Introduction to Transformer

Part-1

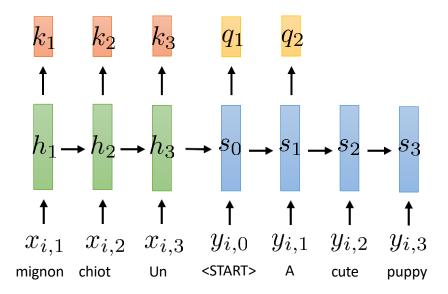
Tanmoy Chakraborty
Associate Professor, IIT Delhi
https://tanmoychak.com/





Is Attention All We Need?

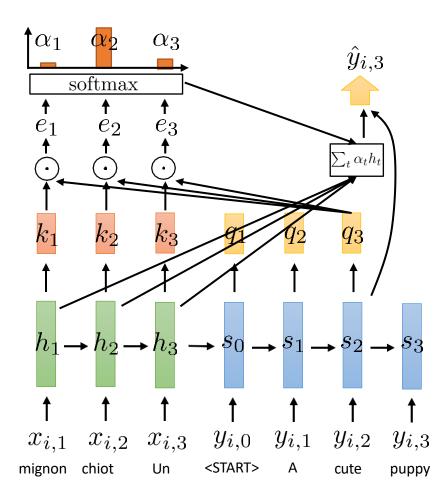
Recap: Attention







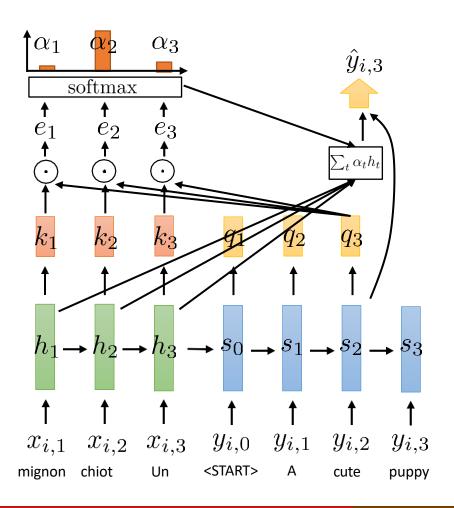
Recap: Attention







Recap: Attention

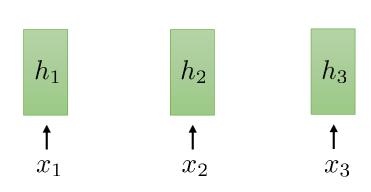


- If we have **attention**, do we even need recurrent connections?
- Can we transform our RNN into a purely attention-based model?
- Attention can access all time steps simultaneously, potentially doing everything that recurrence can, and even more. However, this approach presents some challenges:

The encoder lacks temporal dependencies at all!



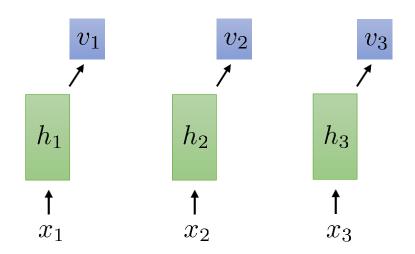




this is *not* a recurrent model! but still weight sharing:

$$h_t = \sigma(Wx_t + b)$$
 shared weights at all time steps



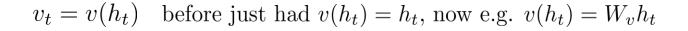


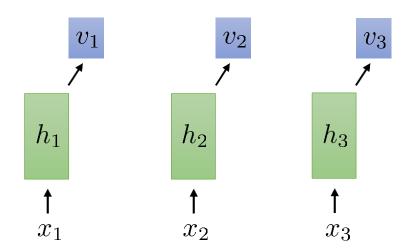
this is *not* a recurrent model! but still weight sharing:

$$h_t = \sigma(Wx_t + b)$$
 shared weights at all time steps







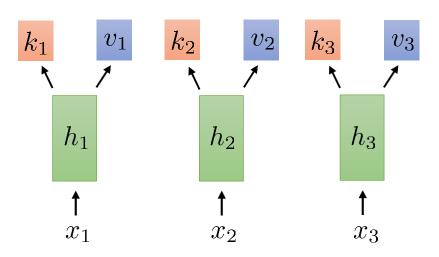


this is *not* a recurrent model! but still weight sharing:

$$h_t = \sigma(Wx_t + b)$$
 shared weights at all time step



$$v_t = v(h_t)$$
 before just had $v(h_t) = h_t$, now e.g. $v(h_t) = W_v h_t$

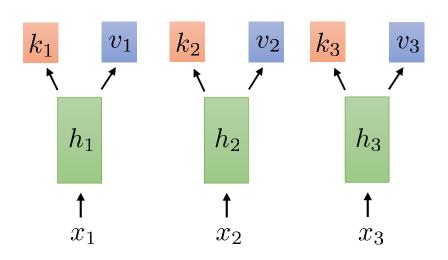


this is *not* a recurrent model! but still weight sharing:

$$h_t = \sigma(Wx_t + b)$$
 shared weights at all time steps







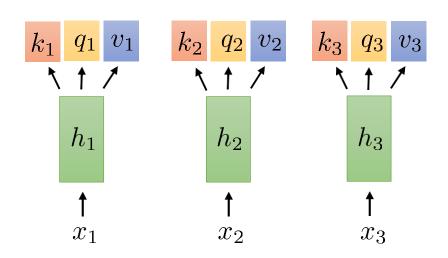
$$v_t = v(h_t)$$
 before just had $v(h_t) = h_t$, now e.g. $v(h_t) = W_v h_t$
 $k_t = k(h_t)$ (just like before) e.g., $k_t = W_k h_t$

this is *not* a recurrent model! but still weight sharing:

$$h_t = \sigma(Wx_t + b)$$
 shared weights at all time steps







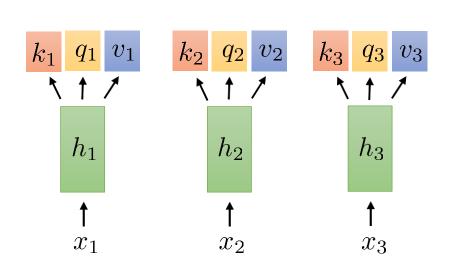
$$v_t = v(h_t)$$
 before just had $v(h_t) = h_t$, now e.g. $v(h_t) = W_v h_t$
 $k_t = k(h_t)$ (just like before) e.g., $k_t = W_k h_t$

this is *not* a recurrent model! but still weight sharing:

$$h_t = \sigma(Wx_t + b)$$
 shared weights at all time steps







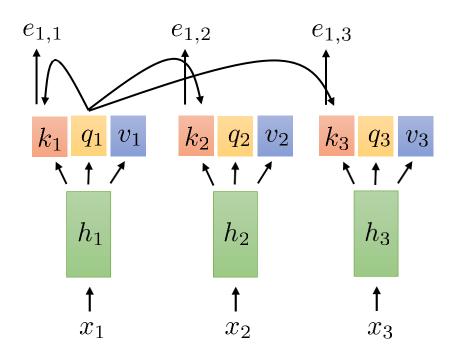
$$v_t = v(h_t)$$
 before just had $v(h_t) = h_t$, now e.g. $v(h_t) = W_v h_t$
 $k_t = k(h_t)$ (just like before) e.g., $k_t = W_k h_t$
 $q_t = q(h_t)$ e.g., $q_t = W_q h_t$

this is *not* a recurrent model! but still weight sharing:

$$h_t = \sigma(Wx_t + b)$$
 shared weights at all time steps







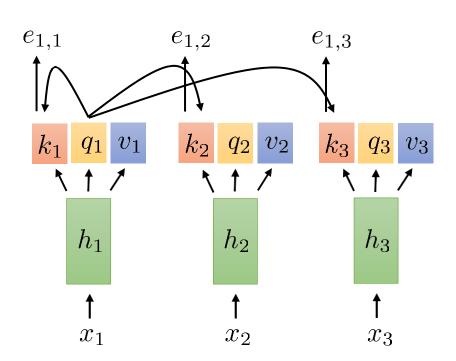
$$v_t = v(h_t)$$
 before just had $v(h_t) = h_t$, now e.g. $v(h_t) = W_v h_t$
 $k_t = k(h_t)$ (just like before) e.g., $k_t = W_k h_t$
 $q_t = q(h_t)$ e.g., $q_t = W_q h_t$

this is *not* a recurrent model! but still weight sharing:

$$h_t = \sigma(Wx_t + b)$$
 shared weights at all time steps





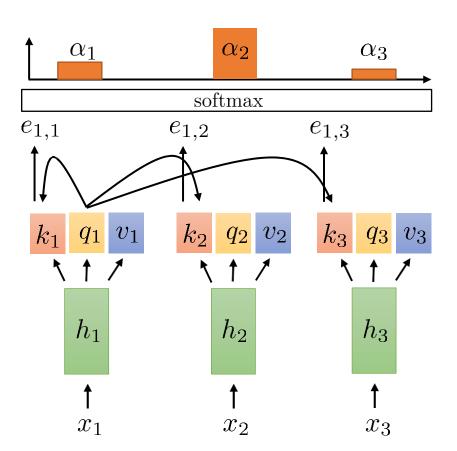


$$e_{l,t} = q_l \cdot k_t$$
 $v_t = v(h_t)$ before just had $v(h_t) = h_t$, now e.g. $v(h_t) = W_v h_t$
 $k_t = k(h_t)$ (just like before) e.g., $k_t = W_k h_t$
 $q_t = q(h_t)$ e.g., $q_t = W_q h_t$
this is not a recurrent model!
but still weight sharing:

$$h_t = \sigma(Wx_t + b)$$
 shared weights at all time steps







$$e_{l,t} = q_l \cdot k_t$$

 $v_t = v(h_t)$ before just had $v(h_t) = h_t$, now e.g. $v(h_t) = W_v h_t$

$$k_t = k(h_t)$$
 (just like before) e.g., $k_t = W_k h_t$

$$q_t = q(h_t)$$
 e.g., $q_t = W_q h_t$

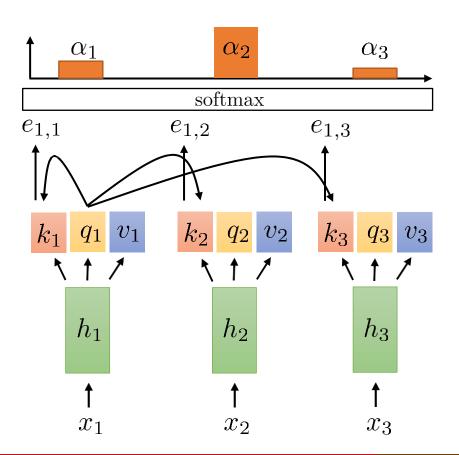
this is *not* a recurrent model!

but still weight sharing:

$$h_t = \sigma(Wx_t + b)$$
 shared weights at all time steps







$$\alpha_{l,t} = \exp(e_{l,t}) / \sum_{t'} \exp(e_{l,t'})$$

$$e_{l,t} = q_l \cdot k_t$$

$$v_t = v(h_t) \text{ before just had } v(h_t) = h_t, \text{ now e.g. } v(h_t) = W_v h_t$$

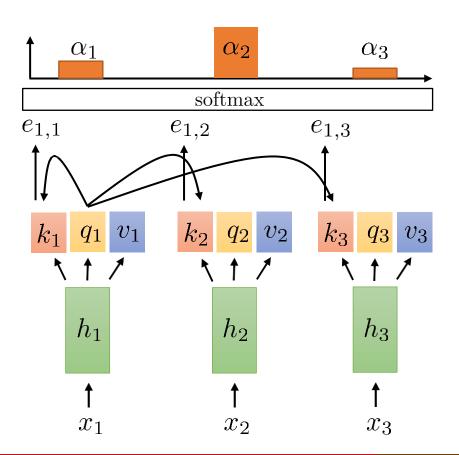
$$k_t = k(h_t) \text{ (just like before)} \quad \text{e.g., } k_t = W_k h_t$$

$$q_t = q(h_t) \quad \text{e.g., } q_t = W_q h_t$$
this is not a recurrent model!
but still weight sharing:

$$h_t = \sigma(Wx_t + b)$$
 shared weights at all time steps







$$\alpha_{l,t} = \exp(e_{l,t}) / \sum_{t'} \exp(e_{l,t'})$$

$$e_{l,t} = q_l \cdot k_t$$

$$v_t = v(h_t) \text{ before just had } v(h_t) = h_t, \text{ now e.g. } v(h_t) = W_v h_t$$

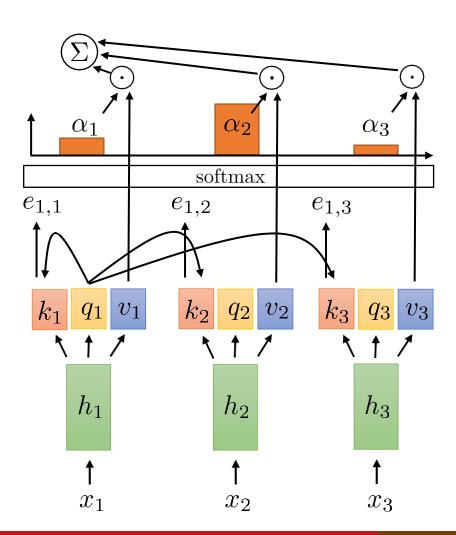
$$k_t = k(h_t) \text{ (just like before)} \quad \text{e.g., } k_t = W_k h_t$$

$$q_t = q(h_t) \quad \text{e.g., } q_t = W_q h_t$$
this is not a recurrent model!
but still weight sharing:

$$h_t = \sigma(Wx_t + b)$$
 shared weights at all time steps







$$\alpha_{l,t} = \exp(e_{l,t}) / \sum_{t'} \exp(e_{l,t'})$$

$$e_{l,t} = q_l \cdot k_t$$

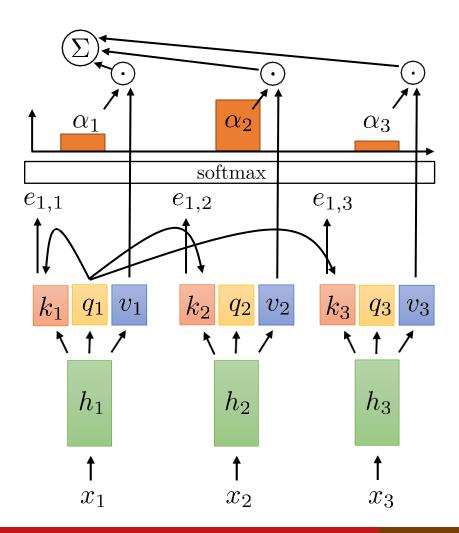
$$v_t = v(h_t) \text{ before just had } v(h_t) = h_t, \text{ now e.g. } v(h_t) = W_v h_t$$

