Attention-based architectures

INTELLIGENT SYSTEMS FOR PATTERN RECOGNITION (ISPR)

DAVIDE BACCIU – DIPARTIMENTO DI INFORMATICA - UNIVERSITA’ DI PISA

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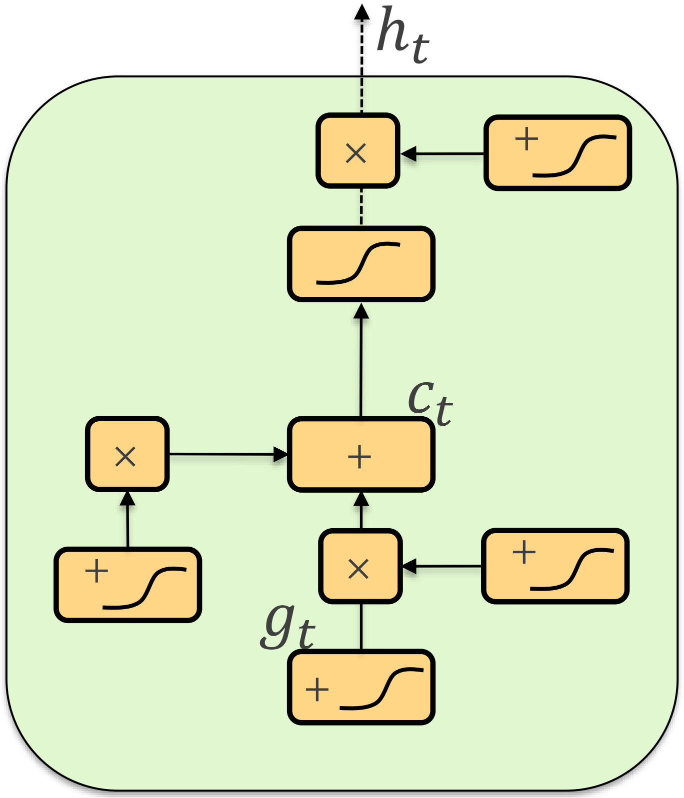
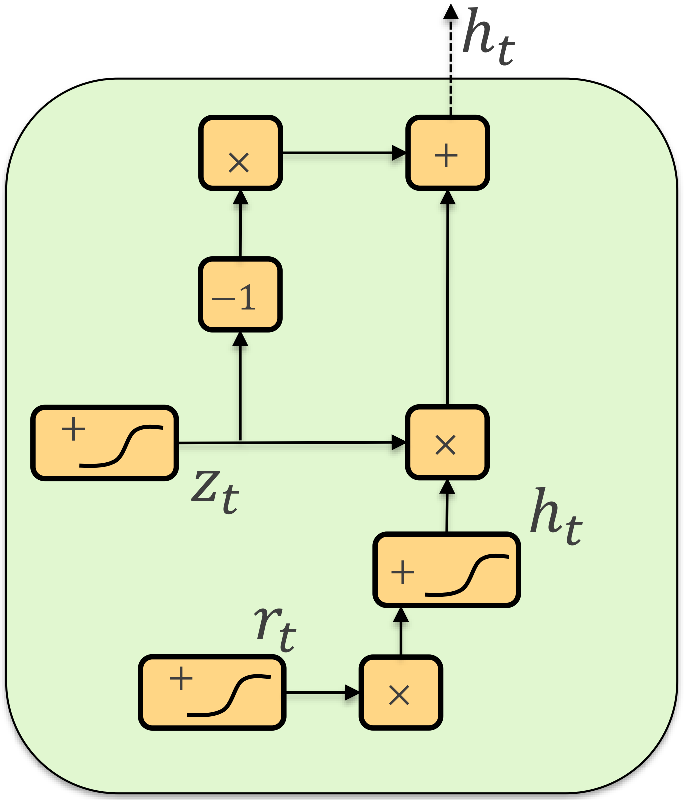
Lecture Outline

- Neural attention for structured/compound data
  - Sequence-to-sequence paradigm
  - Cross-attention
  - Self-attention and transformers
  - Attention in vision tasks

Gated RNN Refresher

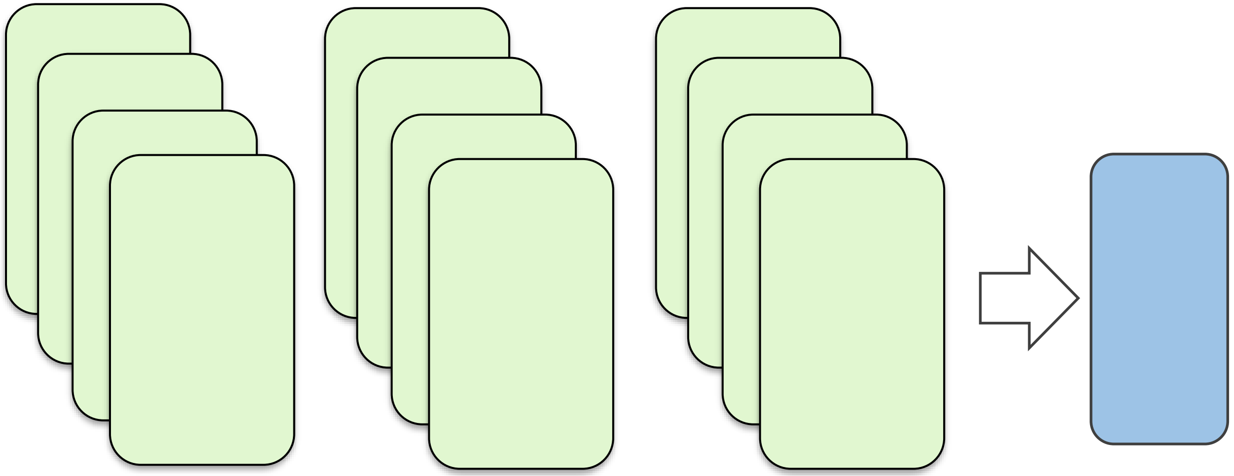


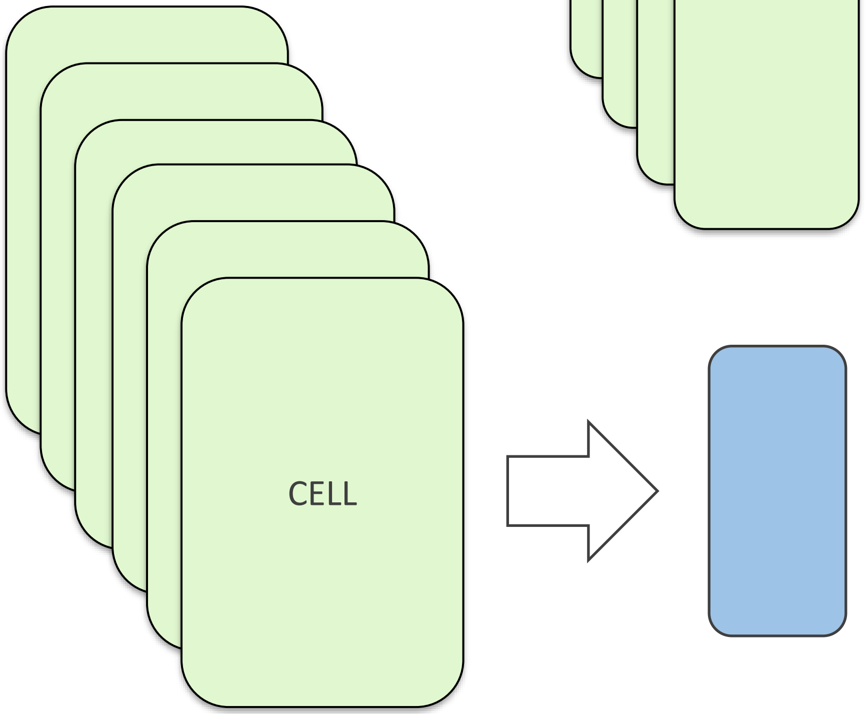
LSTM Cell



GRU Cell

Graphical Notation for Compositionality





Use a simplified (and overloaded) graphical notation to represent GRNN layers and stacks of GRNN

Dealining with Compound Data

- GRNN are excellent to handle size/topology varying data in input
  - How can we handle size/topology varying outputs?
  - Sequence-to-sequence
- Structured data is compound information
  - Efficient processing needs the ability to focus on certain parts of such information
  - Attention mechanism

Sequence-to-sequence

Sequence Transduction

- Input and output are both sequences
- They may have different lengths
- Example: machine translation

The cat is on the table → **Il gatto è sul tavolo**

How do we model the context here?

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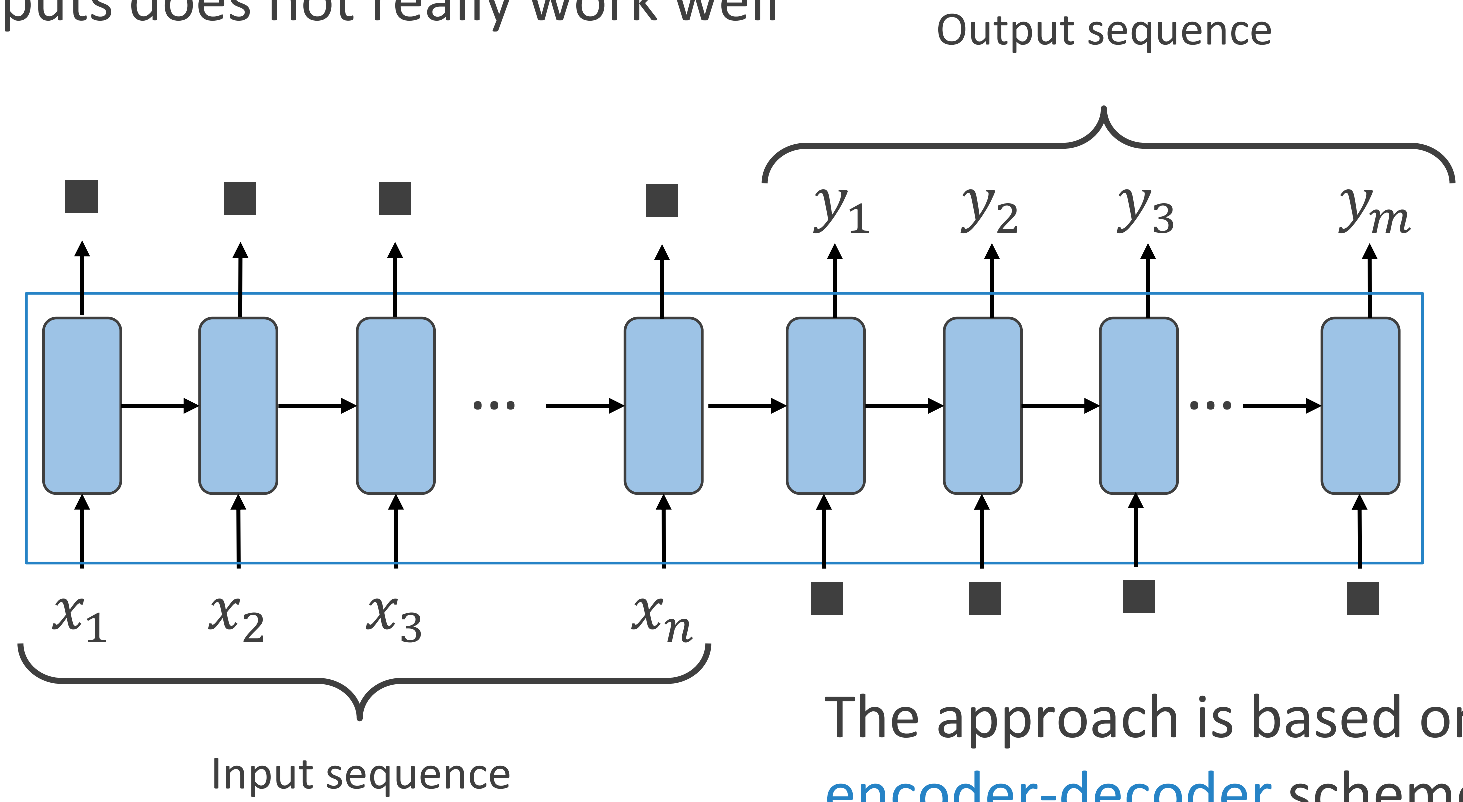
Learning to Output Variable Length Sequences

