PURDUE UNIVERSITY NORTHWEST

Natural Language Processing
CS 52570

Lecture 15 ----- Self-Attention and Transformers

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Part of this course is derived using resources from Stanford CS 224N, originated by Dr. Manning and others.

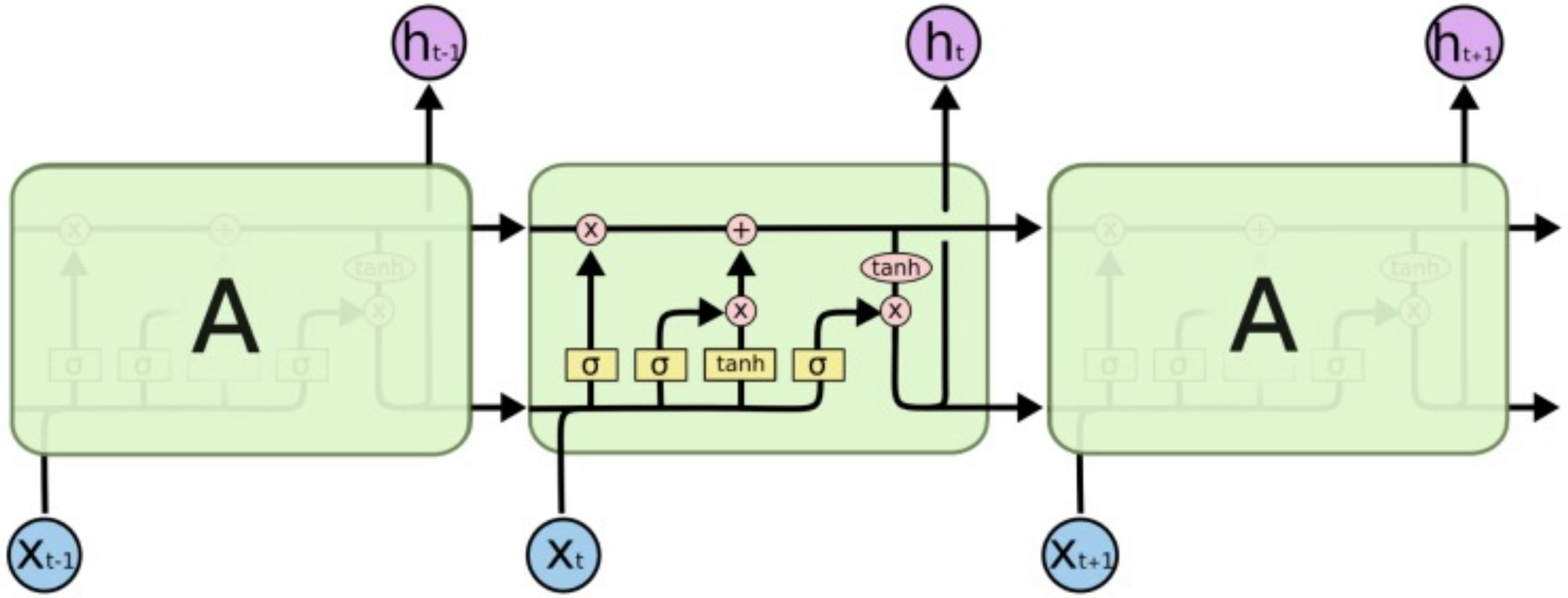
Recap Questions:

- If the gradient becomes too big, then the SGD update step becomes too big:

$$\theta^{new} = \theta^{old} - \overbrace{\alpha}^{\text{learning rate}} \underbrace{\nabla_\theta J(\theta)}_{\text{gradient}}$$

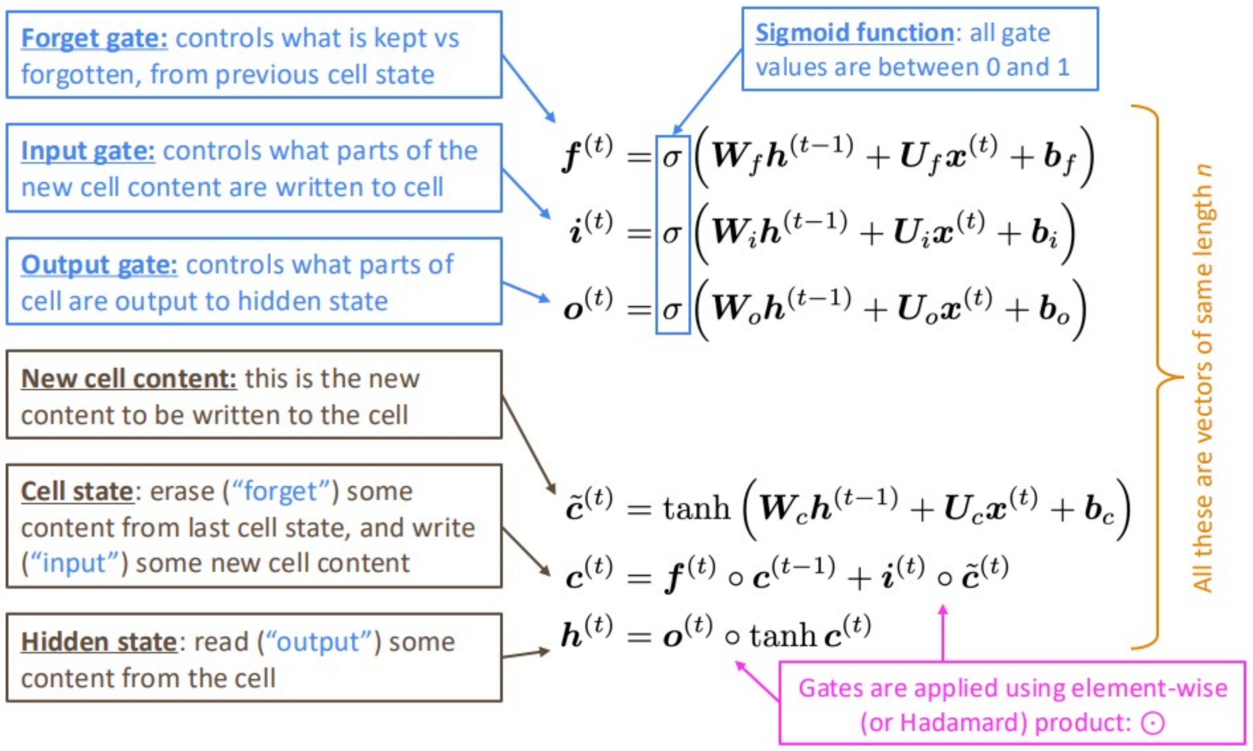
- This can cause bad updates: we take too large a step and reach a weird and bad parameter configuration (with large loss)
- In the worst case, this will result in **Inf** or **NaN** in your network (then you have to restart training from an earlier checkpoint)

What are the components in LSTM?



