Recurrent Neural Networks

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Master in Artificial Intelligence (FIB-UPC)

Introduction

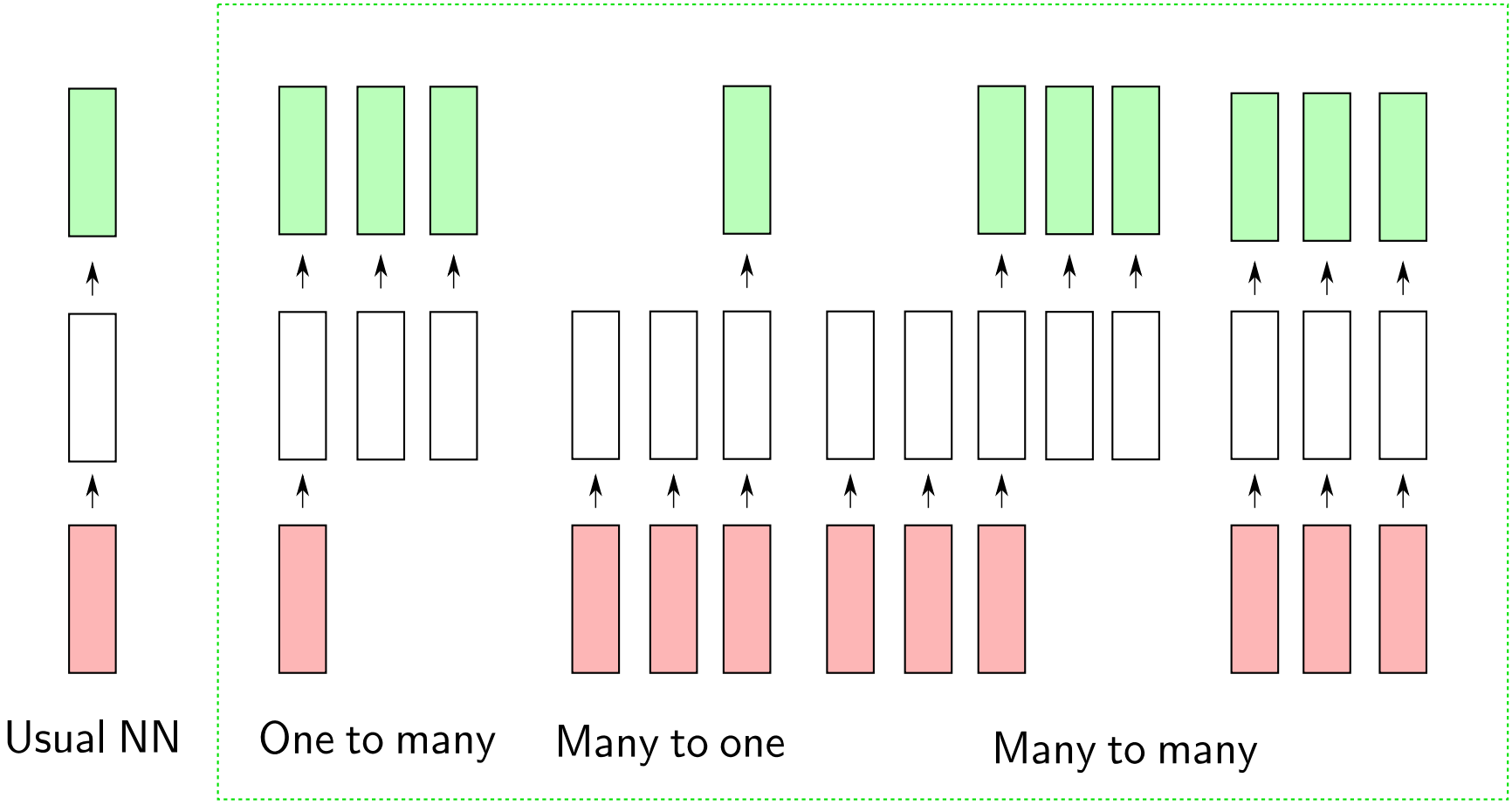
Sequential data

- Many problems are described by sequences
  - Time series
  - Video/audio processing
  - Natural Language Processing (translation, dialogue)
  - Bioinformatics (DNA/protein)
  - Process control
- Model the problem = Extract elements sequence dependencies

Long time dependences

- Sequences can be modeled using non sequential ML methods (e.g. sliding windows), but
  - All sequences must have the same length
  - Order of the elements always matters
  - We cannot model dependencies longer than the chosen sequence length
- We need methods that explicitly model time/order dependencies capable of:
  - Processing arbitrary length examples
  - Providing different mappings (one to many, many to one, many to many)

Input-Output mapping



One to many - Image captioning

$\Rightarrow$ Black and white dog jumps over bar

from Deep Visual-Semantic Alignments for Generating Image Descriptions Andrej Karpathy, Li Fei-Fei

Many to One - Sentiment Analysis

My flight was just delayed, s**t	$\Rightarrow$	Negative
Never again BA, thanks for the dreadful flight	$\Rightarrow$	Negative
We arrived on time, yeehaaa!	$\Rightarrow$	Positive
Another day, another flight	$\Rightarrow$	Neutral
Efficient, quick, delightful, always with BA	$\Rightarrow$	Positive

[How, many, programmers, for, changing, a, lightbulb,?]

⇒ [Wie, viele, Programmierer, zum, Wechseln, einer, Glühbirne,?]

⇒ [Combien, de, programmeurs, pour, changer, une, ampoule,?]

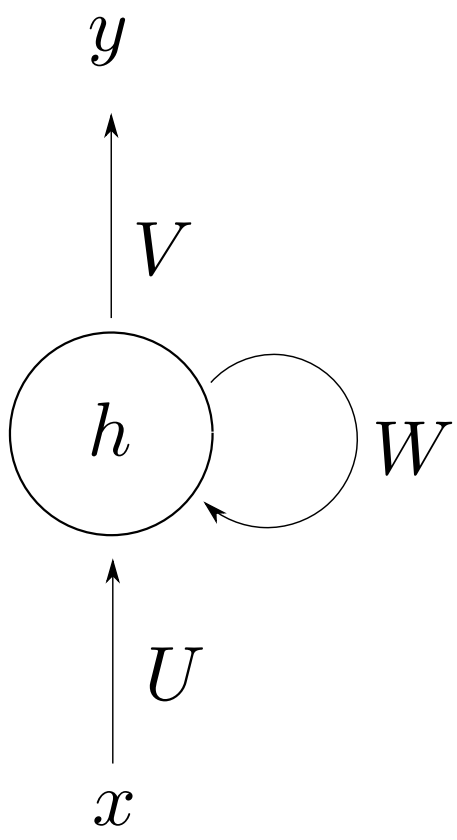
⇒ [¿,Cuántos, programadores, para, cambiar, una, bombilla,?]

⇒ [Zenbat, bonbilla, bat, aldatzeko, programatzaileak,?]

Recurrent Networks

- RNN are feed forward NN with edges that span adjacent time steps (recurrent edges)
- At each time step nodes receive input from the current data and from the previous state
- This makes that input data from previous time steps can influence the output at the current time step
- RNN are universal function approximators (Turing Complete)

Recurrent Node

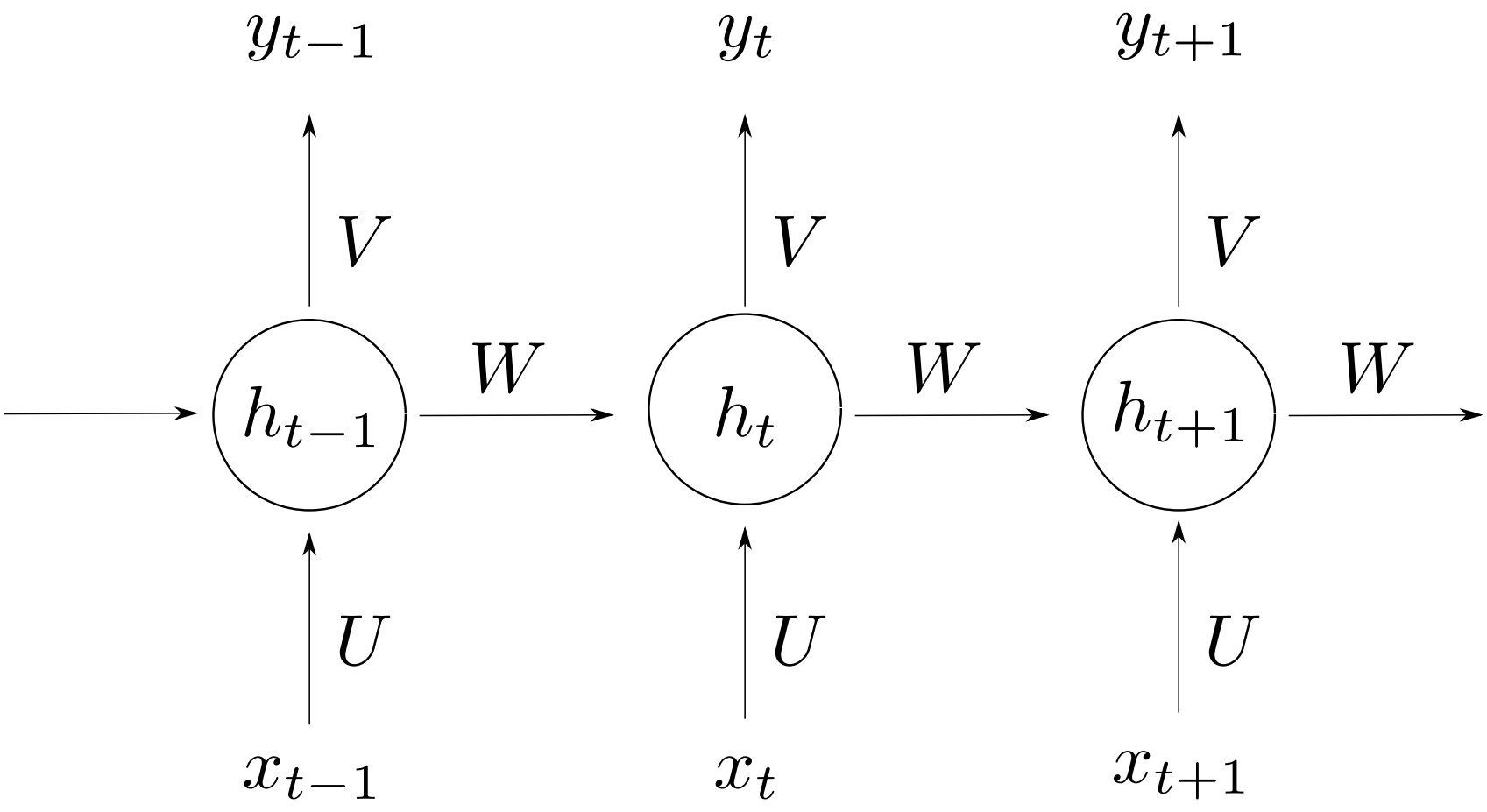


- Input (x) is a vector of values for time t
- The hidden node (h) stores the state
- Weights are shared through time
- Each step the computation uses the previous step

$$h^{(t+1)} = f(h^{(t)}, x_{t+1}; \theta) = f(f(h^{(t-1)}, x_t; \theta), x_{t+1}; \theta) = \cdots$$

