UNIVERSITY OF TECHNOLOGY
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CHEMNITZ

Neurocomputing

Recurrent neural networks

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https://tu-chemnitz.de/informatik/KI/edu/neurocomputing

1 - RNN

Problem with feedforward networks

- **Feedforward neural networks** learn to associate an input vector to an output.

$$\mathbf{y} = F_\theta(\mathbf{x})$$

- If you present a sequence of inputs $\mathbf{x}_0, \mathbf{x}_1, \dots, \mathbf{x}_t$ to a feedforward network, the outputs will be independent from each other:

$$\mathbf{y}_0 = F_\theta(\mathbf{x}_0)$$

$$\mathbf{y}_1 = F_\theta(\mathbf{x}_1)$$

$$\dots$$

$$\mathbf{y}_t = F_\theta(\mathbf{x}_t)$$

- Many problems depend on time series, such as predicting the future of a time series by knowing its past values.

$$x_{t+1} = F_\theta(x_0, x_1, \dots, x_t)$$

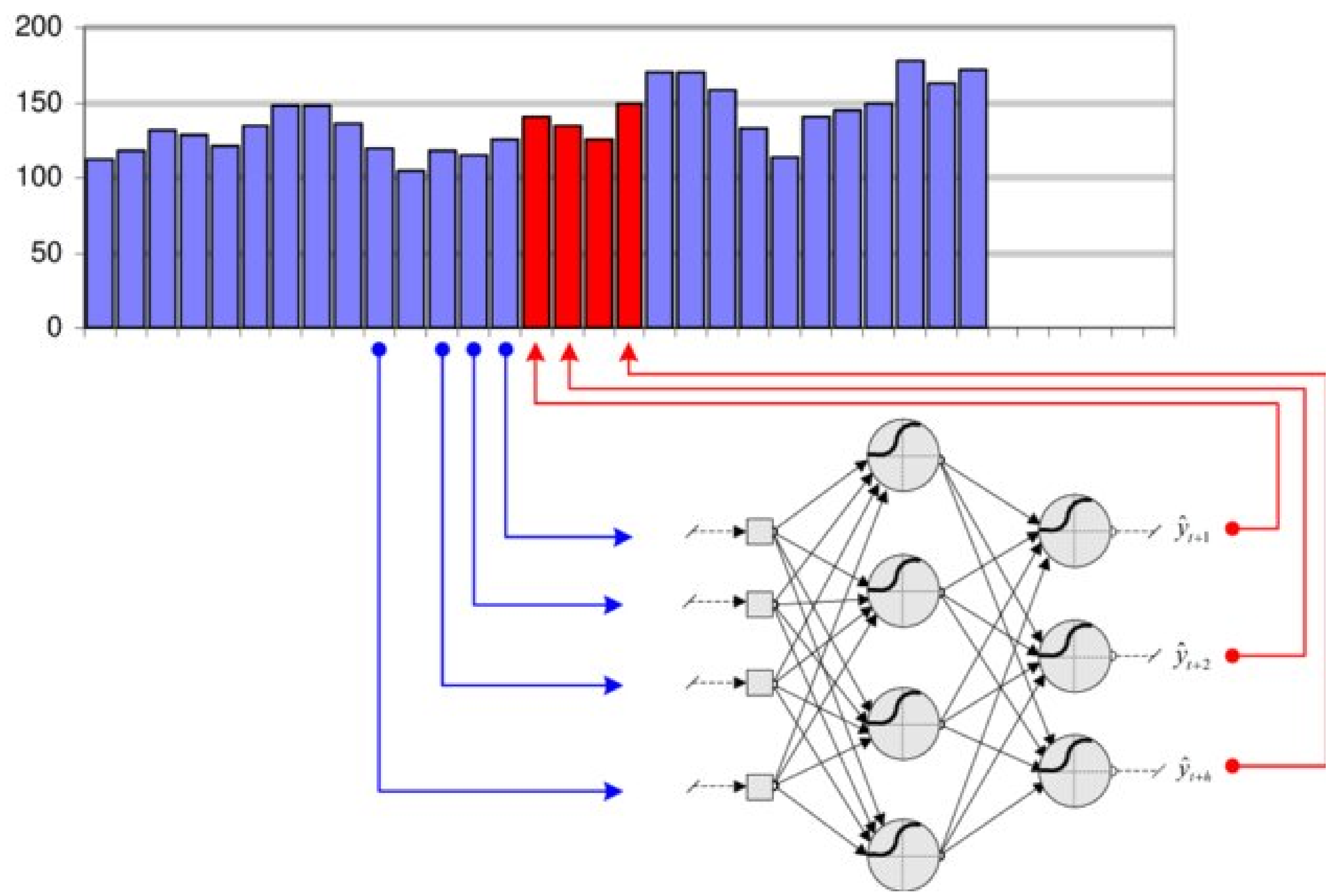
- Example: weather forecast, financial prediction, predictive maintenance, video analysis…

Input aggregation

- A naive solution is to **aggregate** (concatenate) inputs over a sufficiently long window and use it as a new input vector for the feedforward network.

$$\mathbf{X} = \begin{bmatrix} \mathbf{x}_{t-T} & \mathbf{x}_{t-T+1} & \dots & \mathbf{x}_t \end{bmatrix}$$

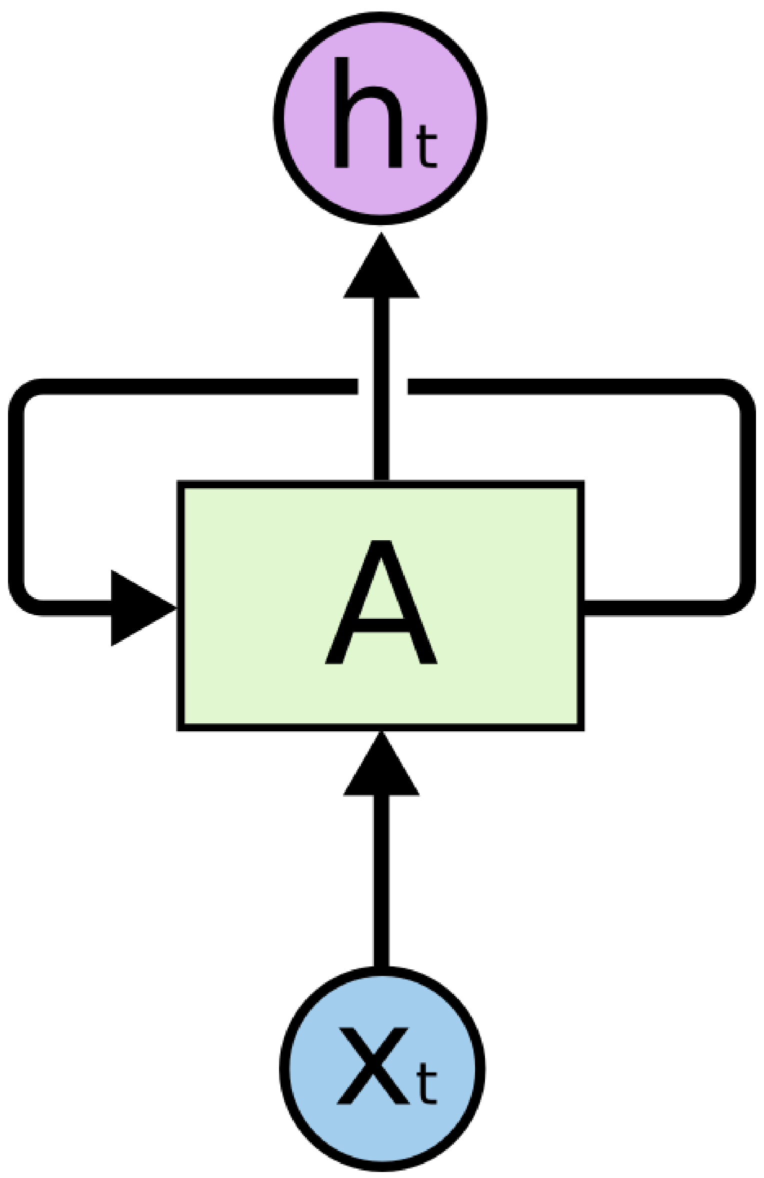
$$\mathbf{y}_t = F_\theta(\mathbf{X})$$



- **Problem 1:** How long should the window be?
- **Problem 2:** Having more input dimensions increases dramatically the complexity of the classifier (VC dimension), hence the number of training examples required to avoid overfitting.

https://www.researchgate.net/publication/220827486_A_study_on_the_ability_of_Support_Vector_Regression_and_Neural_Networks_to_Forecast_Basic_Time_Ser

Recurrent neural network



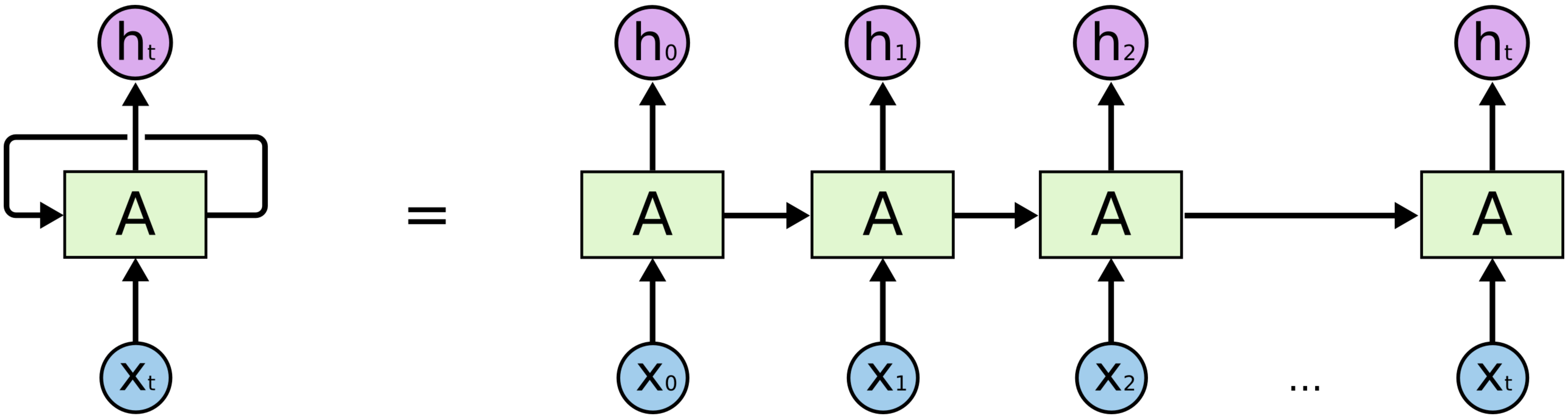
Source: http://colah.github.io/posts/2015-08-Understanding-LSTMs

- A **recurrent neural network** (RNN) uses it previous output as an additional input (*context*).
- All vectors have a time index t denoting the time at which this vector was computed.
- The input vector at time t is $\mathbf{x}_t$, the output vector is $\mathbf{h}_t$:

$$\mathbf{h}_t = \sigma(W_x \times \mathbf{x}_t + W_h \times \mathbf{h}_{t-1} + \mathbf{b})$$

- σ is a transfer function, usually logistic or tanh.
- The input $\mathbf{x}_t$ and previous output $\mathbf{h}_{t-1}$ are multiplied by **learnable weights**:
  - W_x is the input weight matrix.
  - W_h is the recurrent weight matrix.

