Recurrent Neural Networks

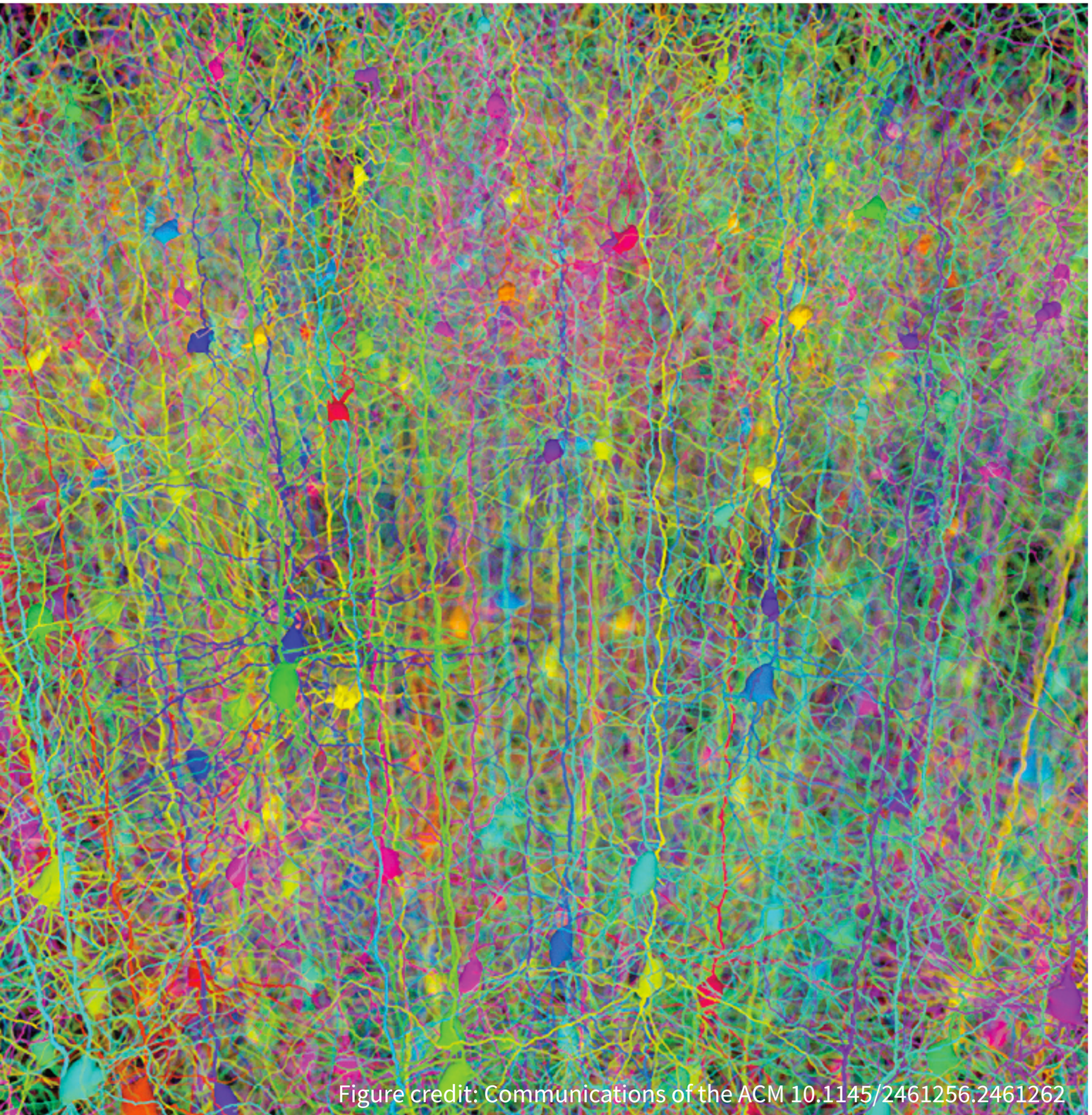

Figure credit: Communications of the ACM 10.1145/2461256.2461262

GRAHAM TAYLOR

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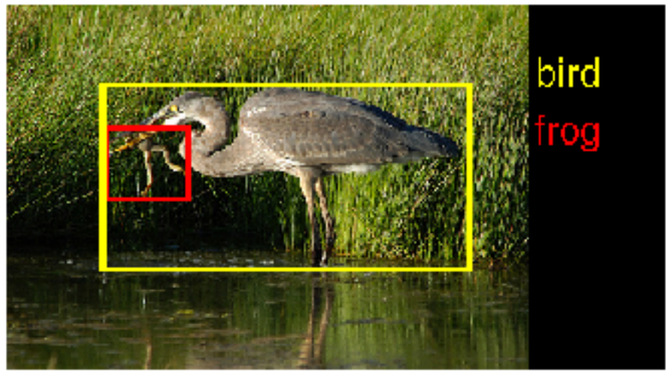
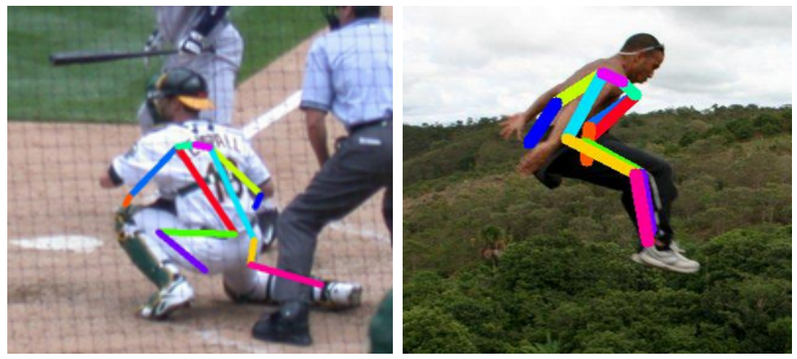
Deep Learning Successes

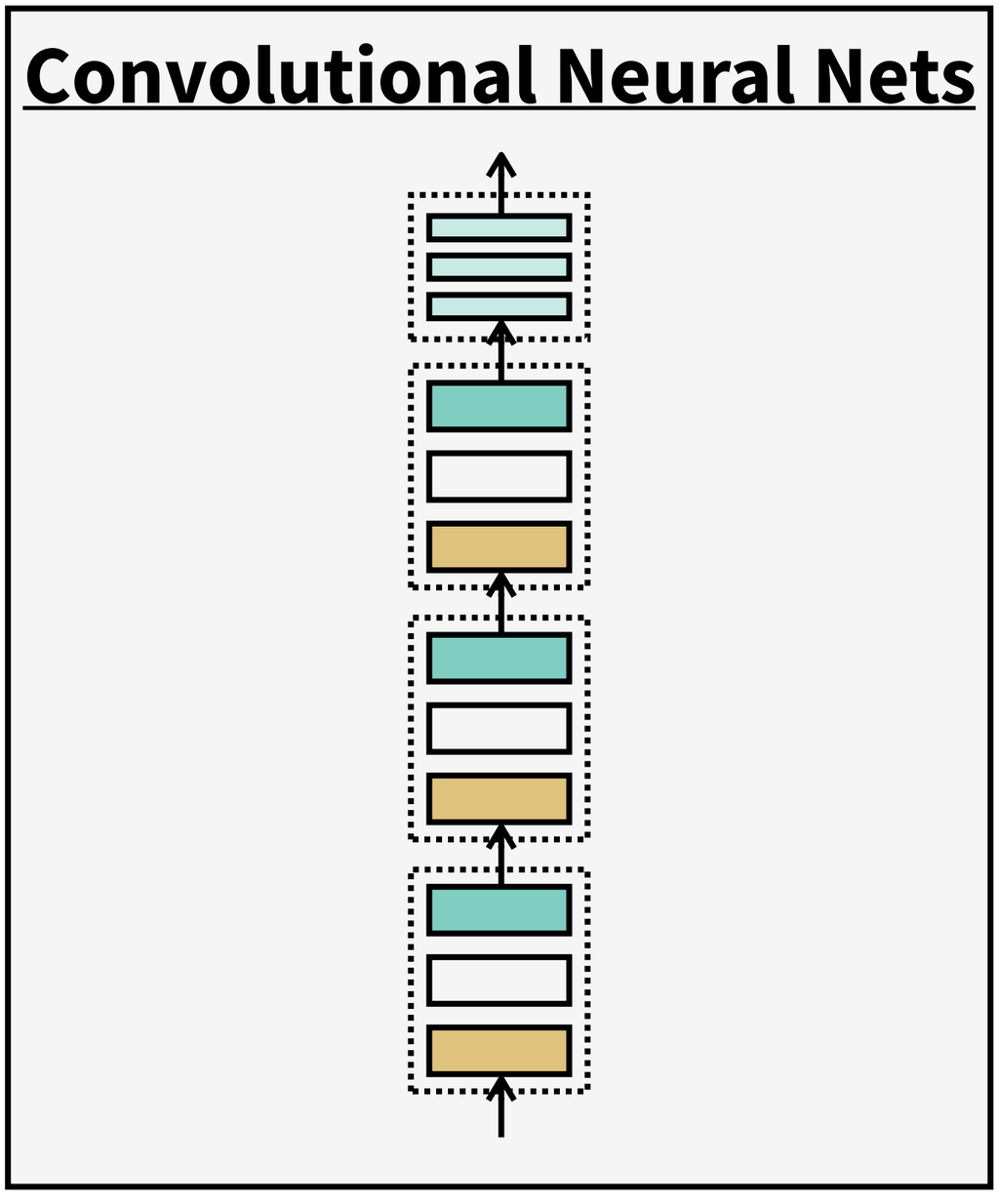
- Vision
  - Object recognition and detection
  - Pose estimation and activity recognition
- Speech
  - Speech recognition
  - Speaker authentication
- Natural Language Processing
  - Question answering
  - Machine translation





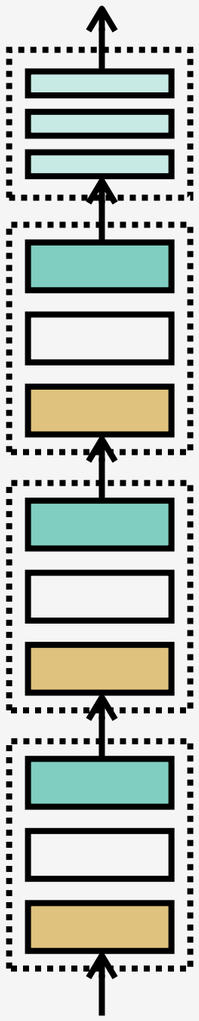
Two “Hammers”

Two “Hammers”

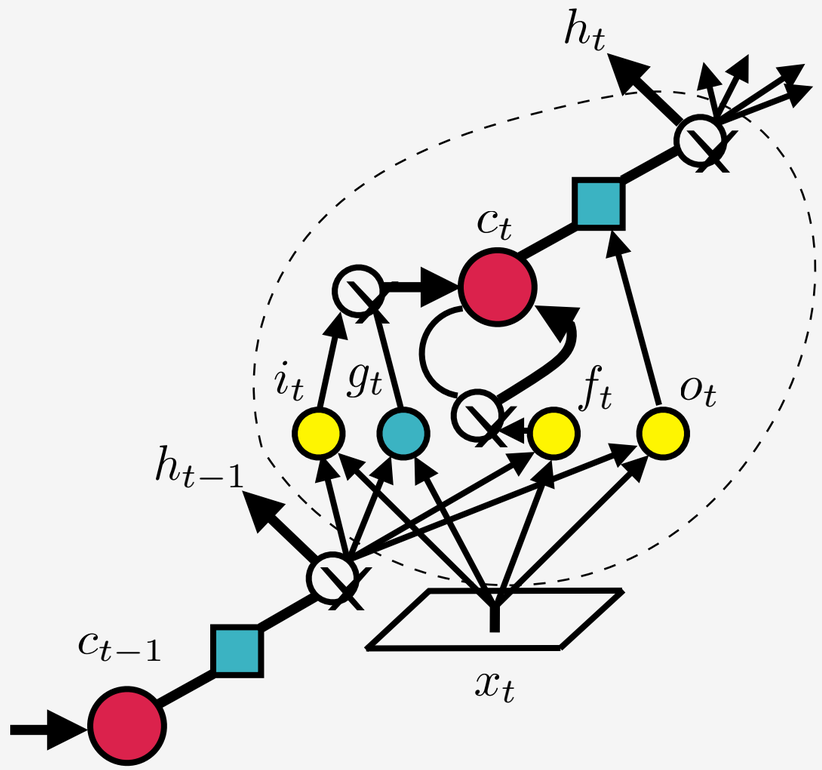


Two “Hammers”

Convolutional Neural Nets



Recurrent Neural Nets

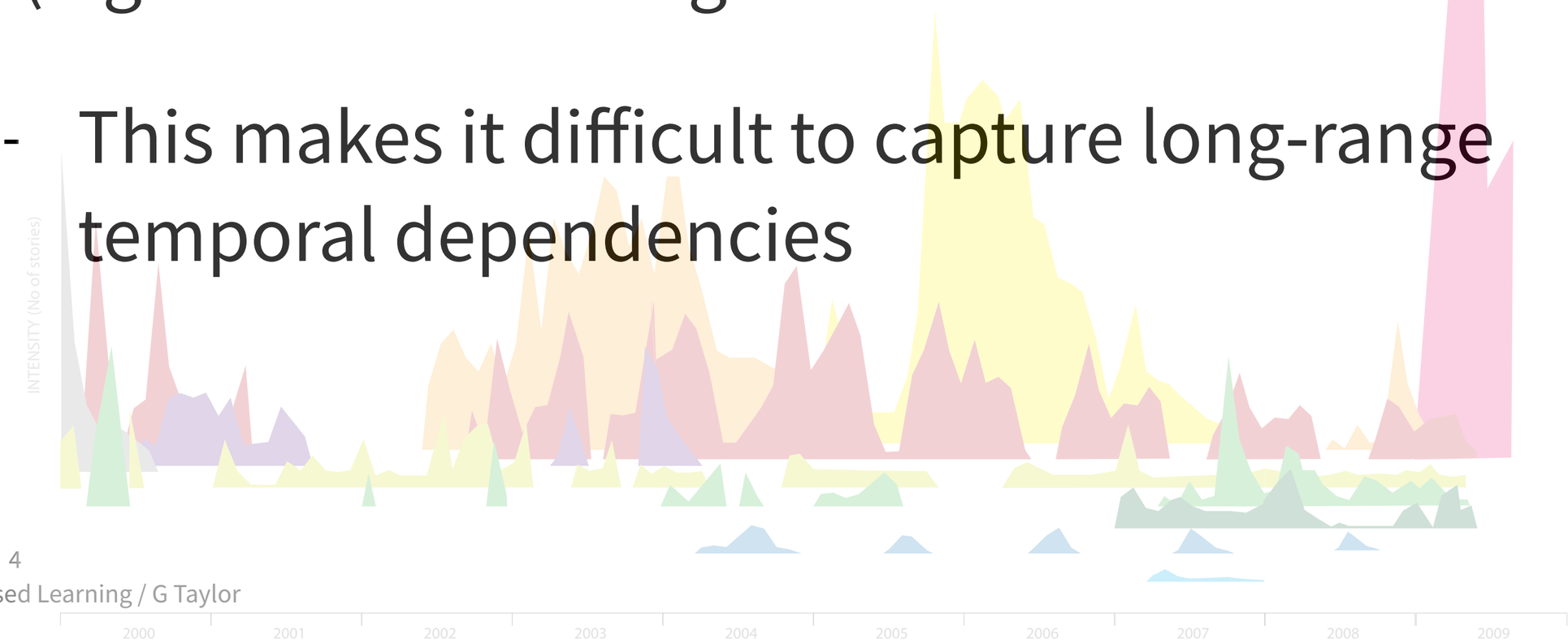


Learning Sequence Representations

- Time is an integral part of many human behaviours (e.g. motion, reasoning, dialogue)

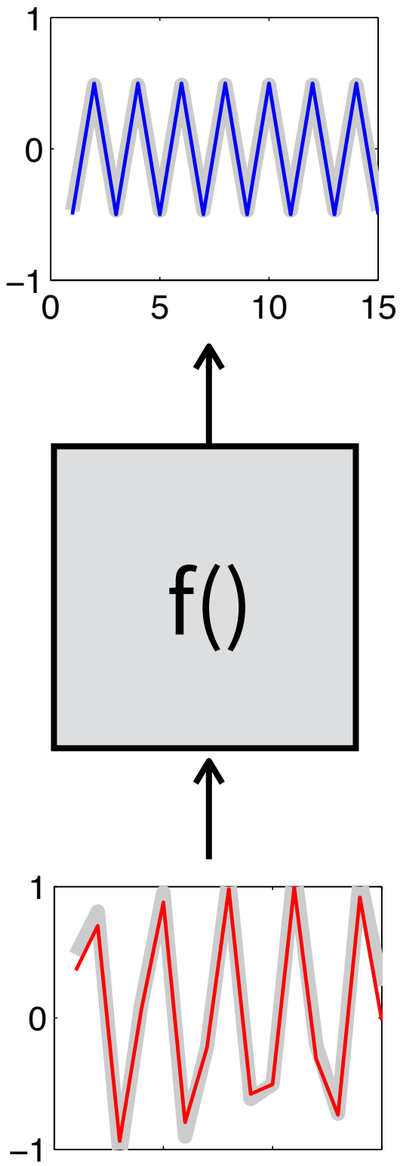
- Easiest way to cope with time is to simply ignore it (e.g. model fixed-length windows of observations)

