Deep Learning:

Recurrent Neural Networks

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Deep Learning VO - WS 23/24

Lecture 8 - November 27th, 2023

Today

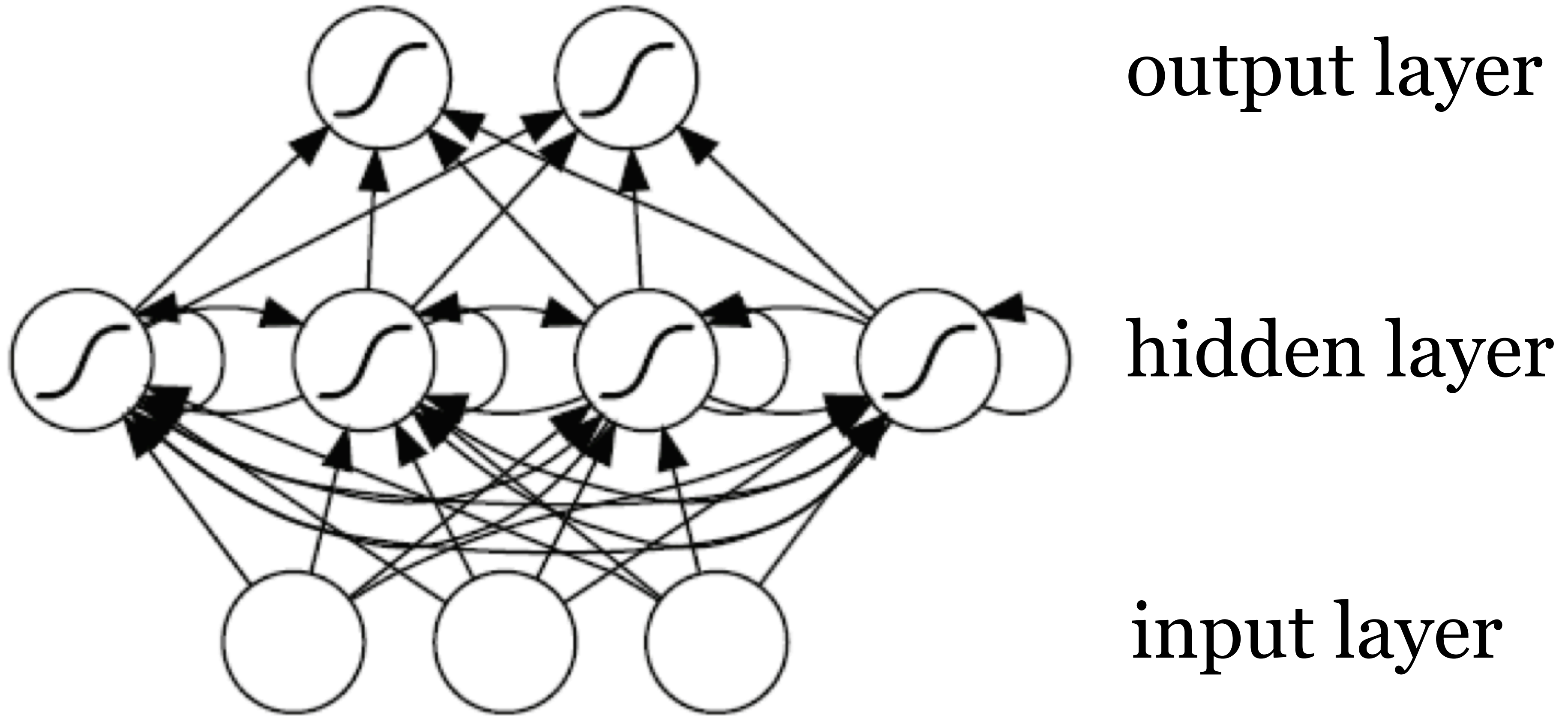
- Recurrent Neural Networks
  - Simple RNNs
  - Backpropagation Through Time
  - Architectural Variants
  - Gated RNNs (LSTM & GRU)

Recurrent Neural Networks (RNNs)

Typical input: Sequence of values (vectors) $\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(\tau)}$

Typical output: Sequence of values (vectors) $\mathbf{o}^{(1)}, \ldots, \mathbf{o}^{(\tau)}$

Network graph includes recurrent connections.



At each discrete time step t,

- input $\mathbf{x}^{(t)}$ is presented,
- hidden state $\mathbf{h}^{(t)}$ is updated,
- output $\mathbf{o}^{(t)}$ is computed,
- loss $L^{(t)}$ is evaluated, and
- gradient is backpropagated through time.

(Simple) RNNs were introduced in the 1980s.

Advantages:

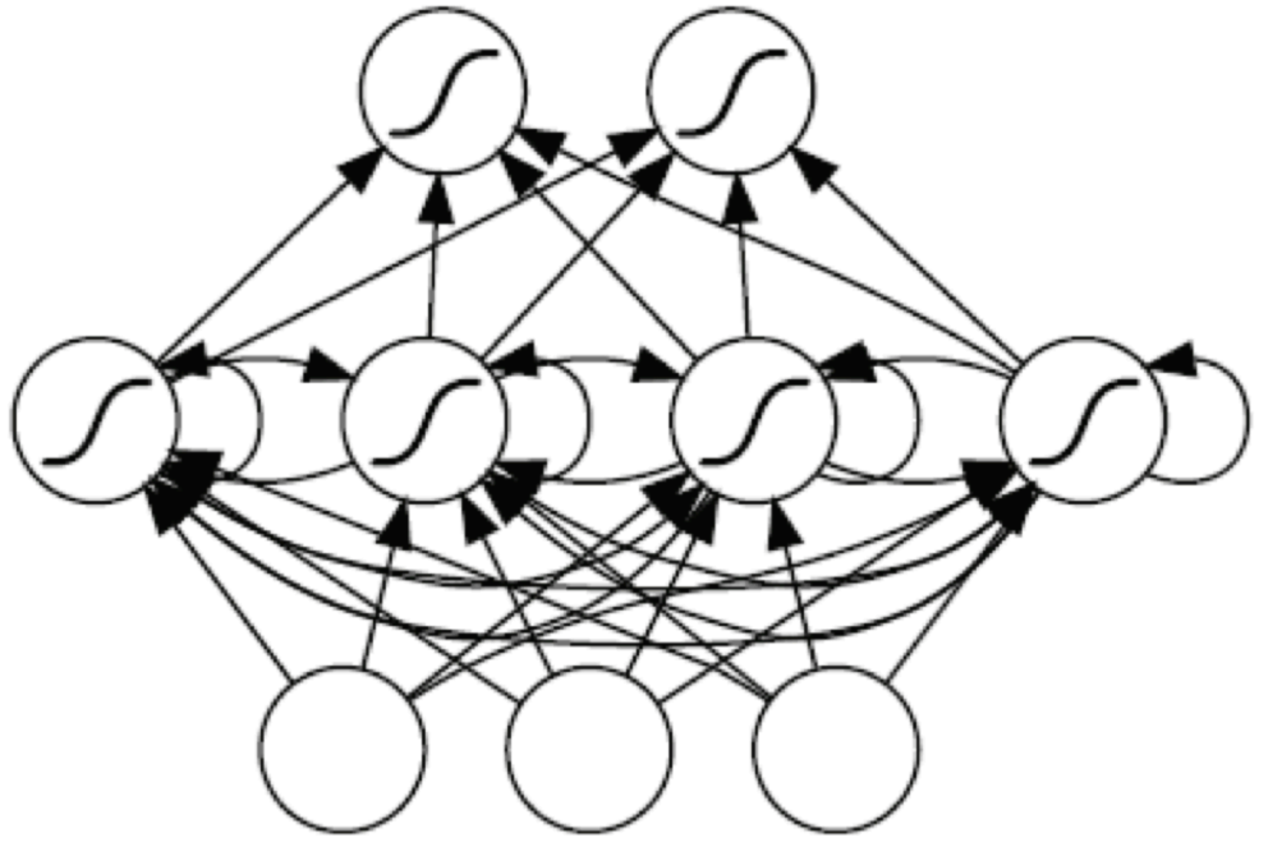
- Can process inputs of variable length.
- Implements parameter sharing over time.
- Can therefore generalize over time (compare to CNNs).

Simple RNNs: Computation

Typical input: Sequence of values (vectors) $\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(\tau)}$

Typical output: Sequence of values (vectors) $\mathbf{o}^{(1)}, \ldots, \mathbf{o}^{(\tau)}$

Network graph includes recurrent connections.



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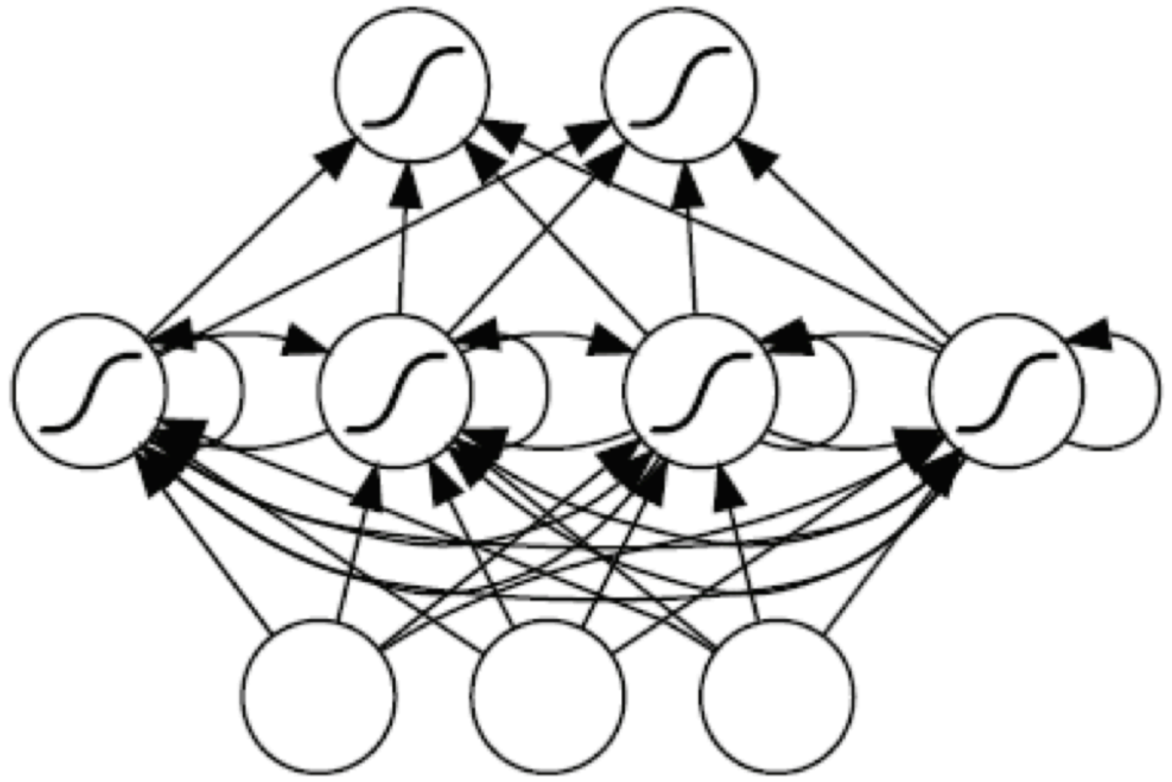
- hidden state $\mathbf{h}^{(t)}$ is updated,
- output $\mathbf{o}^{(t)}$ is computed,
- loss $L^{(t)}$ is evaluated, and
- gradient is backpropagated through time.

$$\mathbf{a}^{(t)} = \mathbf{b} + W\mathbf{h}^{(t-1)} + U\mathbf{x}^{(t)}$$
$$\mathbf{h}^{(t)} = \tanh(\mathbf{a}^{(t)})$$
$$\mathbf{o}^{(t)} = \mathbf{c} + V\mathbf{h}^{(t)}$$
$$\hat{\mathbf{y}}^{(t)} = \text{softmax}\left(\mathbf{o}^{(t)}\right)$$

Unfolding in Time



View the RNN as a dynamical system driven by external input:

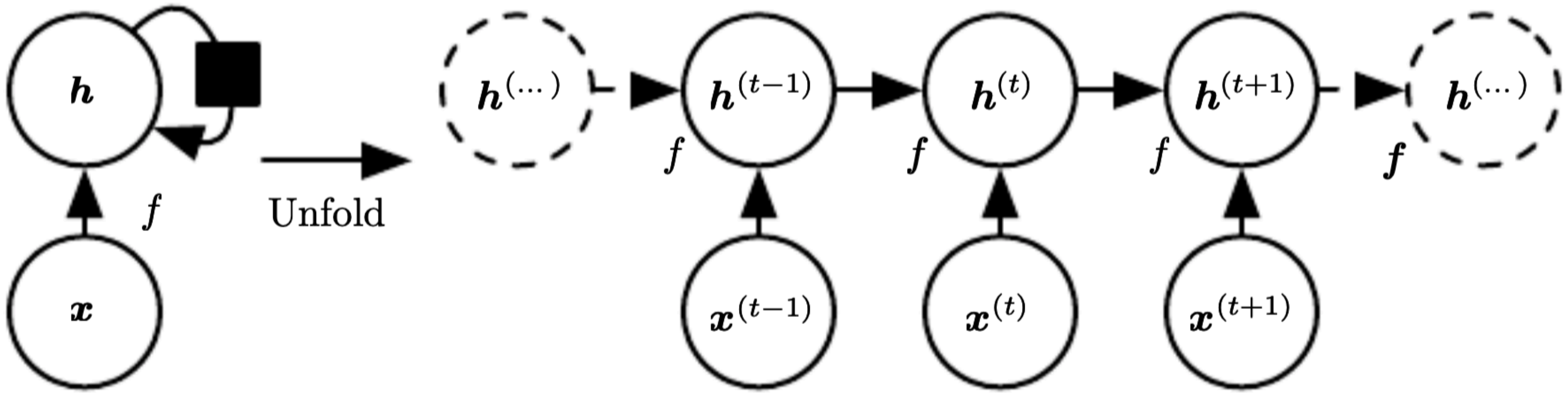
$$\mathbf{h}^{(t)} = f\left(\mathbf{h}^{(t-1)}, \mathbf{x}^{(t)}; \theta\right)$$

We can unfold the equation in time:

$$\mathbf{h}^{(3)} = f\left(\mathbf{h}^{(2)}, \mathbf{x}^{(3)}; \theta\right) = f\left(f\left(\mathbf{h}^{(1)}, \mathbf{x}^{(2)}; \theta\right), \mathbf{x}^{(3)}; \theta\right) = f\left(f\left(f\left(\mathbf{h}^{(0)}, \mathbf{x}^{(1)}; \theta\right), \mathbf{x}^{(2)}; \theta\right), \mathbf{x}^{(3)}; \theta\right)$$

