Transformers

Designing, Visualizing and Understanding Deep Neural Networks

CS W182/282A

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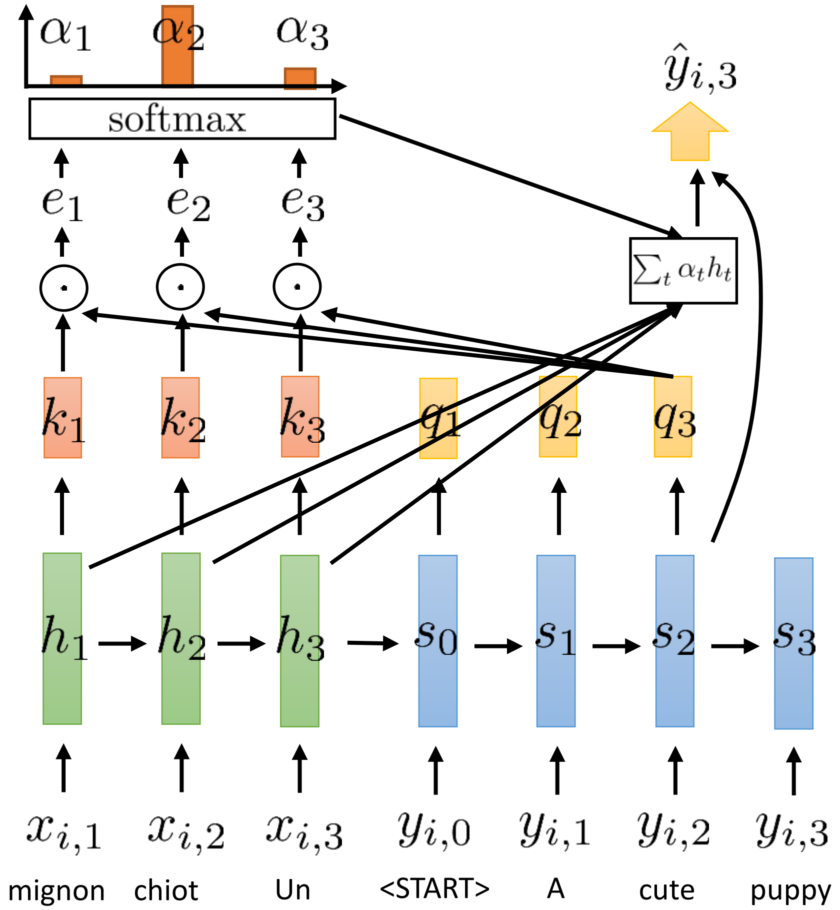
UC Berkeley

Is Attention All We Need?

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 **every** time step

Can in principle do **everything** that recurrence can, and more!

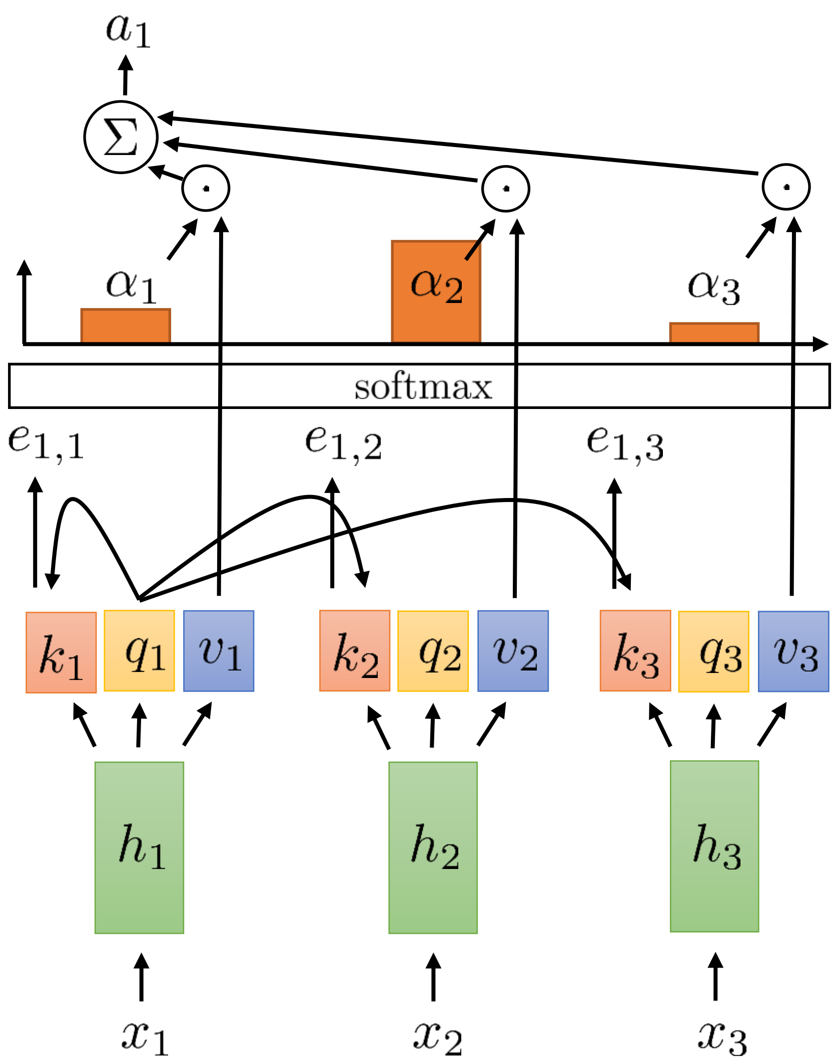
This has a few issues we must overcome:

Problem 1: now step $l = 2$ can't access s_1 or s_0

The encoder has no temporal dependencies at all!

We **must** fix this first

Self-Attention



$$a_l = \sum_t \alpha_{l,t} v_t$$

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

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

we'll see why this is important soon

$v_t = v(h_t)$ 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!

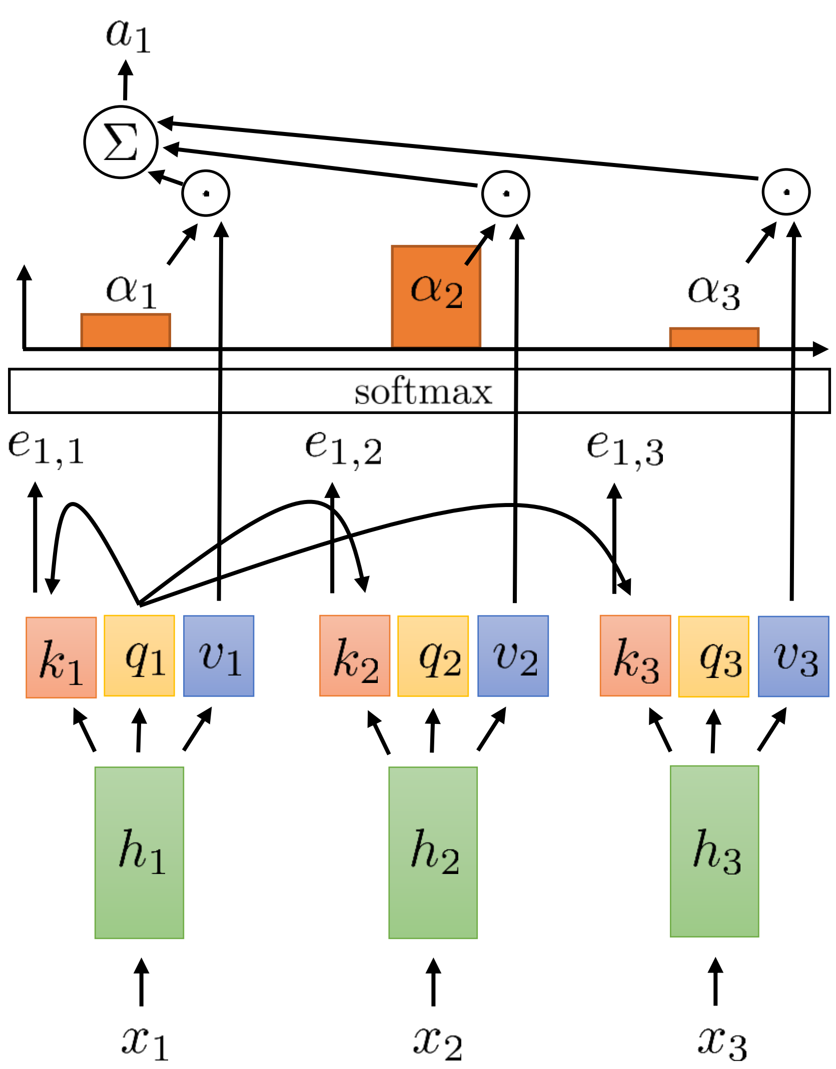
but still weight sharing:

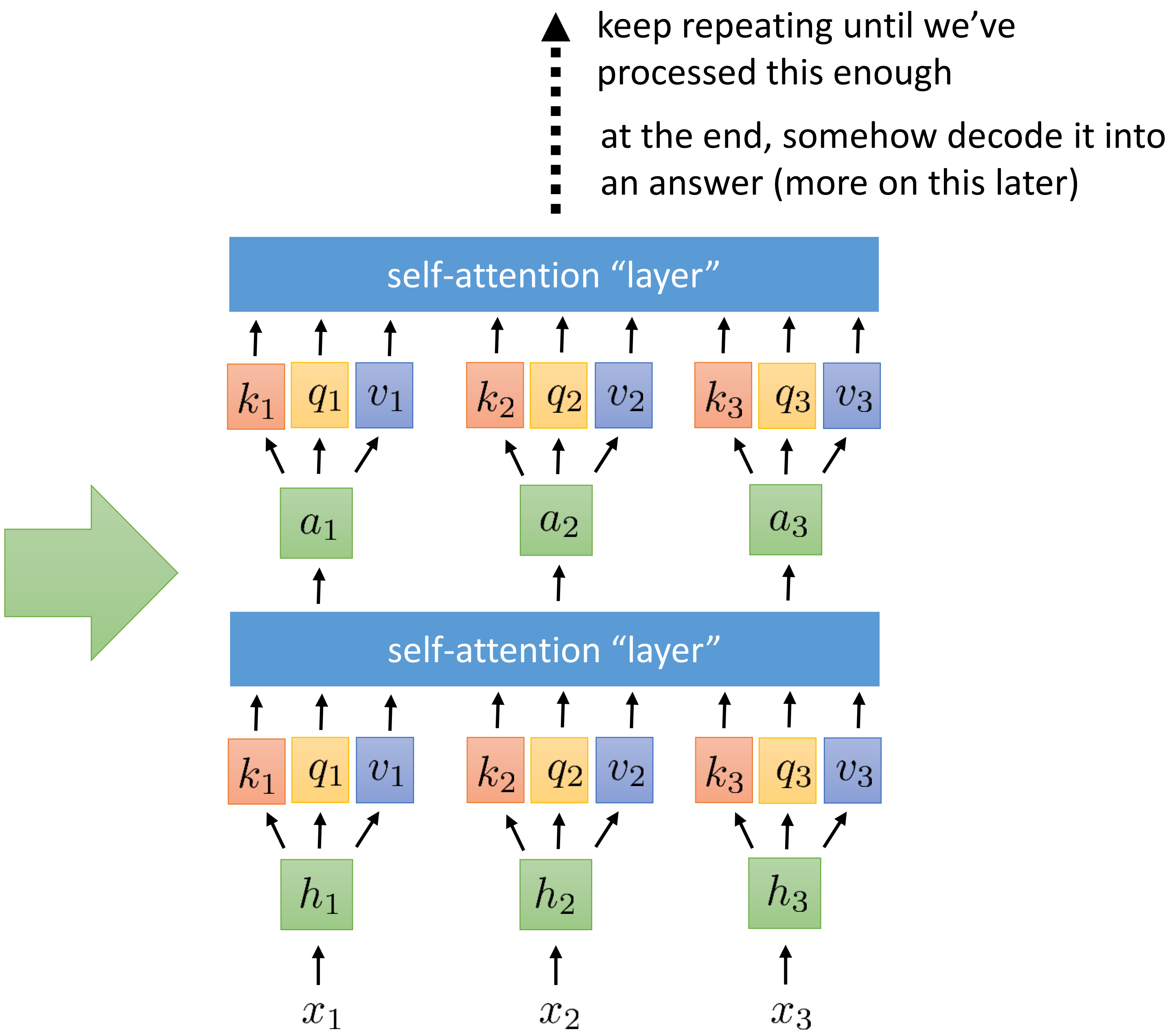
$$h_t = \sigma(W x_t + b)$$

shared weights at all time steps

(or any other nonlinear function)

Self-Attention





From Self-Attention to Transformers

The basic concept of **self-attention** can be used to develop a very powerful type of sequence model, called a **transformer**

But to make this actually work, we need to develop a few additional components to address some fundamental limitations

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?

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$$v_t = W_v h_t$$

Sequence Models with Self-Attention

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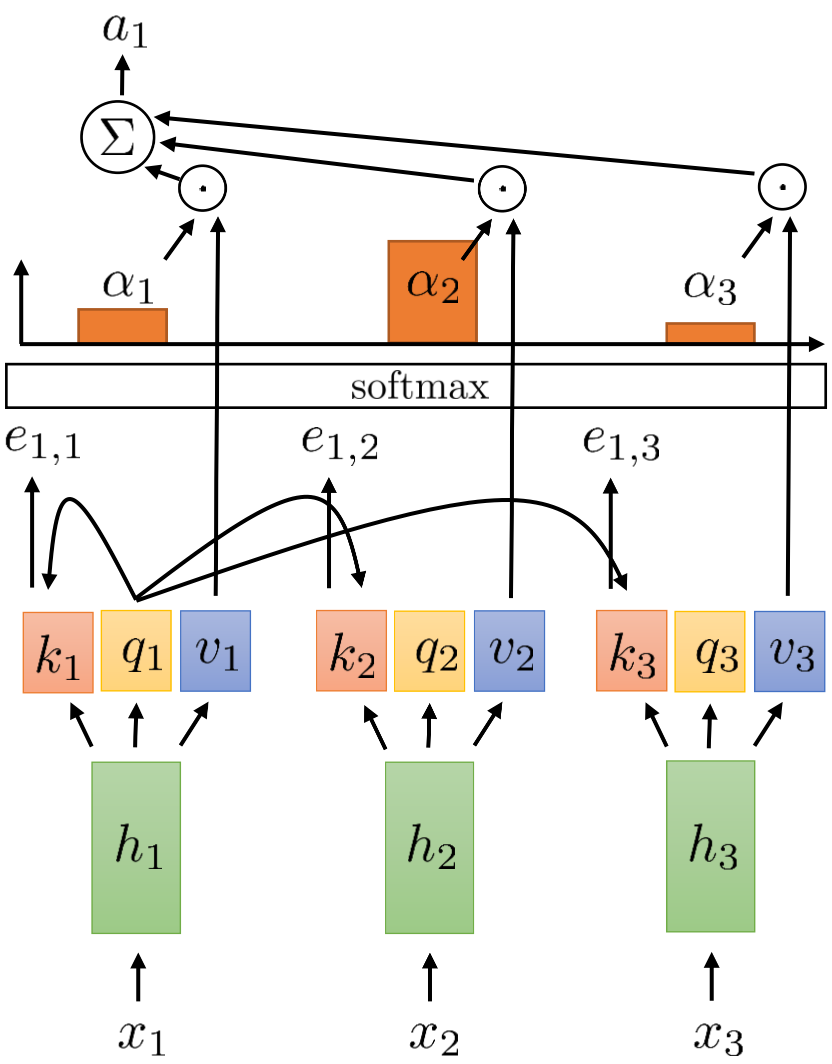
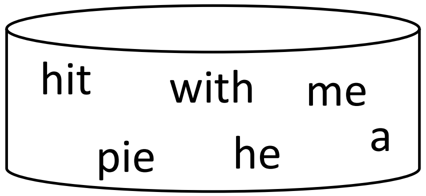
Positional encoding: what is the order?