Recurrent neural networks



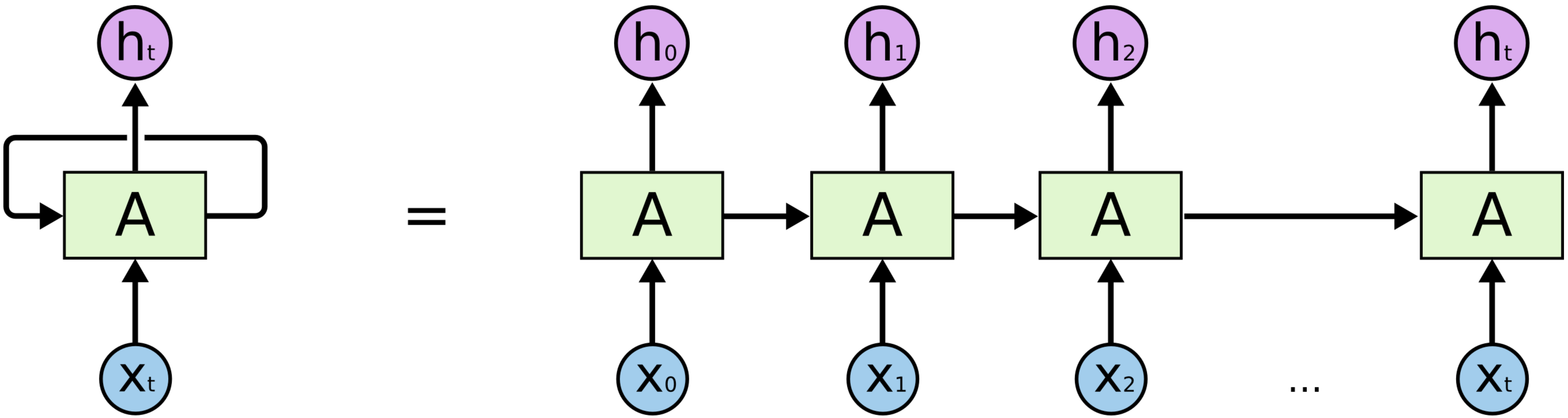
Source: http://colah.github.io/posts/2015-08-Understanding-LSTMs

- One can **unroll** a recurrent network: the output $\mathbf{h}_t$ depends on the whole history of inputs from $\mathbf{x}_0$ to $\mathbf{x}_t$.

$$
\begin{aligned}
\mathbf{h}_t & = \sigma(W_x \times \mathbf{x}_t + W_h \times \mathbf{h}_{t-1} + \mathbf{b}) \\
& = \sigma(W_x \times \mathbf{x}_t + W_h \times \sigma(W_x \times \mathbf{x}_{t-1} + W_h \times \mathbf{h}_{t-2} + \mathbf{b}) + \mathbf{b}) \\
& = f_{W_x, W_h, \mathbf{b}} (\mathbf{x}_0, \mathbf{x}_1, \dots, \mathbf{x}_t)
\end{aligned}
$$

- A RNN is considered as part of **deep learning**, as there are many layers of weights between the first input $\mathbf{x}_0$ and the output $\mathbf{h}_t$.
- The only difference with a DNN is that the weights W_x and W_h are **reused** at each time step.

BPTT: Backpropagation through time



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

$$\mathbf{h}_t = f_{W_x, W_h, \mathbf{b}} (\mathbf{x}_0, \mathbf{x}_1, \dots, \mathbf{x}_t)$$

- The function between the history of inputs and the output at time t is differentiable: we can simply apply gradient descent to find the weights!
- This variant of backpropagation is called **Backpropagation Through Time** (BPTT).
- Once the loss between $\mathbf{h}_t$ and its desired value is computed, one applies the **chain rule** to find out how to modify the weights W_x and W_h using the history $(\mathbf{x}_0, \mathbf{x}_1, \dots, \mathbf{x}_t)$.

BPTT: Backpropagation through time

- Let's compute the gradient accumulated between $\mathbf{h}_{t-1}$ and $\mathbf{h}_t$:

$$\mathbf{h}_t = \sigma(W_x \times \mathbf{x}_t + W_h \times \mathbf{h}_{t-1} + \mathbf{b})$$

- As for feedforward networks, the gradient of the loss function is decomposed into two parts:

$$\frac{\partial \mathcal{L}(W_x, W_h)}{\partial W_x} = \frac{\partial \mathcal{L}(W_x, W_h)}{\partial \mathbf{h}_t} \times \frac{\partial \mathbf{h}_t}{\partial W_x}$$
$$\frac{\partial \mathcal{L}(W_x, W_h)}{\partial W_h} = \frac{\partial \mathcal{L}(W_x, W_h)}{\partial \mathbf{h}_t} \times \frac{\partial \mathbf{h}_t}{\partial W_h}$$

- The first part only depends on the loss function (mse, cross-entropy):

$$\frac{\partial \mathcal{L}(W_x, W_h)}{\partial \mathbf{h}_t} = -(\mathbf{t}_t - \mathbf{h}_t)$$

- The second part depends on the RNN itself.

BPTT: Backpropagation through time

- Output of the RNN:

$$\mathbf{h}_t = \sigma(W_x \times \mathbf{x}_t + W_h \times \mathbf{h}_{t-1} + \mathbf{b})$$

- The gradients w.r.t the two weight matrices are given by this **recursive** relationship (product rule):

$$\frac{\partial \mathbf{h}_t}{\partial W_x} = \mathbf{h'}_t \times (\mathbf{x}_t + W_h \times \frac{\partial \mathbf{h}_{t-1}}{\partial W_x})$$

$$\frac{\partial \mathbf{h}_t}{\partial W_h} = \mathbf{h'}_t \times (\mathbf{h}_{t-1} + W_h \times \frac{\partial \mathbf{h}_{t-1}}{\partial W_h})$$

- The derivative of the transfer function is noted $\mathbf{h'}_t$:

$$\mathbf{h'}_t = \begin{cases} \mathbf{h}_t \, (1 - \mathbf{h}_t) \quad \text{for logistic} \\ (1 - \mathbf{h}_t^2) \quad \text{for tanh.} \end{cases}$$

BPTT: Backpropagation through time

- If we **unroll** the gradient, we obtain:

$$\frac{\partial \mathbf{h}_t}{\partial W_x} = \mathbf{h'}_t \, (\mathbf{x}_t + W_h \times \mathbf{h'}_{t-1} \, (\mathbf{x}_{t-1} + W_h \times \mathbf{h'}_{t-2} \, (\mathbf{x}_{t-2} + W_h \times \ldots (\mathbf{x}_0))))$$

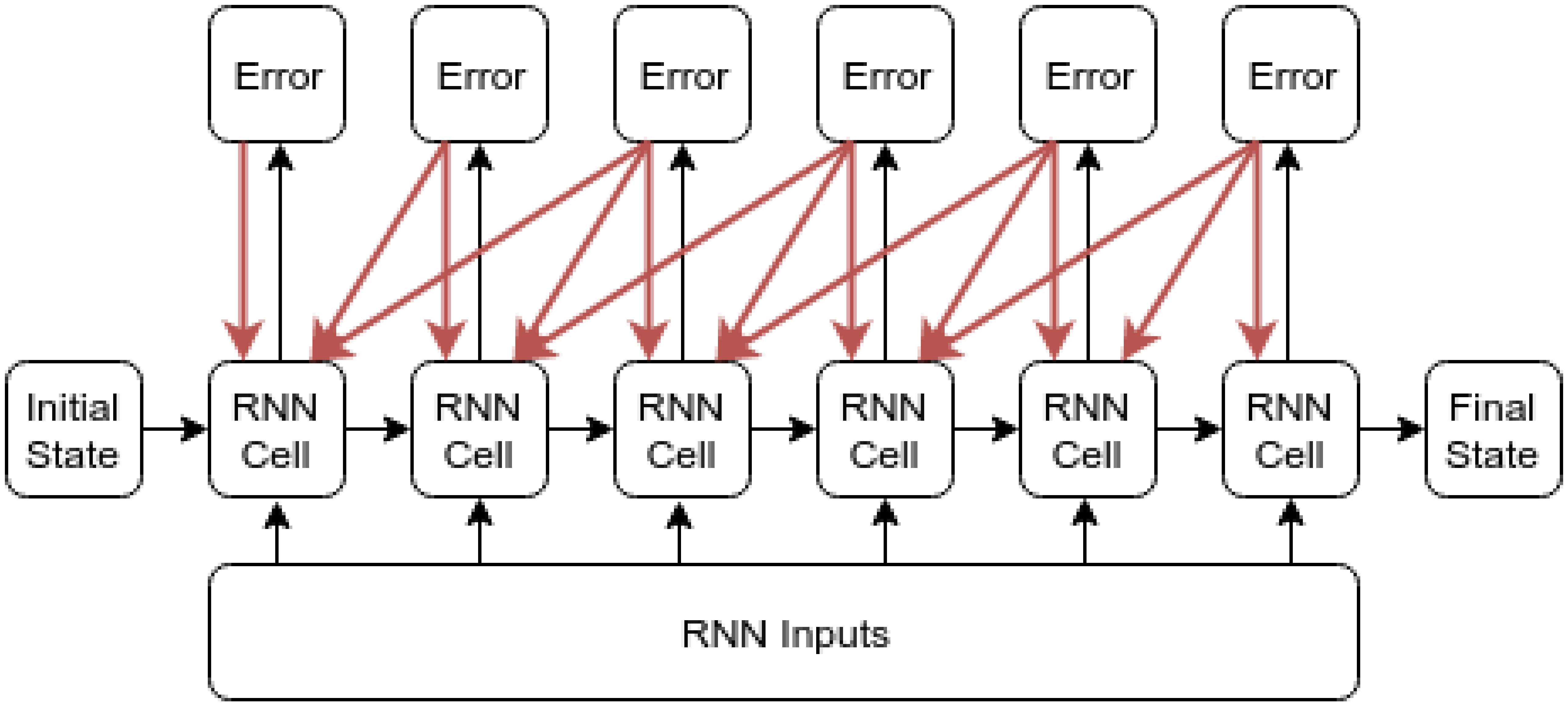
$$\frac{\partial \mathbf{h}_t}{\partial W_h} = \mathbf{h'}_t \, (\mathbf{h}_{t-1} + W_h \times \mathbf{h'}_{t-1} \, (\mathbf{h}_{t-2} + W_h \times \mathbf{h'}_{t-2} \, \ldots (\mathbf{h}_0)))$$

- When updating the weights at time t, we need to store in memory:
  - the complete history of inputs $\mathbf{x}_0$, $\mathbf{x}_1$, ... $\mathbf{x}_t$.
  - the complete history of outputs $\mathbf{h}_0$, $\mathbf{h}_1$, ... $\mathbf{h}_t$.
  - the complete history of derivatives $\mathbf{h'}_0$, $\mathbf{h'}_1$, ... $\mathbf{h'}_t$.

before computing the gradients iteratively, starting from time t and accumulating gradients **backwards** in time until $t = 0$.

- Each step backwards in time adds a bit to the gradient used to update the weights.

