Quebec
Artificial
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# 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**
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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.

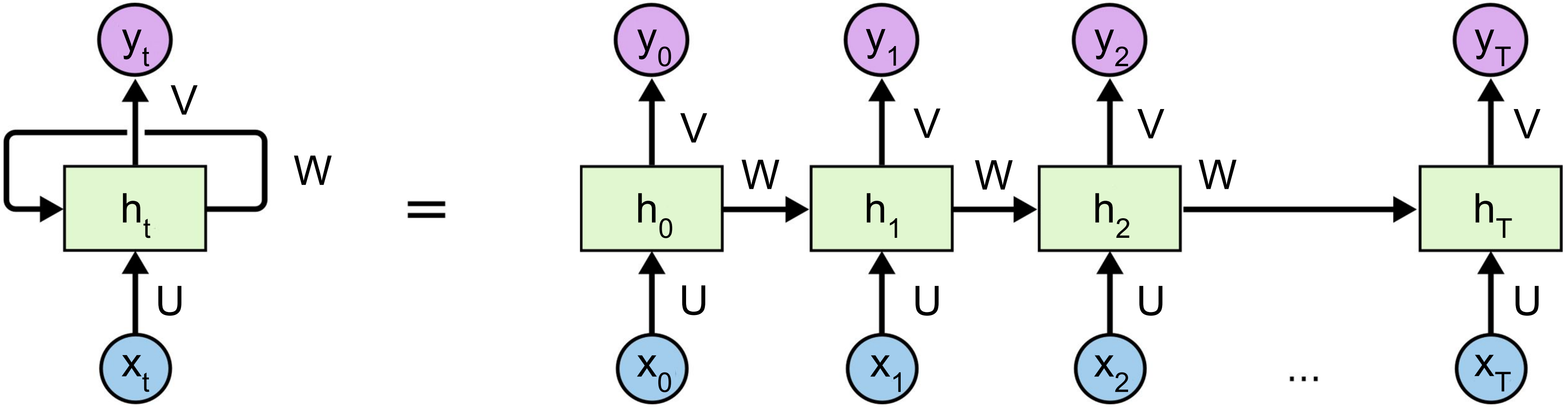



Image from Christopher Olah's blog

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:

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

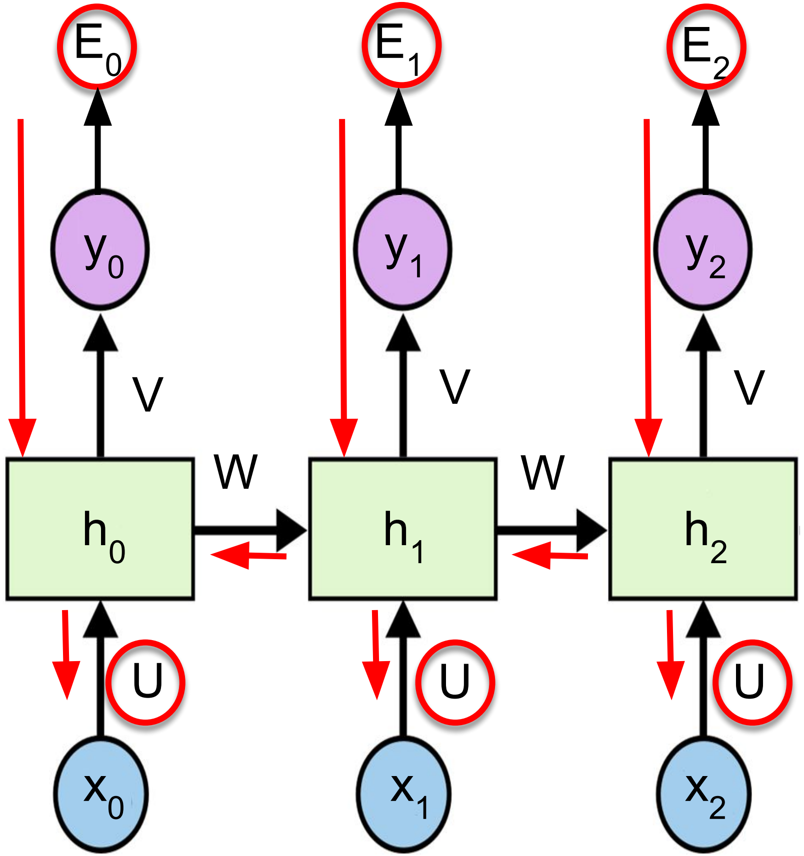



Image from Christopher Olah's blog

# 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

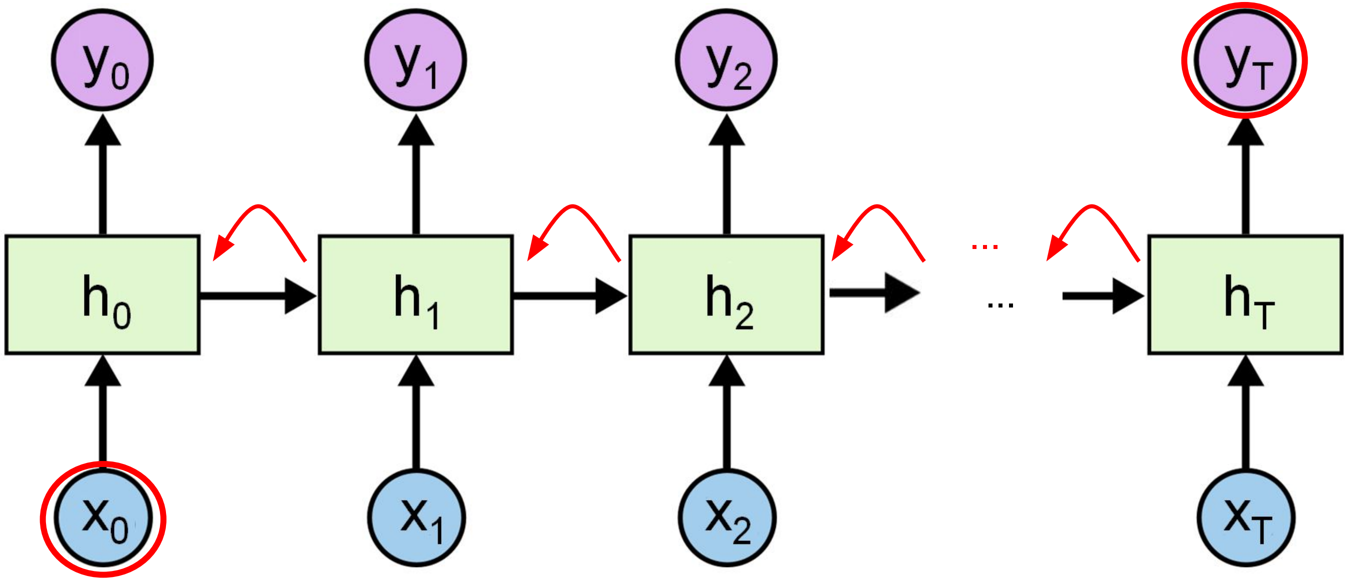
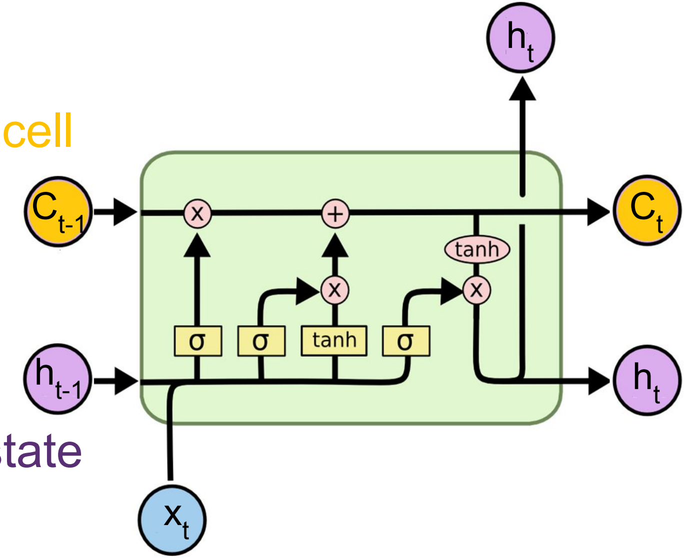



Image from Christopher Olah's blog

# Long Short-Term Memory (LSTM)

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

Memory cell



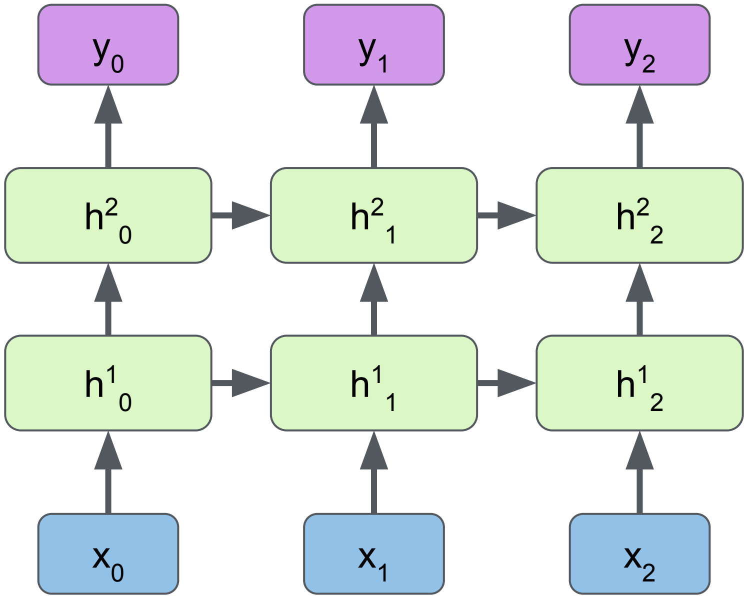

Internal state

$$i_t = \sigma(U_i x_t + W_i h_{t-1} + b_i)$$
$$f_t = \sigma(U_f x_t + W_f h_{t-1} + b_f)$$
$$o_t = \sigma(U_o x_t + W_o h_{t-1} + b_o)$$
$$g_t = tanh(U_g x_t + W_g h_{t-1} + b_g)$$
$$C_t = i_t \times g_t + f_t \times C_{t-1}$$
$$h_t = o_t \times tanh(C_t)$$

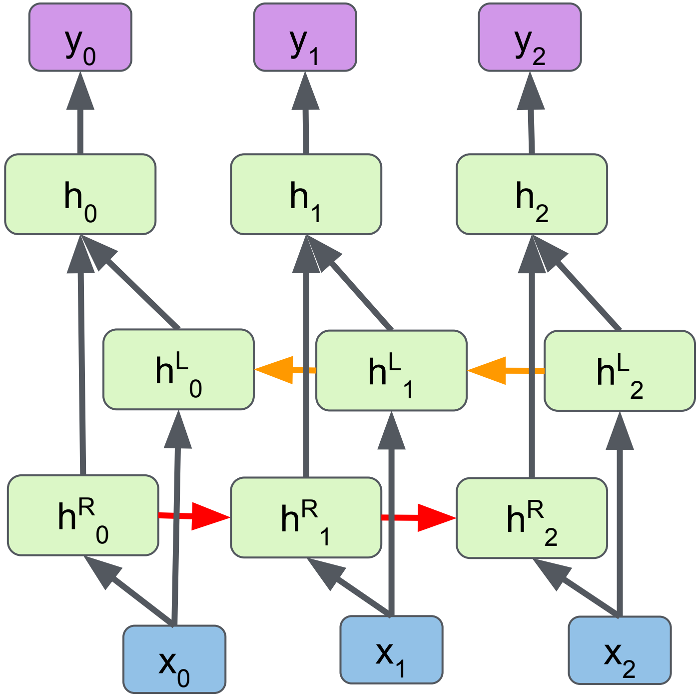
Image from Christopher Olah's blog

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

# Multi-Layer and Bidirectional RNNs




Layers of RNNs




Bidirectional RNNs

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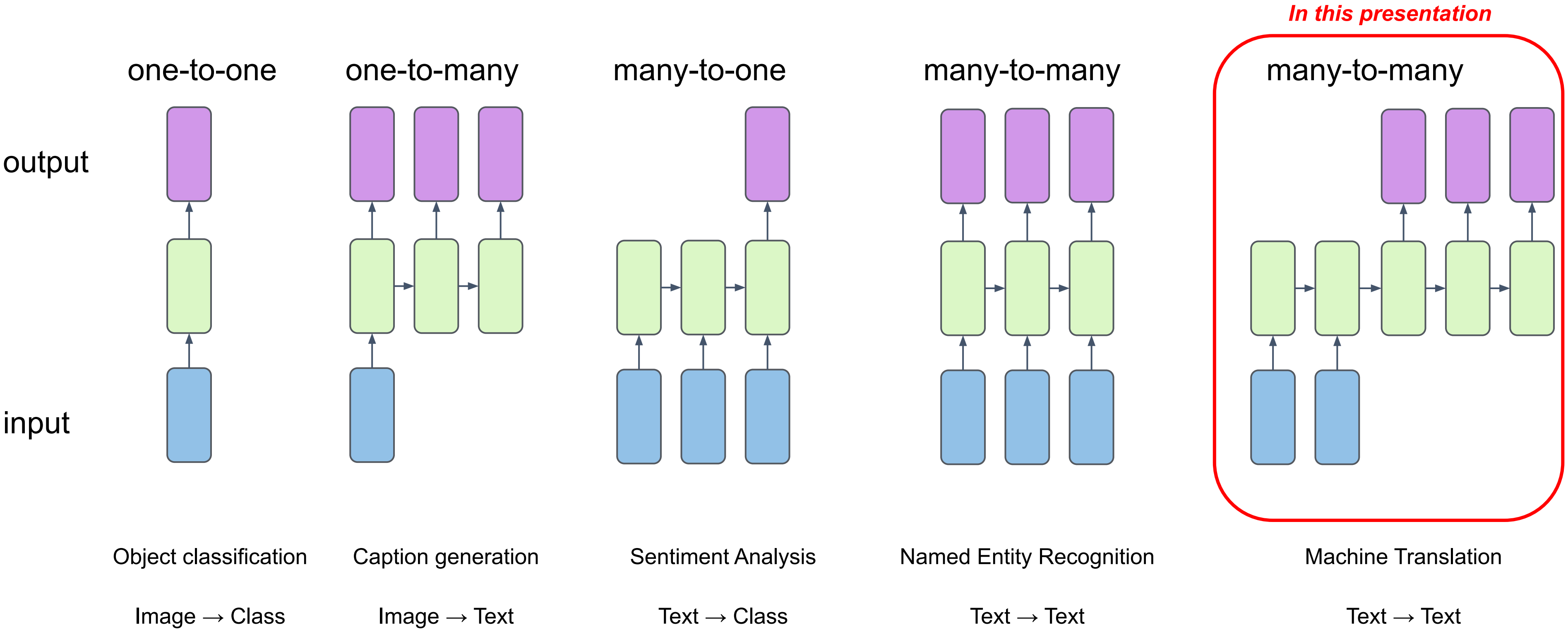
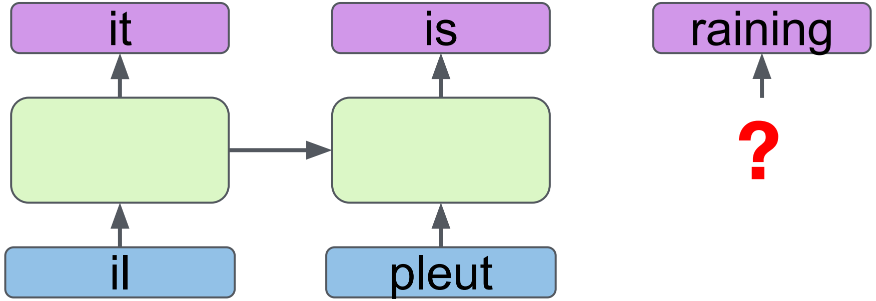
# Modeling Sequences



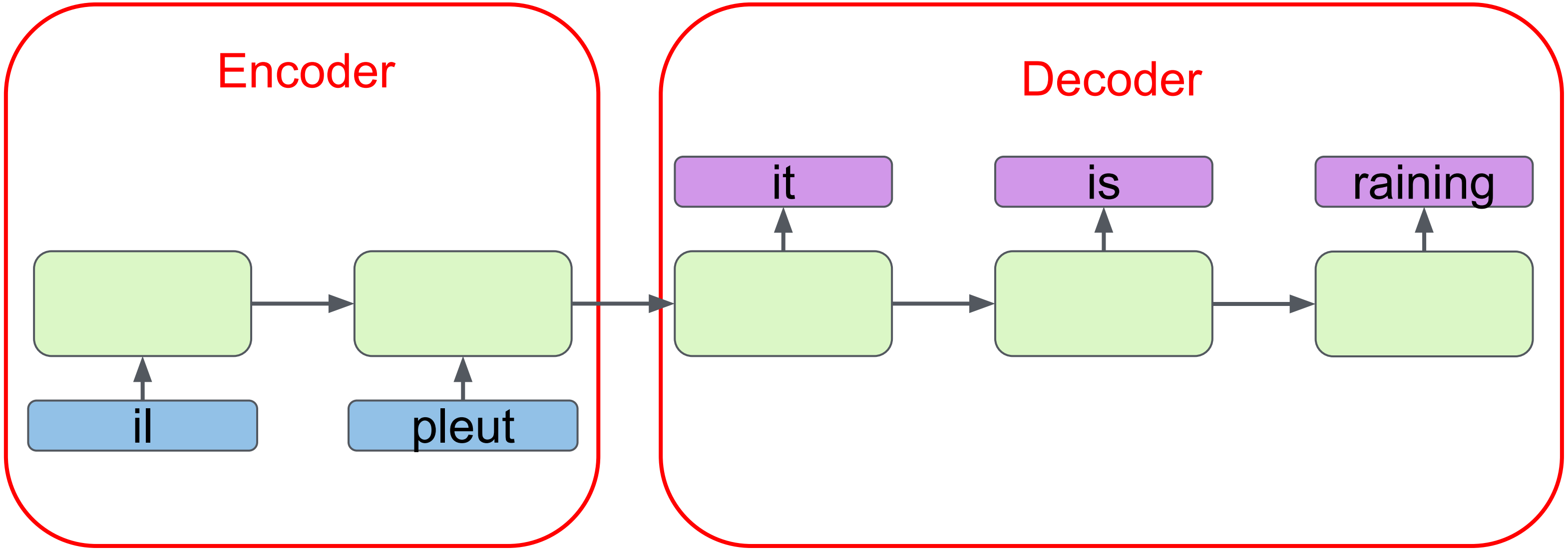
# Modeling Sequences

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



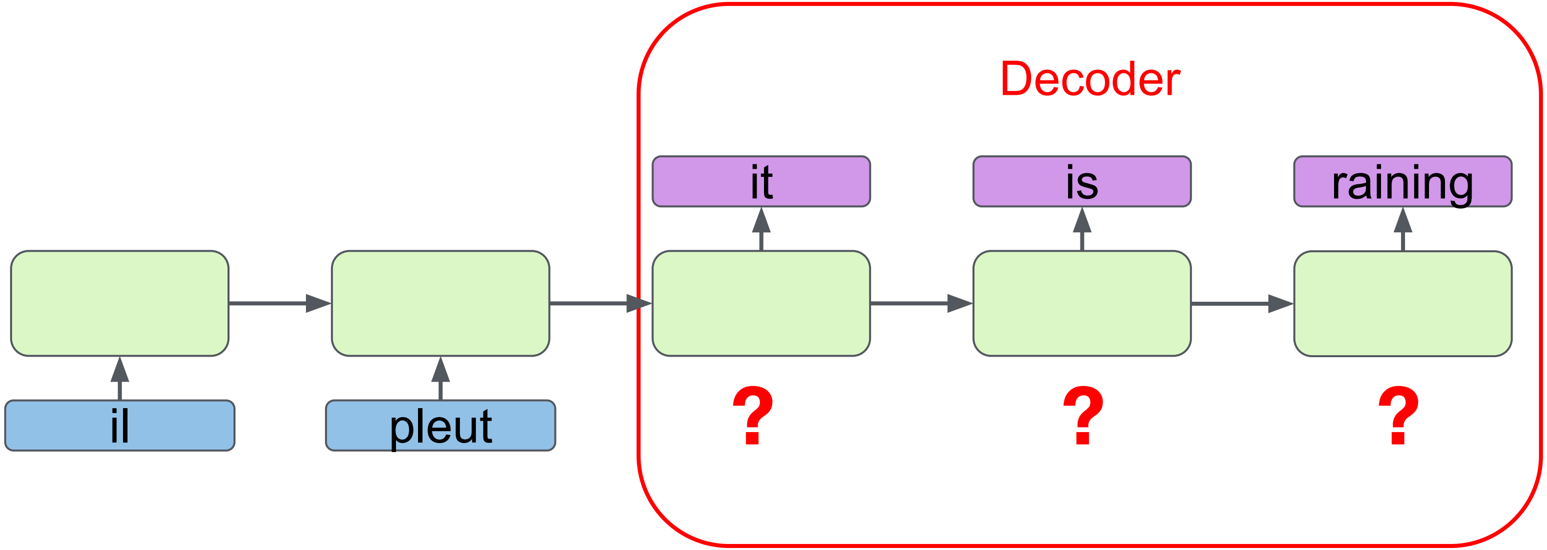
# Different input-output sequence sizes

- 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.