what we see:

he hit me with a pie

what naïve self-attention sees:



a pie hit me with he

a hit with me he pie

he pie me with a hit

most alternative orderings are nonsense, but some change the meaning

in general the position of words in a sentence carries information!

Idea: add some information to the representation at the beginning that indicates where it is in the sequence!

$$h_t = f(x_t, t)$$

some function

Positional encoding: sin/cos

Naïve positional encoding: just append t to the input $\qquad \bar{x}_t = \begin{bmatrix} x_t \\ t \end{bmatrix}$

This is not a great idea, because **absolute** position is less important than **relative** position

I walk my dog every day

every single day I walk my dog

The fact that “my dog” is right after “I walk” is the important part, not its absolute position

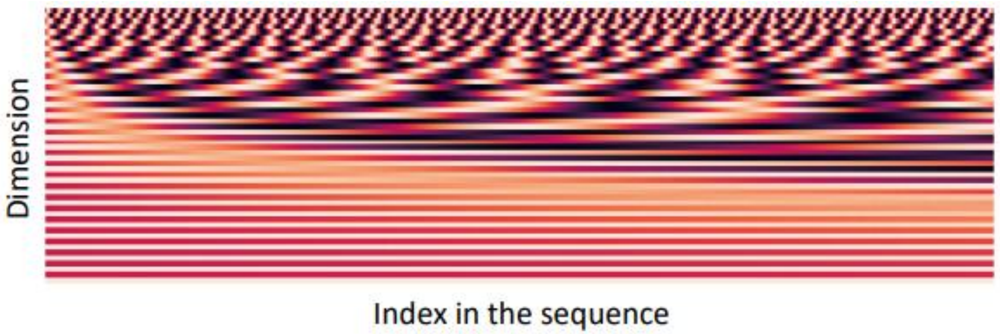
we want to represent **position** in a way that tokens with similar **relative** position have similar **positional encoding**

Idea: what if we use **frequency-based** representations?

$$p_t = \begin{bmatrix} \sin(t/10000^{2*1/d}) \\ \cos(t/10000^{2*1/d}) \\ \sin(t/10000^{2*2/d}) \\ \cos(t/10000^{2*2/d}) \\ \cdots \\ \sin(t/10000^{2*\frac{d}{2}/d}) \\ \cos(t/10000^{2*\frac{d}{2}/d}) \end{bmatrix}$$

dimensionality of positional encoding

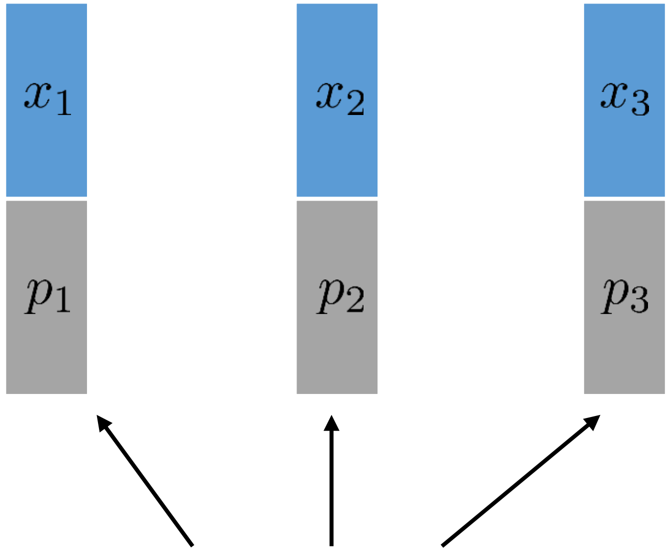
“even-odd” indicator



“first-half vs. second-half” indicator

Positional encoding: learned

Another idea: just learn a positional encoding



Different for every input sequence

The same learned values for every sequence

but different for different time steps

dimensionality

max sequence length

How many values do we need to learn?

$$P = [p_1, p_2, \ldots, p_T] \in R^{d \times T}$$

+ more flexible (and perhaps more optimal) than sin/cos encoding

+ a bit more complex, need to pick a max sequence length (and can't generalize beyond it)

How to incorporate positional encoding?

At each step, we have x_t and p_t

Simple choice: just concatenate them $\bar{x}_t = \begin{bmatrix} x_t \\ p_t \end{bmatrix}$

More often: just add after **embedding** the input

input to self-attention is $\mathrm{emb}(x_t) + p_t$

some learned function (e.g., some fully connected layers with linear layers + nonlinearities)

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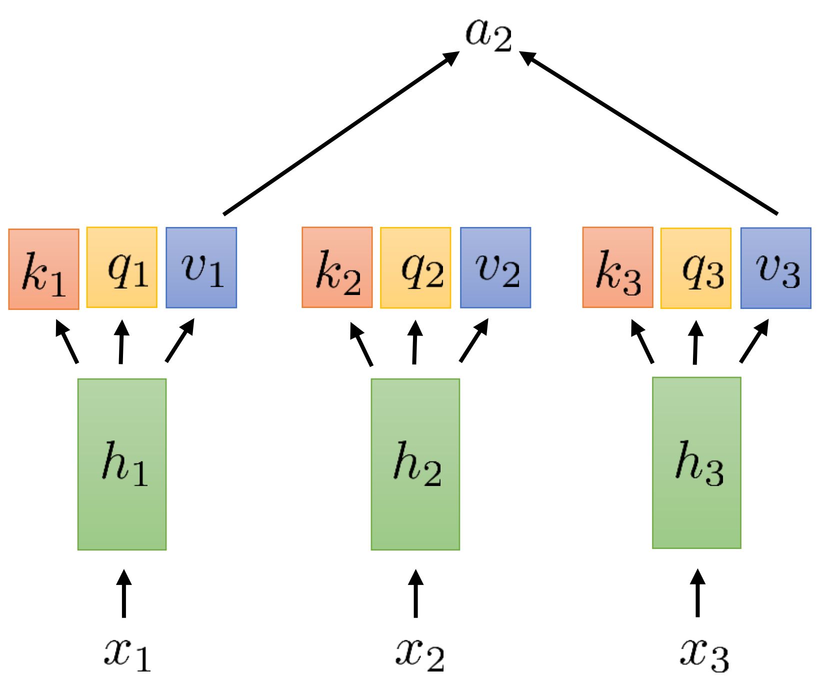
Multi-head attention