Long Short-Term Memory (LSTM)

We have a sequence of inputs $x\,(t)$, and we will compute a sequence of hidden states $h\,(t)$ and cell states $c\,(t)$. On timestep t:



Forget gate: controls what is kept vs forgotten, from previous cell state

Input gate: controls what parts of the new cell content are written to cell

Output gate: controls what parts of cell are output to hidden state

New cell content: this is the new content to be written to the cell

Cell state: erase ("forget") some content from last cell state, and write ("input") some new cell content

Hidden state: read ("output") some content from the cell

Sigmoid function: all gate values are between 0 and 1

$$\boldsymbol{f}^{(t)} = \boxed{\sigma}\left(\boldsymbol{W}_f \boldsymbol{h}^{(t-1)} + \boldsymbol{U}_f \boldsymbol{x}^{(t)} + \boldsymbol{b}_f\right)$$

$$\boldsymbol{i}^{(t)} = \boxed{\sigma}\left(\boldsymbol{W}_i \boldsymbol{h}^{(t-1)} + \boldsymbol{U}_i \boldsymbol{x}^{(t)} + \boldsymbol{b}_i\right)$$

$$\boldsymbol{o}^{(t)} = \boxed{\sigma}\left(\boldsymbol{W}_o \boldsymbol{h}^{(t-1)} + \boldsymbol{U}_o \boldsymbol{x}^{(t)} + \boldsymbol{b}_o\right)$$

$$\tilde{\boldsymbol{c}}^{(t)} = \tanh\left(\boldsymbol{W}_c \boldsymbol{h}^{(t-1)} + \boldsymbol{U}_c \boldsymbol{x}^{(t)} + \boldsymbol{b}_c\right)$$

$$\boldsymbol{c}^{(t)} = \boldsymbol{f}^{(t)} \circ \boldsymbol{c}^{(t-1)} + \boldsymbol{i}^{(t)} \circ \tilde{\boldsymbol{c}}^{(t)}$$

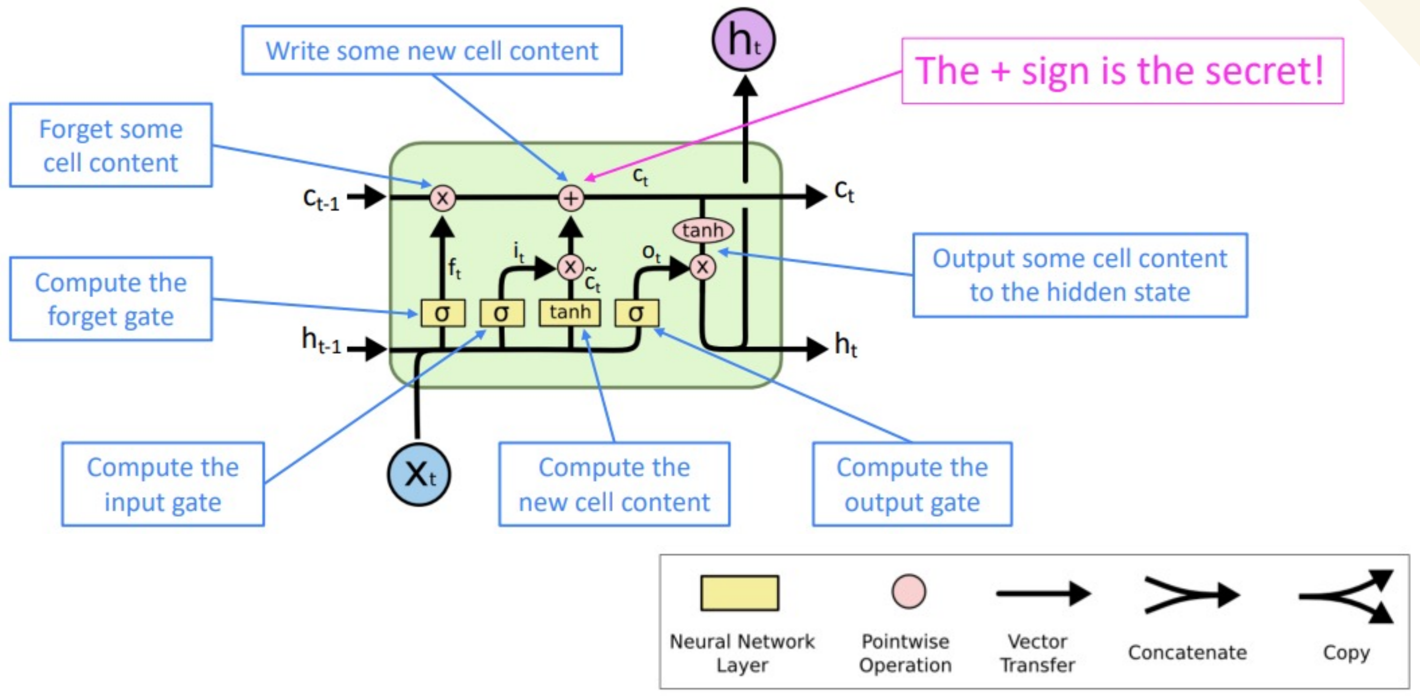
$$\boldsymbol{h}^{(t)} = \boldsymbol{o}^{(t)} \circ \tanh \boldsymbol{c}^{(t)}$$

All these are vectors of same length n

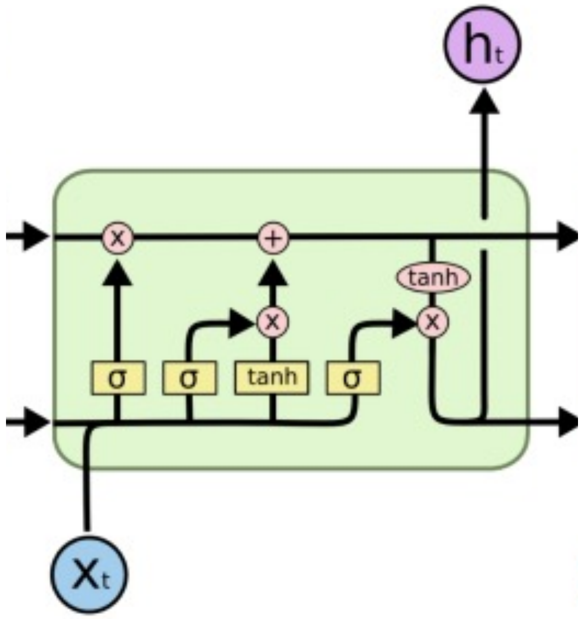
Gates are applied using element-wise (or Hadamard) product: $\odot$

