STAT 453: Introduction to Deep Learning and Generative Models

Ben Lengerich

Lecture 20: Attention & Transformers

November 12, 2025

Reading: See course homepage

Last time: Recurrent Neural Networks (RNNs)

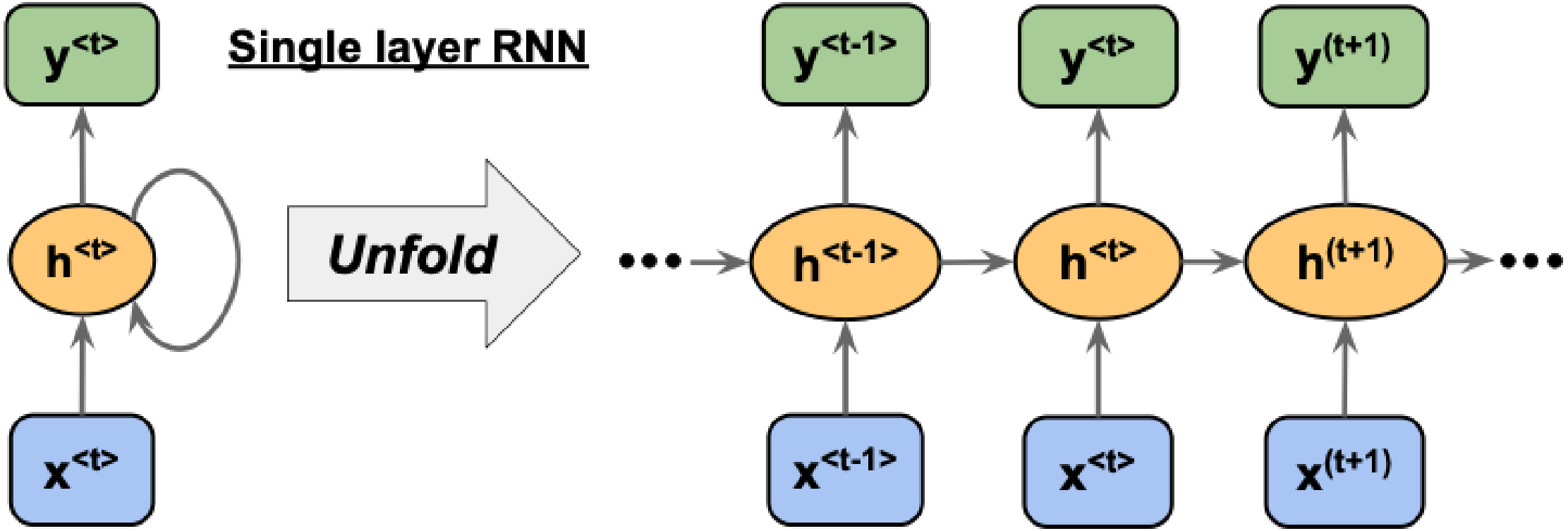


Image source: Sebastian Raschka, Vahid Mirjalili. Python Machine Learning. 3rd Edition. Packt, 2019

From RNN…

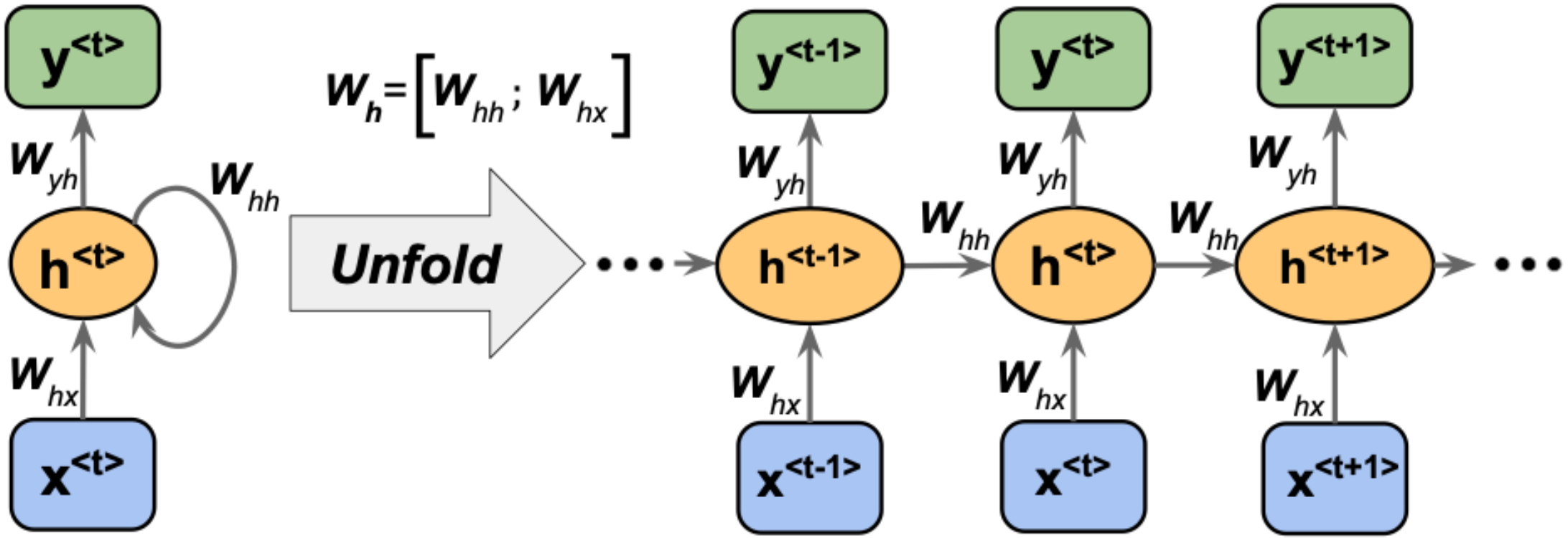


Image source: Sebastian Raschka, Vahid Mirjalili. Python Machine Learning. 3rd Edition. Packt, 2019

From RNN…to GPT

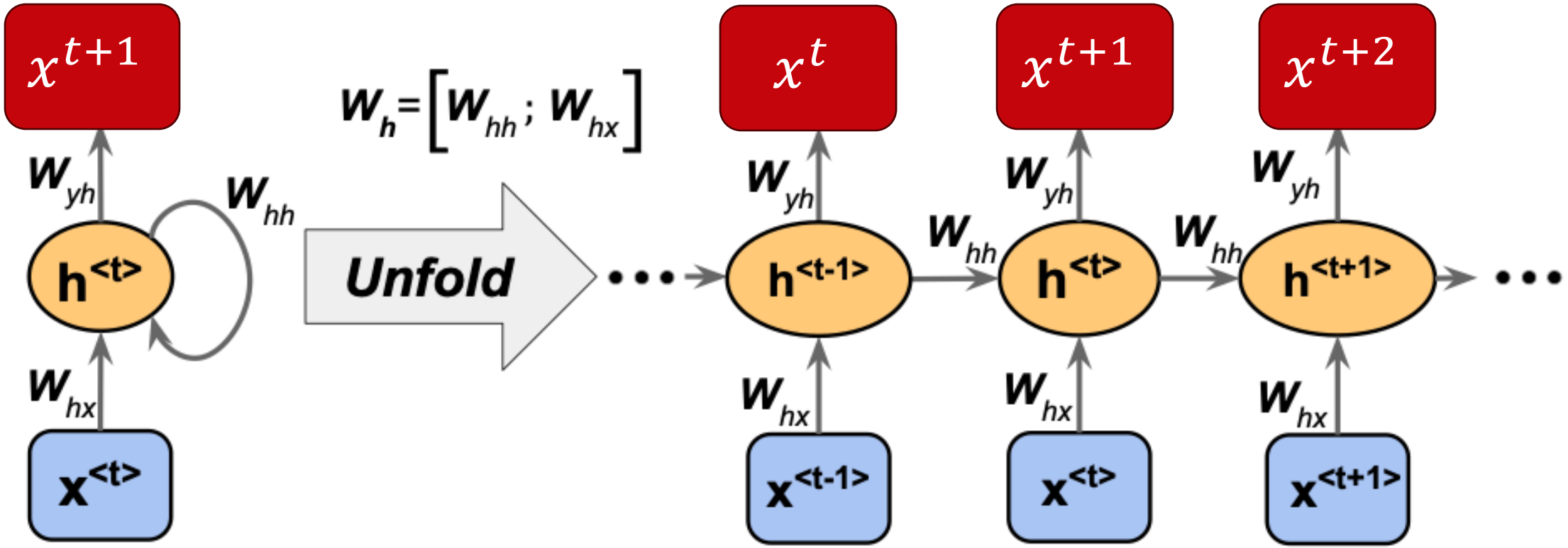
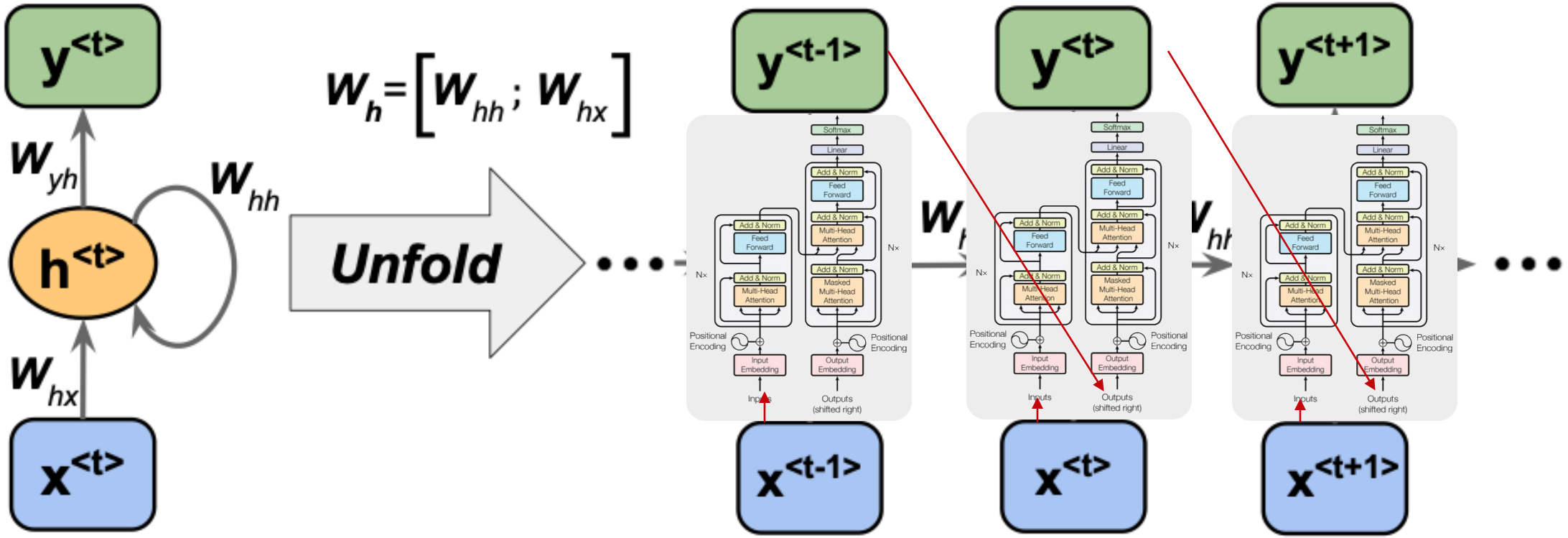


Image source: Sebastian Raschka, Vahid Mirjalili. Python Machine Learning. 3rd Edition. Packt, 2019

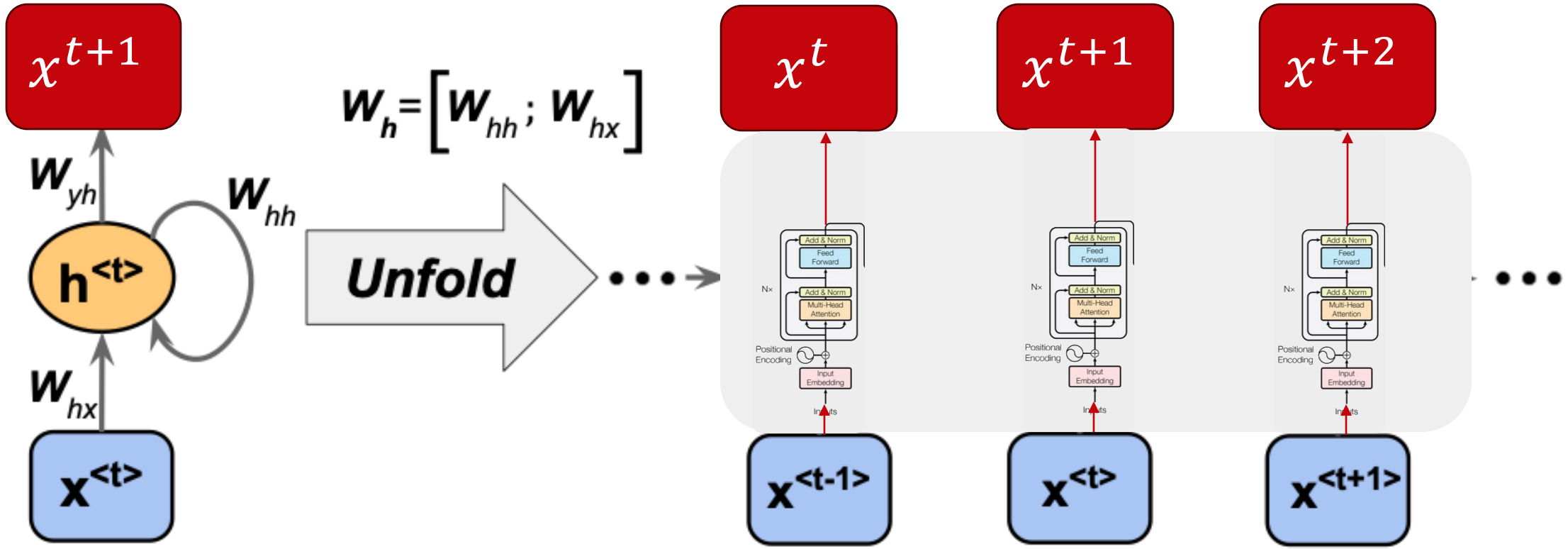
From RNN…to GPT…by Transformers



Vaswani, A., Shazeer, N., Parmar, N., Uszkoreit, J., Jones, L., Gomez, A.N., Kaiser, L. and Polosukhin, I., 2017. Attention Is All You Need.

Image source: Sebastian Raschka, Vahid Mirjalili. Python Machine Learning. 3rd Edition. Packt, 2019

From RNN…to GPT…by Transformers



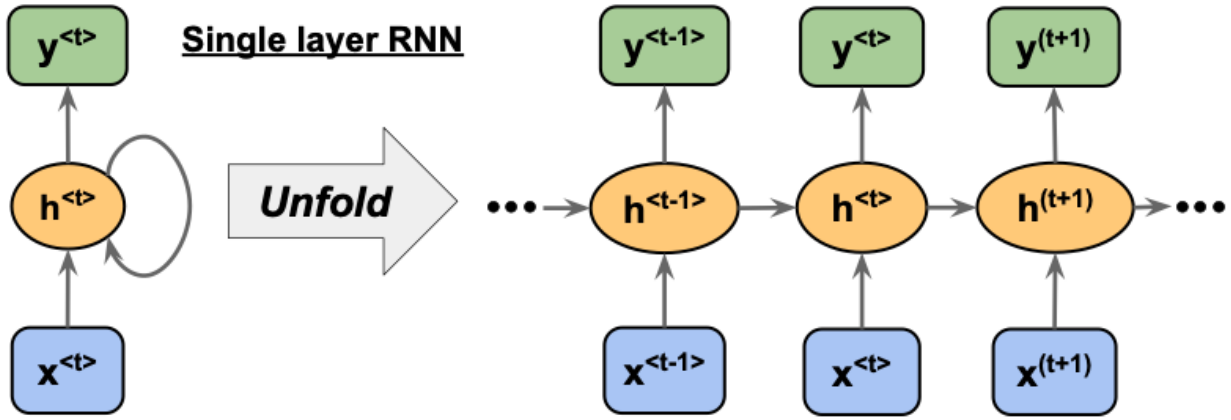
Vaswani, A., Shazeer, N., Parmar, N., Uszkoreit, J., Jones, L., Gomez, A.N., Kaiser, L. and Polosukhin, I., 2017. Attention Is All You Need.

Image source: Sebastian Raschka, Vahid Mirjalili. Python Machine Learning. 3rd Edition. Packt, 2019

The Attention Mechansism

Why Attention?