# 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.



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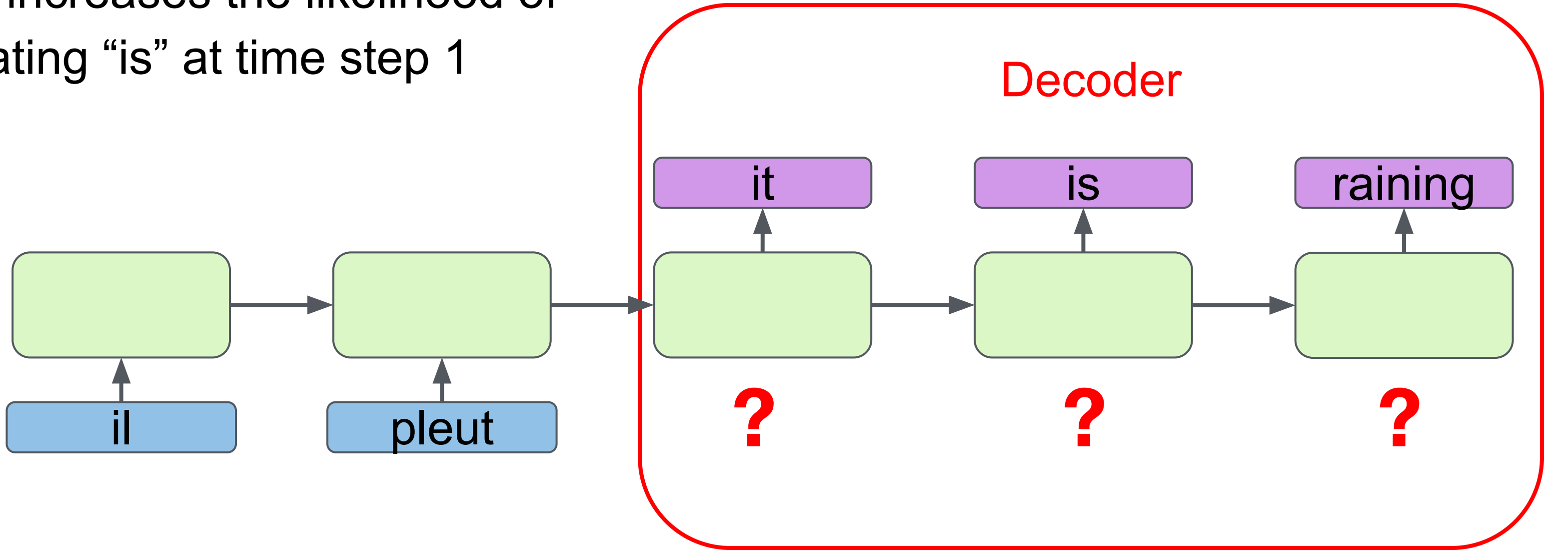
# Different input-output sequence sizes

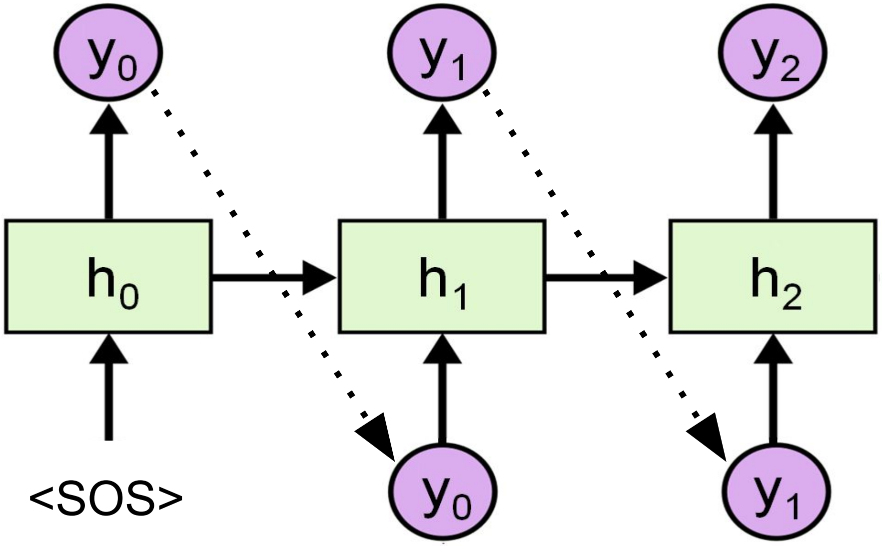
Example: knowing that the decoder generated “it” at time step 0 increases the likelihood of generating “is” at time step 1



# Autoregressive RNNs

<SOS> *Start of sequence*

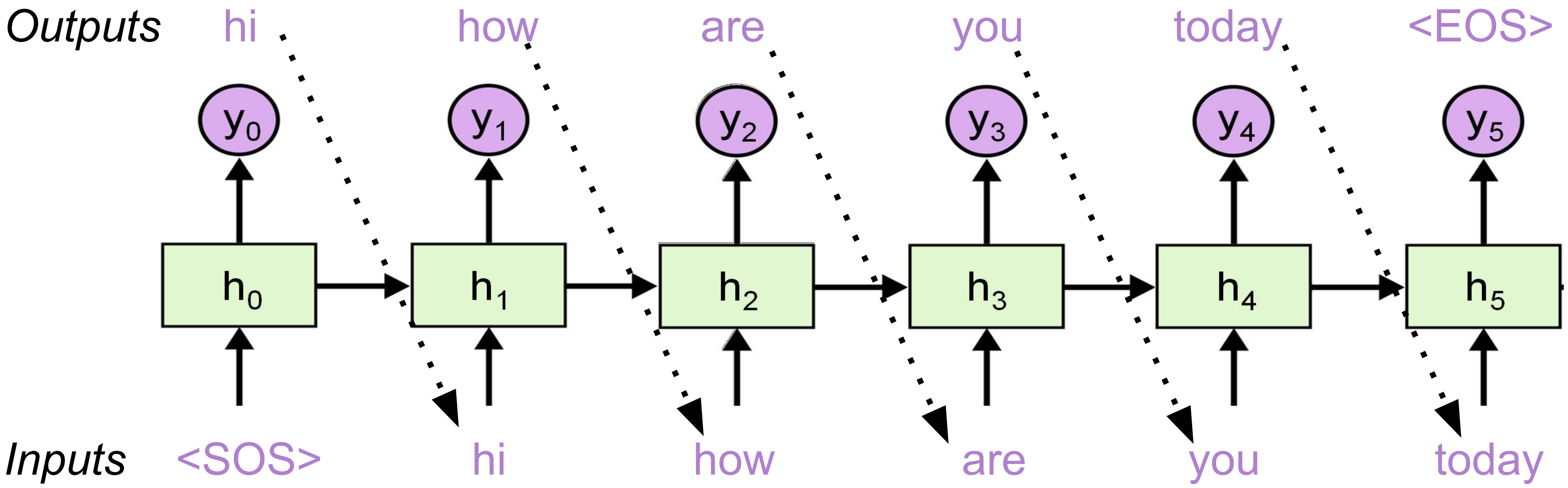
- We can use a RNN to **generate** a sequence.
- In order to generate consistent outputs across time, we can condition each output on previously generated outputs.
- Such a model is called **autoregressive**.



# Autoregressive RNNs

*<SOS> Start of sequence*

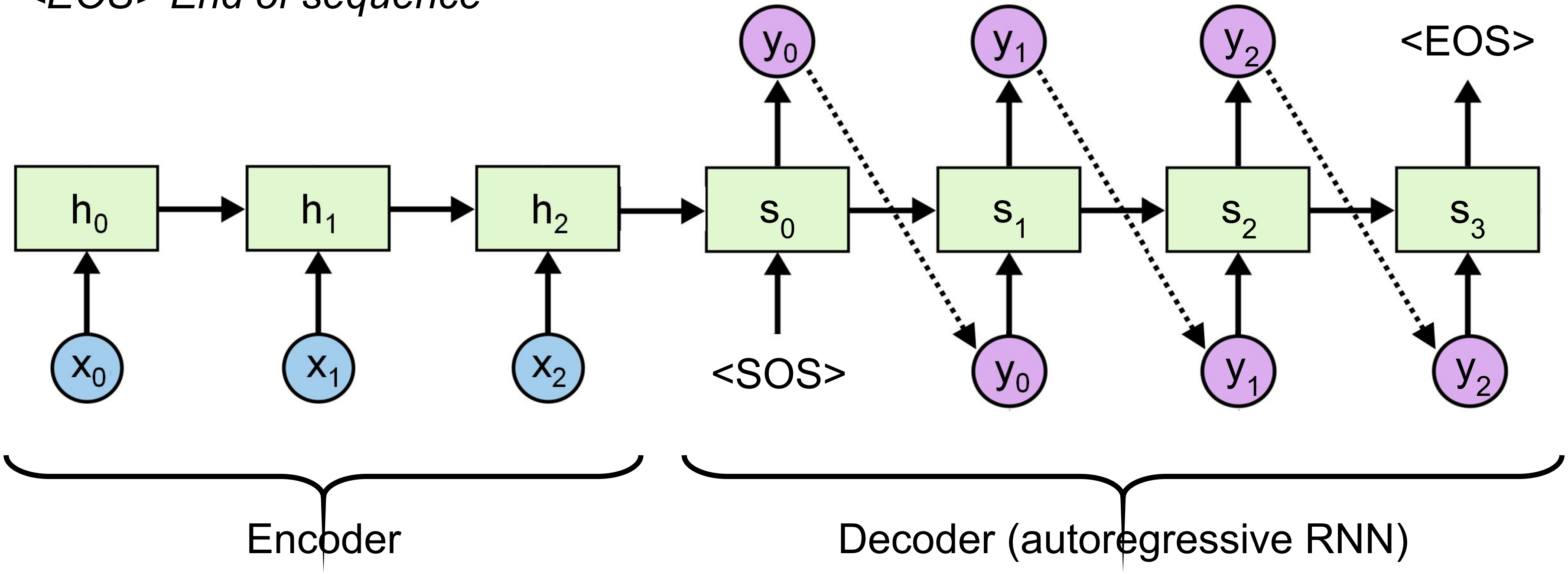
*<EOS> End of sequence*



# Sequence-to-Sequence Models

*<SOS> Start of sequence*

*<EOS> End of sequence*



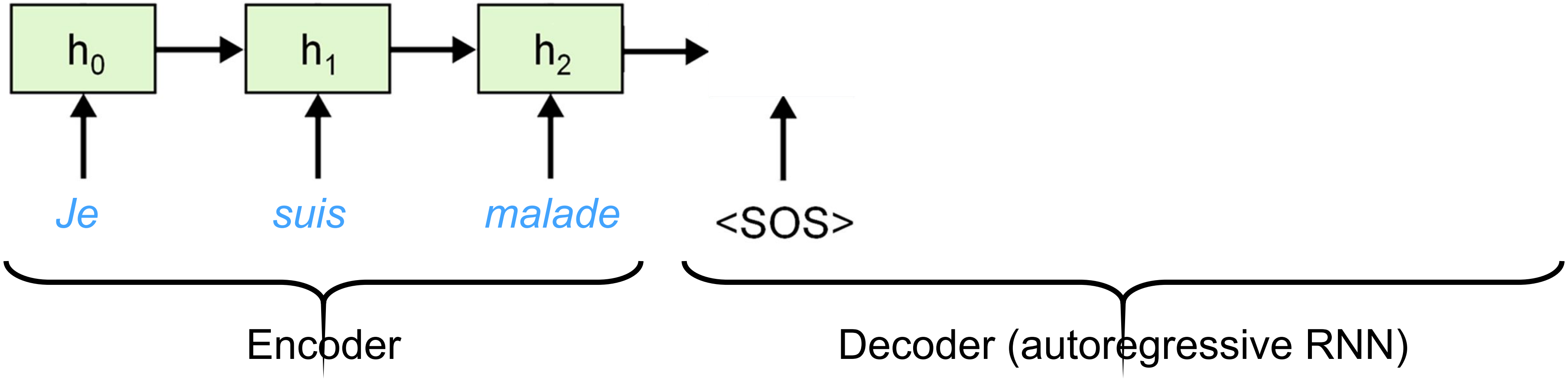

Sutskever et al., Sequence to Sequence Learning with Neural Networks

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

# Sequence-to-Sequence Models - Example

<SOS> Start of sequence

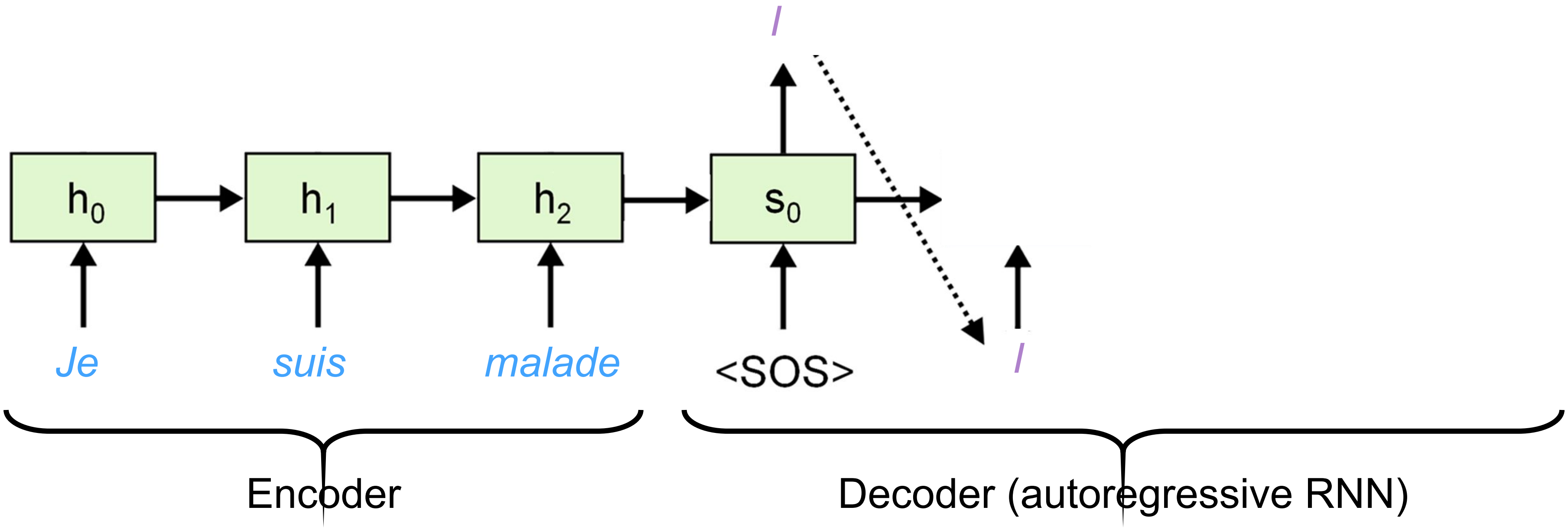
<EOS> End of sequence



# Sequence-to-Sequence Models - Example

<SOS> Start of sequence

<EOS> End of sequence



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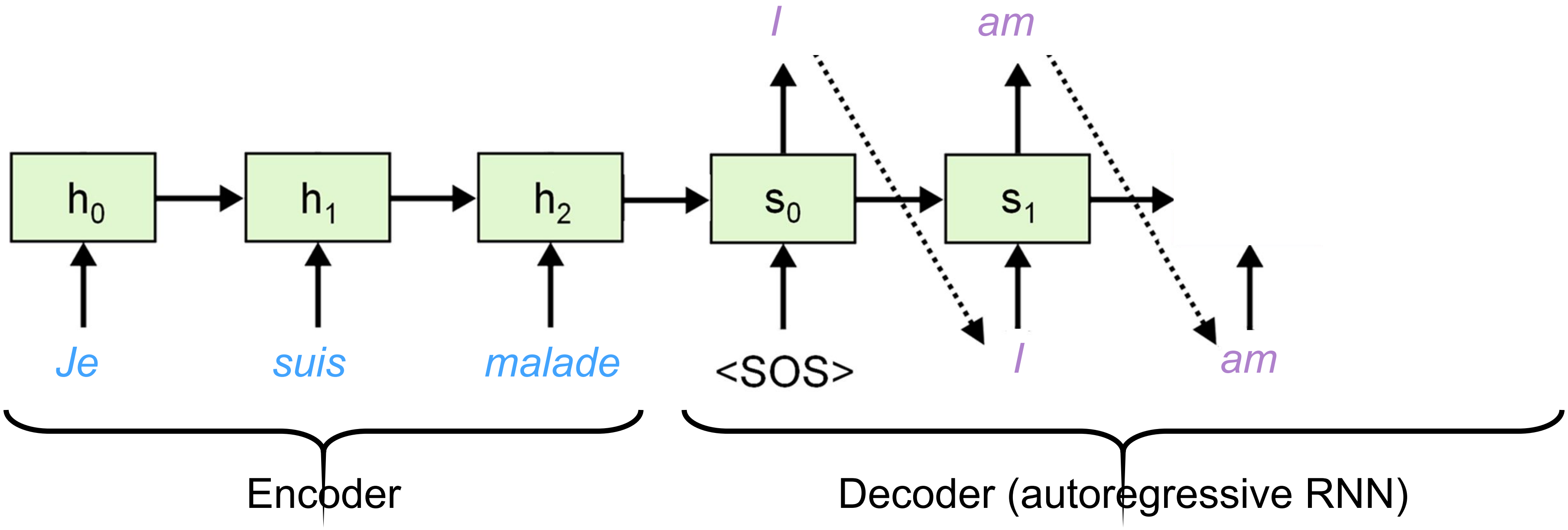
# Sequence-to-Sequence Models - Example