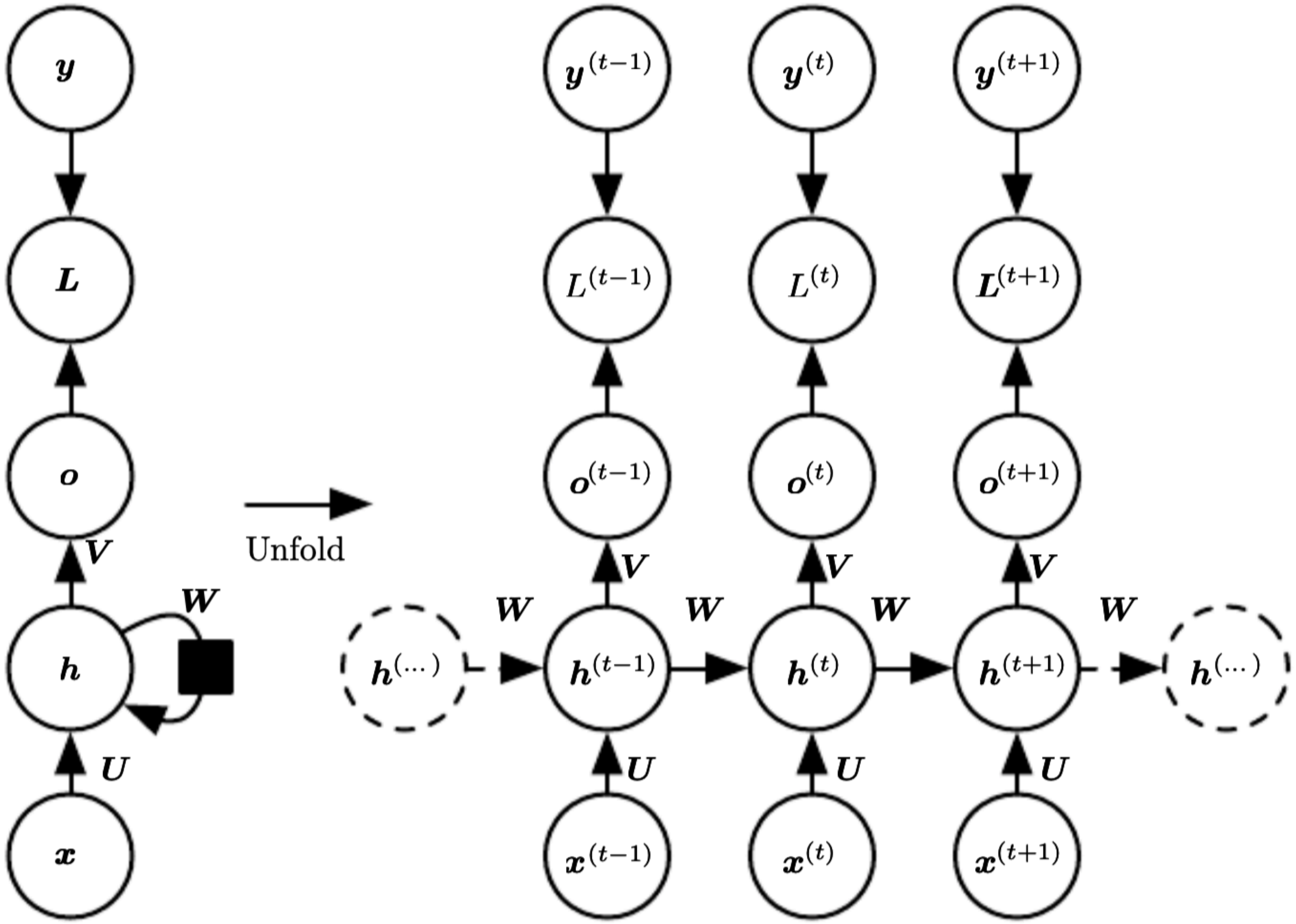
Unfolding the computational graph:

(square indicates unit time delay)



Network typically learns to use $\mathbf{h}^{(t)}$ as a lossy summary of the task-relevant aspects of the past sequence up to t.

RNN Equations and Training



$$\mathbf{a}^{(t)} = \mathbf{b} + W\mathbf{h}^{(t-1)} + U\mathbf{x}^{(t)}$$
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$$\mathbf{o}^{(t)} = \mathbf{c} + V\mathbf{h}^{(t)}$$
$$\hat{\mathbf{y}}^{(t)} = \text{softmax}\left(\mathbf{o}^{(t)}\right)$$

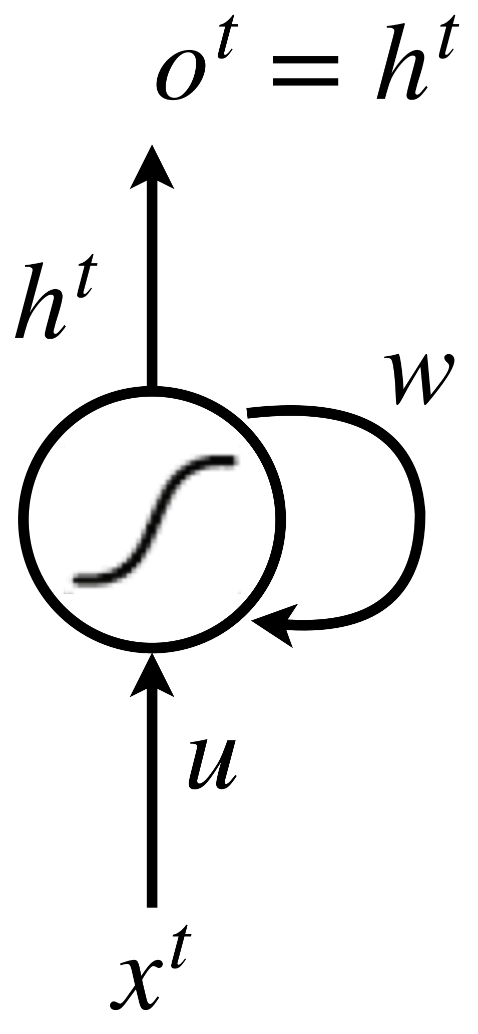
Training is via **backpropagation through time:** Compute the gradients in the unfolded computational graph.

Today

- [ ] Recurrent Neural Networks
  - [x] Simple RNNs
  - [ ] Backpropagation Through Time
  - [ ] Architectural Variants
  - [ ] Gated RNNs (LSTM & GRU)

Backpropagation Through Time

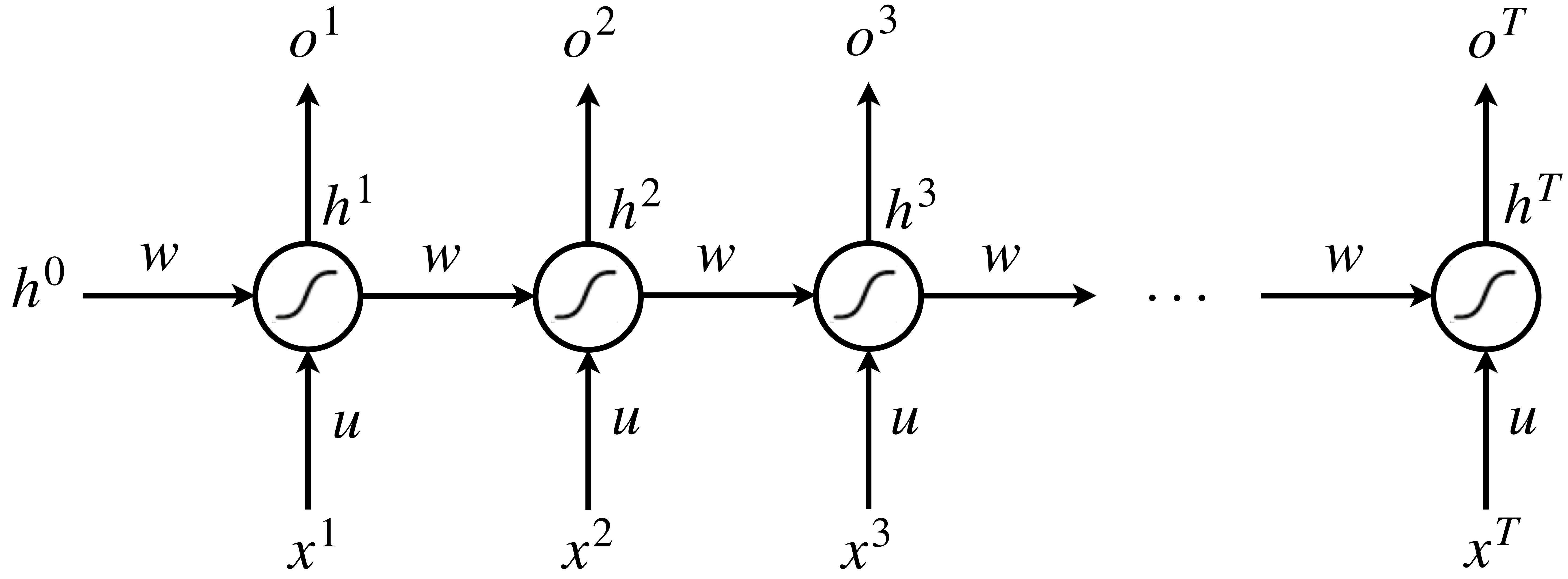
An example: a single neuron with a recurrent connection to itself.



$$h^0 = 0$$

$$h^t = \sigma\left(\underbrace{ux^t + wh^{t-1}}_{a^t = ux^t + wh^{t-1}}\right)$$

Unfolded Network:

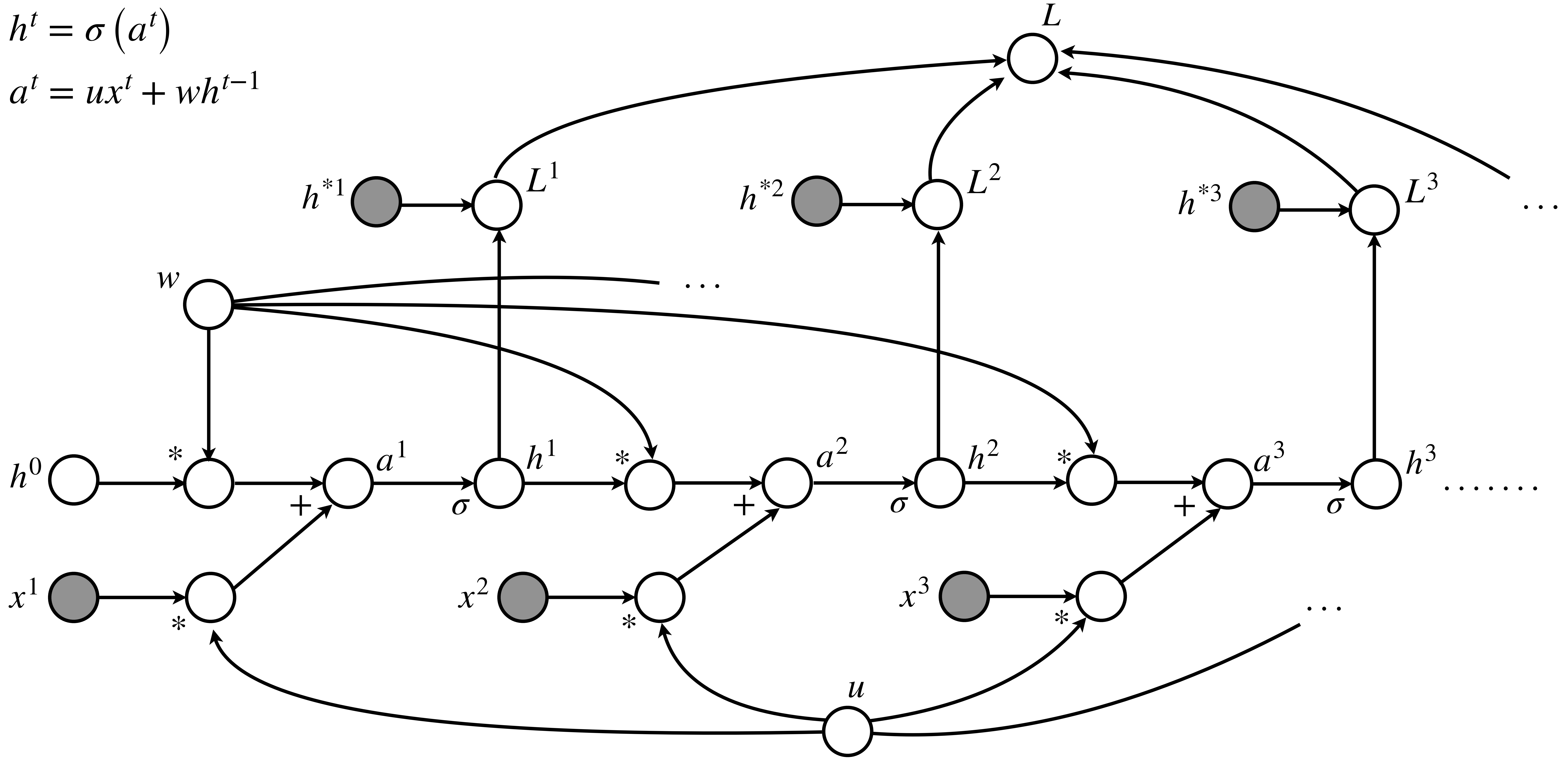


Unfolded Computational Graph

$$L = \sum_{t=1}^{T} L^t \quad L^t = \frac{1}{2}\left(h^t - h^{*t}\right)^2$$

$$h^t = \sigma\left(a^t\right)$$

$$a^t = ux^t + wh^{t-1}$$



Backpropagation Through Time

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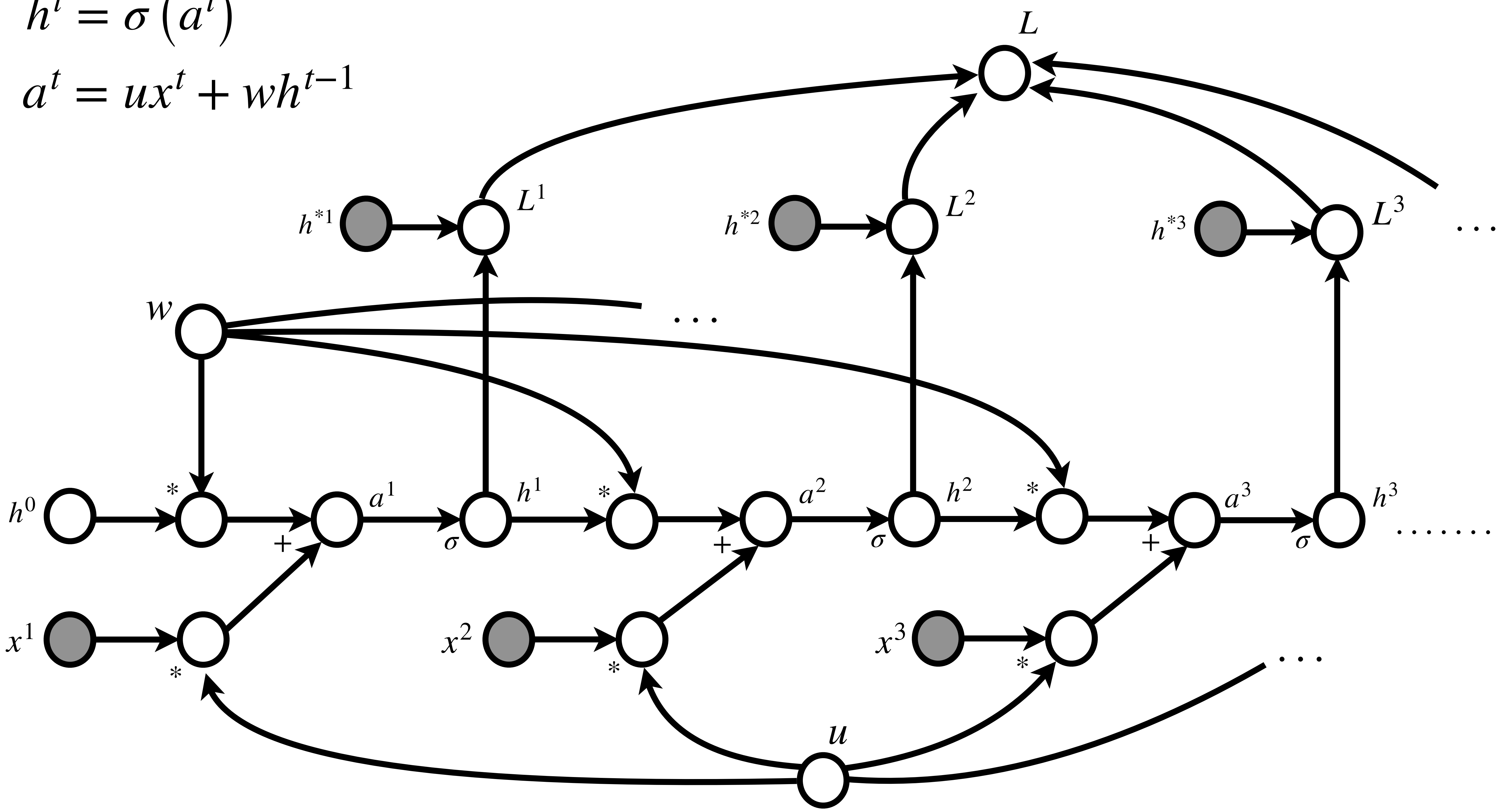

- We need $\frac{\partial L}{\partial w}$ and $\frac{\partial L}{\partial u}$ for parameter updates.
- To sketch the idea, we will show for $\frac{\partial L}{\partial w}$.

Backpropagation Through Time

$$L = \sum_{t=1}^{T} L^t \quad L^t = \frac{1}{2}\left(h^t - h^{*t}\right)^2$$

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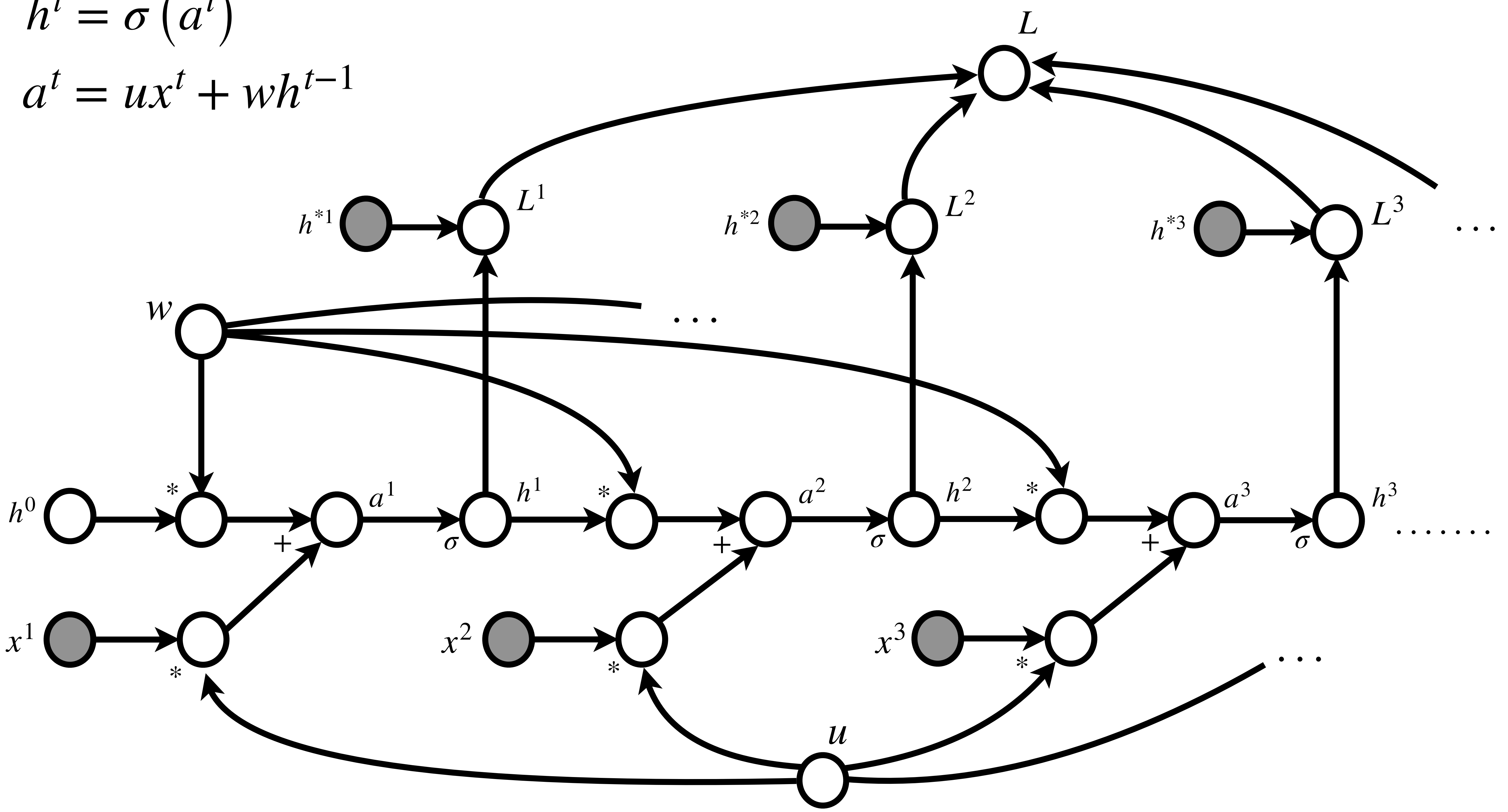

$$\frac{\partial L}{\partial w} = \sum_{t=1}^{T} \frac{\partial L}{\partial a^t}\frac{\partial a^t}{\partial w} = \sum_{t=1}^{T} \frac{\partial L}{\partial a^t} h^{t-1} = \sum_{t=1}^{T} \delta^t h^{t-1}$$

$$\boxed{\delta^t \stackrel{\text{def}}{=} \frac{\partial L}{\partial a^t}}$$

Backpropagation Through Time

$$L = \sum_{t=1}^{T} L^t \quad L^t = \frac{1}{2}\left(h^t - h^{*t}\right)^2$$

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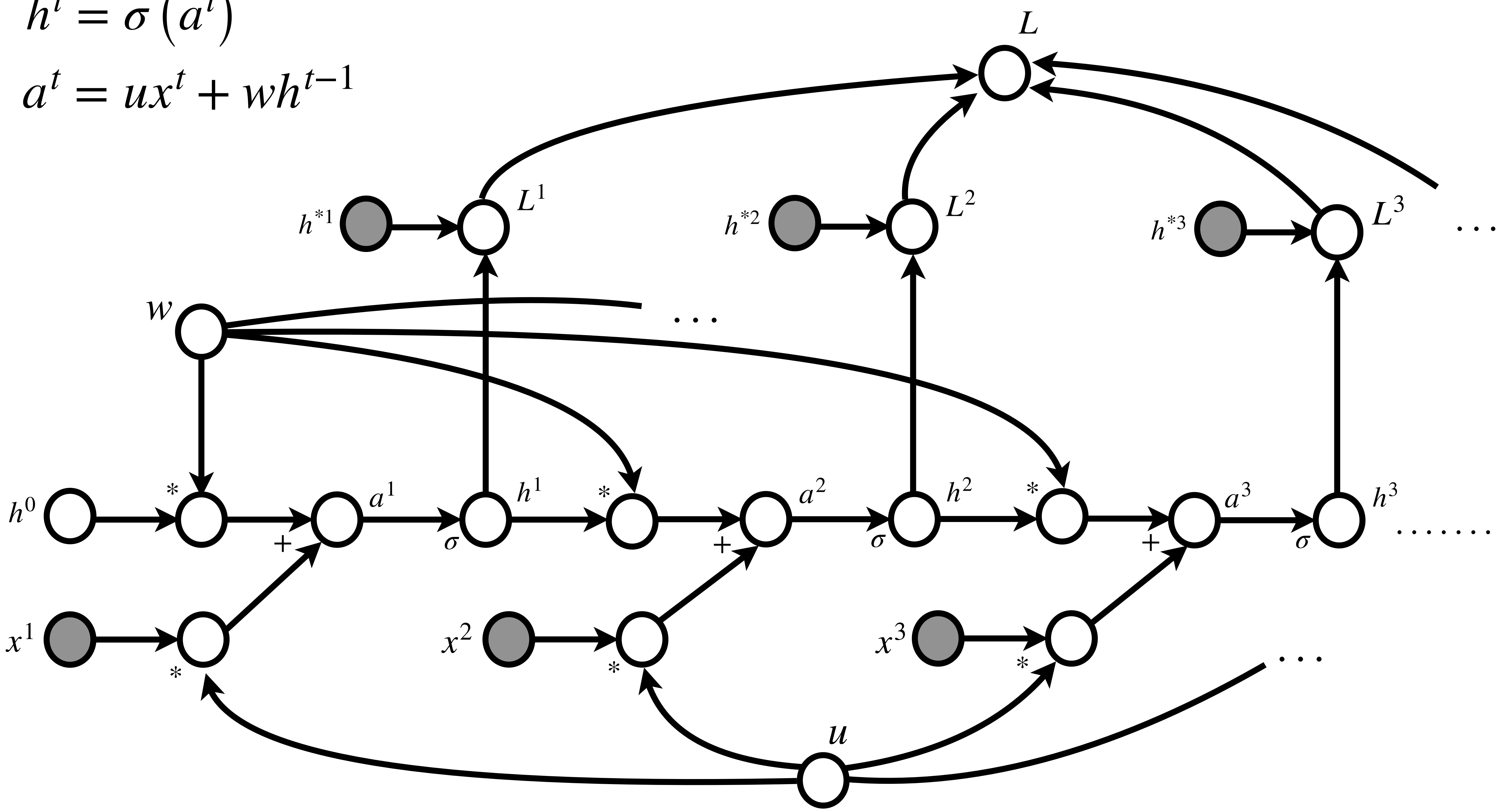

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$$\delta^t \overset{\mathbf{def}}{=} \frac{\partial L}{\partial a^t} = \frac{\partial L}{\partial h^t}\frac{\partial h^t}{\partial a^t} = \frac{\partial L}{\partial h^t}\dot{\sigma}\left(a^t\right)$$

$$\frac{\partial L}{\partial h^t} = \underbrace{\frac{\partial L}{\partial L^t}}_{1}\frac{\partial L^t}{\partial h^t} + \underbrace{\frac{\partial L}{\partial a^{t+1}}}_{\delta^{t+1}}\underbrace{\frac{\partial a^{t+1}}{\partial h^t}}_{w} = \frac{\partial L^t}{\partial h^t} + \delta^{t+1}\cdot w$$

Backpropagation Through Time

$$L = \sum_{t=1}^{T} L^t \quad L^t = \frac{1}{2}\left(h^t - h^{*t}\right)^2$$

$h^t = \sigma\left(a^t\right)$

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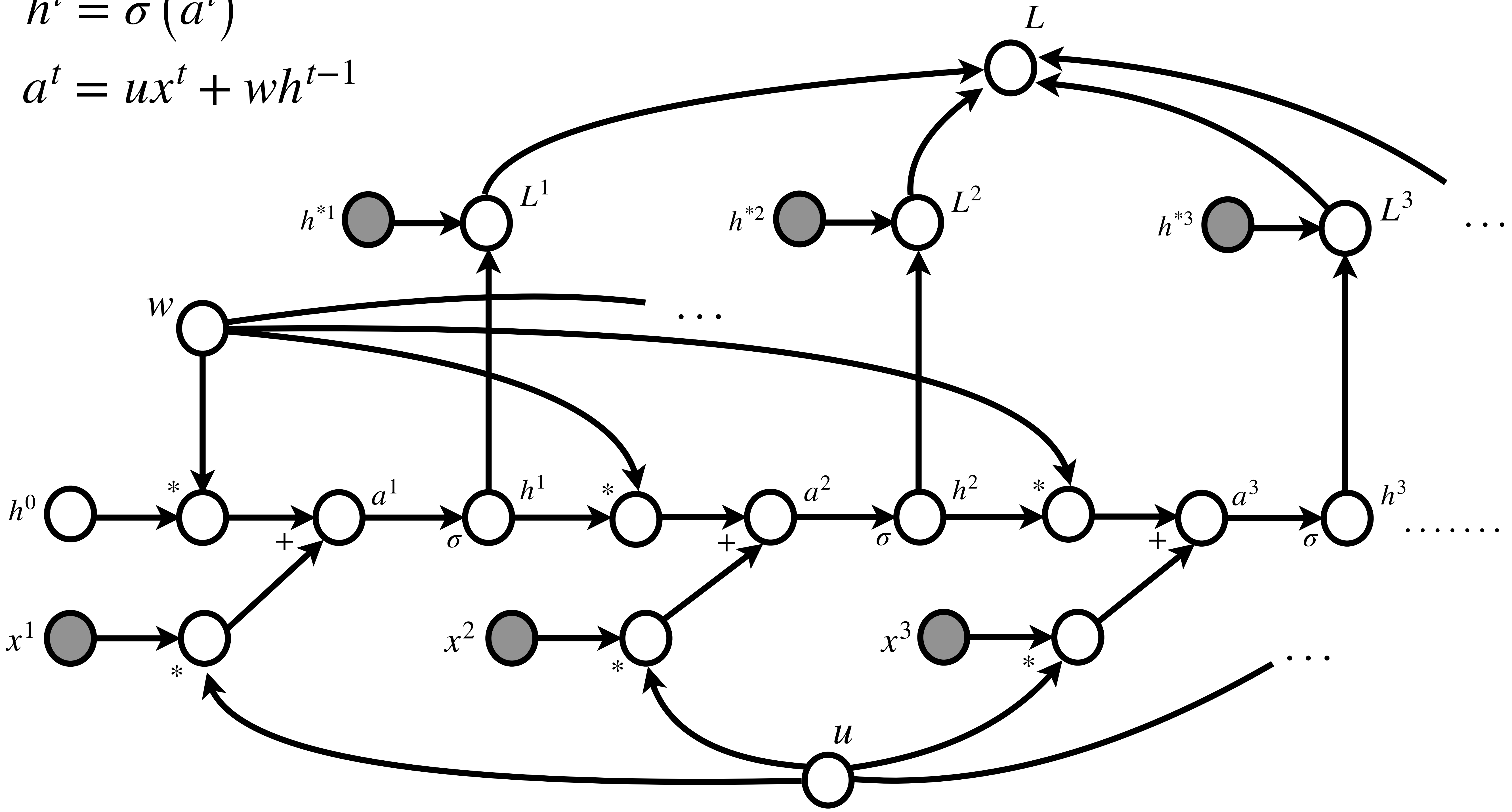

$$\frac{\partial L}{\partial w} = \sum_{t=1}^{T} \frac{\partial L}{\partial a^t}\frac{\partial a^t}{\partial w} = \sum_{t=1}^{T} \frac{\partial L}{\partial a^t} h^{t-1} = \sum_{t=1}^{T} \delta^t h^{t-1}$$