- Consider machine translation:
  - Do we really need the whole sequence to translate each word?
  - Where is **the** library? →
    - Donde esta **la** biblioteca?
  - Where is **the** huge public library? →
    - Donde esta **la** enorme biblioteca publica?
- Problem: RNNs compress all information into a fixed-length vector. Long-range dependencies are tricky.



“Attention”

- Originally developed for language translation:
  Bahdanau, D., Cho, K., & Bengio, Y. (2014). Neural machine translation by jointly learning to align and translate. https://arxiv.org/abs/1409.0473
- *"... allowing a model to automatically (soft-)search for parts of a source sentence that are relevant to predicting a target word ..."*

"traditional"
encoder+decoder
RNN

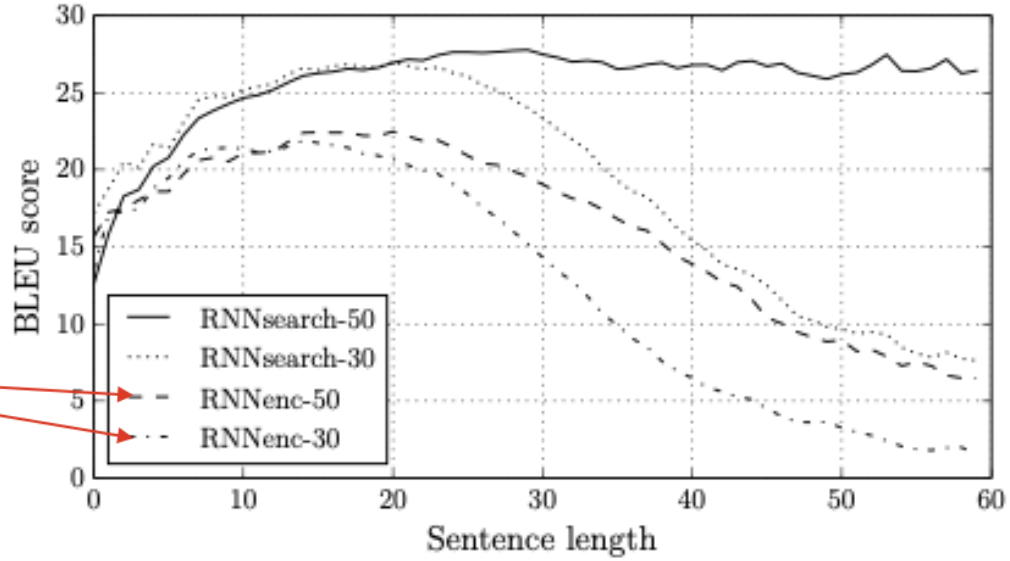


Figure 2: The BLEU scores of the generated translations on the test set with respect to the lengths of the sentences. The results are on the full test set which includes sentences having unknown words to the models.

“Attention”

Main idea:

Assign attention weight to each word, to know how much "attention" the model should pay to each word

“Attention”

Main idea:

Assign attention weight to each word, to know how much "attention" the model should pay to each word

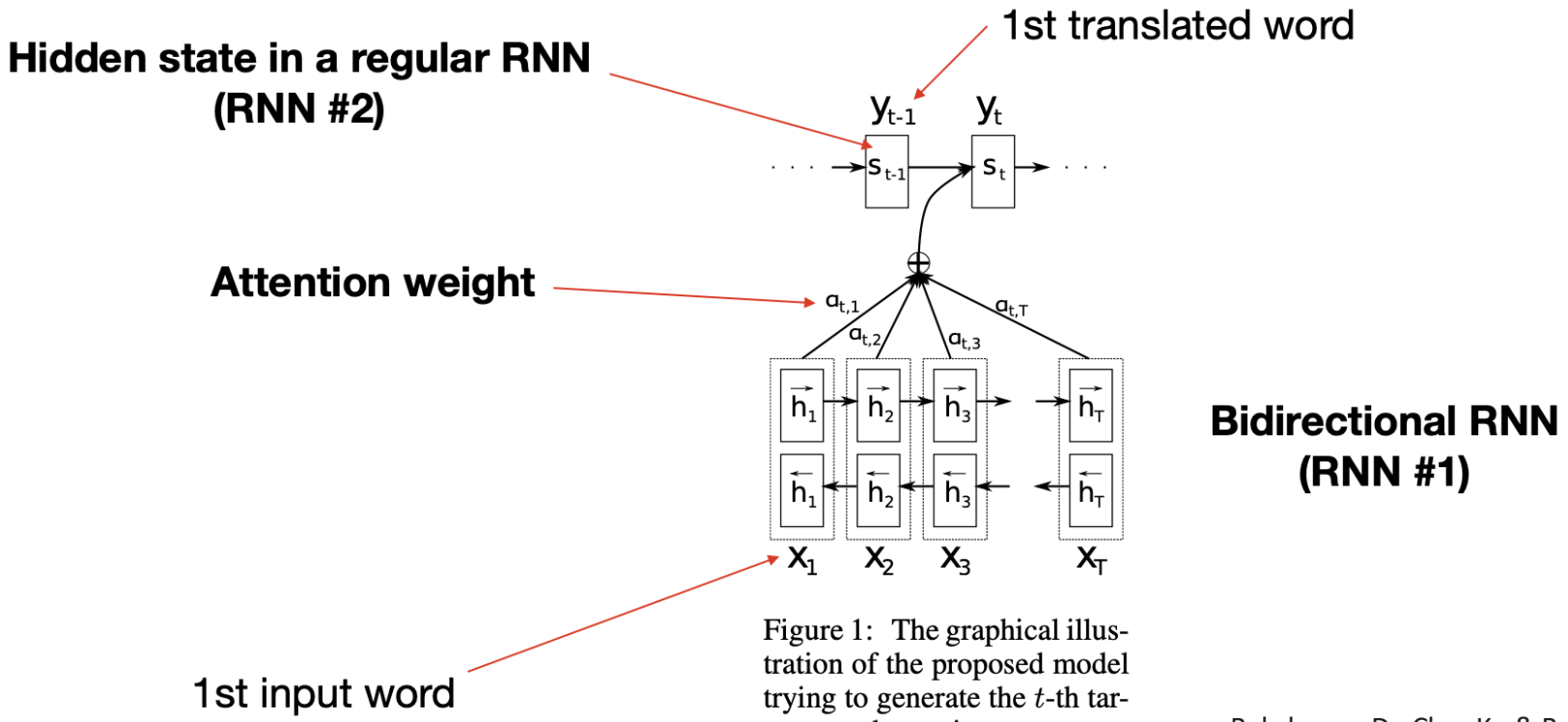


Figure 1: The graphical illustration of the proposed model trying to generate the t-th target word y_t given a source sentence $(x_1, x_2, \ldots, x_T)$.

Bahdanau, D., Cho, K., & Bengio, Y. (2014). Neural machine translation by jointly learning to align and translate. https://arxiv.org/abs/1409.0473

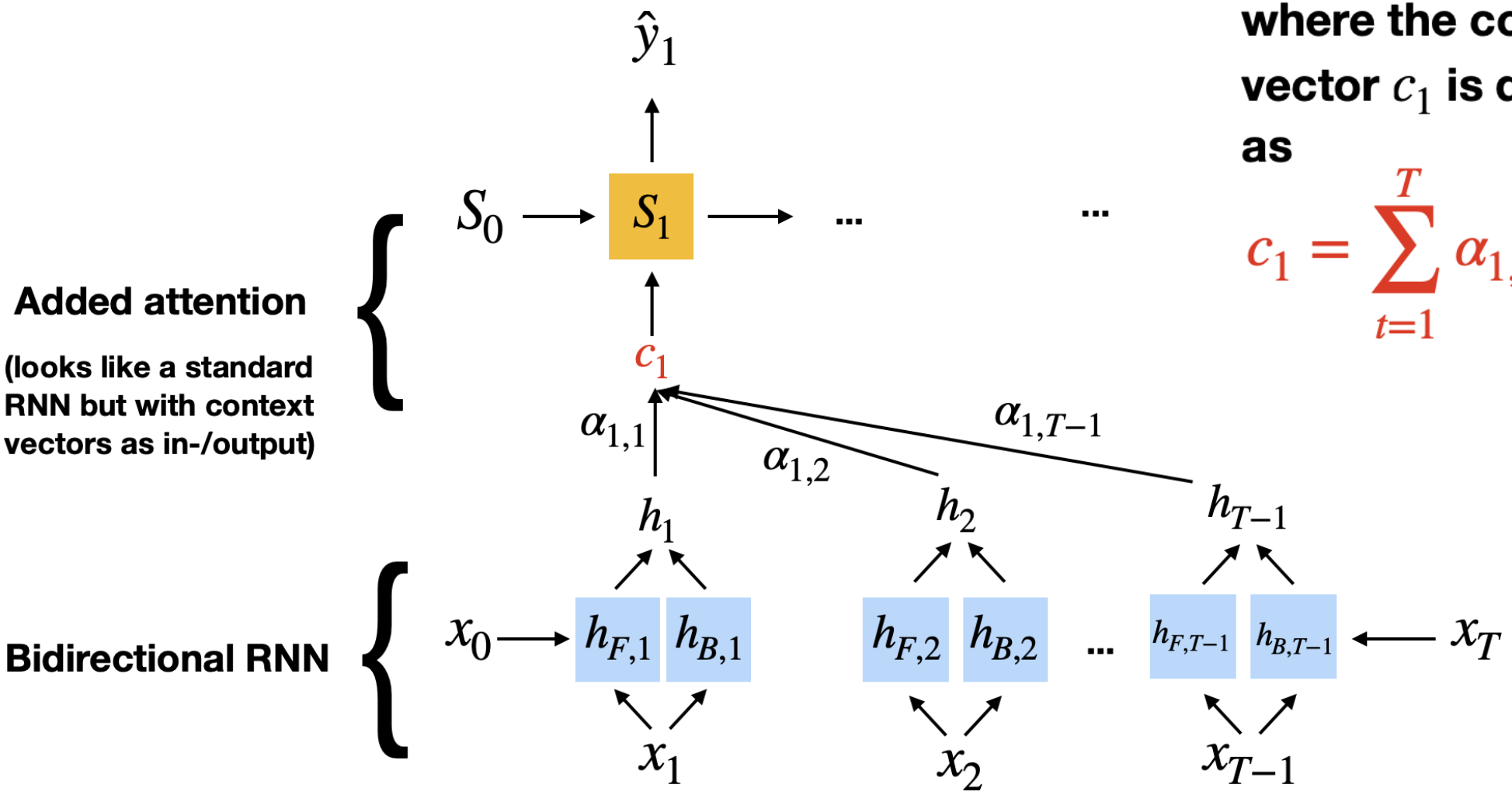
Hard attention?

- Make a zero-one decision about where to attend.
- Problem: Hard to train. Requires methods such as reinforcement learning

Benefit: Interpretable?

Lei et al 2016

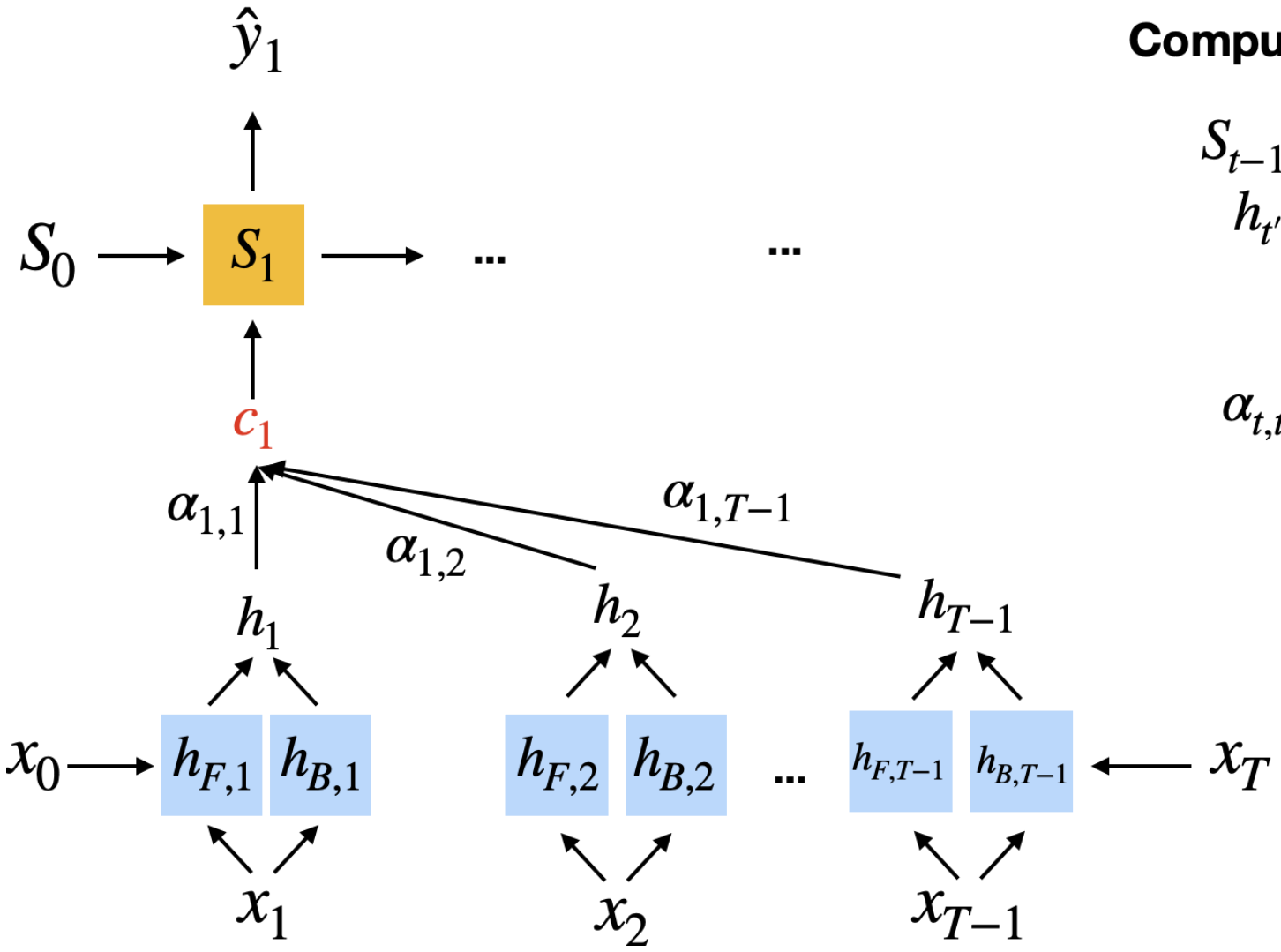
Soft attention



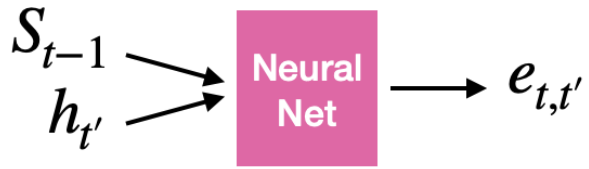
where the context vector c_1 is defined as

