ST449 Artificial Intelligence and Deep Learning

Lecture 5

Sequence modeling

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https://github.com/lse-st449/lectures

Topics of this lecture

- Recurrent neural networks
- Exploding and vanishing gradients
- Vector to sequence models
- Bidirectional recurrent neural networks
- Long short-term memory networks
- Gated recurrent units
- Sequence transduction models
- Encoder-decoder architecture
  - w and w/o alignment
- Transformer (attention) networks

Recurrent neural networks

Recurrent neural networks overview

- Recurrent neural networks (RNNs): a family of neural networks for sequential data
  - Specialized for processing a sequence of vectors $\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}, \dots, \boldsymbol{x}^{(T)}$

- Most RNNs can process sequences of variable length

- Key idea: parameter sharing
  - Parameter sharing across different parts of the model

- Similarities to convolutional neural networks:
  - Convolutional neural networks also use parameter sharing
  - Use of convolution for 1-dimensional temporal sequences

Unfolding computational graphs

- Computational graph: defines application of a set of computations
    - Mapping of inputs to outputs
    - Mapping parameters to a loss function value

- Consider a non-linear dynamical system, defined by the recursive equation:

$$\boldsymbol{h}^{(t+1)} = f_\theta\left(\boldsymbol{h}^{(t)}\right)$$

where $\boldsymbol{h}^{(t)}$ is the state of the system, f_θ is a given function with θ parameter

- This is an autonomous system because the mapping f_θ does not depend on an independent variable (ex. time t)

- Unfolded equation:

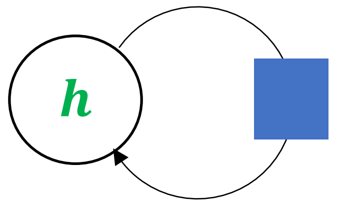
$$\boldsymbol{h}^{(1)} = f_\theta\left(\boldsymbol{h}^{(0)}\right), \boldsymbol{h}^{(2)} = f_\theta \circ f_\theta\left(\boldsymbol{h}^{(0)}\right), \dots, \boldsymbol{h}^{(t)} = f_\theta \circ \cdots \circ f_\theta\left(\boldsymbol{h}^{(0)}\right)$$

Unfolding computational graphs (cont'd)

- Recurrence equation:

$$\boldsymbol{h}^{(t+1)} = f_{\theta}\left(\boldsymbol{h}^{(t)}\right)$$

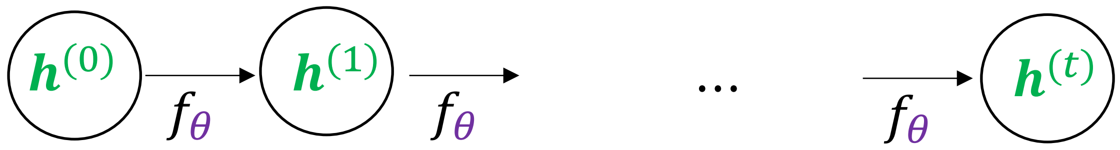
Recurrent graph



- Unfolded representation:

$$\boldsymbol{h}^{(t)} = f_{\theta} \circ \cdots \circ f_{\theta}(\boldsymbol{h}^{(0)})$$

Unfolded graph



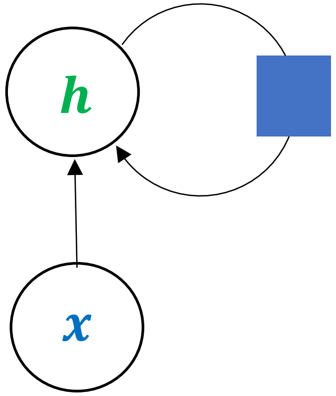
Unfolding computational graphs (cont’d)

- Non-autonomous dynamical system:

$$\boldsymbol{h}^{(t+1)} = f_\theta\left(\boldsymbol{h}^{(t)}, \boldsymbol{x}^{(t+1)}\right)$$

Input sequence
“driving sequence”

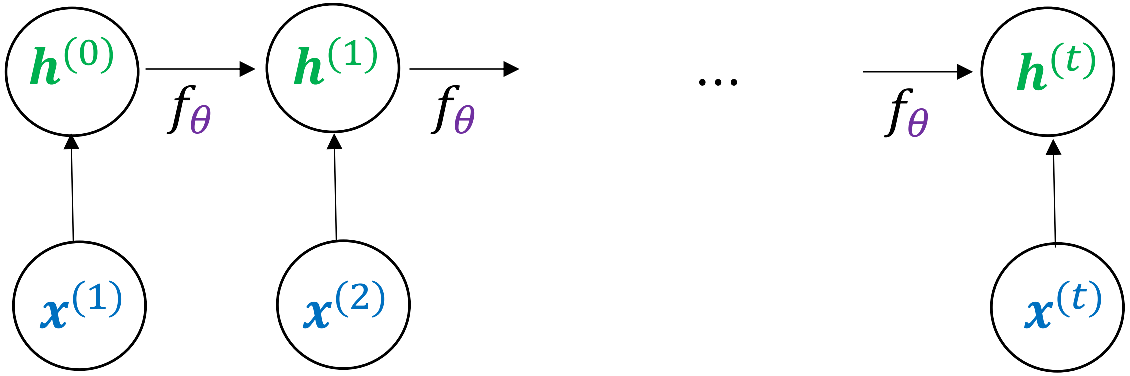
Recurrent graph



- Unfolded representation:

$$\boldsymbol{h}^{(t)} = f_\theta(f_\theta(\cdots f_\theta\left(\boldsymbol{h}^{(0)}, \boldsymbol{x}^{(1)}\right)\cdots, \boldsymbol{x}^{(t-1)}), \boldsymbol{x}^{(t)})$$

Unfolded graph



Unfolding computational graphs (cont’d)

- Recurrent graphs
  - Provide succinct representations

- Unfolded graphs
  - Provide explicit description of which computations to perform
  - Show paths along which information flows
    - Forward in time: for computing outputs and loss function
    - Backward in time: for computing gradients