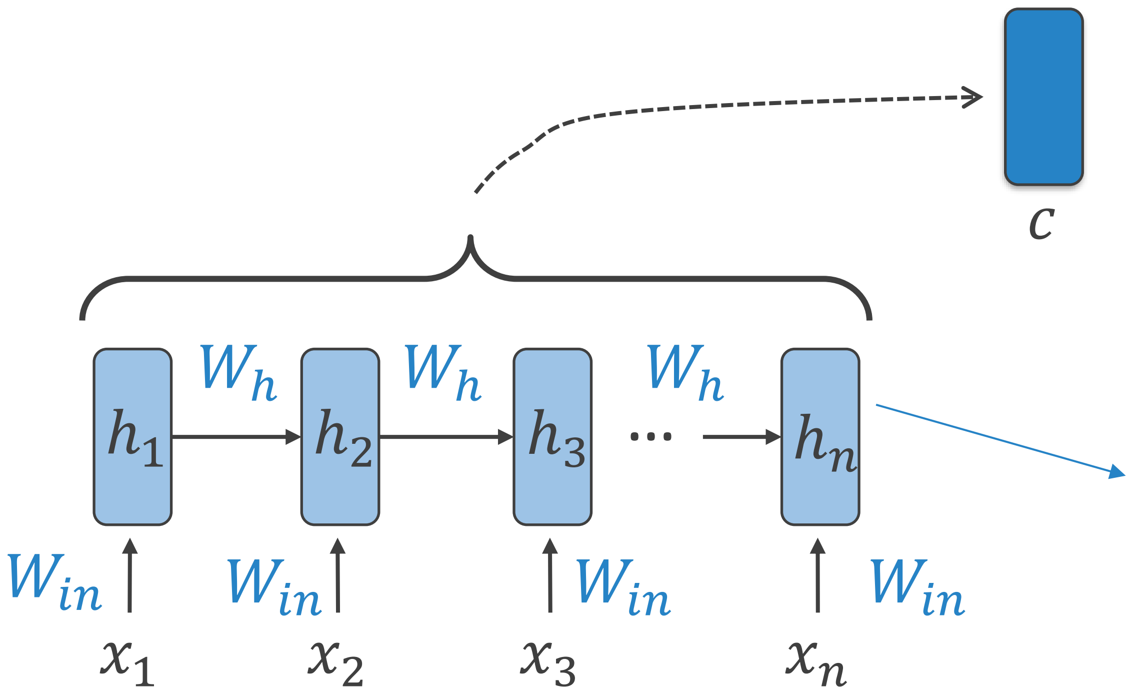
The idea of an unfolded RNN with blank inputs-outputs does not really work well



The approach is based on an encoder-decoder scheme

Encoder

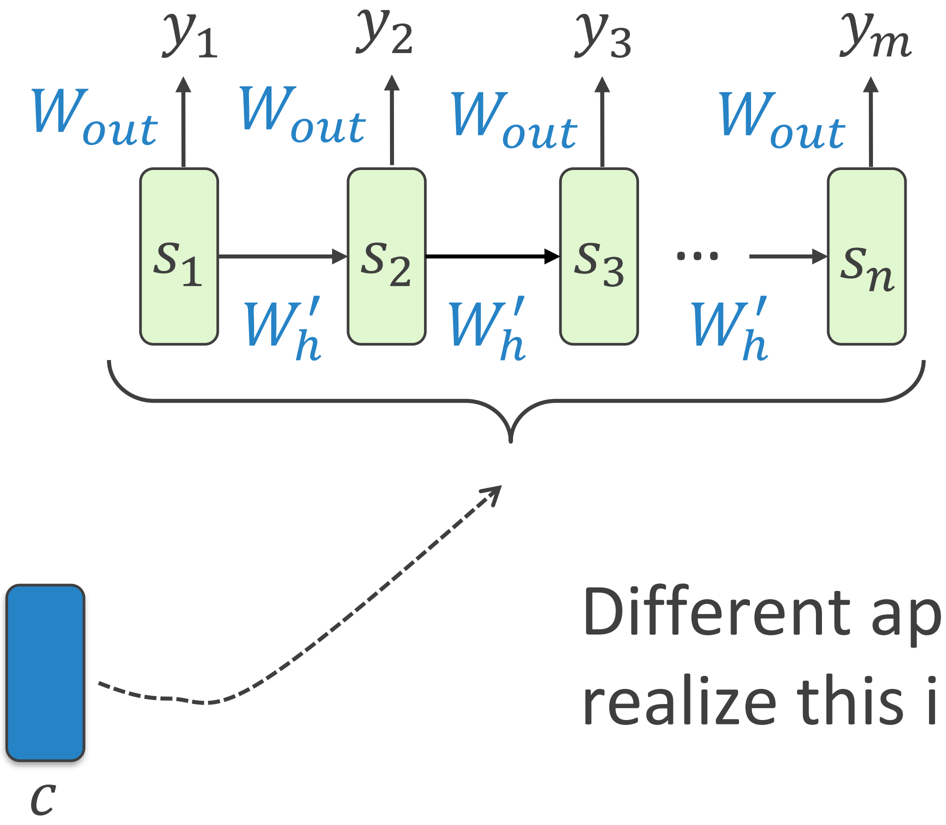
Produce a compressed and fixed length representation c of all the input sequence $x_1, \dots, x_n$



Originally $c = h_n$

Activations of an LSTM/GRU layer of K cells

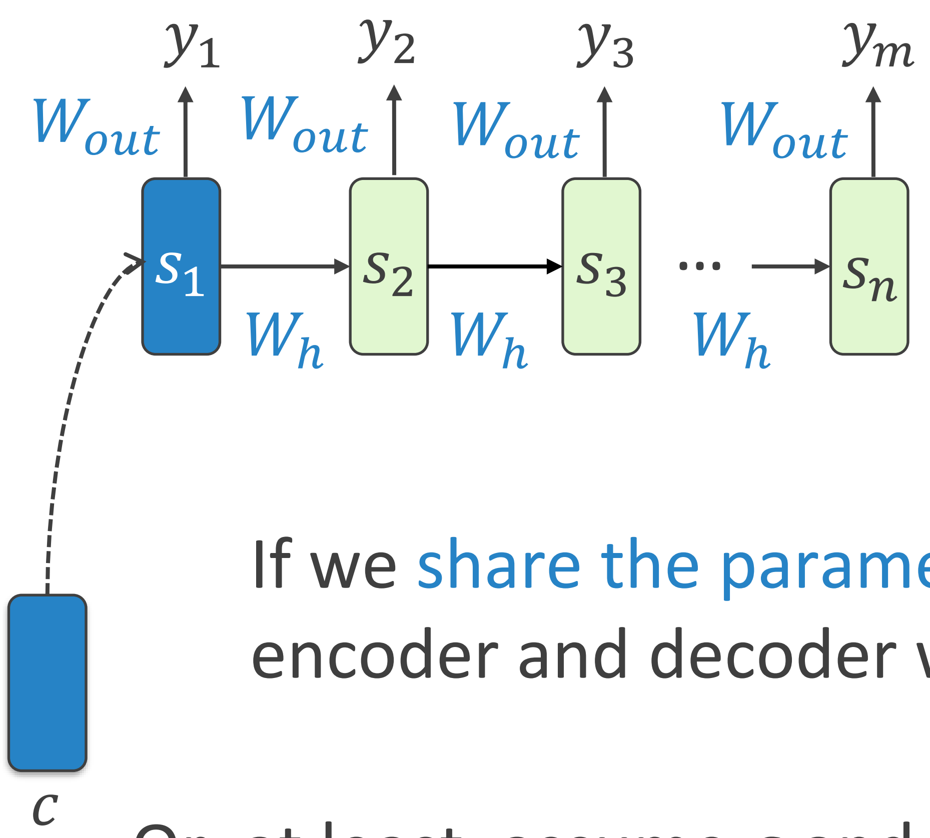
Decoder



A LSTM/GRU layer of K cells seeded by the context vector c

Different approaches to realize this in practice

Decoder

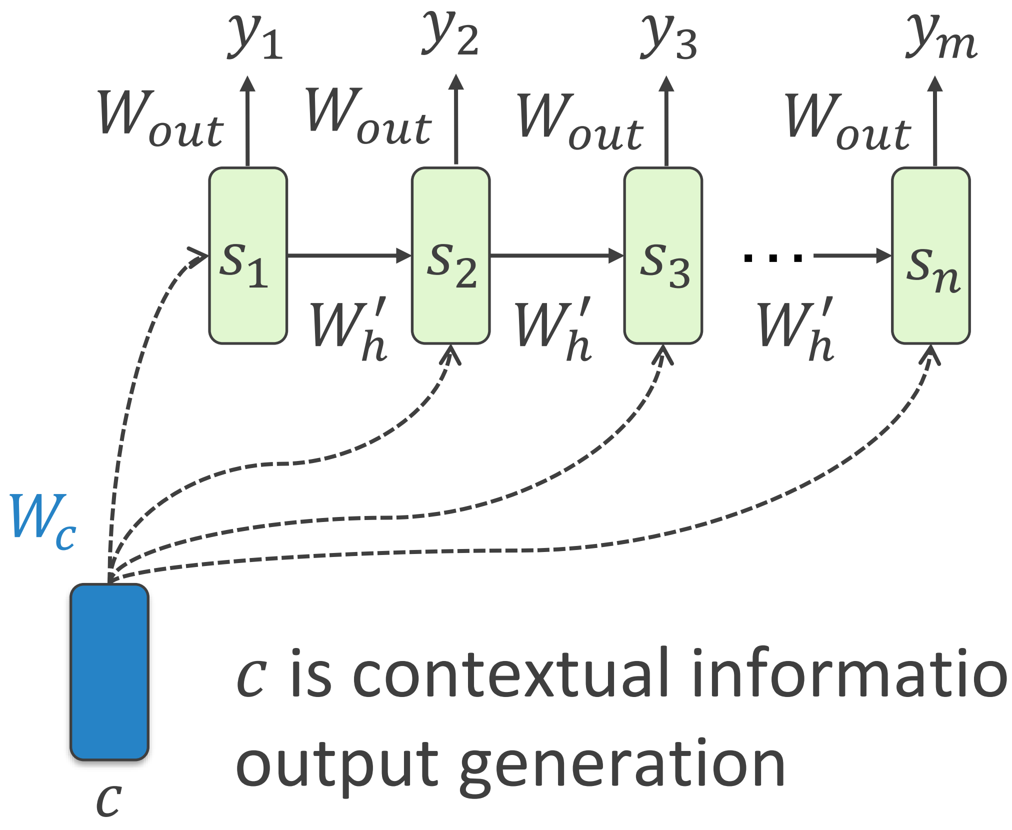


We risk to lose memory of c soon

If we share the parameters between encoder and decoder we can take $s_1 = c$

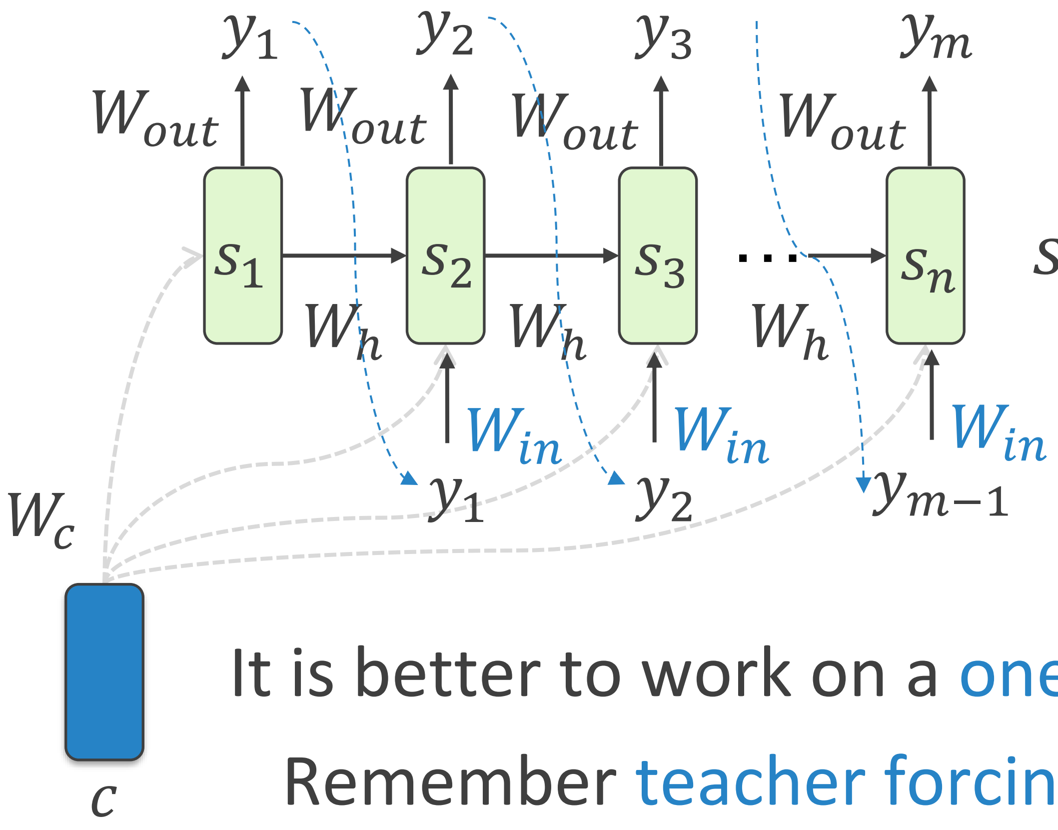
Or, at least, assume c and s_1 have compatible size