$$c_1 = \sum_{t=1}^{T} \alpha_{1,t} \, h_t$$

Soft attention

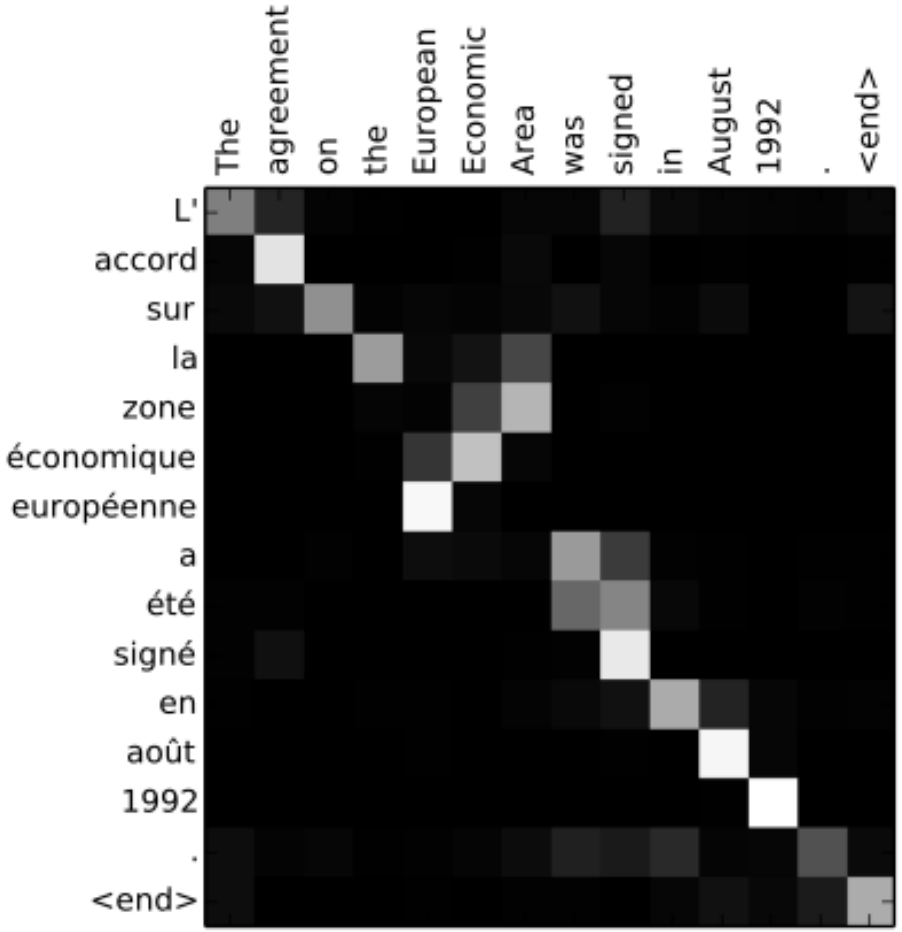


Computing attention weights

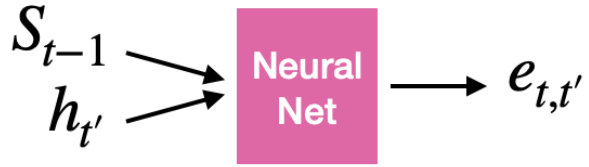


$$\alpha_{t,t'} = \frac{\exp(e_{t,t'})}{\sum_{t'=1}^{T} \exp(e_{t,t'})}$$

Soft attention



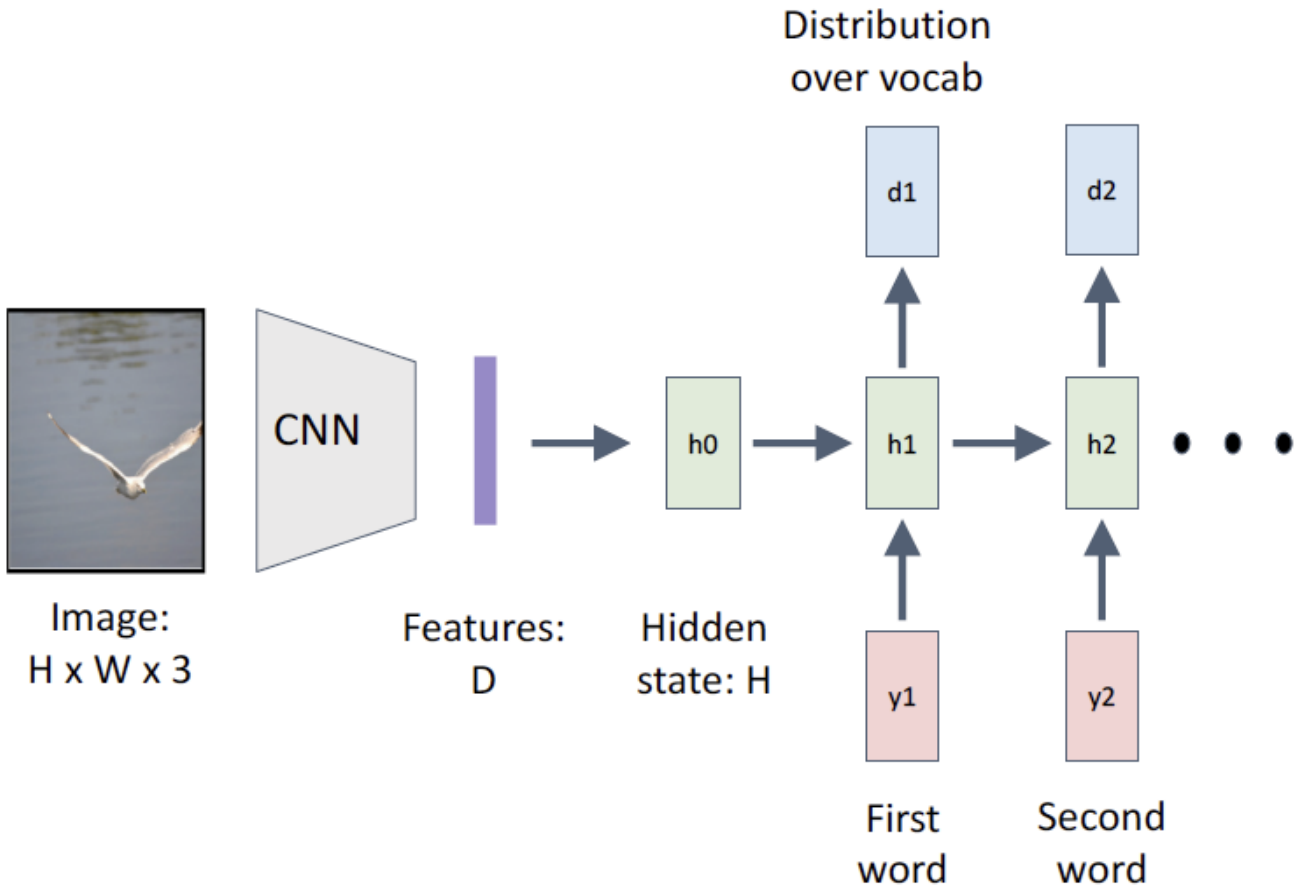
Computing attention weights



$$\alpha_{t,t'} = \frac{\exp(e_{t,t'})}{\sum_{t'=1}^{T} \exp(e_{t,t'})}$$

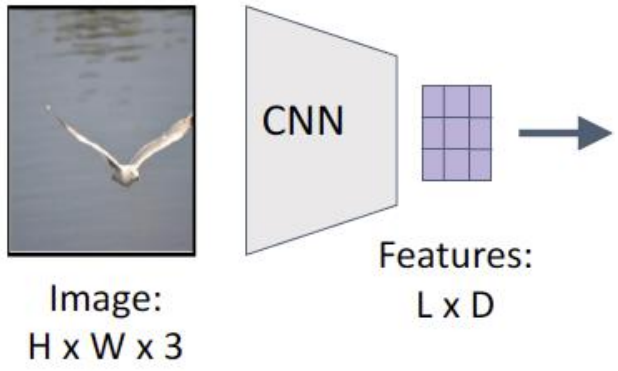
Bahdanau, D., Cho, K., & Bengio, Y. (2014). Neural machine translation by jointly learning to align and translate. https://arxiv.org/abs/1409.0473

Example: Soft Attention for Image Captioning



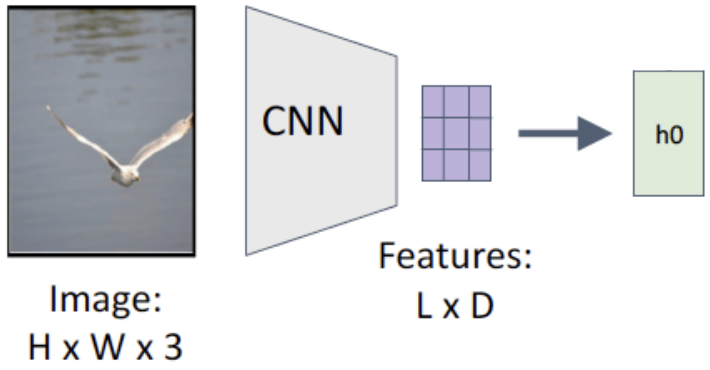
RNN only looks at whole image once…but different parts of the image are important for different parts of the caption.

Example: Soft Attention for Image Captioning



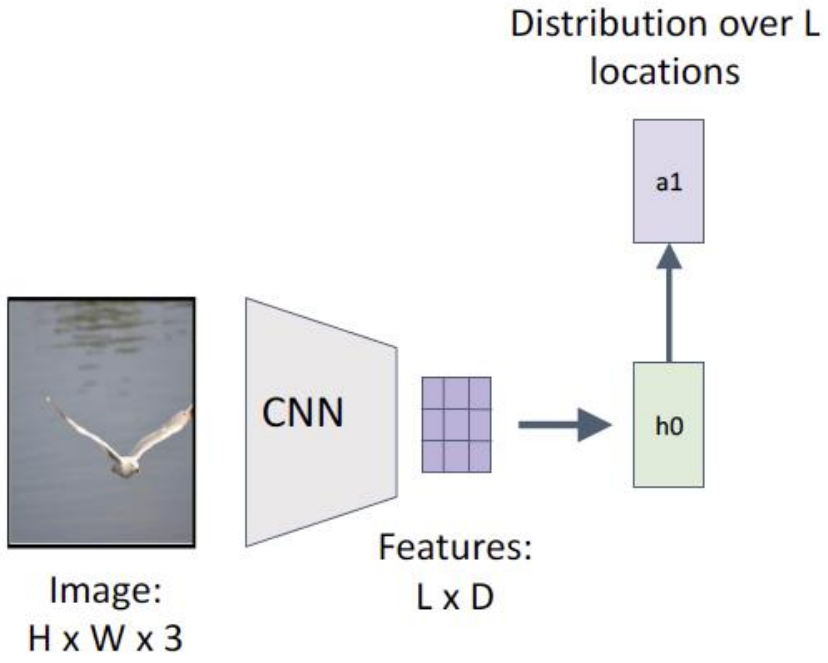
Xu et al, "Show, Attend and Tell: Neural Image Caption Generation with Visual Attention", ICML 2015

Example: Soft Attention for Image Captioning



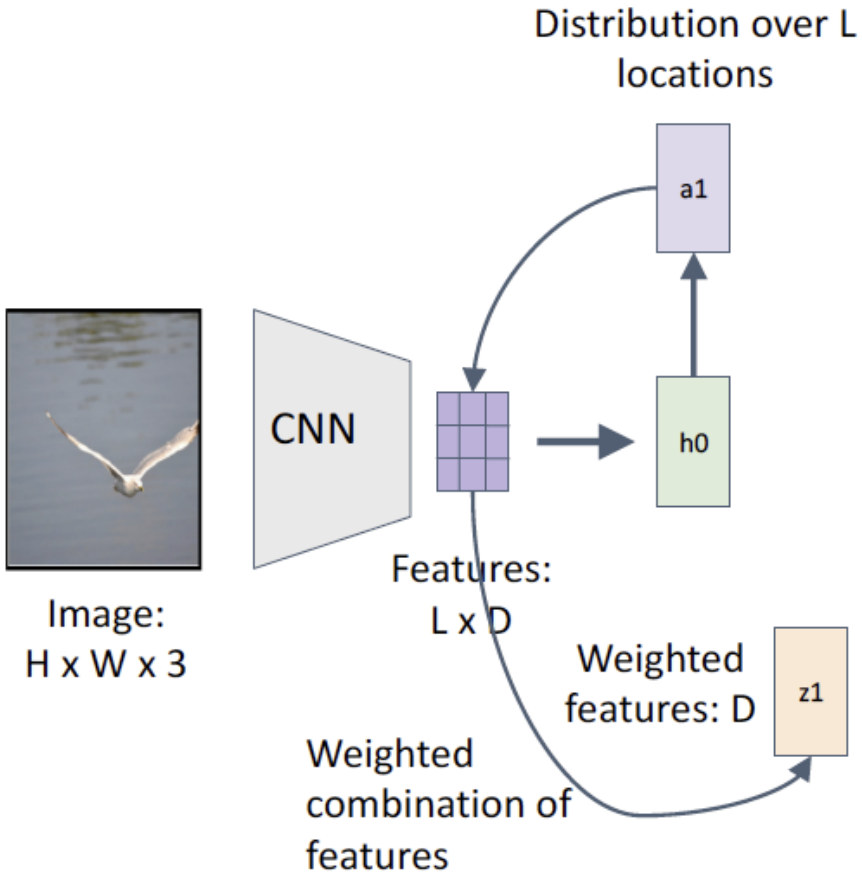
Xu et al, "Show, Attend and Tell: Neural Image Caption Generation with Visual Attention", ICML 2015

Example: Soft Attention for Image Captioning

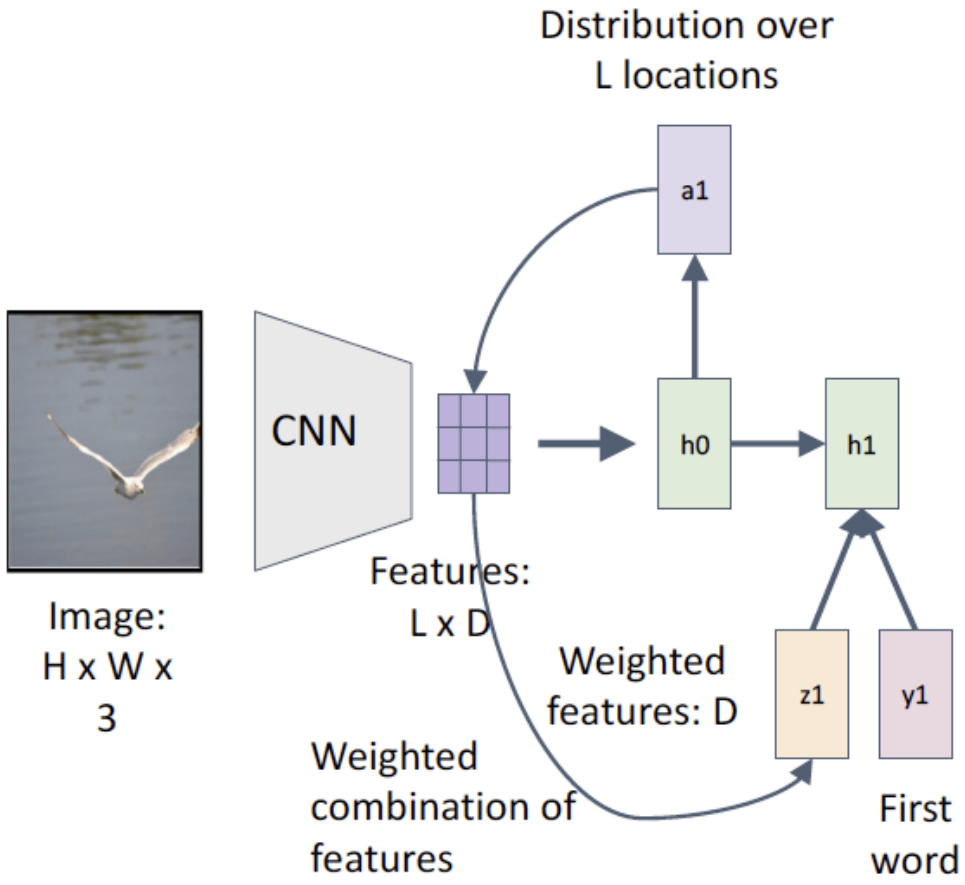


Xu et al, "Show, Attend and Tell: Neural Image Caption Generation with Visual Attention", ICML 2015

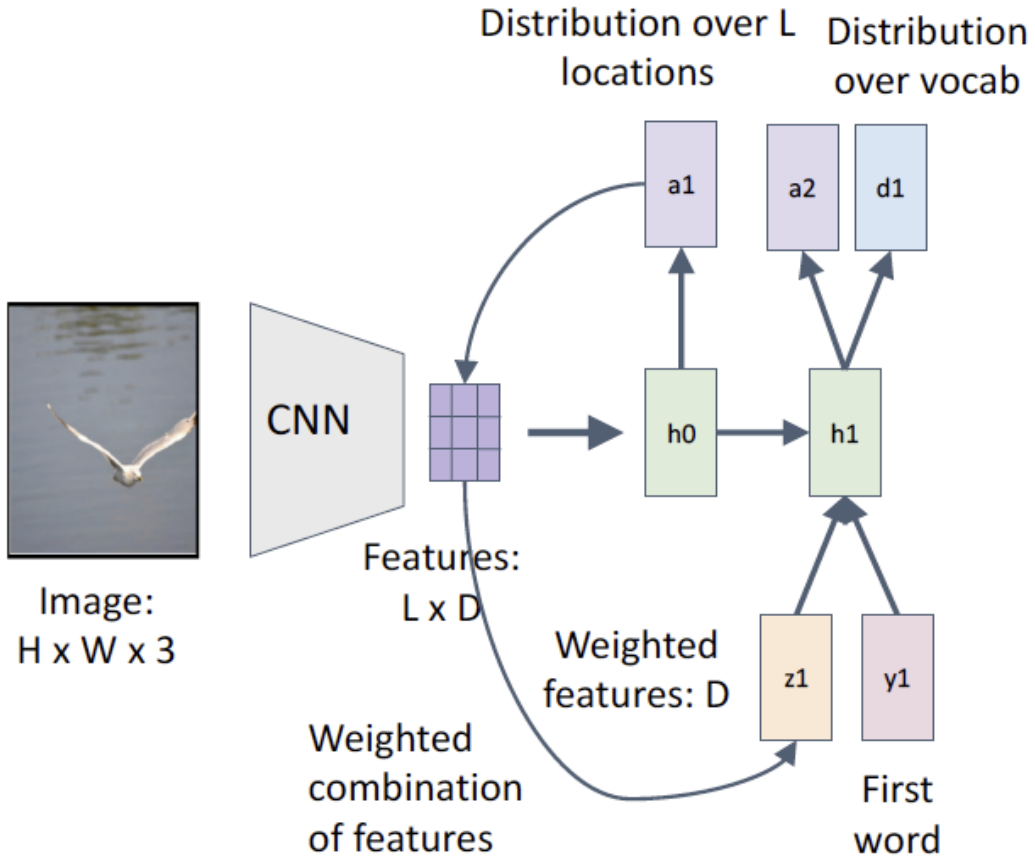
Example: Soft Attention for Image Captioning