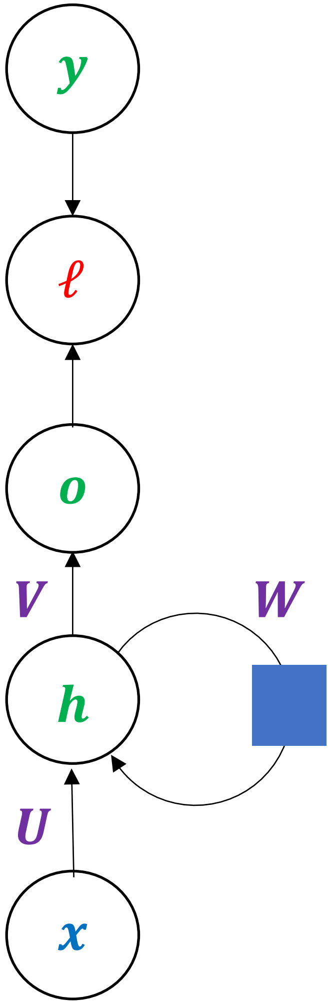
Common RNN architecture: A

True output

Loss function

Hidden state

Input



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

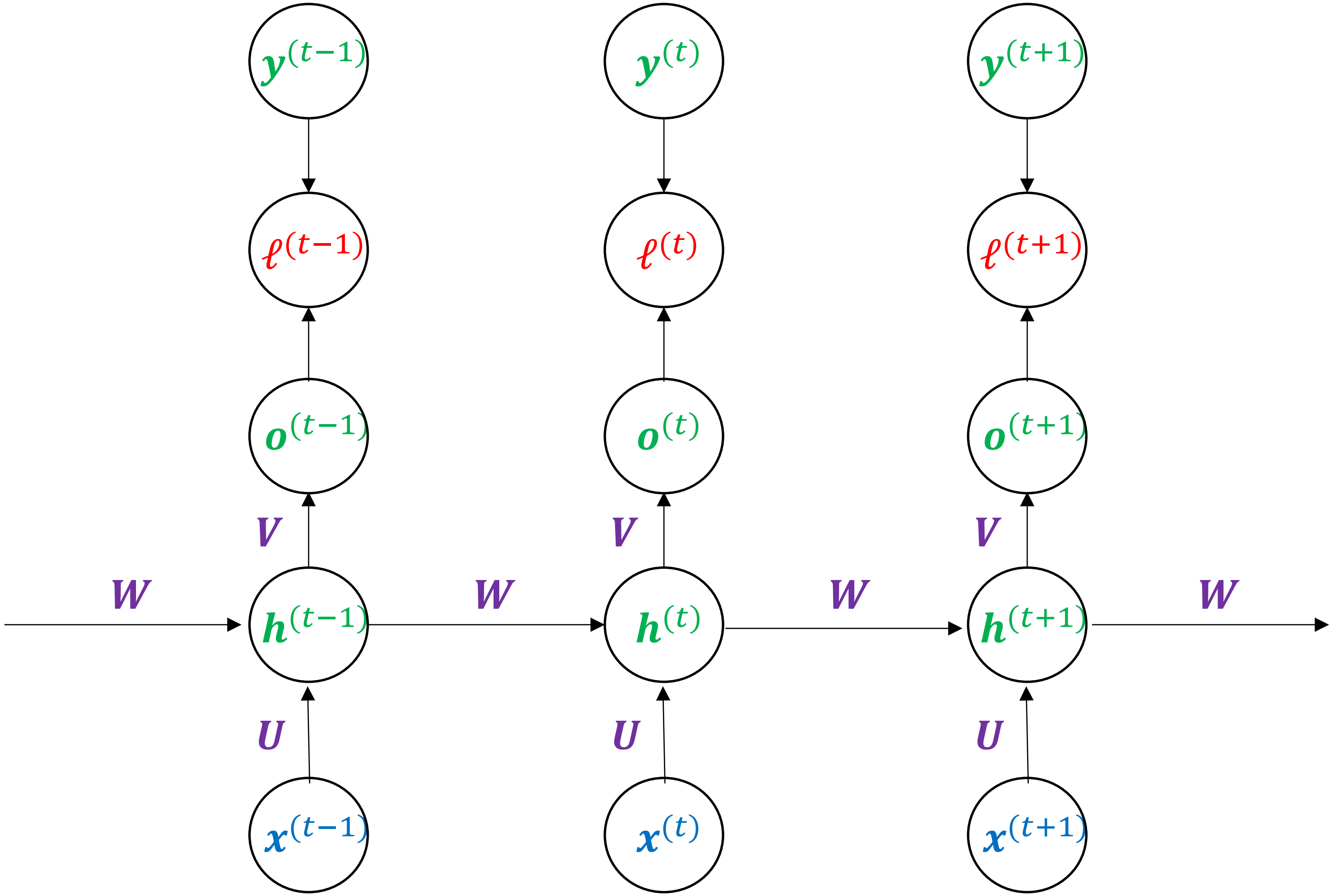
$$\boldsymbol{o}^{(t)} = \boldsymbol{V}\boldsymbol{h}^{(t)} + \boldsymbol{c}$$

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

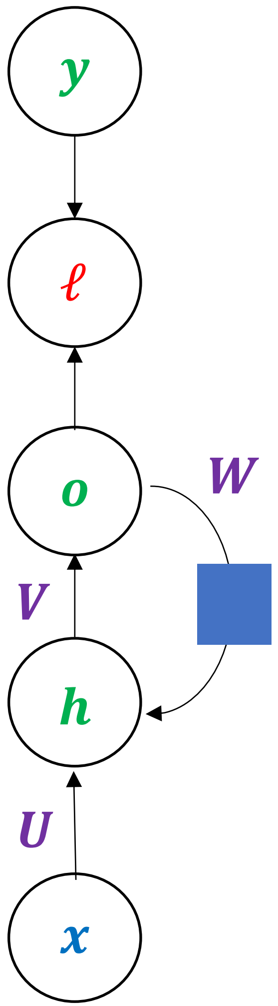
$$\boldsymbol{a}^{(t)} = \boldsymbol{W}\boldsymbol{h}^{(t-1)} + \boldsymbol{U}\boldsymbol{x}^{(t)} + \boldsymbol{b}$$

- Output: each time step
- Recurrent connections: between hidden units at successive time steps

Common RNN architecture: A (unfolded)



Common RNN architecture: B



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

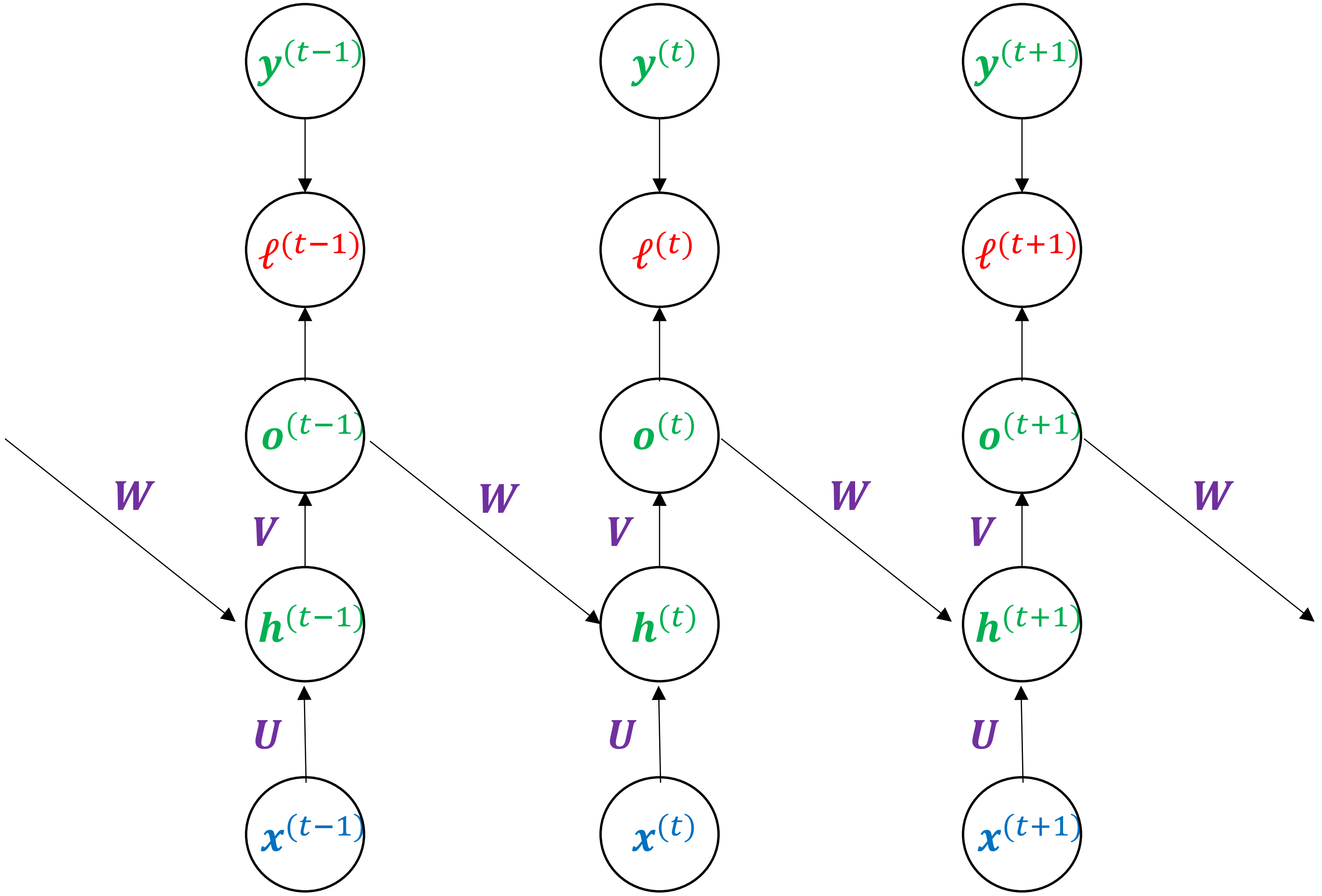
$$\boldsymbol{o}^{(t)} = \boldsymbol{V}\boldsymbol{h}^{(t)} + \boldsymbol{c}$$