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$$\delta^t = \left(\frac{\partial L^t}{\partial h^t} + \delta^{t+1} \cdot w\right) \cdot \dot{\sigma}\left(a^t\right)$$

Backpropagating error through time

Backpropagation Through Time

$$L = \sum_{t=1}^{T} L^t \quad L^t = \frac{1}{2}\left(h^t - h^{*t}\right)^2$$

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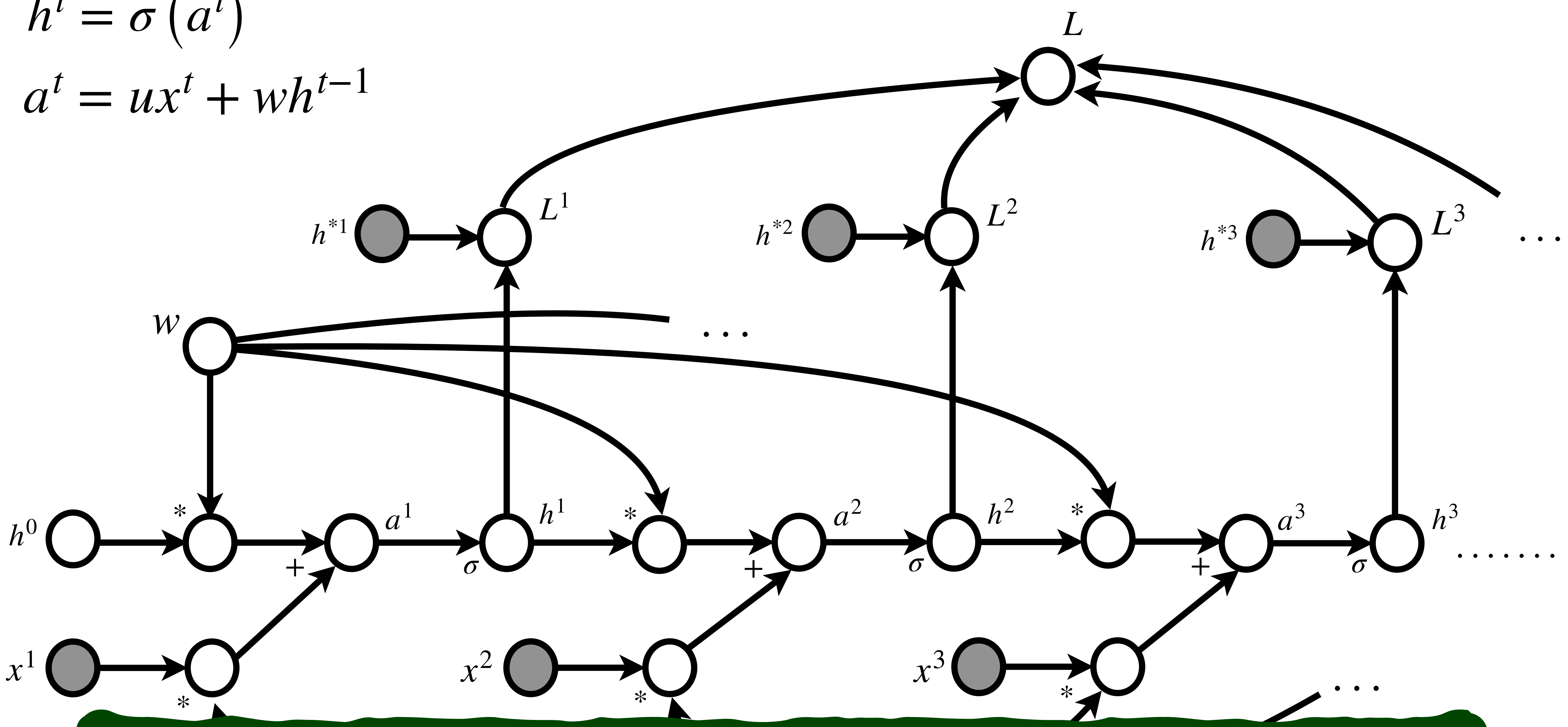

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$$\delta^t = \left(\frac{\partial L^t}{\partial h^t} + \delta^{t+1}\cdot w\right)\cdot\dot{\sigma}\left(a^t\right)$$

Backpropagating error through time

Notes on backpropagation through time:

- Depends on the number of time steps.
- Before each parameter update, we need to wait and store everything until all computations are done.
  - Memory demanding for longer sequences.
  - Alternative: “truncated backprop through time”.

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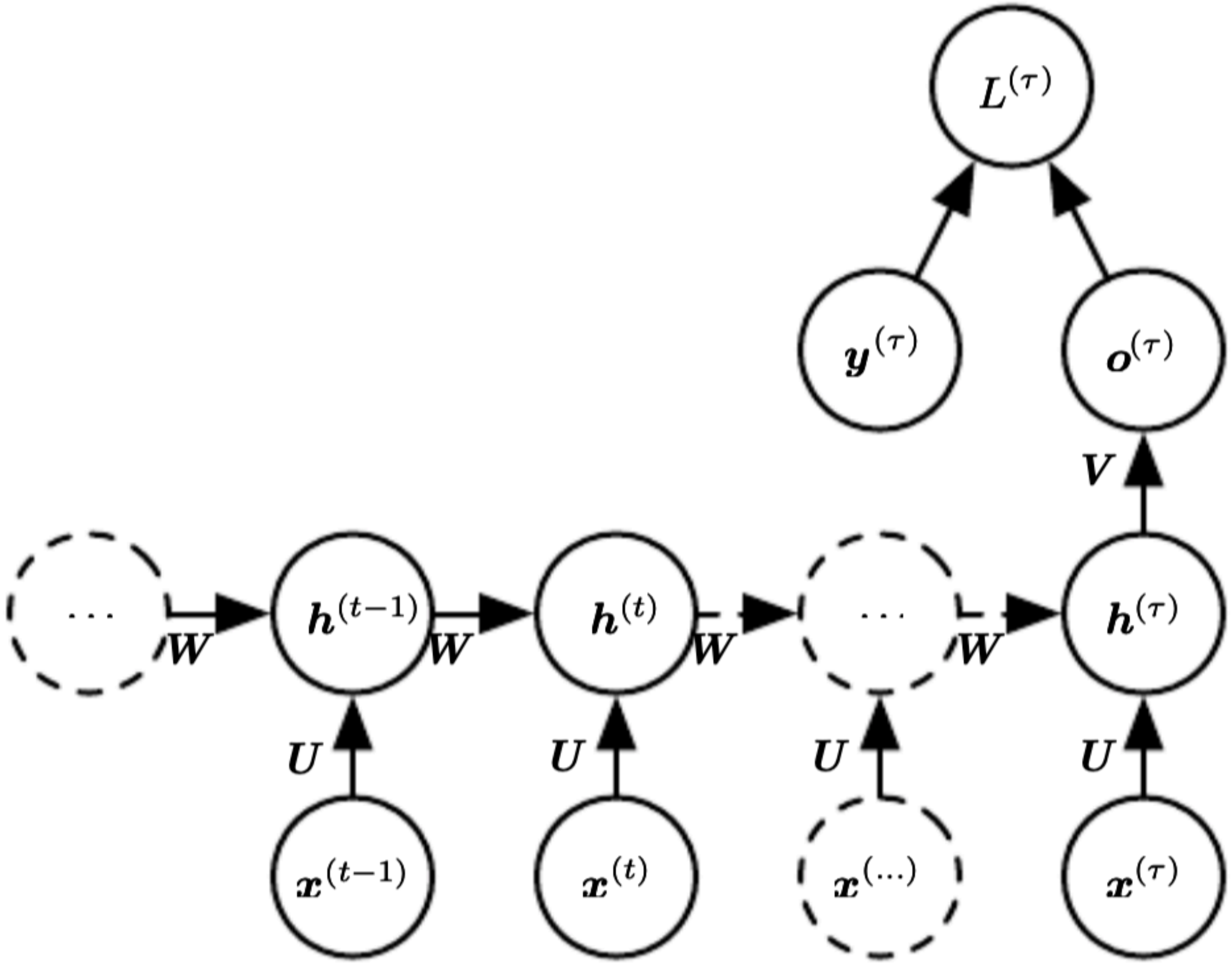
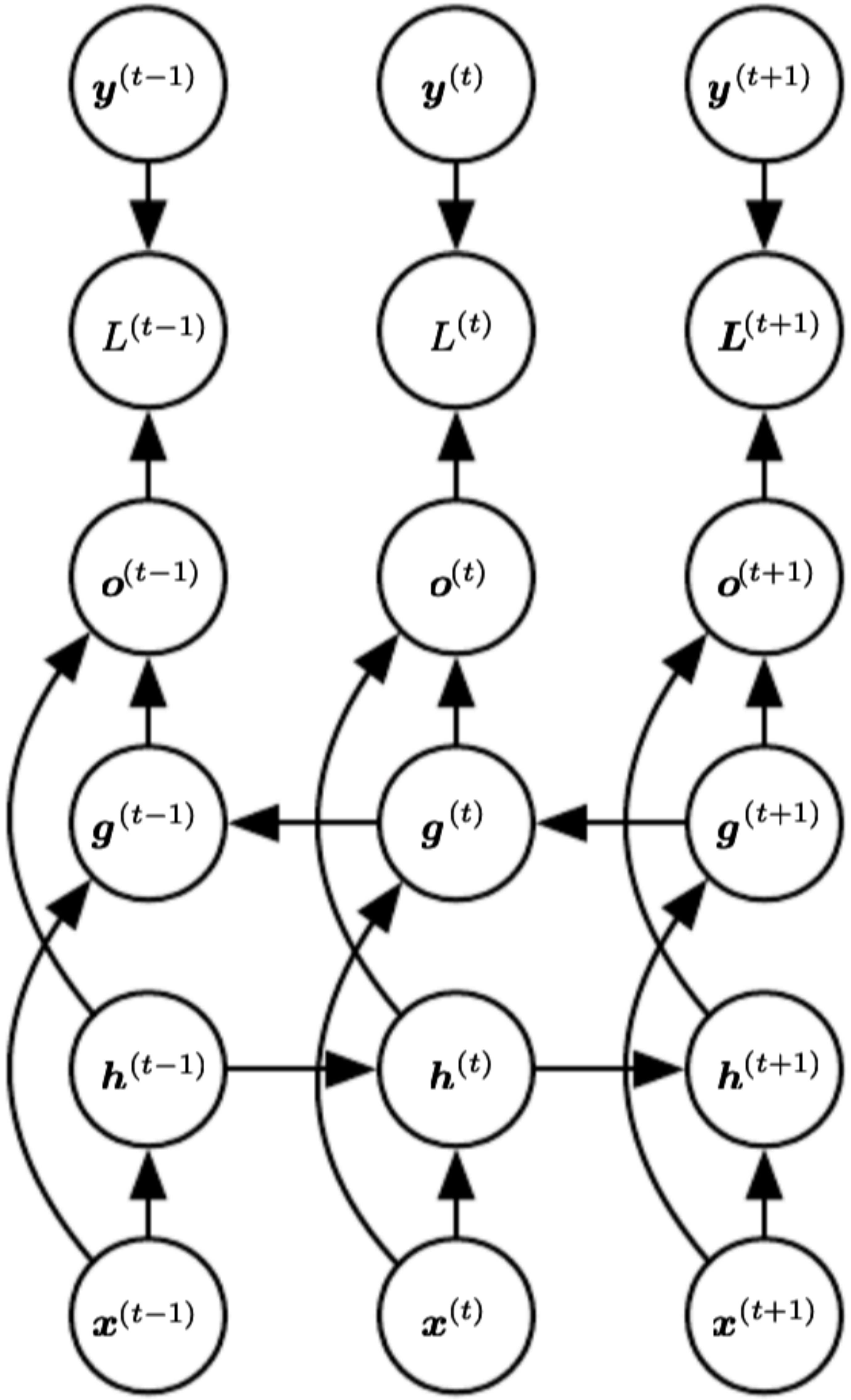
(1) Single output at the end of the sequence



Some potential use cases:

- Text classification.
- Detecting anomalies from a given measurement sequence.
- Summarize a sequence and produce a fixed-size representation, then use this as input for further processing.