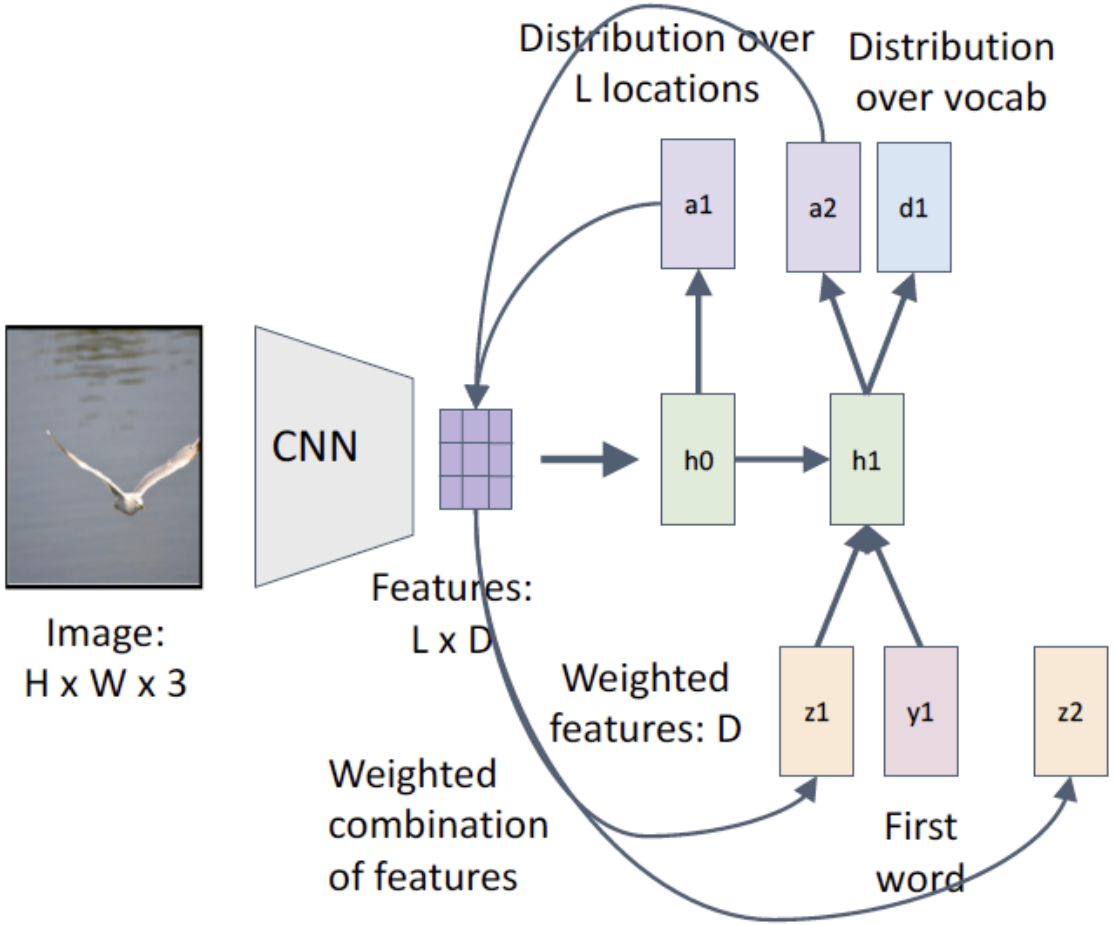
Example: Soft Attention for Image Captioning



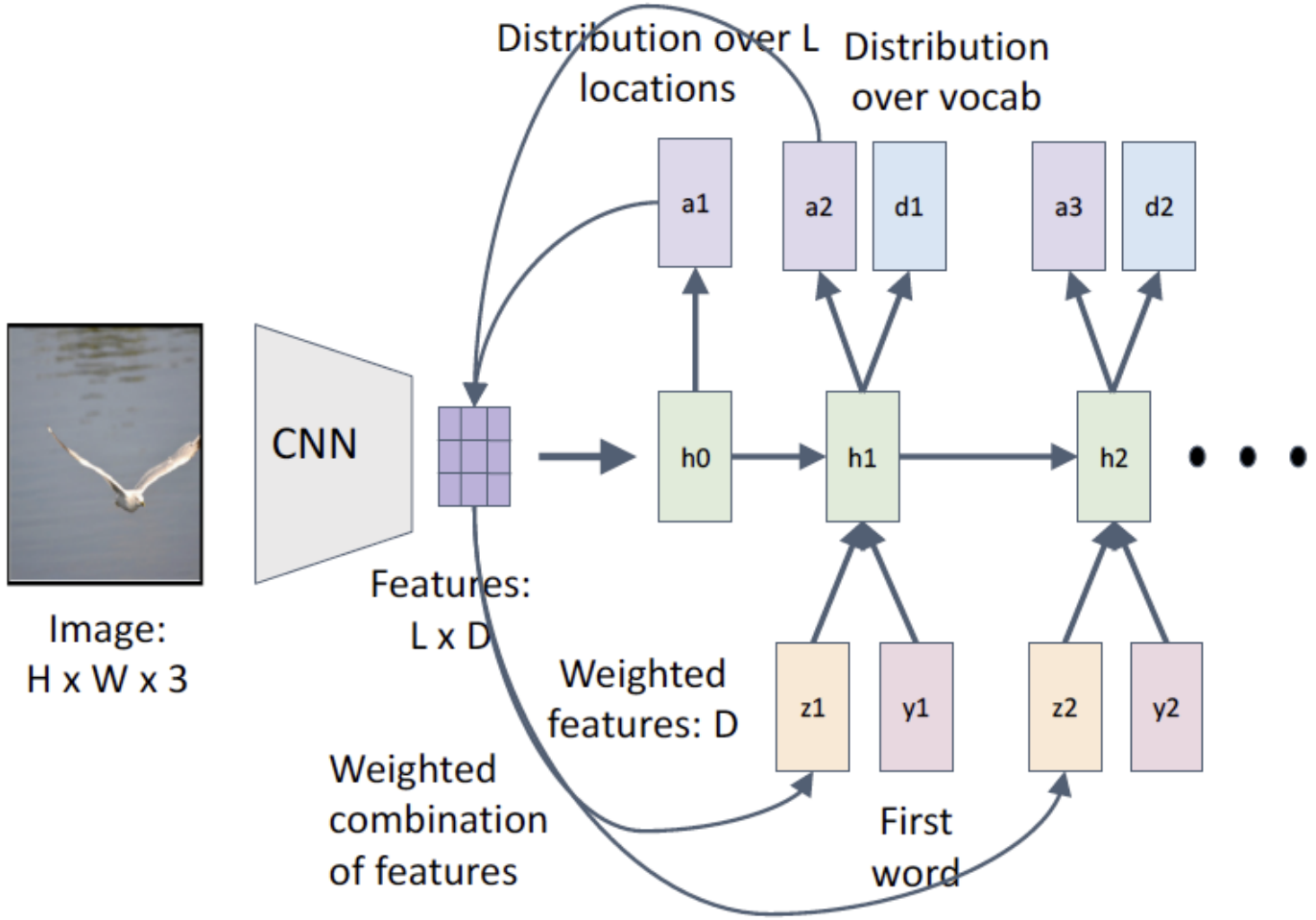
Example: Soft Attention for Image Captioning



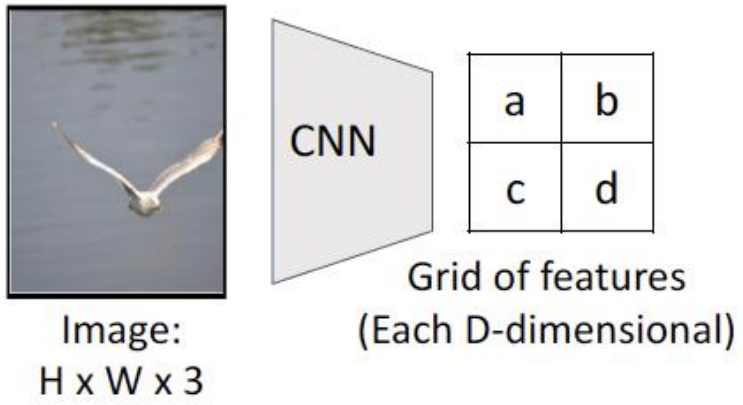
Example: Soft Attention for Image Captioning



Example: Soft Attention for Image Captioning



Aside: CNNs were an example of hard attention



Xu et al, "Show, Attend and Tell: Neural Image Caption Generation with Visual Attention", ICML 2015

Aside: CNNs were an example of hard attention

Image:
H x W x 3

CNN

a	b
c	d

Grid of features
(Each D-dimensional)

Context vector z
(D-dimensional)

From
RNN:

p_a	p_b
p_c	p_d

Distribution over
grid locations
$p_a + p_b + p_c + p_c = 1$

Xu et al, "Show, Attend and Tell: Neural Image Caption Generation with Visual Attention", ICML 2015

Hard attention:
Sample ONE location
according to p, z = that vector

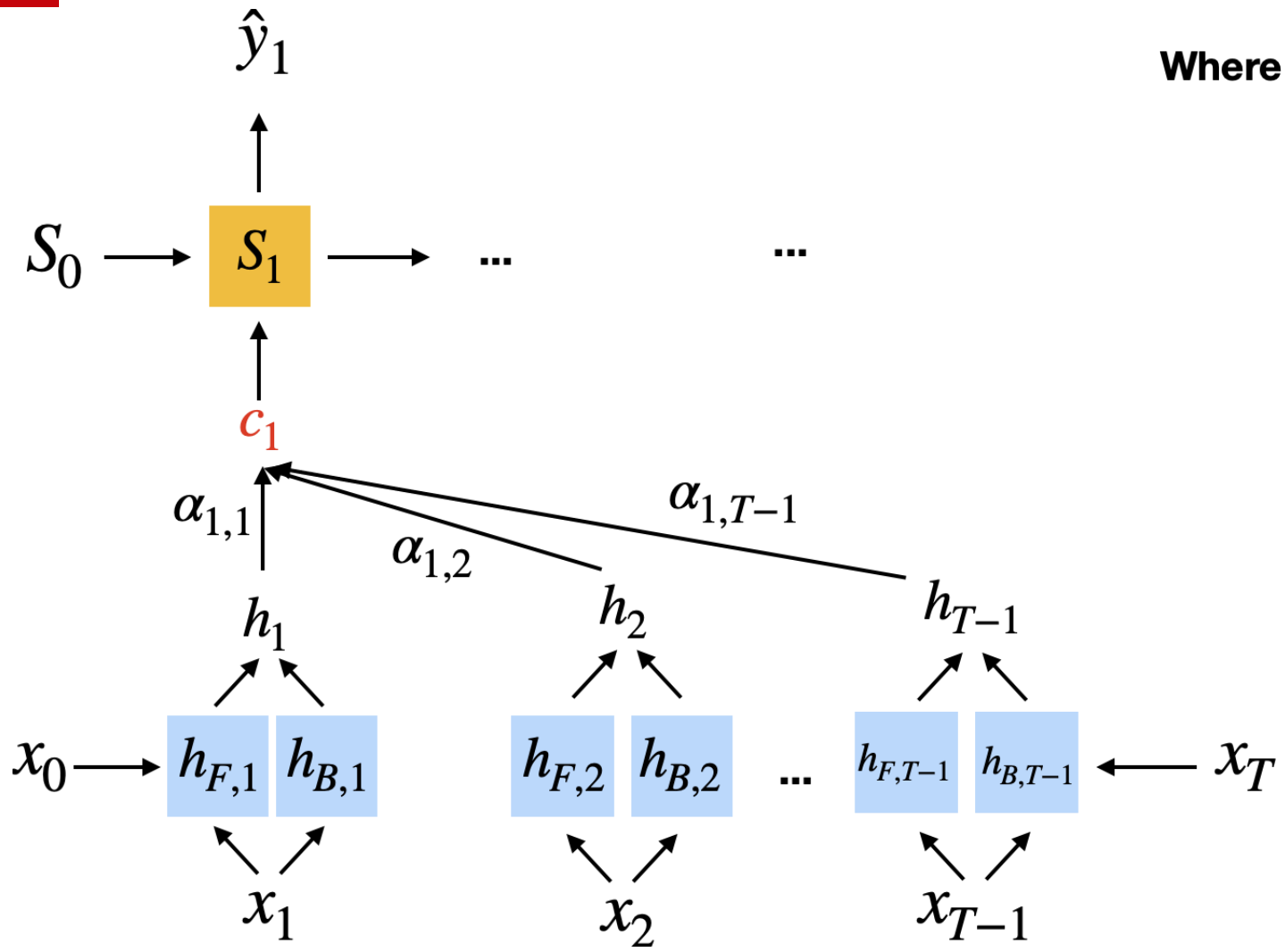
With argmax, dz/dp is zero
almost everywhere …
Can't use gradient descent;
need reinforcement learning

Soft attention:
Summarize ALL locations
$z = p_a a + p_b b + p_c c + p_d d$

Derivative dz/dp is nice!
Train with gradient descent

Self-Attention

”Original” (RNN) Attention Mechanism

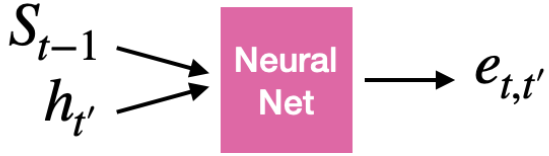


Where the context vector c_1 is defined as

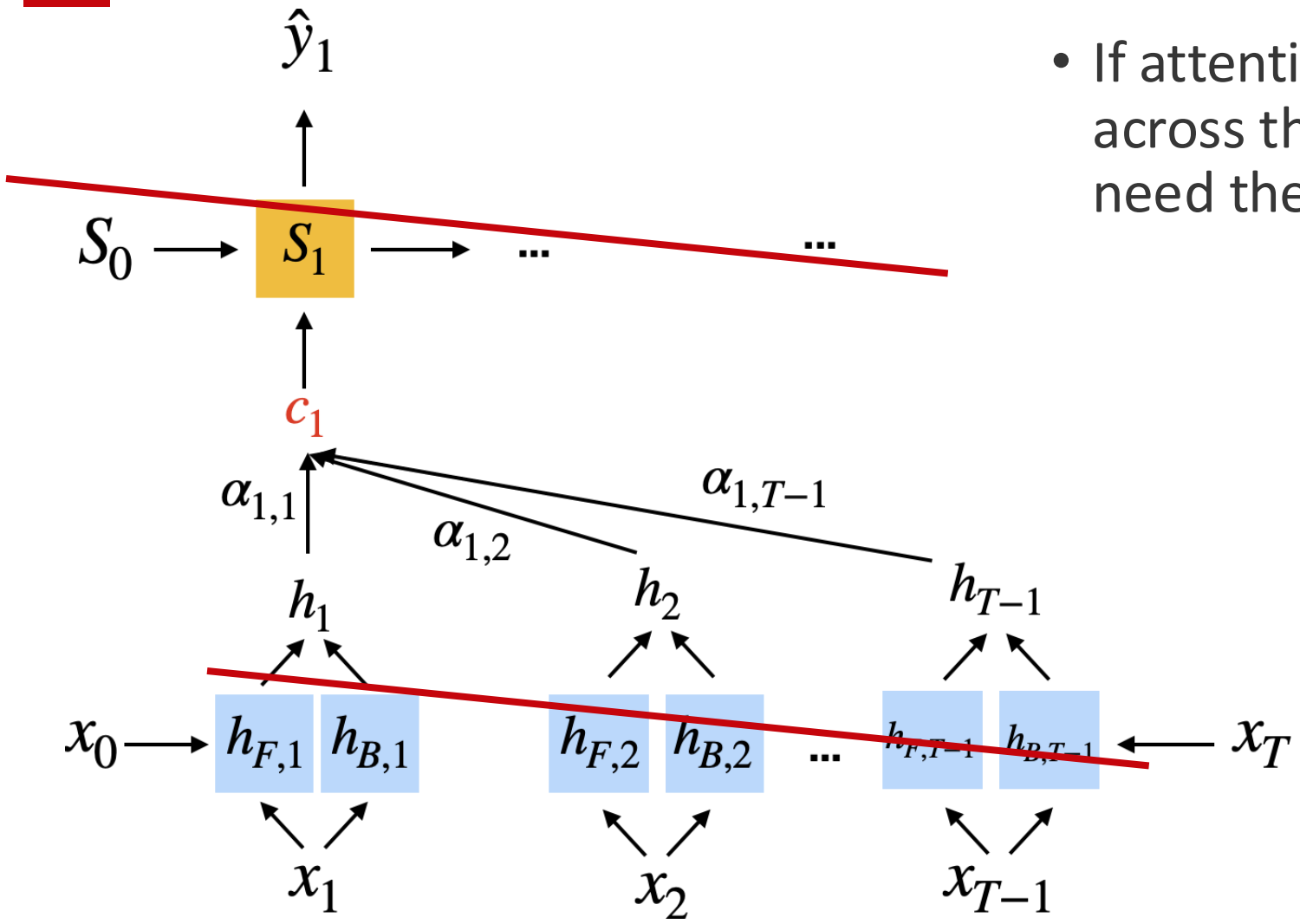
$$c_1 = \sum_{t=1}^{T} \alpha_{1,t}\, h_t$$

And the attention weights are

$$\alpha_{t,t'} = \frac{\exp(e_{t,t'})}{\sum_{t'=1}^{T} \exp(e_{t,t'})}$$



Can we get rid of the sequential parts?



