

Recurrent Neural Networks

deep learning 3

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Motivation

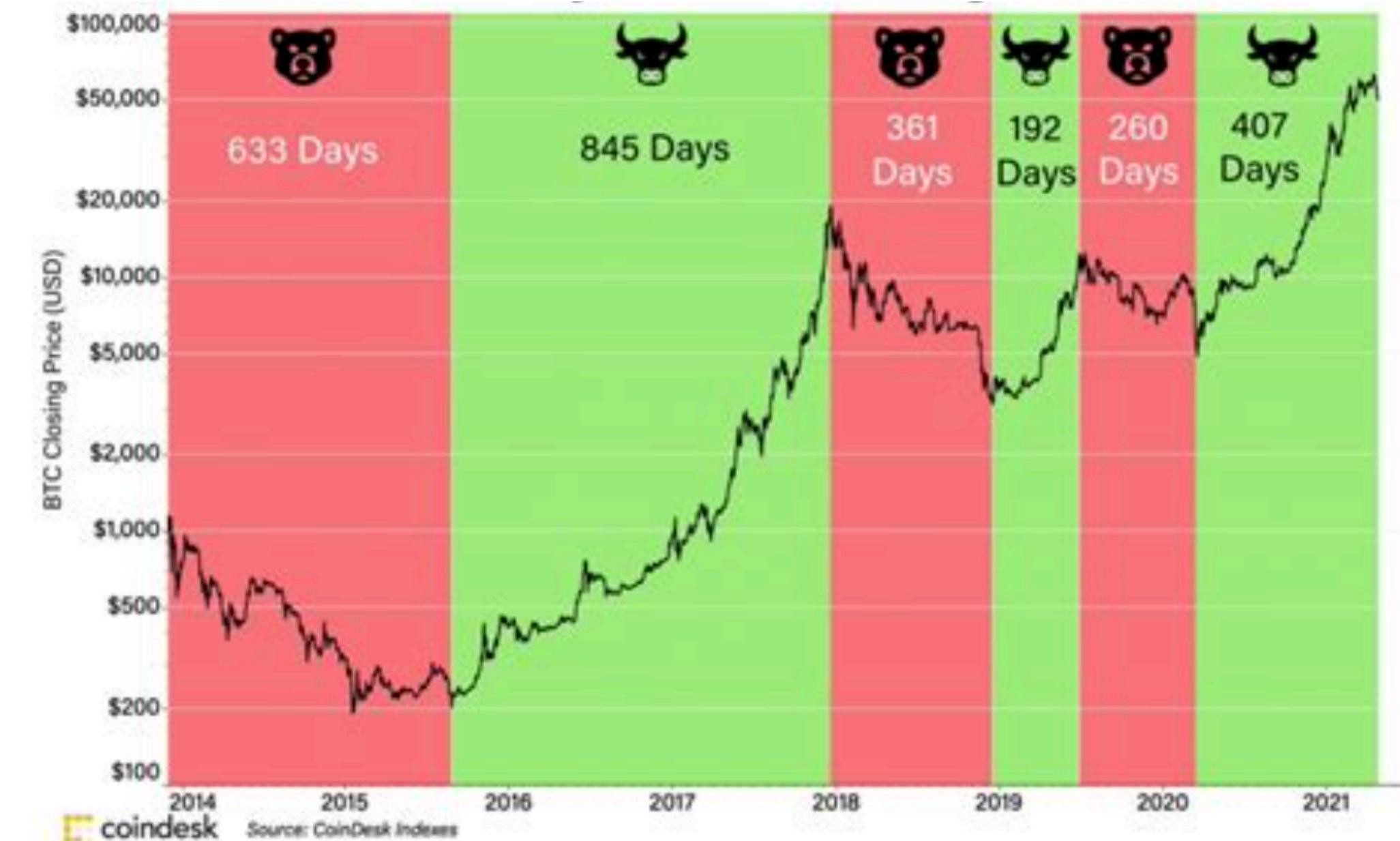
A lot of data is sequential, varying over time:

- Sentences
- Music
- EEG
- Movement
- Markets

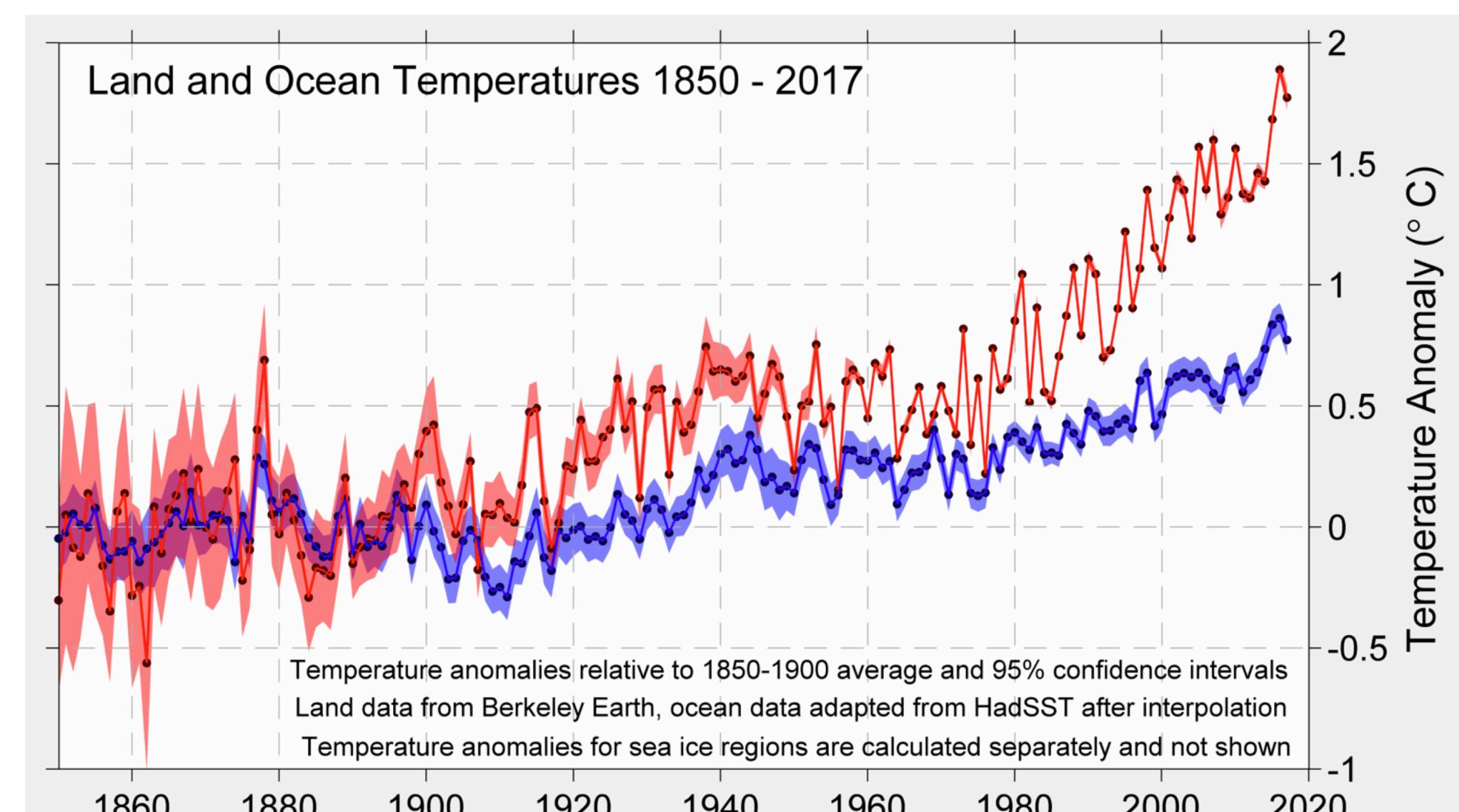
Motivation

With sequences, the past offers context:

- Ik krijg geld van de **bank**
- Ik wil een nieuwe **bank** aanschaffen



We need the past to make sense of the future.



Data considerations

We need to worry about:

- How much of the past will we need (window)
- How much of the future do we want to predict (horizon)
- How to prepare the data without leaking data

For the last point, we need to be very careful not to “leak” the future back into the present.