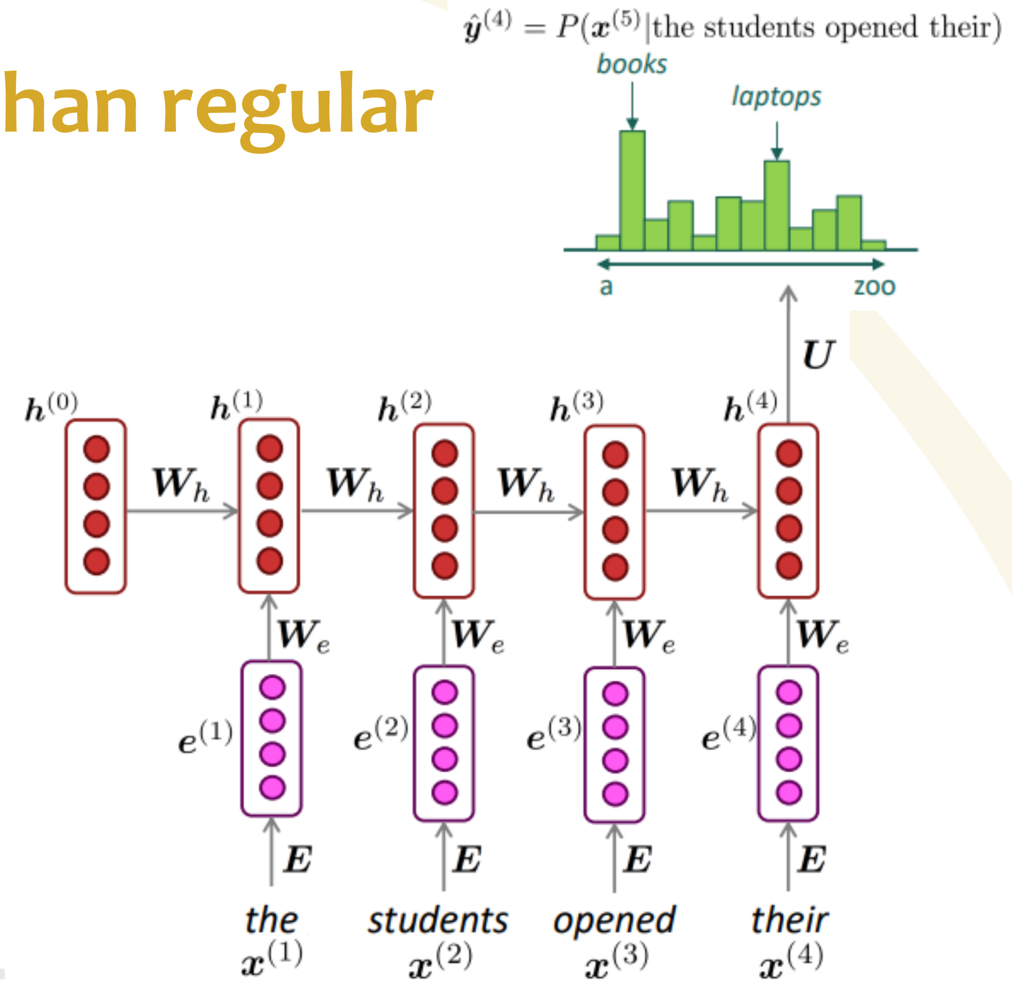
Long Short-Term Memory (LSTM)

You can think of the LSTM equations visually like this:

