Attention and Transformer Architectures

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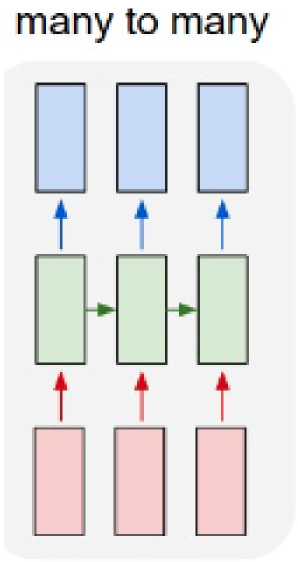
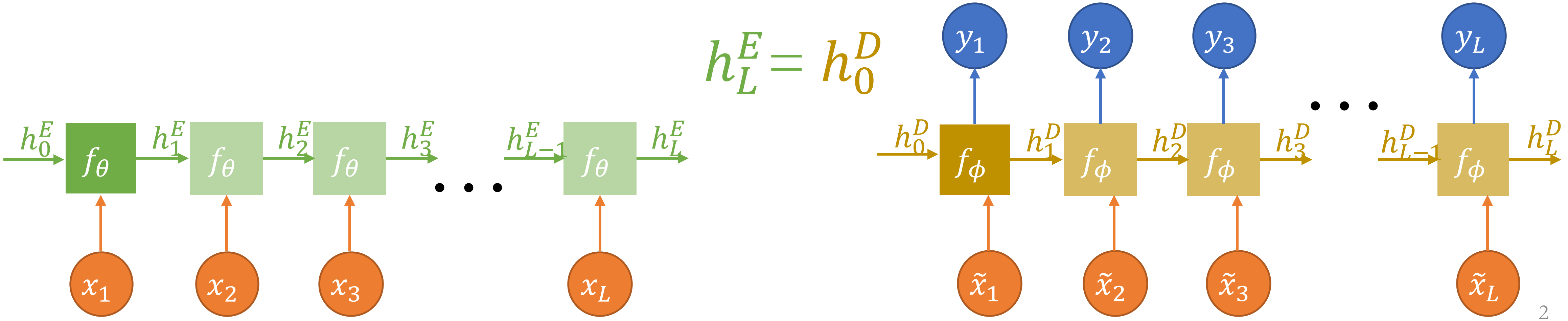
Standard RNNs struggle for **sequence-to-sequence** tasks because of limited hidden state capacity

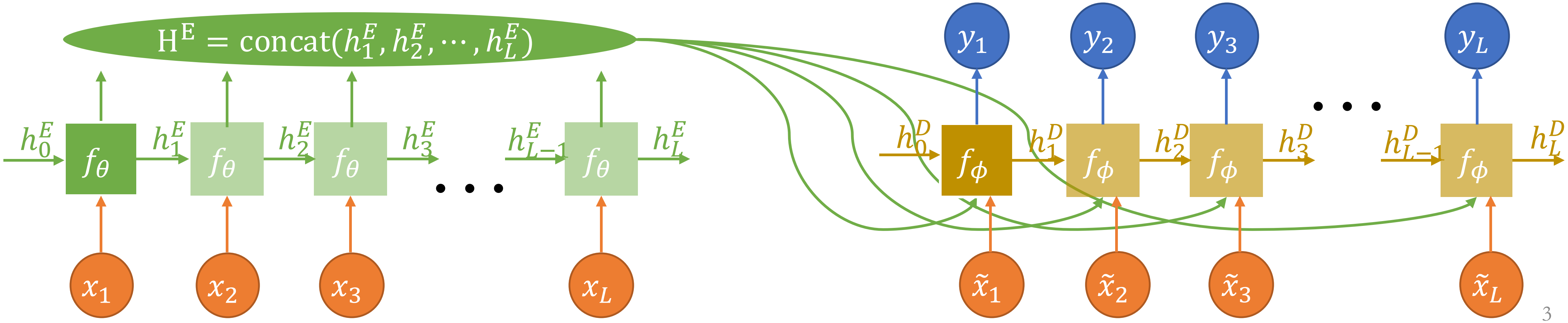
- Example: Translation between French and English
- Could we use a one-to-one input/output RNN?
  - Problem: Input sequence could have different length.
  - Problem: The order of words is not the same in French and English.
- More common to use autoencoder structure with 2 RNNs.
  - Problem: Challenging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





