Quebec
Artificial
Intelligence
Institute

Mila

Sequence to Sequence Models

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Plan

- RNN Recap
- Sequence to Sequence Models
- Attention Mechanism
- Transformer
- Libraries and References

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- **RNN Recap**
- Sequence to Sequence
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Recurrent Neural Networks

- The parameters of the model are **shared** over time.
- The internal state (h_t) is updated at each time step.

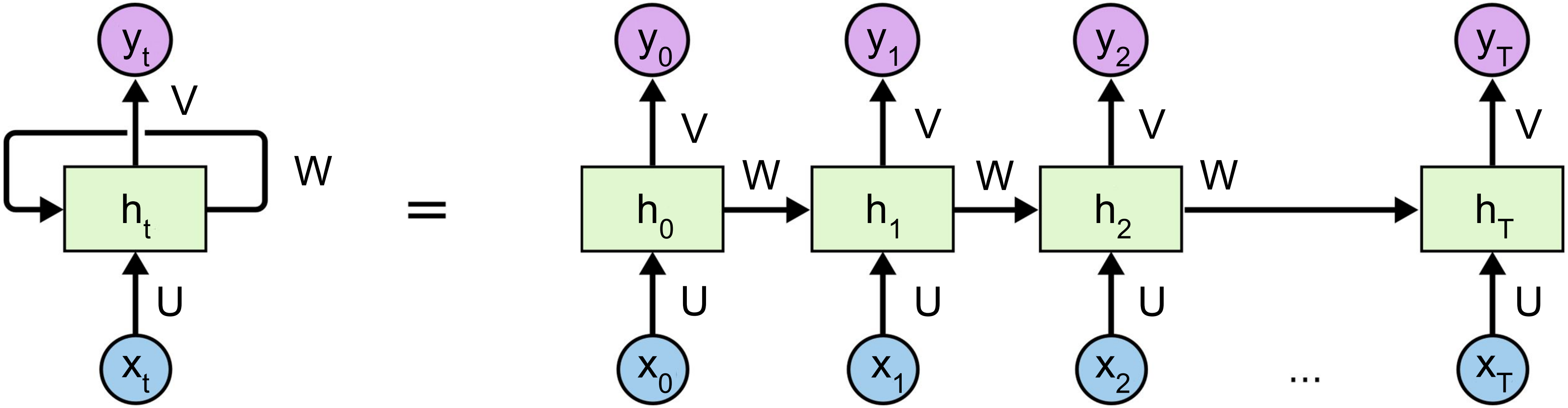

Image from Christopher Olah's blog

The initial internal state (h_{-1}) is dropped for simplicity

Backpropagation Through Time

- The global error is:

$$E = \sum_{t=0}^{T} E_t$$

- To compute the gradient of the global error with respect to a parameter, we compute the gradient of the individual error at each time step, and then sum all those values. For example:

$$\frac{\partial E}{\partial U} = \sum_{t=0}^{T} \frac{\partial E_t}{\partial U}$$

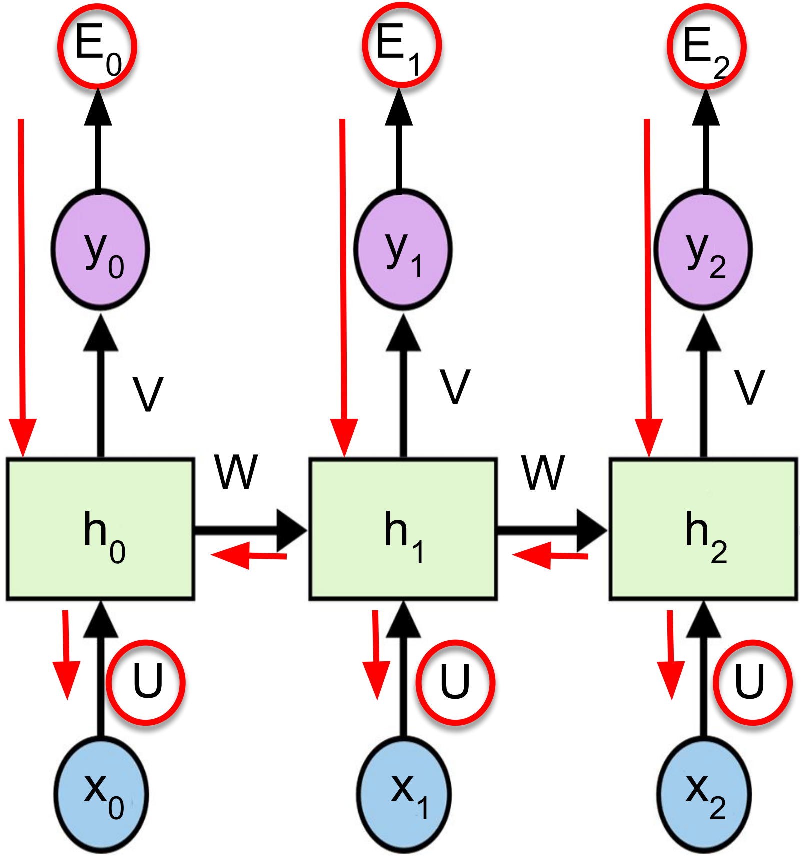

Image from Christopher Olah's blog

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Long-Term Dependencies

- Long-term dependencies are difficult to learn due to the long chain of gradients $\frac{\partial h_T}{\partial h_{T-1}} \cdots \frac{\partial h_3}{\partial h_2} \cdot \frac{\partial h_2}{\partial h_1} \cdot \frac{\partial h_1}{\partial h_0}$ that can lead to vanishing gradients

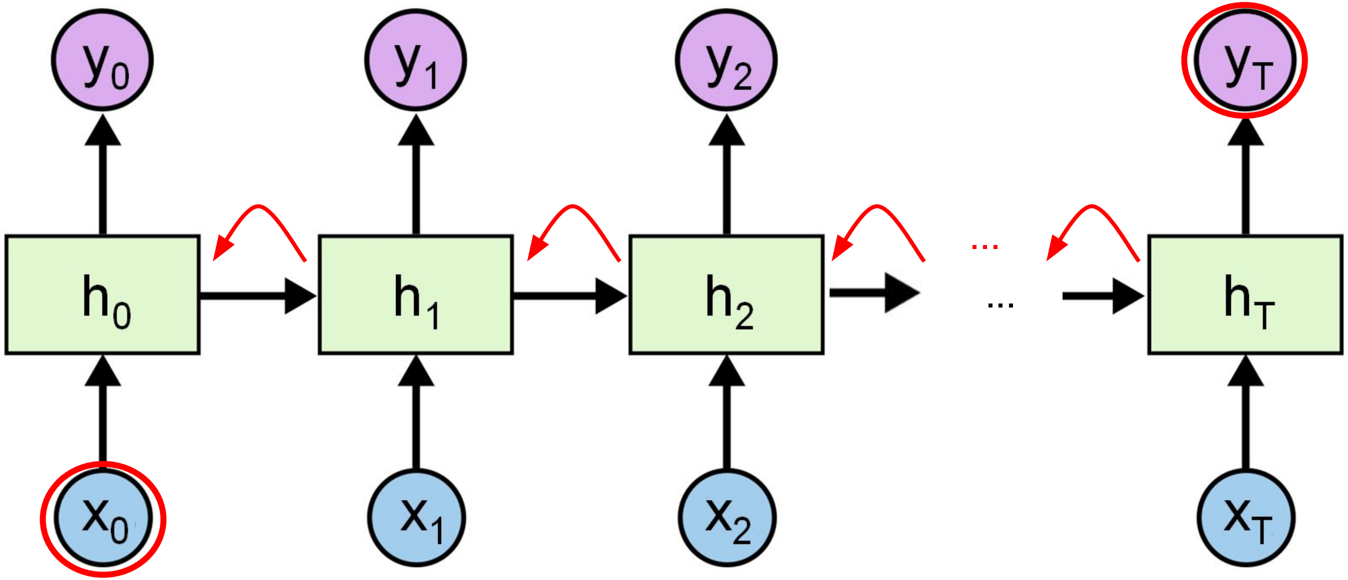

Image from Christopher Olah's blog

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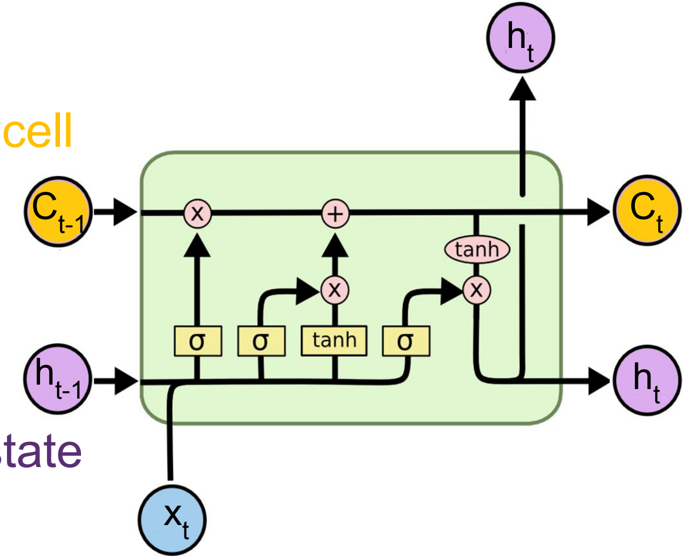
Long Short-Term Memory (LSTM)

- Reduce the vanishing gradient problem using a gate mechanism and adding a memory cell.

Memory cell

Internal state



$$i_t = \sigma(U_i x_t + W_i h_{t-1} + b_i)$$

$$f_t = \sigma(U_f x_t + W_f h_{t-1} + b_f)$$

$$o_t = \sigma(U_o x_t + W_o h_{t-1} + b_o)$$

$$g_t = tanh(U_g x_t + W_g h_{t-1} + b_g)$$

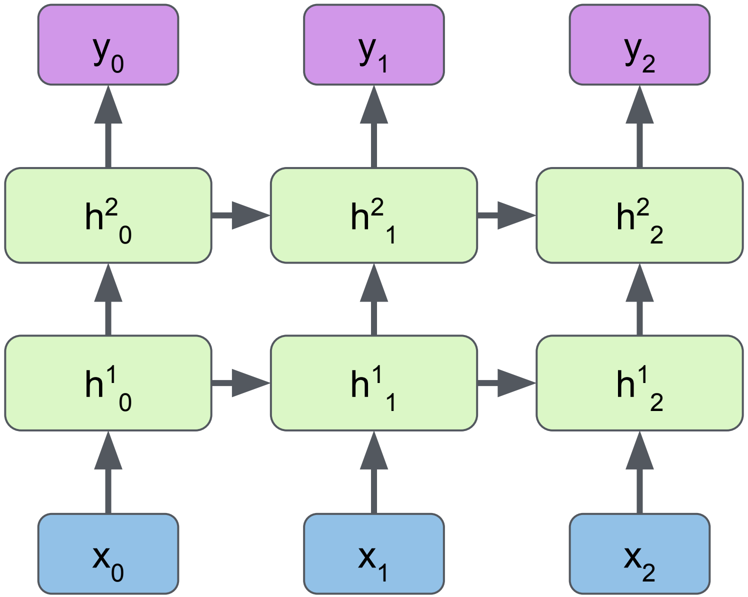
$$C_t = i_t \times g_t + f_t \times C_{t-1}$$

$$h_t = o_t \times tanh(C_t)$$

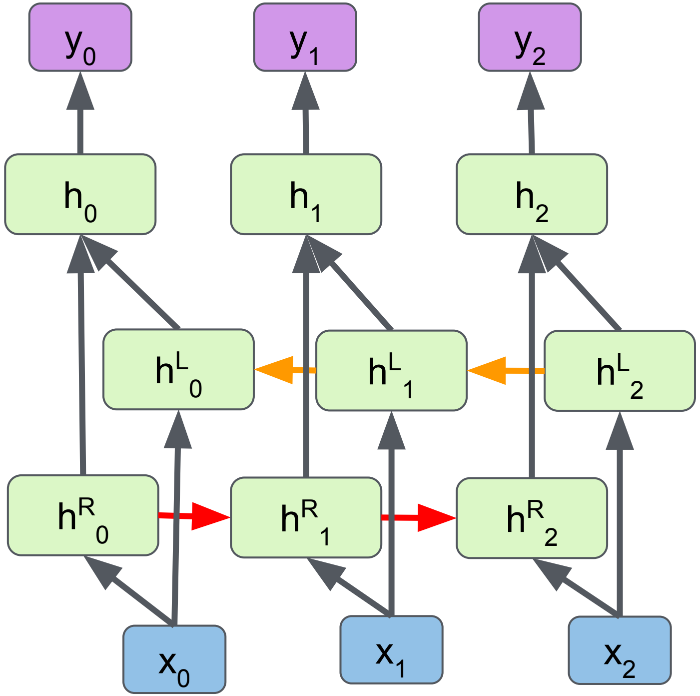
Image from Christopher Olah's blog

Hochreiter et al., Long short-term memory, Neural Computation 1997

Multi-Layer and Bidirectional RNNs



Layers of RNNs



Bidirectional RNNs

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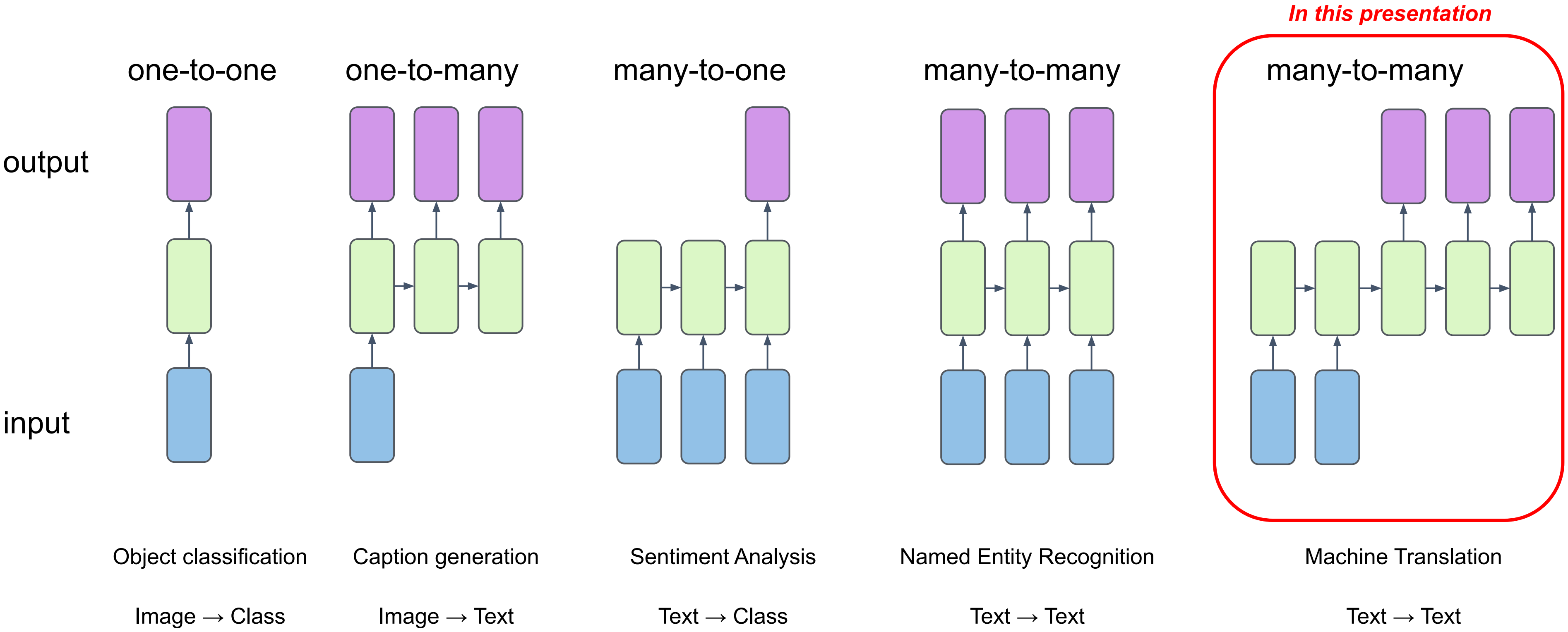
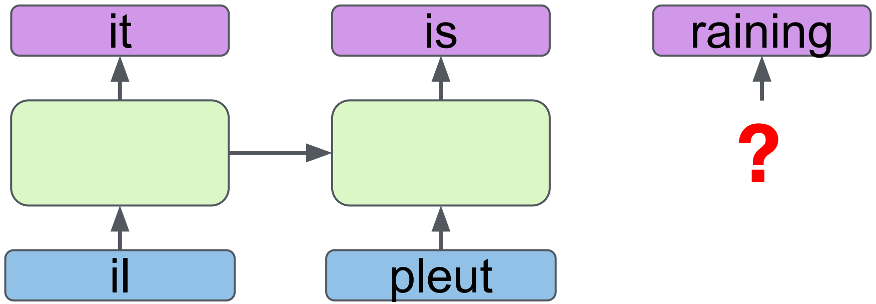
Modeling Sequences



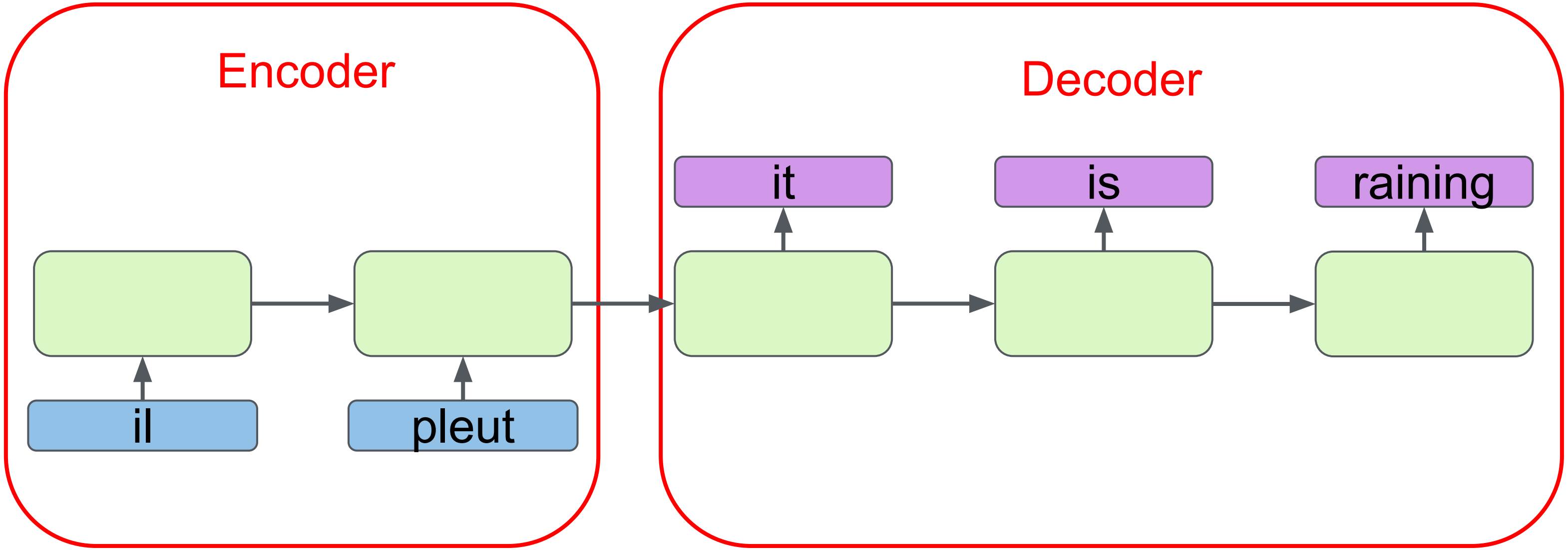
Modeling Sequences

- How to handle input and output sequences of different lengths?
  - Machine translation.
  - Text summarization.
  - …



Different input-output sequence sizes

- Create an architecture composed of two components (e.g. two different RNNs):
    - Encoder that processes the input sequence.
    - Decoder that generates the output sequence based on the encoded input.