$$k_t = k(h_t) \text{ (just like before)} \quad \text{e.g., } k_t = W_k h_t$$

$$q_t = q(h_t) \quad \text{e.g., } q_t = W_q h_t$$
this is not a recurrent model!
but still weight sharing:

$$h_t = \sigma(Wx_t + b)$$
 shared weights at all time steps





$$a_{l} = \sum_{t} \alpha_{l,t} v_{t}$$

$$\alpha_{l,t} = \exp(e_{l,t}) / \sum_{t'} \exp(e_{l,t'})$$

$$e_{l,t} = q_{l} \cdot k_{t}$$

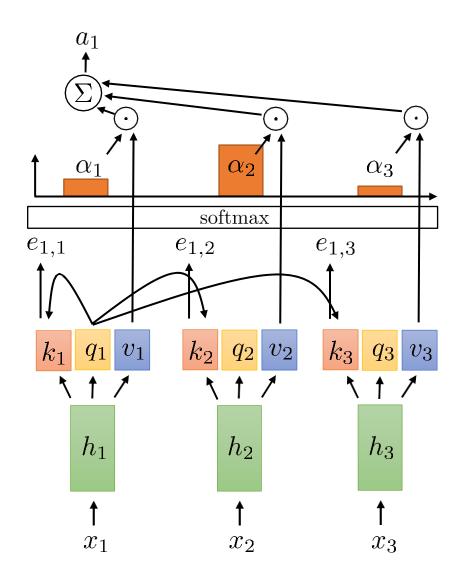
$$v_{t} = v(h_{t}) \quad \text{before just had } v(h_{t}) = h_{t}, \text{ now e.g. } v(h_{t}) = W_{v}h_{t}$$

$$k_{t} = k(h_{t}) \text{ (just like before)} \quad \text{e.g., } k_{t} = W_{k}h_{t}$$

$$q_{t} = q(h_{t}) \quad \text{e.g., } q_{t} = W_{q}h_{t}$$
this is not a recurrent model!
but still weight sharing:
$$h_{t} = \sigma(W_{t}x_{t} + b)$$

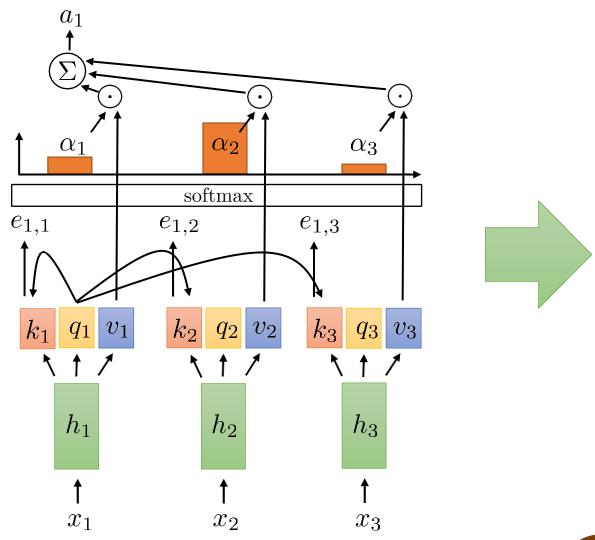
$$h_t = \sigma(Wx_t + b)$$
 shared weights at all time steps

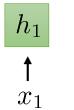


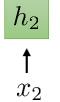


$$\begin{aligned} a_l &= \sum_t \alpha_{l,t} v_t \\ \alpha_{l,t} &= \exp(e_{l,t}) / \sum_{t'} \exp(e_{l,t'}) \\ e_{l,t} &= q_l \cdot k_t \\ v_t &= v(h_t) \quad \text{before just had } v(h_t) = h_t, \text{ now e.g. } v(h_t) = W_v h_t \\ k_t &= k(h_t) \text{ (just like before)} \quad \text{e.g., } k_t = W_k h_t \\ q_t &= q(h_t) \quad \text{e.g., } q_t = W_q h_t \\ \text{this is } not \text{ a recurrent model!} \\ \text{but still weight sharing:} \\ h_t &= \sigma(W_t x_t + b) \\ \text{shared weights at all time steps} \end{aligned}$$





