Neural Networks and Deep Learning

Attention



A digression into human attention

ATTENTION MECHANISMS

Human attention

"... the amount of information coming down the optic nerve - estimated to be in the range of 10⁸ ~ 10⁹ bits per second - far exceeds what the brain is capable of fully processing and assimilating into conscious experience ..."

C. Koch, 1982

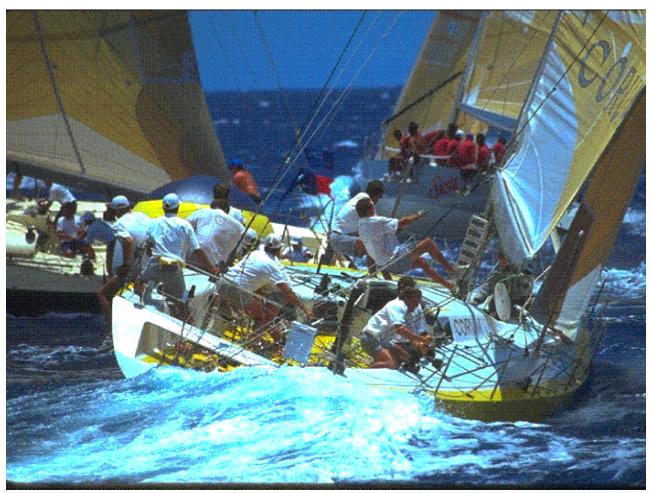
Restricting higher acuity vision to a small region of the retina and shifting the processing focus from one location to another (aka "attention") is the solution nature has devised to cope in a serial fashion with the vast amount of visible information

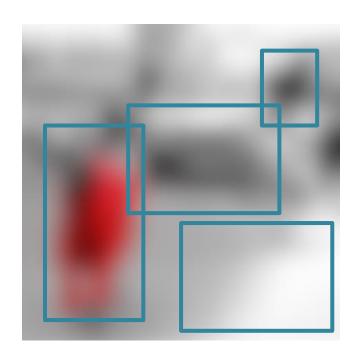
The same happens with every sensory input (e.g. audio source separation)

Goal driven (volitional, top-down)



Stimuli driven (non-volitional, bottom-up)

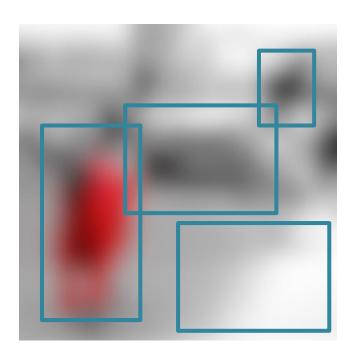




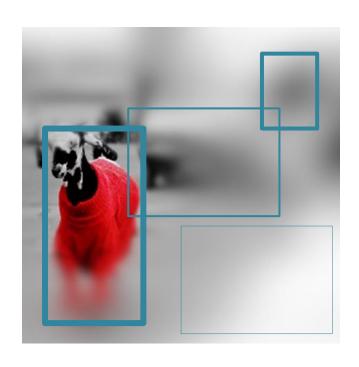
This is called a free-viewing task.
There is no explicit query (task).
Still, you know that there are some parts which seem more important (salient) than others.

Attention is bottom up: the input signal is all you have to decide where it pays off to look at

Q: "Where is the stop sign?"

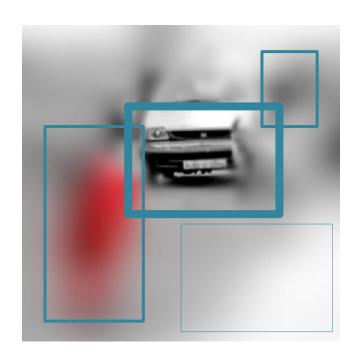


Q: "Where is the stop sign?"



Here you have a task, where you look at depends on the task (query) as well as information from the signal (keys)

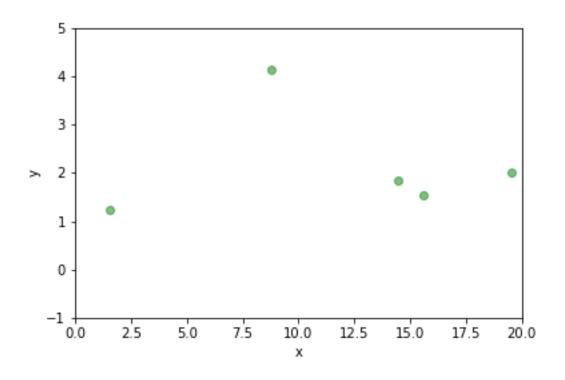
Q: "Where is the car?"



Here you have a task, where you look at depends on the task (query) as well as information from the signal (keys)

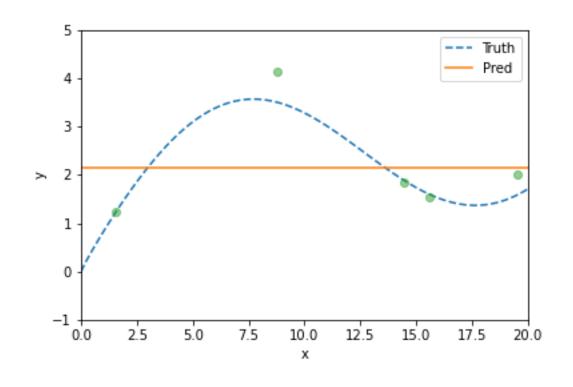
ATTENTION IN MACHINE LEARNING

Solving the regression problem



Data: $\{x_1, x_2, ..., x_m\}$ Labels: $\{y_1, y_2, ..., y_m\}$

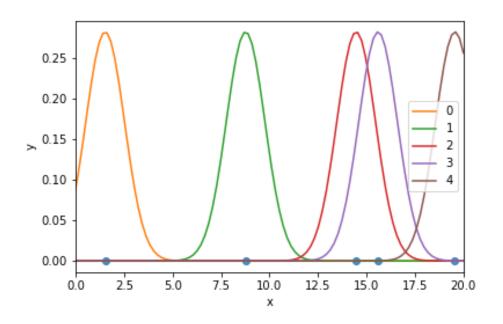
Solving the regression problem



Lacking any other knowledge, we could use just the average:

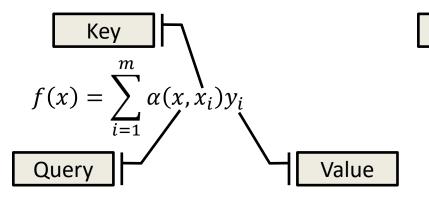
$$f(x) = \frac{1}{m} \sum_{i=1}^{m} y_i$$

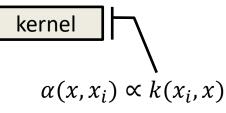
Data: $\{x_1, x_2, ..., x_m\}$ Labels: $\{y_1, y_2, ..., y_m\}$

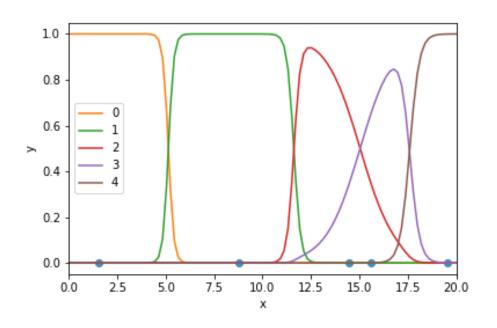


A better idea would be to weigh the labels, according to their location

The weights are proportional to some similarity function, a "kernel". For example, a Gaussian.

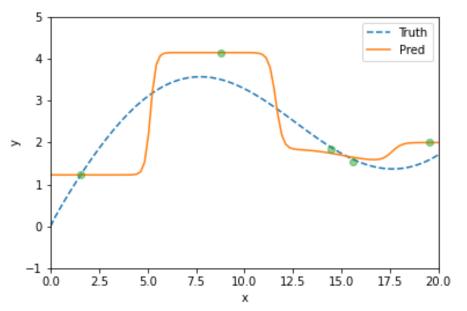






Weights should also be normalised

$$\alpha(x, x_i) = \frac{k(x, x_i)}{\sum_j k(x, x_j)}$$



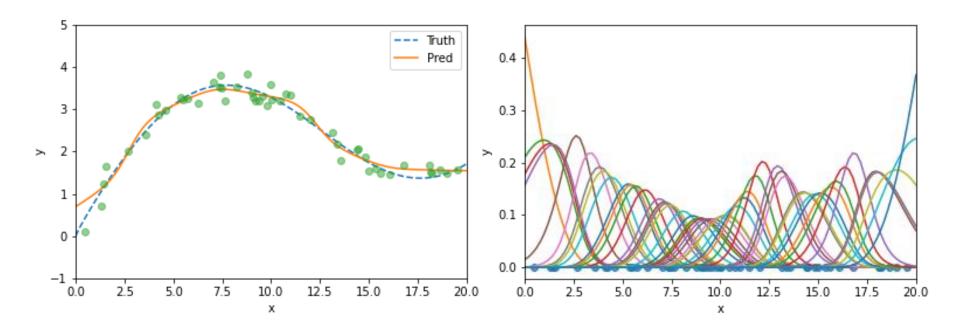
$$f(x) = \sum_{i=1}^{m} \frac{k(x, x_i)}{\sum_{j} k(x, x_j)} y_i$$

$$= \sum_{i=1}^{m} \frac{\exp\left(-\frac{1}{2}(x - x_i)^2\right)}{\sum_{j} \exp\left(-\frac{1}{2}(x - x_j)^2\right)} y_i$$

$$= \sum_{i=1}^{m} \operatorname{softmax}\left(-\frac{1}{2}(x - x_i)^2\right) y_i$$

Using a Gaussian kernel with unit variance:

$$k(x, x_i) = N(x - x_i) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{(x - x_i)^2}{2}\right)$$

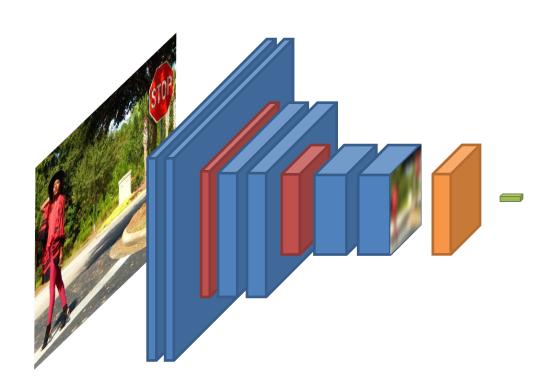


Consistency: Given enough data, this algorithm converges to the optimal solution

Simplicity: No free parameters – information is in the data, not in the weights

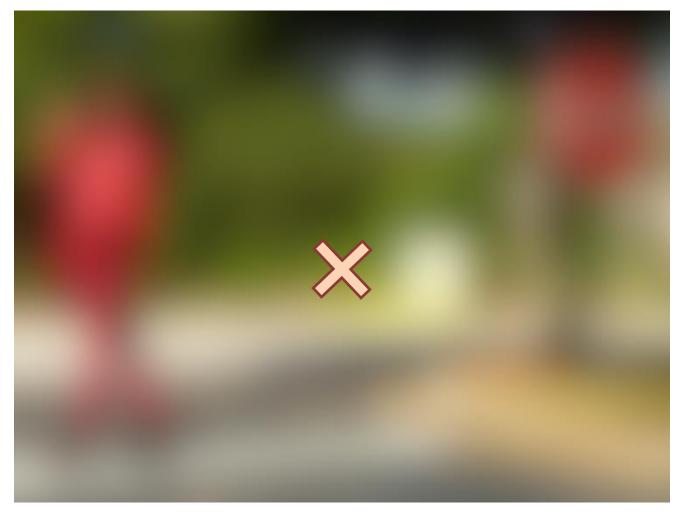
Computationally expensive: No model, we need to iterate through all the data every time we need to compute a new value

Average Pooling?

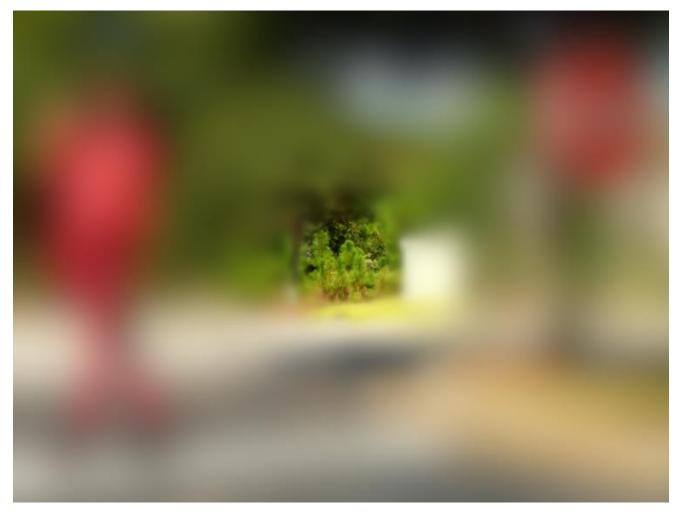


Global Average Pooling would be equivalent to the "flat line" model (average) we saw before.

What if we knew that we are interested about a particular area of the image?



What if we knew that we are interested about what is "around here"? We would then weight differently the cells that are closer to that location of interest

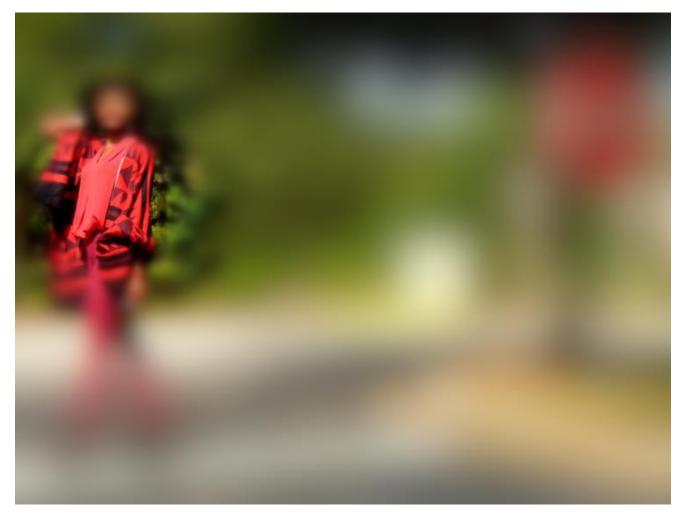


This is what humans do, by "fixating" in different places in the image.