History of RNNs

The timeseries of timeseries

- 1982 RNN are discovered by John Hopfield
- 1995 The LSTM architecture was proposed with input and output gates
- 1999 Forget gates were added
- 2009 LSTM won the handwriting recognition competition
- 2013 LSTM outperformed other models at natural speech recognition
- 2014 GRU architecture was introduced
- 2017 probabilistic forecasting (DeepAR, MQRNN, TFT)

Simple RNN

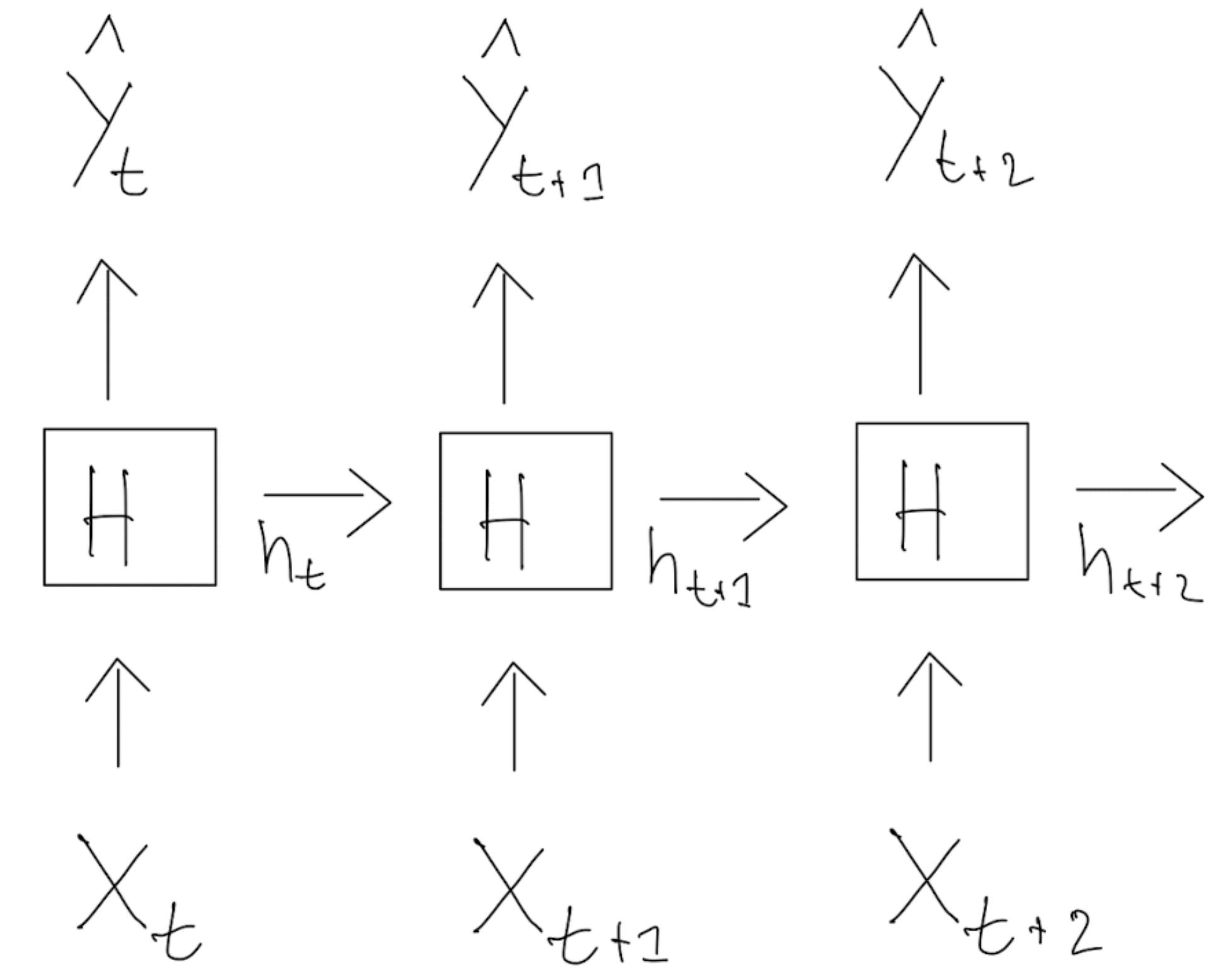
We start with a simple neural network H

To add time, we introduce the concept of a hidden state h_t that we pass on.

While this might look confusing at first, there is just a small difference with the

$$\hat{y} = \sigma(WX + b)$$

formula we have been using so far.



