Attention and Transformer Architectures

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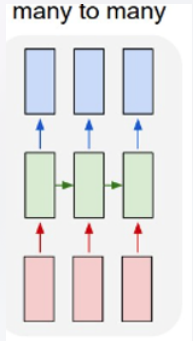
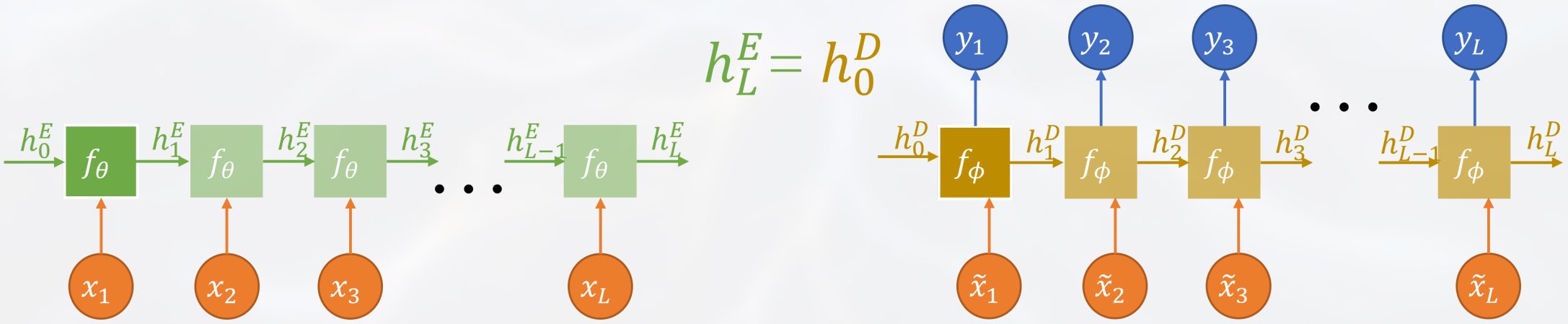
Standard RNNs Struggle for **Sequence-To-Sequence** Tasks Because of Limited Hidden State Capacity

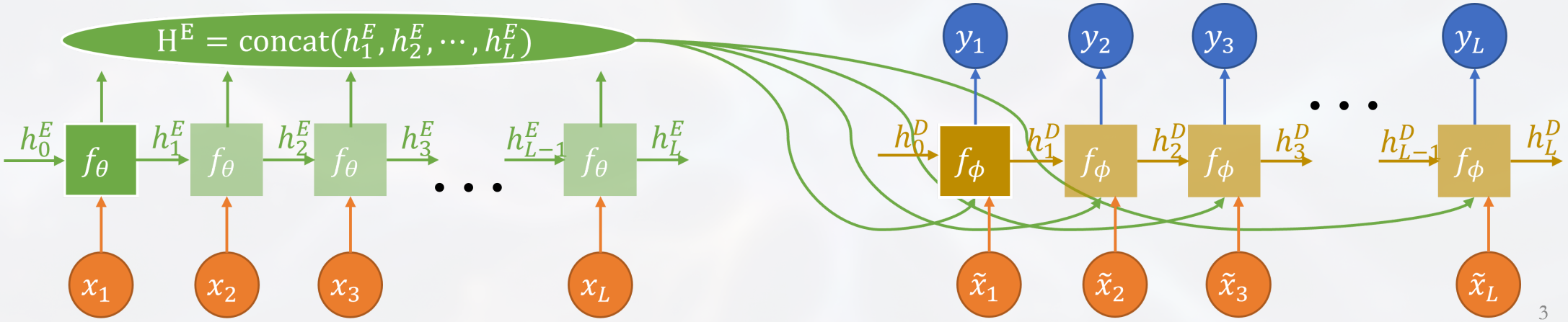
- Example: Translation between French and English
- Could we use a one-to-one input/output RNN?
  - Problem: Input sequence could have different length.
  - Problem: The order of words is not the same in French and English.
- More common to use autoencoder structure with 2 RNNs.
  - Problem: Challenging to encode entire sentence in hidden state.





Attention Is a Model Architecture That Enables the Decoder to Efficiently Use All Encoder Outputs

- Attention overcomes some of the challenges of RNN-based translation.
- Attention allows long-range dependencies and avoids a completely sequential view of the input and output.