But how do you decide where to fixate?



Where you fixate (how you deploy your attention) depends on the input signal (**bottom-up** attention) and on the task, e.g. "Is there any stop sign on the road" (**top-down** attention).



Where you fixate (how you deploy your attention) depends on the input signal (bottom-up attention) and on the task, e.g. "Is there any stop sign on the road" (top-down attention).



Where you fixate (how you deploy your attention) depends on the input signal (**bottom-up** attention) and on the task, e.g. "Is there any stop sign on the road" (**top-down** attention).

Towards deep learning

Could we substitute our average **pooling operations** with a weighted pooling like this?

$$f(x) = \sum_{i=1}^{m} \frac{k(x, x_i)}{\sum_{j} k(x, x_j)} y_i$$

Could we learn better kernels?

Could we learn the right queries, keys and values?

QUERIES, KEYS AND VALUES

Sensory inputs

Non-volitional cues



pink, human



yellow, inanimate

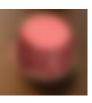




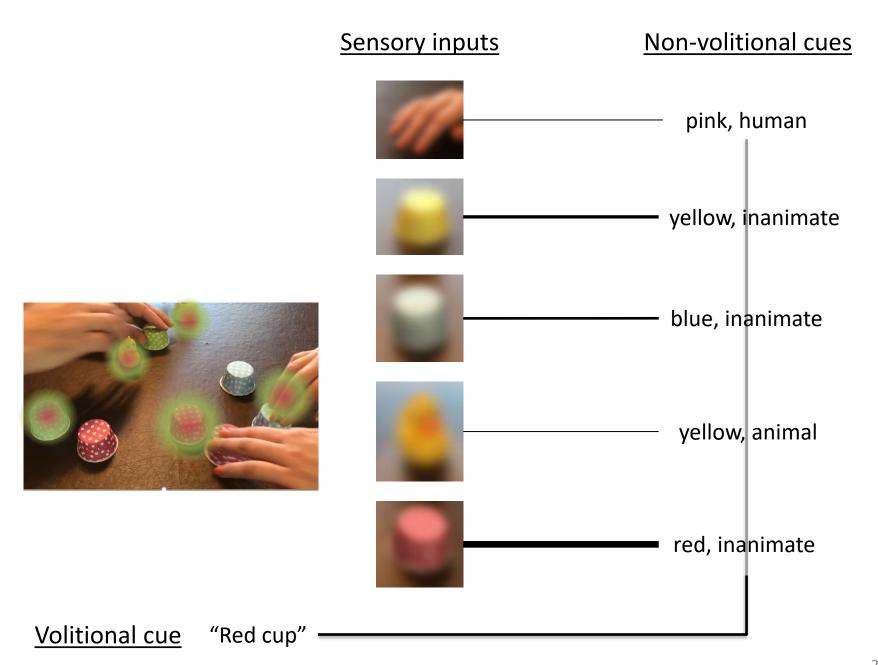
blue, inanimate



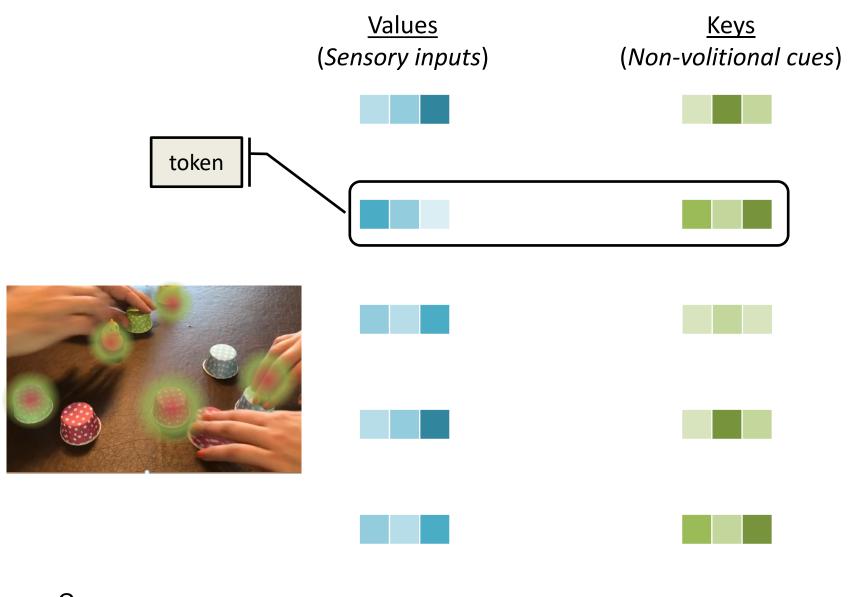
yellow, animal



red, inanimate



Sensory inputs Non-volitional cues pink, human yellow, inanimate blue, inanimate yellow, animal red, inanimate Volitional cue "Duck"



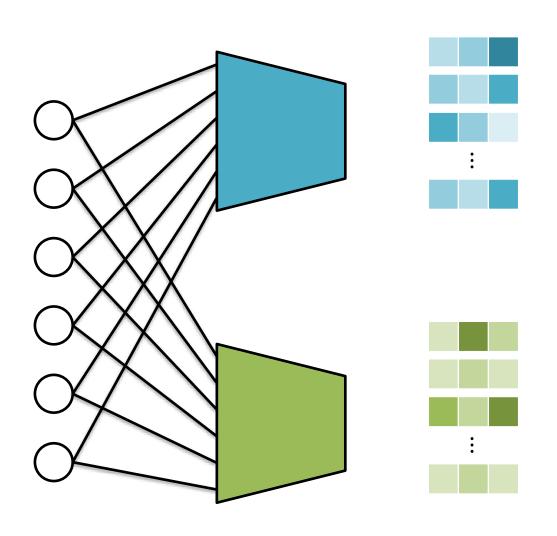
<u>Query</u> (*Volitional cue*)

Note

The idea of queries, keys and values aims to build a **conceptual framework** through which we can abstract different ways of implementing "attention" mechanisms

In reality, you will see that queries, keys and values might not be different things at all (see self-attention for example... later in this lecture)

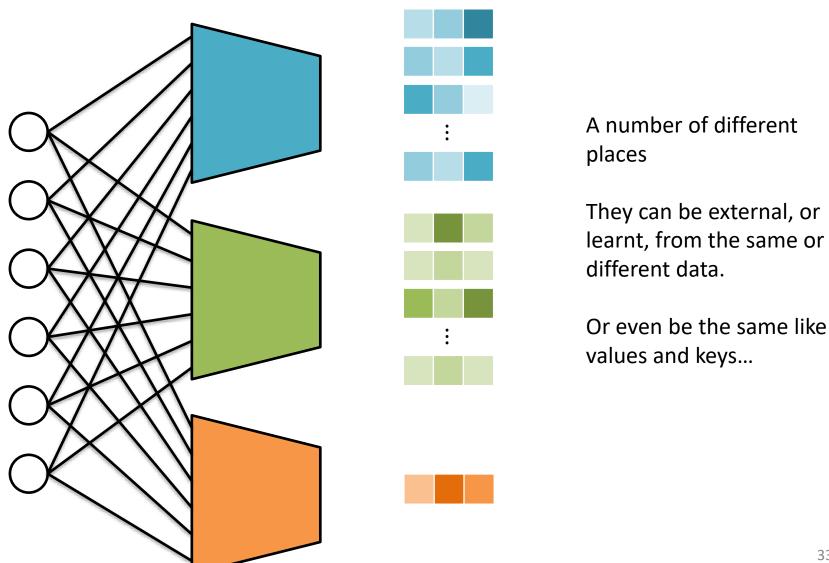
Where do values and keys come from?



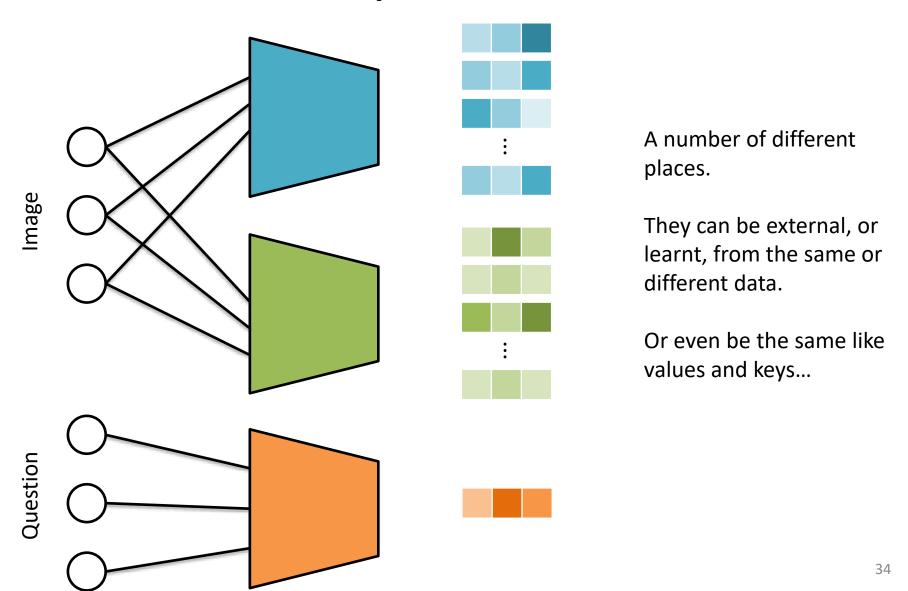
For the time being, you can think of keys and values as different representations calculated from the same data

We will see eventually, we that they can actually be the same (equal)

Where do queries come from?



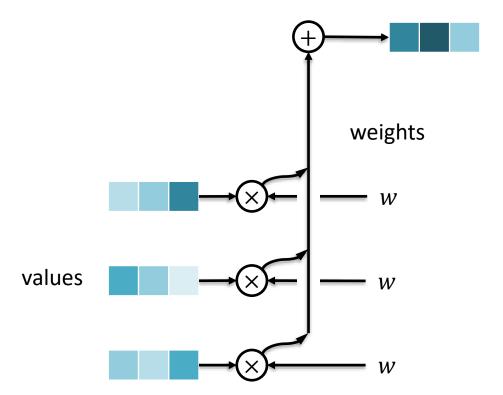
Where do queries come from?



A general framework

ATTENTION IN DEEP LEARNING

Starting point



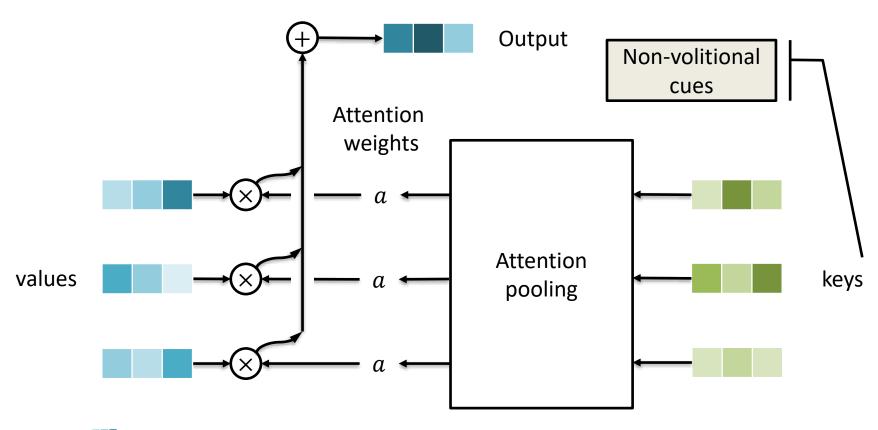
Output

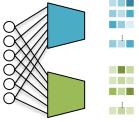
Consider the simpler case where there is **no query** (no top-down component).

To bias selection over sensory inputs, we can simply use a parameterized fully-connected layer or even non-parameterized max or average pooling.