Simple RNN

To incorporate the hidden state, we simply add it:

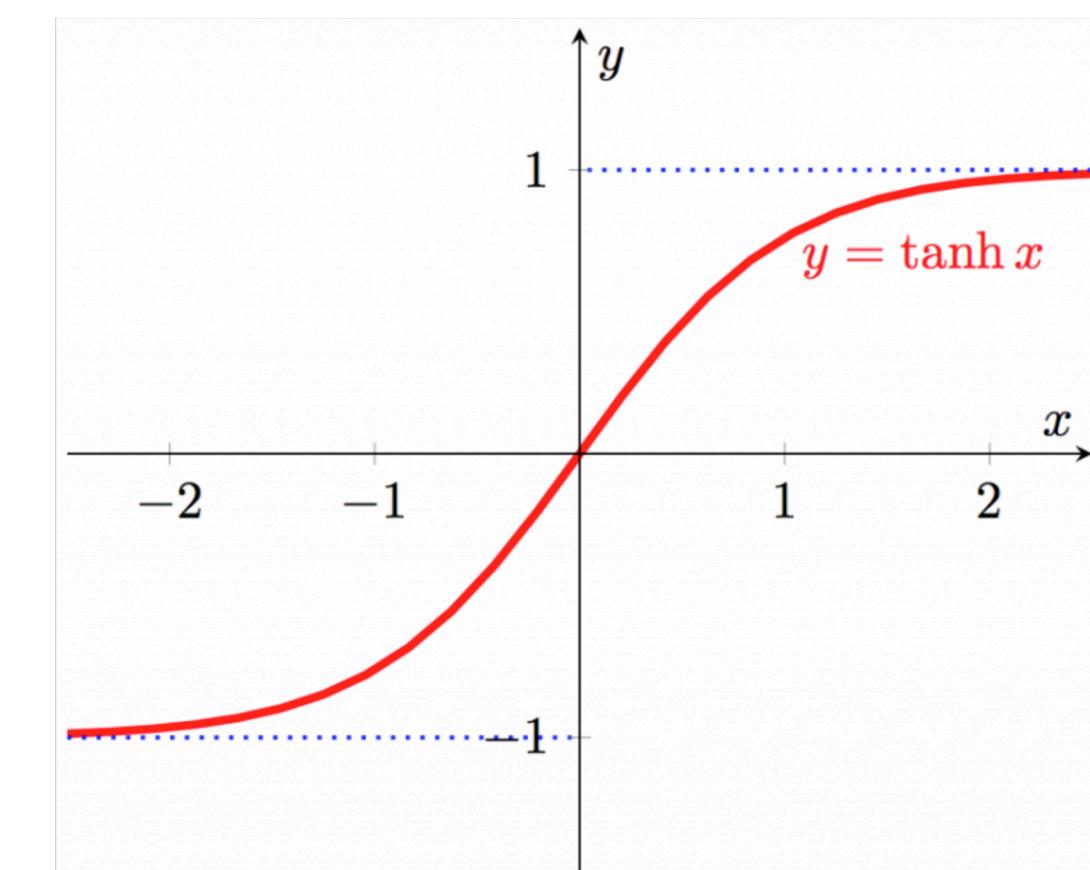