(2) Bidirectional RNNs



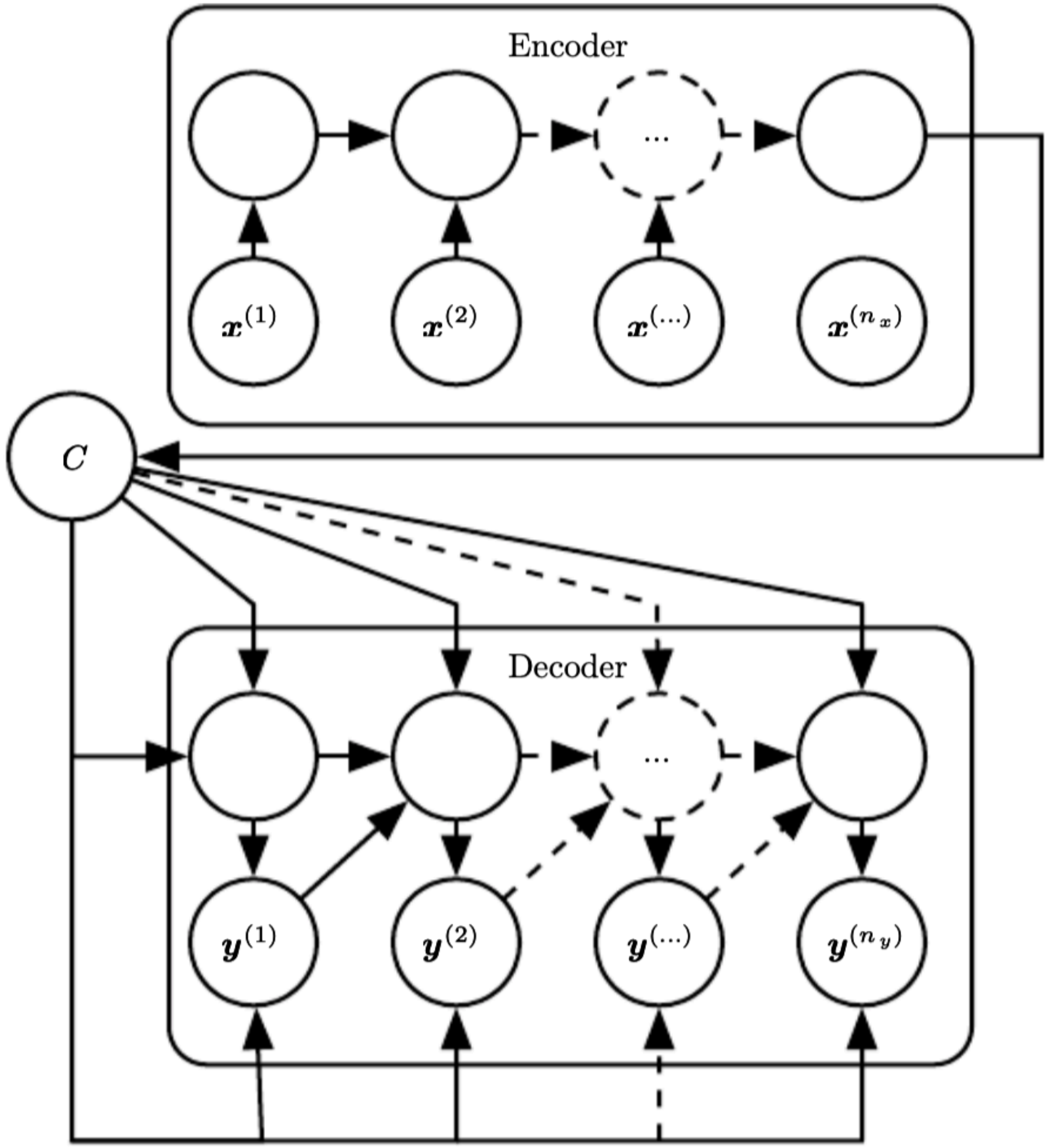
- If the whole sequence is known in advance.
- Future may provide important information.
- When deciding on $\mathbf{o}^{(t)}$, take times around t into account.

$\mathbf{h}^{(t)}$: RNN that moves ***forward*** in time

$\mathbf{g}^{(t)}$: RNN that moves ***backward*** in time

($\mathbf{g}^{(t)}$ sees the sequence in reversed order)

(3) Encoder-Decoder (Sequence-to-Sequence) Architecture



- If the output sequence does not have the same length as input sequence, e.g. in language translation.

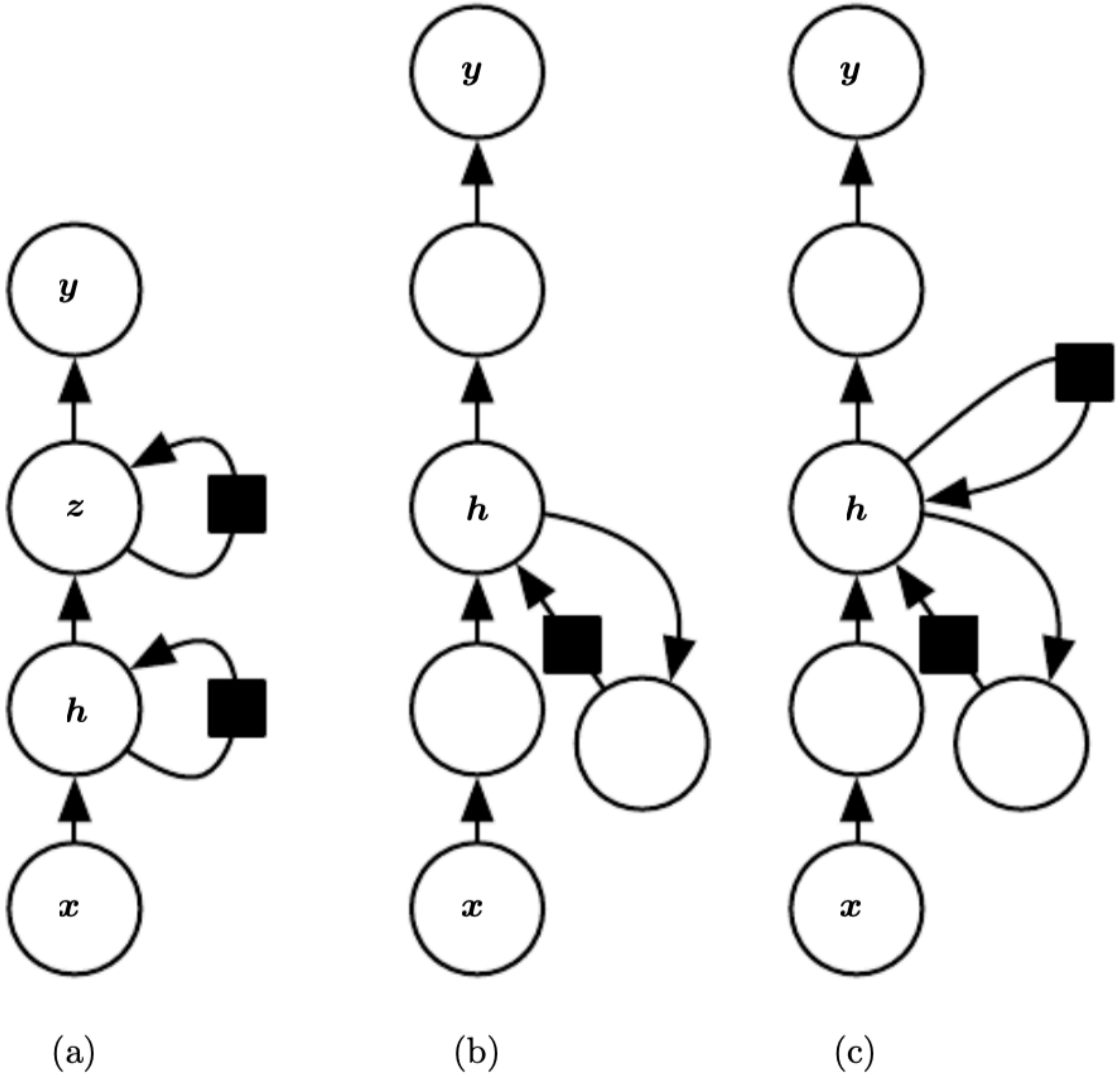
Input: Sequence $\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(n_x)}$

Output: Sequence $\mathbf{y}^{(1)}, \dots, \mathbf{y}^{(n_y)}$

Encoder: Processes input and emits the context C, typically a simple function of its final hidden state.

Decoder: Generates the output sequence conditioned on this context C.

(4) Deep Recurrent Networks



Possible ways to deepen RNNs:

(a) Several recurrent hidden layers.

(b, c) Additional input/output layers.

(b) Deep hidden-to-hidden interactions

(c) Same as (b) but with skip-connections.

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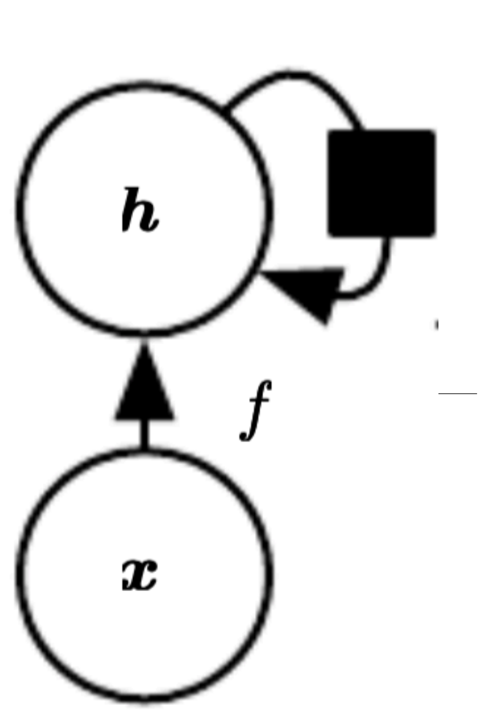
Problem: Challenging long-term dependencies



- *Vanishing/exploding gradients* problem:

Gradients propagated over many stages tend to either vanish or explode.

We can mitigate *exploding gradients* by gradient clipping.

What about *vanishing gradients*?

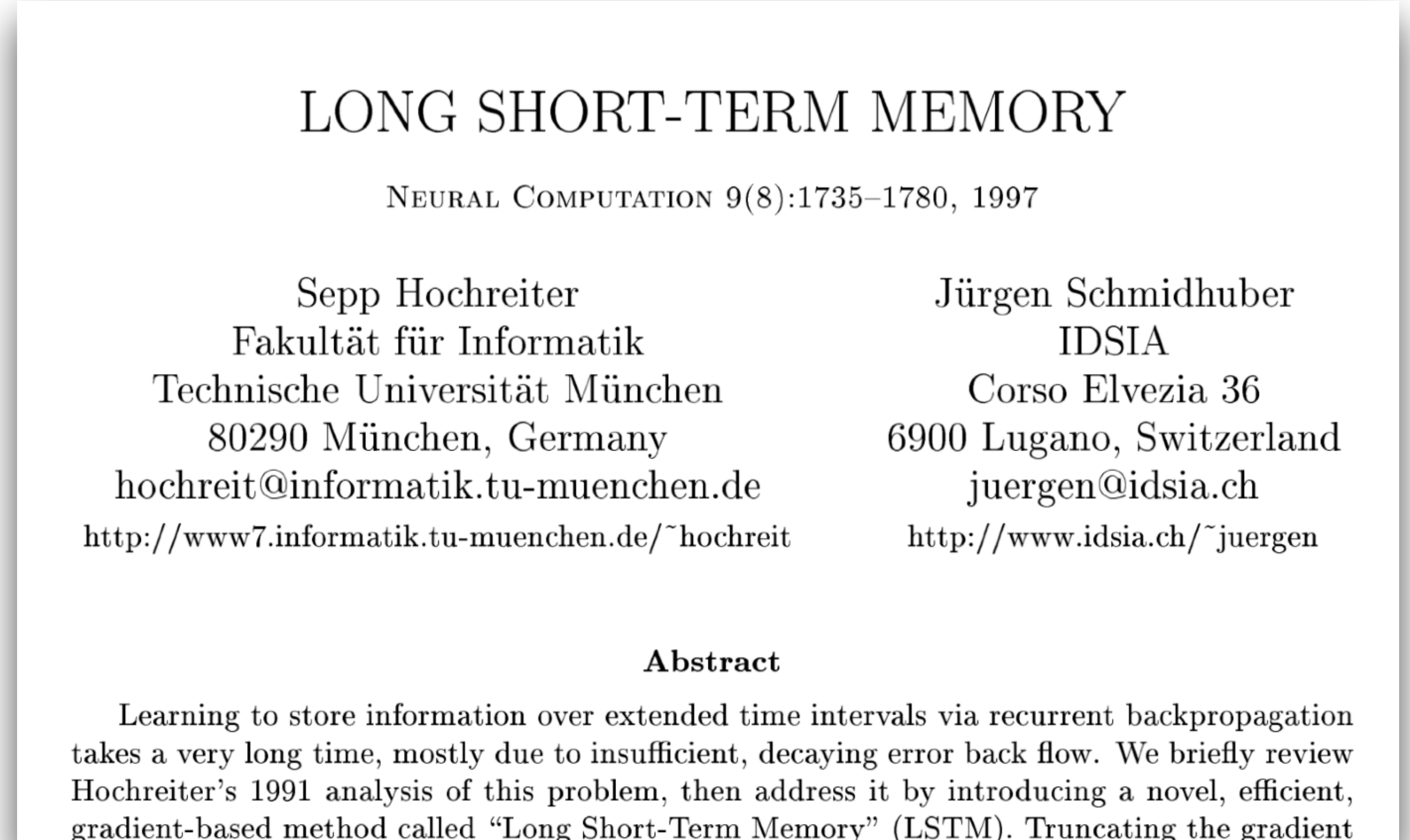
- In order to store memories in a way that is robust to small perturbations, the RNN must enter a region of parameter space where gradients vanish.
- The gradient of a long term interaction has exponentially smaller magnitude than that of a short term interaction.

Long Short-Term Memory (LSTM)

Idea: **Create paths through time that have derivatives that neither vanish nor explode.**

LSTM basic unit: A memory cell

- A linear neuron with a unit-weight self loop, where:
    - an **input gate** controls whether to load something in,
    - an **output gate** controls whether to make the content available to others,
    - a **forget gate** controls whether to forget the content.



LONG SHORT-TERM MEMORY

NEURAL COMPUTATION 9(8):1735–1780, 1997

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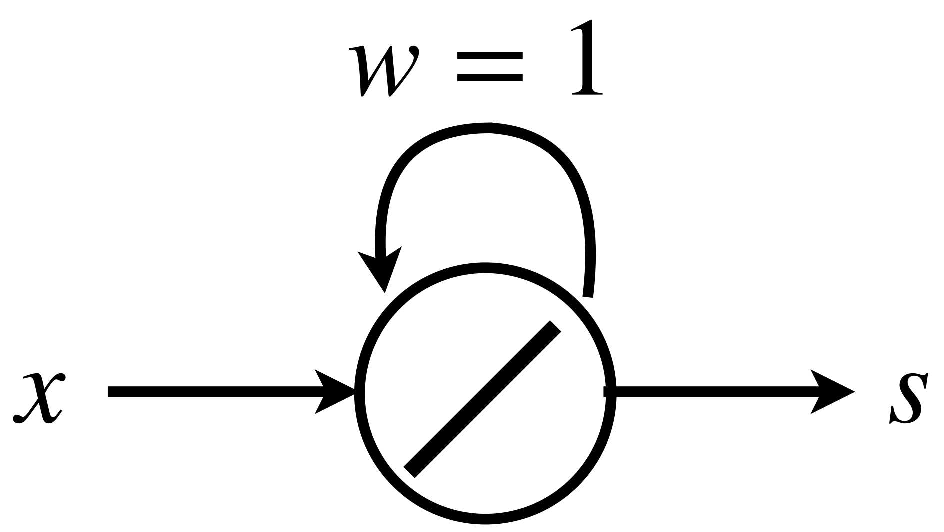
Abstract

Learning to store information over extended time intervals via recurrent backpropagation takes a very long time, mostly due to insufficient, decaying error back flow. We briefly review Hochreiter's 1991 analysis of this problem, then address it by introducing a novel, efficient, gradient-based method called "Long Short-Term Memory" (LSTM). Truncating the gradient

[S. Hochreiter and J. Schmidhuber. "Long short-term memory." *Neural Computation*, 1997.]