Decoder



c is contextual information kept throughout output generation

Decoder



$$s_i = f(c, s_{i-1}, y_{i-1})$$

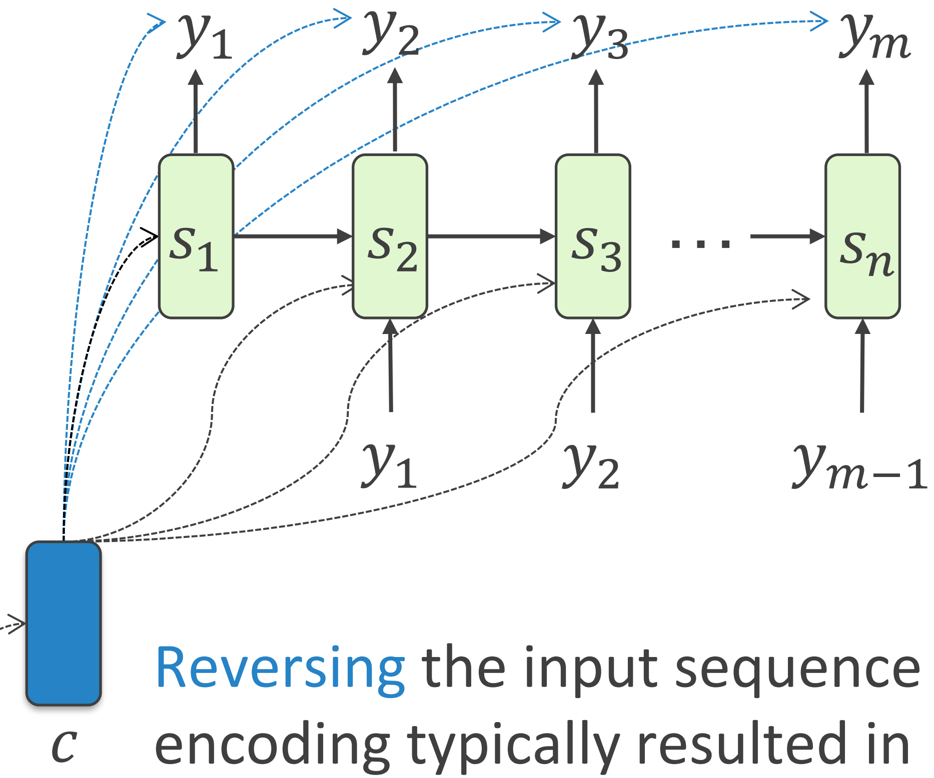
It is better to work on a one-step-ahead scheme

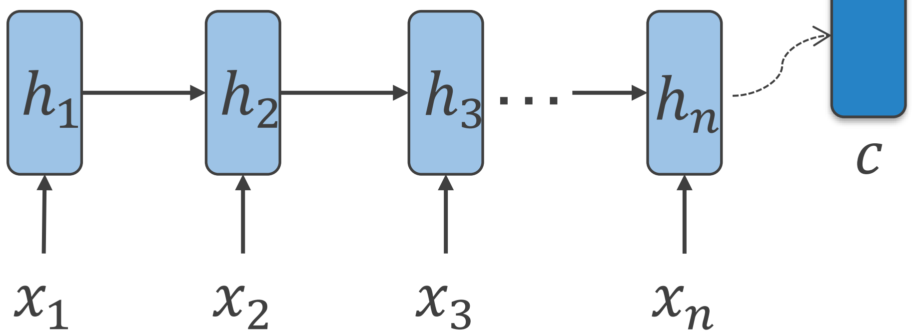
Remember teacher forcing (only) at training time

Sequence-To-Sequence Learning

Encoder-Decoder can share parameters (but it is uncommon)

Encoder-Decoder can be trained end-to-end or independently





Reversing the input sequence in encoding typically resulted in increased performance (?!)

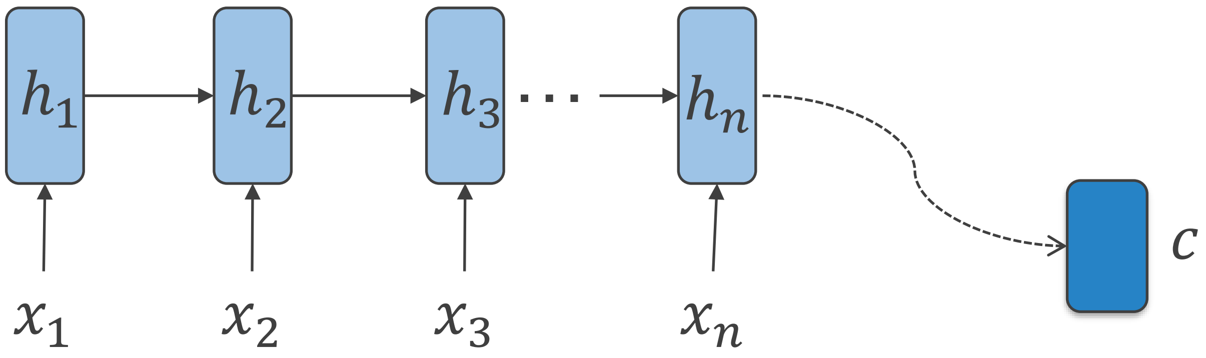
A Motivating Example

The cat is on the table

Il gatto è sul tavolo

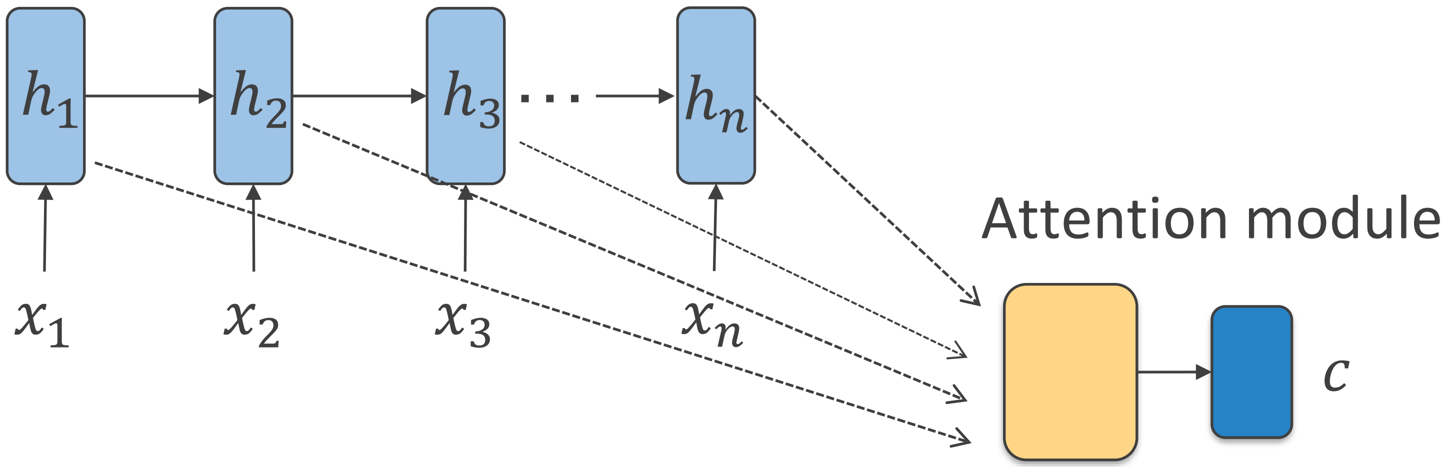
Attention

On the Need of Paying Attention



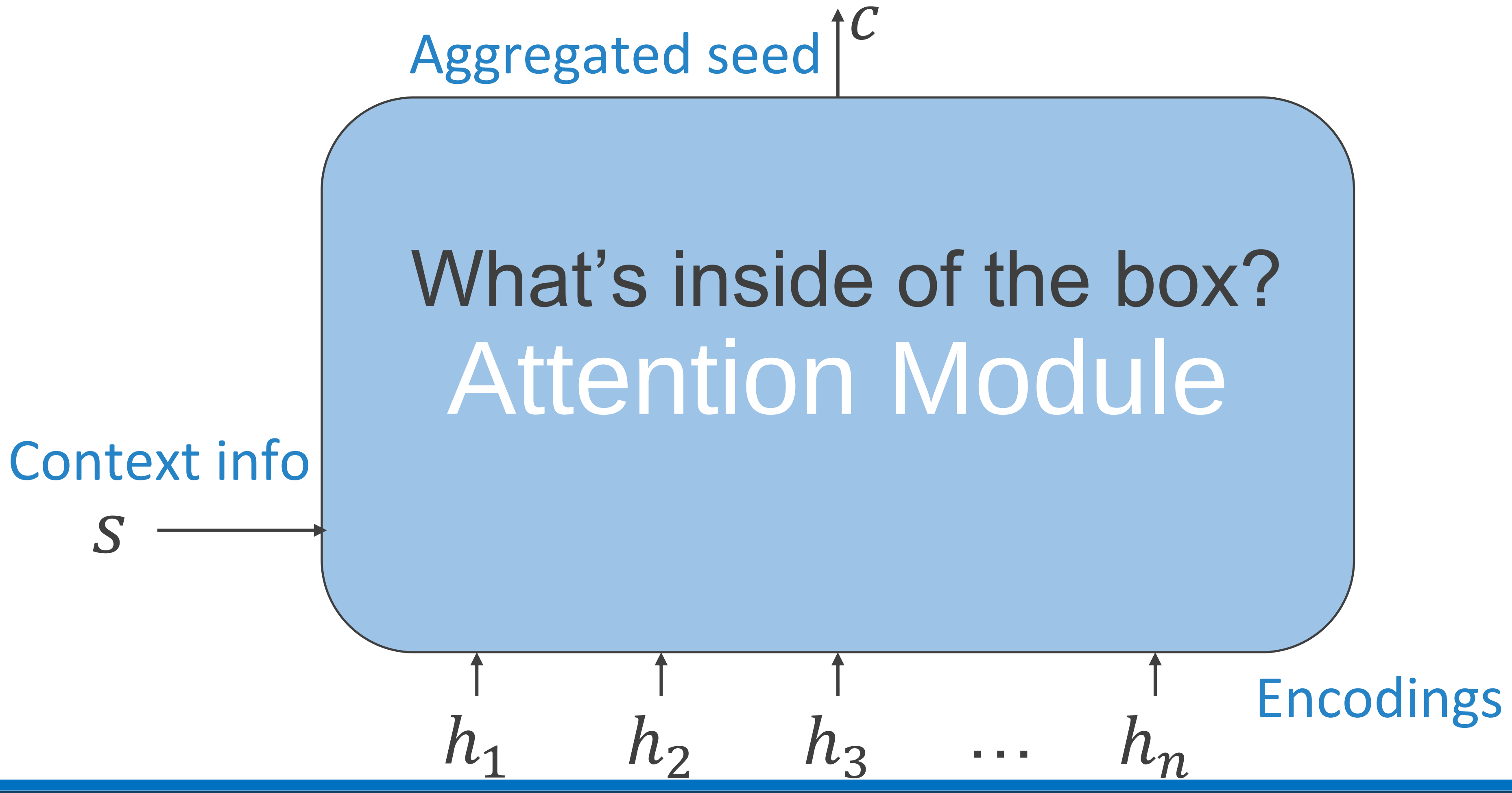
- Encoder-Decoder scheme assumes the hidden activation of the last input element summarizes sufficient information to generate the output
  - Bias toward most recent past
- Other parts of the input sequence might be very informative for the task
  - Possibly elements appearing very far from sequence end

On the Need of Paying Attention



- Attention mechanisms select which part of the sequence to focus on to obtain a good c

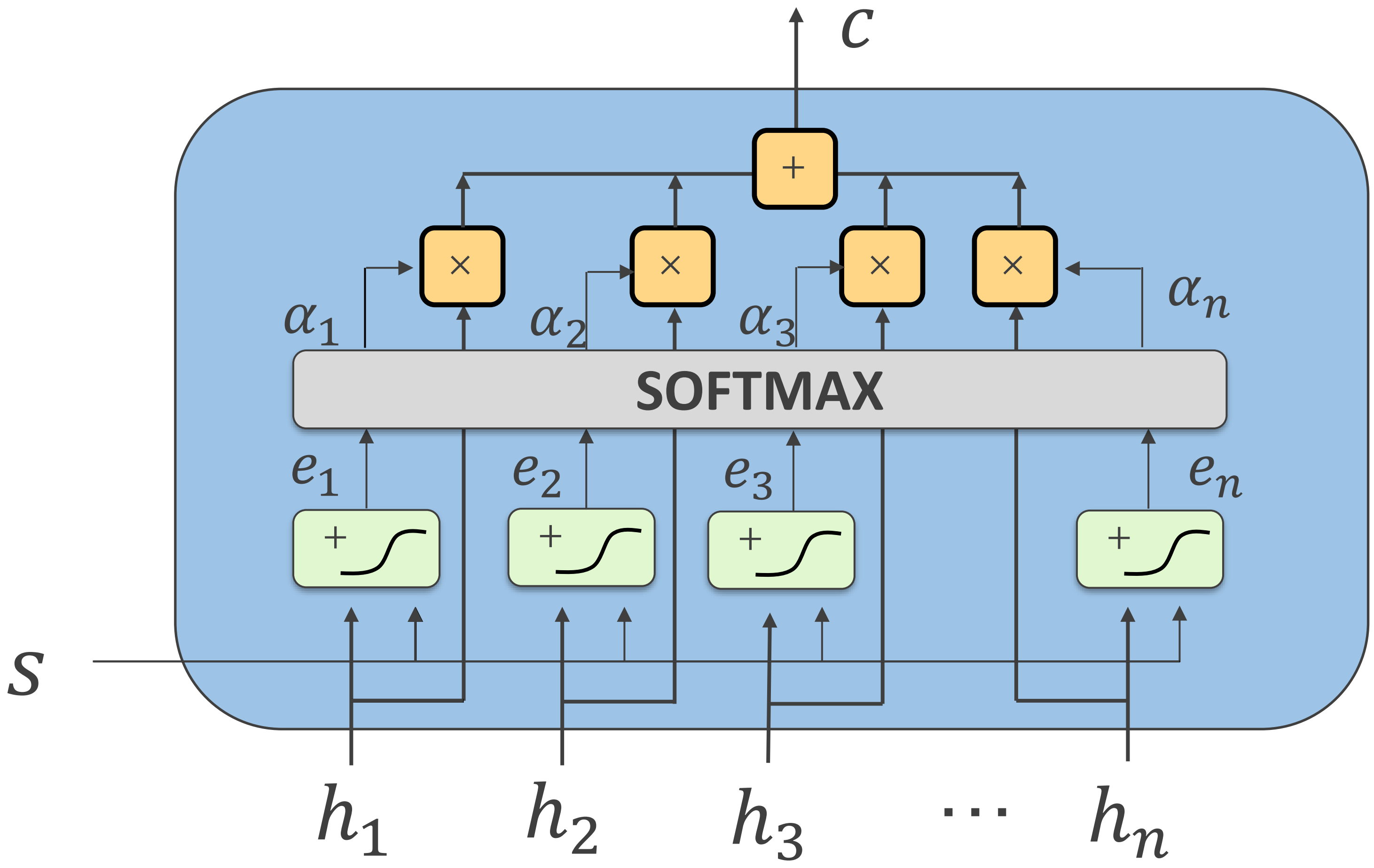
Attention Mechanisms – Blackbox View



What's inside of the box?