- We can think of a RNN as a deep network that stacks layers through time

Training RNN (unfolding)



Activation Functions

- There are different choices for the activation function to compute the hidden state, but:
- The hyperbolic tangent function (*tanh*) is a popular choice versus the usual sigmoid function
- Good results are also achieved using the rectified linear function (ReLU) instead

$$a^{(t)} = b + W \cdot h^{(t-1)} + U \cdot x^{(t)} \quad (1)$$

$$h^{(t)} = tanh(a^{(t)}) \quad (2)$$

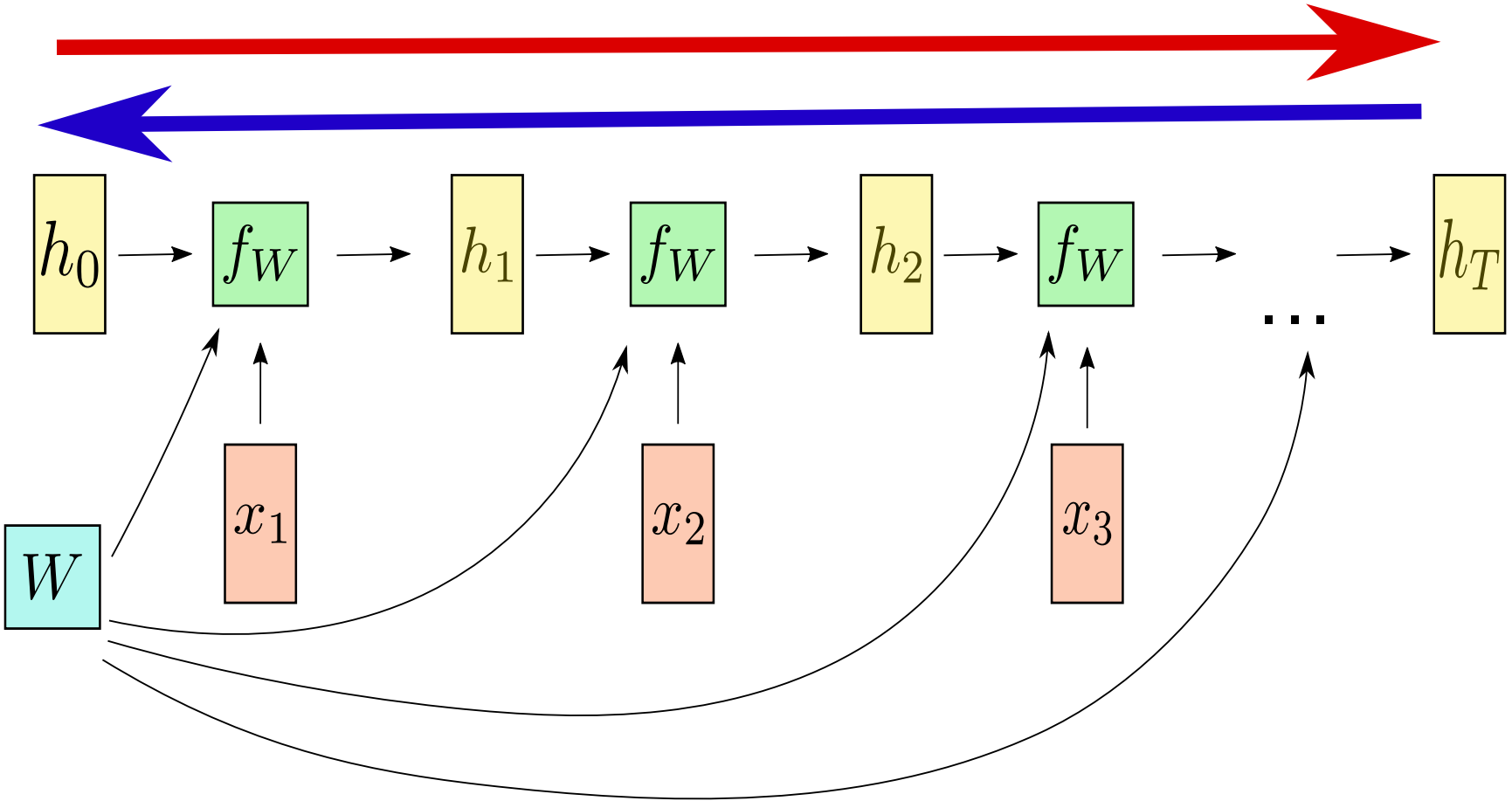
$$y^{(t)} = c + V \cdot h^{(t)} \quad (3)$$

b and c are bias, an additional step can be added depending on the task

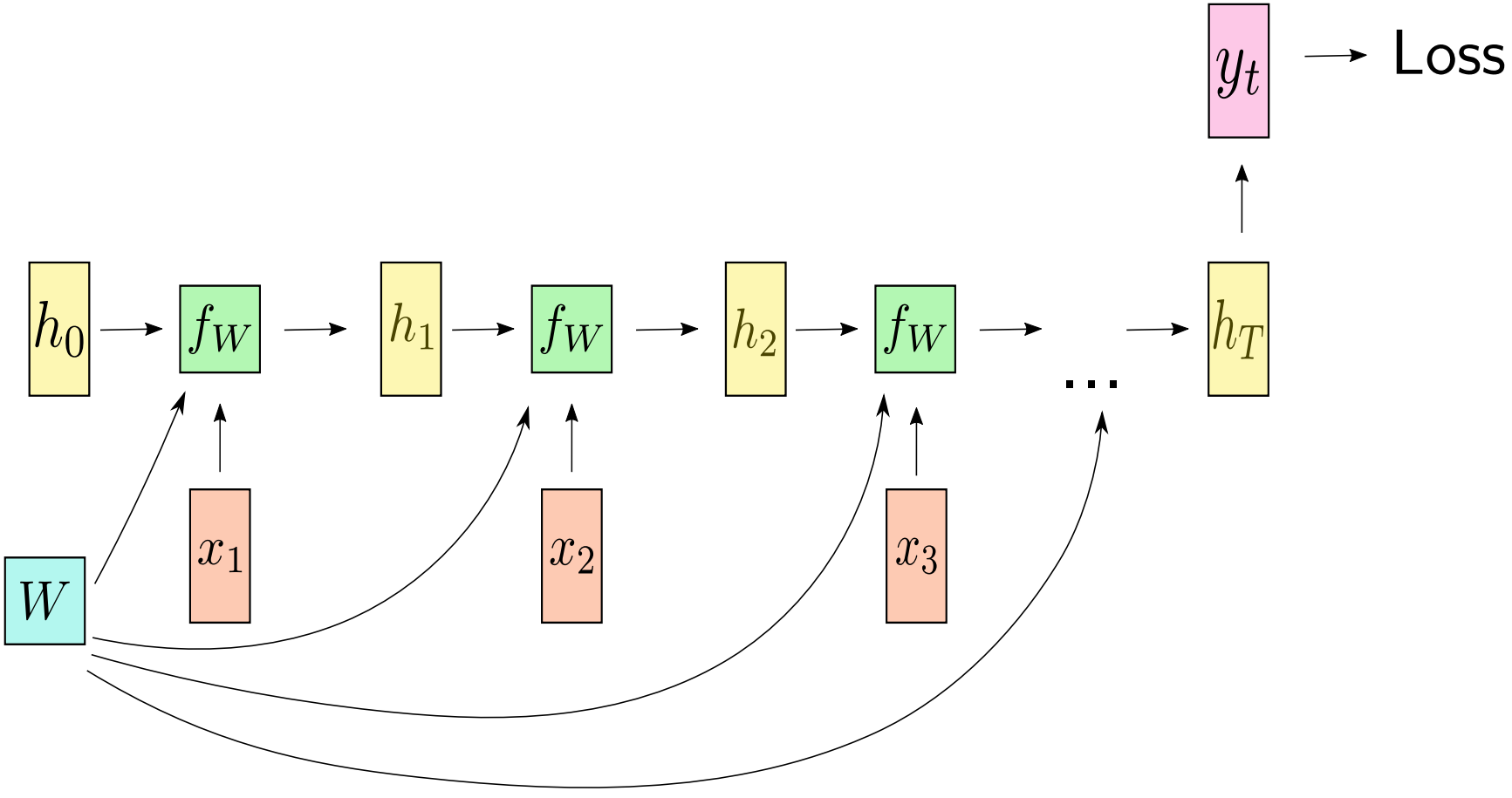
Training RNN

- RNN are trained using backpropagation
- The computation is unfolded through the sequence to propagate the activations and to compute the gradient
- This is known as Backpropagation Through Time (BPTT)
- Usually the input is limited in length to reduce computational cost, this is known as Truncated BPTT
  - Assumes that influence is limited to a time horizon

