CS639 Deep Learning for NLP

Attention and Transformer

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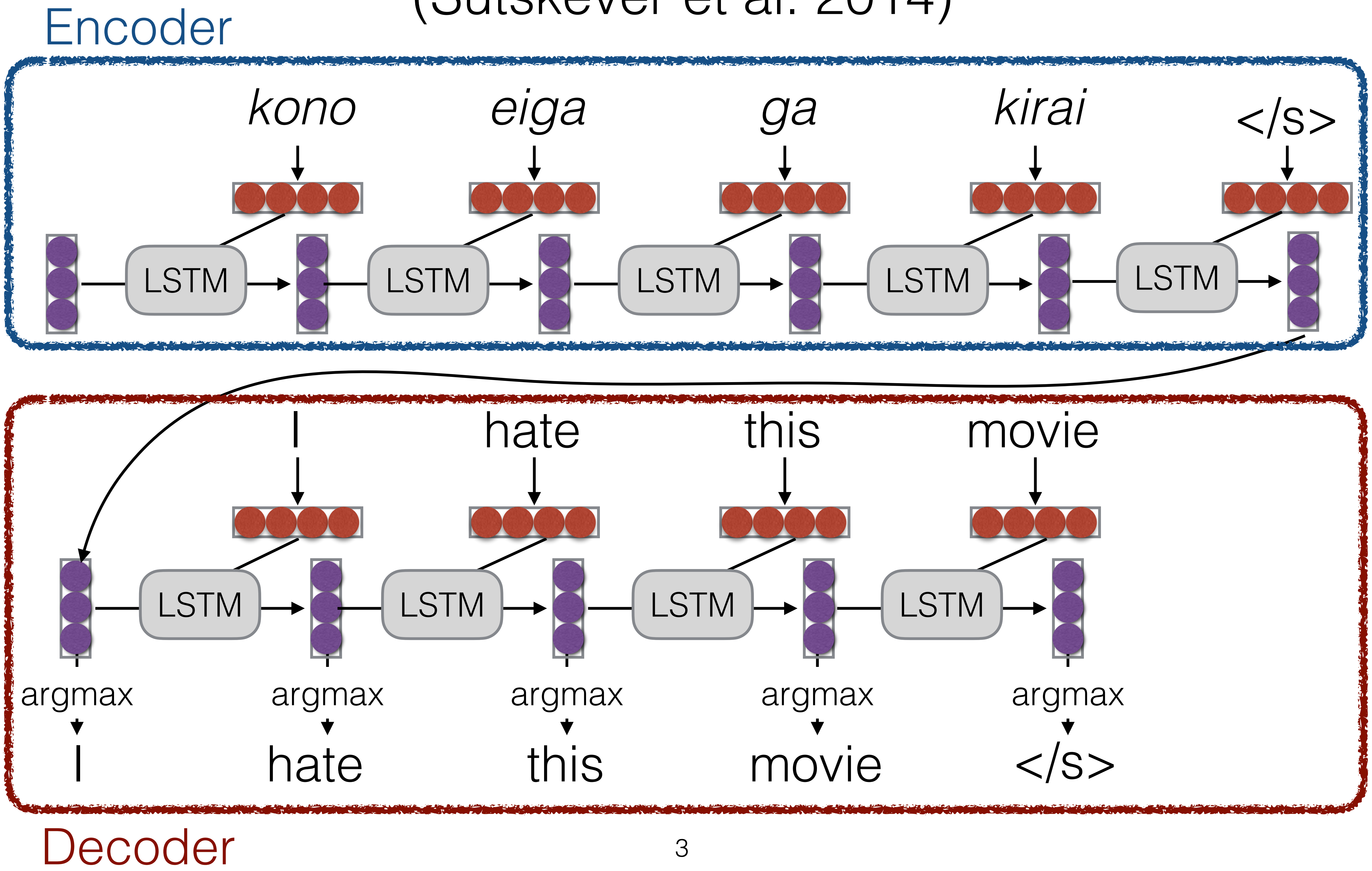
Slides adapted from Graham, Sergey
https://junjiehu.github.io/cs639-spring26

Outline

- Brief Introduction to Attention
- Transformer (Five Key Components)
- Advanced Training And Applications of Attention

Encoder-decoder Models

(Sutskever et al. 2014)

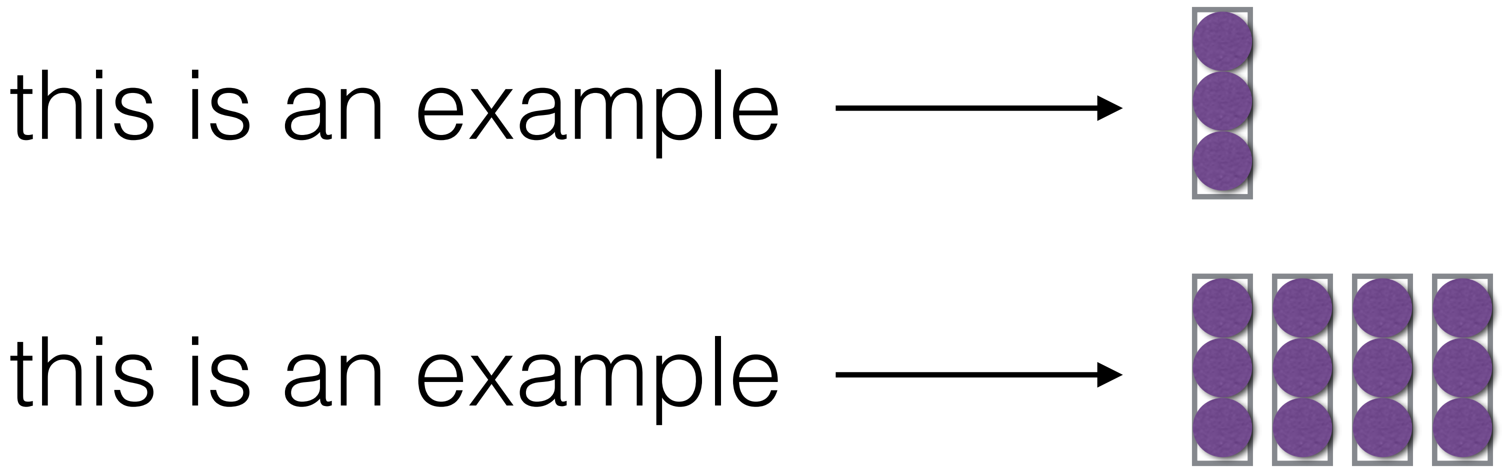


Sentence Representations

Problem!

It's not ideal to compress the meaning of a sentence with variable length into a single vector.

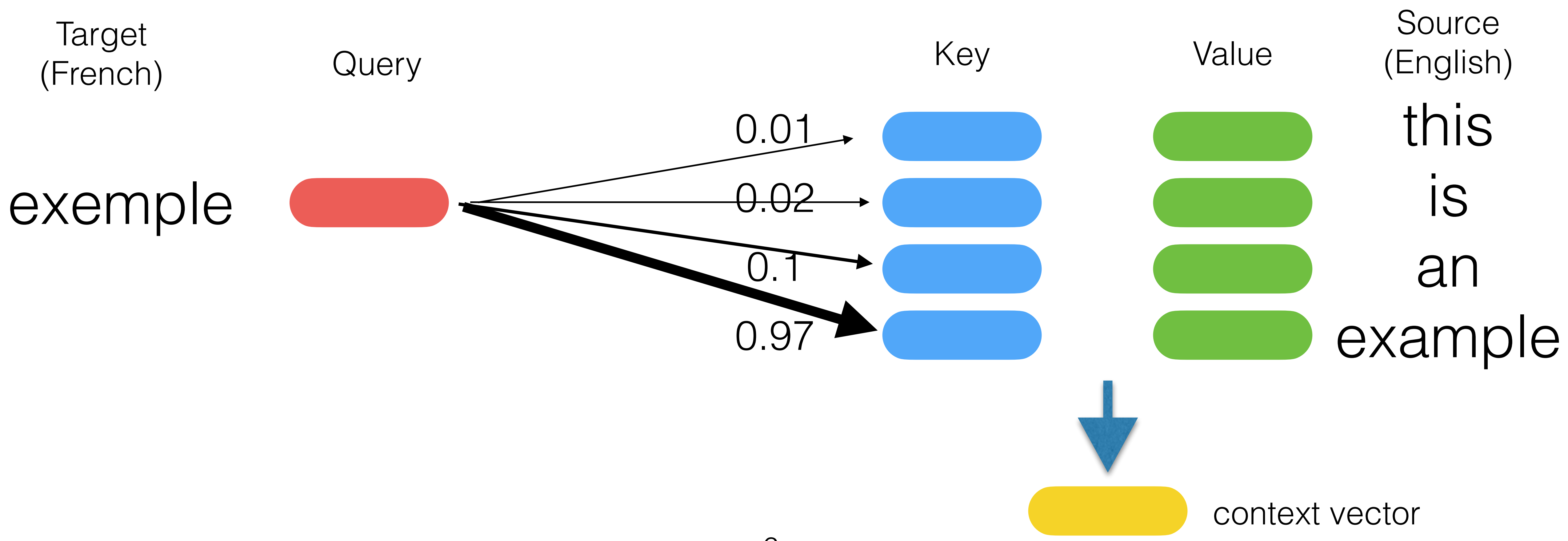
- But what if we could use multiple vectors, based on the length of the sentence.



Attention

Basic Idea of Attention

- Embed the **source elements** (e.g., English words) into a dictionary of (**key, value**) vectors
- When a **query** of a target element (e.g., a French word), pick relevant source elements by comparing **query** and **keys**
- Summarize the relevant **values** into **a context vector**



Basic Idea

(Bahdanau et al. 2015)

- Attention is first used in machine translation
- Encode each word in the sentence into a vector
- When decoding, perform a linear combination of these vectors, weighted by "attention weights"
- Use this combination in picking the next word
- In a sequence-to-sequence model, we sometimes call the attention from *the **target** hidden vector (**query**)* to *all the **source** vectors (**keys**)* as "**target-to-source cross attention**".

Attention: “pick” at the input

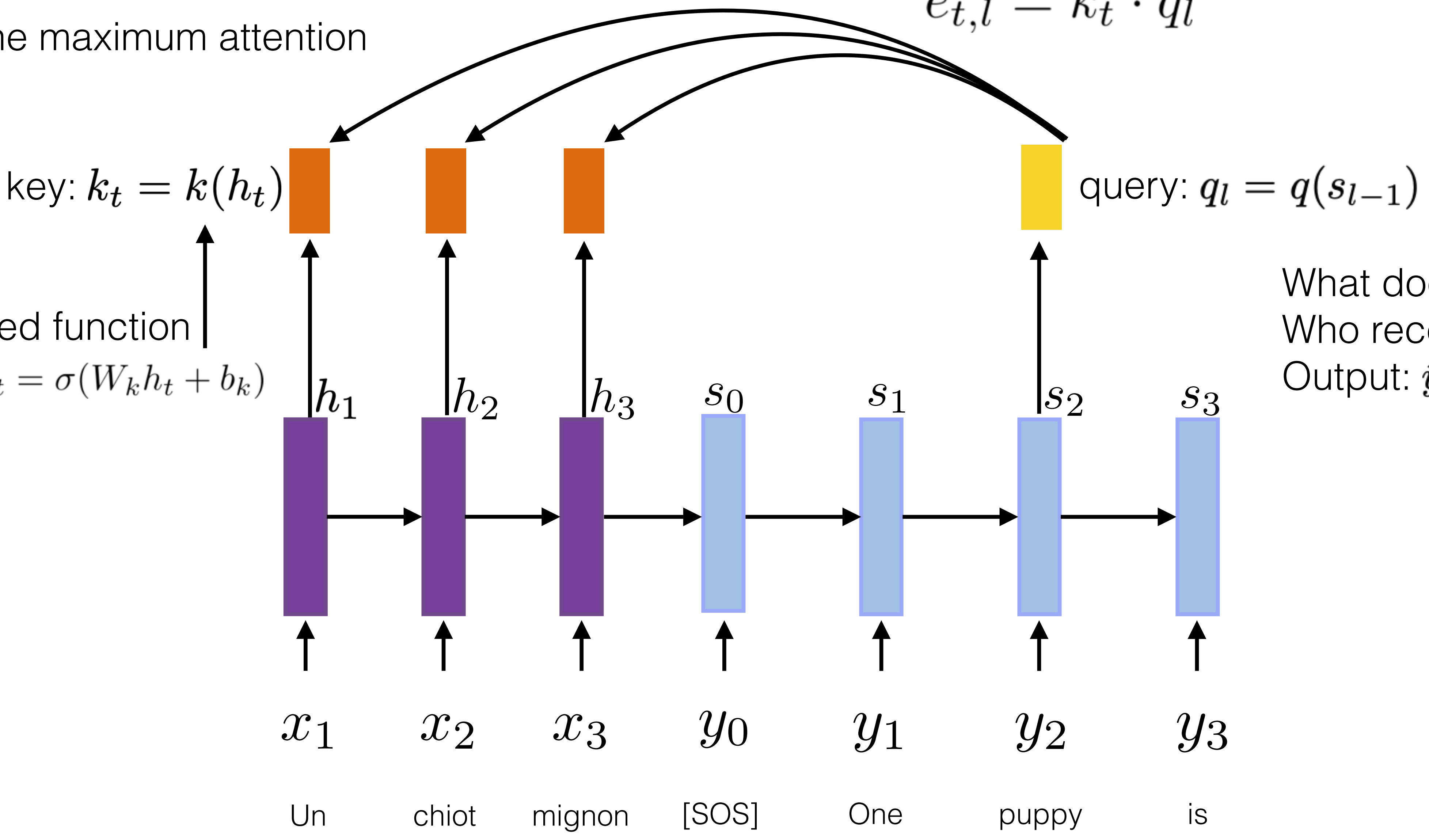
Intuition: **Send** the most relevant h_t by $\arg\max_t e_{t,l}$ **to step** l, however argmax operation is **not differentiable!**

$$\alpha_{\cdot,l} = \mathrm{softmax}(e_{\cdot,l})$$
$$\alpha_{t,l} = \frac{\exp(e_{t,l})}{\sum_{t'} \exp(e_{t',l})}$$

Let $a_l = \sum_t \alpha_{t,l} h_t$ $\rightarrow$ approximate h_t with the maximum attention

Attention score for (encoder) step t to (decoder) step l

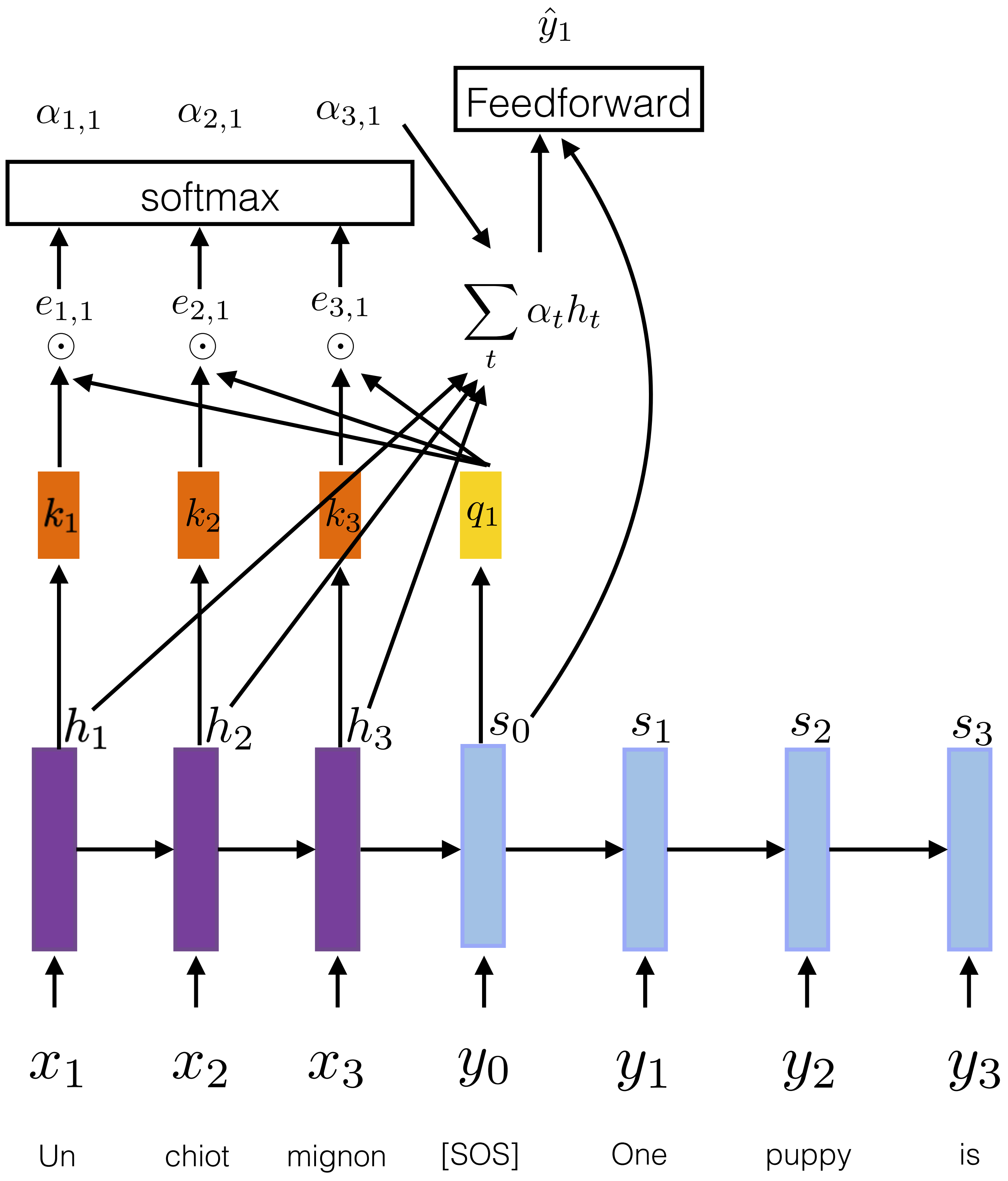
$$e_{t,l} = k_t \cdot q_l$$



What does “send” mean?
Who receives it?
Output: $\hat{y}_l = f(s_{l-1}, a_l)$

Attention (Example)