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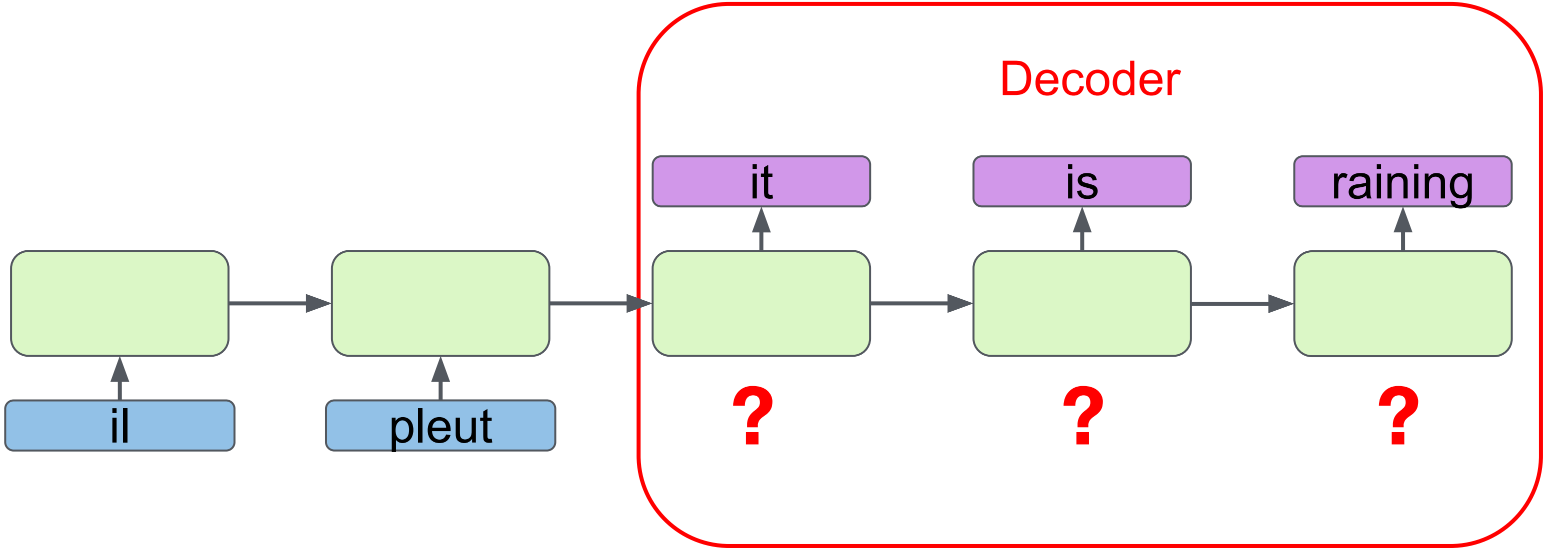
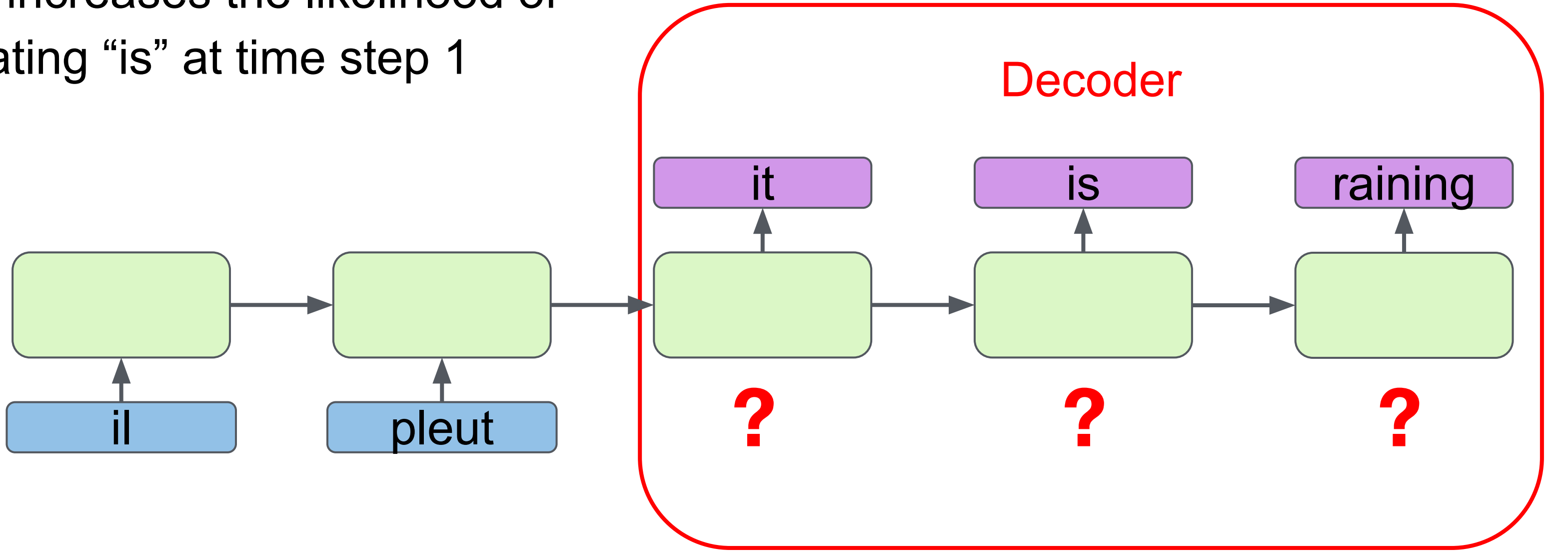
Different input-output sequence sizes

- How to implement the decoder?
- Note the missing input. We need a mechanism that will allow the decoder to generate consistent outputs across time.



Different input-output sequence sizes

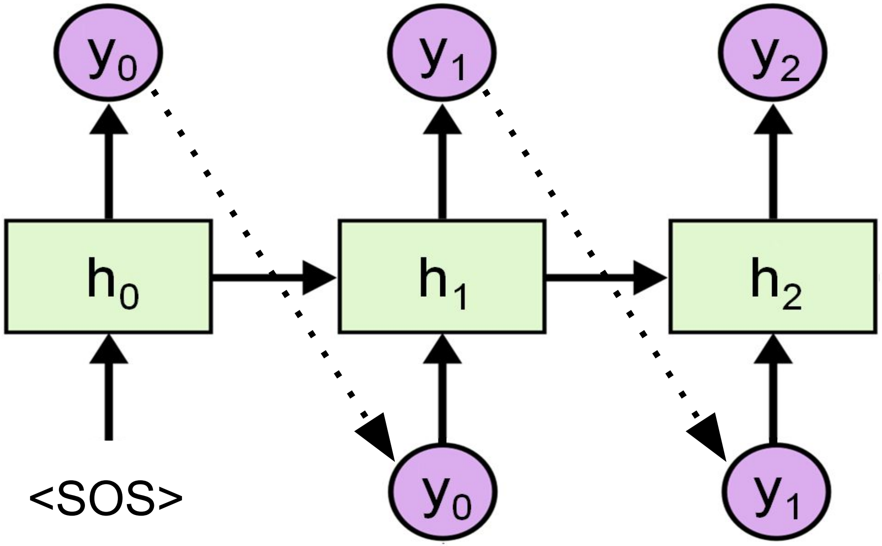
Example: knowing that the decoder generated “it” at time step 0 increases the likelihood of generating “is” at time step 1



Autoregressive RNNs

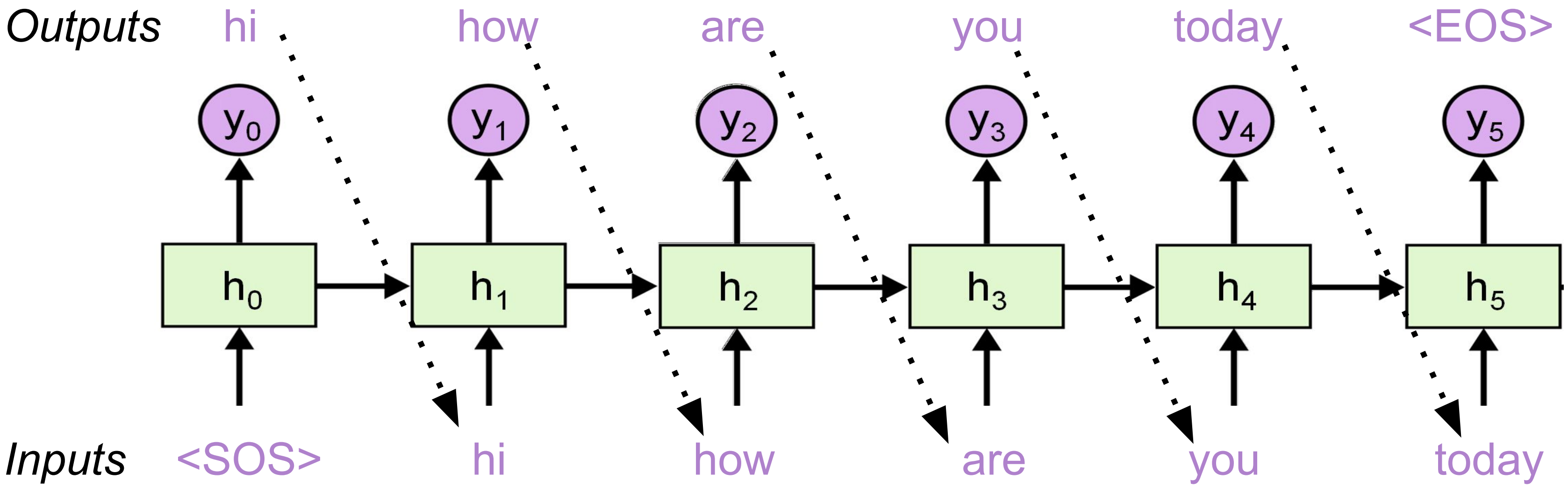
<SOS> *Start of sequence*

- We can use a RNN to **generate** a sequence.
- In order to generate consistent outputs across time, we can condition each output on previously generated outputs.
- Such a model is called **autoregressive**.



Autoregressive RNNs

<SOS> Start of sequence
<EOS> End of sequence



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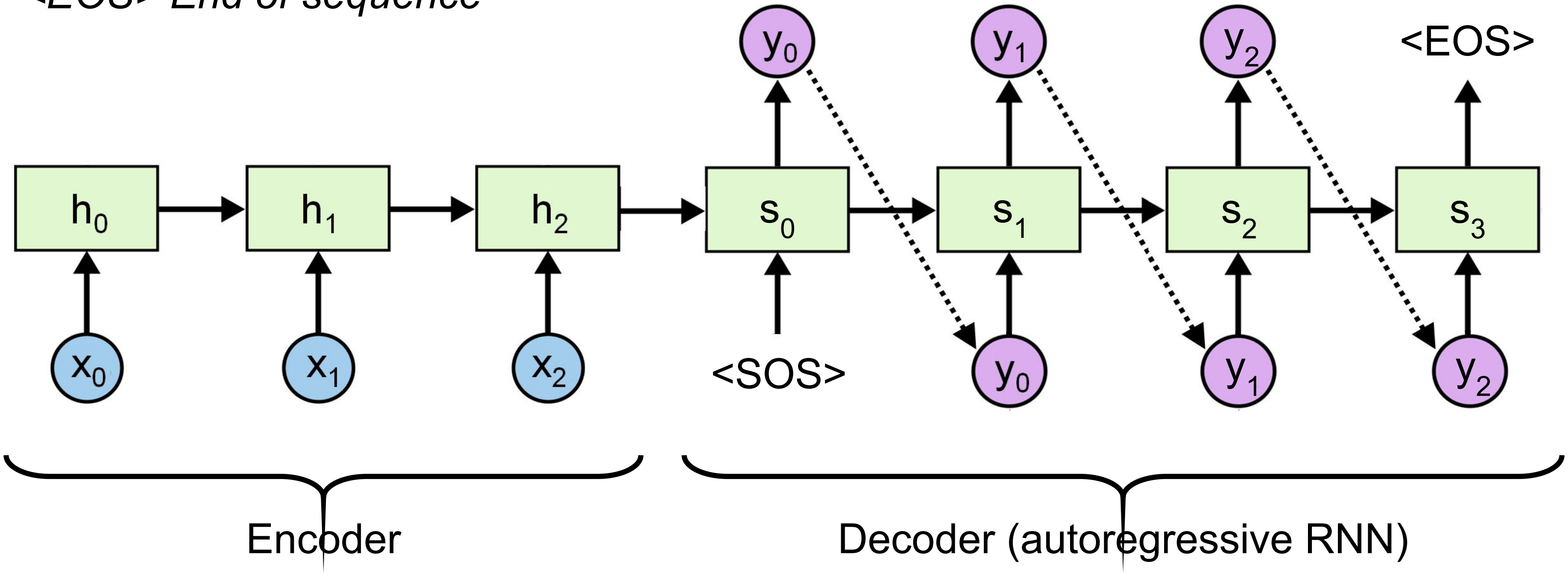
Sequence-to-Sequence Models

<SOS> Start of sequence

<EOS> End of sequence



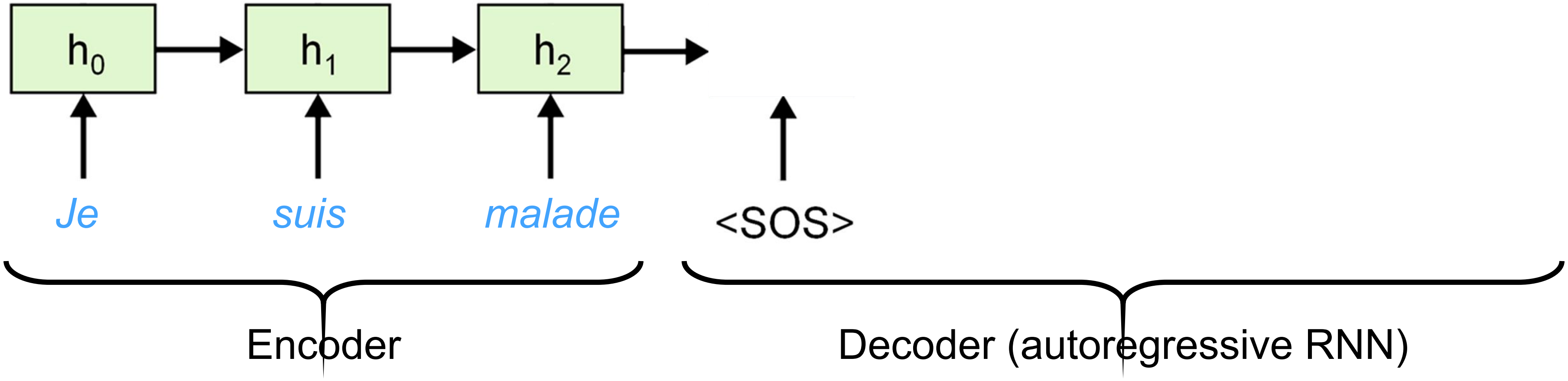
Sutskever et al., Sequence to Sequence Learning with Neural Networks

Cho et al., Learning Phrase Representations using RNN Encoder–Decoder for Statistical Machine Translation