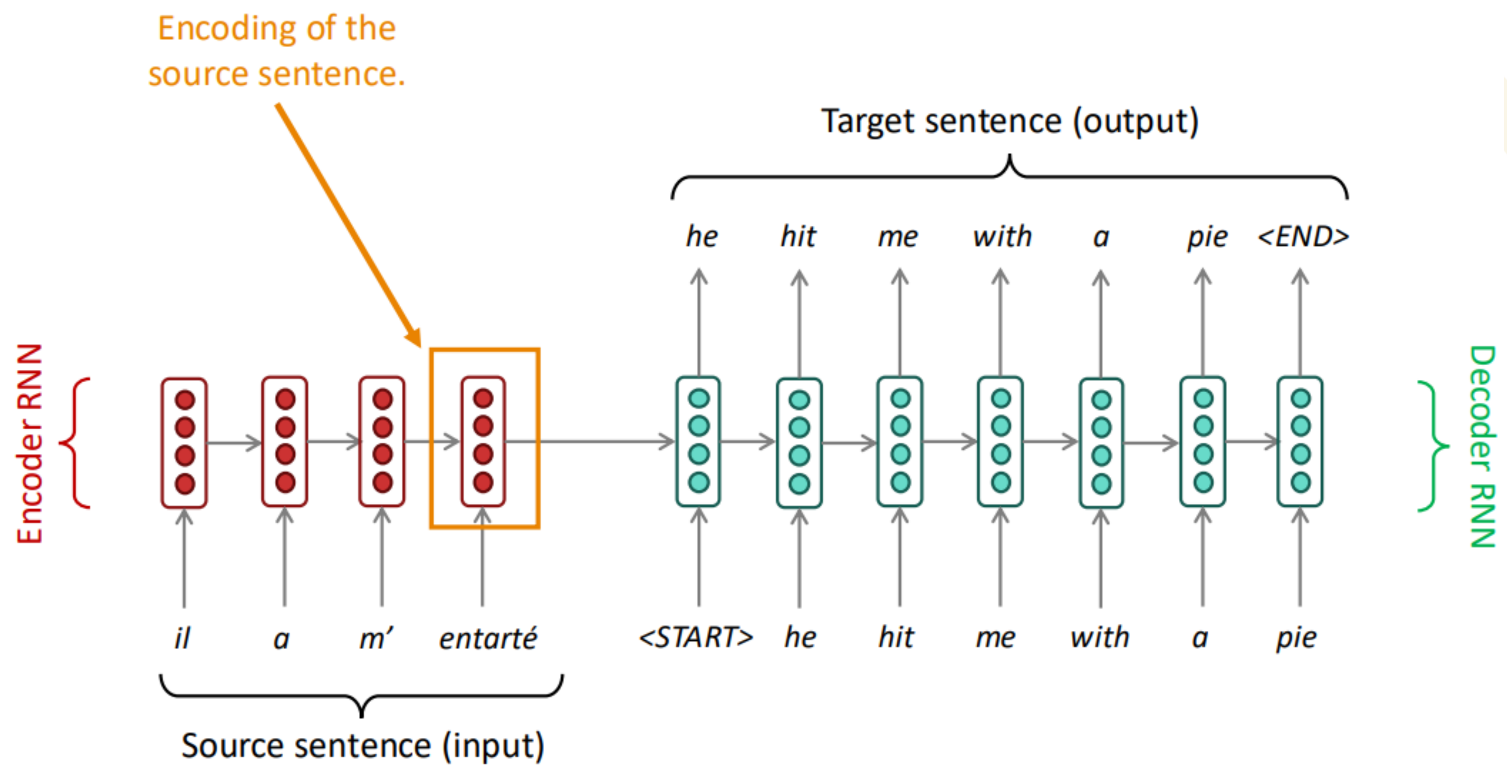


Why LSTM is better than regular

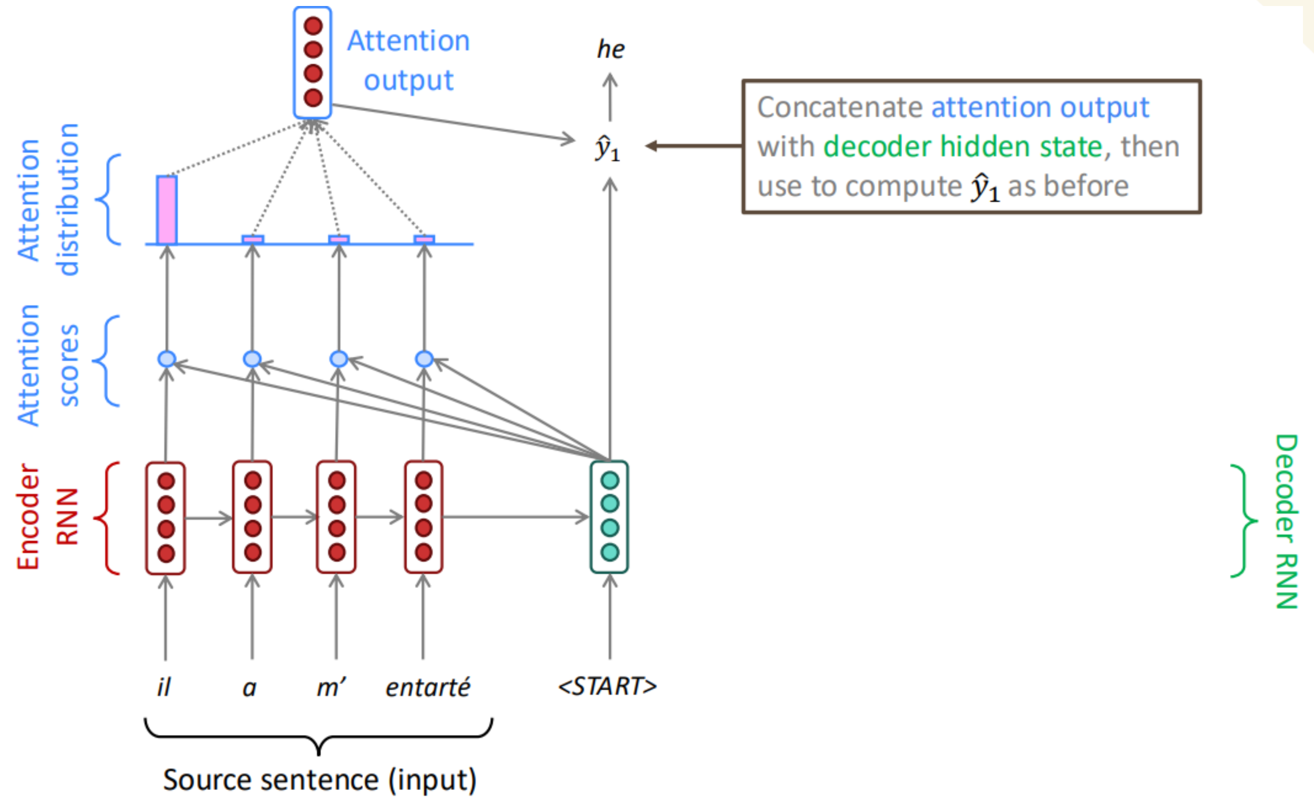




The bottleneck in RNN-based NMT



Sequence-to-sequence with attention



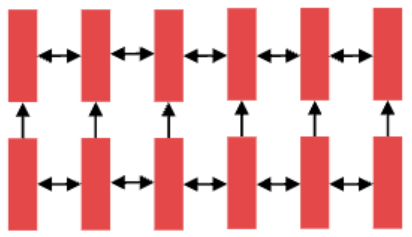
Concatenate attention output with decoder hidden state, then use to compute $\hat{y}_1$ as before

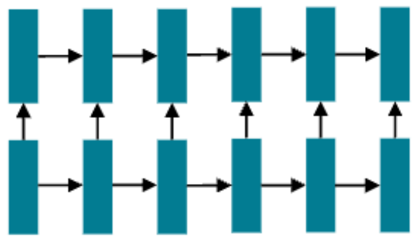
Lecture Plan

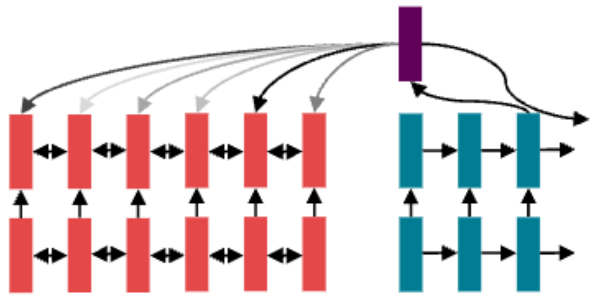
1. From recurrence (RNN) to attention-based NLP models
2. The Transformer model
3. Great results with Transformers
4. Drawbacks and variants of Transformers

In last few lectures: Recurrent models for (most) NLP!

- Around 2016, the de facto strategy in NLP is to encode sentences with a bidirectional LSTM:
  - for example, the source sentence in a translation
- Define your output (parse, sentence, summary) as a sequence and use an LSTM to generate it.
- Use attention to allow flexible access to memory.

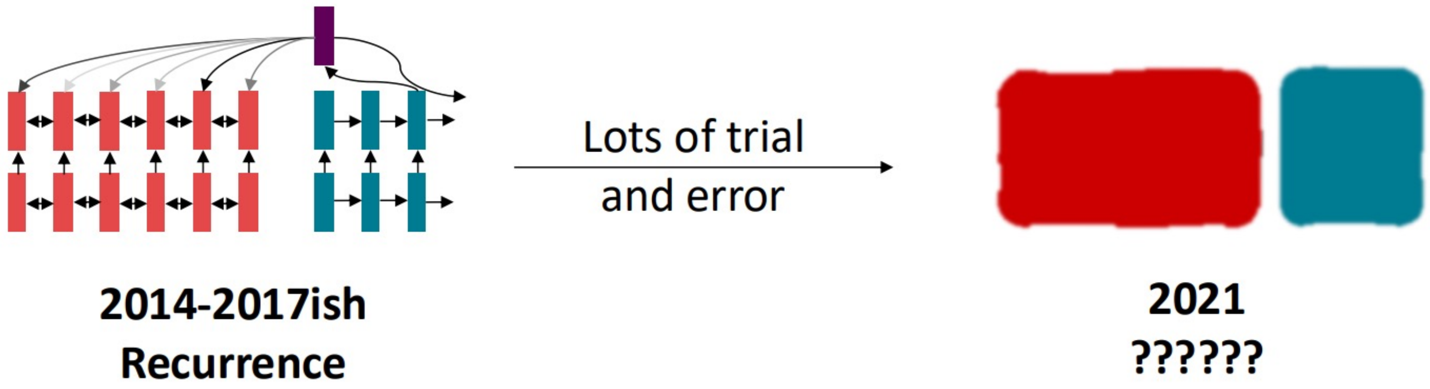






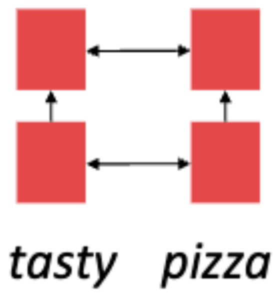
Do we even need recurrence at all?