- This makes it difficult to capture long-range temporal dependencies

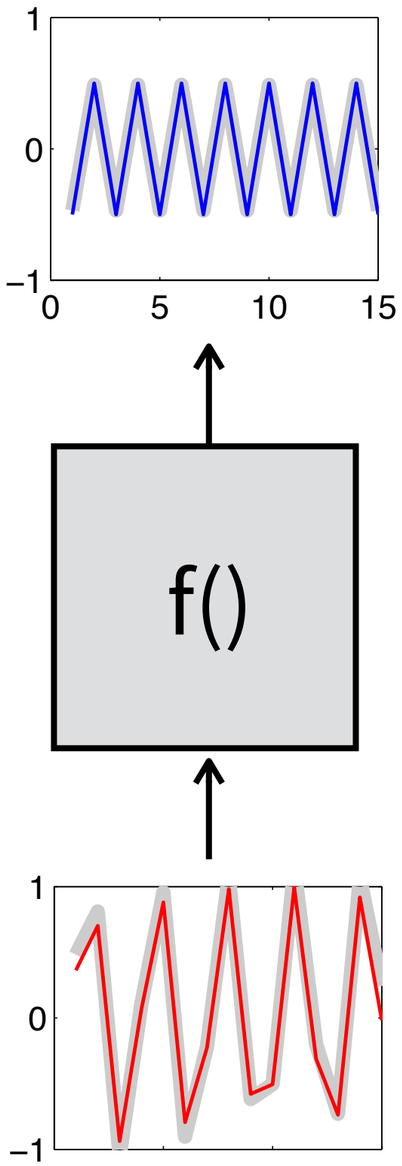


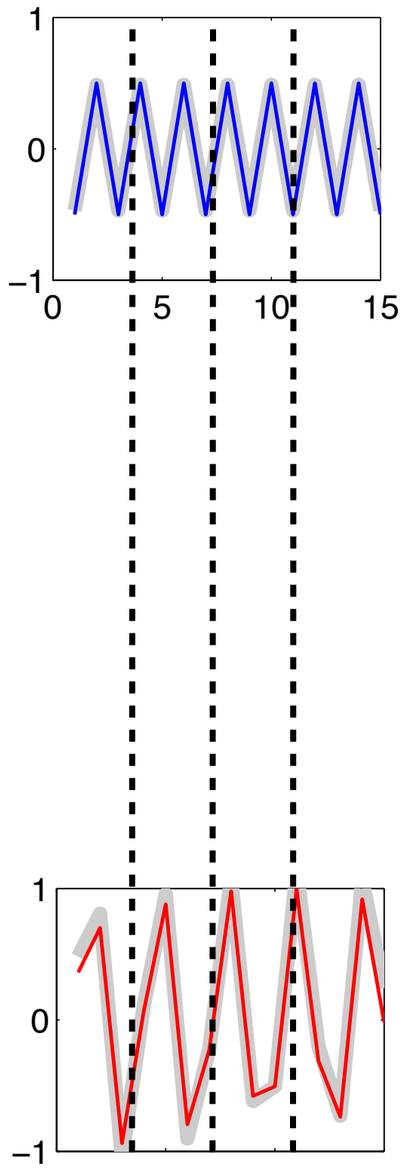
Modeling fixed-length windows?

Modeling fixed-length windows?

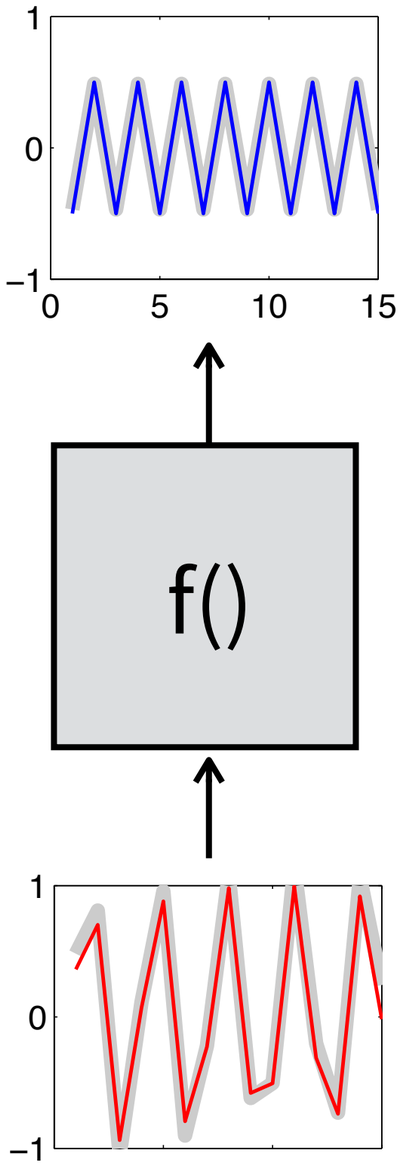


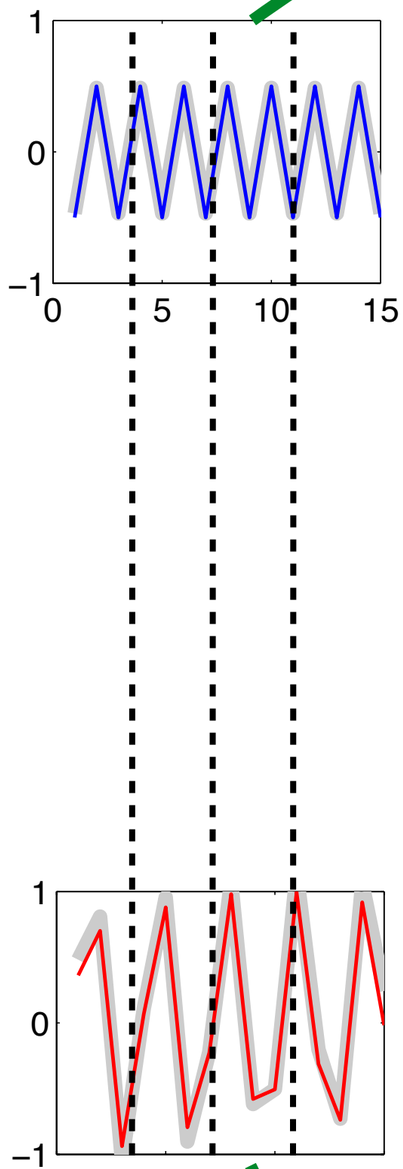
Modeling fixed-length windows?

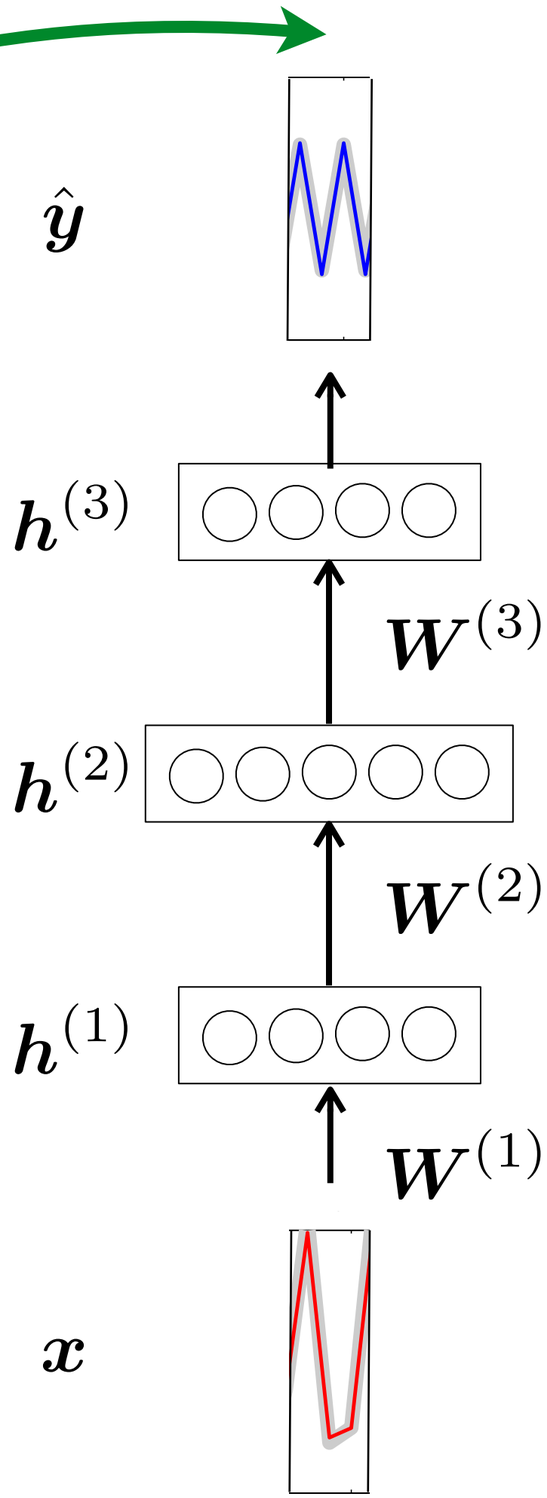




Modeling fixed-length windows?

