Master's degree ICT Internet Multimedia Engineering

ADVANCED NEURAL NETWORK DESIGNS: SELF-ATTENTION & TRANSFORMERS

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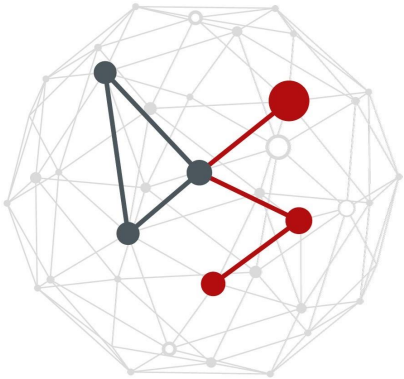

DIPARTIMENTO DI INGEGNERIA DELL'INFORMAZIONE

DIPARTIMENTO MATEMATICA

UNIVERSITÀ DEGLI STUDI DI PADOVA

Outline (1/2)

- Reference papers
- General picture
  - RNN *vs* transformers
  - The transformer building blocks (high level)
  - Encoder/decoder and full picture
- Block-by-block analysis
  - Word embedding
  - Self-attention
  - Multihead self-attention
  - Positional encoding
  - Skip connections and normalization
  - Decoder output: dense layer + softmax
  - Masked self-attention @decoder

Outline (2/2)

- Selected applications & trends
  - Learning to attend and diagnose
  - Large language Models
  - Automatic speech translation
  - Automatics code completion
  - Code generation from descriptive text
  - …
- Concluding remarks

[Vaswani2017]
101185 cit, Jan 2023

Attention Is All You Need

Conference on Neural Information Processing Systems, NeurIPS 2017

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Abstract

The dominant sequence transduction models are based on complex recurrent or convolutional neural networks that include an encoder and a decoder. The best performing models also connect the encoder and decoder through an attention mechanism. We propose a new simple network architecture, the Transformer, based solely on attention mechanisms, dispensing with recurrence and convolutions entirely. Experiments on two machine translation tasks show these models to be superior in quality while being more parallelizable and requiring significantly less time to train. Our model achieves 28.4 BLEU on the WMT 2014 English-to-German translation task, improving over the existing best results, including ensembles, by over 2 BLEU. On the WMT 2014 English-to-French translation task, our model establishes a new single-model state-of-the-art BLEU score of 41.0 after training for 3.5 days on eight GPUs, a small fraction of the training costs of the best models from the literature.

Transformers in Time-series Analysis: A Tutorial

Sabeen Ahmed[1], Ian E. Nielsen[1], Aakash Tripathi[1]
Shamoon Siddiqui[1], Ghulam Rasool[1], Ravi P. Ramachandran[1]
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Abstract

Transformer architecture has widespread applications, particularly in Natural Language Processing and computer vision. Recently Transformers have been employed in various aspects of time-series analysis. This tutorial provides an overview of the Transformer architecture, its applications, and a collection of examples from recent research papers in time-series analysis. We delve into an explanation of the core components of the Transformer, including the self-attention mechanism, positional encoding, multi-head, and encoder/decoder. Several enhancements to the initial, Transformer architecture are highlighted to tackle time-series tasks. The tutorial also provides best practices and techniques to overcome the challenge of effectively training Transformers for time-series analysis.

1 Introduction and Background

Transformers belong to a class of machine learning models that use self-attention or the scaled dot-product operation as their primary learning mechanism. Transformers were initially proposed for neural machine translation - one of the most challenging natural language processing (NLP) tasks [64]. Recently, transformers have been successfully employed to tackle various problems in machine learning and achieve state-of-the-art performance. Apart from classical NLP tasks, examples from other areas include image classification, object detection & segmentation, image & language generation, sequential decision making in reinforcement learning, multi-modal (text, speech, and image) data processing, and analysis of tabular and time-series data. This tutorial paper focuses on time-series analysis using Transformers.

The time-series data consist of ordered samples, observations, or features recorded sequentially over time. Time-series datasets often arise naturally in many real-world applications where data is recorded over a fixed sampling interval. Examples include stock prices, digitized speech signals, traffic measurements, sensor data for weather patterns, biomedical measurements, and various kinds of population data recorded over time. The time-series analysis may include processing the numeric data for multiple tasks, including

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[Sabeem2023] Springer. Circuits, Systems and Signal Processing, 25 July 2023

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Acknowledgments

Gerard I. Gállego, Universitat Politècnica de Catalunya, Barcelona, Spain – “The Transformer Revolution,” CTTC, November 2022.

[Alammar2018] Jay Alammar, “The Illustrated Transformer,” (blog) June 27, 2018.

Transformer – what it is

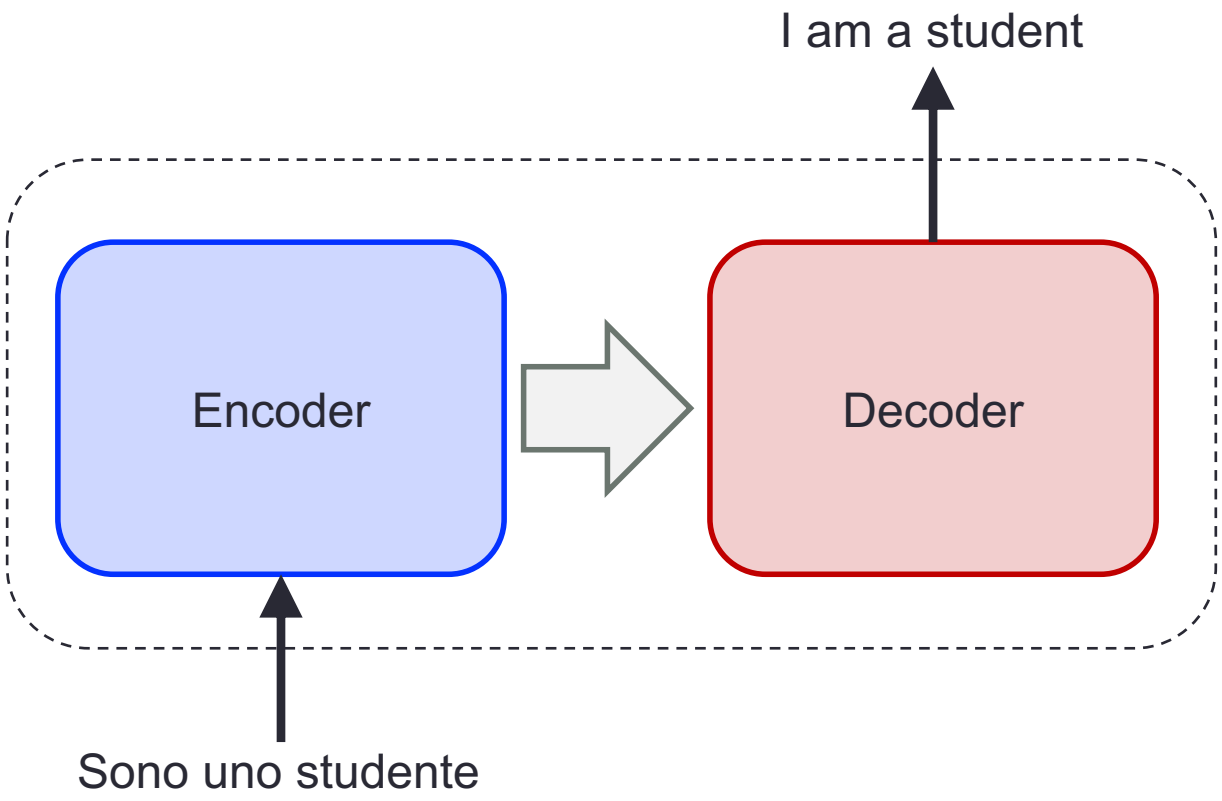
- Sequence-to-sequence architecture
- Implemented via an encoder-decoder model
- Designed based on FFNNs (***no recursion***, ***no memory cells***)
- Takes a sequence S_I of data items as input
- Returns a sequence S_O of data items as output
- Sequences do not necessarily have the same length
- S_I is then compressed into a fixed-length code
- The code is used by the decoder to generate S_O
- Original transformer [Vaswani2017]
  - Proposed for language translation
  - Takes a sequence of words from one language
  - Returns the corresponding sentence in another language

RNN *vs* transformers (high level)

- RNNs
  - Implicitly capture position of words/items in a sequence by passing one item at a time to the RNN – past memory is used to process the current input
  - Time correlation is modeled and retained by the internal cell memory
- Transformers
  - Are FFNNs
  - They do not use RNN memory cells
  - The sentence/data sequence is fed all at once to the NN

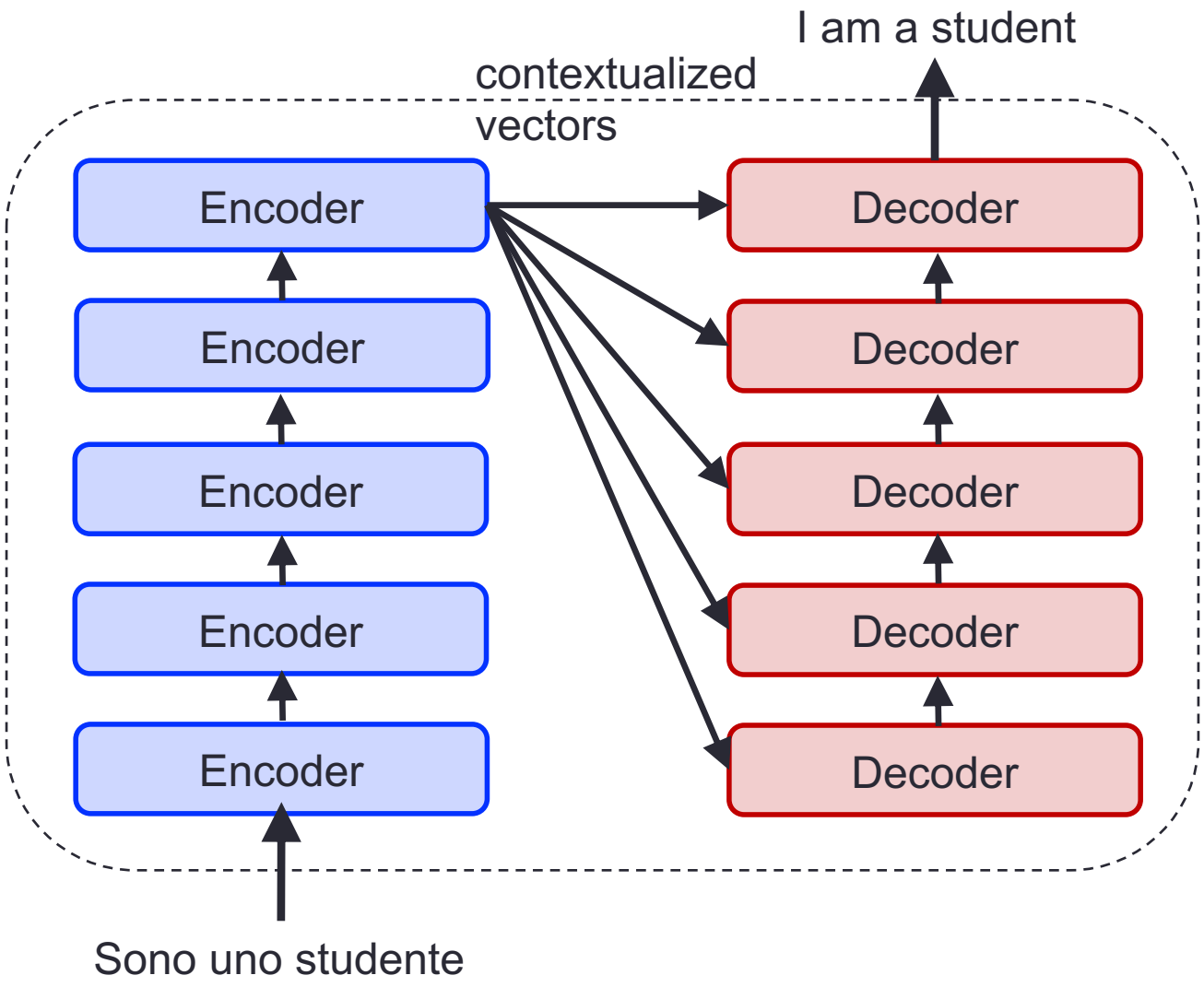
- ADVANTAGES
  - Getting rid of RNN cells (dense, slow to train, memory expensive)
  - Transformers better exploit the parallelism of modern GPUs

The transformer (very high-level)



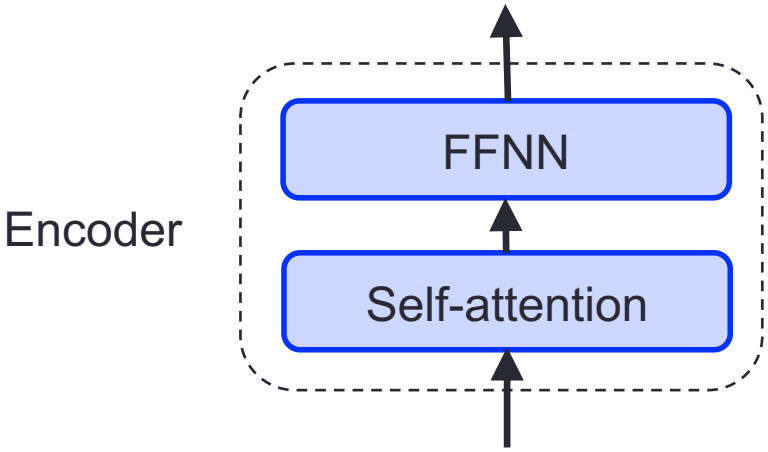
Encoder and decoder are a stack of components

The transformer (high-level)



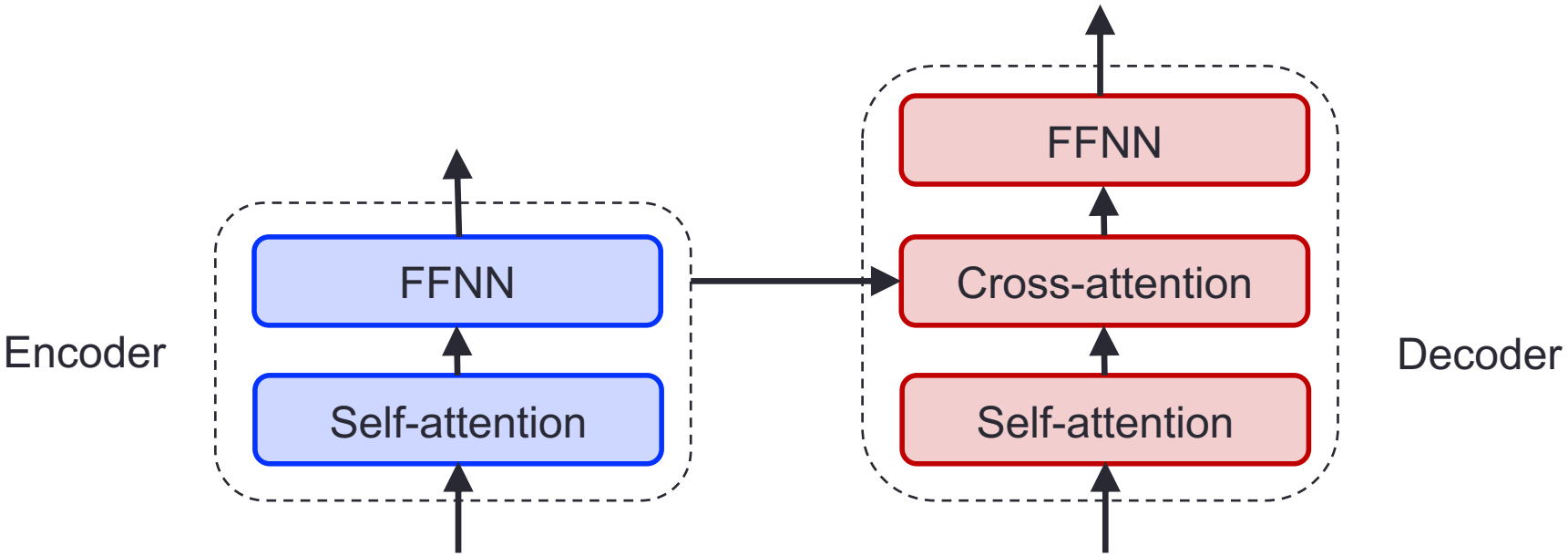
Encoder

- The encoders are all identical
  - They do not share weights among them
  - Each one is composed of 2 sub-layers
    - **Bottom:** Self-attention (**linear**, correlation)
    - **Top:** Feed forward neural networks (**non-linear**) – it is *independently applied* to each vector from the underlyining attention block (see shortly)

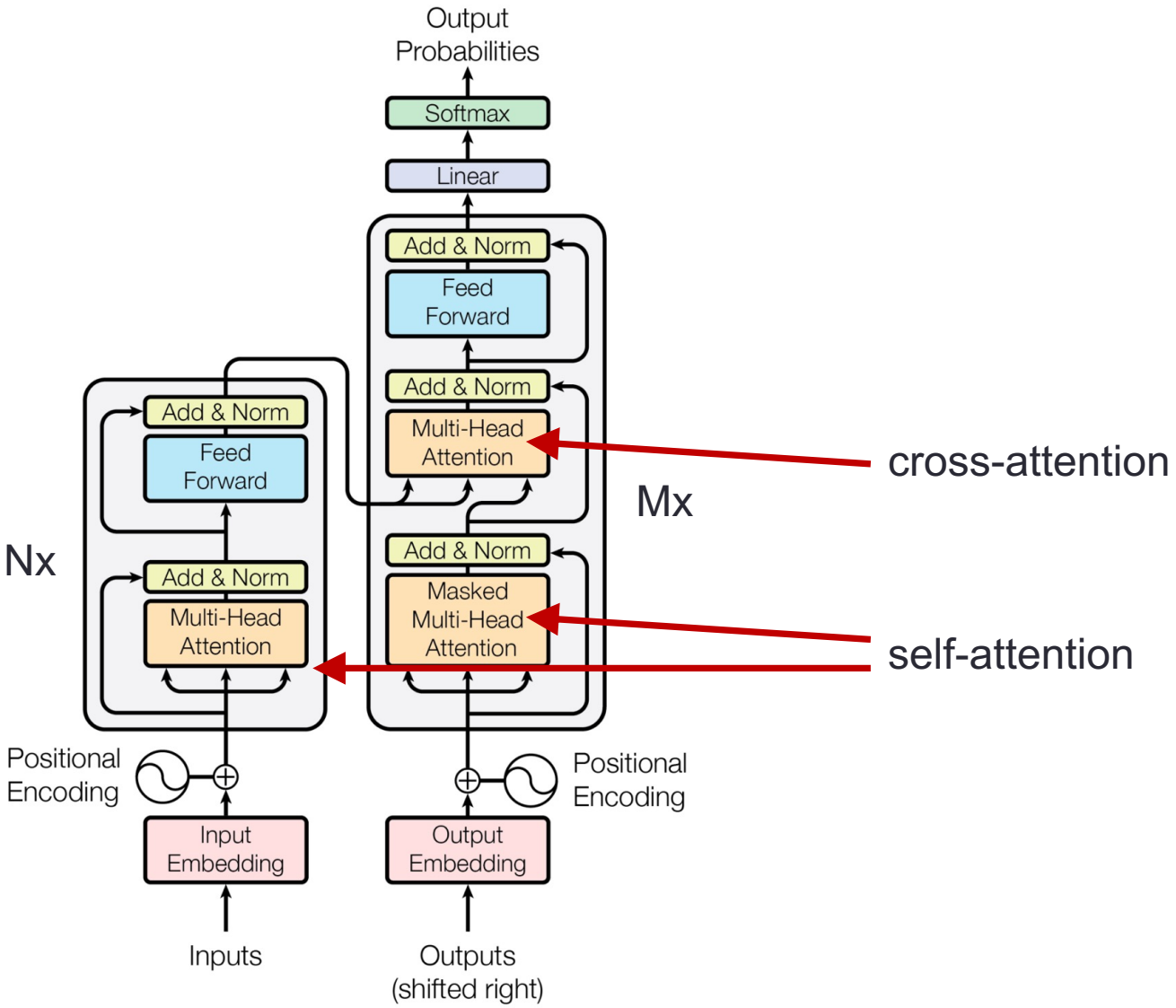


Decoder

- The decoder additionally uses a cross-attention layer
- To exploit the contextualized info learned by the encoder



The full picture [Vaswani2017]



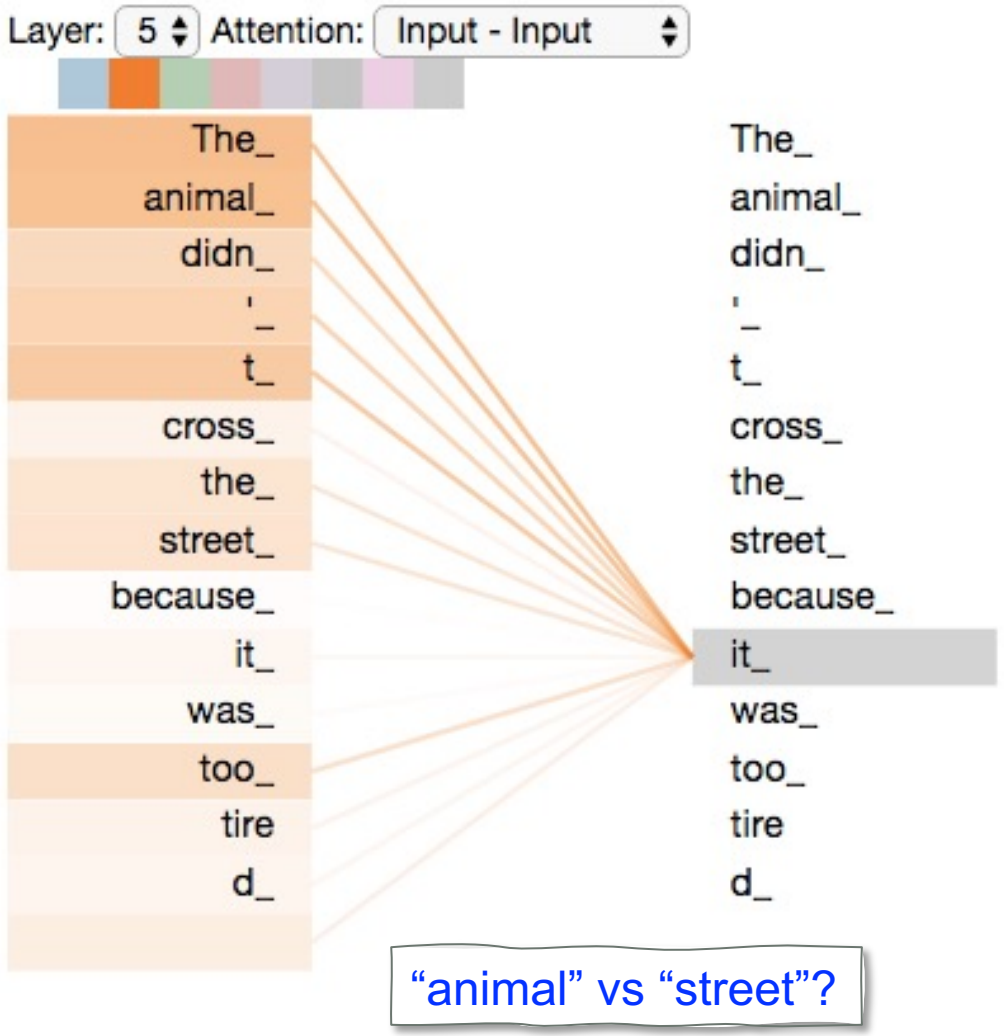
BLOCK-BY BLOCK ANALYSIS

Key ingredients

- Self attention
  - Queries, keys and values are the input data themselves
  - Obtained via dot products (basically, to automatically discover correlations within the input sequence)
- Positional encoding
  - Needed as data sequence is fed *all at once*
  - **Desiderata: 1)** unique encoding value for each time step in a sequence of items, **2)** consistent distance across time steps for seqs of various length **3)** encoding results must be independent of the length of the sequence, **4)** the encoding must be deterministic
  - Allows the model to learn the data temporal correlation structure
- New things to look at wrt RNNs
  - Self-attention, multi-head attention, positional encoding, masked multi-head attention

Self-attention (intuition)

- Let's take the work "it" as the target word in a sentence
- A relation is built (correlation) between each target word and any other word in the same sentence
- This relation is stored in the form of a probability distribution (softmax)
- A single word **attends to** multiple words in the same sentence (sequence)



Example

The word “she” in this sentence

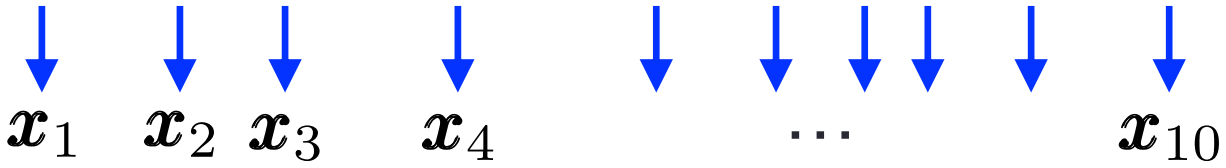
- Is semantically connected with the subject “Noa”
- Is connected with the noun “cat”
- And also with the state of being verb “is”