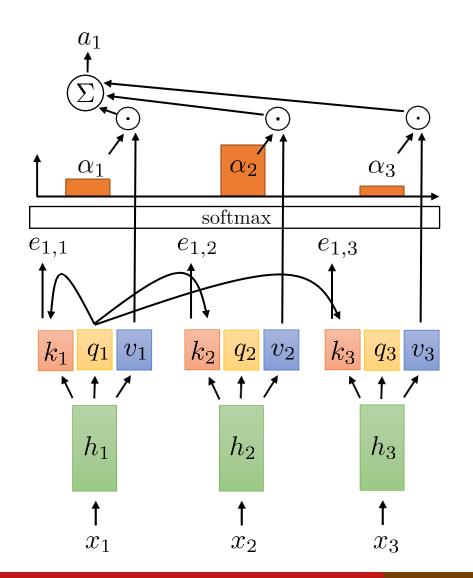


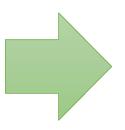


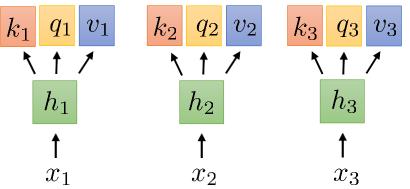






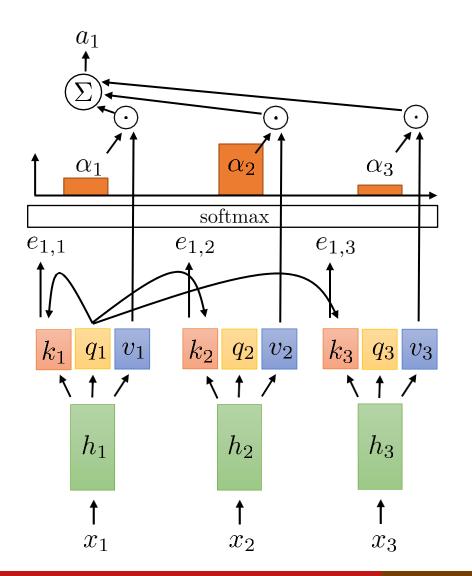




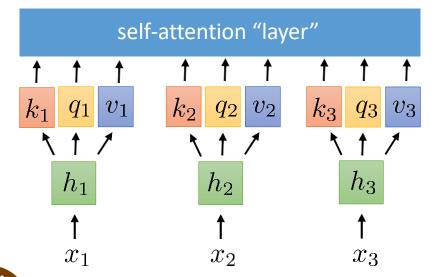






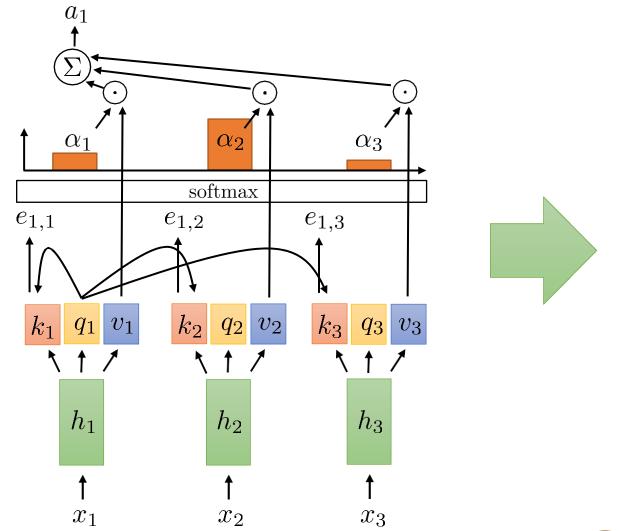


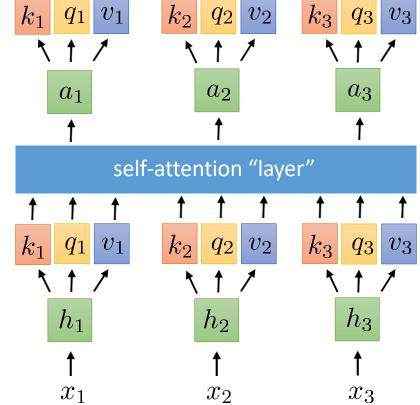






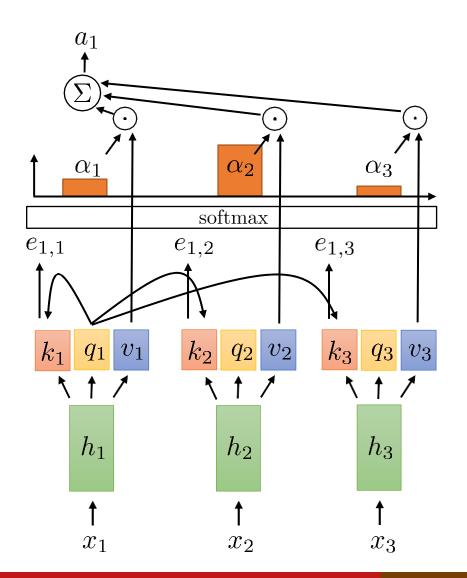


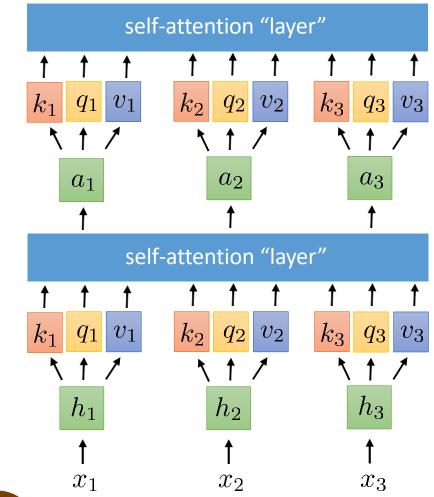






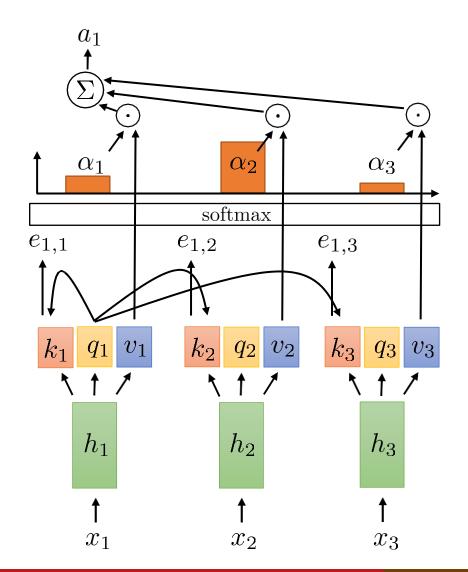


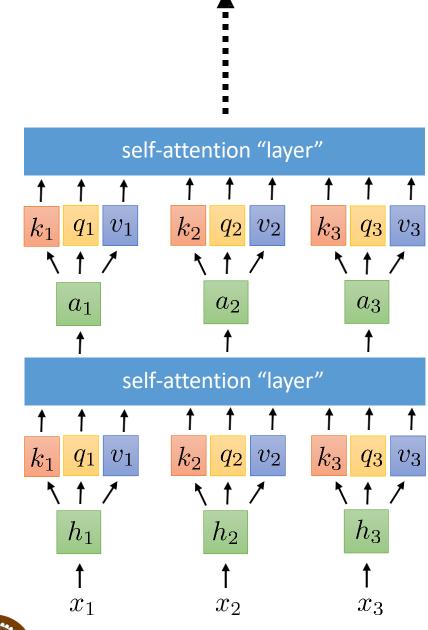






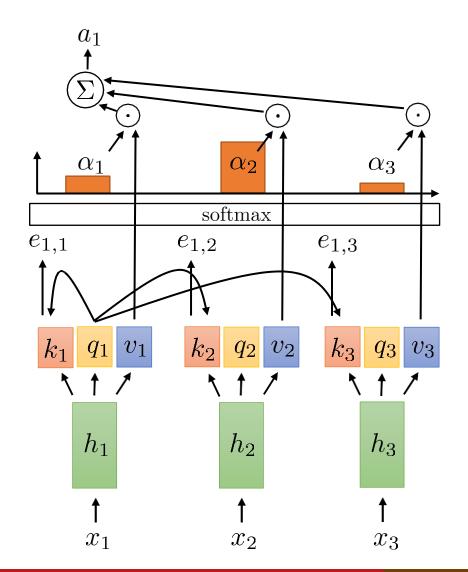


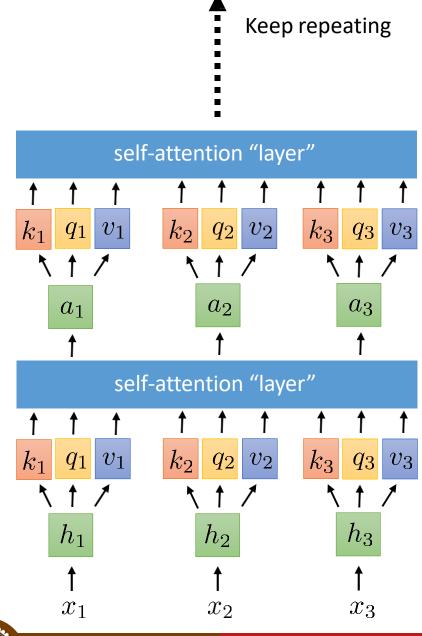
















From Self-Attention to Transformers

- We will talk about a class of models for processing sequences that does not use recurrent connections but instead relies entirely on attention and will build up towards a class of models called **Transformers**.
- To address a few key limitations, we need to add certain elements:

1. Positional encoding addresses lack of sequence information

2. Multi-headed attention allows querying multiple positions at each layer

3. Adding nonlinearities so far, each successive layer is *linear* in the previous one

4. Masked decoding how to prevent attention lookups into the future?





From Self-Attention to Transformers

- We will talk about a class of models for processing sequences that does not use recurrent connections but instead relies entirely on attention and will build up towards a class of models called **Transformers**.
- To address a few key limitations, we need to add certain elements:

1. Positional encoding

2. Multi-headed attention

3. Adding nonlinearities

4. Masked decoding

addresses lack of sequence information

allows querying multiple positions at each layer

so far, each successive layer is *linear* in the previous one

how to prevent attention lookups into the future?