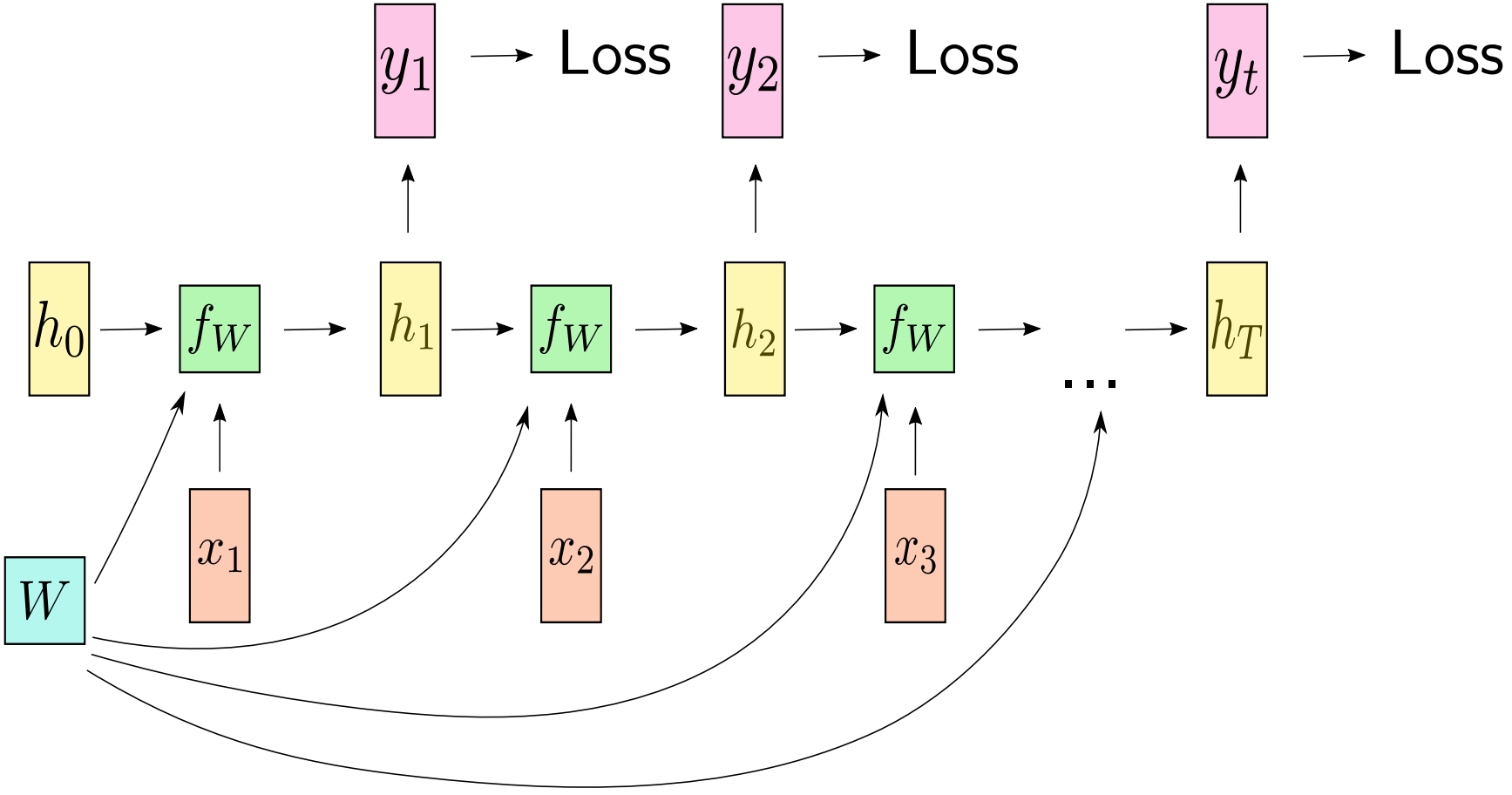
Recurrent NN unfolded



Recurrent NN (Regresssion/Classification)

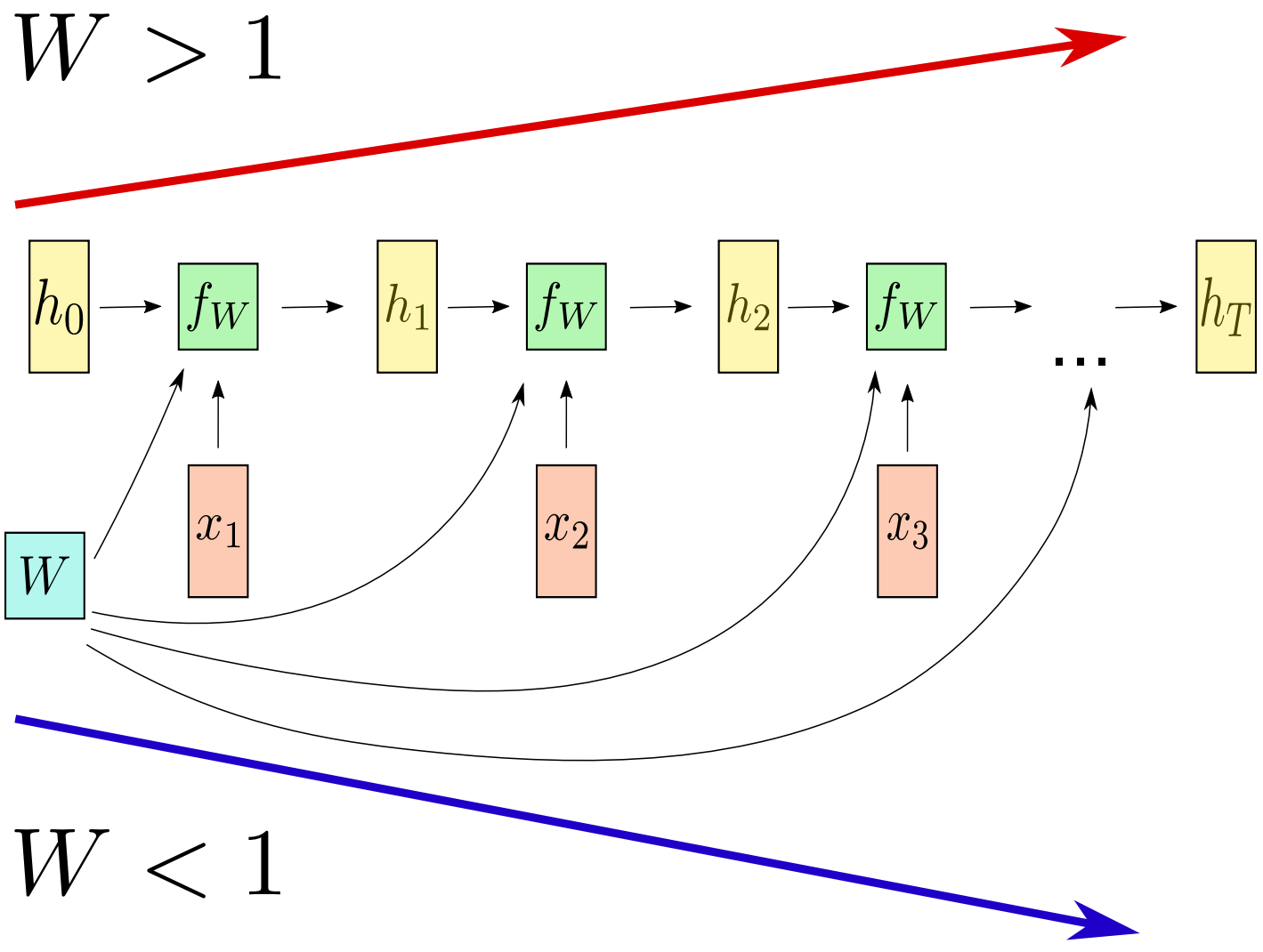


Recurrent NN (Sequence to Sequence)



Gradient problems

- Two main problems during training
  - Exploding Gradient
  - Vanishing Gradient
- Problems appear because of the sharing of weights
- Recurrent edge weights in combination with activation function magnify ($W > 1$) or shrink ($W < 1$) the gradient exponentially with the length of the sequence
- Clipping gradients and regularization are usual solutions to exploding gradient


$W > 1$
h_0
f_W
h_1
f_W
h_2
f_W
...
h_T
x_1
x_2
x_3
W
$W < 1$

- Learning long time dependencies is difficult for vanilla RNN
- More sophisticated recurrent architectures allow reducing gradient problems
- **Gated RNNs** introduce memory and gating mechanisms
  - When to store information in the state
  - How much new information changes the state

LSTMs

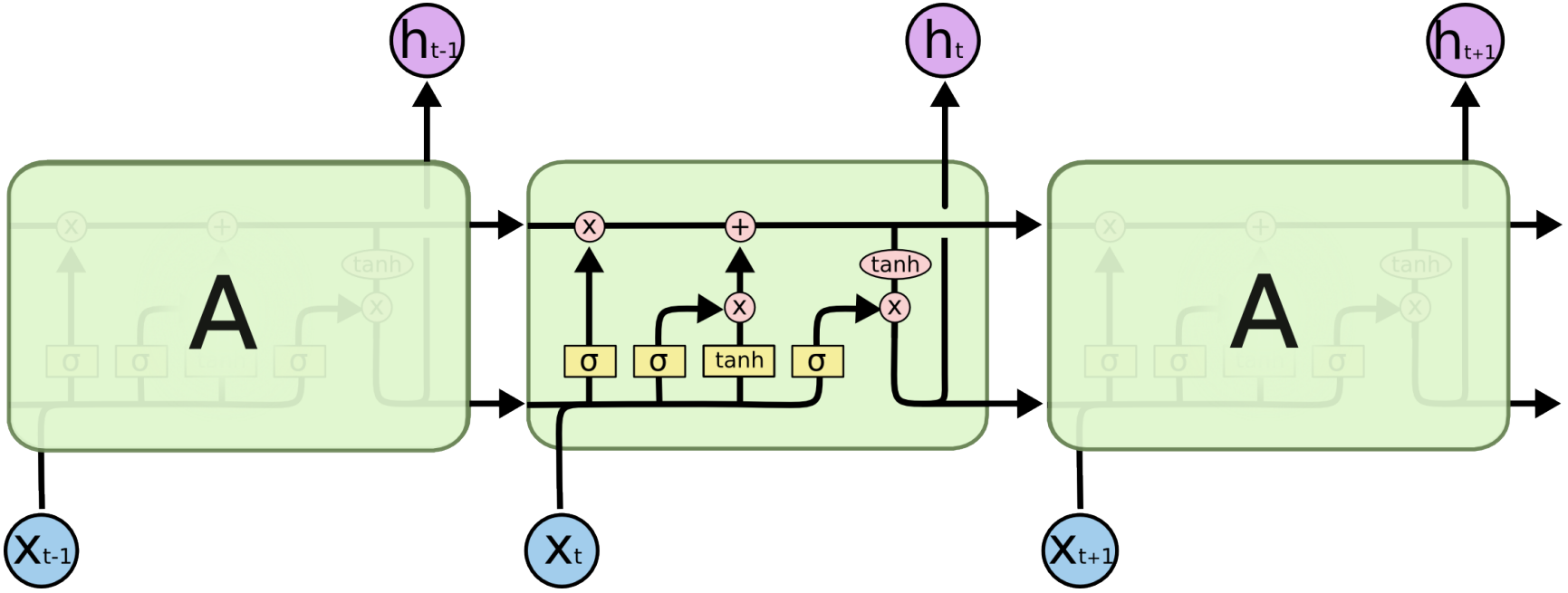
Long Short Term Memory units (LSTMs)

- LSTMs specialize on learning long time dependencies
- They are composed by a memory cell and control gates
- Gates allow regulating how much the new information changes the state and flows to the next step
  - Forget Gate
  - Input Gate
  - Update Gate
  - Output Gate

Long Short Term Memory units (LSTMs)

LSTMs propagate a hidden state (h_t) and a cell state (c_t)

- The hidden state acts as a short-term memory (large updates)
- The cell state acts as a long-term memory (small updates)
- Gates control updates from previous time steps to the current one
- Information can flow between short-term and long-term memory