We would like to re-express words

- Contextualizing them wrt other words data items
- A proximity based metrix cannot be the way
  - As shown in the example, words that are far apart may be correlated

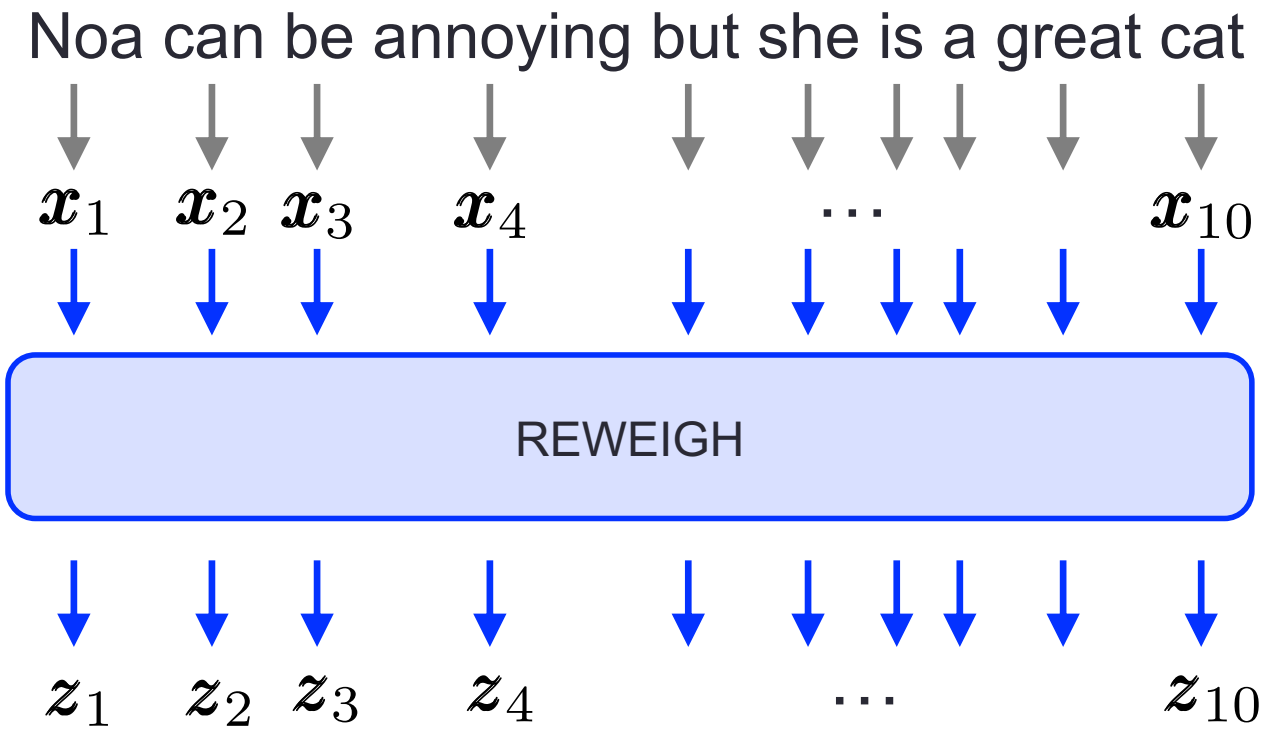
Self-attention

Noa can be annoying but she is a great cat



STEP 1: from words to vectors
→ embeddings

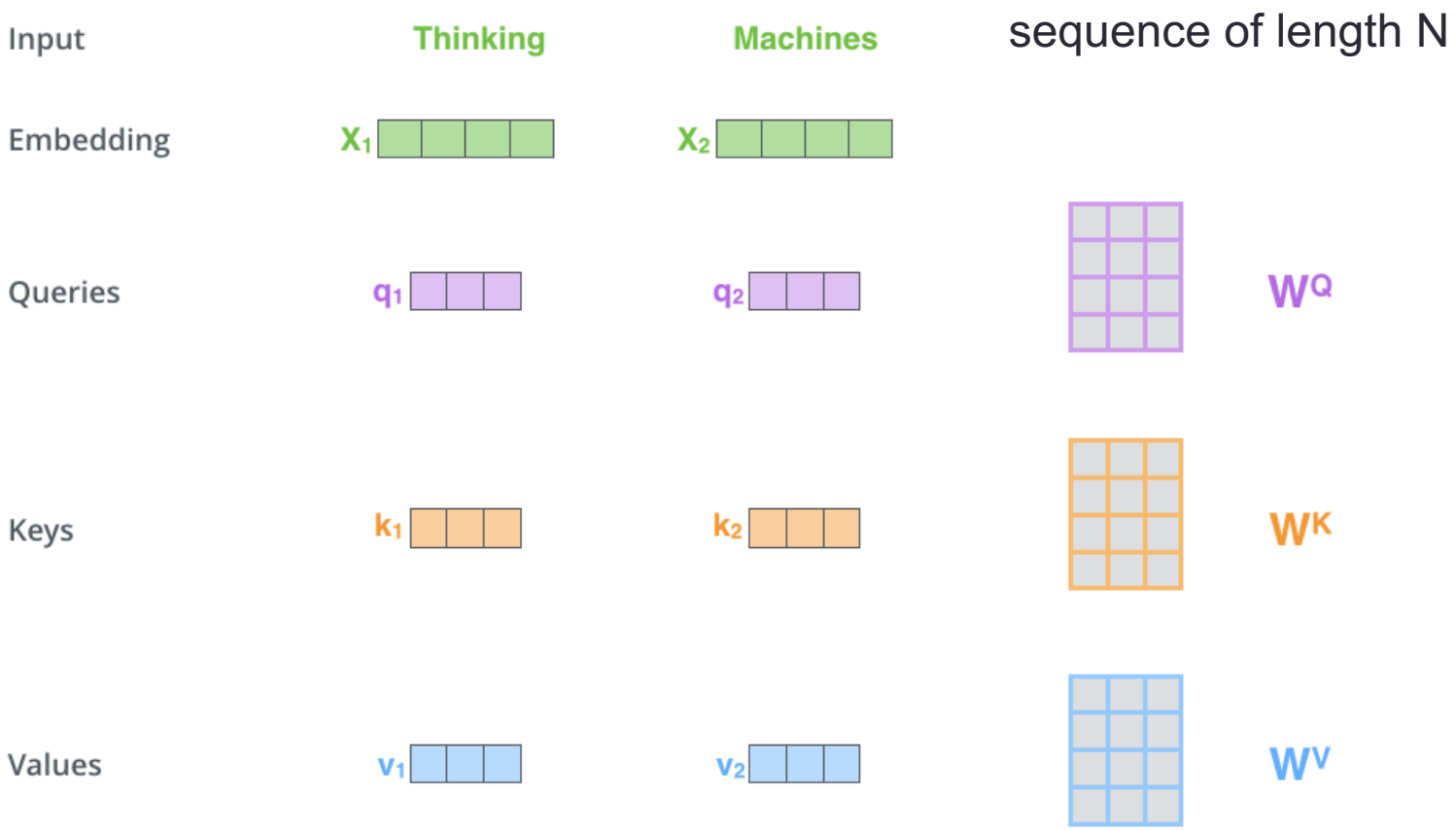
Self-attention



STEP 2: reweigh words

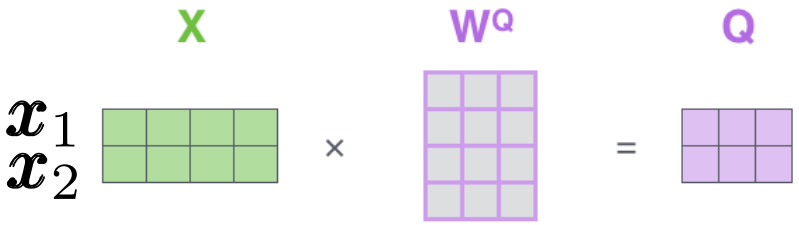
- Reweighing process is done via self-attention
- The new vectors/words are contextualized representations

Self-attention: queries, keys, values



Multiply the $\mathbf{x}_i$ vectors by 3 different matrices $\mathbf{W}^Q$, $\mathbf{W}^K$, $\mathbf{W}^V$ to obtain Query, Key and Value vectors

Self-attention: queries, keys, values

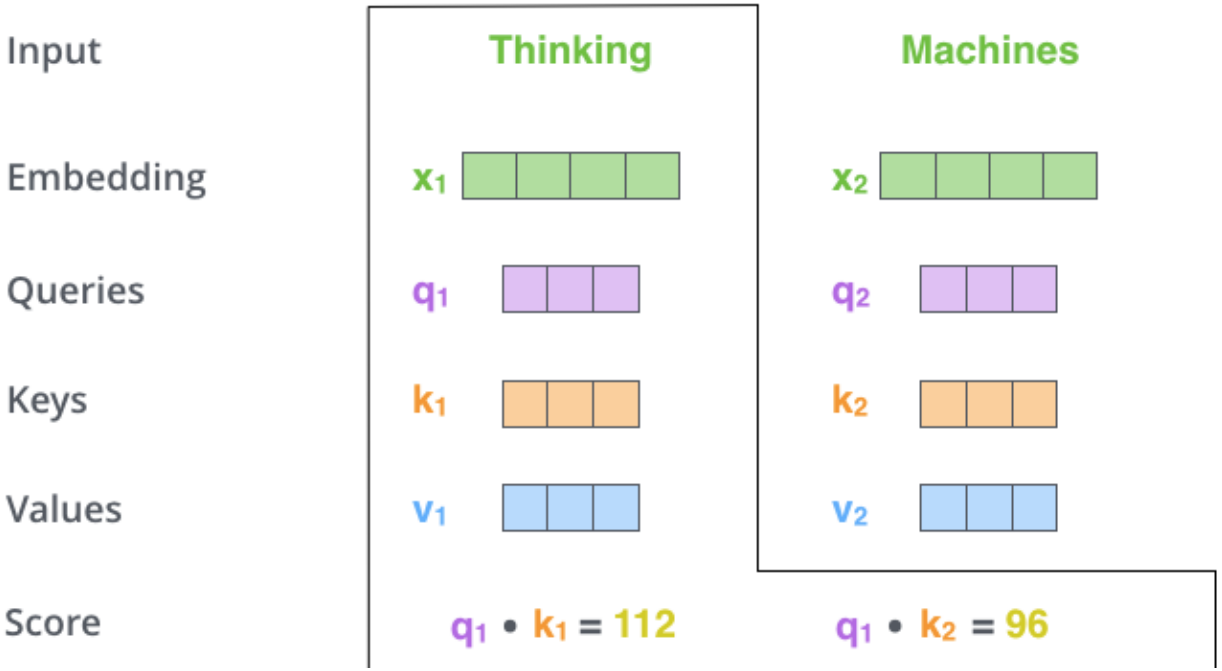


in matrix form

Note: for this slideset we use row vectors – the same calculations apply verbatim with column vectors

Queries, Keys and Values: are 3 linearly weighed vectors of the input. The weights in these matrices are to be learned

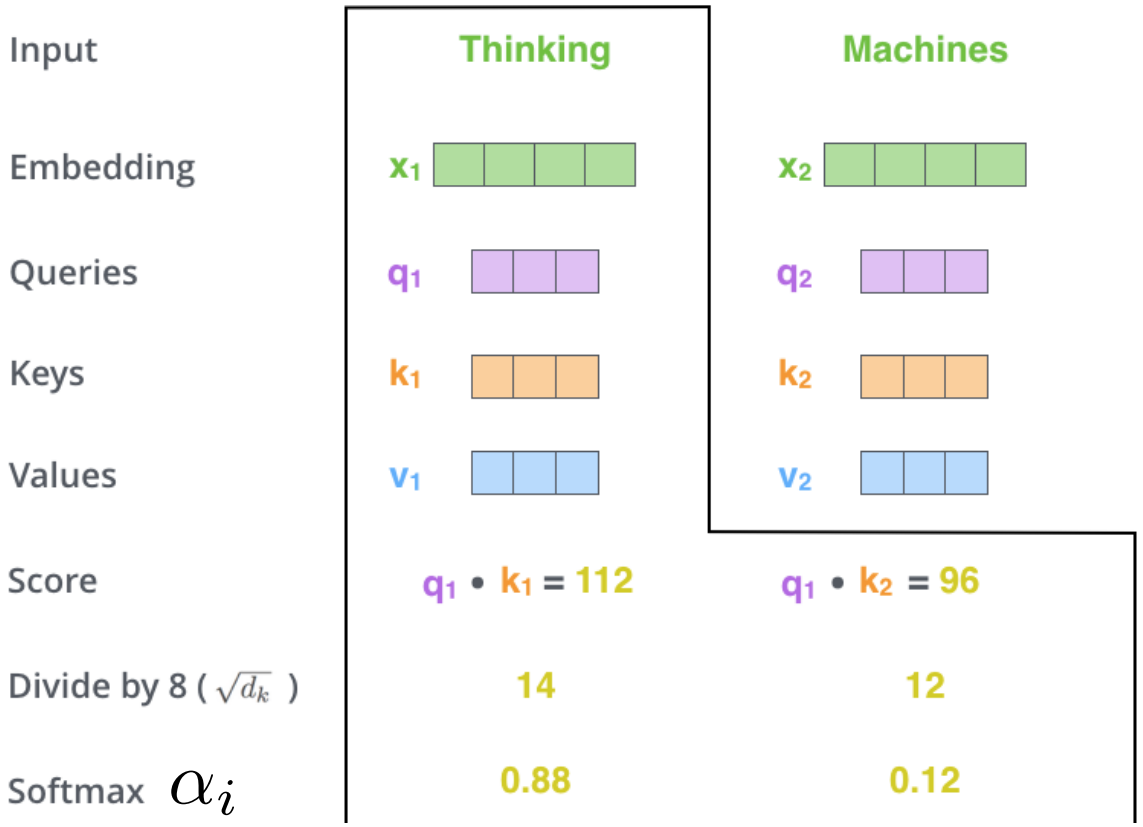
Self-attention: scores



For every $\mathbf{x}_i$ in the sequence: compute the dot product of $\mathbf{q}_i$ and all the N keys $\mathbf{k}_j$, this returns the so called scores

- N scores (one for each word)
- It is a correlation measure

Self-attention: normalized scores

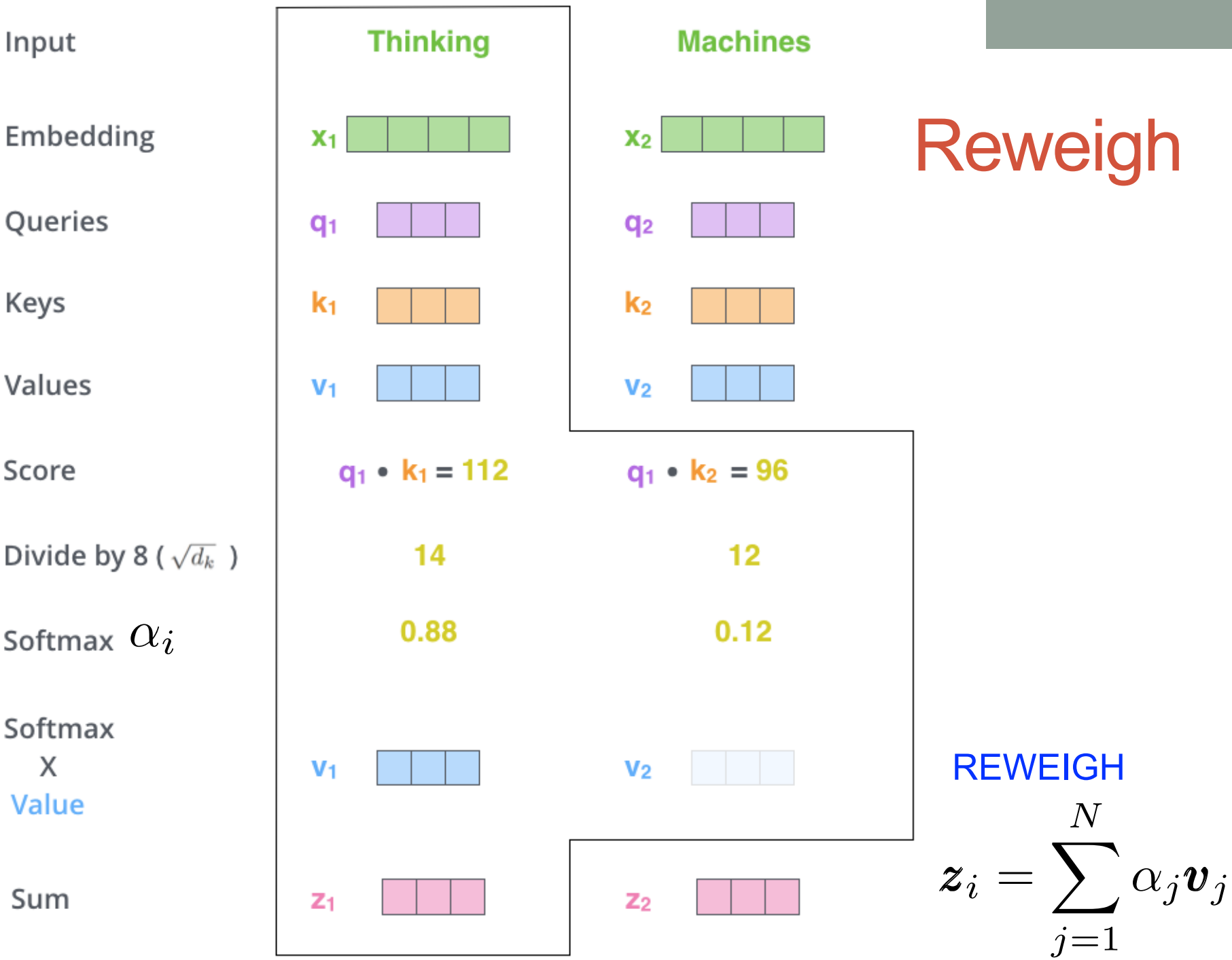


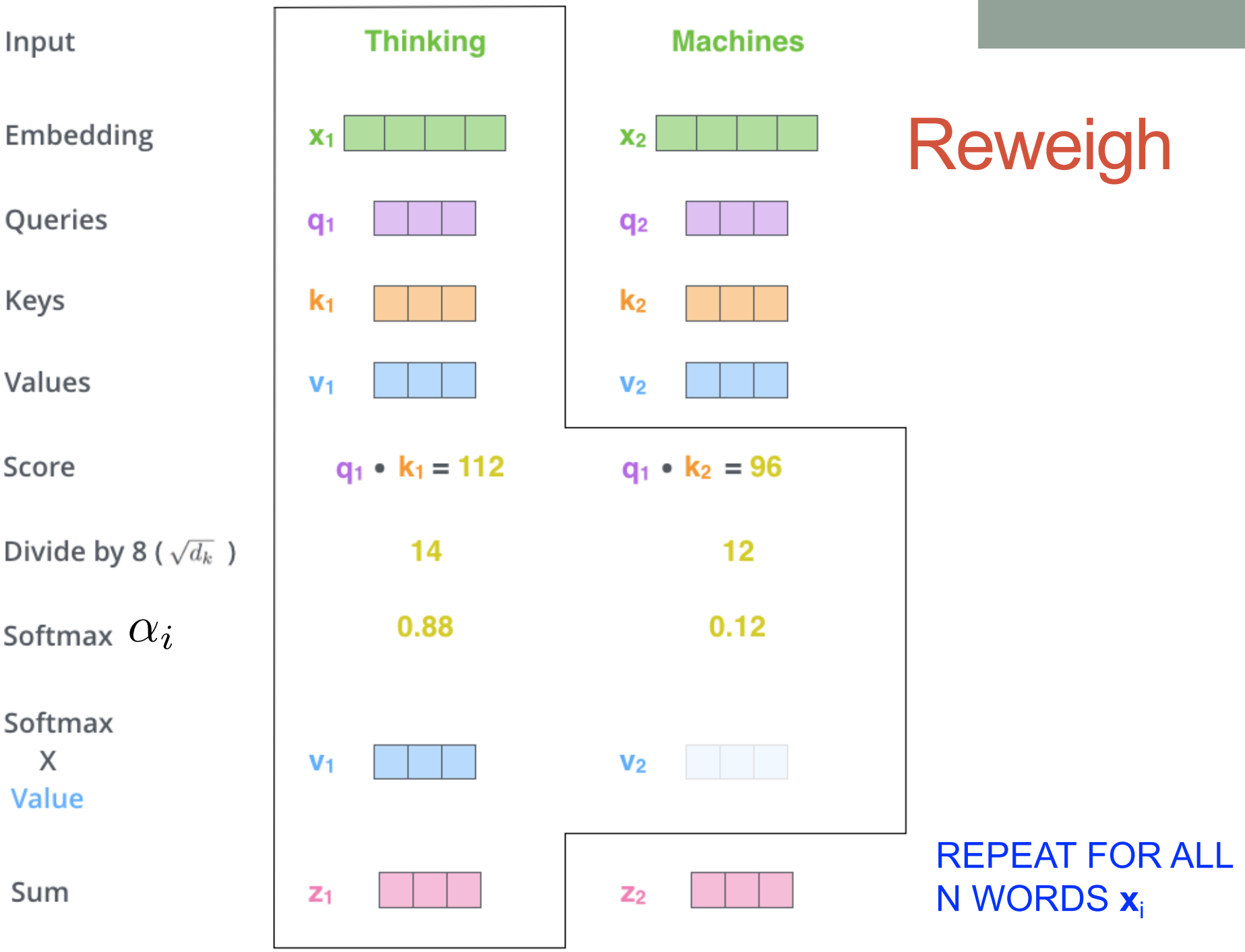
WEIGHTS

$$\alpha_j \in [0,1], \forall j$$

$$\sum_{j=1}^{N} \alpha_j = 1$$

Normalize (see later), this returns a vector of N real values (one for each element). Use softmax to obtain weights in [0,1]


Input
Thinking
Machines
Embedding
x1
x2
Queries
q1
q2
Keys
k1
k2
Values
v1
v2
Score
q1 • k1 = 112
q1 • k2 = 96
Divide by 8 (√dk)
14
12
Softmax αi
0.88
0.12
Softmax X Value
v1
v2
Sum
z1
z2
Reweigh
REWEIGH
$$z_i = \sum_{j=1}^{N} \alpha_j v_j$$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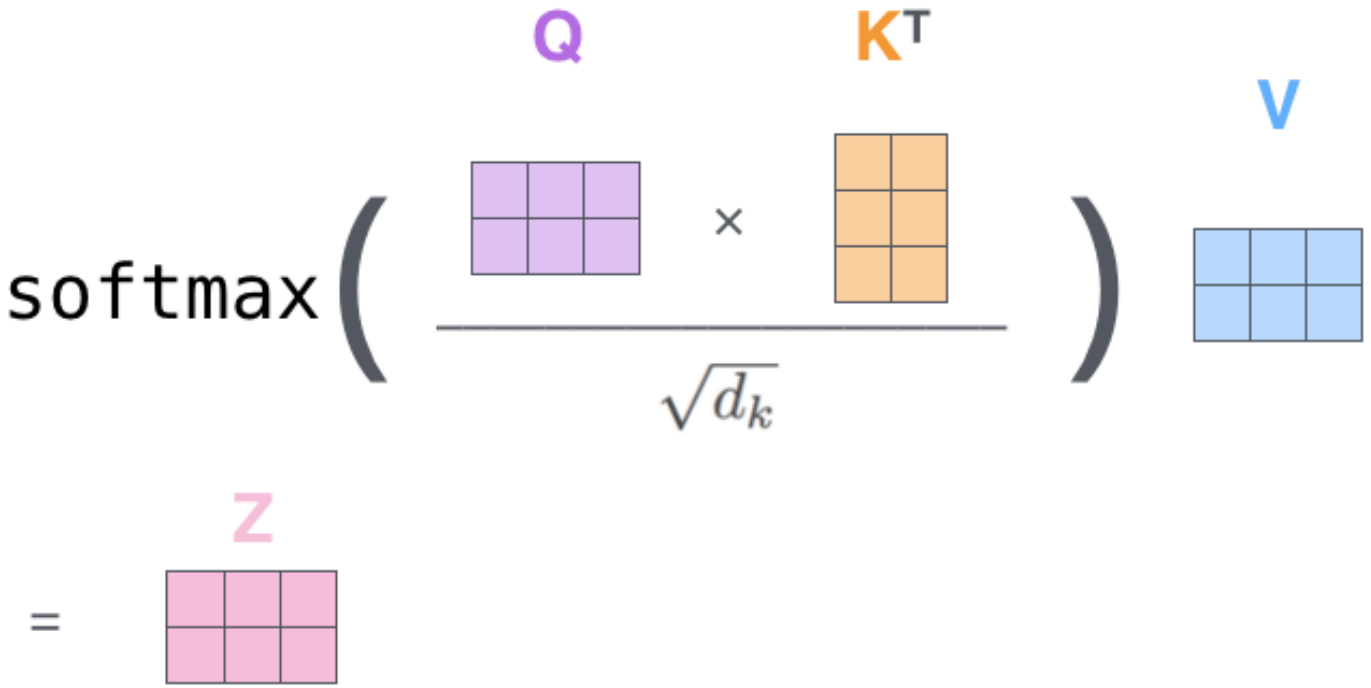
Reweigh
REPEAT FOR ALL N WORDS xi