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

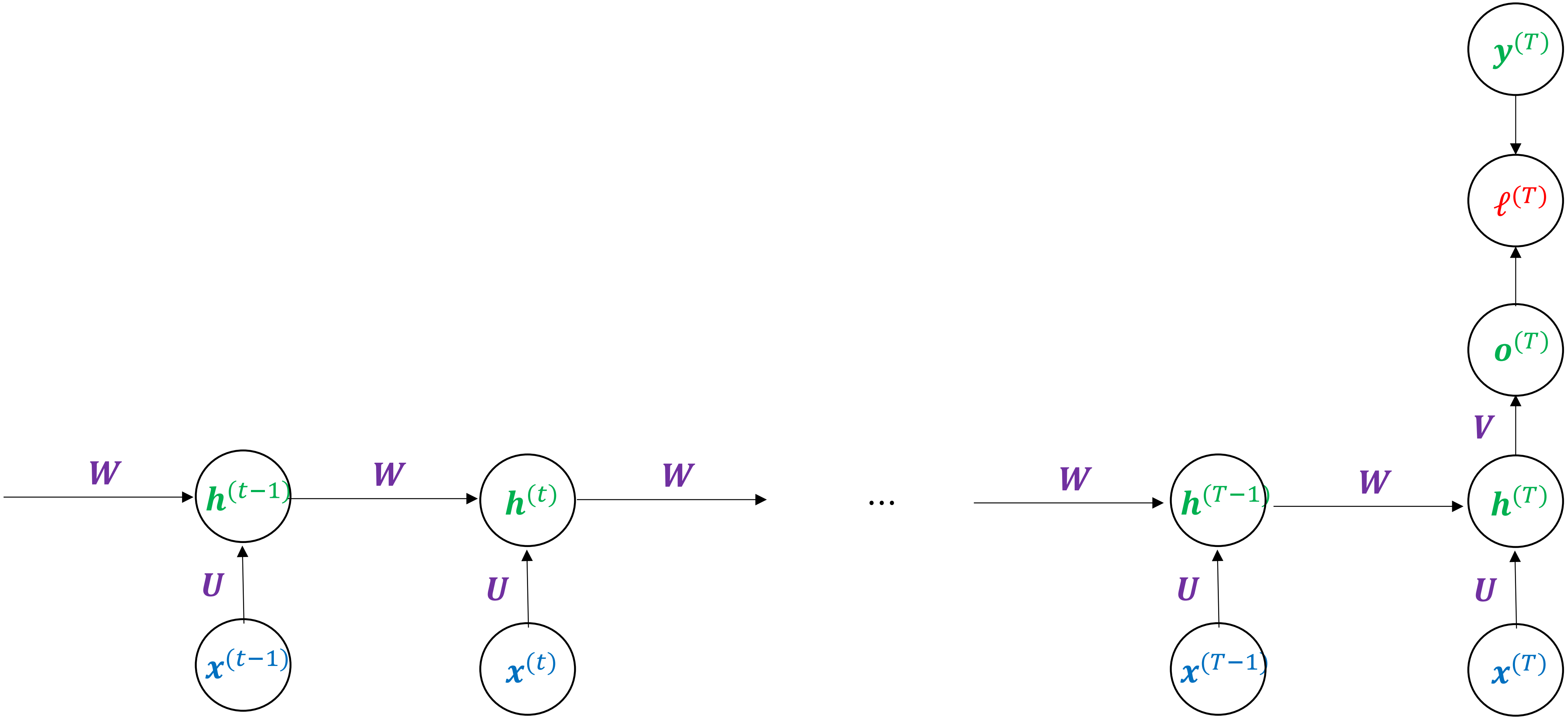
$$\boldsymbol{a}^{(t)} = \boldsymbol{W}\boldsymbol{h}^{(t-1)} + \boldsymbol{U}\boldsymbol{x}^{(t)} + \boldsymbol{b}$$

- Output: each time step
- Recurrent connections: from output at a time step to the hidden unit at next time step

Common RNN architecture: B (unfolded)



Common RNN architectures: C



- Output: after an input sequence is read
- Recurrent connections: between hidden units