Since we are relying **entirely** on attention now, we might want to incorporate **more than one** time step



$$a_l = \sum_t \alpha_{l,t} v_t$$

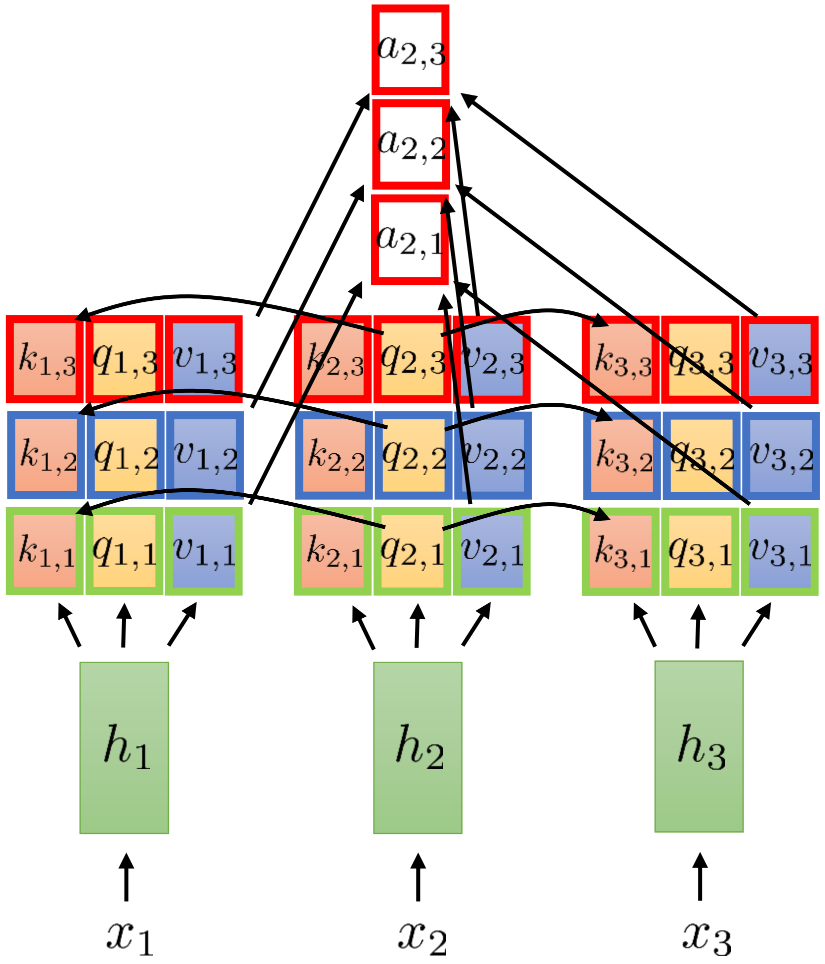
because of softmax, this will be dominated by one value

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

hard to specify that you want two different things (e.g., the subject and the object in a sentence)

Multi-head attention

Idea: have multiple keys, queries, and values for every time step!



full attention vector formed by concatenation:

$$a_2 = \begin{bmatrix} a_{2,1} \\ a_{2,2} \\ a_{2,3} \end{bmatrix}$$

compute weights **independently** for each head

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

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

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

around **8** heads seems to work pretty well for big models

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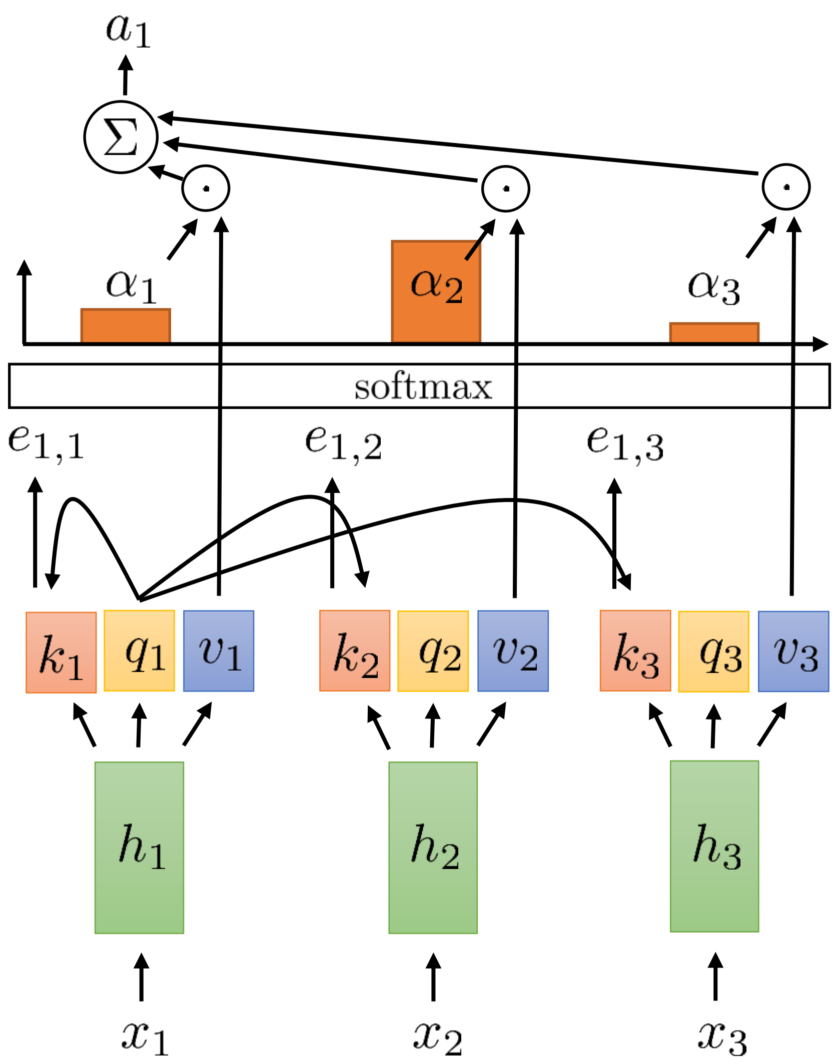
Self-Attention is **Linear**



$$k_t = W_k h_t \qquad q_t = W_q h_t \qquad v_t = W_v h_t$$

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

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

$$a_l = \sum_t \alpha_{l,t} v_t = \sum_t \alpha_{l,t} W_v h_t = W_v \sum_t \alpha_{l,t} h_t$$