In matrix form



As for the normalization inside the softmax

- “Leap of faith” for now

Self-attention block – recap

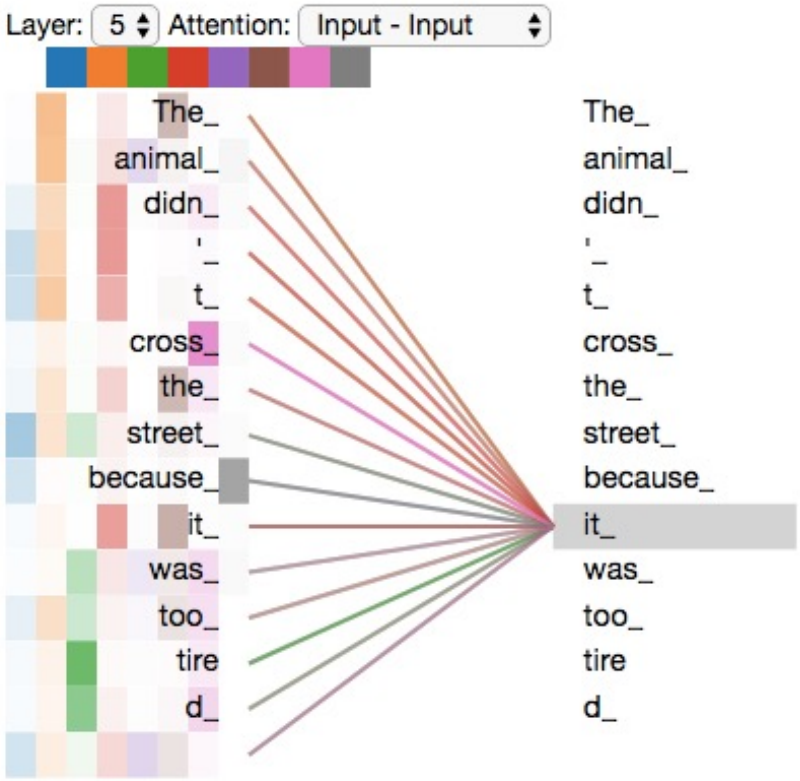
- So, attention captures the degree of dependence (”correlation”) among the data items (e.g., words) in a data sequence (e.g., sentence)
- This dependence can be related to semantic meaning in the language, similarity in an embedded/ferature space, proximity of points in the data space
- It is captured by
  - Computing a distribution of weights (probabilities) expressing how much each item attends to (relates to) each other item in the same sequence, and then,
  - Reweighing the data items themselves using the weights (the probabilities)

Aspects worth of note

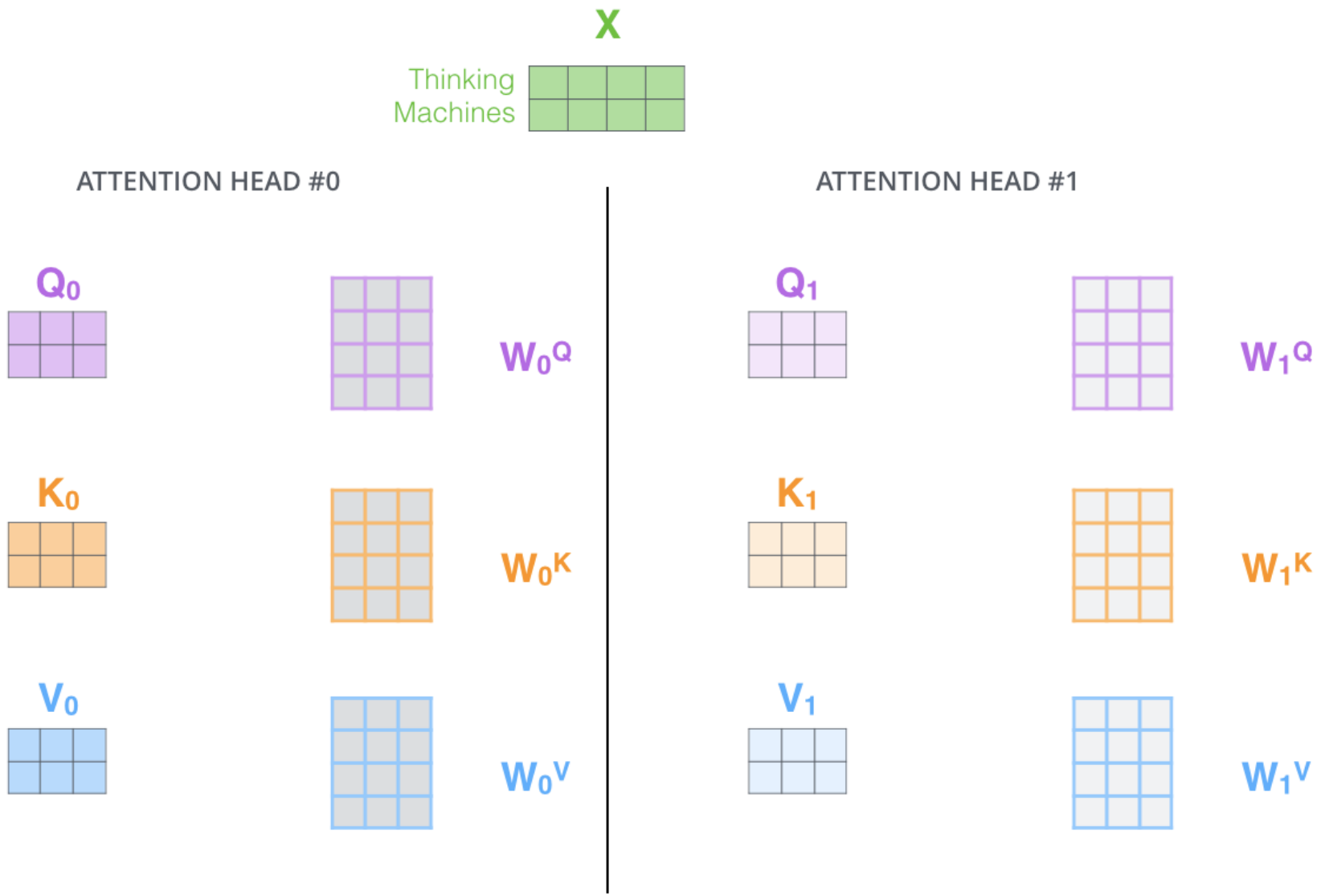
- Order has no influence on the calculation of the $\mathbf{z}_i$
- Proximity has no influence in the calculation of the $\mathbf{z}_i$
- The approach does not depend on the sequence length N
- Complexity scales as $O(N^2)$
  - For each data item $\mathbf{x}_i$ → compute N weights to rexpress it into $\mathbf{z}_i$
  - Repeat for N data items
  - This is a drawback for long sequences (price to pay)

Multihead attention

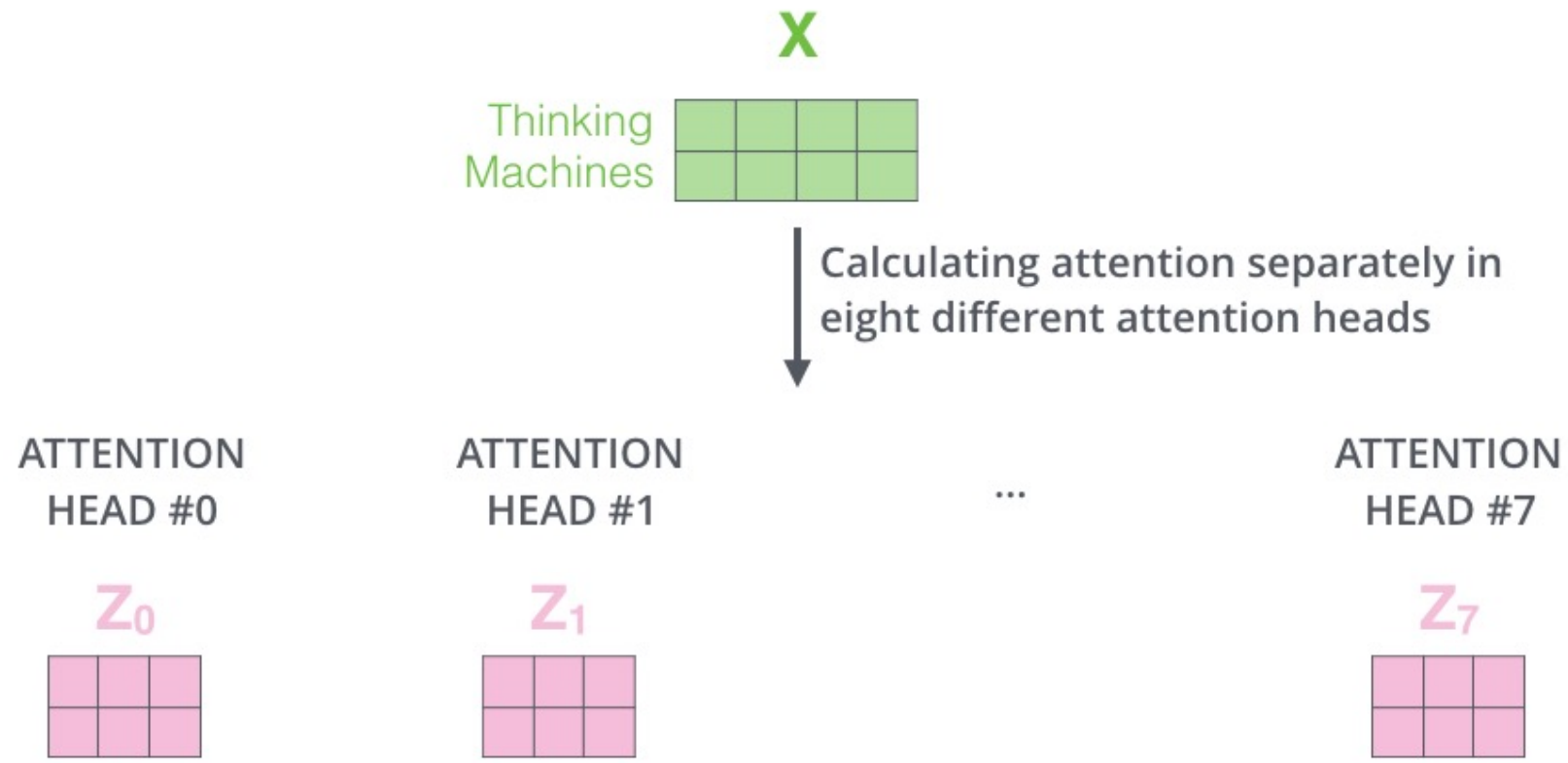
- Merely: using multiple self-attention in parallel
- Same idea as adding multiple CNN filters for a convolutional layer
- Each head may be (possibly) capturing different correlation properties of the input – at different semantic levels



Multihead attention (2 heads)

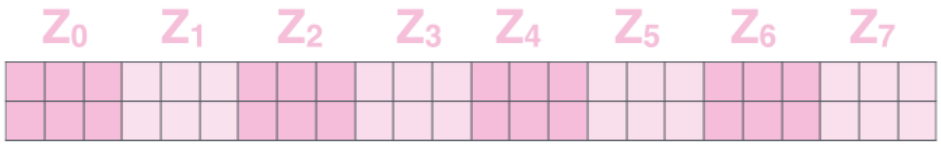


Multihead attention (8 heads)



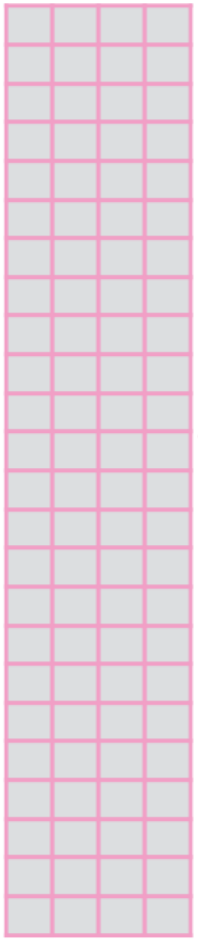
Multihead attention (8 heads)

1) Concatenate all the attention heads



2) Multiply with a weight matrix W^O that was trained jointly with the model

X



3) The result would be the Z matrix that captures information from all the attention heads. We can send this forward to the FFNN

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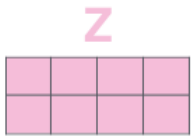


Multihead attention: full pipeline

1) This is our input sentence*

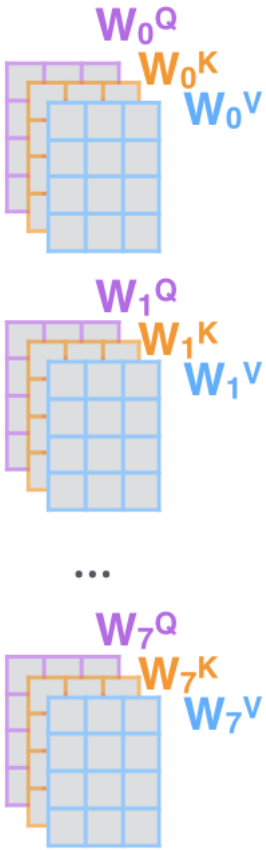
2) We embed each word*

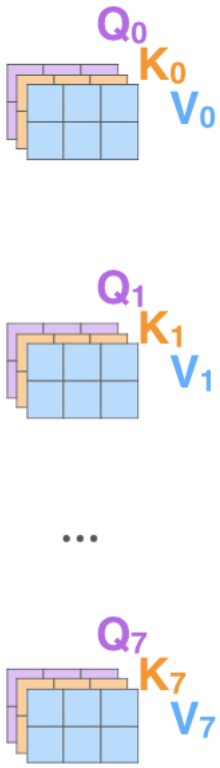
3) Split into 8 heads. Multiply **X** by weight matrices

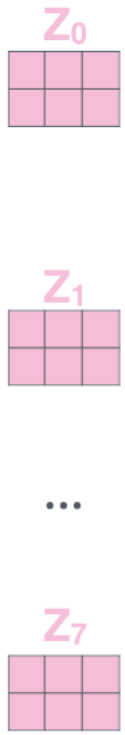
4) Calculate attention using the resulting Q/K/V matrices

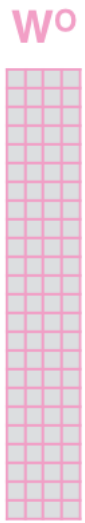
5) Concatenate the resulting Z matrices, then multiply with weight matrix W^O to produce the output of the layer

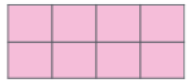
Thinking Machines



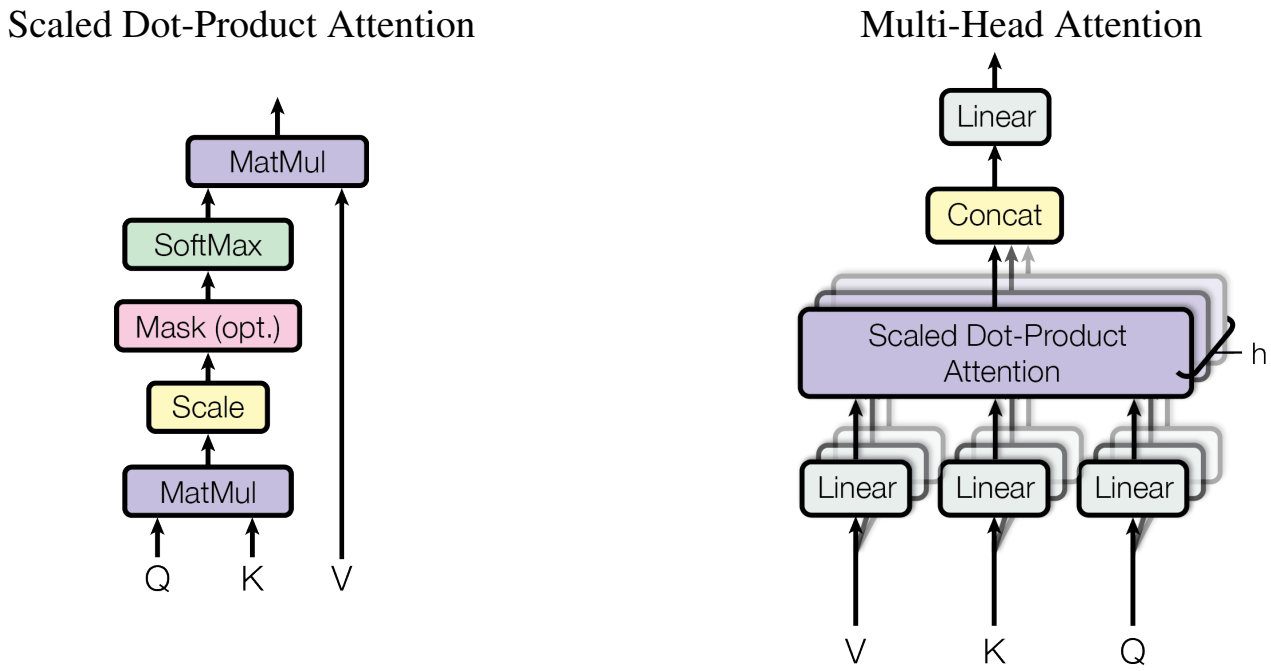






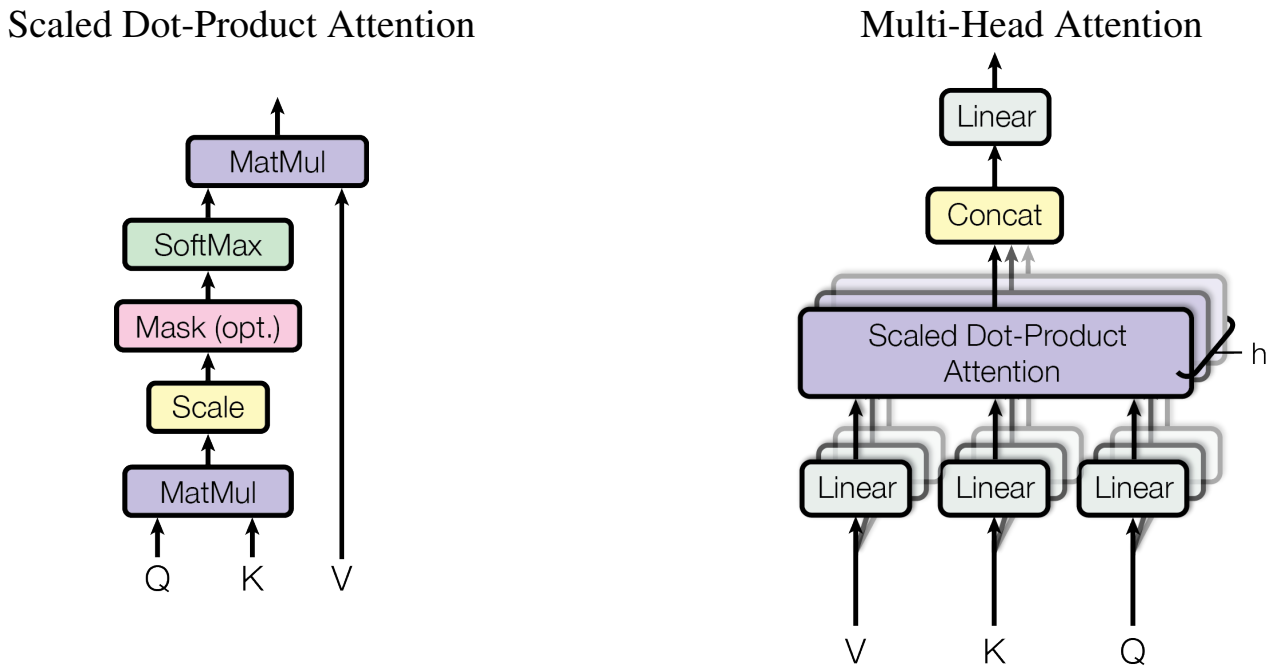


Attention mechanism



- Wait a minute… attention does not contain any weights!!!
- But it will make it so the weights in matrices $\mathbf{W}^Q$, $\mathbf{W}^K$, $\mathbf{W}^V$ will be learned so as to extract meaningful projections of the input data – projections that will make sense when self-attention is used with them

Attention mechanism



- Wait a minute… attention does not contain any weights!!!
- But it will make it so the weights in matrices $\mathbf{W}^Q$, $\mathbf{W}^K$, $\mathbf{W}^V$ will be learned so as to extract meaningful projections of the input data – projections that will make sense when self-attention is used with them

Problem

- Nothing of what we have seen so far (self-attention) depends on the ordering of data items (words)
- The output representations $\mathbf{z}_i$ are order-independent
- However, we are processing time series and, as such, we would like to track temporal dependencies

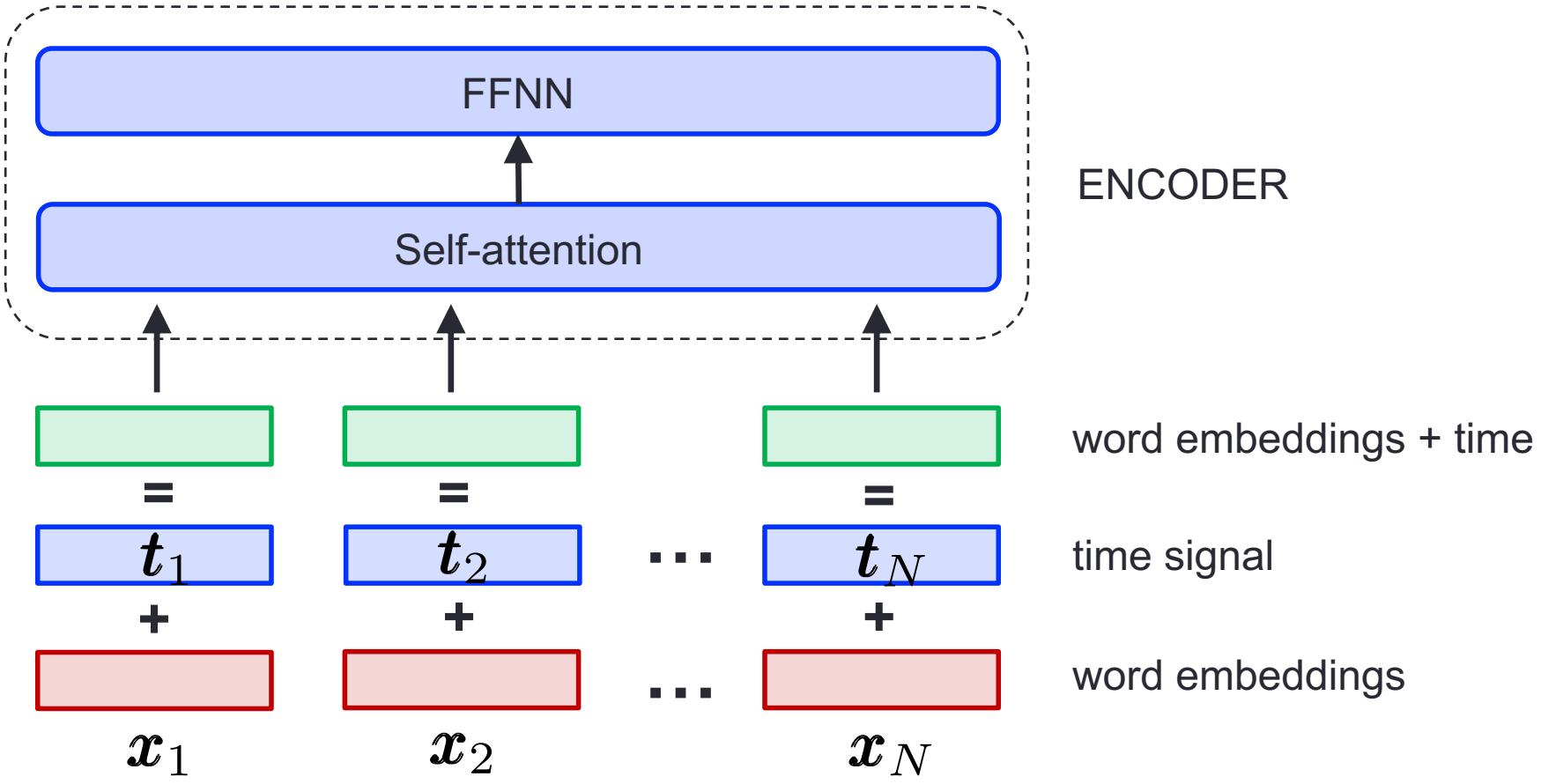
Solution: time signal

- For the model to make use of the order of the sequence
- We add timing information to the data
  - Generating a (deterministic) time signal and adding it to the input items
  - Such time signal is called positional encoding (PE)
- PE vectors have the same dimension of word embeddings
  - So that the two can be summed
  - Let m be the size of the input vectors $|\mathbf{x}_n|=m$
  - Let $\mathbf{t}(n,i)$ be the element i of the PE vector for data item n
    - With n=1,…,N and i=1,…,m