- Abstractly: Attention is a way to pass information from a sequence (x) to a neural network input. (h_t)
- This is also exactly what RNNs are used for – to pass information!
- Can we just get rid of the RNN entirely? Maybe attention is just a better way to pass information!

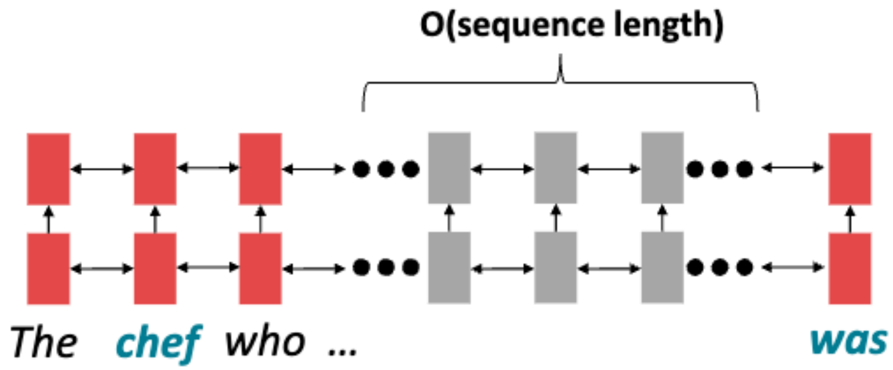


Issues with recurrent models: Linear interaction distance

- RNNs are unrolled “left-to-right”.
  - This encodes linear locality: a useful heuristic, and nearby words often affect each other’s meanings



- However, this also brings a problem:
- RNNs take O(sequence length) steps for distant word pairs to interact.



If not recurrence, how about word windows?

- **Word window models aggregate local contexts**
- Just like 1D convolution
- Number of unparallelizable operations does not increase sequence length

- Problem: What about long-distance dependencies?

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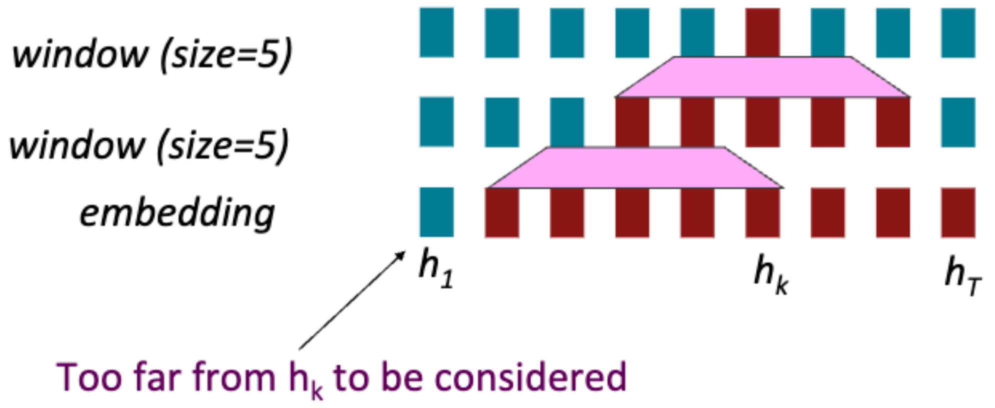
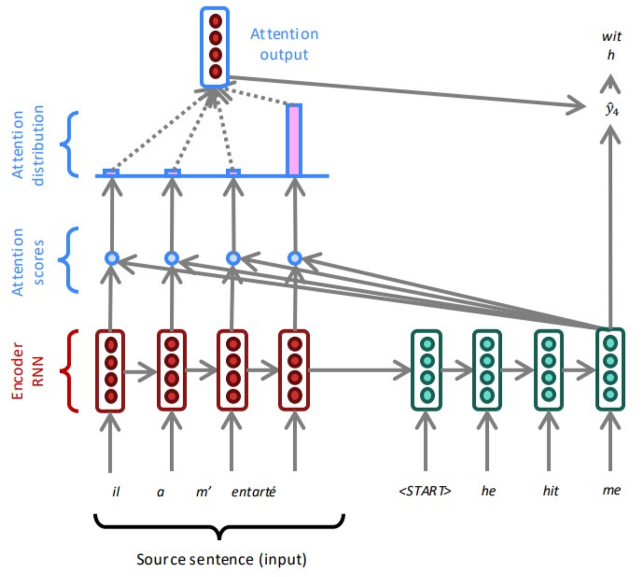


Red states indicate those "visible" to h_k

The building block we need: self attention

- What we talked about
  – Cross attention: paying attention to the input x to generate y_t



- What we need
  – Self attention: to generate y_t , we need to pay attention to $y_{<t}$

Self-Attention: keys, queries, values from the same sequence

Let $\boldsymbol{w}_{1:n}$ be a sequence of words in vocabulary V. For each $\boldsymbol{w}_i$, let $\boldsymbol{x}_i = E\boldsymbol{w}_i$, where $E \in \mathbb{R}^{d\times|V|}$is an embedding matrix.

1. Transform each word embedding with weight matrices Q, K, V , each in $\mathbb{R}^{d\times d}$

$$\boldsymbol{q}_i = Q\boldsymbol{x}_i(\text{queries}) \qquad \boldsymbol{k}_i = K\boldsymbol{x}_i(\text{keys}) \qquad \boldsymbol{v}_i = V\boldsymbol{x}_i(\text{values})$$

2. Compute pairwise similarities between keys and queries; normalize with softmax

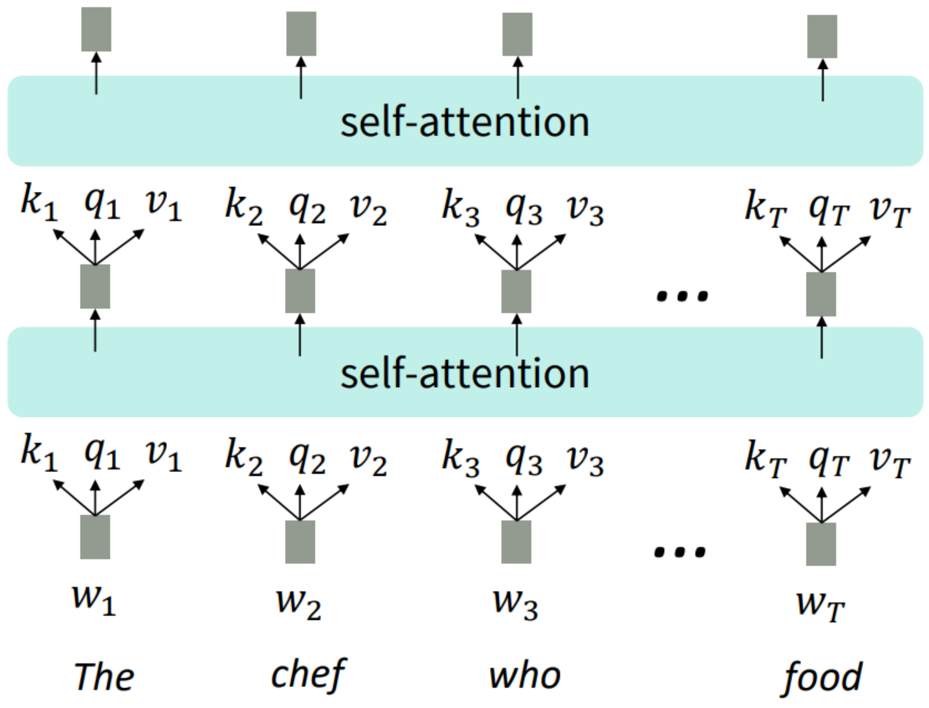
$$\boldsymbol{e}_{ij} = \boldsymbol{q}_i^T \boldsymbol{k}_j \qquad \boldsymbol{\alpha}_{ij} = \frac{exp(\boldsymbol{e}_{ij})}{\sum_{j'} exp(\boldsymbol{e}_{ij'})}$$