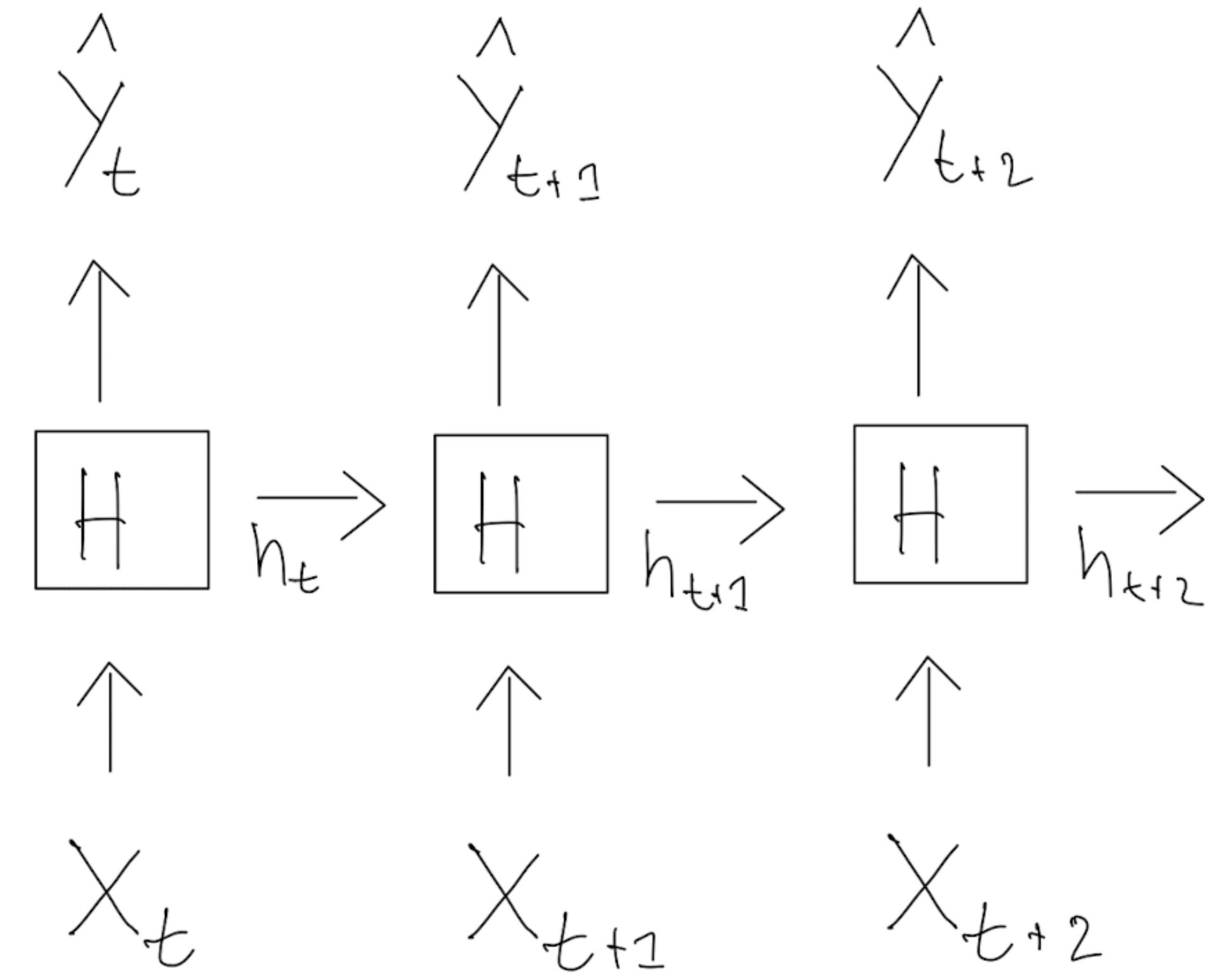
$$h_t = \sigma(W_x X_t + W_h h_{t-1} + b)$$