- If attention already ties inputs across the sequence, do we really need the recurrence?

Self-attention (very basic form)

Main procedure:

1) Derive attention weights: similarity between current input and all other inputs (next slide)
2) Normalize weights via softmax (next slide)
3) Compute attention value from normalized weights and corresponding inputs (below)

Self-attention as weighted sum:

$$A_i = \sum_{j=1}^{T} a_{ij} \boldsymbol{x}_j$$

output corresponding to the i-th input

weight based on similarity between current input $\boldsymbol{x}_i$ and all other inputs

Self-attention (very basic form)

Self-attention as weighted sum:

$$A_i = \sum_{j=0}^{T} a_{ij} x_j$$

output corresponding to the i-th input

weight based on similarity between current input x_i and all other inputs

How to compute the attention weights?

here as simple dot product:

$$e_{ij} = x_i^\top x_j$$

repeat this for all inputs $j \in \{1 \ldots T\}$, then normalize

$$a_{ij} = \frac{\exp\left(e_{ij}\right)}{\sum_{j=1}^{T} \exp\left(e_{ij}\right)} = \text{softmax}\left(\left[e_{ij}\right]_{j=1\ldots T}\right)$$

Self-attention (very basic form)

No learnable parameters?

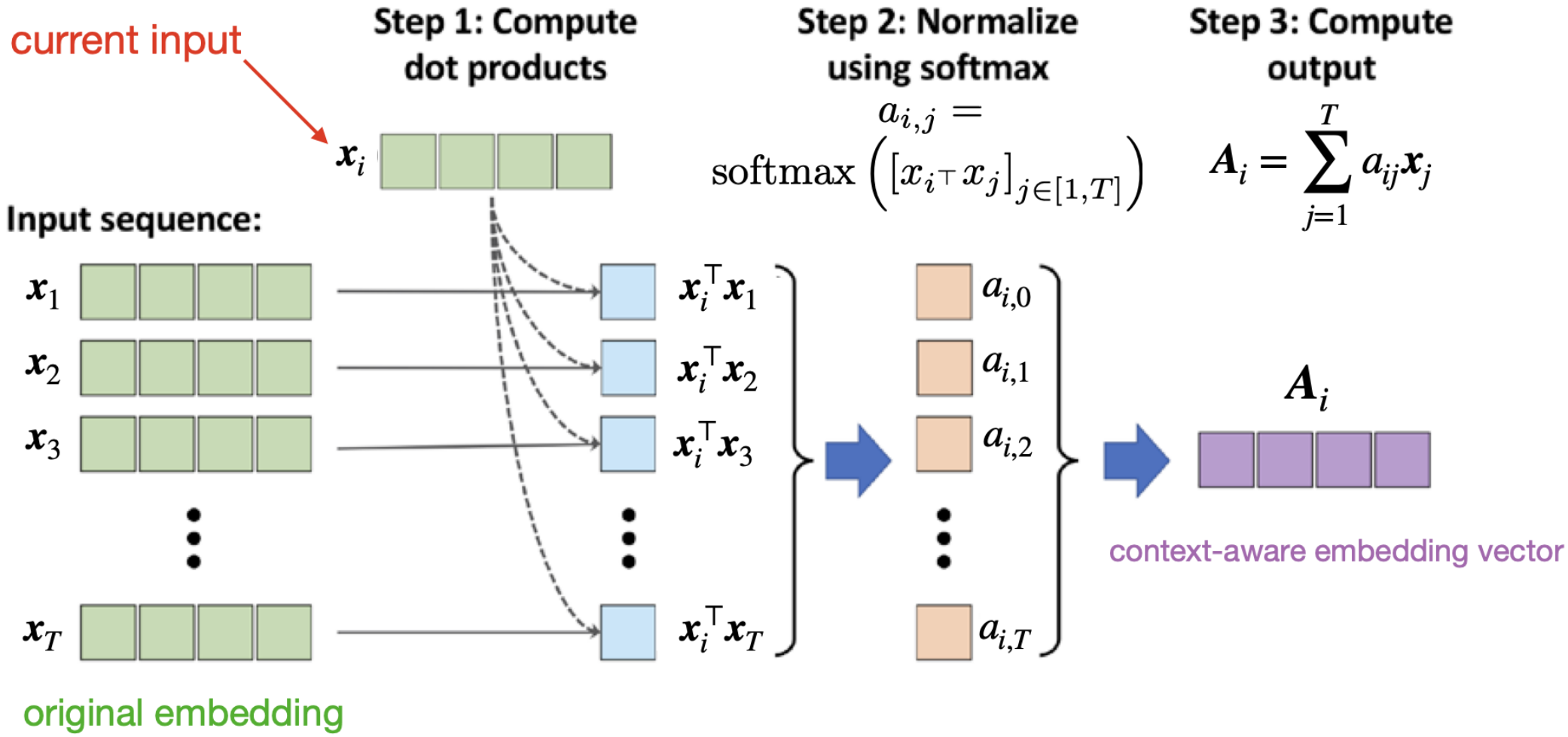


Image source: Raschka & Mirjalili 2019. Python Machine Learning, 3rd edition

Learnable Self-attention

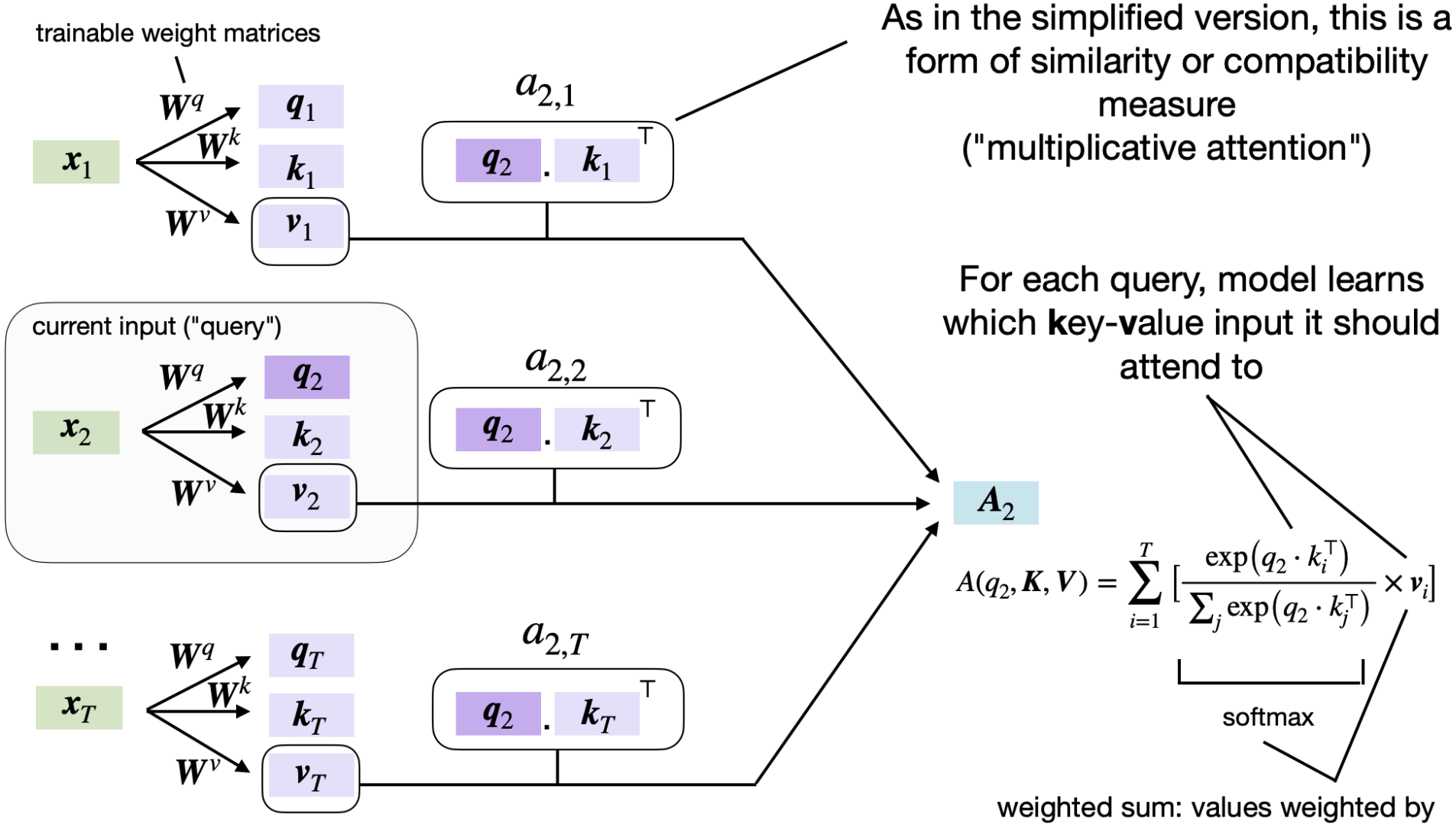
- Previous basic version did not involve any learnable parameters, so not very useful for learning a language model
- We are now adding 3 trainable weight matrices that are multiplied with the input sequence embeddings

$$\text{query} = \boldsymbol{W}^{q}\boldsymbol{x}_i$$

$$\text{key} = \boldsymbol{W}^{k}\boldsymbol{x}_i$$

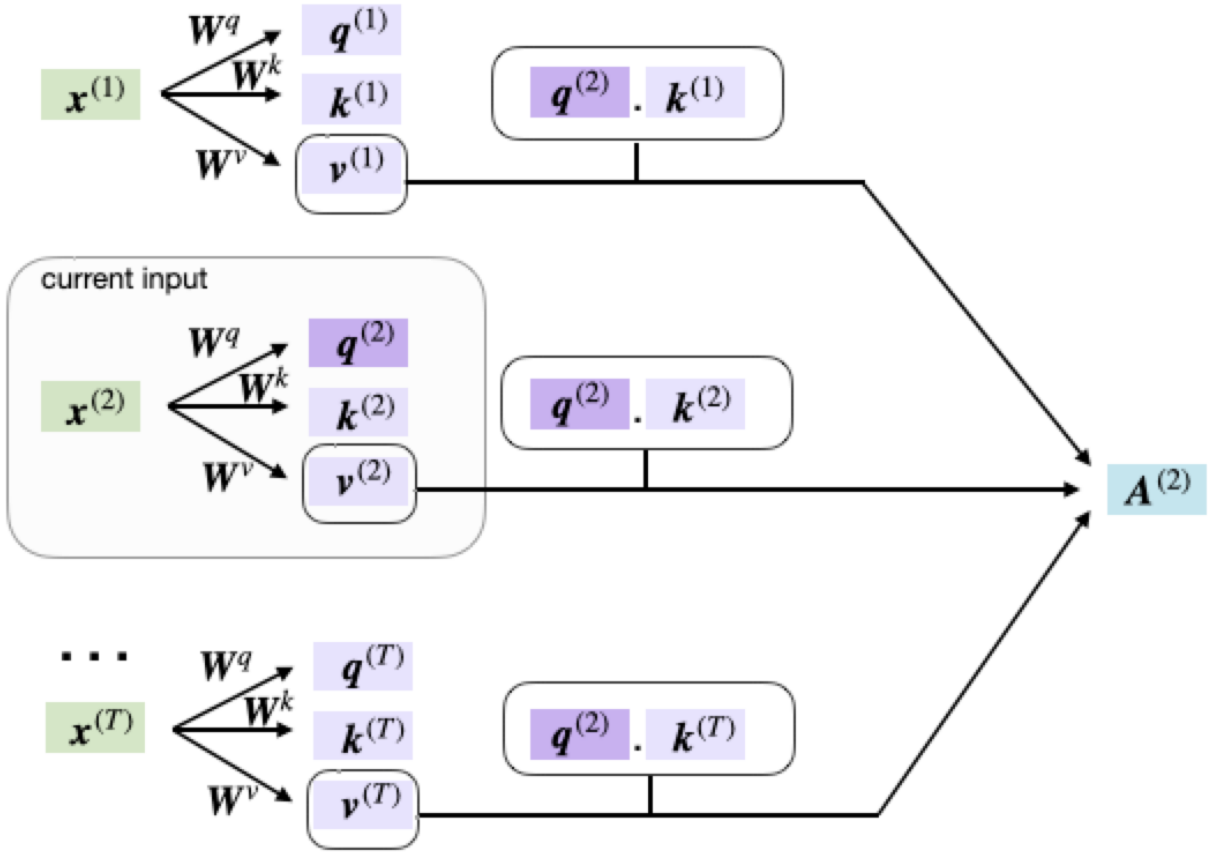
$$\text{value} = \boldsymbol{W}^{v}\boldsymbol{x}_i$$