Positional Encoding - Motivation

- **Problem :** Self-attention processes all the elements of a sequence in parallel without any regard for their order.
 - Example: the sun rises in the east
 - Permuted version: rises in the sun the east

the east rises in the sun

Bag of Words

in , the , rises , east , sun

- Self-attention is permutation invariant.
- In natural language, it is important to take into account the order of words in a sentence.
- Solution: Explicitly add positional information to indicate where a word appears in a sequence



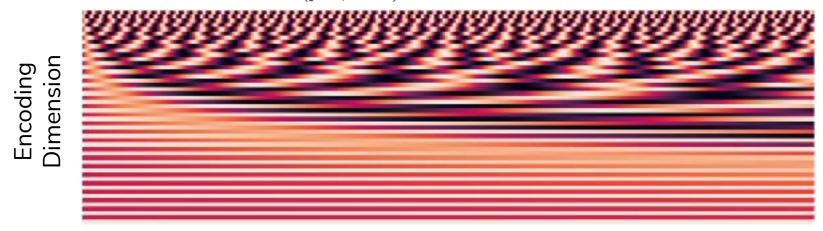


Sinusoidal Positional Encoding

- Helps it determine the position of each word (absolute positional information), or the distance between different words in the sequence (relative positional information)
- The frequency decreases along the encoding dimension.

$$PE_{(pos,2i)} = sin(pos/10000^{2i/d_{\text{model}}})$$

$$PE_{(pos,2i+1)} = cos(pos/10000^{2i/d_{\text{model}}})$$



We will see this in more detail later!

Position





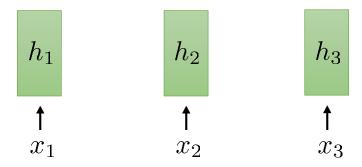
From Self-Attention to Transformers

- We will talk about a class of models for processing sequences that does not use recurrent connections but instead relies entirely on attention and will build up towards a class of models called transformers.
- To address a few key limitations, we need to add certain elements:
- 1. Positional encoding addresses lack of sequence information
- 2. Multi-headed attention allows querying multiple positions at each layer
- 3. Adding nonlinearities so far, each successive layer is *linear* in the previous one
- 4. Masked decoding how to prevent attention lookups into the future?



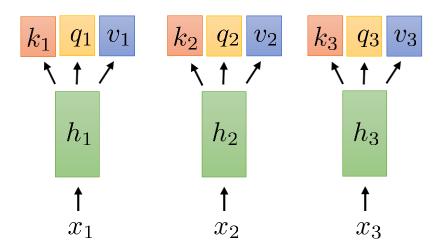


Given that we're fully depending on attention now, it could be beneficial to include more than one time step.





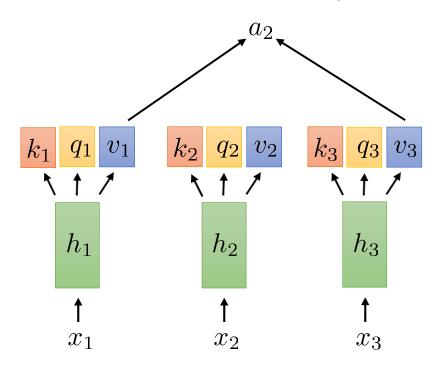
Given that we're fully depending on attention now, it could be beneficial to include more than one time step.

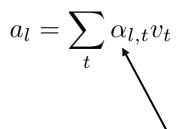






Given that we're fully depending on attention now, it could be beneficial to include more than one time step.

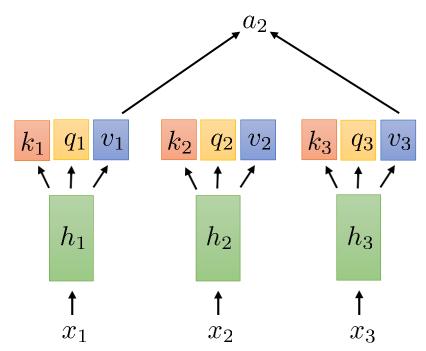


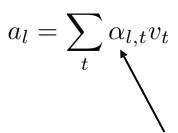


Due to the softmax function, this will be heavily influenced by a single value.



Given that we're fully depending on attention now, it could be beneficial to include more than one time step.





Due to the softmax function, this will be heavily influenced by a single value.

$$e_{l,t} = q_l \cdot k_t$$

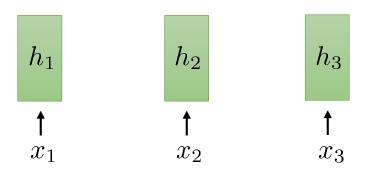
It's challenging to clearly specify that you want two distinct elements, like the subject and object in a sentence.





Multi-Head Attention

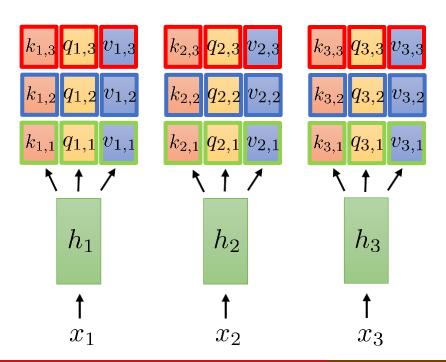
Solution: Use multiple keys, queries, and values for each time step





Multi-Head Attention

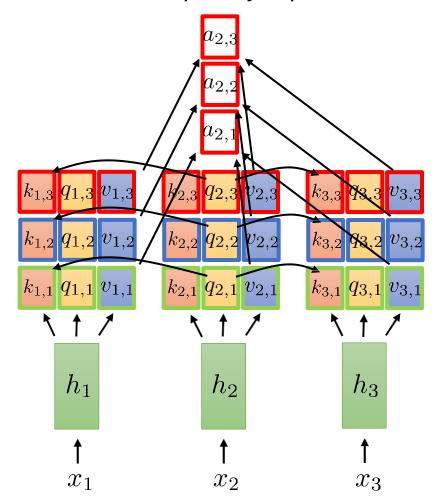
Solution: Use multiple keys, queries, and values for each time step





Multi-Head Attention

Solution: Use multiple keys, queries, and values for each time step



full attention vector formed by concatenation:

$$a_2 = \left[\begin{array}{c} a_{2,1} \\ a_{2,2} \\ a_{2,3} \end{array} \right]$$

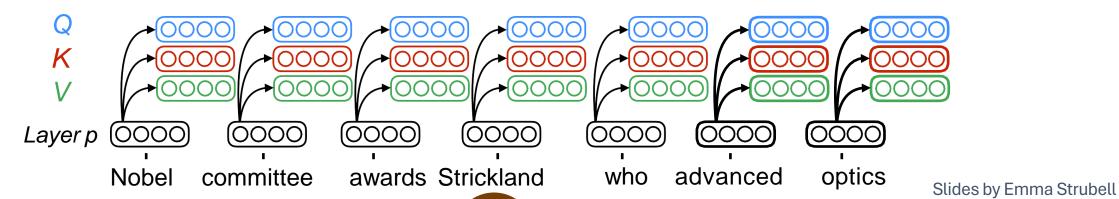
compute weights independently for each head

$$e_{l,t,i} = q_{l,i} \cdot k_{l,i}$$

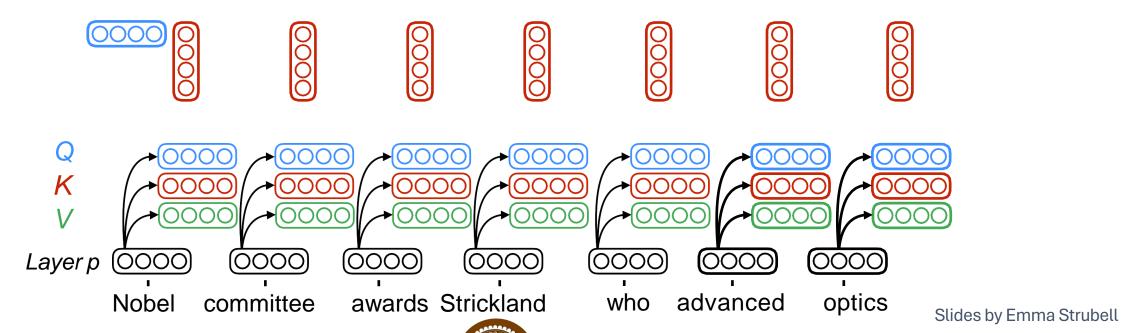
$$\alpha_{l,t,i} = \exp(e_{l,t,i}) / \sum_{t'} \exp(e_{l,t',i})$$