This is equivalent to

$$h_t = \sigma(W[X_t, h_{t-1}] + b)$$

where $[X, h]$ means concatenate

σ is an activation function, typically *tanh*



The art of forgetting

Even E.Coli has a memory

RNNs have not explicit way to forget or retain memory.

We can make this a bit more advanced by adding gates.

A gate Γ controls

- what part of the past we retain
- what part we forget.

GRU - Gated Residual Unit

I keep forgetting how GRUs work

We need to be able to:

- *Remember* the past, and completely ignore the new state
- *Forget* the past, and focus on the present
- *Something in between* where we find a ratio between forgetting and remembering.

We also want to gate to be influenced by both the new input and the old state.

GRU - Gated Residual Unit

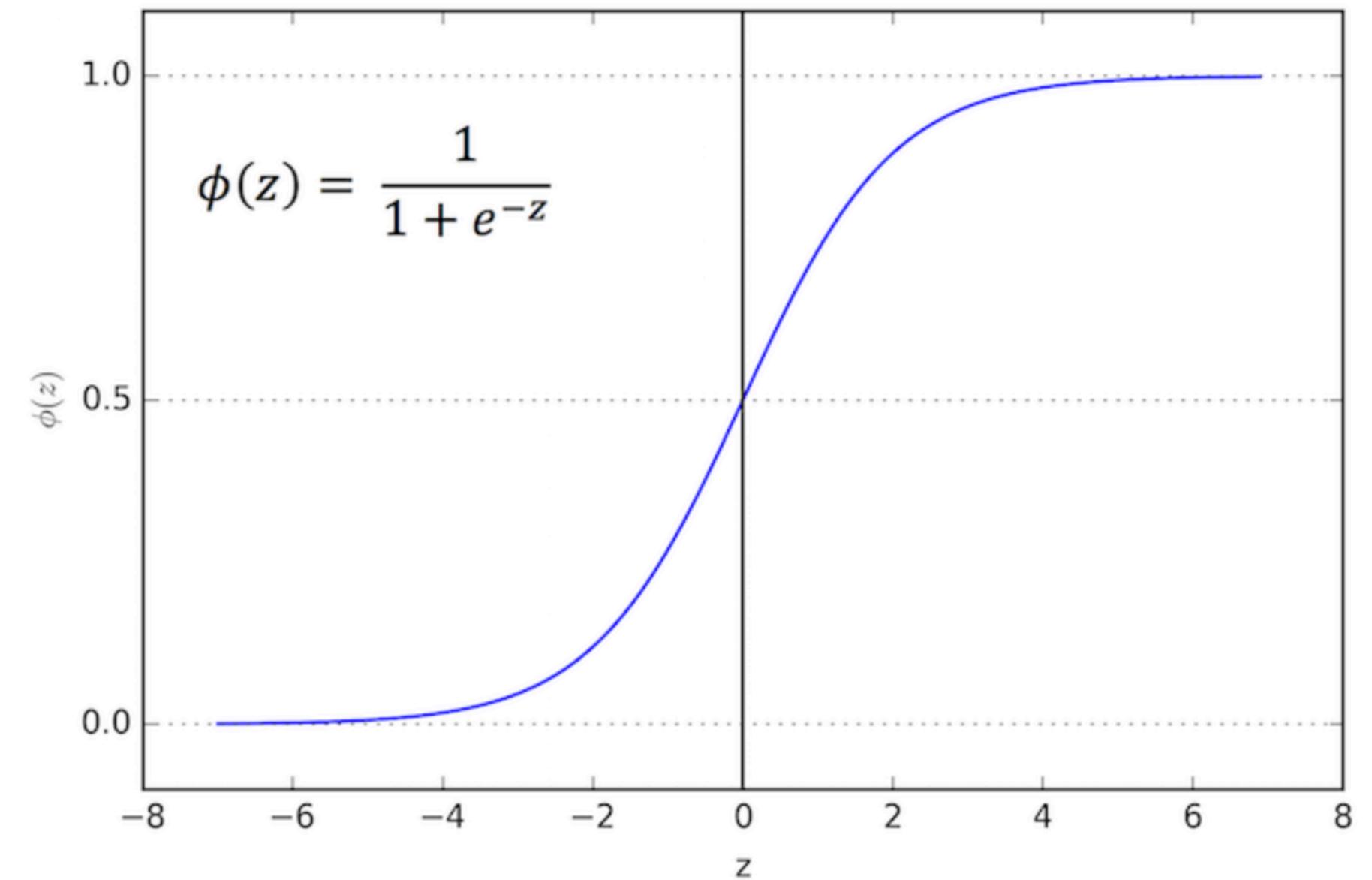
you shall not pass

To create a gate, we will use a sigmoid activation and pick a W such that Γ has the same dimensions as X :

$$\Gamma = \sigma(W[X_t, h_{t-1}] + b)$$

This gives us numbers of the **same shape** as the input, **between [0,1]**

To apply the gate, we will use what is called a Hadamard product \otimes



$$\begin{bmatrix} 1.0 & 2.0 \\ 0.5 & -2.4 \end{bmatrix} \otimes \begin{bmatrix} 0.9 & 0.01 \\ 0.5 & 0.2 \end{bmatrix} = \begin{bmatrix} 0.9 & 0.04 \\ 0.25 & -0.48 \end{bmatrix}$$

X Γ output

GRU - simplified

Concatenate state, create gate, hadamard

The GRU creates

- a *candidate state* \tilde{h}
- a gate Γ

and the gate Γ decides, based on context, how much of the past is remembered. The W and b in the formulas below are different weights, but I left out the subscripts to simplify the formula.