The Revenge of the Gates!

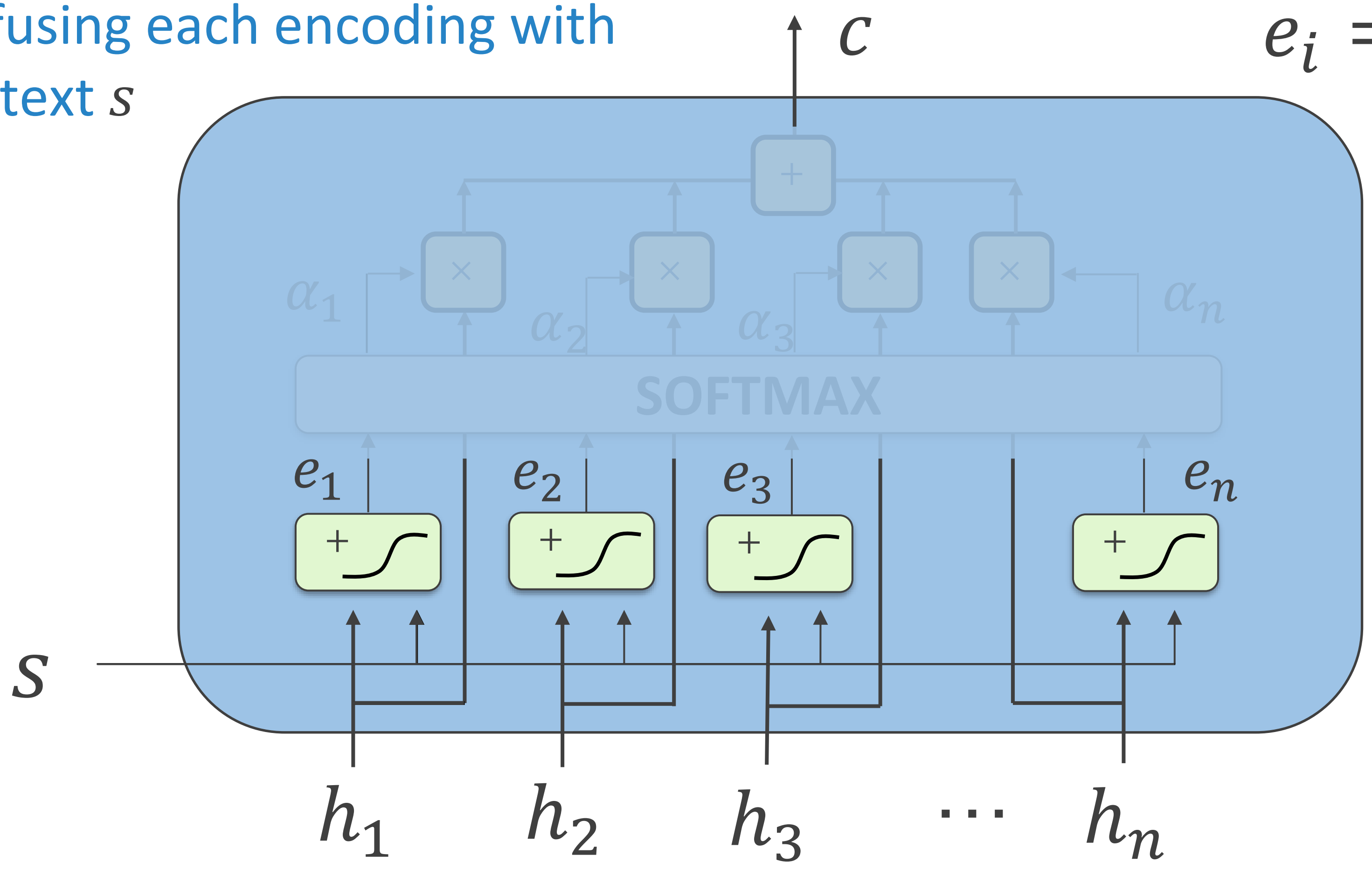
Opening the Box



Opening the Box – Relevance

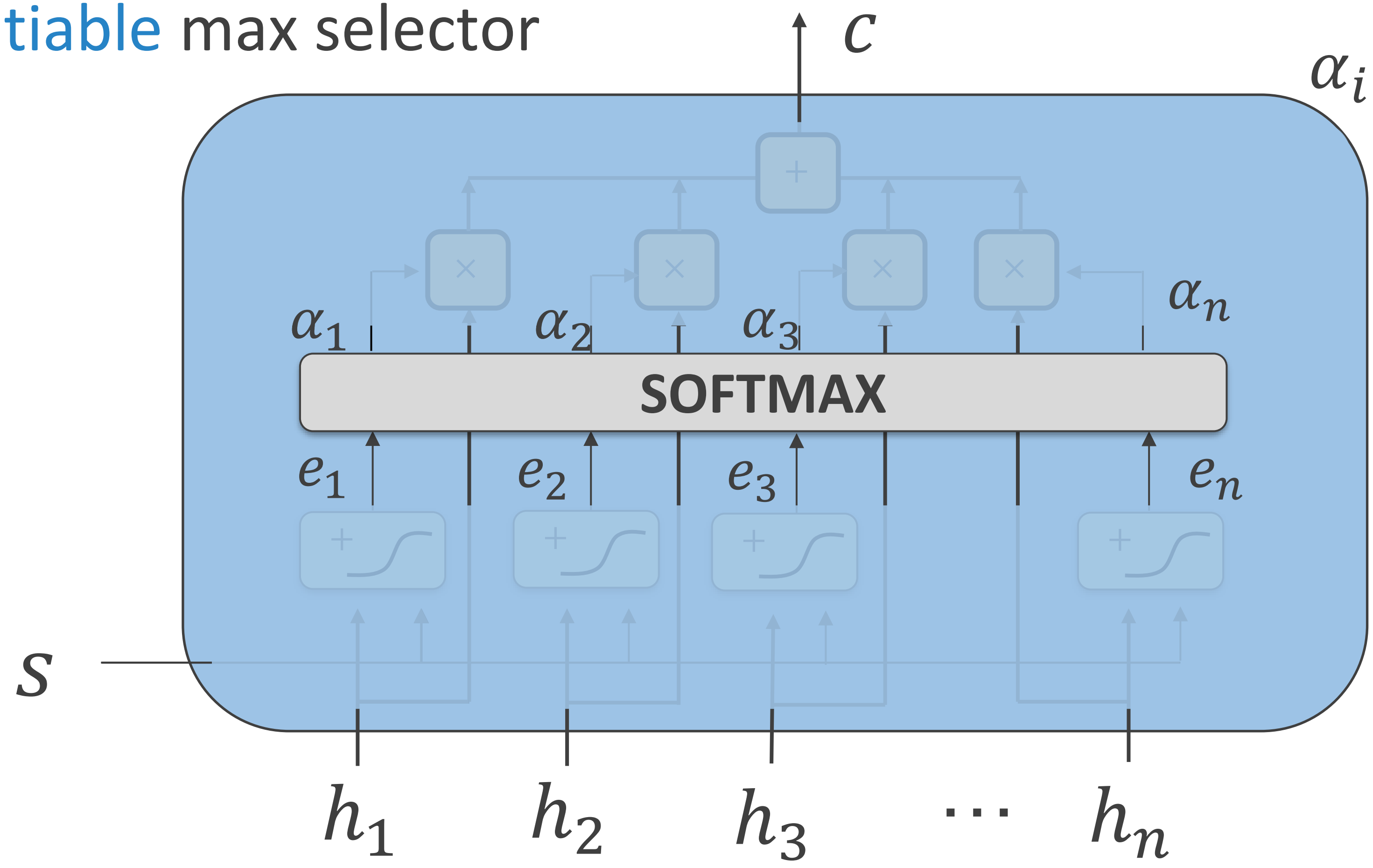
Tanh layer fusing each encoding with current context s

$e_i = \mathrm{a}(s, h_i)$



Opening the Box – Softmax

A differentiable max selector operator

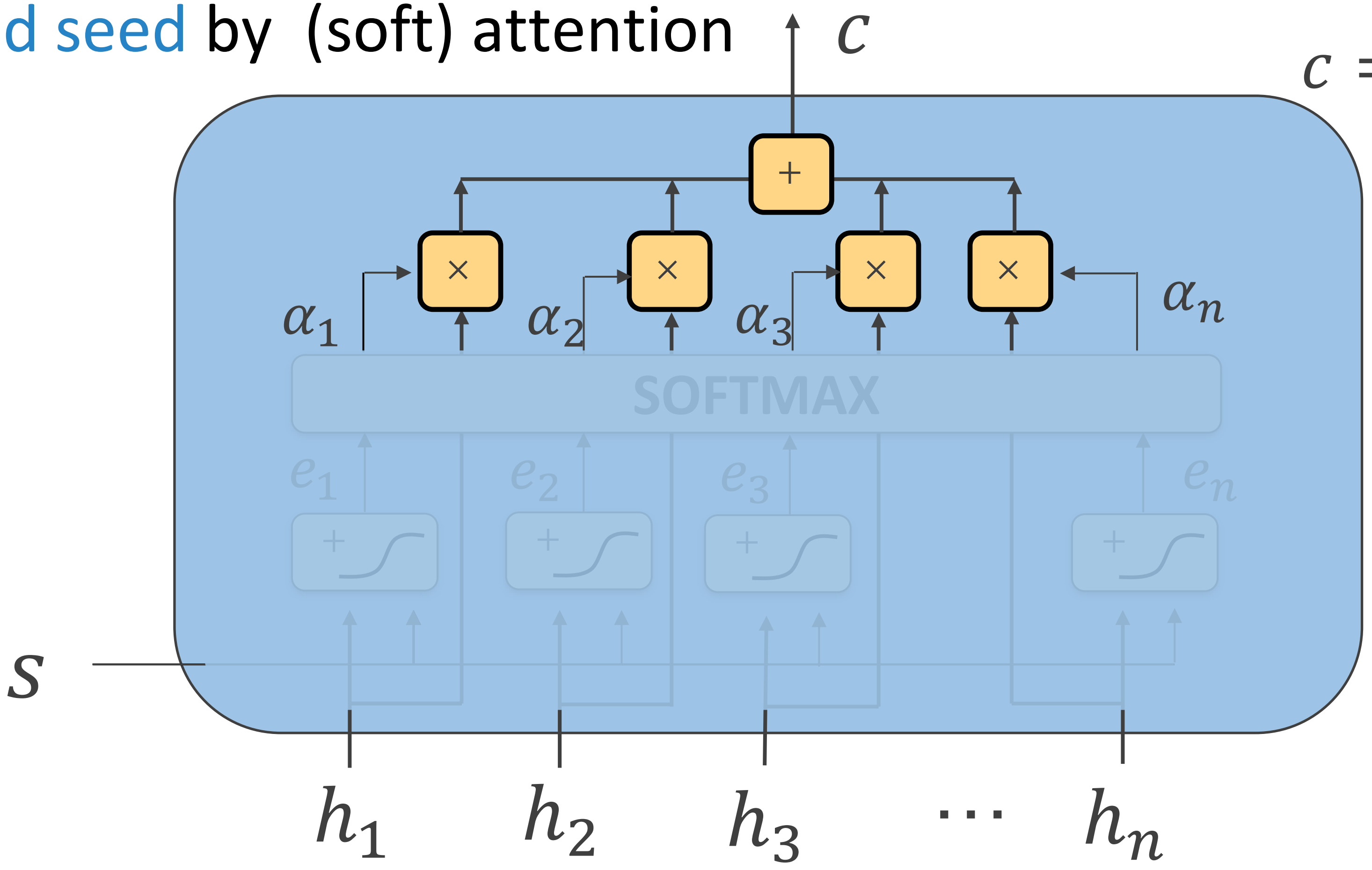


$$\alpha_i = \frac{\exp(e_i)}{\sum_j \exp(e_j)}$$

Opening the Box – Voting

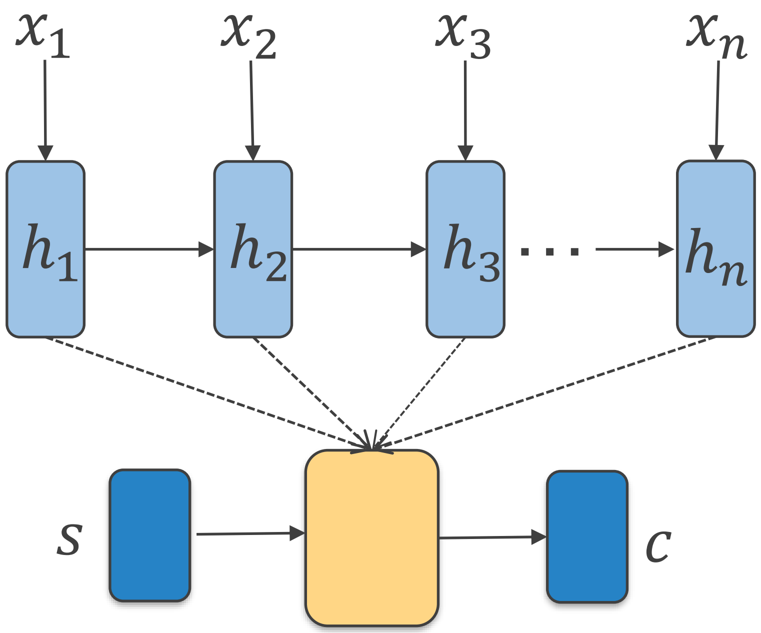
Aggregated seed by (soft) attention voting