$$\boldsymbol{t}(n,2i) = \sin(n/10000^{2i/m})$$

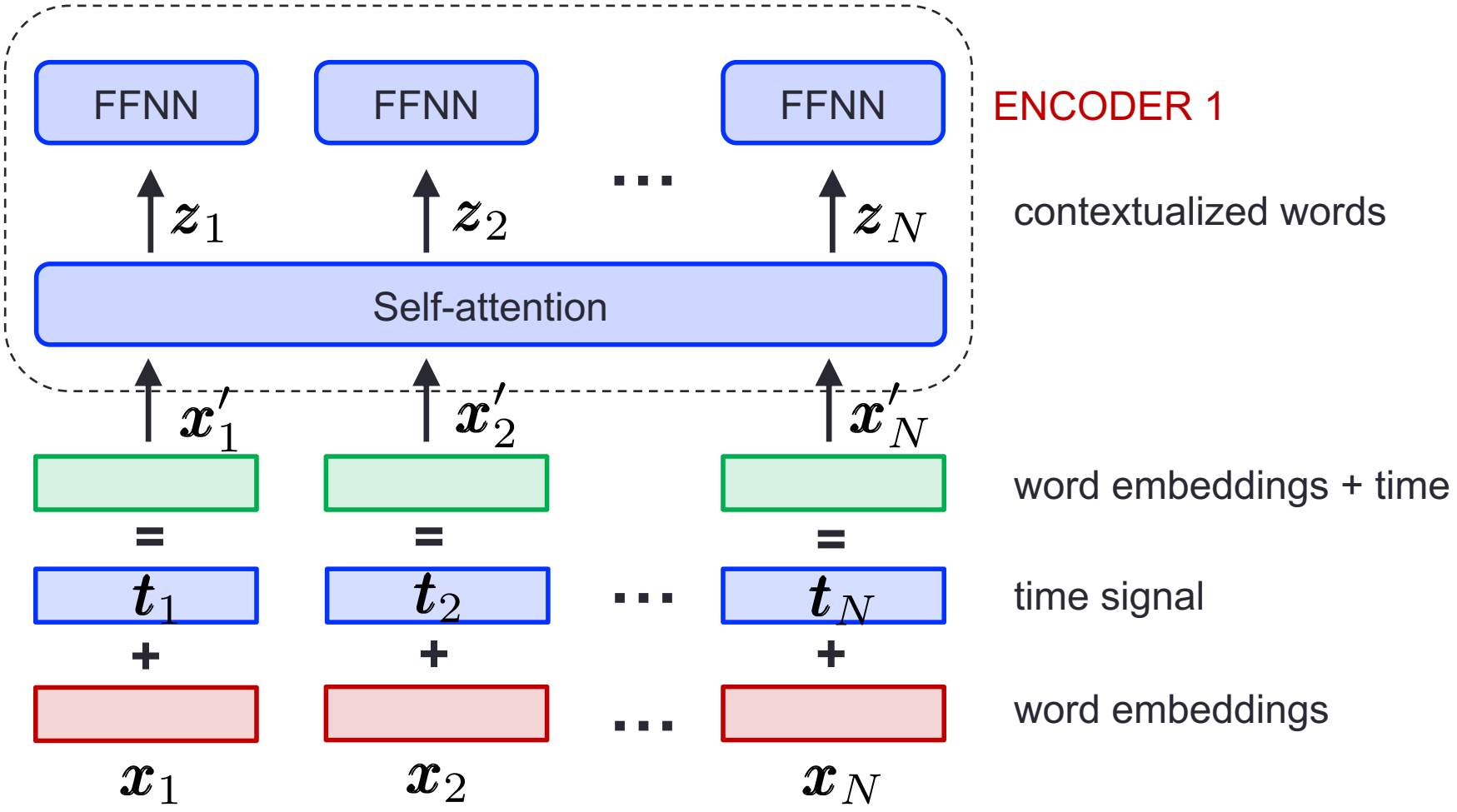
$$\boldsymbol{t}(n,2i+1) = \cos(n/10000^{2i/m})$$

Word embeddings + time signal

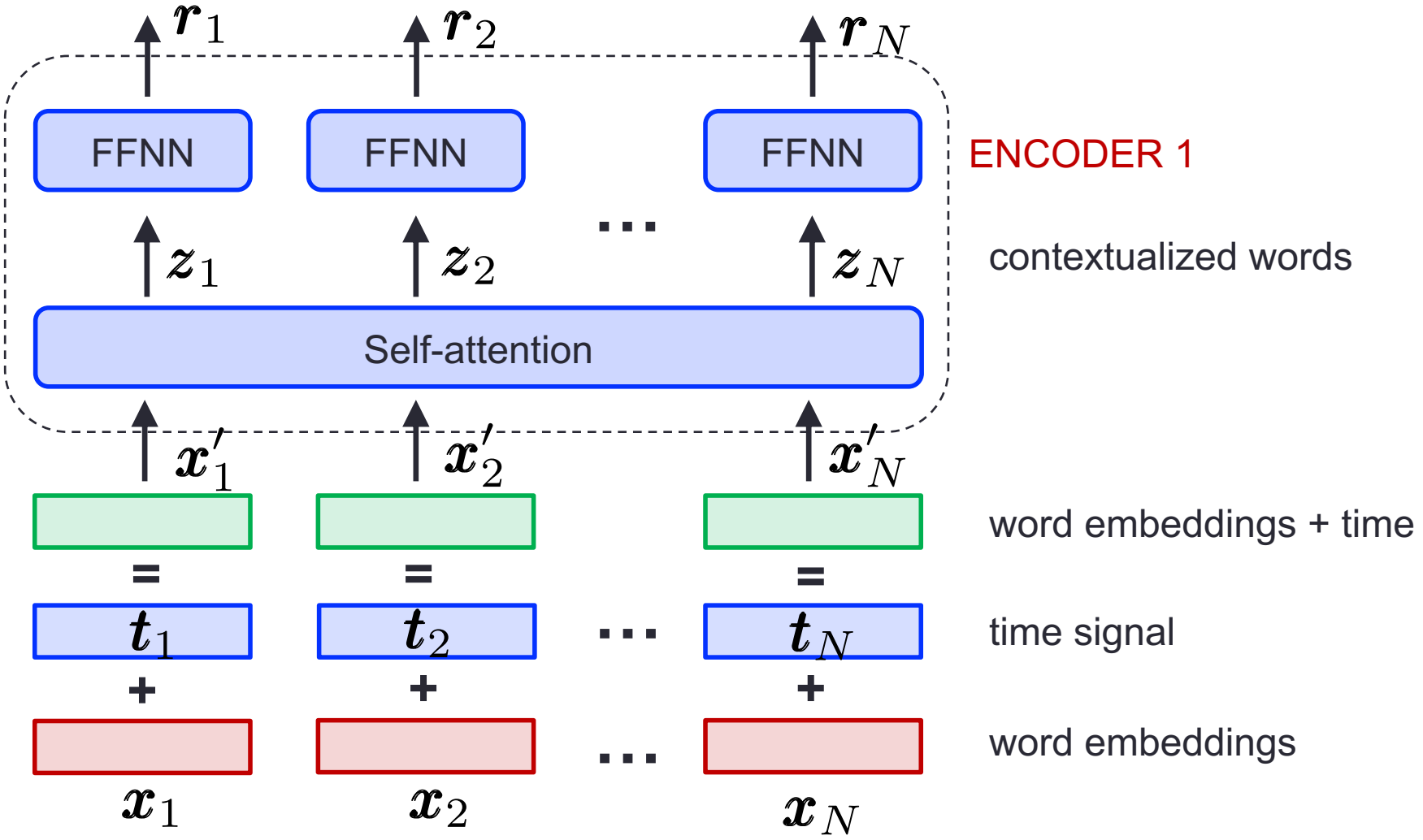


FFNN

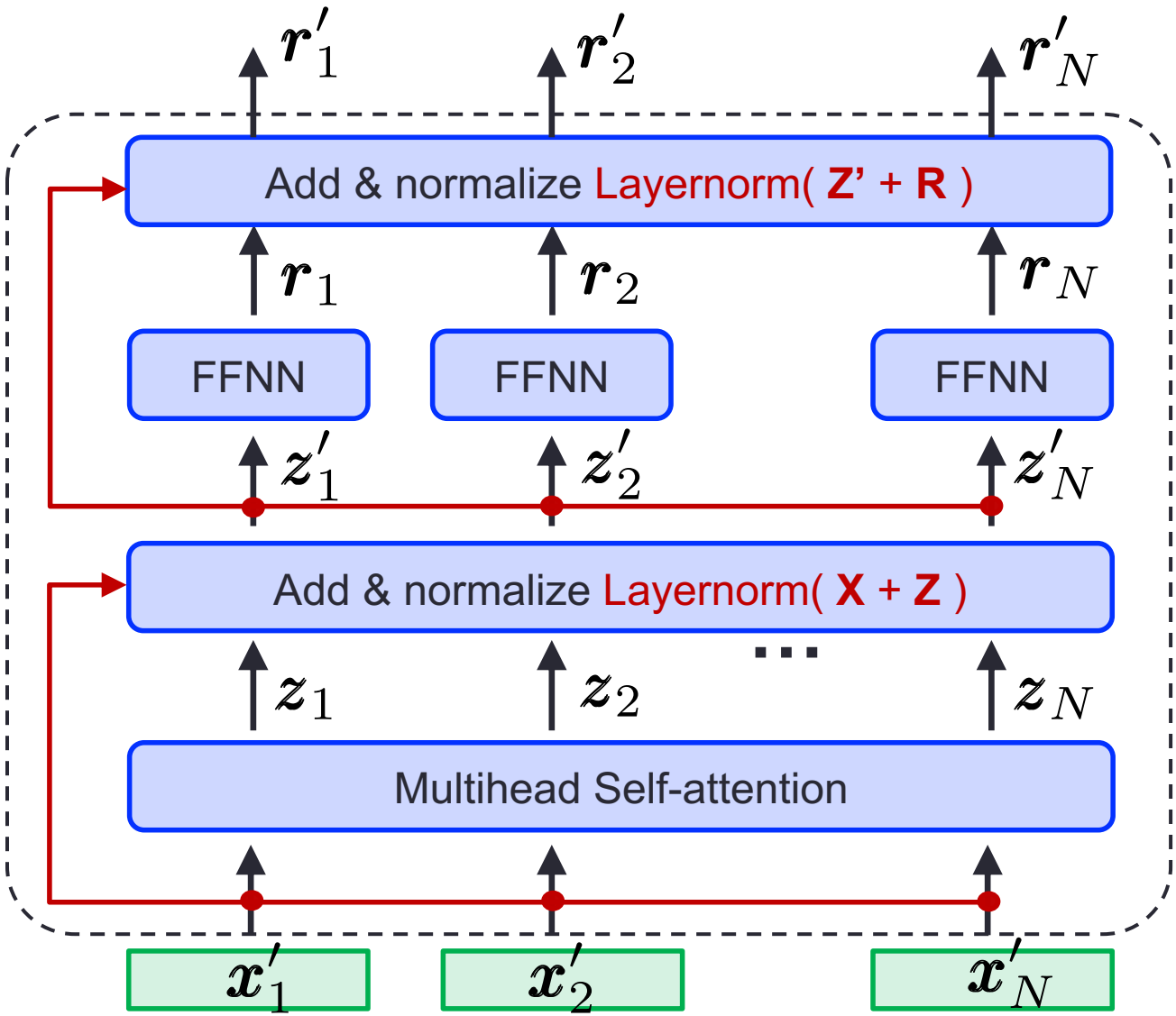
The same FFNN (same weights) is applied to each $\mathbf{z}_i$ independently. It consists of two linear transformations with a ReLU non-linearity in between. FFNN weights are shared across $\mathbf{z}_i$ but differ from layer to layer



$$\boldsymbol{r}_i = \text{FFNN}(\boldsymbol{z}_i) = \max(0, \boldsymbol{z}_i \boldsymbol{W}_1 + \boldsymbol{b}_1)\boldsymbol{W}_2 + \boldsymbol{b}_2$$



Residual connection and normalization



to ENCODER 2

ENCODER 1

REPEAT N TIMES

use **layer normalization**

contextualized words

word embeddings + time

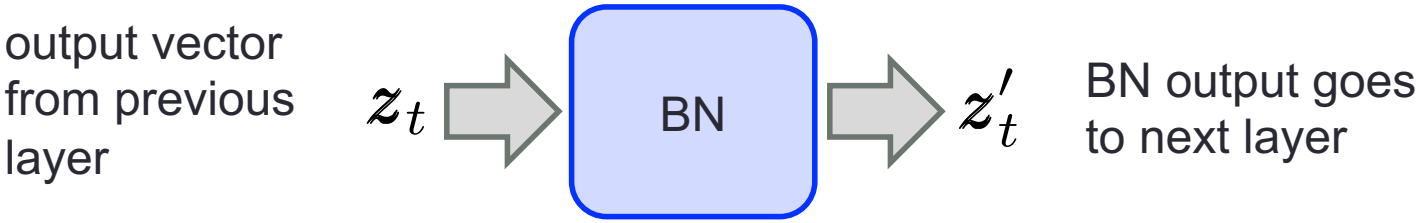
Batchnorm (BN)

- It is a technique proposed by Google in [Ioffe2015]
- Rescales vectors by first bringing them to
  - Zero mean (remove mean over a mini-batch)
  - Unit variance (over a mini-batch)
- Means and variances are computed on mini-batches
  - Two scaling parameters are learned to reshape the output vector
  - So that it works best (range and stdev) with the non-linearities at the following layer in the neural network architecture
- It largely improves learning speed and stability
- Often used in combination with residual (skip) connections

[Ioffe2015] S. Ioffe, C. Szegedy, "Batch Normalization: Accelerating Deep Network Training by Reducing Internal Covariate Shift," Proceedings of the 32nd Int. Conf. on Machine Learning (ICML), Lille, France, July 2015.

BN transform (1/2)

- At training time t, BN transforms input $\boldsymbol{z}_t$ into output $\boldsymbol{z}'_t$



- Input vector $\boldsymbol{z}_t = [z_t^{(1)}\ z_t^{(2)}\ \ldots\ z_t^{(H)}]^\top$ has H activations
- The BN transform is applied to each activation $z_t^{(k)}$ independently
- Next, we refer to activation k, by omitting the apex (k)
- For this specific activation, we refer to a mini-batch

$$\mathcal{B} = \{z_{1\ldots m}\}$$

BN transform (2/2)

- Let us consider any activation k (from 1, …, H)
- Input: values of for such activation over a mini-batch are: $\mathcal{B} = \{z_{1\ldots m}\}$
- Output values for the mini-batch are:

$$\{z_i' = \mathrm{BN}_{\gamma,\beta}(z_i), i = 1, \ldots, m\}$$

1) $\mu_{\mathcal{B}} = \frac{1}{m}\sum_{i=1}^{m} z_i$

2) $\sigma_{\mathcal{B}}^2 = \frac{1}{m}\sum_{i=1}^{m}(z_i - \mu_{\mathcal{B}})^2$

3) $\hat{z}_i \leftarrow \frac{z_i - \mu_{\mathcal{B}}}{\sqrt{\sigma_{\mathcal{B}}^2 + \epsilon}}$

normalize

4) $z_i' \leftarrow \gamma\hat{z}_i + \beta \triangleq \mathrm{BN}_{\gamma,\beta}(z_i)$

scale and shift

Layer normalization (LN) [Ba2016]

- For the transformer, LN is used in place of BN
- Same concept: rescale vectors
- However, mean and variance are *solely* computed using the current vector instead of using all the vectors in the mini-batch
- If a hidden layer has H units (activations) with current vector

$$\boldsymbol{z} = [z^{(1)}\ z^{(2)}\ \dots\ z^{(H)}]^\top$$

- LN computes

$$\mu = \frac{1}{H}\sum_{h=1}^{H} z^{(h)} \qquad \sigma = \sqrt{\frac{1}{H}\sum_{h=1}^{H}(z^{(h)} - \mu)^2}$$

[Ba2016] J. L. Ba, J. R. Kiros, G. E. Hinton, "Layer normalization," *Tech. Report*, arXiv:1607.06450v1, July 21, 2016.

Layer normalization (LN) [Ba2016]

- LN input $\boldsymbol{z} = [z^{(1)}\ z^{(2)}\ \ldots\ z^{(H)}]^\top$
  - LN computes

$$\mu = \frac{1}{H}\sum_{h=1}^{H} z^{(h)} \qquad \sigma = \sqrt{\frac{1}{H}\sum_{h=1}^{H}(z^{(h)} - \mu)^2}$$

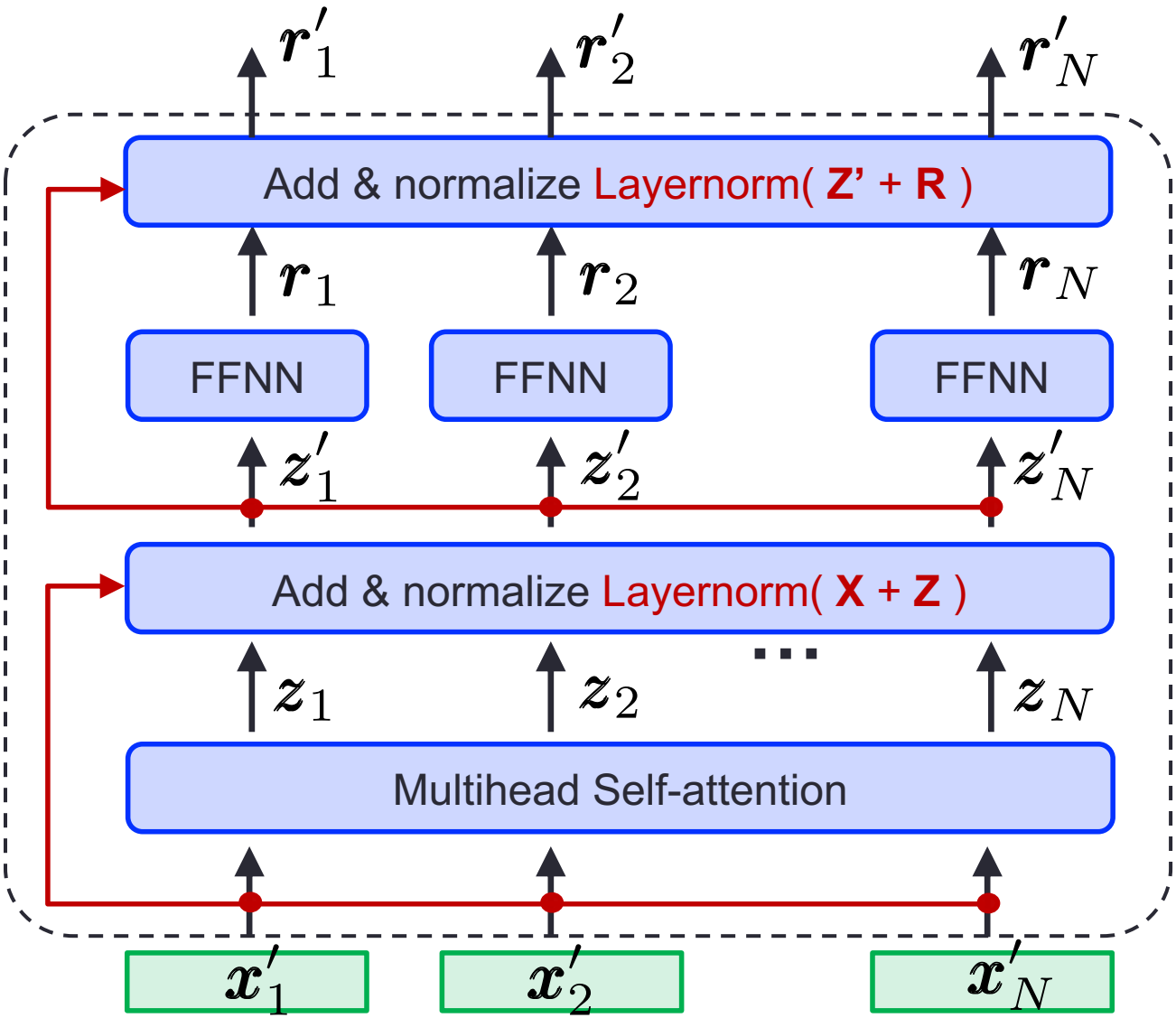
  - LN output is

$$\boldsymbol{z}' = \frac{\boldsymbol{g}}{\sigma} \odot (\boldsymbol{z} - \mu\mathbf{1}) + \boldsymbol{b}$$

  - where $\odot$ is the elementwise product, **g** and **b** are **gain** and **bias** vectors of the same dimension of **z** (**1** is the vector of all 1s)
  - **gain** and **bias**: are learned via backpropagation

[Ba2016] J. L. Ba, J. R. Kiros, G. E. Hinton, "Layer normalization," *Tech. Report*, arXiv:1607.06450v1, July 21, 2016.

LN in the transformer



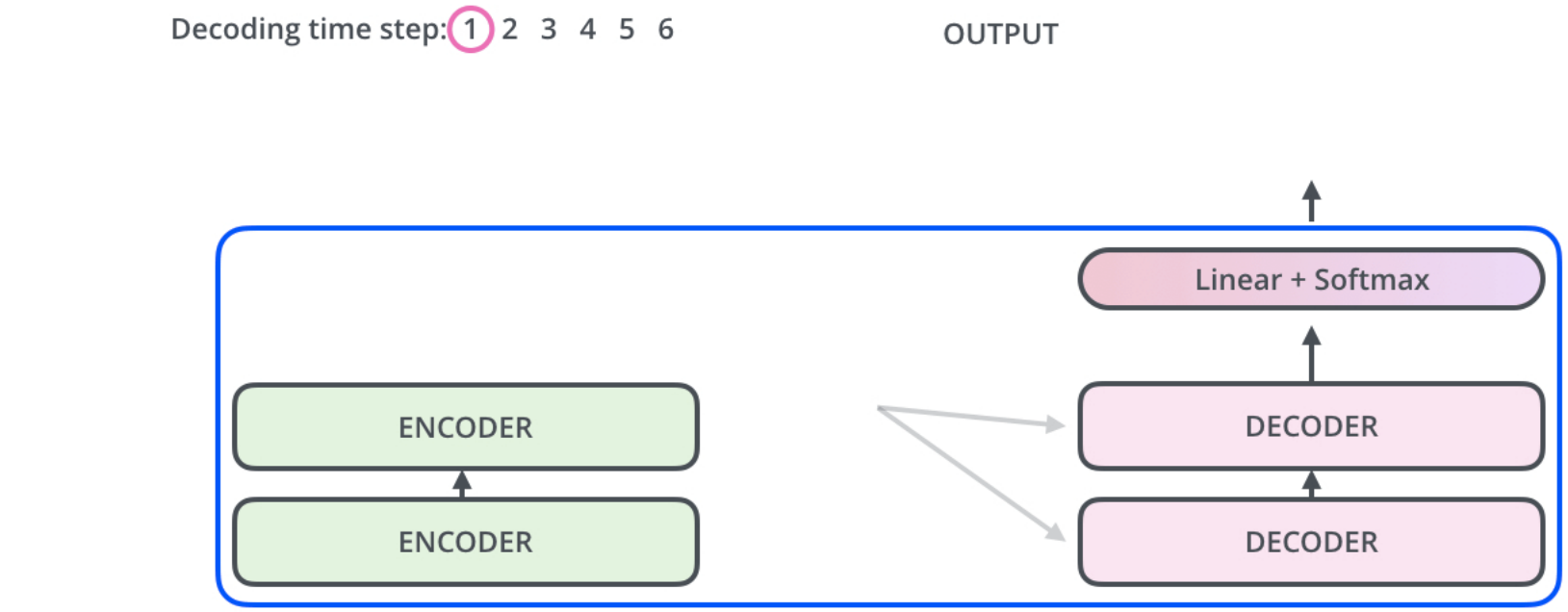
to ENCODER 2

ENCODER 1

LN is applied *element-wise* to all entries of current matrix **X+Z** (H corresponds to the no. of elements in such matrix)