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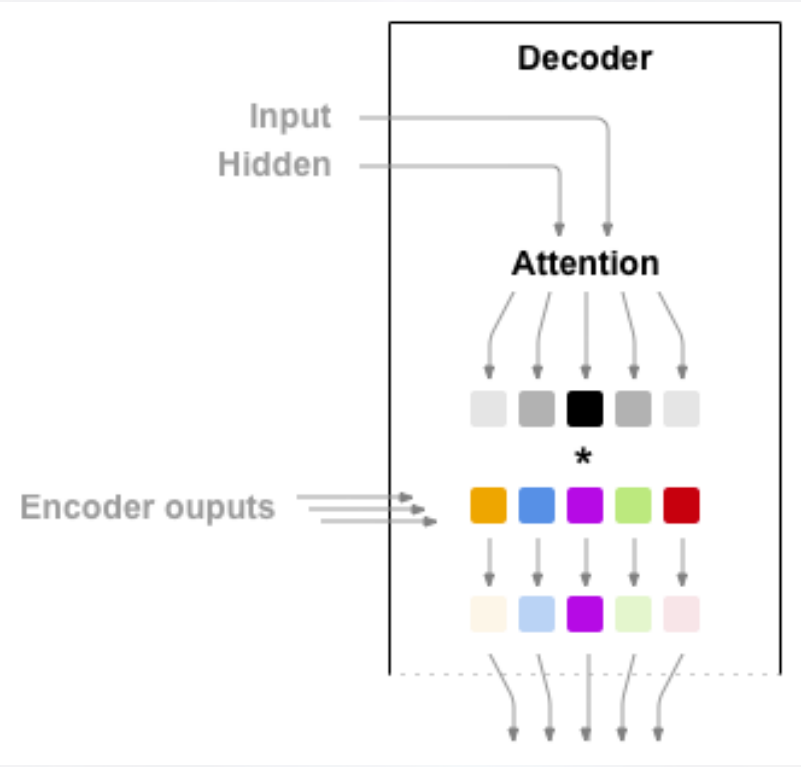
Based on the Input and Hidden State, **Attention** Determines the Weights for Adding the Encoder Outputs

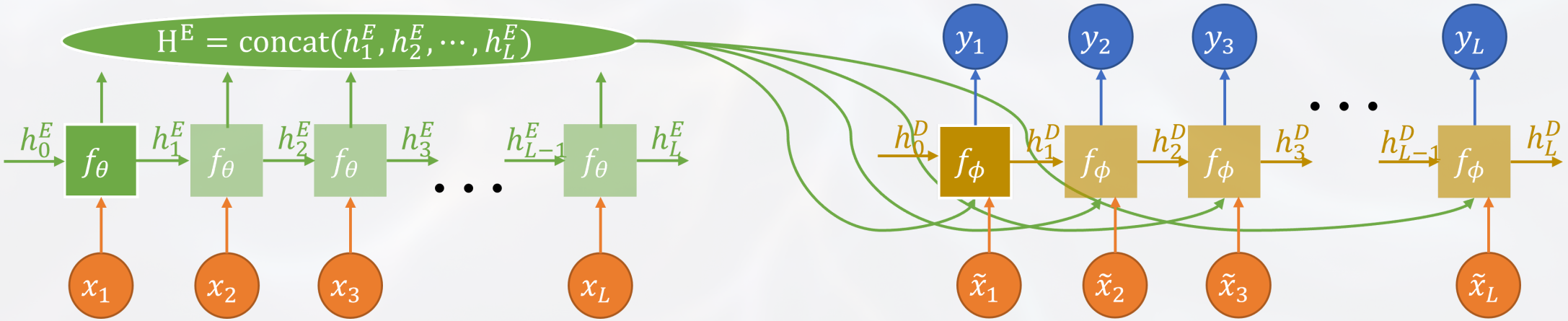
- Informally, the attention mechanism determines which encoder outputs the network should "focus" on (α for attention).
- The weights are normalized to sum to one via softmax, $\sum_l \alpha_l = 1$.
  - Akin to the intuitive idea of "limited attention".
  - In practice, I conjecture this normalization is critical for its training stability.
- The output of attention is a weighted sum of the inputs based on the computed attention weights: $\text{out} = \sum_l \alpha_l h_l^E$.