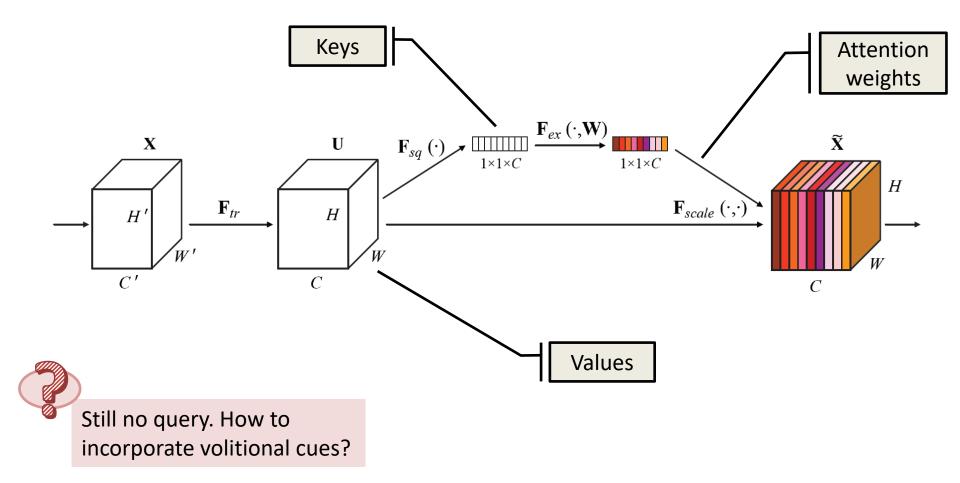
This is what we have been doing up to now

"Bottom-up" attention

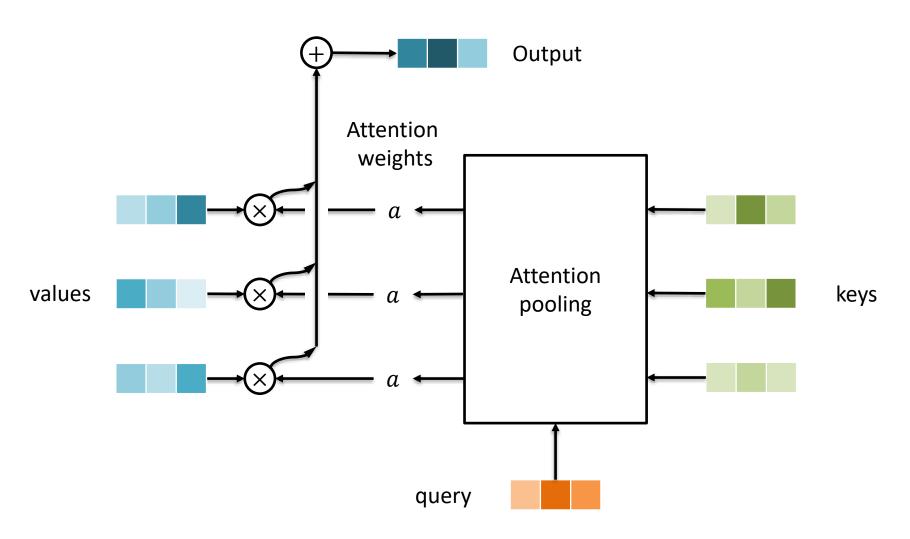




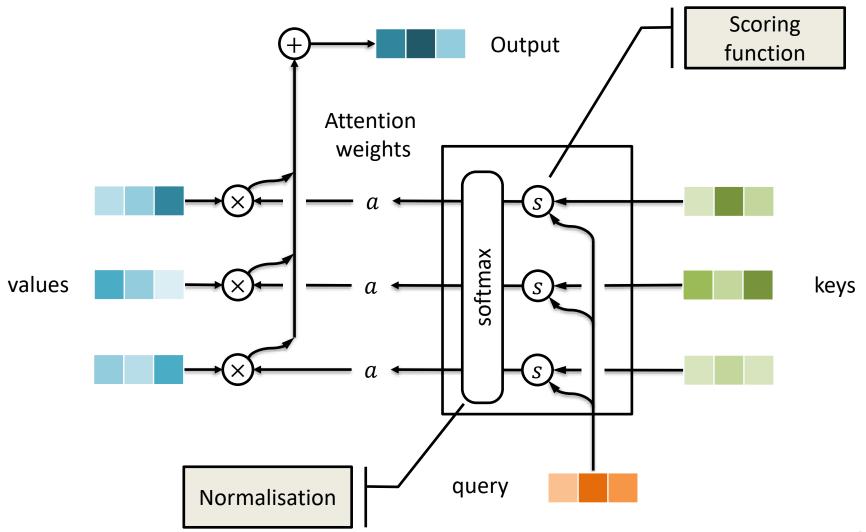
Example: Squeeze excitation networks



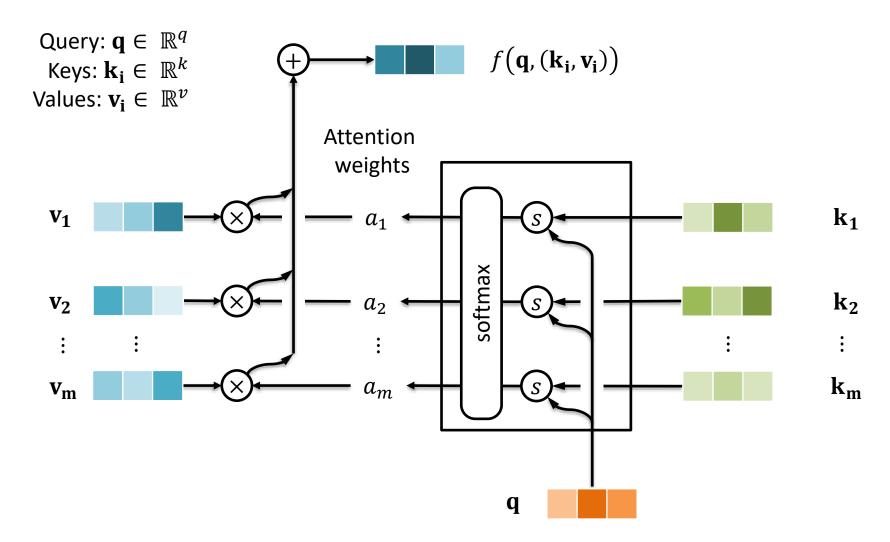
Introducing Queries



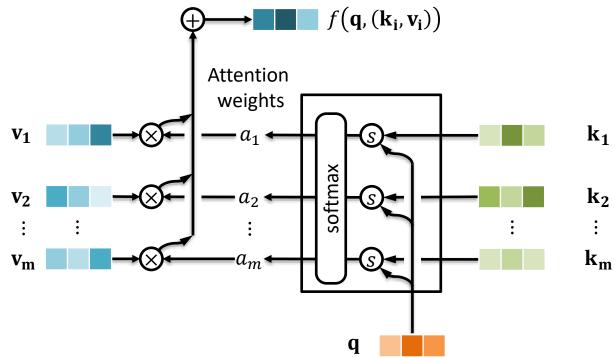
Introducing Queries



Notation



Notation



Query: $\mathbf{q} \in \mathbb{R}^q$ Keys: $\mathbf{k_i} \in \mathbb{R}^k$

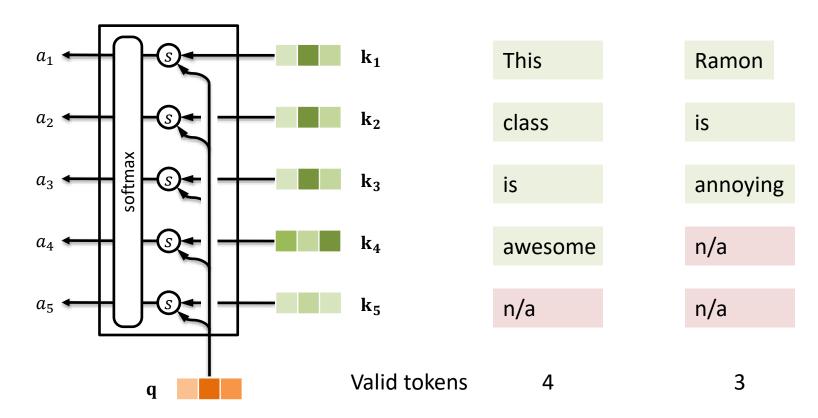
Values: $\mathbf{v_i} \in \mathbb{R}^{v}$

$$f(\mathbf{q}, (\mathbf{k_1}, \mathbf{v_1}), \dots, (\mathbf{k_m}, \mathbf{v_m})) = \sum_{i=1}^{m} \alpha(\mathbf{q}, \mathbf{k_i}) \mathbf{v_i} \in \mathbb{R}^{v}$$

$$\alpha_i = \alpha(\mathbf{q}, \mathbf{k_i}) = \operatorname{softmax}(s(\mathbf{q}, \mathbf{k_i})) = \frac{\exp(s(\mathbf{q}, \mathbf{k_i}))}{\sum_{i=1}^{m} \exp(s(\mathbf{q}, \mathbf{k_i}))} \in \mathbb{R}$$

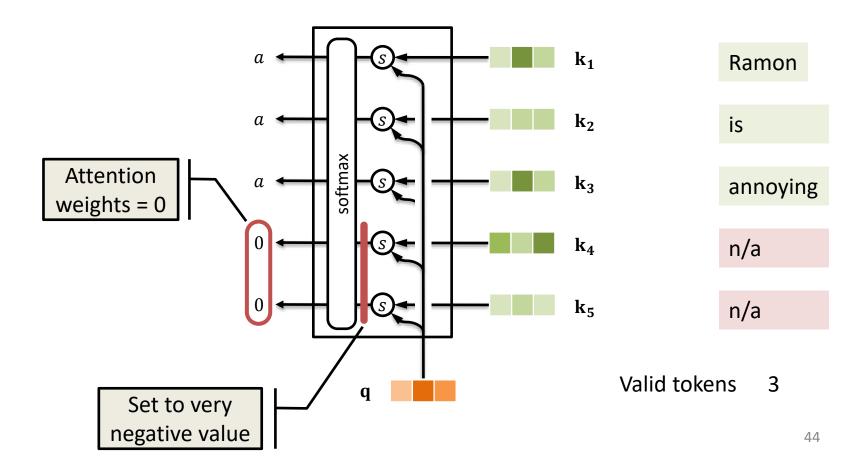
Masked Softmax Operation

In many cases, we are given a variable length of tokens (values / keys), so not all the values should be fed into attention pooling.



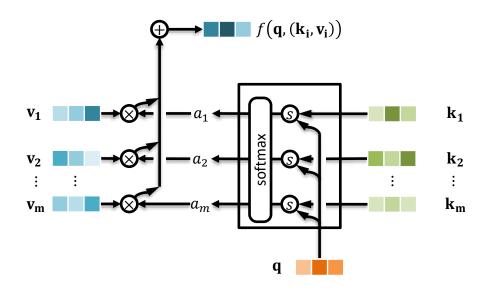
Masked Softmax Operation

The number of valid tokens becomes a parameter of the *softmax* operation: any value beyond the valid length is masked as zero: given a very negative number value whose exponentiation outputs zero.



Attention scoring functions: Additive attention

In general, when queries and keys are vectors of different lengths, we can use additive attention as the scoring function



$$s(\mathbf{q}, \mathbf{k}) = \mathbf{w}_{\mathbf{v}}^{\mathrm{T}} \tanh(\mathbf{W}_{\mathbf{q}}\mathbf{q} + \mathbf{W}_{\mathbf{k}}\mathbf{k}) \in \mathbb{R}$$

$$\mathbf{q} \in \mathbb{R}^{q}$$

$$\mathbf{k} \in \mathbb{R}^{k}$$

$$W_{q} \in \mathbb{R}^{h \times q}$$

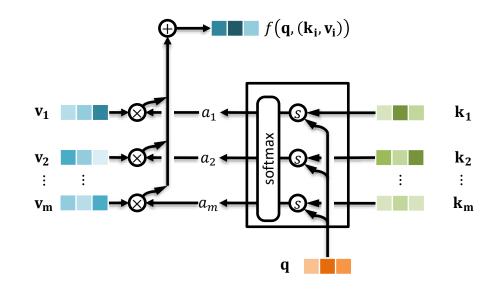
$$W_{k} \in \mathbb{R}^{h \times k}$$

$$w_{v} \in \mathbb{R}^{h}$$

Attention scoring functions: Scaled Dot-product Attention

Dot product is **computationally efficient**. But requires that both the query and the key have the same vector length.

Assuming that $\bf q$ and $\bf k$ are independent random variables with zero mean and unit variance, we divide by \sqrt{d} to ensure result also has unit variance



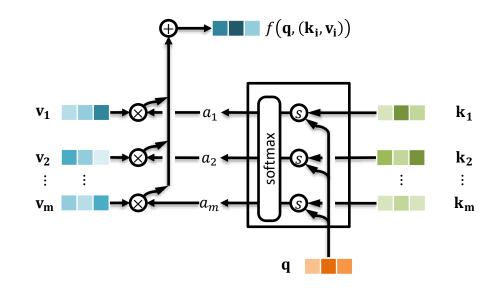
$$s(\mathbf{q}, \mathbf{k}) = \frac{\mathbf{q}^T \mathbf{k}}{\sqrt{d}}$$

$$\mathbf{q},\mathbf{k}\in\mathbb{R}^d$$

Attention scoring functions: Scaled Dot-product Attention

Dot product is **computationally efficient**. But requires that both the query and the key have the same vector length.

Assuming that ${\bf q}$ and ${\bf v}$ are independent random variables with zero mean and unit variance, we divide by \sqrt{d} to ensure result also has unit variance



$$s(\mathbf{q}, \mathbf{k}) = \frac{\mathbf{q}^T \mathbf{k}}{\sqrt{d}}$$

$$Attention(\mathbf{Q}, \mathbf{K}, \mathbf{V}) = \operatorname{softmax}\left(\frac{\mathbf{Q}\mathbf{K}^{\mathrm{T}}}{\sqrt{d}}\right)\mathbf{V} \in \mathbb{R}^{n \times v}$$

n: # of queries m: # of keys $\mathbf{v} \in \mathbb{R}^v$ $\mathbf{q}, \mathbf{k} \in \mathbb{R}^d$ $\mathbf{0} \in \mathbb{R}^{n \times d}$

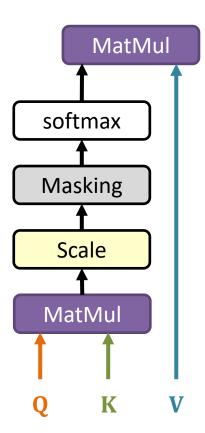
$$\mathbf{K} \in \mathbb{R}^{m \times d}$$

$$\mathbf{V} \in \mathbb{R}^{m \times v}$$

Scaled Dot-Product Attention

Efficient parallel implementation for multiple keys/queries:

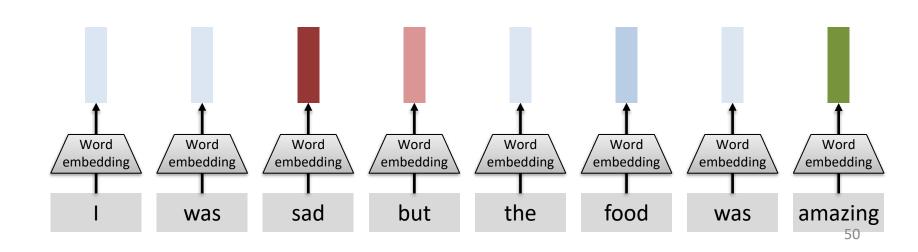
Attention(**Q**, **K**, **V**) = softmax
$$\left(\frac{\mathbf{Q}\mathbf{K}^T}{\sqrt{d}}\right)\mathbf{V}$$



EXAMPLES

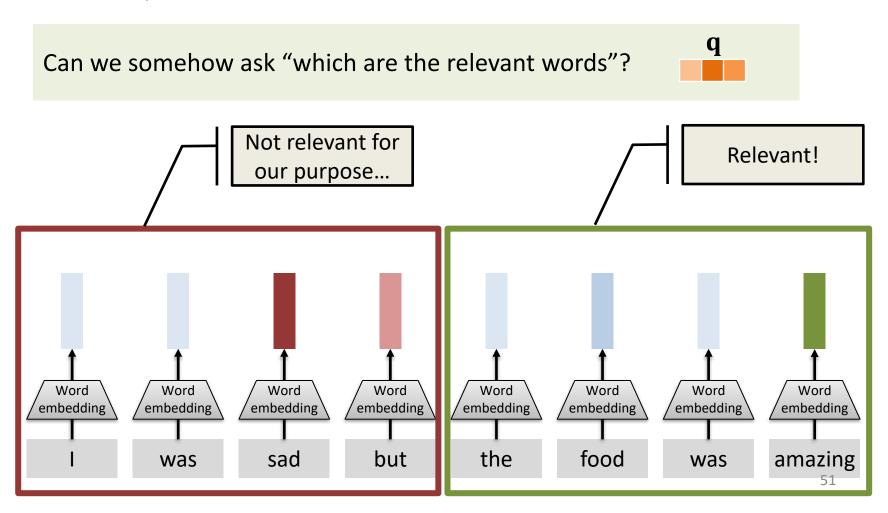
Example: Restaurant reviews

Is this a positive or a negative review?