Learnable Self-attention



Learnable Self-attention

"self"-attention because input to query and key-value pair are the same

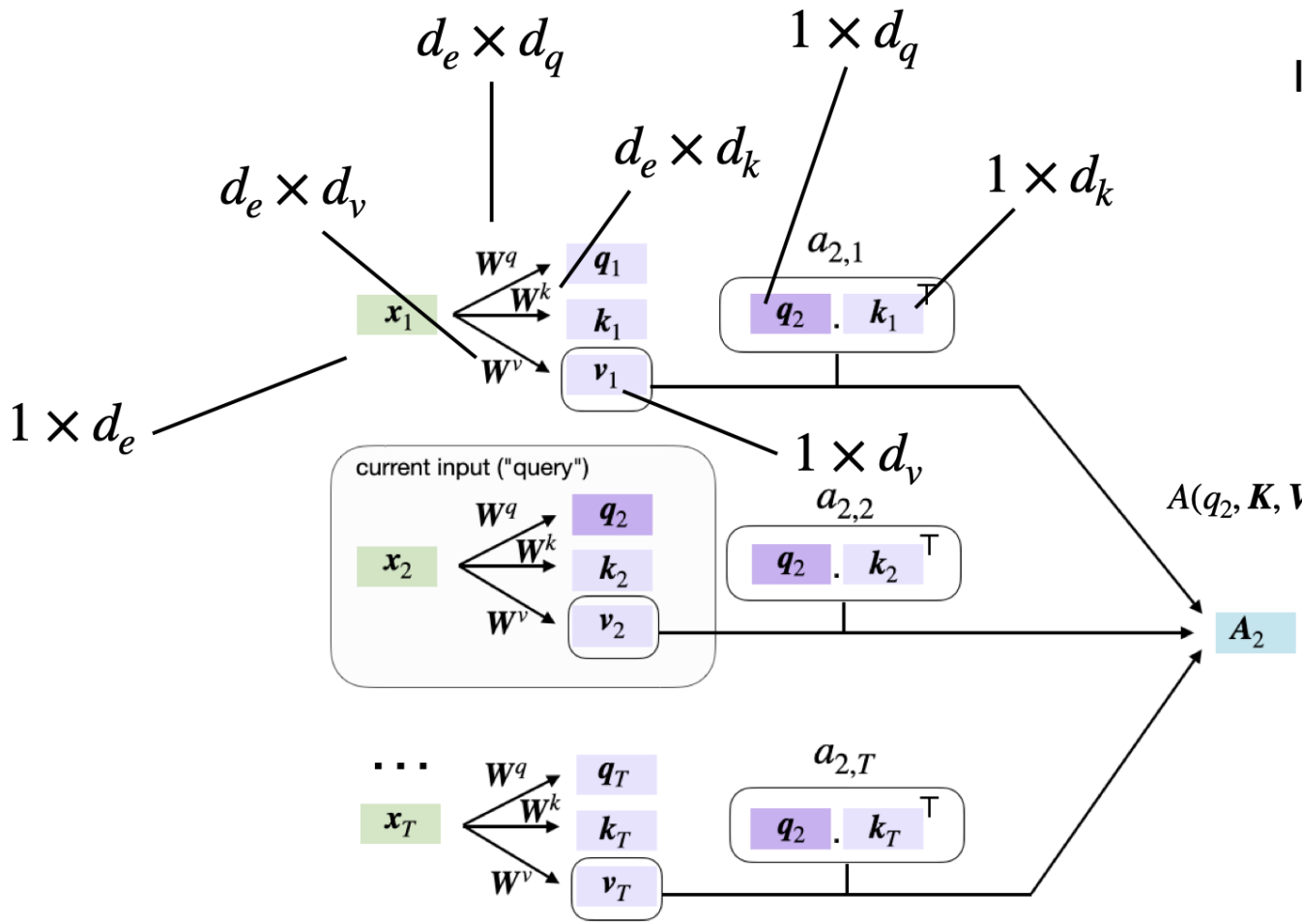


Learnable Self-attention

d_e = embedding size (original transformer = 512)

where $d_q = d_k$

In original transformer, $d_q = d_v$ as well



$$A(q_2, \boldsymbol{K}, \boldsymbol{V}) = \sum_{i=1}^{T} \left[\frac{\exp(q_2 \cdot k_i^\top)}{\sum_j \exp(q_2 \cdot k_j^\top)} \times \boldsymbol{v}_i \right]$$

softmax

1×1

$1 \times d_v$

At the end of the day…

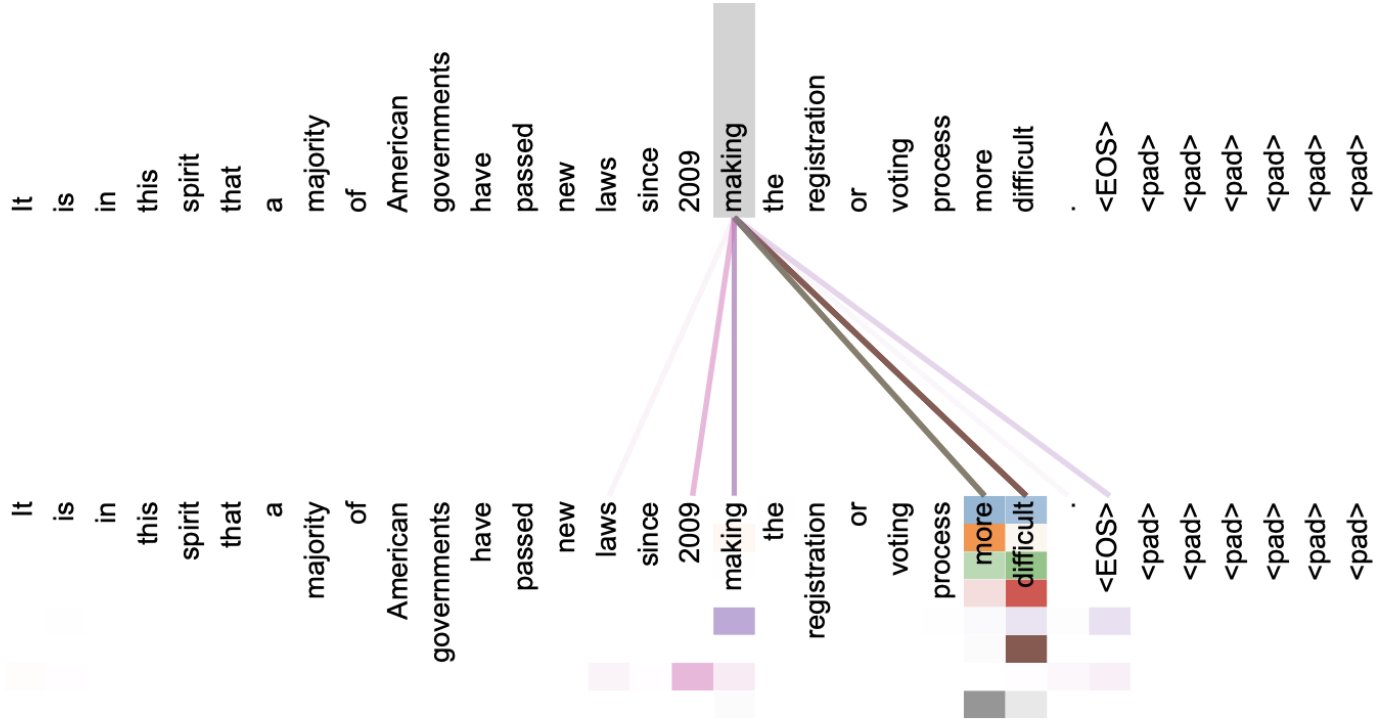


Figure 3: An example of the attention mechanism following long-distance dependencies in the encoder self-attention in layer 5 of 6. Many of the attention heads attend to a distant dependency of the verb 'making', completing the phrase 'making...more difficult'. Attentions here shown only for the word 'making'. Different colors represent different heads. Best viewed in color.

Vaswani, A., Shazeer, N., Parmar, N., Uszkoreit, J., Jones, L., Gomez, A. N., ... & Polosukhin, I. (2017). Attention is all you need. In *Advances in neural information processing systems* (pp. 5998-6008).

The ”Transformer”

Attention Is All You Need

Ashish Vaswani* Google Brain avaswani@google.com

Noam Shazeer* Google Brain noam@google.com

Niki Parmar* Google Research nikip@google.com

Jakob Uszkoreit* Google Research usz@google.com

Llion Jones* Google Research llion@google.com

Aidan N. Gomez* † University of Toronto aidan@cs.toronto.edu

Łukasz Kaiser* Google Brain lukaszkaiser@google.com

Illia Polosukhin* ‡ illia.polosukhin@gmail.com

Attention is all you need

A Vaswani, N Shazeer, N Parmar… - Advances in neural …, 2017 - proceedings.neurips.cc

… to attend to **all** positions in the decoder up to and including that position. **We need** to prevent … **We** implement this inside of scaled dot-product **attention** by masking out (setting to $-\infty$) …

☆ Save 99 Cite Cited by 174852 Related articles All 73 versions »

https://arxiv.org/abs/1706.03762

The Transformer

The ”Transformer”

Attention Is All You Need

Ashish Vaswani* Google Brain avaswani@google.com

Noam Shazeer* Google Brain noam@google.com

Niki Parmar* Google Research nikip@google.com

Jakob Uszkoreit* Google Research usz@google.com

Llion Jones* Google Research llion@google.com

Aidan N. Gomez* † University of Toronto aidan@cs.toronto.edu

Łukasz Kaiser* Google Brain lukaszkaiser@google.com

Illia Polosukhin* ‡ illia.polosukhin@gmail.com

Attention is all you need

A Vaswani, N Shazeer, N Parmar… - Advances in neural …, 2017 - proceedings.neurips.cc

… to attend to **all** positions in the decoder up to and including that position. **We need** to prevent … **We** implement this inside of scaled dot-product **attention** by masking out (setting to $-\infty$) …

☆ Save 99 Cite Cited by 174852 Related articles All 73 versions »

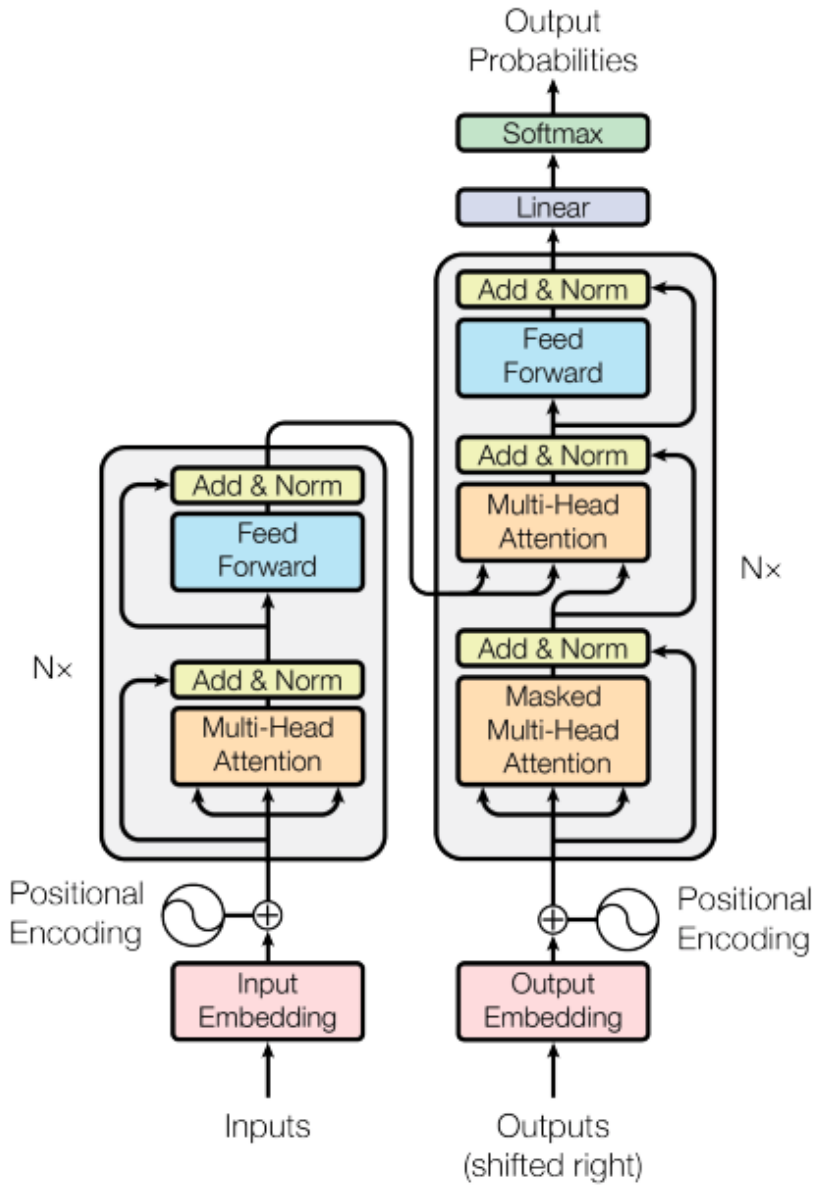
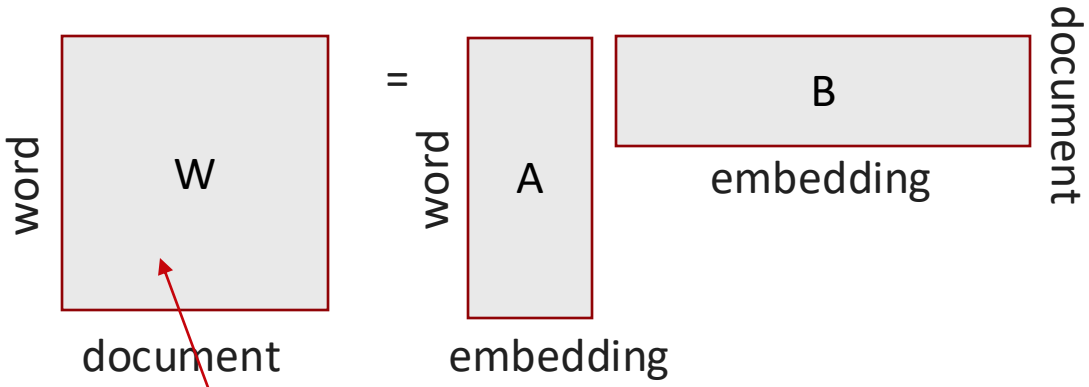


Figure 1: The Transformer - model architecture.

Start with word embeddings…

- Lookup table that translates words (or more formally ”tokens”) into continuous-valued “embeddings”
- Simplest form: random embeddings
- Slightly better: TF-IDF embeddings
- Many ways to improve pre-trained embeddings