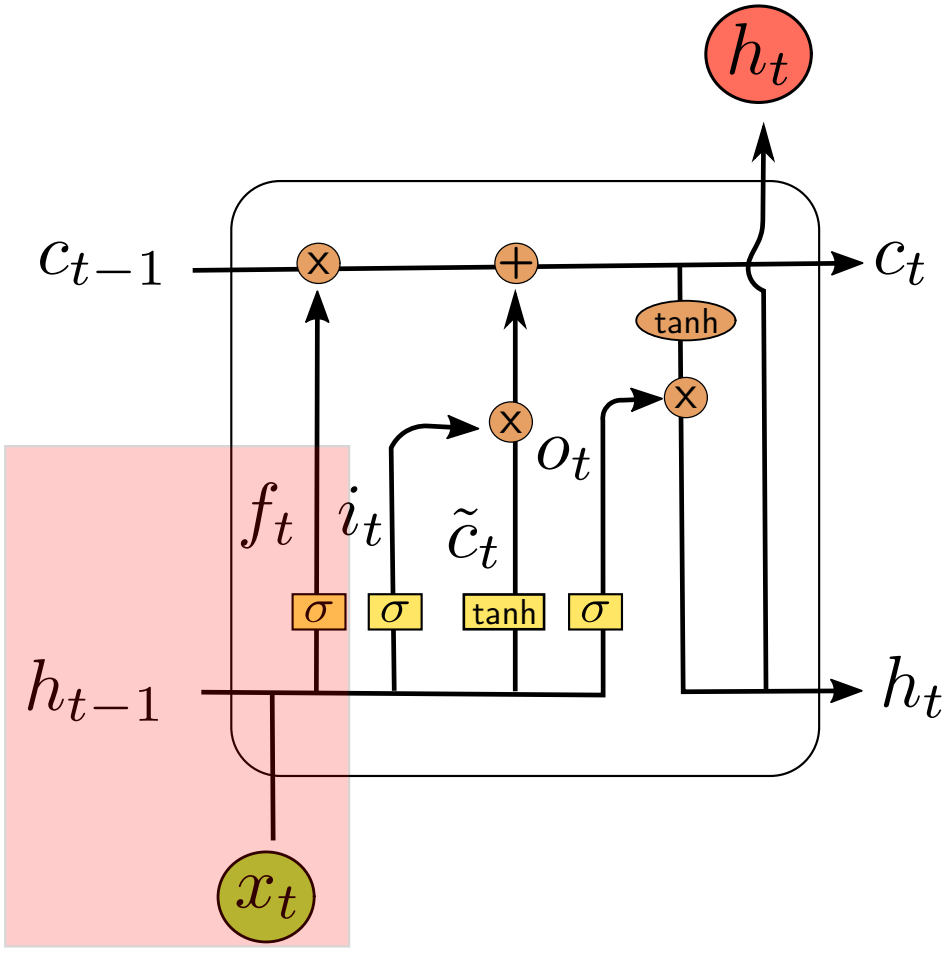


http://colah.github.io/posts/2015-08-Understanding-LSTMs/

Role of activation functions

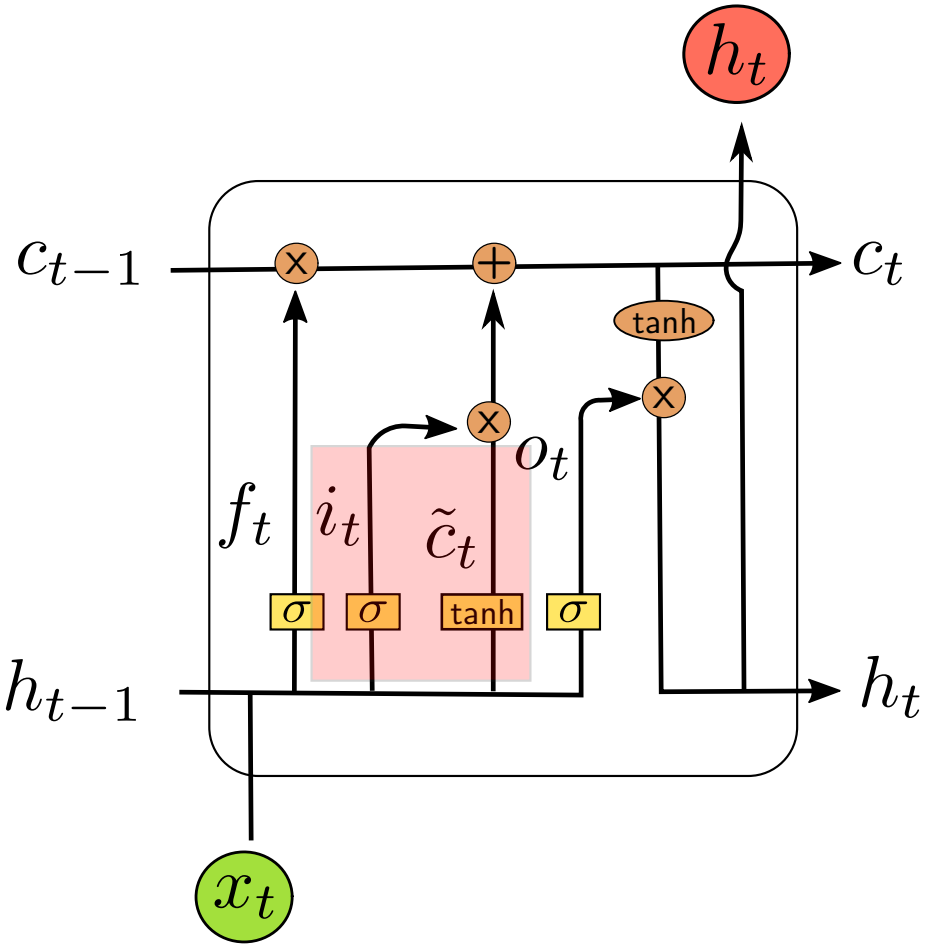
- Gates use as activation functions the sigmoid and tanh functions
- Their role is to perform fuzzy decisions
  - **tanh**: squashes value to range `[-1,1]` (substract, neutral, add)
  - **sigmoid**: squashes value to range `[0,1]` (closed, open)

LSTMs computations



$$f_t = \sigma(W_f \cdot [h_{t-1}, x_t]) \text{ (Forget)}$$

LSTMs computations

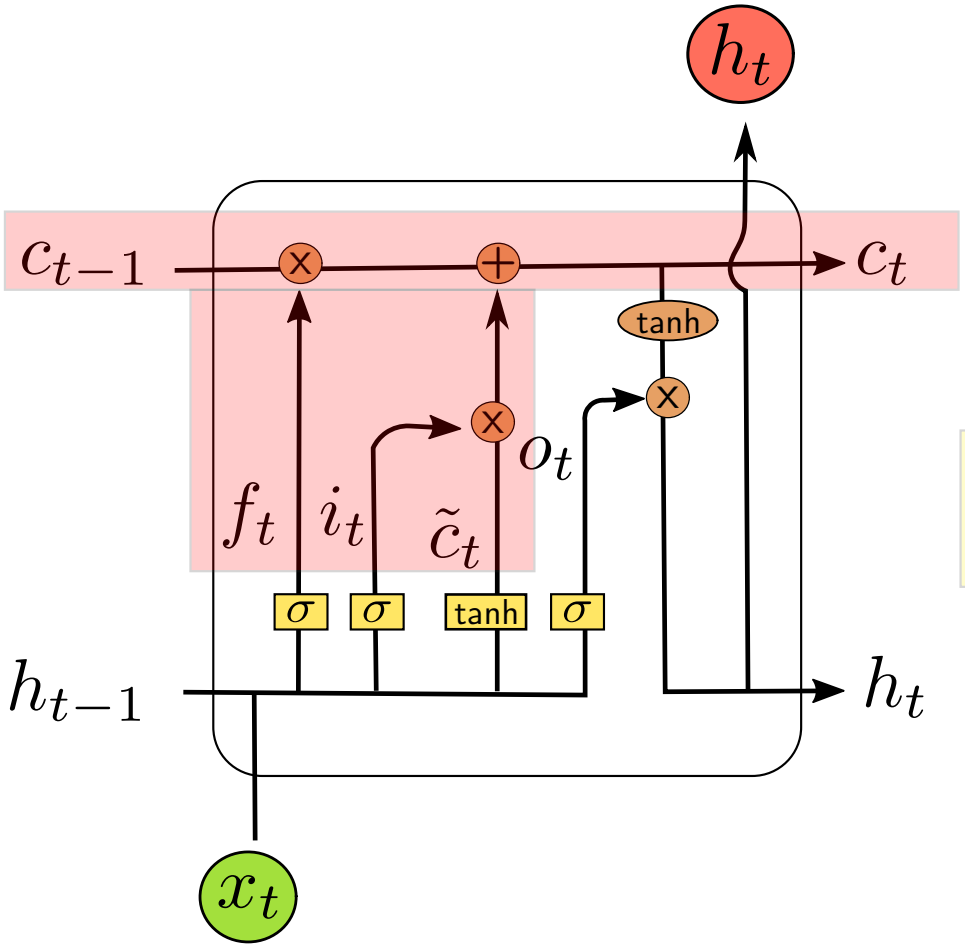


$$f_t = \sigma(W_f \cdot [h_{t-1}, x_t]) \text{ (Forget)}$$

$$i_t = \sigma(W_i \cdot [h_{t-1}, x_t]) \text{ (Input)}$$

$$\tilde{c}_t = tanh(W_c \cdot [h_{t-1}, x_t])$$

LSTMs computations



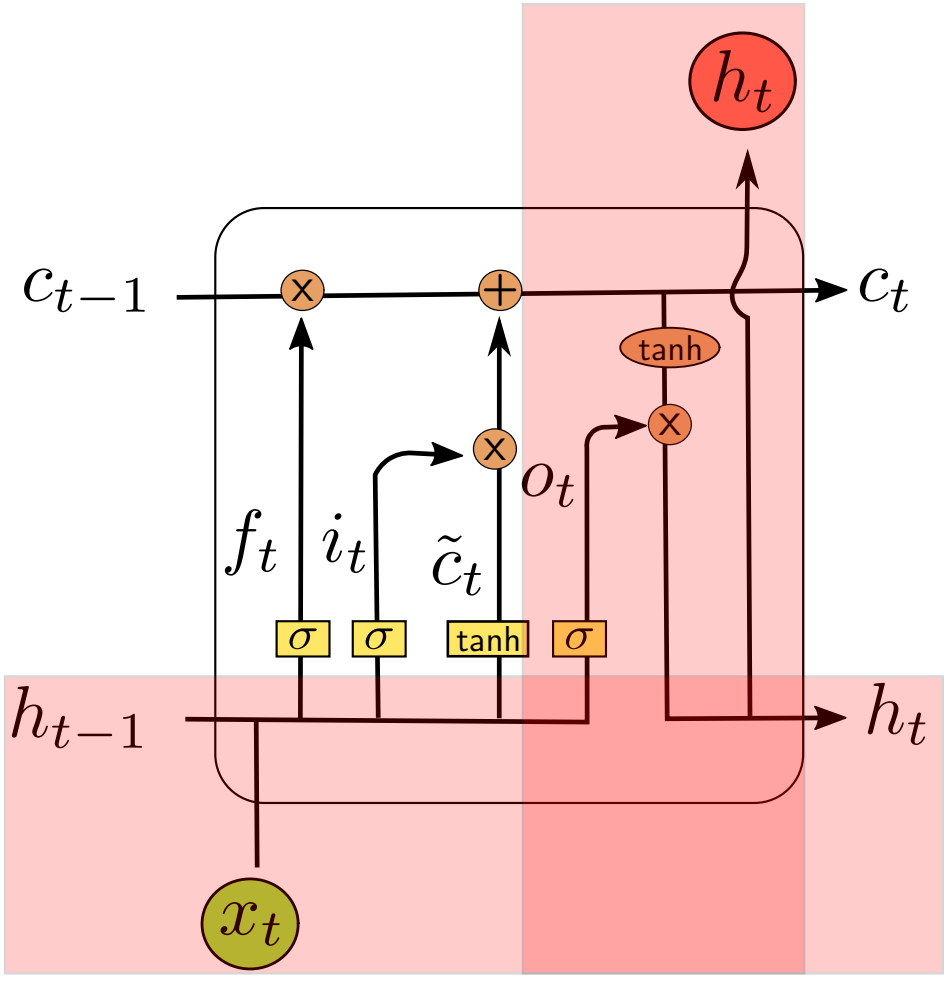
$$f_t = \sigma(W_f \cdot [h_{t-1}, x_t]) \text{ (Forget)}$$