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



A Graphical Example

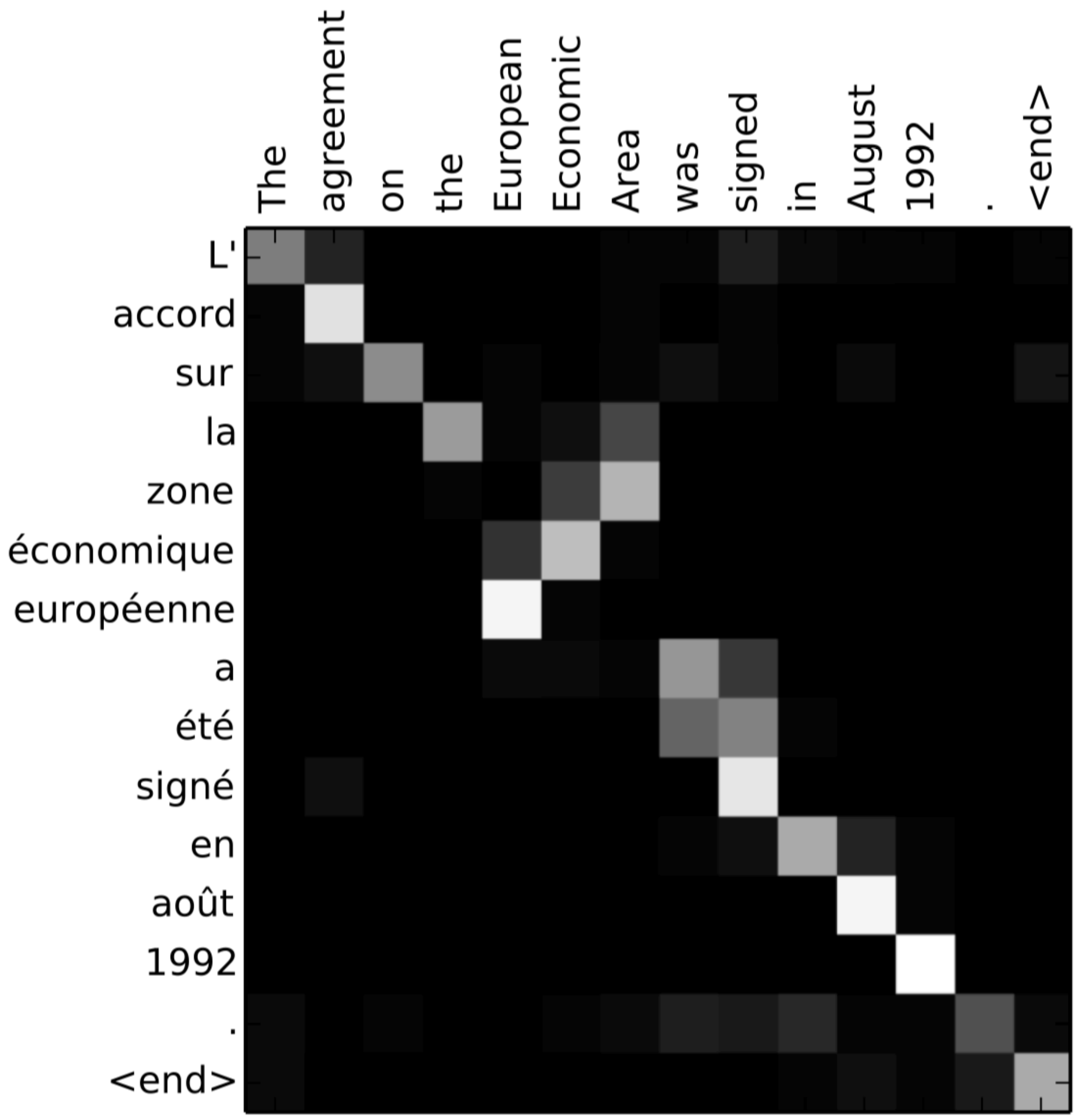


Image from Bahdanau et al. (2015)

Attention Score Functions (1)

- ***q*** is the query and ***k*** is the key
- **Multi-layer Perceptron** (Bahdanau et al. 2015)

$$a(\boldsymbol{q}, \boldsymbol{k}) = \boldsymbol{w}_2^{\intercal} \tanh(W_1[\boldsymbol{q}; \boldsymbol{k}])$$

  - Flexible, often very good with large data
- **Bilinear** (Luong et al. 2015)

$$a(\boldsymbol{q}, \boldsymbol{k}) = \boldsymbol{q}^{\intercal} W \boldsymbol{k}$$

Attention Score Functions (2)

- **Dot Product** (Luong et al. 2015)

$$a(\boldsymbol{q}, \boldsymbol{k}) = \boldsymbol{q}^\intercal \boldsymbol{k}$$

  - No parameters! But requires sizes to be the same.

- **Scaled Dot Product** (Vaswani et al. 2017)
  - *Problem:* scale of dot product increases as dimensions get larger
  - *Fix:* scale by size of the vector

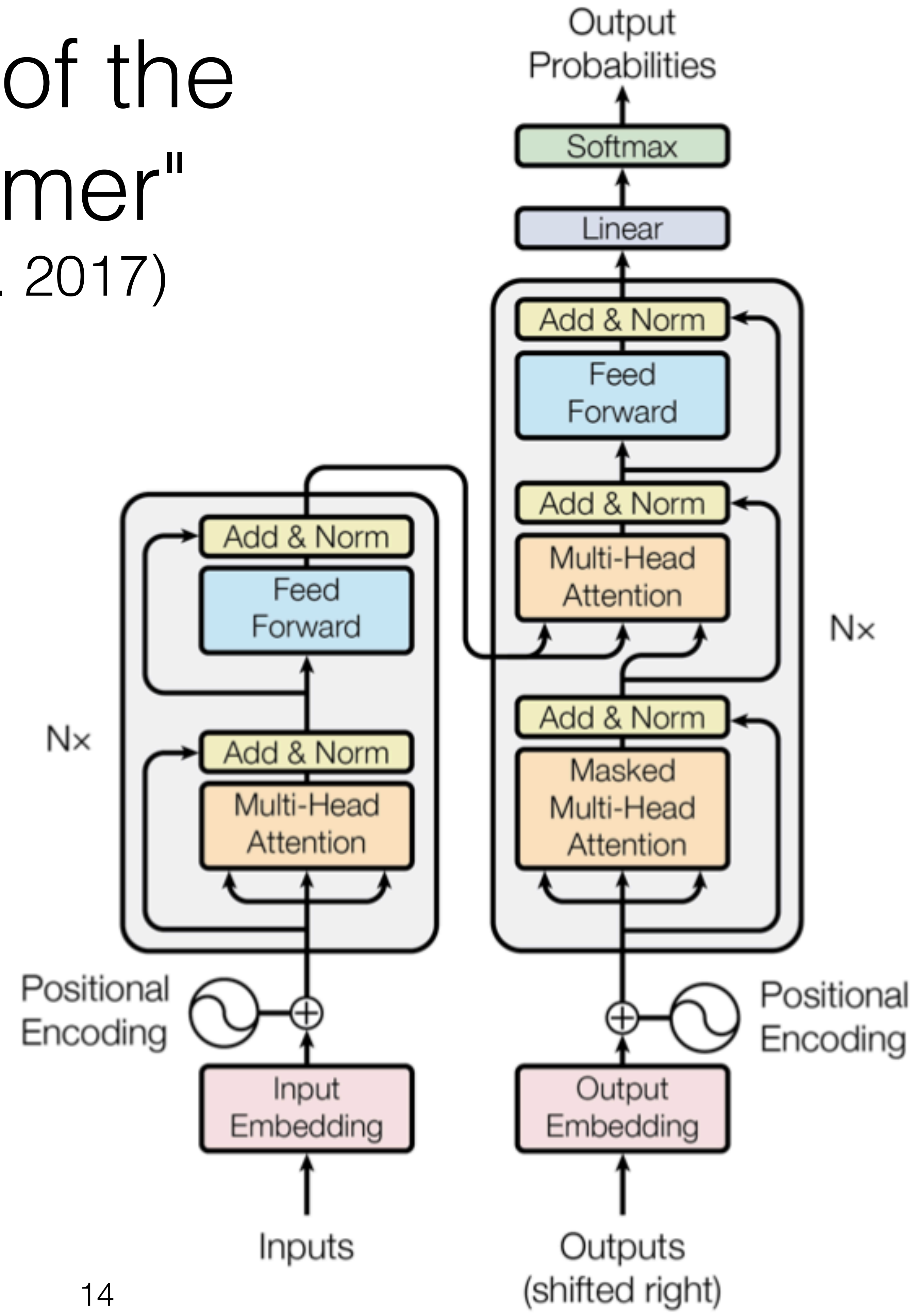
$$a(\boldsymbol{q}, \boldsymbol{k}) = \frac{\boldsymbol{q}^\intercal \boldsymbol{k}}{\sqrt{|\boldsymbol{k}|}}$$

Transformer:
“Attention is All You Need”

(Vaswani et al. 2017)

Summary of the “Transformer" (Vaswani et al. 2017)

- A sequence-to-sequence model based entirely on attention
- Strong results on translation, a wide variety of other tasks
- Fast: only matrix multiplications



Transformers

- A few key components to make Transformer work.

  1. **Self-attention** — allows parallel computing of all tokens

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

  3. **Position encoding** — adds position information to each token

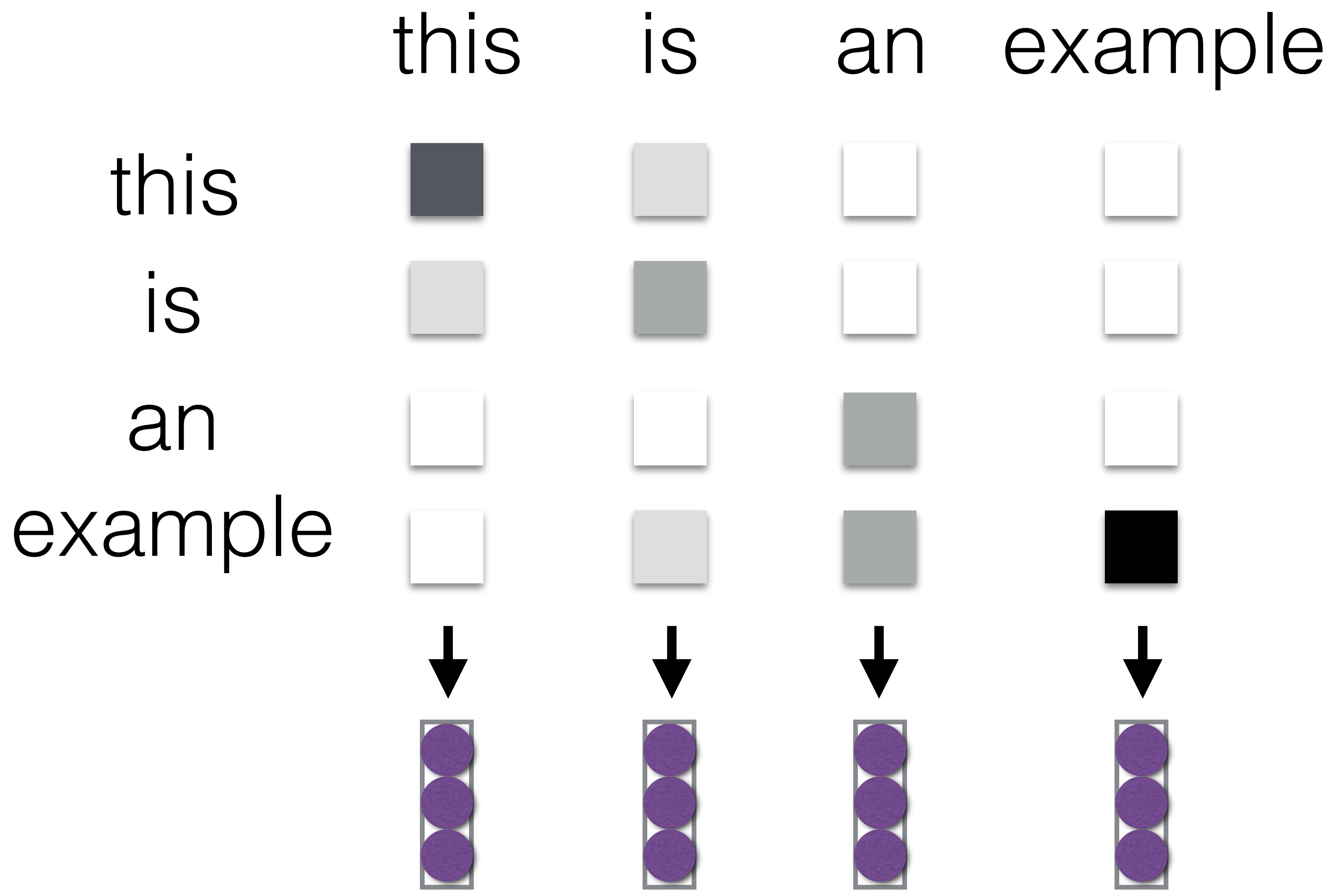
  4. **Adding nonlinearities** — combines features from a self-attention layer

  5. **Masked decoding** — prevents attention lookups in the future tokens

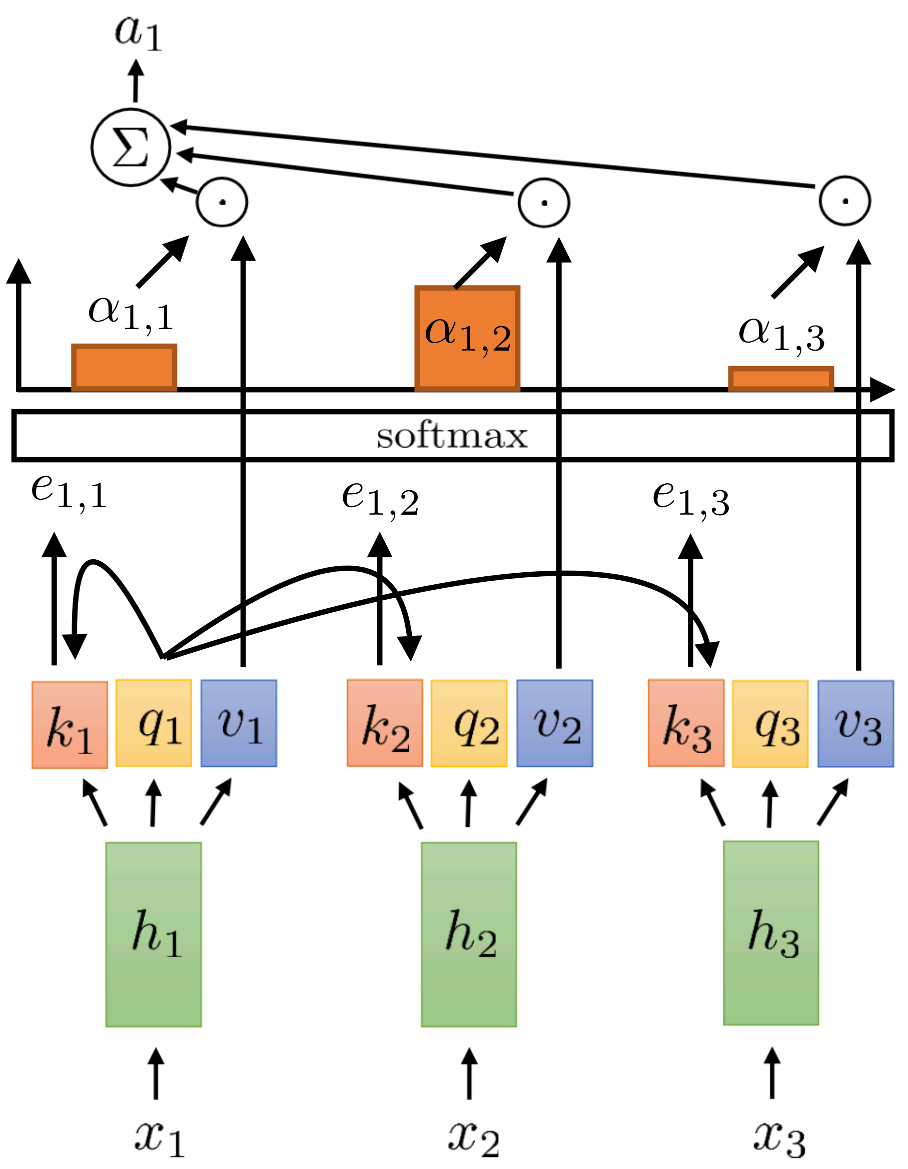
Self Attention

(Cheng et al. 2016, Vaswani et al. 2017)

- **Intuition:** Each element in the sentence attends to all elements including itself → context sensitive encodings!
- Each element will be used as **key, value and query** in self-attention



Self-Attention



Example to compute the attention context for the l-th token

$$a_l = \sum_t \alpha_{l,t} v_t$$
$$\alpha_{l,t} = \exp(e_{l,t}) / \sum_{t'} \exp(e_{l,t'})$$
$$e_{l,t} = q_l \cdot k_t$$

$$v_t = W_v h_t$$
$$k_t = W_k h_t \qquad W_v, W_k, Wq \in \mathbb{R}^{d \times d}$$
$$q_t = W_q h_t, \qquad v_t, k_t, q_t, h_t \in \mathbb{R}^d,$$

this is *not* a recurrent model!