Truncated BPTT

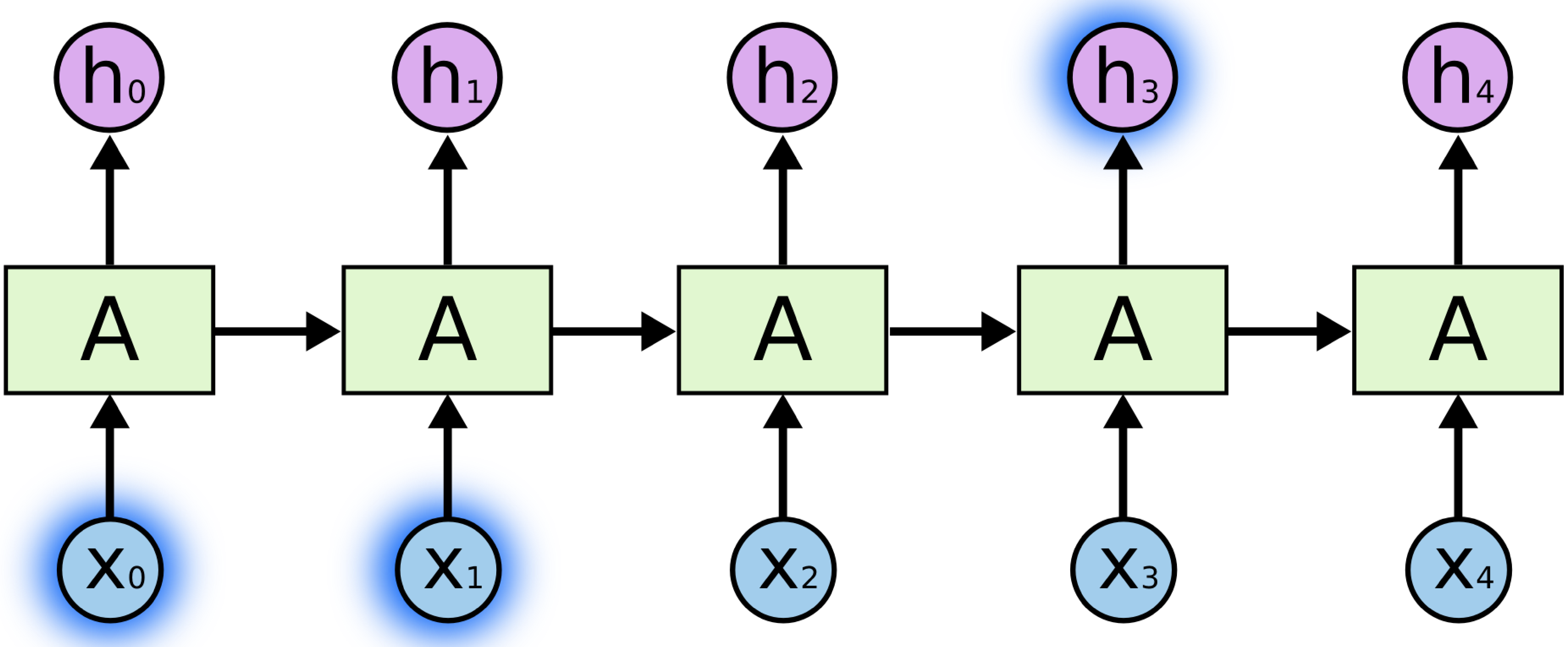


Source: https://r2rt.com/styles-of-truncated-backpropagation.html

- In practice, going back to $t=0$ at each time step requires too many computations, which may not be needed.
- **Truncated BPTT** only updates the gradients up to T steps before: the gradients are computed backwards from t to $t-T$. The partial derivative in $t-T-1$ is considered 0.
- This limits the **horizon** of BPTT: dependencies longer than T will not be learned, so it has to be chosen carefully for the task.
- T becomes yet another hyperparameter of your algorithm...

Temporal dependencies

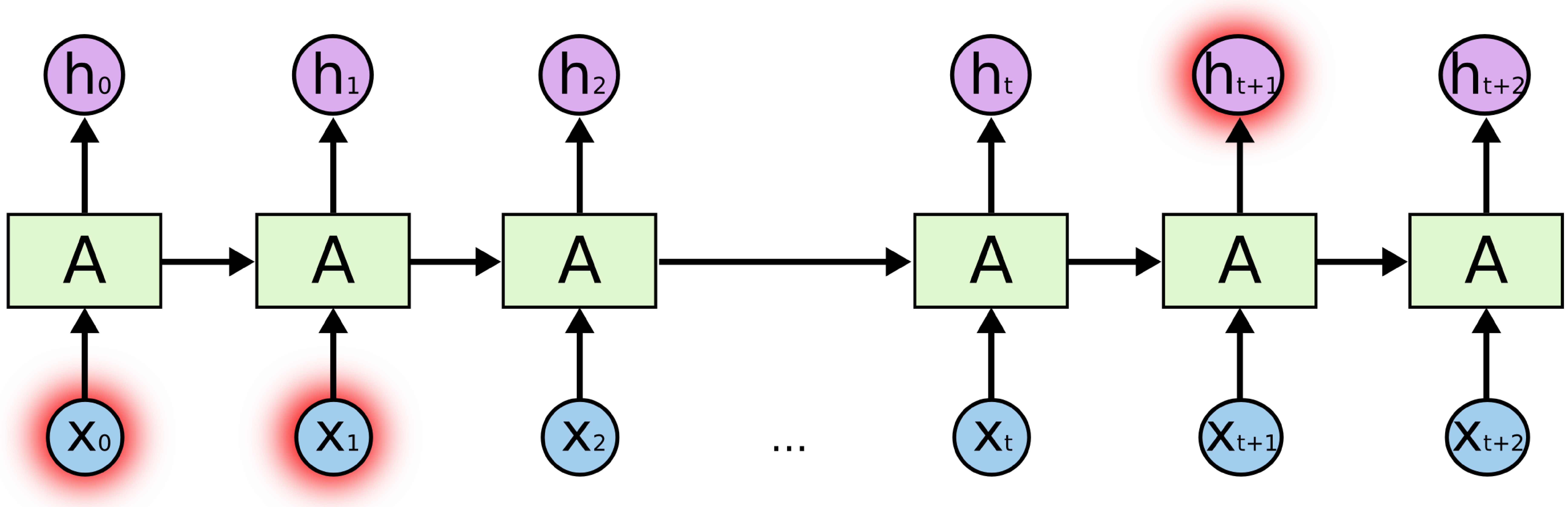
- BPTT is able to find **short-term dependencies** between inputs and outputs: perceiving the inputs $\mathbf{x}_0$ and $\mathbf{x}_1$ allows to respond correctly at $t = 3$.



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

Temporal dependencies

- But it fails to detect **long-term dependencies** because of:
  - the truncated horizon T (for computational reasons).
  - the **vanishing gradient problem**.



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

Vanishing and exploding gradients

- Let’s look at the gradient w.r.t to the input weights:

$$\frac{\partial \mathbf{h}_t}{\partial W_x} = \mathbf{h'}_t \, (\mathbf{x}_t + W_h \times \frac{\partial \mathbf{h}_{t-1}}{\partial W_x})$$

- At each iteration backwards in time, the gradients are multiplied by W_h.
- If you search how $\frac{\partial \mathbf{h}_t}{\partial W_x}$ depends on $\mathbf{x}_0$, you obtain something like:

$$\frac{\partial \mathbf{h}_t}{\partial W_x} \approx \prod_{k=0}^t \mathbf{h'}_k \, ((W_h)^t \, \mathbf{x}_0 + \dots)$$

- If $|W_h| > 1$, $|(W_h)^t|$ increases exponentially with t: the gradient **explodes**.
- If $|W_h| < 1$, $|(W_h)^t|$ decreases exponentially with t: the gradient **vanishes**.

Vanishing and exploding gradients

- **Exploding gradients** are relatively easy to deal with: one just clips the norm of the gradient to a maximal value.

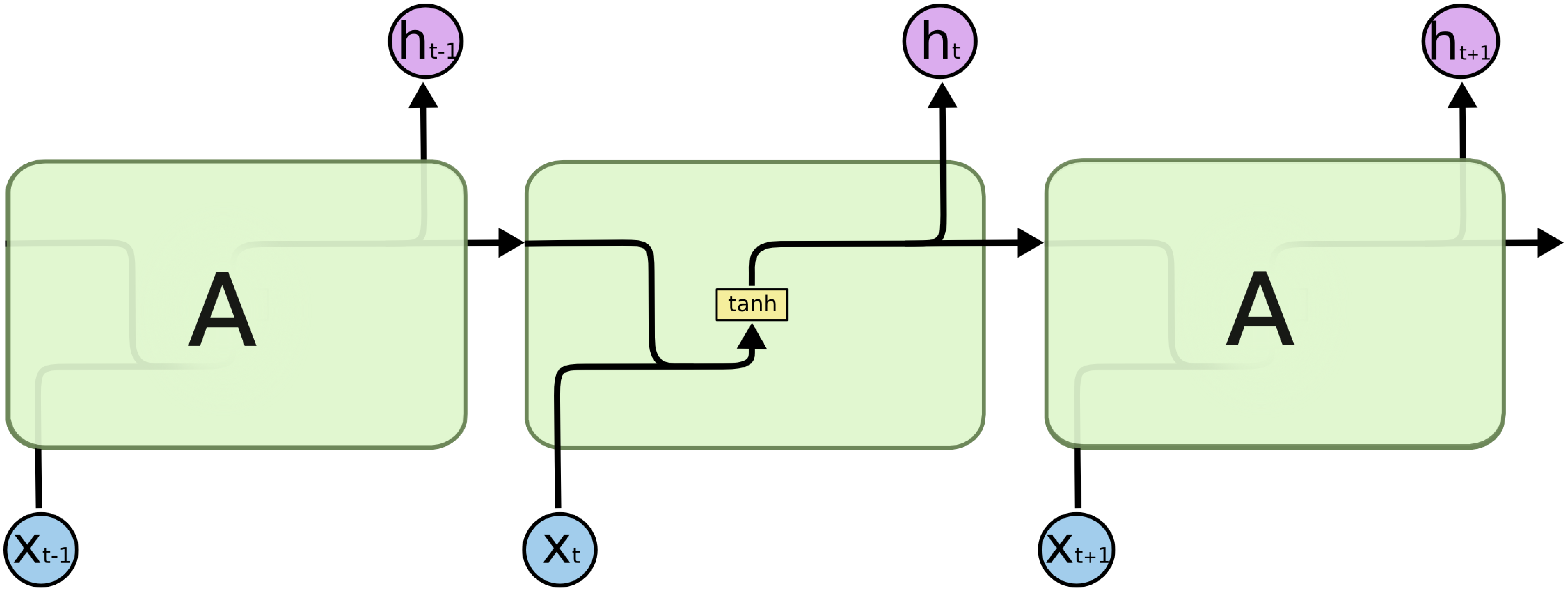
$$||\frac{\partial \mathcal{L}(W_x, W_h)}{\partial W_x}|| \leftarrow \min(||\frac{\partial \mathcal{L}(W_x, W_h)}{\partial W_x}||, T)$$

- But there is no solution to the **vanishing gradient problem** for regular RNNs: the gradient fades over time (backwards) and no long-term dependency can be learned.
- This is the same problem as for feedforward deep networks: a RNN is just a deep network rolled over itself.
- Its depth (number of layers) corresponds to the maximal number of steps back in time.
- In order to limit vanishing gradients and learn long-term dependencies, one has to use a more complex structure for the layer.
- This is the idea behind **long short-term memory** (LSTM) networks.

S. Hochreiter. Untersuchungen zu dynamischen neuronalen Netzen. Diploma thesis, Institut f. Informatik, Technische Univ. Munich, 1991.