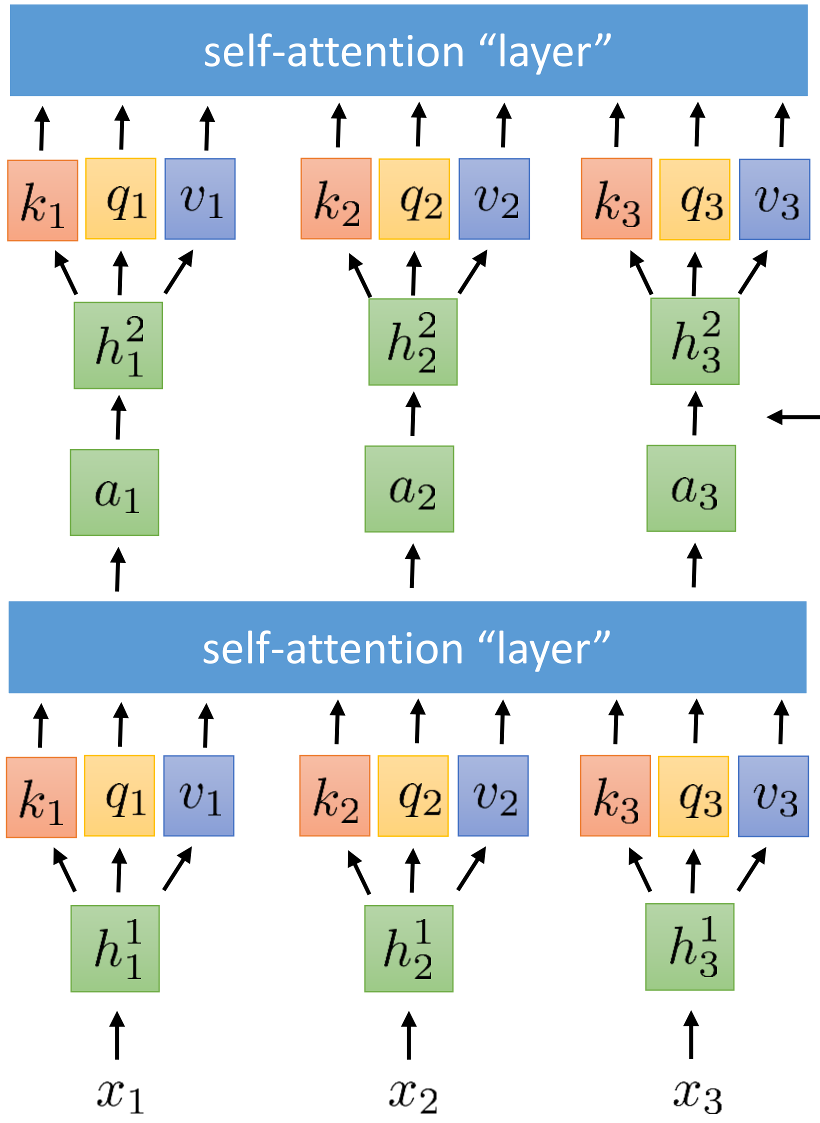
linear transformation

non-linear weights

Every self-attention "layer" is a linear transformation of the previous layer (with non-linear weights)

This is not very expressive

Alternating self-attention & nonlinearity



some non-linear (learned) function
e.g., $h_t^\ell = \sigma(W^\ell a_t^\ell + b^\ell)$

just a neural net applied at every position after every self-attention layer!

Sometimes referred to as "position-wise feedforward network"

We'll describe some specific commonly used choices shortly

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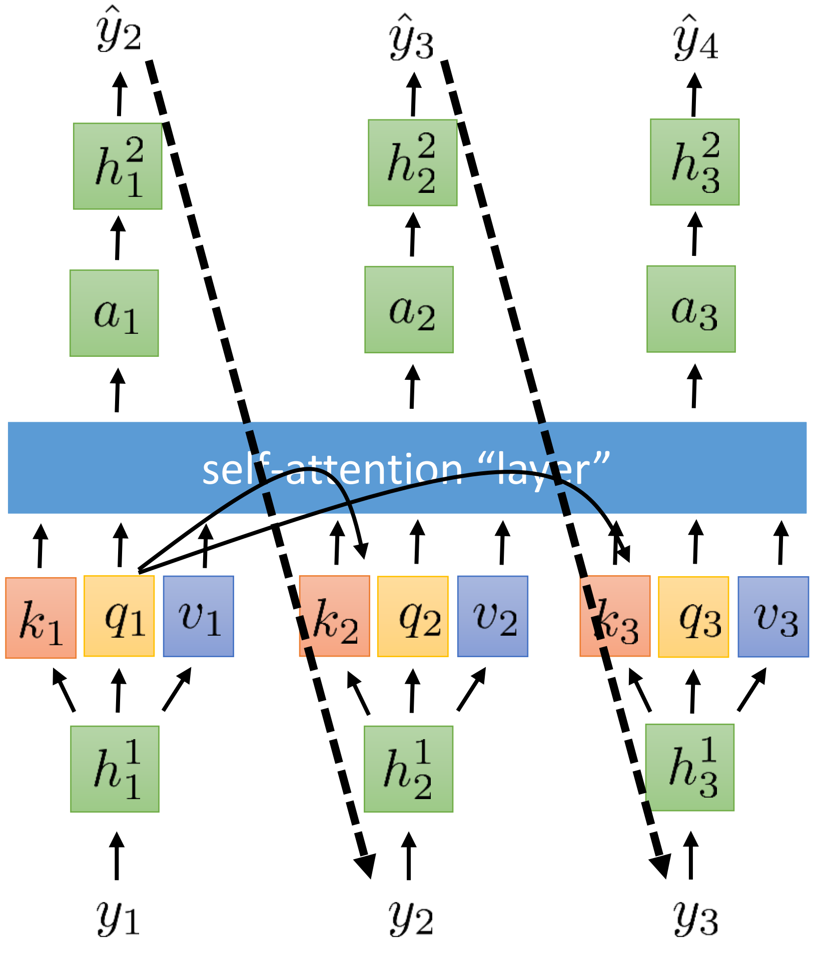
Self-attention can see the future!

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



(in reality, we would have many alternating self-attention layers and position-wise feedforward networks, not just one)

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

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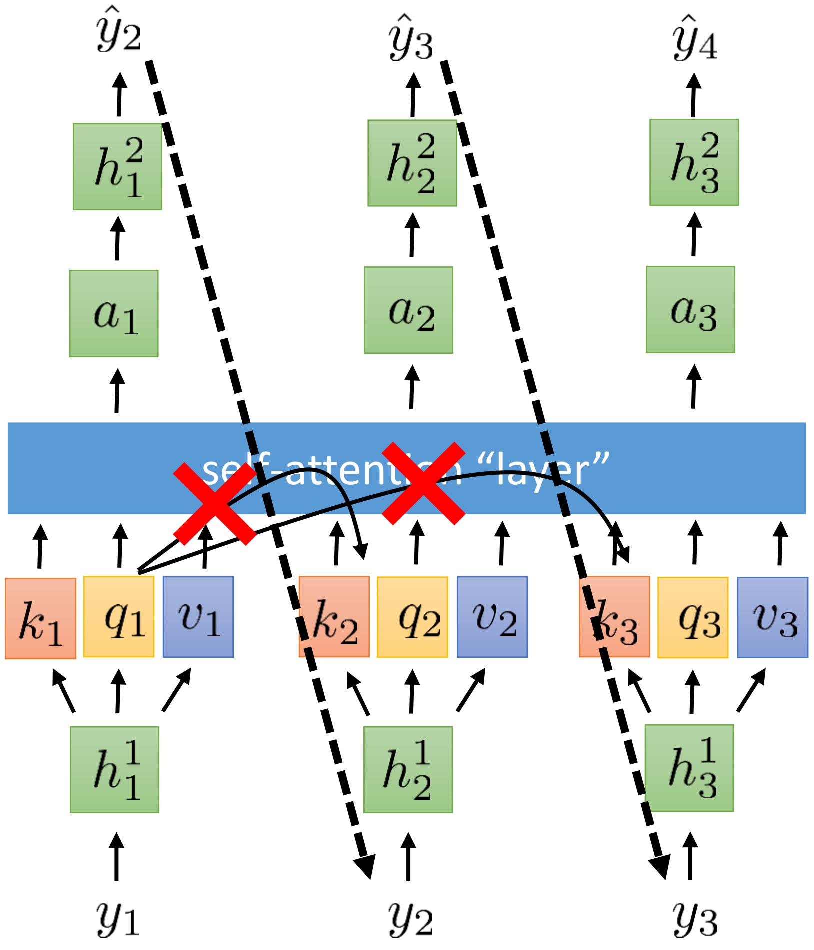