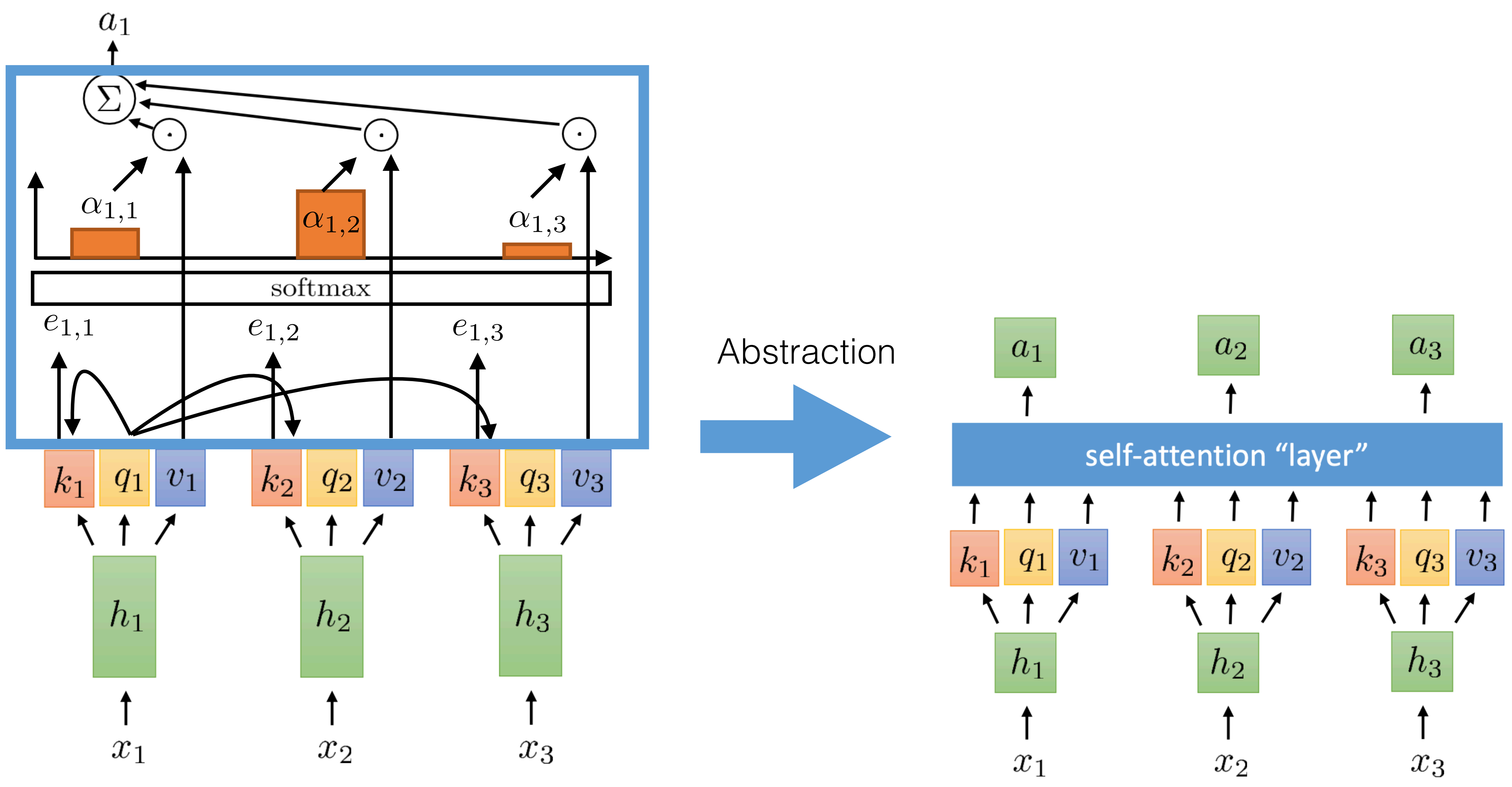
but still weight sharing:

$$h_t = \sigma(Wx_t + b)$$

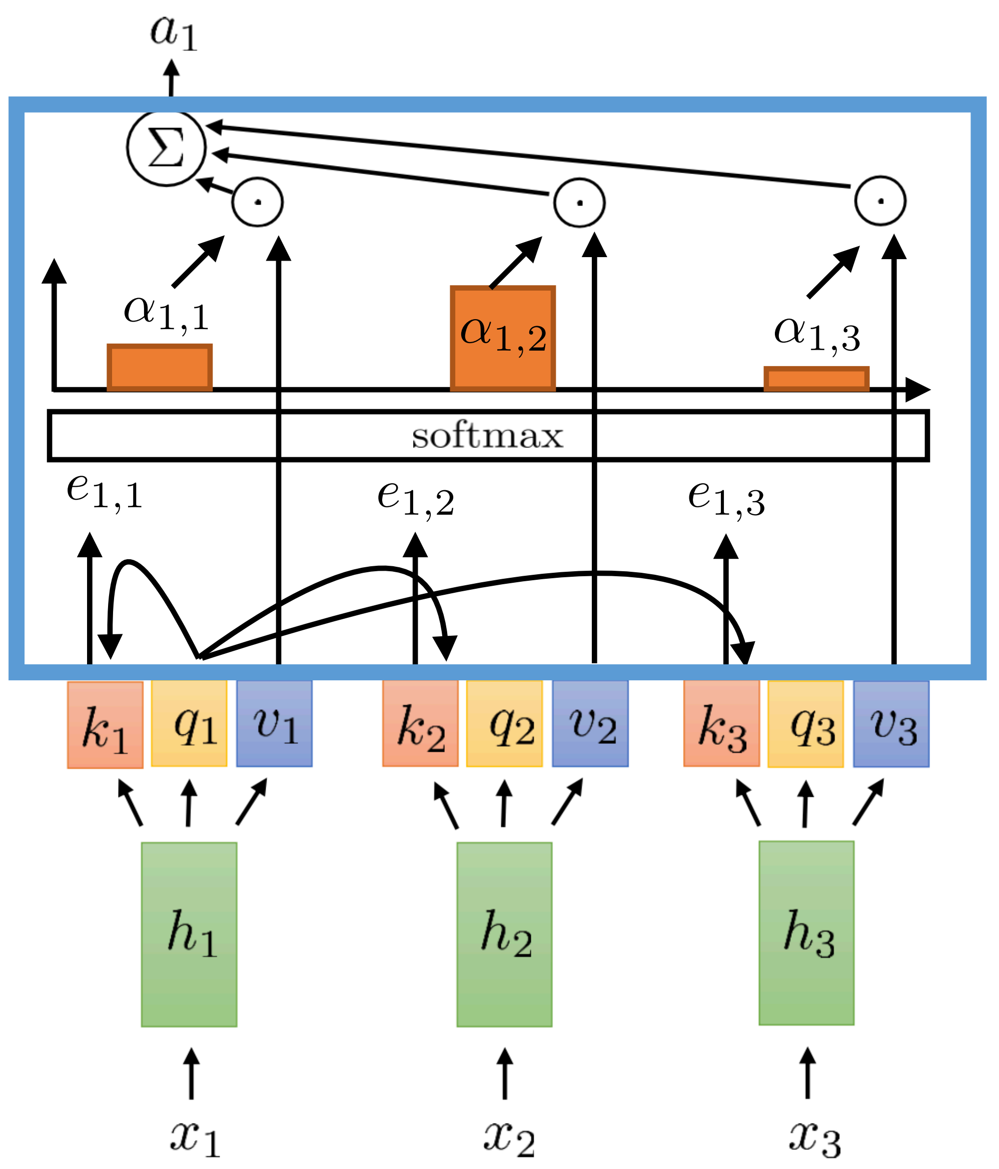
shared weights at all time steps

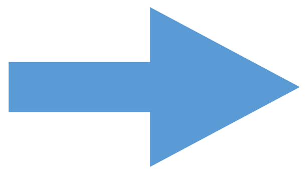
(or any other nonlinear function)

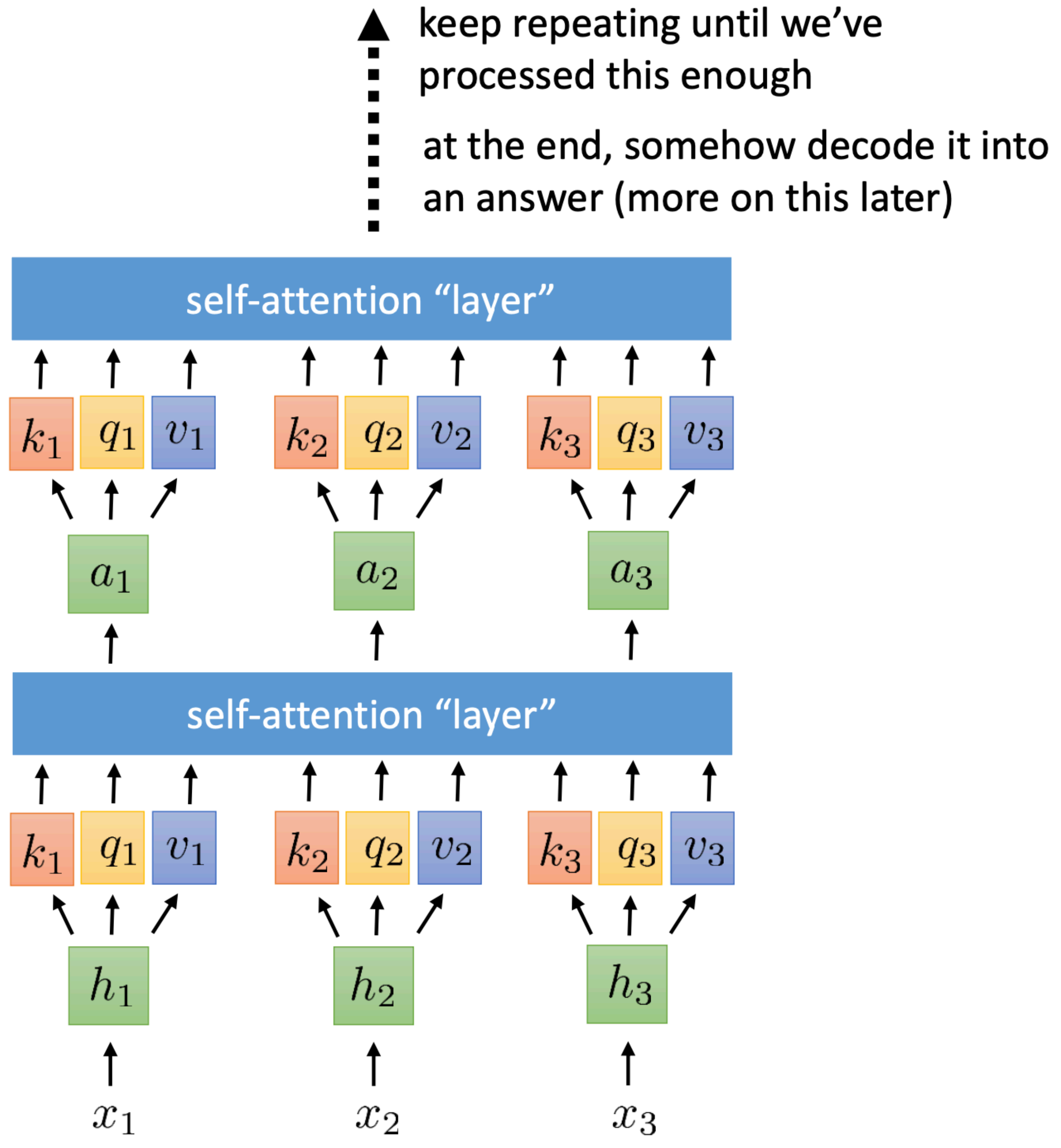
Self-Attention



Self-Attention

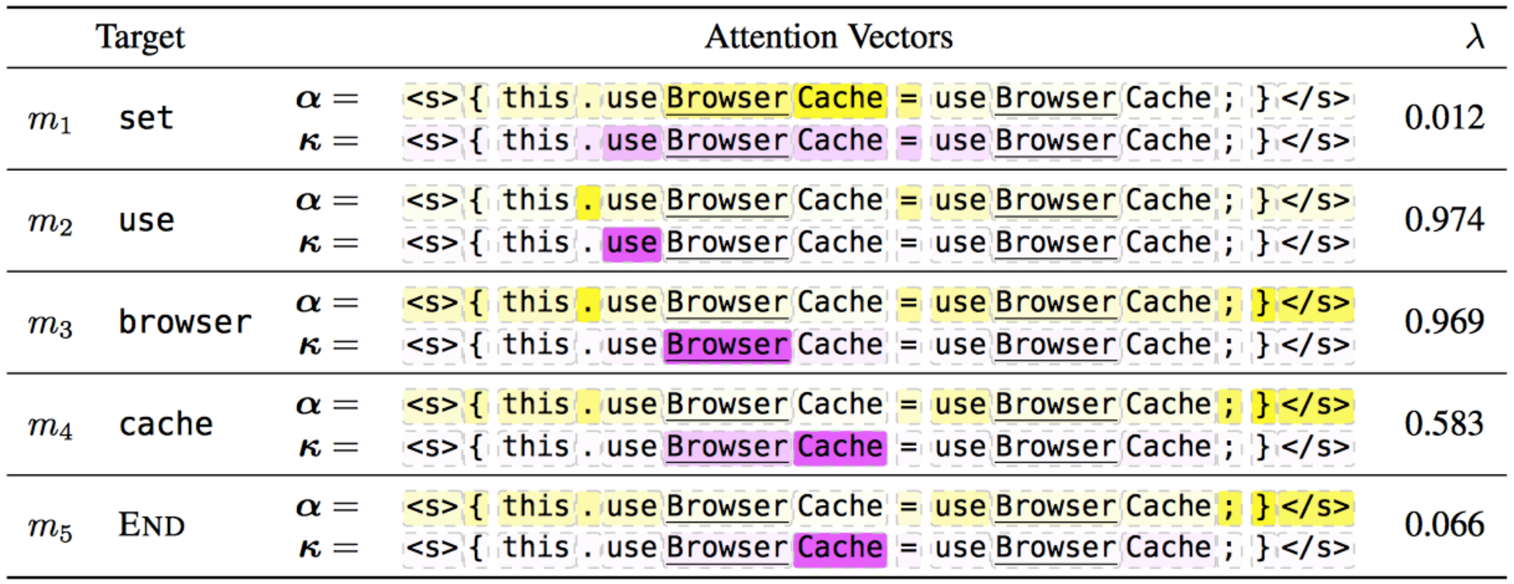






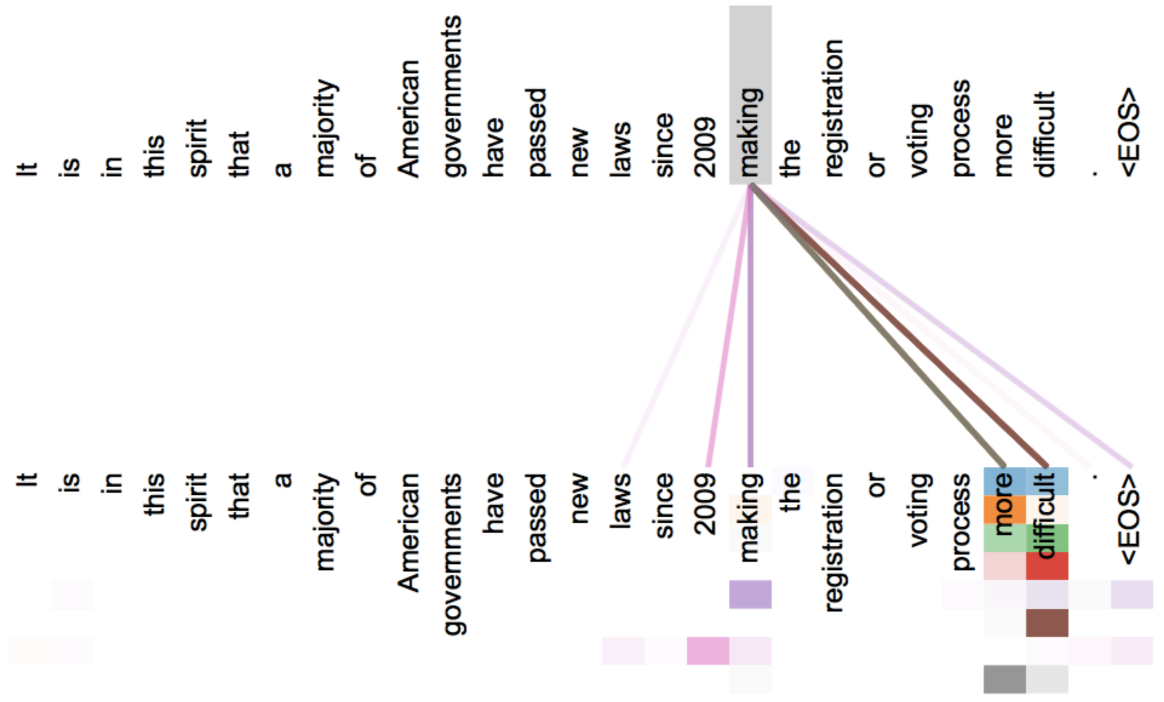
Multi-headed Attention

- **Idea:** multiple attention “heads” focus on different parts of the sentence
- e.g. Different heads for “copy” vs regular (Allamanis et al. 2016)