<SOS> Start of sequence

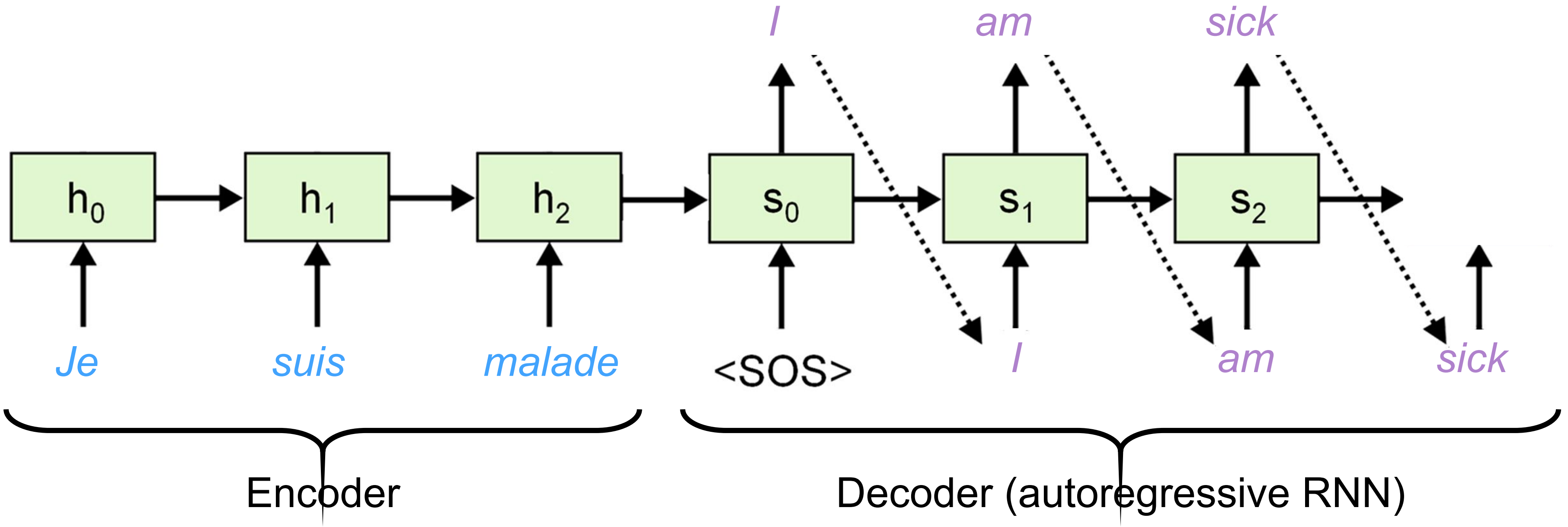
<EOS> End of sequence



# Sequence-to-Sequence Models - Example

<SOS> Start of sequence

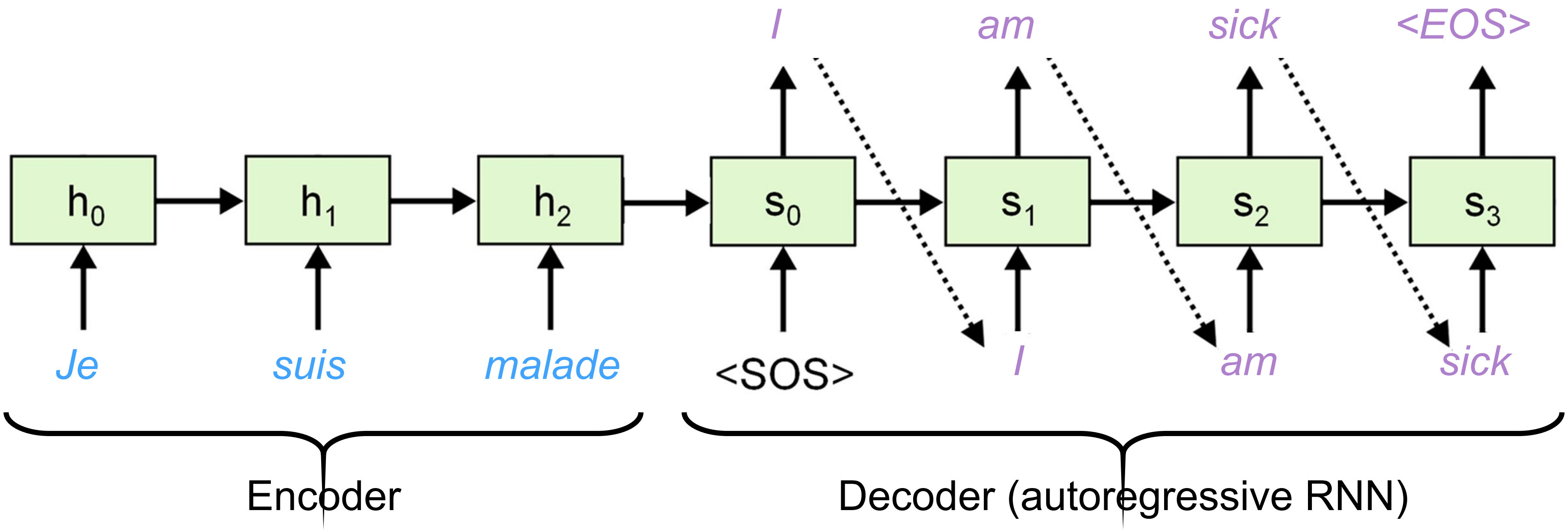
<EOS> End of sequence



# Sequence-to-Sequence Models - Example

<SOS> Start of sequence

<EOS> End of sequence



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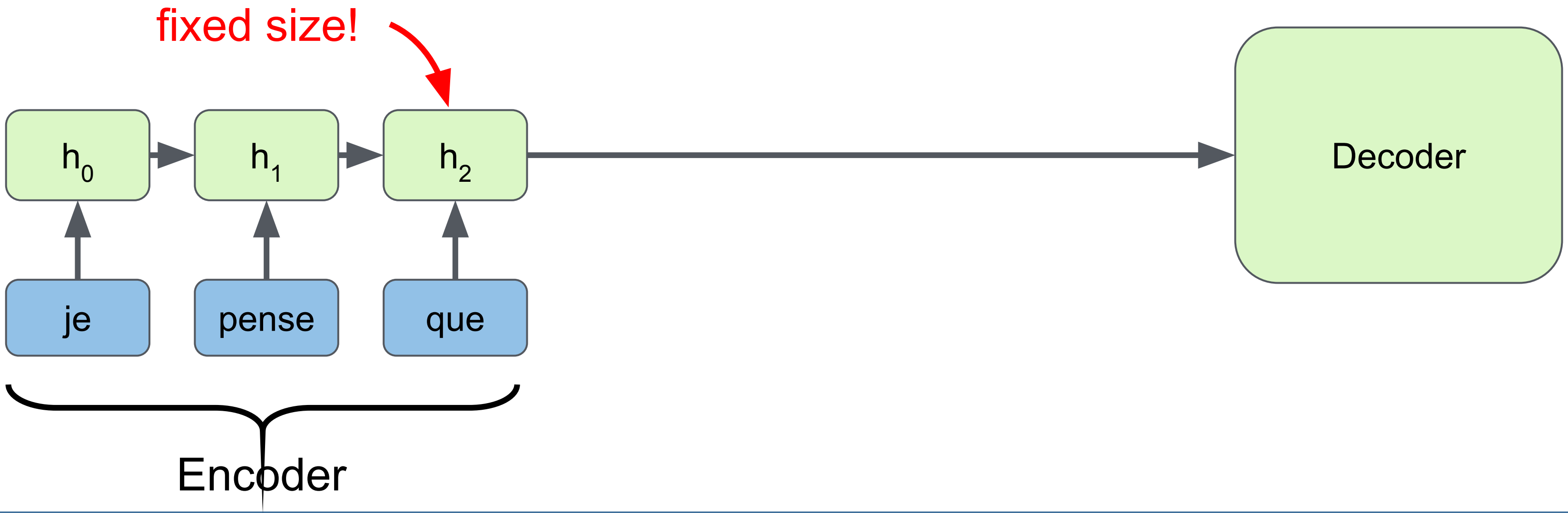
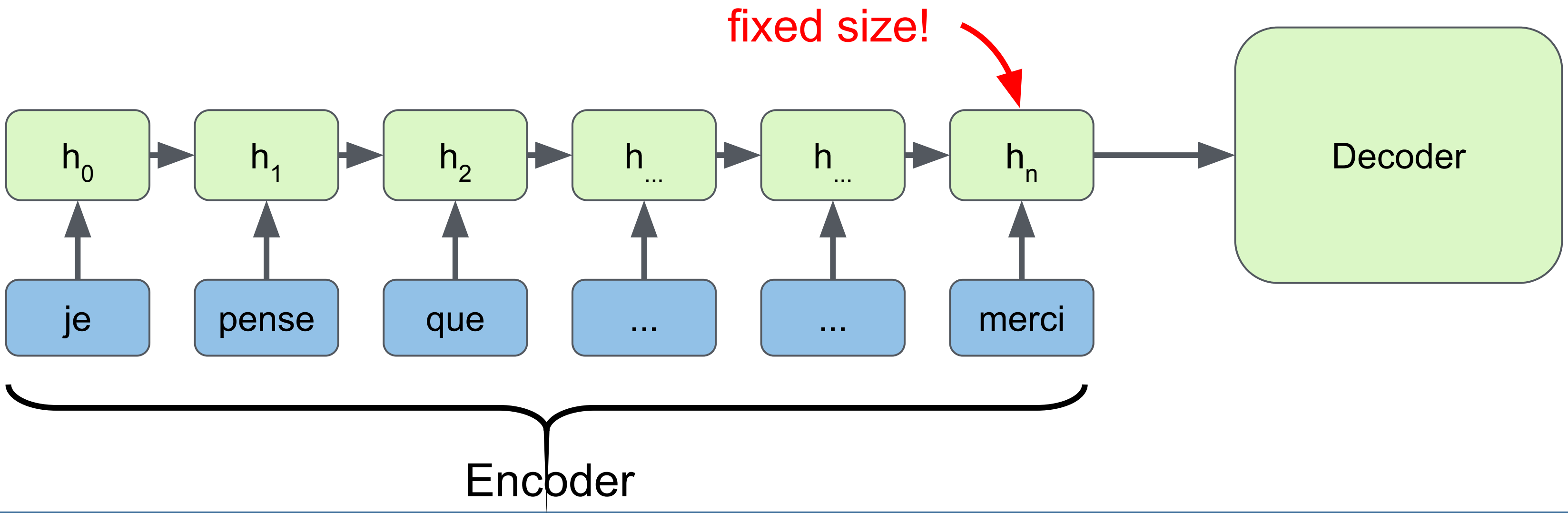
# Sequence-to-Sequence Models - Bottleneck

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



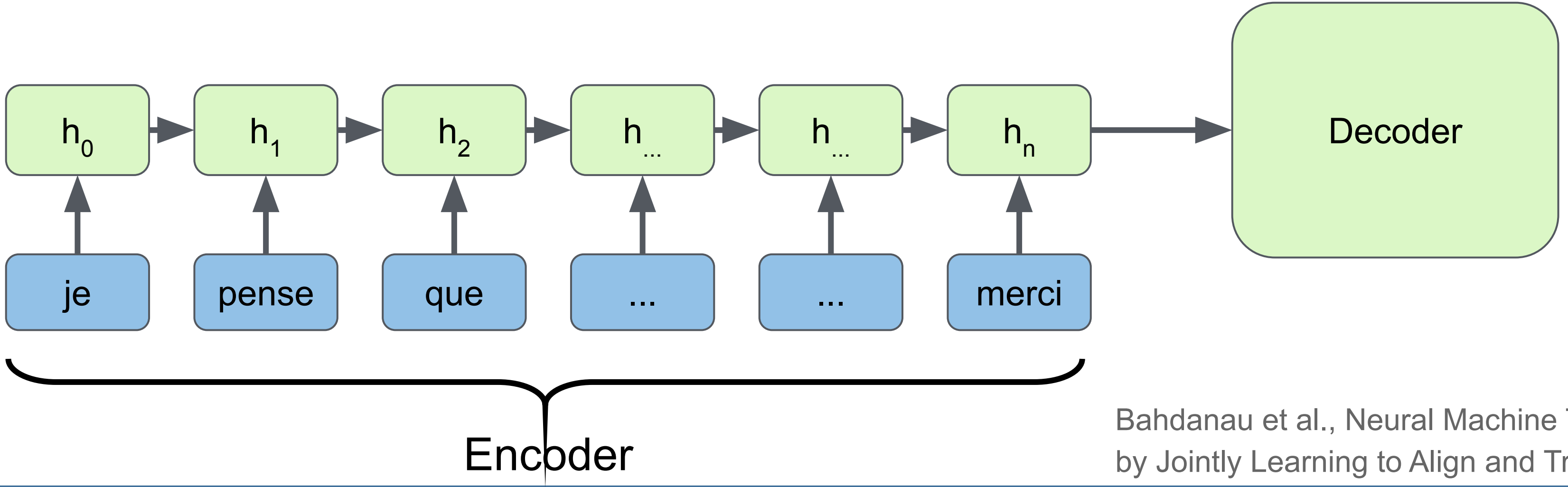
# Sequence-to-Sequence Models - Bottleneck

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



# Attention Mechanism

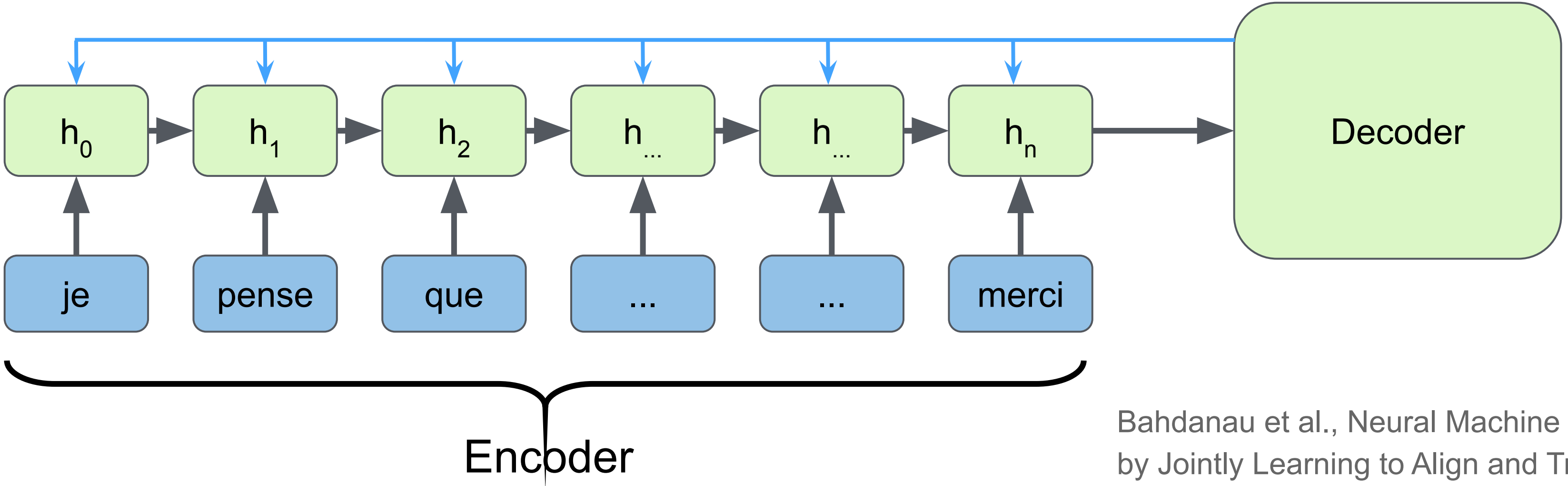
- Problem: it is not easy to store all the necessary information from an **arbitrary long** sequence into a **fixed-size** vector.




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

# Attention Mechanism

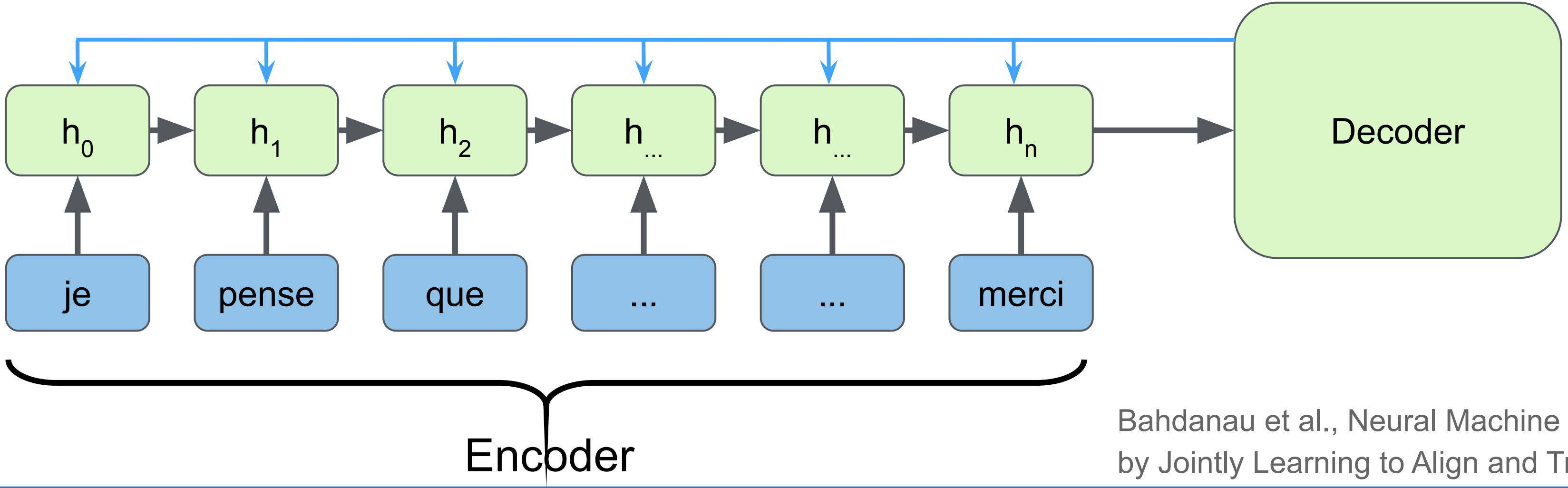
- Problem: it is not easy to store all the necessary information from an **arbitrary long** sequence into a **fixed-size** vector.
- A possible solution can be to allow the decoder to “selectively look back” at the encoded input sequence.