Sequence-to-Sequence Models - Example

<SOS> Start of sequence

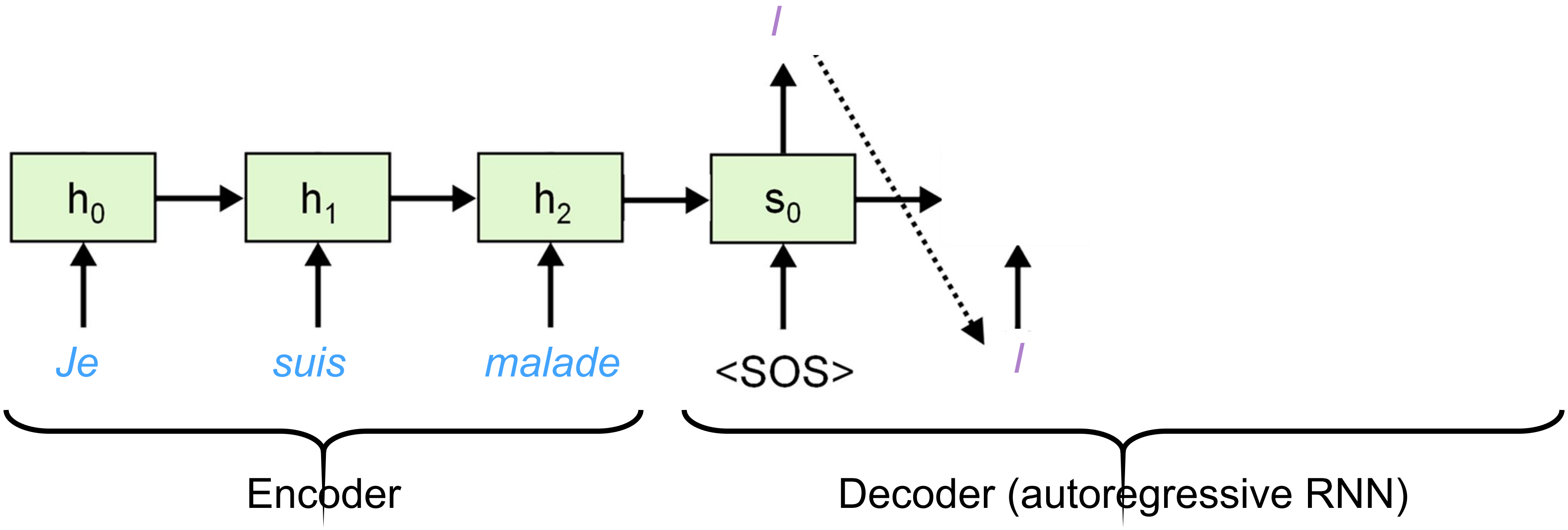
<EOS> End of sequence



Sequence-to-Sequence Models - Example

<SOS> Start of sequence

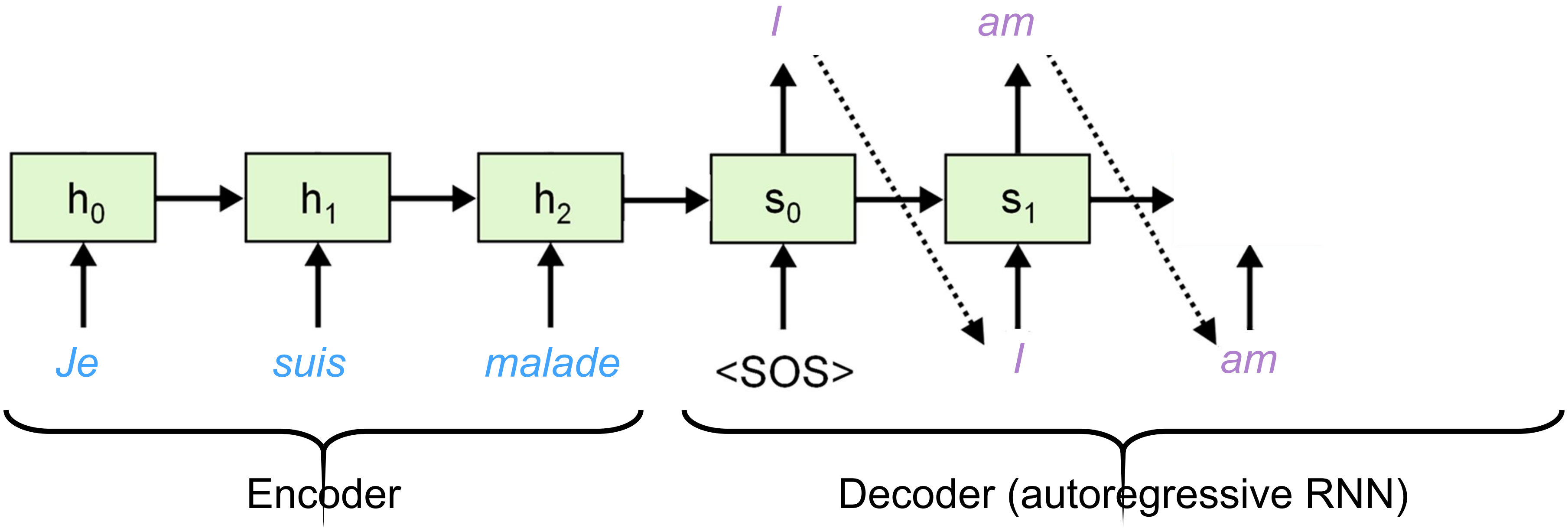
<EOS> End of sequence



Sequence-to-Sequence Models - Example

<SOS> Start of sequence

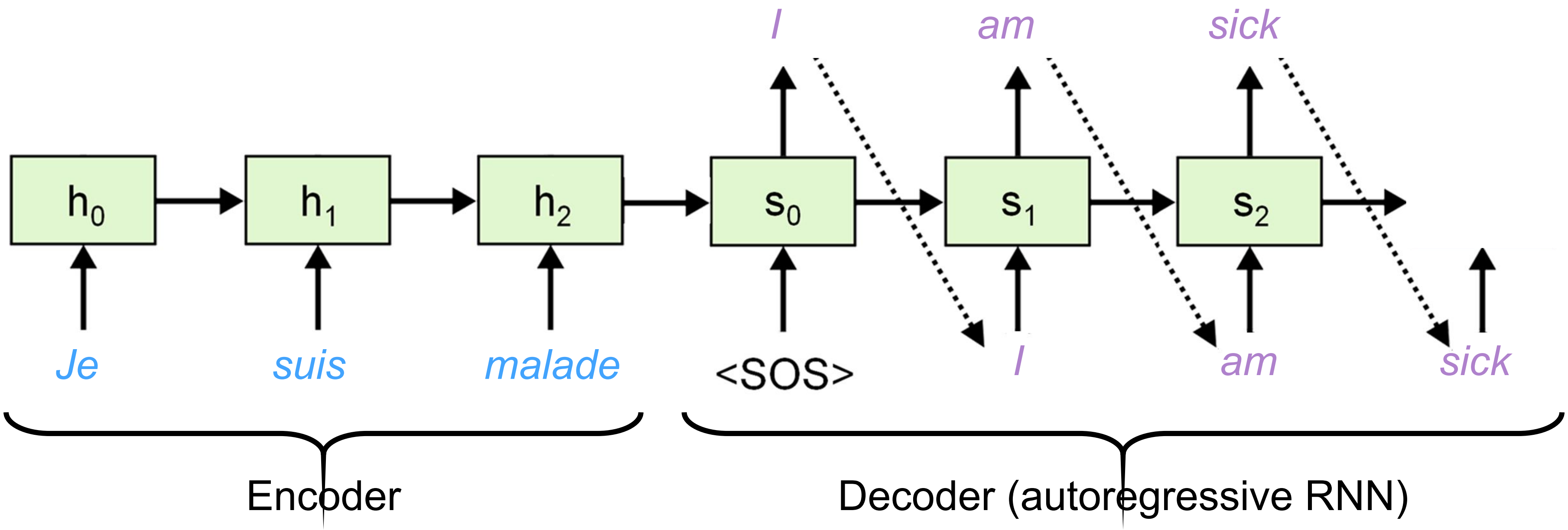
<EOS> End of sequence



Sequence-to-Sequence Models - Example

<SOS> Start of sequence

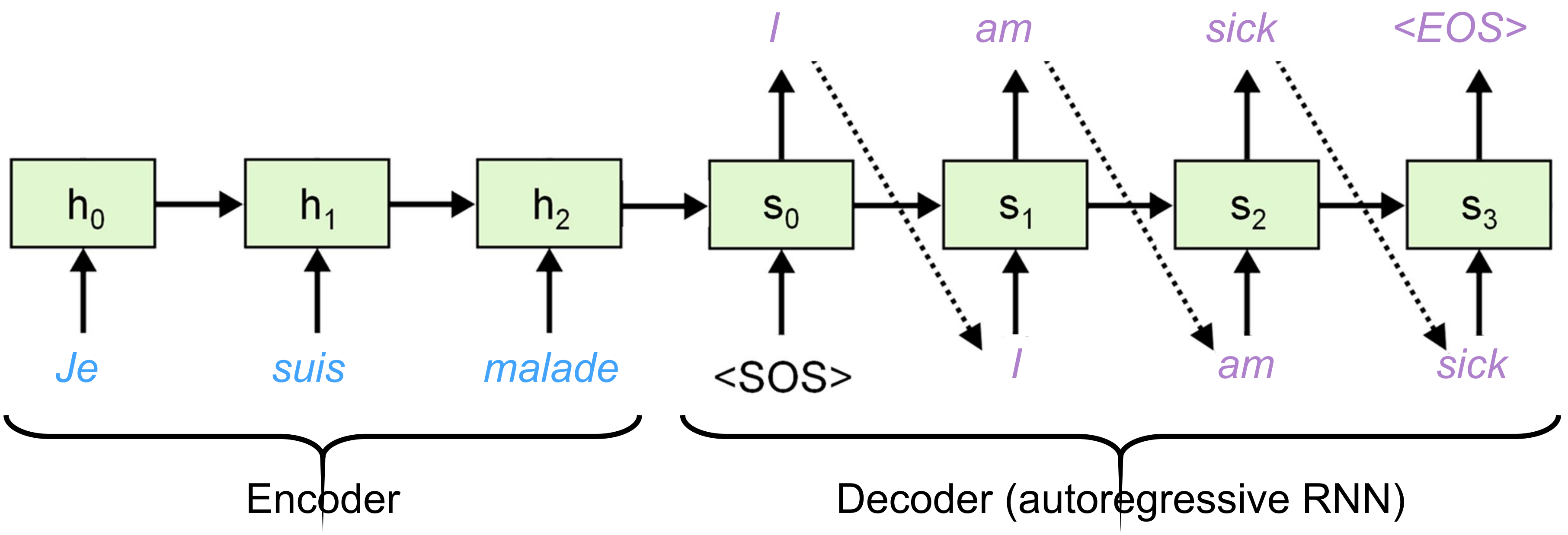
<EOS> End of sequence



Sequence-to-Sequence Models - Example

<SOS> Start of sequence

<EOS> End of sequence



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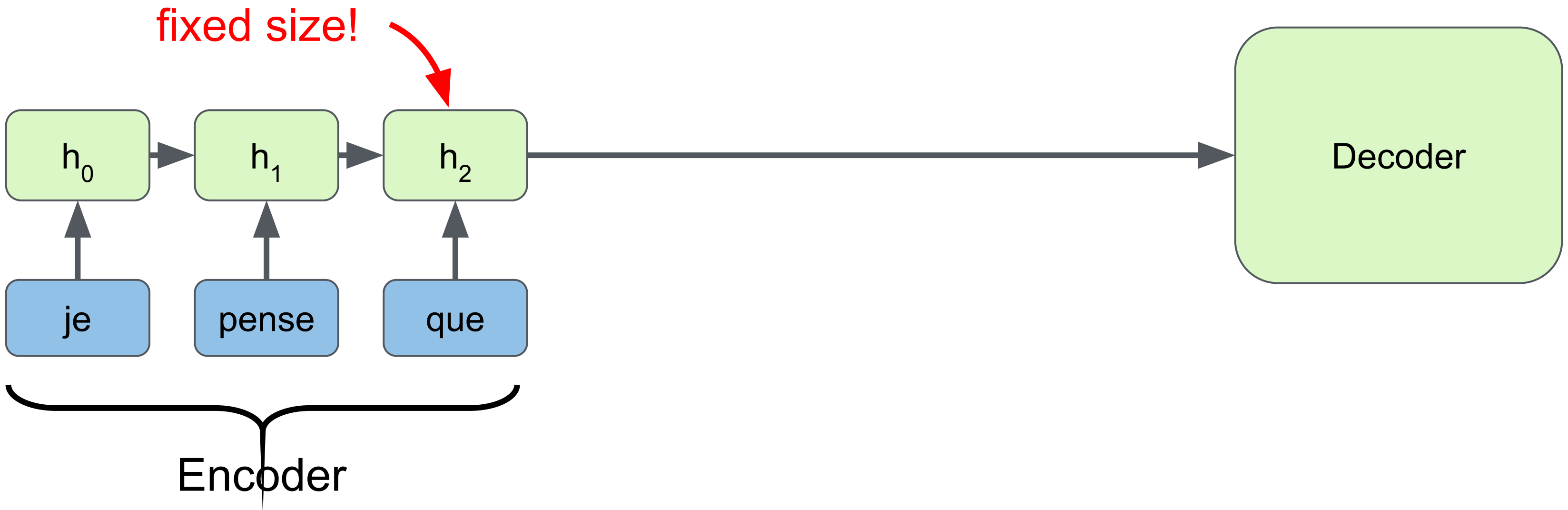
Sequence-to-Sequence Models - Bottleneck

- The encoder has to store/compress all the information from the input into a **fixed size** vector (**h_2** in this example).



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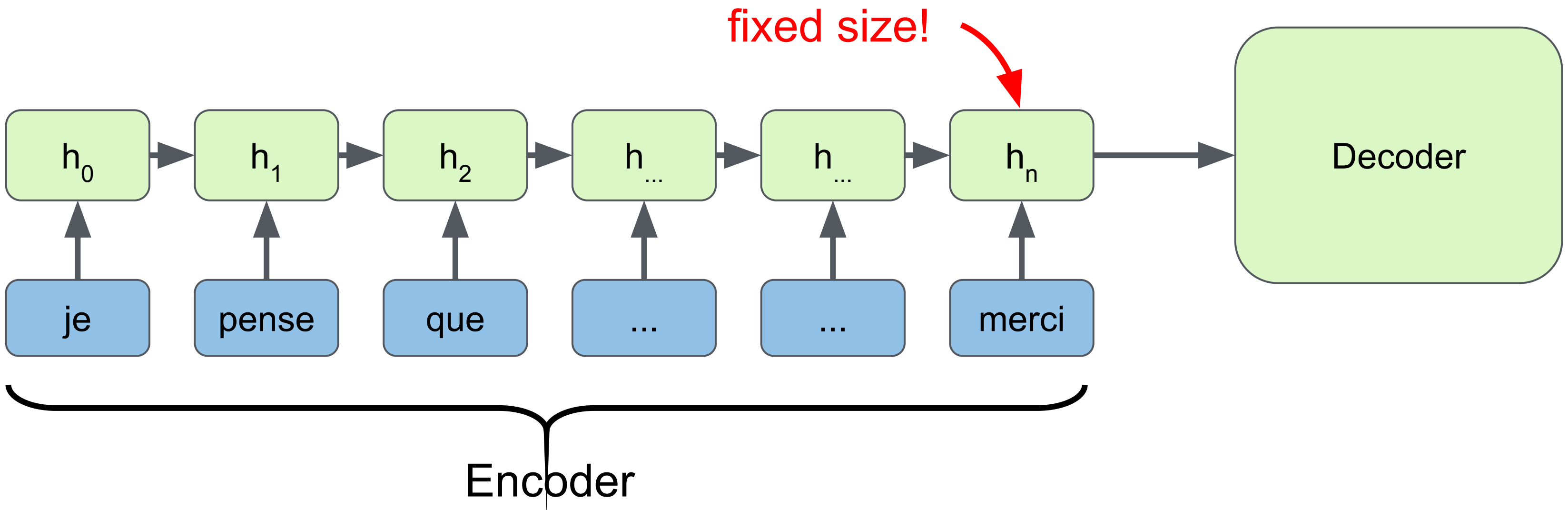
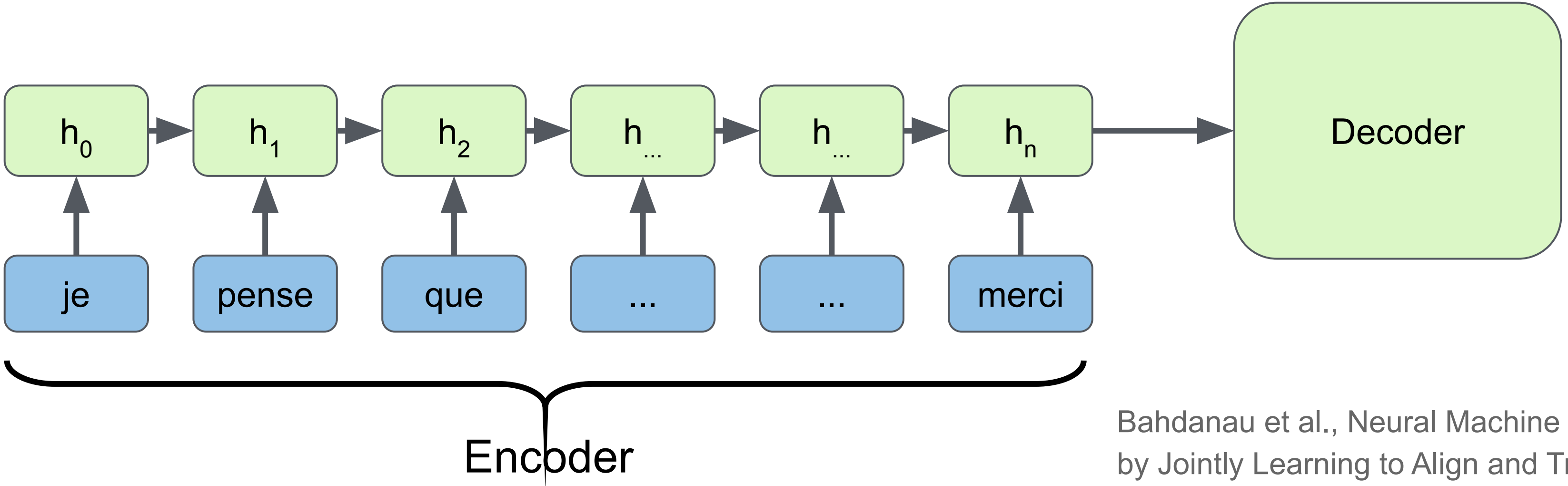
Sequence-to-Sequence Models - Bottleneck

- This is not easy to do with very long input sequences.
- $\mathbf{h_n}$ is a bottleneck.



Attention Mechanism

- Problem: it is not easy to store all the necessary information from an **arbitrary long** sequence into a **fixed-size** vector.



Bahdanau et al., Neural Machine Translation by Jointly Learning to Align and Translate

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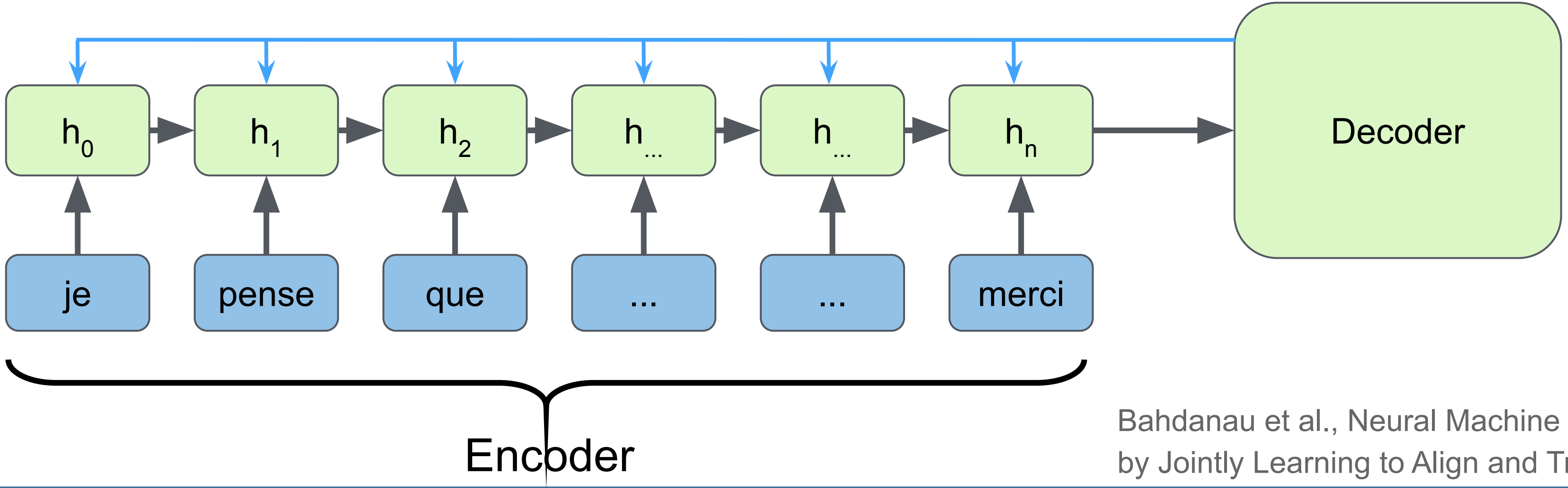
Attention Mechanism

- Problem: it is not easy to store all the necessary information from an **arbitrary long** sequence into a **fixed-size** vector.
- A possible solution can be to allow the decoder to "selectively look back" at the encoded input sequence.



Bahdanau et al., Neural Machine Translation by Jointly Learning to Align and Translate

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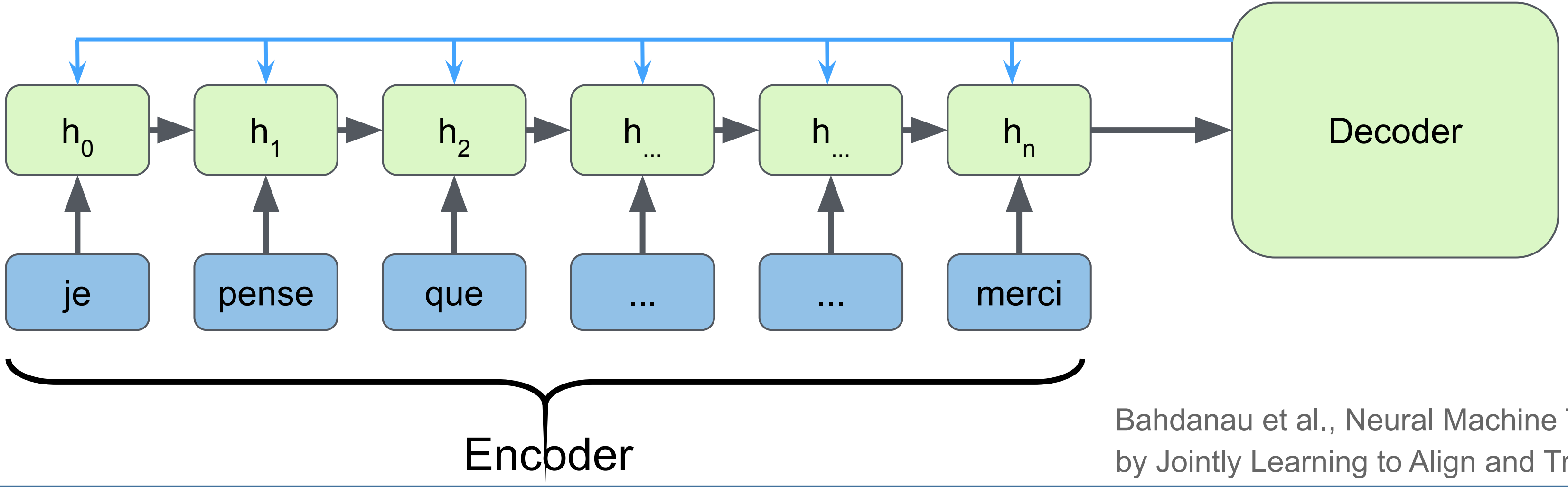
Attention Mechanism

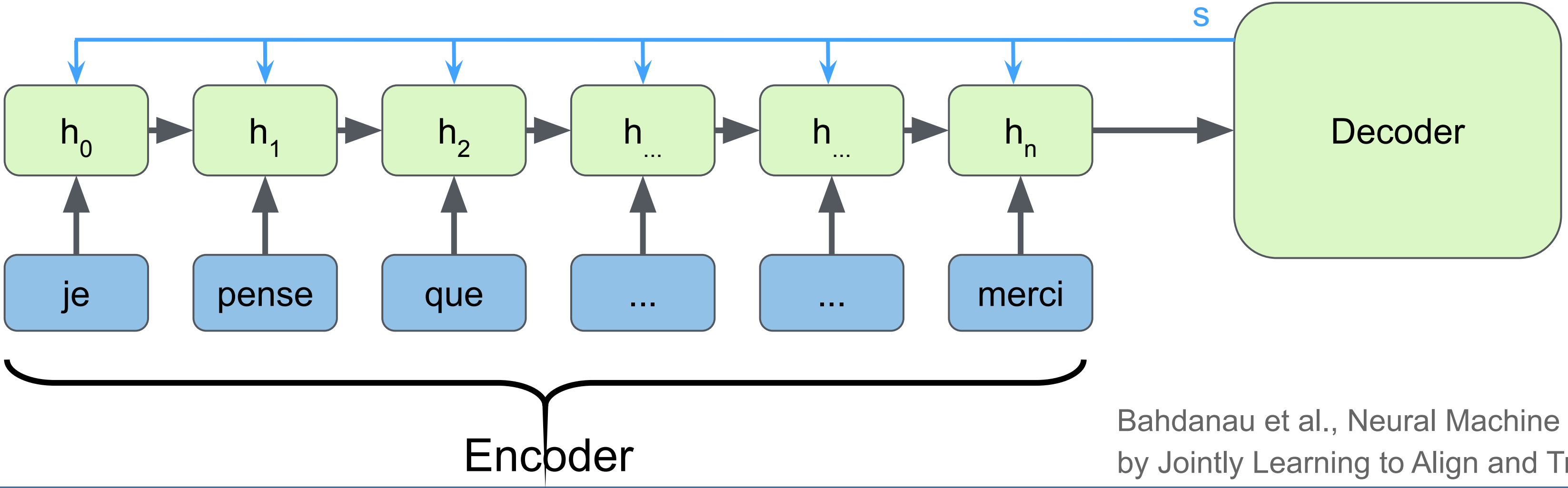
- This can be done with **attention**:
  - At any decoding time step, the decoder can use attention to fetch the relevant information for that step from the encoded input sequence.
- E.g., when producing the output word “think” (in a machine translation task), the decoder can focus on the encoding of the input word “pense”.