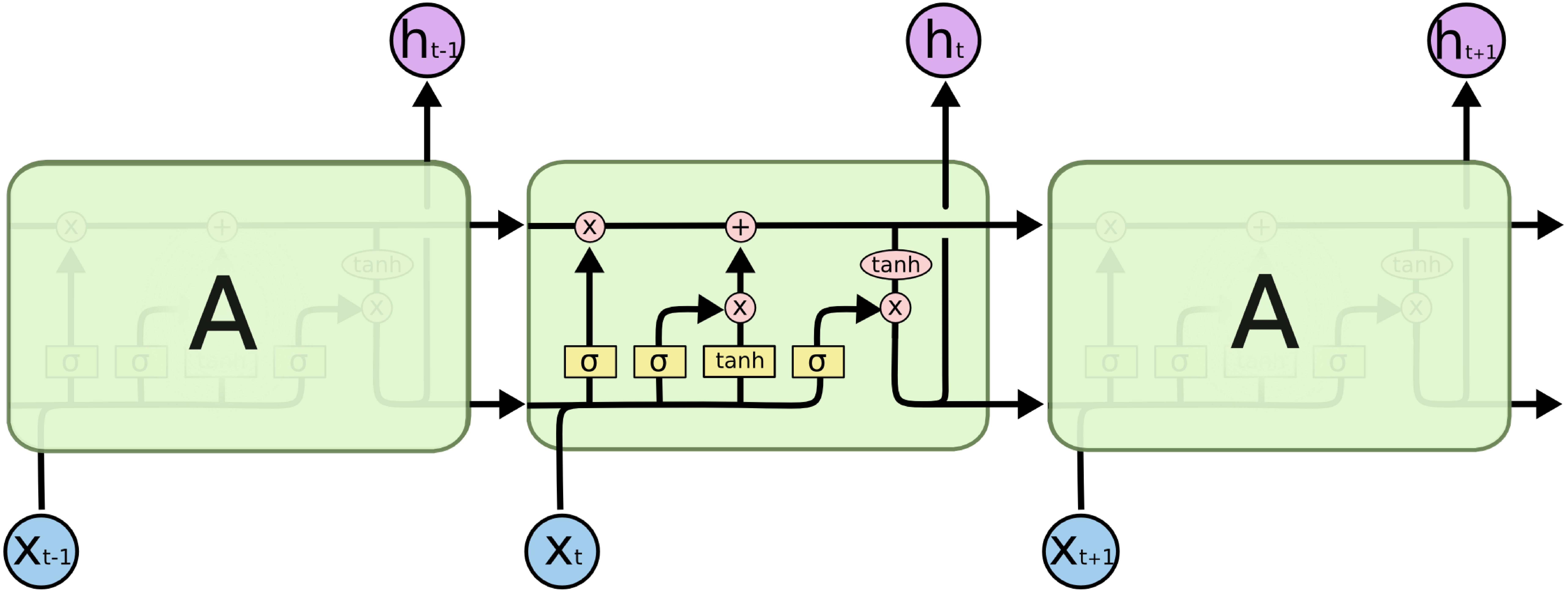
2 - LSTM

Regular RNN



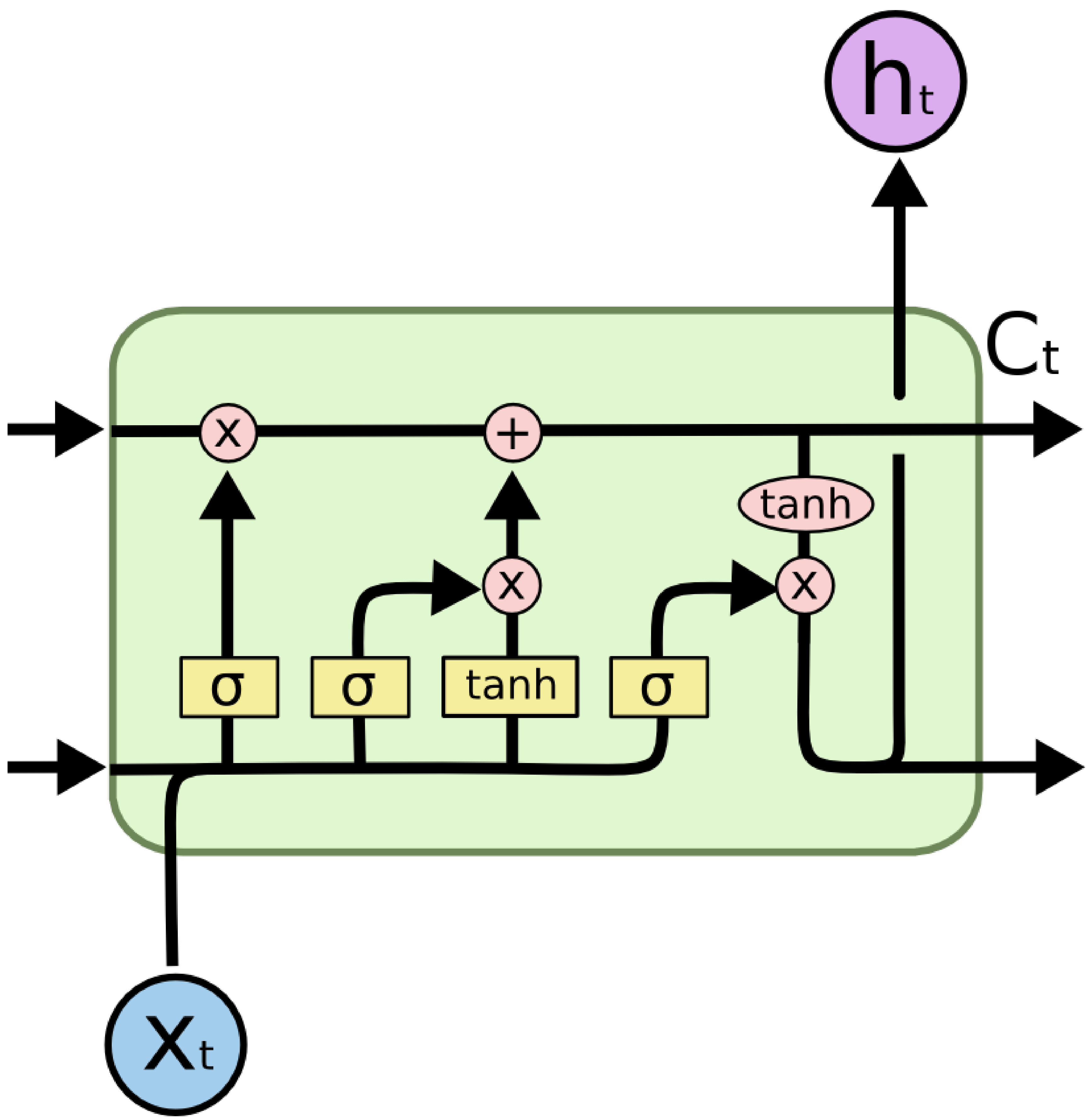
Source: http://colah.github.io/posts/2015-08-Understanding-LSTMs

LSTM



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

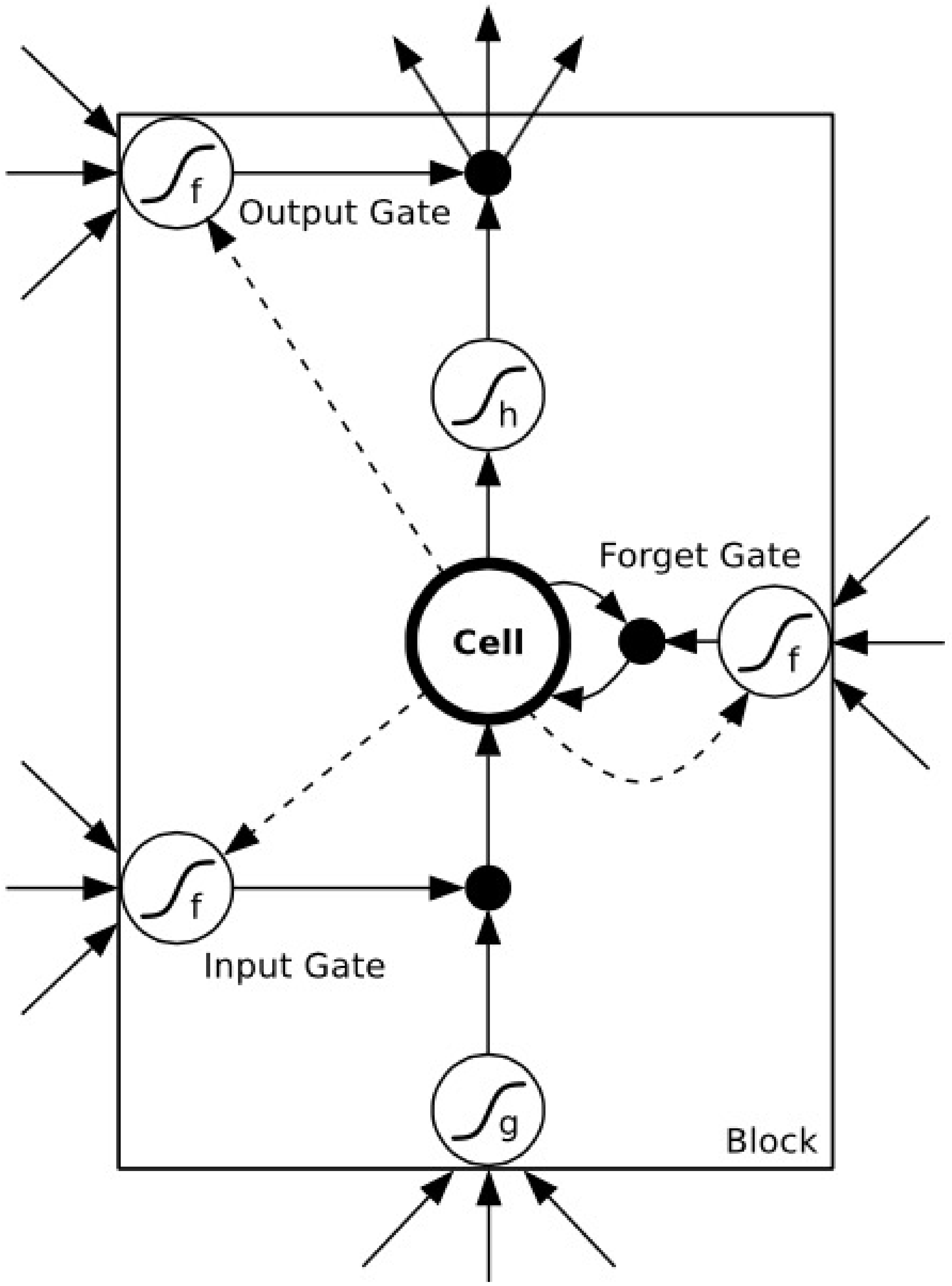
LSTM cell



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

- A **LSTM layer** is a RNN layer with the ability to control what it memorizes.
- In addition to the input $\mathbf{x}_t$ and output $\mathbf{h}_t$, it also has a **state** $\mathbf{C}_t$ which is maintained over time.
- The state is the memory of the layer (sometimes called context).
- It also contains three multiplicative **gates**:
  - The **input gate** controls which inputs should enter the memory.
  - The **forget gate** controls which memory should be forgotten.
  - The **output gate** controls which part of the memory should be used to produce the output.