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

# Attention Mechanism

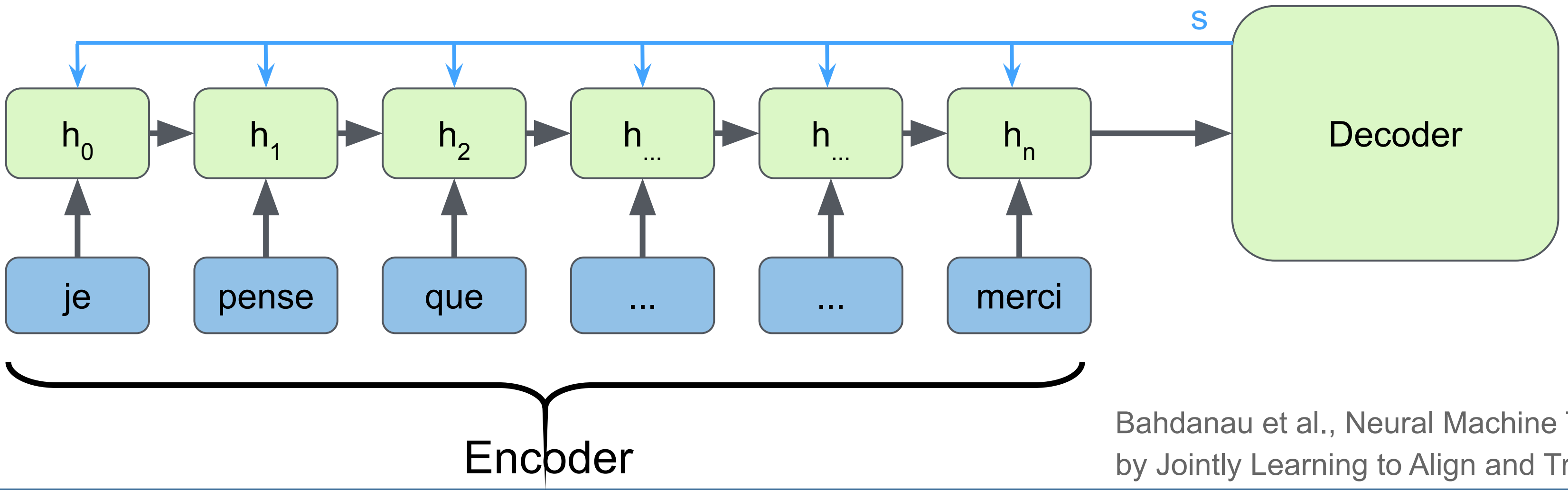
- This can be done with **attention**:
  - At any decoding time step, the decoder can use attention to fetch the relevant information for that step from the encoded input sequence.
- E.g., when producing the output word “think” (in a machine translation task), the decoder can focus on the encoding of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




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

# Attention Mechanism - Formalization

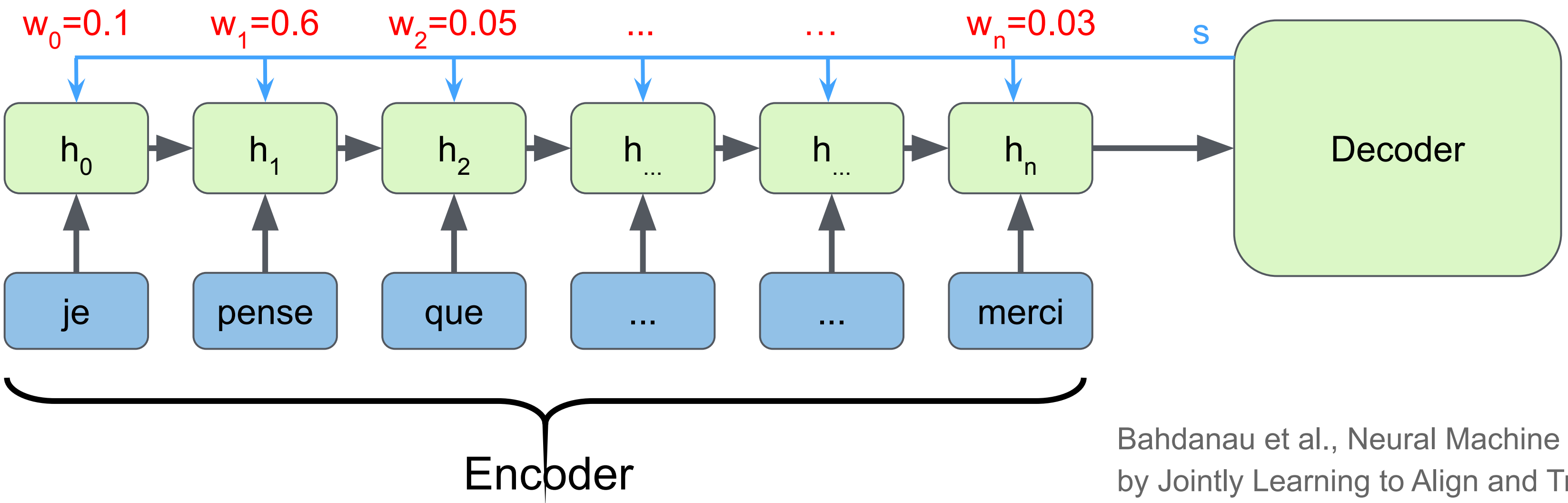
- Attention is a function **A** that, given a decoder state **s** and an encoded input sequence **h**, identifies the elements in **h** that are important at the current decoding time step.




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

# 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).

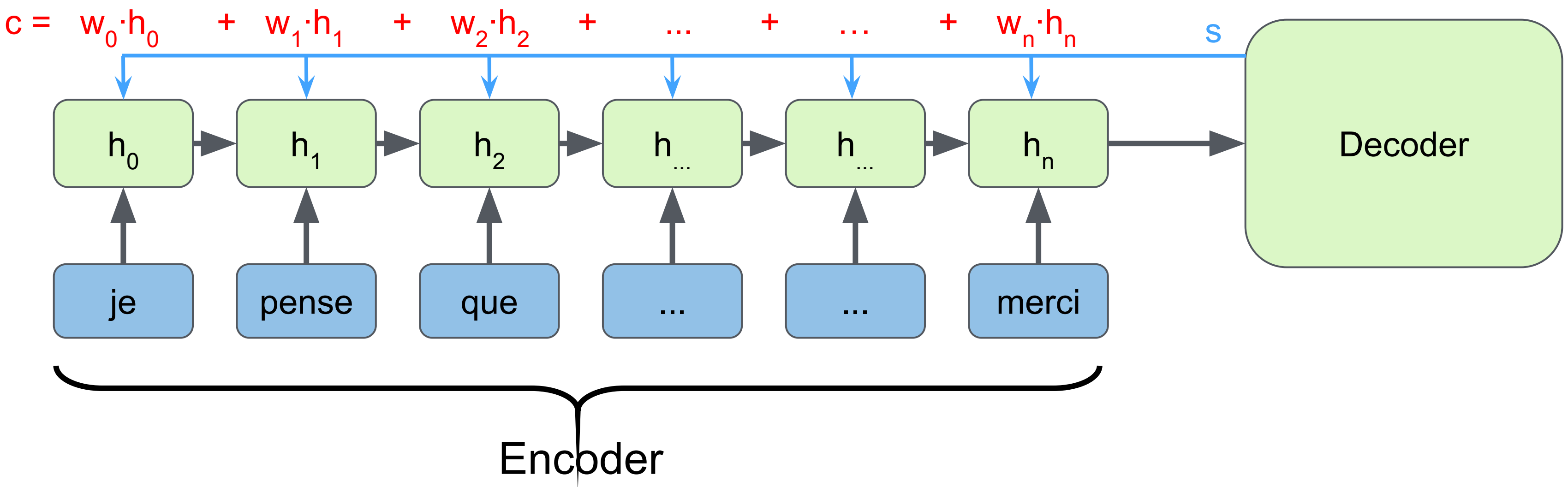



Bahdanau et al., Neural Machine Translation by Jointly Learning to Align and Translate

# Attention Mechanism - Formalization

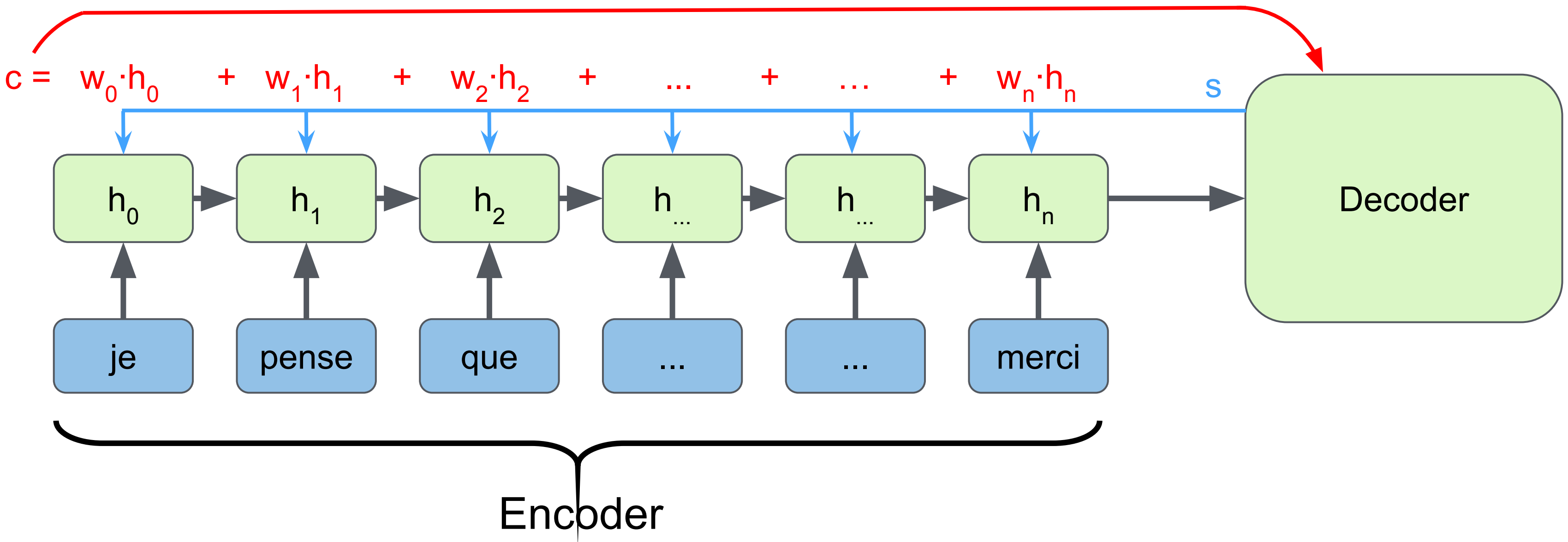
- The weights **w** are used to compute a weighted sum **c** of the elements in the sequence **h**. **c** is called **context vector**.

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



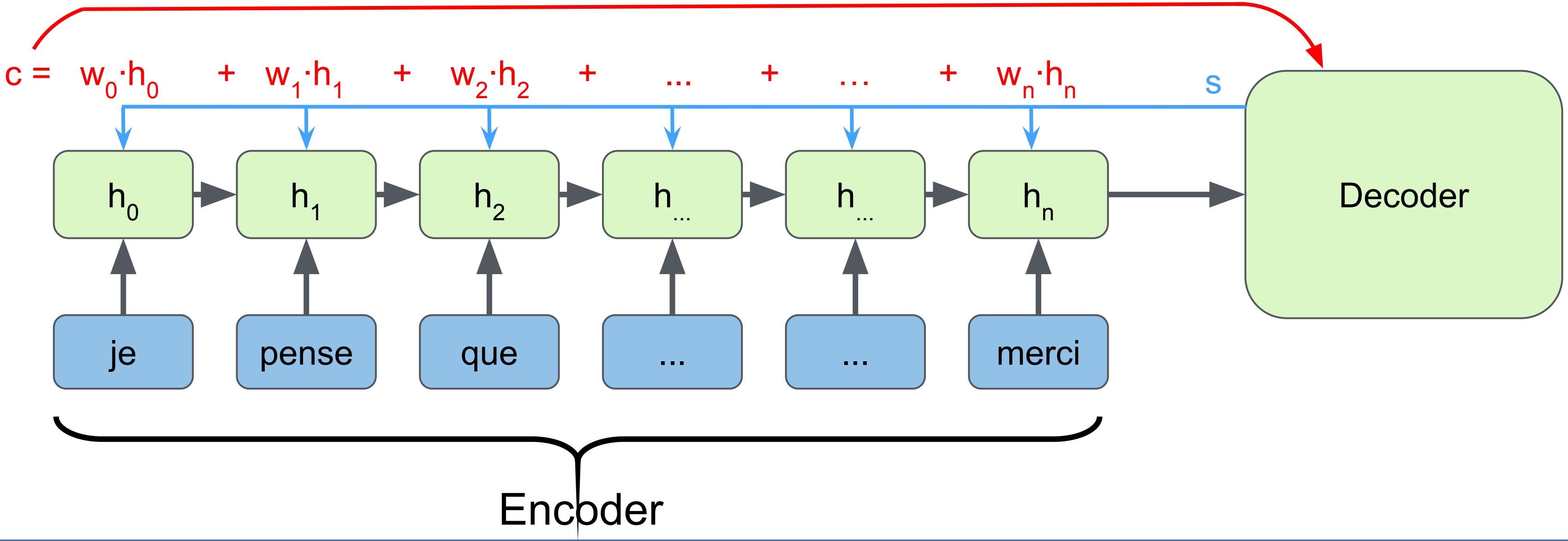
# Attention Mechanism - Formalization

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



# Attention Mechanism - Formalization

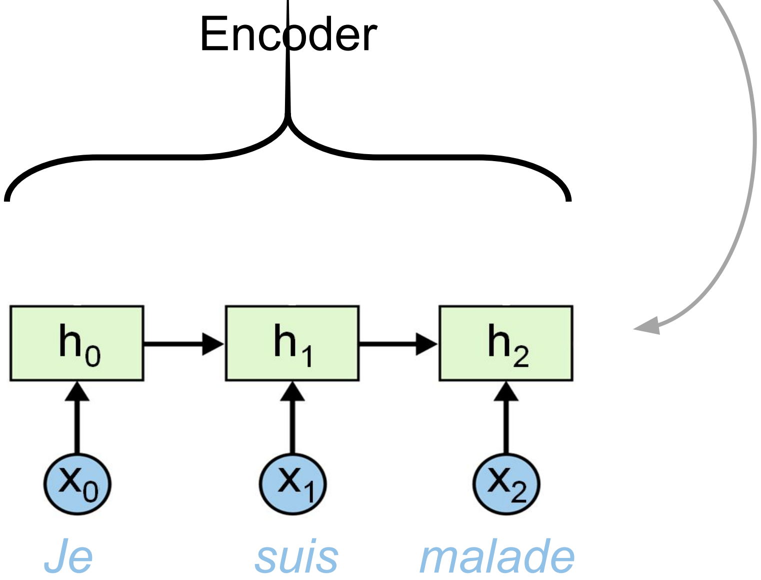
- Let's see a full step-by-step example of the attention mechanism.
- We will then look at how to implement the function **A**.



# Example: Sequence-to-Sequence + Attention

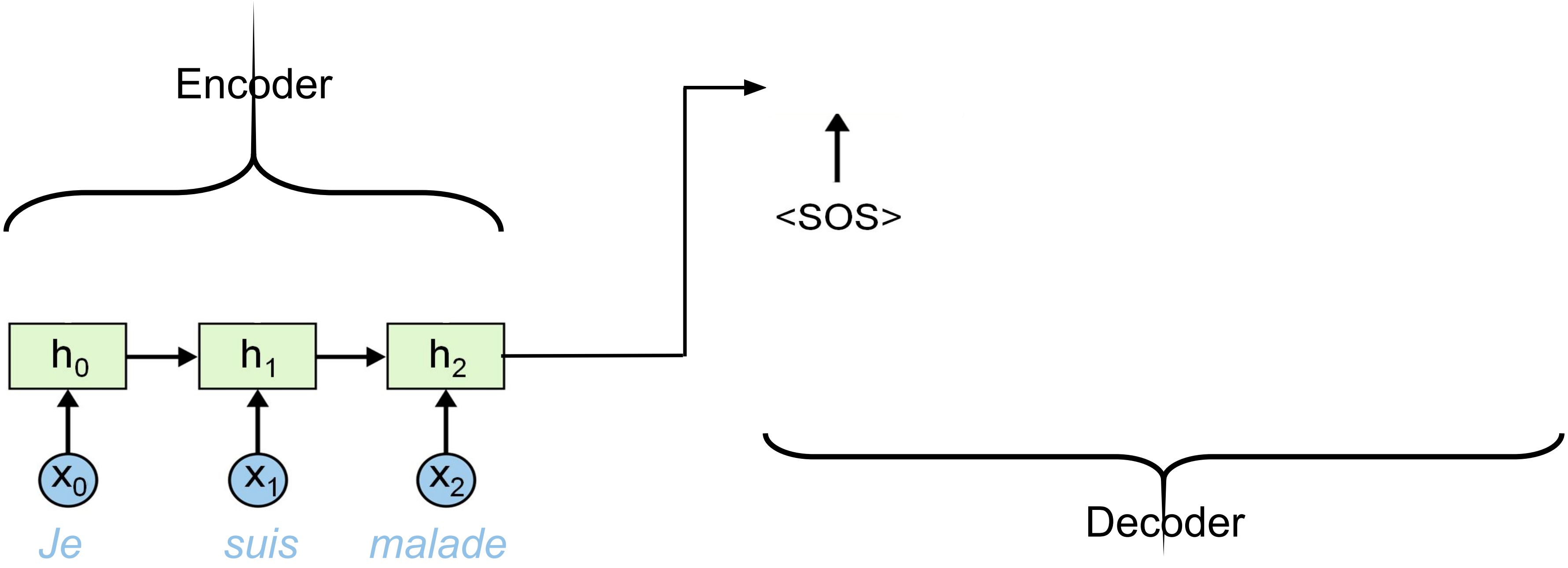
# Example: Sequence-to-Sequence + Attention

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



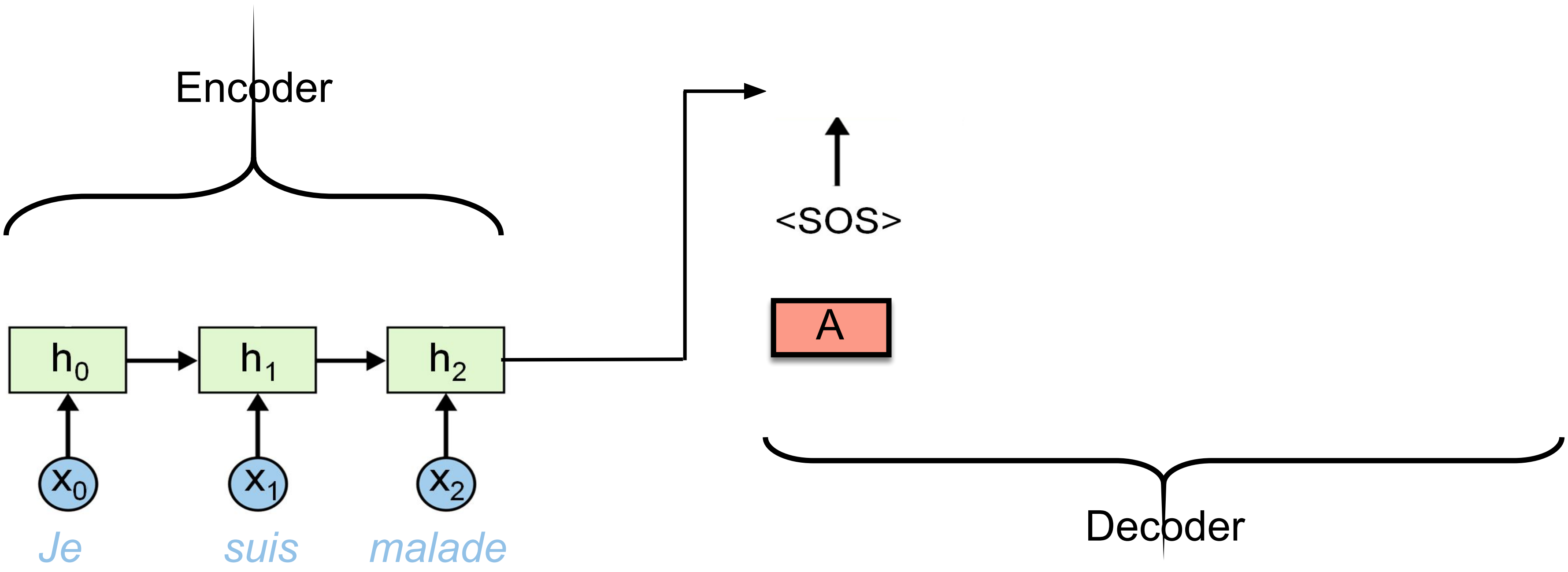
# Example: Sequence-to-Sequence + Attention