https://pytorch.org/tutorials/intermediate/seq2seq_translation_tutorial.html

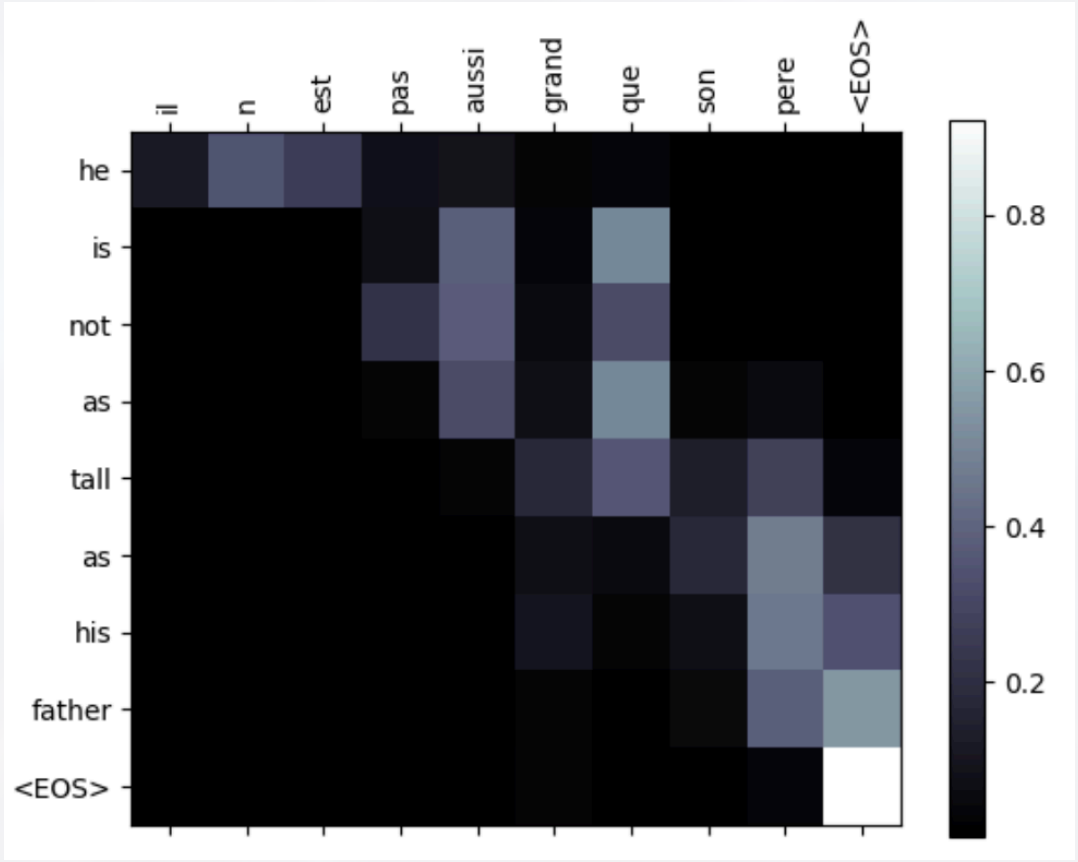
Attention Can Be Represented by Standard Linear Layers and Softmax Functions

- $H^E := [h_1^E, h_2^E, \cdots, h_L^E] \in \mathbb{R}^{k \times L_{max}}$ (hidden state from encoder)
- $h'_{t-1} = [h_{t-1}^D, \tilde{x}_t]$ (concatenate)
- $\alpha_t = \sigma(W_a h'_{t-1} + b_a) \in \mathbb{R}^{L_{max}}$ (softmax for attention weights)
- $c_t = H^E \alpha_t$ (take weighted average of encoder outputs)
- $z_t = \mathrm{ReLU}(W_c[\tilde{x}_t, c_t] + b_c)$ (incorporate input and context)
- $y_t, h_t^D = f_\theta(z_t, h_{t-1}^D)$ (standard RNN)



Because Attention Is a Probability Vector, It Can Enable Some Interpretation of the Model

- A visualization of the attention map can reveal interpretable model structure.
  - Notice the correspondence between input and output words.
- Caution: This is an **abstract view** of the model.
  - It should be interpreted with care as many details are hidden.
  - It does not answer “why” but rather “what” the model is doing.