$$c = \sum_i \alpha_i h_i$$



Attention - Equations

- Relevance: $e_i = \mathrm{a}(s, h_i)$
- Normalization: $\alpha_i = \frac{\exp(e_i)}{\sum_j \exp(e_j)}$
- Aggregation: $c = \sum_i \alpha_i h_i$

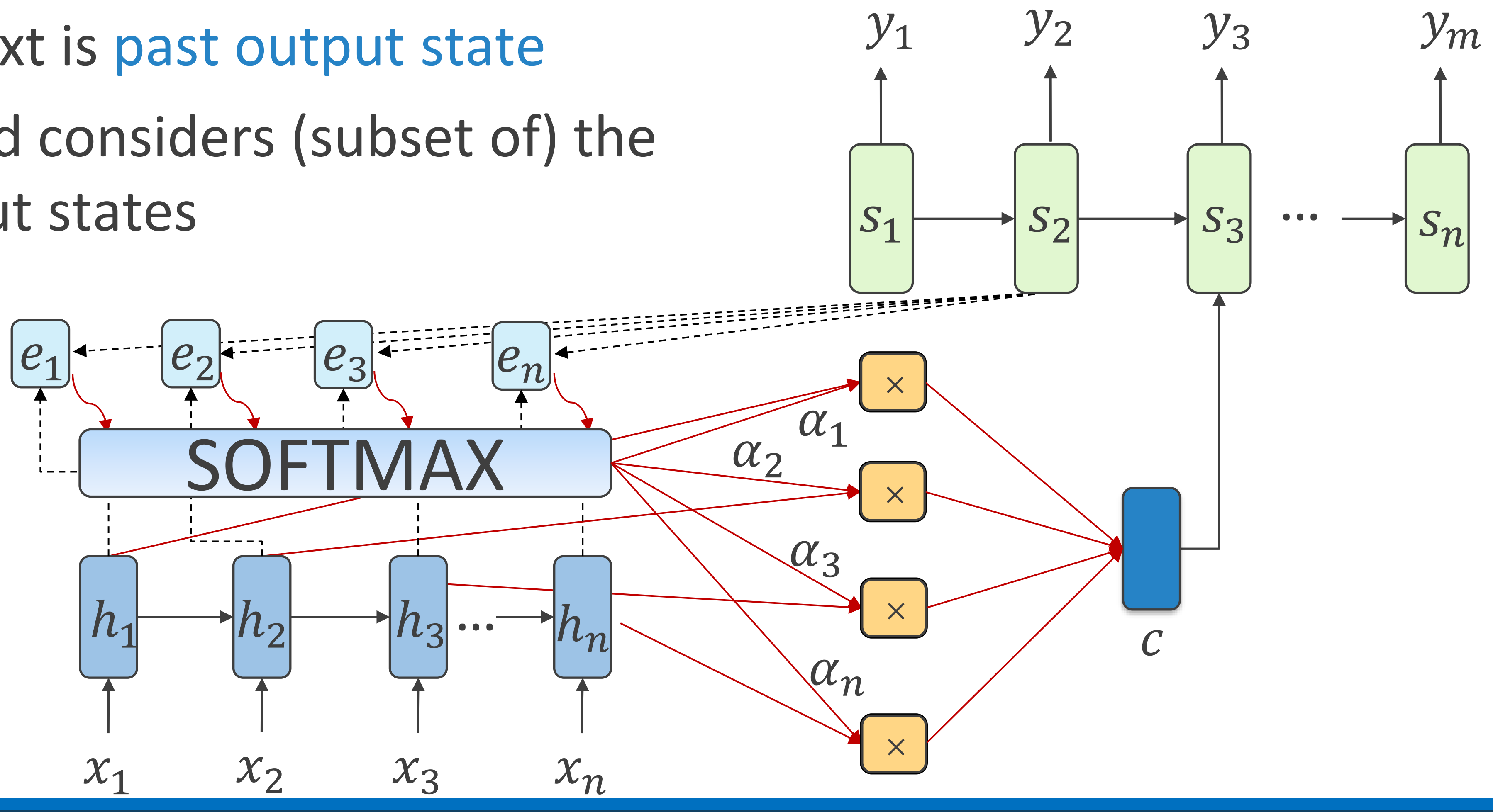


Attention module

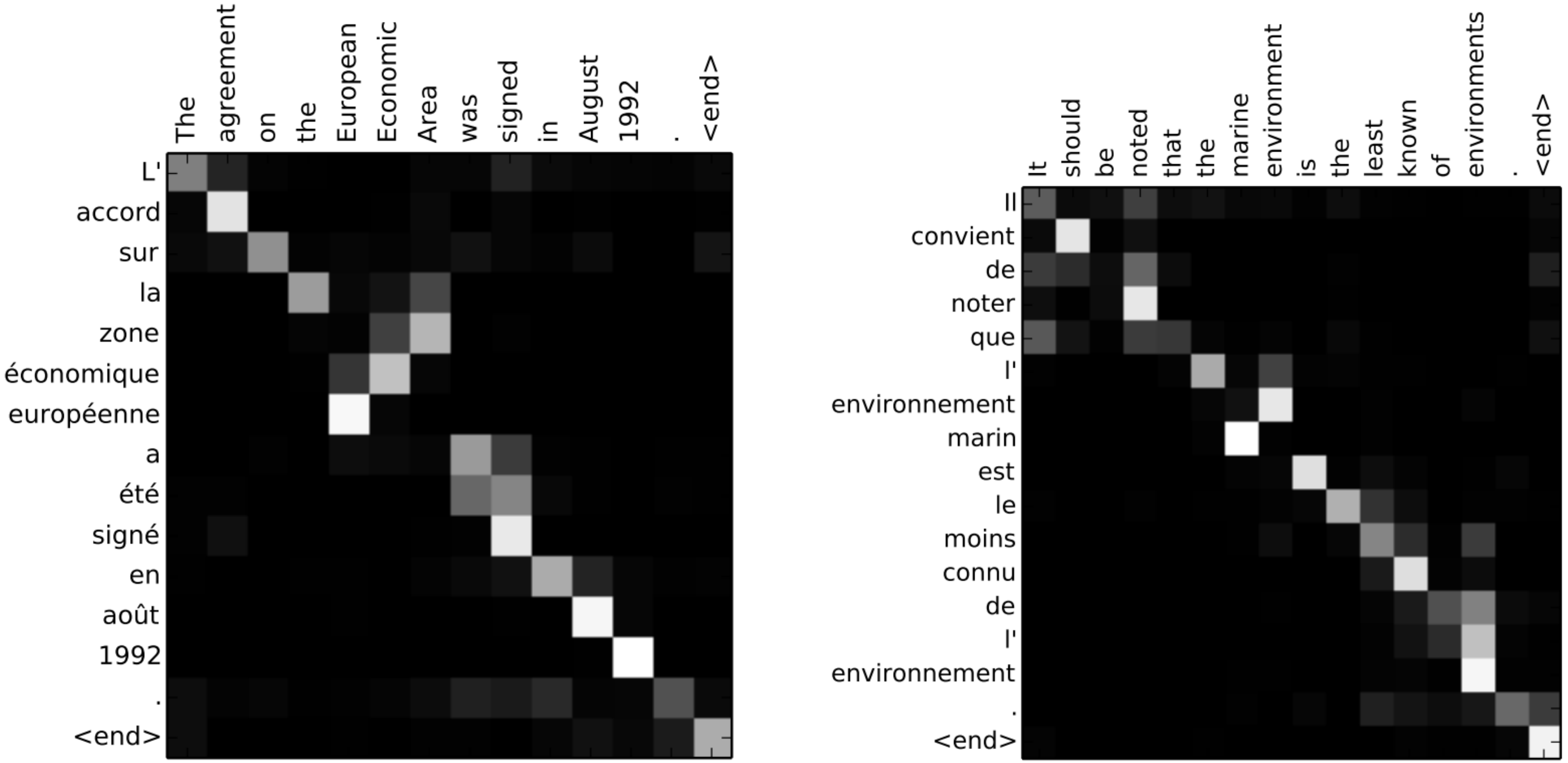
Attention in Seq2Seq

Context is past output state

Seed considers (subset of) the input states



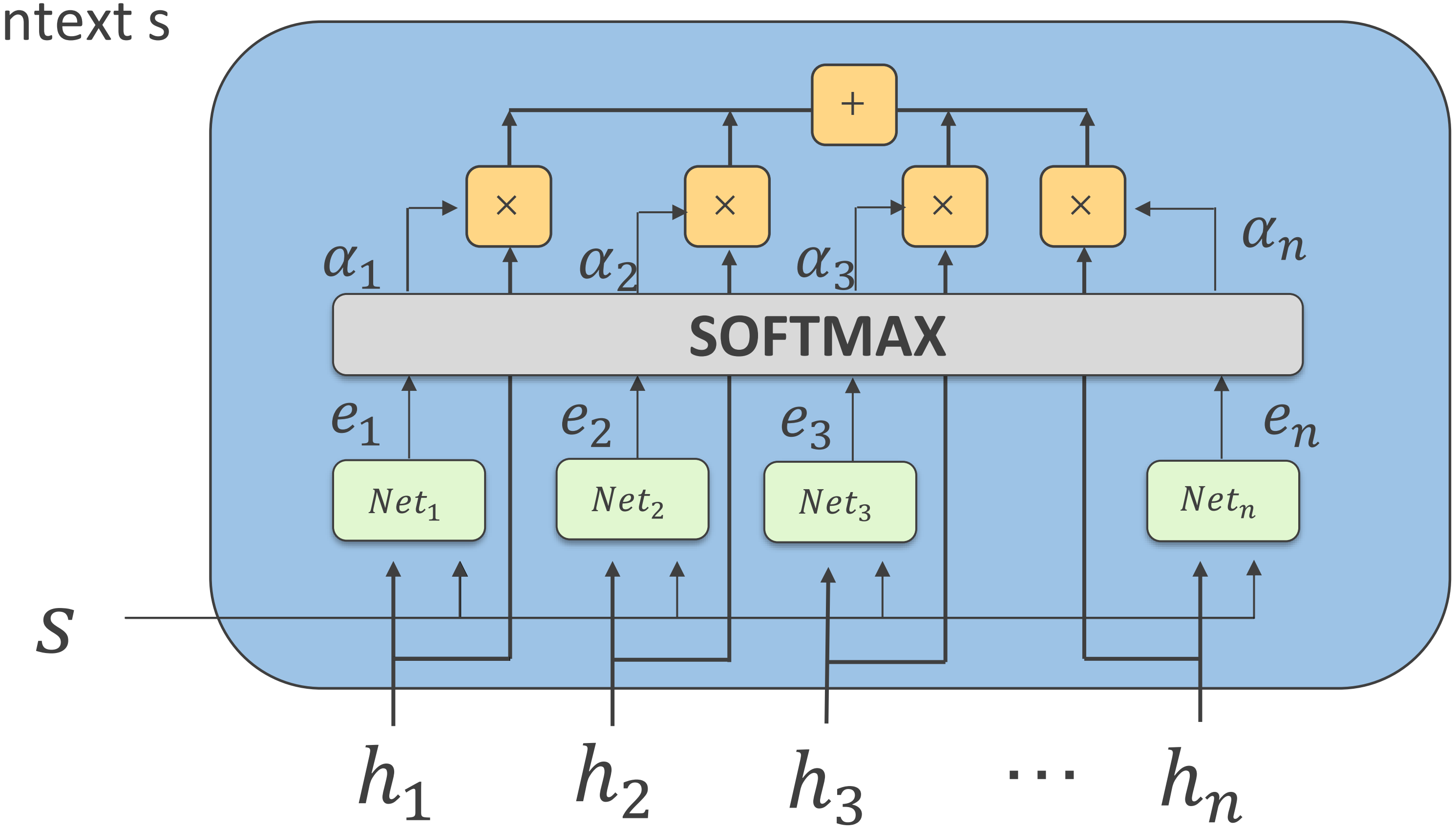
Learning to Translate with Attention



Bahdanau et al, Show, Neural machine translation by jointly learning to align and translate, ICLR 2015