Loss function: negative log-likelihood

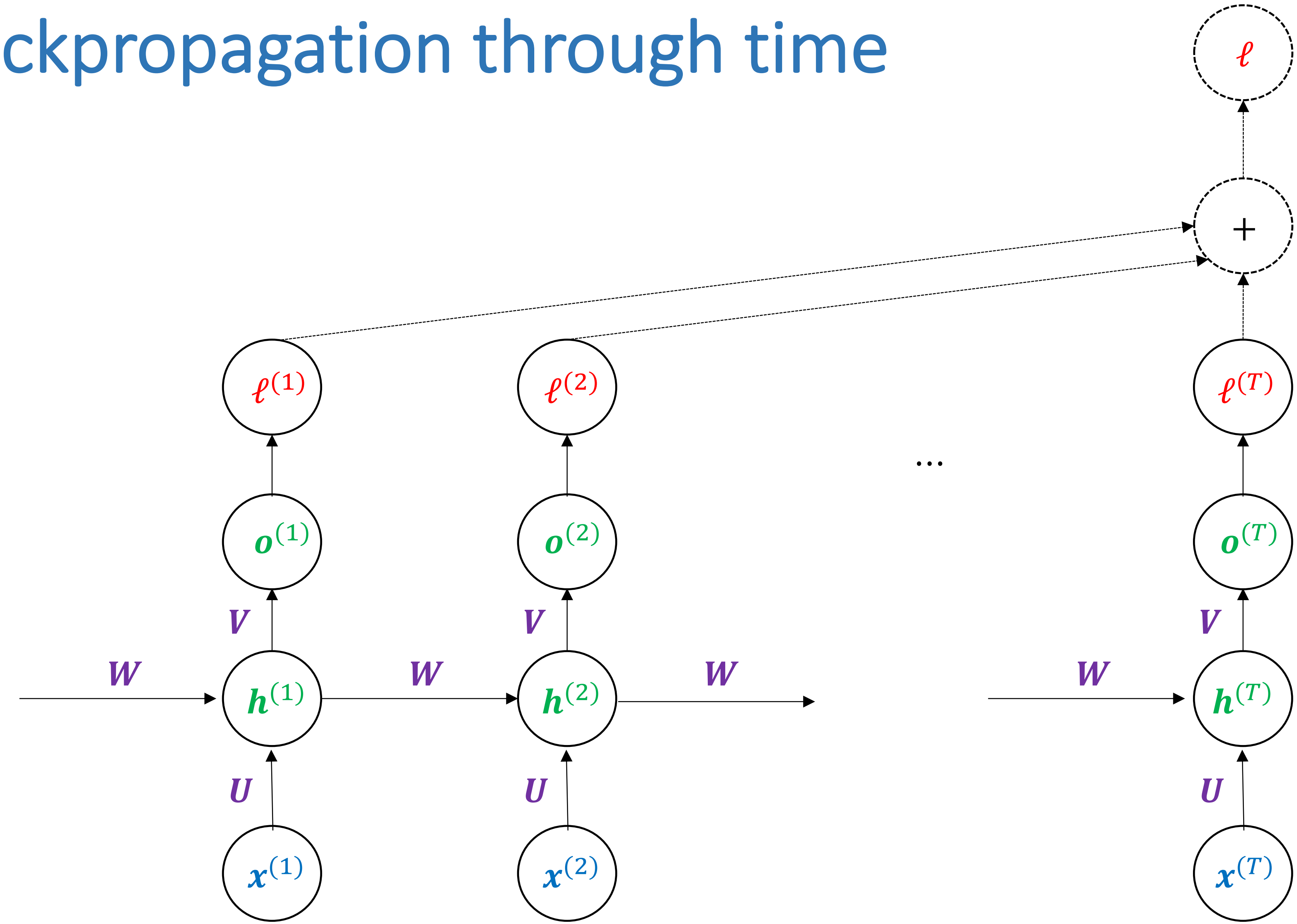
- Negative log-likelihood function:

$$\ell\left(\left(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(T)}\right), \left(\boldsymbol{y}^{(1)}, \dots, \boldsymbol{y}^{(T)}\right)\right) = \sum_{t=1}^{T} \ell^{(t)}$$

where

$$\ell^{(t)} = -\log \underbrace{p_\theta\left(\boldsymbol{y}^{(t)} \mid \boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(t)}\right)}_{= \hat{\boldsymbol{y}}^{(t)}_{\boldsymbol{y}^{(t)}}}$$

Backpropagation through time



Backpropagation through time (cont'd)

- Start with nodes corresponding to loss functions $\ell^{(t)}$:

$$J_{\ell^{(t)}}(\ell) = 1$$

- For nodes corresponding to output functions $\boldsymbol{o}^{(t)}$:

$$J_{\boldsymbol{o}^{(t)}}(\ell) = J_{\ell^{(t)}}(\ell) J_{\boldsymbol{o}^{(t)}}\left(\ell^{(t)}\right) = \hat{\boldsymbol{y}}^{(t)} - \boldsymbol{e}_{y^{(t)}}$$

$\boldsymbol{e}_i$:= vector with the i-th element equal to 1 and other elements 0

- For nodes corresponding to hidden state $\boldsymbol{h}^{(t)}$:

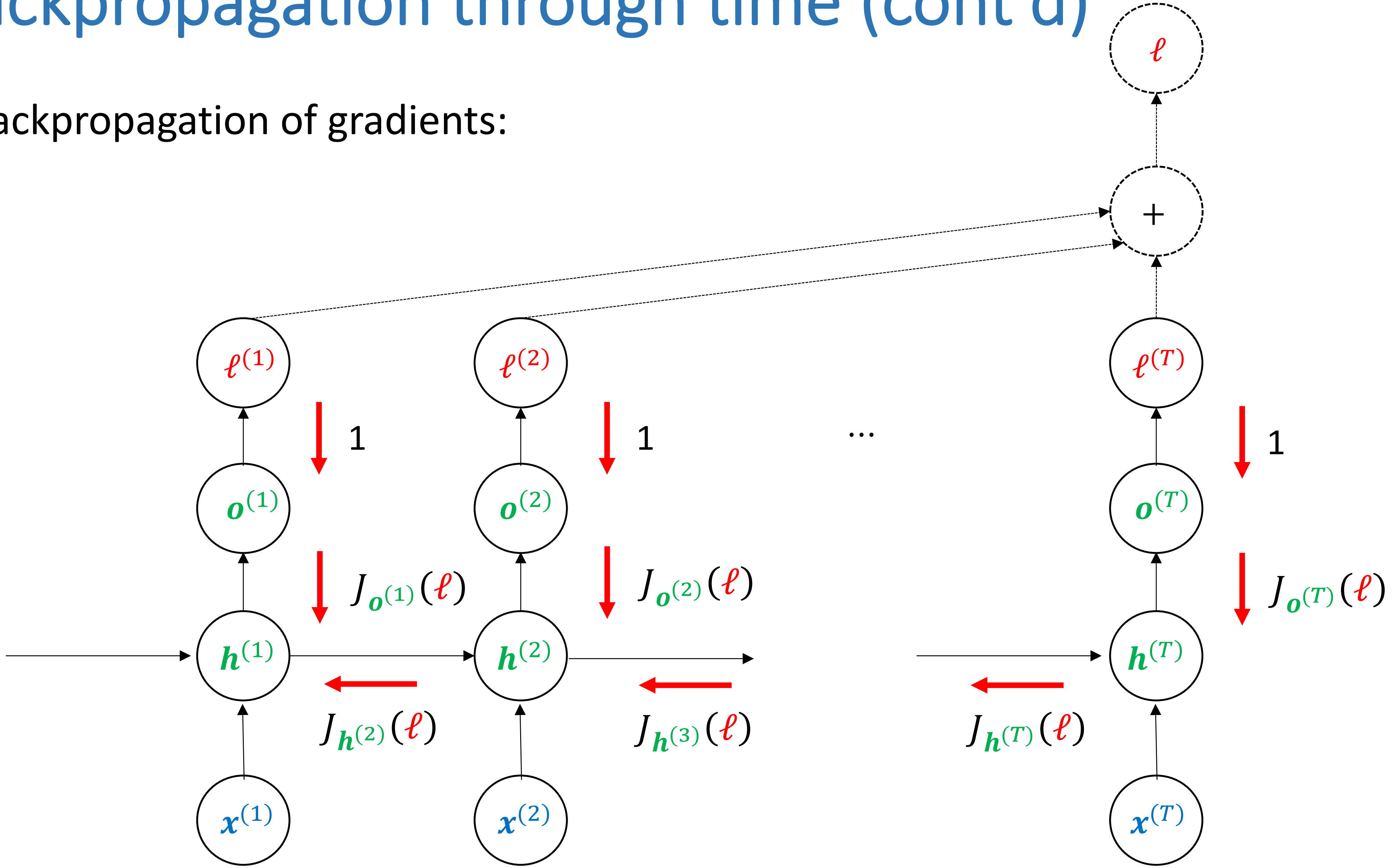
$$J_{\boldsymbol{h}^{(T)}}(\ell) = \boldsymbol{V}^\top J_{\boldsymbol{o}^{(T)}}(\ell)$$