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



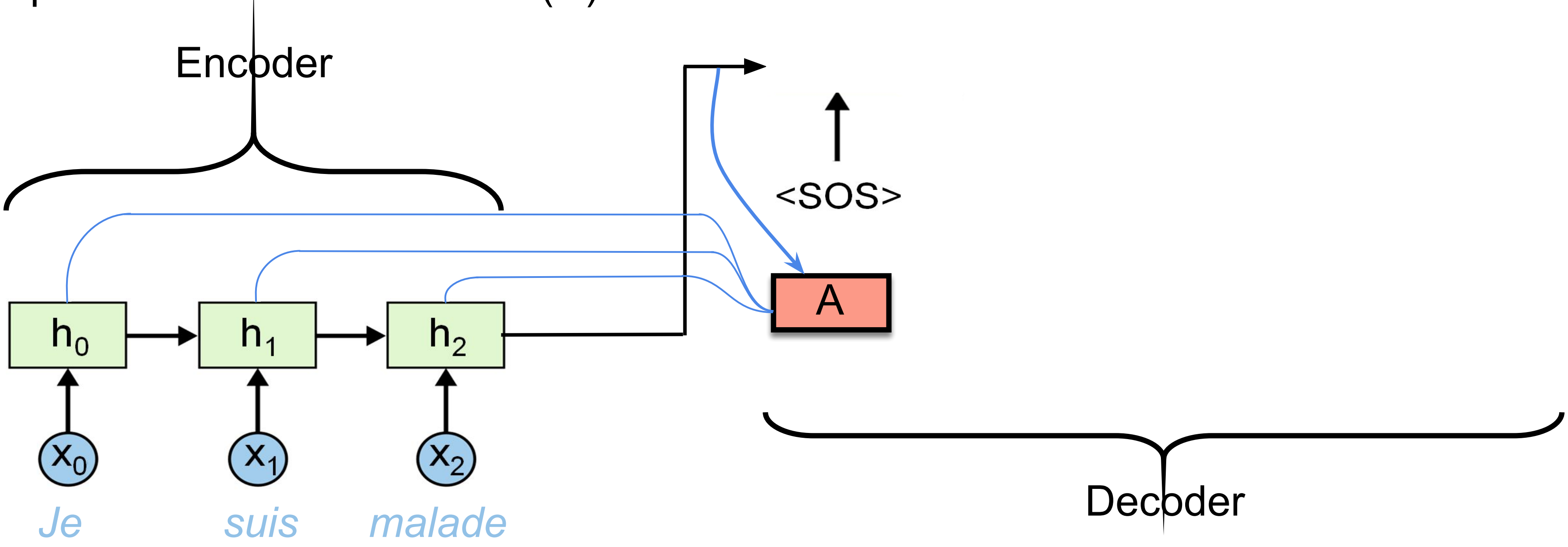
# Example: Sequence-to-Sequence + Attention

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



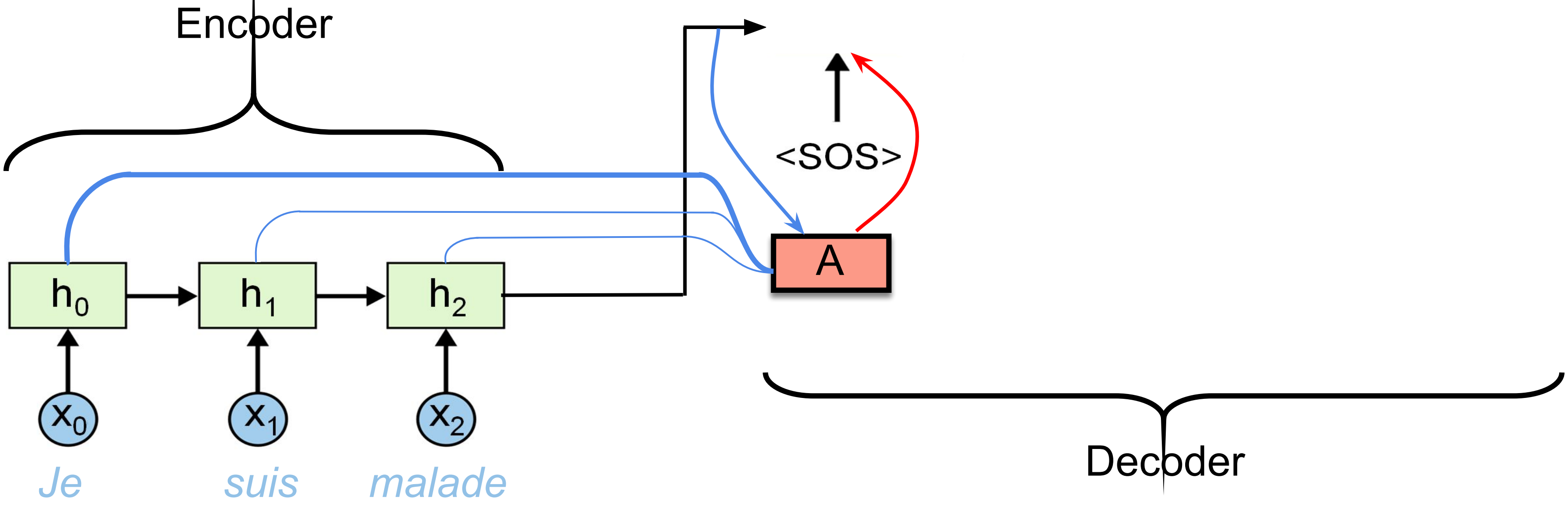
# Example: Sequence-to-Sequence + Attention

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



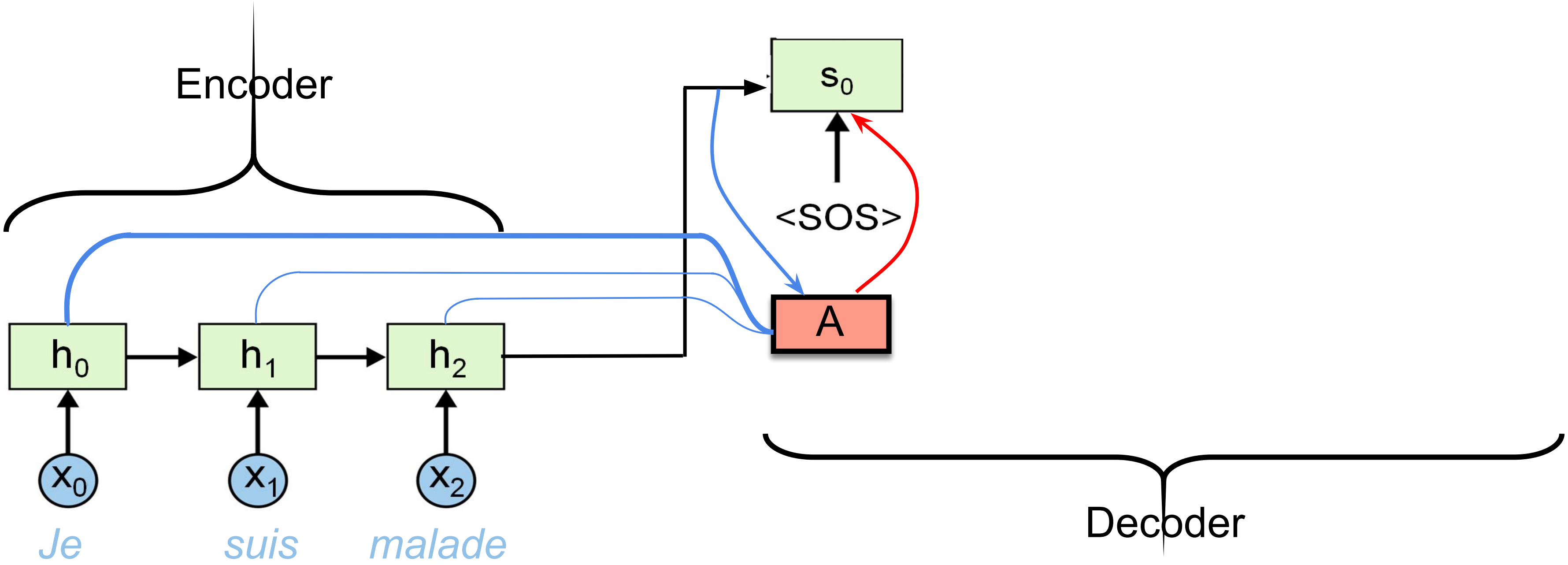
# Example: Sequence-to-Sequence + Attention

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



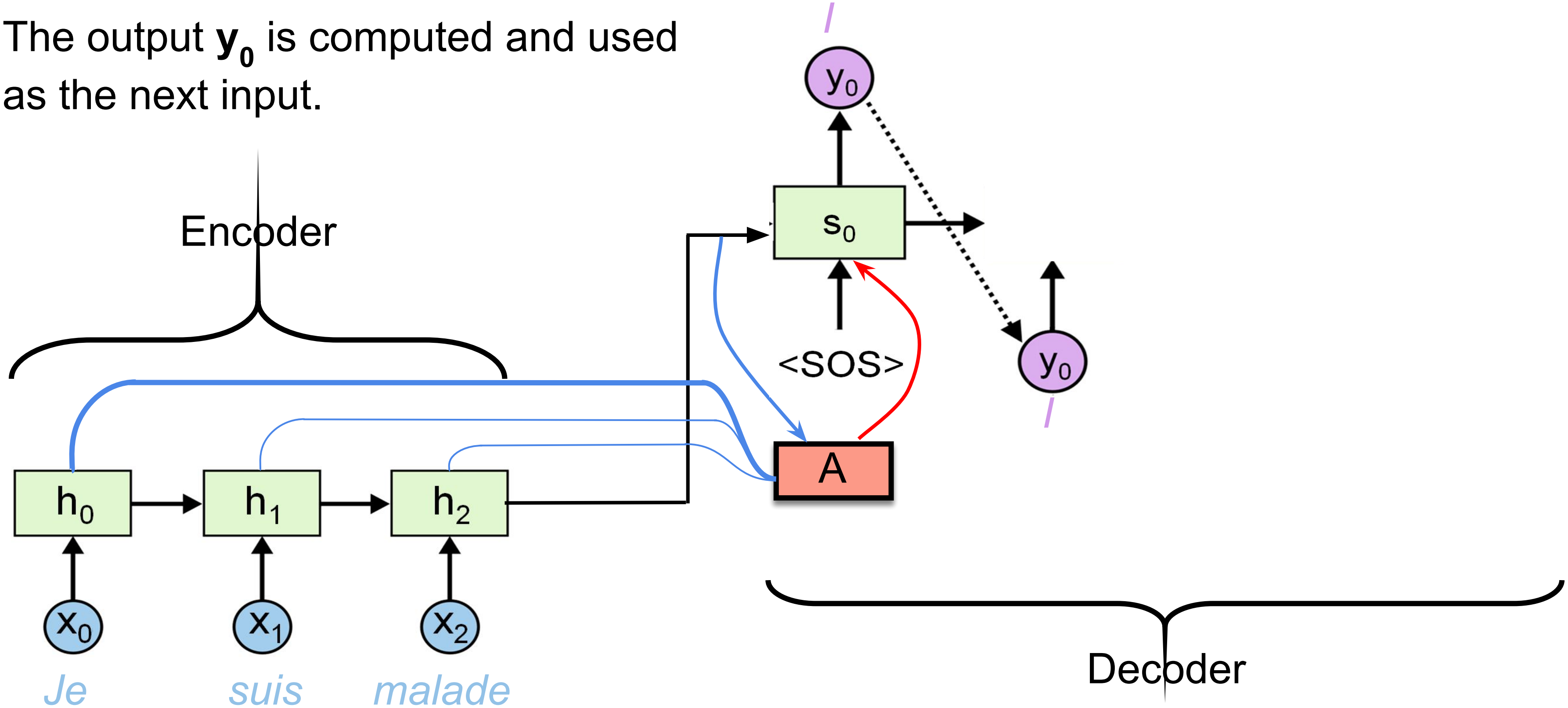
# Example: Sequence-to-Sequence + Attention

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

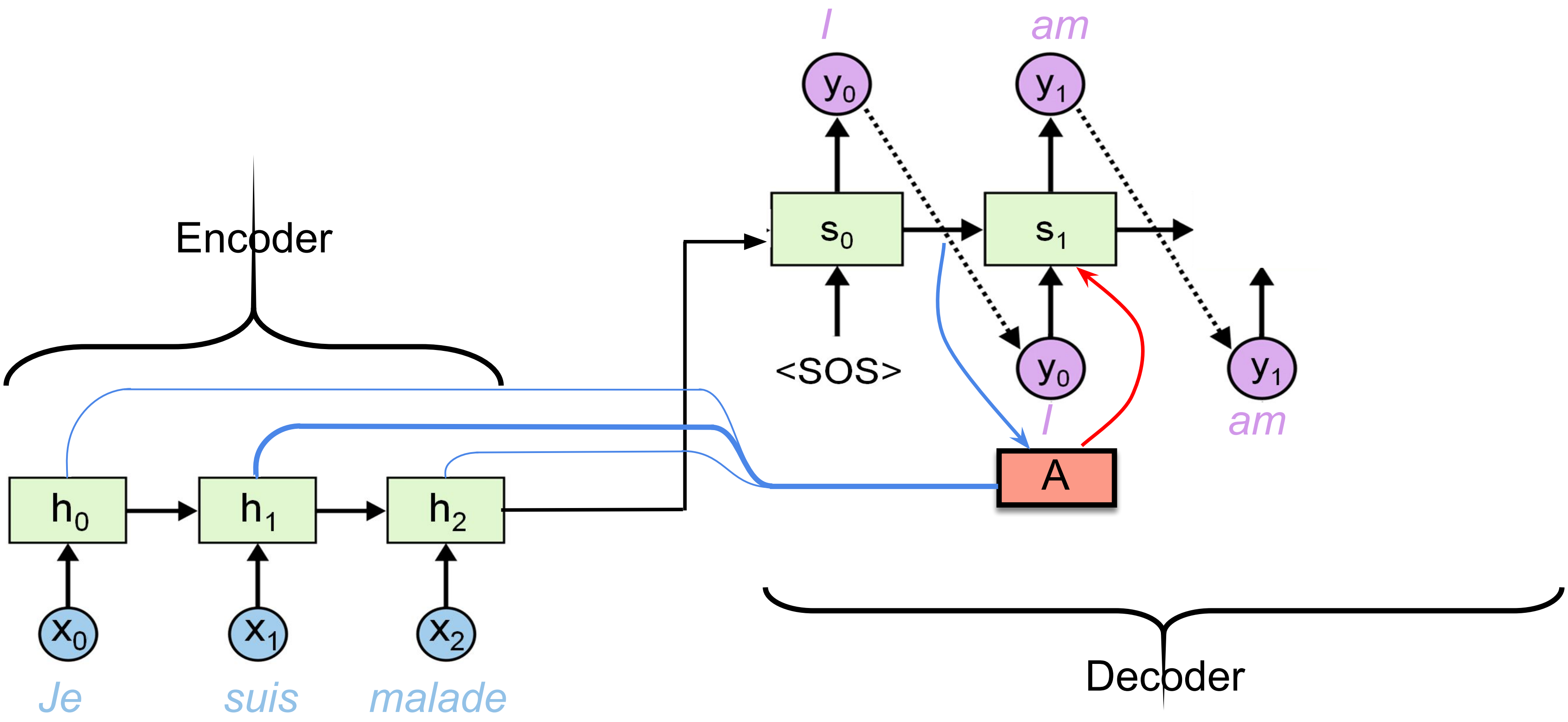


# Example: Sequence-to-Sequence + Attention

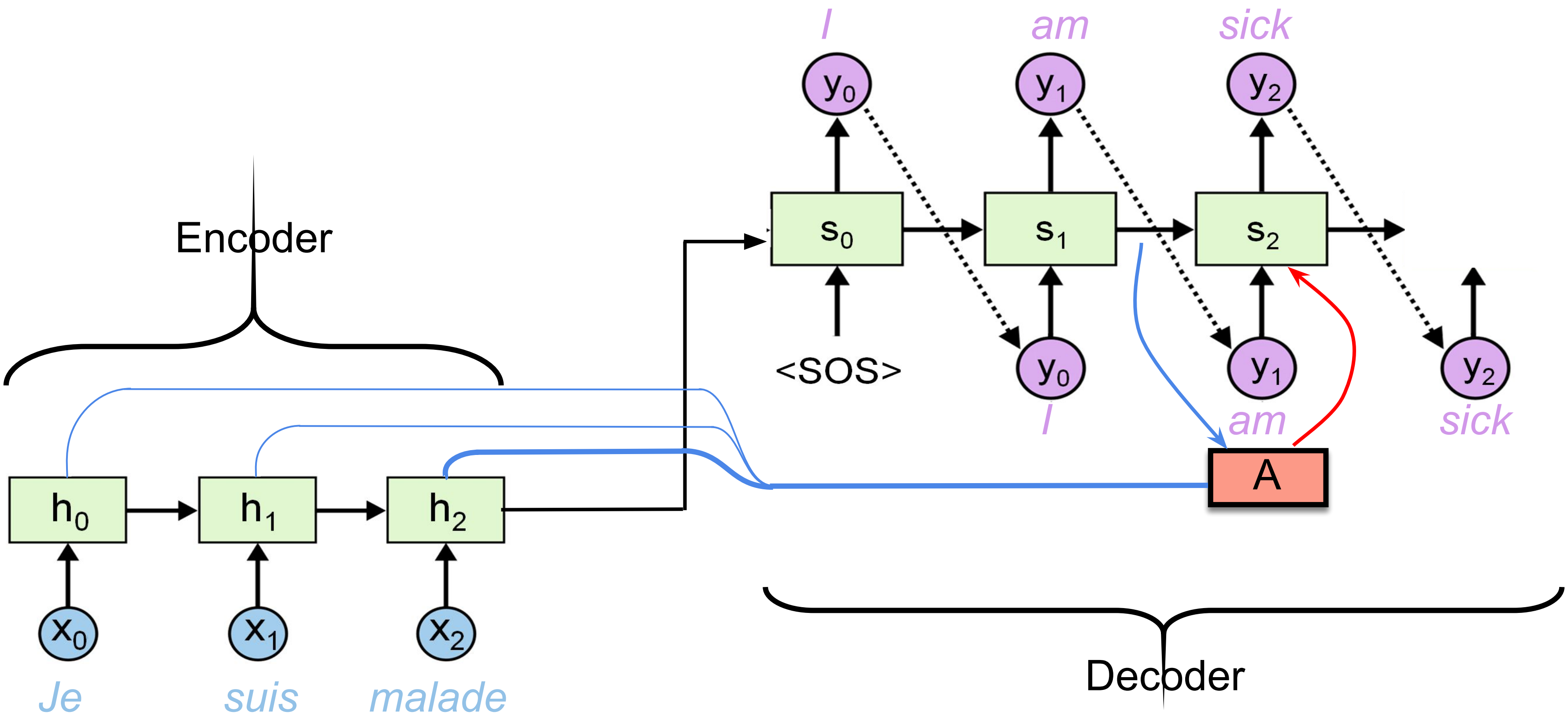
The output $\mathbf{y_0}$ is computed and used as the next input.