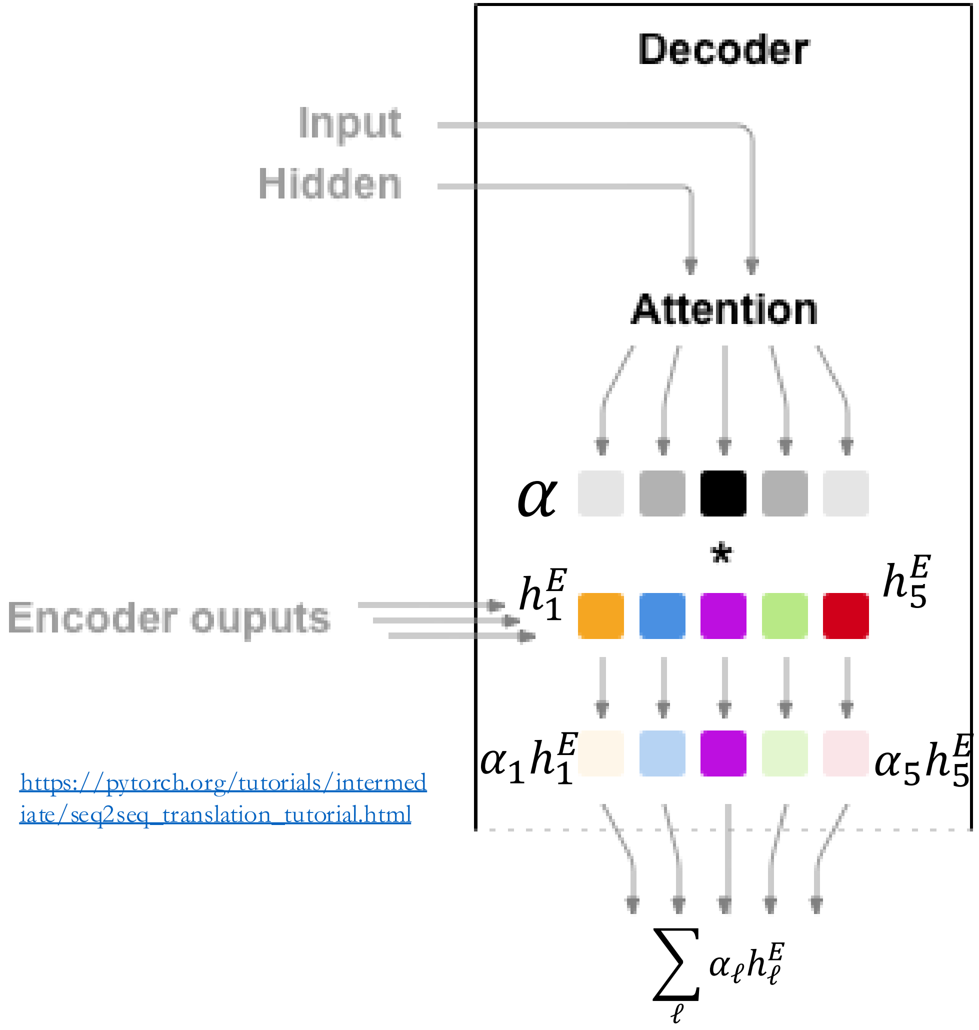
Attention is a model architecture that enables the decoder to efficiently use all encoder outputs

- 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



Based on the input and hidden state, **attention** determines the weights for adding the encoder outputs

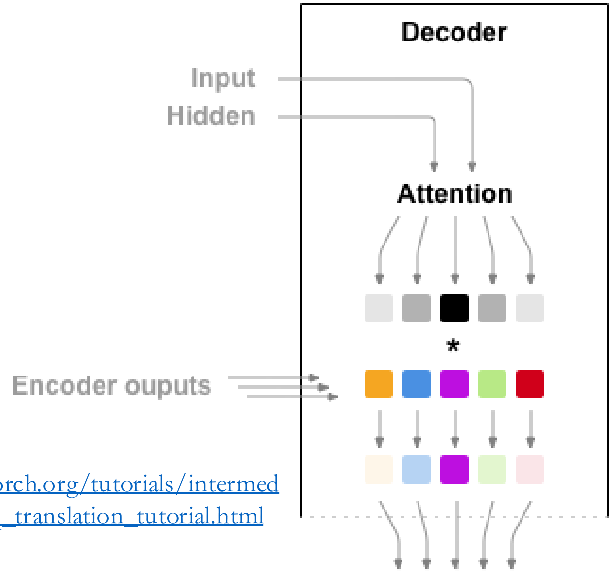
- Informally, the attention mechanism determines which encoder outputs the network should "focus" on (α for attention)
- The weights are normalized to sum to one via softmax, $\sum_\ell \alpha_\ell = 1$
  - Akin to the intuitive idea of "limited attention"
  - In practice, I conjecture this normalization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



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)