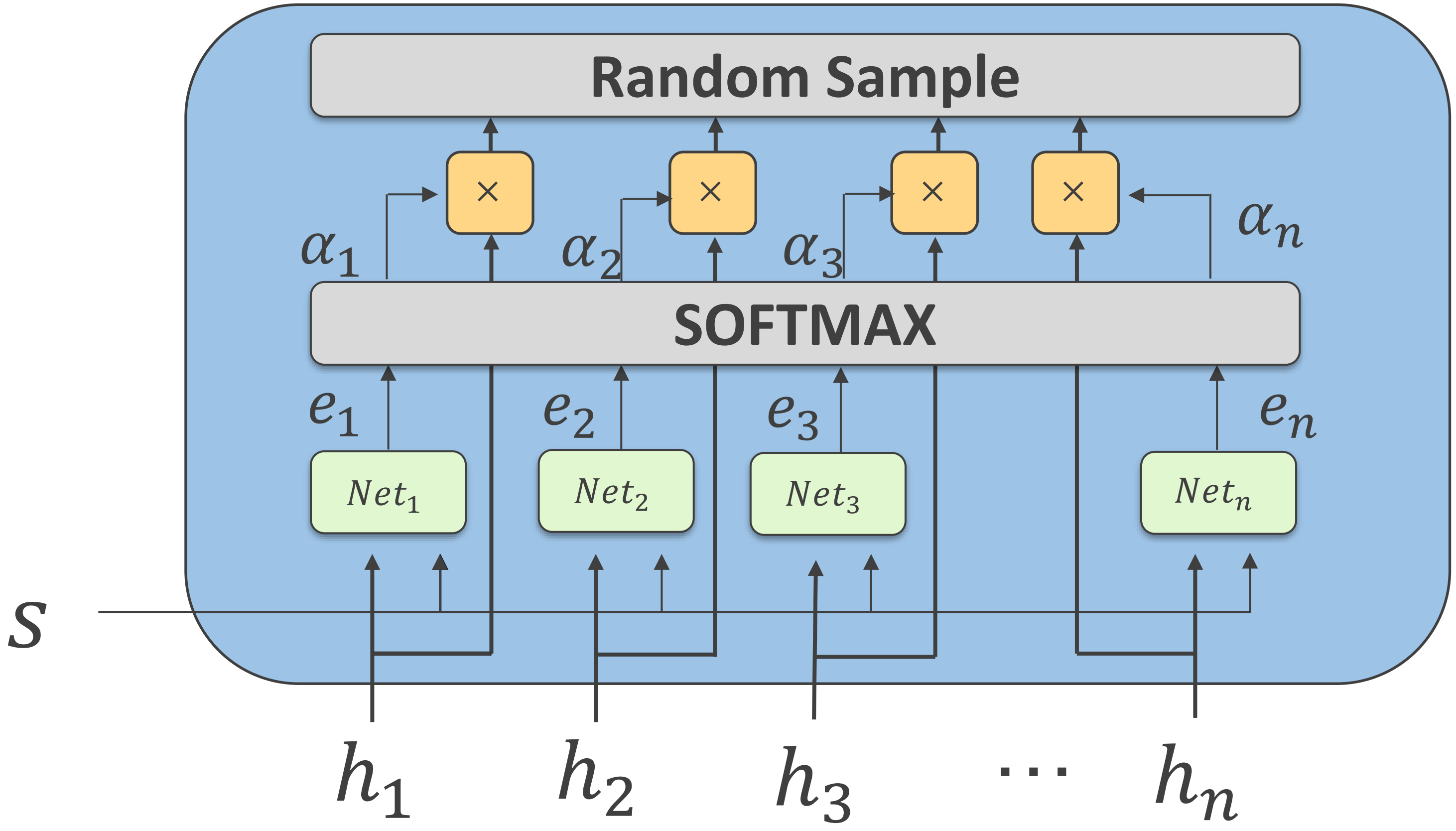
Advanced Attention – Generalize Relevance

This component determines how much each h is correlated/associated with current context s



Advanced Attention – Hard Attention

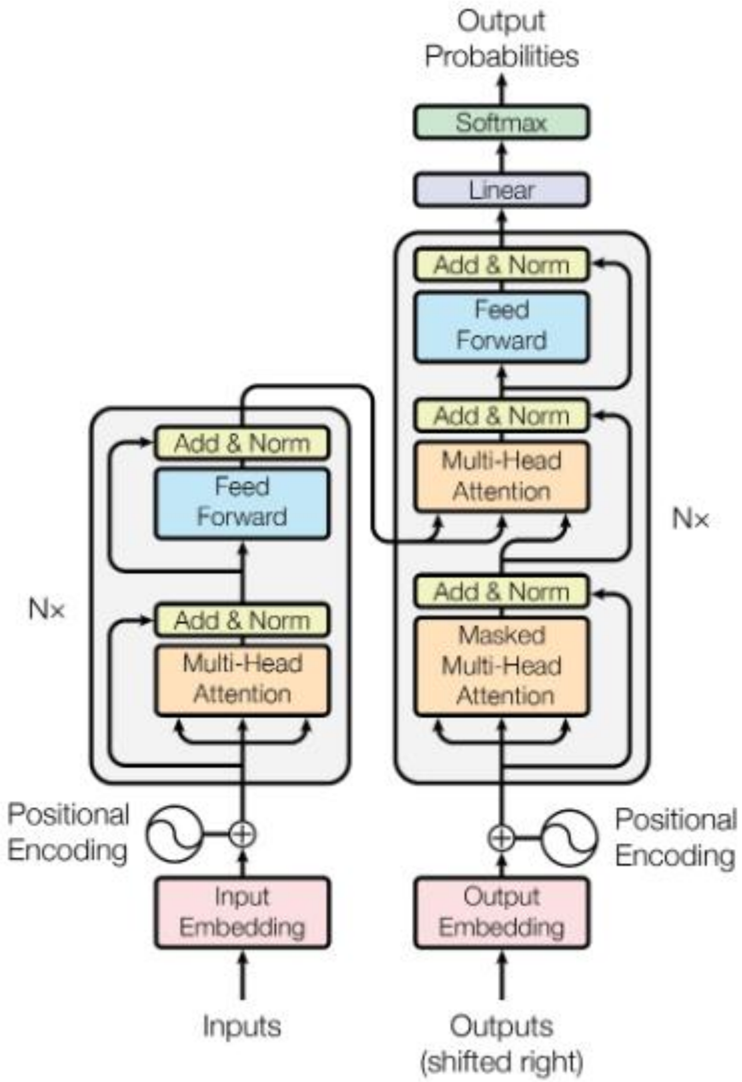
Sample a single encoding using probability α_i



Attention Is All You Need, https://arxiv.org/pdf/1706.03762.pdf

Transformers

- First pure attention-based model
- Self-attention
- No recurrence
- Encoder-decoder architecture



Self Attention

Each element of an input sequence X_i projects into 3 vectors: **query**, **key** and **value**

Self Attention – K,V,Q Generation

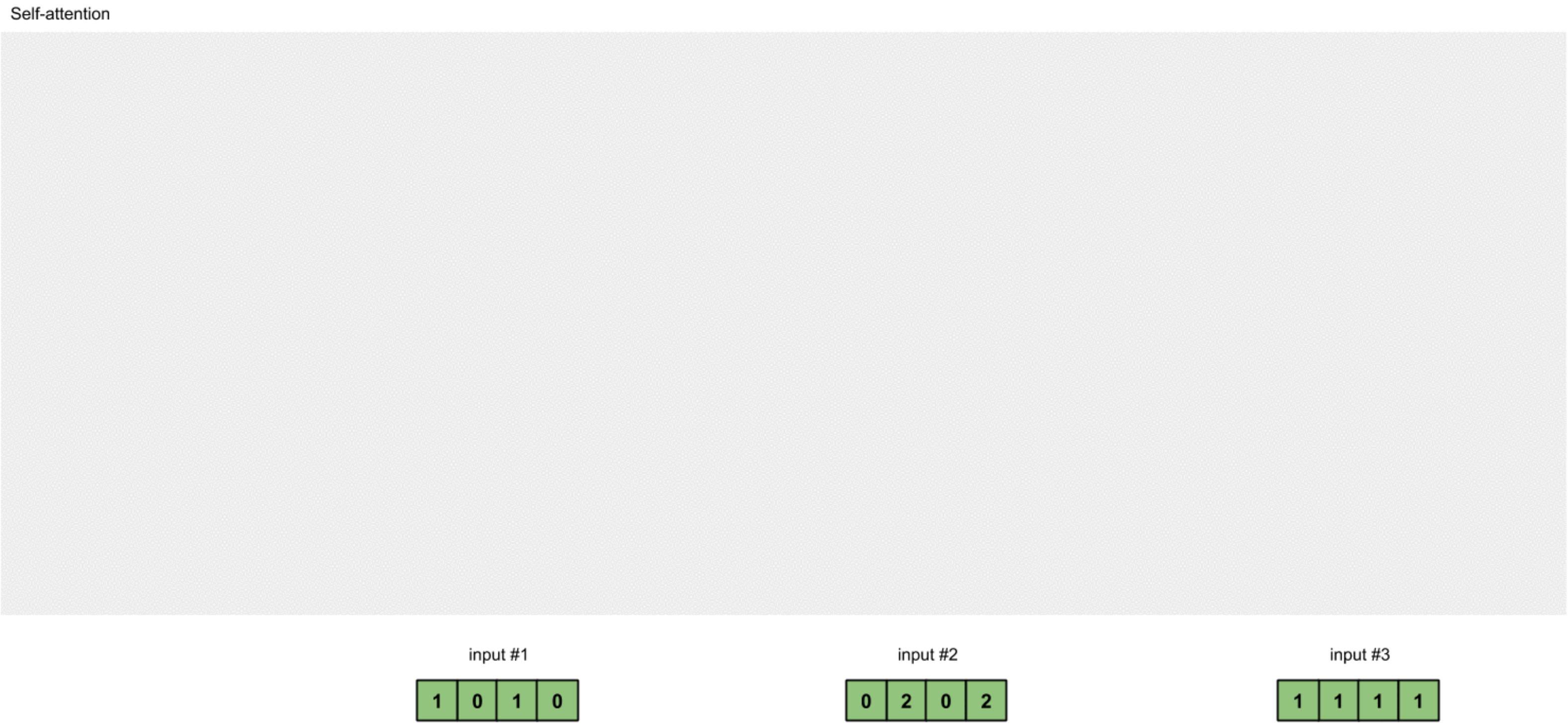
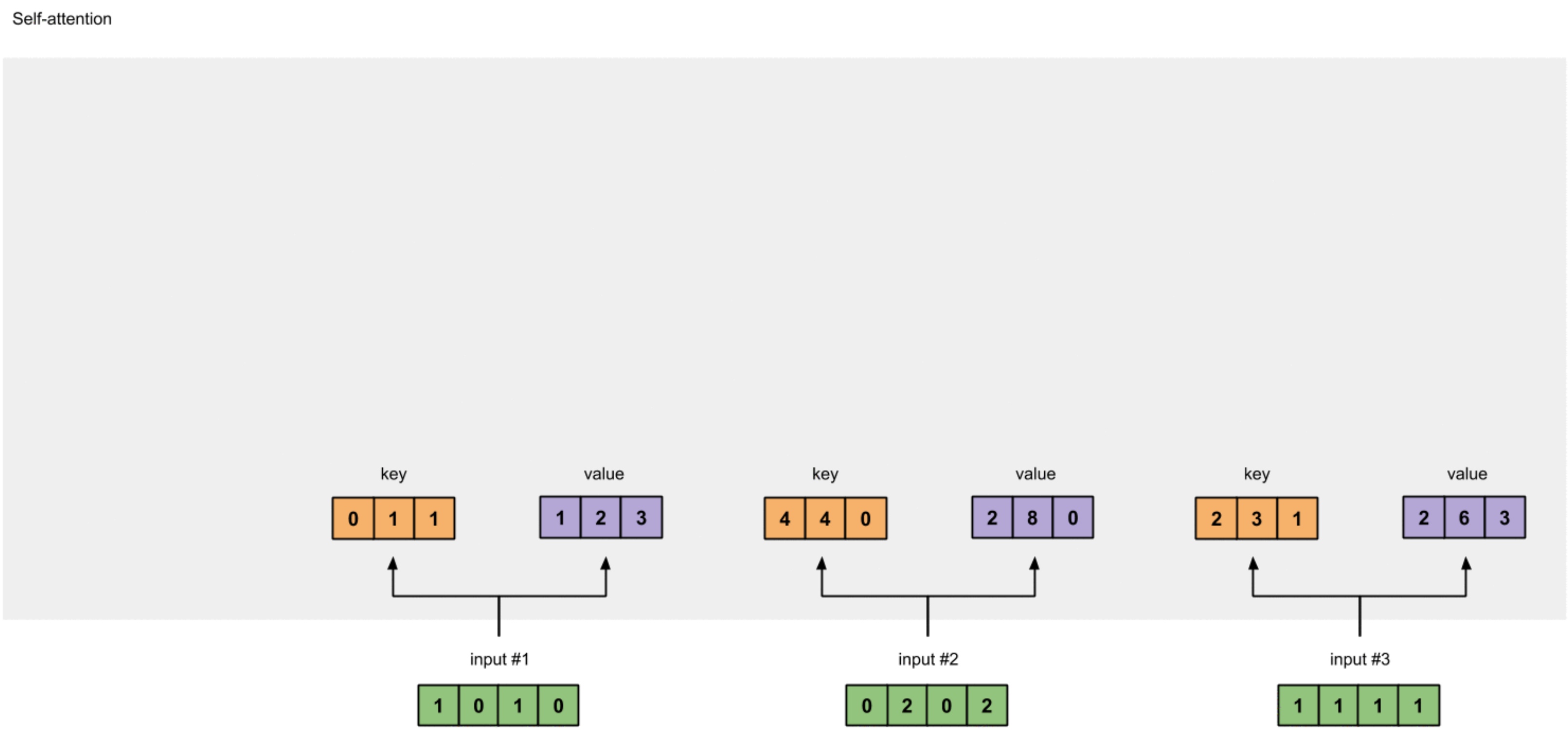
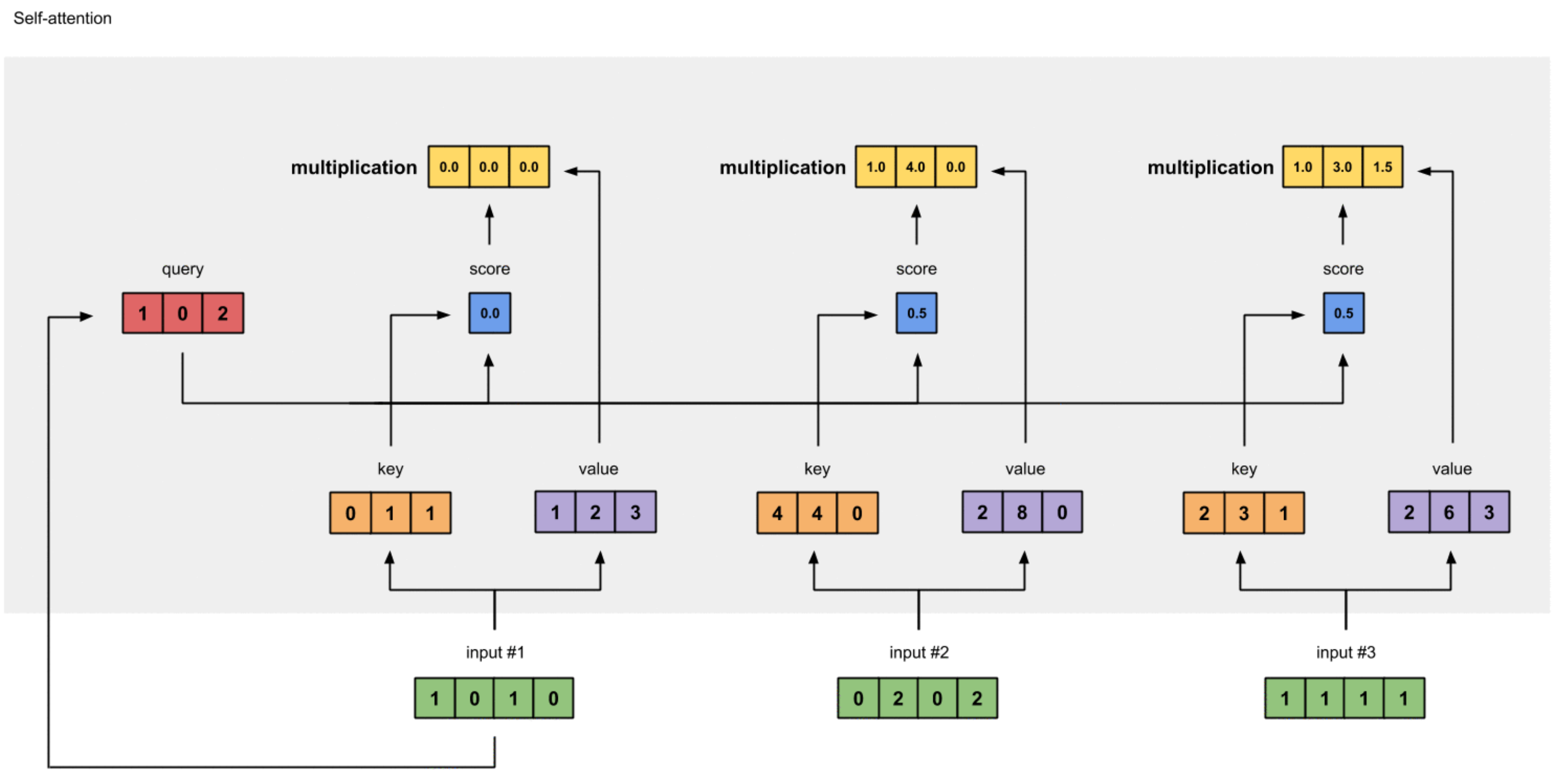