Bahdanau et al., Neural Machine Translation by Jointly Learning to Align and Translate

Attention Mechanism - Formalization

- Attention is a function **A** that, given a decoder state **s** and an encoded input sequence **h**, identifies the elements in **h** that are important at the current decoding time step.



Bahdanau et al., Neural Machine Translation by Jointly Learning to Align and Translate

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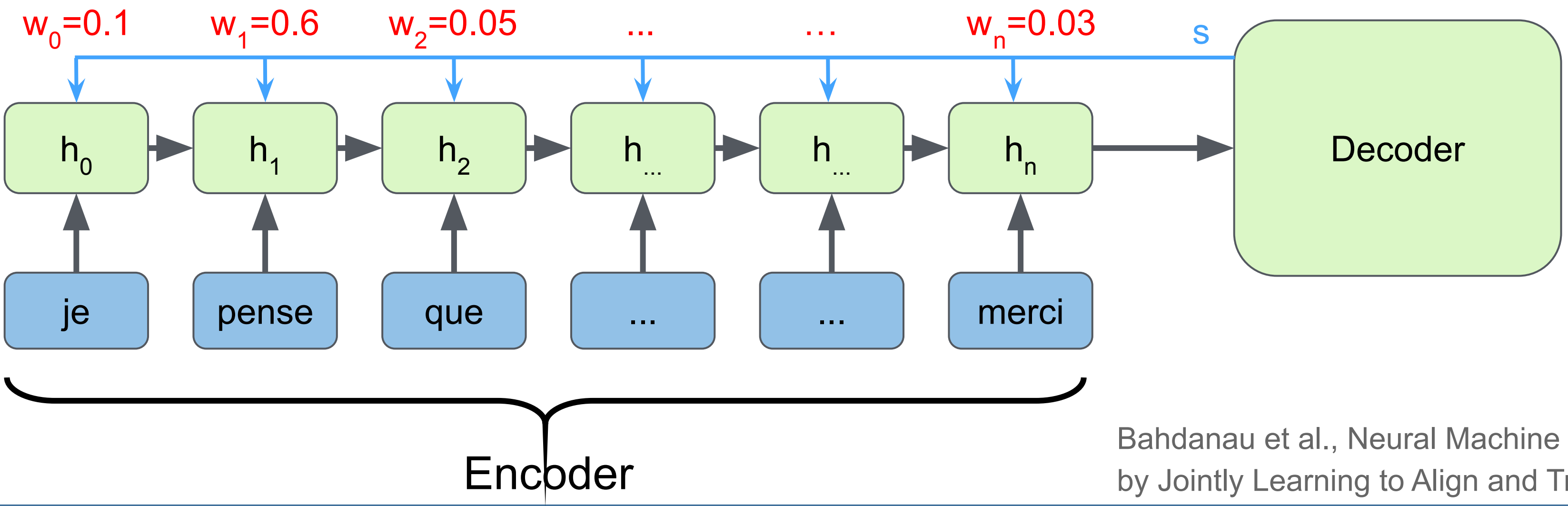
Attention Mechanism - Formalization

- Attention is a function A that, given a decoder state s and an encoded input sequence h, identifies the elements in h that are important at the current decoding time step.
  - **A** assigns weights **w** to the elements in **h**.
  - Those weights are normalized (to sum to 1).

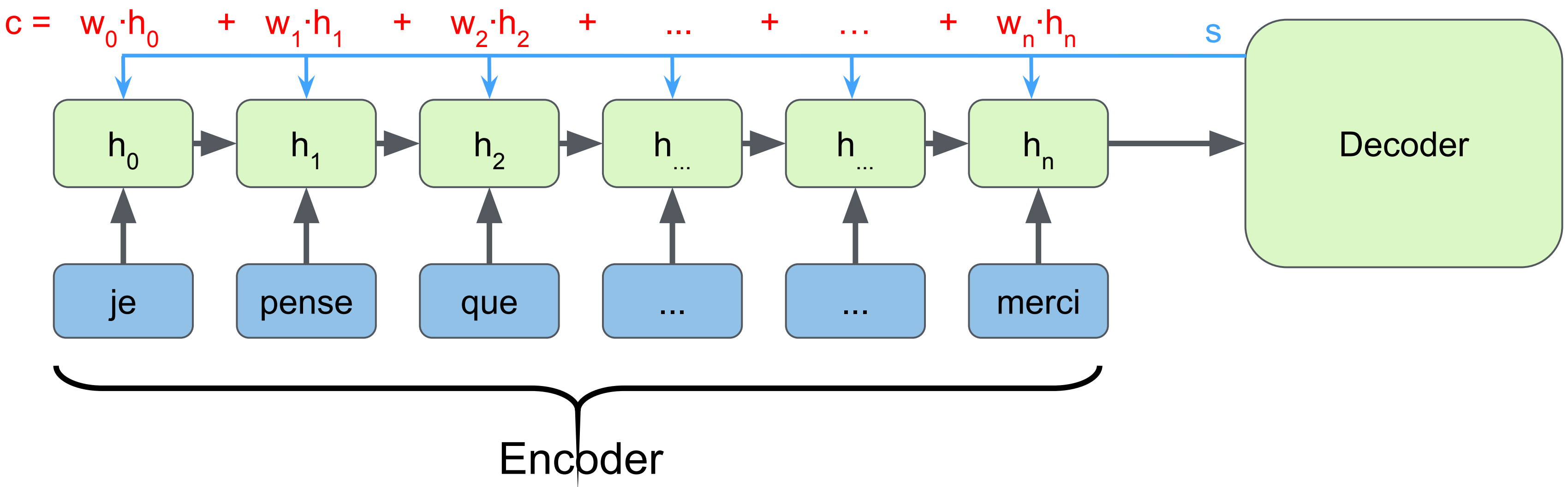


Bahdanau et al., Neural Machine Translation by Jointly Learning to Align and Translate

Attention Mechanism - Formalization

- The weights **w** are used to compute a weighted sum **c** of the elements in the sequence **h**. **c** is called **context vector**.

$$c = \sum_{i=0}^{n} w_i \cdot h_i$$



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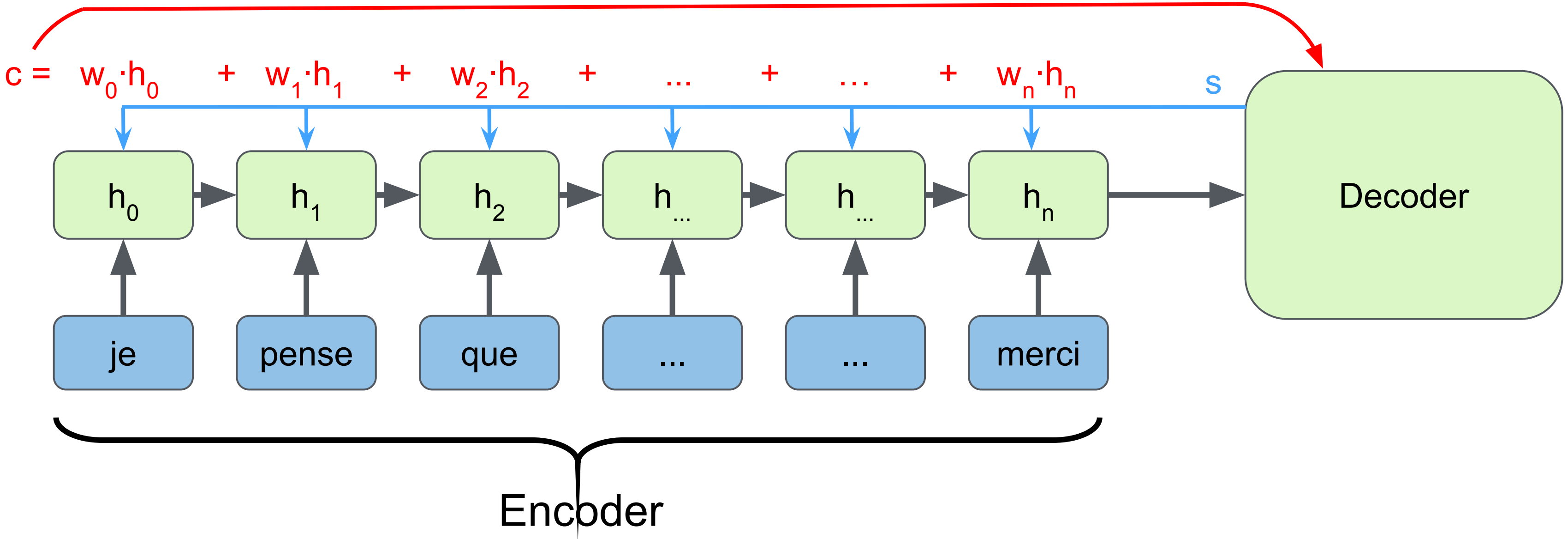
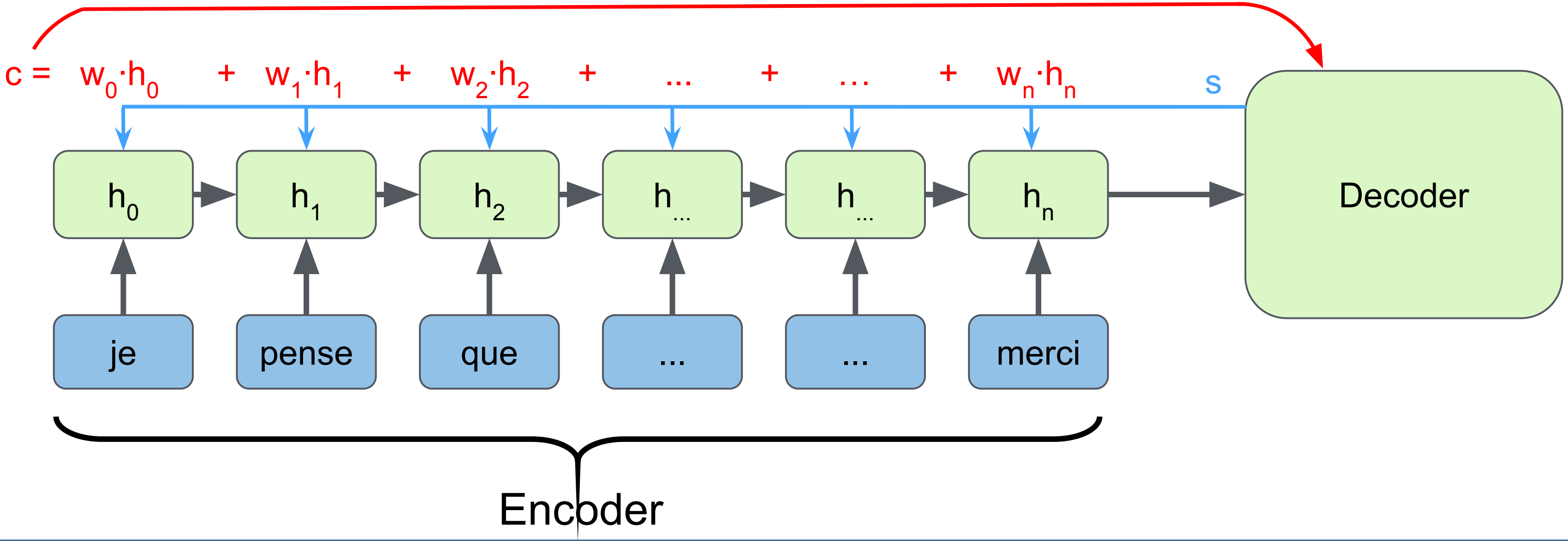
Attention Mechanism - Formalization

- The context vector **c** is then fed to the decoder.



Attention Mechanism - Formalization

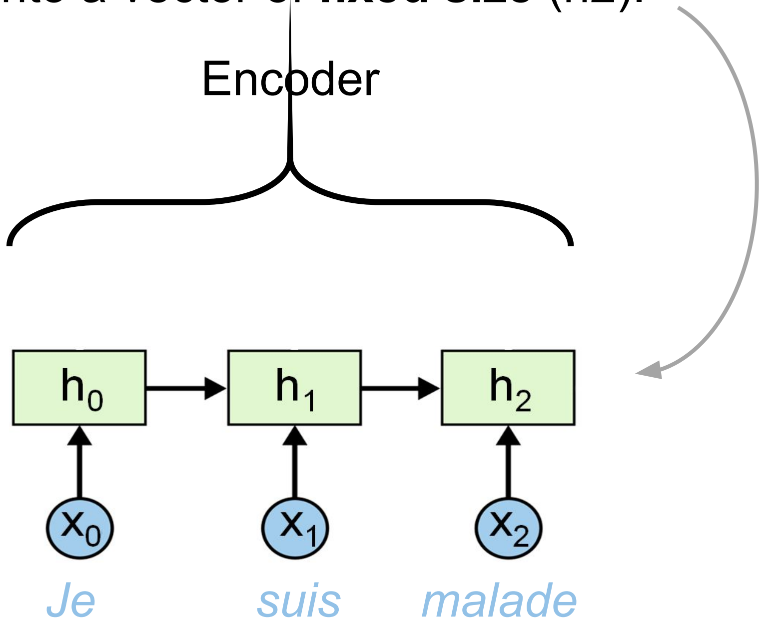
- Let's see a full step-by-step example of the attention mechanism.
- We will then look at how to implement the function **A**.



Example: Sequence-to-Sequence + Attention

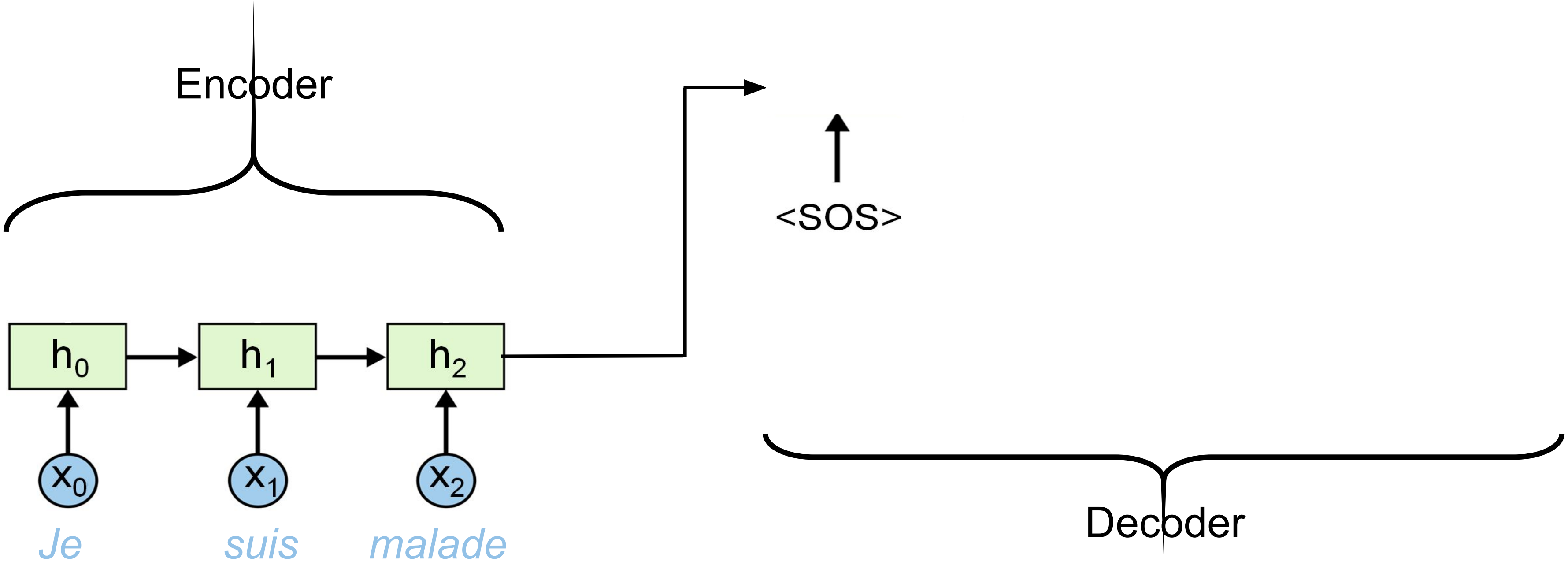
Example: Sequence-to-Sequence + Attention

All the x sequence is encoded into a vector of **fixed size** (h2).



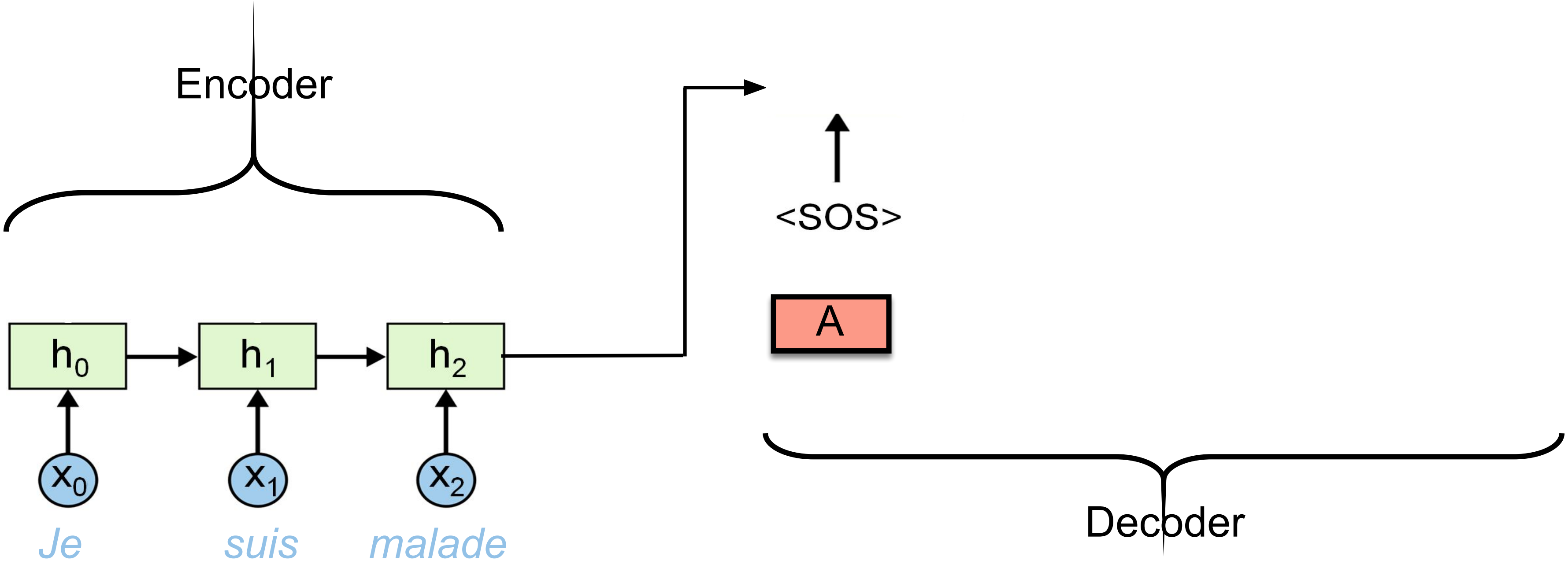
Example: Sequence-to-Sequence + Attention

The decoder starts with the **<SOS>** symbol.