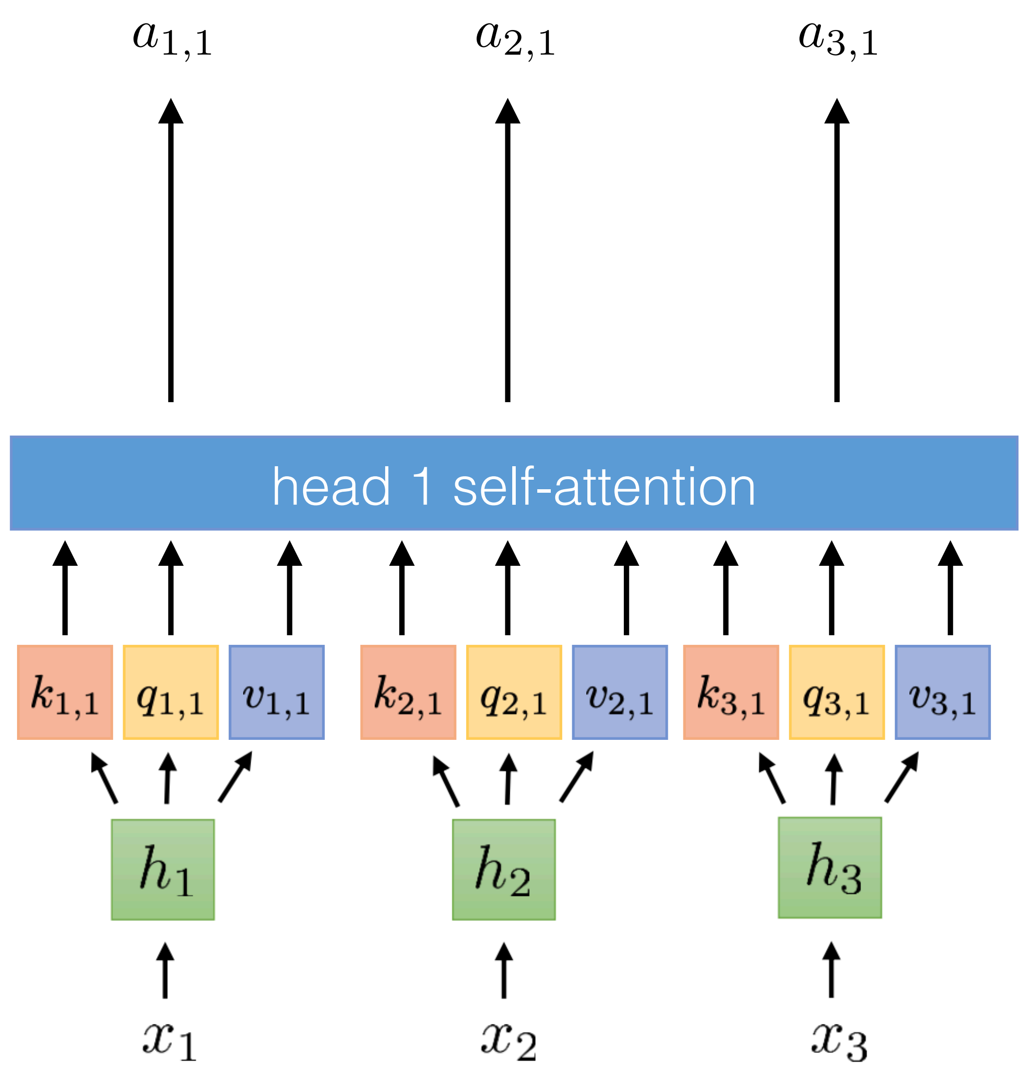
	Target		Attention Vectors	λ
m_1	set	$\boldsymbol{\alpha} =$	<s> { this . use Browser Cache = use Browser Cache ; } </s>	0.012
		$\boldsymbol{\kappa} =$	<s> { this . use Browser Cache = use Browser Cache ; } </s>	
m_2	use	$\boldsymbol{\alpha} =$	<s> { this . use Browser Cache = use Browser Cache ; } </s>	0.974
		$\boldsymbol{\kappa} =$	<s> { this . use Browser Cache = use Browser Cache ; } </s>	
m_3	browser	$\boldsymbol{\alpha} =$	<s> { this . use Browser Cache = use Browser Cache ; } </s>	0.969
		$\boldsymbol{\kappa} =$	<s> { this . use Browser Cache = use Browser Cache ; } </s>	
m_4	cache	$\boldsymbol{\alpha} =$	<s> { this . use Browser Cache = use Browser Cache ; } </s>	0.583
		$\boldsymbol{\kappa} =$	<s> { this . use Browser Cache = use Browser Cache ; } </s>	
m_5	END	$\boldsymbol{\alpha} =$	<s> { this . use Browser Cache = use Browser Cache ; } </s>	0.066
		$\boldsymbol{\kappa} =$	<s> { this . use Browser Cache = use Browser Cache ; } </s>	

- Or multiple independently learned heads (Vaswani et al. 2017)


It is in this spirit that a majority of American governments have passed new laws since 2009 making the registration or voting process more difficult . <EOS>
It is in this spirit that a majority of American governments have passed new laws since 2009 making the registration or voting process more difficult . <EOS>

- Or one head for every hidden node! (Choi et al. 2018)

Multi-head attention


$a_{1,1}$
$a_{2,1}$
$a_{3,1}$
head 1 self-attention
$k_{1,1}$ $q_{1,1}$ $v_{1,1}$ $k_{2,1}$ $q_{2,1}$ $v_{2,1}$ $k_{3,1}$ $q_{3,1}$ $v_{3,1}$
h_1 h_2 h_3
x_1 x_2 x_3

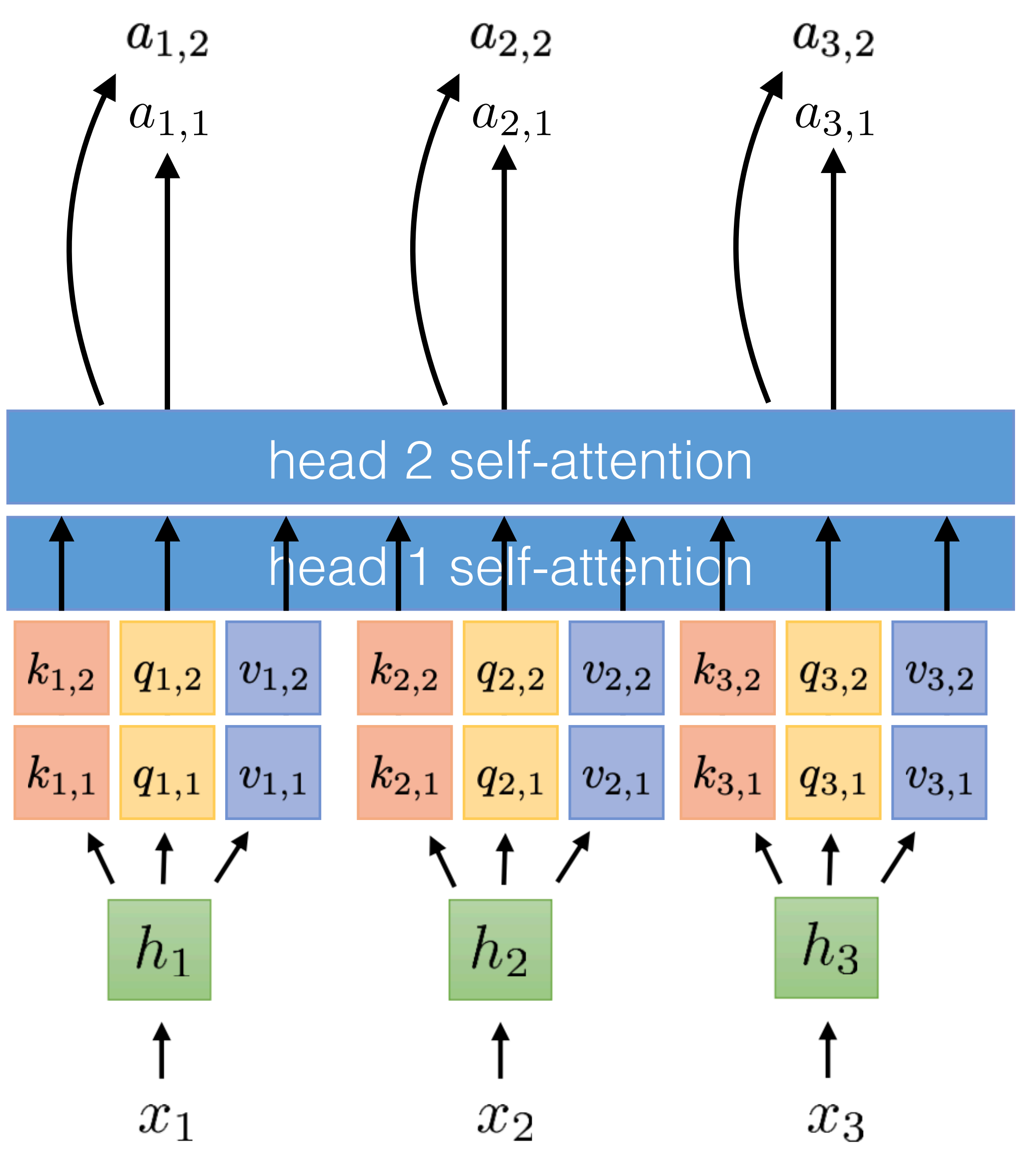
Compute weights independently for each head

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

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

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

Multi-head attention



$a_{1,2}$
$a_{1,1}$
$a_{2,2}$
$a_{2,1}$
$a_{3,2}$
$a_{3,1}$
head 2 self-attention
head 1 self-attention
$k_{1,2}$ $q_{1,2}$ $v_{1,2}$ $k_{2,2}$ $q_{2,2}$ $v_{2,2}$ $k_{3,2}$ $q_{3,2}$ $v_{3,2}$
$k_{1,1}$ $q_{1,1}$ $v_{1,1}$ $k_{2,1}$ $q_{2,1}$ $v_{2,1}$ $k_{3,1}$ $q_{3,1}$ $v_{3,1}$
h_1
h_2
h_3
x_1
x_2
x_3

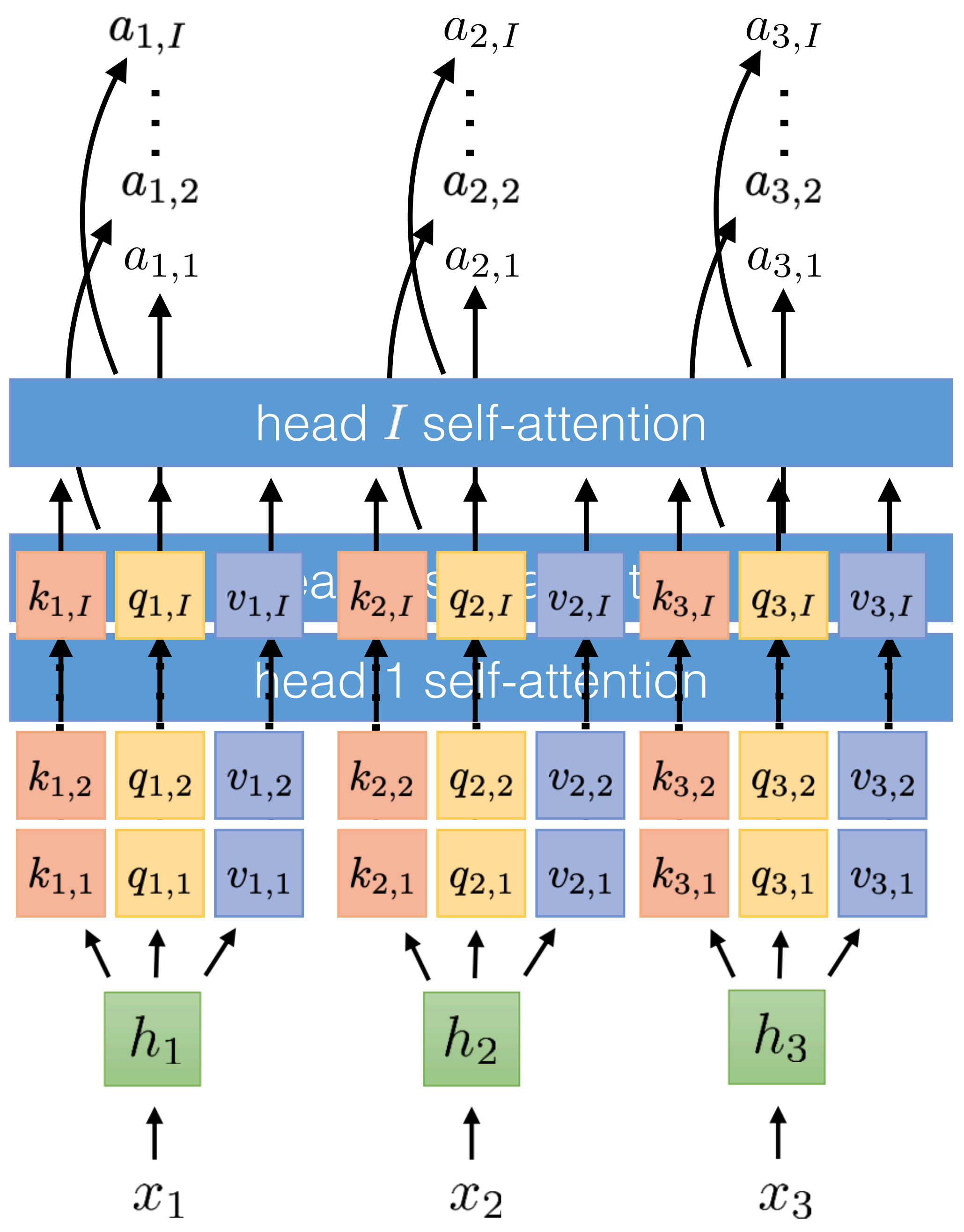
Compute weights independently for each head

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

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

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

Multi-head attention



$a_{1,I}$
$a_{2,I}$
$a_{3,I}$
$a_{1,2}$
$a_{2,2}$
$a_{3,2}$
$a_{1,1}$
$a_{2,1}$
$a_{3,1}$
head I self-attention
$k_{1,I}$ $q_{1,I}$ $v_{1,I}$ $k_{2,I}$ $q_{2,I}$ $v_{2,I}$ $k_{3,I}$ $q_{3,I}$ $v_{3,I}$
head 1 self-attention
$k_{1,2}$ $q_{1,2}$ $v_{1,2}$ $k_{2,2}$ $q_{2,2}$ $v_{2,2}$ $k_{3,2}$ $q_{3,2}$ $v_{3,2}$
$k_{1,1}$ $q_{1,1}$ $v_{1,1}$ $k_{2,1}$ $q_{2,1}$ $v_{2,1}$ $k_{3,1}$ $q_{3,1}$ $v_{3,1}$
h_1
h_2
h_3
x_1
x_2
x_3

$$a_l = \begin{bmatrix} a_{l,I} \\ \cdot \\ \cdot \\ \cdot \\ a_{l,2} \\ a_{l,1} \end{bmatrix} \in \mathbb{R}^d, \quad a_{l,i} \in \mathbb{R}^{\frac{d}{I}}$$

where I is the number of heads. Around 8 heads seems to work pretty well for big models

Compute weights independently for each head

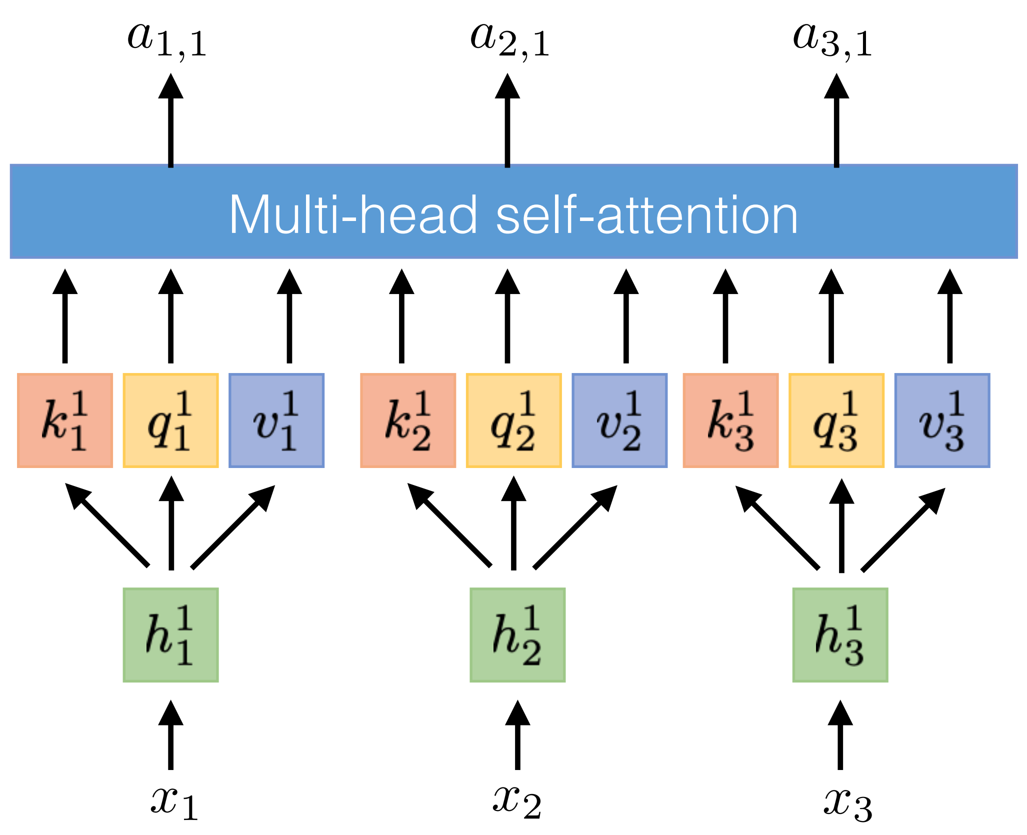
$$e_{l,t,i} = q_{l,i} \cdot k_{l,i}$$

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

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

Self-attention is still linear

- Every self-attention "layer" is a linear transformation of the previous layer (with non-linear attention weights)
- This is not very expressive to learn from the complex data


$a_{1,1}$
$a_{2,1}$
$a_{3,1}$
Multi-head self-attention
k_1^1 q_1^1 v_1^1 k_2^1 q_2^1 v_2^1 k_3^1 q_3^1 v_3^1
h_1^1 h_2^1 h_3^1
x_1 x_2 x_3

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

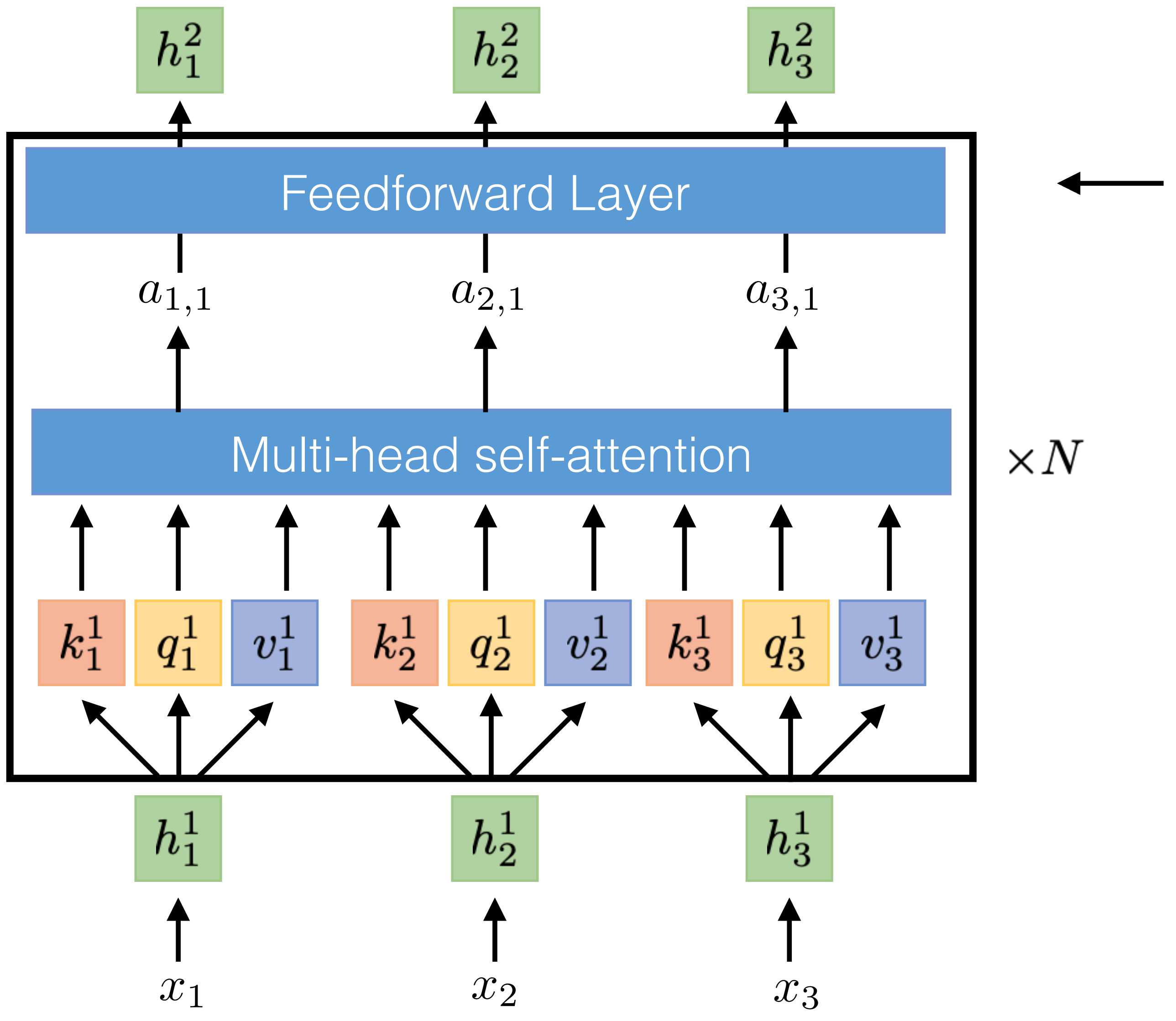
$$\alpha_{l,t} = \exp(e_{l,t}) / \sum_{t'} \exp(e_{l,t'})$$