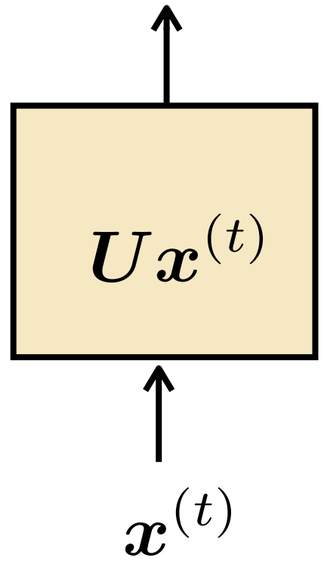




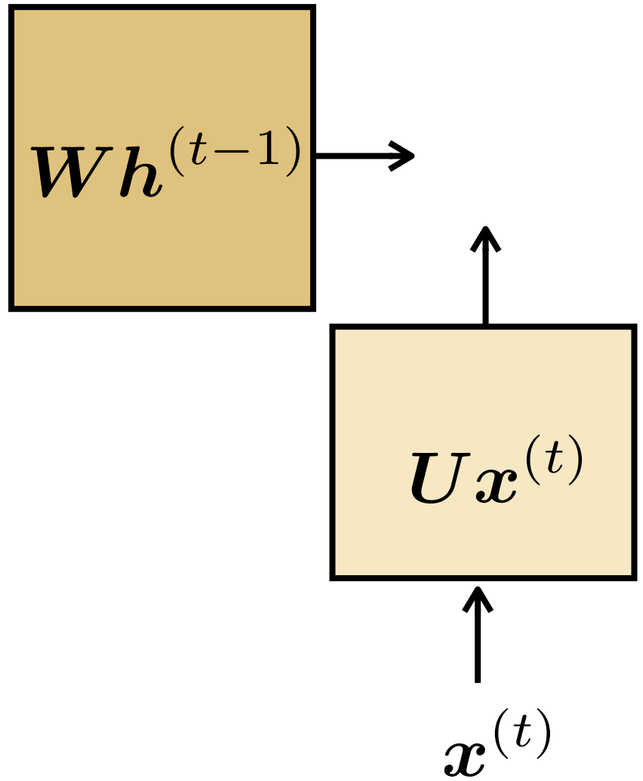


Recurrent Neural Networks

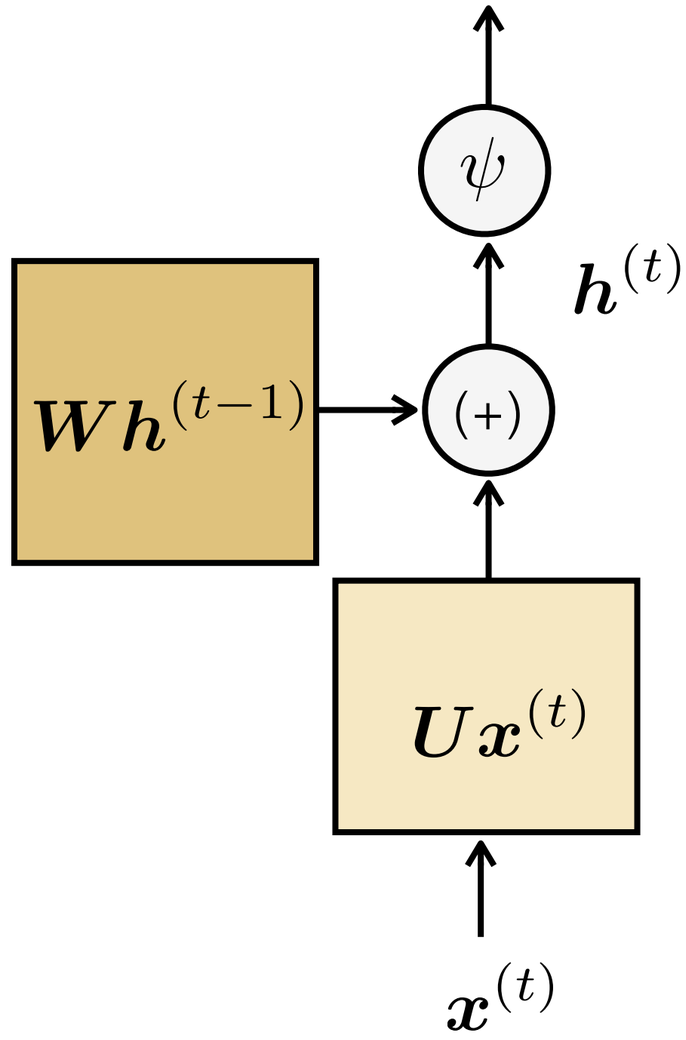
Recurrent Neural Networks



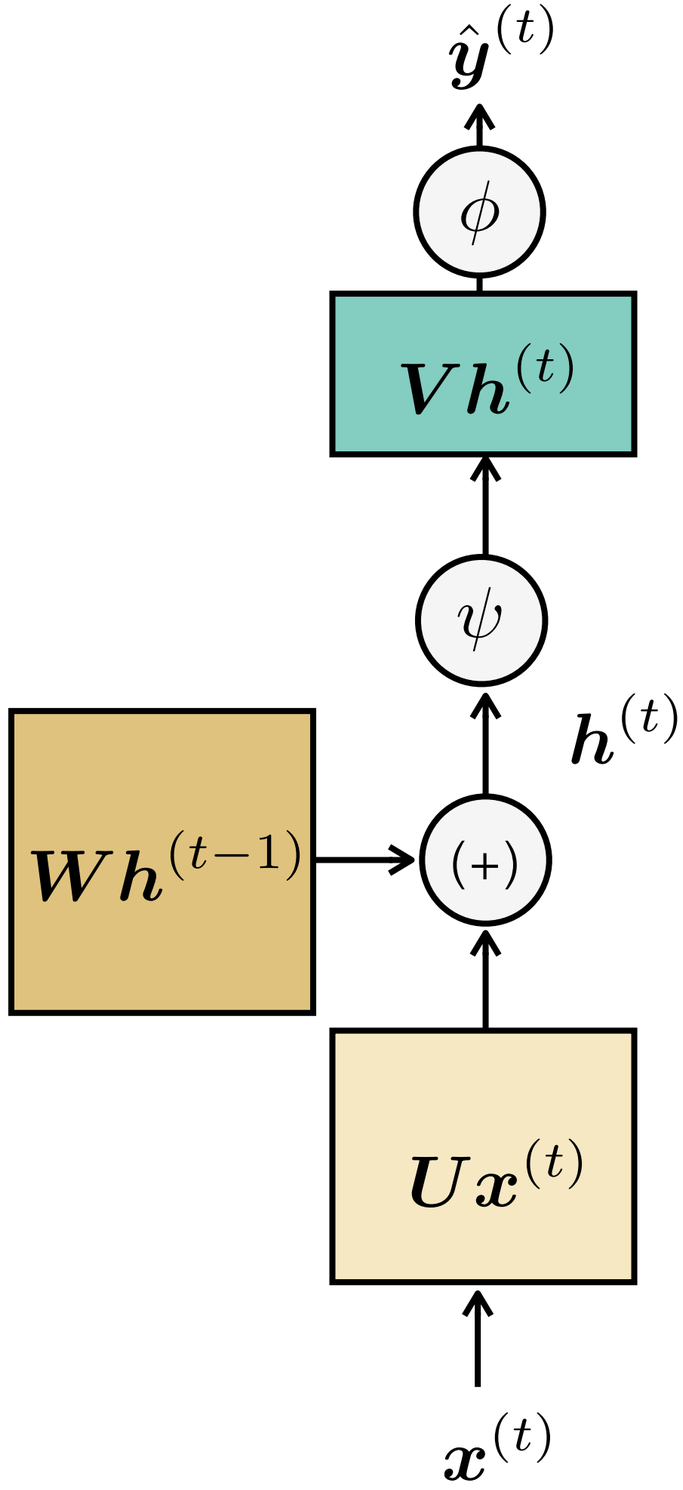
Recurrent Neural Networks



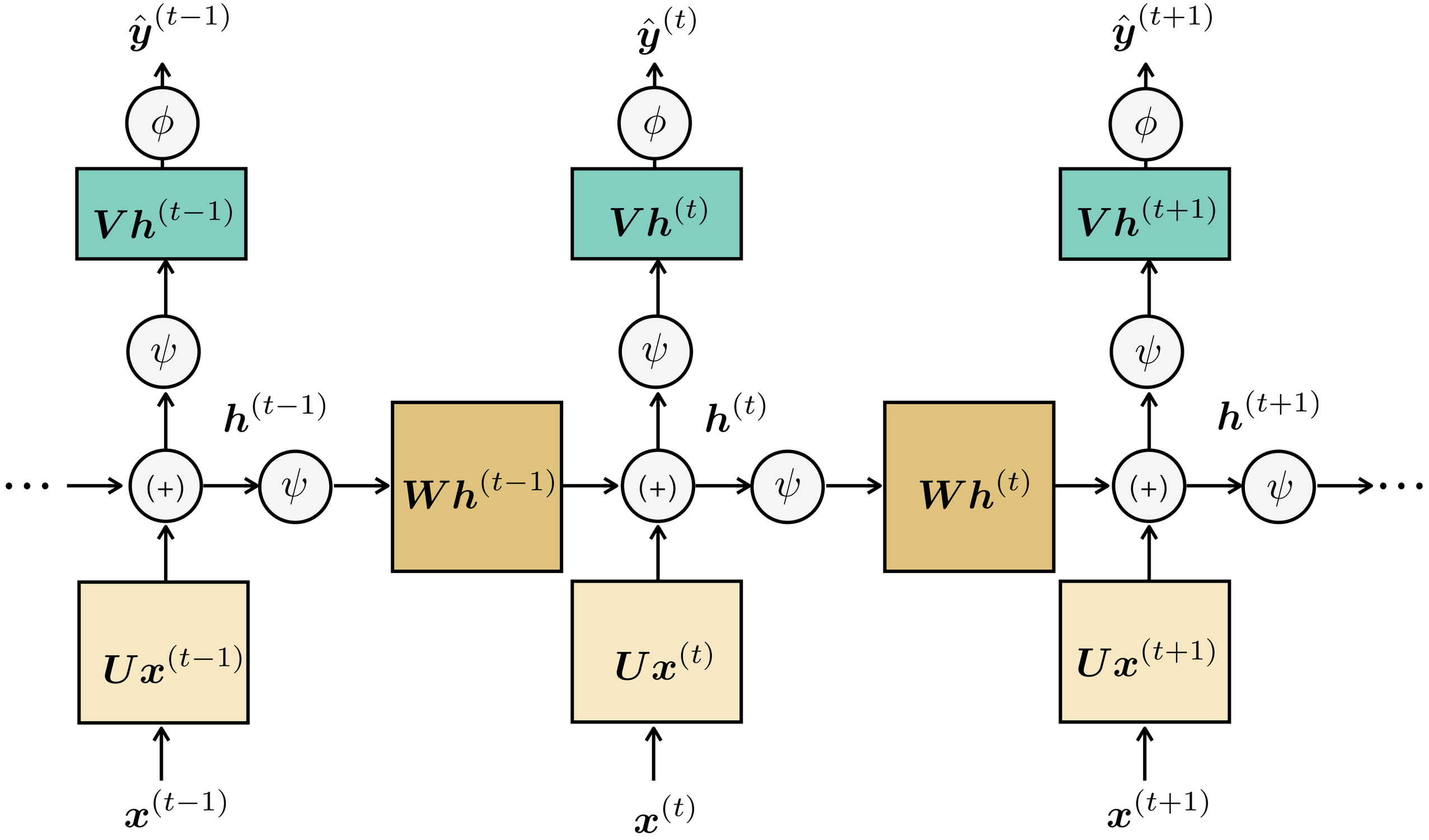
Recurrent Neural Networks



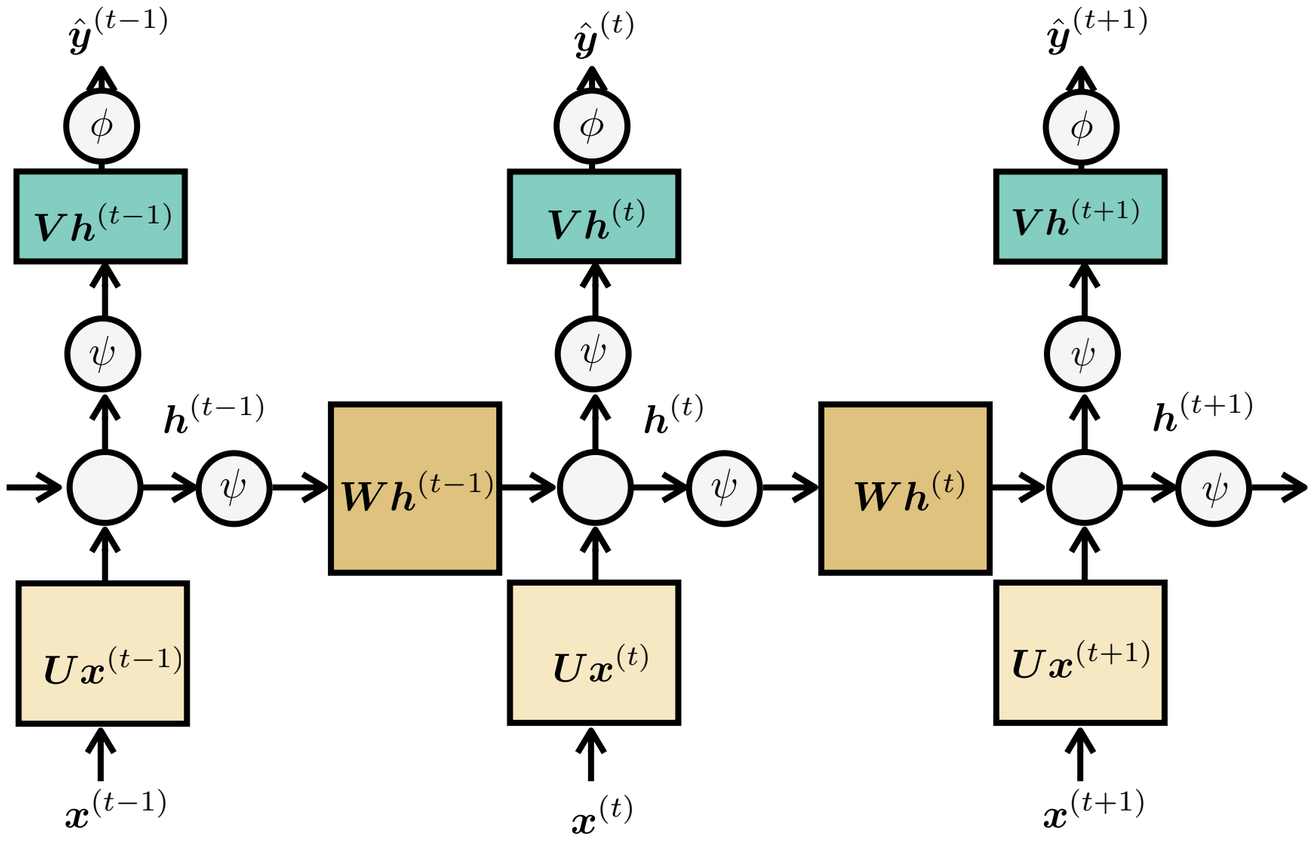
Recurrent Neural Networks



Recurrent Neural Networks



RNN (Update)



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

$$\boldsymbol{h}^{(t)} = \psi(\boldsymbol{a}^{(t)})$$

$$\boldsymbol{o}^{(t)} = \boldsymbol{c} + \boldsymbol{V}\boldsymbol{h}^{(t)}$$

$$\hat{\boldsymbol{y}}^{(t)} = \phi(\boldsymbol{o}^{(t)})$$

RNNs: The Promise

- Possibly high-dimensional, distributed, internal representation and nonlinear dynamics allow model, in theory, model complex time series
  - and capture long-range dependencies!
- Exact gradients can be computed exactly via Backpropagation Through Time

Generality

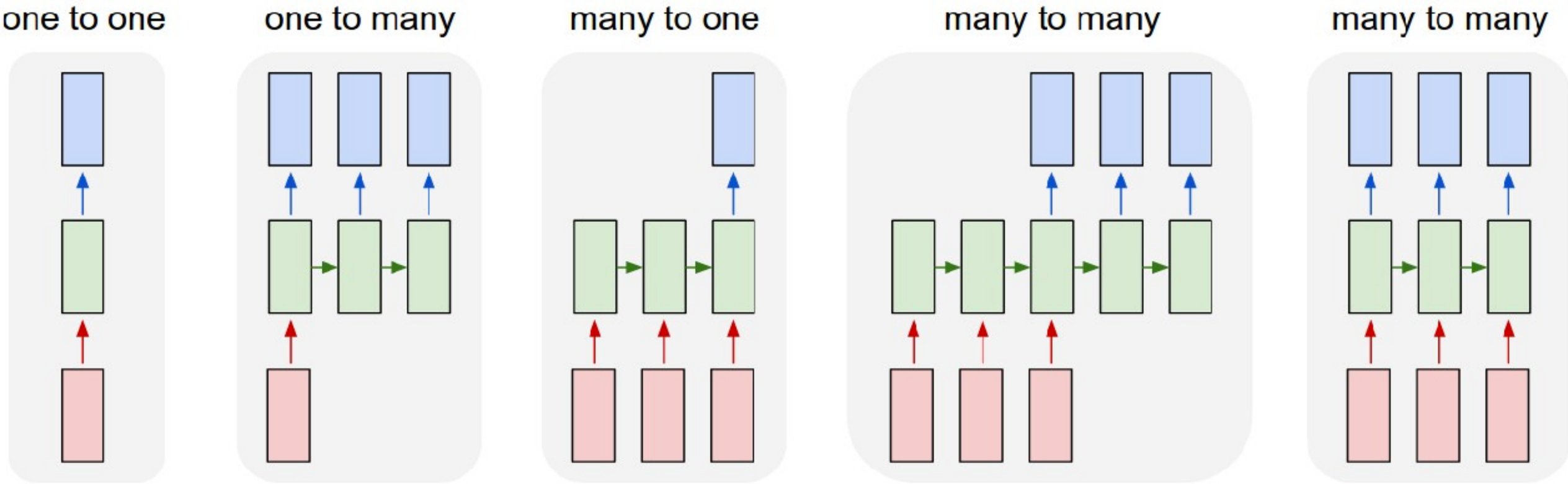
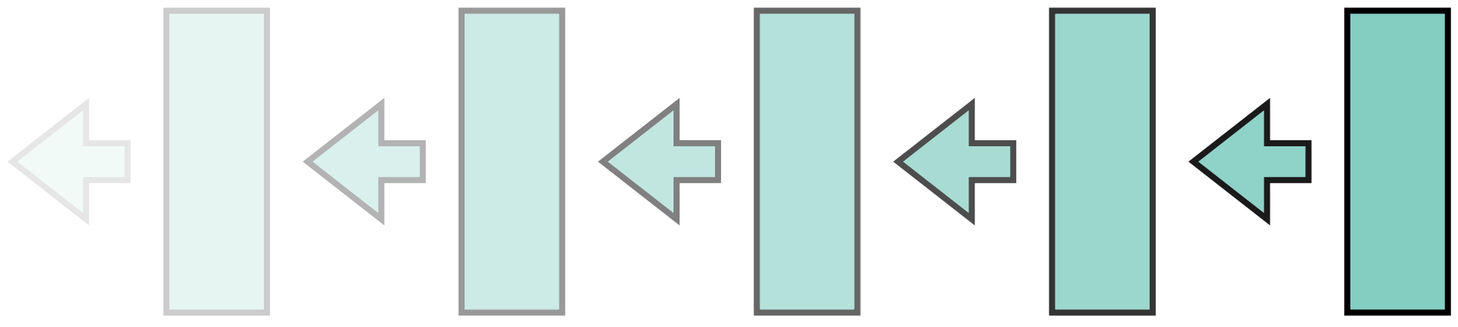


Figure: Andrej Karpathy
http://karpathy.github.io/2015/05/21/rnn-effectiveness/

RNNs: The Reality

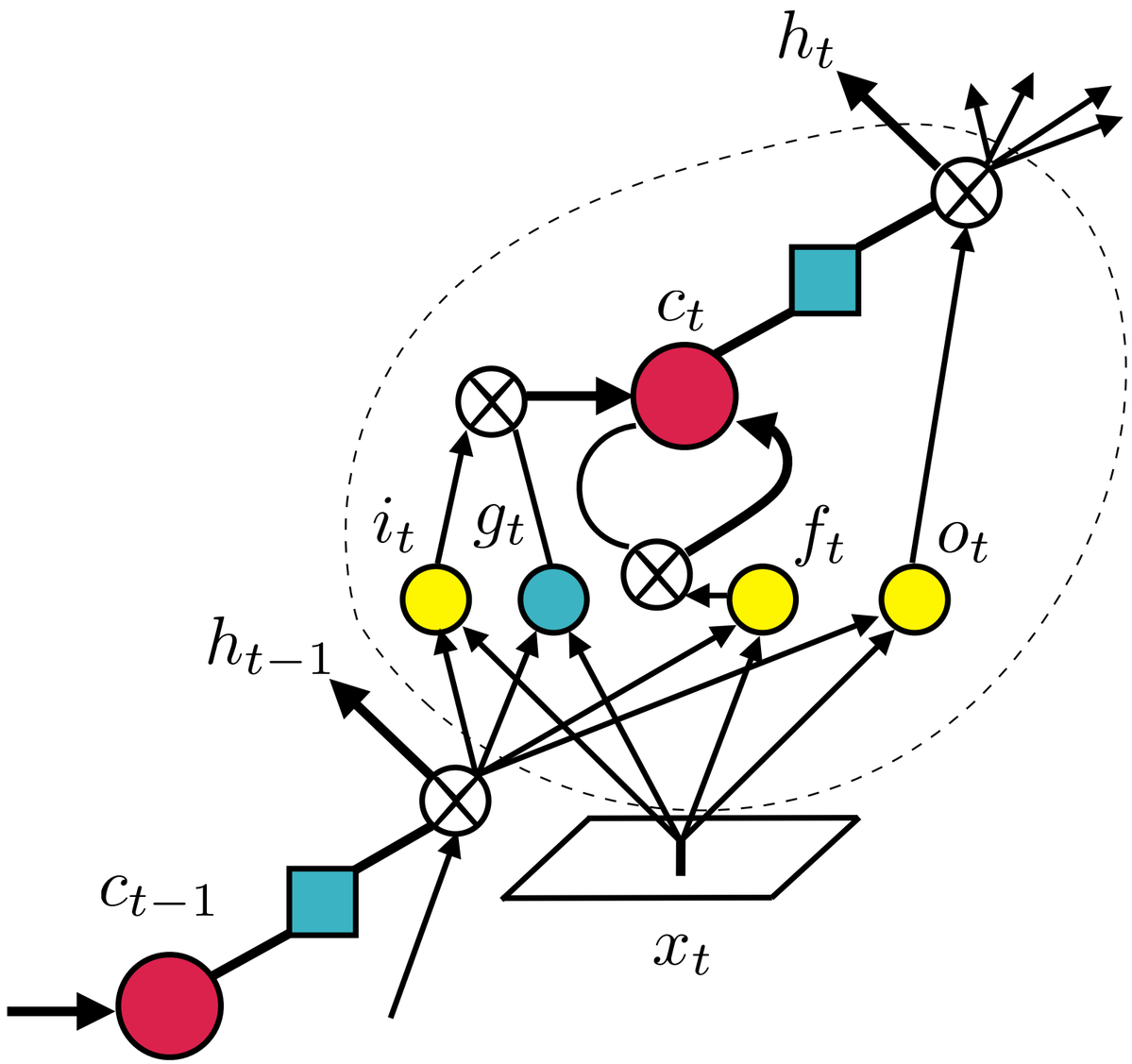
- A powerful and flexible architecture - but?
  - Training RNNs via gradient descent fails on simple problems (typically memorization tasks)
  - Attributed to “vanishing” or “exploding” gradients

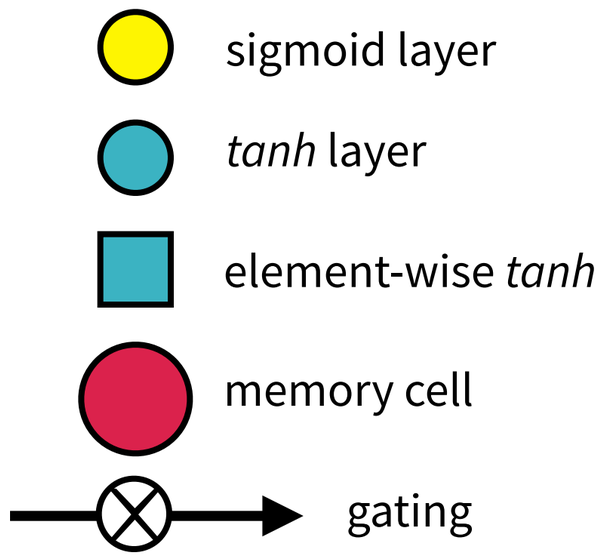


Solutions: Architectural

- Gating 
  - Long Short-term Memory (Hochreiter et al. 1997)
  - Gated Recurrent Units (Chung et al. 2014)
- “Structured” depth (Pascanu et al. 2014)
- Rectifiers (Le, Jaitly and Hinton 2015) 
- Units operating at different timescales (Hihi and Bengio 1996, Koutnik et al. 2014, Chung et al. 2017)