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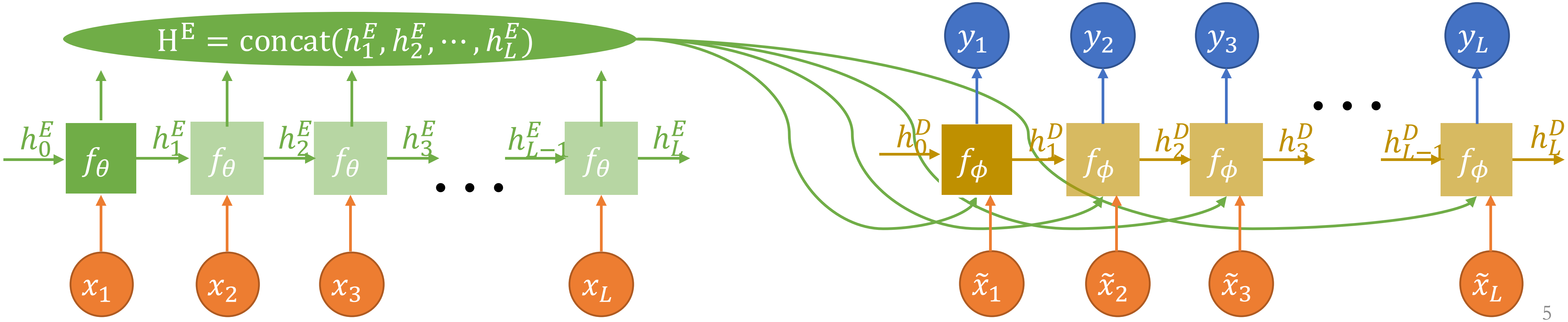

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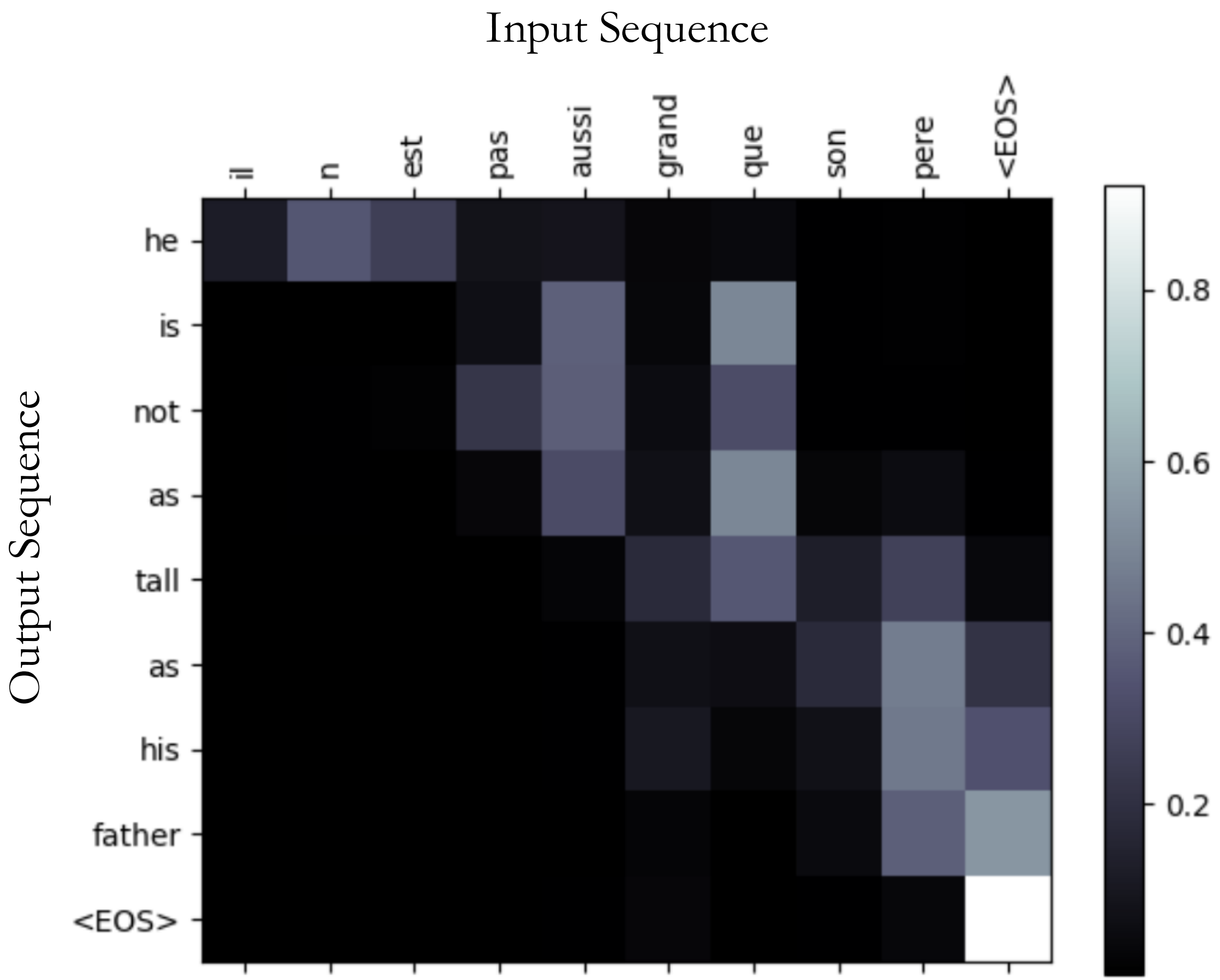
Because attention is a probability vector, it can enable some interpretation of the model