$$i_t = \sigma(W_i \cdot [h_{t-1}, x_t]) \text{ (Input)}$$

$$\tilde{c}_t = tanh(W_c \cdot [h_{t-1}, x_t])$$

$$c_t = f_t \times c_{t-1} + i_t \times \tilde{c}_t \text{ (Update)}$$

LSTMs computations



$$f_t = \sigma(W_f \cdot [h_{t-1}, x_t]) \text{ (Forget)}$$

$$i_t = \sigma(W_i \cdot [h_{t-1}, x_t]) \text{ (Input)}$$

$$\tilde{c}_t = tanh(W_c \cdot [h_{t-1}, x_t])$$

$$c_t = f_t \times c_{t-1} + i_t \times \tilde{c}_t \text{ (Update)}$$

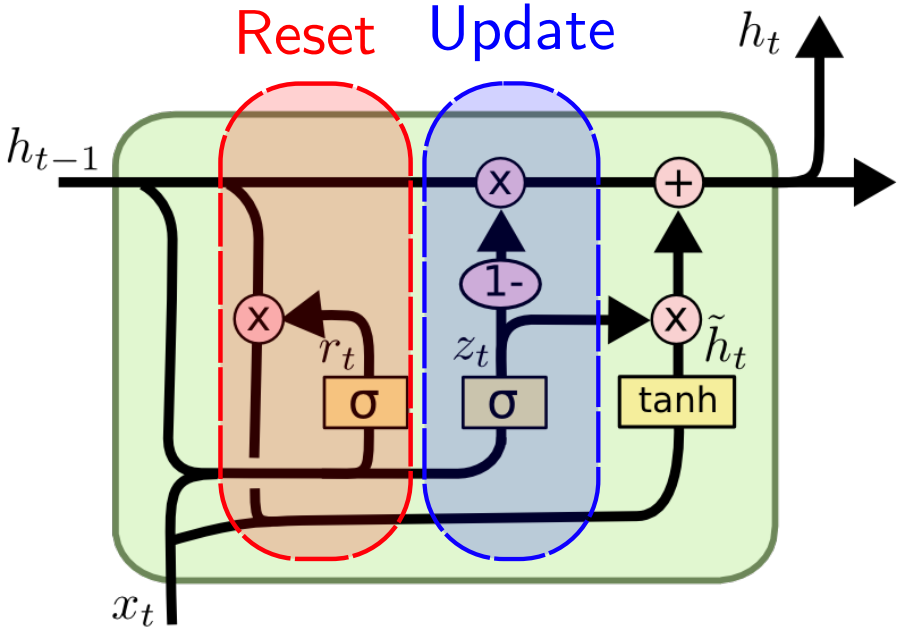
$$o_t = \sigma(W_o \cdot [h_{t-1}, x_t])$$

$$h_t = o_t \times tanh(c_t) \text{ (Output)}$$

GRUs

Gated Recurrent Units

- Reduces the complexity of LSTMs
- Unifies the forgetting and the update gates as a unique update gate
- The update gate computes how the input and previous state are combined
- A reset gate controls the access to the previous state
  - near to one previous state has more effect
  - near to zero new state (updated) has more effect



$$z_t = \sigma(W_z \cdot [h_{t-1}, x_t]) \text{ (upd)}$$

$$r_t = \sigma(W_r \cdot [h_{t-1}, x_t]) \text{ (res)}$$

$$\tilde{h}_t = tanh(W_h \cdot [r_t \times h_{t-1}, x_t])$$

$$h_t = (1 - z_t) \times h_{t-1} + z_t \times \tilde{h}_t$$

Pros/Cons

Vanilla RNN vs LSTMs vs GRUs

- Empirically Vanilla RNN underperforms on complex tasks
- LSTMs are widely used but GRUs are very recent (2014)
- There is not yet theoretical arguments in the LSTMs vs GRUs question
- Empirical studies do not shed light to the question (see references)

- Jozefowicz, R., Zaremba, W., Sutskever, I. (2015). An empirical exploration of recurrent network architectures. In Proceedings of the 32nd International Conference on Machine Learning (ICML-15) (pp. 2342-2350).

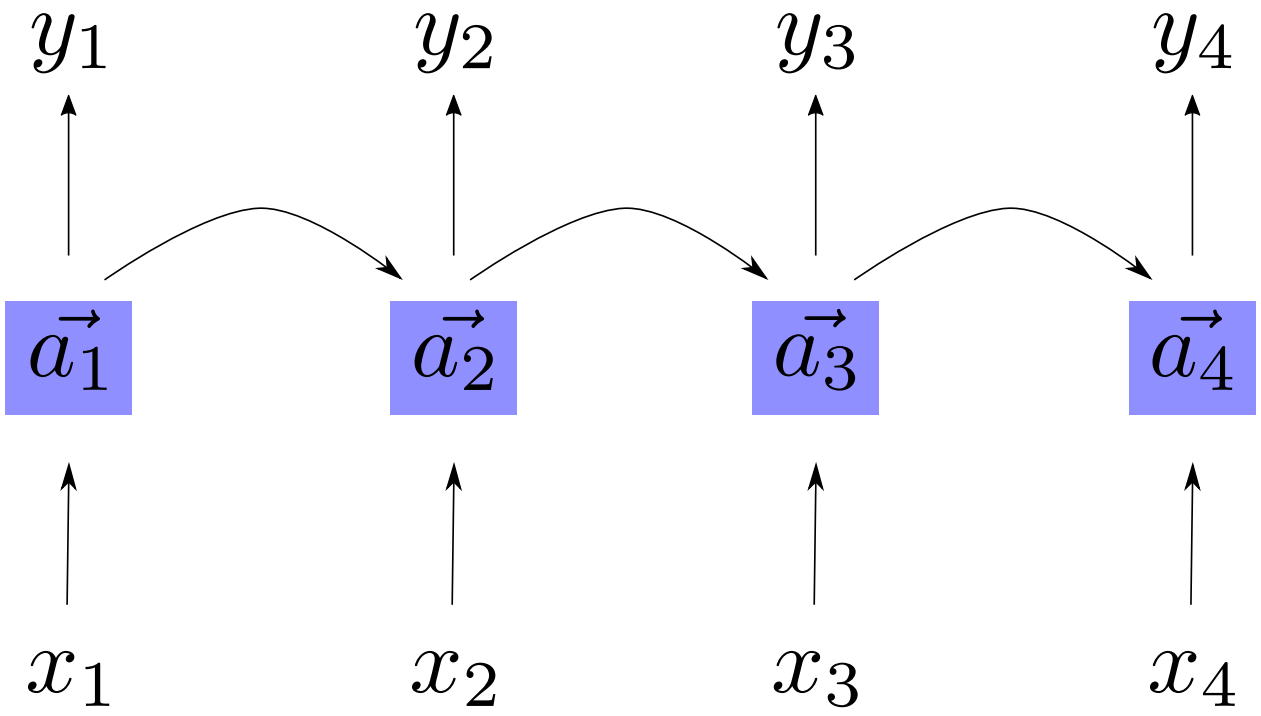
- Chung, J., Gulcehre, C., Cho, K., Bengio, Y. (2014).Empirical evaluation of gated recurrent neural networks on sequence modeling. arXiv preprint arXiv:1412.3555.

RNNs Variations

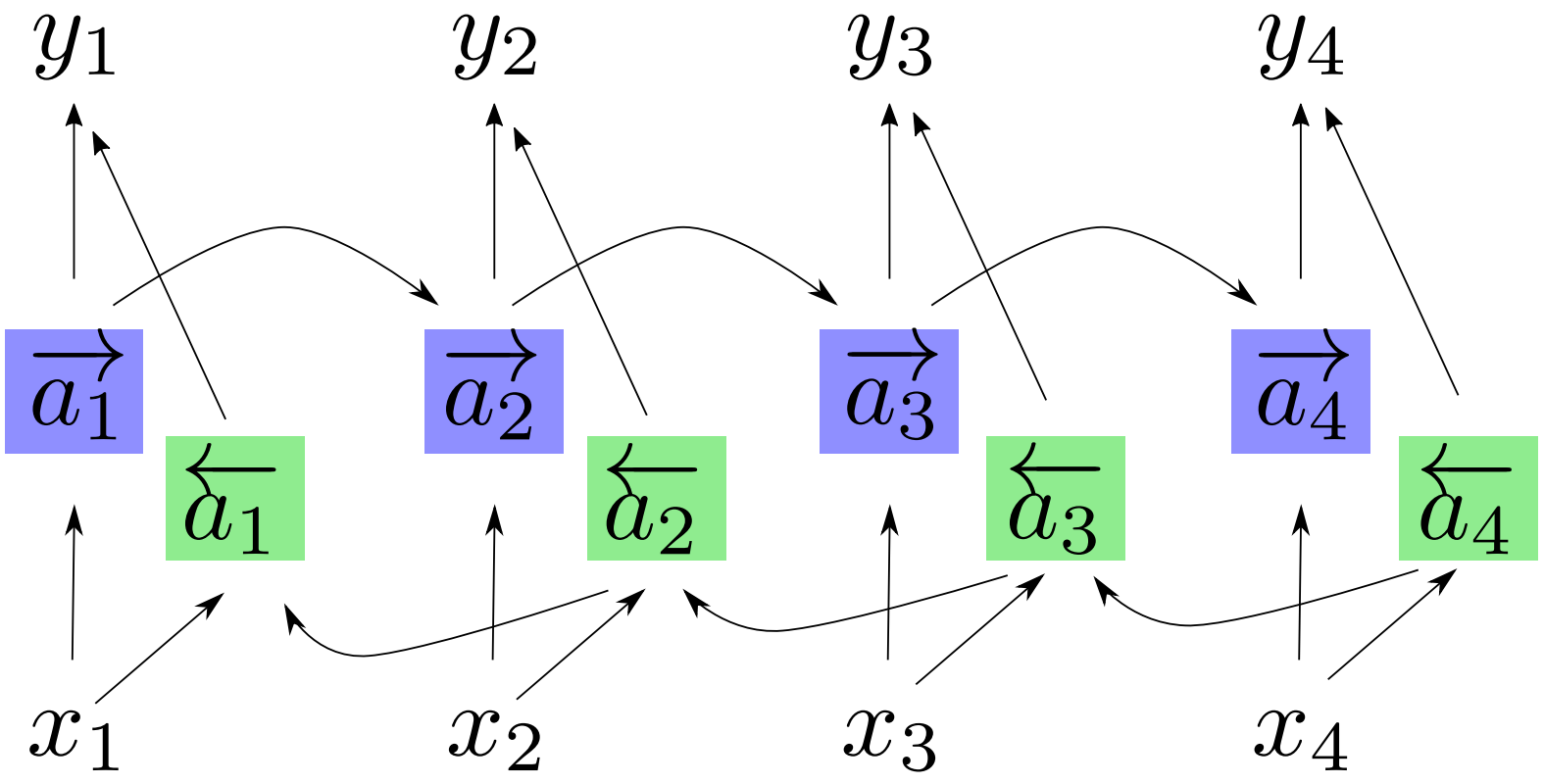
Bidirectional RNNs - Back from the future