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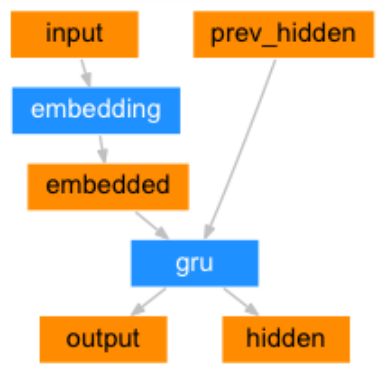
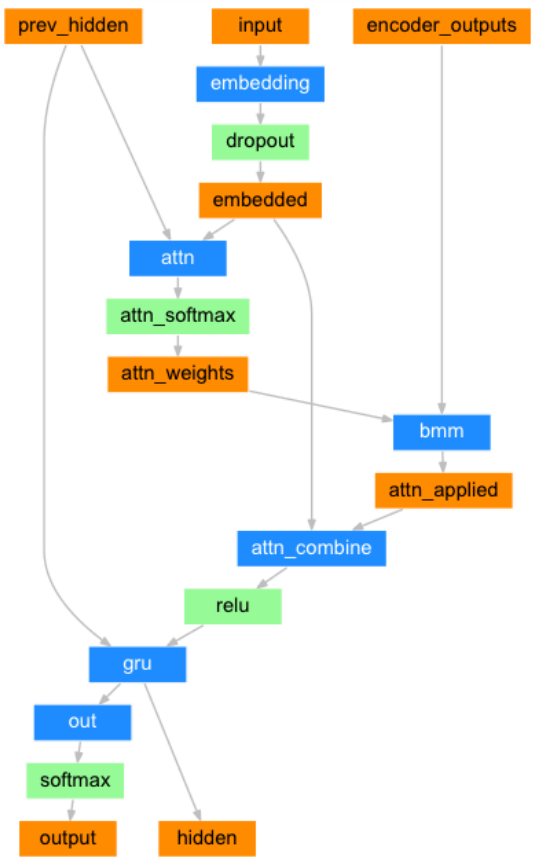
Demo of Seq-2-Seq Task for French to English Translation

- Encoder is simple RNN
- Decoder includes the attention mechanism





Attention Can Be Generalized to Many Other Contexts Beyond Translation

- **Image captioning:** Which pixels of the image should be focused on for generating the caption.
- **Text prediction:** Which previous inputs should be focused on for predicting the next word.
- **Summarization:** Which words in the document should be focused on for generating the next word in the summary.
- ...

Our Seq-2-Seq Attention Is a Special Case of This More General Attention Mechanism

- The output of attention is a weighted average of the values:

$$A(q, K, V) = \sum_i \alpha_i v_i = \sum_i \left(\frac{\exp(e(q, k_i))}{\sum_j \exp(e(q, k_j))} \right) v_i$$

- q is the **query** input, K is the key matrix, V is the value matrix.
- α_i is the **attention weight** for the i-th value.
- $e(q, k_i)$ is the **attention score** (pre-softmax) based on the i-th key.
  - Function of the query q and the i-th key.
  - Intuitively, like a soft/approximate dictionary lookup table (i.e., high value if the query matches the key and low value if the query does not match key).

Our Seq-2-Seq Attention Is a Special Case of This More General Attention Mechanism

- **Generalized attention equation**

$$A(q, K, V) = \sum_i \alpha_i v_i = \sum_i \left(\frac{\exp(e(q, k_i))}{\sum_j \exp(e(q, k_j))} \right) v_i$$