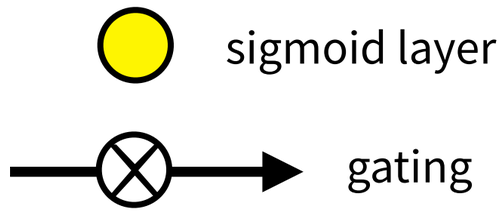
LSTM

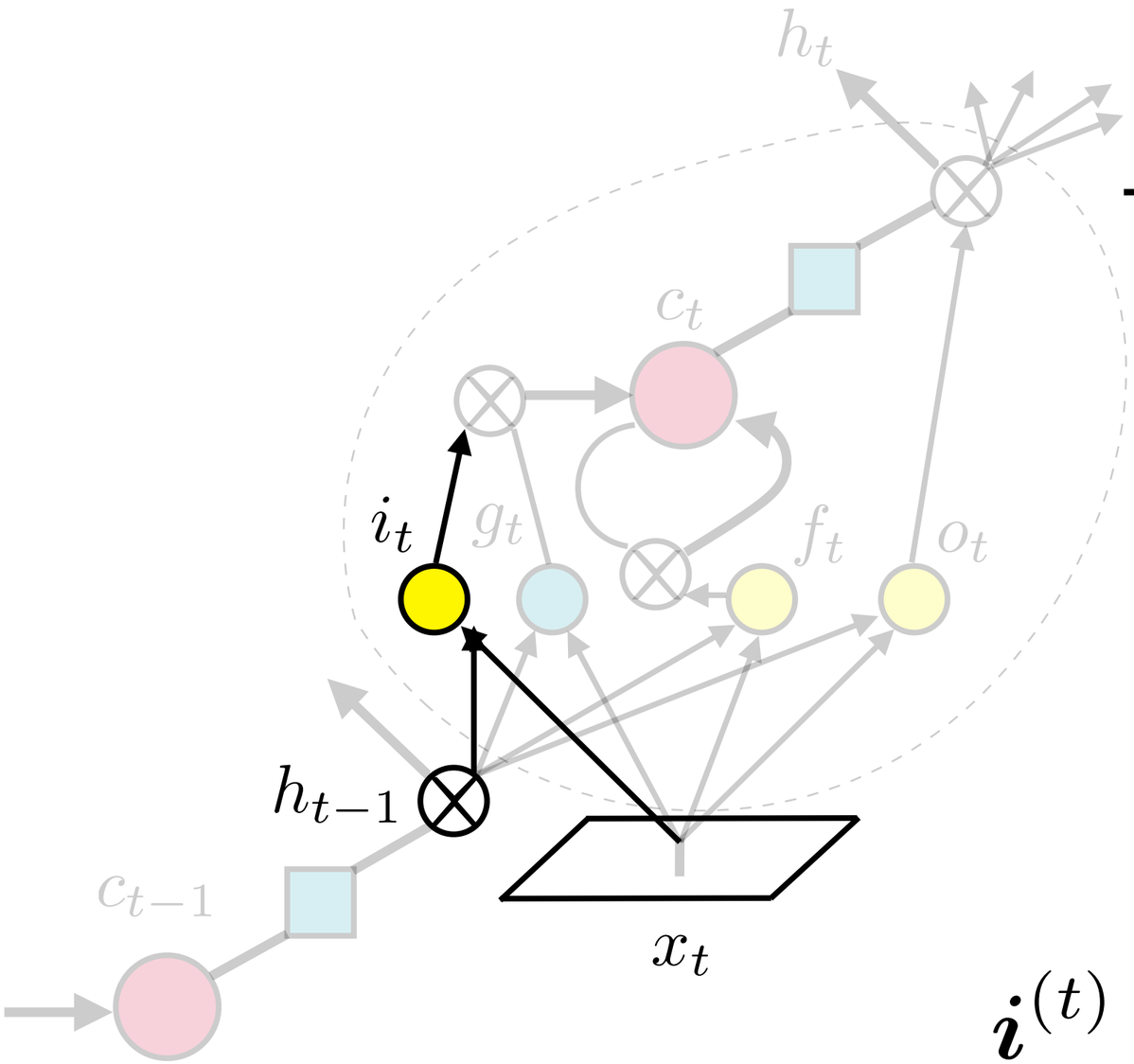




RNN with memory cells
designed to retain long-term information

LSTM - Input gate

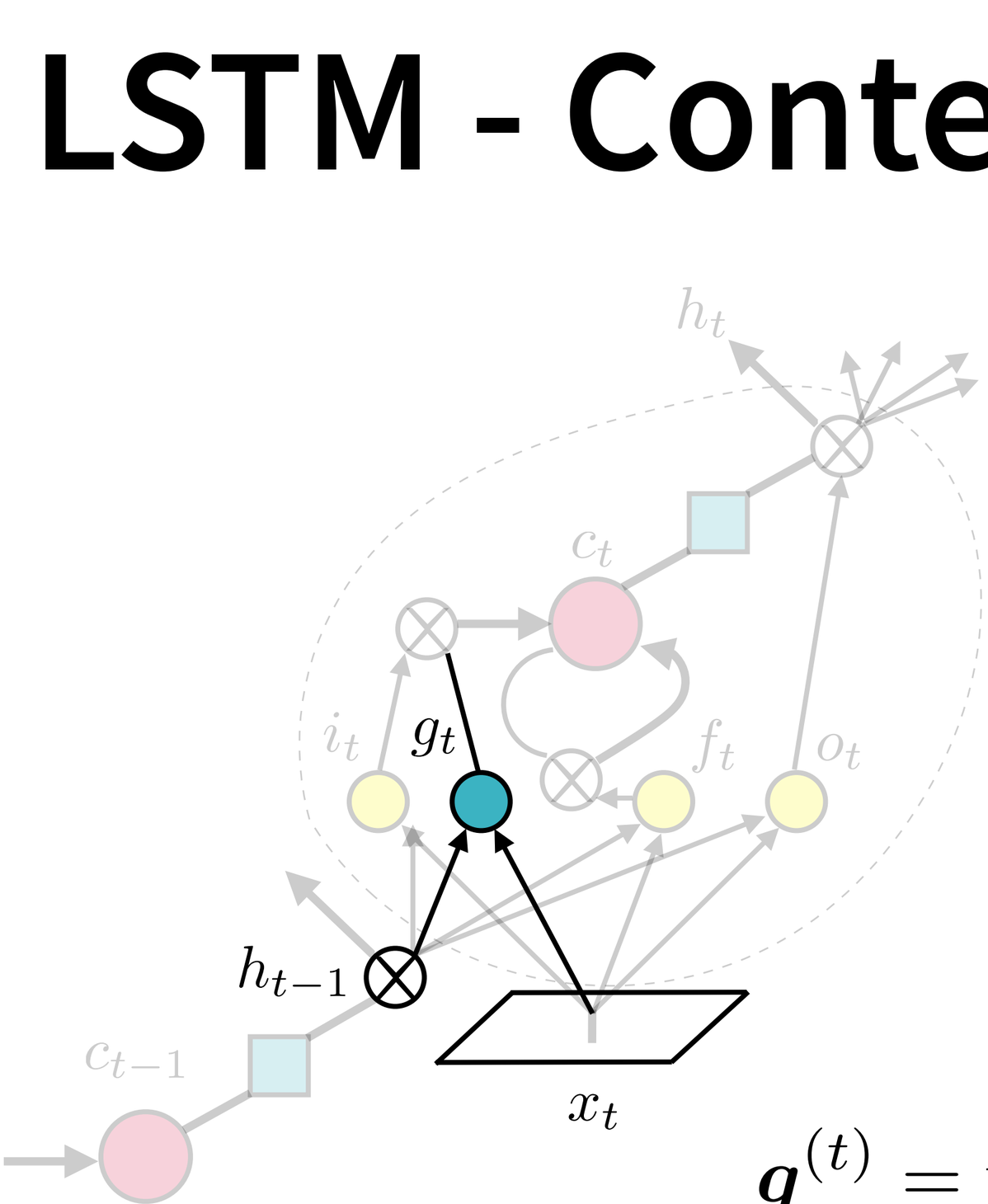




The input gate regulates the flow of new information into the cell

$$\boldsymbol{i}^{(t)} = \sigma\left(\boldsymbol{b}^i + \boldsymbol{W}^i \left[\boldsymbol{h}^{(t-1)}, \boldsymbol{x}^{(t)}\right]\right)$$

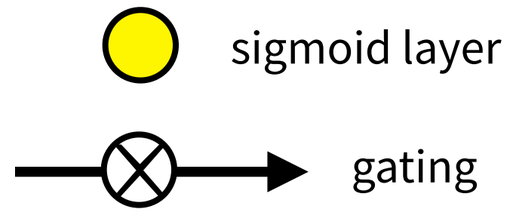
LSTM - Content

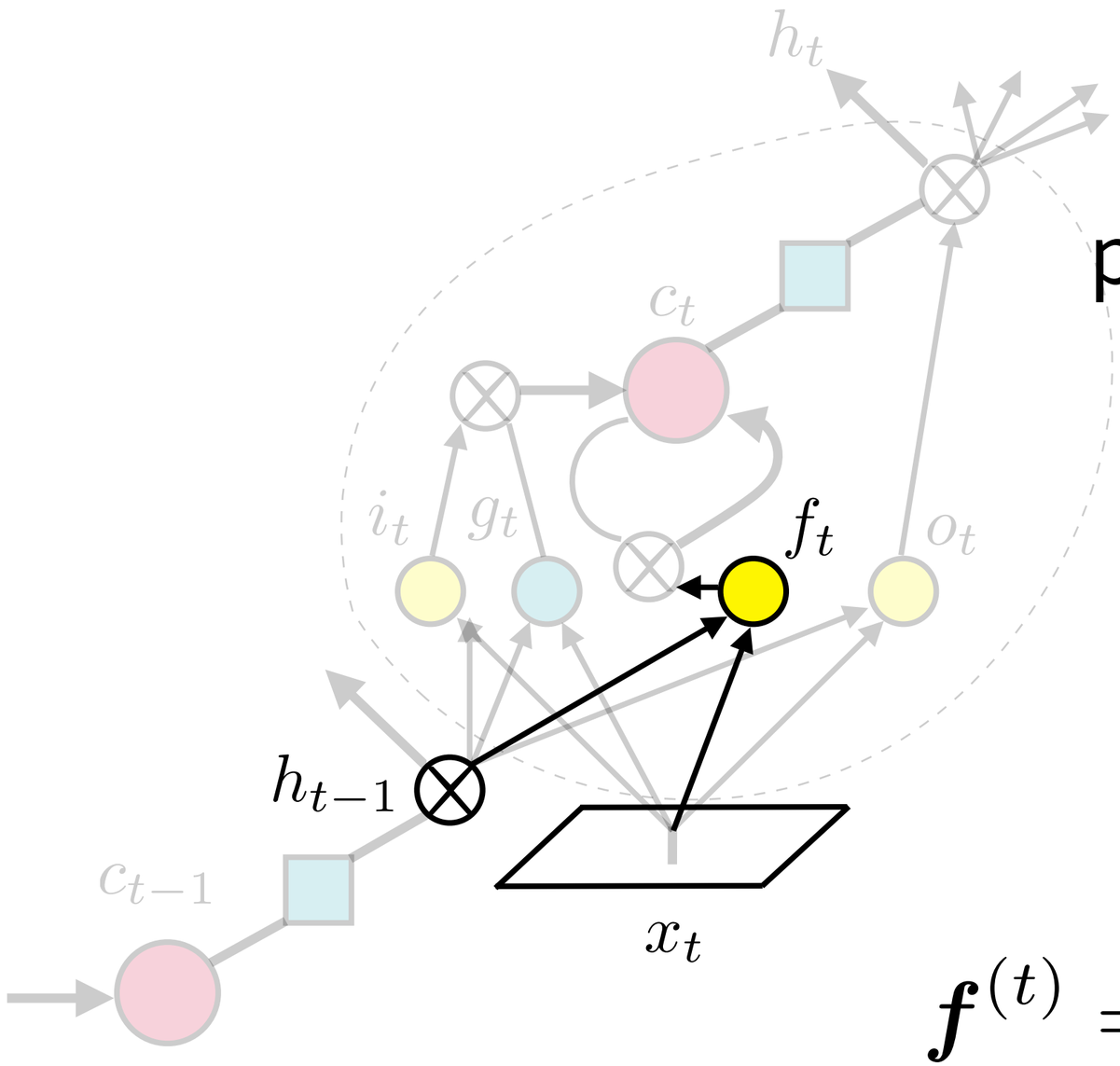


The new information that flows into the cell is a function of the past hidden state and the input (similar to RNN)

$$\boldsymbol{g}^{(t)} = \tanh\left(\boldsymbol{b}^{g} + \boldsymbol{W}^{g}\left[\boldsymbol{h}^{(t-1)}, \boldsymbol{x}^{(t)}\right]\right)$$

LSTM - Forget gate

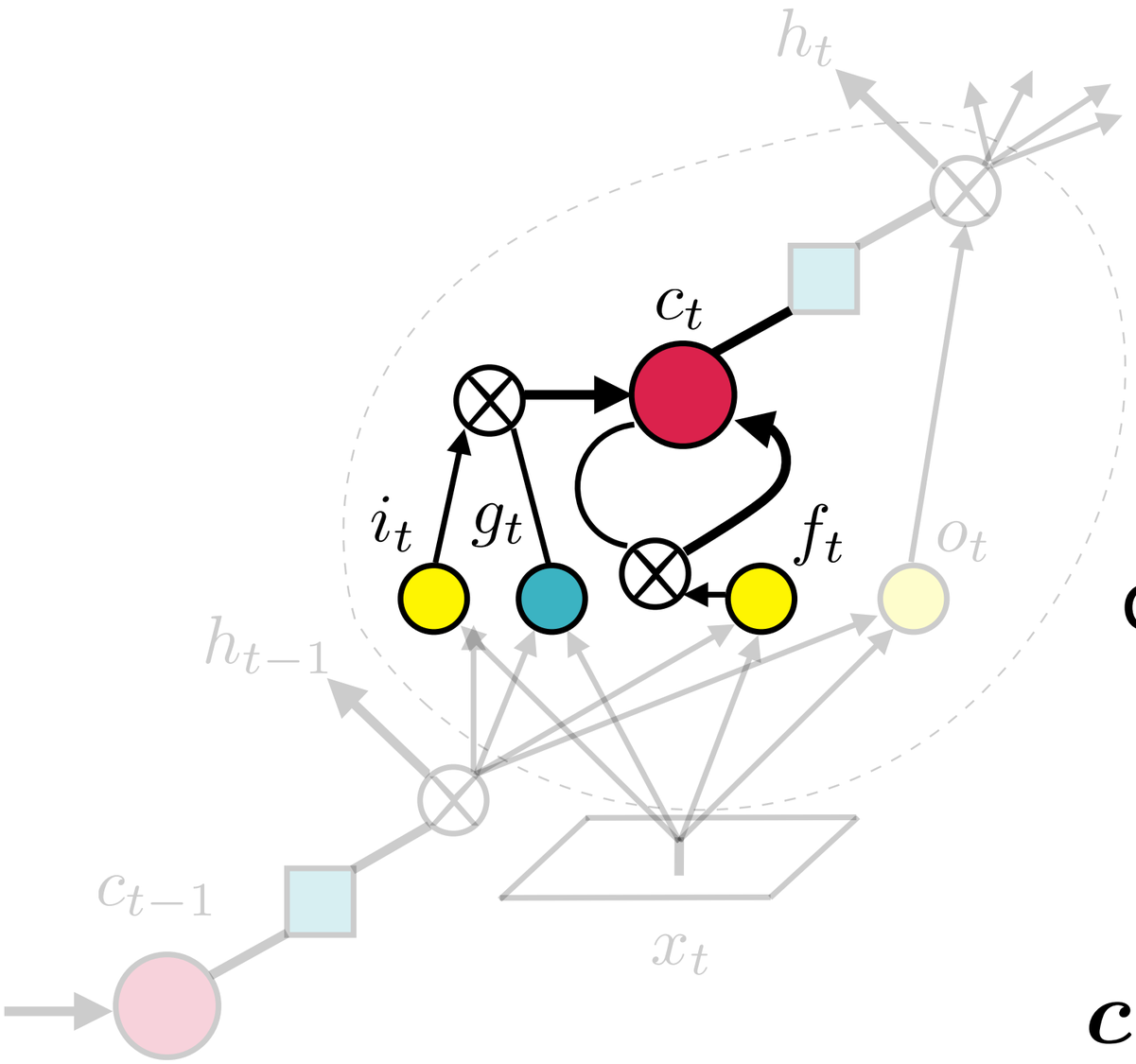


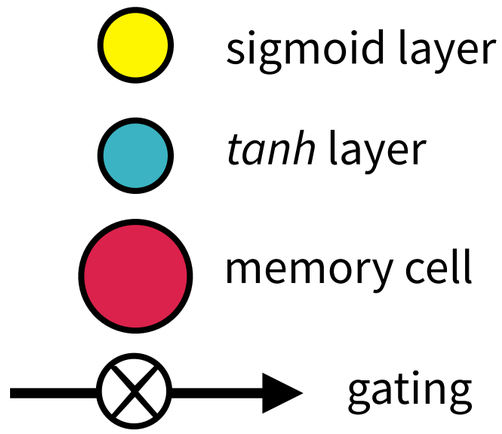


The forget gate regulates preservation of content in the cell

$$\boldsymbol{f}^{(t)} = \sigma\left(\boldsymbol{b}^f + \boldsymbol{W}^f \left[\boldsymbol{h}^{(t-1)}, \boldsymbol{x}^{(t)}\right]\right)$$