- 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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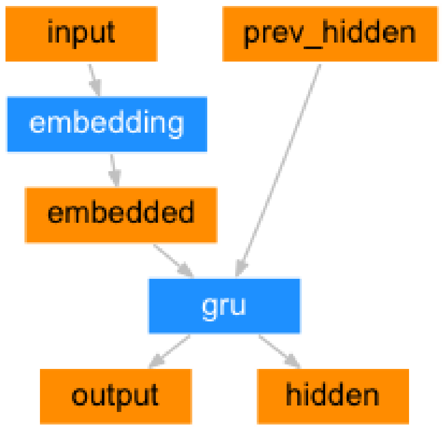
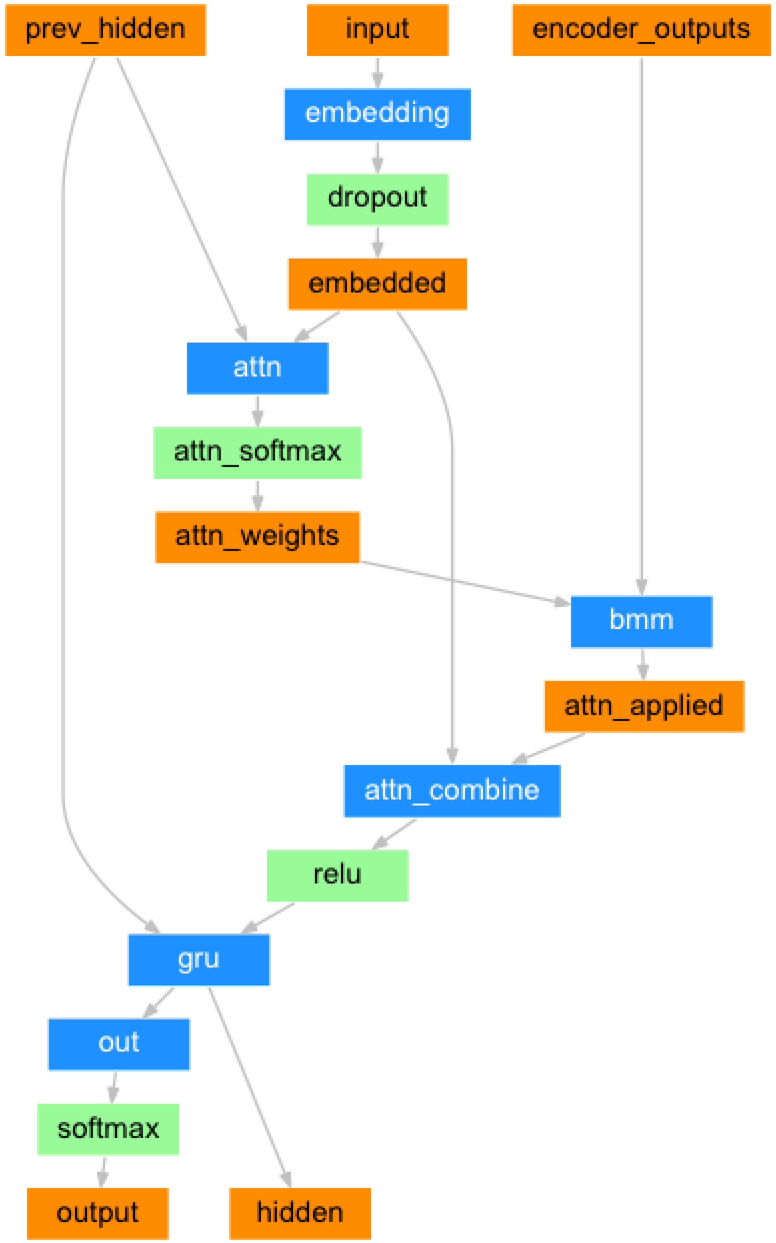
Demo of seq-2-seq task for French to English translation