LSTM - Memory Cell

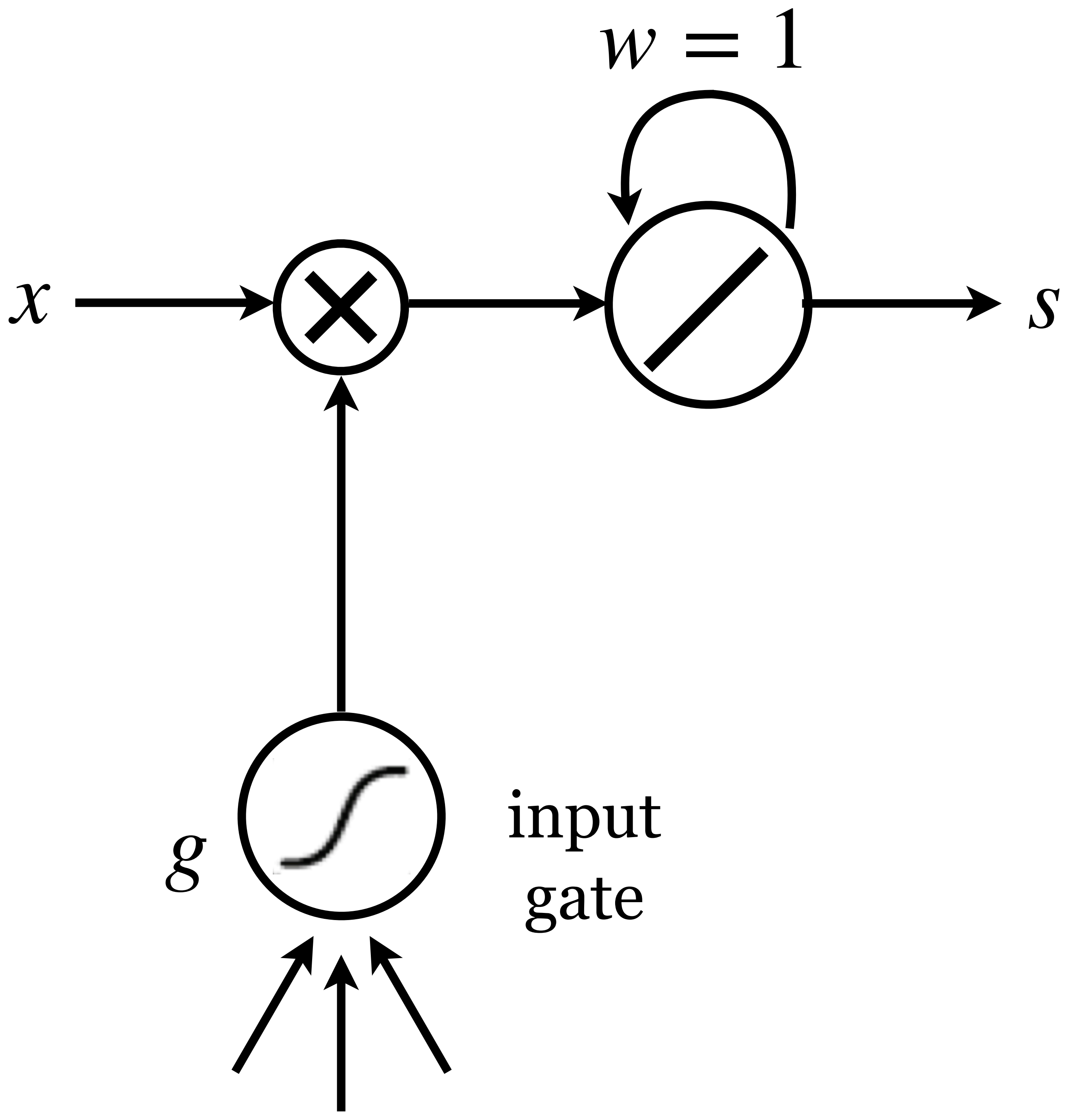


$$s^t = s^{t-1} + x^t$$

[S. Hochreiter and J. Schmidhuber. "Long short-term memory." *Neural Computation*, 1997.]

LSTM - Memory Cell

Input Gate:

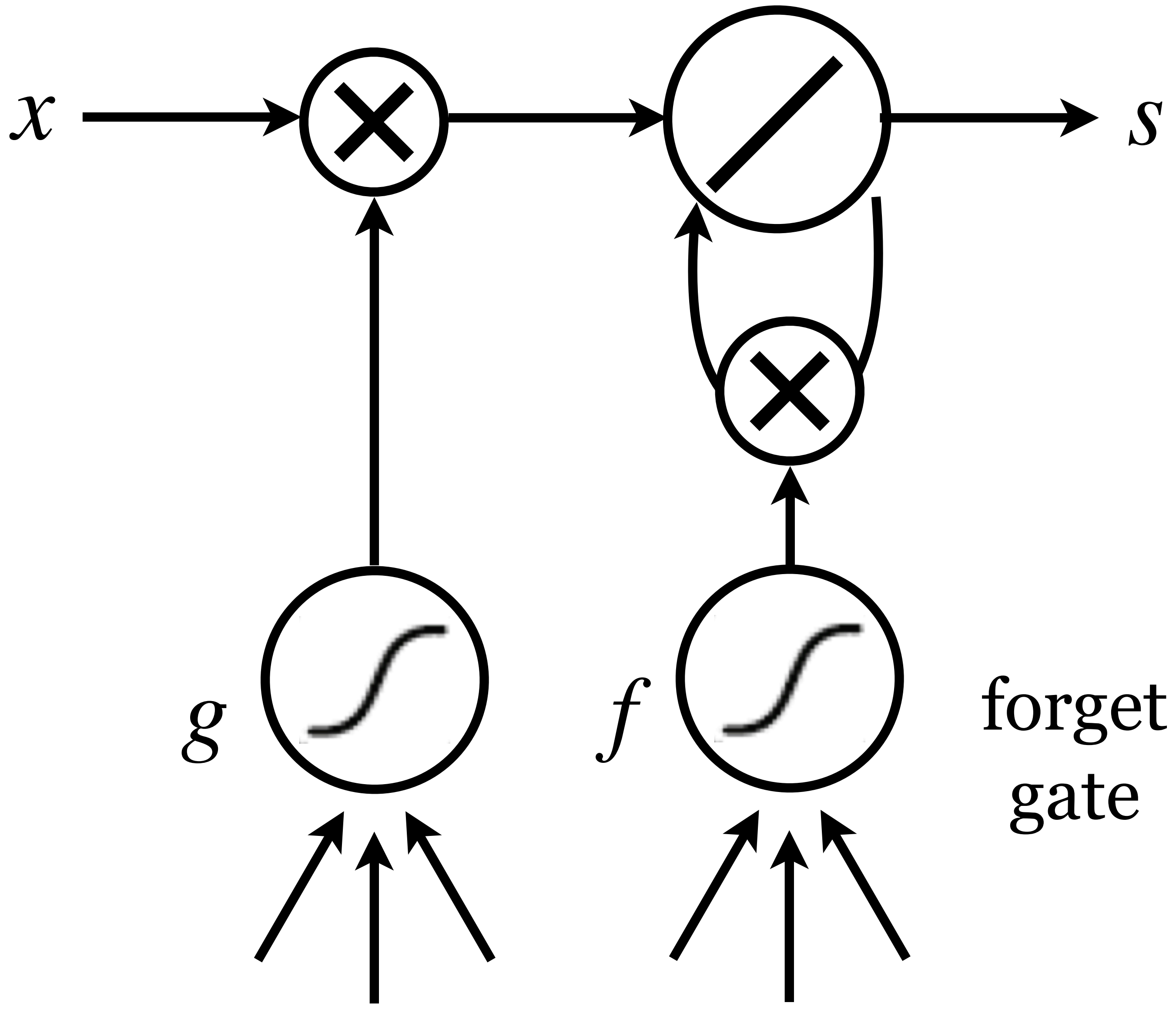


$$s^t = s^{t-1} + g^t x^t$$

[S. Hochreiter and J. Schmidhuber. "Long short-term memory." *Neural Computation*, 1997.]

LSTM - Memory Cell

Forget Gate:

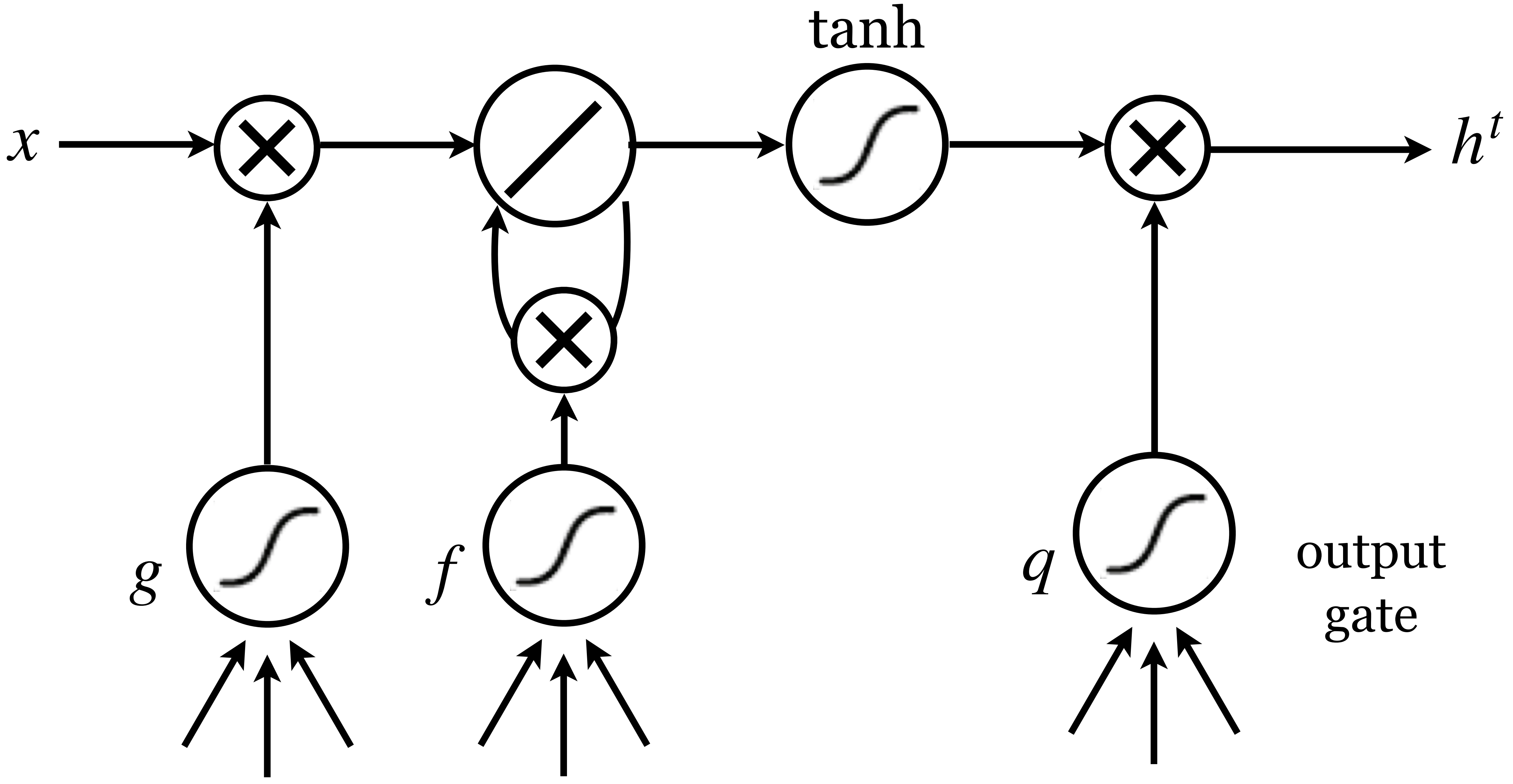


$$s^t = f^t s^{t-1} + g^t x^t$$

[S. Hochreiter and J. Schmidhuber. "Long short-term memory." *Neural Computation*, 1997.]

LSTM - Memory Cell

Output Gate:



$$s^t = f^t s^{t-1} + g^t x^t$$
$$h^t = q^t \cdot \tanh\left(s^t\right)$$

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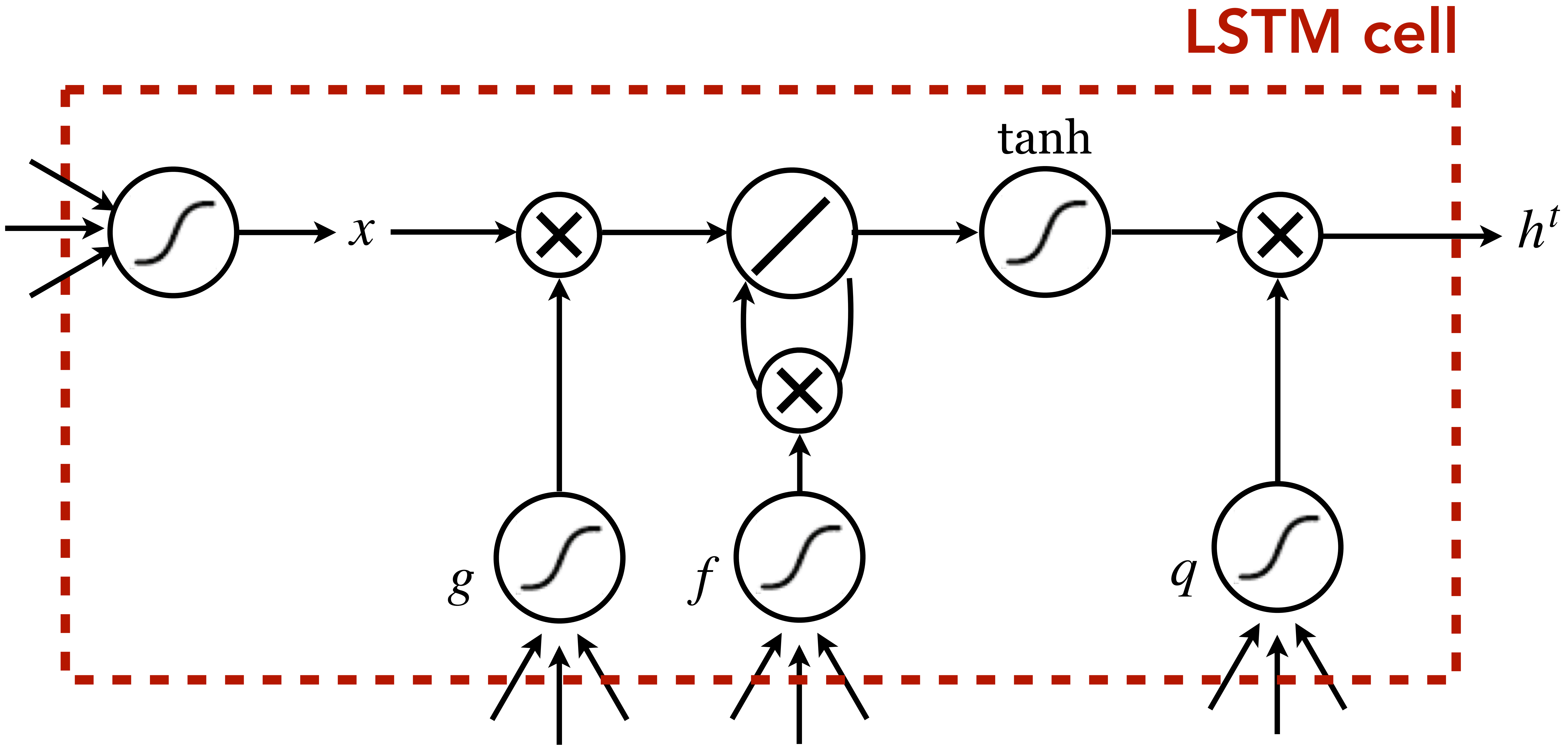
LSTM - Memory Cell