LSTM - Cell update

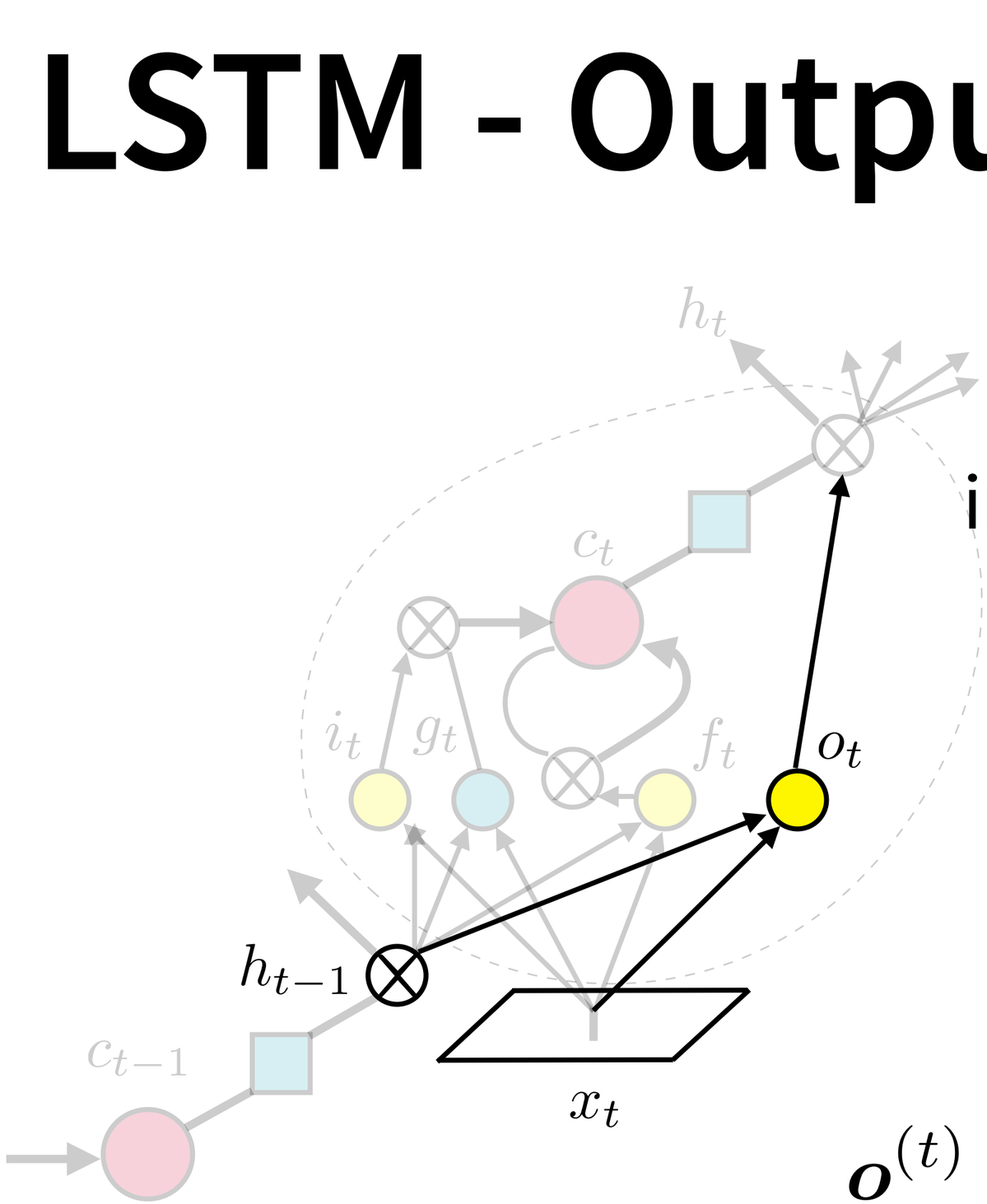




The cell is updated with a combination of new and existing information

$$\boldsymbol{c}^{(t)} = \boldsymbol{f}^{(t)} \odot \boldsymbol{c}^{(t-1)} + \boldsymbol{i}^{(t)} \odot \boldsymbol{g}^{(t)}$$

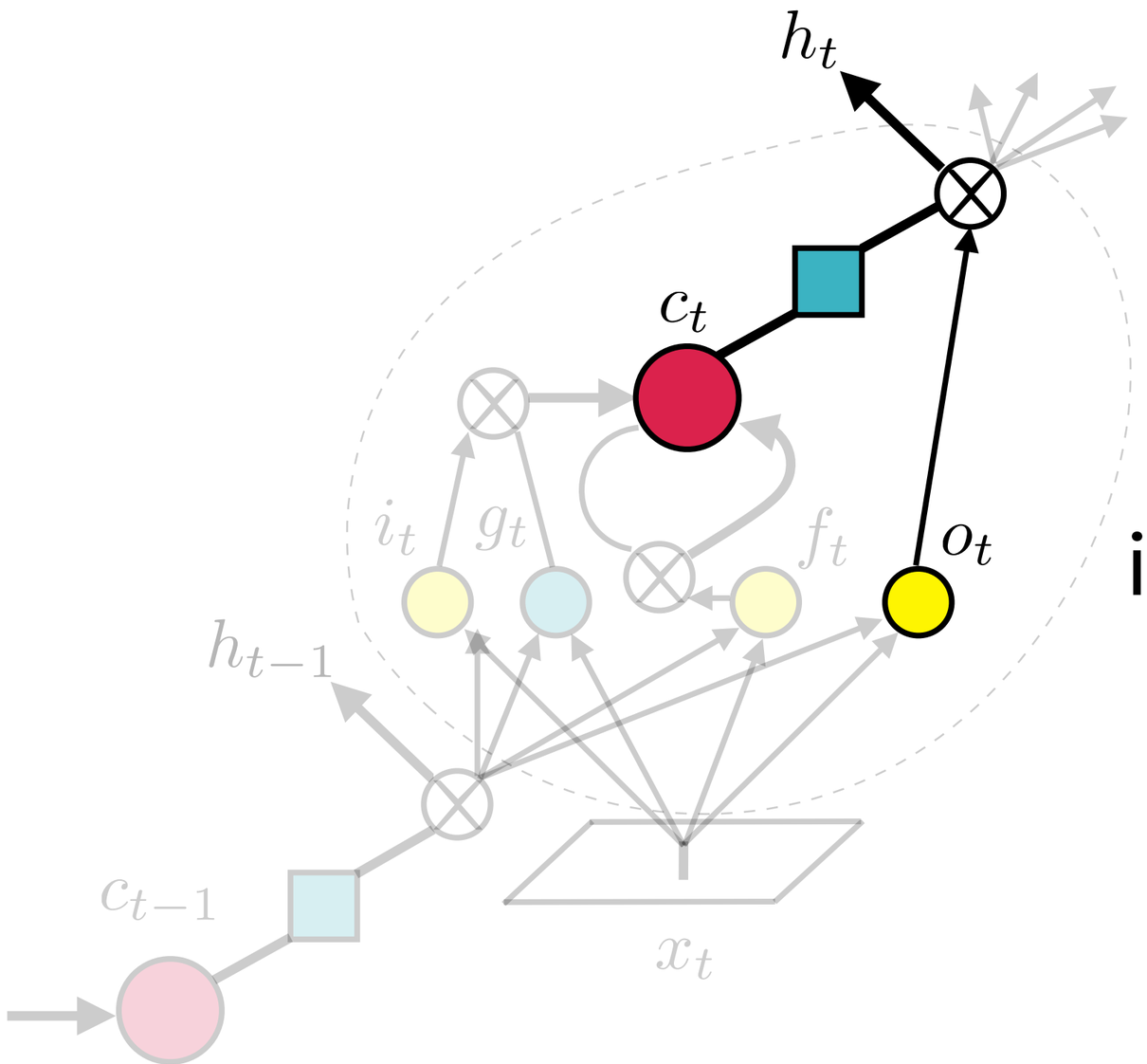
LSTM - Output gate

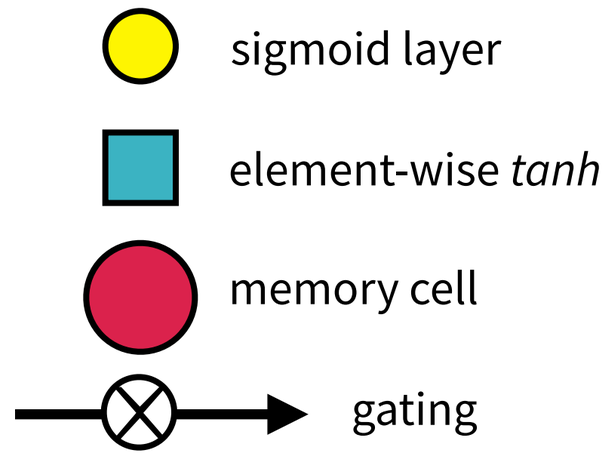


The output gate allows information to flow out of the cell

$$\boldsymbol{o}^{(t)} = \sigma\left(\boldsymbol{b}^o + \boldsymbol{W}^o \left[\boldsymbol{h}^{(t-1)}, \boldsymbol{x}^{(t)}\right]\right)$$

LSTM - New state

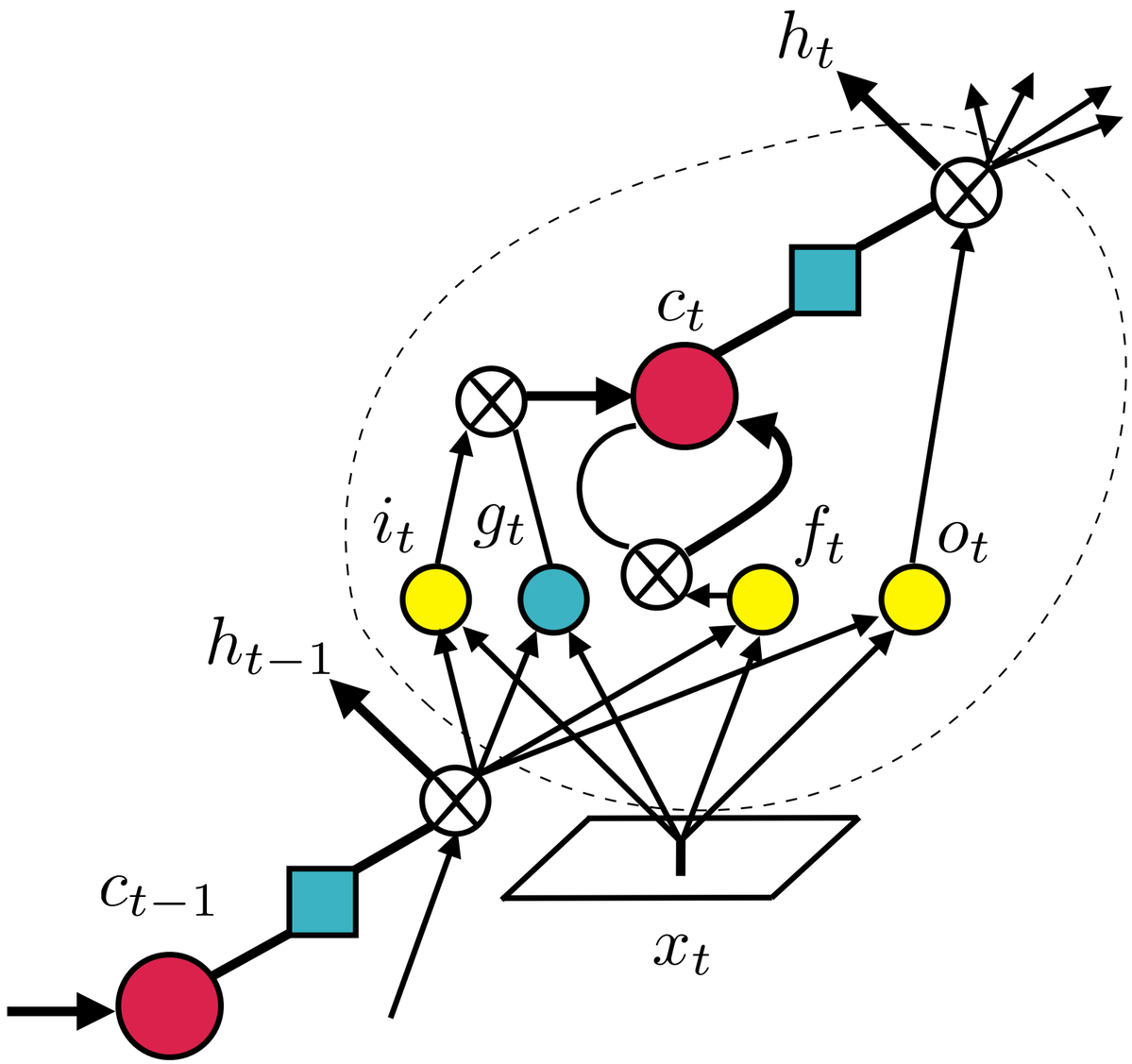


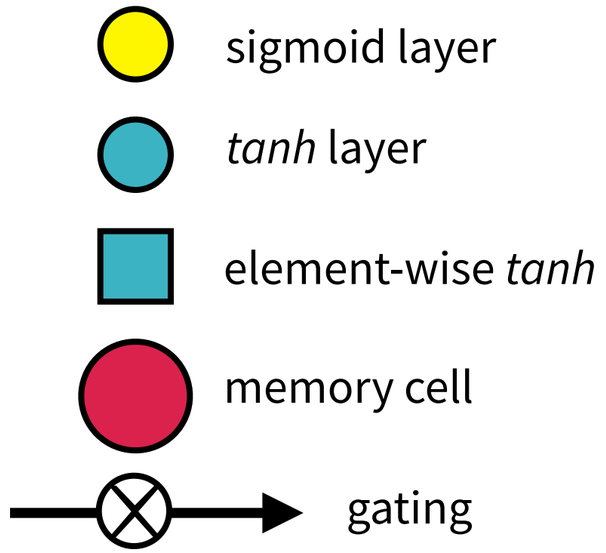


The hidden state update is a nonlinear function of the cell regulated by the output gate

$$\boldsymbol{h}^{(t)} = \boldsymbol{o}^{(t)} \odot \tanh(\boldsymbol{c}^{(t)})$$

LSTM (recap)





$$\boldsymbol{i}^{(t)} = \sigma\left(\boldsymbol{b}^i + \boldsymbol{W}^i \left[\boldsymbol{h}^{(t-1)}, \boldsymbol{x}^{(t)}\right]\right)$$

$$\boldsymbol{g}^{(t)} = \tanh\left(\boldsymbol{b}^g + \boldsymbol{W}^g \left[\boldsymbol{h}^{(t-1)}, \boldsymbol{x}^{(t)}\right]\right)$$

$$\boldsymbol{f}^{(t)} = \sigma\left(\boldsymbol{b}^f + \boldsymbol{W}^f \left[\boldsymbol{h}^{(t-1)}, \boldsymbol{x}^{(t)}\right]\right)$$

$$\boldsymbol{c}^{(t)} = \boldsymbol{f}^{(t)} \odot \boldsymbol{c}^{(t-1)} + \boldsymbol{i}^{(t)} \odot \boldsymbol{g}^{(t)}$$

$$\boldsymbol{o}^{(t)} = \sigma\left(\boldsymbol{b}^o + \boldsymbol{W}^o \left[\boldsymbol{h}^{(t-1)}, \boldsymbol{x}^{(t)}\right]\right)$$

$$\boldsymbol{h}^{(t)} = \boldsymbol{o}^{(t)} \odot \tanh(\boldsymbol{c}^{(t)})$$

Recommended reading:
Chris Olah: Understanding LSTMs (blog)
http://colah.github.io/posts/2015-08-Understanding-LSTMs/