$$J_{\boldsymbol{h}^{(t)}}(\ell) = \underbrace{J_{\boldsymbol{h}^{(t)}}(\boldsymbol{h}^{(t+1)})\, J_{\boldsymbol{h}^{(t+1)}}(\ell)}_{\boldsymbol{D}_{\boldsymbol{h}^{(t+1)}} \boldsymbol{W} J_{\boldsymbol{h}^{(t+1)}}(\ell)} + \underbrace{J_{\boldsymbol{h}^{(t)}}(\boldsymbol{o}^{(t)})}_{\boldsymbol{V}^\top} J_{\boldsymbol{o}^{(t)}}(\ell) \text{ for } 1 \leq t < T$$

$$\boldsymbol{D}_{\boldsymbol{h}^{(t+1)}} = \operatorname{diag}\left(1 - \left(h_1^{(t+1)}\right)^2, \ldots, 1 - \left(h_n^{(t+1)}\right)^2\right)$$

Backpropagation through time (cont'd)

- Backpropagation of gradients:



Backpropagation through time (cont'd)

- Gradients with respect to parameters:

$$J_{\boldsymbol{c}}(\ell) = \sum_{t=1}^{T} J_{\boldsymbol{c}}\left(\boldsymbol{o}^{(t)}\right)^{\top} J_{\boldsymbol{o}^{(t)}}(\ell) = \sum_{t=1}^{T} J_{\boldsymbol{o}^{(t)}}(\ell)$$

$$J_{\boldsymbol{b}}(\ell) = \sum_{t=1}^{T} J_{\boldsymbol{b}}\left(\boldsymbol{h}^{(t)}\right) J_{\boldsymbol{h}^{(t)}}(\ell) = \sum_{t=1}^{T} \boldsymbol{D}_{\boldsymbol{h}^{(t)}} J_{\boldsymbol{h}^{(t)}}(\ell)$$

$$J_{\boldsymbol{V}}(\ell) = \sum_{t=1}^{T} J_{\boldsymbol{o}^{(t)}}(\ell) J_{\boldsymbol{V}}(\boldsymbol{o}^{(t)}) = \sum_{t=1}^{T} J_{\boldsymbol{o}^{(t)}}(\ell)\left(\boldsymbol{h}^{(t)}\right)^{\top}$$

Exercise

- Show that

$$J_{\boldsymbol{o}^{(t)}}(\ell) = \hat{\boldsymbol{y}}^{(t)} - \boldsymbol{e}_{y^{(t)}}$$

- Show that

$$J_{\boldsymbol{h}^{(t)}}\left(\boldsymbol{h}^{(t+1)}\right) J_{\boldsymbol{h}^{(t+1)}}(\ell) = \boldsymbol{D}_{\boldsymbol{h}^{(t+1)}} \boldsymbol{W} J_{\boldsymbol{h}^{(t+1)}}(\ell)$$

Exercise solution

- $\frac{\partial \ell}{\partial \boldsymbol{o}_i^{(t)}} = \frac{\partial \ell}{\partial \ell^{(t)}} \frac{\partial \ell^{(t)}}{\partial \boldsymbol{o}_i^{(t)}} = \frac{\partial \ell^{(t)}}{\partial \boldsymbol{o}_i^{(t)}}$

- $\frac{\partial \ell^{(t)}}{\partial \boldsymbol{o}_i^{(t)}} = \frac{\partial}{\partial \boldsymbol{o}_i^{(t)}} \left(-\log \left(\frac{e^{\boldsymbol{o}_{y^{(t)}}^{(t)}}}{\sum_s e^{\boldsymbol{o}_s^{(t)}}} \right) \right) = -1_{y^{(t)}=i} + \frac{e^{\boldsymbol{o}_i^{(t)}}}{\sum_s e^{\boldsymbol{o}_s^{(t)}}} = -1_{y^{(t)}=i} + \hat{\boldsymbol{y}}_i^{(t)}$

$$\Rightarrow \frac{\partial \ell}{\partial \boldsymbol{o}_i^{(t)}} = \hat{\boldsymbol{y}}_i^{(t)} - 1_{y^{(t)}=i}$$

or, equivalently,

$$J_{\boldsymbol{o}^{(t)}}(\ell) = \hat{\boldsymbol{y}}^{(t)} - \boldsymbol{e}_{y^{(t)}}$$

Exercise solution (cont'd)

- Basic facts: $y = \tanh(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$ and $\tanh'(x) = 1 - y^2$

- $J_{\boldsymbol{h}^{(t)}}\left(\boldsymbol{h}^{(t+1)}\right)_{i,j} = \frac{\partial \boldsymbol{h}_i^{(t+1)}}{\partial \boldsymbol{h}_j^{(t)}} = \frac{\partial}{\partial \boldsymbol{h}_j^{(t)}} \tanh\left(\boldsymbol{a}_i^{(t+1)}\right) = \tanh'\left(\boldsymbol{a}_i^{(t+1)}\right) \boldsymbol{W}_{i,j} = \left(1 - \left(\boldsymbol{h}_i^{(t+1)}\right)^2\right) \boldsymbol{W}_{i,j}$

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

- $\left(J_{\boldsymbol{h}^{(t)}}\left(\boldsymbol{h}^{(t+1)}\right) J_{\boldsymbol{h}^{(t+1)}}(\ell)\right)_i = \sum_j J_{\boldsymbol{h}^{(t)}}\left(\boldsymbol{h}^{(t+1)}\right)_{i,j} J_{\boldsymbol{h}^{(t+1)}}(\ell)_j$

$$= \sum_j \frac{\partial \boldsymbol{h}_i^{(t+1)}}{\partial \boldsymbol{h}_j^{(t)}} J_{\boldsymbol{h}^{(t+1)}}(\ell)_j$$

$$= \sum_j \left(1 - \left(\boldsymbol{h}_i^{(t+1)}\right)^2\right) \boldsymbol{W}_{i,j} J_{\boldsymbol{h}^{(t+1)}}(\ell)_j$$

$$= \sum_j \left(\boldsymbol{D}_{\boldsymbol{h}^{(t+1)}} \boldsymbol{W}\right)_{i,j} J_{\boldsymbol{h}^{(t+1)}}(\ell)_j$$

$$\Rightarrow J_{\boldsymbol{h}^{(t)}}\left(\boldsymbol{h}^{(t+1)}\right) J_{\boldsymbol{h}^{(t+1)}}(\ell) = \boldsymbol{D}_{\boldsymbol{h}^{(t+1)}} \boldsymbol{W} J_{\boldsymbol{h}^{(t+1)}}(\ell)$$

Exploding and vanishing gradients

- RNNs are known to have an issue with exploding and vanishing gradients
  - Exploding gradients: increase of the norm of the gradient during training
  - Vanishing gradients: vanishing long term contributions

- We explain for an RNN with update equations:

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

  and the loss function

$$\ell = \sum_{t=1}^{T} \ell^{(t)}$$

- Note: we can consider $\boldsymbol{s}^{(t)} = a(\boldsymbol{W}\boldsymbol{s}^{(t-1)} + \boldsymbol{U}\boldsymbol{x}^{(t)} + \boldsymbol{b})$ by using $\boldsymbol{s}^{(t)} := a(\boldsymbol{h}^{(t)})$

Exploding and vanishing gradients (cont'd)

- Let θ denote any of the model parameters $\boldsymbol{W}, \boldsymbol{U}, \boldsymbol{b}$

- The Jacobian of the loss function is given by

$$J_\theta(\ell) = \sum_{t=1}^{T} J_\theta(\ell^{(t)})$$

and

$$J_\theta(\ell^{(t)}) = J_{\boldsymbol{h}^{(t)}}(\ell^{(t)}) J_\theta(\boldsymbol{h}^{(t)}) = J_{\boldsymbol{h}^{(t)}}(\ell^{(t)}) \sum_{s=1}^{t} \underbrace{J_{\boldsymbol{h}^{(s)}}(\boldsymbol{h}^{(t)}) J_\theta(\boldsymbol{h}^{(s)})}$$

contributions: long term $s \ll t$
short term $s \approx t$

- By the chain rule

$$J_{\boldsymbol{h}^{(s)}}(\boldsymbol{h}^{(t)}) = \prod_{r=s+1}^{t} J_{\boldsymbol{h}^{(r-1)}}(\boldsymbol{h}^{(r)}) = \prod_{r=s+1}^{t} \boldsymbol{W} \operatorname{diag}(a'(\boldsymbol{h}^{(r-1)}))$$

Special case: $\boldsymbol{a}$ identity mapping

- For a being the identity mapping, we have

$$J_{\boldsymbol{h}^{(s)}}\left(\boldsymbol{h}^{(t)}\right) = \boldsymbol{W}^{t-s}$$

- If the spectral radius $\rho(\boldsymbol{W})$ of $\boldsymbol{W}$ is such that

$$\rho(\boldsymbol{W}) < 1$$

  then the long term components vanish

- Condition $\rho(\boldsymbol{W}) > 1$ is necessary for exploding gradients

General case

- Assume that a is such that $\left\|\mathrm{diag}(a'(\boldsymbol{h}^{(s)}))\right\| \leq \gamma$

- Then, we have

$$\left\|J_{\boldsymbol{h}^{(r)}}(\boldsymbol{h}^{(r-1)})\right\| \leq \|\boldsymbol{W}\| \left\|\mathrm{diag}\left(a'(\boldsymbol{h}^{(r)})\right)\right\| \leq \rho(\boldsymbol{W})\gamma$$

  and, thus,

$$\left\|J_{\boldsymbol{h}^{(s)}}(\boldsymbol{h}^{(t)})\right\| \leq (\rho(\boldsymbol{W})\gamma)^{t-s}$$

- If $\rho(\boldsymbol{W}) < 1/\gamma$, then vanishing gradients occur

Strategies for multiple time scales

- Adding skip connections through time

- Leaky units

- Removing connections

Vector to sequence RNN models

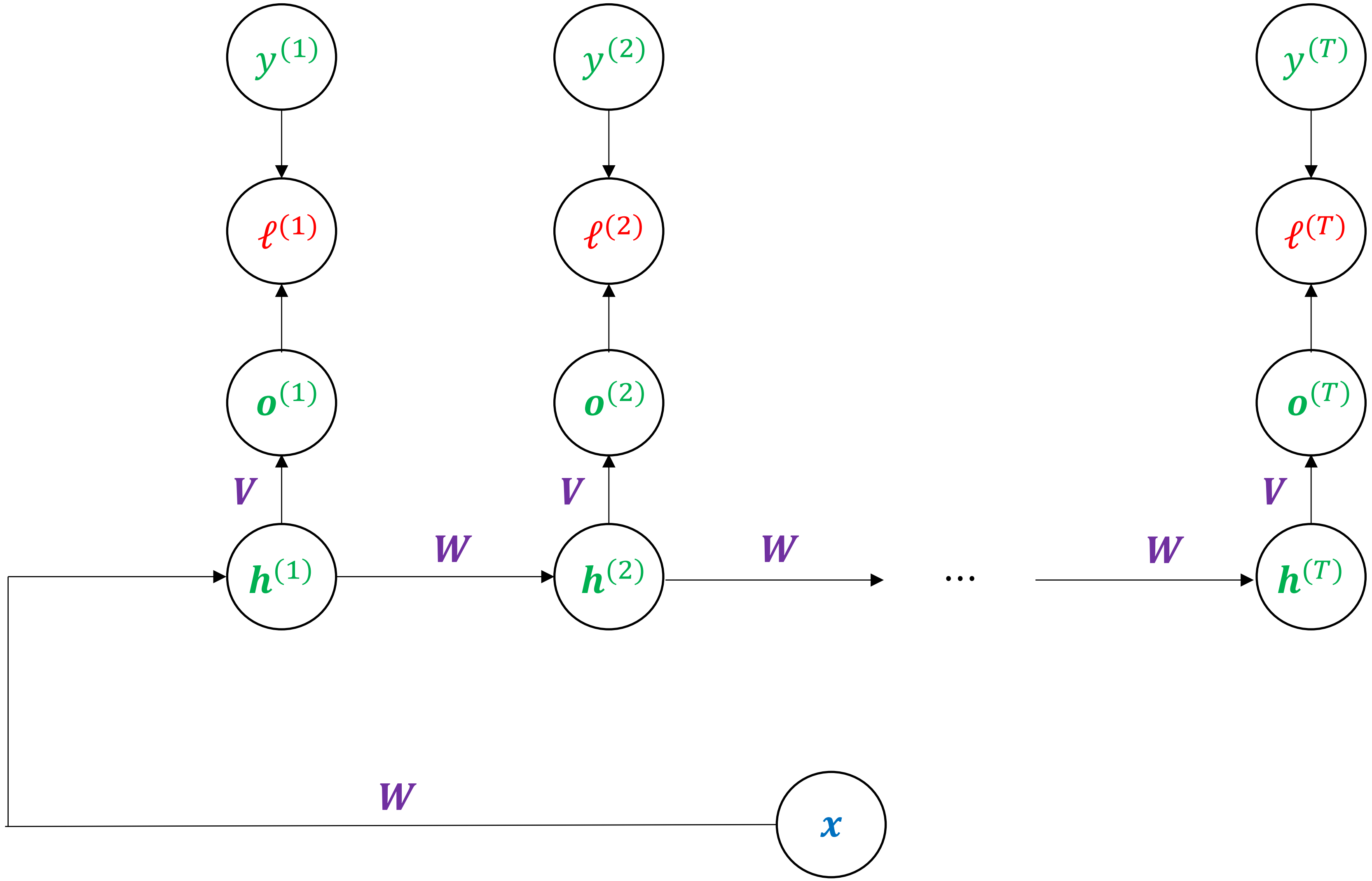
Input: a vector of a fixed dimension $\boldsymbol{x} \longrightarrow \boxed{} \longrightarrow \boldsymbol{y}^{(1)}, \ldots, \boldsymbol{y}^{(T)}$ **Output**: a sequence of some length

- Example applications:
  - Image captioning
  - A module for sequence-to-sequence models