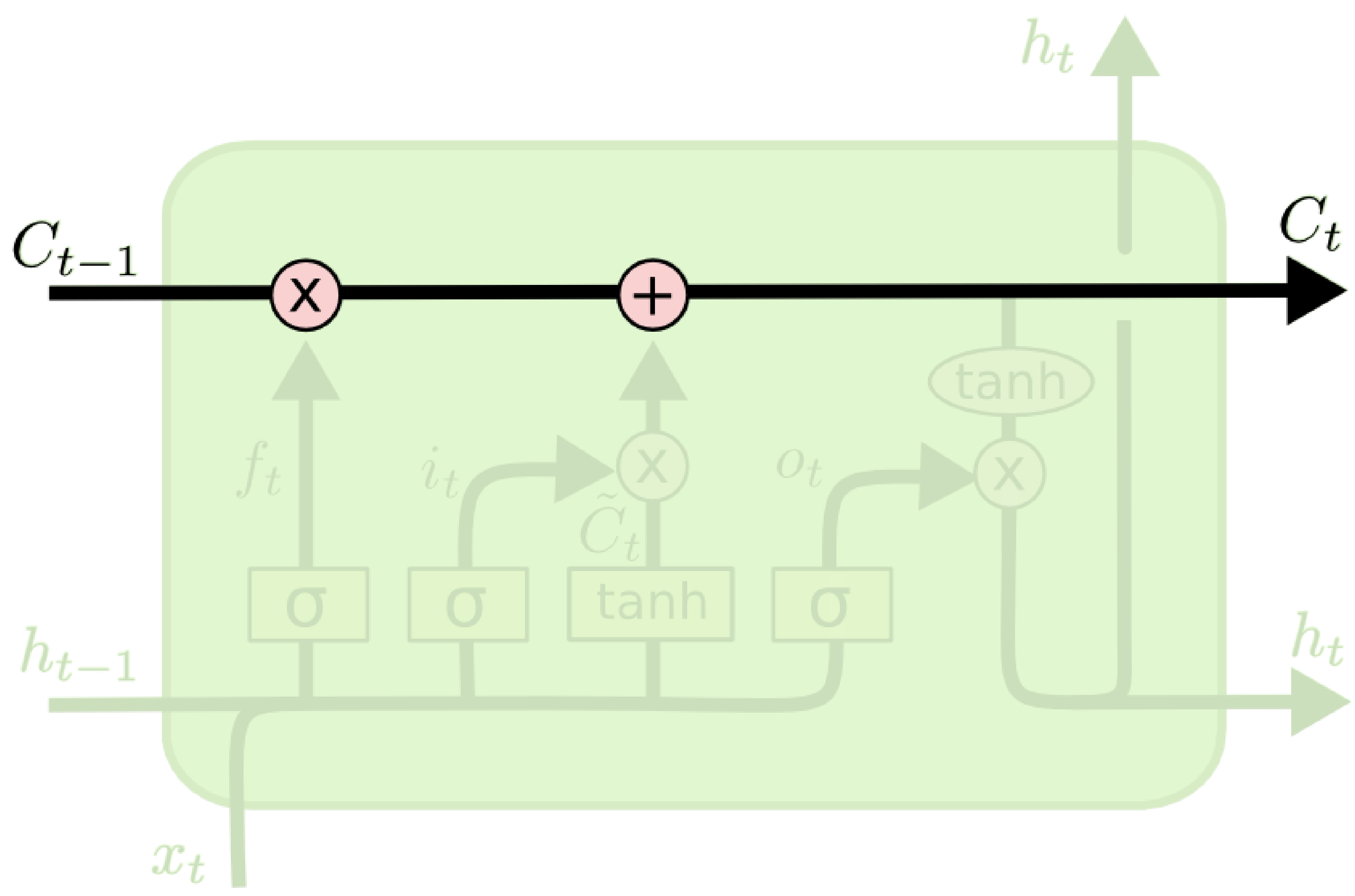
LSTM cell



- The **state** $\mathbf{C}_t$ can be seen as an accumulator integrating inputs (and previous outputs) over time.
    - The **input gate** allows inputs to be stored.
        - *are they worth remembering?*
    - The **forget gate** “empties” the accumulator
        - *do I still need them?*
    - The **output gate** allows to use the accumulator for the output.
        - *should I respond now? Do I have enough information?*
- The gates **learn** to open and close through learnable weights.

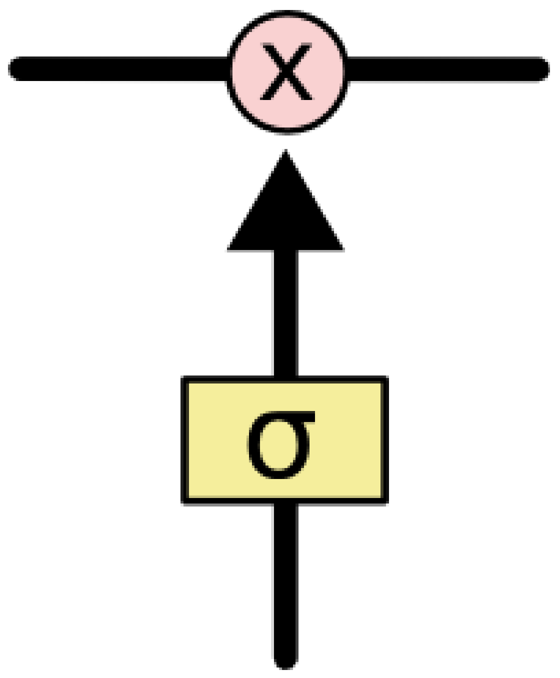
Source: http://eric-yuan.me/rnn2-lstm/

The cell state is propagated over time

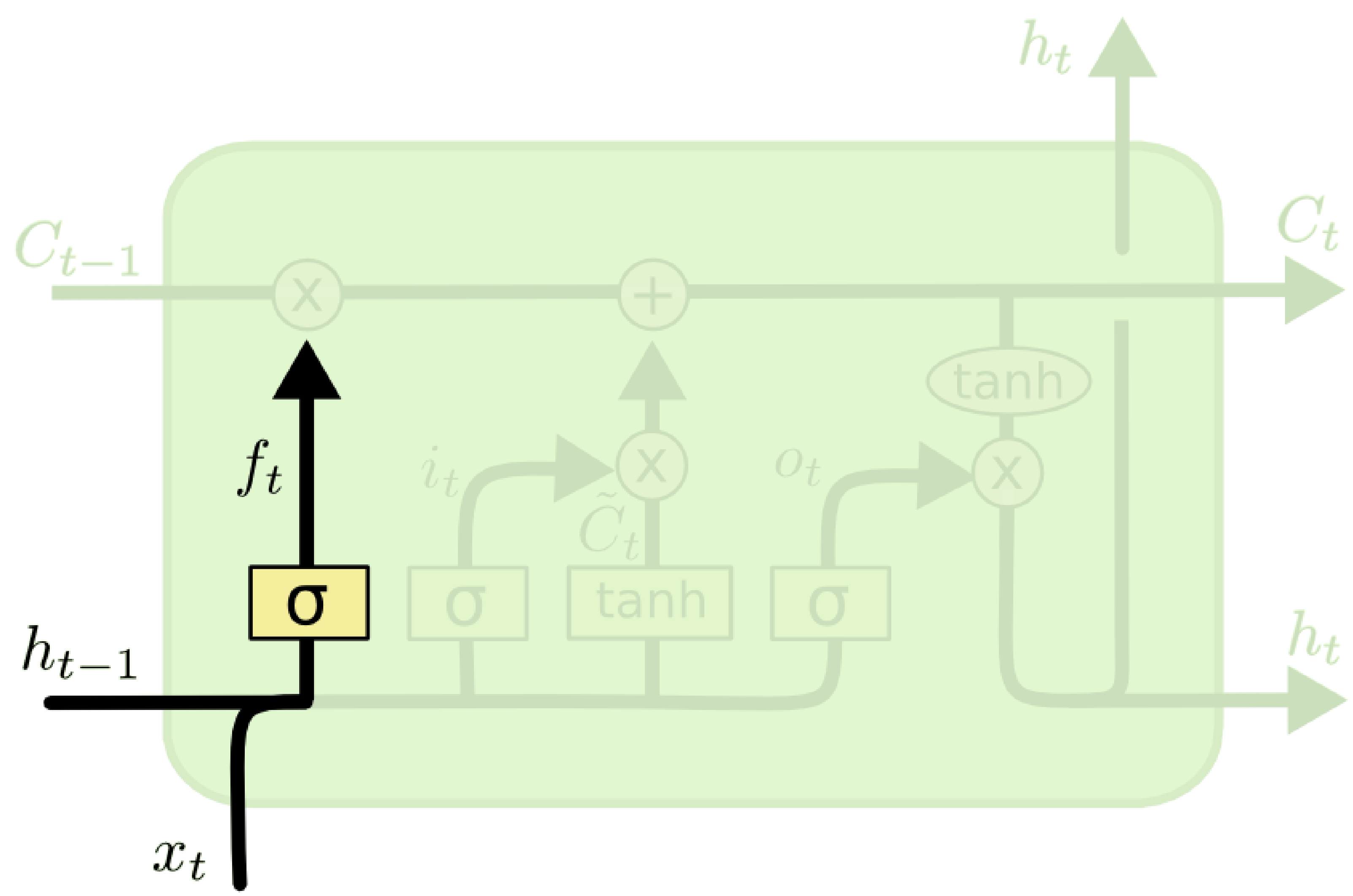


Source: http://colah.github.io/posts/2015-08-Understanding-LSTMs

- By default, the cell state $\mathbf{C}_t$ stays the same over time (*conveyor belt*).
- It can have the same number of dimensions as the output $\mathbf{h}_t$, but does not have to.
- Its content can be erased by multiplying it with a vector of 0s, or preserved by multiplying it by a vector of 1s.
- We can use a **sigmoid** to achieve this:



The forget gate



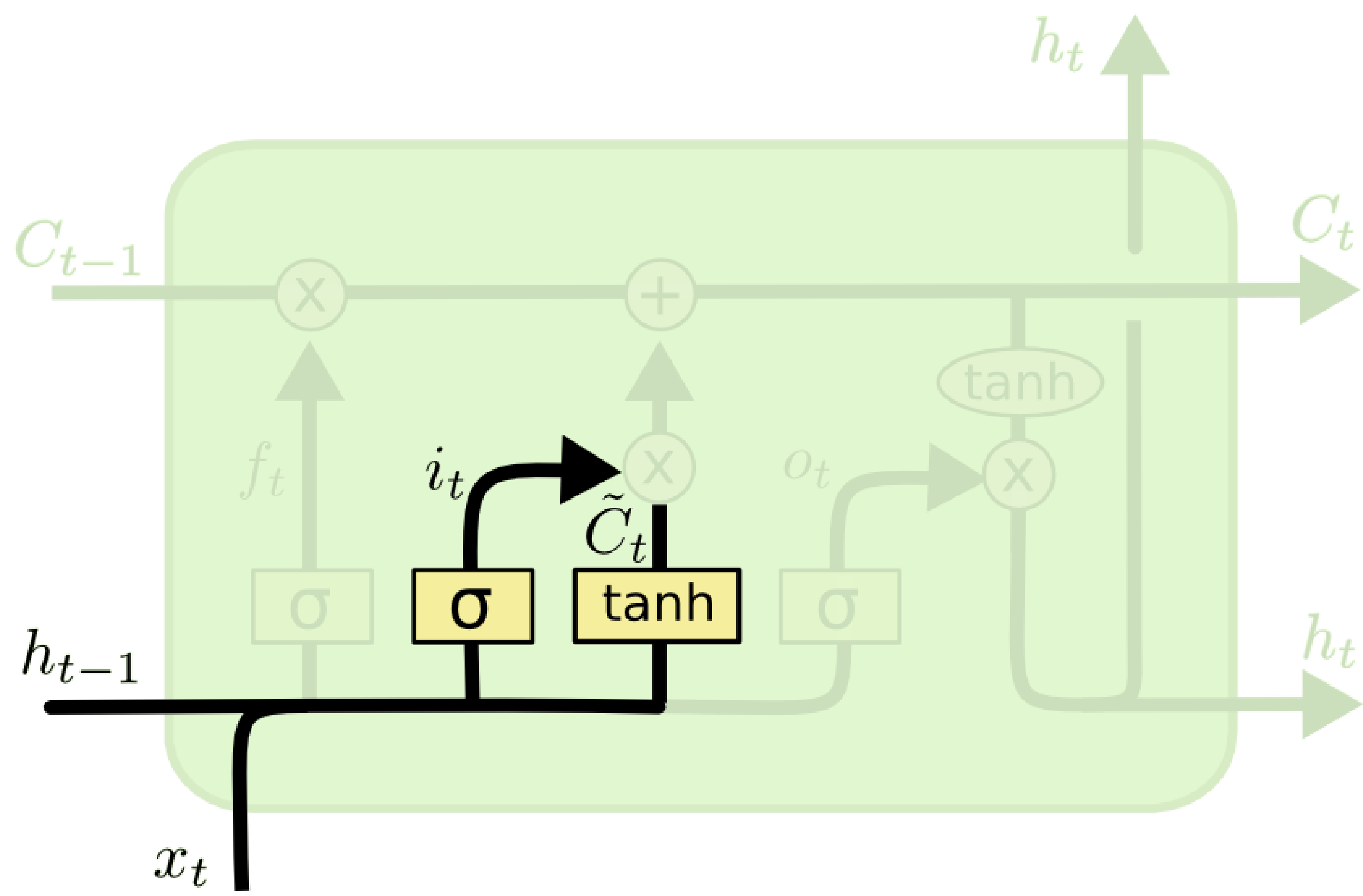
Source: http://colah.github.io/posts/2015-08-Understanding-LSTMs

- Forget weights W_f and a sigmoid function are used to decide if the state should be preserved or not.

$$\mathbf{f}_t = \sigma(W_f \times [\mathbf{h}_{t-1}; \mathbf{x}_t] + \mathbf{b}_f)$$

- $[\mathbf{h}_{t-1}; \mathbf{x}_t]$ is simply the concatenation of the two vectors $\mathbf{h}_{t-1}$ and $\mathbf{x}_t$.
- $\mathbf{f}_t$ is a vector of values between 0 and 1, one per dimension of the cell state $\mathbf{C}_t$.