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

$$a_l = \sum_t \alpha_{l,t} v_t = \sum_t \alpha_{l,t} \underbrace{W_v}_{\text{linear transformation}} h_t = W_v \sum_t \underbrace{\alpha_{l,t}}_{\text{non-linear weights}} h_t$$

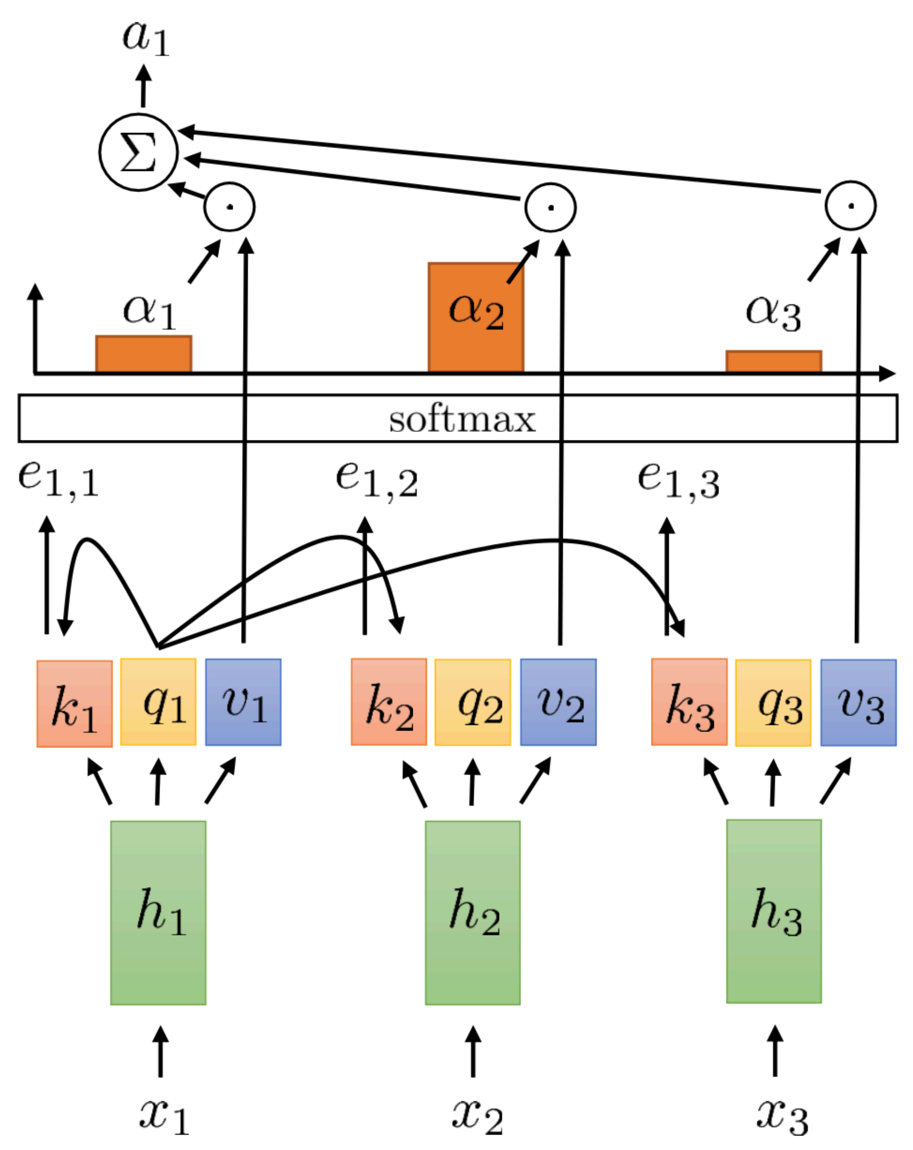
Alternating self-attention & nonlinearity

- Each transformer layer contains a multi-head self-attention layer and a feedforward layer.
- We alternate self-attention and non-linear layer *N* times, namely stack *N* transformer layers.



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

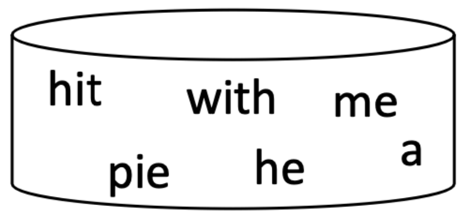
Positional encoding



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!

$$h_t = \underbrace{f}_{\text{some function}}(x_t, t)$$

Positional encoding: sin/cos

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

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

$$\text{I } \underbrace{\text{walk my}}\text{ dog every day} \qquad \text{every single day I } \underbrace{\text{walk my}}\text{ dog}$$

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

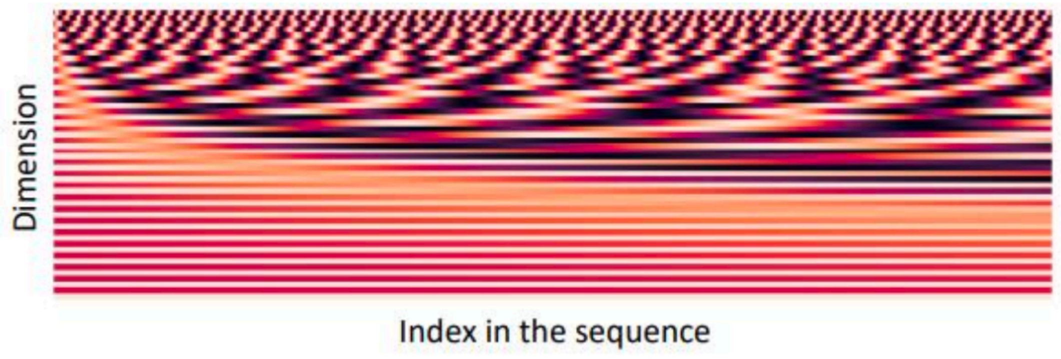
we want to represent **position** in a way that tokens with similar **relative** position have similar **positional encoding**

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

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

dimensionality of positional encoding

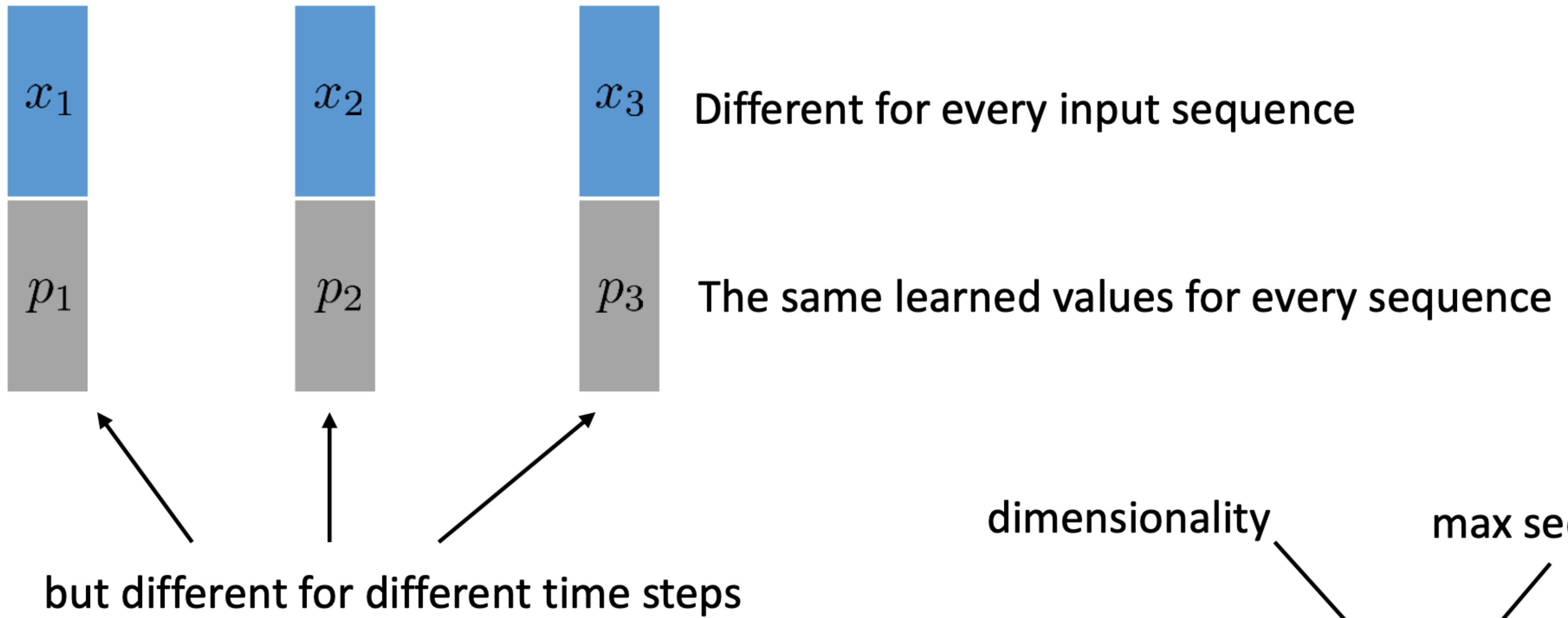
"even-odd" indicator



"first-half vs. second-half" indicator

Positional encoding: learned

Another idea: just learn a positional encoding


x_1
x_2
x_3
Different for every input sequence
p_1
p_2
p_3
The same learned values for every sequence
but different for different time steps

How many values do we need to learn?

dimensionality → d, max sequence length → T

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

+ 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)

Positional encoding: RoPE

- Issue of absolute positional embedding:
  - Sentence 1: I walk my dog every day.
  - Sentence 2: Every day I walk my dog.
- Instead of learning **absolute** positional embedding, model the **relative** positional embedding.

Compare Absolute and Relative Position Embeddings

- Assume query in the m-th position, key and value in the n-th position

$$\begin{aligned}\boldsymbol{q}_m &= f_q(\boldsymbol{x}_m, m)\\ \boldsymbol{k}_n &= f_k(\boldsymbol{x}_n, n)\\ \boldsymbol{v}_n &= f_v(\boldsymbol{x}_n, n),\end{aligned}$$

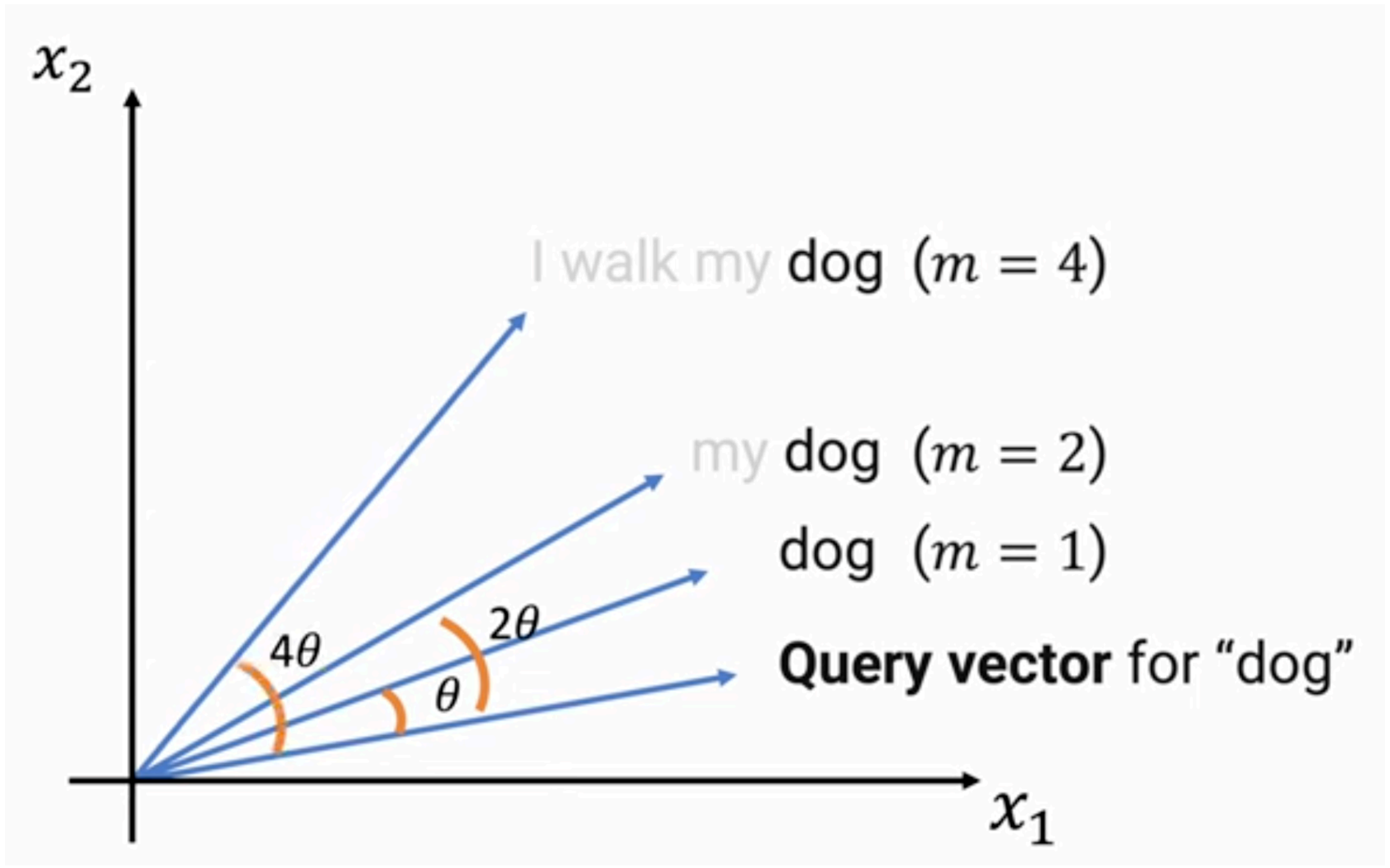
- **Absolute** position encoding in attention:

$$\boldsymbol{q}_m^\intercal \boldsymbol{k}_n = \boldsymbol{x}_m^\intercal \boldsymbol{W}_q^\intercal \boldsymbol{W}_k \boldsymbol{x}_n + \boldsymbol{p}_m^\intercal \mathbf{U}_q^\intercal \mathbf{U}_k \boldsymbol{p}_n + b_{i,j}$$

- **Relative** position encoding in attention:

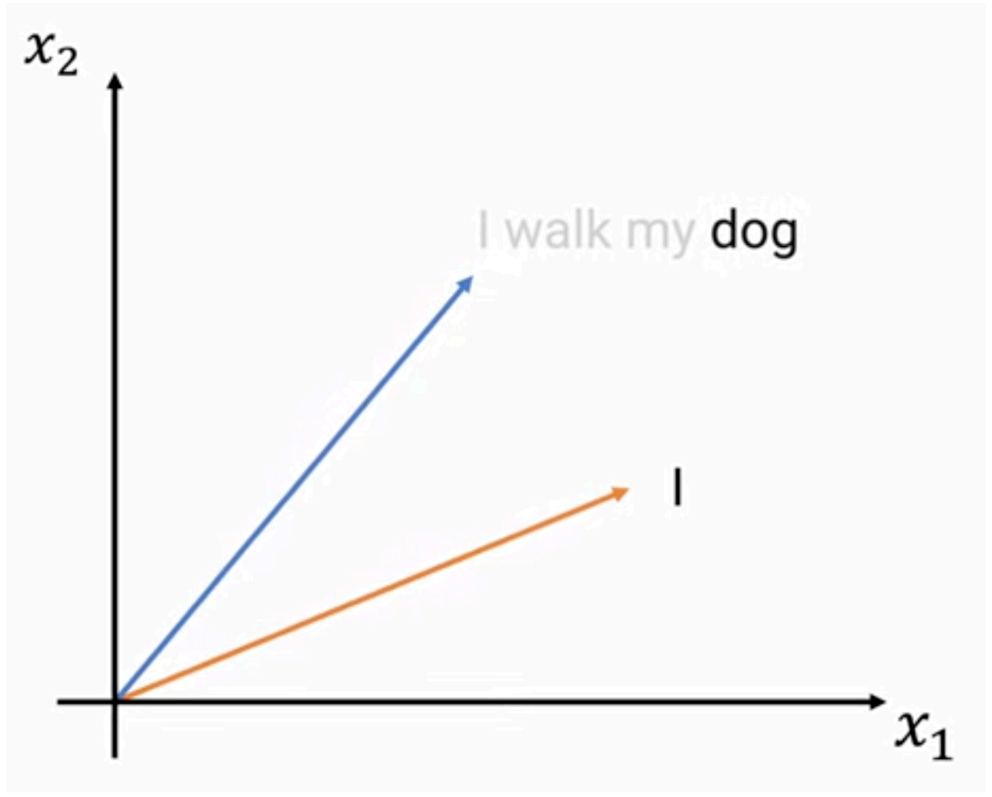
$$\boldsymbol{q}_m^\intercal \boldsymbol{k}_n = \boldsymbol{x}_m^\intercal \boldsymbol{W}_q^\intercal \boldsymbol{W}_k \boldsymbol{x}_n + \boldsymbol{x}_m^\intercal \boldsymbol{W}_q^\intercal \boldsymbol{W}_k \tilde{\boldsymbol{p}}_{m-n} + \tilde{\boldsymbol{p}}_{m-n}^\intercal \boldsymbol{W}_q^\intercal \boldsymbol{W}_k \boldsymbol{x}_n$$