- In some domains it is easier to learn dependencies if information flows in both directions
- For instance, domains where decisions depend on the whole sequence
  - Part of Speech tagging
  - Machine translation
  - Speech/handwritting recognition
- A RNN can be split in two, so sequences are processed in both directions

Regular RNNs (only forward)



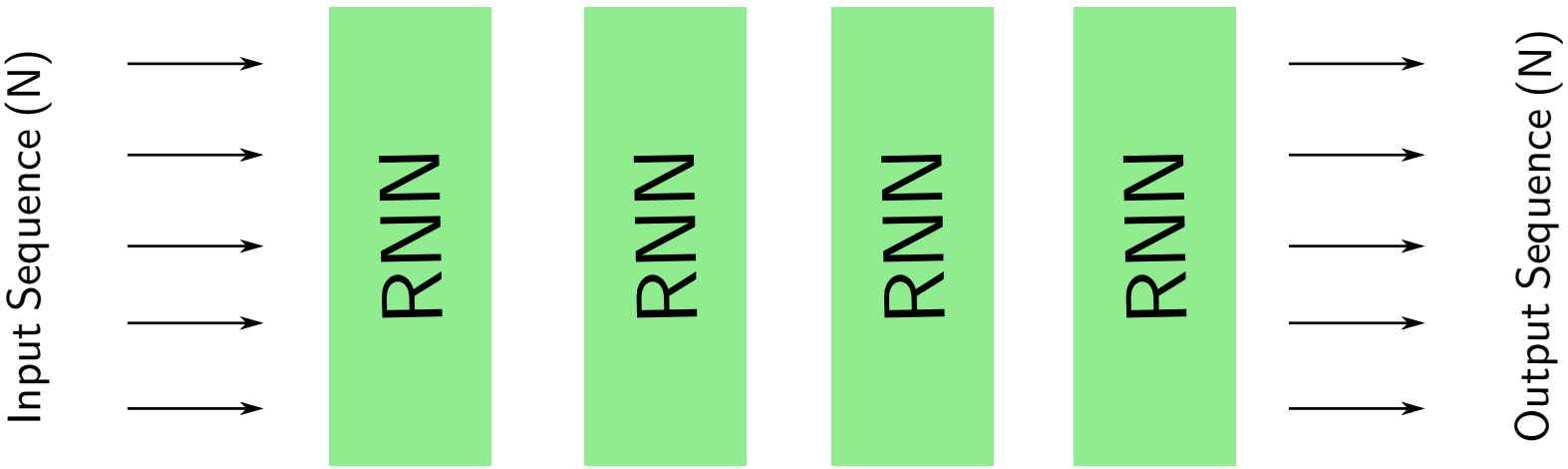
Bidirectional RNNs (forward-backward)



Bidirectional RNNs - Training

- Both directions are independent (no interconnections)
- Backpropagation needs to follow the graph dependencies, not all weights can be updated at the same time
  - Propagating Forward: Pass the input sequence as is and reversed through the RNNs, then compute the outputs using matching steps
  - Propagating Backward:: Pass the error backwards from the outputs through the RNNs (both directions), back propagate to the inputs using matching steps

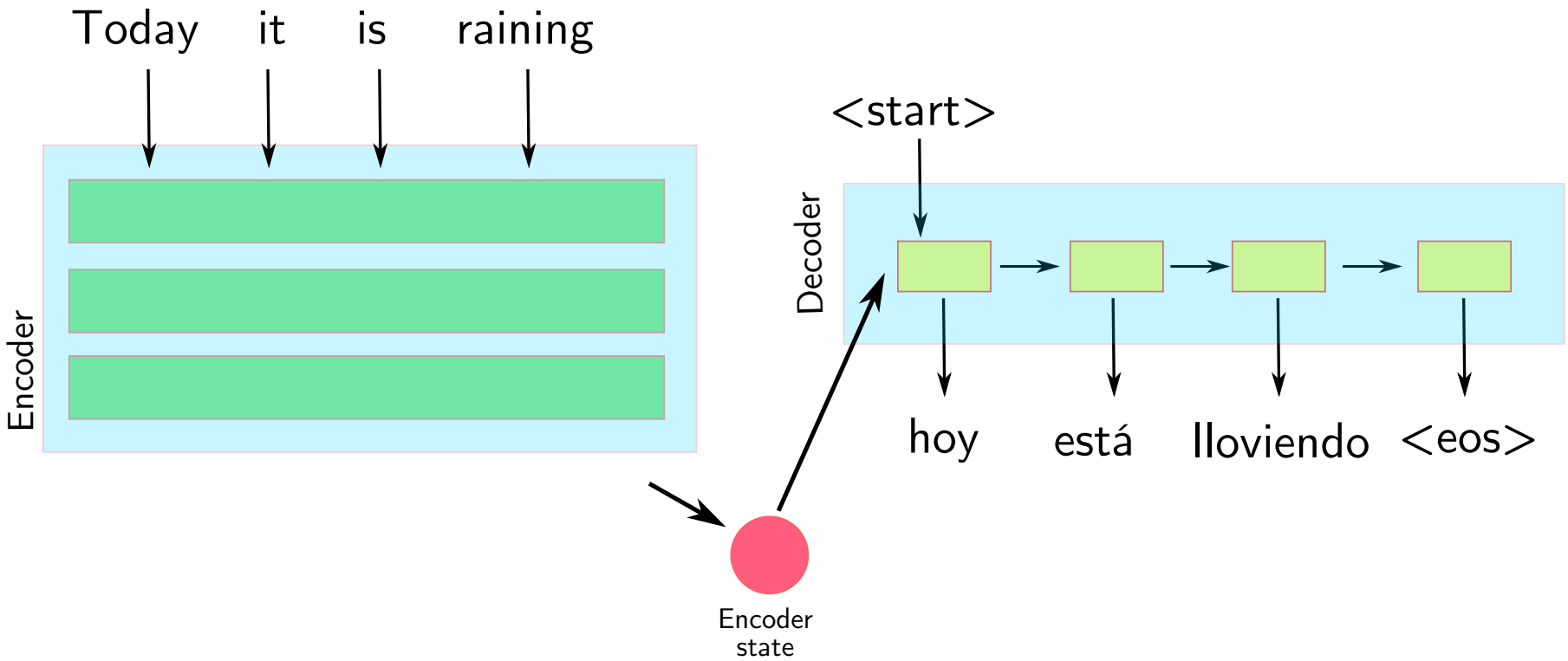
- Direct sequence association
  - Input and output sequences have the same lengths
  - All the outputs of the BPTT are used for the output
  - Training is straightforward



Encoder-decoder architecture

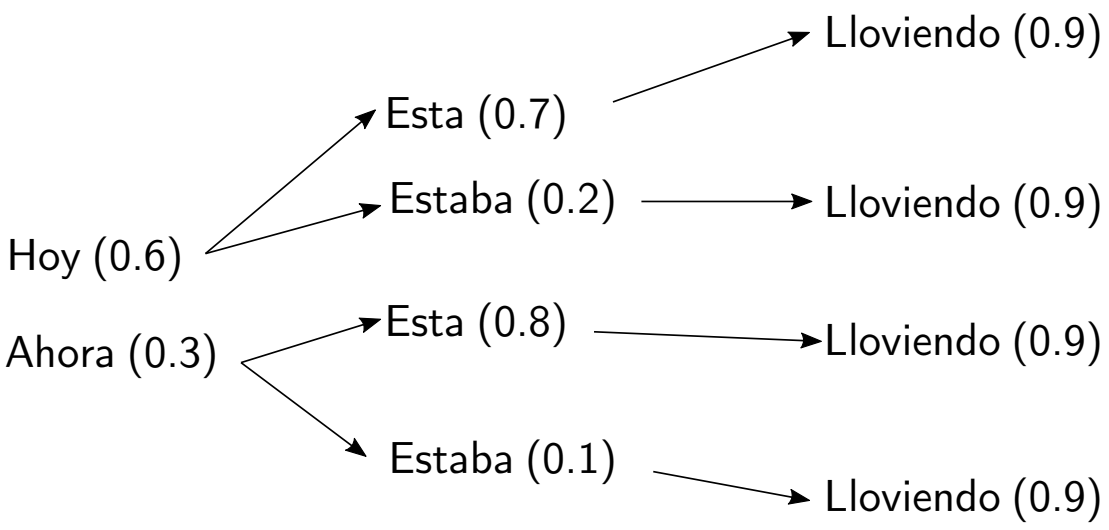
- Input and output sequences can have different lengths
- Encoder RNN summarizes input in a coding state
- Decoder RNN generates output from that state
- Different options connecting Encoder-Decoder (direct, peeking, attention) or training (teacher forcing)
- Inference: The sequence is generated element by element using the output of the previous step or using a beam search

Encoder-Decoder (Plain)