The input gate



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

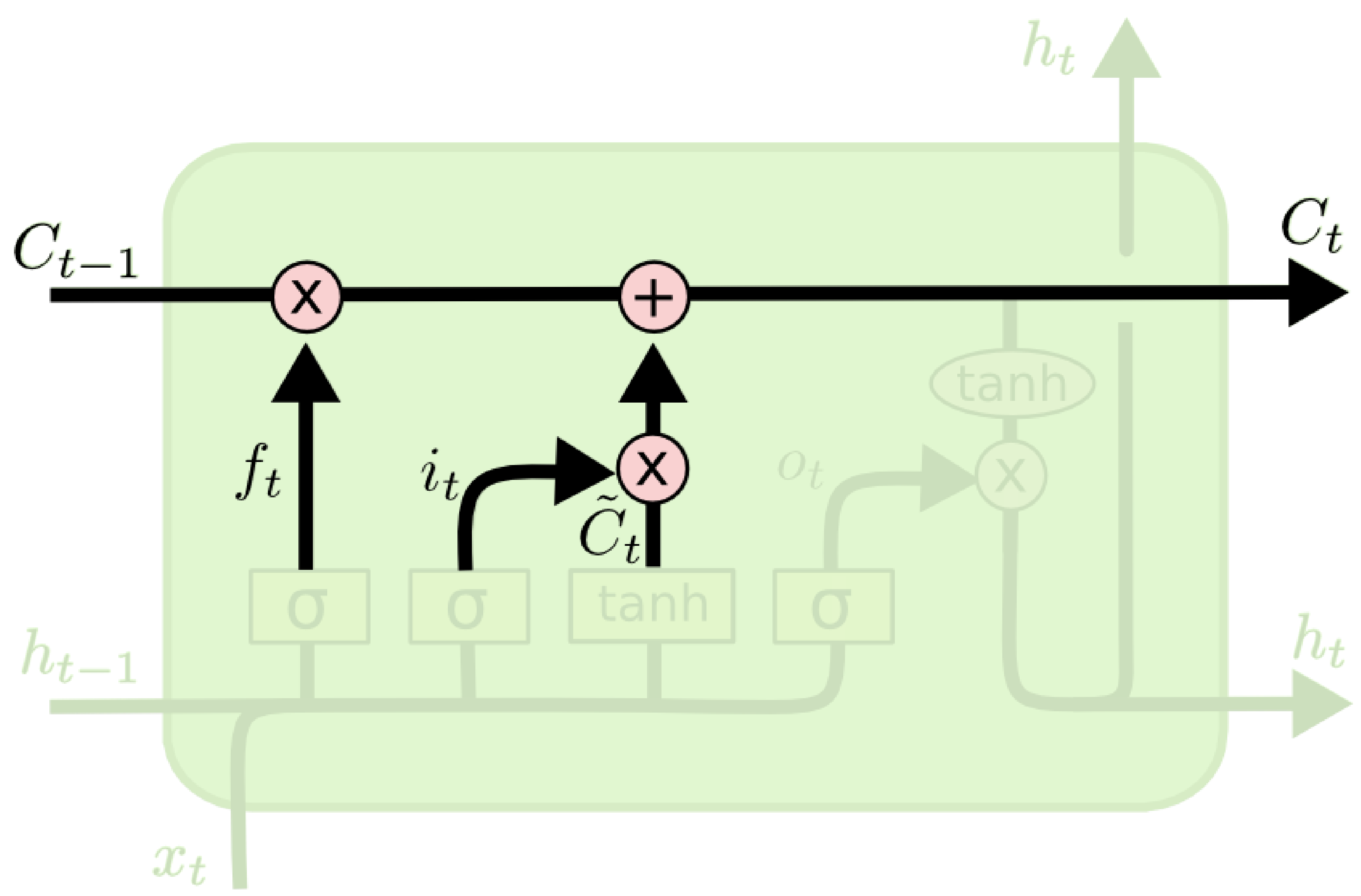
- Similarly, the input gate uses a sigmoid function to decide if the state should be updated or not.

$$\mathbf{i}_t = \sigma(W_i \times [\mathbf{h}_{t-1}; \mathbf{x}_t] + \mathbf{b}_i)$$

- As for RNNs, the input $\mathbf{x}_t$ and previous output $\mathbf{h}_{t-1}$ are combined to produce a **candidate state** $\tilde{\mathbf{C}}_t$ using the tanh transfer function.

$$\tilde{\mathbf{C}}_t = \tanh(W_C \times [\mathbf{h}_{t-1}; \mathbf{x}_t] + \mathbf{b}_c)$$

Updating the state



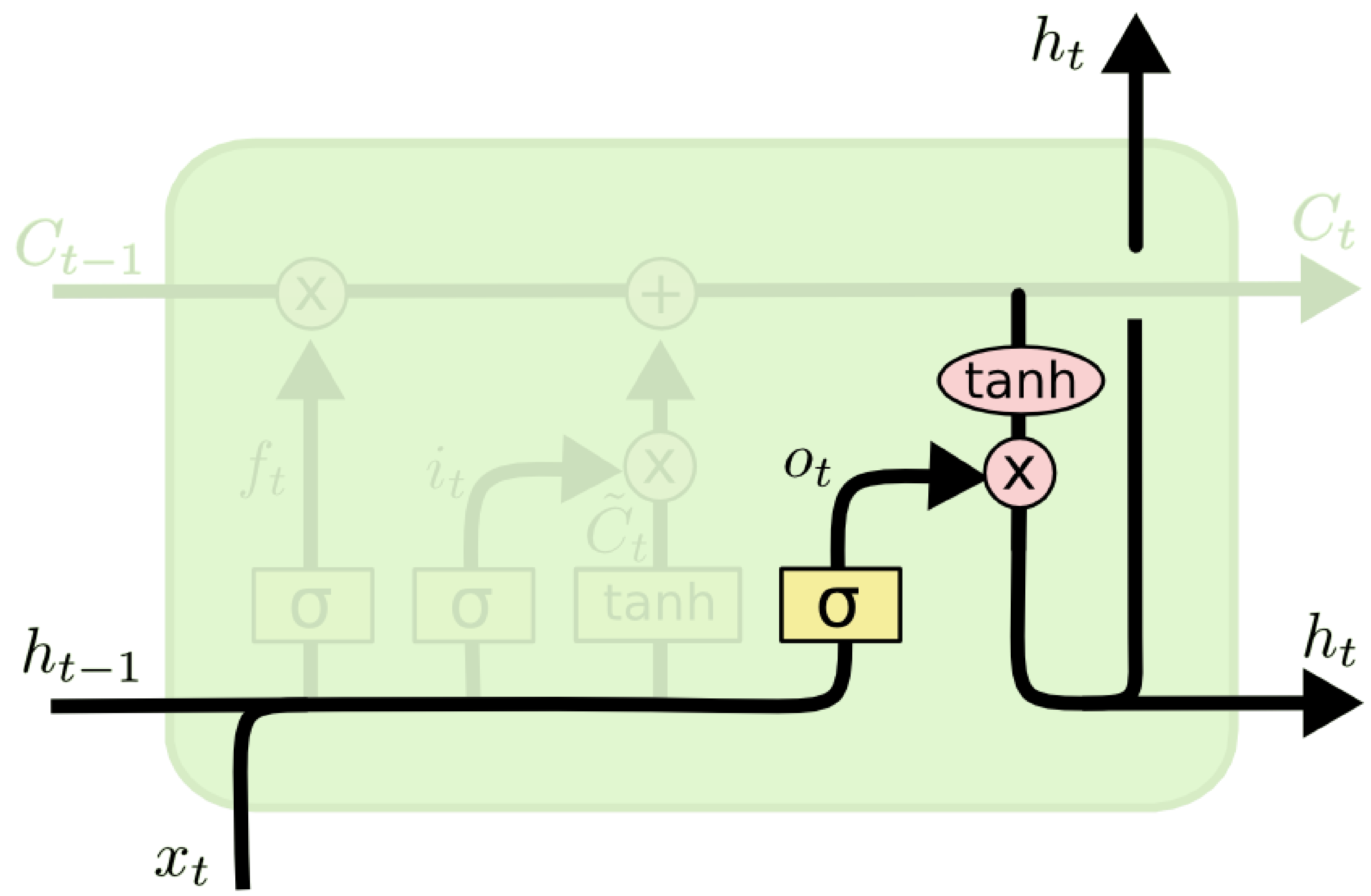
Source: http://colah.github.io/posts/2015-08-Understanding-LSTMs

- The new state $\mathbf{C}_t$ is computed as a part of the previous state $\mathbf{C}_{t-1}$ (element-wise multiplication with the forget gate $\mathbf{f}_t$) plus a part of the candidate state $\tilde{\mathbf{C}}_t$ (element-wise multiplication with the input gate $\mathbf{i}_t$).

$$\mathbf{C}_t = \mathbf{f}_t \odot \mathbf{C}_{t-1} + \mathbf{i}_t \odot \tilde{\mathbf{C}}_t$$

- Depending on the gates, the new state can be equal to the previous state (gates closed), the candidate state (gates opened) or a mixture of both.

The output gate



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

- The output gate decides which part of the new state will be used for the output.

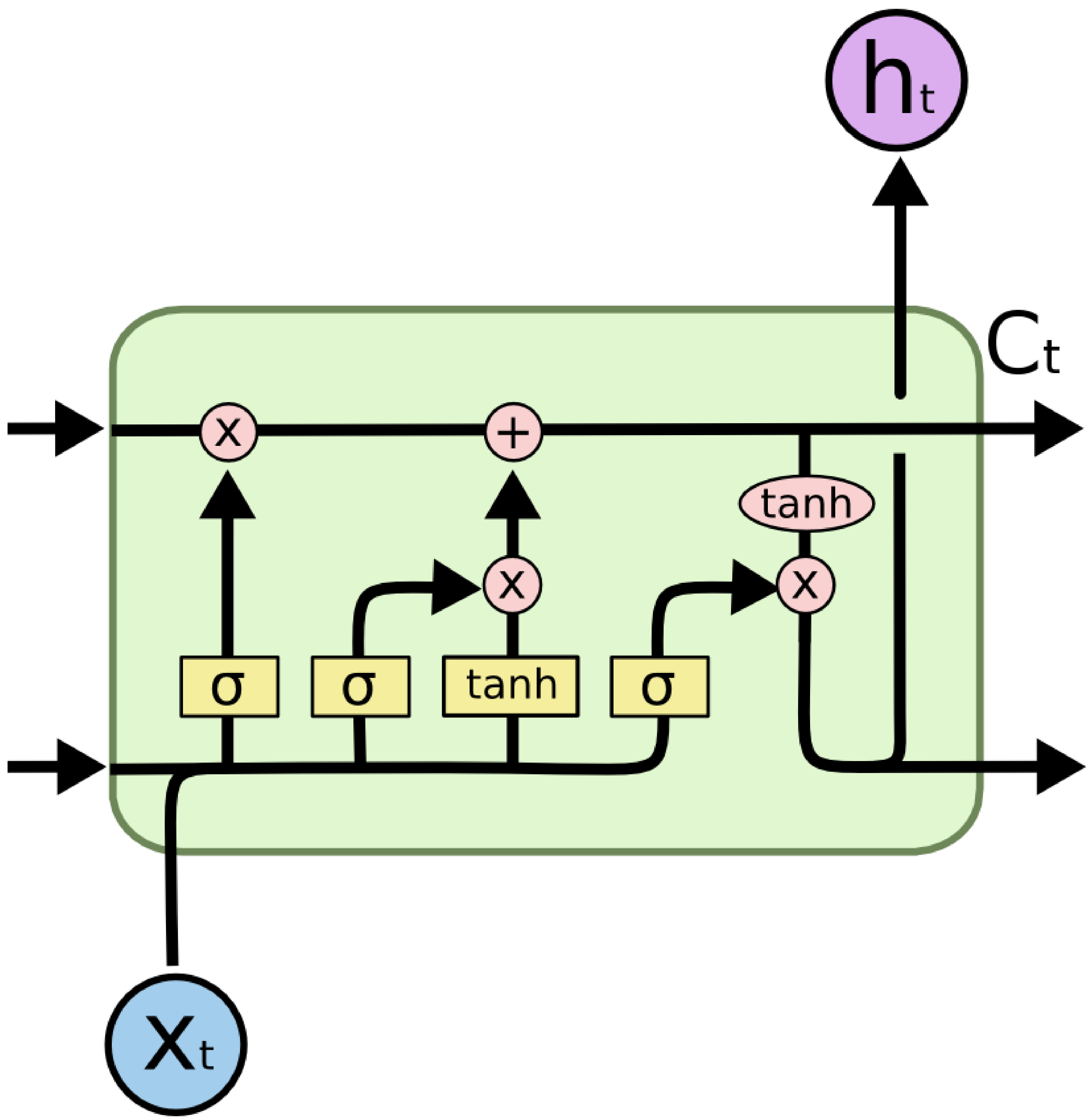
$$\mathbf{o}_t = \sigma(W_o \times [\mathbf{h}_{t-1}; \mathbf{x}_t] + \mathbf{b}_o)$$