A bird flies over the water

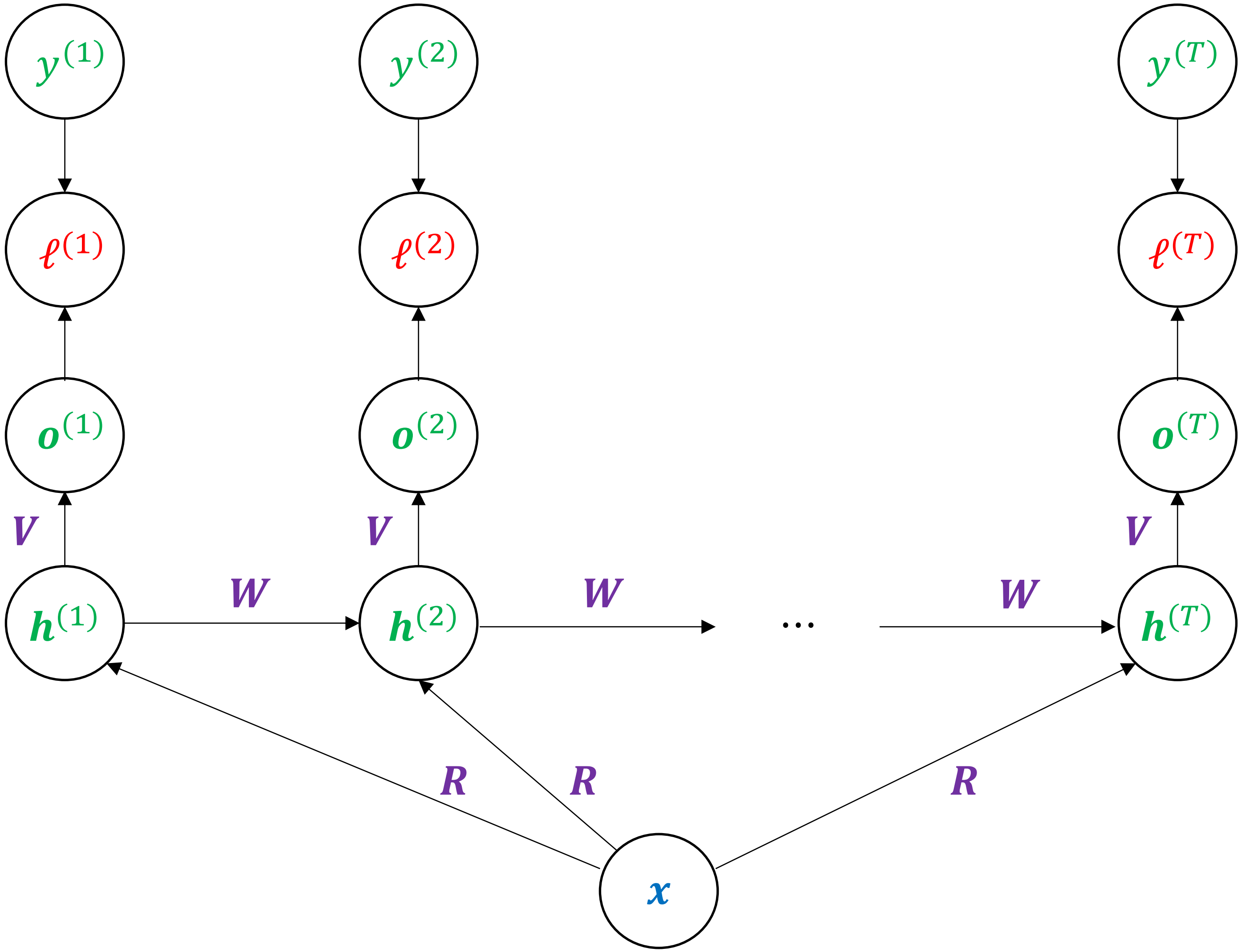
- Common approaches based on using a standard RNN:
  1. Initialize hidden state $\boldsymbol{h}^{(0)}$ to input vector $\boldsymbol{x}$
  2. Feed input vector $\boldsymbol{x}$ as input at each time step
  3. Combine both

Approach 1



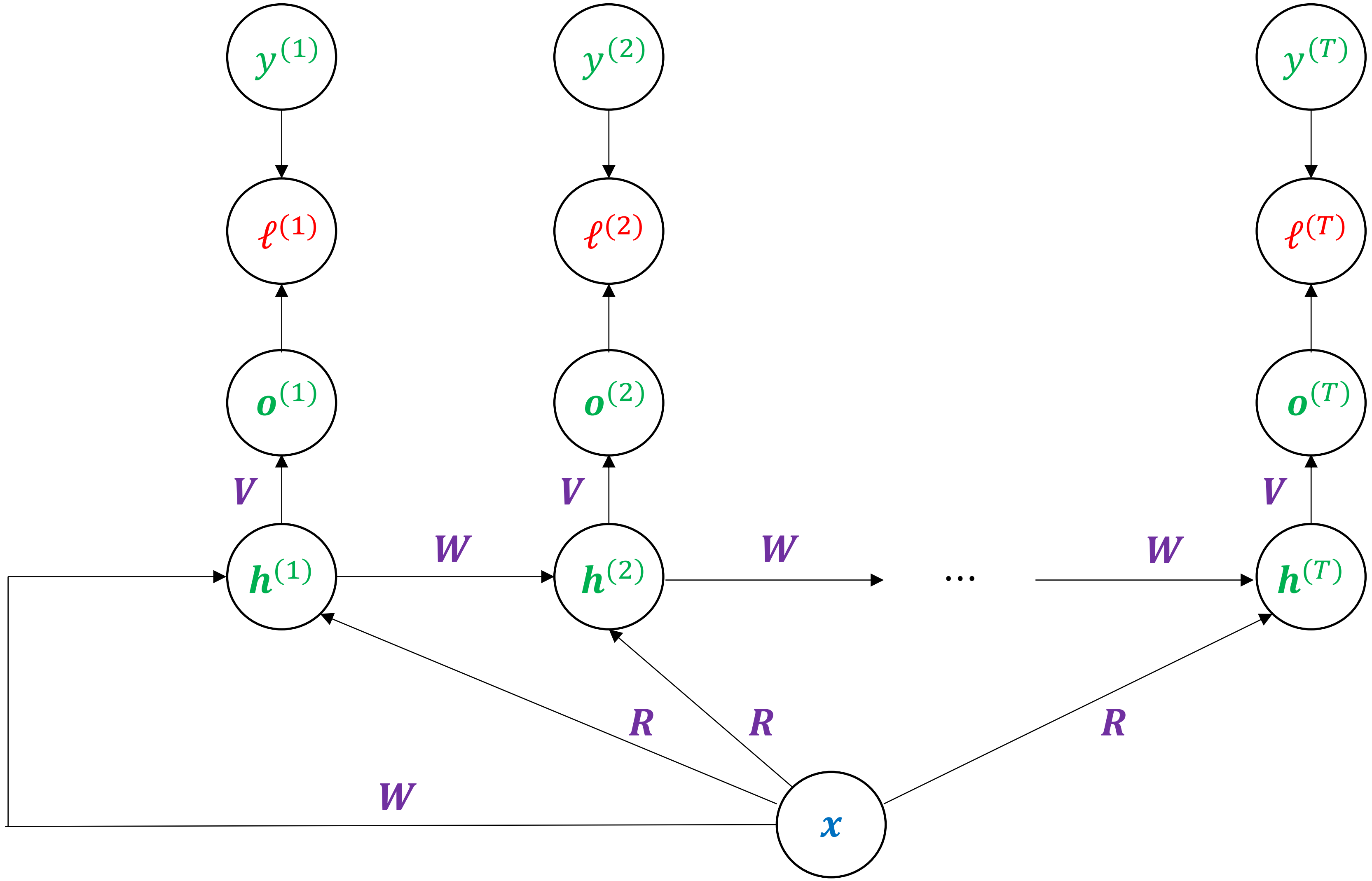
$y^{(1)}$
$y^{(2)}$
$y^{(T)}$
$\ell^{(1)}$
$\ell^{(2)}$
$\ell^{(T)}$
$\boldsymbol{o}^{(1)}$
$\boldsymbol{o}^{(2)}$
$\boldsymbol{o}^{(T)}$
$\boldsymbol{V}$
$\boldsymbol{V}$
$\boldsymbol{V}$
$\boldsymbol{h}^{(1)}$
$\boldsymbol{W}$
$\boldsymbol{h}^{(2)}$
$\boldsymbol{W}$
…
$\boldsymbol{W}$
$\boldsymbol{h}^{(T)}$
$\boldsymbol{W}$
$\boldsymbol{x}$