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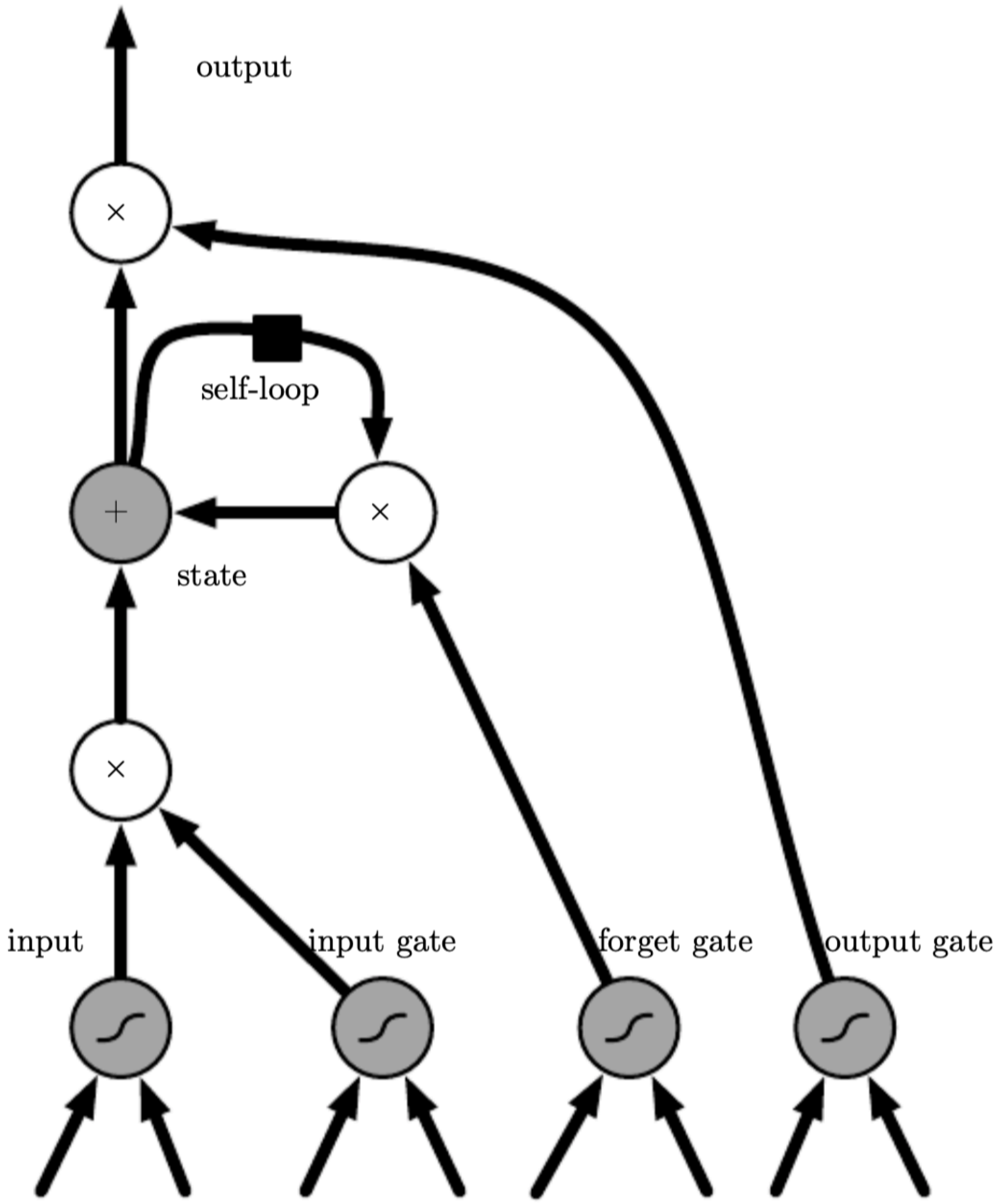
LSTM - Memory Cell - Details



$$h_i^{(t)} = \tanh\left(s_i^{(t)}\right) q_i^{(t)}$$

$$s_i^{(t)} = f_i^{(t)} s_i^{(t-1)} + g_i^{(t)} \sigma \left(b_i + \sum_j U_{i,j} x_j^{(t)} + \sum_j W_{i,j} h_j^{(t-1)} \right)$$

$$g_i^{(t)} = \sigma \left(b_i^g + \sum_j U_{i,j}^g x_j^{(t)} + \sum_j W_{i,j}^g h_j^{(t-1)} \right)$$

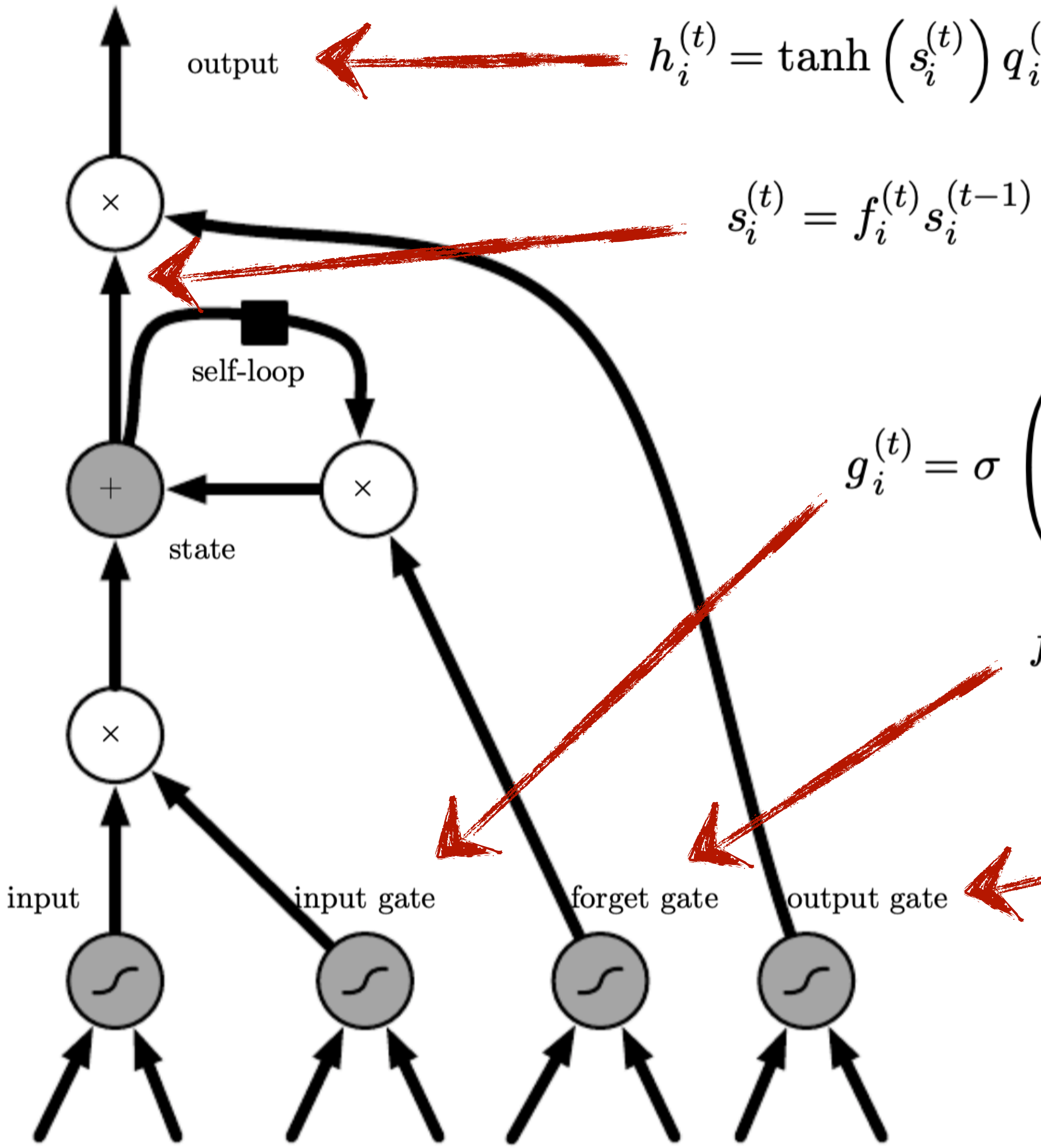
$$f_i^{(t)} = \sigma \left(b_i^f + \sum_j U_{i,j}^f x_j^{(t)} + \sum_j W_{i,j}^f h_j^{(t-1)} \right)$$

$$q_i^{(t)} = \sigma \left(b_i^o + \sum_j U_{i,j}^o x_j^{(t)} + \sum_j W_{i,j}^o h_j^{(t-1)} \right)$$

$\boldsymbol{x}^{(t)}$ is the current input vector.

$\boldsymbol{h}^{(t)}$ is the current hidden layer vector.

LSTM - Memory Cell - Details



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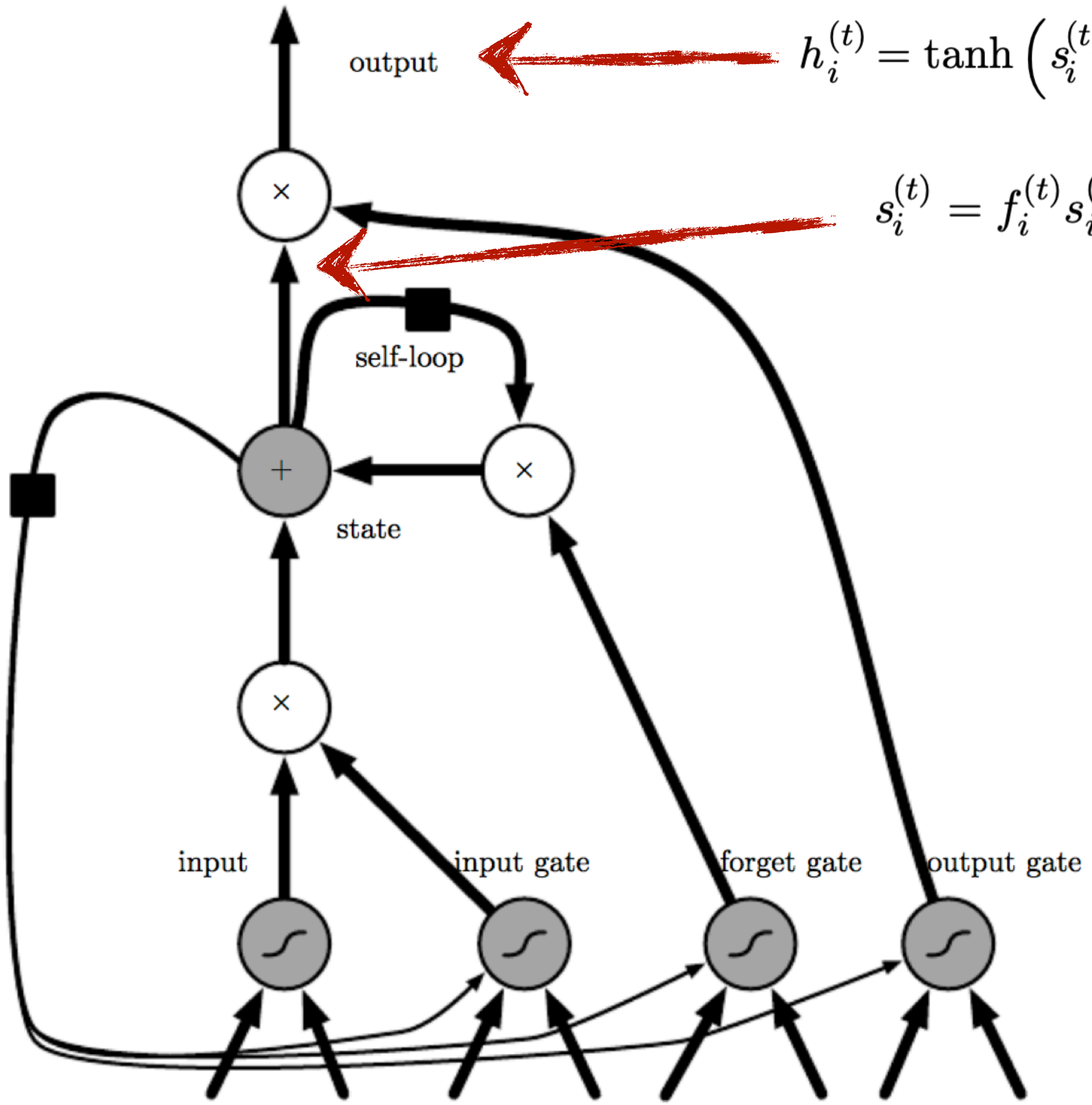
LSTM - Memory Cell - Details



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$$s_i^{(t)} = f_i^{(t)} s_i^{(t-1)} + g_i^{(t)} \sigma\left(b_i + \sum_j U_{i,j} x_j^{(t)} + \sum_j W_{i,j} h_j^{(t-1)}\right)$$

- The state unit can also be used as an extra input to the gating units.

$\boldsymbol{x}^{(t)}$ is the current input vector.

$\boldsymbol{h}^{(t)}$ is the current hidden layer vector.

Gated Recurrent Unit (GRU)

A simplified version of an LSTM cell.

- an **update gate** : u simultaneously controls the forgetting factor and the input gating.
- a **reset gate** : r controls which parts of the hidden state are used for the update.

$$h_i^{(t)} = u_i^{(t-1)} h_i^{(t-1)} + (1 - u_i^{(t-1)}) \sigma \left(b_i + \sum_j U_{i,j} x_j^{(t)} + \sum_j W_{i,j} r_j^{(t-1)} h_j^{(t-1)} \right)$$

- The output values of u_i^t and r_j^t are computed in the usual way.