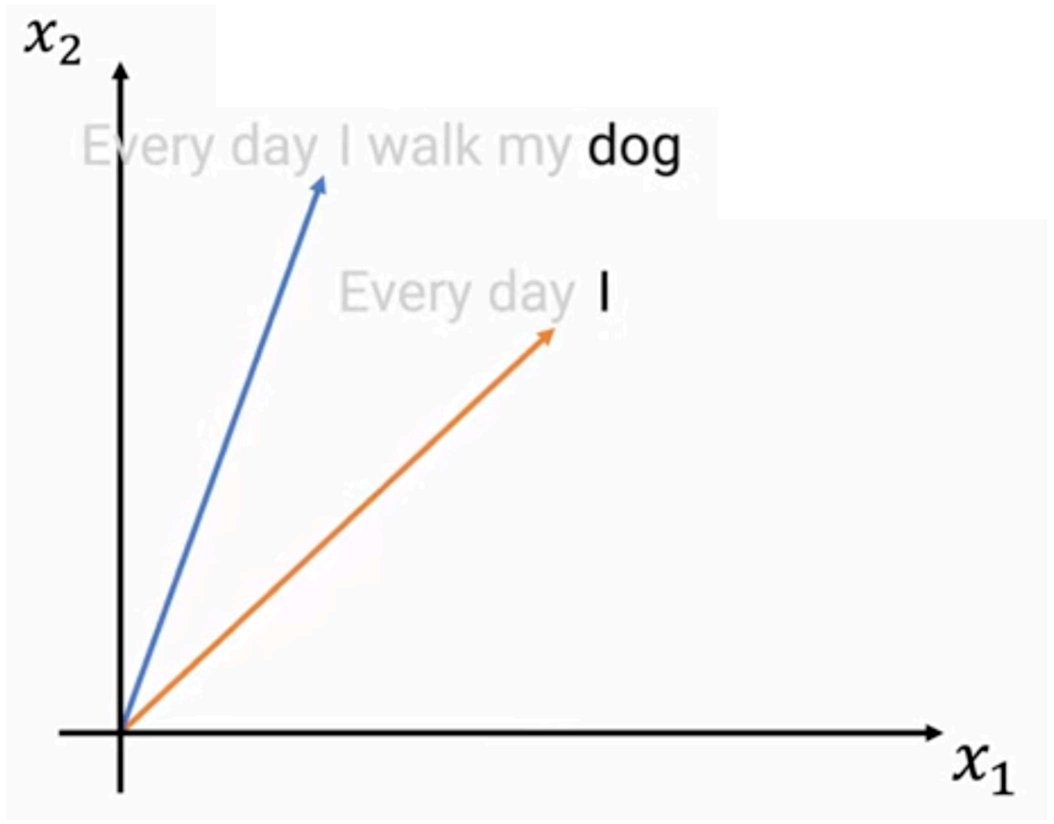
RoPE: Relative Positional Encoding



RoPE: Relative Positional Encoding

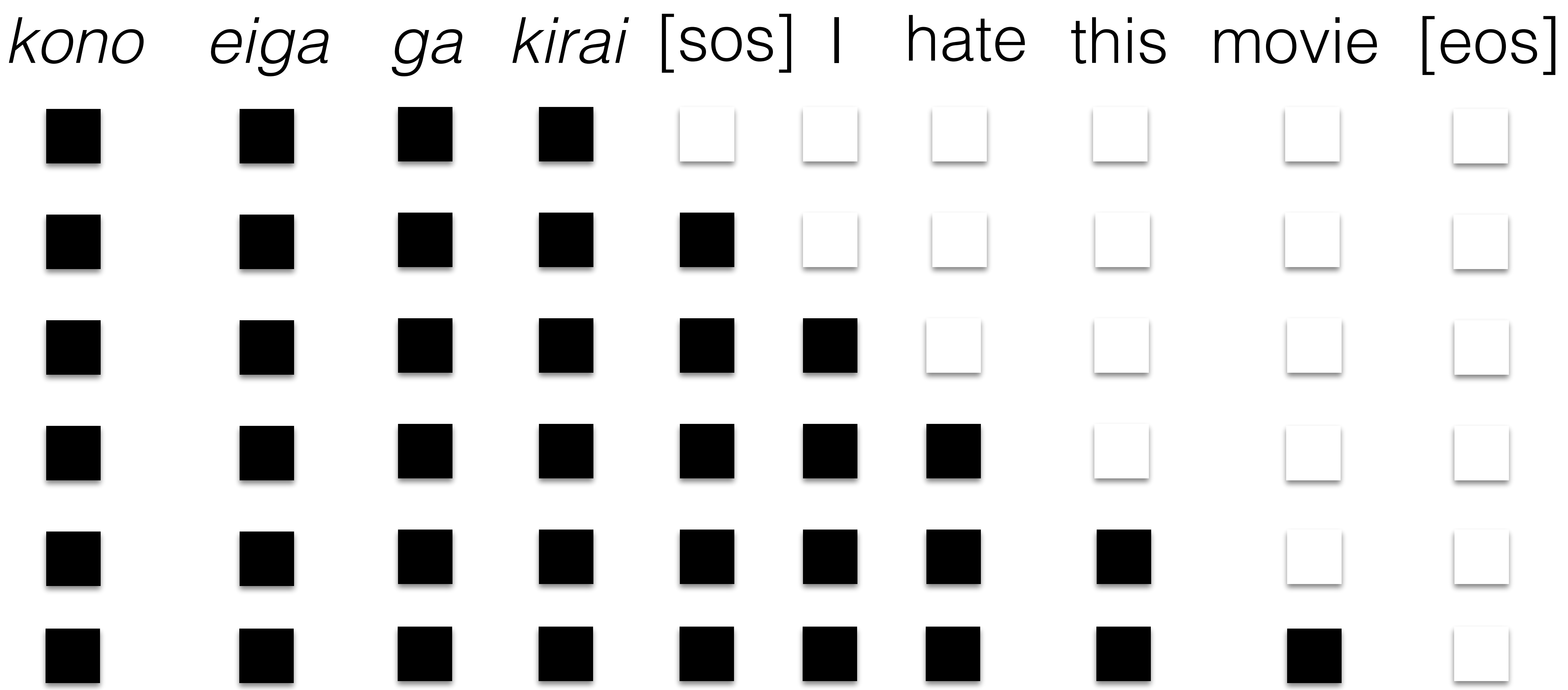
- Relative angle between “I” and “dog” remains the same even after adding two words in the beginning.



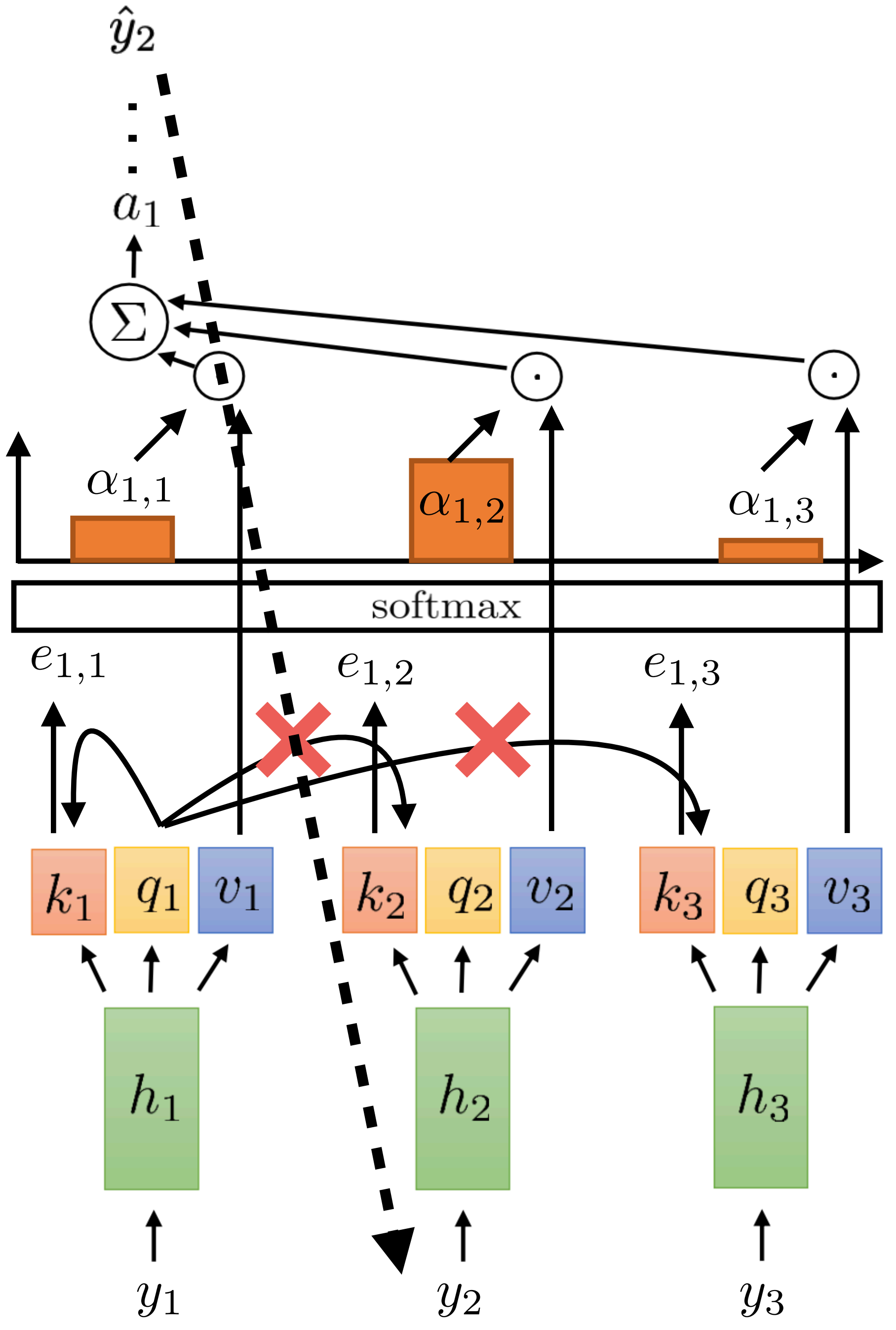


Masked attention for Target sentence

- For the conditioned prediction, we aim to predict the current target word based on its past words and the source input, i.e., $P(y_i|X, y_{<i})$
- We can do so by "masking" the results for the output



Masked attention for Target sentence



- **At test time**, the predicted token will be feed as input to the next time step
- We must design a masking to allow self-attention on the **past tokens**, but not on the **future tokens**.

Easy solution:

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

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

in practice:

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

inside the softmax

Multiply the attention matrix by 0-1 masking matrix

Attention Tricks

- **Self Attention:** Each layer combines words with others
- **Multi-headed Attention:** 8 attention heads learned independently
- **Normalized Dot-product Attention:** Remove bias in dot product when using large networks
- **Positional Encodings:** Make sure that even if we don’t have RNN, can still distinguish positions

Training Tricks

- **Layer Normalization:** Help ensure that layers remain in reasonable range
- **Specialized Training Schedule:** Adjust default learning rate of the Adam optimizer
- **Label Smoothing:** Insert some uncertainty in the training process
- **Masking for Efficient Training**

Code Walk:
The Annotated Transformer

https://nlp.seas.harvard.edu/2018/04/03/attention.html

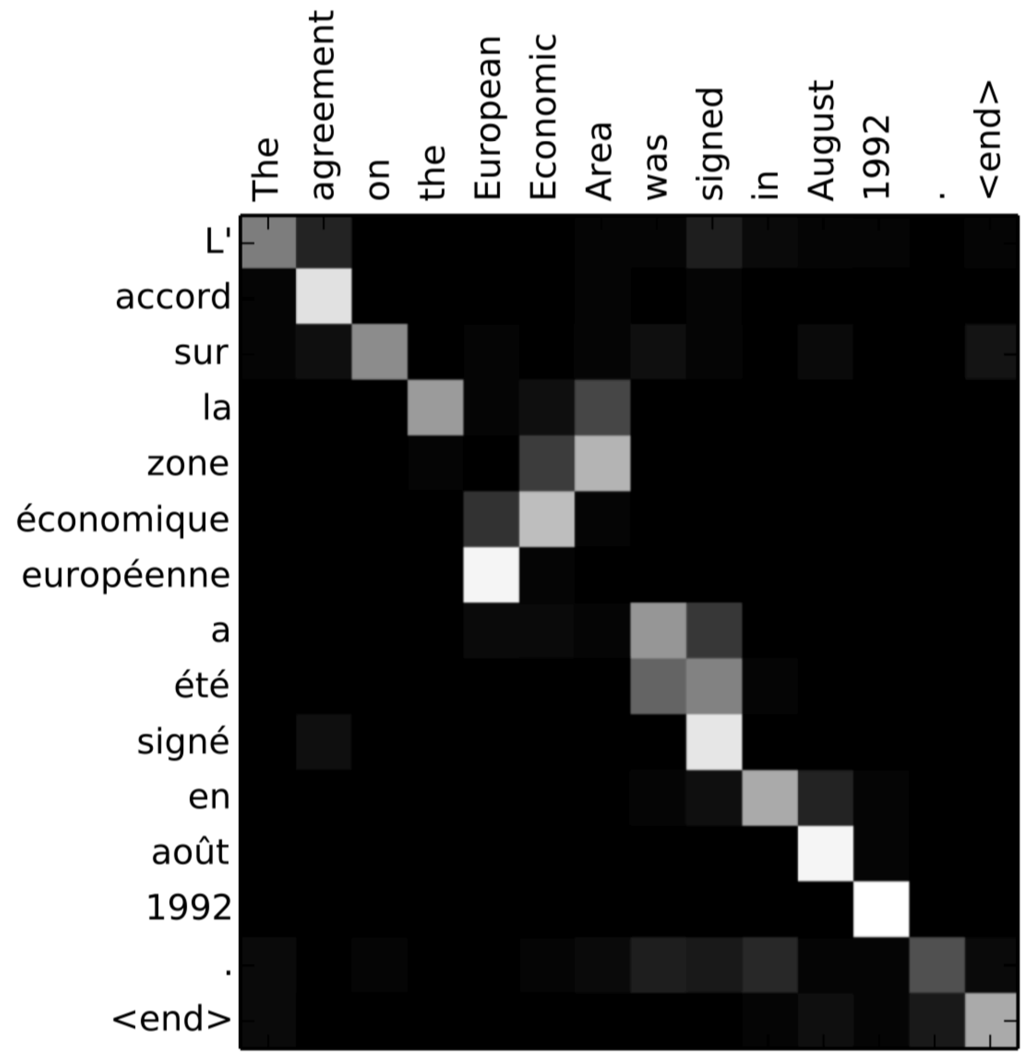
A Caveat: Attention Is Not All You Need?

- Transformers are very popular, for good reason, but
- They can be **slow to decode** at test time (Zhang et al. 2018)
- They **don't necessarily outperform RNNs** on the decoder side of seq2seq tasks (Chen et al. 2018)
- They can be **hard to train on small data** (Nguyen and Salazar 2019)
- Use them, but also be aware of limitations!