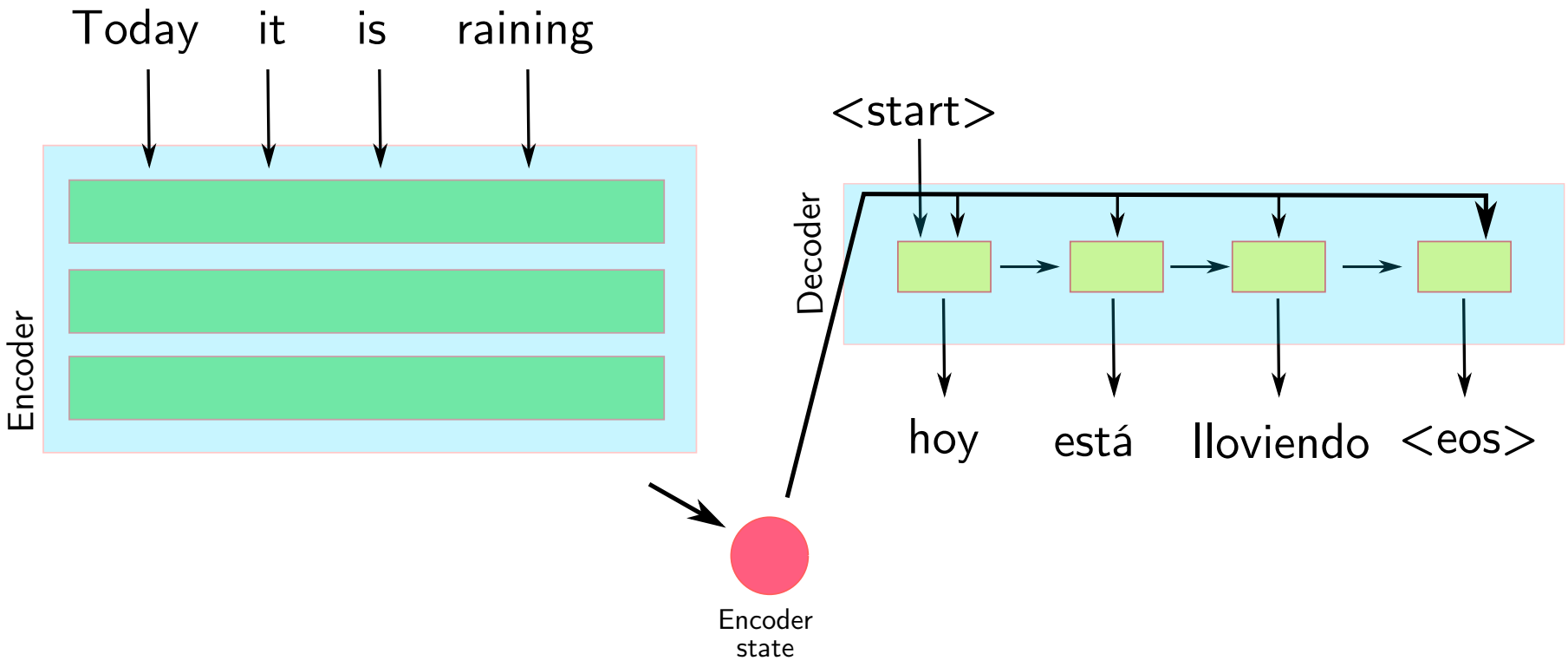


Encoder-Decoder (Plain) - Inference

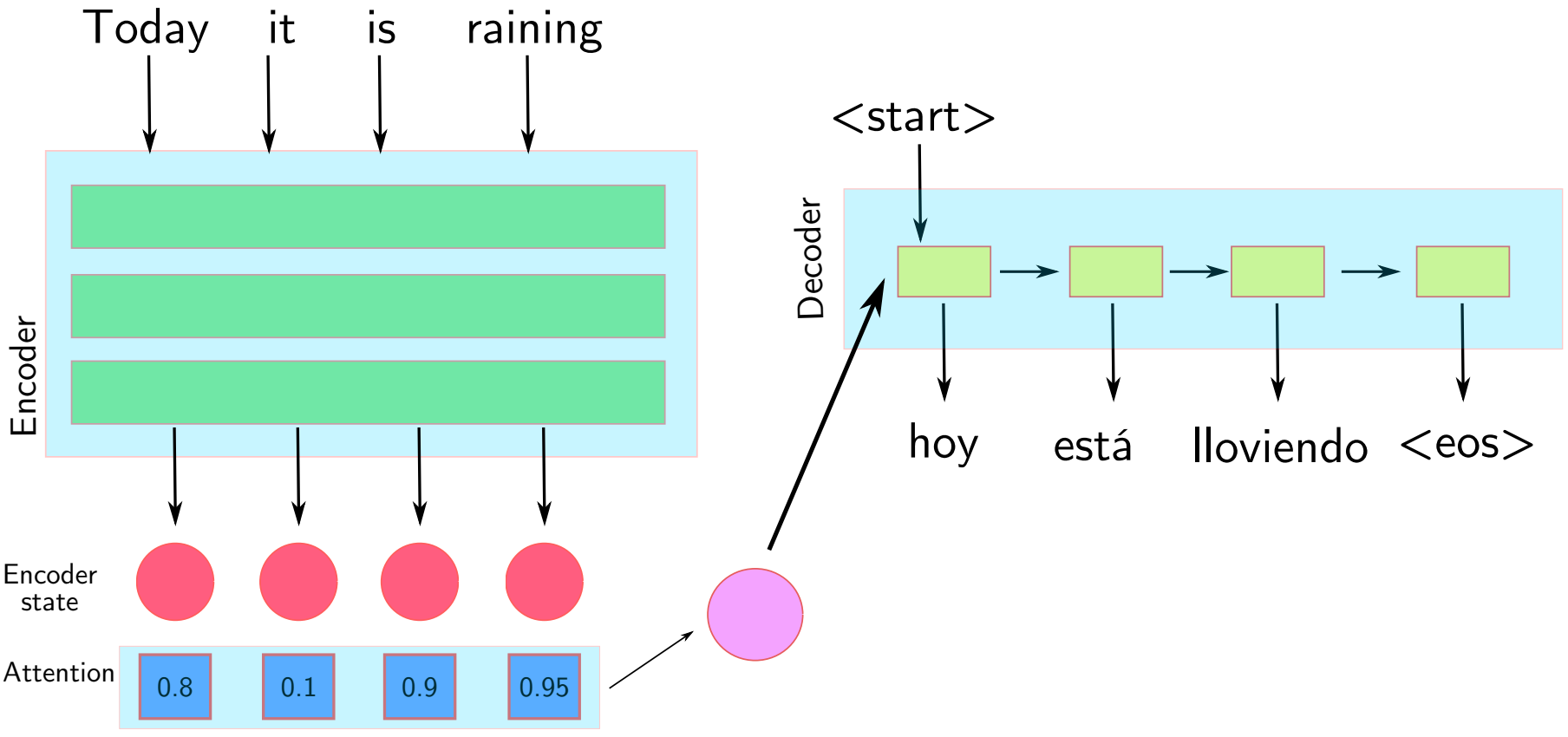
- When generating a sequence of discrete values, the greedy approach could not be the best policy
- A limited exploration of the branching alternatives is needed (beam search)
- The sequence with the largest joint probability is the sequence generated



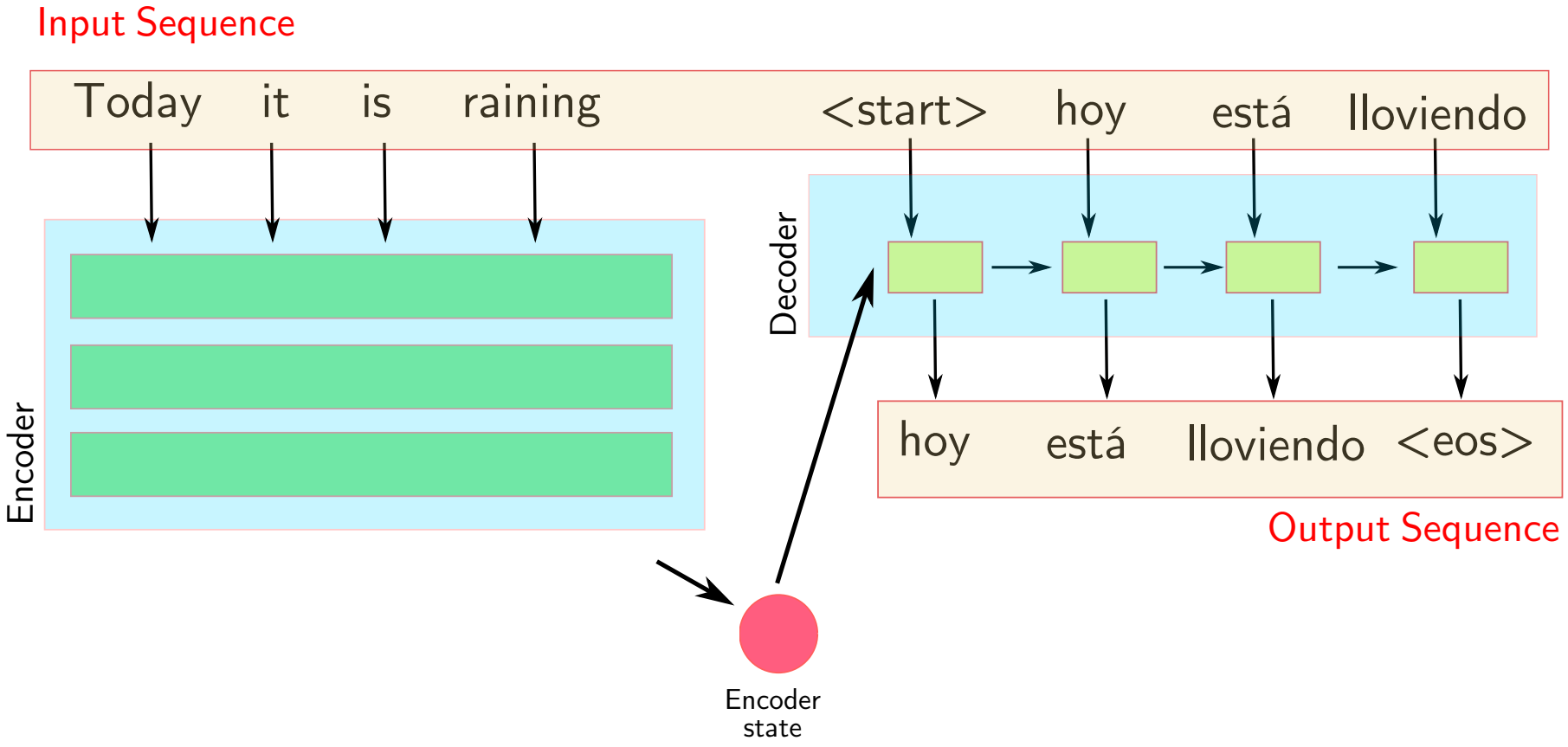
Encoder-Decoder (Peeking)



Encoder-Decoder (Attention)



Encoder-Decoder (Teacher Forcing)



- RNNs are Turing complete, but it is difficult to achieve it in practice
- New architectures include:
  - Data structures to store information (Read/Write Operations)
  - RNNs control the operations
  - Attention mechanisms
- Graves, Wayne, Danihelka **Neural Turing Machines**, ArXiv preprint arXiv:1410.5401
- C. Olah, S. Carter, Attention and Augmented Recurrent Neural Networks, Distill, Sept 9, 2016

Guided Laboratory

Sequence prediction

- Sequence to value
  - Predicting the next step of a time series
  - Classification of time series
  - Predicting sentiment from tweets
  - Text generation (predicting characters)
- Sequence to sequence
  - Learning to add