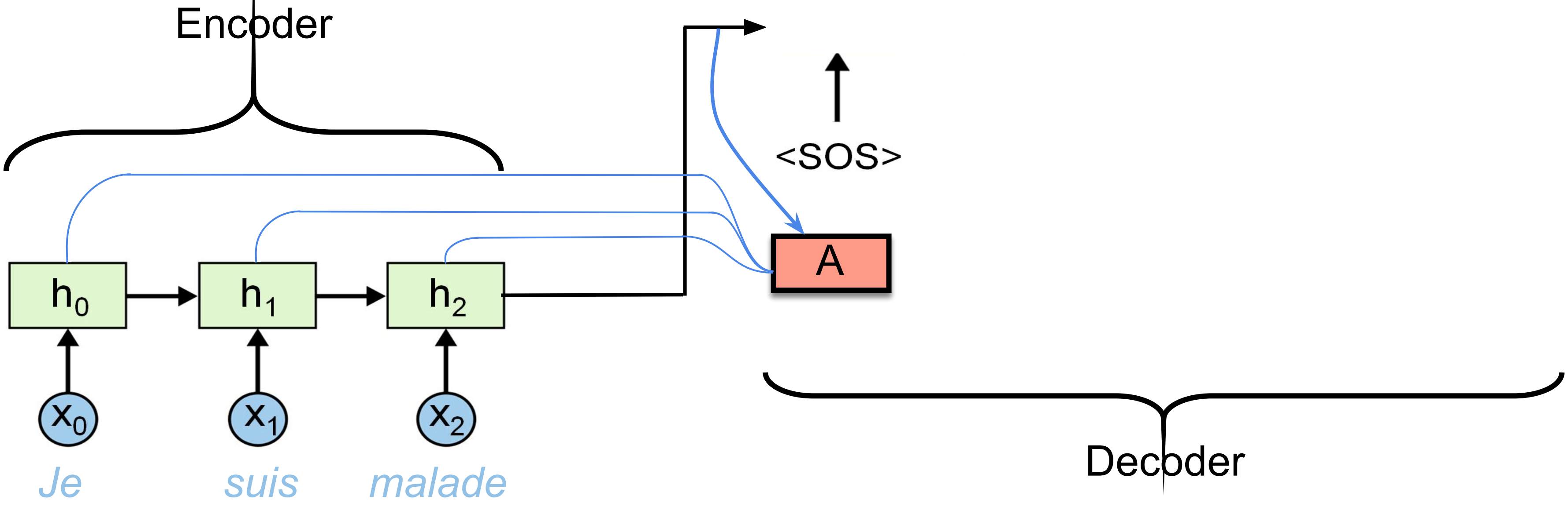
Example: Sequence-to-Sequence + Attention

The attention model **A** is added to the decoder.



Example: Sequence-to-Sequence + Attention

The decoder's previous state and the encoded input sequence **h** are fed as inputs to the attention model (**A**).



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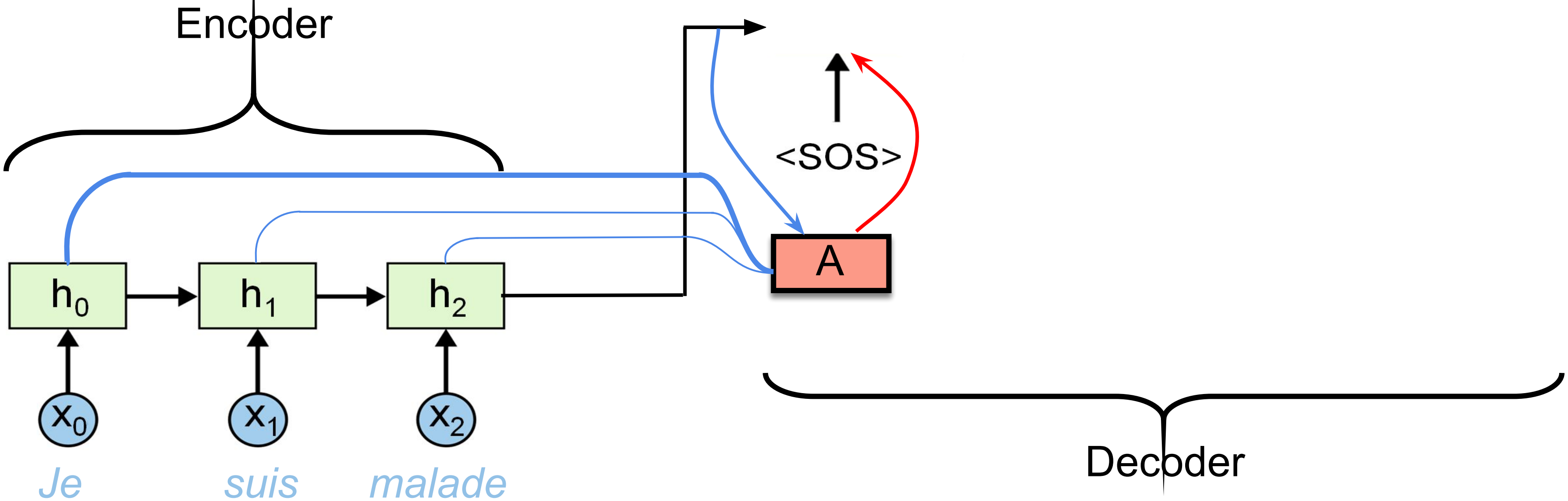
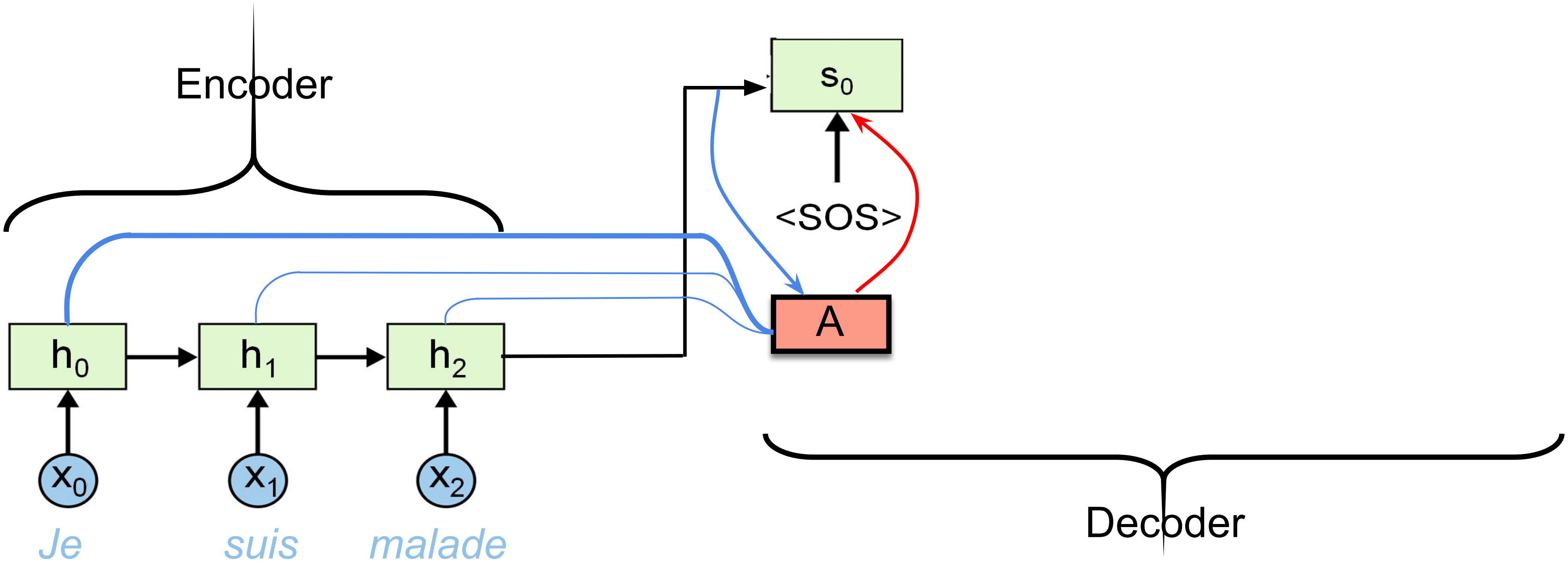
Example: Sequence-to-Sequence + Attention

The context vector (output of the attention) is fed as an input to the decoder.



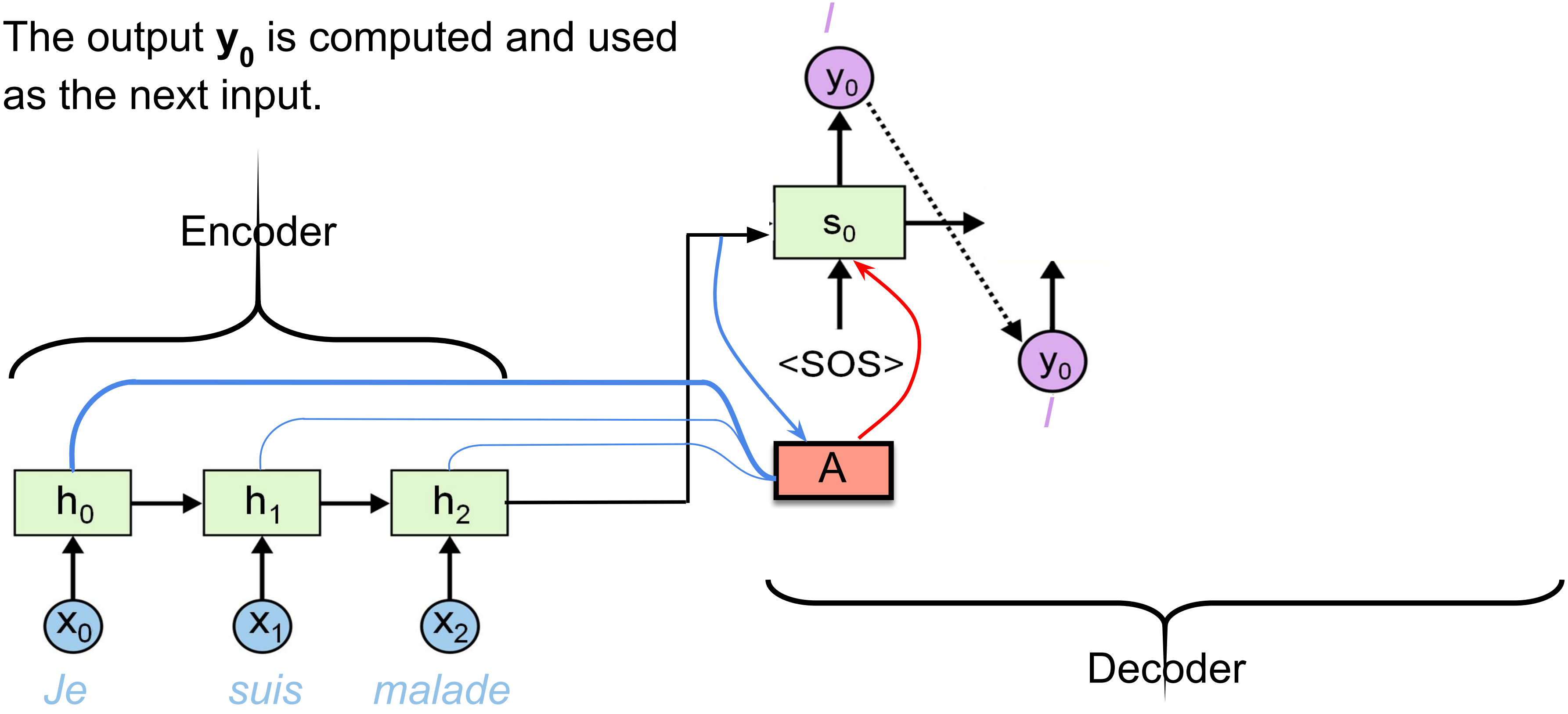
Example: Sequence-to-Sequence + Attention

The internal state $\mathbf{s}_0$ is computed.

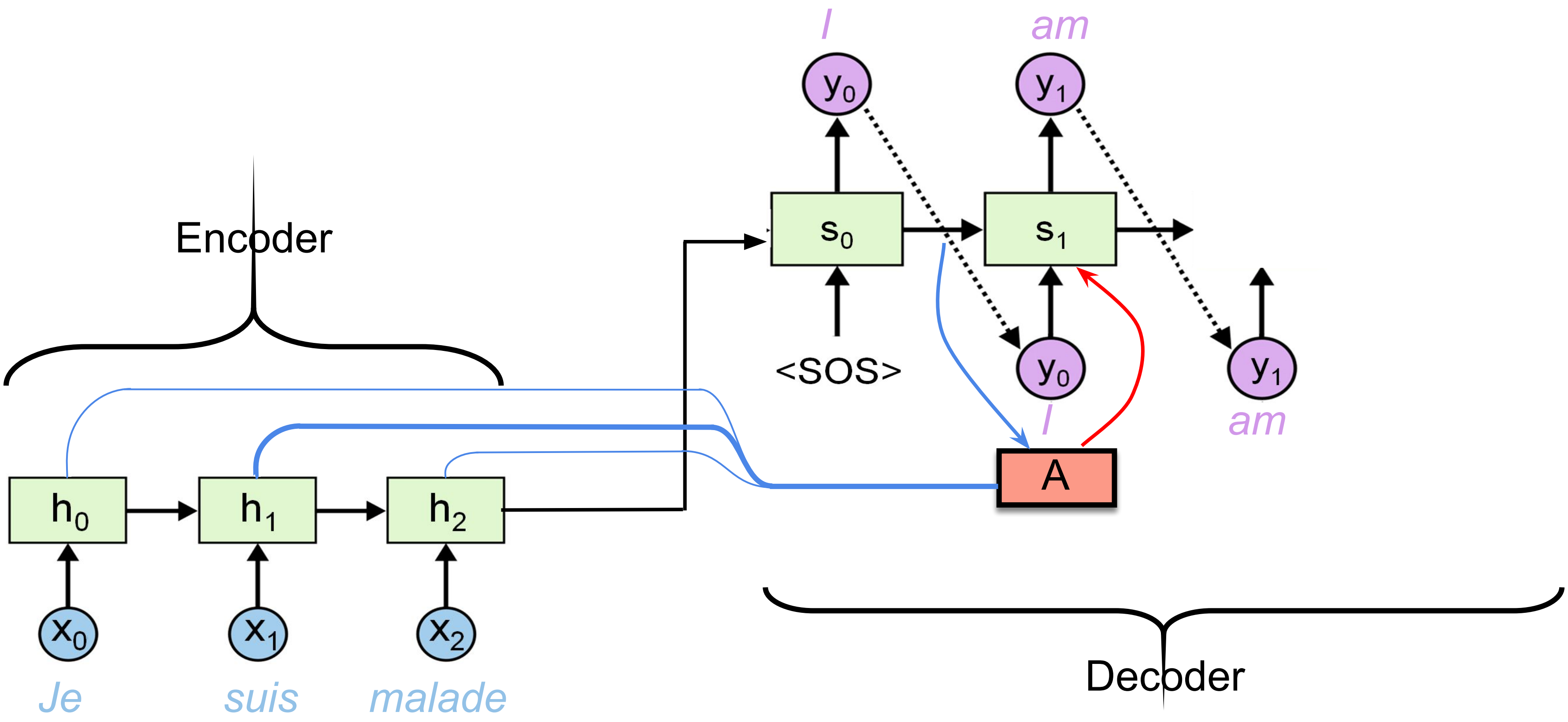


Example: Sequence-to-Sequence + Attention

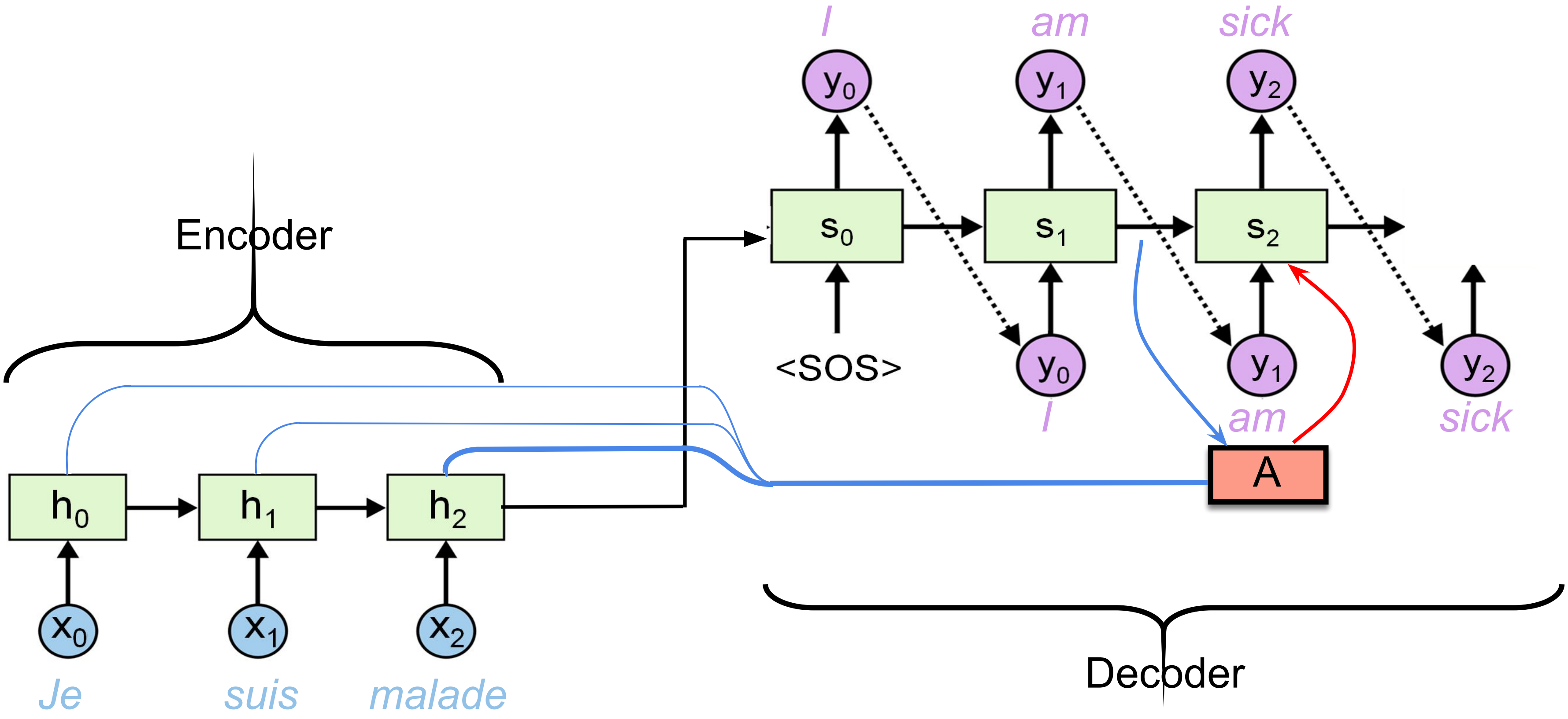
The output $\mathbf{y_0}$ is computed and used as the next input.