Better Modeling for Attention

Incorporating Markov Properties
(Cohn et al. 2015)

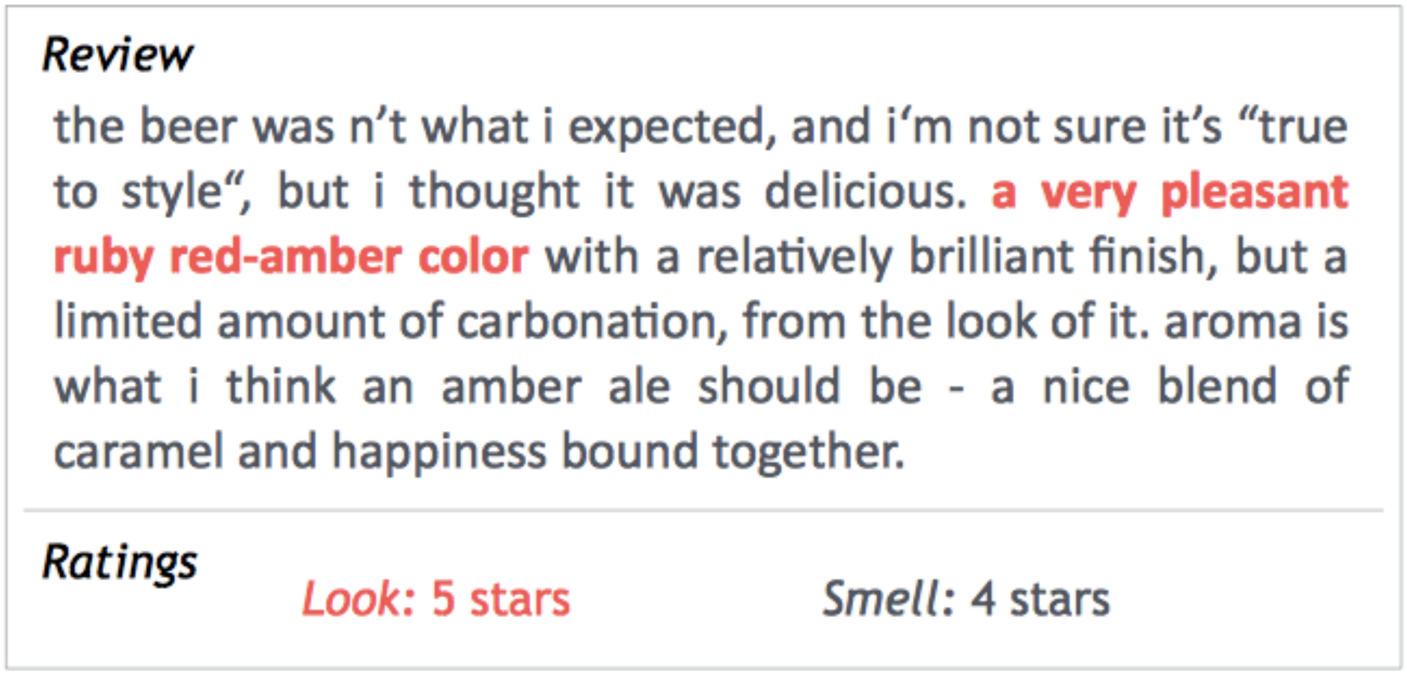
- **Intuition:** attention from last time tends to be correlated with attention this time



- Add information about the last attention when making the next decision

Hard Attention

- Instead of a soft interpolation, make a **zero-one decision** about where to attend (Xu et al. 2015)
  - Harder to train, requires methods such as reinforcement learning (see later classes)
- Perhaps this helps interpretability? (Lei et al. 2016)



Review

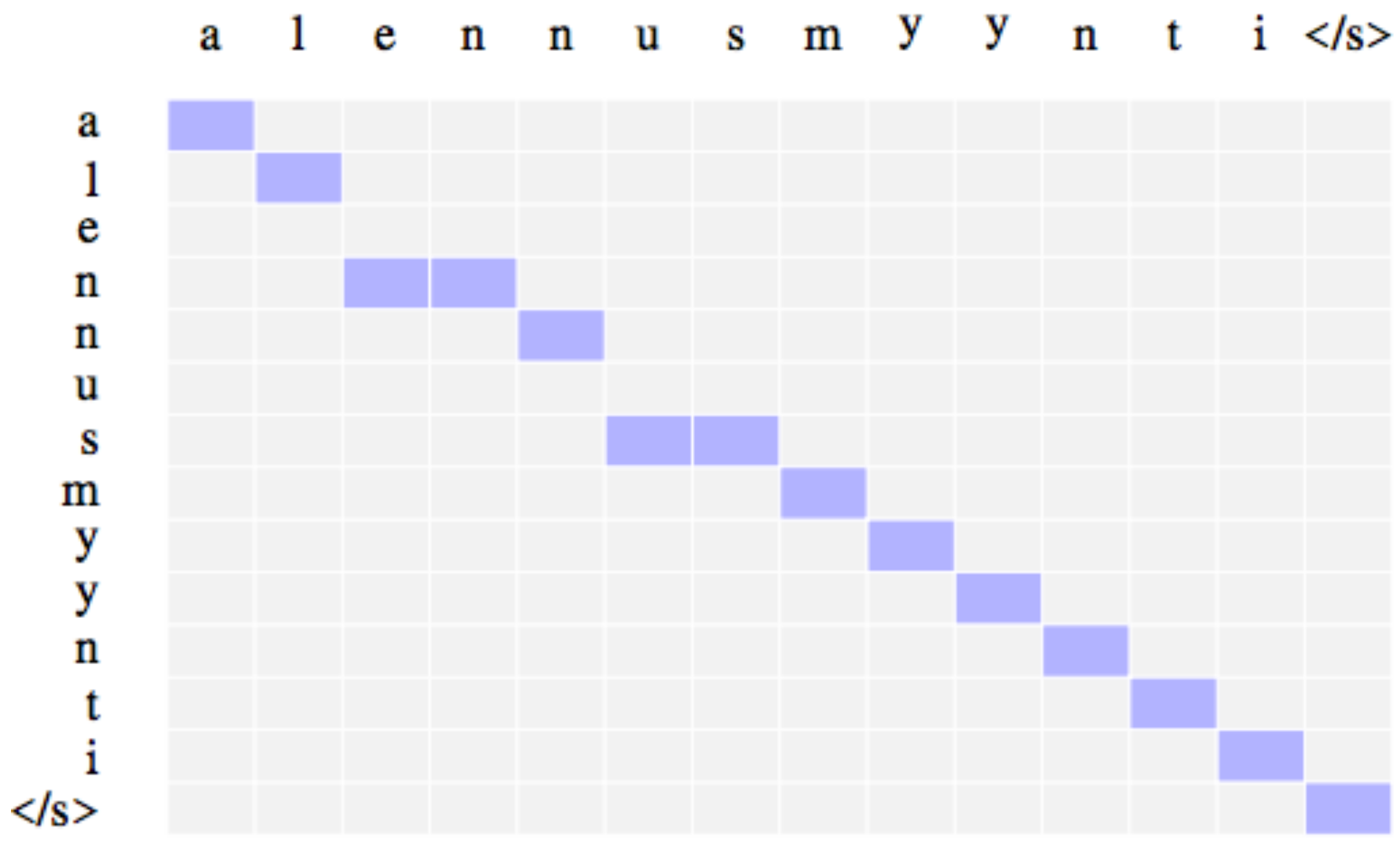
the beer was n't what i expected, and i'm not sure it's "true to style", but i thought it was delicious. **a very pleasant ruby red-amber color** with a relatively brilliant finish, but a limited amount of carbonation, from the look of it. aroma is what i think an amber ale should be - a nice blend of caramel and happiness bound together.

Ratings

Look: 5 stars *Smell:* 4 stars

Monotonic Attention (e.g. Yu et al. 2016)

- In some cases, we might know the output will be the same order as the input
  - Speech recognition, incremental translation, morphological inflection (?), summarization (?)



- **Basic idea:** hard decisions about whether to read more

Better Training for Attention

Coverage

- **Problem:** Neural models tends to drop or repeat content
- **Solution:** Model how many times words have been covered
    - Impose a penalty if attention not approx.1 over each word (Cohn et al. 2015)
    - Add embeddings indicating coverage (Mi et al. 2016)

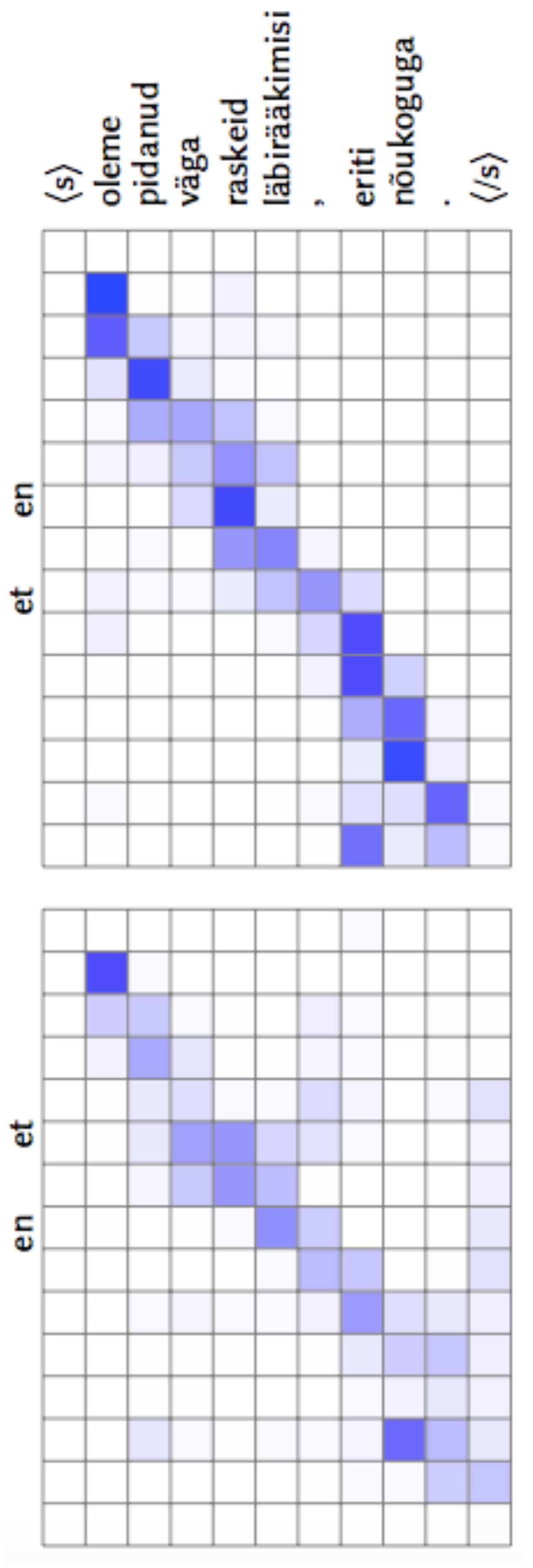
Bidirectional Training

(Cohn et al. 2015)

- **Intuition:** Our attention should be roughly similar in forward and backward directions

- **Method:** Train so that we get a bonus based on the trace of the matrix product for training in both directions

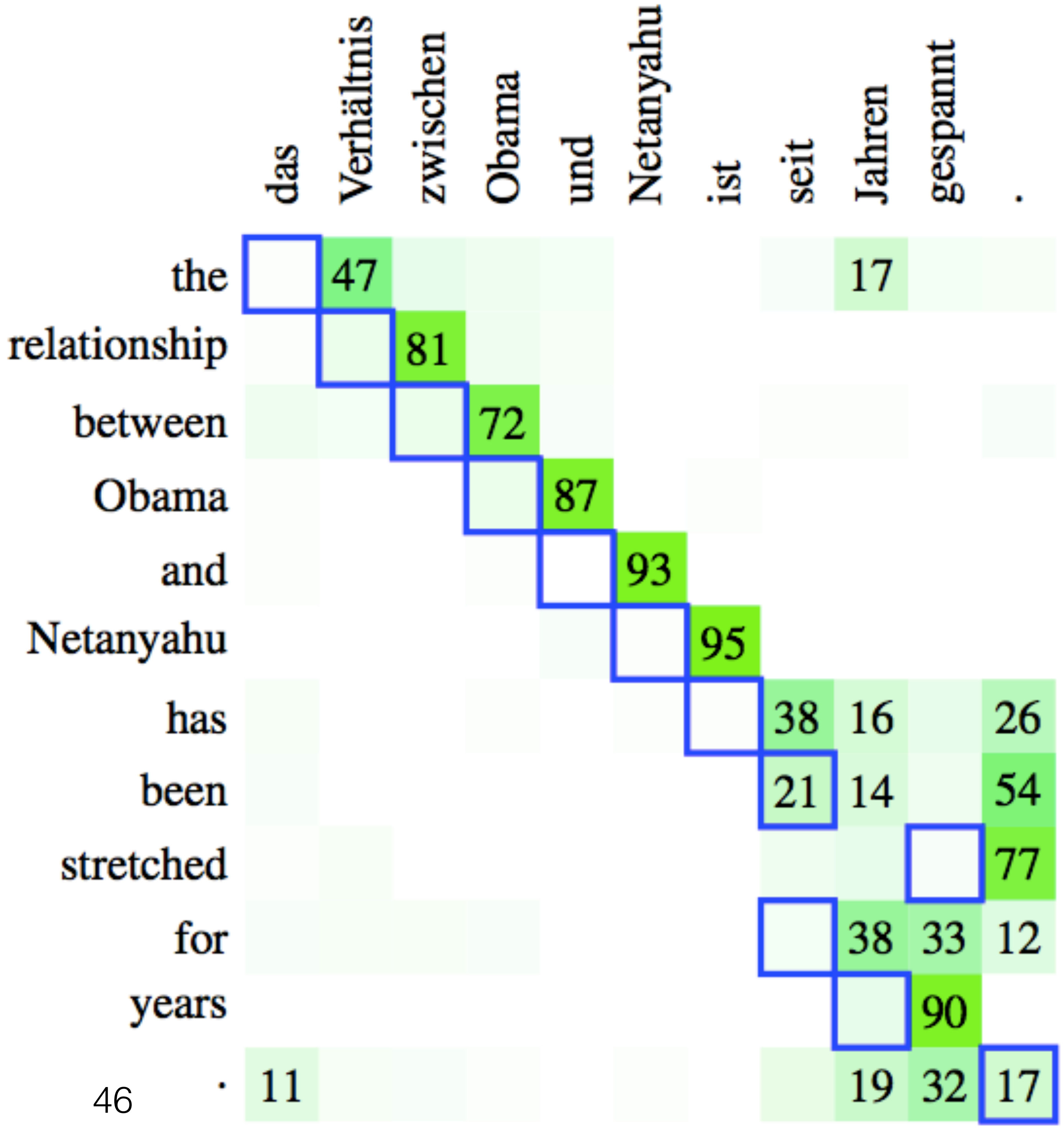
$$\mathrm{tr}(A_{X\rightarrow Y}A^{\intercal}_{Y\rightarrow X})$$



Attention is not Alignment!

(Koehn and Knowles 2017)

- Attention is often blurred
- Attention is often off by one
- It can even be manipulated to be non-intuitive! (Jain and Wallace 2019, Pruthi et al. 2020)



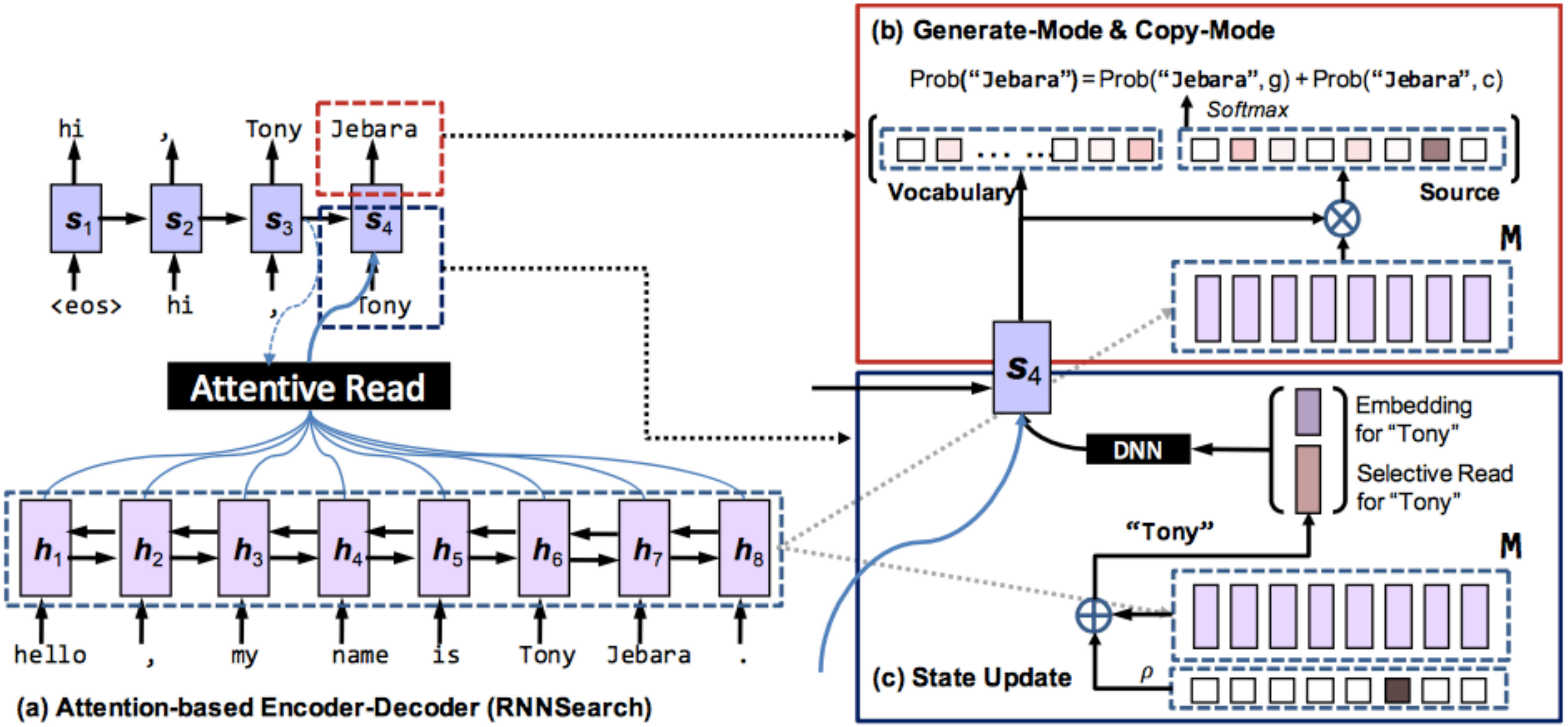
Supervised Training
(Mi et al. 2016)

- Sometimes we can get “gold standard” alignments *a-priori*
    - Manual alignments
    - Pre-trained with strong alignment model
- **Train the model to match** these strong alignments

What Else Can We Attend To?