At test time (when decoding), the **inputs** at steps 2 & 3 will be based on the output at step 1…

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

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

…but not into the **future**

Easy solution:

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

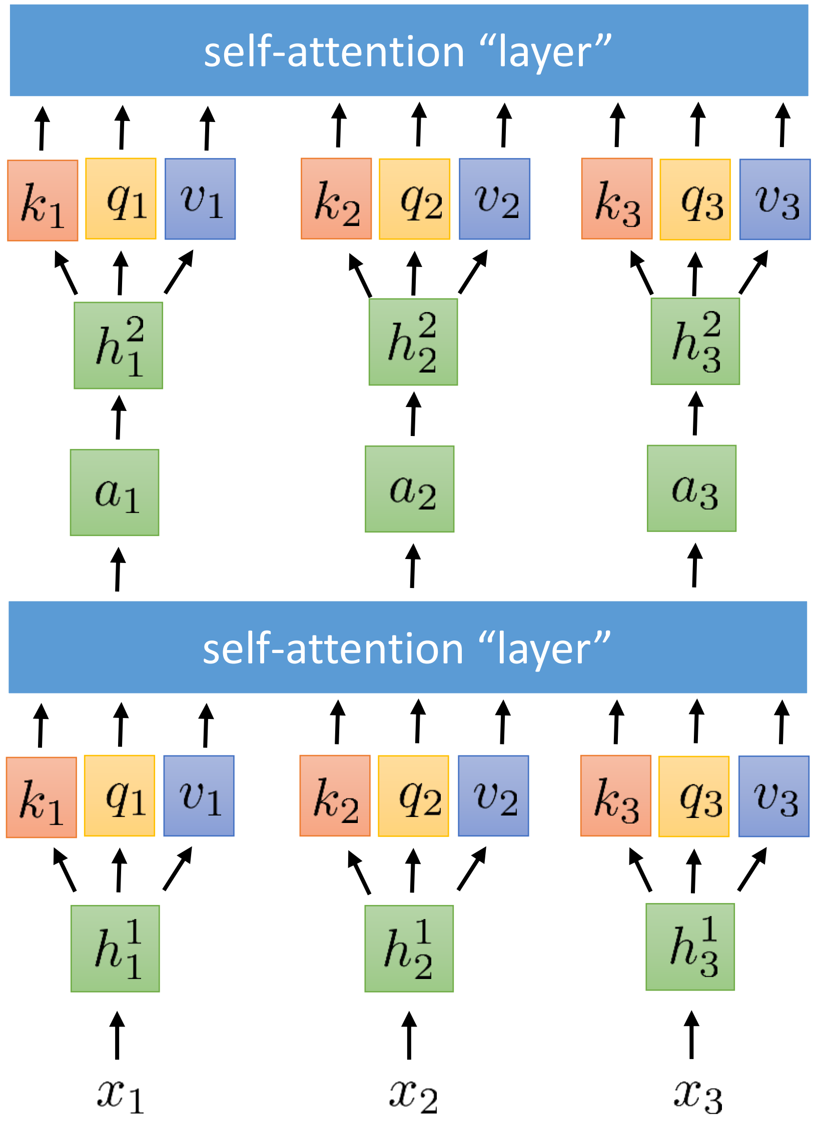
$$e_{l,t} = \begin{cases} q_l \cdot k_t & \text{if } l \geq t \\ -\infty & \text{otherwise} \end{cases}$$

in practice:

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

inside the softmax

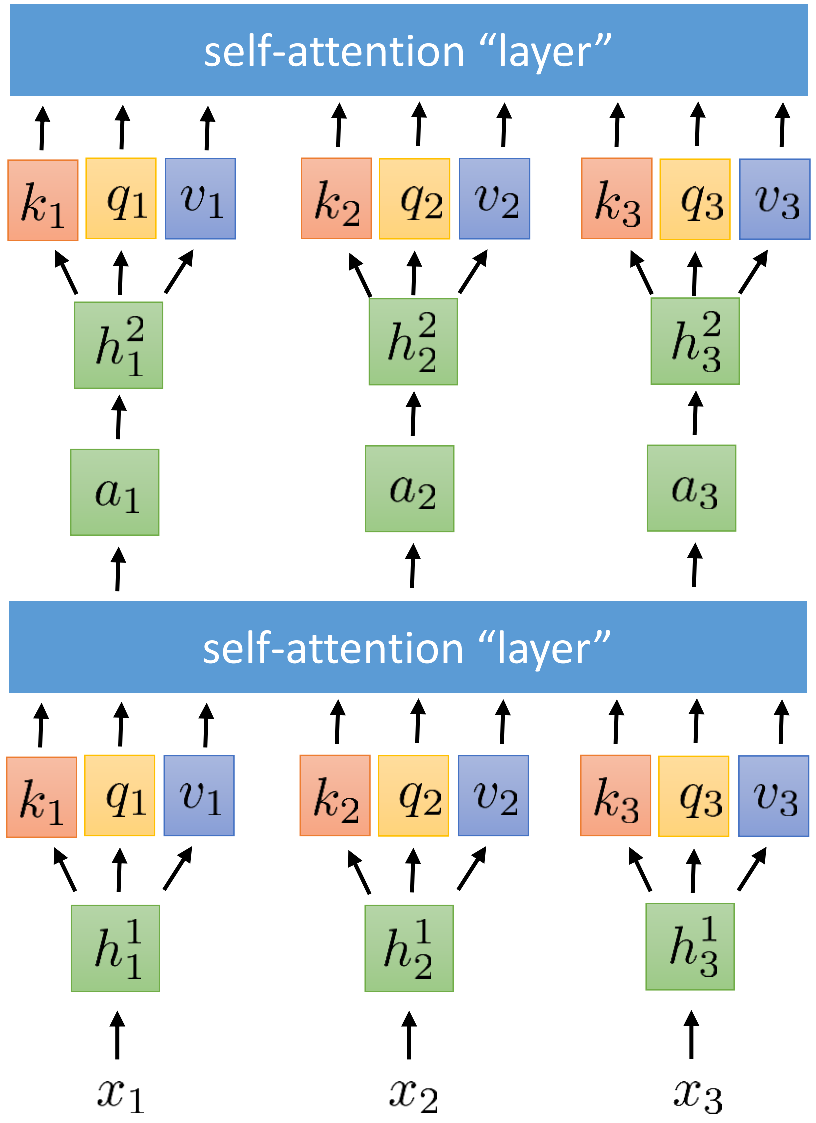
Implementation summary



- We can implement a **practical** sequence model based **entirely** on self-attention
- Alternate self-attention "layers" with nonlinear position-wise feedforward networks (to get nonlinear transformations)
- Use positional encoding (on the input or input embedding) to make the model aware of relative positions of tokens
- Use multi-head attention
- Use masked attention if you want to use the model for decoding