- **Query was hidden state with input**

$$q = h'_{t-1} = [h^D_{t-1}, \tilde{x}_t]$$

- **Attention score function was linear where $K = (W, b)$**

$$e(q, k_i) = w_i^T q + b_i = w_i^T h'_{t-1} + b_i$$

- **Values was encoder values**

$$V = H^E$$

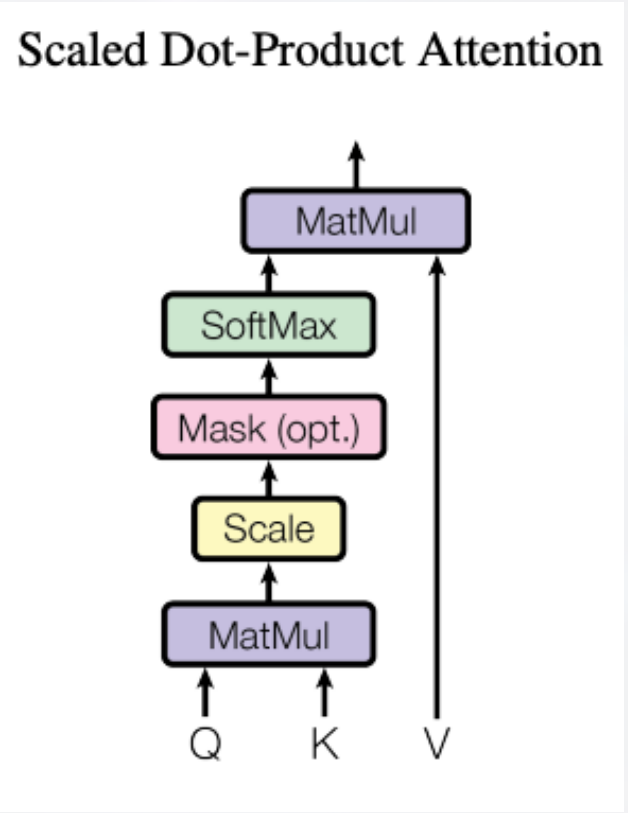
(Attention eqs from before)

- $H^E := [h^E_1, h^E_2, \cdots, h^E_L] \in \mathbb{R}^{k \times L_{max}}$ (hidden state from encoder)
- $h'_{t-1} = [h^D_{t-1}, \tilde{x}_t]$ (concatenate)
- $\alpha_t = \sigma(W_a h'_{t-1} + b_a) \in \mathbb{R}^{L_{max}}$ (softmax for attention weights)
- $c_t = H^E \alpha_t$ (take weighted average of encoder outputs)

A **Self-Attention** Module Computes the Queries, Keys and Values Using the Input Sequence Itself

- $X = [x_1, x_2, ..., x_L]^T \in \mathbb{R}^{L \times D_{in}}$
- Self attention to compute Q, K and V:
  - $Q = XW_Q \in \mathbb{R}^{L \times H}$ (ignoring bias term for simplicity)
  - $K = XW_K \in \mathbb{R}^{L \times H}$
  - $V = XW_V \in \mathbb{R}^{L \times D_{out}}$
- Dot product attention scores: $A(Q, K, V) = \sigma(QK^T)V$
  - $QK^T \in \mathbb{R}^{L \times L}$ are the **attention scores**.
  - The softmax σ is taken over the first dimension.
- A single output for a single query has a simple form:

$$A(q, K, V) = \sigma([q^T k_1, ..., q^T k_L])V = \sum_l \sigma_l([q^T k_1, ..., q^T k_L])v_l$$



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

Self-Attention Has Quadratic Form Inside the Softmax and a Linear Form Outside

- We can expand the attention mechanism as just a function of the sequence X:

$$A_{self}(X) = \sigma(QK^T)V$$

$$= \sigma(XW_Q(XW_K)^T)(XW_V)$$

$$= \sigma(XW_QW_K^TX^T)(XW_V)$$

- Do not be afraid of attention, it's mostly just matrix multiplications :-)

Self-Attention Is a **Permutation-Equivariant** Neural Network Module

- What is the key difference between a set and a sequence?
- In sets, the order of the elements doesn't matter!
- The input-output relationship of transformers behave more like sets than a sequences.
- Formally, self-attention is **equivariant** to the input order of the sequence: $A_{self}(PX) = PA_{self}(X)$ where P is a permutation matrix that permutes L rows.
- **Initial example:**
  - $X = [1, 2, 3, 4]^T$
  - $A_{self}(X) = [6, 7, 8, 9]^T$
- **Permuted input produces the same output but permuted:**
  - $X' = PX = [4, 3, 2, 1]^T$
  - $A_{self}(X') = [9, 8, 7, 6]^T = PA_{self}(X)$

Simple Proof of **Equivariance** Property

- $A_{self}(X) = \sigma(XW_Q W_K^T X^T)(XW_V)$
- $A_{self}(PX) = \sigma((PX)W_Q W_K^T (PX)^T)((PX)W_V)$
- $= \sigma(P(XW_Q W_K^T X^T)P^T)PXW_V$
- $= P\sigma(XW_Q W_K^T X^T P^T)PXW_V$ (permuting rows and then softmax is equivalent to softmax and then permuting rows)
- $= P\sigma(XW_Q W_K^T X^T)P^T PXW_V$ (permuting scores and then softmax is equivalent to softmax and then permuting outputs)
- $= P\sigma(XW_Q W_K^T X^T)XW_V$
- $= PA_{self}(X)$