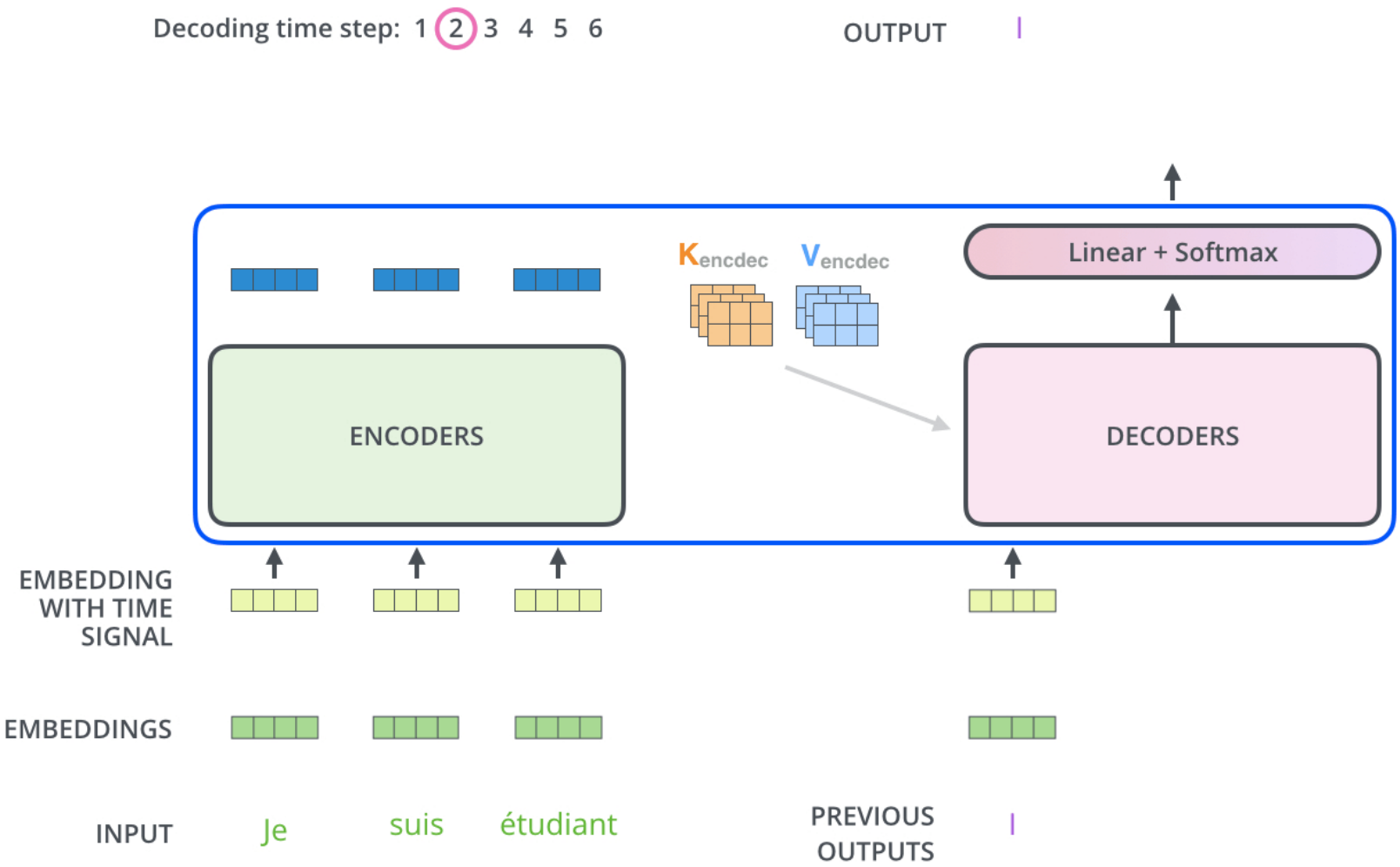
word embeddings + time

Encoder + decoder



The encoder start by processing the input sequence. The output of the top encoder is transformed into a set of attention vectors **K** and **V** (via linear projections). These are to be used by each decoder in its "encoder-decoder attention" layer which helps the decoder focus on appropriate places in the input sequence

Decoding: autoregressive process



Decoder output

- The decoder stack outputs vectors of floats
- How do we turn it into a final word?
- We use a linear (dense) layer
  - It is a simple fully connected NN: projects the vector produced by the stack of decoders into a much larger vector called the logits vector
  - If our vocabulary is, e.g., 10,000 words: this will be the size of the logits vector
- After that: a softmax layer turns the logits vector
  - into a vector of probabilities (one for each word in dictionary)
  - the cell with the highest probability is chosen as the output for the next time step

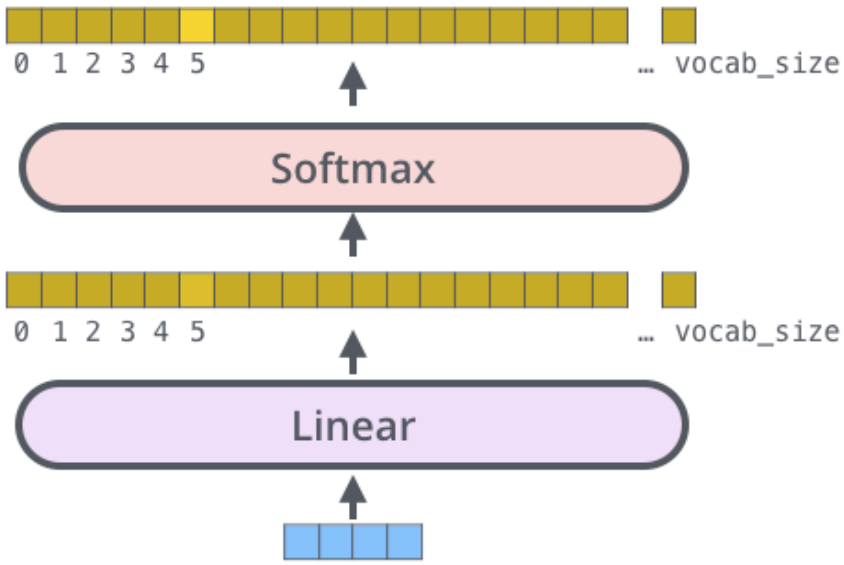
Decoder output

Which word in our vocabulary is associated with this index?

am

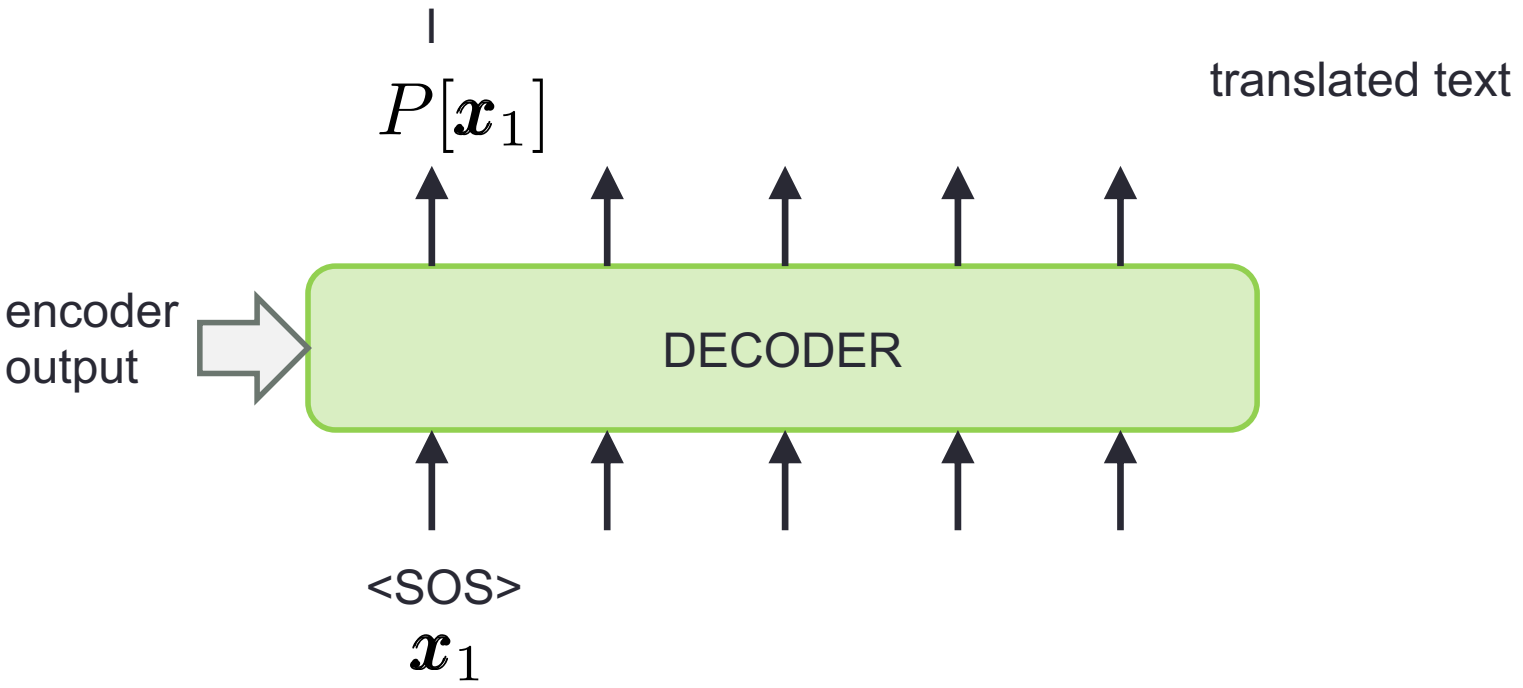
Get the index of the cell with the highest value (**argmax**)

5



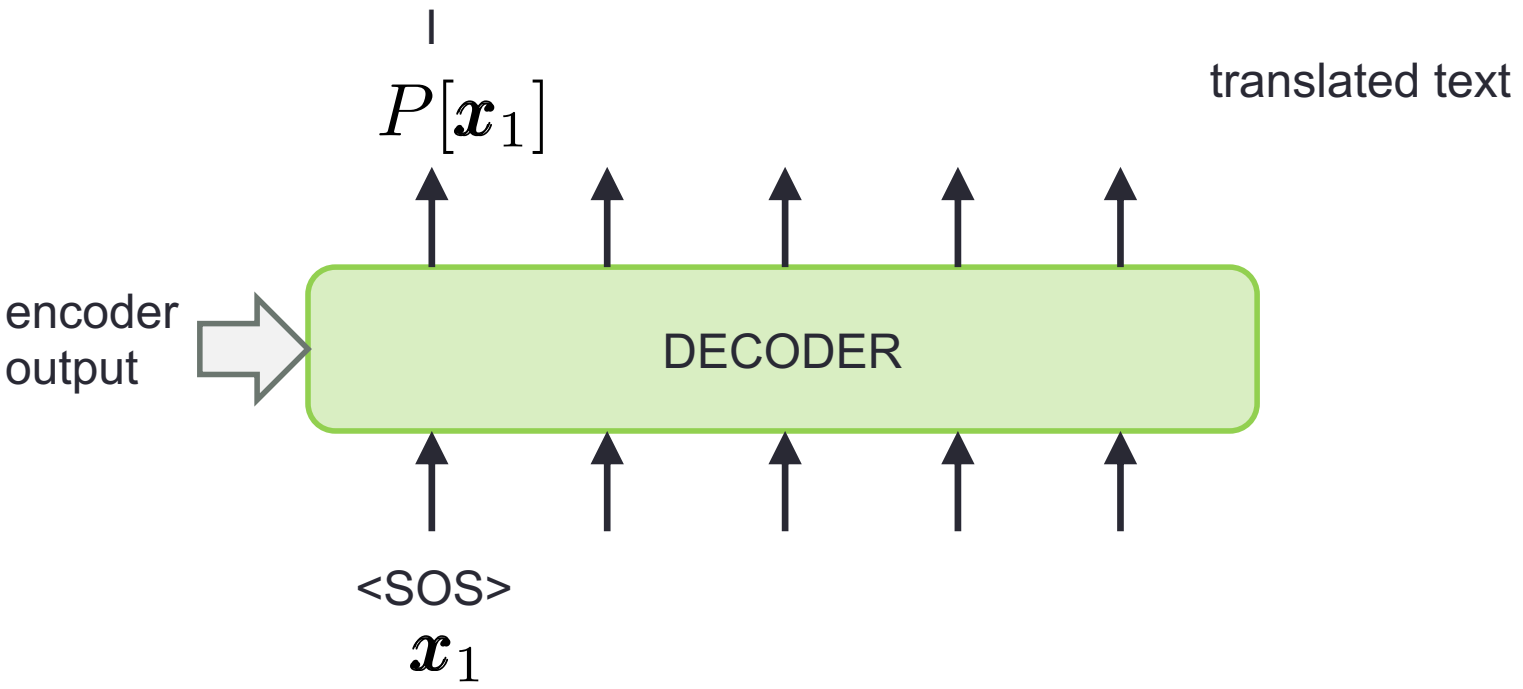
Decoder: masked self-attention

- The encoders obtain contextualized information over the whole sequence - it is used by the cross-attention blocks at the decoder to infer the next word in the translation
- Let's look at the traslation of the italian sequence "io ho una macchina" into English "I have a car"



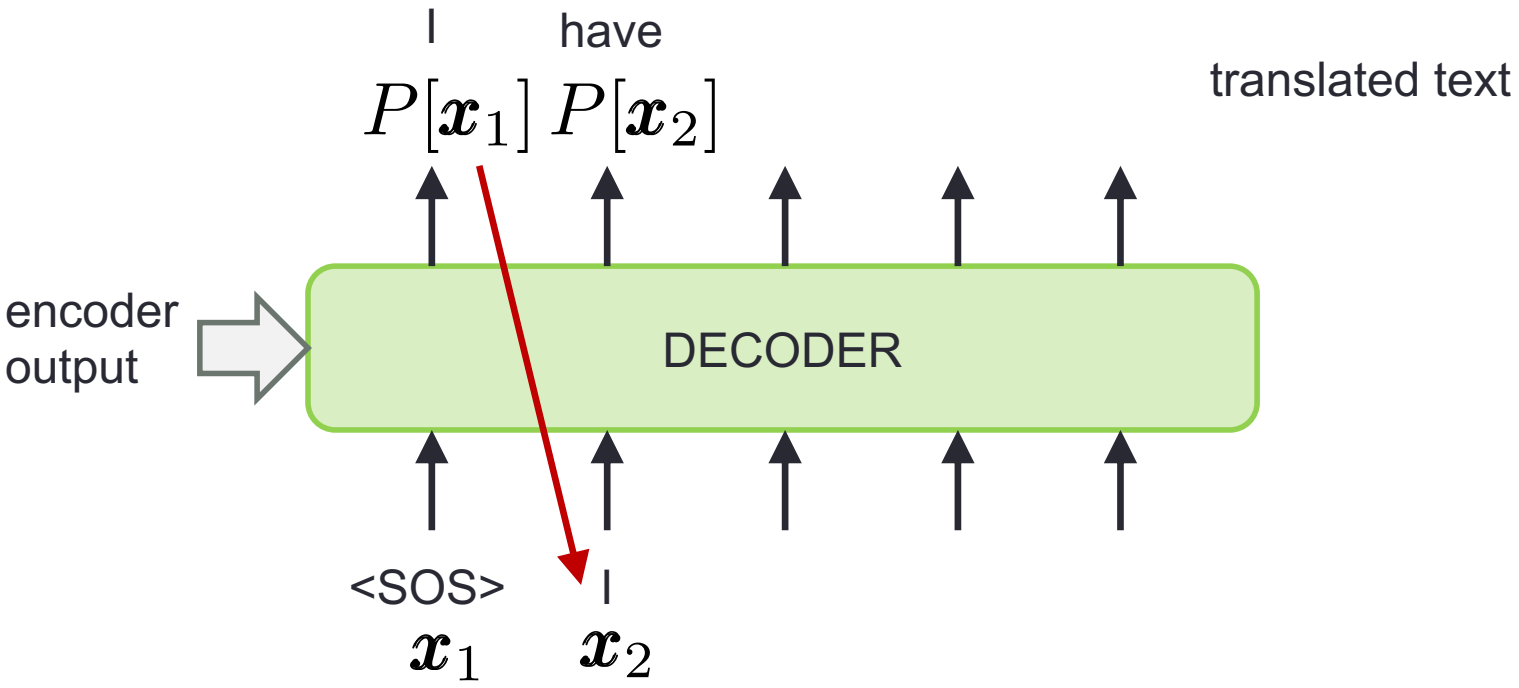
Decoder: masked self-attention

- As a first step, we input the start of sequence <SOS> symbol to the decoder: the first output should be “I” → the softmax should peak at the “I” word from the dictionary
- The output in this case is solely inferred from the encoder output



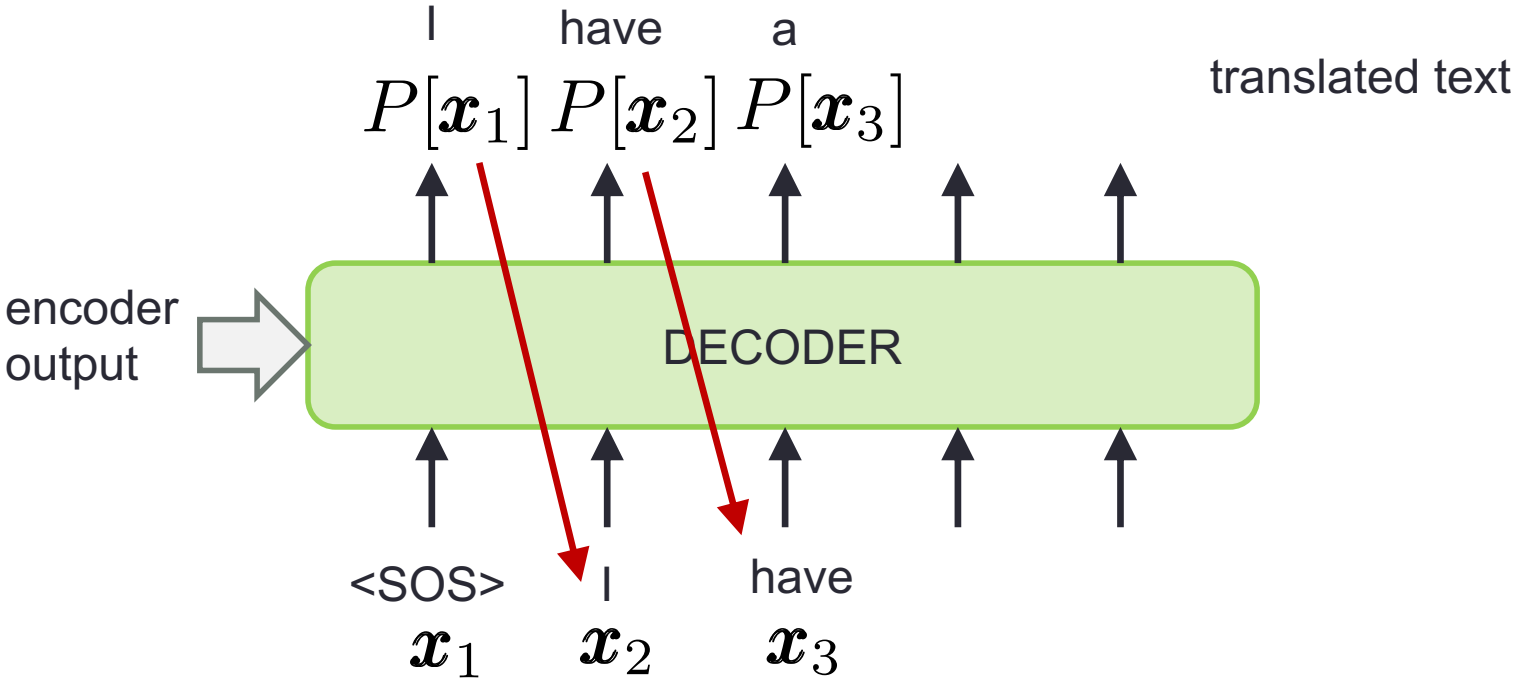
Decoder: masked self-attention

- **Step 2**: we autoregressively copy the word “I” to the next decoder input – the word “have” should now be inferred from
  - 1) the context from the encoder
  - 2) the previous decoded words <SOS> and “I”



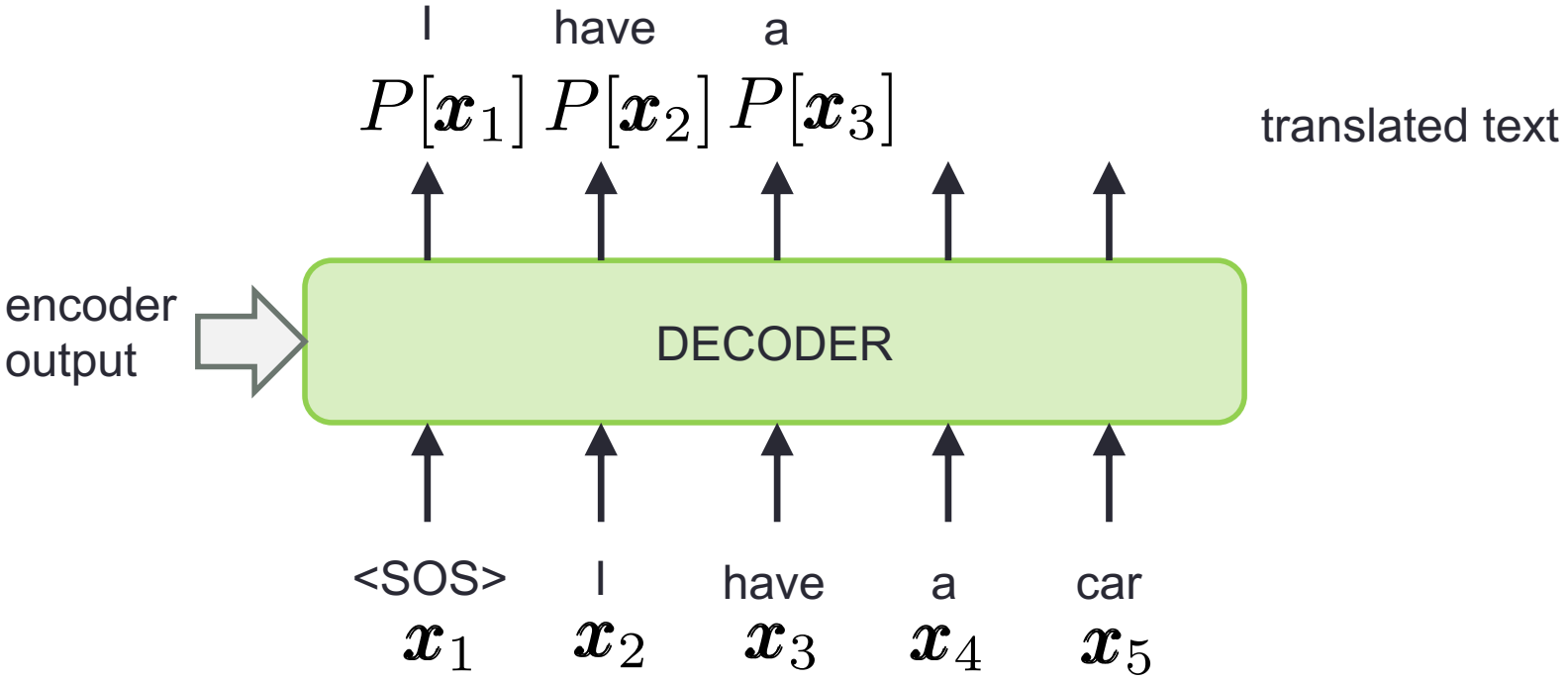
Decoder: masked self-attention

- **Step 3**: we autoregressively copy the word “have” to the next decoder input – the word “a” should now be inferred from
  - 1) the context from the encoder
  - 2) the previous decoded words <SOS>, “I” and “have”



Decoder: masked self-attention

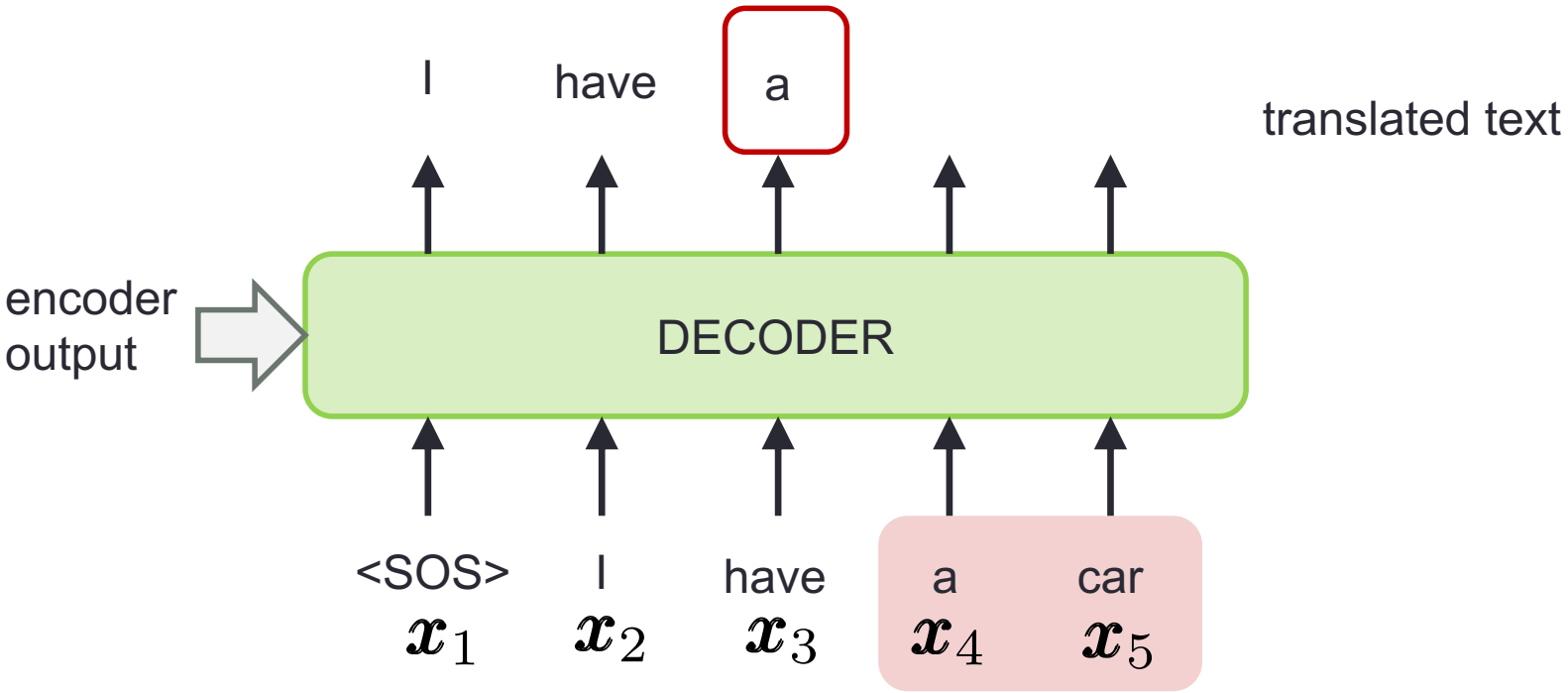
- At training time, the full translated sequence is available (label)
- However, we should train the decoder in order not to cheat