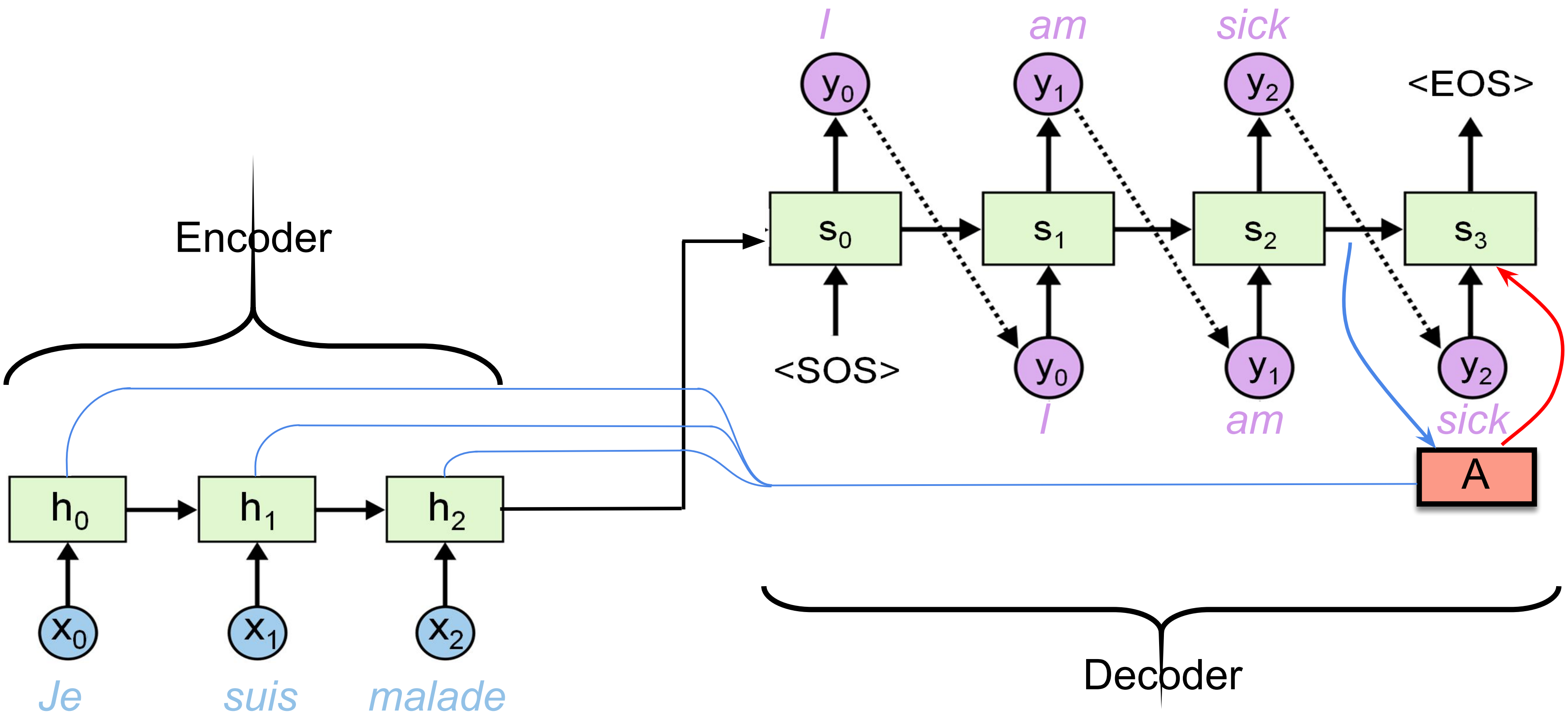
# Example: Sequence-to-Sequence + Attention



# Example: Sequence-to-Sequence + Attention



# Example: Sequence-to-Sequence + Attention



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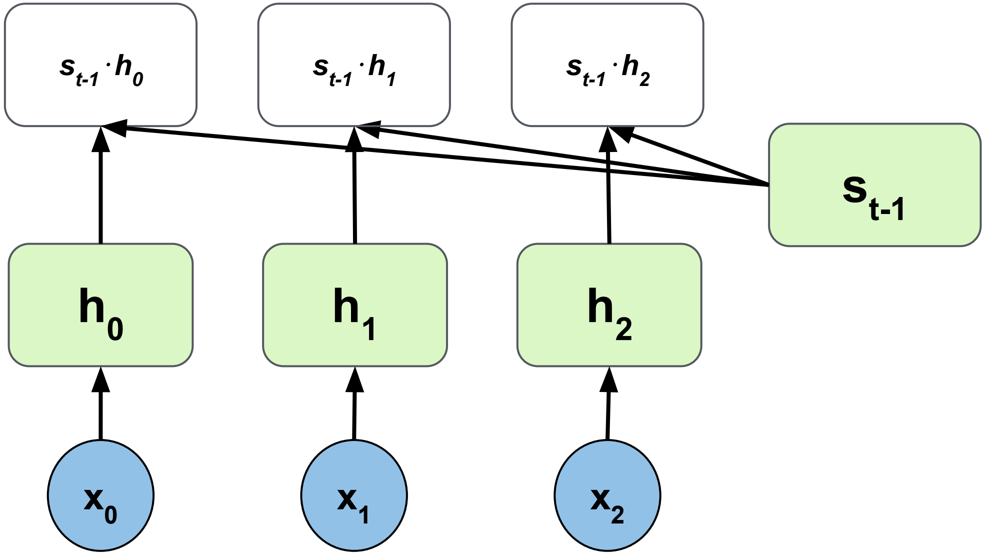
# Attention Function

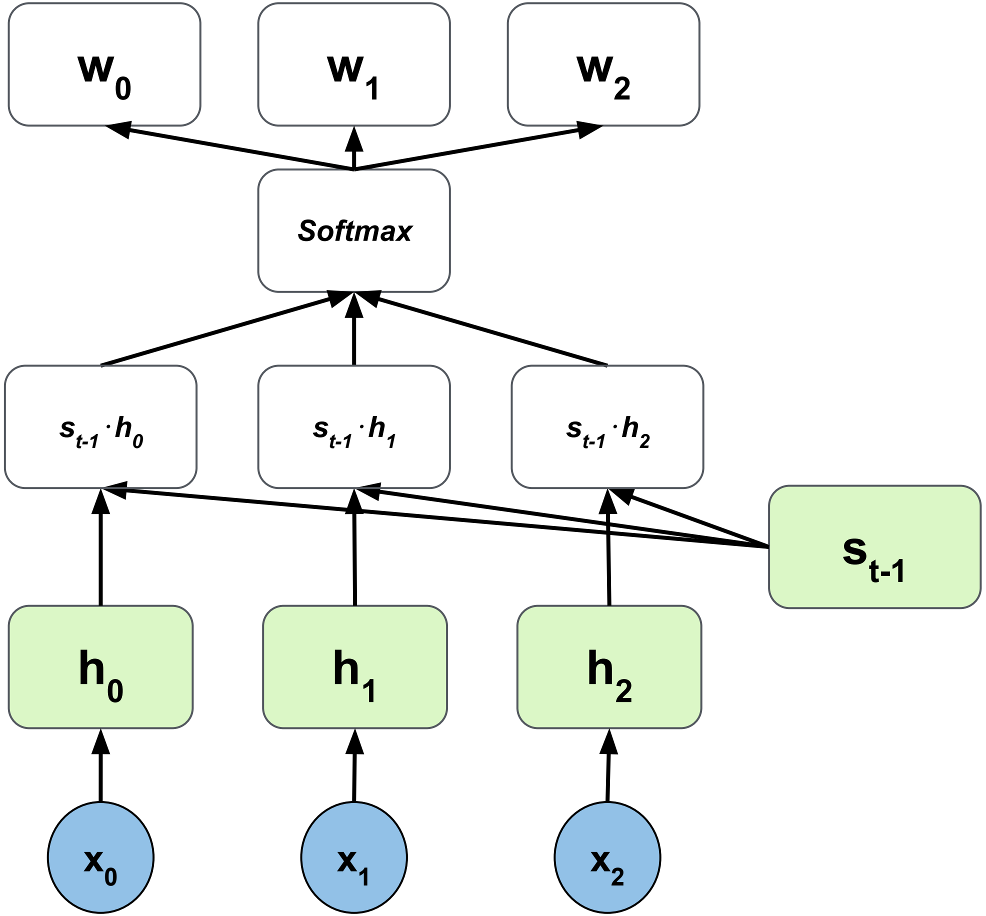
- There are several possible implementations for **A**.
- The most simple version is based on a dot product, i.e., $\mathbf{e_i = s_{t-1} \cdot h_i}$ .



# 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**.

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





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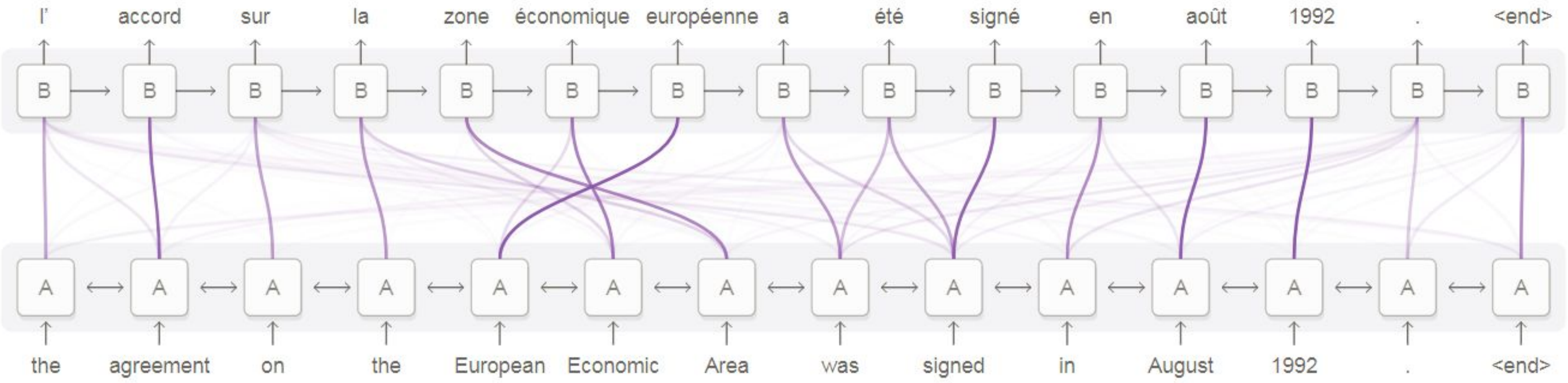
# Visualizing Attention

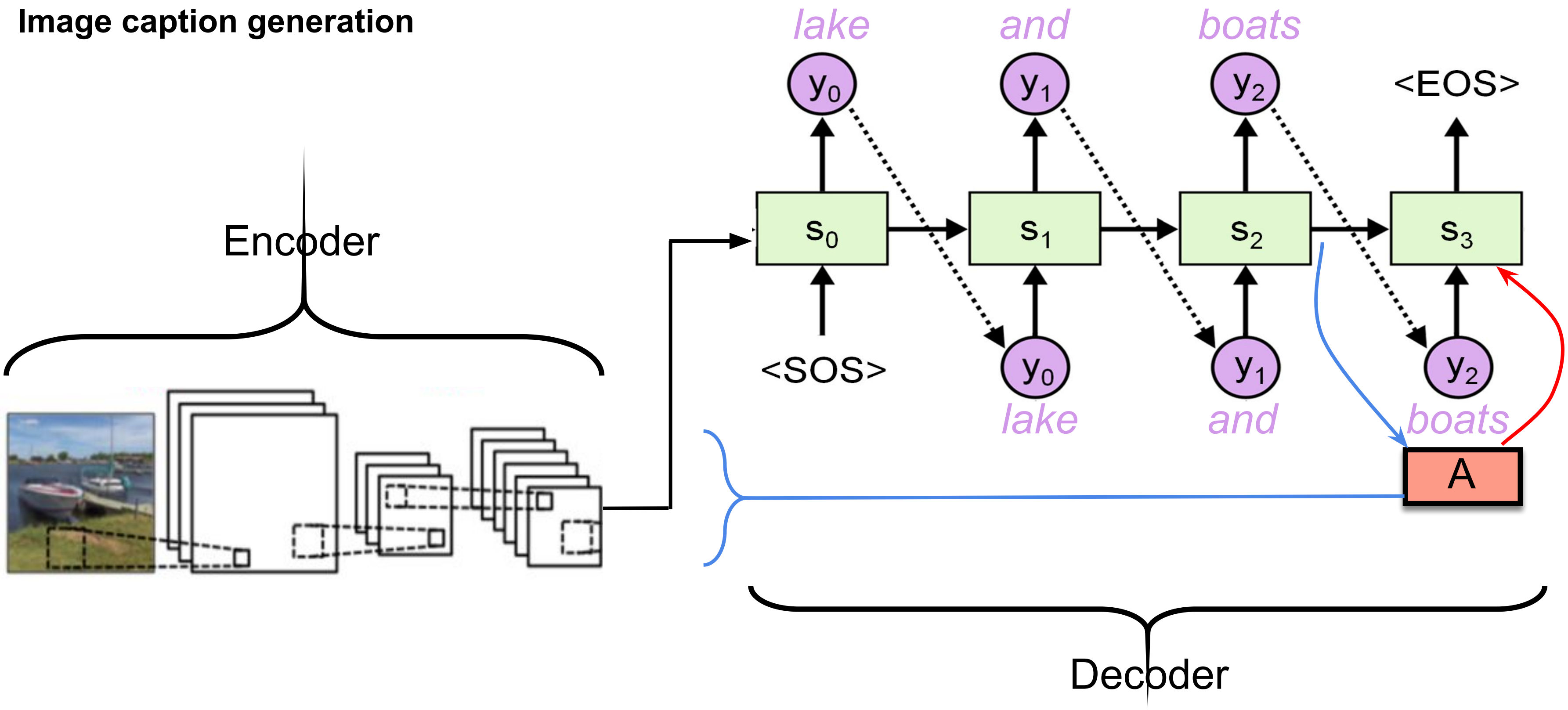



- The thick lines show where the decoder is focusing its attention when analyzing the encoded input sequence.

Image from Christopher Olah's blog

# Other Examples

**Image caption generation**



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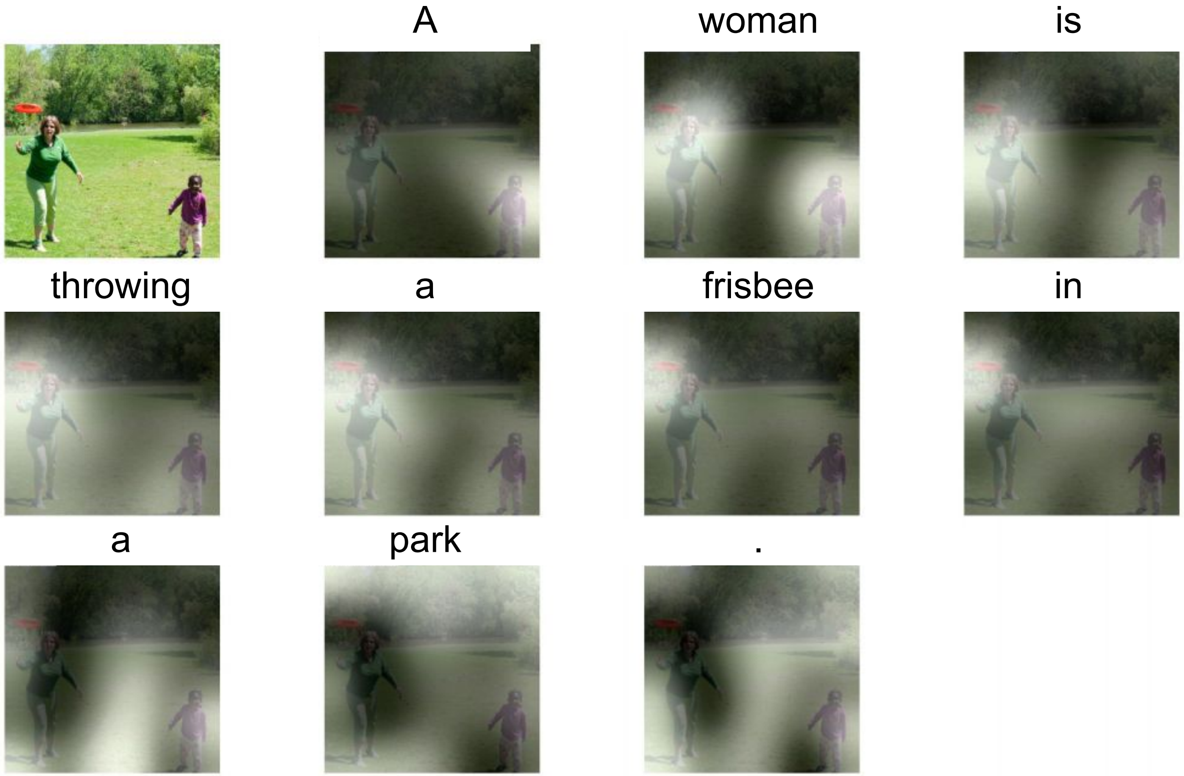
# Other Examples

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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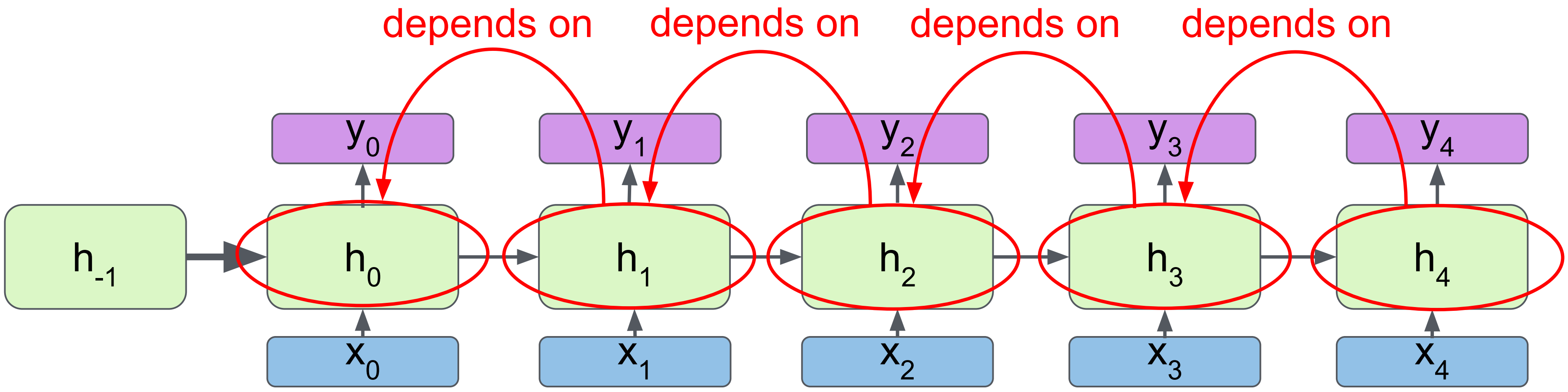
# Beyond RNNs

- 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.