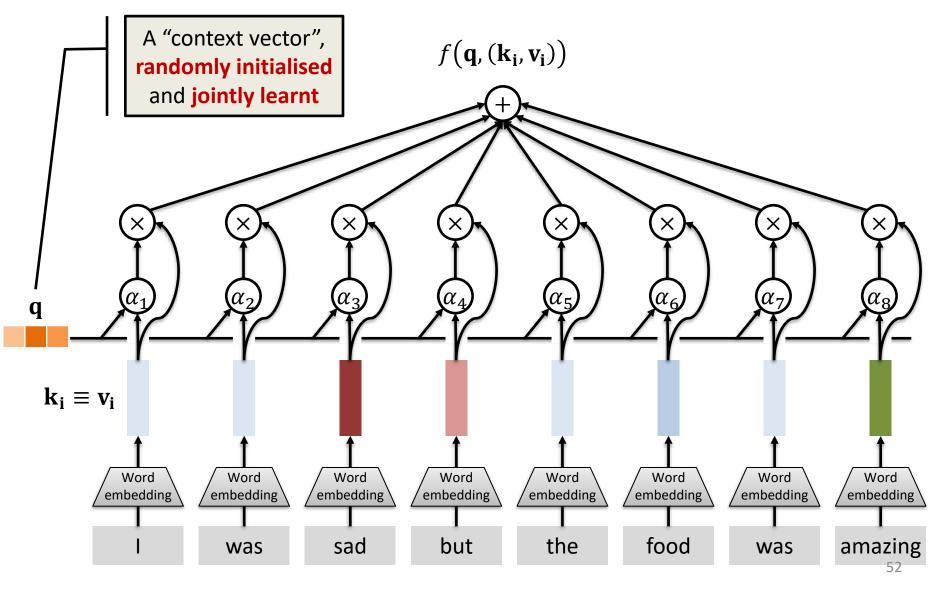


Example: Restaurant reviews

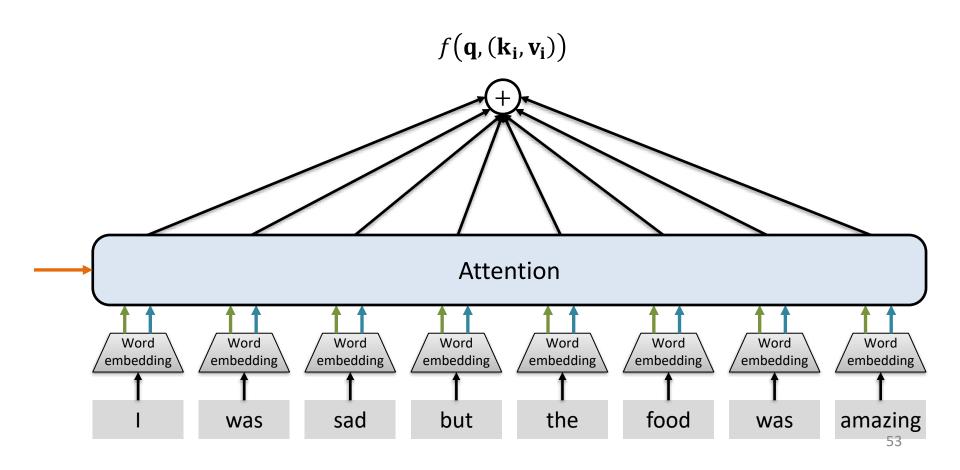
In this example, not all words are relevant to understand if this review is positive or not



Example: Sentiment Analysis



Example: Sentiment Analysis



Example: Hierarchical Attention

Casa Lolea es un lugarcito fantástico hermoso riquísimo bello simple puro amor
Caímos con mi novio para cenar porque estaba cerca del hotel
Cuando entramos nos dijeron que hay que reservar con dos noches de anticipación
El día siguiente era nuestra última noche en Barcelona
Muy amablemente accedieron a darnos una mesita para el otro día
Volvimos llenos de expectativas porque no sabíamos a qué se debía tanto revuelo
Y lo entendimos

Me sabe mal ver que lugares que me gusten tanto tengan reseñas tan encontradas...

Al parecer las personas que han ido han tenido una mala experiencia.

No me gusta que otros reciban un mal servicio/comida cuando yo la paso tan bien.

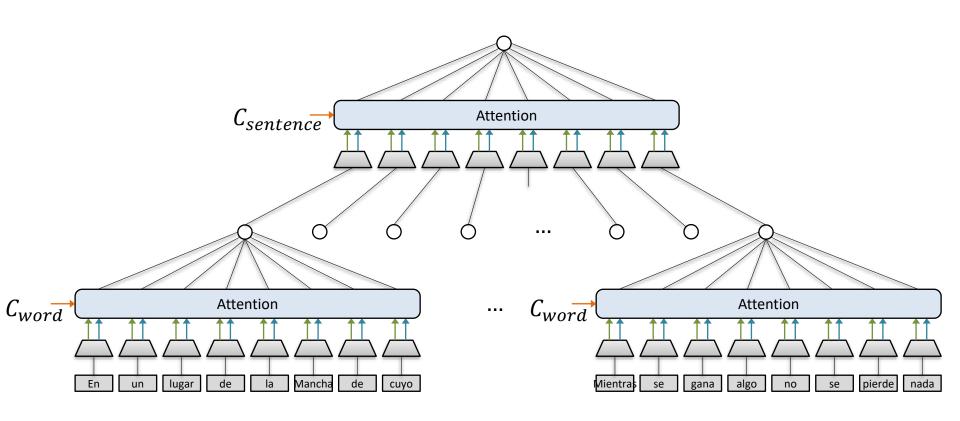
Por eso he ido unas cuatro veces a Casa Lolea antes de escribir esta reseña

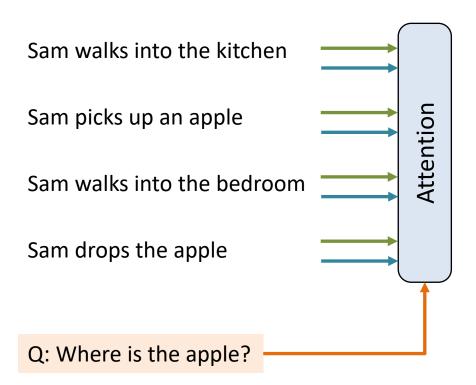
La verdad es que no tengo ni el más mínimo pero

Las tapas son exquisitas, las recomiendo sobre las conservas

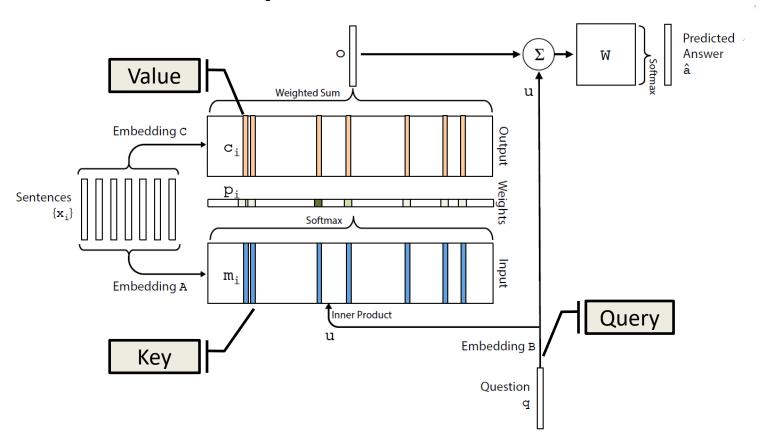
(¿por qué comer conservas en un restaurante? ya esto es una duda MUY personal.)

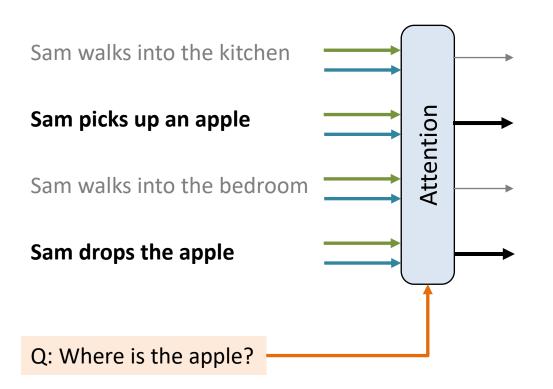
Example: Hierarchical Attention





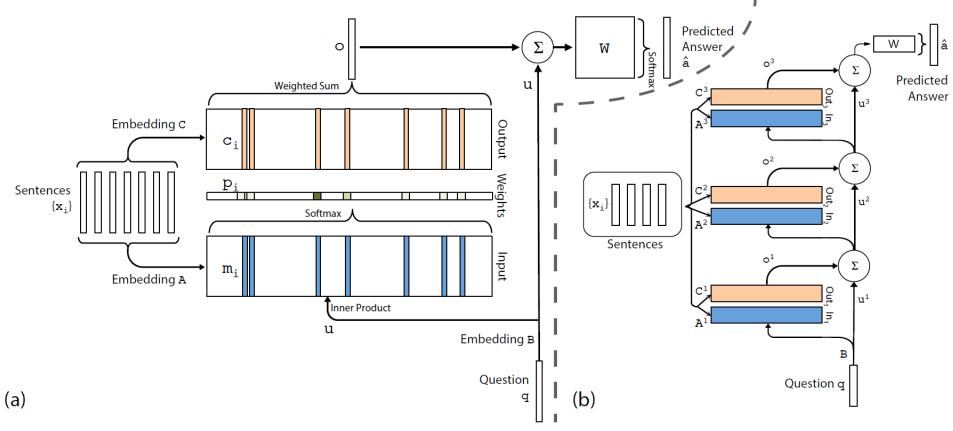
This is a typical question-answering problem. You are given a passage and a question, and you need to come up with an answer





Simple attention selects sentences with "apple"

Hierarchical attention does not work as it misses intermediate steps



Sam walks into the kitchen. Sam picks up an apple. Sam walks into the bedroom.

Sam drops the apple.

Q: Where is the apple?

A. Bedroom

Brian is a lion. Julius is a lion. Julius is white. Bernhard is green.

O: What color is Brian?

A. White

Mary journeyed to the den.

Mary went back to the kitchen.

John journeyed to the bedroom.

Mary discarded the milk.

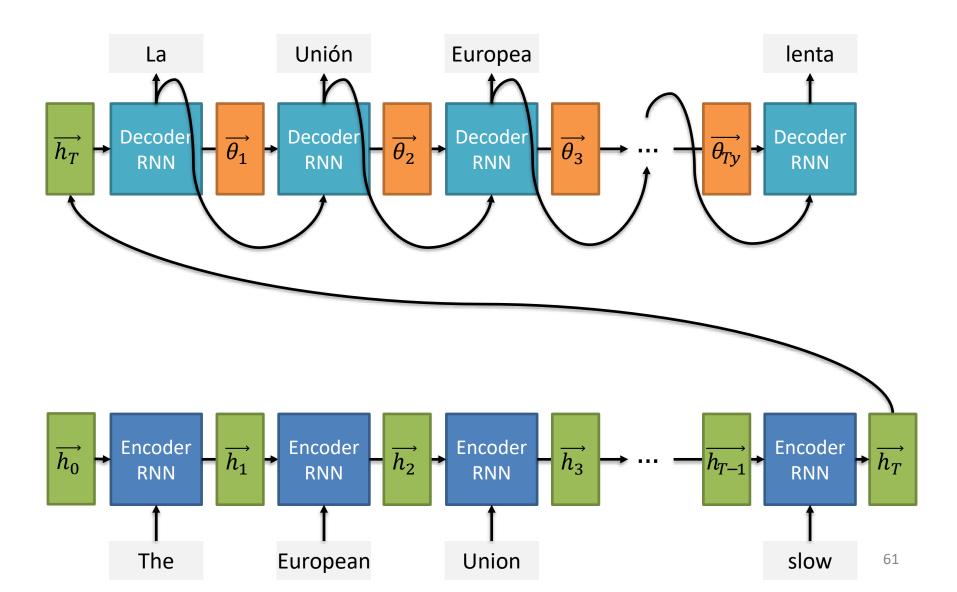
O: Where was the milk before the den?