- 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

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

  - q is the <u>**query**</u> input, K is the key matrix, V is the value matrix
  - α_i is the <u>**attention weight**</u> for the i-th value
  - $e(q,k_i)$ is the <u>**attention score**</u> (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

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

- 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

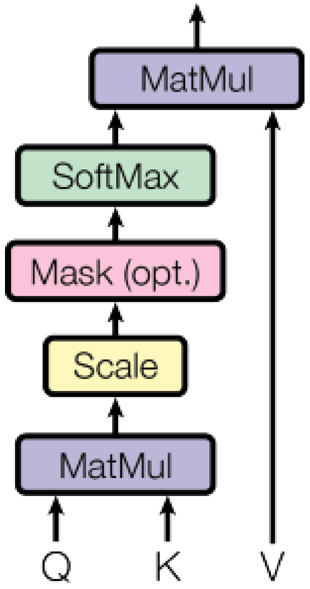
- $X = [x_1, x_2, \dots, x_L]^T \in \mathbb{R}^{L \times D_{in}}$
- Self attention to compute Q, K and V
  - $Q = XW_Q \in \mathbb{R}^{L \times H}$ (ignoring bias term for simplicity)
  - $K = XW_K \in \mathbb{R}^{L \times H}$
  - $V = XW_V \in \mathbb{R}^{L \times D_{out}}$
- Dot product attention scores

$$A(Q, K, V) = \sigma(QK^T)V$$

  - $QK^T \in \mathbb{R}^{L \times L}$ are the **attention scores**
  - The softmax σ is taken over the first dimension
- A single output for a single query has a simple form:

$$A(q, K, V) = \sigma([q^T k_1, \dots, q^T k_L])V = \sum_{\ell} \sigma_\ell([q^T k_1, \dots, q^T k_L]) v_\ell$$

Scaled Dot-Product Attention



Vaswani, A., Shazeer, N., Parmar, N., Uszkoreit, J., Jones, L., Gomez, A. N., ... & Polosukhin, I. (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
- $A_{self}(X) = \sigma(QK^T)V$
- $= \sigma\big(XW_Q(XW_K)^T\big)(XW_V)$
- $= \sigma\big(XW_QW_K^TX^T\big)(XW_V)$
- 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

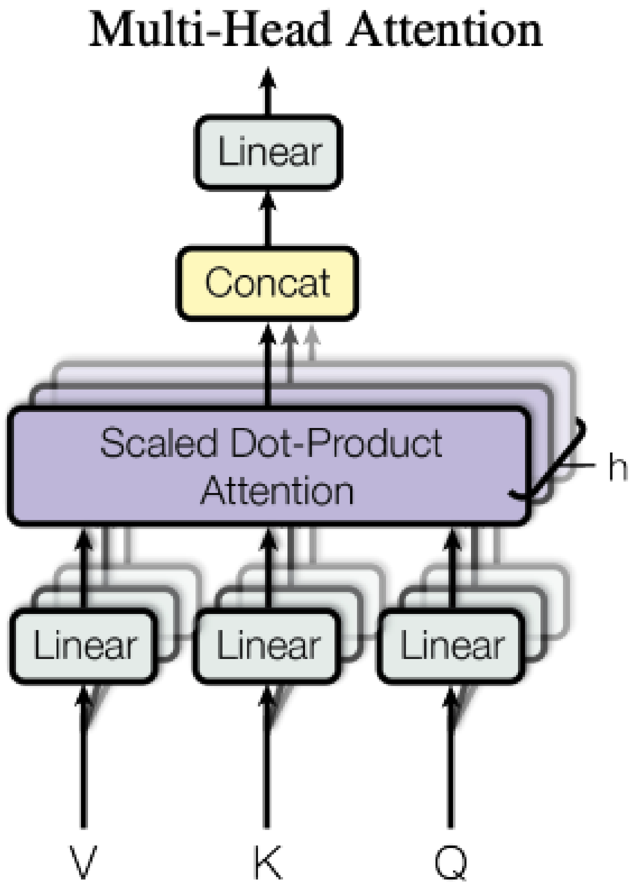
- $A_{self}(X) = \sigma\left(XW_Q W_K^T X^T\right)(XW_V)$
- $A_{self}(PX) = \sigma\left((PX)W_Q W_K^T (PX)^T\right)\left((PX)W_V\right)$
- $= \sigma\left(P\left(XW_Q W_K^T X^T\right)P^T\right)PXW_V$
- $= P\sigma\left(XW_Q W_K^T X^T P^T\right)PXW_V$
  (permuting rows and then softmax is equivalent to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