Figure credit to this article

Self Attention – Compute Attention Score

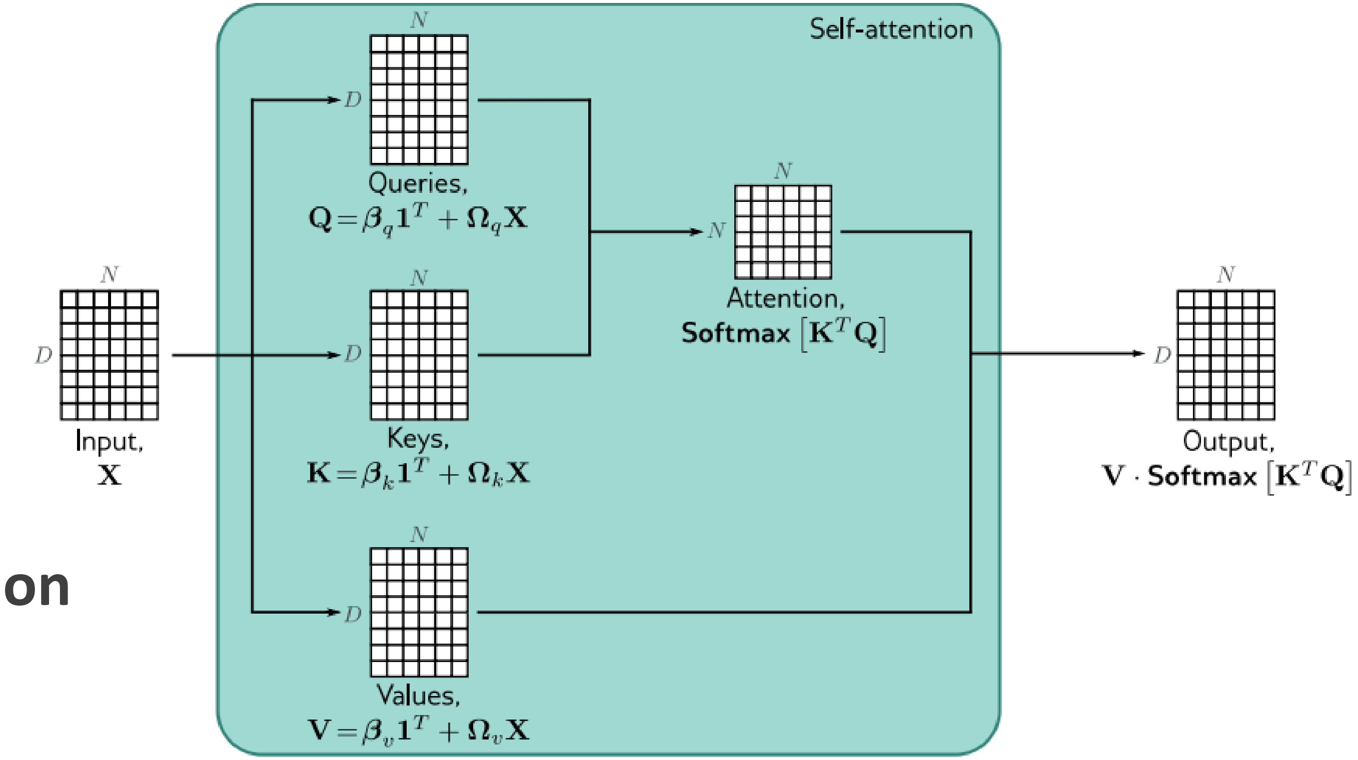


Self Attention – Produce Output



Self Attention

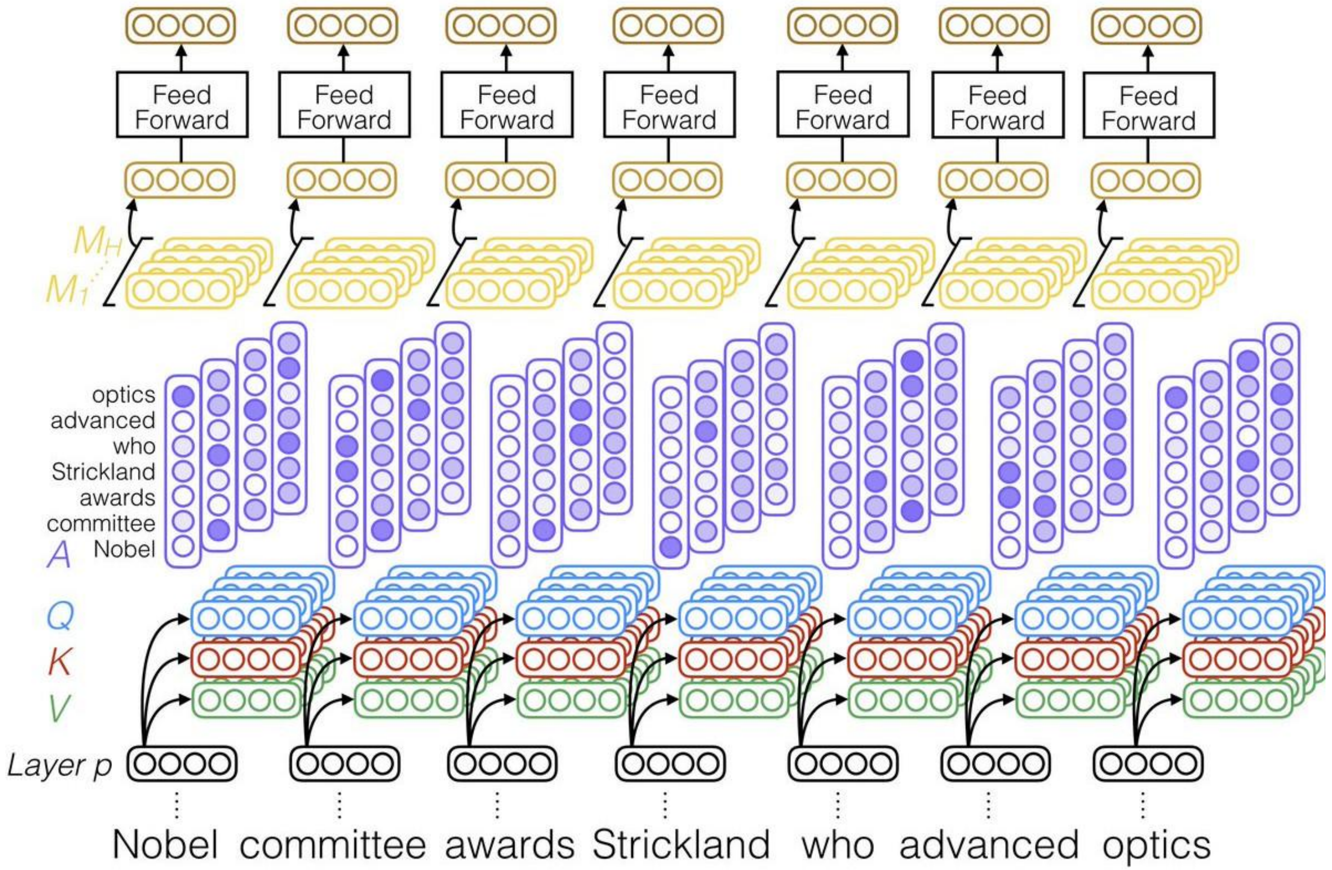
Each element of an input sequence X_i projects into 3 vectors: **query**, **key** and **value**

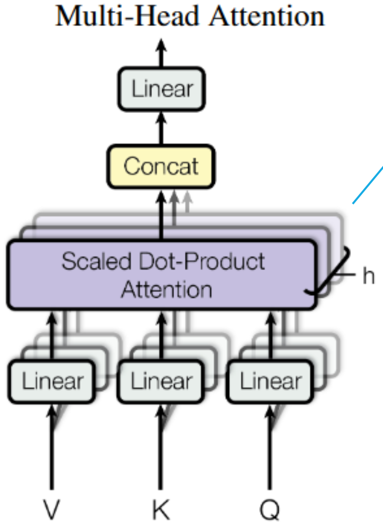


Scaled (multiplicative) self-attention

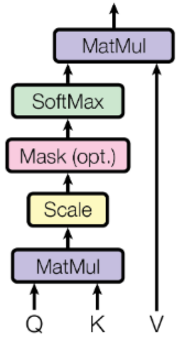
$$\sum_j softmax_j \left(\frac{Q_i \cdot \boldsymbol{K}^T}{\sqrt{d_k}} \right) V_j$$

Self Attention – MultiHead





concat



Strubell et al, Linguistically-Informed Self-Attention for Semantic Role Labeling, EMNLP 2018

Is self-attention a good mechanism to model temporal dependencies?