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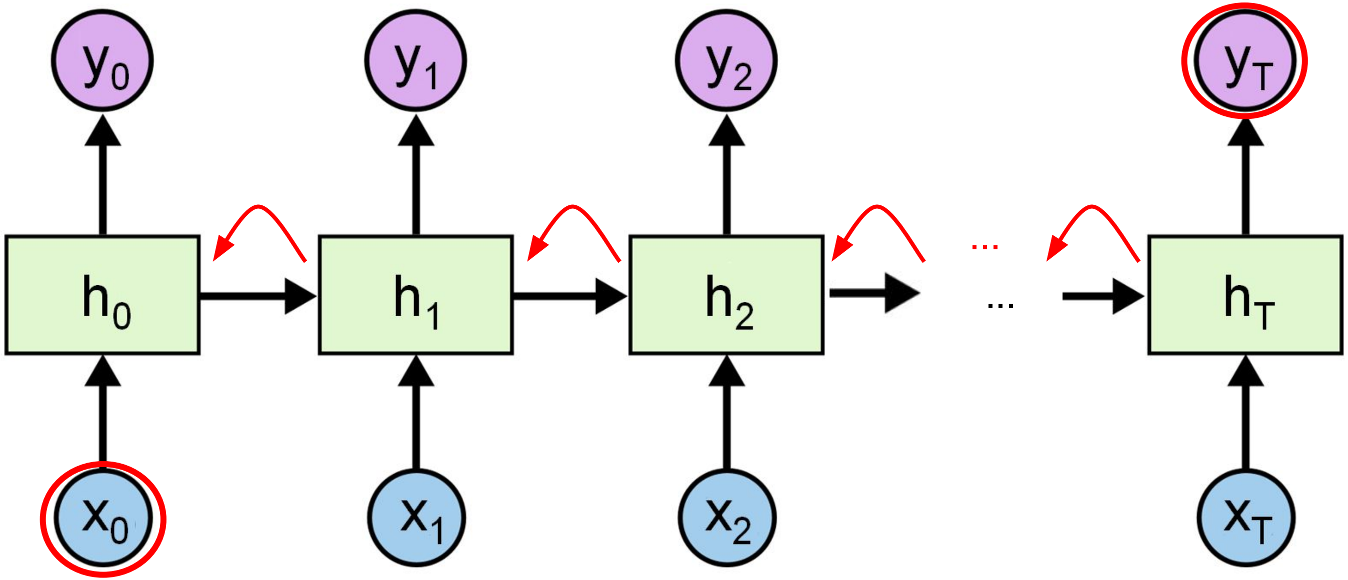
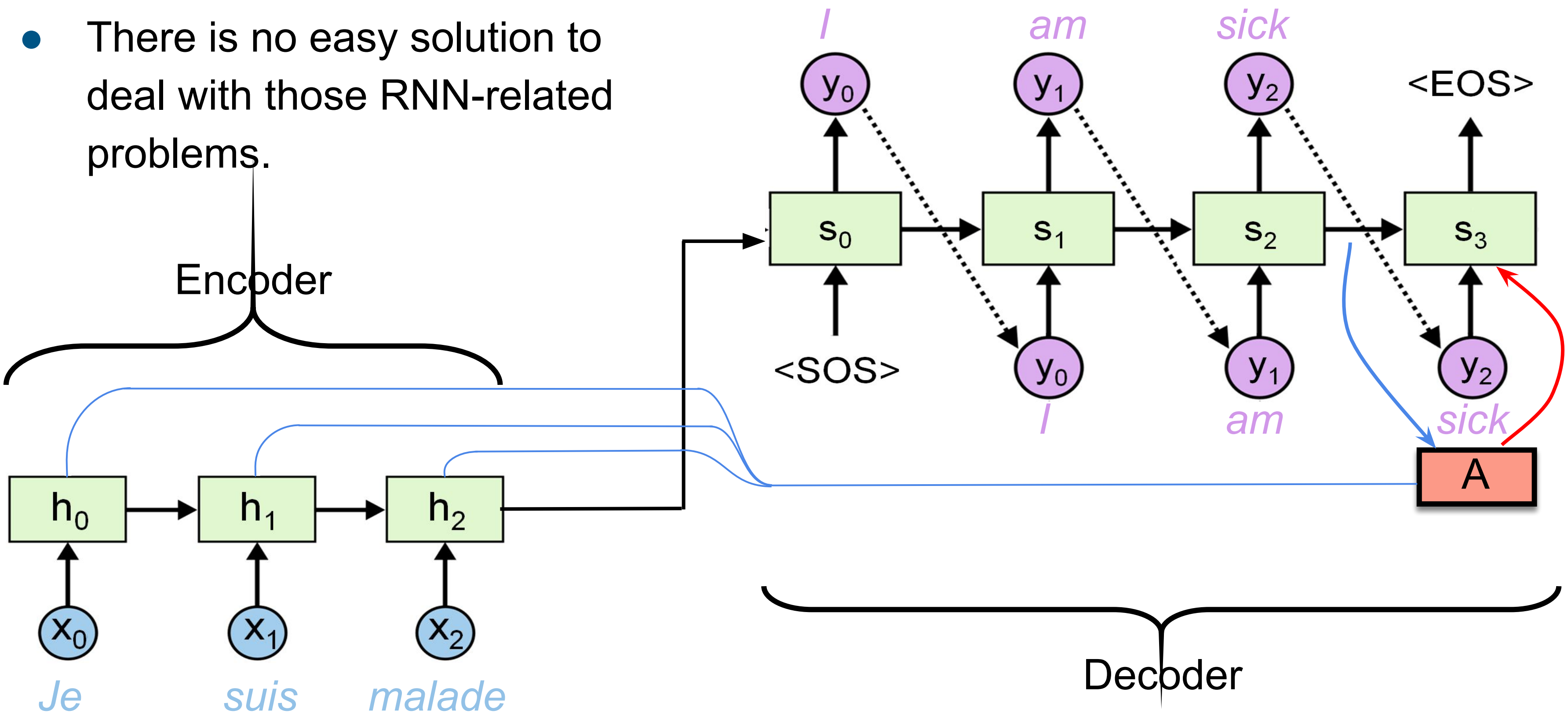
# Beyond RNNs

- 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.



# Beyond RNNs

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





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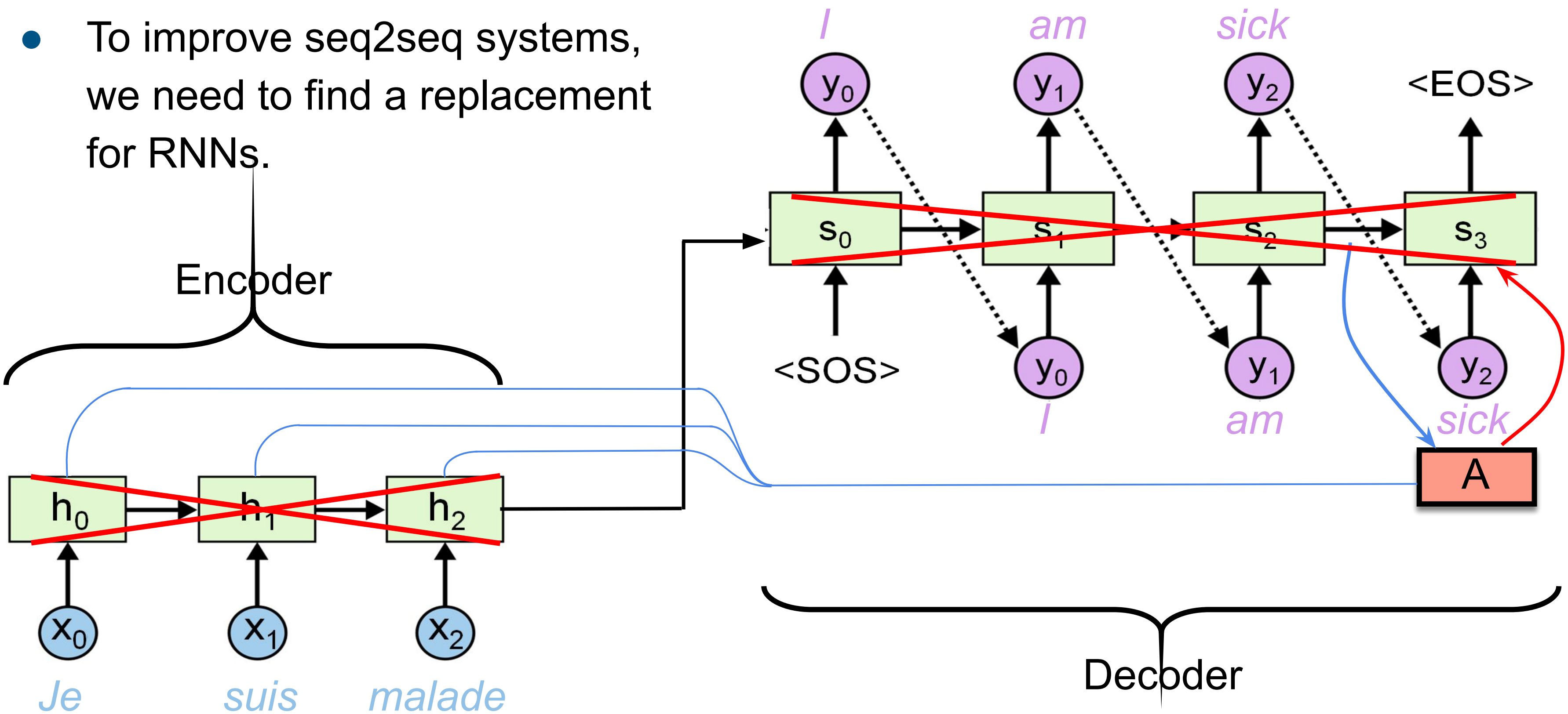
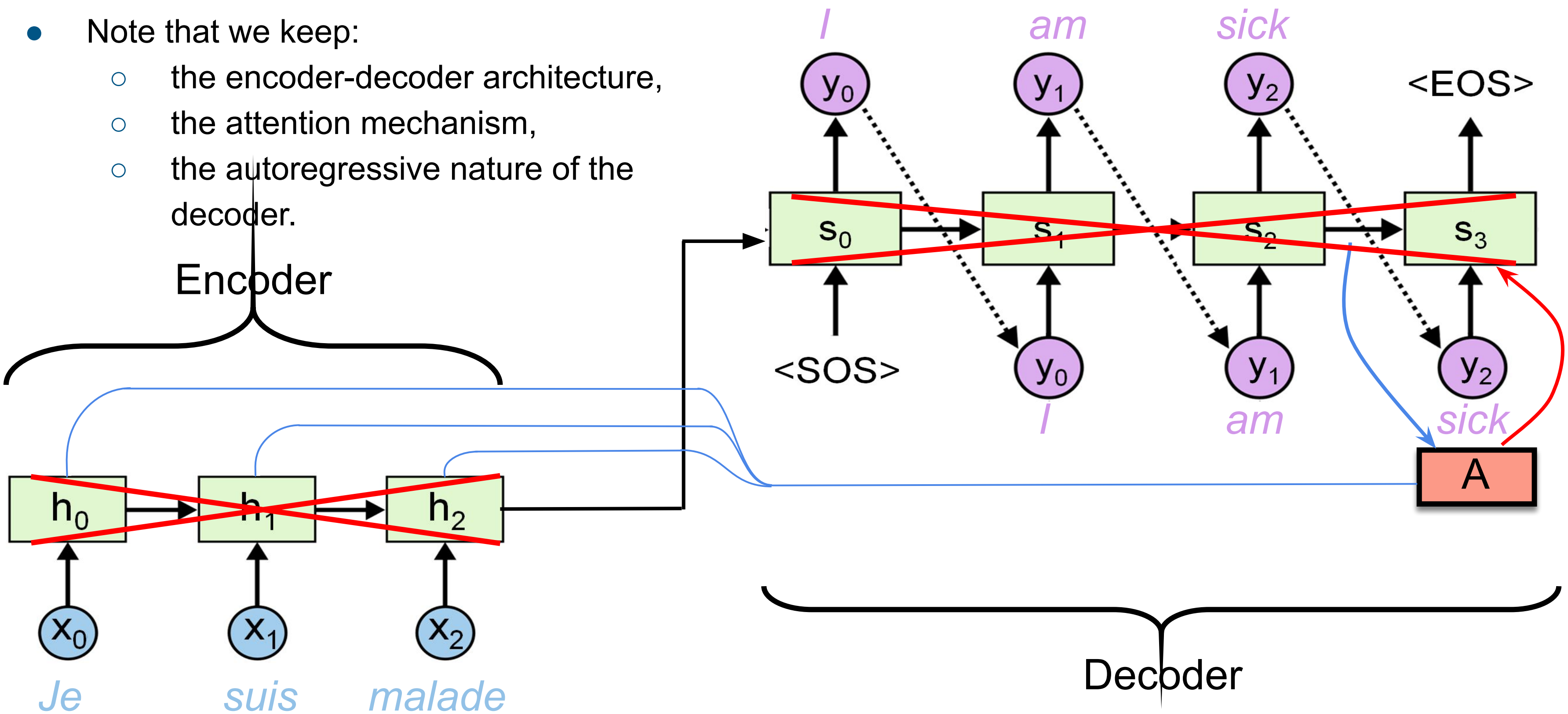
# Beyond RNNs

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



# Beyond RNNs

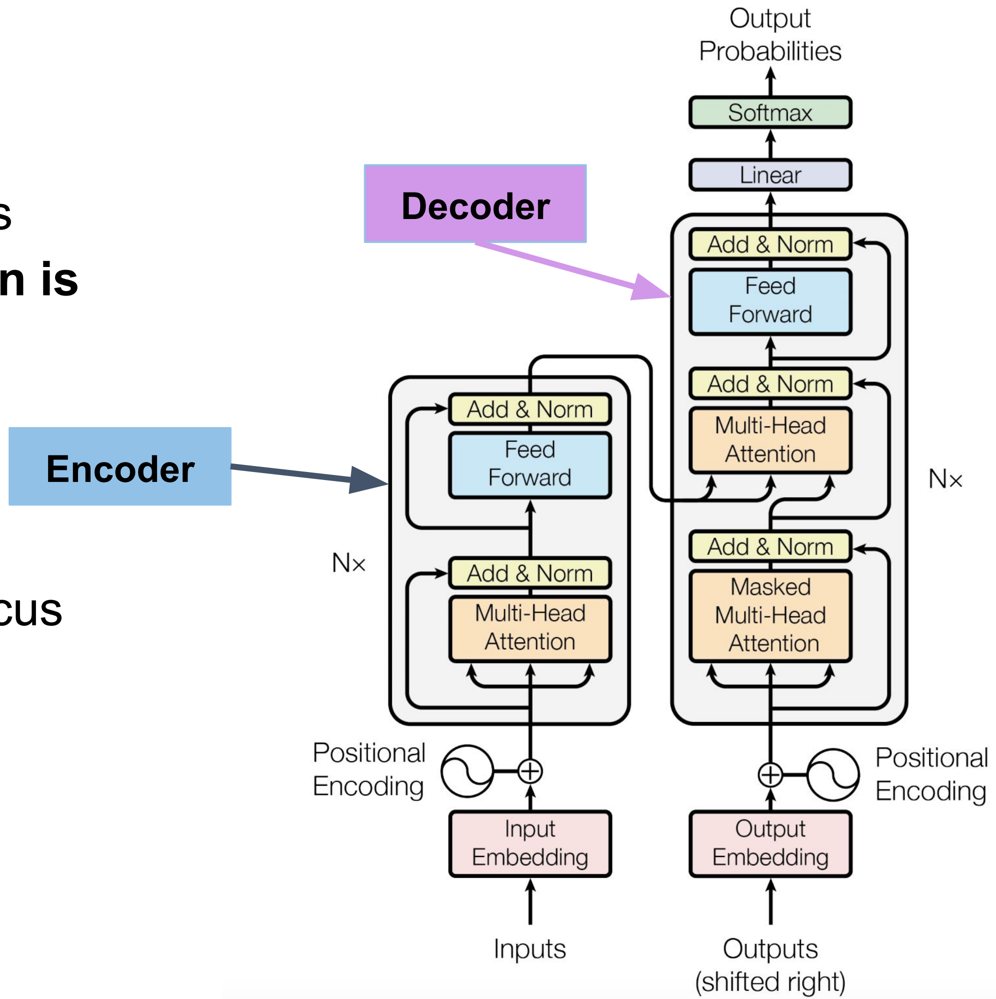
- Note that we keep:
  - the encoder-decoder architecture,
  - the attention mechanism,
  - the autoregressive nature of the decoder.



# Transformer

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

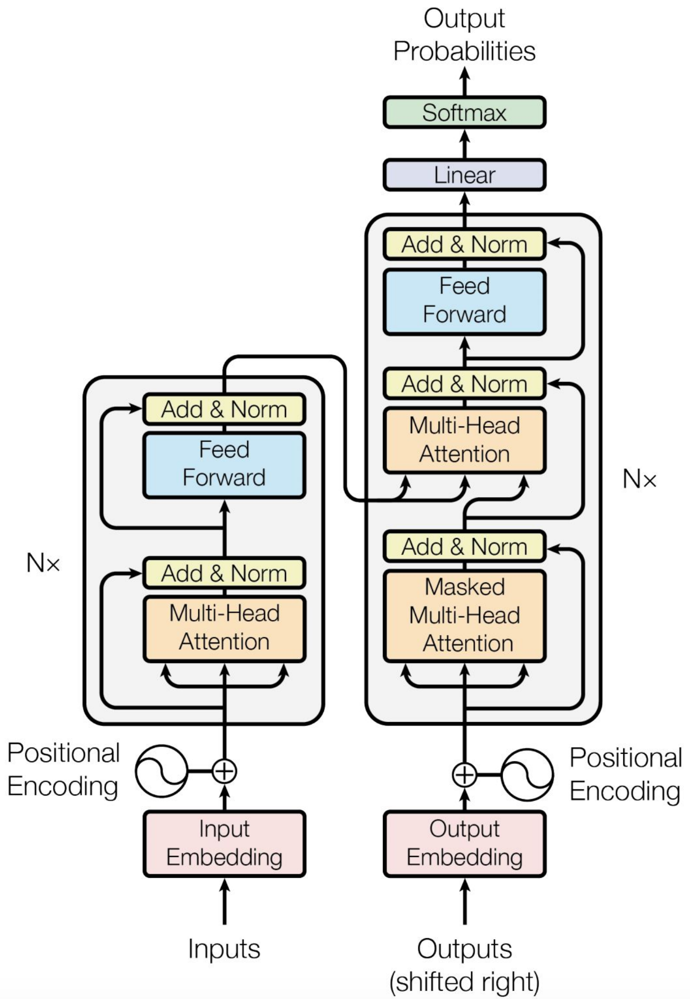
- Note: in the next slides we will focus on providing the intuition, thus simplifying some aspects of the architecture.