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}
$$A_1(X), A_2(X), \cdots, A_H(X)$$
- Multiheaded attention simply concatenates the output of each attention and applies a linear function
$$A_{multi-head}(X) = [A_1(X), A_2(X), \cdots, A_H(X)]\mathrm{W_H}$$
  - The concatenated dimension is $D_{head} \cdot H$
  - $W_H \in \mathbb{R}^{(D_{head} \cdot H) \times D_{out}}$



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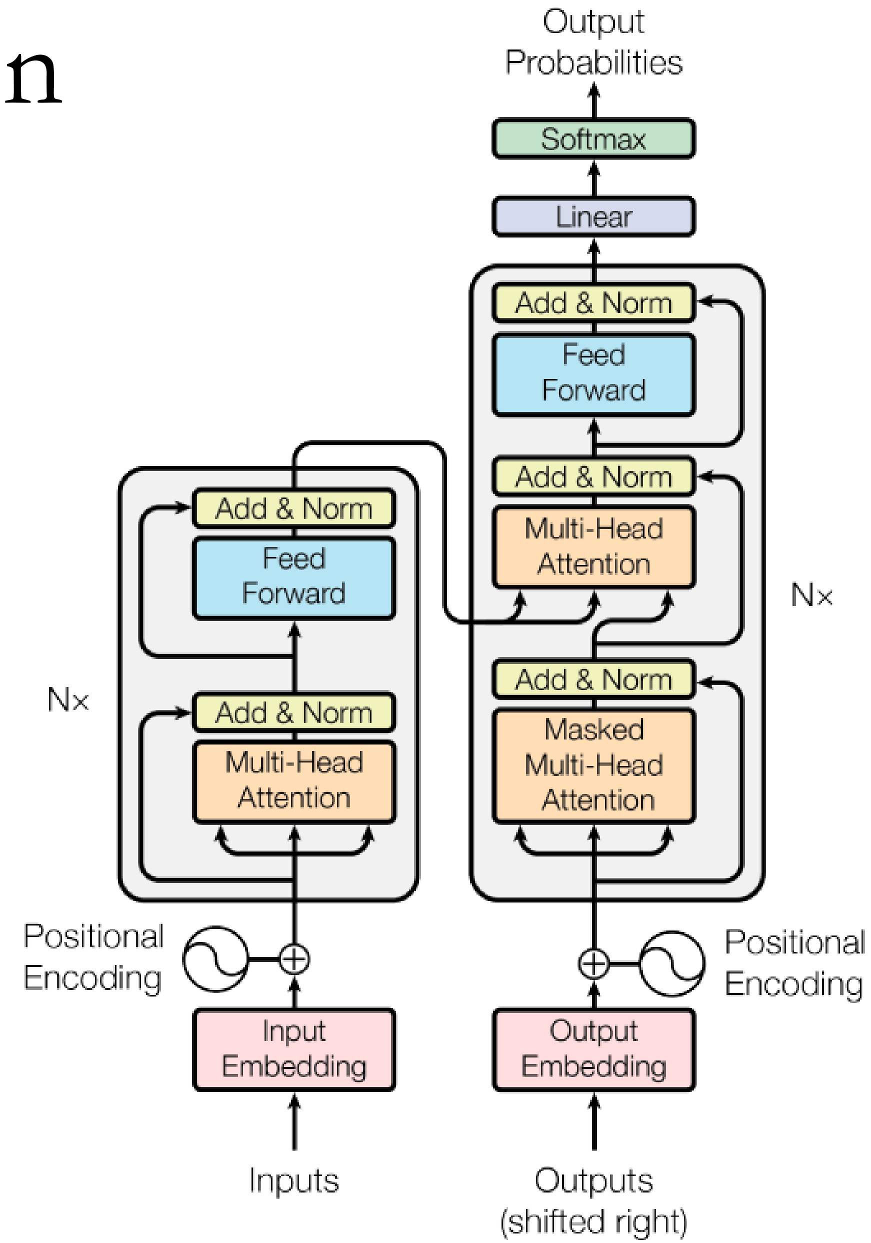
Transformers uses only attention instead of RNN structure