$$a_{l,i} = \sum_{t} \alpha_{l,t,i} v_{t,i}$$

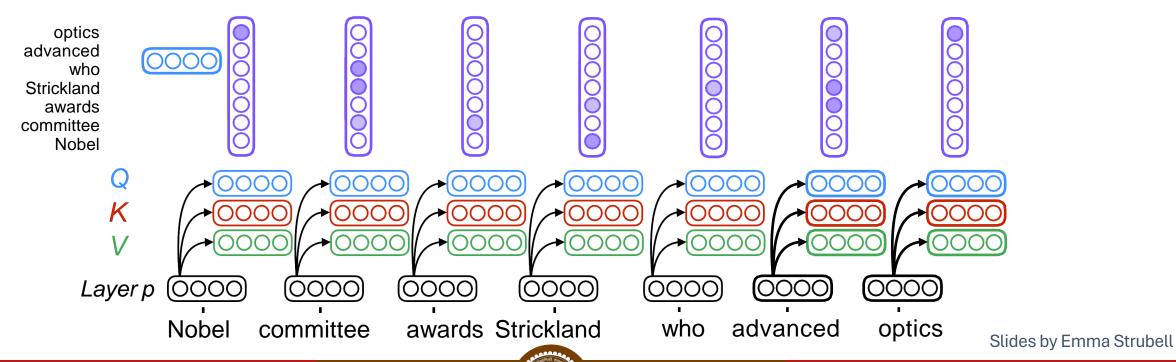




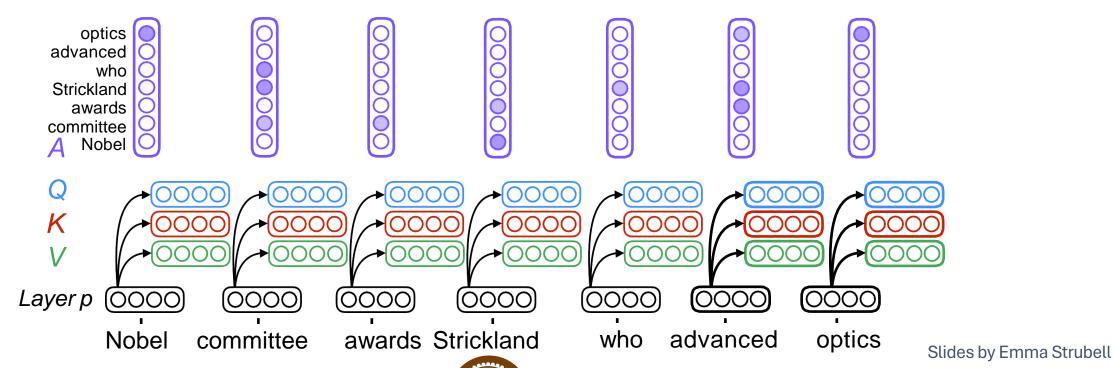




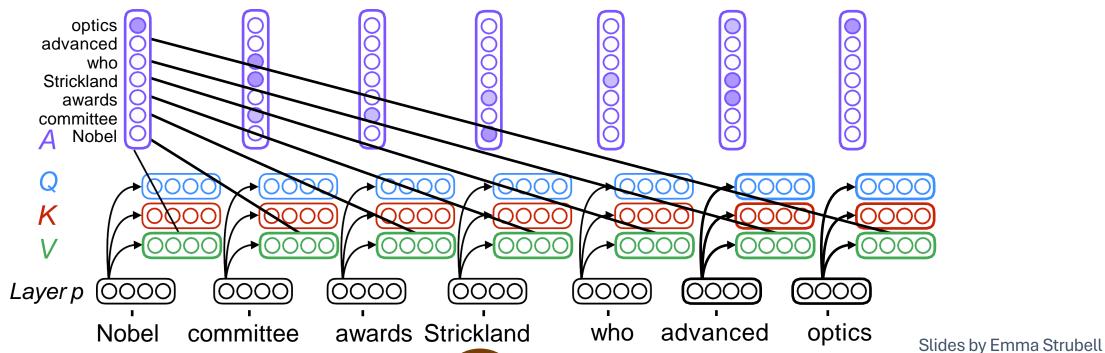




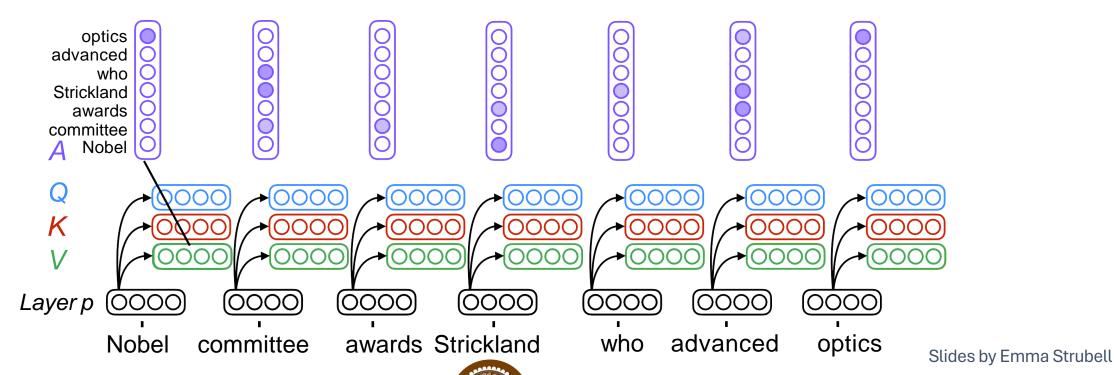




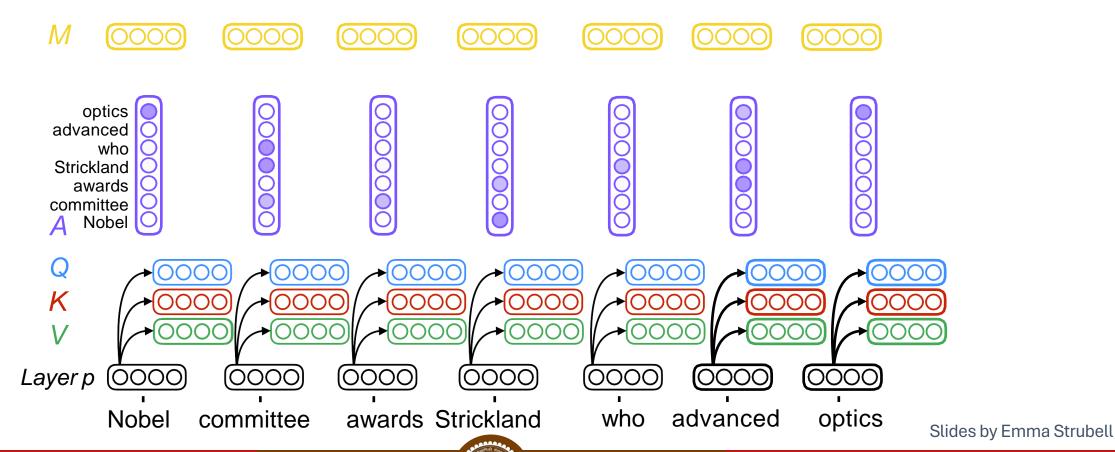




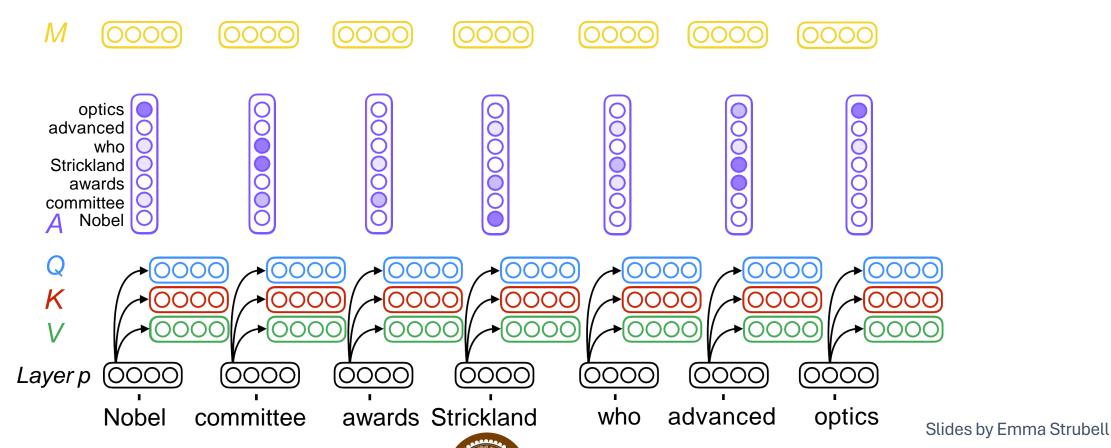








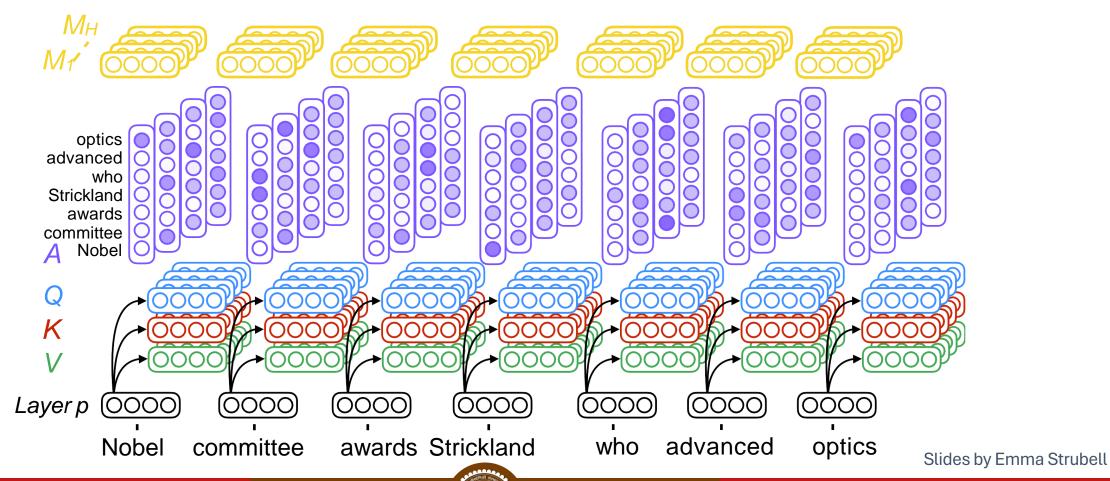






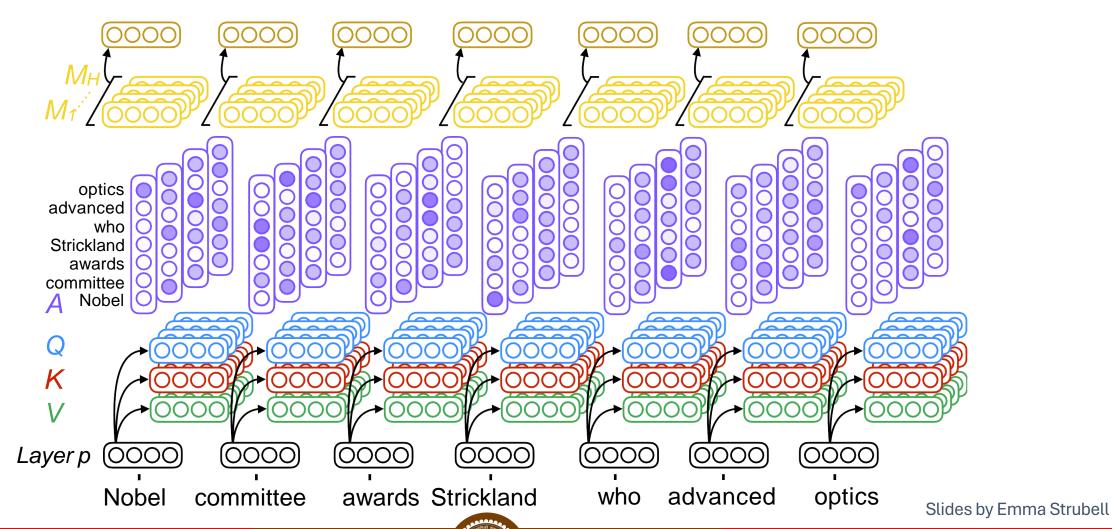
Tanmoy Chakraborty

Multi-Head Self-Attention





Multi-Head Self-Attention





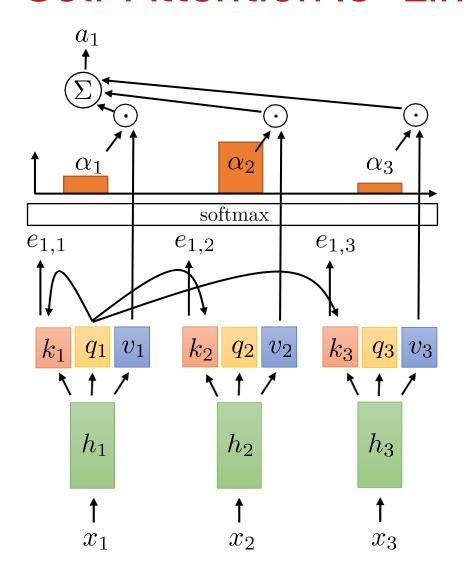
From Self-Attention to Transformers

- We will talk about a class of models for processing sequences that does not use recurrent connections but instead relies entirely on attention and will build up towards a class of models called transformers.
- To address a few key limitations, we need to add certain elements:
- 1. Positional encoding addresses lack of sequence information
- 2. Multi-headed attention allows querying multiple positions at each layer
- 3. Adding nonlinearities so far, each successive layer is *linear* in the previous one
- 4. Masked decoding how to prevent attention lookups into the future?