- The output not only influences the decision, but also how the gates will updated at the next step.

$$\mathbf{h}_t = \mathbf{o}_t \odot \tanh(\mathbf{C}_t)$$

LSTM

- The function between $\mathbf{x}_t$ and $\mathbf{h}_t$ is quite complicated, with many different weights, but everything is differentiable: BPTT can be applied.



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

Forget gate

$$\mathbf{f}_t = \sigma(W_f \times [\mathbf{h}_{t-1}; \mathbf{x}_t] + \mathbf{b}_f)$$

Input gate

$$\mathbf{i}_t = \sigma(W_i \times [\mathbf{h}_{t-1}; \mathbf{x}_t] + \mathbf{b}_i)$$

Output gate

$$\mathbf{o}_t = \sigma(W_o \times [\mathbf{h}_{t-1}; \mathbf{x}_t] + \mathbf{b}_o)$$

Candidate state

$$\tilde{\mathbf{C}}_t = \tanh(W_C \times [\mathbf{h}_{t-1}; \mathbf{x}_t] + \mathbf{b}_c)$$

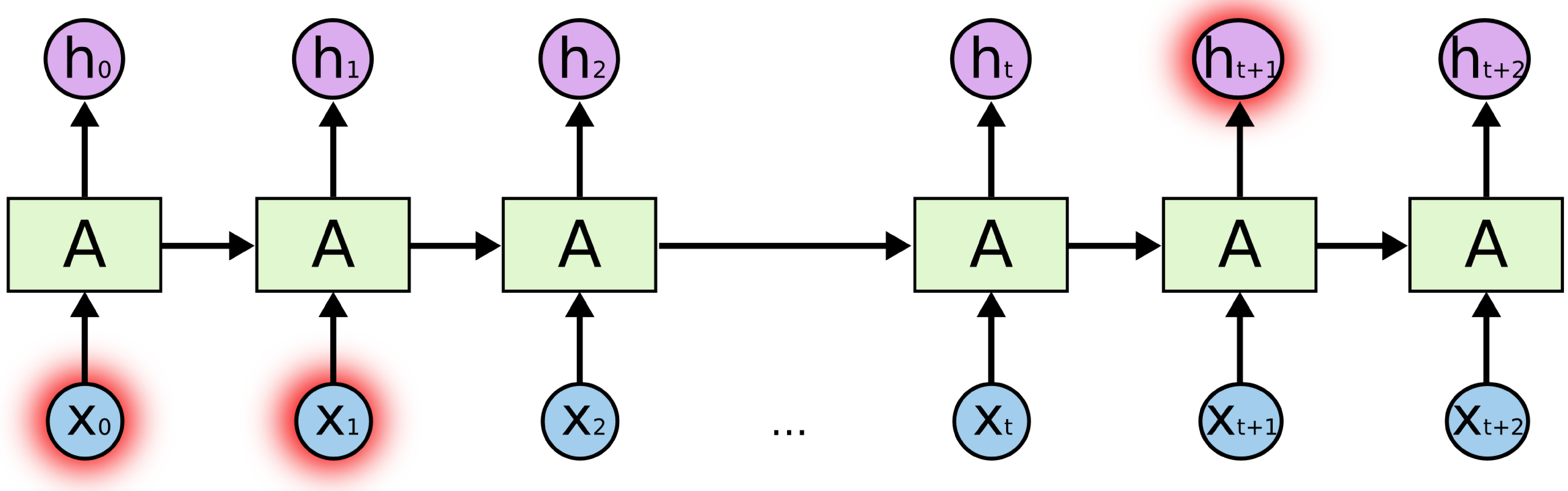
New state

$$\mathbf{C}_t = \mathbf{f}_t \odot \mathbf{C}_{t-1} + \mathbf{i}_t \odot \tilde{\mathbf{C}}_t$$

Output

$$\mathbf{h}_t = \mathbf{o}_t \odot \tanh(\mathbf{C}_t)$$

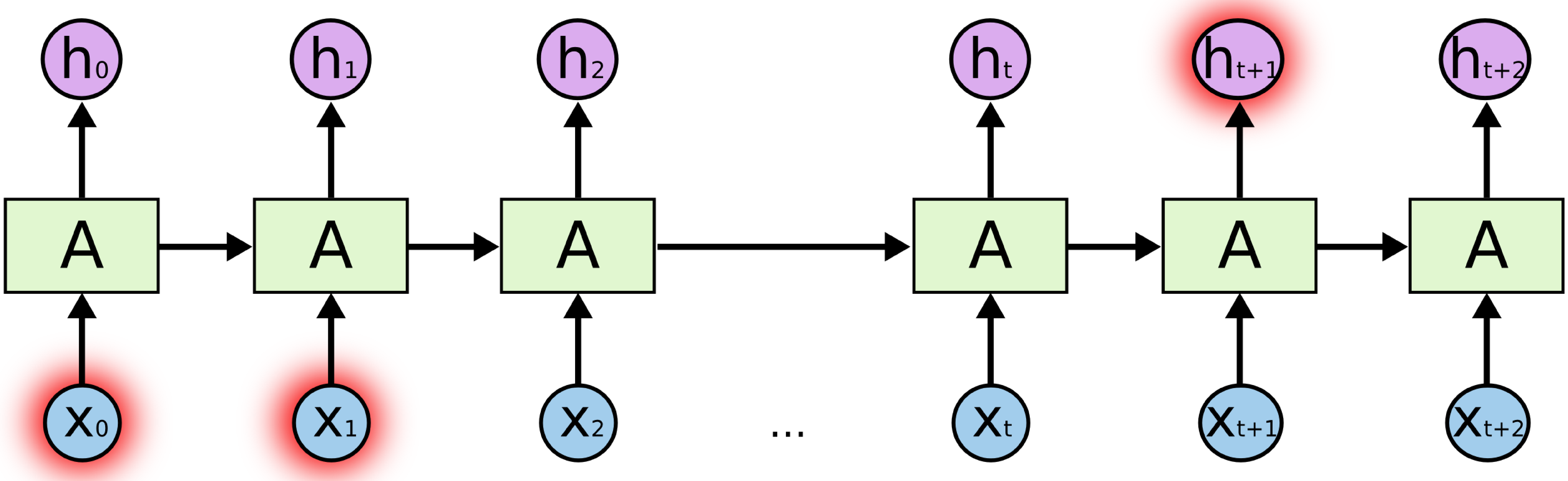
How do LSTM solve the vanishing gradient problem?



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

- Not all inputs are remembered by the LSTM: the input gate controls what comes in.
- If only $\mathbf{x}_0$ and $\mathbf{x}_1$ are needed to produce $\mathbf{h}_{t+1}$, they will be the only ones stored in the state, the other inputs are ignored.

How do LSTM solve the vanishing gradient problem?



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

- If the state stays constant between $t = 1$ and t, the gradient of the error will not vanish when backpropagating from t to $t = 1$, because nothing happens!

$$\mathbf{C}_t = \mathbf{C}_{t-1} \rightarrow \frac{\partial \mathbf{C}_t}{\partial \mathbf{C}_{t-1}} = 1$$

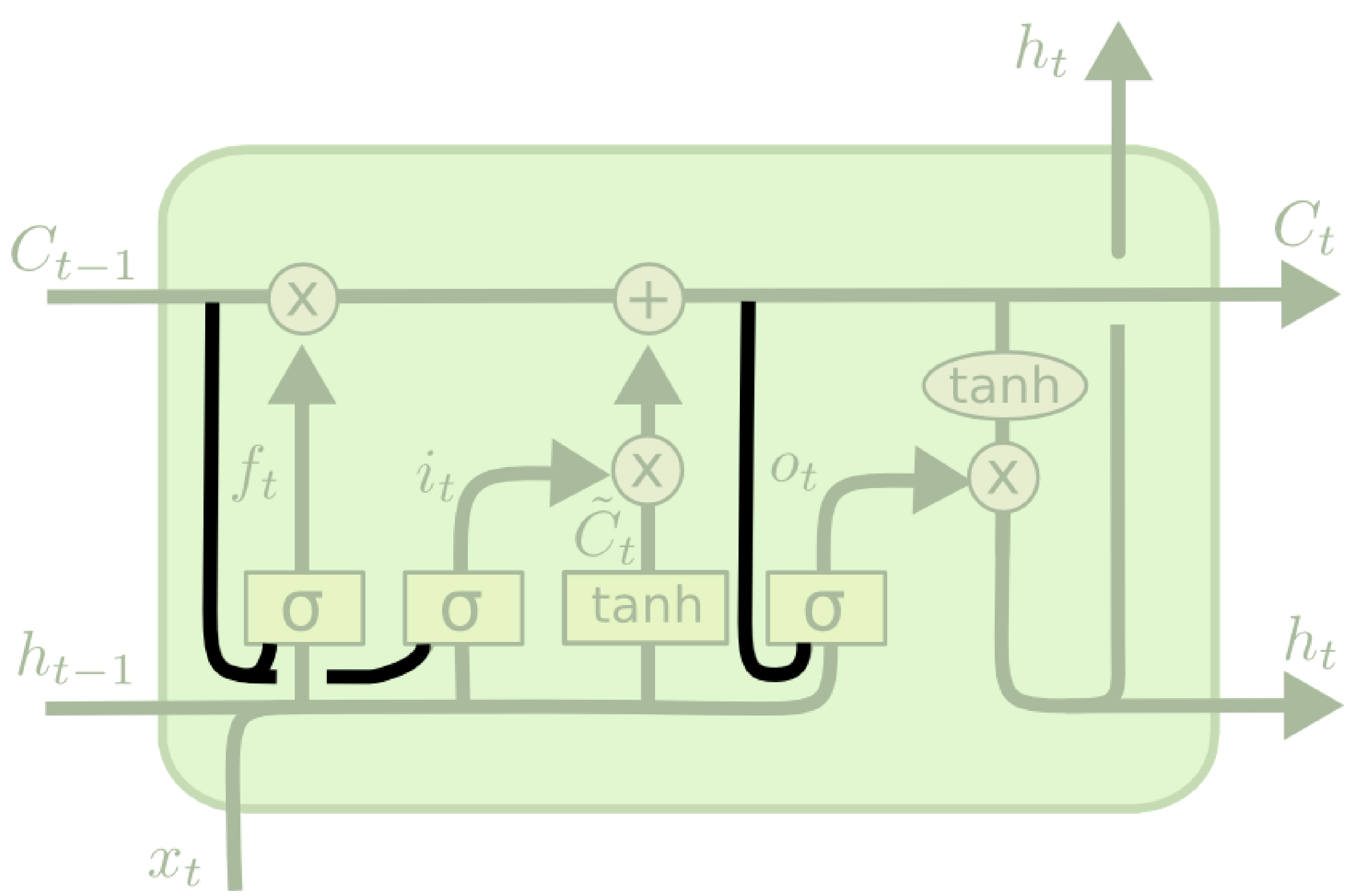
- The gradient is multiplied by exactly one when the gates are closed.