Masked Attention Forces Attention Weights on Future Values to Be 0

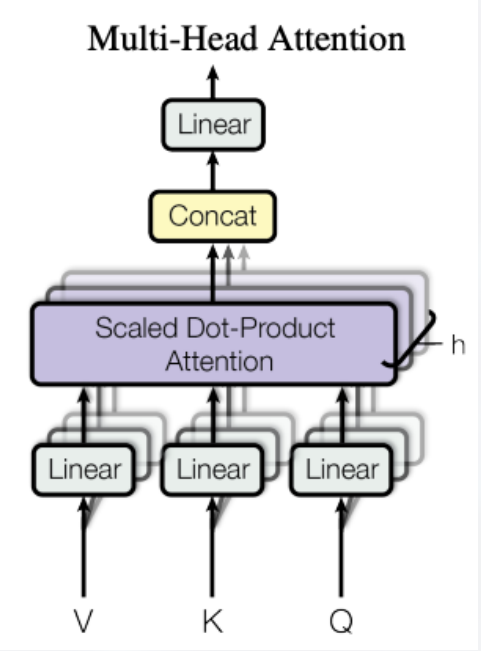
- For generating the output sequence, we cannot let the current word depend on future words, it should only depend on past words.
- To enforce this, we add a mask to the attention scores before applying the softmax.
- The mask has $-\infty$ where the value should be 0.
- This ensures that decoder outputs only depend on previous words/outputs.

Multi-Headed Attention Combines Multiple Attention Mechanisms Via Concatenation

- Suppose we have H attention modules with an output dimension of D_{head}: $A_1(X), A_2(X), \ldots, A_H(X)$.
- Multiheaded attention simply concatenates the output of each attention and applies a linear function:

$$A_{multi-head}(X) = [A_1(X), A_2(X), \cdots, A_H(X)]W_H$$

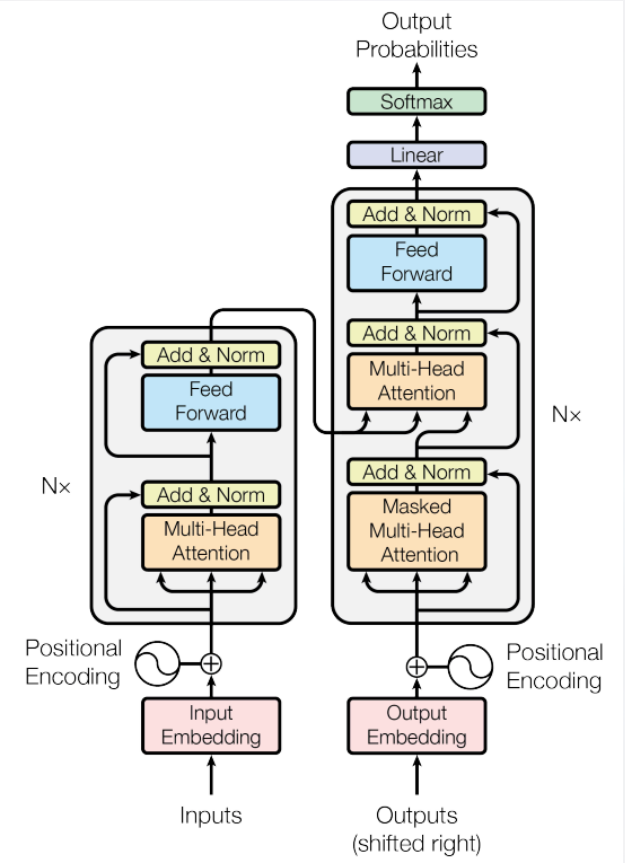
- The concatenated dimension is $D_{head} \cdot H$.
- $W_H \in \mathbb{R}^{(D_{head} \cdot H) \times D_{out}}$