Decoder: masked self-attention

- Let training be at time 3 at the decoder side
- For this, only $\boldsymbol{x}_1$, $\boldsymbol{x}_2$ and $\boldsymbol{x}_3$ should be used

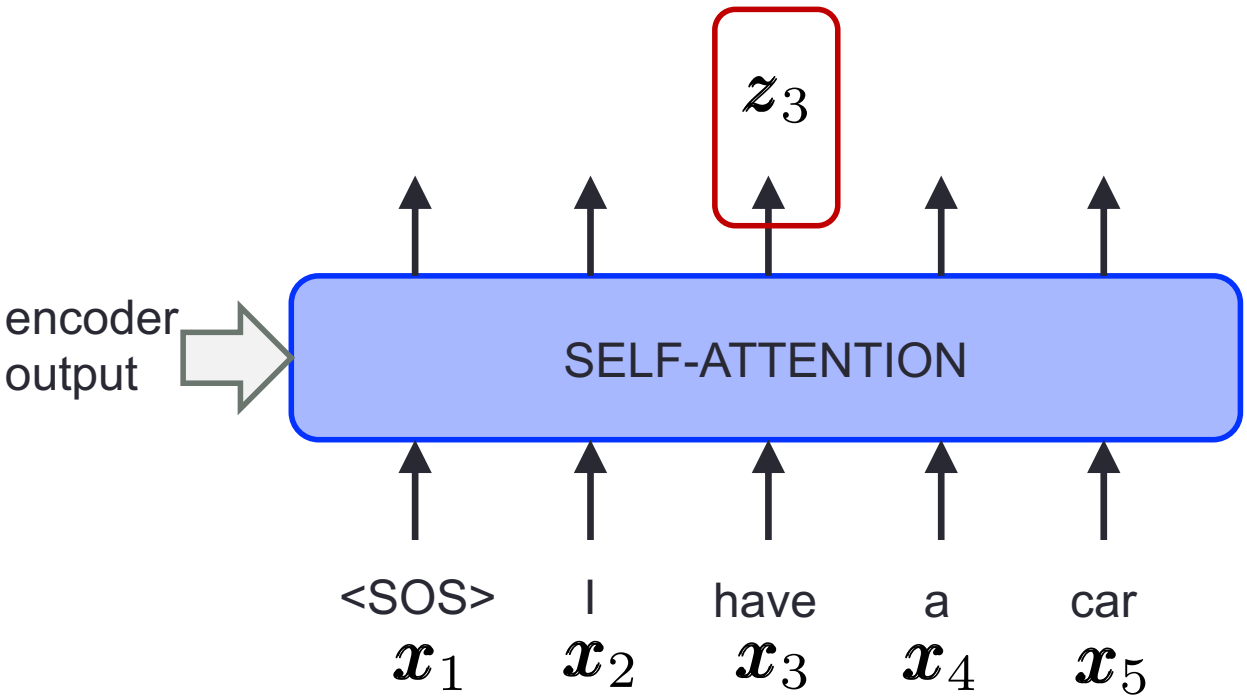
  → no access to $\boldsymbol{x}_4$ and $\boldsymbol{x}_5$



Decoder: masked self-attention

- Compute queries, keys, values. The scores are:

$$s_{31} = \frac{\boldsymbol{k}_1 \boldsymbol{q}_3^\top}{\sqrt{d}}, \ldots, s_{35} = \frac{\boldsymbol{k}_5 \boldsymbol{q}_3^\top}{\sqrt{d}}$$



Masked (normalized) weights

$$\begin{bmatrix} \alpha_{31} \\ \alpha_{32} \\ \alpha_{33} \\ \alpha_{34} \\ \alpha_{35} \end{bmatrix}^\top = \begin{bmatrix} \exp(s_{31})/S \\ \exp(s_{32})/S \\ \exp(s_{33})/S \\ 0 \\ 0 \end{bmatrix}^\top$$

$$S = \sum_{i=1}^{3} \exp(s_{3i})$$

$$\boldsymbol{z}_3 = \sum_{j=1}^{5} \alpha_{3j} \boldsymbol{v}_j$$

Decoder: masked self-attention

- Repeating for all $\mathbf{z}_i$
- The sofmax weights expressed in terms of matrix product are (sequence length = 5)

$$\boldsymbol{K} \times \boldsymbol{Q}^T = \begin{bmatrix} \alpha_{11} & 0 & 0 & 0 & 0 \\ \alpha_{21} & \alpha_{22} & 0 & 0 & 0 \\ \alpha_{31} & \alpha_{32} & \alpha_{33} & 0 & 0 \\ \alpha_{41} & \alpha_{42} & \alpha_{43} & \alpha_{44} & 0 \\ \alpha_{51} & \alpha_{52} & \alpha_{53} & \alpha_{54} & \alpha_{55} \end{bmatrix}$$

- It is implemented as a mask applied to the softmax weights
- by setting the weights s_{ij} = -infinity in the positions with 0 in the above matrix

Discussion

- The paper title says “Attention is all you need”
- This may be replaced with “Correlation is all you need”
- It looks like the correlation structure that is embedded into data sequences, images, sentences is the most important aspect to capture
- There are signs that (with advanced transformer architectures) this correlation also enables computational thinking and reasoning as a (rather unexpected) result

- Future results will unveil whether this is the case

Large Language Models (LLMs) Landscape

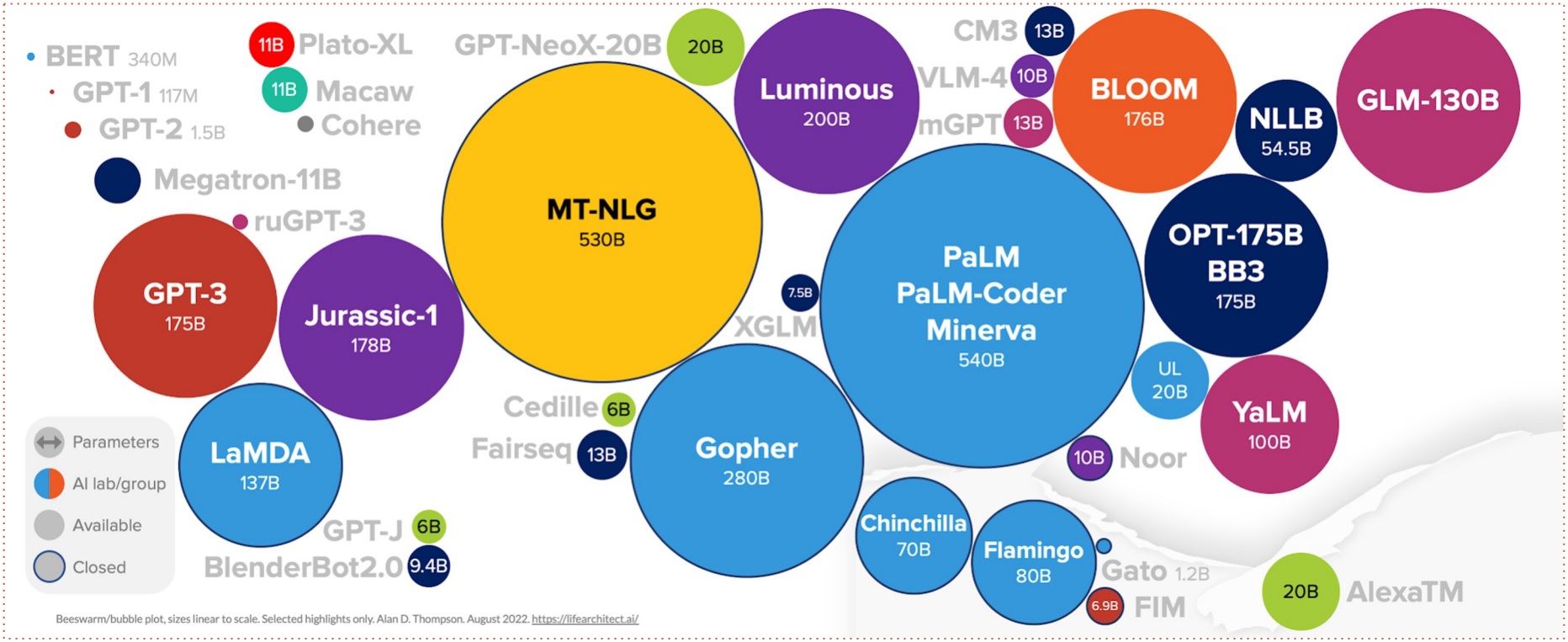


Figure: Alan D. Thompson, "Inside language models (from GPT-3 to PaLM)" (2022).

Optimal Large Language Models

DeepMind

Training Compute-Optimal Large Language Models

Jordan Hoffmann*, Sebastian Borgeaud*, Arthur Mensch*, Elena Buchatskaya, Trevor Cai, Eliza Rutherford, Diego de Las Casas, Lisa Anne Hendricks, Johannes Welbl, Aidan Clark, Tom Hennigan, Eric Noland, Katie Millican, George van den Driessche, Bogdan Damoc, Aurelia Guy, Simon Osindero, Karen Simonyan, Erich Elsen, Jack W. Rae, Oriol Vinyals and Laurent Sifre*

*Equal contributions

We investigate the optimal model size and number of tokens for training a transformer language model under a given compute budget. We find that current large language models are significantly under-trained, a consequence of the recent focus on scaling language models whilst keeping the amount of training data constant. By training over 400 language models ranging from 70 million to over 16 billion parameters on 5 to 500 billion tokens, we find that for compute-optimal training, the model size and the number of training tokens should be scaled equally: for every doubling of model size the number of training tokens should also be doubled. We test this hypothesis by training a predicted compute-optimal model, *Chinchilla*, that uses the same compute budget as *Gopher* but with 70B parameters and 4× more more data. *Chinchilla* uniformly and significantly outperforms *Gopher* (280B), GPT-3 (175B), Jurassic-1 (178B), and Megatron-Turing NLG (530B) on a large range of downstream evaluation tasks. This also means that *Chinchilla* uses substantially less compute for fine-tuning and inference, greatly facilitating downstream usage. As a highlight, *Chinchilla* reaches a state-of-the-art average accuracy of 67.5% on the MMLU benchmark, greater than a 7% improvement over *Gopher*.

CL] 29 Mar 2022

Optimal Large Language Models

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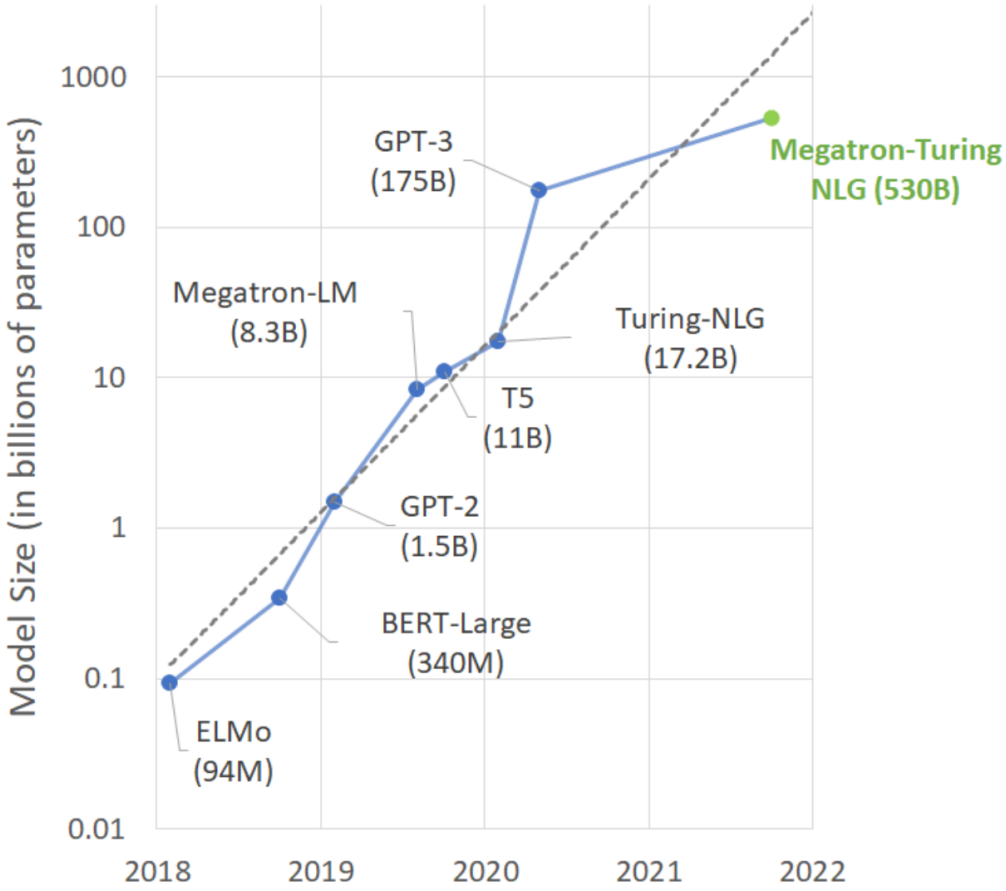
Table 1 | **Current LLMs**. We show five of the current largest dense transformer models, their size, and the number of training tokens. Other than LaMDA (Thoppilan et al., 2022), most models are trained for approximately 300 billion tokens. We introduce *Chinchilla*, a substantially smaller model, trained for much longer than 300B tokens.

Model	Size (# Parameters)	Training Tokens
LaMDA (Thoppilan et al., 2022)	137 Billion	168 Billion
GPT-3 (Brown et al., 2020)	175 Billion	300 Billion
Jurassic (Lieber et al., 2021)	178 Billion	300 Billion
Gopher (Rae et al., 2021)	280 Billion	300 Billion
MT-NLG 530B (Smith et al., 2022)	530 Billion	270 Billion
Chinchilla	70 Billion	1.4 Trillion

A new Moore law?



[Brown2022] Brown, T., Mann, B., Ryder, N., Subbiah, M., Kaplan, J. D., et al. "Using DeepSpeed and Megatron to Train Megatron-Turing NLG 530B, A Large-Scale Generative Language Model," arXiv 2201.11990v3 [cs.CL] 4 Feb 2022.

WHY *SCALED* DOT PRODUCTS?

Scaled dot products

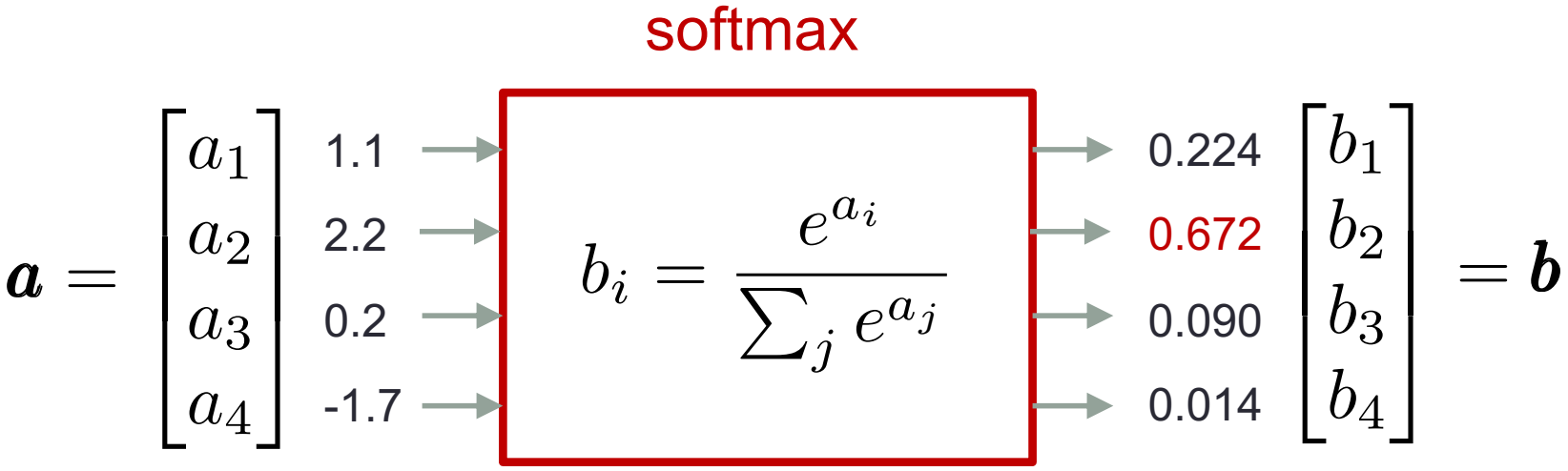
- In papers and books, you often read something like:

  "As you increase the number of dimensions, the dot products grows larger in magnitue → pushing the softmax function into regions where it has extreme gradients" [Kamath2022]

  EXTREME GRADIENTS?

Scaled dot products: softmax

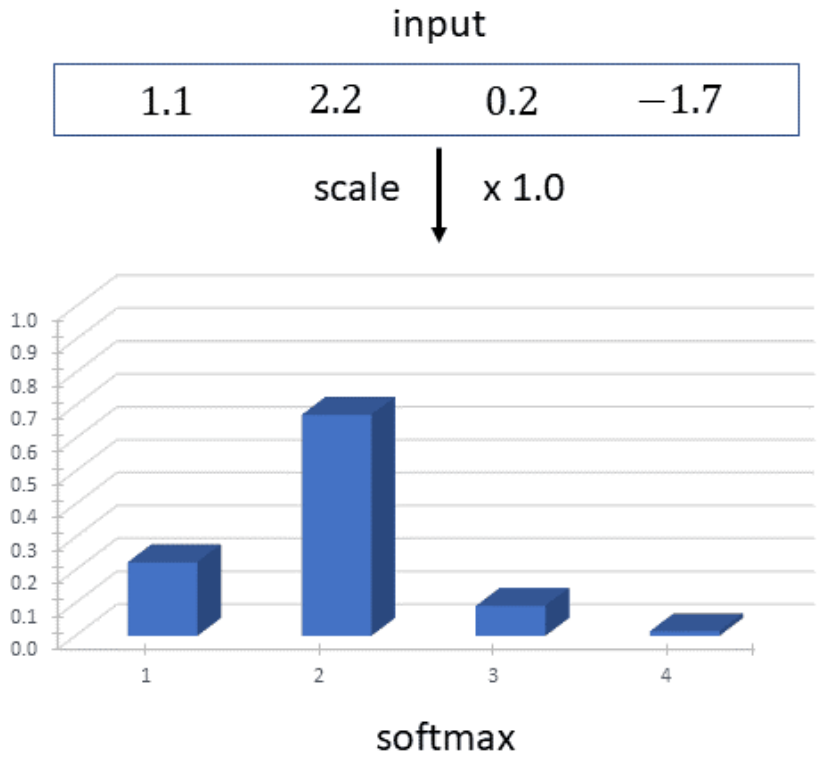
- To see this, let us take a look at the softmax function
- It is a vector function $\texttt{softmax} : \mathbb{R}^n \rightarrow \mathbb{R}^n$



$$b_i \in [0, 1], \sum_i b_i = 1$$

Scaled dot products: softmax

- softmax is NOT scale invariant, as shown here below



The higher we scale the input, the more the largest input dominates the softmax output → getting close to 1

If we reduce the scale factor, the outputs become very similar

Let's verify this

- Vectors of size n, pick an index j, γ=constant →

$$a_j = \gamma\,,\; a_i = \gamma - \varepsilon\,,\;\; \text{for } i \neq j\,,\; \text{with } 0 < \varepsilon \ll \gamma$$

- Now consider a scaled version (by factor K>0) of vector **a**

$$a'_i = K a_i\,,\; i = 1, \ldots, n\,,\; \text{with } K > 0$$

- The softmax applied to this scaled vector leads to

$$b_i = \frac{e^{-K\varepsilon}}{1 + (n-1)e^{-K\varepsilon}} \underset{K\to\infty}{\to} 0\,,\; i \neq j$$

$$b_j = \frac{1}{1 + (n-1)e^{-K\varepsilon}} \underset{K\to\infty}{\to} 1$$

- This means that small differences gets amplified for large K

Scaled dot products: softmax

- softmax
  - computing the Jacobian (gradient for a vector function)

$$\boldsymbol{J} = \begin{bmatrix} \frac{\partial b_1}{\partial a_1} & \frac{\partial b_1}{\partial a_2} & \cdots & \frac{\partial b_1}{\partial a_n} \\ \frac{\partial b_2}{\partial a_1} & \frac{\partial b_2}{\partial a_2} & \cdots & \frac{\partial b_2}{\partial a_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial b_n}{\partial a_1} & \frac{\partial b_n}{\partial a_2} & \cdots & \frac{\partial b_n}{\partial a_n} \end{bmatrix}$$

  - It can be proven than (see Appendix B)

$$\frac{\partial b_i}{\partial a_j} = b_i(\delta_{i,j} - b_j)\,,\; i,j = 1,\ldots,n$$

Scaled dot products: softmax

- softmax
  - computing the Jacobian (gradient for a vector function), with n=4

$$\boldsymbol{J} = \begin{bmatrix} b_1(1-b_1) & -b_1 b_2 & -b_1 b_3 & -b_1 b_4 \\ -b_2 b_1 & b_2(1-b_2) & -b_2 b_3 & -b_2 b_4 \\ -b_3 b_1 & -b_3 b_2 & b_3(1-b_3) & -b_3 b_4 \\ -b_4 b_1 & -b_4 b_2 & -b_4 b_3 & b_4(1-b_4) \end{bmatrix}$$

  - Where it holds:

$$\frac{\partial b_i}{\partial a_j} = b_i(\delta_{i,j} - b_j)\,,\; i,j = 1,\ldots,n$$

Kronecker delta

Scaled dot products: softmax

- softmax
  - computing the Jacobian (gradient for a vector function), with n=4

$$\boldsymbol{J} = \begin{bmatrix} b_1(1-b_1) & -b_1 b_2 & -b_1 b_3 & -b_1 b_4 \\ -b_2 b_1 & b_2(1-b_2) & -b_2 b_3 & -b_2 b_4 \\ -b_3 b_1 & -b_3 b_2 & b_3(1-b_3) & -b_3 b_4 \\ -b_4 b_1 & -b_4 b_2 & -b_4 b_3 & b_4(1-b_4) \end{bmatrix}$$

- The Jacobian is symmetric
- Diagonal elements become zero when any of the b_j takes the value 0 or 1

Scaled dot products: softmax

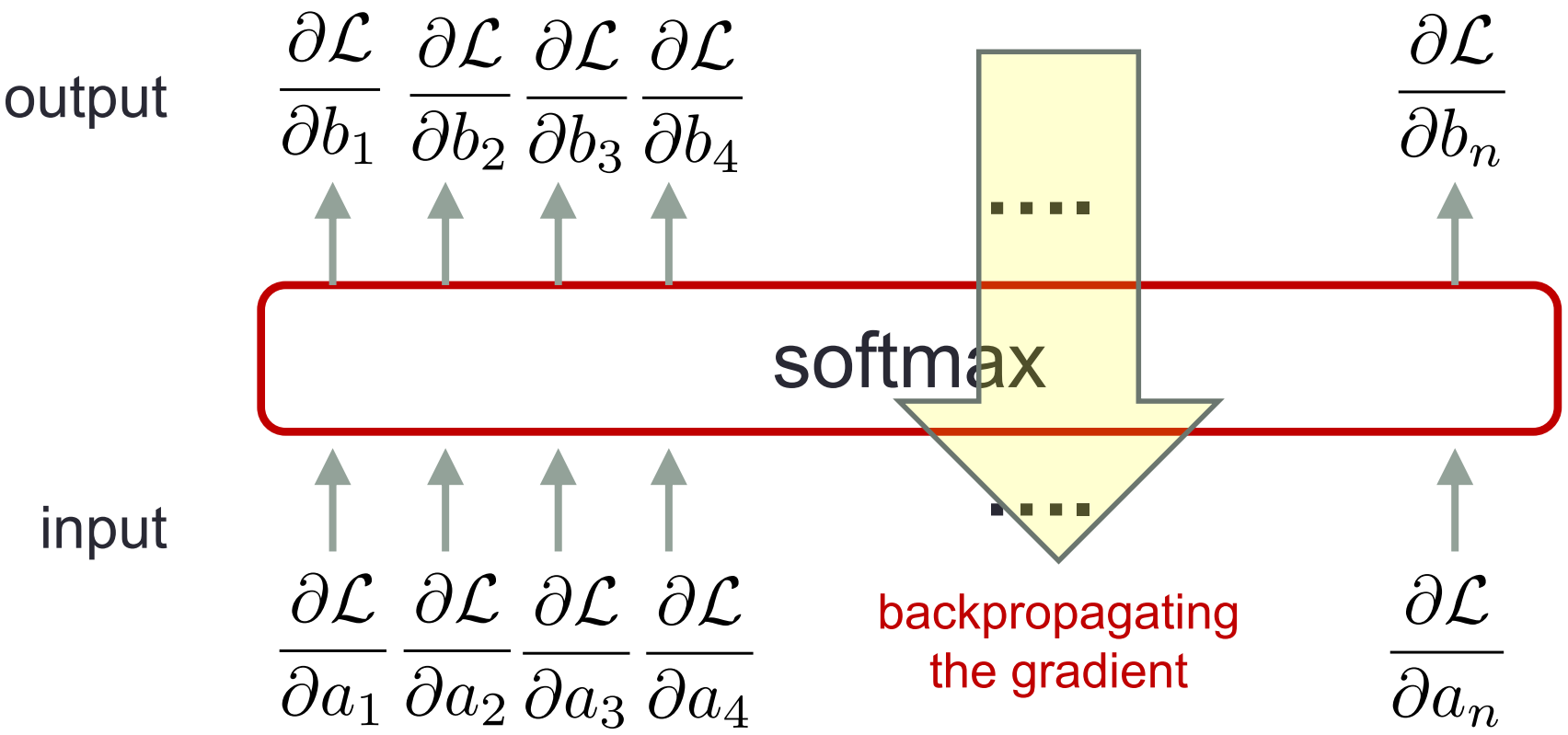
- It follows that
  - **J** becomes the zero matrix in any of the following four output vector cases

$$\boldsymbol{b}_a = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad \boldsymbol{b}_b = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} \quad \boldsymbol{b}_c = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} \quad \boldsymbol{b}_d = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