$$\Gamma = \sigma(W[X_t, h_{t-1}] + b)$$

$$\tilde{h}_t = \tanh(W[X_t, h_{t-1}] + b)$$

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

GRU - full

The full GRU has two gates, but the principle is the same

$$\Gamma_u = \sigma(W[X_t, h_{t-1}] + b)$$

$$\Gamma_r = \sigma(W[X_t, h_{t-1}] + b)$$

$$\tilde{h}_t = \tanh(W[X_t, \Gamma_r \otimes h_{t-1}] + b)$$

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

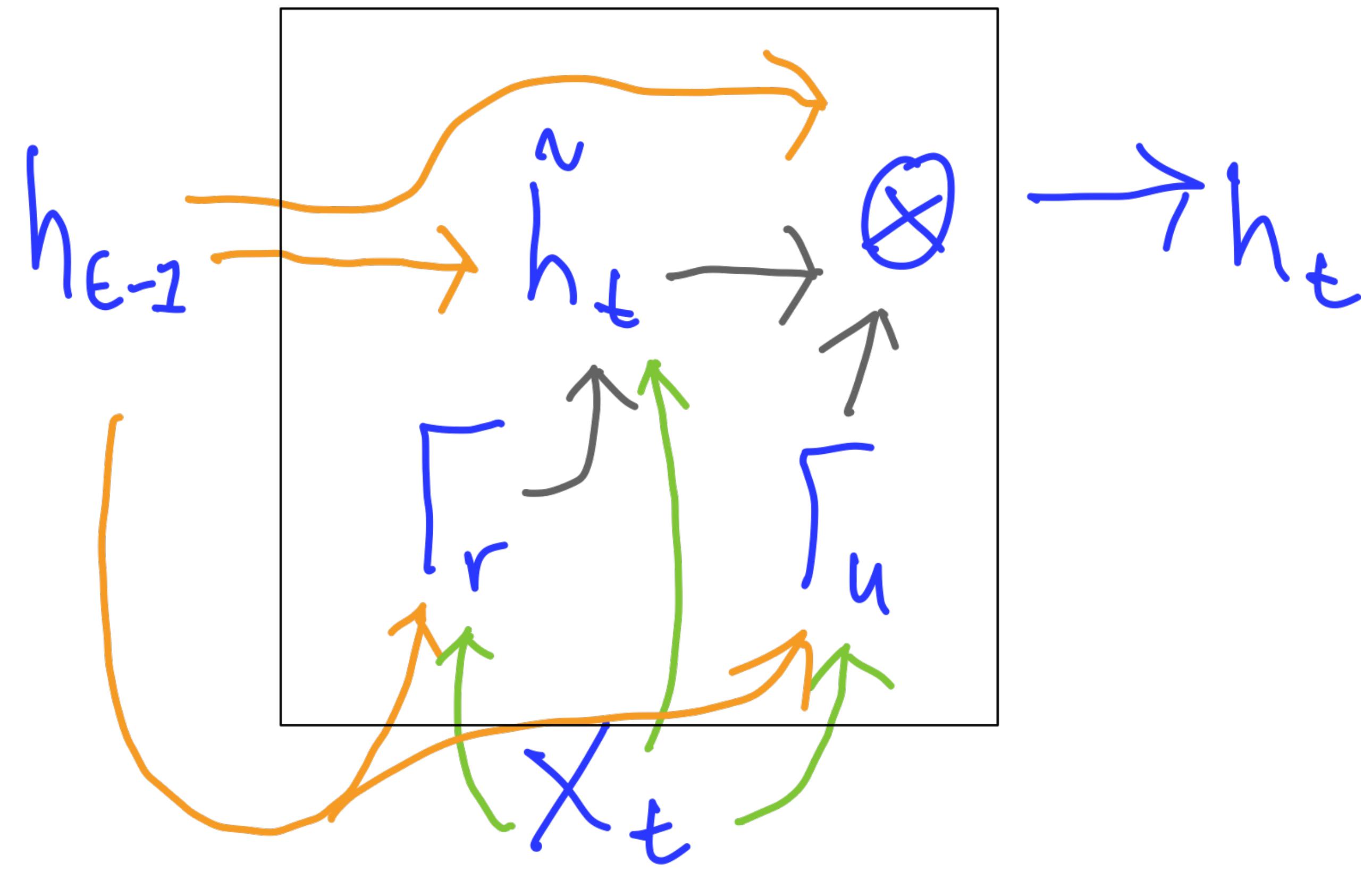
GRU

The same, but rephrased

We use the hidden state h_{t-1} and X_t to create two gates.