Self-Attention Is "Linear"



$$k_{t} = W_{k}h_{t} \quad q_{t} = W_{q}h_{t} \quad v_{t} = W_{v}h_{t}$$

$$\alpha_{l,t} = \exp(e_{l,t}) / \sum_{t'} \exp(e_{l,t'})$$

$$e_{l,t} = q_{l} \cdot k_{t}$$

$$a_{l} = \sum_{t} \alpha_{l,t}v_{t} = \sum_{t} \alpha_{l,t}W_{v}h_{t} = W_{v} \sum_{t} \alpha_{l,t}h_{t}$$

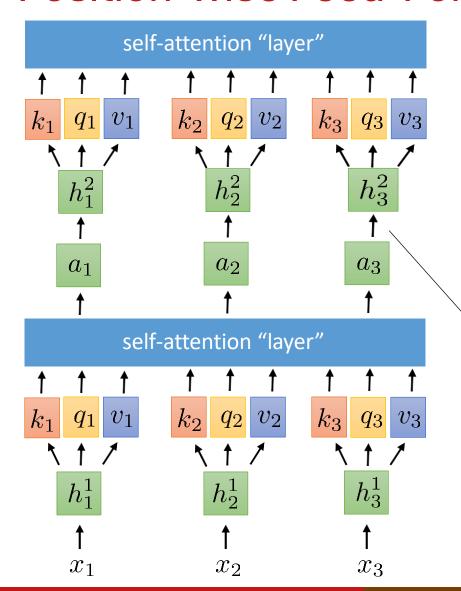
linear transformation

Problem: Every self-attention layer is a linear transformation of the previous layer with non-linear weights.



non-linear weights

Position-wise Feed-Forward Networks

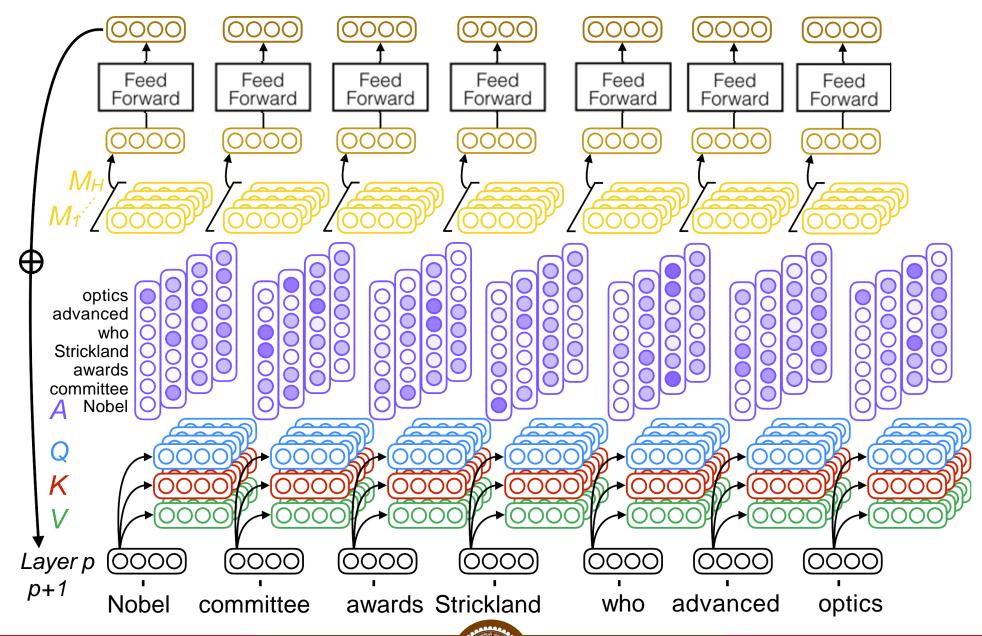


- **Solution :** Make the model more expressive is by alternating use of self-attention and non-linearity.
- Non-linearity is incorporated by means of a feedforward network which consists of two linear transformations with a ReLU activation in between.

$$FFN(x) = \max(0, xW_1 + b_1)W_2 + b_2$$

• The same non-linearity is utilized across various positions but they differ from layer to layer.







From Self-Attention to Transformers

- We will talk about a class of models for processing sequences that does not use recurrent connections but instead relies entirely on attention and will build up towards a class of models called transformers.
- To address a few key limitations, we need to add certain elements:

1. Positional encoding addresses lack of sequence information

2. Multi-headed attention allows querying multiple positions at each layer

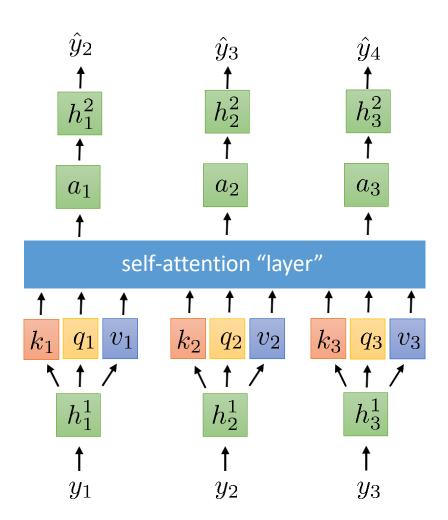
3. Adding nonlinearities so far, each successive layer is *linear* in the previous one

4. Masked decoding how to prevent attention lookups into the future?





Self-attention can see the future!

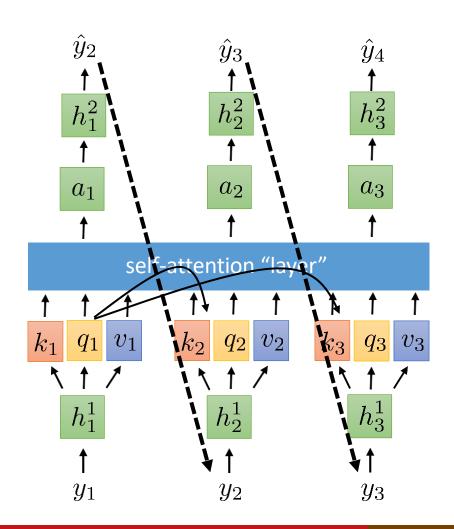


A **crude** self-attention "language model":

In practice, there would be several alternating self-attention layers and position-wise feedforward networks



Self-attention can see the future!



A **crude** self-attention "language model":

In practice, there would be several alternating self-attention layers and position-wise feedforward networks

Big problem: self-attention at step 1 can look at the value at steps 2 & 3, which is based on the **inputs** at steps 2 & 3

At test time (when decoding), the inputs at steps 2 & 3 will be based on the output at step 1...

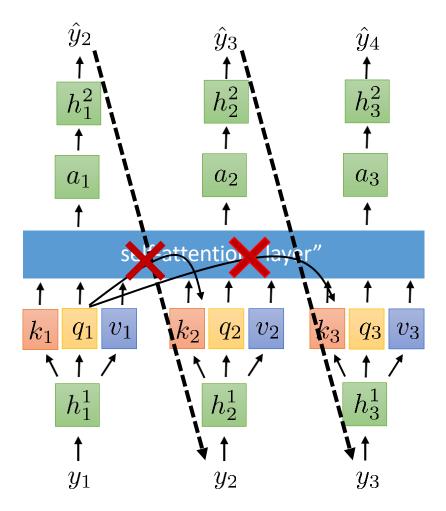
...which requires knowing the **input** at steps 2 & 3





Masked Attention

A **crude** self-attention "language model":



At test time (when decoding), the inputs at steps 2 & 3 will be based on the output at step 1...

...which requires knowing the input at steps 2 & 3

Must allow self-attention into the **past**...

...but not into the **future**

Easy solution:

$$e_{l,t} = a_l \cdot k_t$$

$$e_{l,t} = \begin{cases} q_l \cdot k_t & \text{if } l \ge t \\ -\infty & \text{otherwise} \end{cases}$$

in practice:

just replace $\exp(e_{l,t})$ with 0 if l < t inside the softmax