- No RNN structure, parallel
- **Positional encoding (next slide)**
- 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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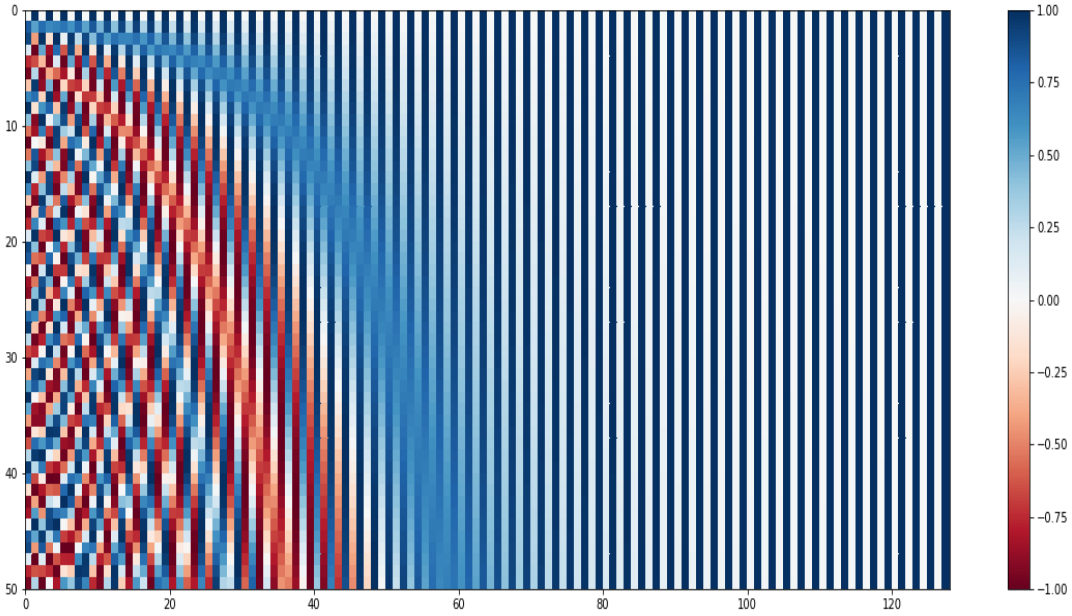
Without positional encoding, the model would be unable to leverage word position information

- 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

Position in sentence (up to 50)



Dimension index at most D

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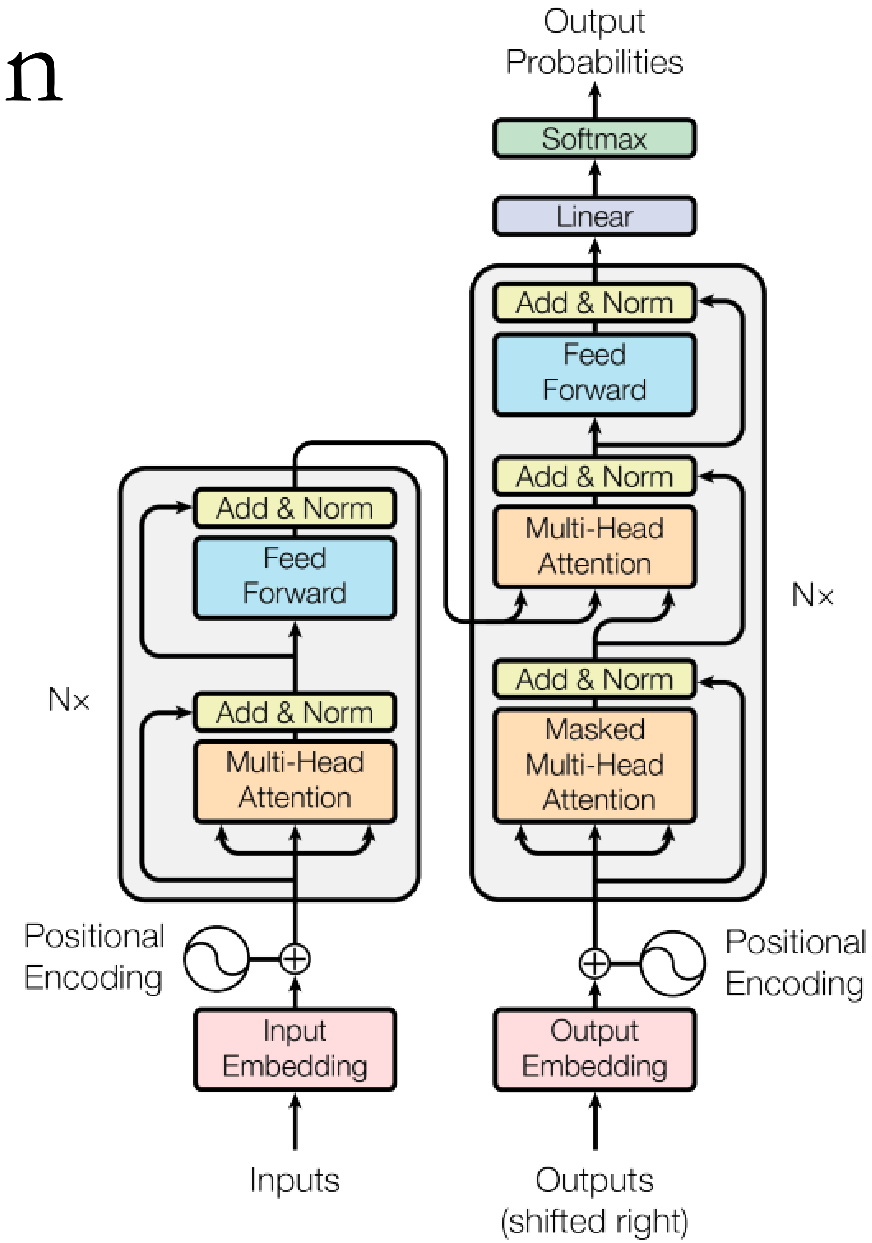