3. Compute output for each word as weighted sum of values

$$\boldsymbol{o}_i = \sum_j \boldsymbol{\alpha}_{ij}\boldsymbol{v}_i$$

Self-attention as an NLP building block

- In the diagram at the right, we have stacked self-attention blocks, like we might stack LSTM layers.
- Can self-attention be a drop-in replacement for recurrence?
  - ➢ No. It has a few issues, which we'll go through. First, self-attention is an operation on sets. It has no inherent notion of order.



Self-attention doesn't know the order of its inputs

Barriers and solutions for Self-Attention as a building block

Barriers		**Solutions**
1. Doesn't have an inherent notion of order!	$\longrightarrow$	**?**

Fixing the first self-attention problem: sequence order

- Since self-attention doesn't build in order information, we need to encode the order of the sentence in our keys, queries, and values.
- Consider representing each sequence index as a vector

$$\boldsymbol{p}_i \in \mathbb{R}^{\mathrm{d}}, \text{ for } i \in \{1,2, \dots, n\} \text{ are position vectors}$$

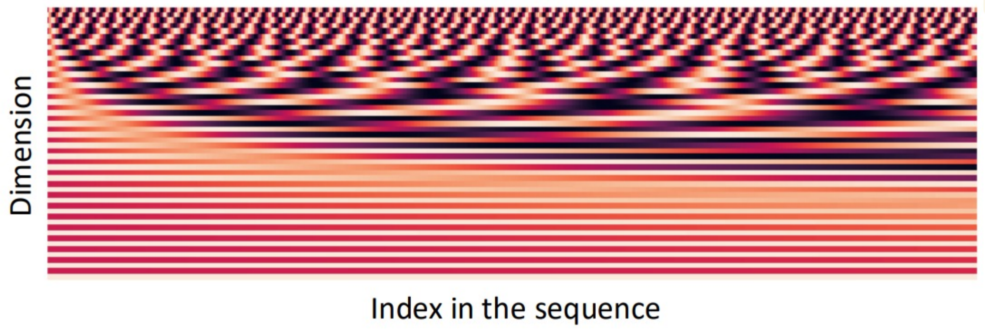
- Don't worry about what the $\boldsymbol{p}_i$ are made of yet!
- Easy to incorporate this info into our self-attention block: just add the $\boldsymbol{p}_i$ to our inputs!
- Recall that $\boldsymbol{x}_i$ is the embedding of the word at index i.

The positioned embedding: $\tilde{\boldsymbol{x}}_i = \boldsymbol{x}_i + \boldsymbol{p}_i$

Position representation vectors through sinusoids

- **Sinusoidal position representations:** concatenate sinusoidal functions of varying periods:

$$\boldsymbol{p}_i = \begin{pmatrix} \sin(i/10000^{2*1/d}) \\ \cos(i/10000^{2*1/d}) \\ \vdots \\ \sin(i/10000^{2*\frac{d}{2}/d}) \\ \cos(i/10000^{2*\frac{d}{2}/d}) \end{pmatrix}$$



Pros:

- Periodicity indicates that maybe "absolute position" isn't as important
- Maybe can extrapolate to longer sequences as periods restart!

Cons:

- Not learnable
- The extrapolation doesn't really work!

Position representation vectors learned from scratch

- Learned absolute position representations: Let all $\boldsymbol{p}_i$ be learnable parameters! Learn a matrix $\boldsymbol{p} \in \mathbb{R}^{\mathrm{d} \times \mathrm{n}}$, and let each $\boldsymbol{p}_i$ be a column of that matrix!
- Pros: Flexibility--each position gets to be learned to fit the data
- Cons: Definitely can't extrapolate to indices outside 1, … , n.
- Most systems use this!
  - This often leads to strong empirical results, especially when the training and test sequence lengths are similar.
- Sometimes people try more flexible representations of position:
  - Relative linear position attention [Shaw et al., 2018]
  - Dependency syntax-based position [Wang et al., 2019]

Common, modern relative position embeddings

- **High level thought process**: a relative position embedding should be some $f(x, i)$ subject to:

$$\langle f(x,i), f(y,j)\rangle = g(x,y,i-j)$$

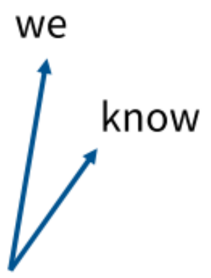
- That is, the attention score (dot product between query and key) only gets to depend on the relative position $(i - j)$.
- How do existing embeddings not fulfill this goal?
  1. **Sinusoidal**: the attention score has various cross-terms that are not just dependent on relative position (they depend on i or j, like sin(i)cos(j))
  2. **Absolute:** the positional embeddings are added to the input token embeddings, the resulting attention score will depend on individual position i or j, not the relative position.

$$e_{ij} = \frac{x_i W^Q (x_j W^K + a_{ij}^K)^T}{\sqrt{d_z}}$$

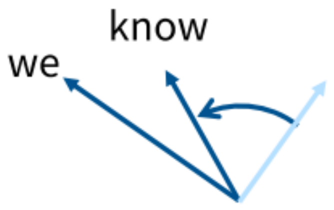
RoPE – Relative position embedding via rotation

How can we solve this problem?