The reset gate Γ_r controls how much of the past h_{t-1} is mixed into X_t to create a new candidate context \tilde{h}

The other gate is the update gate Γ_u and this balances the old h_{t-1} and the new \tilde{h}_t



GRU

Implemented in Python

Compare the [Trax implementation](#) with the formulas

$$\Gamma_u = \sigma(W[X_t, h_{t-1}] + b)$$

$$\Gamma_r = \sigma(W[X_t, h_{t-1}] + b)$$

$$\tilde{h}_t = \tanh(W[X_t, \Gamma_r \otimes h_{t-1}] + b)$$

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

```
def forward(self, inputs):
    x, gru_state = inputs

    # Dense layer on the concatenation of x and h.
    w1, b1, w2, b2 = self.weights
    y = jnp.dot(jnp.concatenate([x, gru_state], axis=-1), w1) + b1

    # Update and reset gates.
    u, r = jnp.split(fastmath.sigmoid(y), 2, axis=-1)

    # Candidate.
    c = jnp.dot(jnp.concatenate([x, r * gru_state], axis=-1), w2) + b2

    new_gru_state = u * gru_state + (1 - u) * jnp.tanh(c)
    return new_gru_state, new_gru_state
```

LSTM

The LSTM has

- three gates (update, input and forget) instead of two (update and reset)
- Has both a context C and a hidden state h

$$\Gamma_u = \sigma(W[X_t, h_{t-1}] + b)$$

$$\Gamma_r = \sigma(W[X_t, h_{t-1}] + b)$$

$$\tilde{h}_t = \tanh(W[X_t, \Gamma_r \otimes h_{t-1}] + b)$$

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

$$\Gamma_u = \sigma(W[X_t, h_{t-1}] + b)$$

$$\Gamma_i = \sigma(W[X_t, h_{t-1}] + b)$$

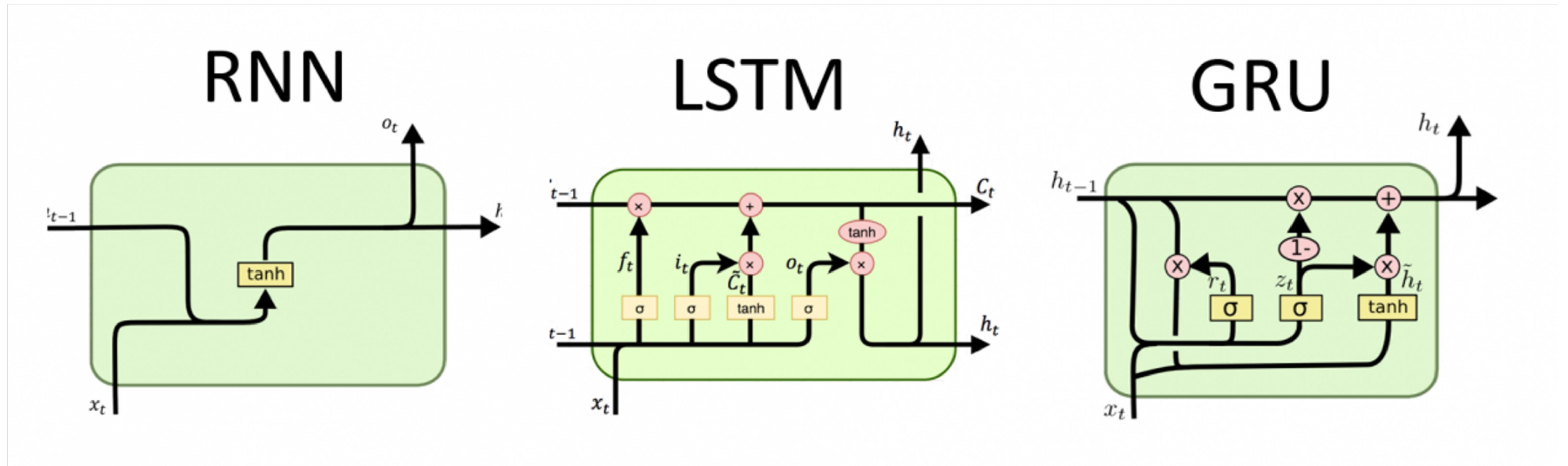
$$\Gamma_f = \sigma(W[X_t, h_{t-1}] + b)$$

$$\tilde{h} = \Gamma_i \otimes \tanh(W[X_t, h_{t-1}] + b)$$

$$\tilde{C} = \tanh(\Gamma_f \otimes C + \tilde{h})$$

$$h_t = \Gamma_u \otimes \tilde{C}$$

Overview



Overview

No free lunch

- The Simple RNN is the most basic, but does not have good ways to control memory
- LSTM has more parameters with three gates and two hidden states, and thus more complexity
- GRU is a simplified version of the LSTM with two gates and one hidden state.

There is no “best” Recurrent Neural Network, this depends on your usecase.