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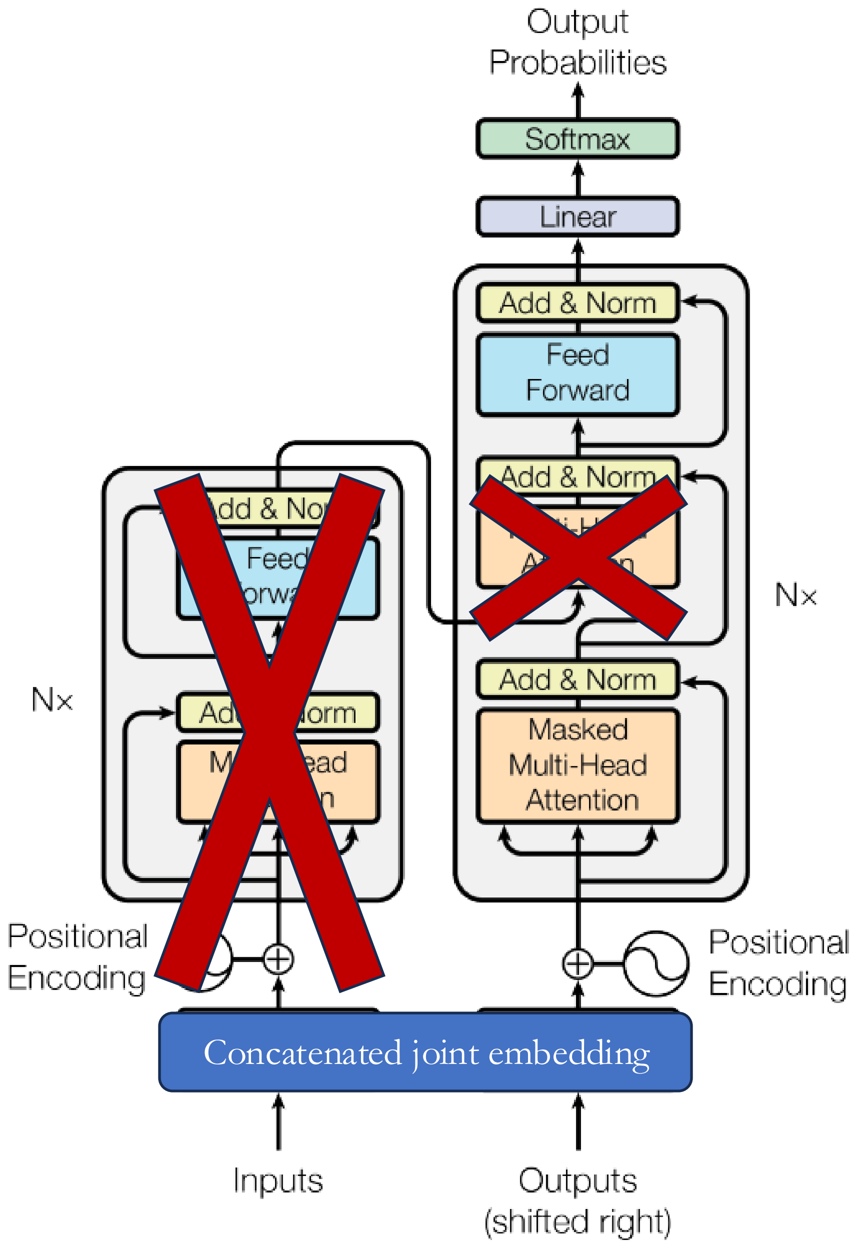
Decoder-only transformers have become the mainstream design

- 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



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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