LSTM networks

- LSTM are particularly good at learning long-term dependencies, because the gates protect the cell from vanishing gradients.
- Its problem is how to find out which inputs (e.g. $\mathbf{x}_0$ and $\mathbf{x}_1$) should enter or leave the state memory.
- Truncated BPTT is used to train all weights: the weights for the candidate state (as for RNN), and the weights of the three gates.
- LSTM are also subject to overfitting. Regularization (including dropout) can be used.
- The weights (also for the gates) can be convolutional.
- The gates also have a bias, which can be fixed (but hard to find).
- LSTM layers can be stacked to detect dependencies at different scales (deep LSTM network).

Hochreiter and Schmidhuber (1997). Long short-term memory. Neural computation, 9(8).

Peephole connections



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

- A popular variant of LSTM adds *peephole* connections, where the three gates have additionally access to the state $\mathbf{C}_{t-1}$.

$$\mathbf{f}_t = \sigma(W_f \times [\mathbf{C}_{t-1}; \mathbf{h}_{t-1}; \mathbf{x}_t] + \mathbf{b}_f)$$

$$\mathbf{i}_t = \sigma(W_i \times [\mathbf{C}_{t-1}; \mathbf{h}_{t-1}; \mathbf{x}_t] + \mathbf{b}_i)$$

$$\mathbf{o}_t = \sigma(W_o \times [\mathbf{C}_t; \mathbf{h}_{t-1}; \mathbf{x}_t] + \mathbf{b}_o)$$

- It usually works better, but it adds more weights.

Gers and Schmidhuber (2000). Recurrent nets that time and count. IJCNN.

GRU: Gated Recurrent Unit

- Another variant is called the **Gated Recurrent Unit** (GRU).

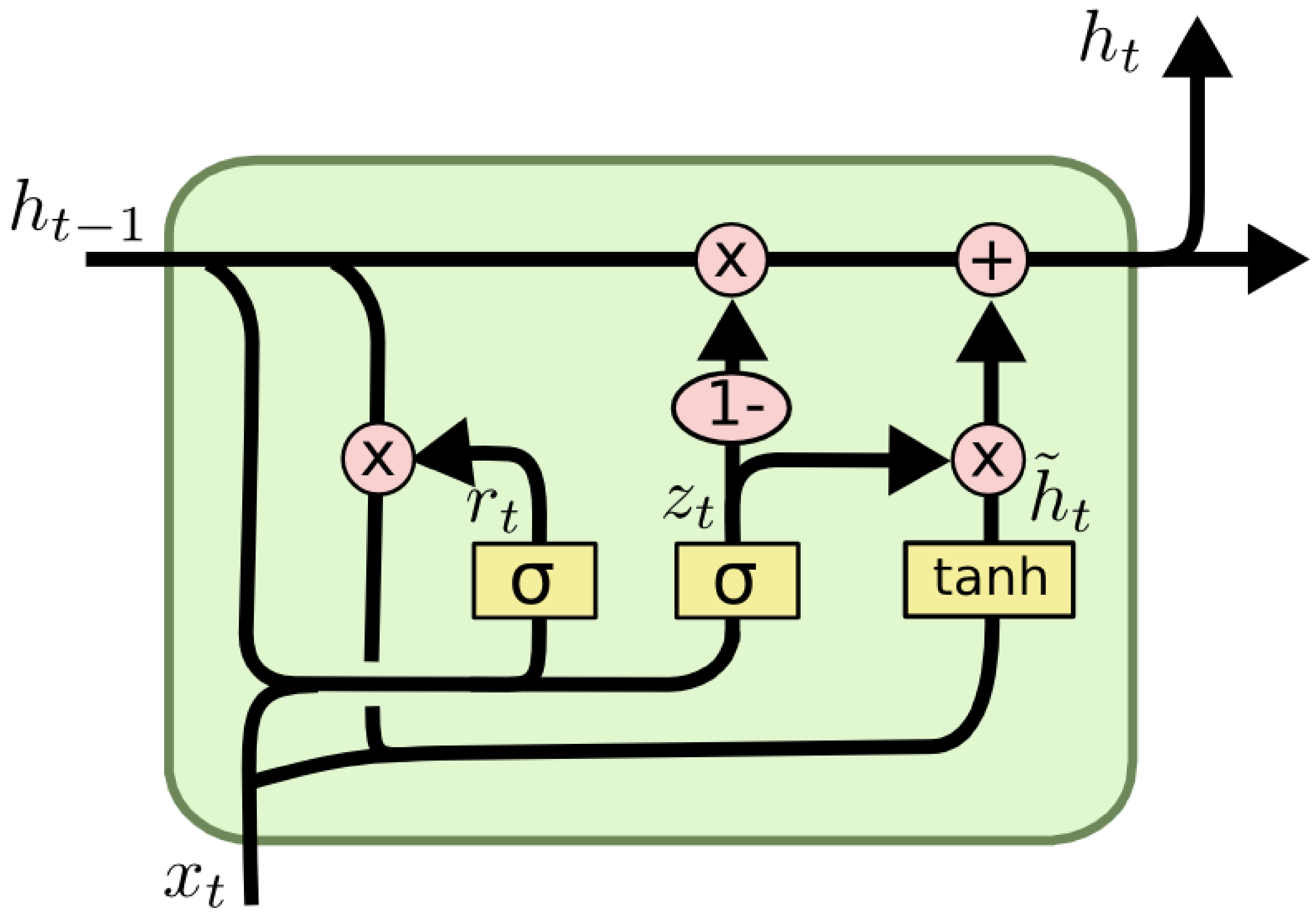
- It uses directly the output $\mathbf{h}_t$ as a state, and the forget and input gates are merged into a single gate $\mathbf{r}_t$.

$$\mathbf{z}_t = \sigma(W_z \times [\mathbf{h}_{t-1}; \mathbf{x}_t])$$

$$\mathbf{r}_t = \sigma(W_r \times [\mathbf{h}_{t-1}; \mathbf{x}_t])$$

$$\tilde{\mathbf{h}}_t = \tanh(W_h \times [\mathbf{r}_t \odot \mathbf{h}_{t-1}; \mathbf{x}_t])$$

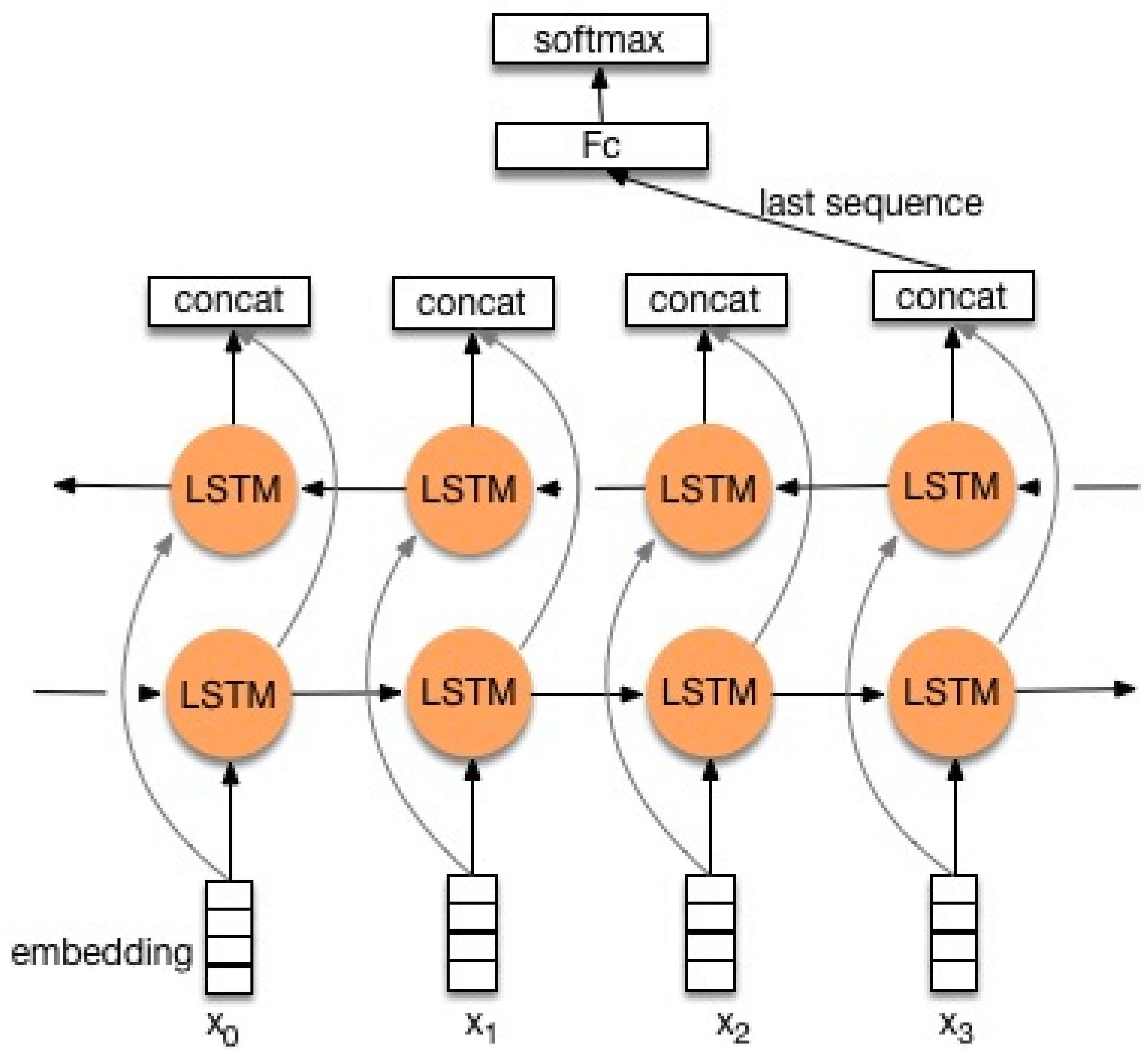
$$\mathbf{h}_t = (1 - \mathbf{z}_t) \odot \mathbf{h}_{t-1} + \mathbf{z}_t \odot \tilde{\mathbf{h}}_t$$



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

- It does not even need biases (mostly useless in LSTMs anyway).
- Much simpler to train as the LSTM, and almost as powerful.

Bidirectional LSTM



- A **bidirectional LSTM** learns to predict the output in two directions:
  - The **feedforward** line learns using the past context (classical LSTM).
  - The **backforward** line learns using the future context (inputs are reversed).
- The two state vectors are then concatenated at each time step to produce the output.
- Only possible offline, as the future inputs must be known.
- Works better than LSTM on many problems, but slower.

Source:
http://www.paddlepaddle.org/doc/demo/sentiment_analysis/sentiment_analysis.html

References

- A great blog post by Christopher Olah to understand recurrent neural networks, especially LSTM:

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

- Shi Yan built on that post to explain it another way:

https://medium.com/@shiyan/understanding-lstm-and-its-diagrams-37e2f46f1714#.m7fxgvjwf