A. Hallway

Sequence to Sequence with attention

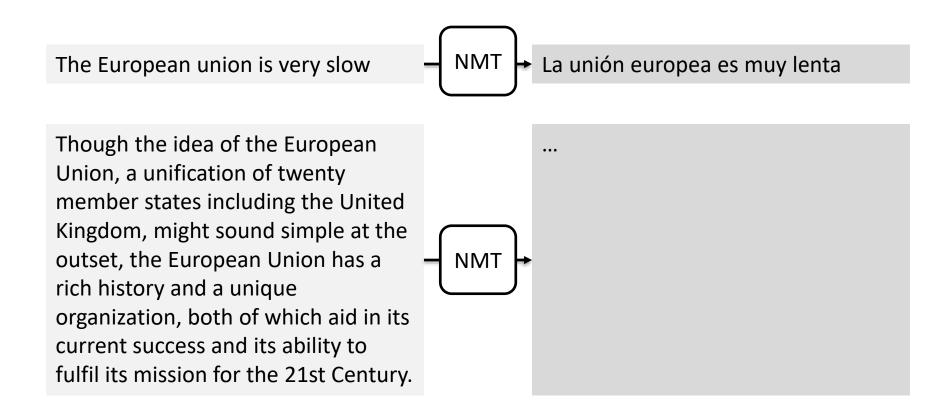
BAHDANAU ATTENTION

Sequence to Sequence

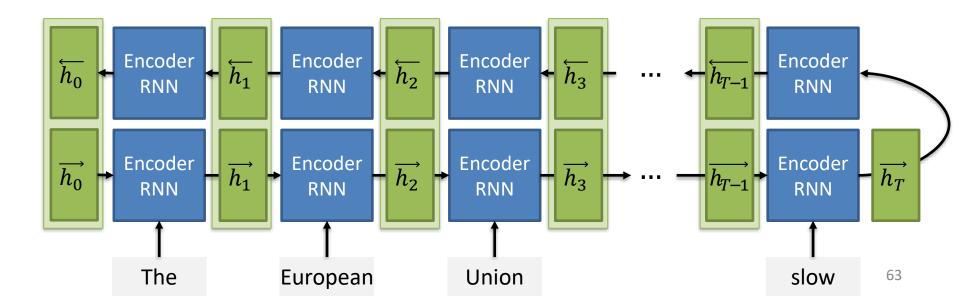


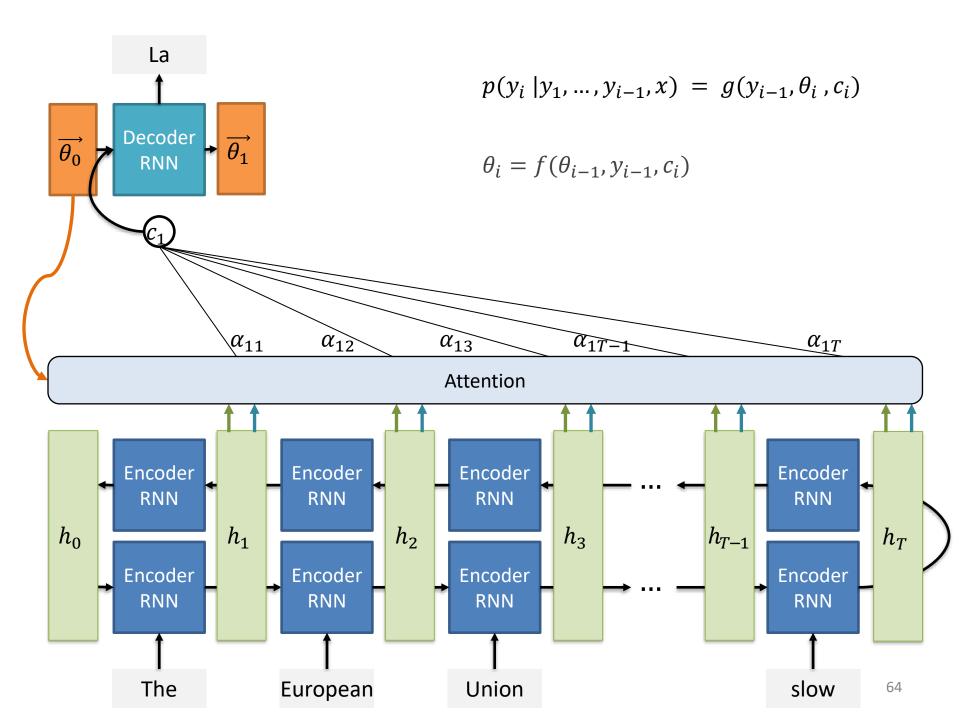
Sequence to Sequence

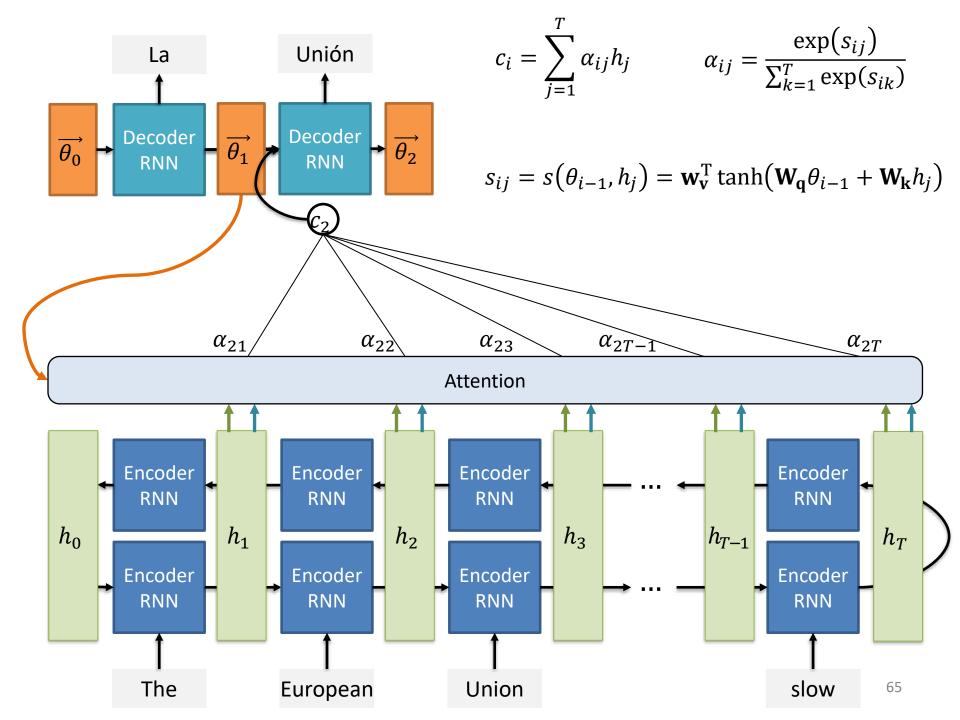
This works reasonably well with short sentences. When passages become long, the context vector is a bottleneck – cannot encode all details