The Transformer

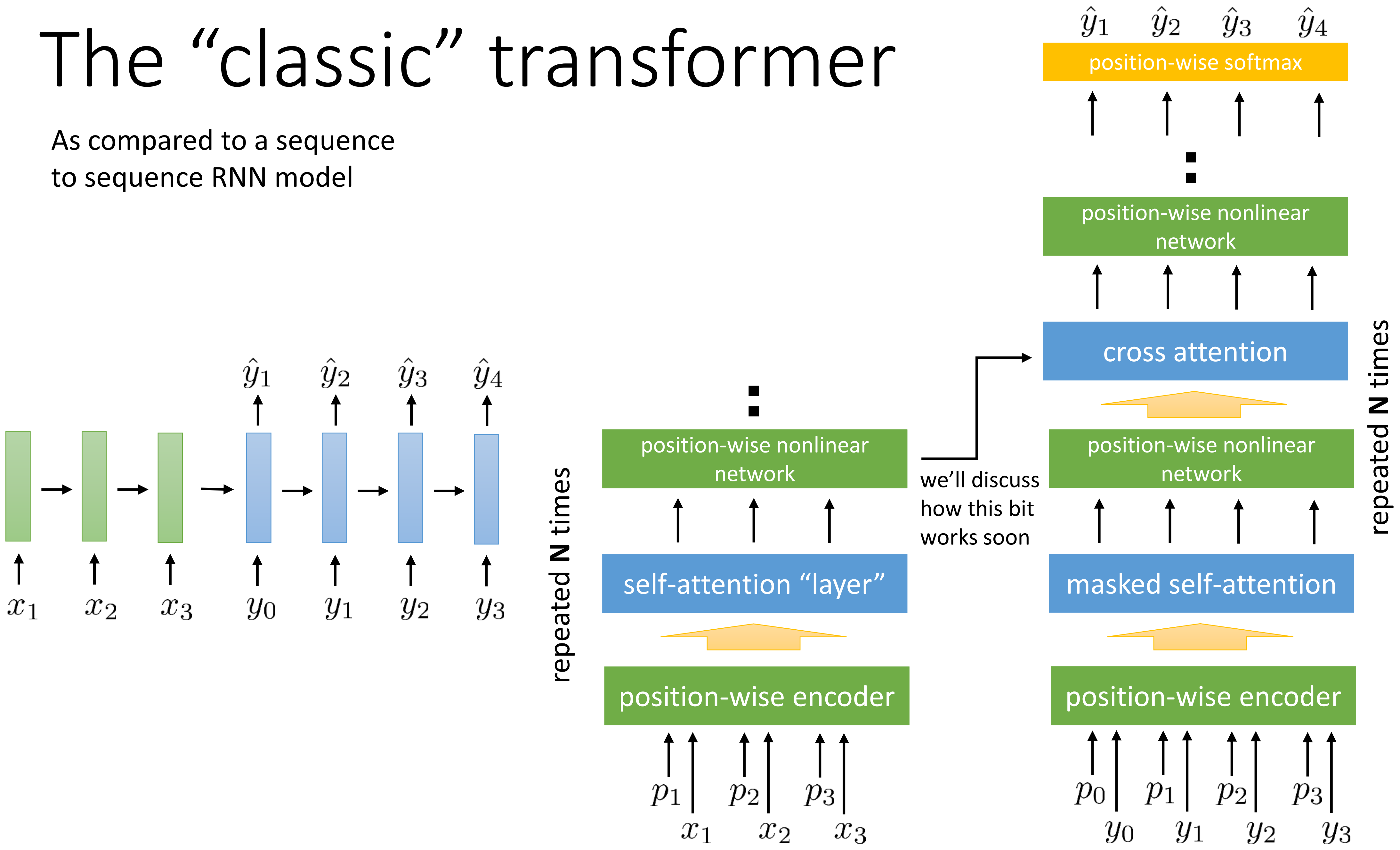
Sequence to sequence with self-attention



- There are a number of model designs that use successive self-attention and position-wise nonlinear layers to process sequences
- These are generally called “Transformers” because they transform one sequence into another at **each** layer
  - See Vaswani et al. **Attention Is All You Need.** 2017
- The “classic” transformer (Vaswani et al. 2017) is a **sequence to sequence** model
- A number of well-known follow works also use transformers for language modeling (BERT, GPT, etc.)

The “classic” transformer

As compared to a sequence
to sequence RNN model



Combining encoder and decoder values

"Cross-attention"

Much more like the **standard** attention from the previous lecture

$$\text{query: } q_l^\ell = W_q^\ell s_l^\ell$$

output of position-wise nonlinear network at (decoder) layer ℓ, step l

$$\text{key: } k_t^\ell = W_k^\ell h_t^\ell$$

output of position-wise nonlinear network at (encoder) layer ℓ, step t

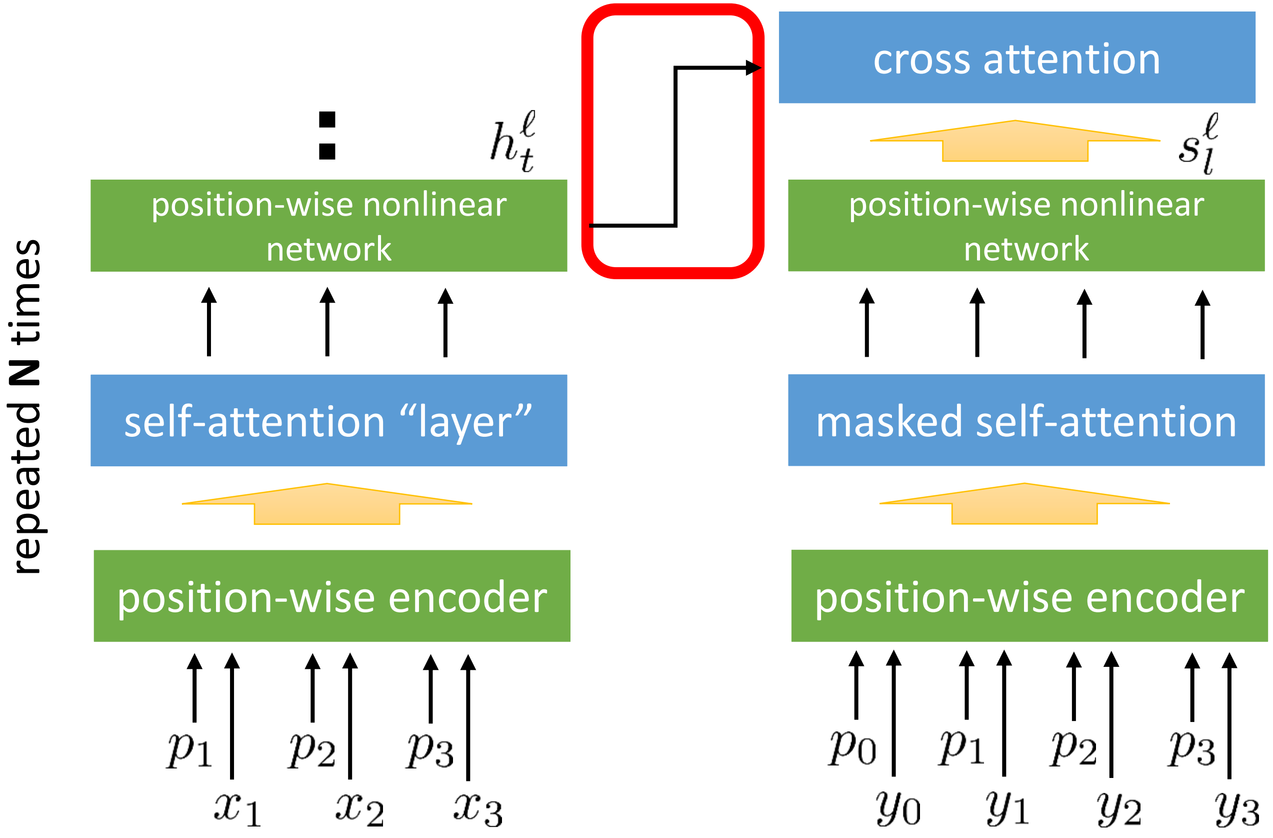
$$\text{value: } v_t^\ell = W_k^\ell h_t^\ell$$

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

$$\alpha_{l,t}^\ell = \frac{\exp(e_{l,t}^\ell)}{\sum_{t'} \exp(e_{l,t'}^\ell)}$$

$$c_l^\ell = \sum_t \alpha_{l,t}^\ell v_t^\ell$$

cross attention output



in reality, cross-attention is **also** multi-headed!