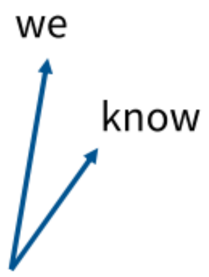
- We want our embeddings to be invariant to absolute position
- We know that inner products are invariant to arbitrary rotation



Position independent embedding



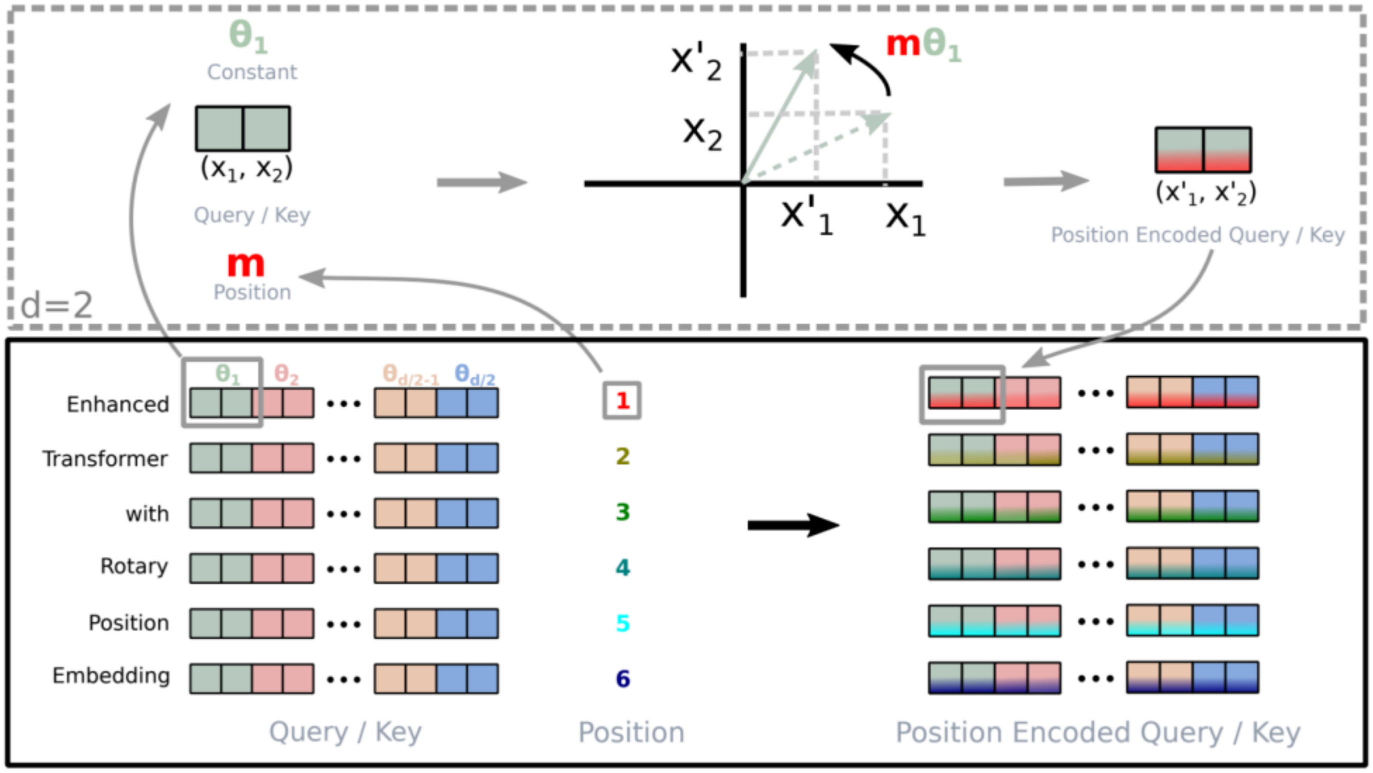
Embedding
“of course we know”
Rotate by ‘2 rotations’



Embedding
“we know that”
Rotate by ‘0 rotation’

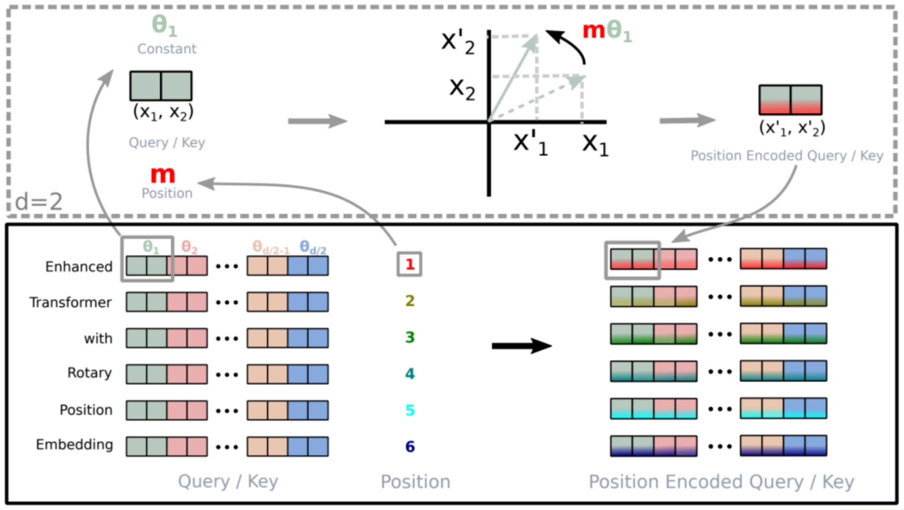
RoPE – From 2 to many dimensions

- Just pair up the coordinates and rotate them in 2d (motivation: complex numbers)



[Su et al 2021]

RoPE in equations



- Get the 2-D pairs
  - Each pair of dimensions (x_{2k}, x_{2k+1}) forms a 2-D vector (or complex number): $z_k = x_{2k} + jx_{2k+1}$
- Apply position-dependent rotation
  - For position p and input token embedding x: $\mathrm{RoPE}(x, p) = R(p)x$
  - For each pair, RoPE is defined as $R_k(p) = \begin{bmatrix} \cos(p\theta_k) & -\sin(p\theta_k) \\ \sin(p\theta_k) & \cos(p\theta_k) \end{bmatrix}, \theta_k = 10000^{-2k/d}$
  - For each pair, this matrix transformation equals to a rotation: $z'_k = z_k e^{jp\theta_k}$
- Finally, apply RoPE to queries and keys embeddings: $Q'_i = R(i)Q_i, K'_j = R(j)K_j$
  - Then the attention uses: $(Q'_i)^\top K'_j = Q_i^\top R(i-j)K_j$
  - Attention depends only on relative distance $(i-j)$