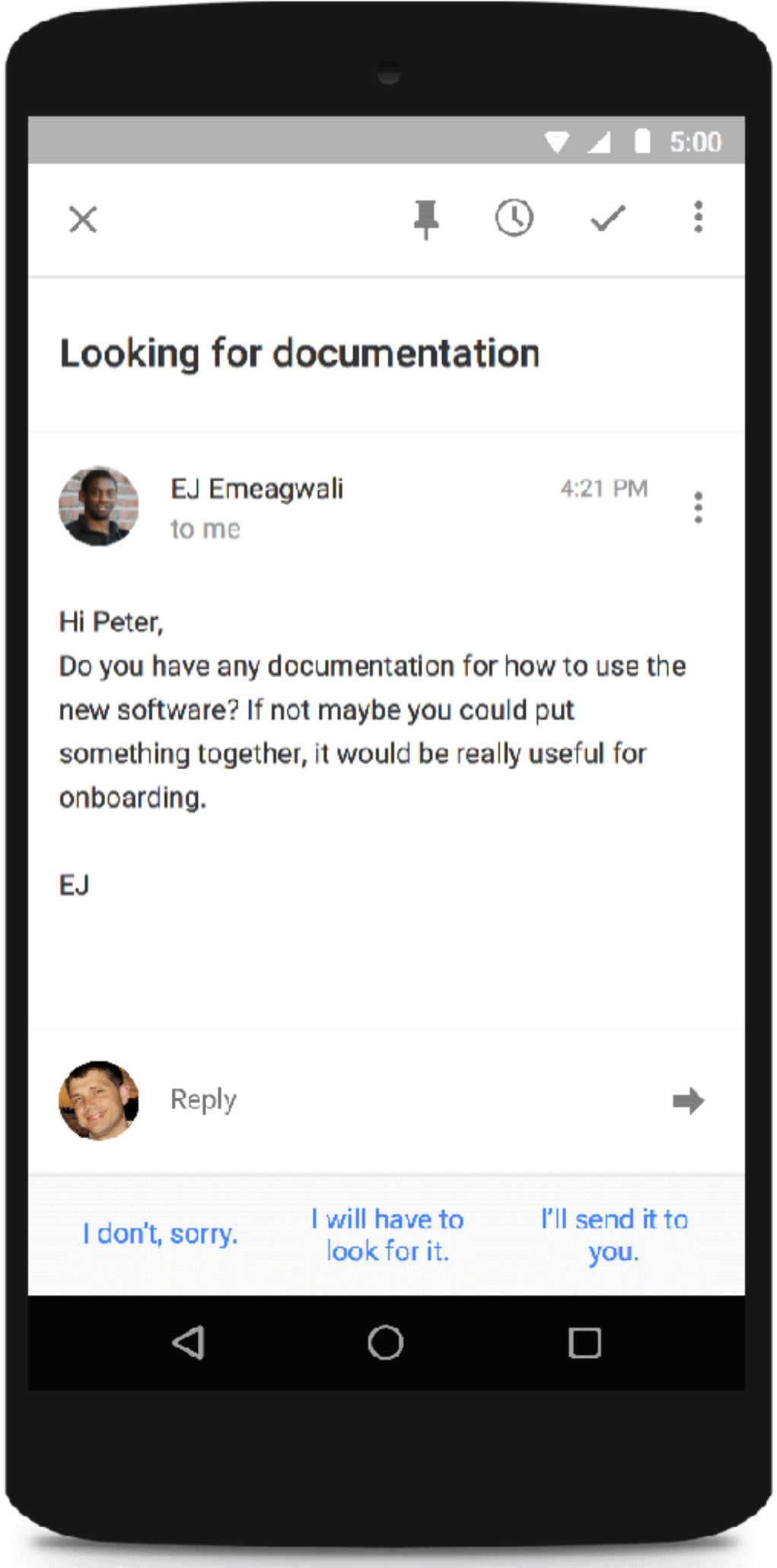


Figure: Google

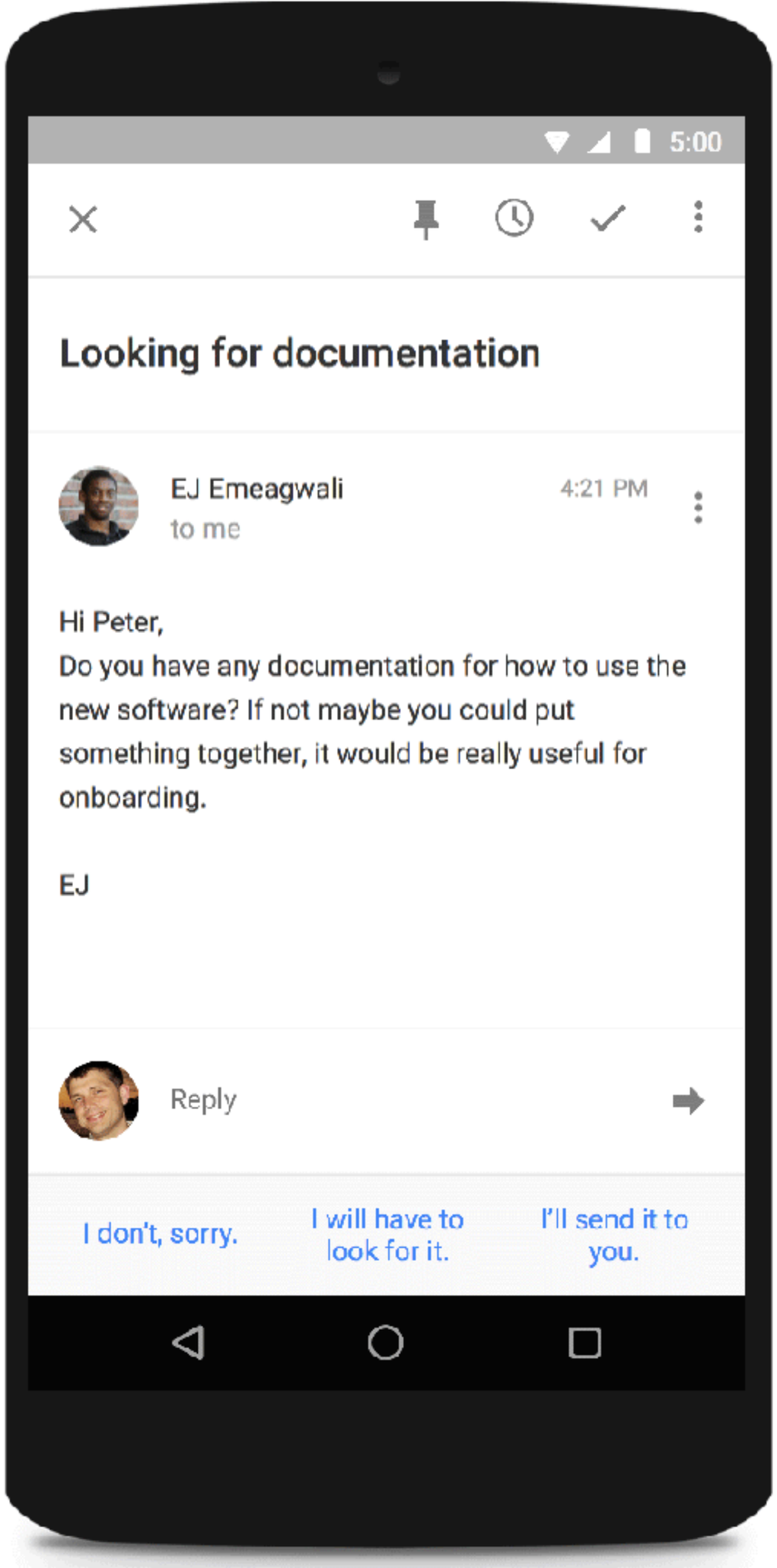
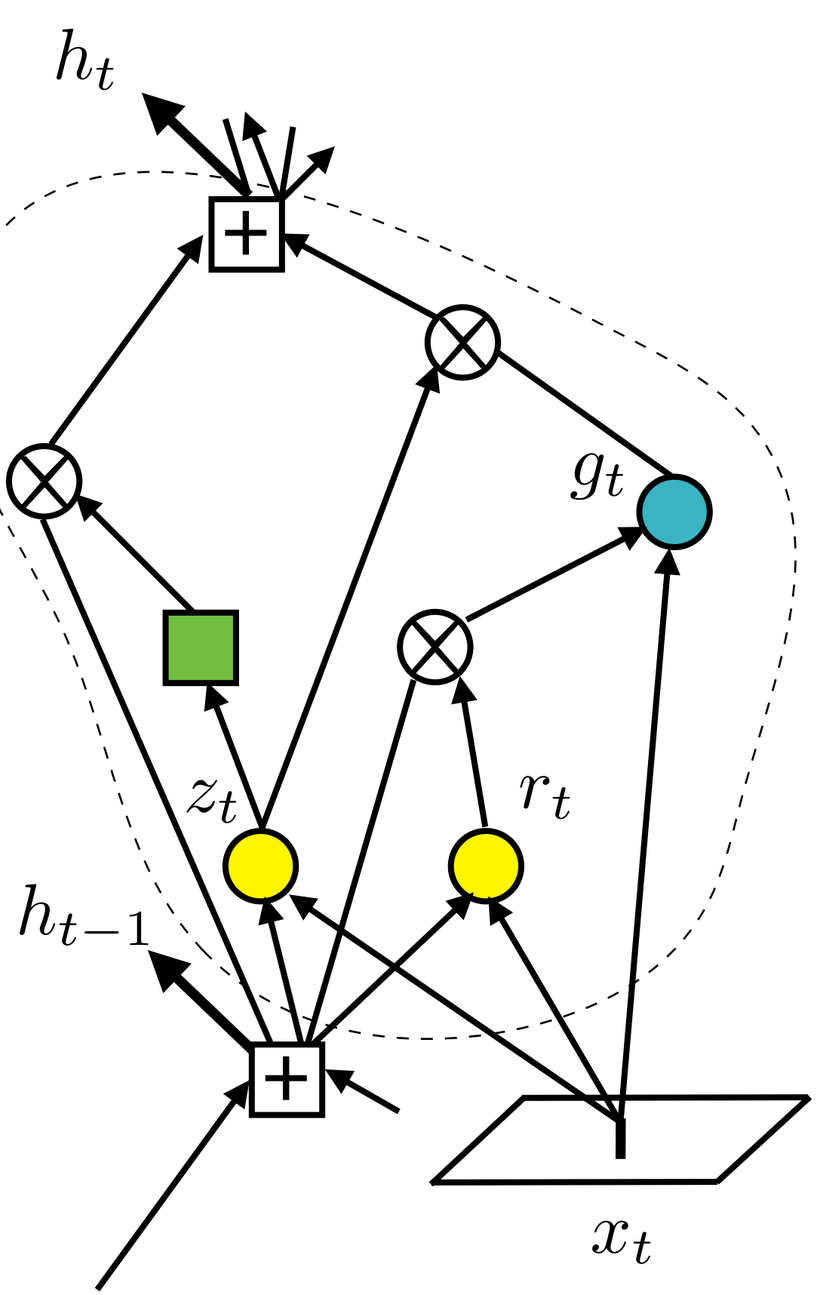
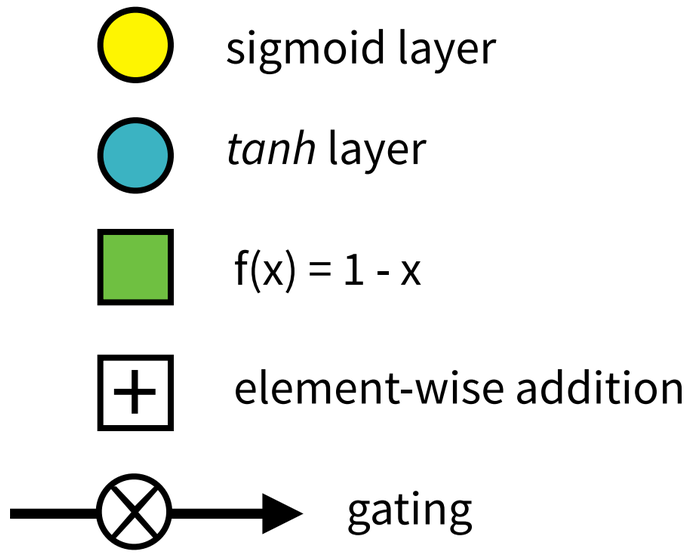


Figure: Google

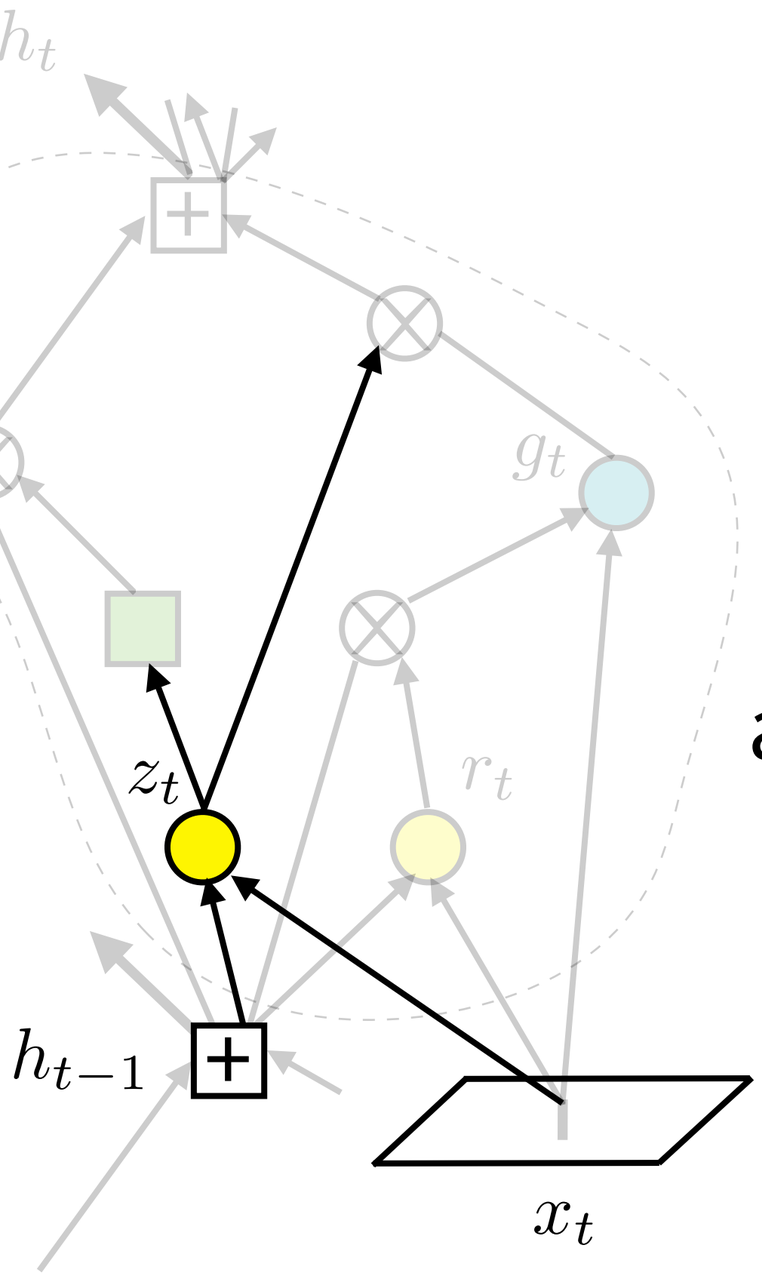
Gated Recurrent Units (GRU)

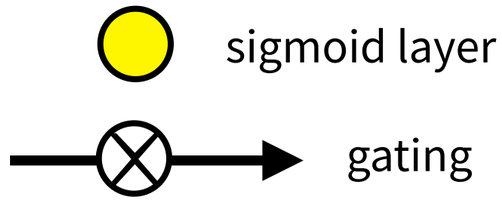




Combine forget and input gates into a single “update gate”
Merges cell state and hidden state

GRU - Update gate

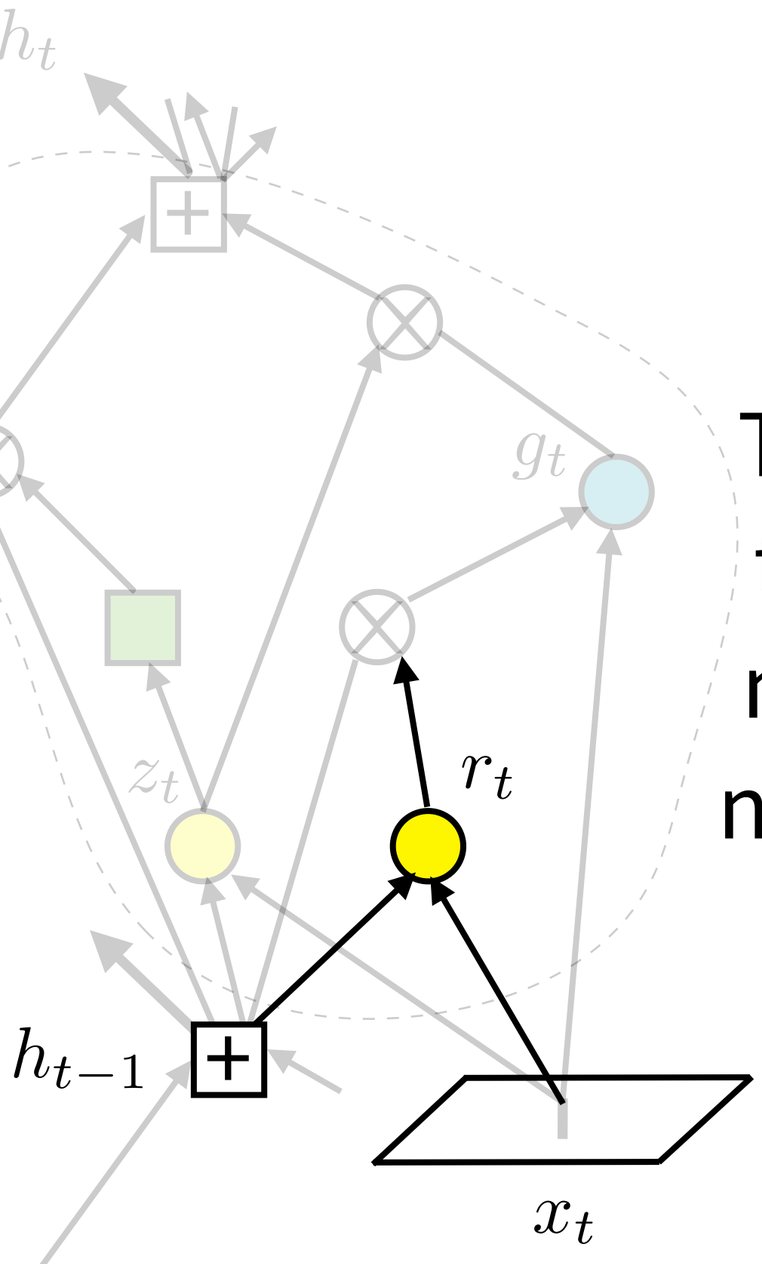


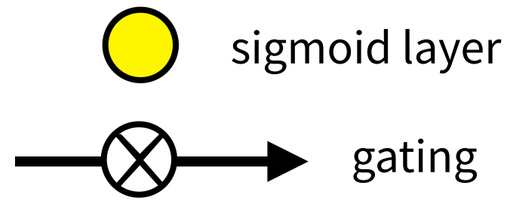


The update gate simultaneously controls the forgetting factor and the decision to update the state

$$\boldsymbol{z}^{(t)} = \sigma\left(\boldsymbol{b}^z + \boldsymbol{W}^z \left[\boldsymbol{h}^{(t-1)}, \boldsymbol{x}^{(t)}\right]\right)$$