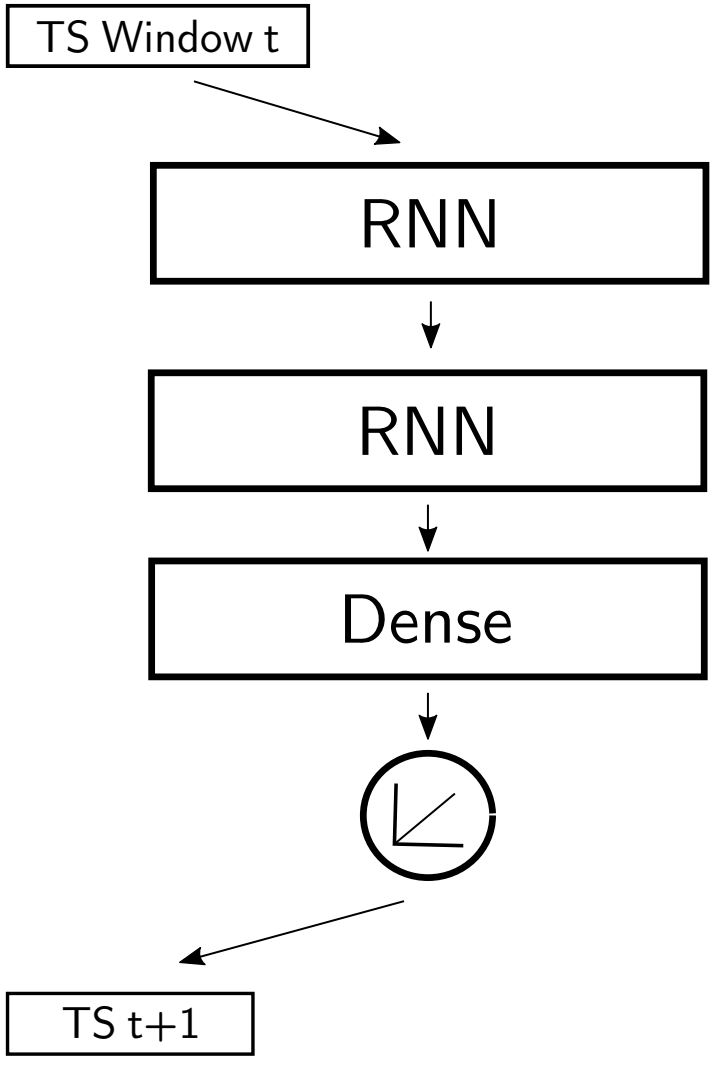
- Time series regression
- Dataset: Air Quality every hour
- Goal: Predict air quality next hour

Training time

35064 Train/ 8784 Test/6 lag

32 Neurons /1 Layer/30 epochs

$\sim$ 30 sec

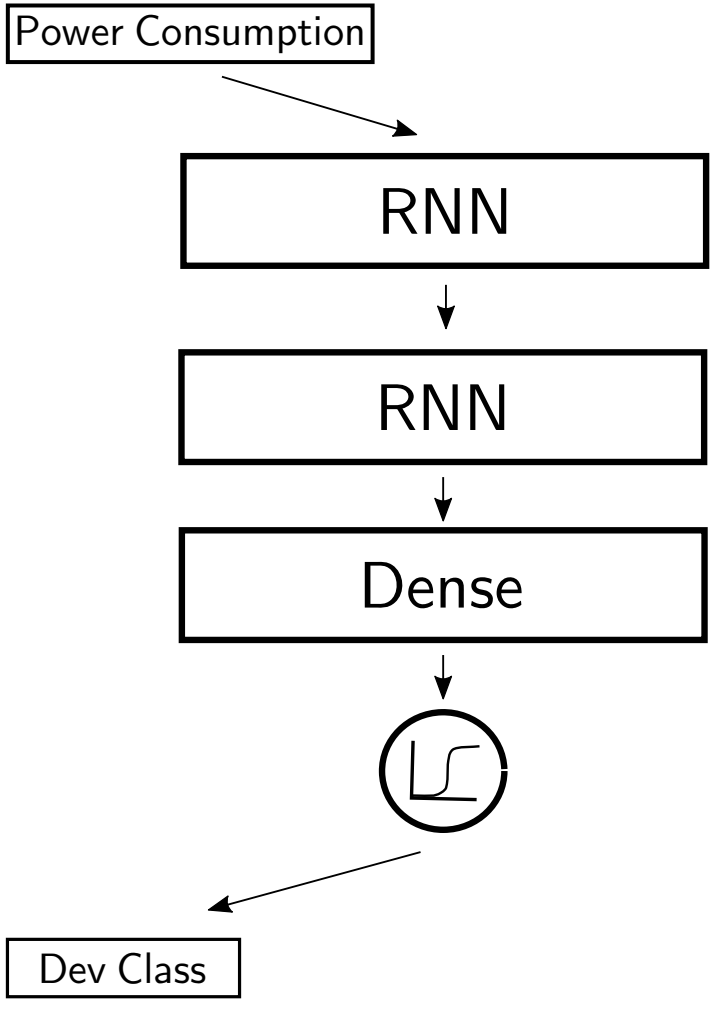


- Time series classification
- Daily power consumption of household devices (7 classes, 96 attributes)
- Goal: Predict household device class

Training time

64 Neurons /2 Layers/30 epochs

$\sim$ 1 min



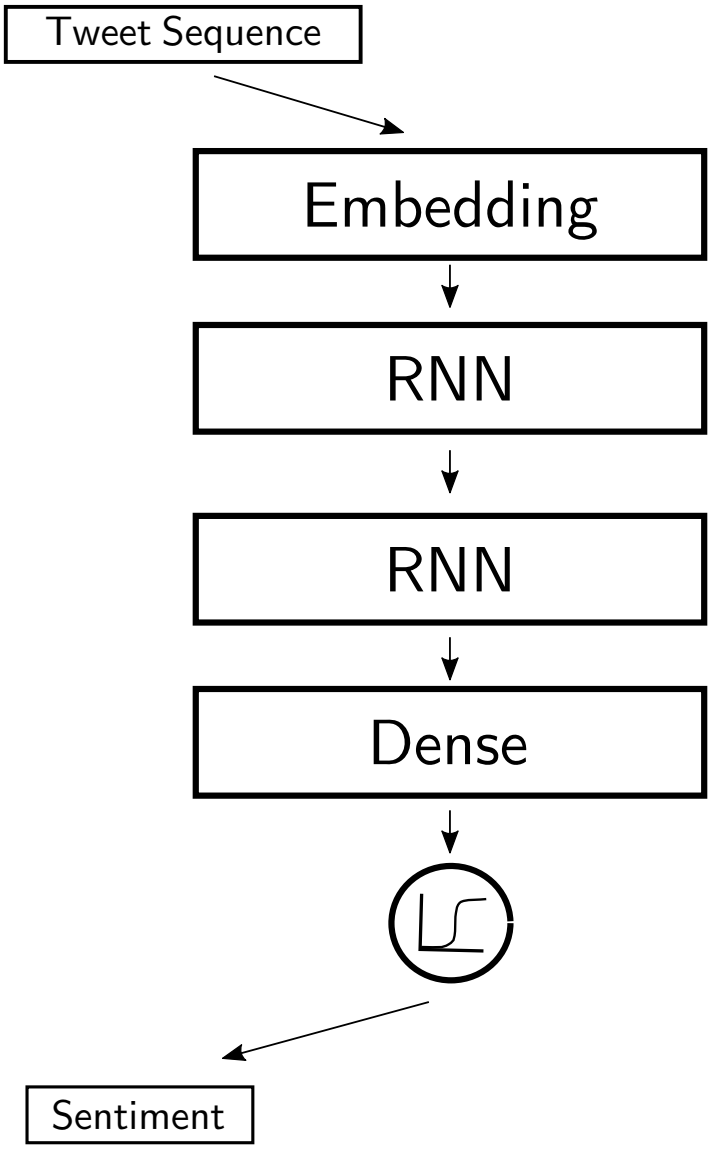
- Tweets (neg, pos, neutral)
- Tweets as sequences of words
- Preprocess: Generate vocabulary, recode sequences
- Embed sequences to a more convenient space

Training time

5000 words/ 40 dim embedding

64 Neurons /1 Layer/50 epochs

$\sim$ 3 min



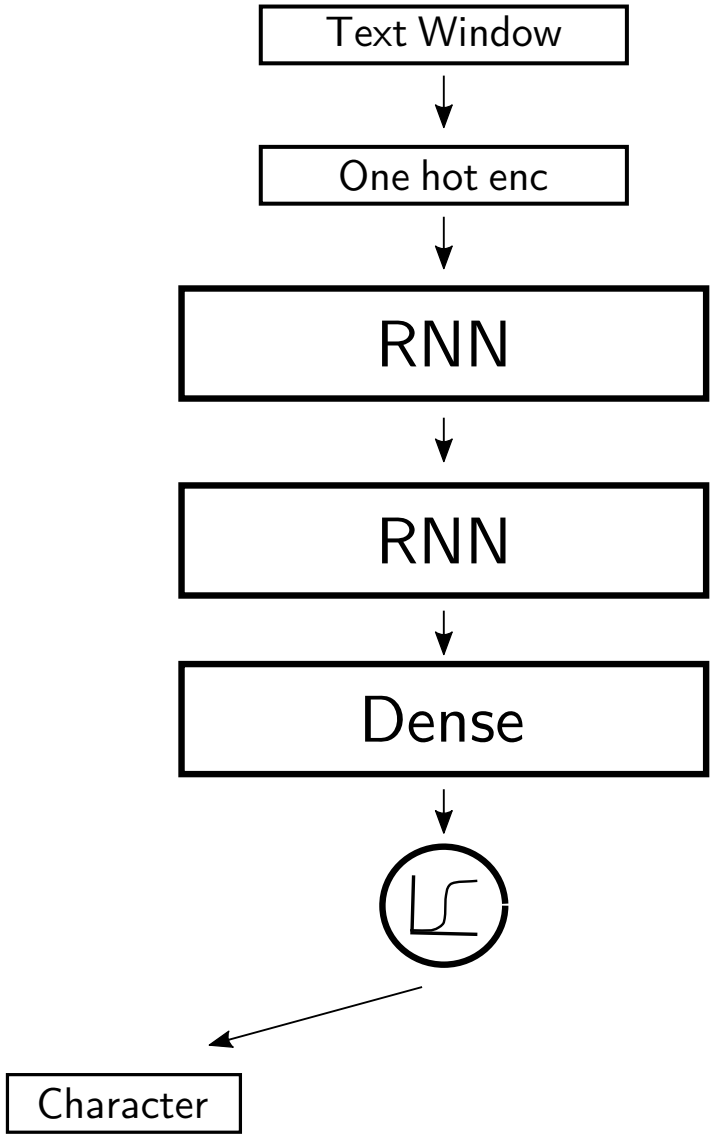
- Poetry text
- Character prediction from text windows
- Preprocess: sequences of characters' one hot encoding
- Text generation by predicting characters iteratively

Training time

poetry1/50 chars/3 skip

64 Neu/1 Ly/10 it/10 ep_it

$\sim$ 23 min



- Predicting addition results from text
- Input sequence: `NUMBER+NUMBER`
- Output sequence: `NUMBER`
- Preprocess: sequences of characters' one hot encoding
- RNN Encode + RNN Decode

Training time

50000 ex/3 digits

128 Neu/1 Ly/50 ep

$\sim$ 5 min 30 sec

Task 5: Learning to add