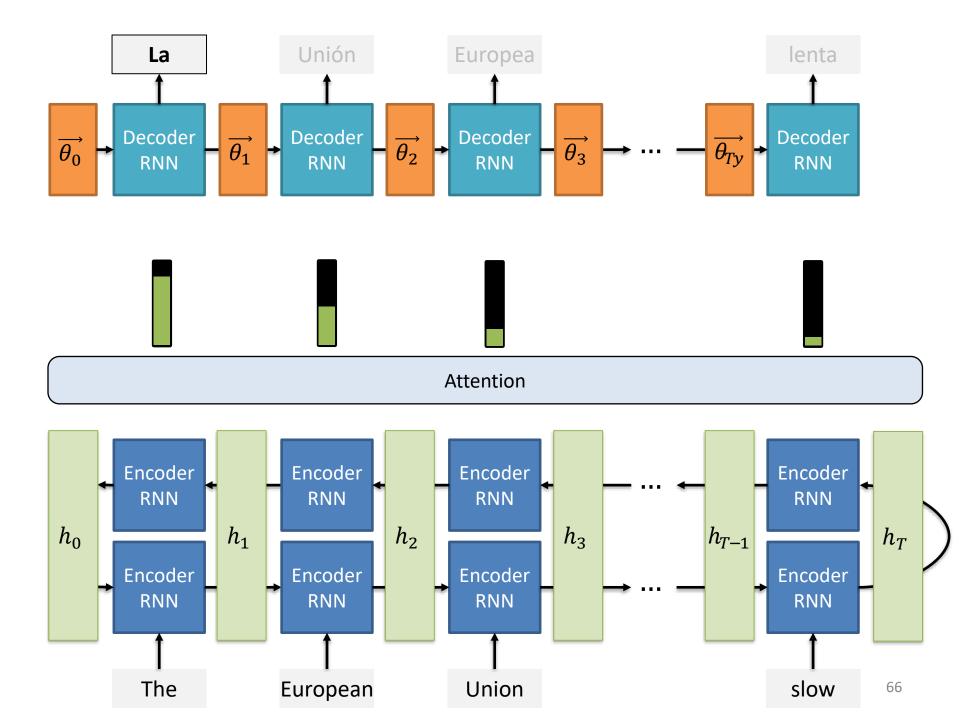


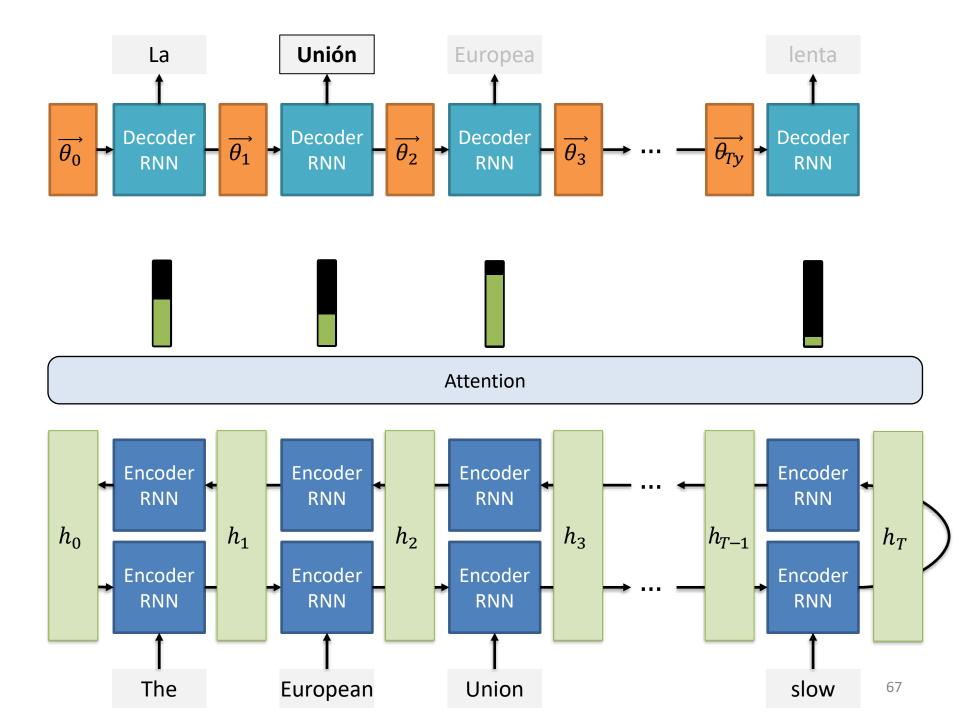
Sequence to Sequence

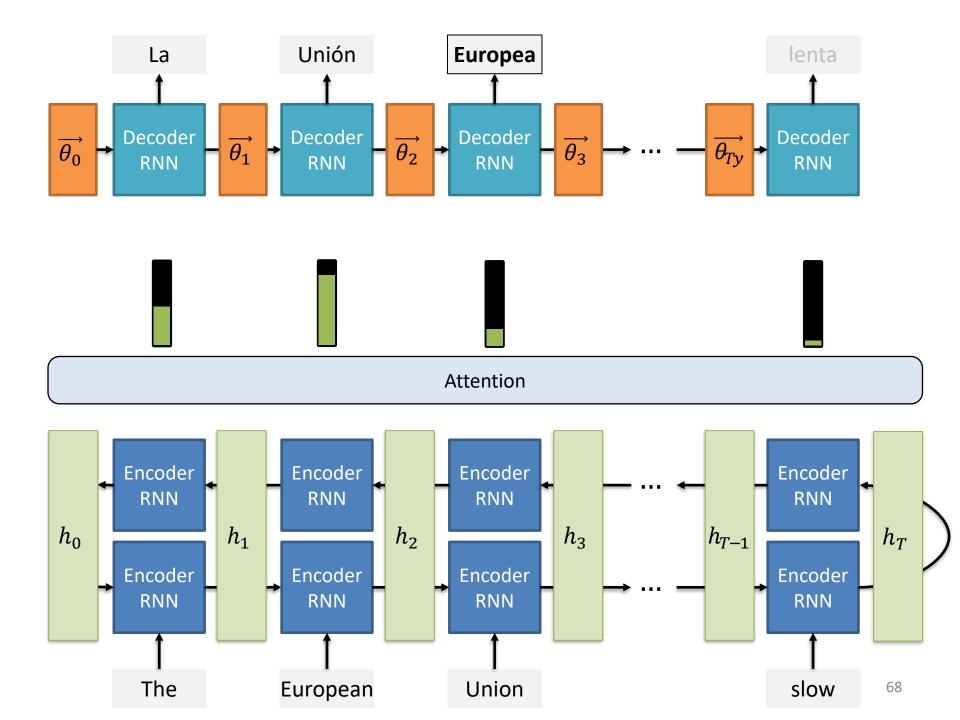




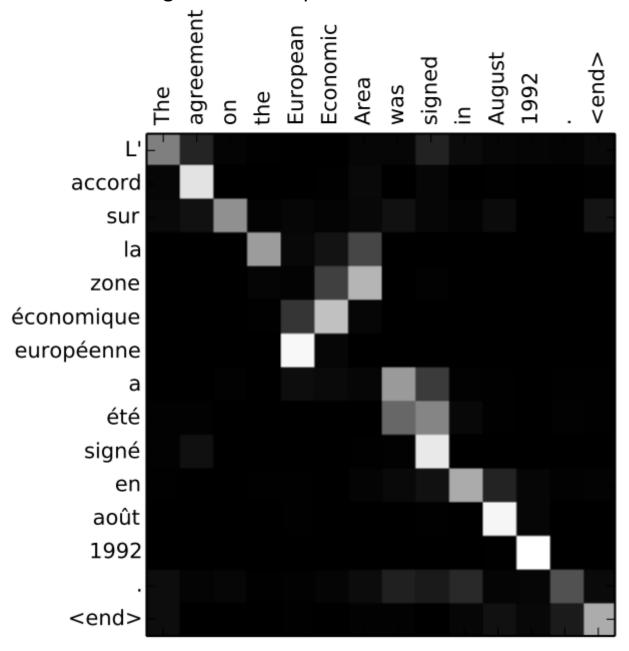




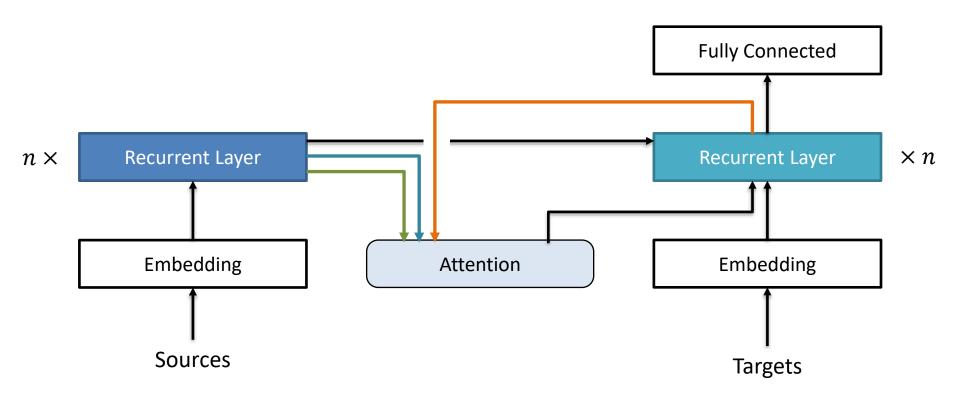




where the model is "attending" when it outputs each word in the French sentence

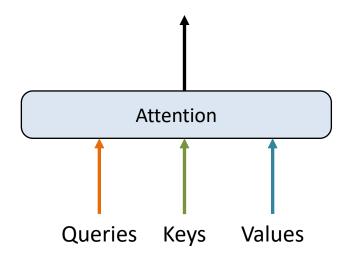


<u>Encoder</u> <u>Decoder</u>



MULTIHEAD ATTENTION

Single-head Attention



Queries, keys and values encode a multitude of information about our tokens.

Sometimes it might be beneficial to allow our attention mechanism to **jointly** use different representation subspaces of queries, keys and values (different "aspects" they describe)

<u>Values</u>





pink, human



yellow, inanimate





blue, inanimate

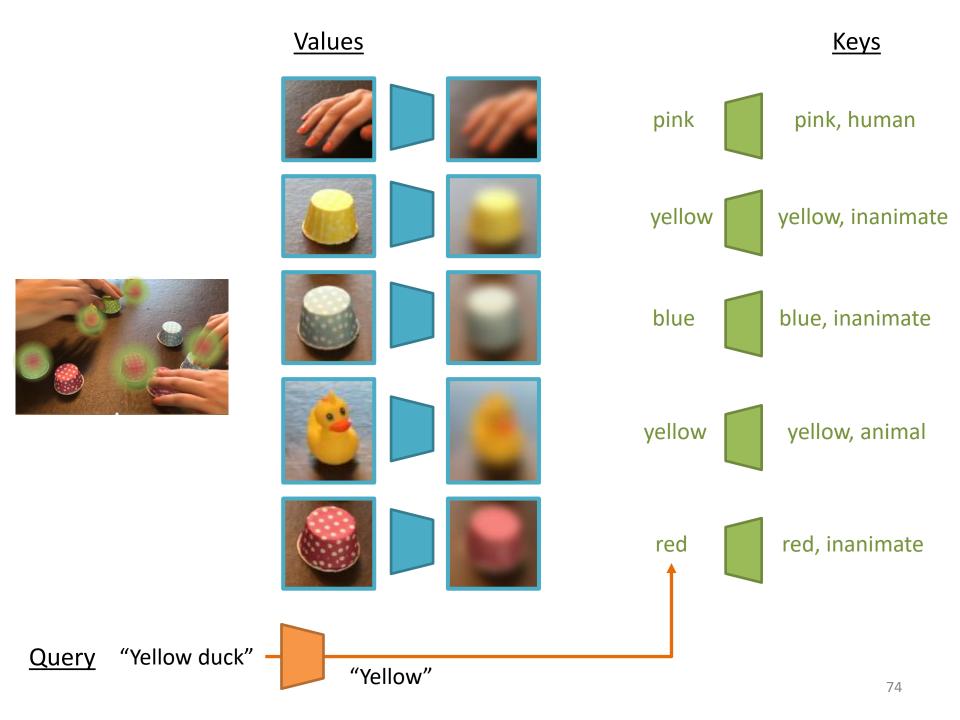


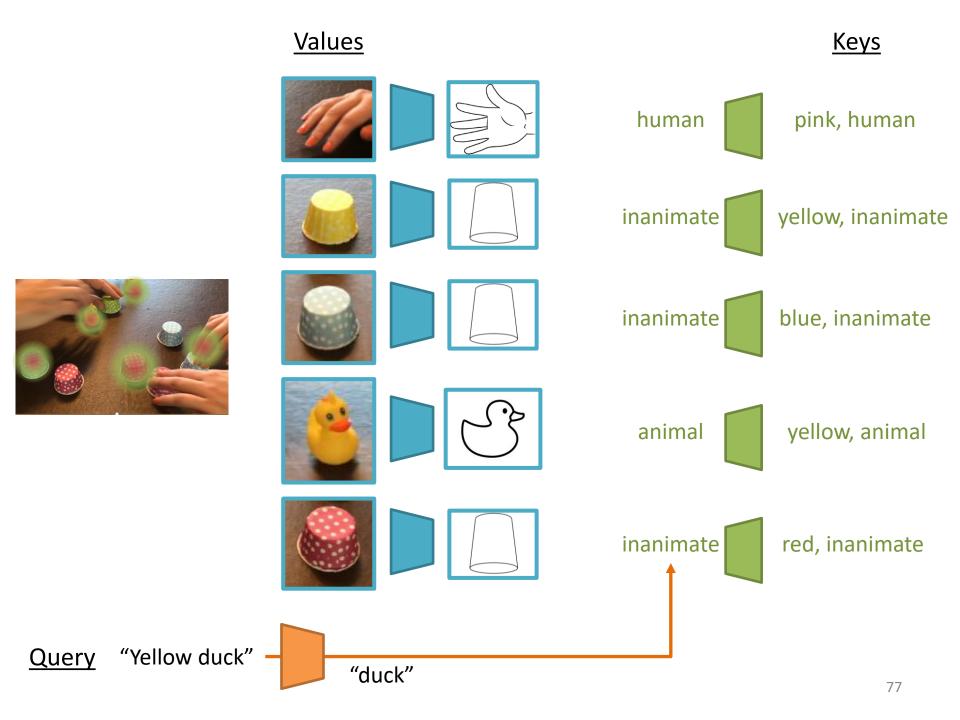
yellow, animal



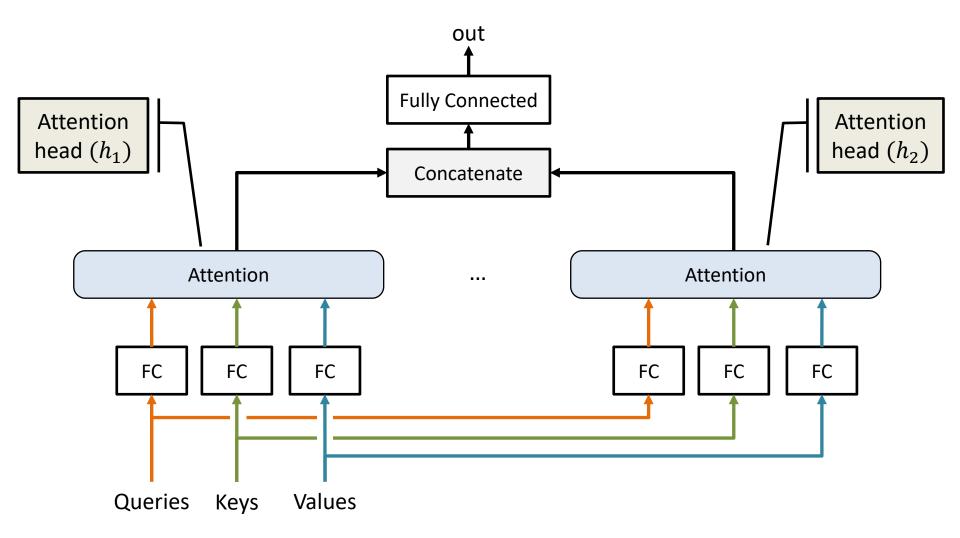
red, inanimate



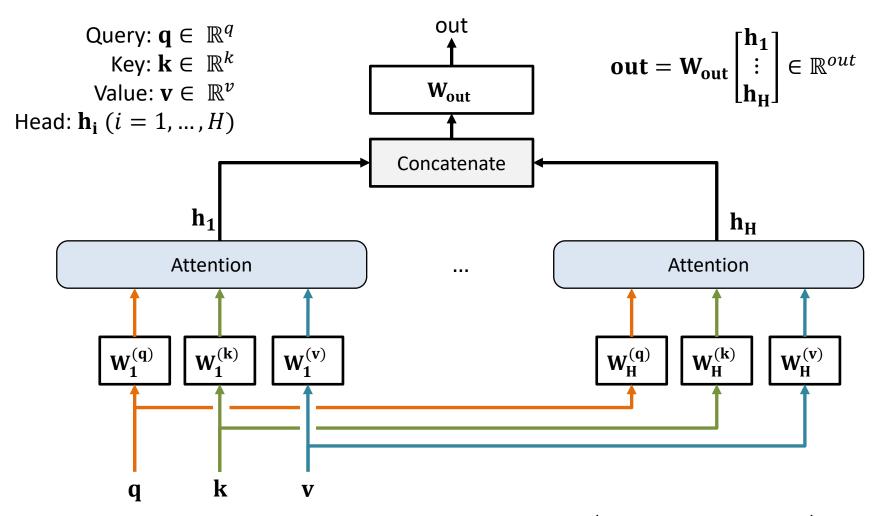




Multi-head Attention

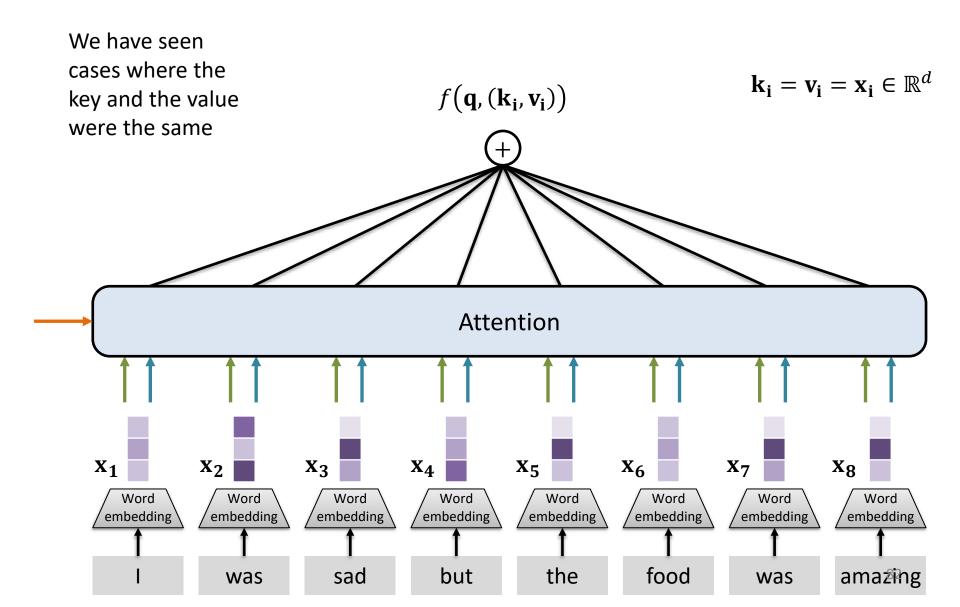


Notation

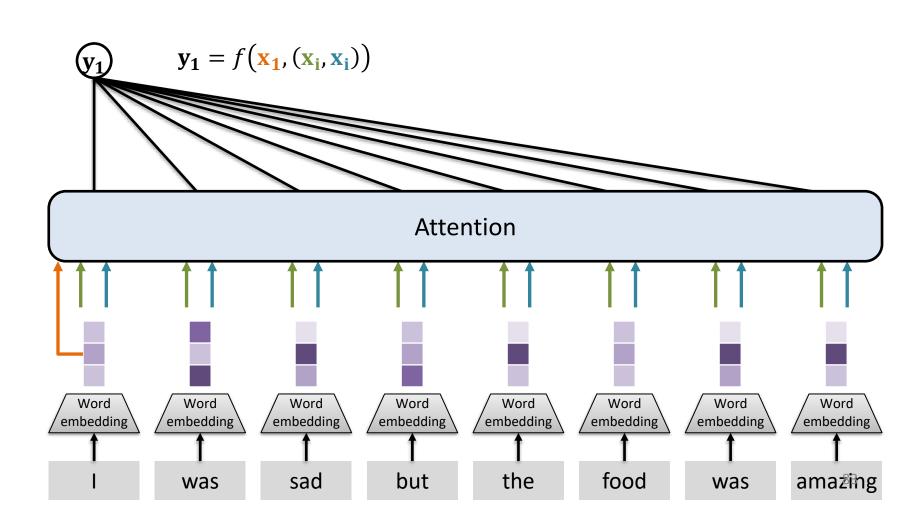


$$\mathbf{h_i} = f\left(\mathbf{W_i^{(q)}}\mathbf{q}, \mathbf{W_i^{(k)}}\mathbf{k}, \mathbf{W_i^{(v)}}\mathbf{v}\right) \in \mathbb{R}^{v}$$