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.

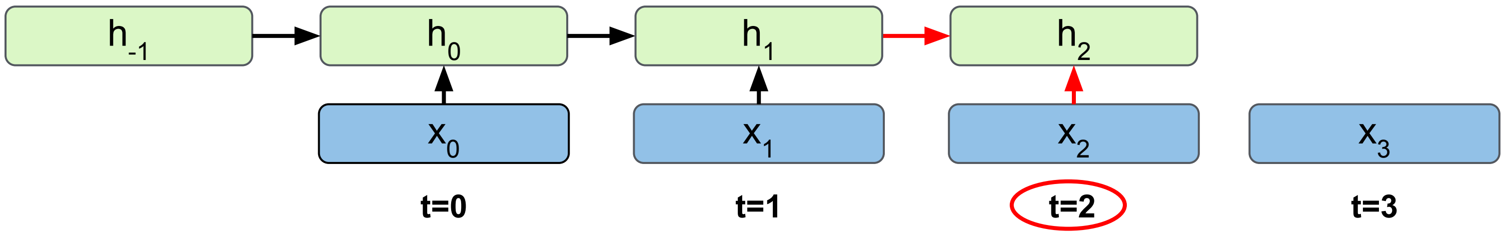



Vaswani et al, “Attention Is All You Need”, 2017

# 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.

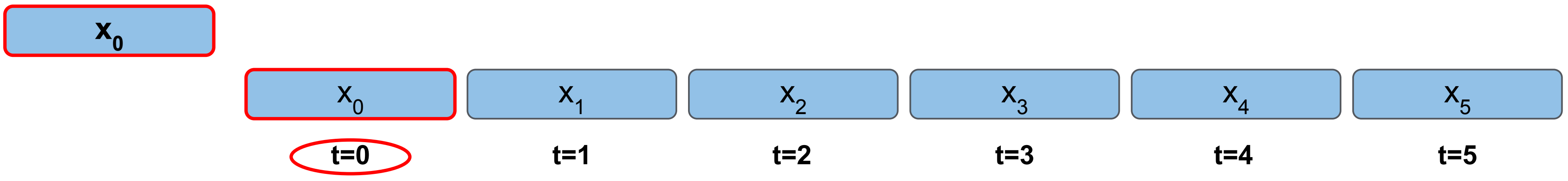


# Self-Attention

- 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.

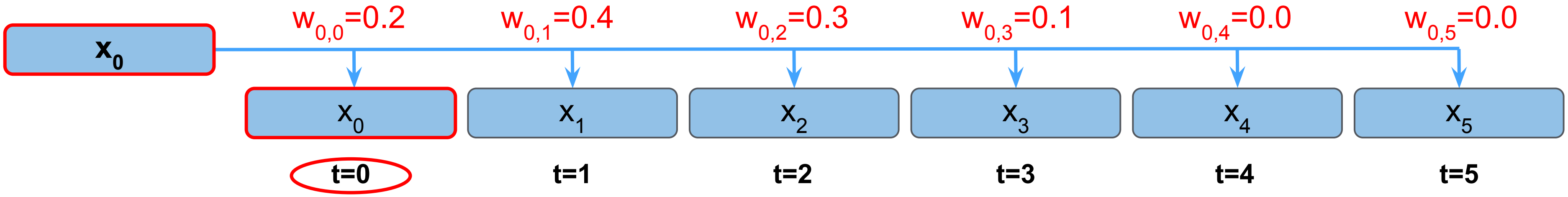
# Self-Attention

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



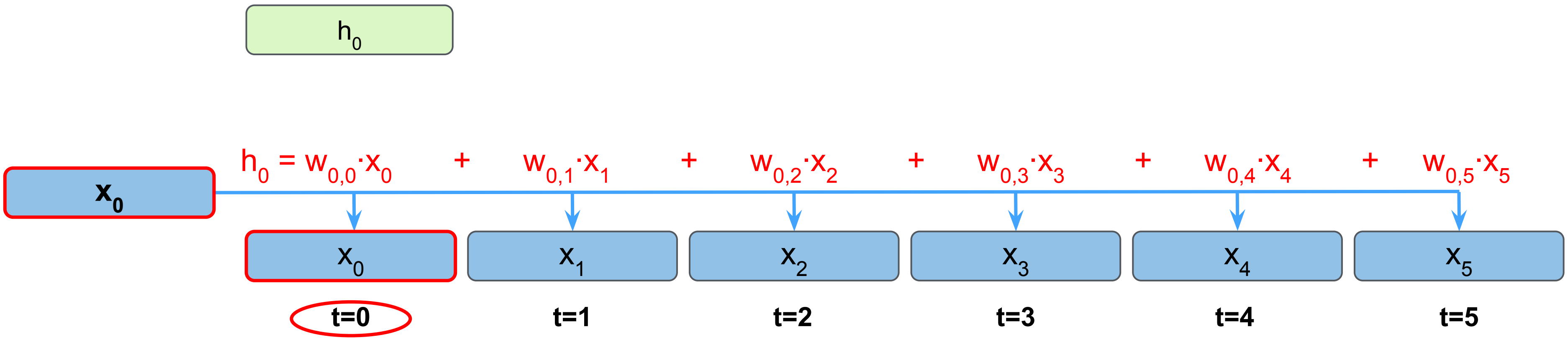
# Self-Attention

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



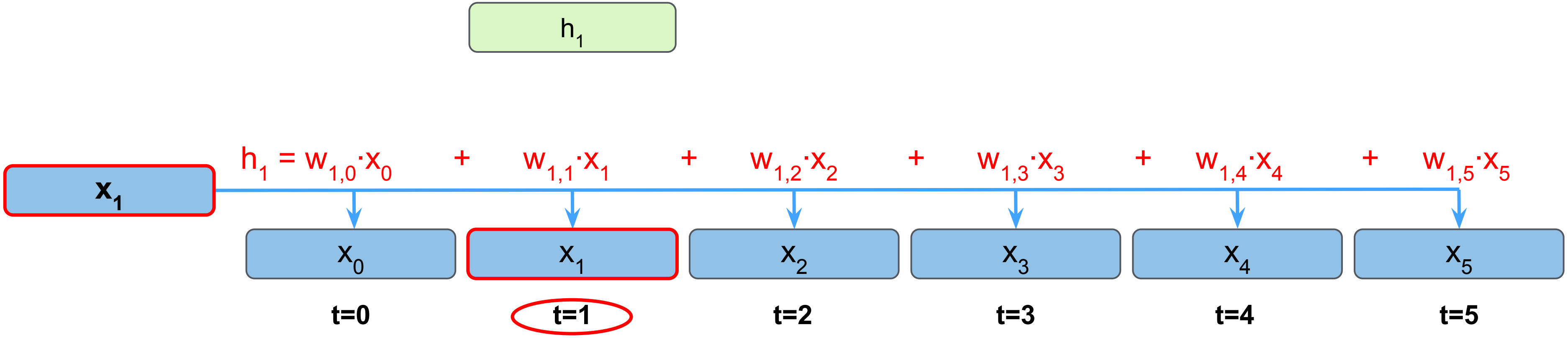
# Self-Attention

- 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.



# Self-Attention

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





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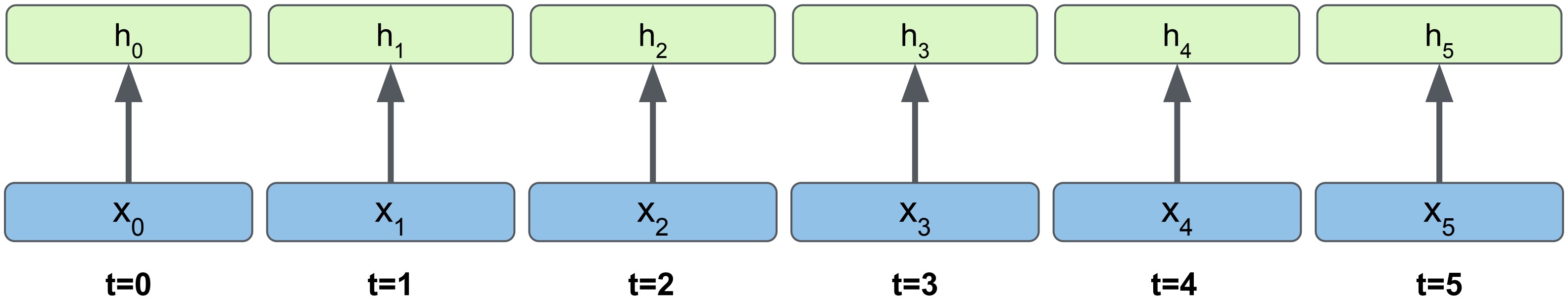
# Self-Attention

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



# Self-Attention - Multiple Heads

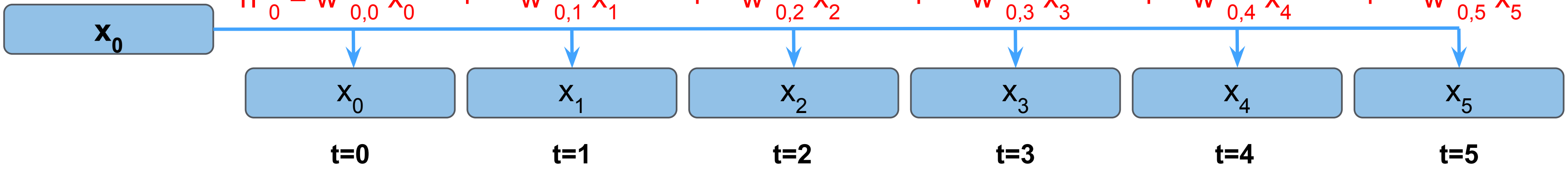
- The self-attention is meant to identify all elements in a sequence which are “relevant” to encode $x_t$.
- Given that there can be several types of relevant information, we can have several attention mechanisms.

# 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.

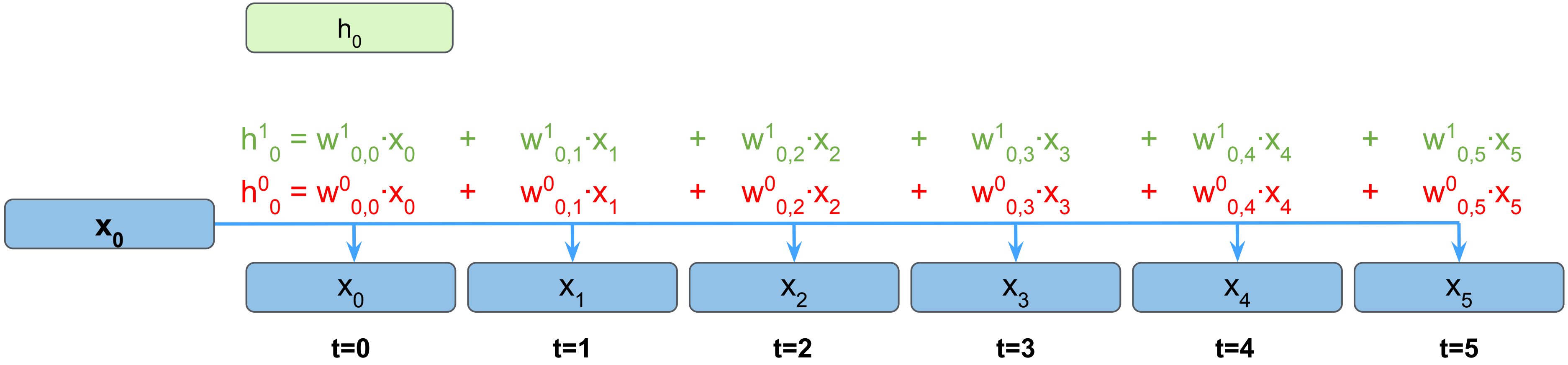
$$h^1_0 = w^1_{0,0}\cdot x_0 + w^1_{0,1}\cdot x_1 + w^1_{0,2}\cdot x_2 + w^1_{0,3}\cdot x_3 + w^1_{0,4}\cdot x_4 + w^1_{0,5}\cdot x_5$$

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



# 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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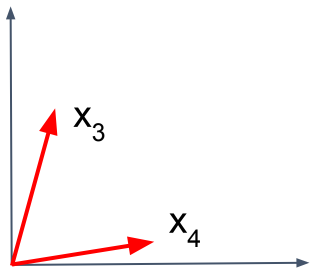
# Self-Attention - Multiple Heads

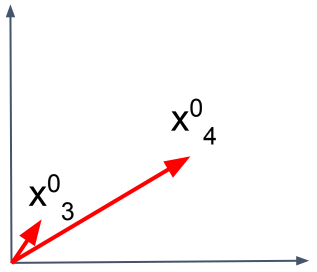
- The weights for a given head are based on a dot-product.
    - E.g., $\mathbf{w^0_{3,4} = x^0_3 \cdot x^0_4}$

- 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.

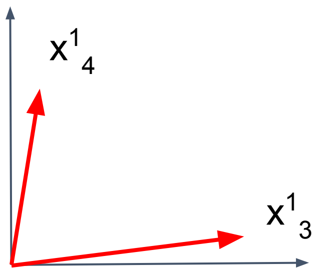
**Original** space



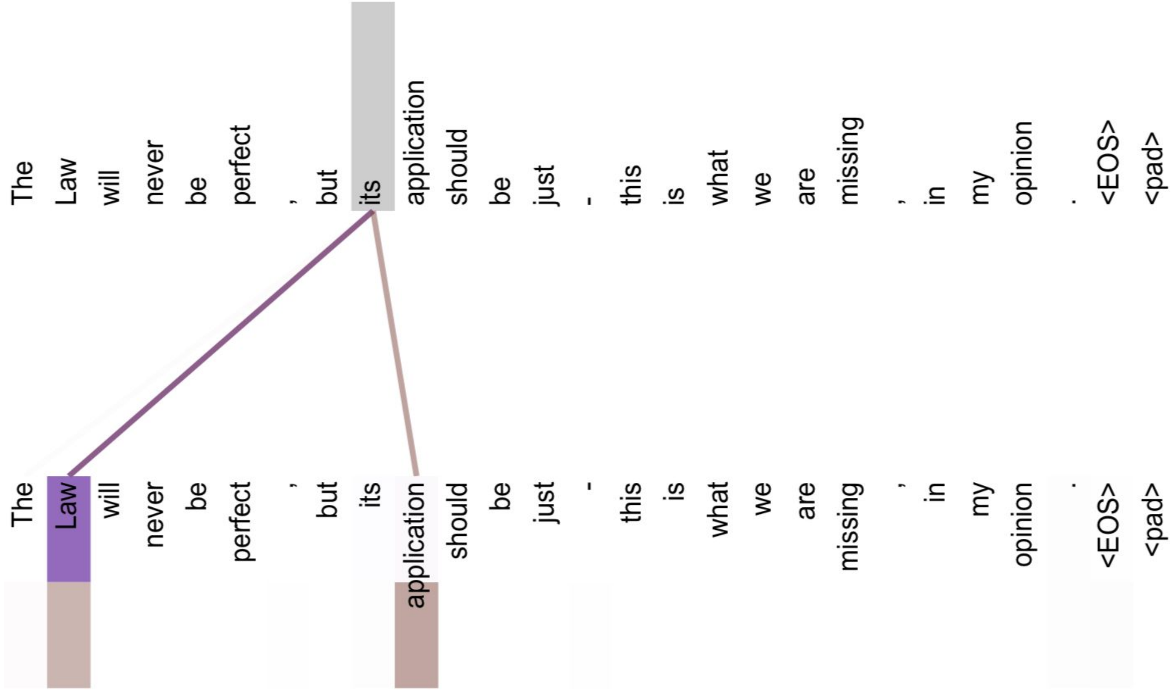

**head#0** space




**head#1** space



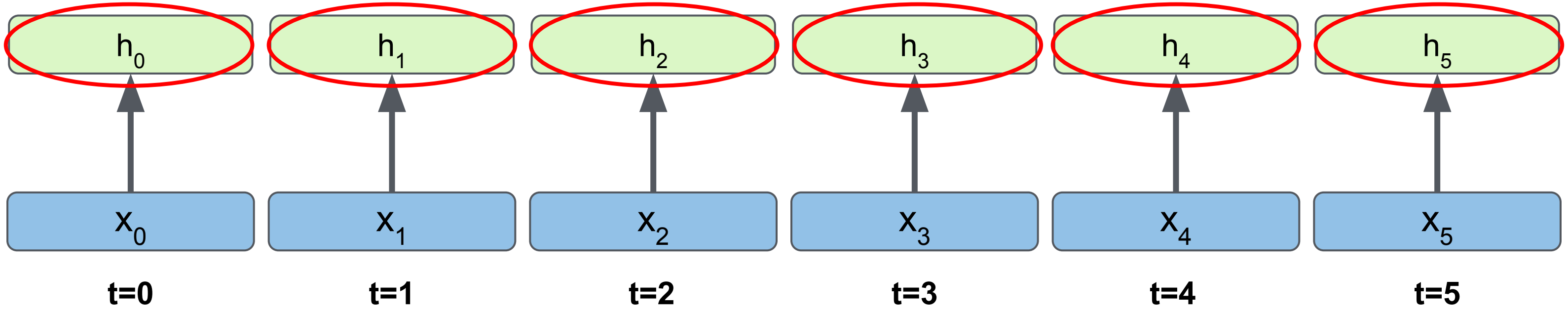
# Self-Attention - Visualization




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

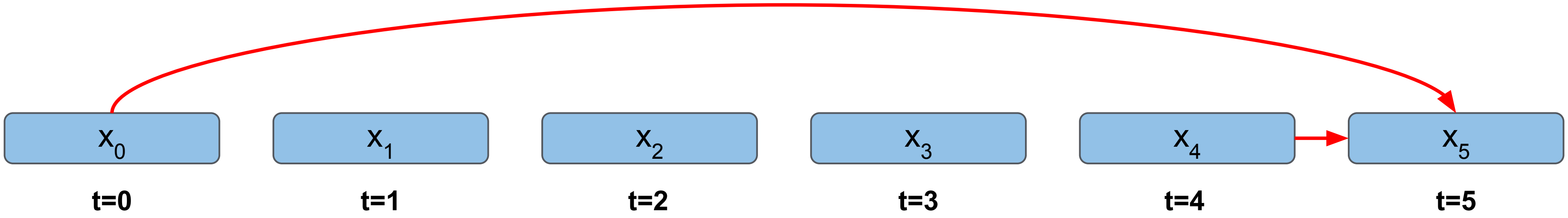
# Self-Attention - Advantages

- 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?