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

Transformers Uses Only Attention Instead of RNN Structure

- No RNN structure, parallel
- **Positional encoding**
- Multi-headed **scaled** attention
  - Masked version ensures current output does not depend on "future" outputs
  - Cross attention and self-attention
- Includes feed forward layers that operate on each input independently
  - Think of applying a simple NN to a batch of samples (where each sample corresponds to one element of the sequence)



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Without Positional Encoding, the Model Would Be Unable to Leverage Word Position Information

- Remember that self-attention is **permutation-equivariant** operator.
- Similarly, the feed-forward layers are just like operating on a batch of samples so they are also a **permutation-equivariant** operator.
- Therefore, it would be impossible for the model to reason about absolute or relative word positions.
  - (Slight caveat: the masked attention removes the permutation equivariant property, but it is not explicit.)
- Yet reasoning about word positions is critical for language understanding.
- Adding positional encoding to the word representation overcomes this issue so that the order of words is embedded in the sequences.
  - Positional encodings are very important for transformers to work.

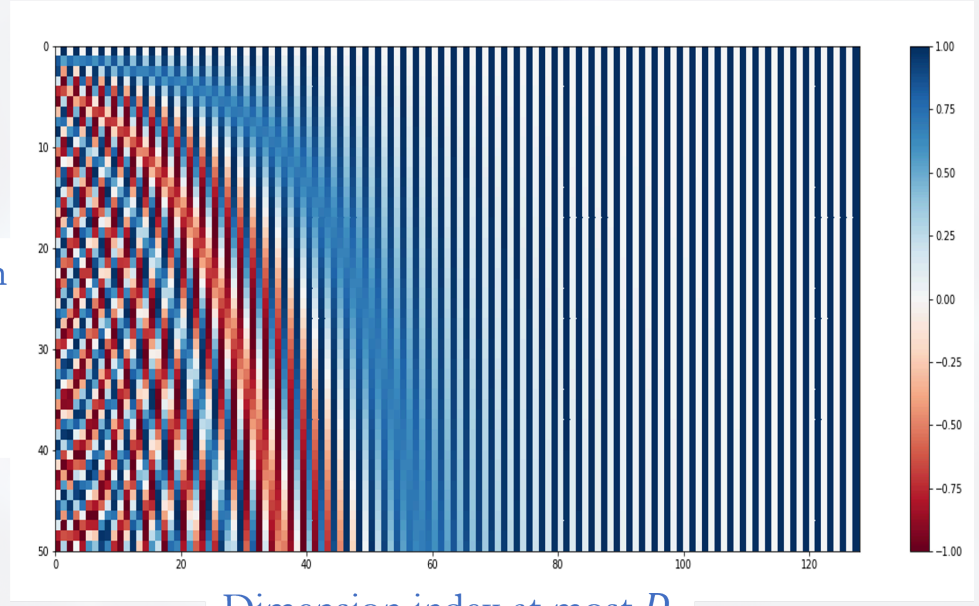
Without Positional Encoding, the Model Would Be Unable to Leverage Word Position Information

- Positional encoding has the same dimension D as the word embedding.
- It alternates between sine and cosine with a geometric progression of wavelengths from 2π to $10,000 \cdot 2\pi$.

$$PE_{2i}(t) = \sin\left(\frac{t}{10{,}000^{2i/D}}\right)$$

$$PE_{2i+1}(t) = \cos\left(\frac{t}{10{,}000^{2i/D}}\right)$$

- This enables relative and absolute positioning information to be encoded.



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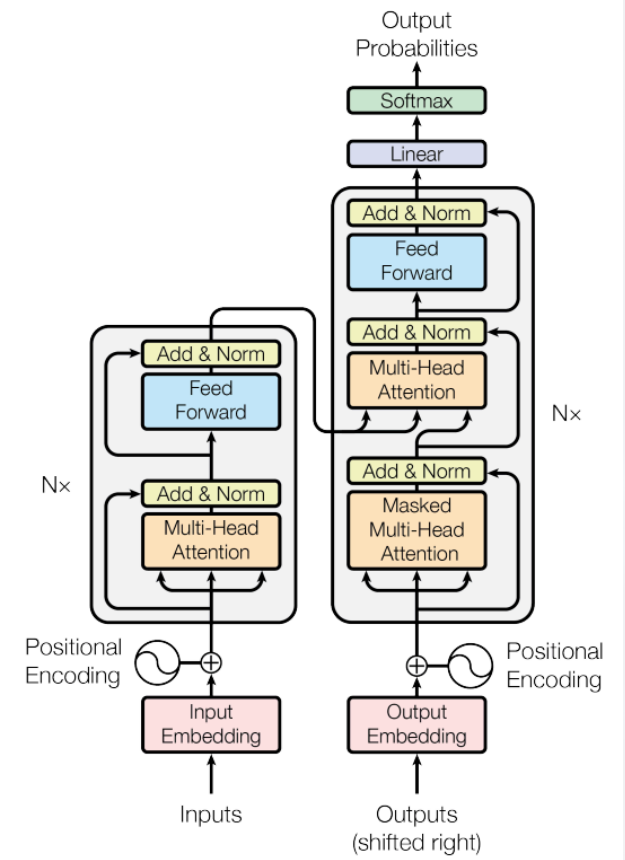