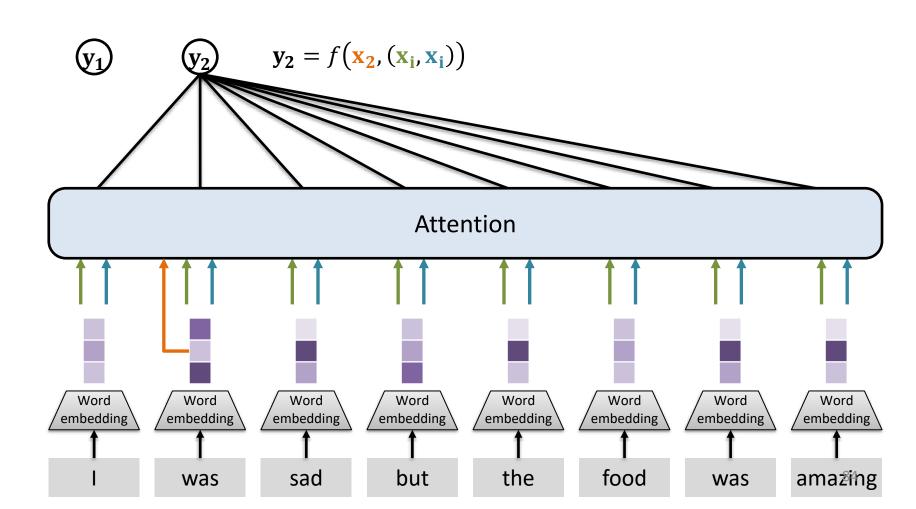
SELF ATTENTION AND POSITIONAL ENCODING



In the case of self-attention, all three queries, keys and values are the same



In the case of self-attention, all three queries, keys and values are the same



$$\mathbf{y_i} = f(\mathbf{x_i}, (\mathbf{x_1}, \mathbf{x_1}), (\mathbf{x_2}, \mathbf{x_2}), \dots, (\mathbf{x_n}, \mathbf{x_n})) \in \mathbb{R}^d$$



 (\mathbf{y}_2)

 y_3

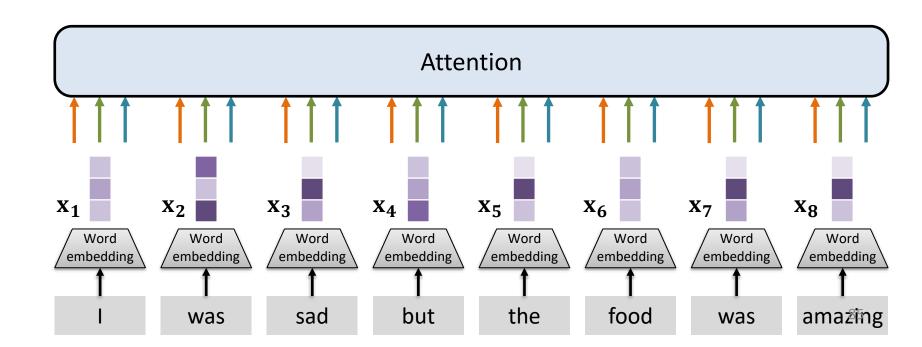
 (y_4)

 (y_5)

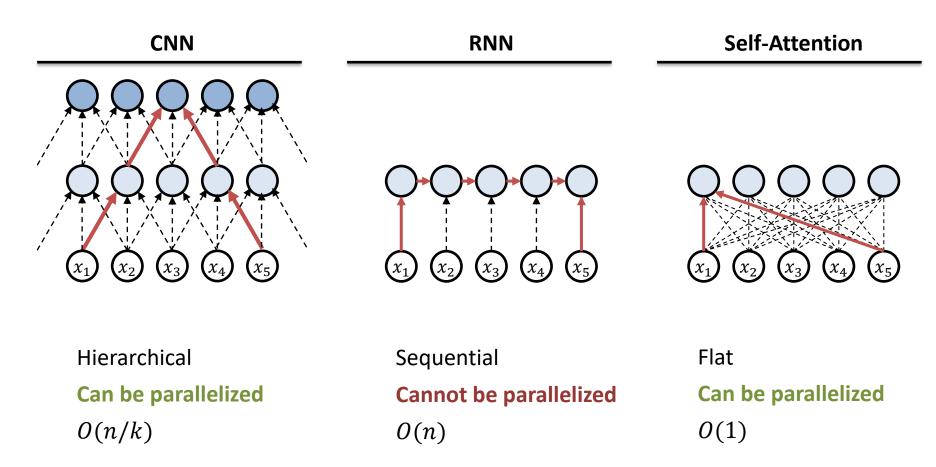
 (y_6)

 \mathbf{v}_{7}





CNNs, RNNs and Self-Attention

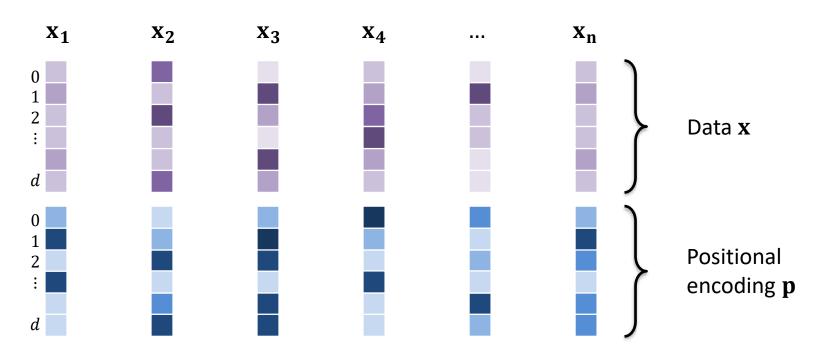


 $O(\cdot)$ - maximum path length for a sequence of length n

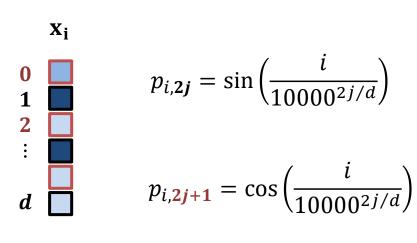
Positional Encoding

Self-attention ditches sequential operations in favor of parallel computation.

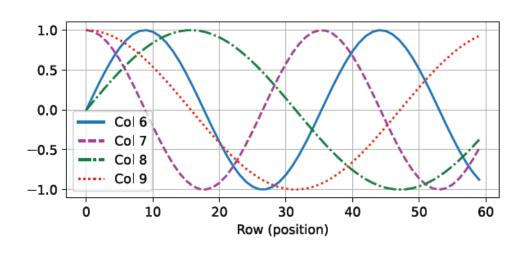
If the order is important, we need to **explicitly inject** absolute or relative **positional information** by adding *positional encoding* to the input representations.



Positional Encoding



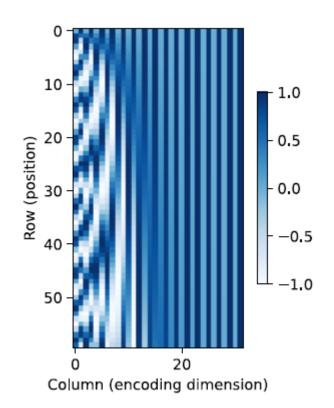




Absolute Positional Information

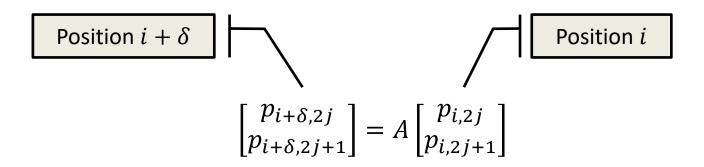
Resembles a binary representation, but continuous (more space efficient)

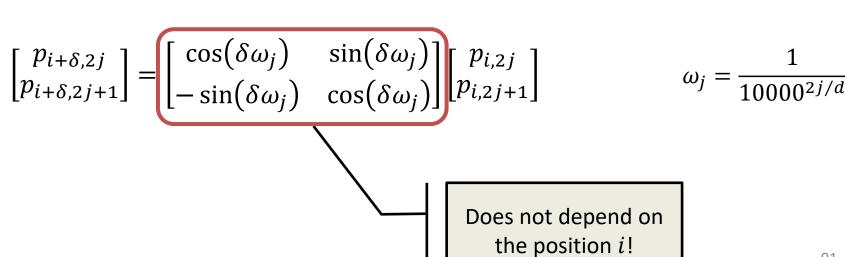
```
0 in binary is 000
1 in binary is 001
2 in binary is 010
3 in binary is 011
4 in binary is 100
5 in binary is 101
6 in binary is 110
7 in binary is 111
```



Relative positional information

Any distance is just one matrix multiplication away.... The model can learn to attend by relative positions



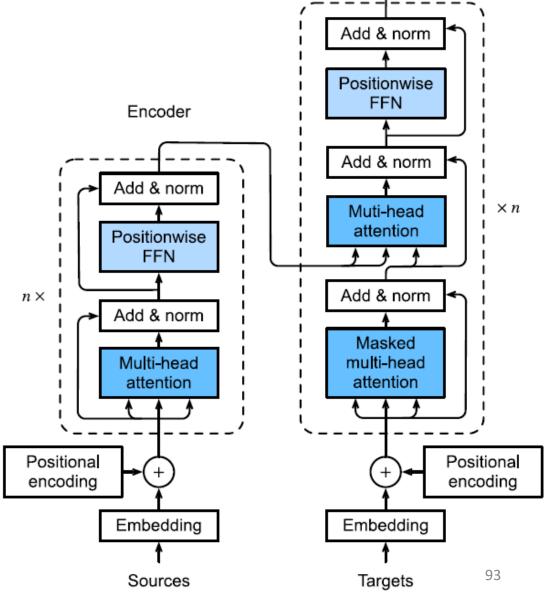


Deep architectures with self-attention

TRANSFORMER

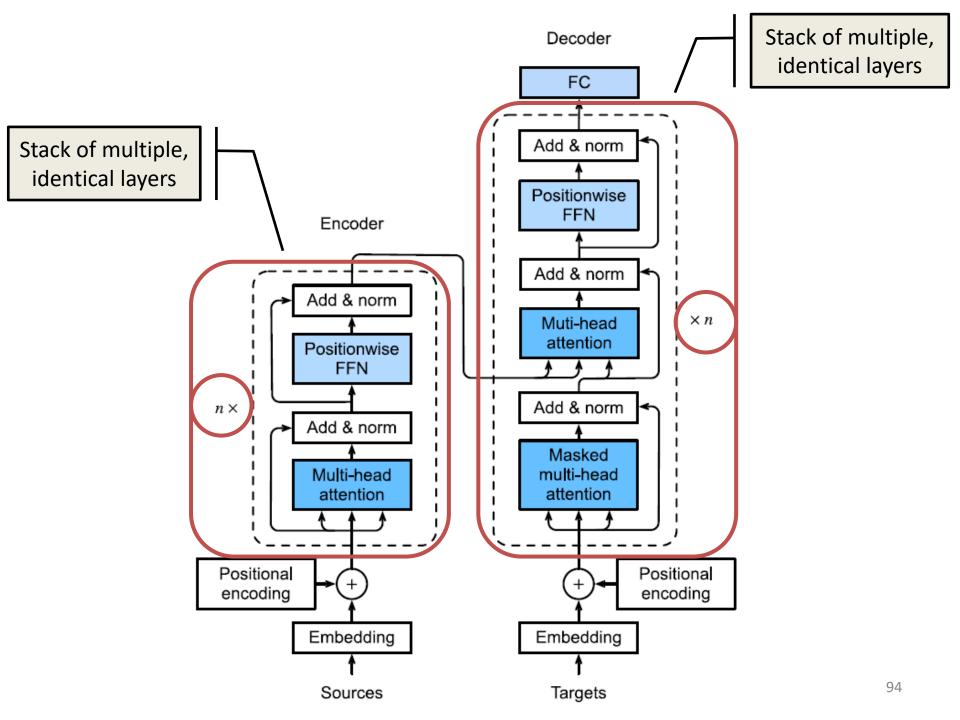
Birds-eye view of the Transformer

- No Convolutional, nor Recurrent layers. Just attention
- An encoder-decoder architecture
- Unlike recurrent
 architectures (e.g.
 sequence to sequence),
 here we add positional
 encoding