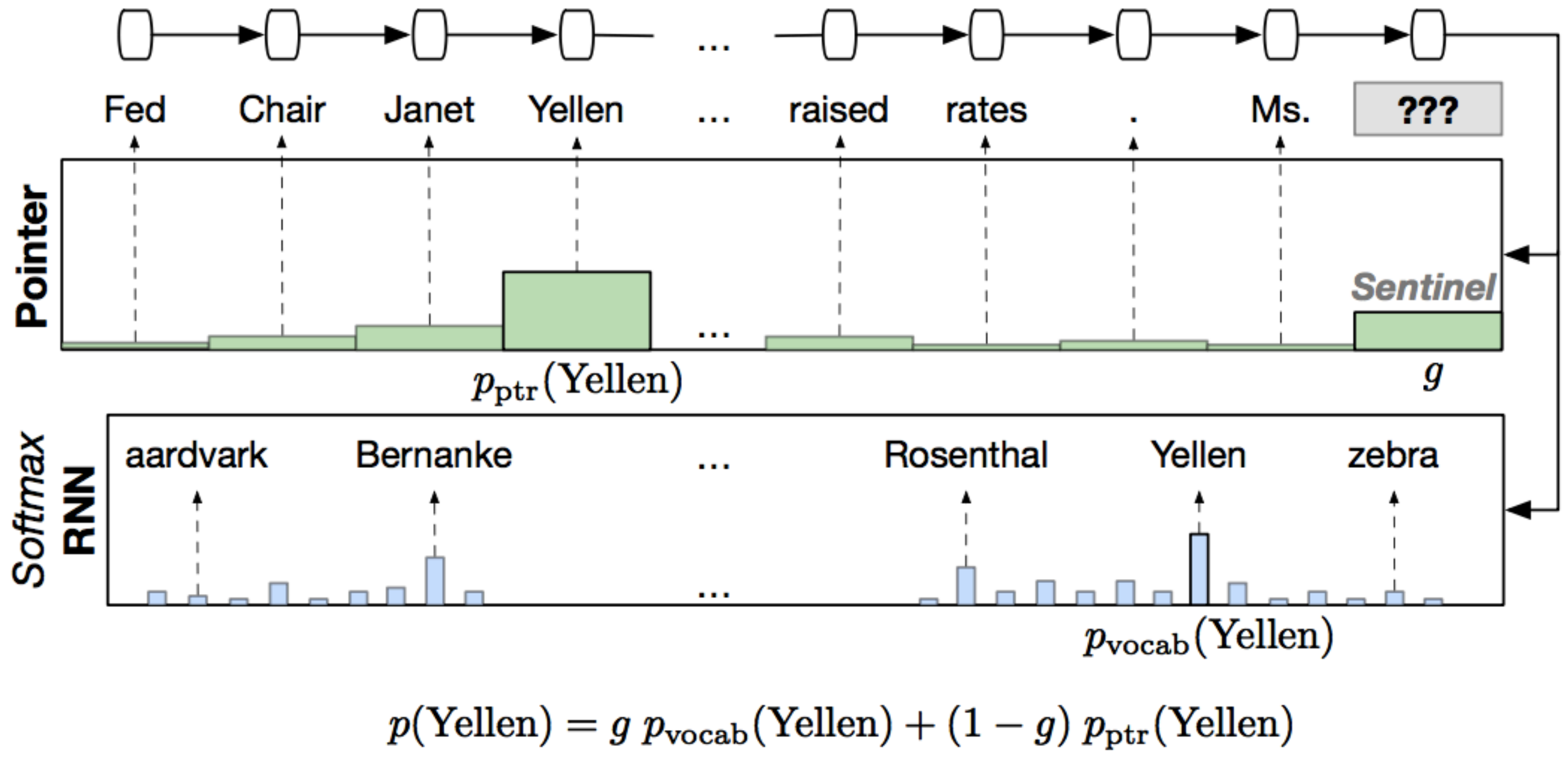
Copy Mechanisms

- Like the previous explanation
- But also, more directly through a *copy mechanism* (Gu et al. 2016)



Copying from History

- In language modeling, attend to the previous words (Merity et al. 2016)

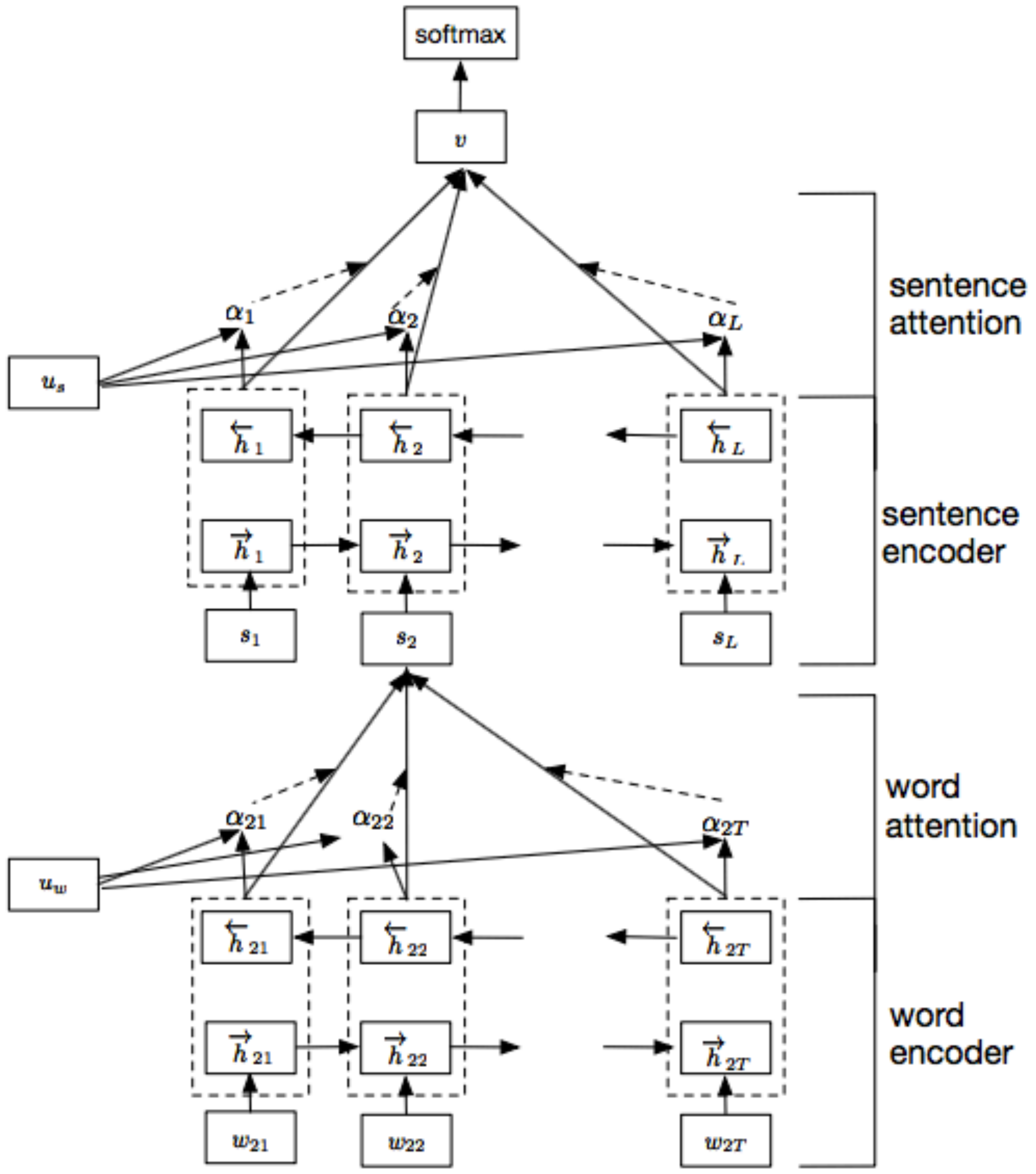


$$p(\text{Yellen}) = g\, p_{\text{vocab}}(\text{Yellen}) + (1-g)\, p_{\text{ptr}}(\text{Yellen})$$

- In translation, attend to either input or previous output (Vaswani et al. 2017)

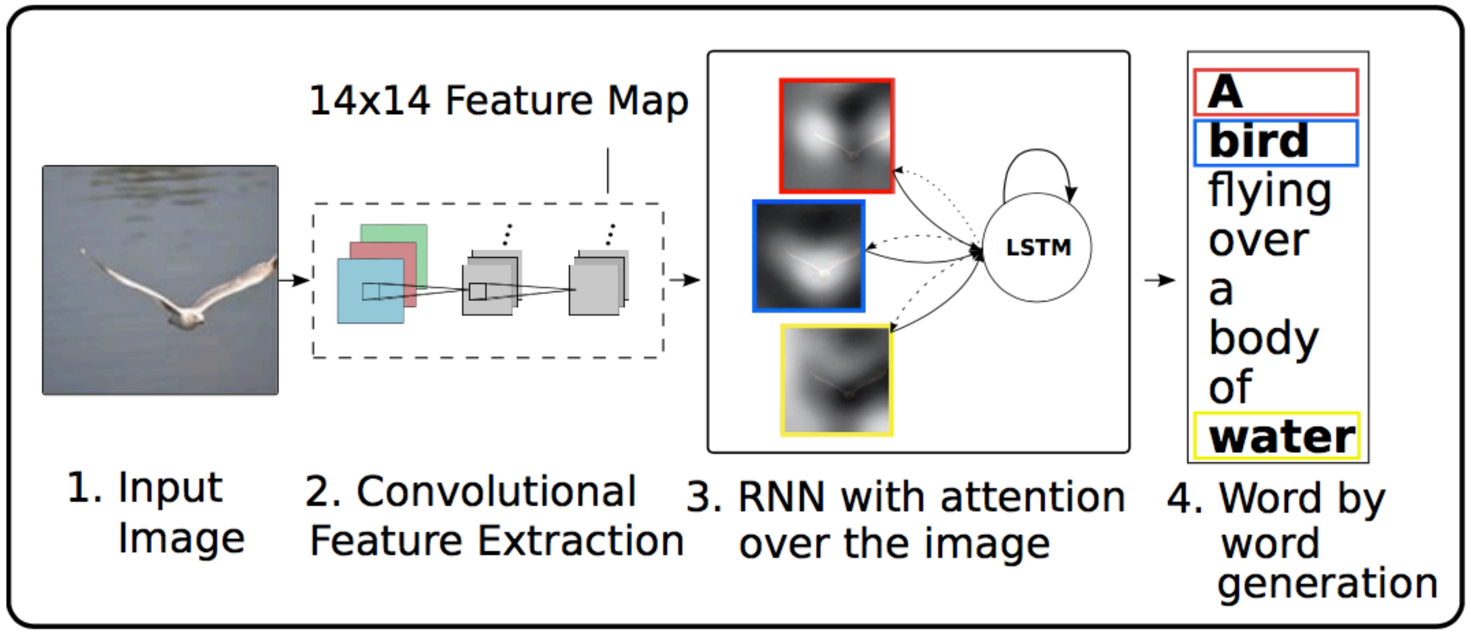
Hierarchical Structures
(Yang et al. 2016)

- Encode with attention over each sentence, then attention over each sentence in the document

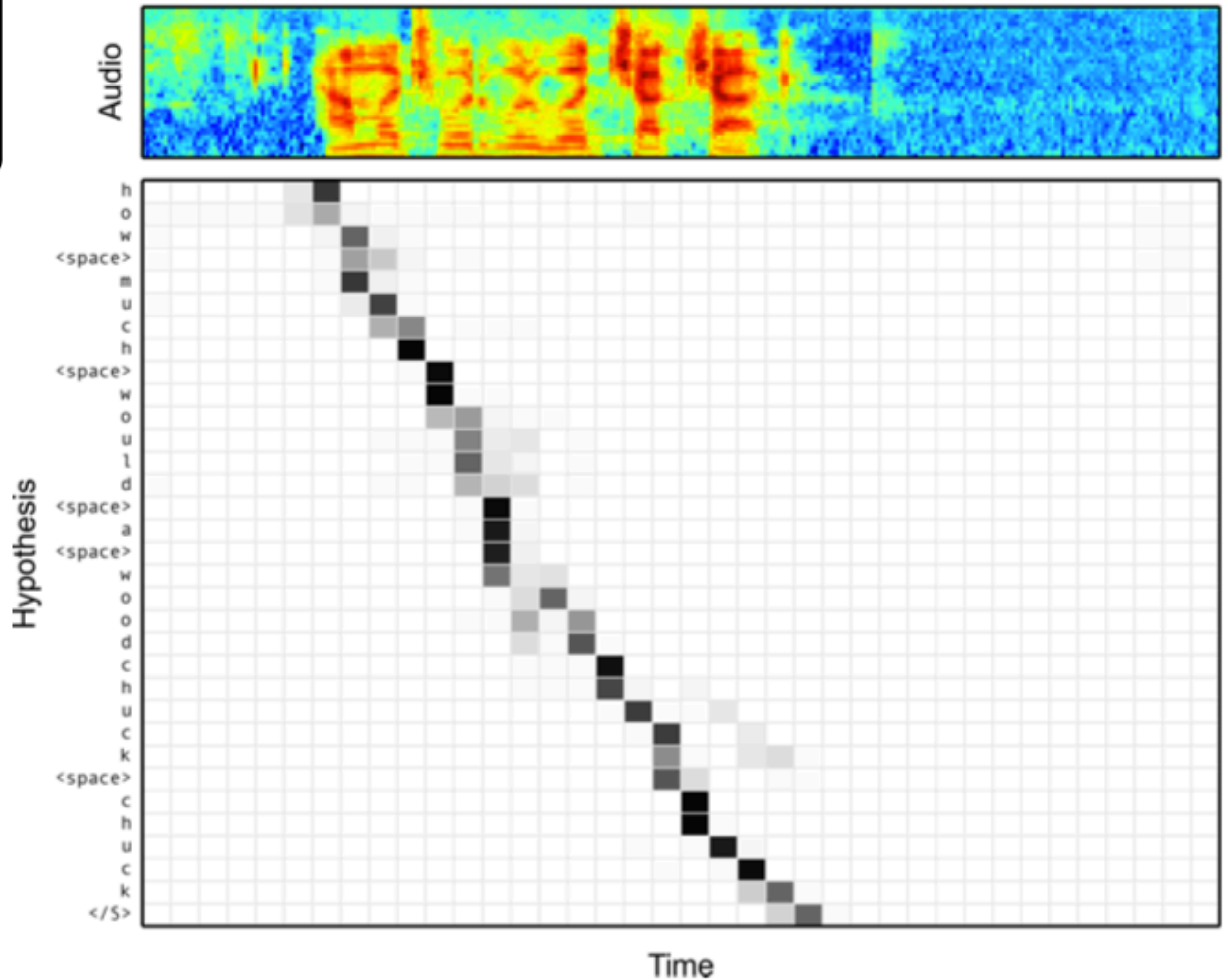


Various Modalities

- Images (Xu et al. 2015)

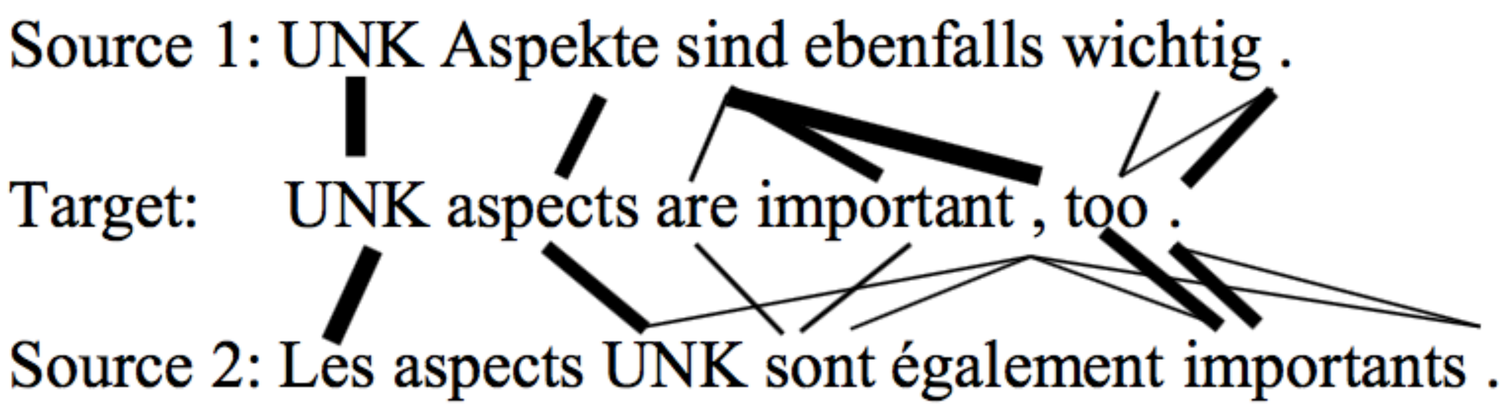

14x14 Feature Map
LSTM
A
bird
flying
over
a
body
of
water
1. Input Image
2. Convolutional Feature Extraction
3. RNN with attention over the image
4. Word by word generation

- Speech (Chan et al. 2015)



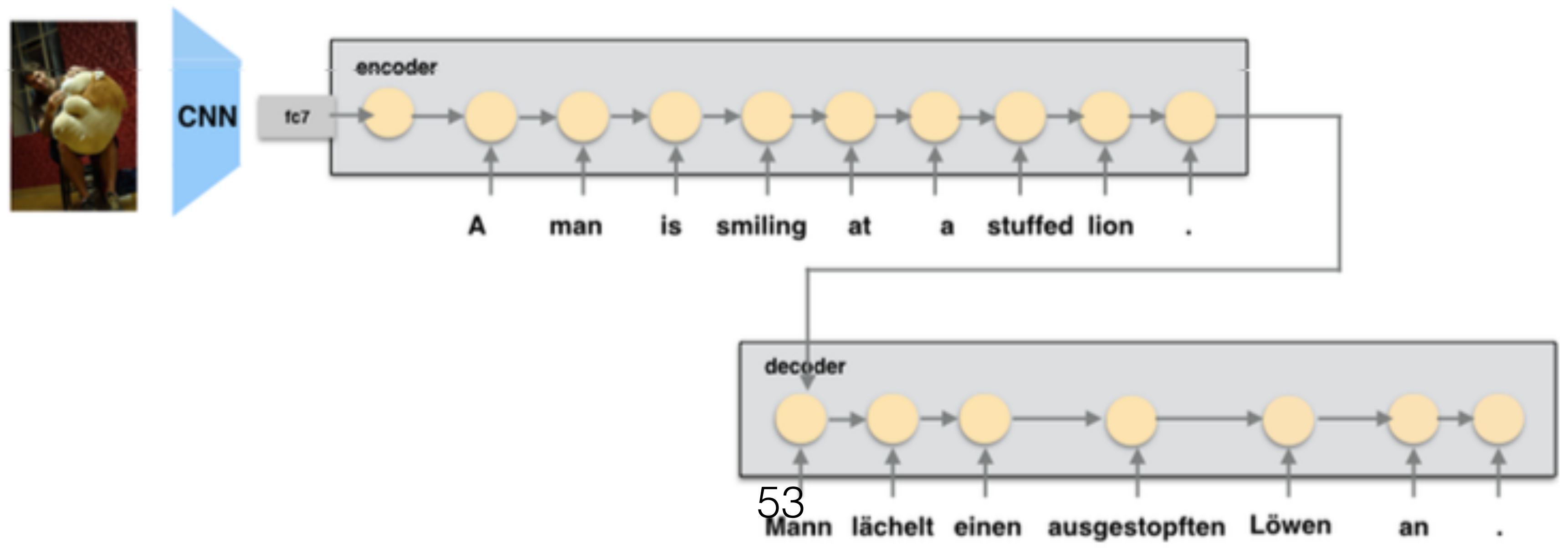
Multiple Sources

- Attend to multiple sentences (Zoph et al. 2015)


Source 1: UNK Aspekte sind ebenfalls wichtig .
Target: UNK aspects are important , too .
Source 2: Les aspects UNK sont également importants .

  - Libovicky and Helcl (2017) compare multiple strategies

- Attend to a sentence and an image (Huang et al. 2016)


CNN
fc7
encoder
A man is smiling at a stuffed lion .
decoder
Mann lächelt einen ausgestopften Löwen an .

Questions?