$$w_{x,y} = tf_{x,y} \times \log\left(\frac{N}{df_x}\right)$$

TF-IDF

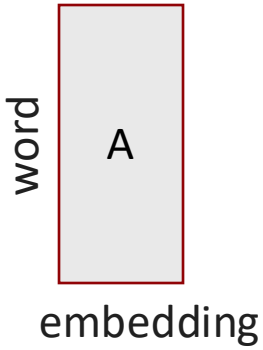
Term x within document y

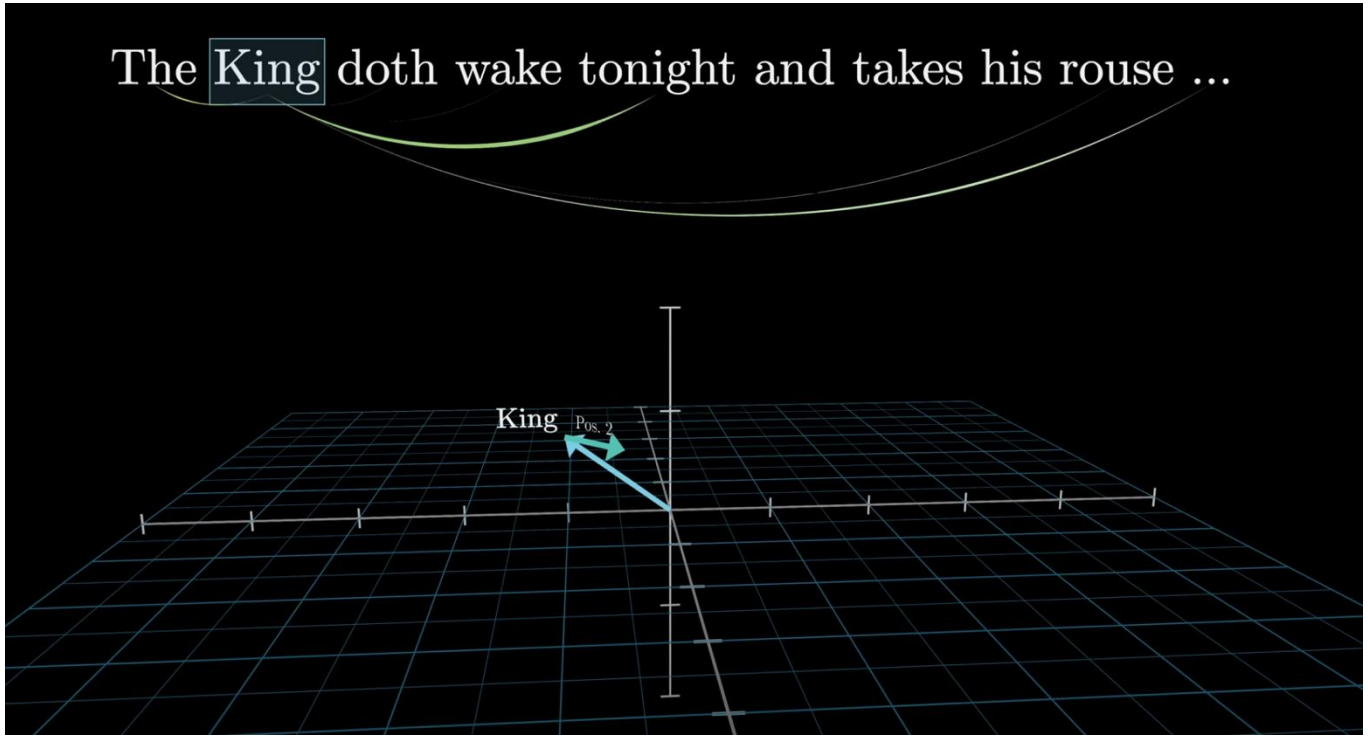
$tf_{x,y}$ = frequency of x in y

df_x = number of documents containing x

N = total number of documents

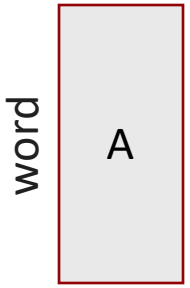
Start with word embeddings…

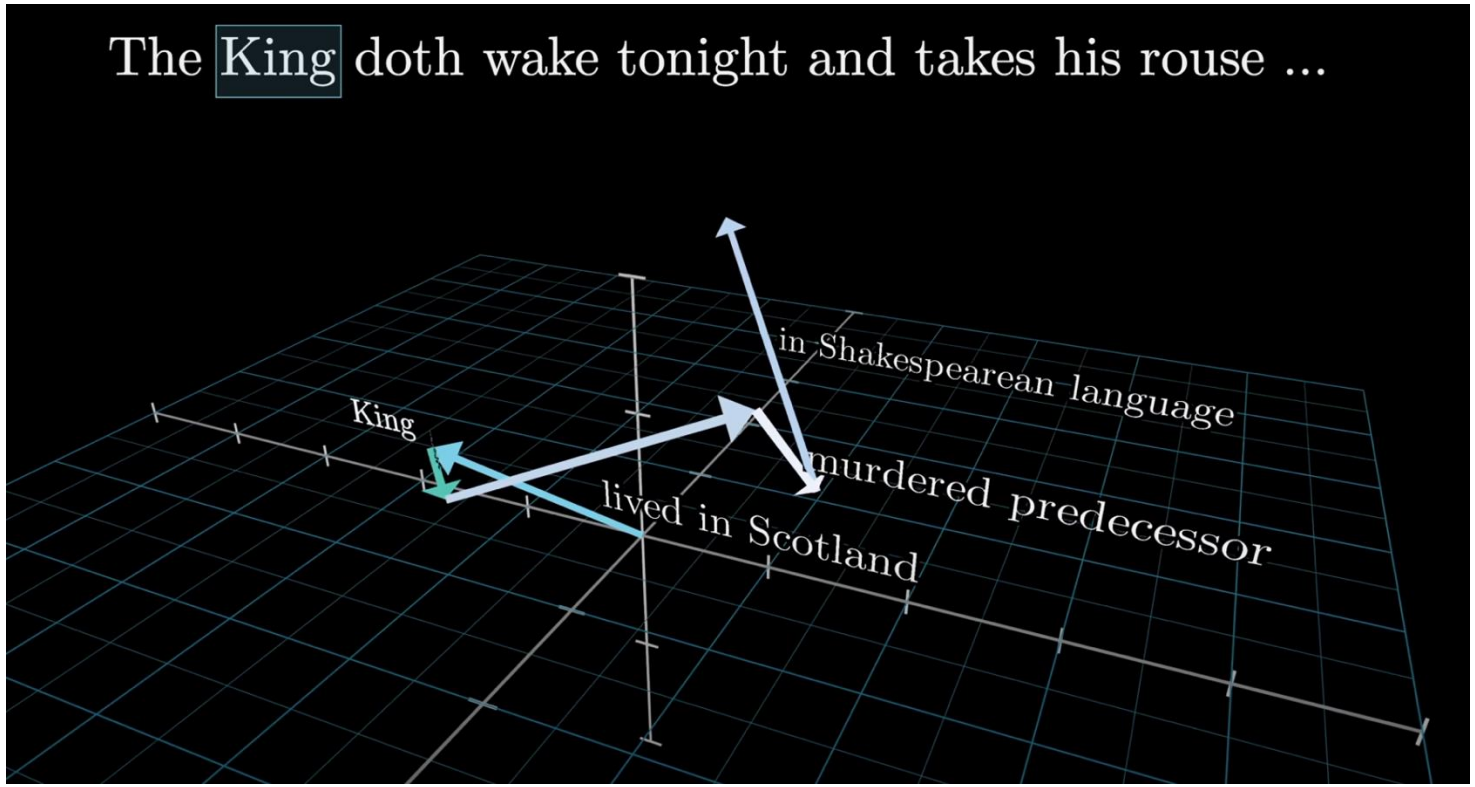




3Blue1Brown "Attention in Transformers"

Update embeddings by context





3Blue1Brown "Attention in Transformers"

Multi-headed Attention

- Apply self-attention multiple times in parallel (similar to multiple kernels for channels in CNNs)
- For each head (self-attention layer), use different , then concatenate the results,
- 8 attention heads in the original transformer
- Allows attending to different parts in the sequence differently

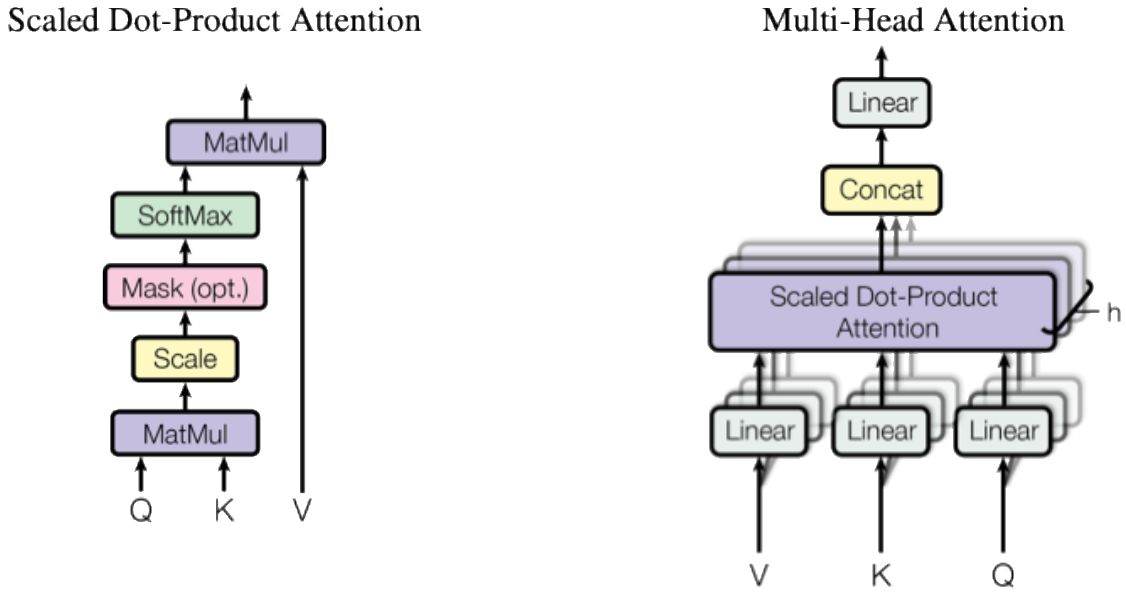
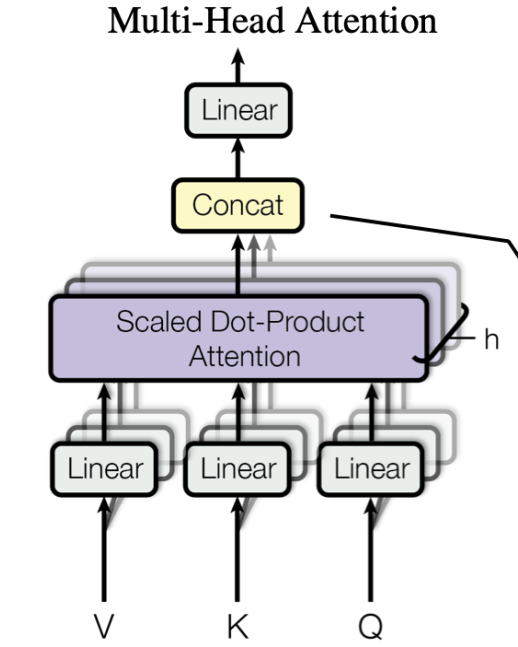


Figure 2: (left) Scaled Dot-Product Attention. (right) Multi-Head Attention consists of several attention layers running in parallel.

Vaswani, A., Shazeer, N., Parmar, N., Uszkoreit, J., Jones, L., Gomez, A.N., Kaiser, L. and Polosukhin, I., 2017. Attention Is All You Need.

Multi-headed Attention



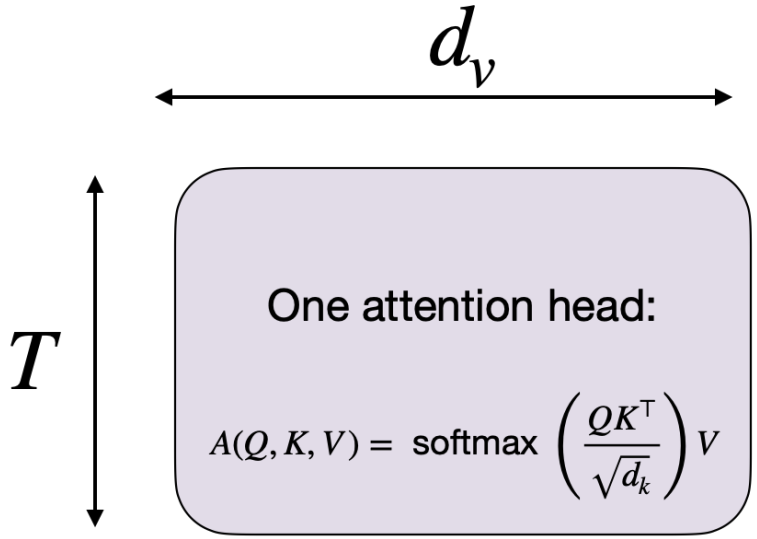
Vaswani, A., Shazeer, N., Parmar, N., Uszkoreit, J., Jones, L., Gomez, A.N., Kaiser, L. and Polosukhin, I., 2017. Attention Is All You Need.

Input sequence dim.
in original transformer:

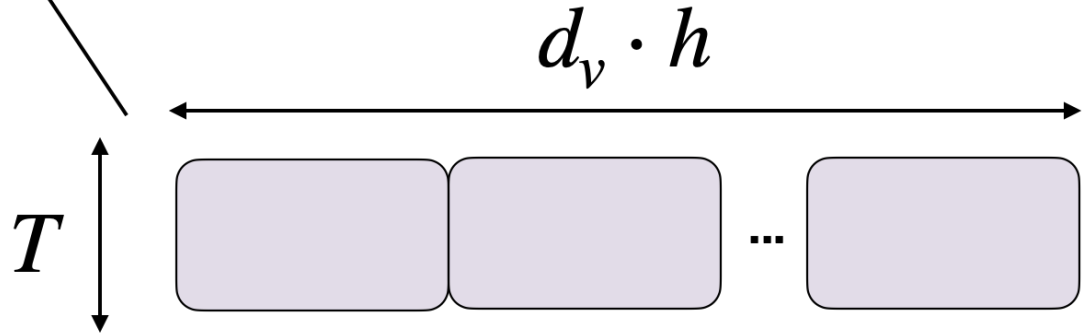
$T \times d_e = T \times 512$

and

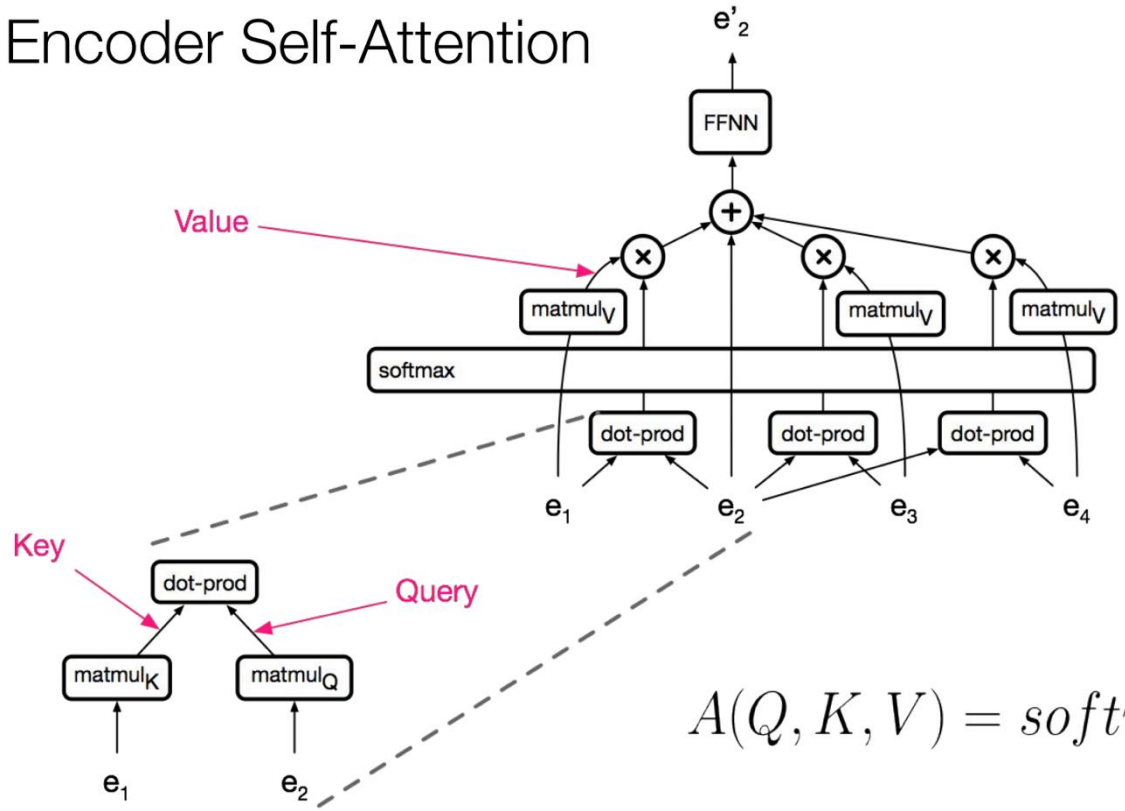
$d_v = 512/h = 64$



Concatenated:



The ”Transformer”: Encoder



$$A(Q,K,V) = softmax(\frac{QK^T}{\sqrt{d_k}})V$$

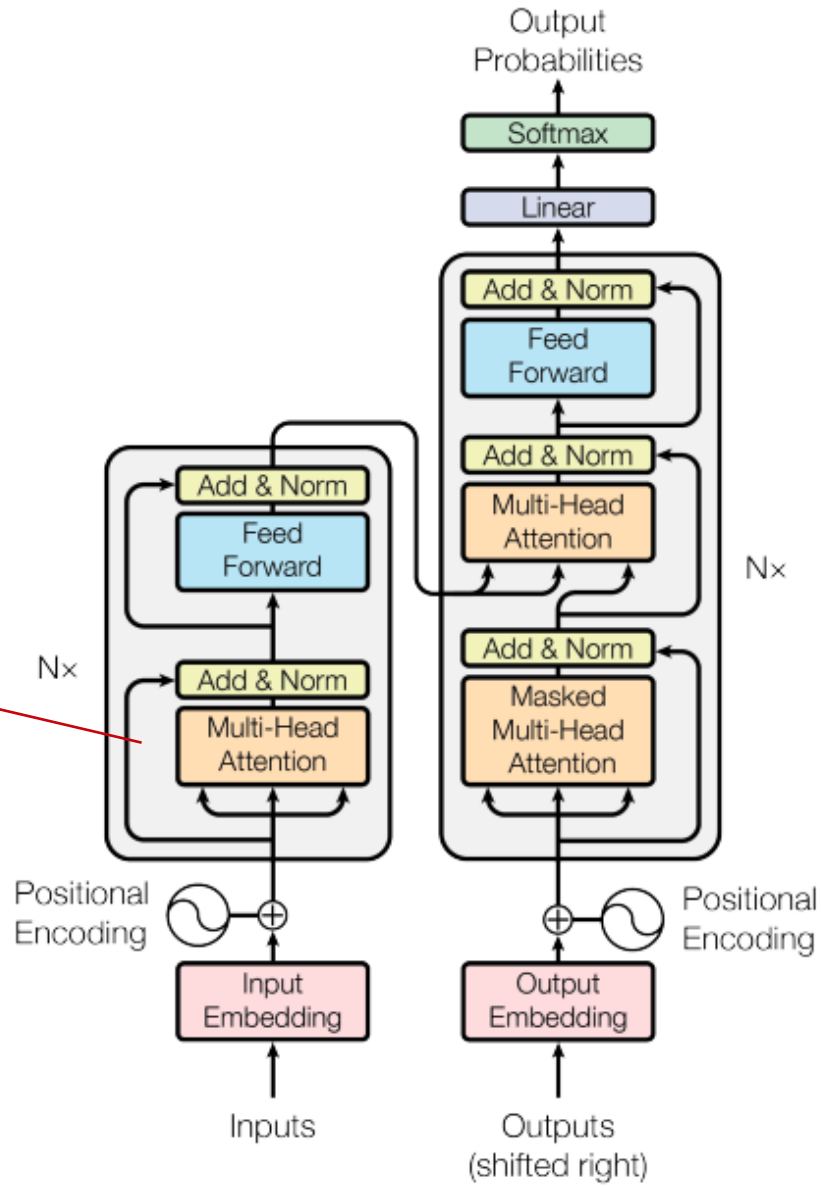
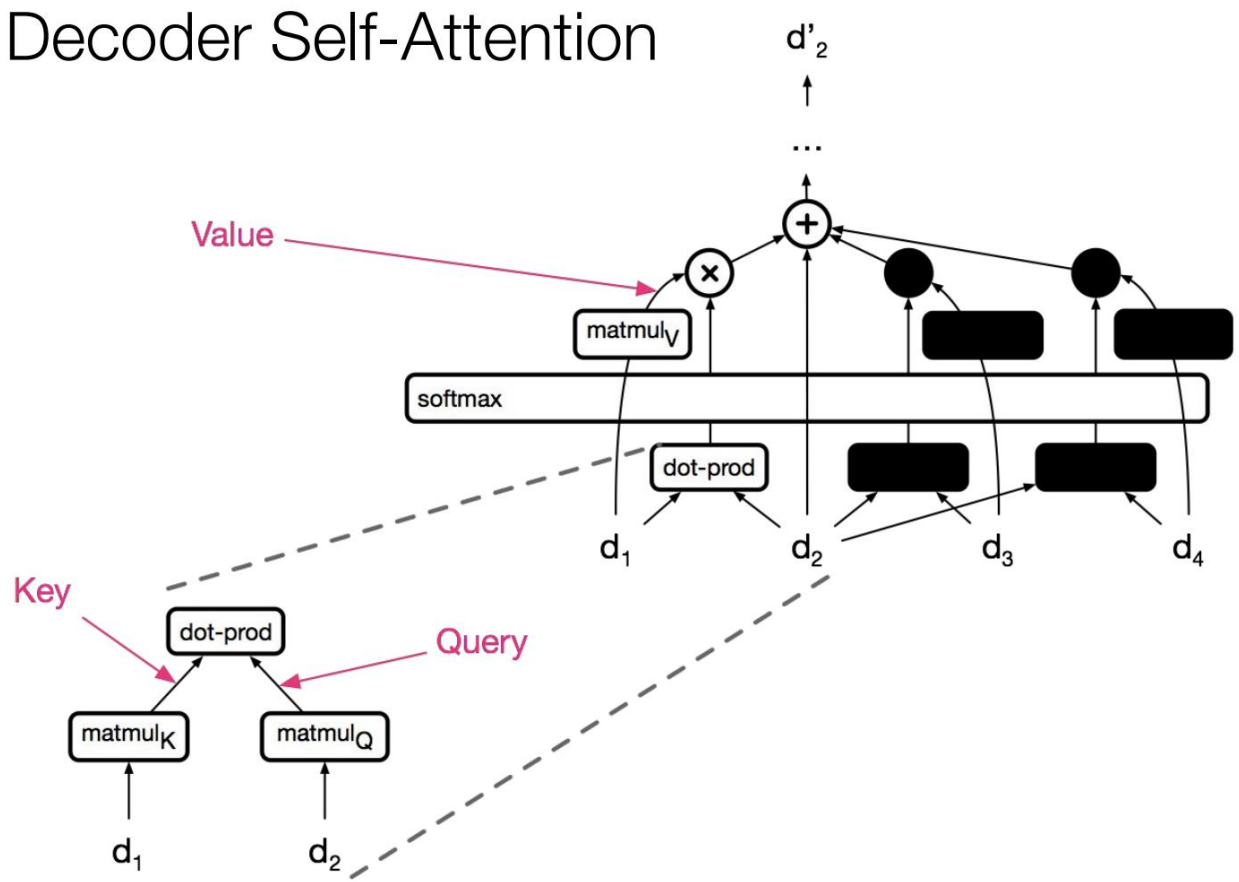


Figure 1: The Transformer - model architecture.

Vasvani [“Self-Attention for Generative Models”]

The ”Transformer”: Decoder



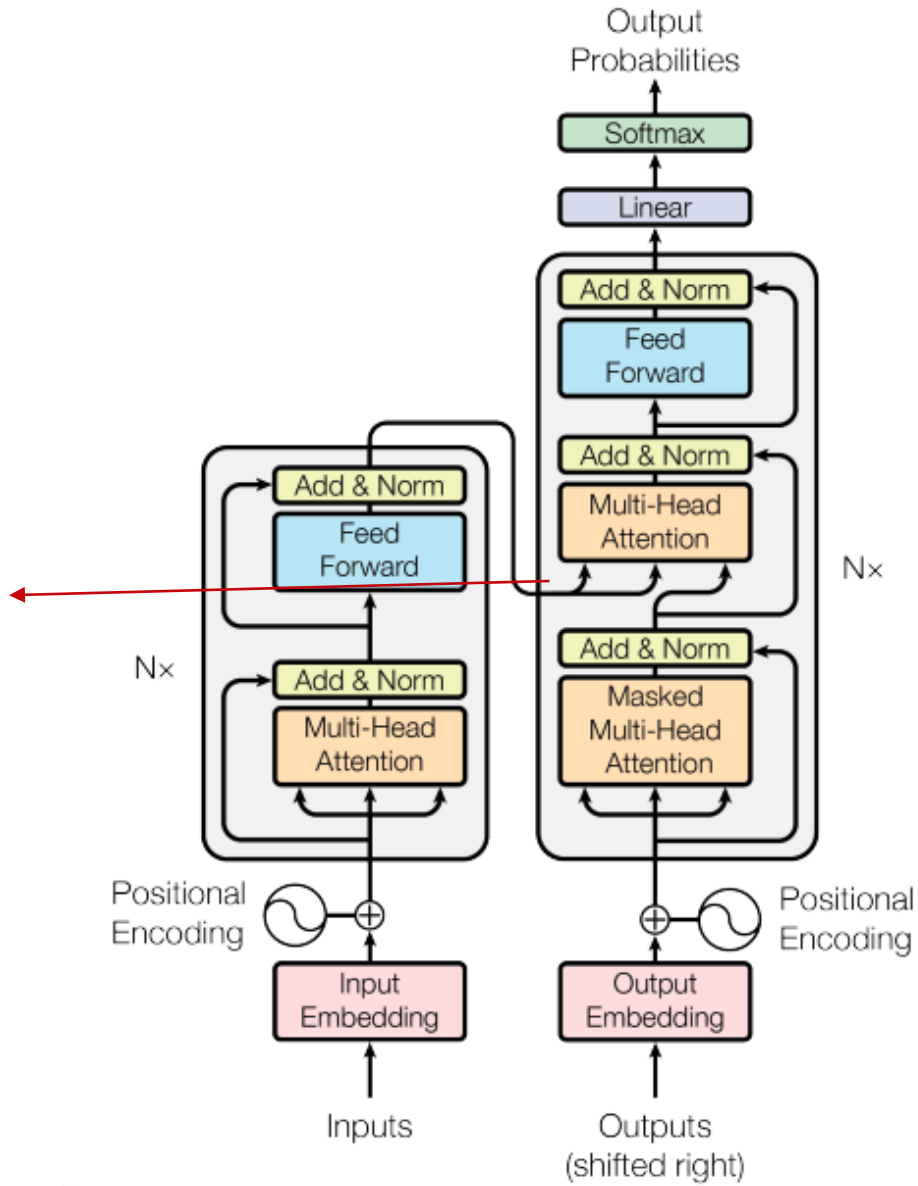


Figure 1: The Transformer - model architecture.

Vasvani [“Self-Attention for Generative Models”]

Transformer Tricks (4?)

- **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

Transformer Tricks – Positional Encodings

- Scaled dot-product and fully-connected layer are permutation invariant
- Sinusoidal positional encoding is a vector of small values (constants) added to the embeddings
- As a result, same word will have slightly different embeddings depending on where they occur in the sentence

$$PE_{pos,2i} = \sin\left(\frac{pos}{10000^{2i/d}\text{model}}\right)$$

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

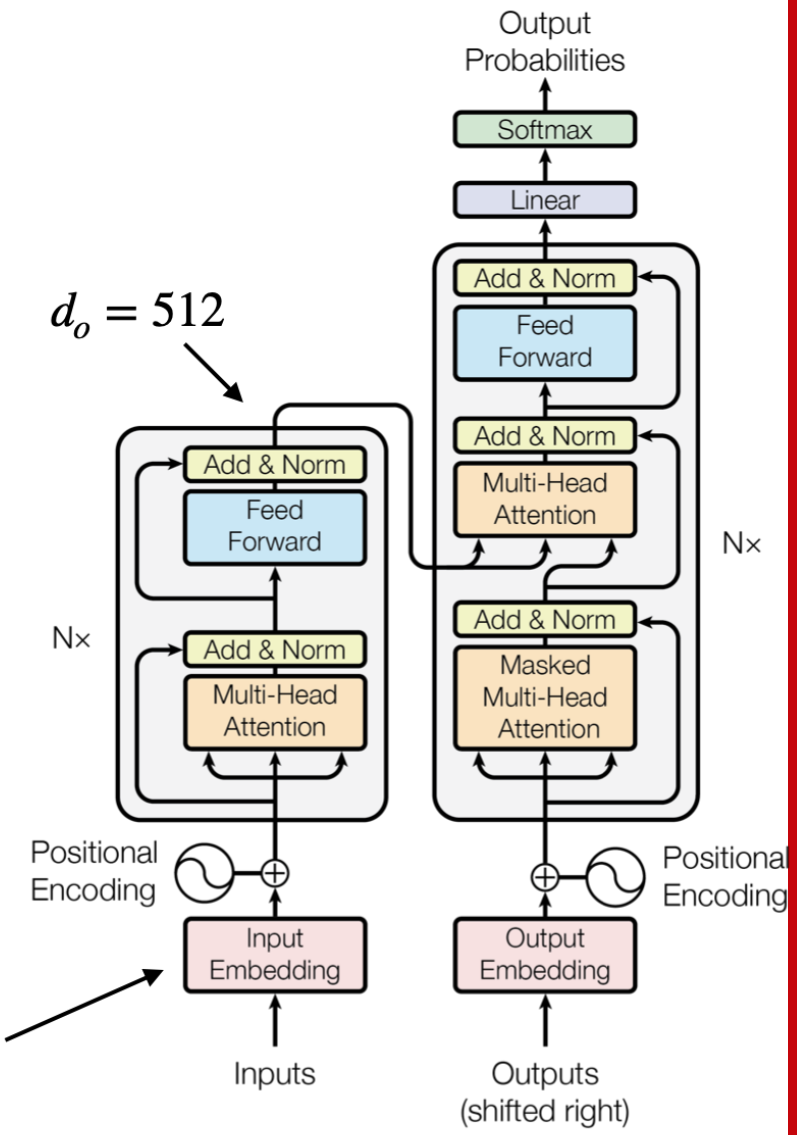


Figure 1: The Transformer - model architecture.

Vaswani, A., Shazeer, N., Parmar, N., Uszkoreit, J., Jones, L., Gomez, A.N., Kaiser, L. and Polosukhin, I., 2017. Attention Is All You Need.

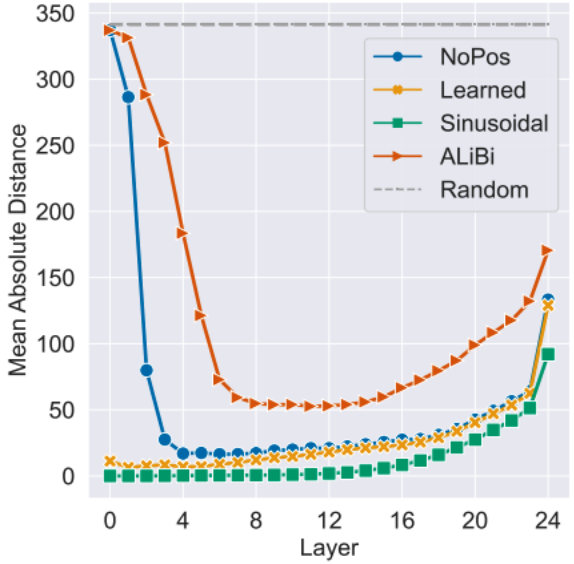
Transformer Tricks (3?)

Transformer Language Models without Positional Encodings Still Learn Positional Information

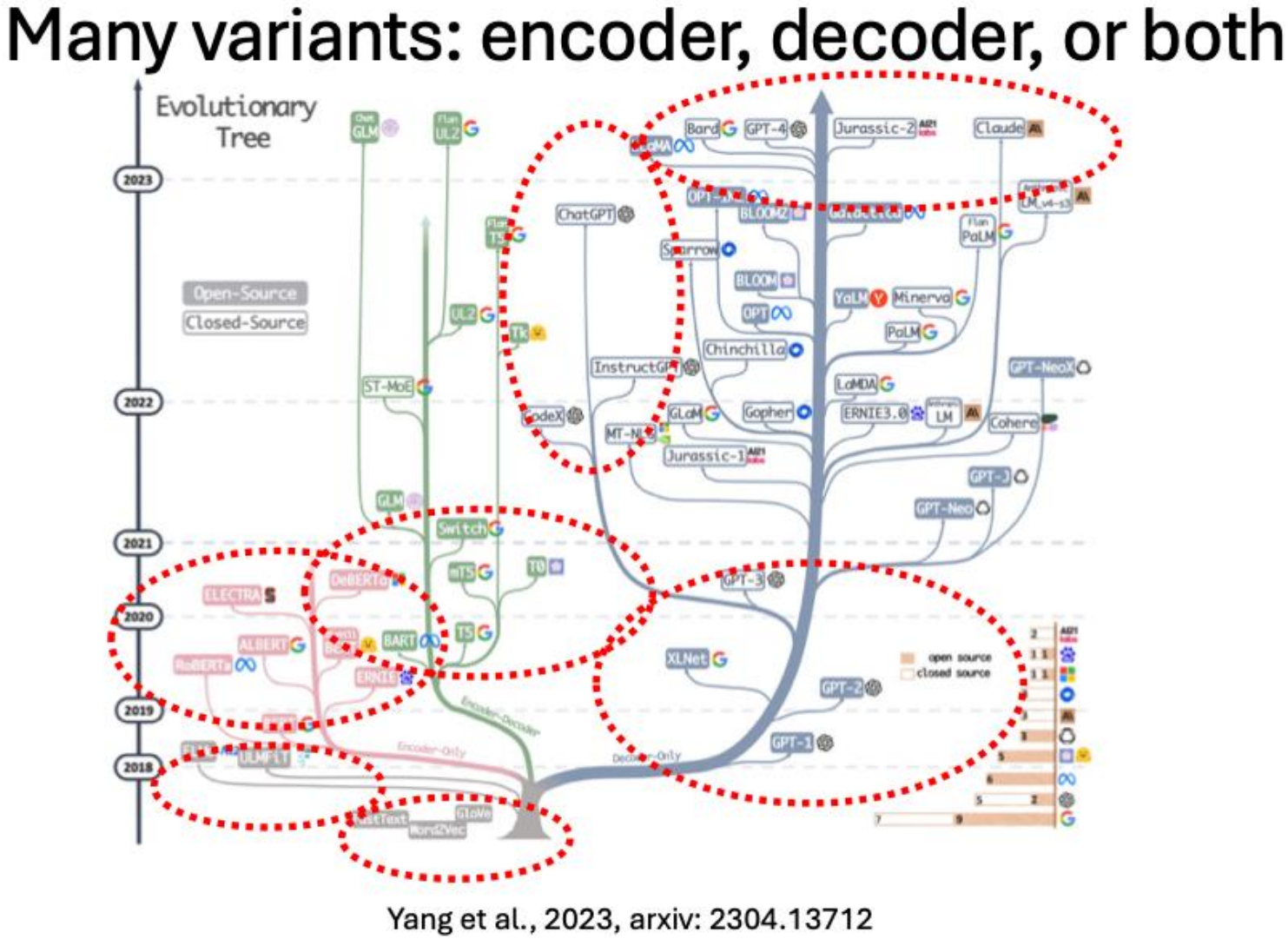
Adi Haviv[τ] **Ori Ram**[τ] **Ofir Press**[ω] **Peter Izsak**[ι] **Omer Levy**[τμ]

[τ]Tel Aviv University [ω]University of Washington [ι]Intel Labs [μ]Meta AI

{adi.haviv, ori.ram, levyomer}@cs.tau.ac.il, ofirp@cs.washington.edu, peter.izsak@intel.com



Many variants of transformer architectures



Yang et al., 2023, arxiv: 2304.13712

Next Time: GPT

Generative Pre-Trained Transformer

Questions?