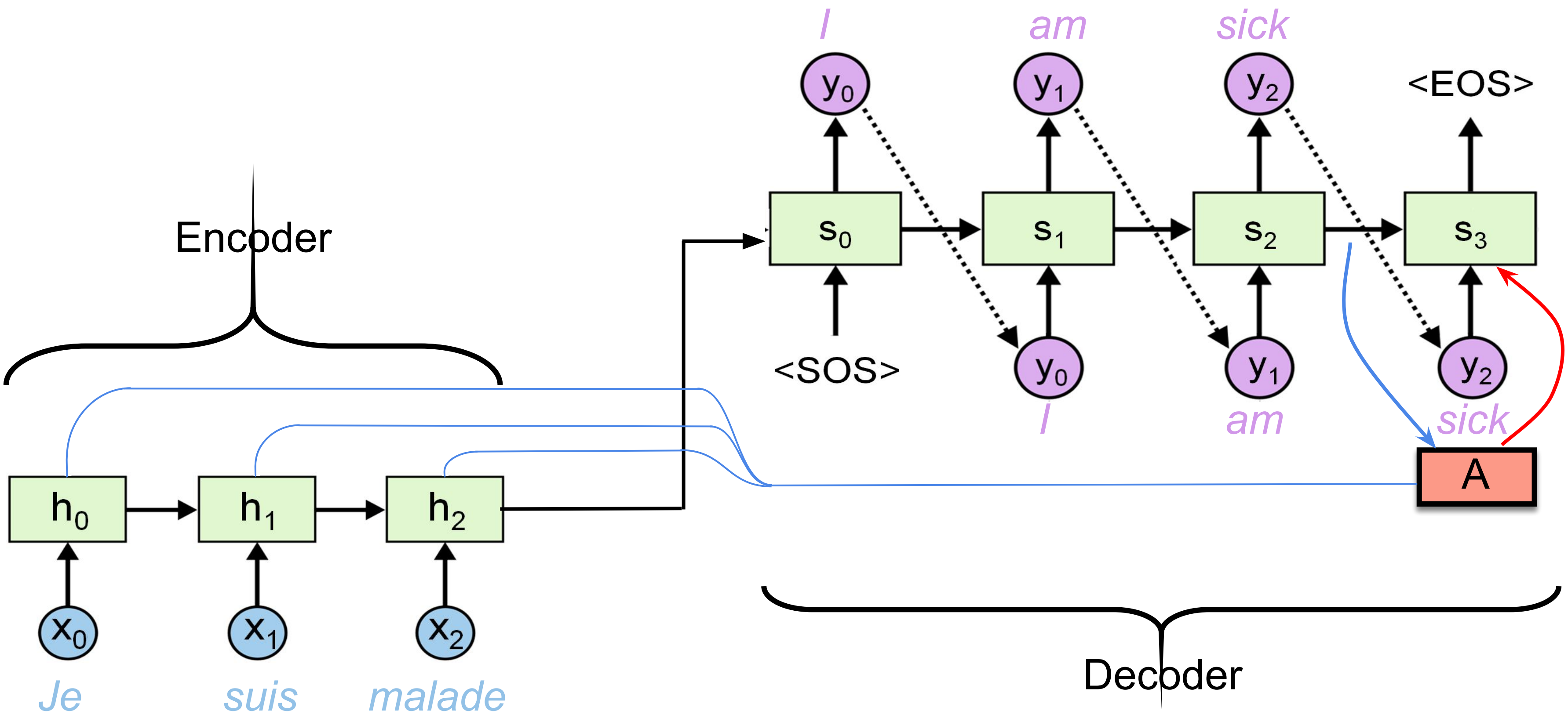
Example: Sequence-to-Sequence + Attention



Example: Sequence-to-Sequence + Attention



Example: Sequence-to-Sequence + Attention



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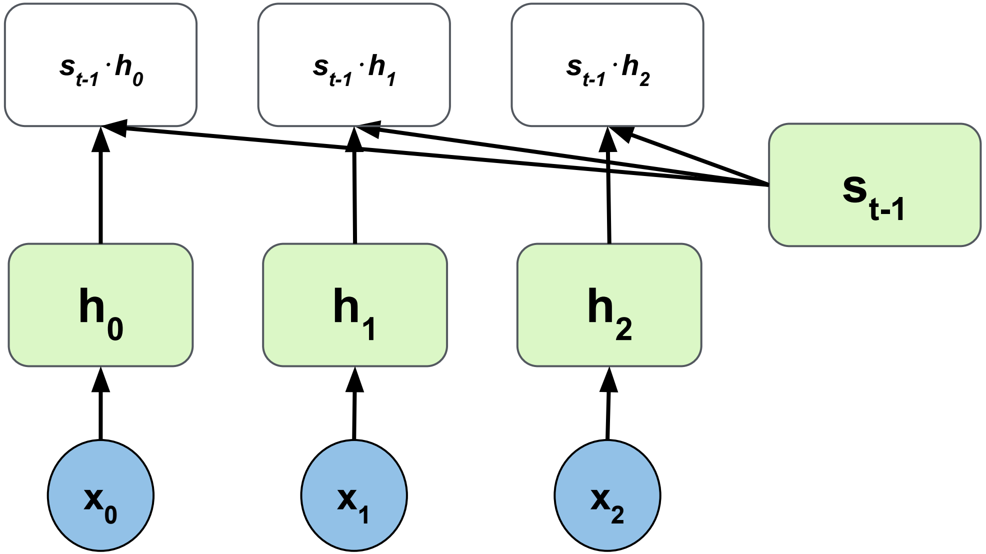
Attention Function

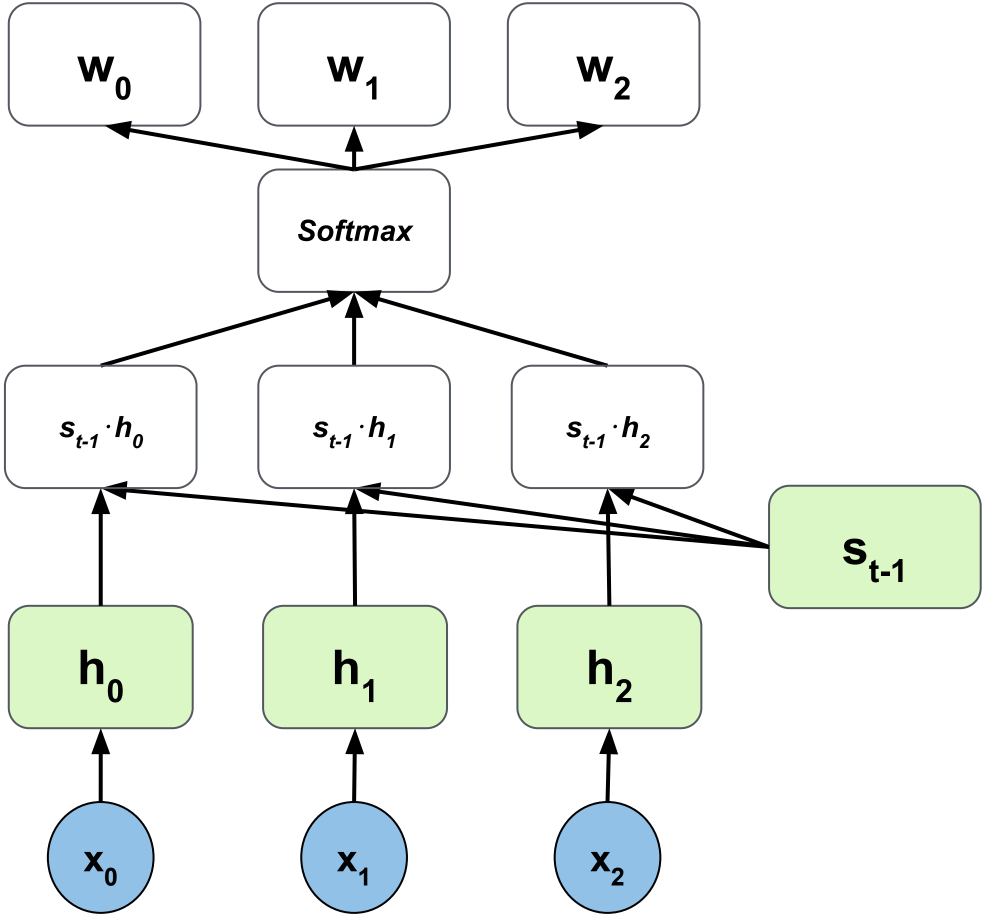
- There are several possible implementations for **A**.
- The most simple version is based on a dot product, i.e., $\mathbf{e_i = s_{t-1} \cdot h_i}$.



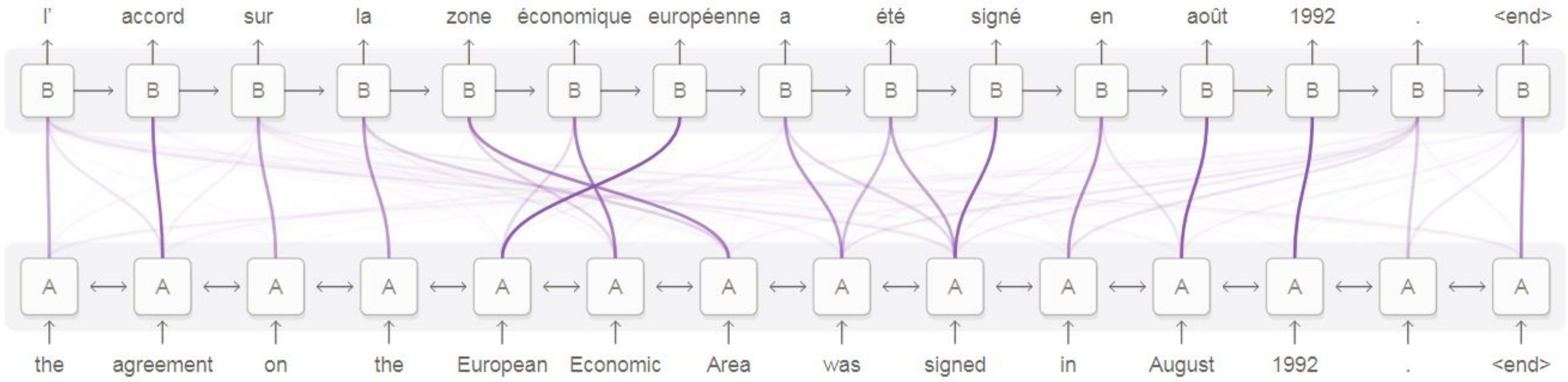
Attention Function

- The dot product results are passed through a Softmax to get normalized weights **w=[w$_0$, ..., w$_n$]**, which indicate how "important" the various elements are.
- The final result is the weighted sum of **h**.

$$c = \sum_{i=0}^{n} w_i \cdot h_i$$



Visualizing Attention

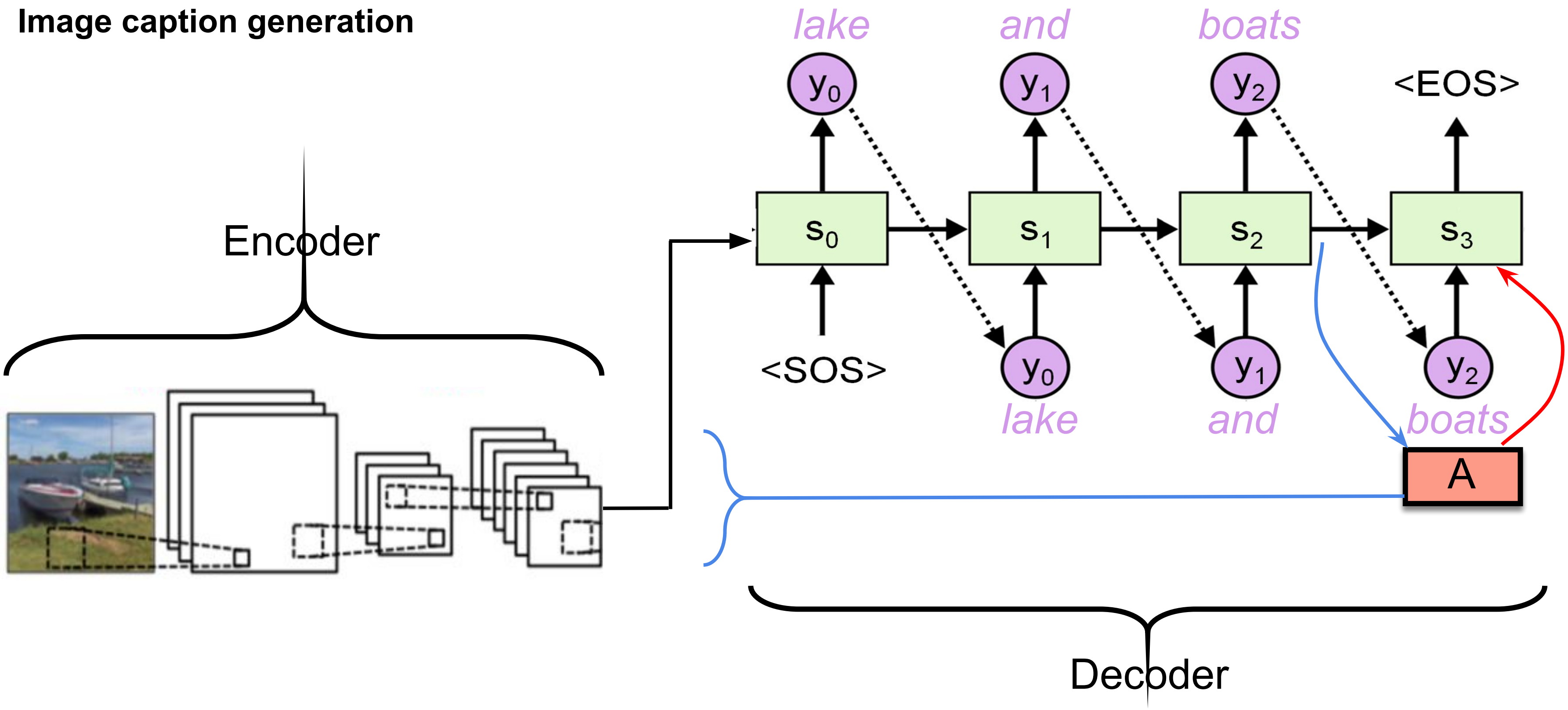


- The thick lines show where the decoder is focusing its attention when analyzing the encoded input sequence.

Image from Christopher Olah's blog

Other Examples

Image caption generation



Other Examples

A woman is throwing a frisbee in a park .

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

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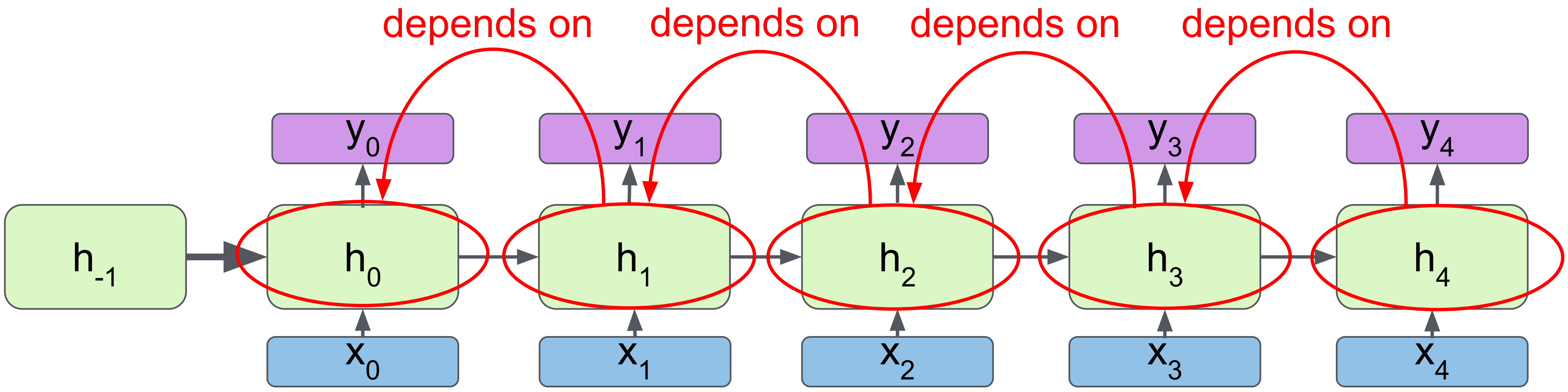
Beyond RNNs

- Sequence-to-Sequence + Attention systems perform well, but they are based on RNNs (simple RNNs / LSTMs / GRUs).
- RNNs suffer from two problems:
  - Not easy to parallelize.
  - Even in the more “complex” implementations (e.g. LSTMs), they struggle to capture (very) long-term dependencies.

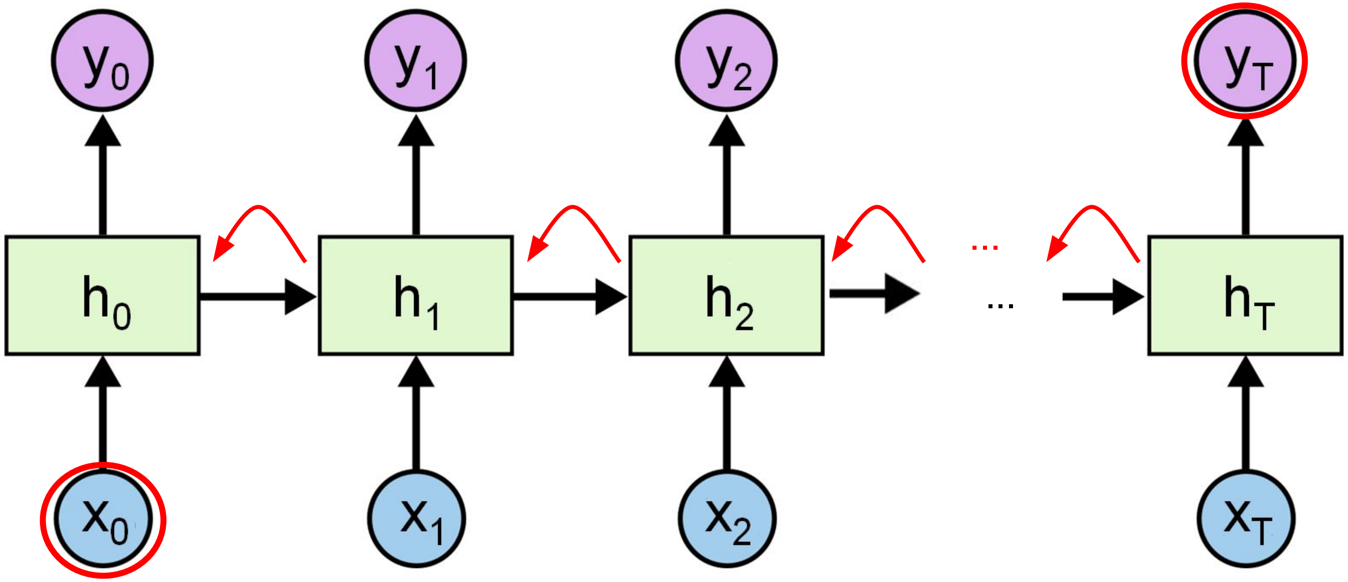
Beyond RNNs

- Every state in an RNN depends on the previous internal state.
- This creates a chain of computation which prevents parallelization.



Beyond RNNs

- Long-term dependencies are hard to capture with RNNs.
- This problem is strongly mitigated using LSTMs / GRUs, but it's still there for very long sequences.



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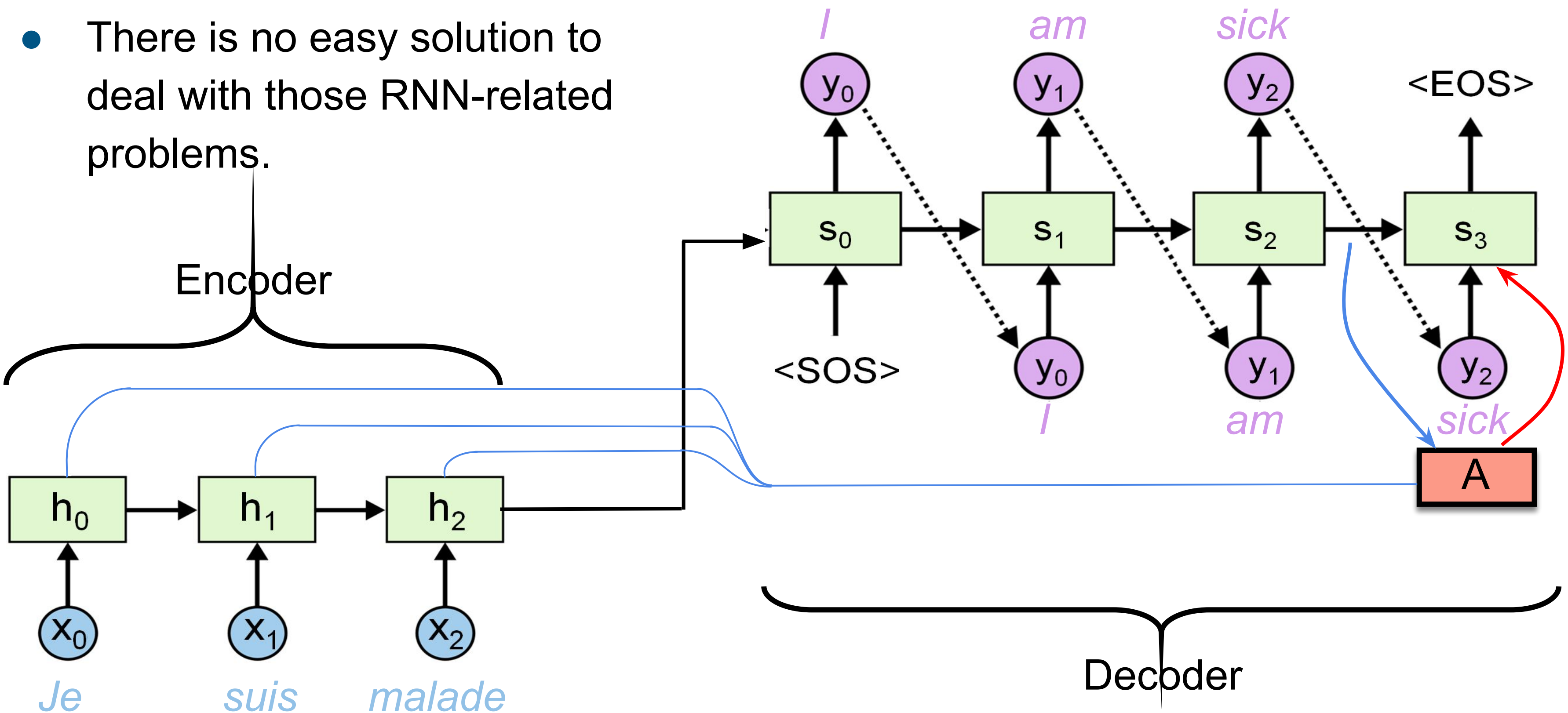
Beyond RNNs

- There is no easy solution to deal with those RNN-related problems.