  - For large input values → softmax generates outputs that closely resemble the above configurations (the largest input value tends to dominate the sofmax output)

Backpropagation through a softmax layer

- During backpropagation
  - We backpropagate the error gradient from output to input of the softmax layer (as we do for any other layer)



Backpropagation through a softmax layer

- Using the chain rule of derivatives, we write

$$\frac{\partial \mathcal{L}}{\partial a_j} = \sum_{i=1}^{n} \frac{\partial \mathcal{L}}{\partial b_i} \times \frac{\partial b_i}{\partial a_j} = \begin{bmatrix} \frac{\partial b_1}{\partial a_j} & \frac{\partial b_2}{\partial a_j} & \cdots & \frac{\partial b_n}{\partial a_j} \end{bmatrix} \cdot \begin{bmatrix} \frac{\partial \mathcal{L}}{\partial b_1} \\ \frac{\partial \mathcal{L}}{\partial b_2} \\ \vdots \\ \frac{\partial \mathcal{L}}{\partial b_n} \end{bmatrix}$$

- The row vector on the right size of this equation is the j-th column (transposed) of the Jacobian matrix **J**

- Given this, in vector form it holds

$$\frac{\partial \mathcal{L}}{\partial \boldsymbol{a}} = \boldsymbol{J}^T \cdot \frac{\partial \mathcal{L}}{\partial \boldsymbol{b}}$$

Backprop outcome

- Backprop works by moving the error gradient from output layer to input layer according to

$$\frac{\partial \mathcal{L}}{\partial \boldsymbol{a}} = \boldsymbol{J}^T \cdot \frac{\partial \mathcal{L}}{\partial \boldsymbol{b}}$$

- When softmax input values grow in magnitude → the output emphasizes the largest input element that gets close to 1 and the remaining elements get close to 0
- In this situation the **J** matrix tends to the **0** matrix and the gradient gets killed by the softmax layer
- As a consequence, all elements coming before the softmax layer slow down learning or even stop learning all together

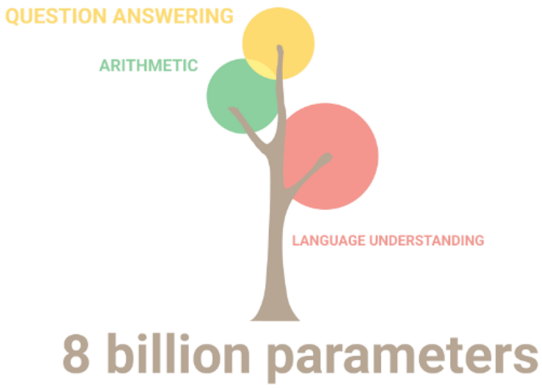
Solution to vanishing softmax gradient

- In the original transformer paper [Vaswani2017]
  - The input to the softmax corresponds to the result of the **dot product** between *key vectors* and *query vectors* (of the same dimension d=64)
  - The larger the dimension d of such vectors, the larger the dot product will tend to be
  - The remedy used by the authors is to divide the dot product by the square root of the dimension d
  - In this way, learning will not be affected by the gradient vanishing problem

This shows how a small detail can have a huge impact

MORE APPLICATIONS AND TRENDS

The growing tree of capabilities…

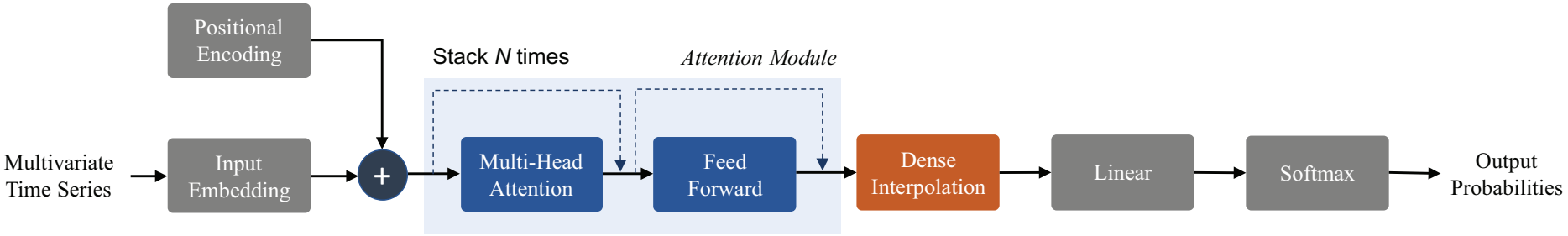


Chowdhery, A., Narang, S., Devlin, J., Bosma, M., Mishra, G., Roberts, A., et al. (2022). "PaLM: Scaling Language Modeling with Pathways," arXiv2203.

https://blog.research.google/2022/04/pathways-language-model-palm-scaling-to.html

Attend and diagnose [Song2018]

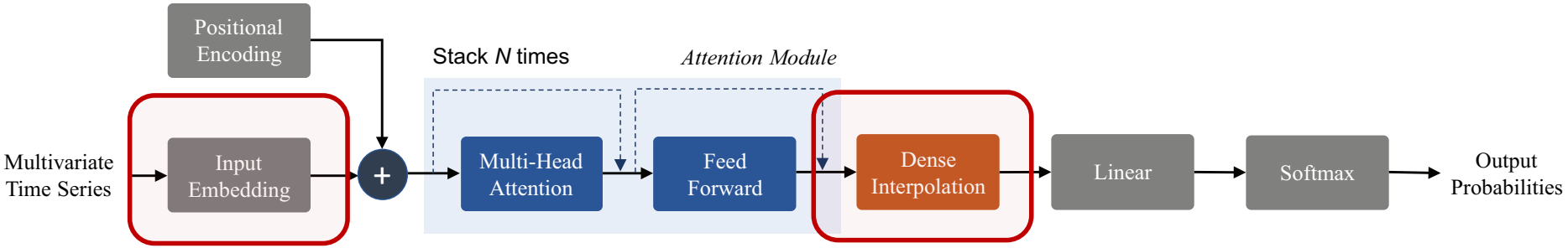
- Uses transformer model: encoder-only architecture
- Takes multivariate time series (input)
- Returns class probability estimates or regression
  - Depending on the configuration of the last layer



[Song2018] H. Song, D. Rajan, J.J. Thiagarajan, A. Spanias, "Attend and diagnose: clinical time-series analysis using attention models," Proc. of Thirty-Second AAAI Conference on Artificial Intelligence (AAAI-18), 2018. Github: https://github.com/khirotaka/SAnD/

Attend and diagnose [Song2018]

- Only two differences with respect to transformer are
  - Input embedding
  - Dense interpolation



[Song2018] H. Song, D. Rajan, J.J. Thiagarajan, A. Spanias, “Attend and diagnose: clinical time-series analysis using attention models,” Proc. of Thirty-Second AAAI Conference on Artificial Intelligence (AAAI-18), 2018.

Input embedding

- T time steps
- Input vectors at time t are $\boldsymbol{x}_t \in \mathbb{R}^m$, with t=1,…,T
- Input embedding
  - Transform (1D convolution) from input vectors to output vector
  - Using a kernel size of 1, this is equivalent to projecting the input vector into a higher dimensional space of size d>m
  - Number of output channels C_{in}=m
  - Number of input channels C_{out}=d

cross-correlation

$$\boldsymbol{y}_t[j] = \text{bias}[j] + \sum_{k=0}^{C_{\text{in}}-1} w(j,k) \star \boldsymbol{x}_t[k]\,,\; j = 0, \ldots, C_{\text{out}} - 1$$

output vector

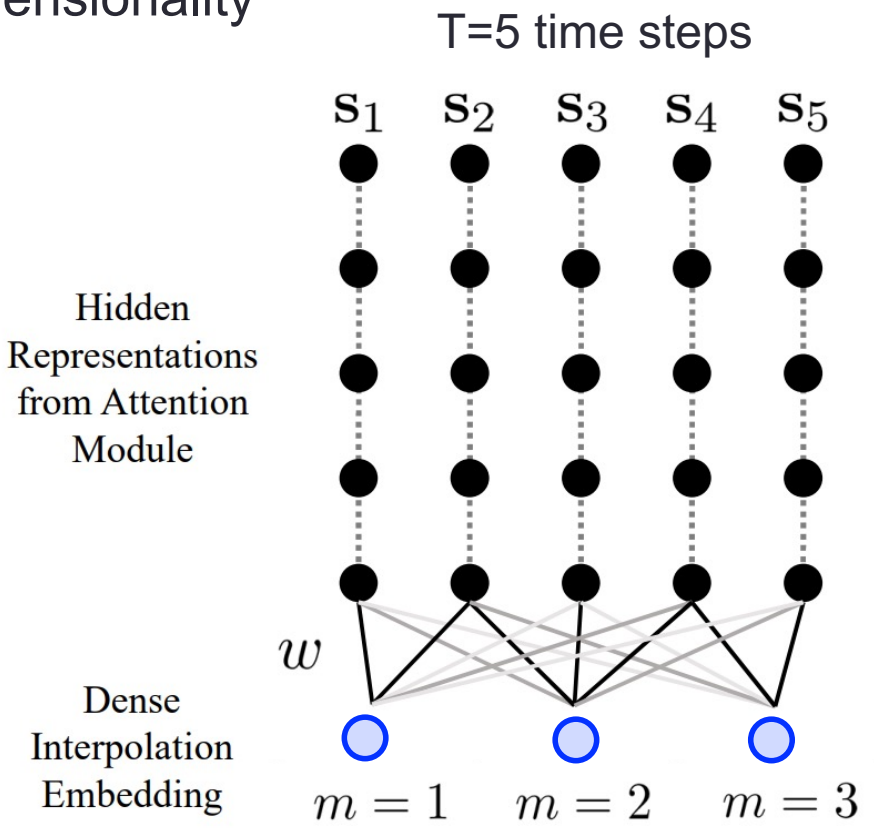
bias for out channel j

convolution weights

input vector k-th element

Dense interpolation

- Interpolation of hidden vectors from the last attention block
  - Interpolation weights predefined
  - implemented to reduce the dimensionality



The speech transformer

SPEECH-TRANSFORMER: A NO-RECURRENCE SEQUENCE-TO-SEQUENCE MODEL FOR SPEECH RECOGNITION

Linhao Dong[1,2], *Shuang Xu*[1], *Bo Xu*[1]

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ABSTRACT

Recurrent sequence-to-sequence models using encoder-decoder architecture have made great progress in speech recognition task. However, they suffer from the drawback of slow training speed because the internal recurrence limits the training parallelization. In this paper, we present the Speech-Transformer, a no-recurrence sequence-to-sequence model entirely relies on attention mechanisms to learn the positional dependencies, which can be trained faster with more efficiency. We also propose a 2D-Attention mechanism, which can jointly attend to the time and frequency axes of the 2-dimensional speech inputs, thus providing more expressive representations for the Speech-Transformer. Evaluated on the Wall Street Journal (WSJ) speech recognition dataset, our best model achieves competitive word error rate (WER) of 10.9%, while the whole training process only takes 1.2 days on 1 GPU, significantly faster than the published results of recurrent sequence-to-sequence models.

Index Terms— Speech Recognition, Sequence-to-Sequence, Attention, Transformer

1. INTRODUCTION

In speech recognition field, sequence-to-sequence (seq2seq) mod-

Recently, Vaswani et al. [17] proposed a no-recurrence sequence-to-sequence model, called the Transformer, which achieved state-of-the-art performance on WMT 2014 English-to-French translation task with markedly less training cost. Its fundamental module is self-attention, a mechanism relates all the position-pairs of a sequence to extract a more expressive sequence representation. Since the self-attention can draw the dependencies between different positions through the position-pair computation rather than the position-chain computation of RNNs, it just needs to be calculated once to obtain the transformed representation, rather than be computed one by one in RNNs. Therefore, the Transformer relying solely on attention mechanisms can be trained faster with more parallelization, which is exactly needed by the seq2seq models in automatic speech recognition (ASR).

In this paper, we successfully introduce the Transformer to ASR task and we term our model the Speech-Transformer, a new seq2seq model that transforms speech feature sequences to the corresponding character sequences. Additionally, we propose a 2D-Attention mechanism, which is inspired by the time-frequency LSTM in [18] but replaces the time-frequency recurrence with both the temporal and spectral dependencies captured by attention. By deploying the WSJ speech recognition dataset, we find our proposed 2D-Attention mechanism achieves better performance than the convolutional networks in [5], thus providing a more discriminated representation for

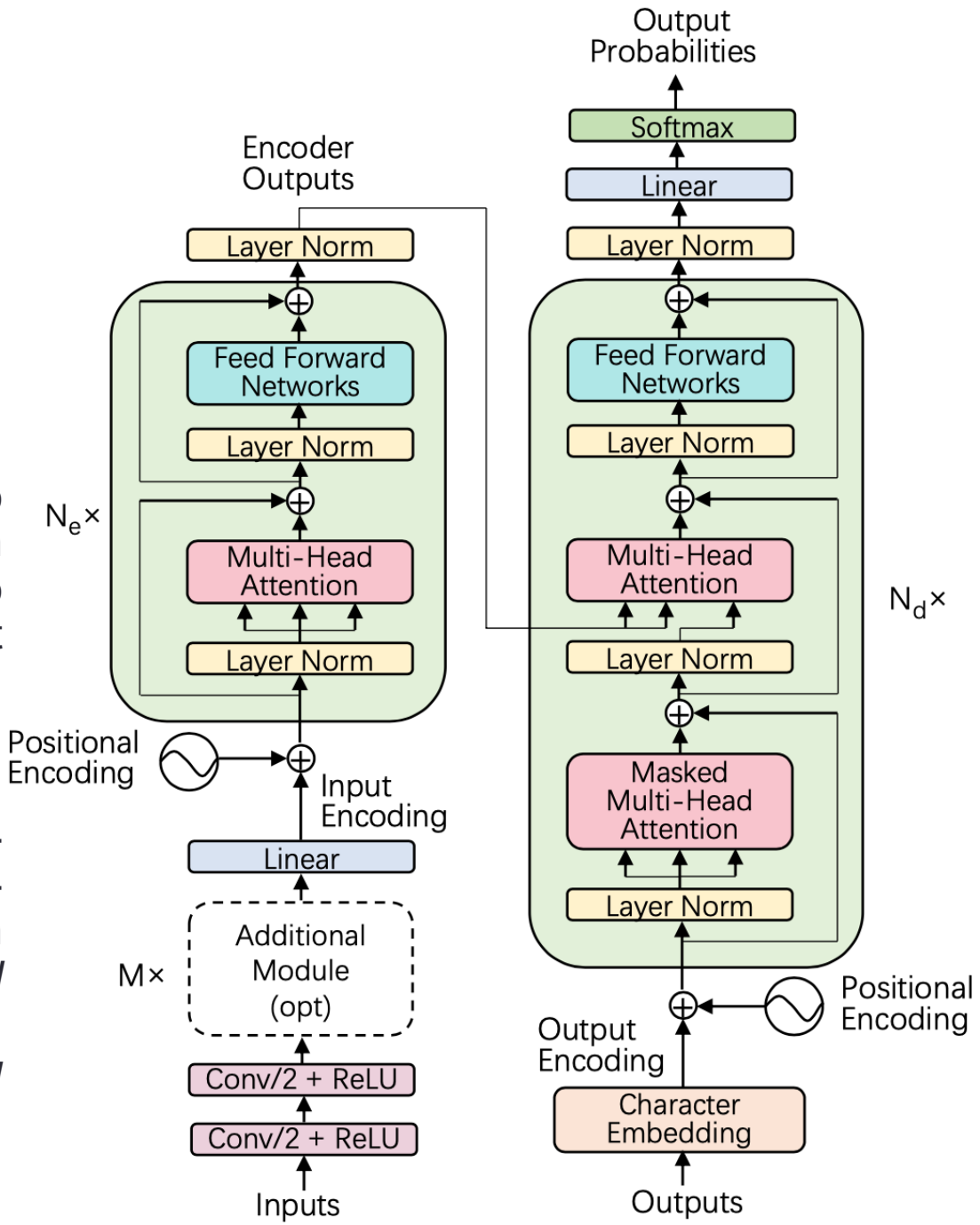
Architecture

Standard transformer model

Only differences are

- Input is a spectrogram
- 2D convolutions used to process it (stride 2 along both time and frequency axes to reduce size and make it comparable with that of output)

[Dong2018] L. Dong, S. Xu, B. Xu, "Speech transformer: a no-recurrence sequence-to-sequence model for speech recognition," *IEEE International Conference on Acoustics, Speech and Signal Processing (ICASSP)*, 2018.



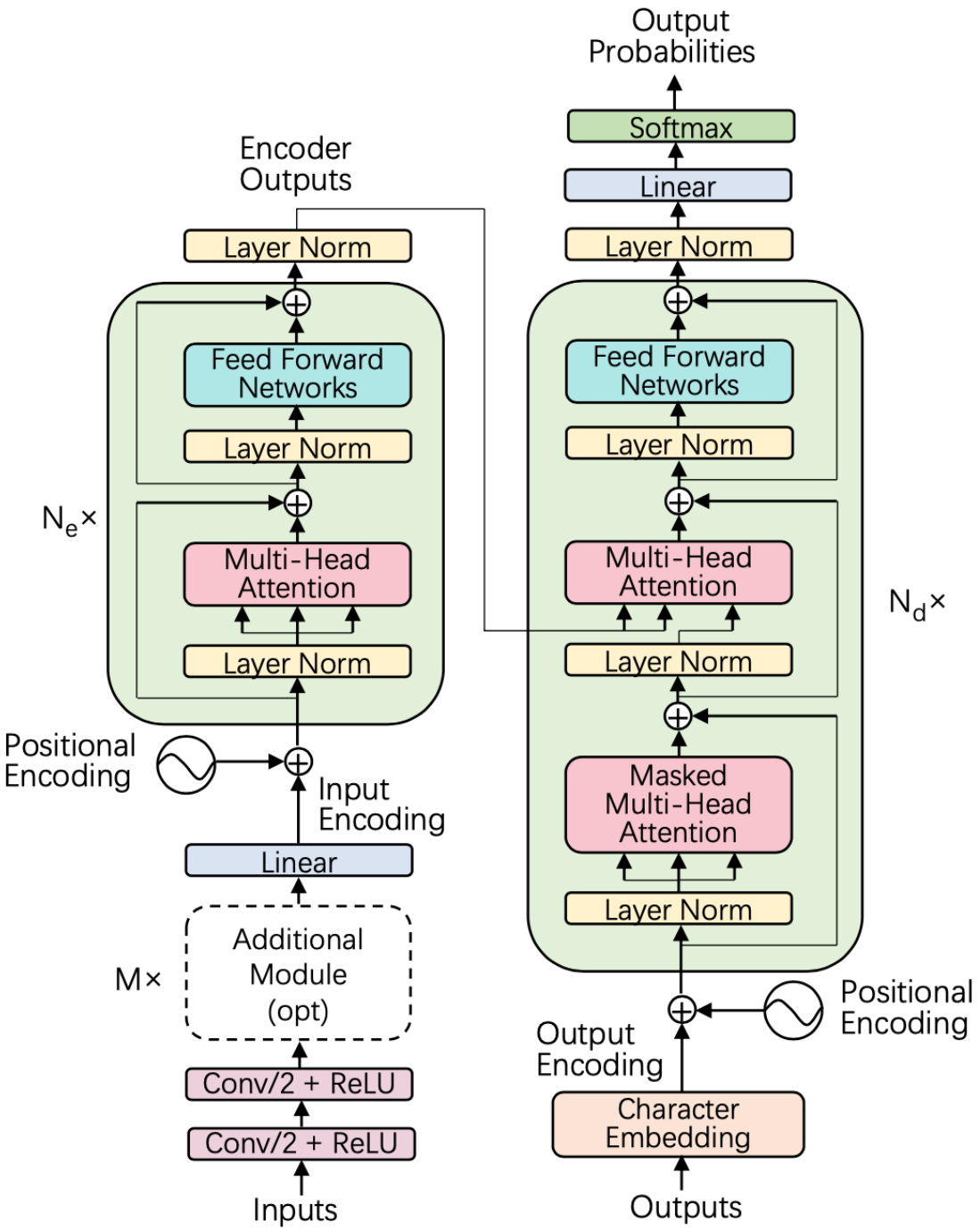
Architecture

Convolution: 3x3 with stride 2

Linear layer:

- Applied to the flattened conv output
- To obtain input encoding vectors (of the same size d_{model})

All the rest is identical to original transformer from [Vaswani2017]



Word error rate (WER) performance

Parameters

- N_e no. of encoder blocks
- N_d no. of decoder blocks
- d_{ff} inner dimension of feed-forward networks (FFN)
- d_{model} = 256 model dimension (size of vectors at input of FFN)
- h=8 no. of heads for the attention block

Model	N_e	N_d	d_{ff}	WER
6Enc6Dec (base model)	6	6	1024	12.20
12Enc6Dec-wide (big model)	12	6	2048	**10.92**
4Enc8Dec	4	8	1024	13.26
8Enc4Dec	8	4	1024	11.95
8Enc4Dec-wide	8	4	2048	11.56
10Enc5Dec-wide	10	5	2048	11.01

[Dong2018] L. Dong, S. Xu, B. Xu, “Speech transformer: a no-recurrence sequence-to-sequence model for speech recognition,” *IEEE International Conference on Acoustics, Speech and Signal Processing (ICASSP)*, 2018.

INTERSPEECH 2020
October 25–29, 2020, Shanghai, China

Conformer: Convolution-augmented Transformer for Speech Recognition

Anmol Gulati, James Qin, Chung-Cheng Chiu, Niki Parmar, Yu Zhang, Jiahui Yu, Wei Han, Shibo Wang, Zhengdong Zhang, Yonghui Wu, Ruoming Pang

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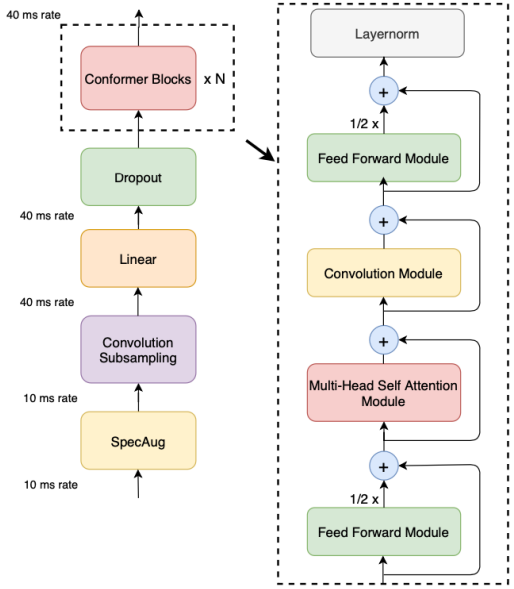
Abstract

Recently Transformer and Convolution neural network (CNN) based models have shown promising results in Automatic Speech Recognition (ASR), outperforming Recurrent neural networks (RNNs). Transformer models are good at capturing content-based global interactions, while CNNs exploit local features effectively. In this work, we achieve the best of both worlds by studying how to combine convolution neural networks and transformers to model both local and global dependencies of an audio sequence in a parameter-efficient way. To this regard, we propose the convolution-augmented transformer for speech recognition, named *Conformer*. *Conformer* significantly outperforms the previous Transformer and CNN based models achieving state-of-the-art accuracies. On the widely used LibriSpeech benchmark, our model achieves WER of 2.1%/4.3% without using a language model and 1.9%/3.9% with an external language model on test/testother. We also observe competitive performance of 2.7%/6.3% with a small model of only 10M parameters.