GRU - Reset gate

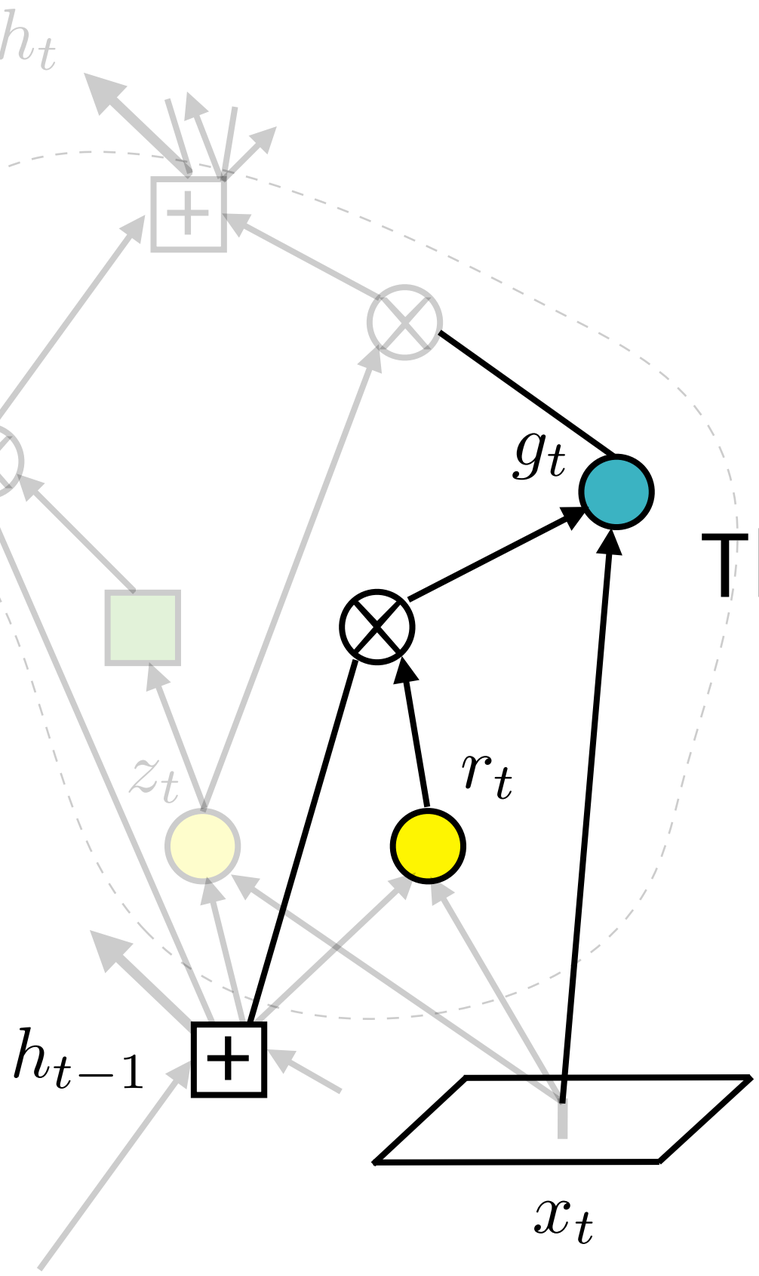


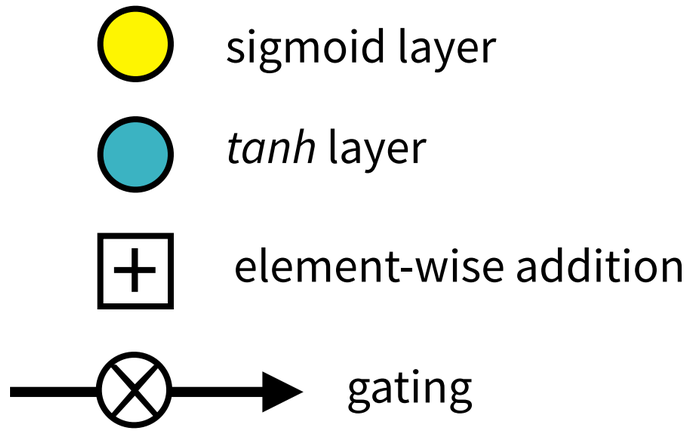


The reset gate controls which part of the old state is used to compute the next state, introducing an additional nonlinear effect b/w past and present

$$\boldsymbol{r}^{(t)} = \sigma\left(\boldsymbol{b}^r + \boldsymbol{W}^r \left[\boldsymbol{h}^{(t-1)}, \boldsymbol{x}^{(t)}\right]\right)$$

GRU - Target state

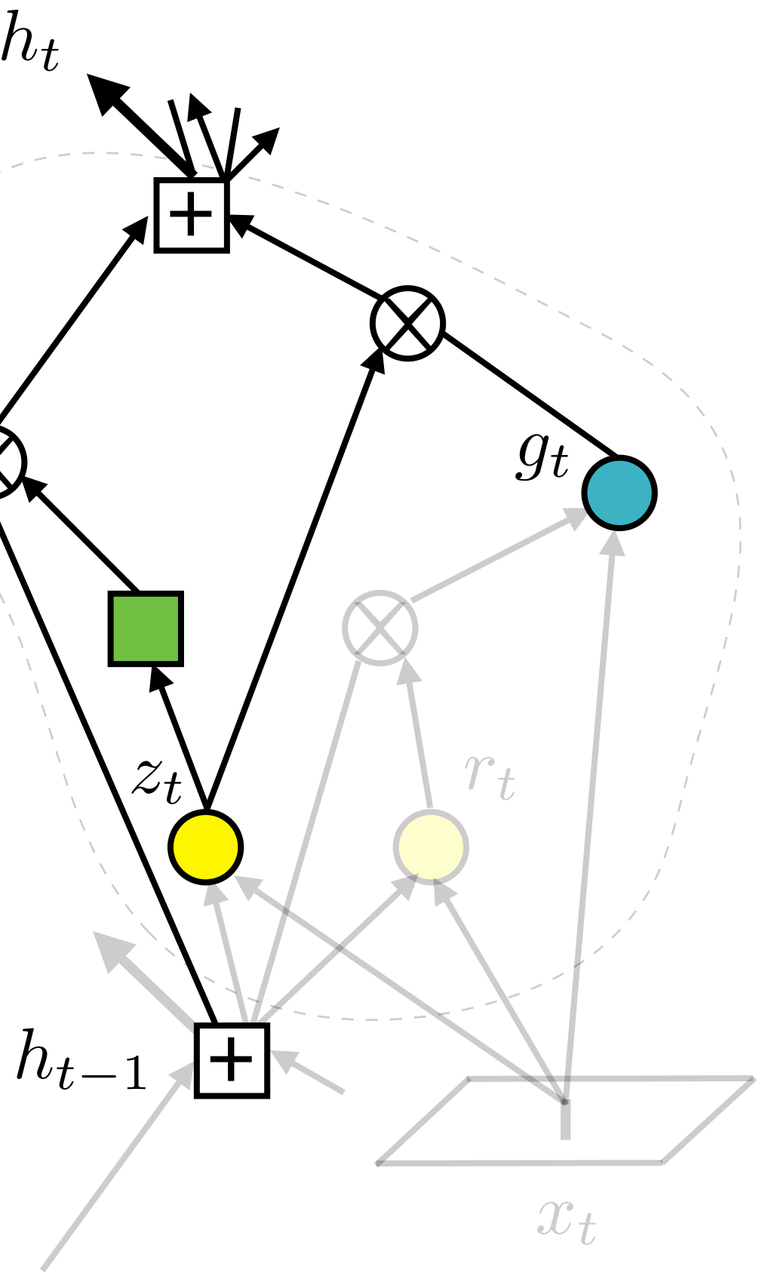


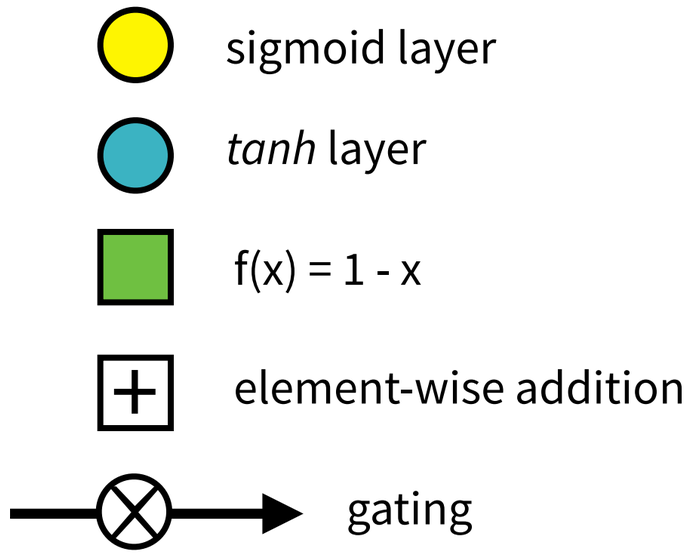


The target state is a nonlinear function of the previous state and input

$$\boldsymbol{g}^{(t)} = \tanh\left(\boldsymbol{b}^g + \boldsymbol{W}^g \left[\boldsymbol{r}^{(t)} \odot \boldsymbol{h}^{(t-1)}, \boldsymbol{x}^{(t)}\right]\right)$$

GRU - New state

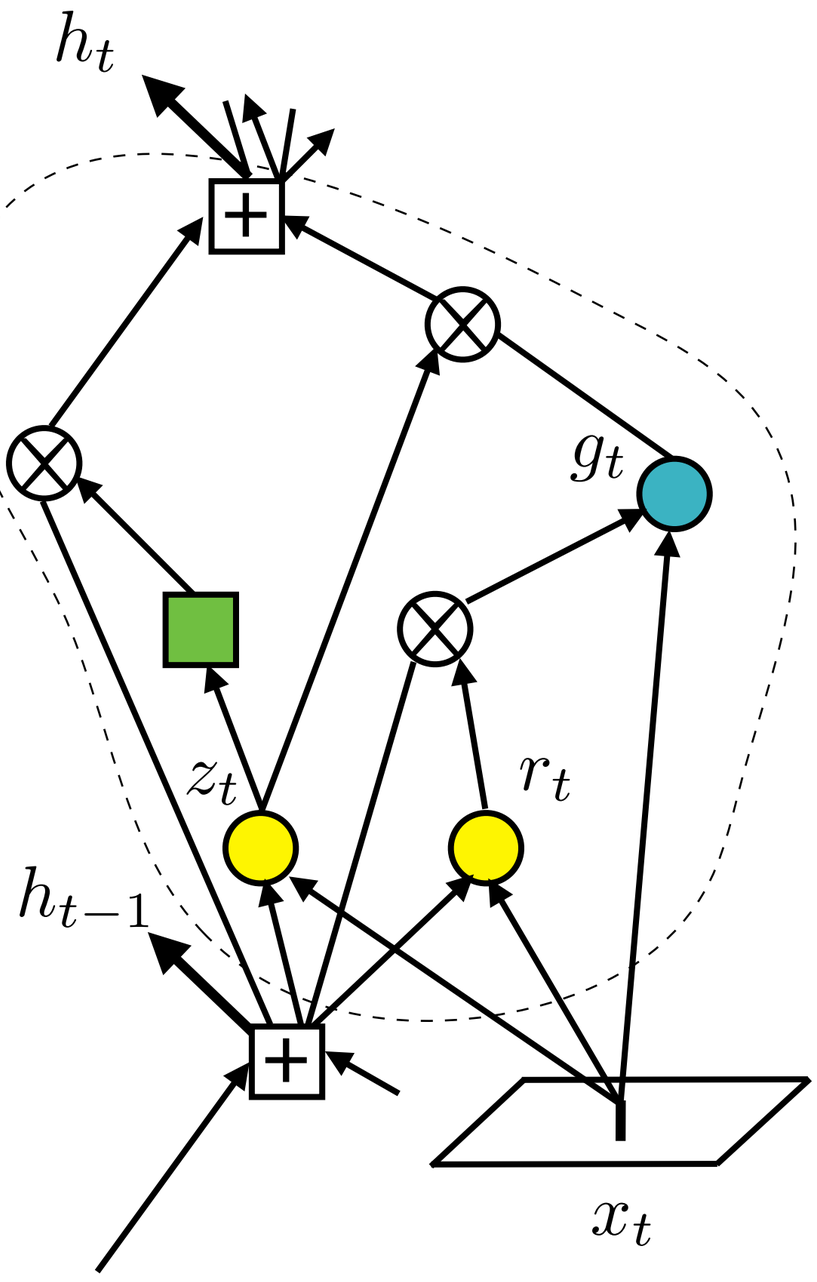


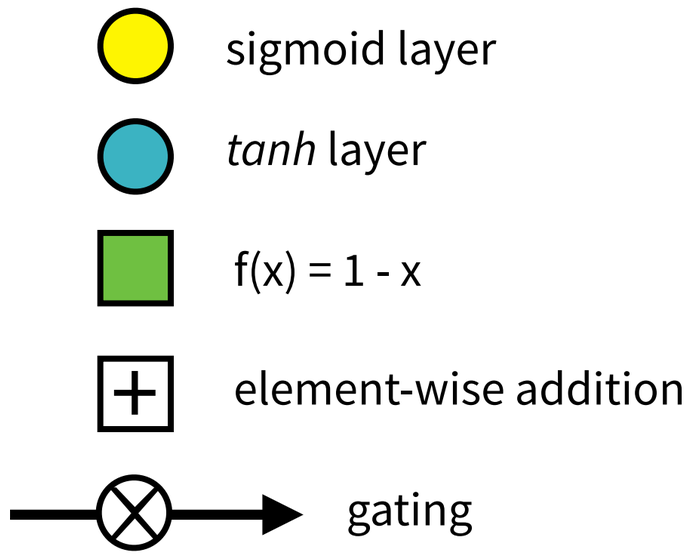


The new state is a function of the target state and previous state

$$\boldsymbol{h}^{(t)} = (1 - \boldsymbol{z}^{(t)}) \odot \boldsymbol{h}^{(t-1)} + \boldsymbol{z}^{(t)} \odot \boldsymbol{g}^{(t)}$$

GRU (recap)





$$\boldsymbol{z}^{(t)} = \sigma\left(\boldsymbol{b}^z + \boldsymbol{W}^z \left[\boldsymbol{h}^{(t-1)}, \boldsymbol{x}^{(t)}\right]\right)$$

$$\boldsymbol{r}^{(t)} = \sigma\left(\boldsymbol{b}^r + \boldsymbol{W}^r \left[\boldsymbol{h}^{(t-1)}, \boldsymbol{x}^{(t)}\right]\right)$$

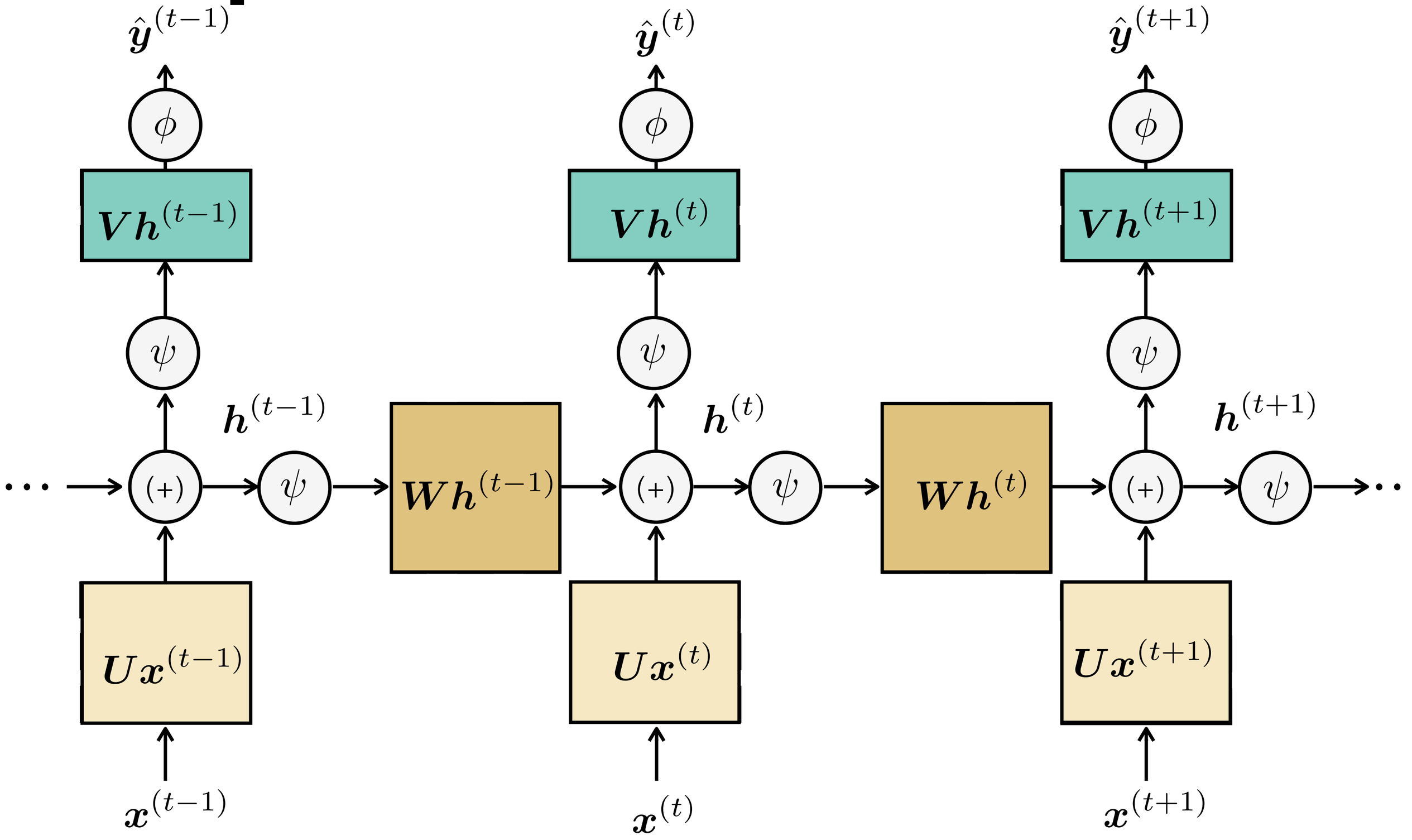
$$\boldsymbol{g}^{(t)} = \tanh\left(\boldsymbol{b}^g + \boldsymbol{W}^g \left[\boldsymbol{r}^{(t)} \odot \boldsymbol{h}^{(t-1)}, \boldsymbol{x}^{(t)}\right]\right)$$

$$\boldsymbol{h}^{(t)} = (1 - \boldsymbol{z}^{(t)}) \odot \boldsymbol{h}^{(t-1)} + \boldsymbol{z}^{(t)} \odot \boldsymbol{g}^{(t)}$$