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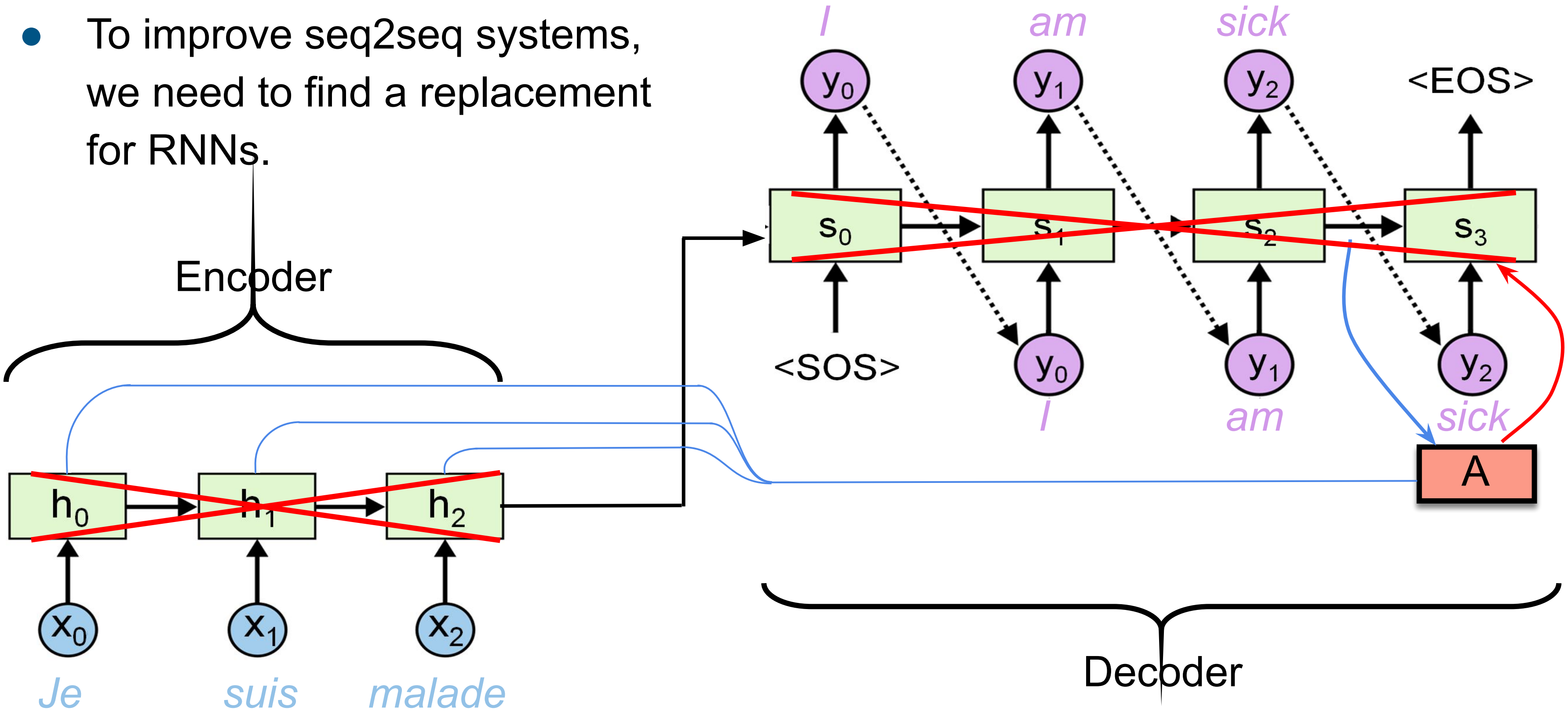
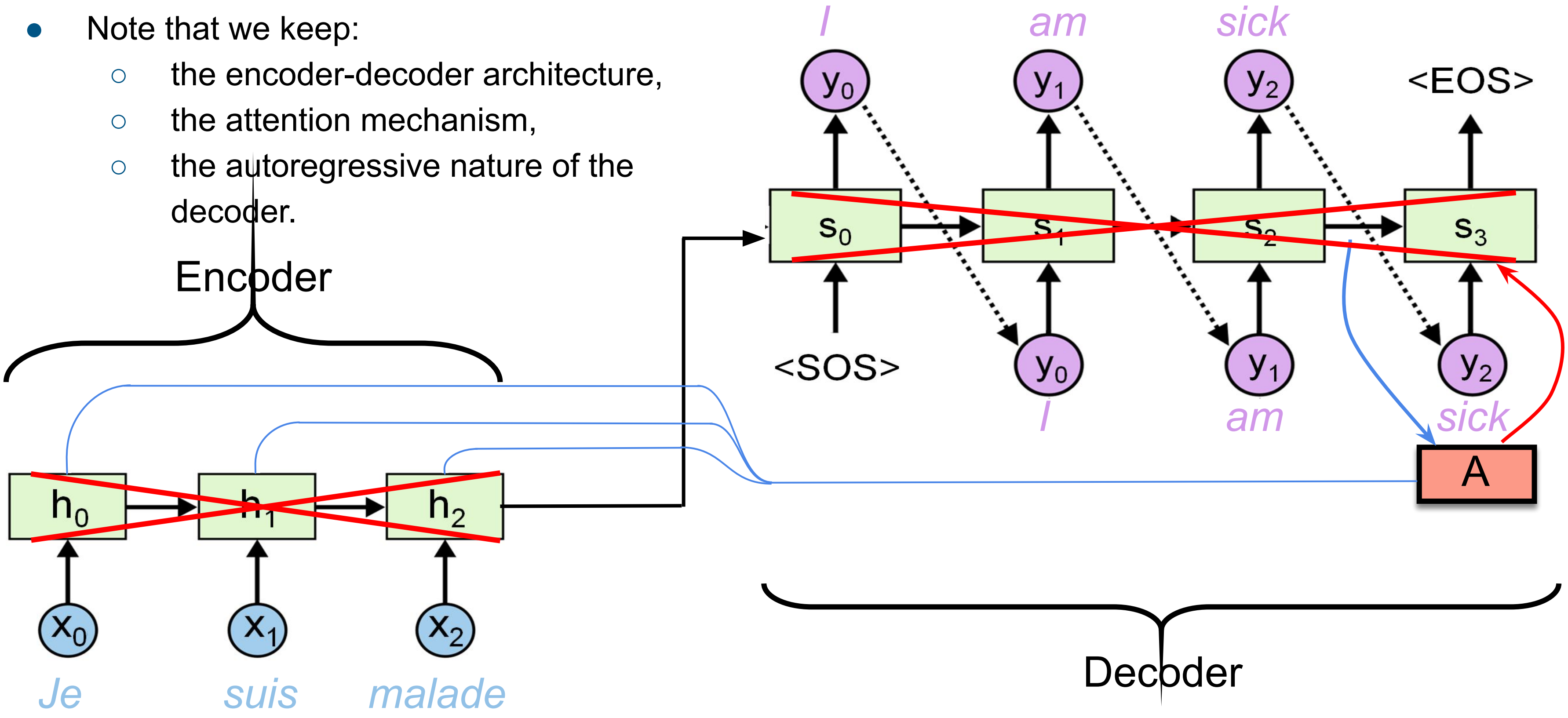
Beyond RNNs

- To improve seq2seq systems, we need to find a replacement for RNNs.



Beyond RNNs

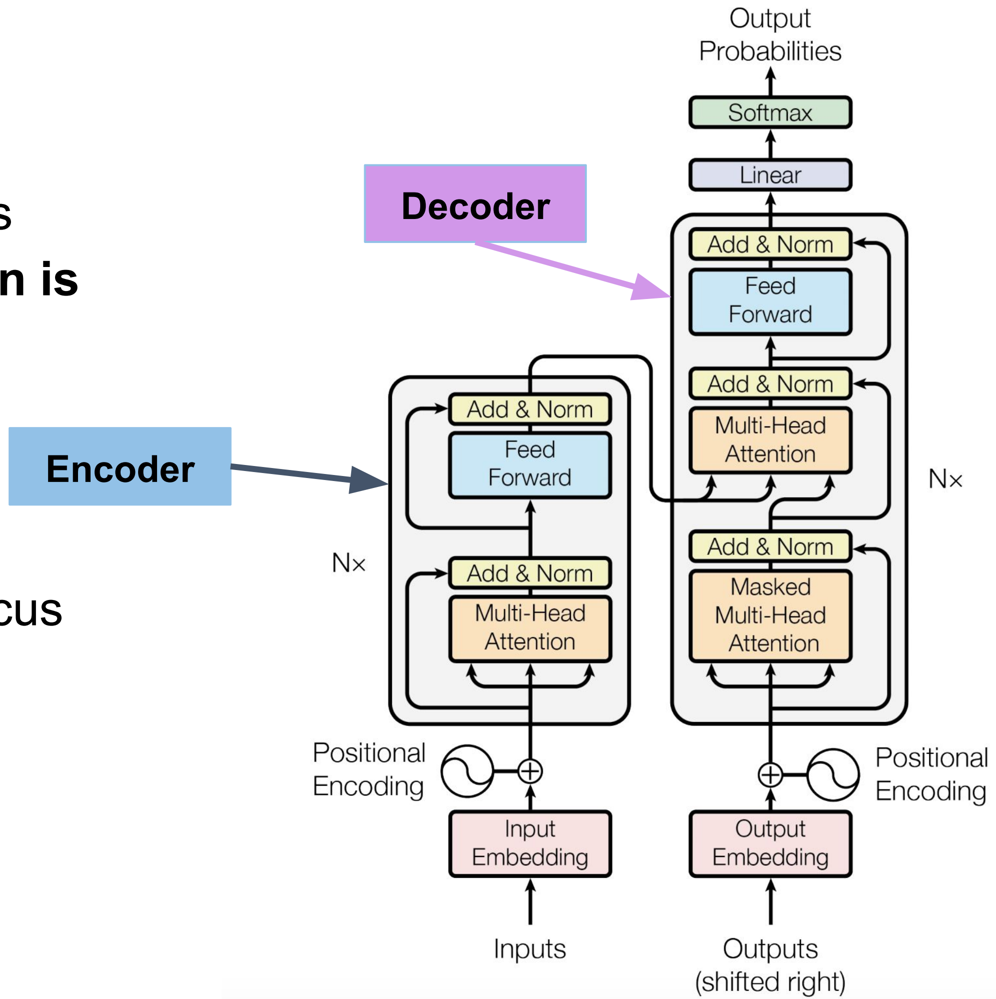
- Note that we keep:
  - the encoder-decoder architecture,
  - the attention mechanism,
  - the autoregressive nature of the decoder.



Transformer

- The Transformer architecture was introduced in the paper "**Attention is all you need**".

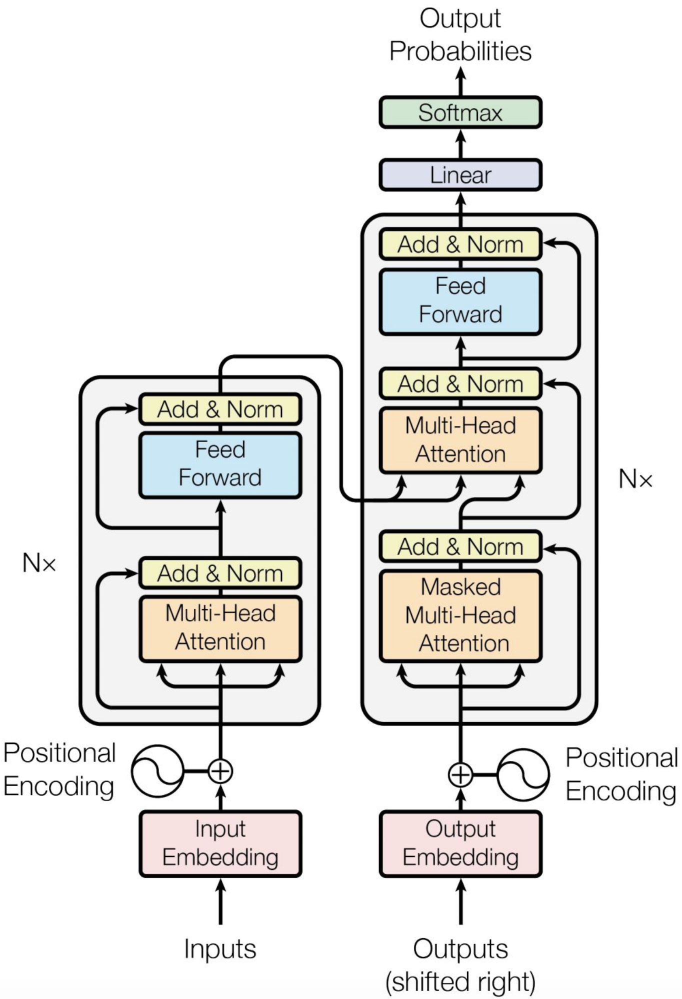
- Note: in the next slides we will focus on providing the intuition, thus simplifying some aspects of the architecture.



Vaswani et al, "Attention Is All You Need", 2017

Transformer

- Several key points:
  - Recurrence replaced with self-attention and multi-head attention.
  - Positional encodings.
  - Residual connections.
  - Layer normalization.
  - Position-wise feed-forward networks.
- We will focus on the self-attention and the multi-head attention.

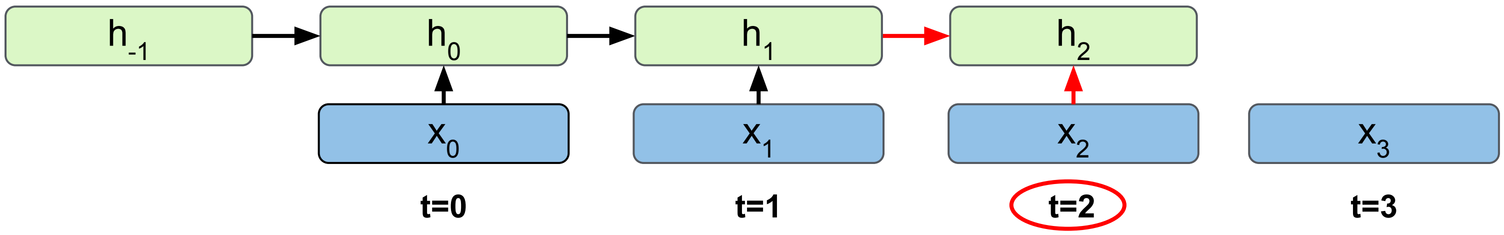


Vaswani et al, “Attention Is All You Need”, 2017

Self-Attention

- Before introducing Self-Attention, let's recap how a RNN works.
- At each time step, a RNN encodes the current input taking into consideration the past context (or the future context for right-to-left models).

- Example: the hidden state h_2 is encoding the information from the current input x_2 as well as the previous context.

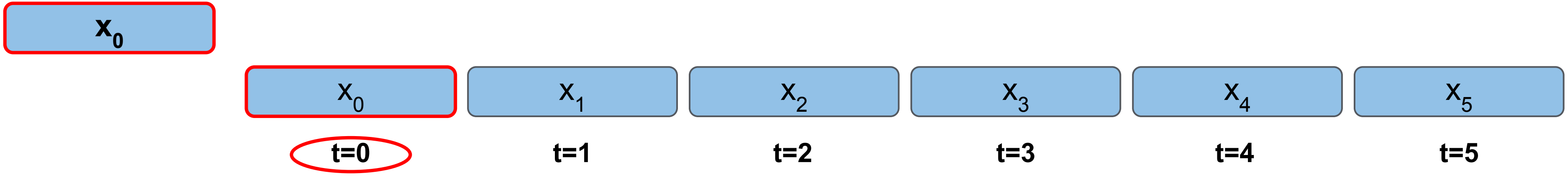


Self-Attention

- We want to do something similar with self attention:
  - encode the current input taking into consideration the surrounding context.
- The attention mechanism is used to identify the elements in a sequence which are “relevant” to encode the current one.

Self-Attention

- Let's consider time step 0 with its element x_0.
- We will identify all elements in the sequence which are "relevant" to encode x_0.



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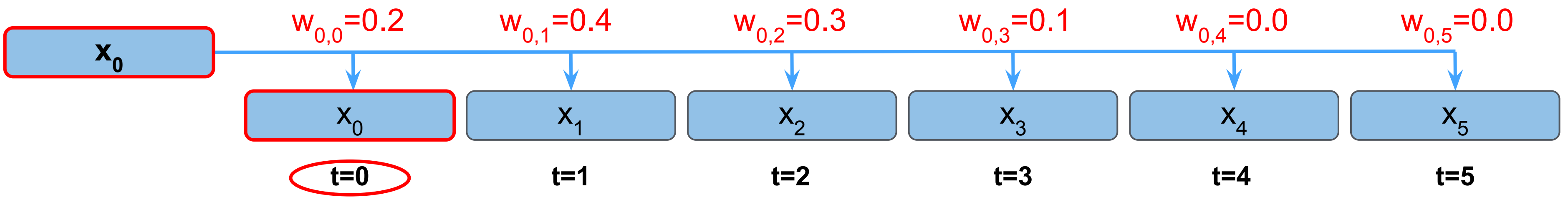
Self-Attention

- This is done by assigning a weight to each element (by computing a dot product between the element and x_0)…



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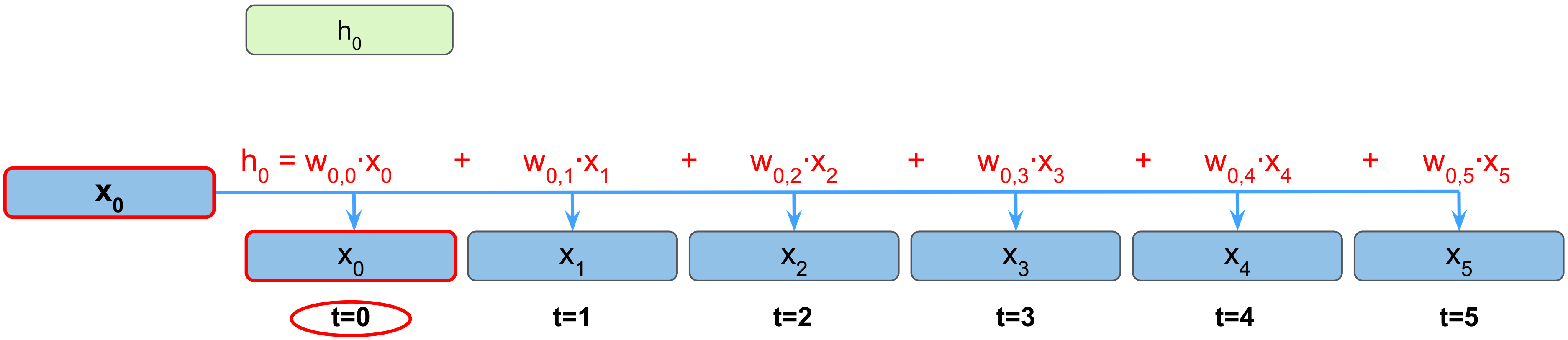
Self-Attention

- This is done by assigning a weight to each element (by computing a dot product between the element and x0)…
- ... and then computing a normalized weighted sum.