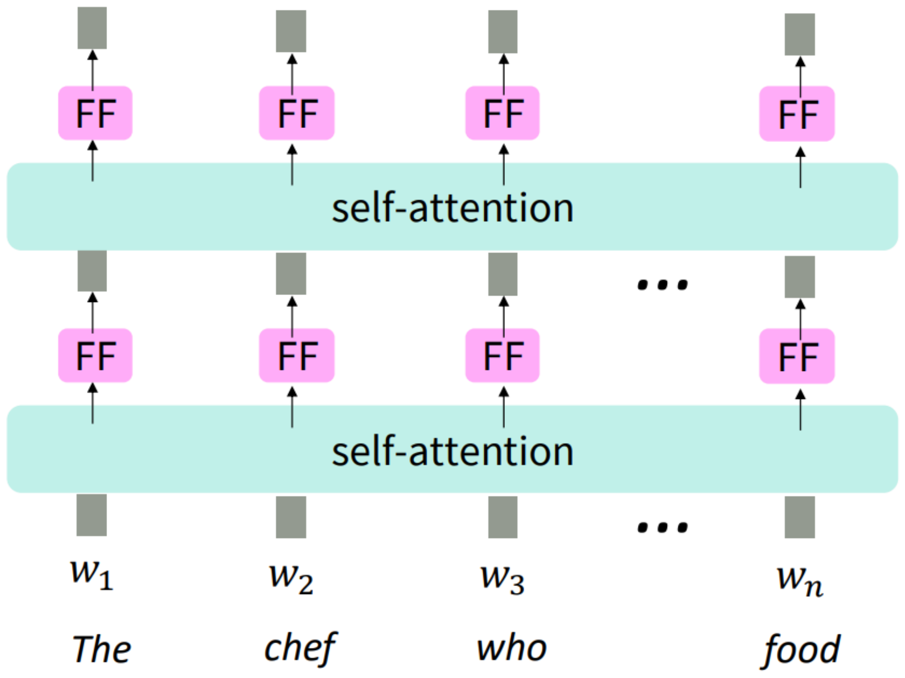
Barriers and solutions for Self-Attention as a building block

Barriers		**Solutions**
1. Doesn’t have an inherent notion of order!	$\longrightarrow$	1. Add position representations to the inputs.
2. No nonlinearities for deep learning magic! It’s all just weighted averages.	$\longrightarrow$	**?**

Adding nonlinearities in self-attention

- Note that there are no elementwise nonlinearities in self-attention; stacking more self-attention layers just re-averages value vectors
- Easy fix: add a feed-forward network to post-process each output vector.

$$\begin{aligned} m_i &= MLP(\text{output}_i) \\ &= W_2 * \text{ReLU}(W_1 \, \text{output}_i + b_1) + b_2 \end{aligned}$$



Intuition: the FF network processes the result of attention

Barriers and solutions for Self-Attention as a building block

Barriers

1. Doesn't have an inherent notion of order! →
2. No nonlinearities for deep learning magic! It's all just weighted averages →
3. Need to ensure we don't "look at the future" when predicting a sequence →
    - Like in machine translation
    - Or language modeling

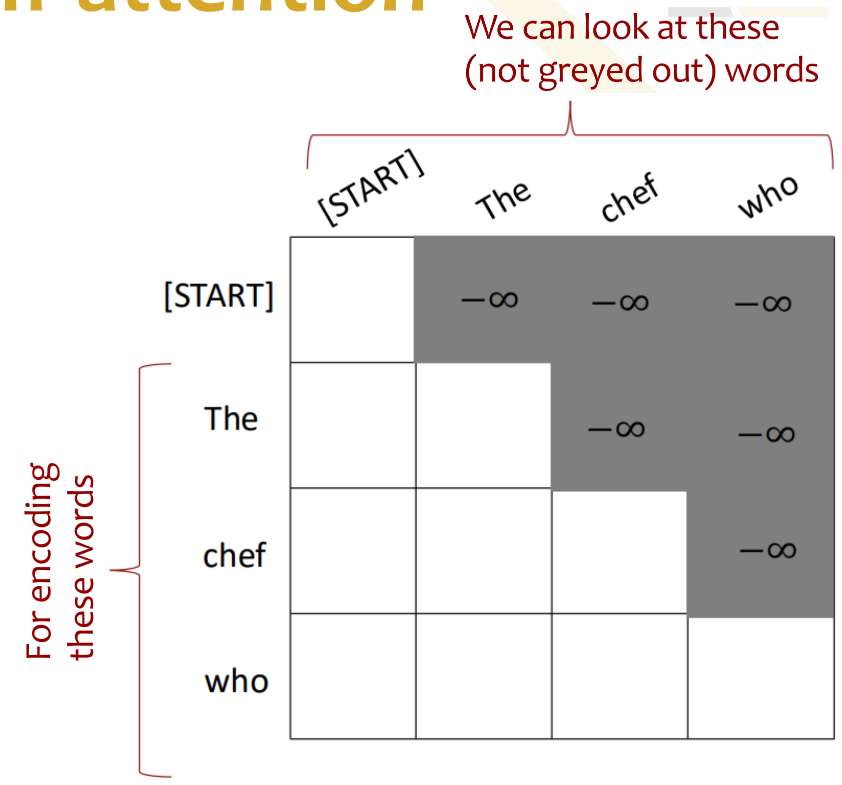
Solutions

1. Add position representations to the inputs
2. Easy fix: apply the same feedforward network to each self-attention output.
3. ?

Masking the future in self-attention

- To use self-attention in decoders, we need to ensure we can't peek at the future.
- At every timestep, we could change the set of keys and queries to include only past words. (Inefficient!)
- To enable parallelization, we mask out attention to future words by setting attention scores to $-\infty$.

$$e_{ij} = \begin{cases} q_i^\top k_j, j \le i \\ -\infty, j > i \end{cases}$$



Barriers and solutions for Self-Attention as a building block

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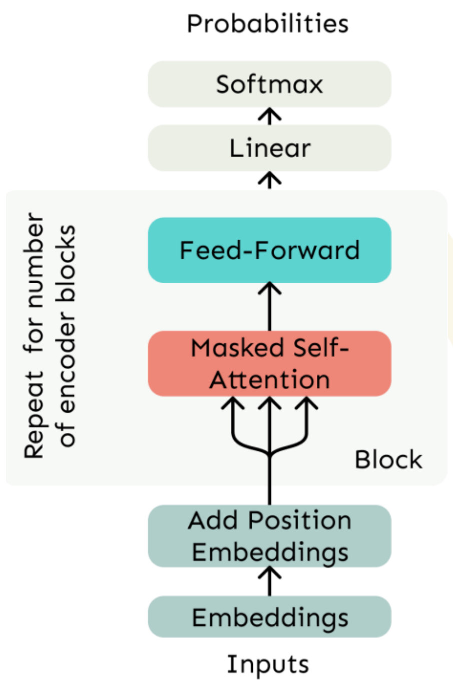
    - Like in machine translation
    - Or language modeling

Solutions

1. Add position representations to the inputs.
2. Easy fix: apply the same feedforward network to each self-attention output.
3. Mask out the future by artificially setting attention weights to zero.

Necessities for a self-attention building block

1. Self-attention:
   - The basis of the method.
2. Position representations:
   - Specify the sequence order, since self-attention is an unordered function of its inputs.
3. Nonlinearities:
   - At the output of the self-attention block.
   - Frequently implemented as a simple feedforward network.
4. Masking:
   - To parallelize operations while not looking at the future.
   - Keeps information about future from "leaking" to the past.


Probabilities
Softmax
Linear
Repeat for number of encoder blocks
Feed-Forward
Masked Self-Attention
Block
Add Position Embeddings
Embeddings
Inputs