Recall LSTMs: $h_i^{(t)} = \tanh\left(s_i^{(t)}\right) q_i^{(t)}$

$$s_i^{(t)} = f_i^{(t)} s_i^{(t-1)} + g_i^{(t)} \sigma \left(b_i + \sum_j U_{i,j} x_j^{(t)} + \sum_j W_{i,j} h_j^{(t-1)} \right)$$

- GRUs have only two gates (instead of three with LSTMs).
- A single "update gate". (LSTMs: input & forget gates).
- Therefore usually less parameters than LSTMs.

Example: Application to Text Translation

- **LSTMs** became popular after they achieved state-of-the-art results in text translation.

Sequence to Sequence Learning with Neural Networks

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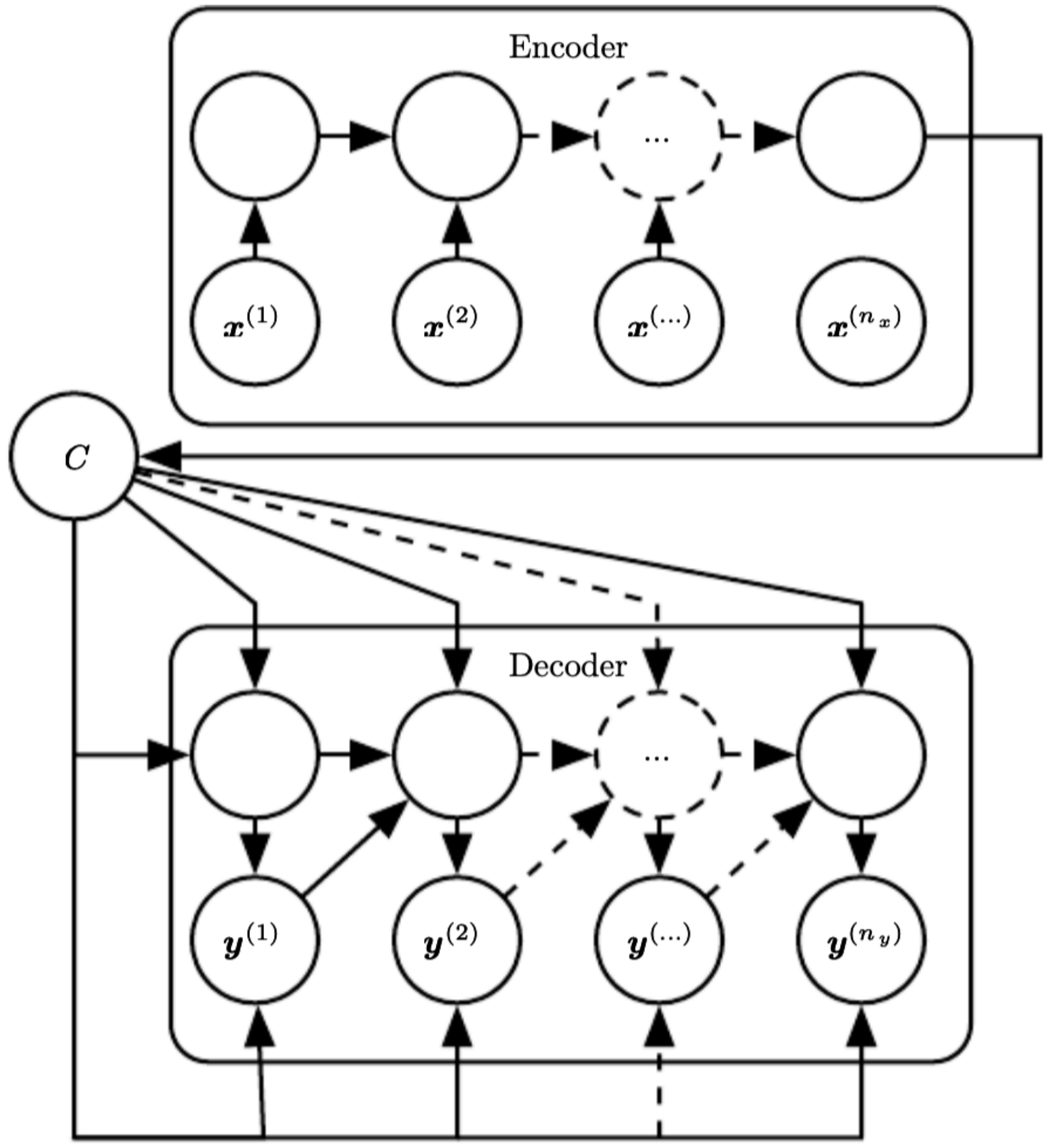
Input: Sentence in language A as a sequence of words.

Output: Sentence in language B as a sequence of words.

Length of input and output sequence may differ.

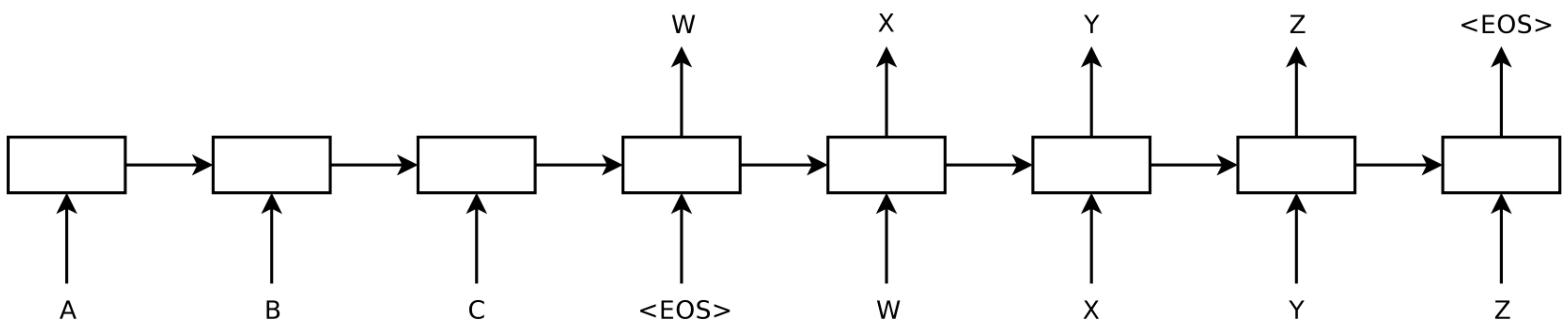
The model uses two LSTM-based network blocks:

- **Encoder:** Reads the input sequence and produces a fixed-size vector representation (its hidden state).
- **Decoder:** Starting with the hidden state of the encoder, it produces the output sequence.



Example: Application to Text Translation

- **Dataset**: WMT’14 English-to-French
- Vector representation for each word:
  - 160k words for source language.
  - 80k words for target language.
  - Words are embedded in 1000-dim embeddings.
  - Out-of-vocabulary words: <UNK> token.
  - End-of-sentence: <EOS> token.



- **Network** (384M parameters):
  - Deep LSTM with 4 layers.
  - 1000 cells per layer.
  - 1000-dim word embeddings.
  - Output: Softmax over 80k words.
  - Decoding the output as sentences:
    - Left-to-right beam search decoder.
- **Training**:
  - SGD for 7.5 epochs with gradient clipping.
  - After epoch 5, half the learning rate each epoch.

Example: Application to Text Translation

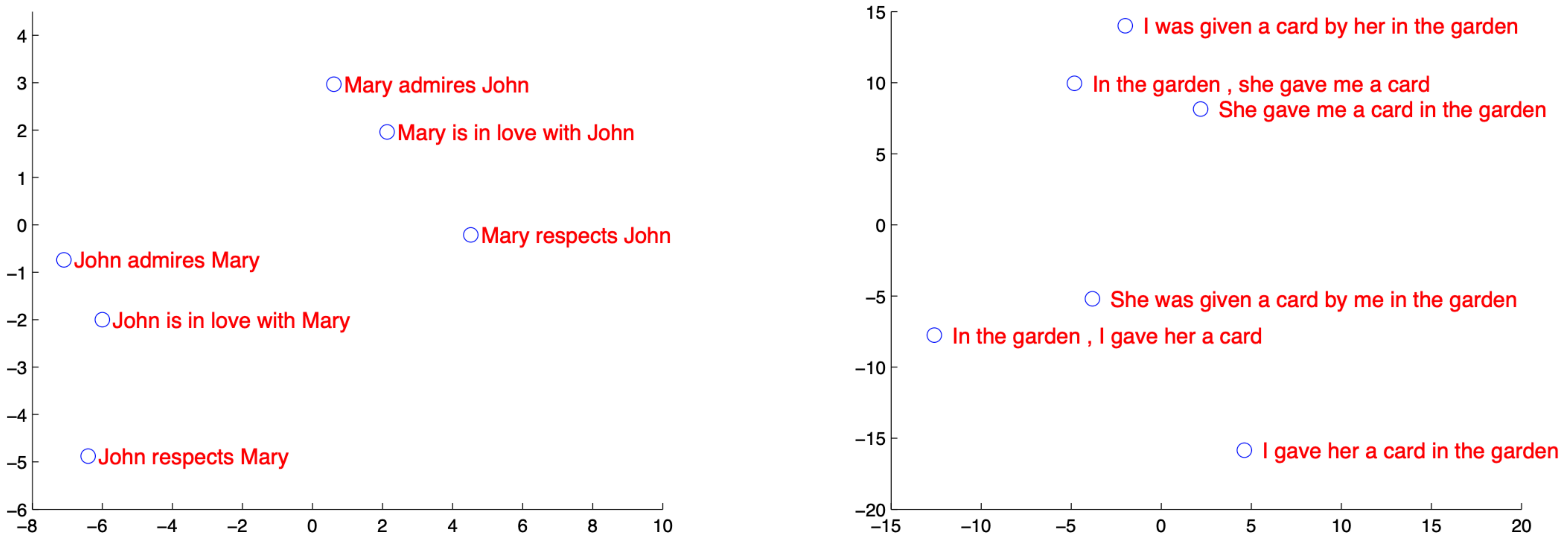
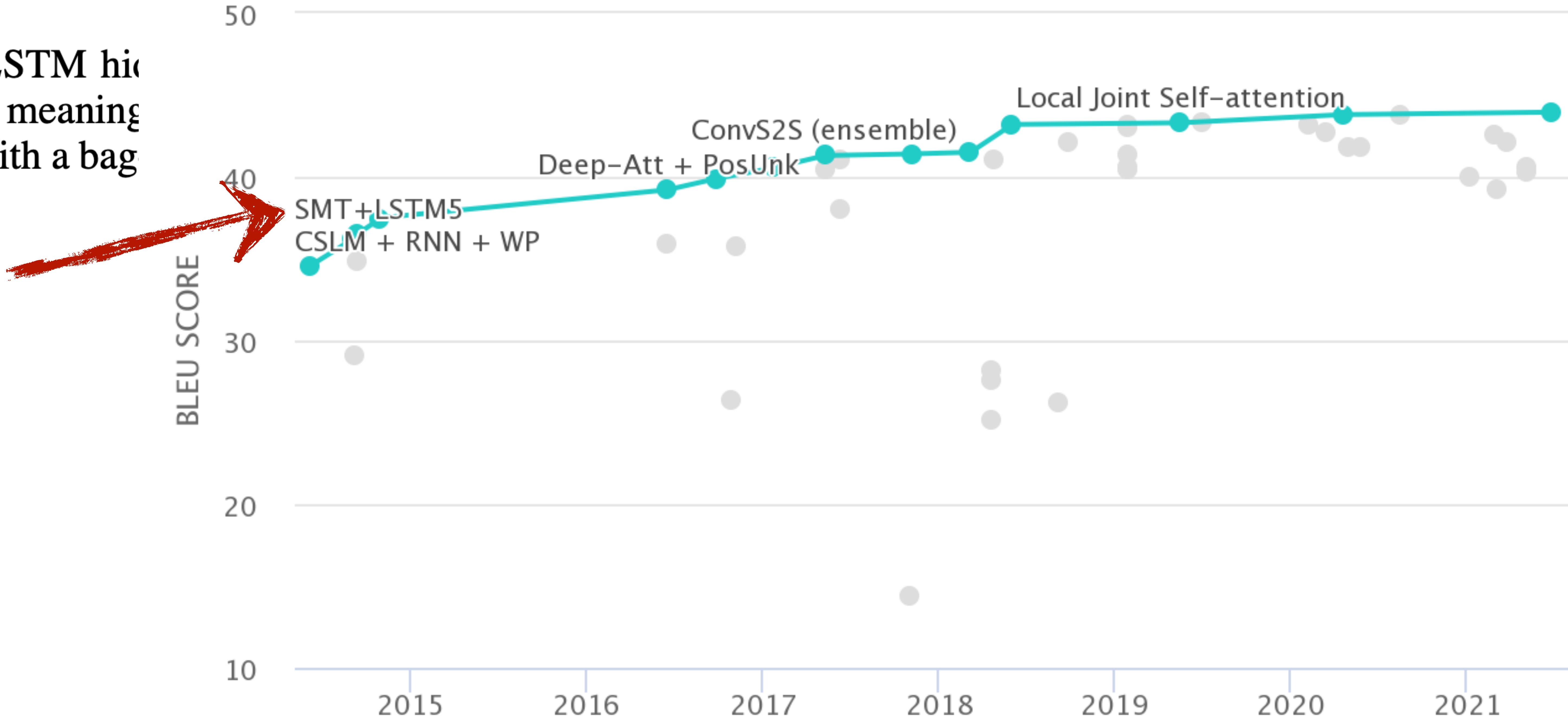


Figure 2: The figure shows a 2-dimensional PCA projection of the LSTM hi
after processing the phrases in the figures. The phrases are clustered by meaning
primarily a function of word order, which would be difficult to capture with a bag
both clusters have similar internal structure.

Source: https://paperswithcode.com/sota/machine-translation-on-wmt2014-english-french/



Summary

- RNN graphs include **recurrent connections** & implement **parameter sharing over time**.
    - Can process input sequences of variable length.
- Simple RNNs use standard neurons in the recurrent layer.
    - Architectural variants (e.g., bidirectional RNNs, encoder-decoder, …) exist.
- Training is via **backpropagation through time.**
    - Compute the gradients over the unrolled network & unrolled computation graph.
- Problems in training (simple) RNNs: **vanishing/exploding gradients**.
    - Memory units can overcome that!
    - **LSTMs & GRUs** use gating mechanisms in the recurrent layer units.
- Around 2010s, LSTMs became popular with state-of-the-art results in text translation.
    - Today, transformers have become the dominating model for such language processing tasks.

[Vaswani et al. "Attention is all you need." NeurIPS 2017.]

Today

- ☑ Recurrent Neural Networks
  - ☑ Simple RNNs
  - ☑ Backpropagation Through Time
  - ☑ Architectural Variants
  - ☑ Gated RNNs (LSTM & GRU)

Questions?