewitt

• Self-supervised Transformer based models shattered language understanding benchmarks in NLP in 2018.

Decoder only

Can't condition on future words, good for generation GPT-2, GPT-3, LaMDA

Encoder-Decoder



- Combine benefits of both
- Original Transformer, UniLM, BART, T5, Meena