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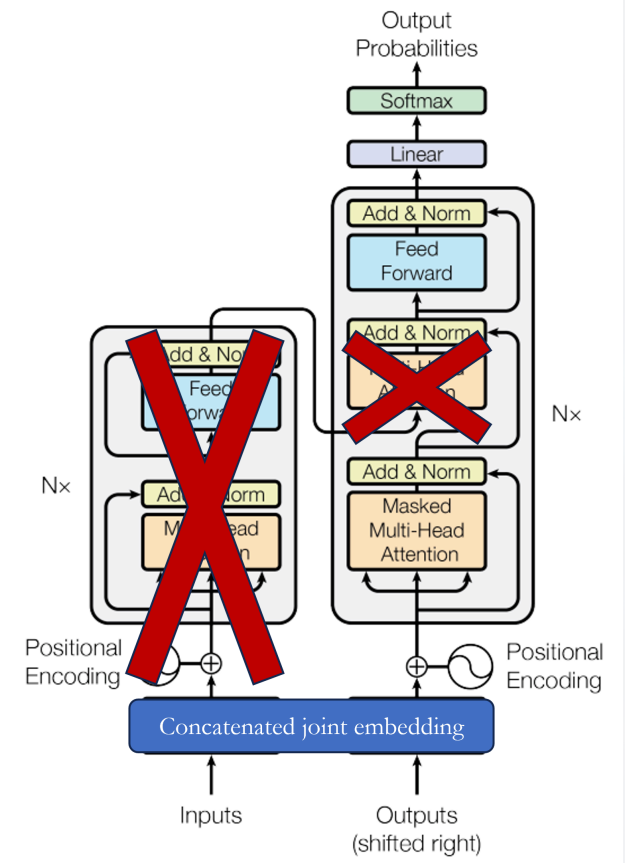
Decoder-Only Transformers Have Become the Mainstream Design

- To form a decoder-only transformer:
  - Simply concatenate the input to the output of the decoder part.
  - Remove cross attention and simply use masked attention.
- This forms a simpler and more versatile architecture.
  - One potential issue is that it cannot reason back and forth across the words but must think in a “forward only” direction.
- Overall, this simpler Decoder-only architecture has become the de-facto standard.



Comparison Between RNNs and Attention-Based Models for Sequences

- **RNNs**
  - Pro: For generation, RNNs have a small hidden state so they require less memory.
  - Pro: They are also quite natural for next-token generation.
  - Con: During training, they must process the sequence sequentially.
  - Con: May lose long-range dependencies when compressing into a single hidden state.
- **Transformers / Attention-based models**
  - Pro: During training, they can process an entire sequence in parallel.
  - Pro: Allows complex long-range dependencies across the whole sequence.
  - Con: More computationally expensive both in terms of memory and computation.
  - Memory and computation scales quadratically in sequence length L.
  - State-space models (e.g., Mamba) provide an alternative that reduces the computational complexity but preserves longer-range dependencies.

Summary

- **RNN-based sequence to sequence** models previously struggled because the transferred hidden state was too small.
- **Cross attention** allowed the RNN to leverage the hidden states of all parts of the input sequence.
- **Masked self-attention** and **positional encoding** allowed for sequence models without RNNs for stable long-range dependencies.

Other References

- Illustration of self-attention
  - https://towardsdatascience.com/illustrated-self-attention-2d627e33b20a
- Simple explanation with entire architecture of GPT
  - https://dugas.ch/artificial_curiosity/GPT_architecture.html