LSTM: A Search Space Odyssey

- So many possibilities!
- Several investigations over architectural variations of the LSTM and GRU found that no variant beat the "baseline" over a wide variety of tasks (Greff et al., 2015), (Jozefowicz et al., 2015)
- Grief et al. (2015) found the forget gate and output activation function to be the LSTM's most critical parts

Deep RNNs


$\hat{\boldsymbol{y}}^{(t-1)}$
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$\boldsymbol{V}\boldsymbol{h}^{(t)}$
$\boldsymbol{V}\boldsymbol{h}^{(t+1)}$
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$\boldsymbol{h}^{(t-1)}$
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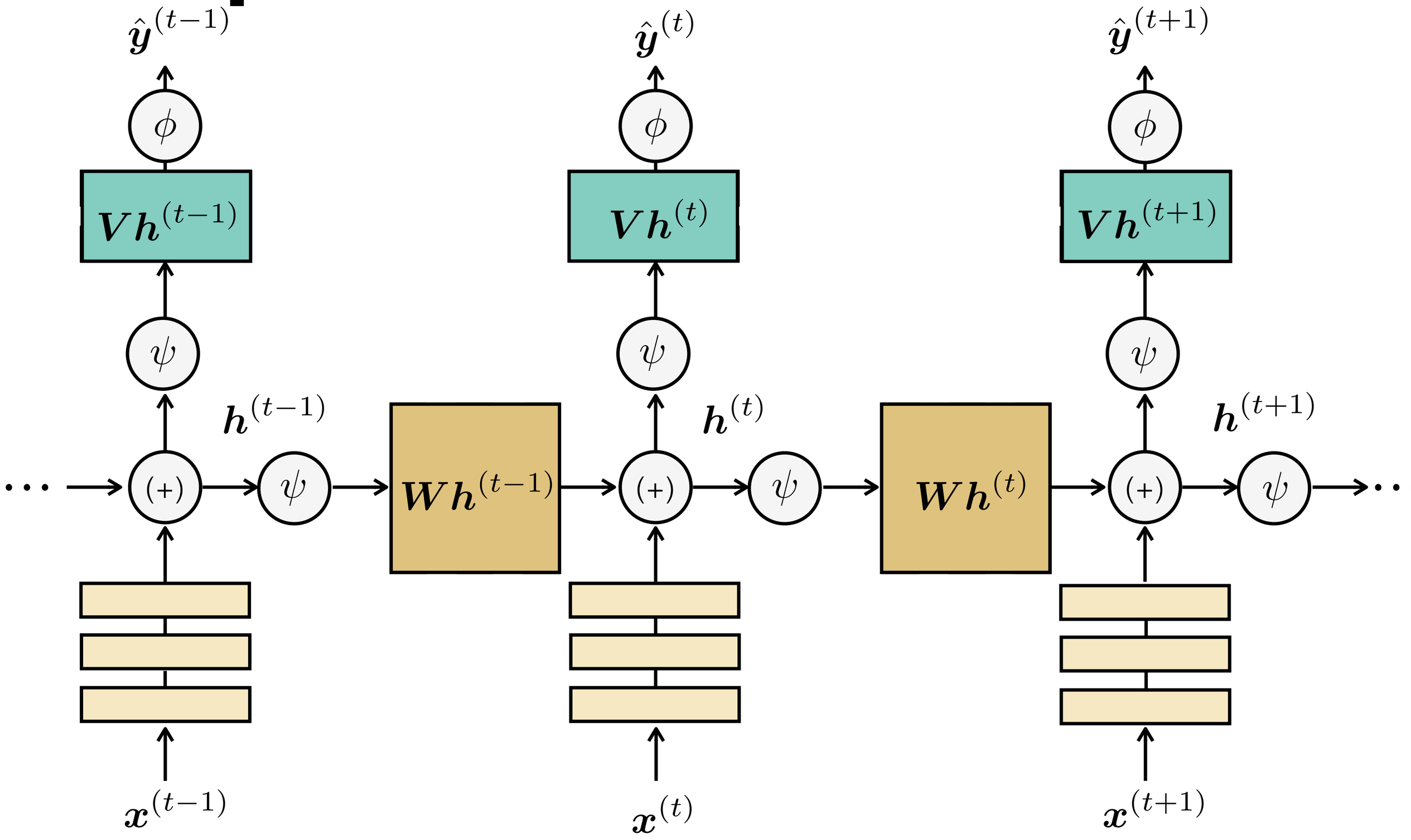
$\boldsymbol{W}\boldsymbol{h}^{(t)}$
$\boldsymbol{U}\boldsymbol{x}^{(t-1)}$
$\boldsymbol{U}\boldsymbol{x}^{(t)}$
$\boldsymbol{U}\boldsymbol{x}^{(t+1)}$
$\boldsymbol{x}^{(t-1)}$
$\boldsymbol{x}^{(t)}$
$\boldsymbol{x}^{(t+1)}$

Deep RNNs


$\hat{\boldsymbol{y}}^{(t-1)}$
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$\boldsymbol{h}^{(t-1)}$
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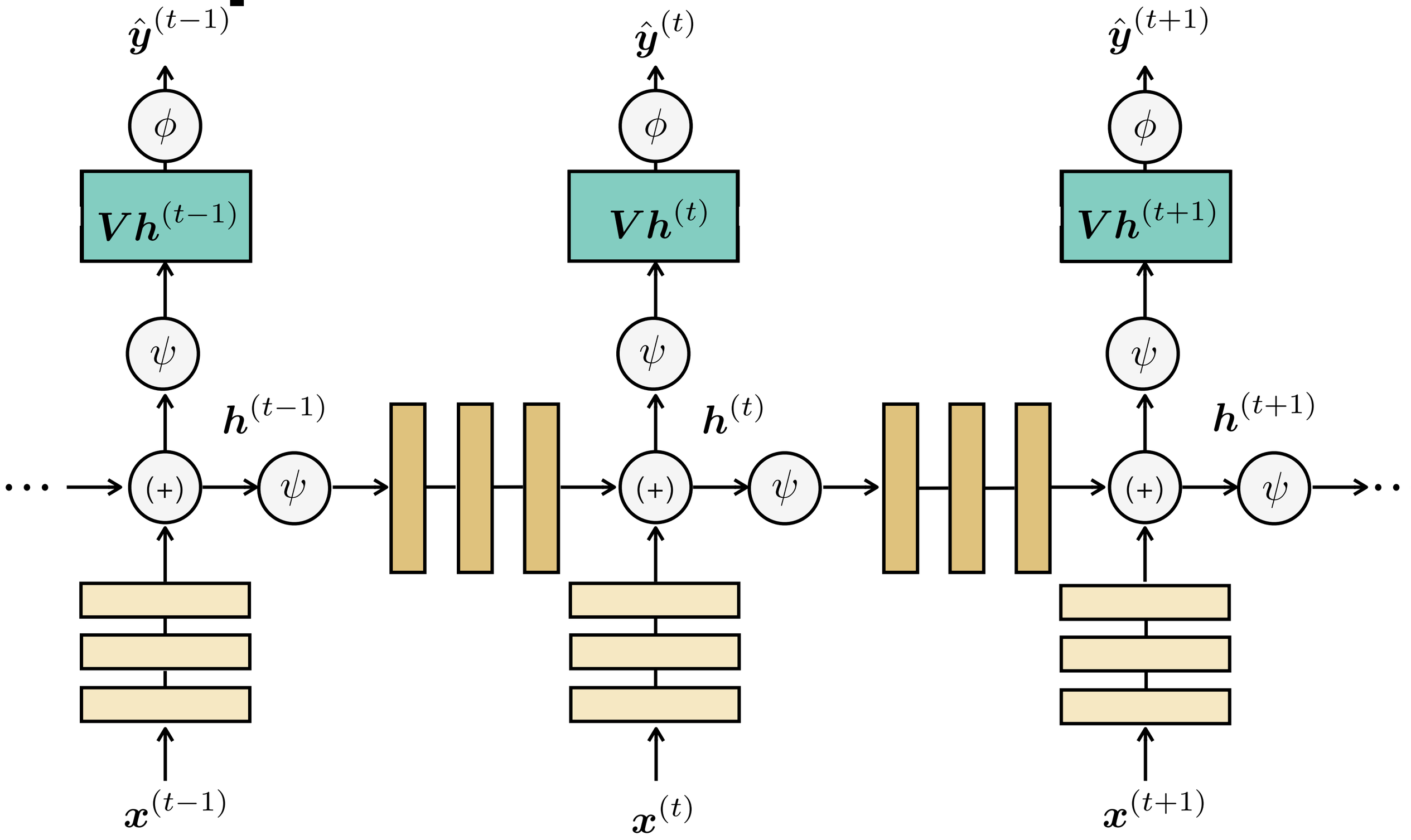
$\boldsymbol{W}\boldsymbol{h}^{(t-1)}$
$\boldsymbol{W}\boldsymbol{h}^{(t)}$
$\boldsymbol{x}^{(t-1)}$
$\boldsymbol{x}^{(t)}$
$\boldsymbol{x}^{(t+1)}$

Deep RNNs


$\hat{\boldsymbol{y}}^{(t-1)}$
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$\boldsymbol{x}^{(t)}$
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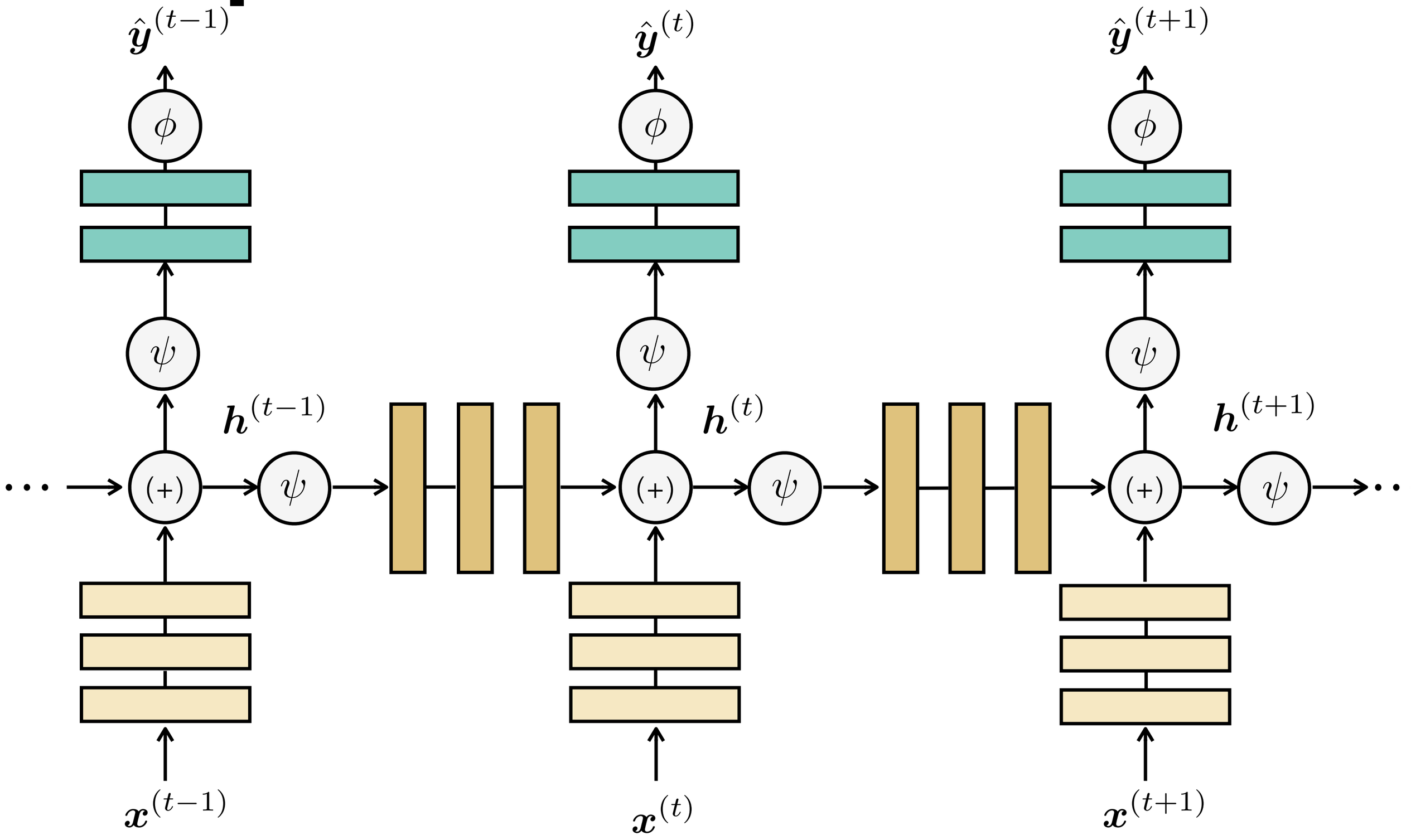
Deep RNNs


$\hat{\boldsymbol{y}}^{(t-1)}$
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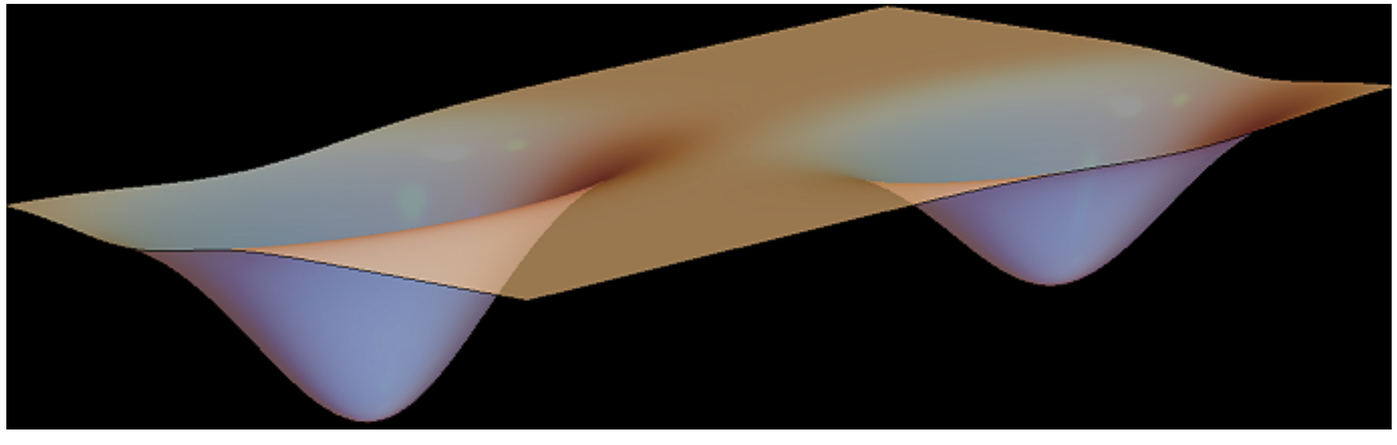
$\boldsymbol{x}^{(t-1)}$
$\boldsymbol{x}^{(t)}$
$\boldsymbol{x}^{(t+1)}$

Solutions: Optimization



- 2nd-order methods (Martens and Sutskever 2011)
- Reservoirs (Jaeger and Haas 2004)
- Gradient clipping/normalization (Pascanu et al. 2012, Mikolov 2012)
- Careful initialization (Sutskever et al. 2013)

Summary (and Advice!)

- Keep the architecture simple!
  - GRUs, gradient clipping, careful initialization
- Use well-tested, well-supported open-source tools:
  - Tensor Flow, PyTorch, Caffe
- Don’t forget the flexibility of input-output structure