Index Terms: speech recognition, attention, convolutional neu-



Conformer

- Input
  - Spectrograms: contain features along time and frequency dimensions
- Self-attention (transformer)
  - good to extract large scale temporal features across time samples
  - does not track local (fine grained features) at each time sample
- Solution
  - use convolution operation to track local features
  - applied after self-attention and before the following FF module

[Gulati2020] A. Gulati, C-C. Chiu, J. Qin, J. Yu, N. Parmar, R. Pang, S. Wang, W. Han, Y. Wu, Y. Zhang, Z. Zhang, "Conformer: Convolution-augmented Transformer for Speech Recognition," 21st Annual Conference of the International Speech Communication Association (INTERSPEECH), 2020. [2197 Citations, Dec. 2023]

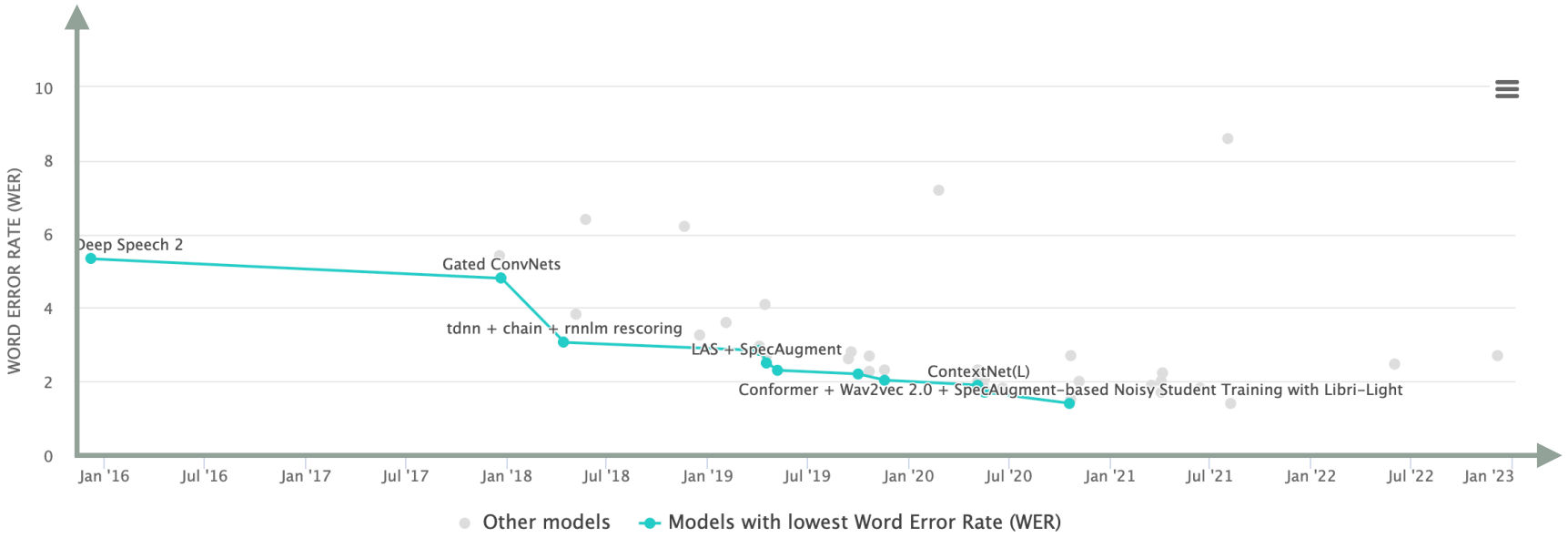
Models and data

- Evaluation on LibriSpeech dataset
  - 970 hours of labeled speech data (http://www.openslr.org/12)
  - **Cepstral** coeff: 80-filterbanks, windows of 25ms, with 10ms overlap
- Three models were identified
  - Small (10 M pars), medium (30 M), large (118 M)
  - Changing network depth, model dimension, no. of transformer heads
- Subsampling
  - Two 3x3 CNN models with stride 2 → 4x temporal subsampling
  - This reduces the sampling period from 10ms to 40ms
- Dropout
  - Applied as *regularizer* in each residual unit of the comformer module (at the output of each module, before it is added to the residual input)

Performance

Method	#Params (M)	WER Without LM		WER With LM	
		testclean	testother	testclean	testother
Hybrid					
Transformer [33]	-	-	-	2.26	4.85
CTC					
QuartzNet [9]	19	3.90	11.28	2.69	7.25
LAS					
Transformer [34]	270	2.89	6.98	2.33	5.17
Transformer [19]	-	2.2	5.6	2.6	5.7
LSTM	360	2.6	6.0	2.2	5.2
Transducer					
Transformer [7]	139	2.4	5.6	2.0	4.6
ContextNet(S) [10]	10.8	2.9	7.0	2.3	5.5
ContextNet(M) [10]	31.4	2.4	5.4	**2.0**	4.5
ContextNet(L) [10]	112.7	**2.1**	4.6	**1.9**	4.1
Conformer (Ours)					
Conformer(S)	10.3	**2.7**	**6.3**	**2.1**	**5.0**
Conformer(M)	30.7	**2.3**	**5.0**	**2.0**	**4.3**
Conformer(L)	118.8	**2.1**	**4.3**	**1.9**	**3.9**

Plenty of models are being proposed…



https://paperswithcode.com/sota/speech-recognition-on-librispeech-test-clean

Code completion

GitHub Copilot

Code completion

arXiv:2107.03374v2 [cs.LG] 14 Jul 2021

Evaluating Large Language Models Trained on Code

Mark Chen [*1] Jerry Tworek [*1] Heewoo Jun [*1] Qiming Yuan [*1] Henrique Ponde de Oliveira Pinto [*1]
Jared Kaplan [*2] Harri Edwards [1] Yuri Burda [1] Nicholas Joseph [2] Greg Brockman [1] Alex Ray [1] Raul Puri [1]
Gretchen Krueger [1] Michael Petrov [1] Heidy Khlaaf [3] Girish Sastry [1] Pamela Mishkin [1] Brooke Chan [1]
Scott Gray [1] Nick Ryder [1] Mikhail Pavlov [1] Alethea Power [1] Lukasz Kaiser [1] Mohammad Bavarian [1]
Clemens Winter [1] Philippe Tillet [1] Felipe Petroski Such [1] Dave Cummings [1] Matthias Plappert [1]
Fotios Chantzis [1] Elizabeth Barnes [1] Ariel Herbert-Voss [1] William Hebgen Guss [1] Alex Nichol [1] Alex Paino [1]
Nikolas Tezak [1] Jie Tang [1] Igor Babuschkin [1] Suchir Balaji [1] Shantanu Jain [1] William Saunders [1]
Christopher Hesse [1] Andrew N. Carr [1] Jan Leike [1] Josh Achiam [1] Vedant Misra [1] Evan Morikawa [1]
Alec Radford [1] Matthew Knight [1] Miles Brundage [1] Mira Murati [1] Katie Mayer [1] Peter Welinder [1]
Bob McGrew [1] Dario Amodei [2] Sam McCandlish [2] Ilya Sutskever [1] Wojciech Zaremba [1]

Abstract

We introduce Codex, a GPT language model fine-tuned on publicly available code from GitHub, and study its Python code-writing capabilities. A distinct production version of Codex powers GitHub Copilot. On HumanEval, a new evaluation set we release to measure functional correctness for synthesizing programs from docstrings, our model solves 28.8% of the problems, while GPT-3 solves 0% and GPT-J solves 11.4%. Furthermore, we find that repeated sampling from the model is a surprisingly effective strategy for producing working solutions to difficult prompts. Using this method, we solve 70.2% of our problems with 100 samples per problem. Careful investigation of our model reveals its limitations, including difficulty with docstrings describing long chains of operations and with binding operations to variables. Finally, we discuss the potential broader impacts of deploying powerful code generation technologies, covering safety, security, and economics.

1. Introduction

Scalable sequence prediction models (Graves, 2014; Vaswani et al., 2017; Child et al., 2019) have become a general-purpose method for generation and representation learning in many domains, including natural language processing (Mikolov et al., 2013; Sutskever et al., 2014; Dai & Le, 2015; Peters et al., 2018; Radford et al., 2018; Devlin et al., 2018), computer vision (Van Oord et al., 2016; Menick & Kalchbrenner, 2018; Chen et al., 2020; Bao et al., 2021), audio and speech processing (Oord et al., 2016; 2018; Dhariwal et al., 2020; Baevski et al., 2020), biology (Alley et al., 2019; Rives et al., 2021), and even across multiple modalities (Das et al., 2017; Lu et al., 2019; Ramesh et al., 2021; Zellers et al., 2021). More recently, language models have also fueled progress towards the longstanding challenge of program synthesis (Simon, 1963; Manna & Waldinger, 1971), spurred by the presence of code in large datasets (Husain et al., 2019; Gao et al., 2020) and the resulting programming capabilities of language models trained on these datasets (Wang & Komatsuzaki, 2021). Popular language modeling objectives like masked language modeling (Devlin et al., 2018) and span prediction (Raffel et al., 2020) have also been adapted to train their programming counterparts CodeBERT (Feng et al., 2020) and PyMT5 (Clement et al., 2020).

Generating code from text description

```python
def incr_list(l: list):
    """Return list with elements incremented by 1.
    >>> incr_list([1, 2, 3])
    [2, 3, 4]
    >>> incr_list([5, 3, 5, 2, 3, 3, 9, 0, 123])
    [6, 4, 6, 3, 4, 4, 10, 1, 124]
    """
    return [i + 1 for i in l]
```

```python
def solution(lst):
    """Given a non-empty list of integers, return the sum of all of the odd elements
    that are in even positions.

    Examples
    solution([5, 8, 7, 1]) ==>12
    solution([3, 3, 3, 3, 3]) ==>9
    solution([30, 13, 24, 321]) ==>0
    """
    return sum(lst[i] for i in range(0,len(lst)) if i % 2 == 0 and lst[i] % 2 == 1)
```

```python
def encode_cyclic(s: str):
    """
    returns encoded string by cycling groups of three characters.
    """
    # split string to groups. Each of length 3.
    groups = [s[(3 * i):min((3 * i + 3), len(s))] for i in range((len(s) + 2) // 3)]
    # cycle elements in each group. Unless group has fewer elements than 3.
    groups = [(group[1:] + group[0]) if len(group) == 3 else group for group in groups]
    return "".join(groups)

def decode_cyclic(s: str):
    """
    takes as input string encoded with encode_cyclic function. Returns decoded string.
    """
    # split string to groups. Each of length 3.
    groups = [s[(3 * i):min((3 * i + 3), len(s))] for i in range((len(s) + 2) // 3)]
    # cycle elements in each group.
    groups = [(group[-1] + group[:-1]) if len(group) == 3 else group for group in groups]
    return "".join(groups)
```

M. Chen et al. “Evaluating Large Language Models Trained on Code”. [Blog 1][Blog 2]

Multimodal

arXiv:2205.06175v2 [cs.AI] 19 May 2022

DeepMind

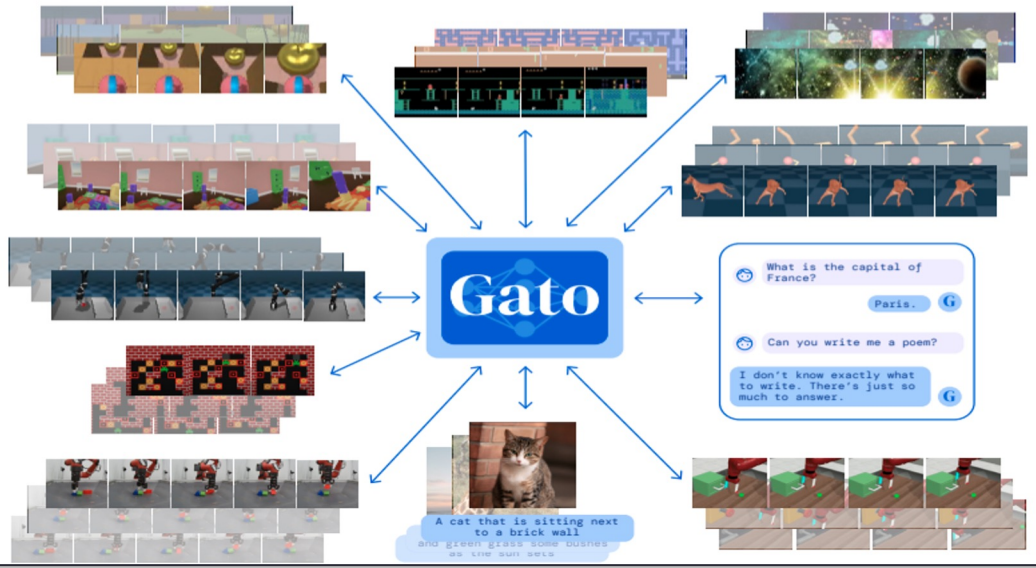
2022-5-19

A Generalist Agent

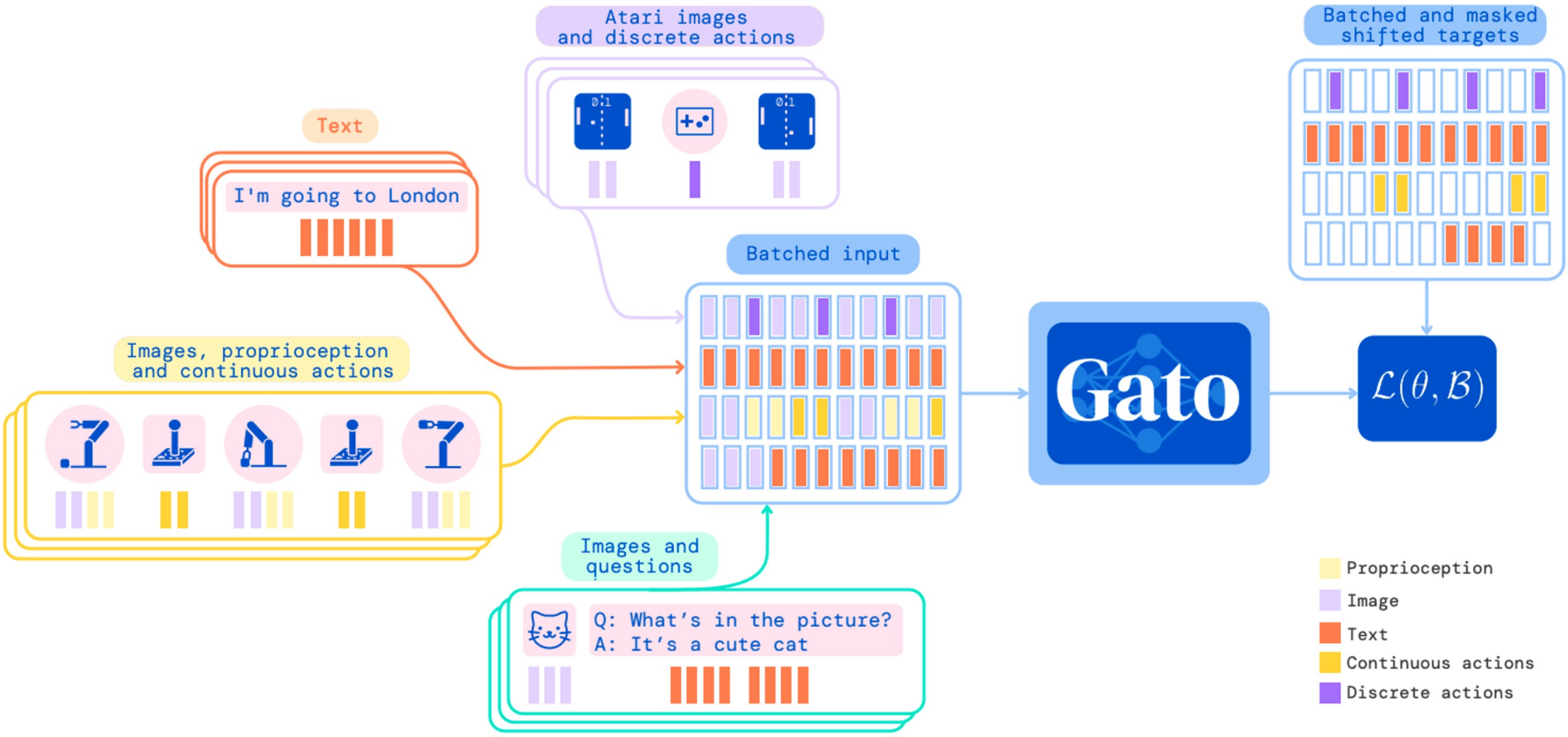
Scott Reed*,†, Konrad Żołna*, Emilio Parisotto*, Sergio Gómez Colmenarejo†, Alexander Novikov, Gabriel Barth-Maron, Mai Giménez, Yury Sulsky, Jackie Kay, Jost Tobias Springenberg, Tom Eccles, Jake Bruce, Ali Razavi, Ashley Edwards, Nicolas Heess, Yutian Chen, Raia Hadsell, Oriol Vinyals, Mahyar Bordbar and Nando de Freitas†

*Equal contributions, †Equal senior contributions, All authors are affiliated with DeepMind

Inspired by progress in large-scale language modeling, we apply a similar approach towards building a single generalist agent beyond the realm of text outputs. The agent, which we refer to as Gato, works as a multi-modal, multi-task, multi-embodiment generalist policy. The same network with the same weights can play Atari, caption images, chat, stack blocks with a real robot arm and much more, deciding based on its context whether to output text, joint torques, button presses, or other tokens. In this report we describe the model and the data, and document the current capabilities of Gato.



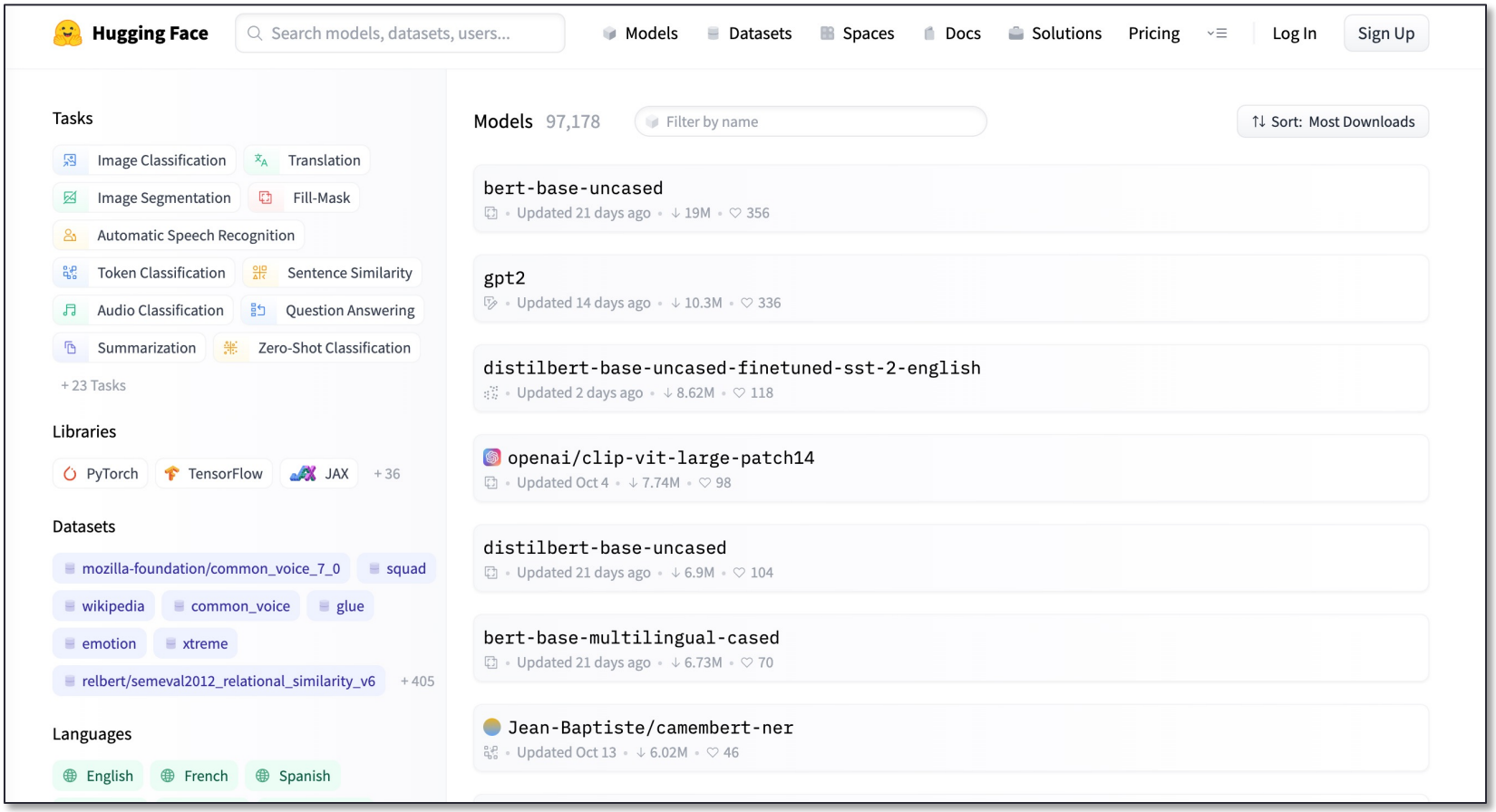
Gato



S. Reed et al. "A Generalist Agent". [Blog]

Repo for models and datasets

https://huggingface.co/models



Additional resources

[Kamath2022] Uday Kamath, Kenneth L. Graham, Wael Emara, “Transformers for Machine Learning: a Deep Dive,” CRC Press, 2022.

[Ahmed2022] S. Ahmed, I. E. Nielsen, A. Tripathi, S. Siddiqui, G. Rasool, R. P. Ramachandran,“Transformers in Time Series Analysis: a Tutorial,” Springer. Circuits, Systems and Signal Processing, 25 July 2023.

[Cristina2022] Stefania Cristina “Training the transformer model,” (blog and book), Nov. 16, 2022.

APPENDIX A: DERIVATIVE OF SOFTMAX

Derivative of softmax (1/4)

- For softmax output node i, we have

$$y_i = \frac{\exp(a_i)}{\sum_k \exp(a_k)} \qquad \frac{\partial y_i}{\partial a_j} = ?$$

- Derivative of a quotient:

$$f(x) = \frac{g(x)}{h(x)} \rightarrow f'(x) = \frac{g'(x)h(x) - h'(x)g(x)}{h(x)^2}$$

- We use:

$$g(x) = \exp(a_i)\,,\; h(x) = \sum_k \exp(a_k)$$

Derivative of softmax (2/4)

if $i = j$

$$\frac{\partial y_i}{\partial a_j} = \frac{\exp(a_i)\sum_k \exp(a_k) - \exp(a_j)\exp(a_i)}{\left(\sum_k \exp(a_k)\right)^2} =$$

$$= \frac{\exp(a_i)\left(\sum_k \exp(a_k) - \exp(a_j)\right)}{\left(\sum_k \exp(a_k)\right)^2} =$$

$$= \frac{\exp(a_i)}{\sum_k \exp(a_k)} \times \frac{\left(\sum_k \exp(a_k) - \exp(a_j)\right)}{\sum_k \exp(a_k)} =$$

$$= y_i(1 - y_j) = y_i(1 - y_i) \text{ (as } i = j)$$

Derivative of softmax (3/4)

if $i \neq j$

$$\frac{\partial y_i}{\partial a_j} = \frac{0 - \exp(a_j)\exp(a_i)}{\left(\sum_k \exp(a_k)\right)^2} =$$

$$= \frac{-\exp(a_j)}{\left(\sum_k \exp(a_k)\right)} \times \frac{\exp(a_i)}{\left(\sum_k \exp(a_k)\right)} =$$

$$= -y_j y_i$$

Derivative of softmax (4/4)

- Thus, we get:

$$\frac{\partial y_i}{\partial a_j} = \begin{cases} y_i(1 - y_i) & i = j \\ -y_j y_i & i \neq j \end{cases}$$

- Compactly, using the Kronecker delta

$$\delta_{ij} = 1 \text{ if } i = j, \delta_{ij} = 0 \text{ otherwise}$$

$$\frac{\partial y_i}{\partial a_j} = y_i(\delta_{ij} - y_j)$$

Master's degree ICT Internet Multimedia Engineering

ADVANCED NEURAL NETWORK DESIGNS: SELF-ATTENTION & TRANSFORMERS

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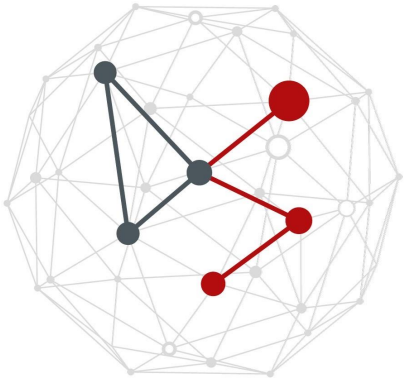

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