One last detail: layer normalization

Main idea: batch normalization is very helpful, but hard to use with sequence models

Sequences are different lengths, makes normalizing across the batch hard

Sequences can be very long, so we sometimes have small batches

Simple solution: "layer normalization" – like batch norm, but not across the batch

Batch norm

d-dimensional vectors for each sample in batch

$a_1, a_2, \ldots, a_B$

d-dim

$$\mu = \frac{1}{B}\sum_{i=1}^{B} a_i \quad \sigma = \sqrt{\frac{1}{B}\sum_{i=1}^{B}(a_i - \mu)^2}$$

$$\bar{a}_i = \frac{a_i - \mu}{\sigma}\gamma + \beta$$

Layer norm

different *dimensions* of a

a

$$\mu = \frac{1}{d}\sum_{i=1}^{d} a_j \quad \sigma = \sqrt{\frac{1}{d}\sum_{i=1}^{d}(a_j - \mu)^2}$$

1-dim

$$\bar{a} = \frac{a - \mu}{\sigma}\gamma + \beta$$

Putting it all together

Decoder decodes one position at a time with masked attention

The Transformer

6 layers, each with d = 512

multi-head attention keys and values $k^\ell_{t,1}, \ldots, k^\ell_{t,m}$ and $v^\ell_{t,1}, \ldots, v^\ell_{t,m}$

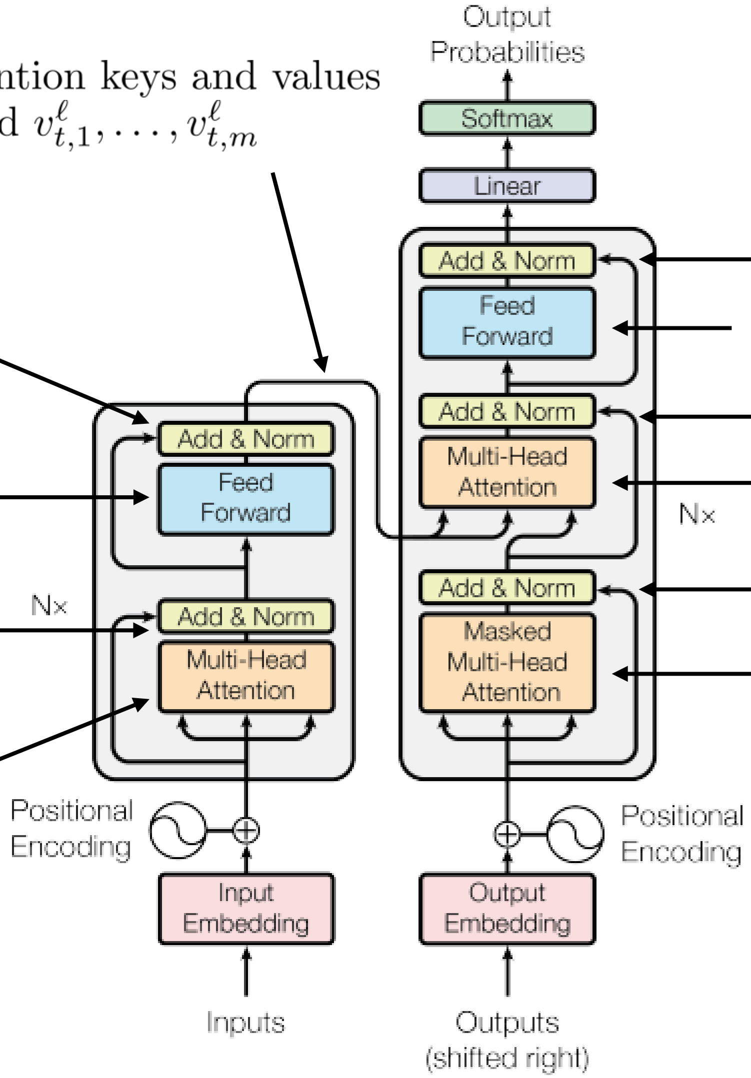
$\bar{h}^\ell_t = \text{LayerNorm}(\bar{a}^\ell_t + h^\ell_t)$
passed to next layer $\ell + 1$

$h^\ell_t = W^\ell_2 \text{ReLU}(W^\ell_1 \bar{a}^\ell_t + b^\ell_1) + b^\ell_2$
2-layer neural net at each position

$\bar{a}^\ell_t = \text{LayerNorm}(\bar{h}^{\ell-1}_t + a^\ell_t)$
essentially a residual connection with LN

input: $\bar{h}^{\ell-1}_t$
output: a^ℓ_t

concatenates attention from all heads



residual connection with LN

$h^\ell_t = W^\ell_2 \text{ReLU}(W^\ell_1 \bar{a}^\ell_t + b^\ell_1) + b^\ell_2$

residual connection with LN

multi-head cross attention

residual connection with LN

same as encoder only **masked**

Vaswani et al. **Attention Is All You Need.** 2017.

Why transformers?

Downsides:

- **Attention computations are technically $O(n^2)$**
- **Somewhat more complex to implement (positional encodings, etc.)**

Benefits:

+ Much better long-range connections

+ Much easier to parallelize

+ In practice, can make it much deeper (more layers) than RNN

The benefits seem to **vastly** outweigh the downsides, and transformers work **much** better than RNNs (and LSTMs) in many cases

Arguably one of the most important sequence modeling improvements of the past decade

Why transformers?

In practice, this means we can use larger models for the same cost

larger model = better performance

much faster training

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	$2.3 \cdot 10^{19}$	$1.4 \cdot 10^{20}$
ConvS2S [9]	25.16	40.46	$9.6 \cdot 10^{18}$	$1.5 \cdot 10^{20}$
MoE [32]	26.03	40.56	$2.0 \cdot 10^{19}$	$1.2 \cdot 10^{20}$
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**	$7.7 \cdot 10^{19}$	$1.2 \cdot 10^{21}$
Transformer (base model)	27.3	38.1	$\mathbf{3.3 \cdot 10^{18}}$	
Transformer (big)	**28.4**	**41.8**	$2.3 \cdot 10^{19}$	

great translation results

Vaswani et al. **Attention Is All You Need.** 2017.

Text summarization

previous state of the art seq2seq model

Model	Test perplexity	ROUGE-L
seq2seq-attention, $L = 500$	5.04952	12.7
Transformer-ED, $L = 500$	2.46645	34.2
Transformer-D, $L = 4000$	2.22216	33.6
Transformer-DMCA, no MoE-layer, $L = 11000$	2.05159	36.2
Transformer-DMCA, MoE-128, $L = 11000$	1.92871	37.9
Transformer-DMCA, MoE-256, $L = 7500$	1.90325	38.8

lower is better (this metric is similar to 1/likelihood)

We'll learn more about the power of transformers as **language models** next time!

Liu et al. **Generating Wikipedia by summarizing long sequences.** 2018.