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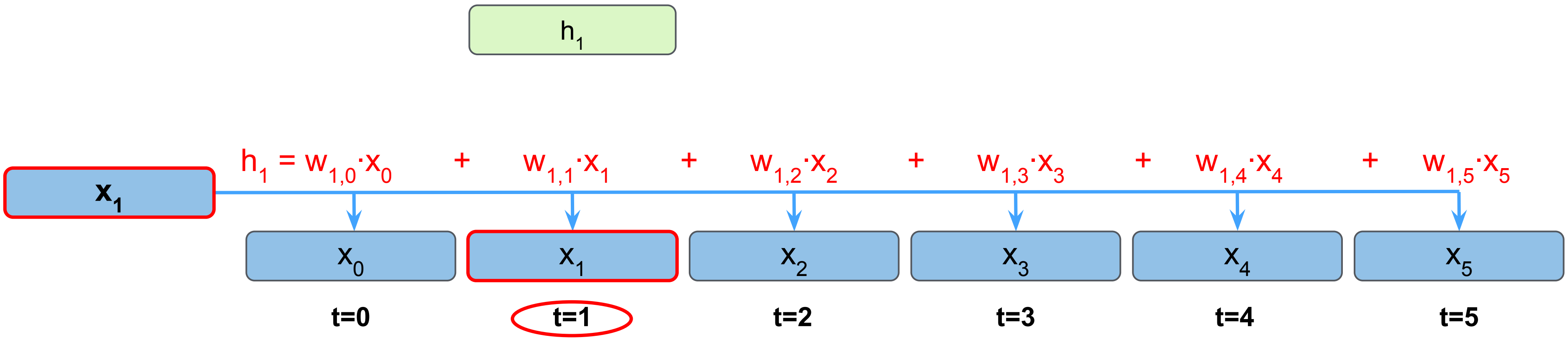
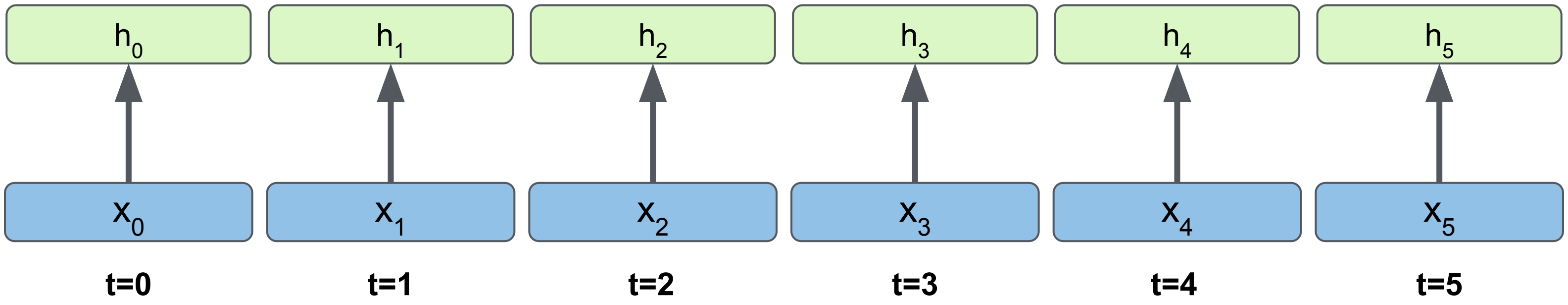
Self-Attention

- This is repeated for every step… (note that the weights vary across steps)



Self-Attention

- This is repeated for every step… (note that the weights vary across steps)
- … until all the steps are completed.



Self-Attention - Multiple Heads

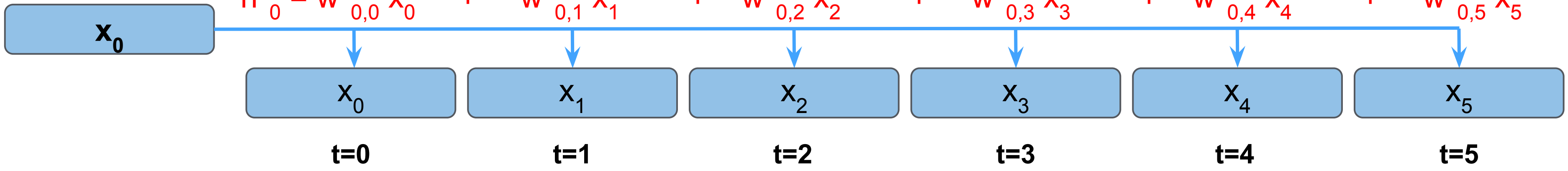
- The self-attention is meant to identify all elements in a sequence which are "relevant" to encode x_t.
- Given that there can be several types of relevant information, we can have several attention mechanisms.

Self-Attention - Multiple Heads

- The self-attention is meant to identify all elements in a sequence which are “relevant” to encode x_t.
- Given that there can be several types of relevant information, we can have several attention mechanisms.
- Each attention mechanism is called a **head**, leading to a **multi-head self-attention**.
    - In this example, there are head#0 and head#1, each with different weights.

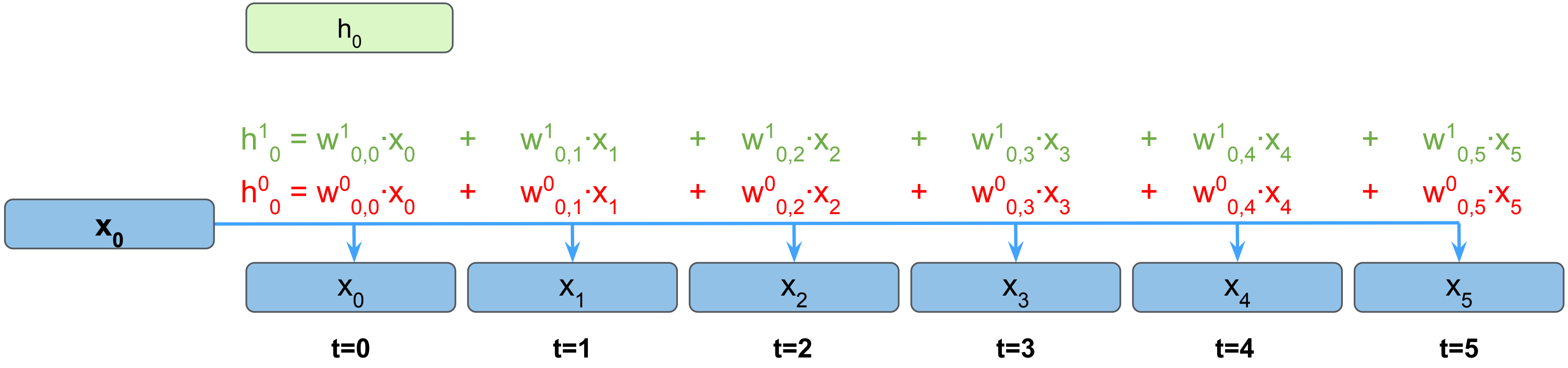
$$h^1_0 = w^1_{0,0} \cdot x_0 + w^1_{0,1} \cdot x_1 + w^1_{0,2} \cdot x_2 + w^1_{0,3} \cdot x_3 + w^1_{0,4} \cdot x_4 + w^1_{0,5} \cdot x_5$$

$$h^0_0 = w^0_{0,0} \cdot x_0 + w^0_{0,1} \cdot x_1 + w^0_{0,2} \cdot x_2 + w^0_{0,3} \cdot x_3 + w^0_{0,4} \cdot x_4 + w^0_{0,5} \cdot x_5$$



Self-Attention - Multiple Heads

- The various heads are then merged together.
  - E.g., they are concatenated, $\mathbf{h_0 = [h^0_0, h^1_0]}$.



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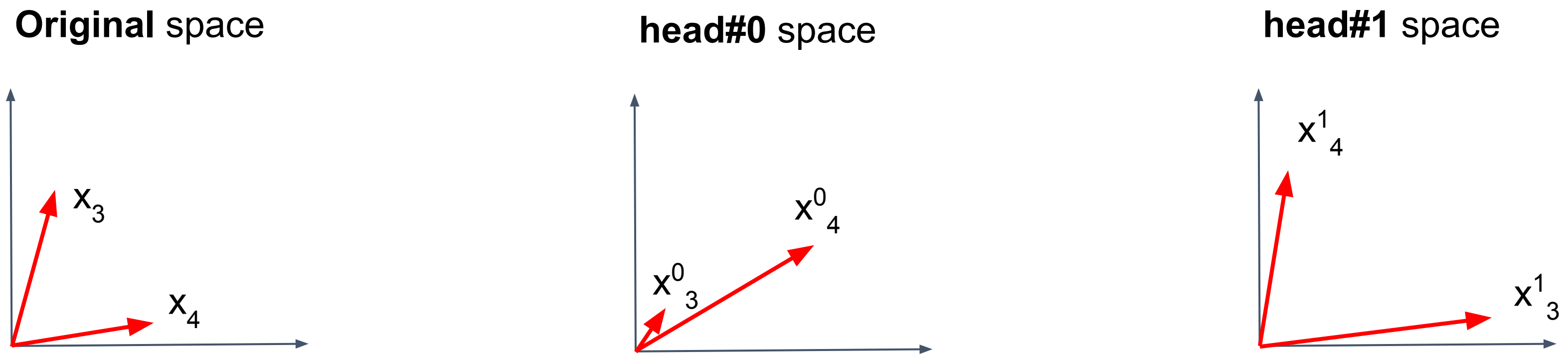
Self-Attention - Multiple Heads

- The weights for a given head are based on a dot-product.
  - E.g., $\mathbf{w^0_{3,4} = x^0_3 \cdot x^0_4}$

- The dot-product is computed in a different space for each attention head. This space is obtained by learning a projection from the original space to the one dedicated to a particular head.



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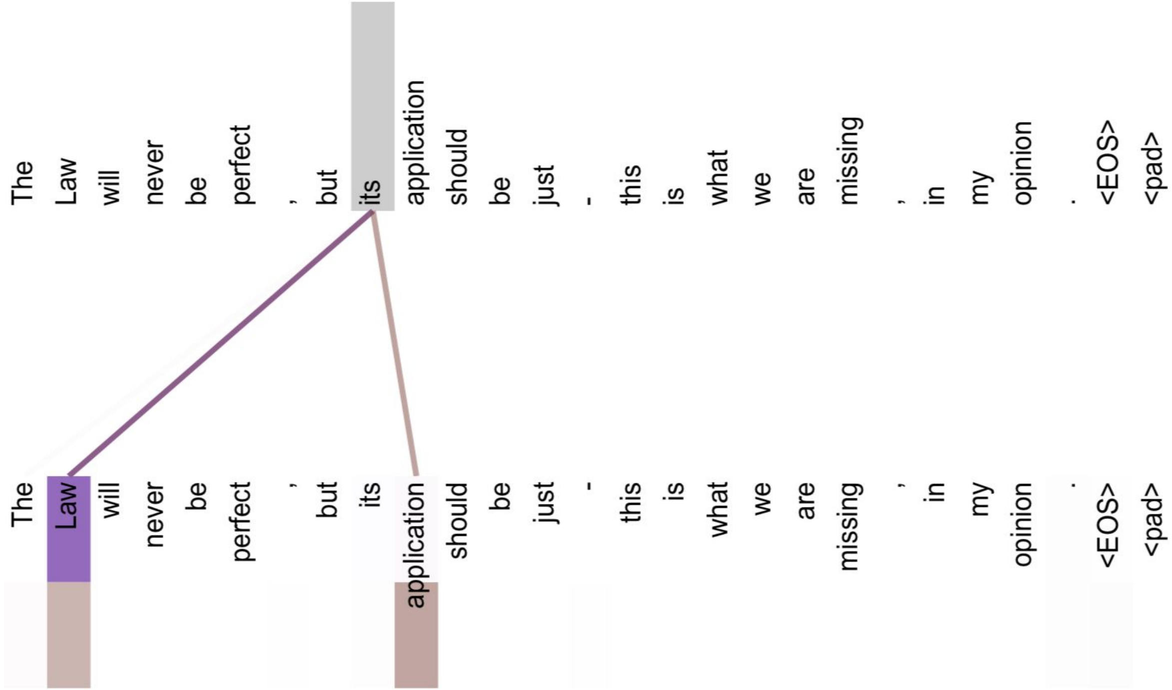
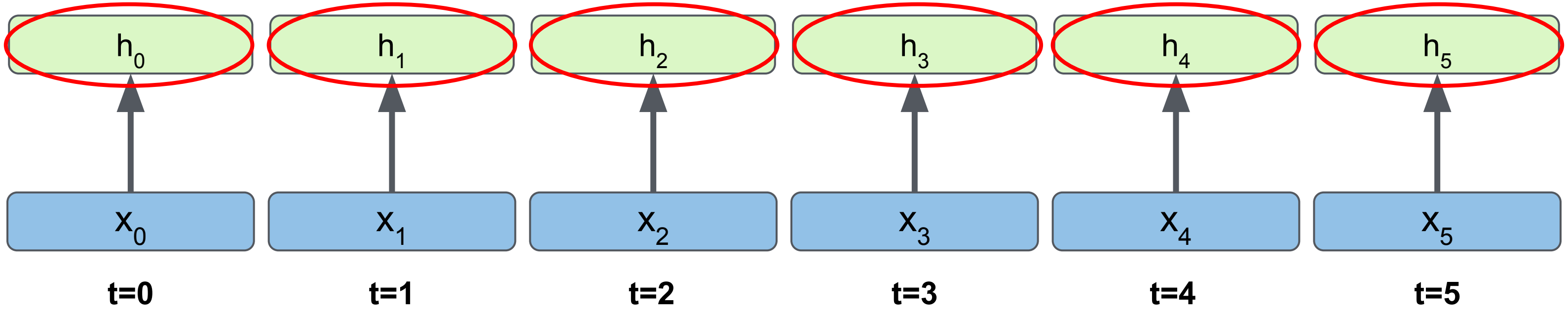
Self-Attention - Visualization



Vaswani et al, “Attention Is All You Need”, 2017

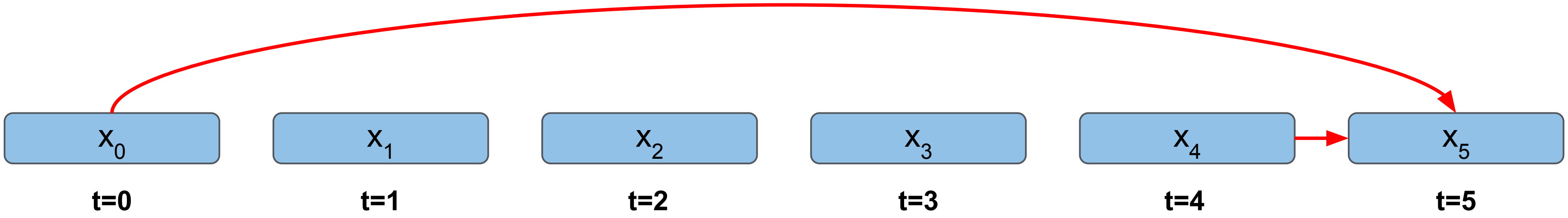
Self-Attention - Advantages

- The multi-head self-attention can be computed in parallel at all time steps.
- There are no dependencies between time steps.



Self-Attention - Advantages

- The RNN chain of computation is **not** there anymore.
- The information does **not** need to flow over a long chain of elements.
- E.g., $\mathbf{x_5}$ has direct access to both $\mathbf{x_0}$ and $\mathbf{x_4}$.



Plan

- RNN Recap
- Sequence to Sequence models
- Attention Mechanism
- Transformer
- **Libraries and References**

Libraries

- RNNs are included in the main DL frameworks:
  - PyTorch : https://pytorch.org/docs/stable/nn.html#recurrent-layers
  - Tensorflow: https://www.tensorflow.org/tutorials/recurrent
- There are several Transformer implementations:
  - in Tensorflow: https://github.com/tensorflow/tensor2tensor
  - in PyTorch: https://github.com/huggingface/pytorch-transformers

References

- Christopher Olah's blog about LSTMs: http://colah.github.io/posts/2015-08-Understanding-LSTMs/
- Christopher Olah's publications on the attention mechanism: https://distill.pub/2016/augmented-rnns/
- Andrej Karpathy's blog about RNNs: http://karpathy.github.io/2015/05/21/rnn-effectiveness/
- The Deep Learning Book (Goodfellow et al.): http://www.deeplearningbook.org/

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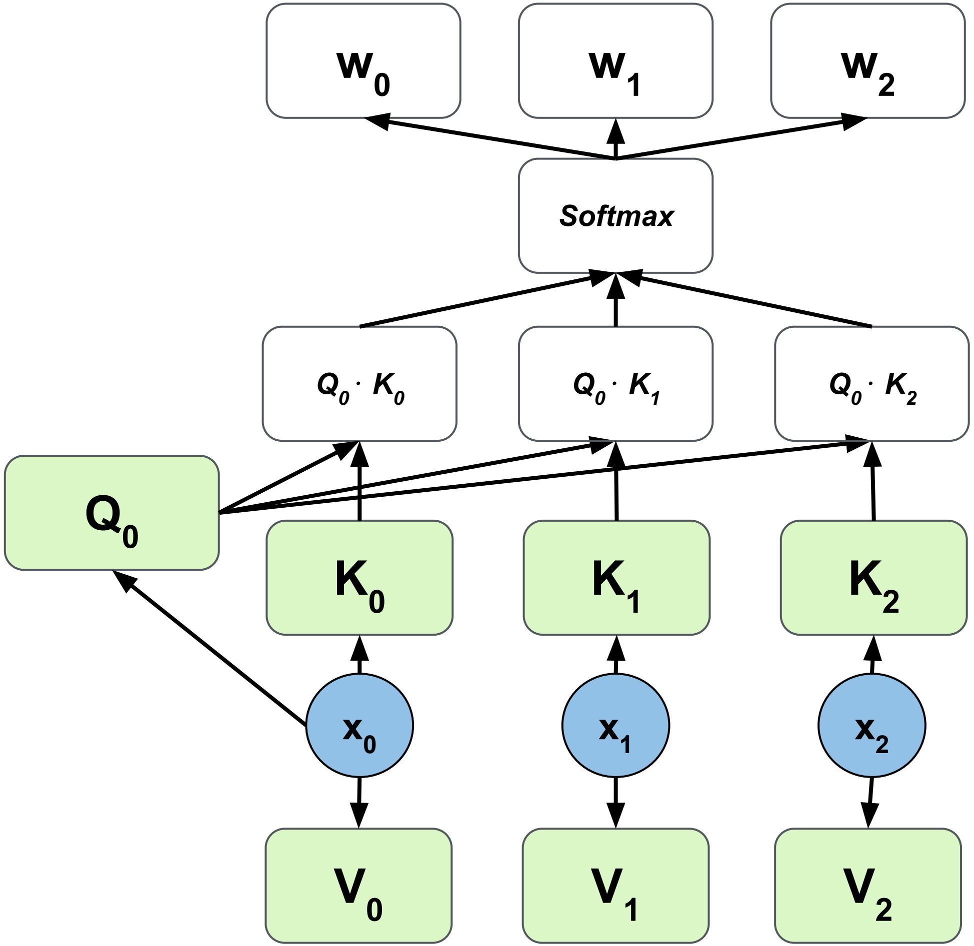
Questions?

Self-Attention

- In reality, every input (x) has 3 different “views”: Q, K, V.
  - Q: query - used to represent the current state (called **s** before).
  - K: keys - used for the dot-product (to compute the weights - called **h** before).
  - V: values - used in the final weighted sum.
- In this example, we are focusing on x_0 .

$$x'_0 = \sum_{i=0}^{n} w_i \cdot V_i$$



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Decoder Probabilities

- Want to maximize:

$$p(y_1, y_2, \ldots, y_n | x)$$

- We can decompose as:

$$p(y_1, y_2, \ldots, y_n | x) = p(y_1 | x)p(y_2, \ldots, y_n | x, y_1)$$

and again:

$$p(y_1, y_2, \ldots, y_n | x) = p(y_1 | x)p(y_2 | x, y_1)p(y_3, \ldots, y_n | x, y_1, y_2)$$

until:

$$p(y_1, y_2, \ldots, y_n | x) = p(y_1 | x)p(y_2 | x, y_1) \ldots p(y_n | x, y_1, \ldots y_{n-1})$$

Results - Seq2Seq W/ and W/O Attention

Model	Max sequence length	BLEU score
Seq2seq	30	13.9
Seq2seq + attention	30	**21.5**
Seq2seq	50	17.8
Seq2seq + attention	50	**26.7**

- The BLEU score (BiLingual Evaluation Understudy) measures the quality of the translation (the higher the score the better).
  - BLEU is a modified form of the Precision metric based on the overlap between output and target.
- Attention improves the score significantly.

Bahdanau et al., Neural Machine Translation by Jointly Learning to Align and Translate

Results - Transformer

- Better results than previous systems (left column)...
- … with a fraction of the training cost (right column).

Model	BLEU		Training cost (FLOP)	
	EN-DE	EN_FR	EN-DE	EN_FR
GNMT (RNNs)	24.6	39.92	$2.3*10^{19}$	$1.4*10^{20}$
Transformer (base)	27.3	38.1	$3.3*10^{18}$	
Transformer (big)	28.4	41.0	$2.3*10^{19}$	

- BLEU score (BiLingual Evaluation Understudy): the higher the score the better.

Self-Attention - Word Order

- The (weighted) sum leads to the loss of the elements' order.
  - E.g., $w_0 \cdot x_0 + w_1 \cdot x_1 = w_1 \cdot x_1 + w_0 \cdot x_0$
- Solution: attach the position information to every word.
  - E.g., $x'_0 = [x_0 + p_0]$, $x'_1 = [x_1 + p_1]$
- Now the order of the elements has an impact on the results:

$$w_0 \cdot [x_0 + p_0] + w_1 \cdot [x_1 + p_1] \neq w_1 \cdot [x_1 + p_0] + w_0 \cdot [x_0 + p_1]$$

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