What happens if I randomly shuffle some tokens?

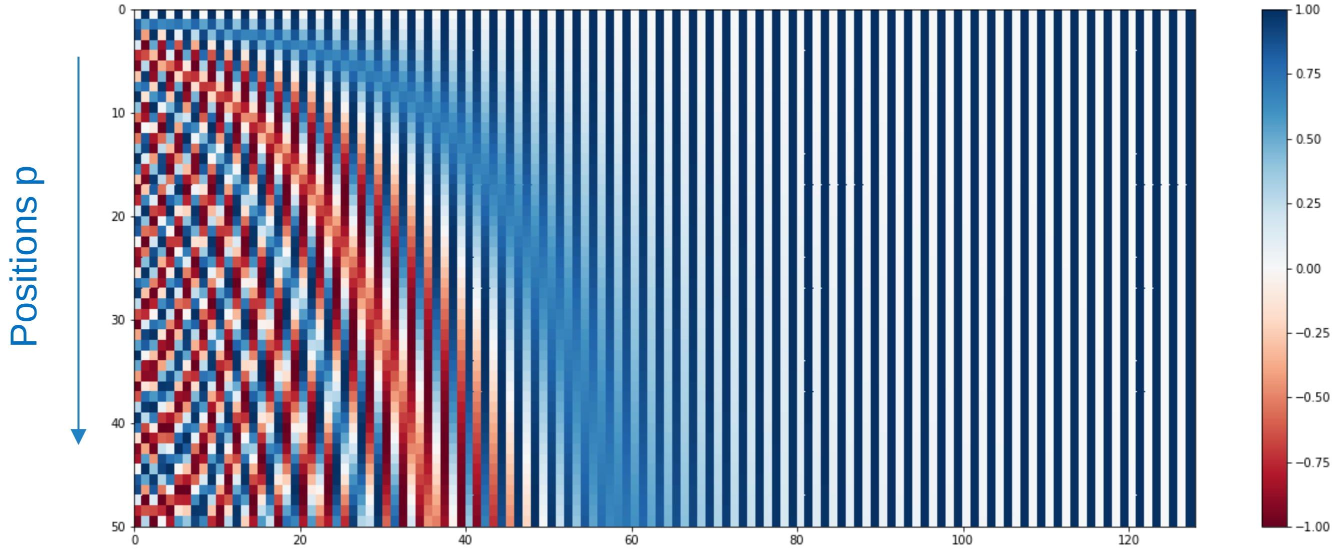
Attention Is All You Need,
https://arxiv.org/pdf/1706.03762.pdf

(Absolute) Positional Encoding

- Self-attention is order-independent
- But in sequences we need ordering information
- Word embedding + positional embedding

$$\underbrace{PE(p, 2i) = \sin(p/10000^{2i/d})}_{\text{frequency}}$$
$$PE(p, 2i+1) = cos(p/10000^{2i/d})$$

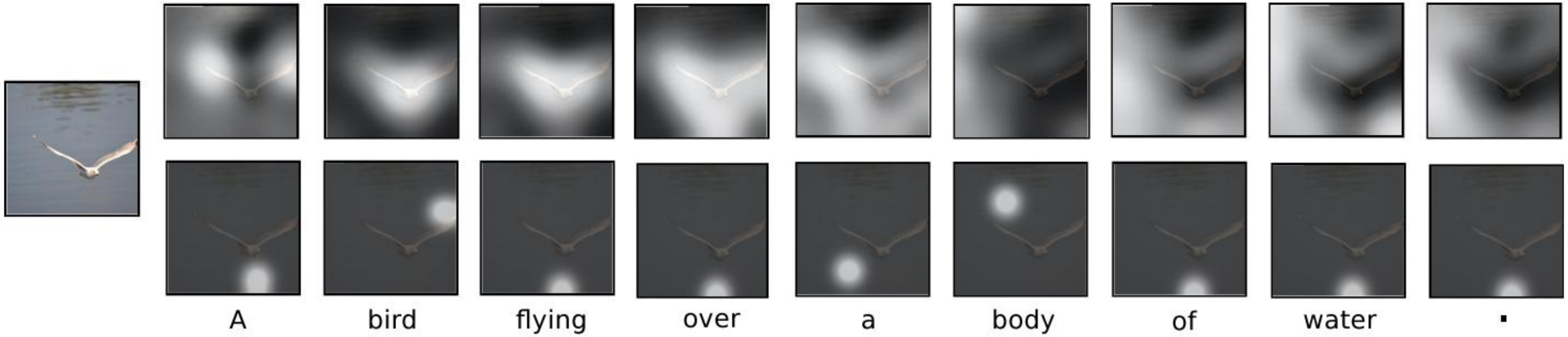
embedding dimensions $i \in \{1, d\}$



Attention in Vision

Attention-Based Captioning – Focus Shifting

Soft Attention



Hard Attention

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

Attention-Based Captioning - Generation

Learns to correlate textual and visual concepts

A woman is throwing a frisbee in a park.

A dog is standing on a hardwood floor.

A stop sign is on a road with a mountain in the background.

Helps understanding why the model fails

A large white bird standing in a forest.

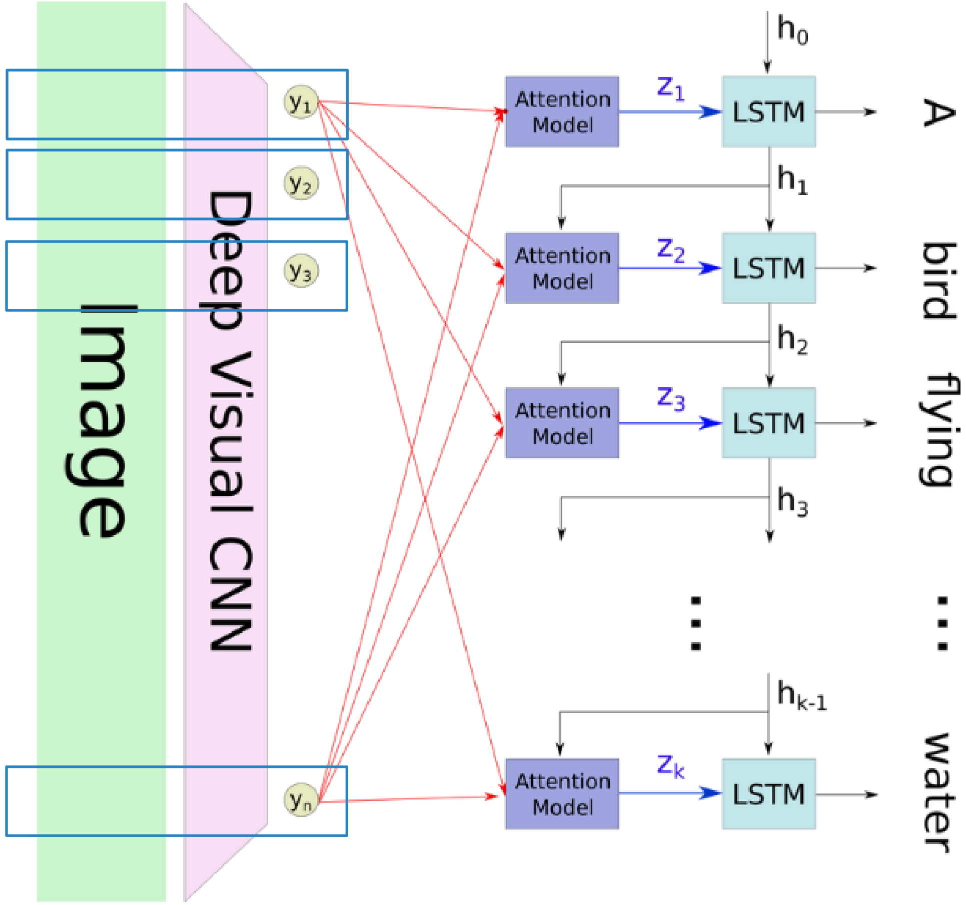
A woman holding a clock in her hand.

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

Attention-Based Captioning – The Model

Encodings associated to *n* image regions

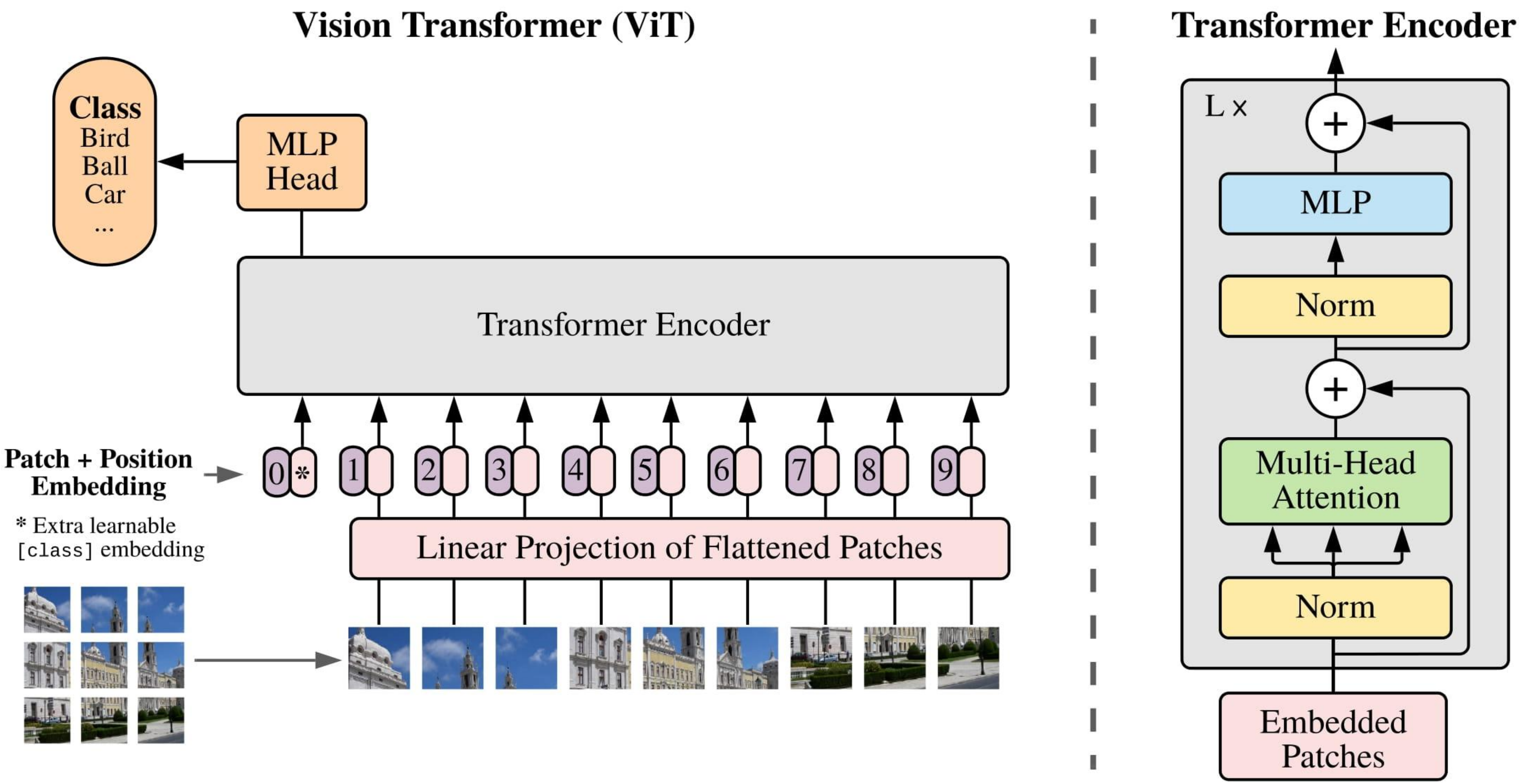
From convolutional layers rather than from fully connected



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

The Vision Transformer (ViT)

A. Dosovitskiy et al, ICLR 2021



Take Home Messages

- Attention.. Attention.. and, again, attention
  - Soft attention is nice because makes everything fully differentiable
  - Hard attention is stochastic hence cannot Backprop
  - Empirical evidences of them being sensitive to different things
- Encoder-Decoder scheme
  - A general architecture to compose heterogeneous models and data
  - Decoding allows sampling complex predictions from an encoding conditioned distribution
- Transformers as low-inductive bias architectures
  - Need huge amounts of data to generalize

Upcoming lectures

- Wed 16/04 - Coding I (Pytorch)
- Thu 17/04 – Coding II (Keras/TF)
- Apr. 18 – Apr 28 – Spring Break (no lectures)

- Bonus track
  - AI Meets Psychiatry: fMRI-Based Multi-Disorder Diagnosis
  - Lecture by Elisa Ferrari at the AI for Health course
  - Today 15/04/2025 h. 16.15-17.30 – ~~Room L1~~ Room C

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