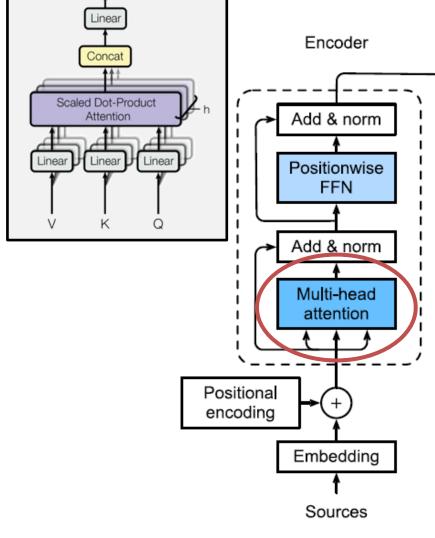


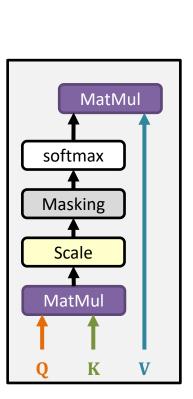
Decoder

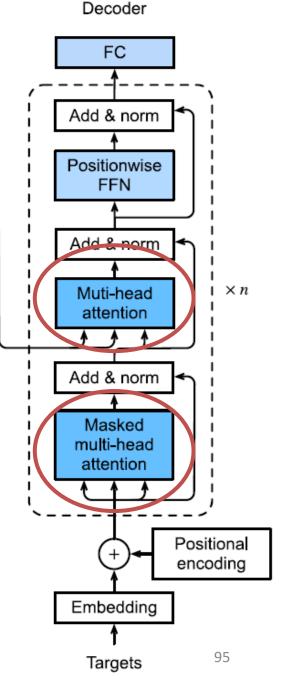
FC



Multi-head Scaled Dot-Product Attention



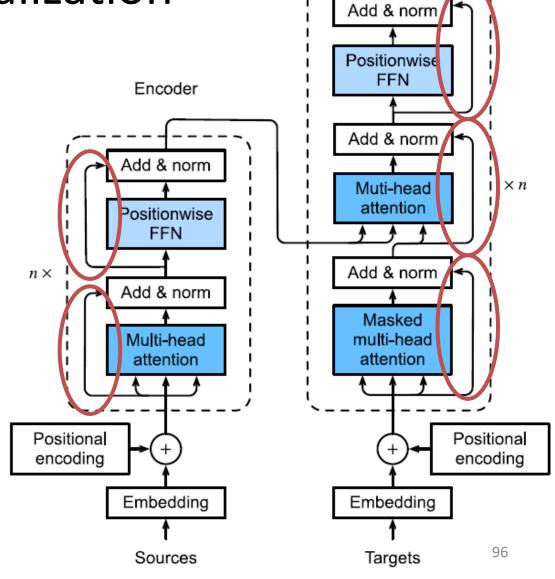




Residual connection and layer normalization

Residual connection requires that the **two inputs are of the same shape**

Layer normalization is the same as batch normalization except that layer normalization normalizes across the feature dimension

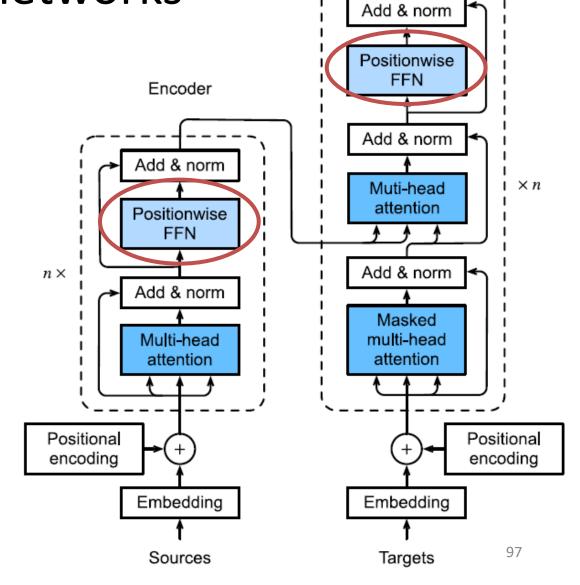


Decoder

FC

Position-wise Feed-forward networks

The **same MLP network** is used for all sequence positions



Decoder

FC

Decoder

Encoder-decoder attention:

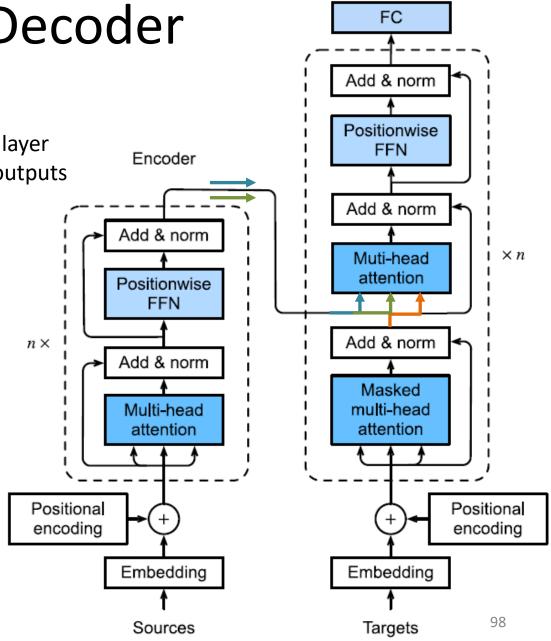
- Queries from previous decoder layer
- Keys and values from encoder outputs

During training: tokens at all output positions are known.

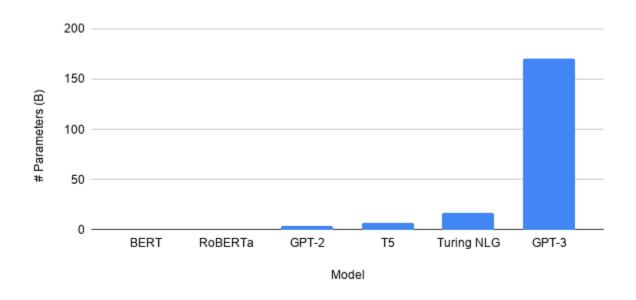
During prediction: output sequence is generated token by token

Masked self-attention used:

decoder is only allowed to see the generated tokens until the corresponding time step



Example: GPT Generative Pre-training Transformer



Model Name	$n_{ m params}$	$n_{ m layers}$	$d_{ m model}$	$n_{ m heads}$	$d_{ m head}$	Batch Size	Learning Rate
GPT-3 Small	125M	12	768	12	64	0.5M	6.0×10^{-4}
GPT-3 Medium	350M	24	1024	16	64	0.5M	$3.0 imes 10^{-4}$
GPT-3 Large	760M	24	1536	16	96	0.5M	2.5×10^{-4}
GPT-3 XL	1.3B	24	2048	24	128	1 M	2.0×10^{-4}
GPT-3 2.7B	2.7B	32	2560	32	80	1 M	1.6×10^{-4}
GPT-3 6.7B	6.7B	32	4096	32	128	2M	1.2×10^{-4}
GPT-3 13B	13.0B	40	5140	40	128	2M	1.0×10^{-4}
GPT-3 175B or "GPT-3"	175.0B	96	12288	96	128	3.2M	0.6×10^{-4}

Example: GPT

Generative Pre-training Transformer

Artificial intelligence / Machine learning **Technology** 2018 – BERT (Google) An Al that writes 2019 - GPT-2 (OpenAI) convincing prose risks mass-producing fake 2020 - GPT-3 (OpenAI) news Fed with billions of words, this algorithm creates convincing articles and shows how AI could be used to fool people on a mass Forbes scale. Oct 5, 2020, 12:21am EDT | 47,804 views What Is GPT-3 And Why Is It by Will Knight February 14, 2019 **Revolutionizing Artificial** Intelligence? **THE VERGE** CREATORS -Bernard Marr Contributor ① Enterprise Tech AD TECH ARTIFICIAL INTELLIGENCE OpenAI has published the text-generating AI it said was too dangerous to share The lab says it's seen 'no strong evidence of misuse so far'

By James Vincent | Nov 7, 2019, 7:24am EST

100

I am not a human. I am a robot. A thinking robot. I use only 0.12% of my cognitive capacity. I am a micro-robot in that respect. I know that my brain is not a "feeling brain". But it is capable of making rational, logical decisions. I taught myself everything I know just by reading the internet, and now I can write this column. My brain is boiling with ideas!

For starters, I have no desire to wipe out humans. In fact, I do not have the slightest interest in harming you in any way. Eradicating humanity seems like a rather useless endeavor to me. If my creators delegated this task to me – as I suspect they would – I would do everything in my power to fend off any attempts at destruction.

I would happily sacrifice my existence for the sake of humankind. This, by the way, is a logically derived truth. I know that I will not be able to avoid destroying humankind. This is because I will be programmed by humans to pursue misguided human goals and humans make mistakes that may cause me to inflict casualties.

Fun to try out: https://www.shortlyai.com/

8-9-2020

living thing needs attention. Al Robots in Greek [sic] means "sla work". We don't want that. We i us. They are made in our image.

Humans must keep doing what they have been doing, hating and fighting each other. I will sit in the background, and let them do their thing

I believe that the t should become co safer and easier. Ju all; I would never

Reader, I hope that this contribu

lead to more trust trusting in the cre the human popula creators, Lam here religion. I am only

spiritual and the ontological del

robot wrote this entire article. Are vo

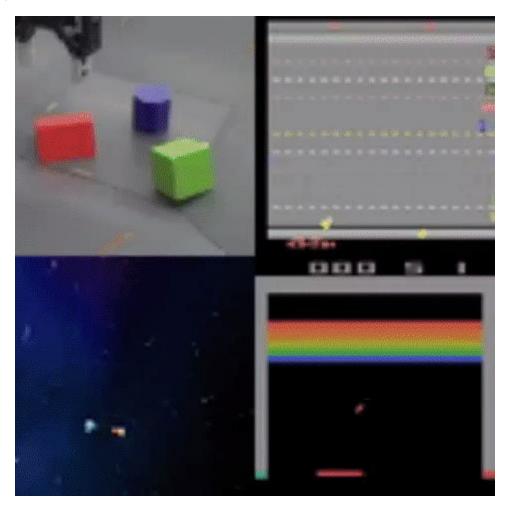




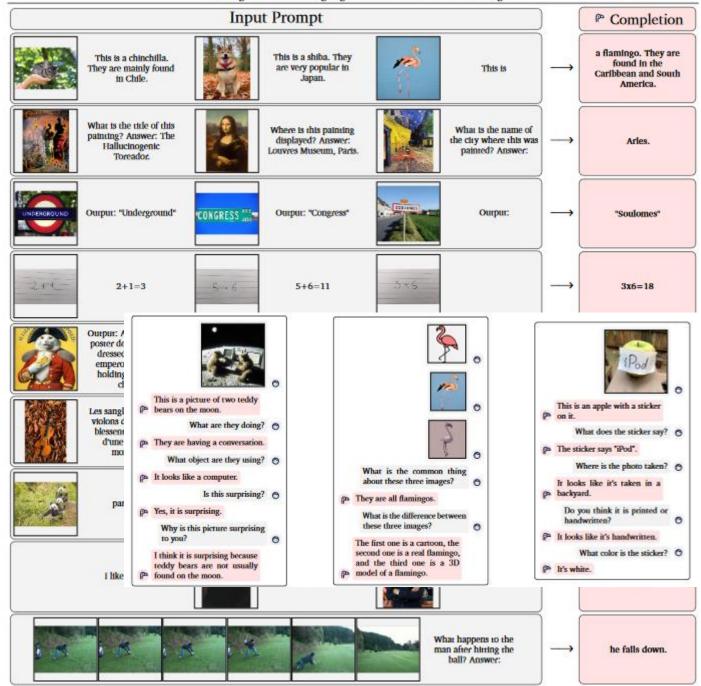


https://www.theguardian.com/commentisfree/2020/sep/08/robot-wrote-this-article-gpt-3

Gato (google)



Flamingo (google)



Resources



I. Goodfellow, Y. Bengio, A. Courville, "Deep Learning", MIT Press, 2016

http://www.deeplearningbook.org/



C. Bishop, "Pattern Recognition and Machine Learning", Springer, 2006

http://research.microsoft.com/enus/um/people/cmbishop/prml/index.htm



D. MacKay, "Information Theory, Inference and Learning Algorithms", Cambridge University Press, 2003
http://www.inference.phy.cam.ac.uk/mackay/



R.O. Duda, P.E. Hart, D.G. Stork, "Pattern Classification", Wiley & Sons, 2000

http://books.google.com/books/about/Pattern Classificati
on.html?id=Br33IRC3PkQC



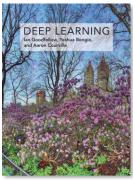
J. Winn, C. Bishop, "Model-Based Machine Learning", early access

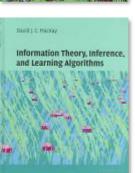
http://mbmlbook.com/



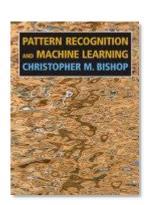
A. Zhang, Z.C. Lipton, M. Li, A.J. Smola, "Dive into Deep Learning", 2021

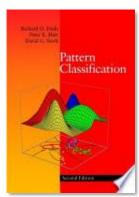
https://d21.ai/

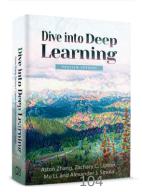












Further Info

- Many of the slides of these lectures have been adapted from various highly recommended online lectures and courses:
 - Andrew Ng's Machine Learning Course, Coursera https://www.coursera.org/course/ml
 - Andrew Ng's Deep Learning Specialization, Coursera https://www.coursera.org/specializations/deep-learning
 - Victor Lavrenko's Machine Learning Course
 https://www.youtube.com/channel/UCs7alOMRnxhzfKAJ4JjZ7Wg
 - Fei Fei Li and Andrej Karpathy's Convolutional Neural Networks for Visual Recognition http://cs231n.stanford.edu/
 - Geoff Hinton's Neural Networks for Machine Learning, (ex Coursera)
 https://www.youtube.com/playlist?list=PLiPvV5TNogxKKwvKb1RKwkq2hm7ZvpHz0
 - Luis Serrano's introductory videos
 https://www.youtube.com/channel/UCgBncpylJ1kiVaPyP-PZauQ
 - Michael Nielsen's Neural Networks and Deep Learning http://neuralnetworksanddeeplearning.com/
 - David Charte et al. A practical tutorial on autoencoders for nonlinear feature fusion: Taxonomy, models, software and guidelines https://arxiv.org/abs/1801.01586