Approach 2



$y^{(1)}$
$y^{(2)}$
$y^{(T)}$
$\ell^{(1)}$
$\ell^{(2)}$
$\ell^{(T)}$
$\boldsymbol{o}^{(1)}$
$\boldsymbol{o}^{(2)}$
$\boldsymbol{o}^{(T)}$
$\boldsymbol{V}$
$\boldsymbol{V}$
$\boldsymbol{V}$
$\boldsymbol{h}^{(1)}$
$\boldsymbol{W}$
$\boldsymbol{h}^{(2)}$
$\boldsymbol{W}$
$\cdots$
$\boldsymbol{W}$
$\boldsymbol{h}^{(T)}$
$\boldsymbol{R}$
$\boldsymbol{R}$
$\boldsymbol{R}$
$\boldsymbol{x}$

Approach 3



$y^{(1)}$
$y^{(2)}$
$y^{(T)}$
$\ell^{(1)}$
$\ell^{(2)}$
$\ell^{(T)}$
$\boldsymbol{o}^{(1)}$
$\boldsymbol{o}^{(2)}$
$\boldsymbol{o}^{(T)}$
$\boldsymbol{V}$
$\boldsymbol{V}$
$\boldsymbol{V}$
$\boldsymbol{h}^{(1)}$
$\boldsymbol{W}$
$\boldsymbol{h}^{(2)}$
$\boldsymbol{W}$
...
$\boldsymbol{W}$
$\boldsymbol{h}^{(T)}$
$\boldsymbol{R}$
$\boldsymbol{R}$
$\boldsymbol{R}$
$\boldsymbol{W}$
$\boldsymbol{x}$

Bidirectional RNNs

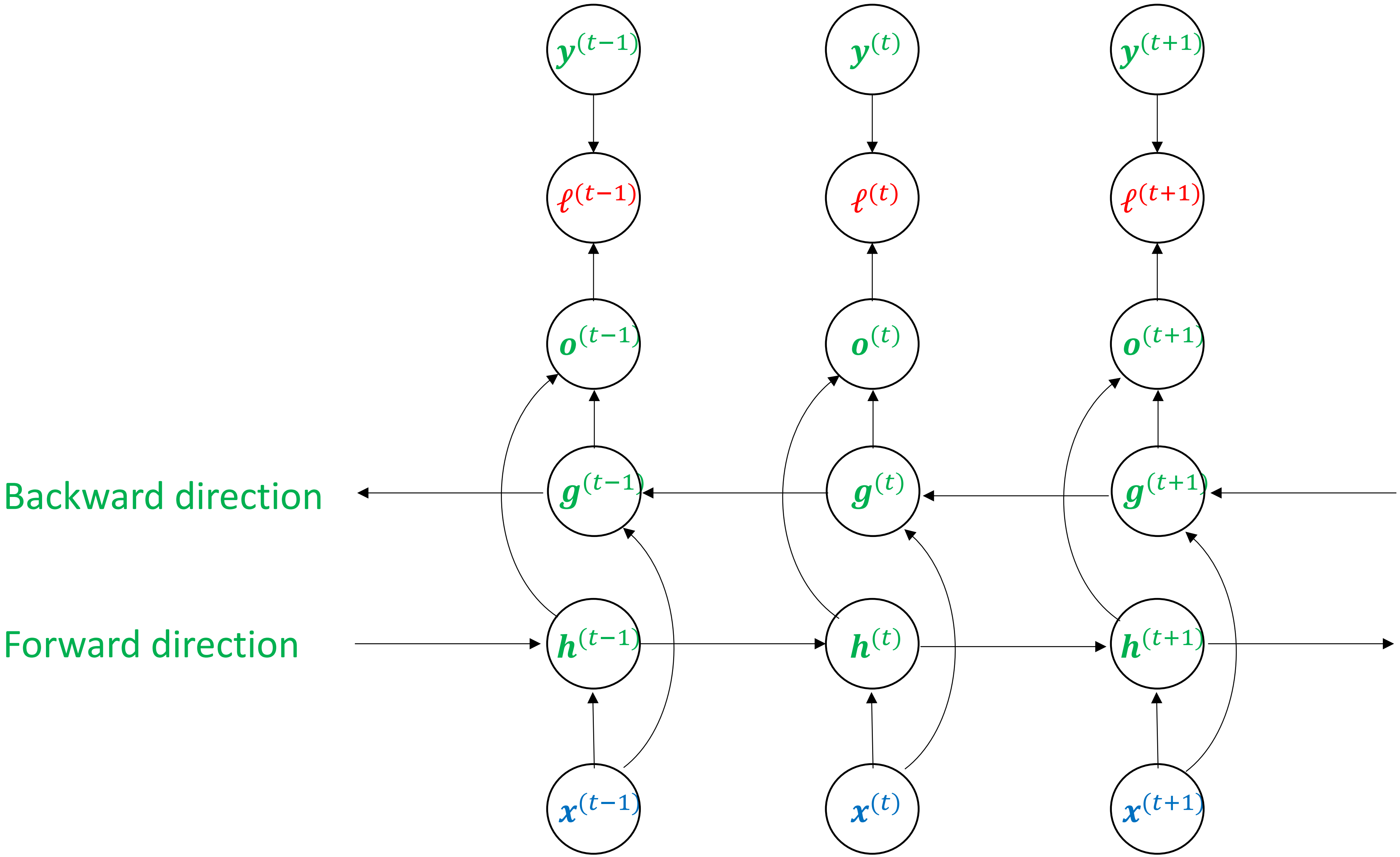
- Bidirectional RNNs: output predictions depend on the whole input sequence

- Example use cases:
  - Speech recognition: interpretation of a phoneme may depend on the next few phonemes (co-articulation) or even next few words (linguistic dependencies)
  - Handwriting recognition
  - Bioinformatics

- Introduced by Schuster and Paliwan 1997

- Key idea: combine two RNNs
  - One having connections forward in time
  - Other having connections backward in time

Common bidirectional RNN architecture



Gated RNNs

Gated RNNs: key ideas

- Create paths through time along which derivatives of parameters neither vanish nor explode

- Connection weights may change at each time step

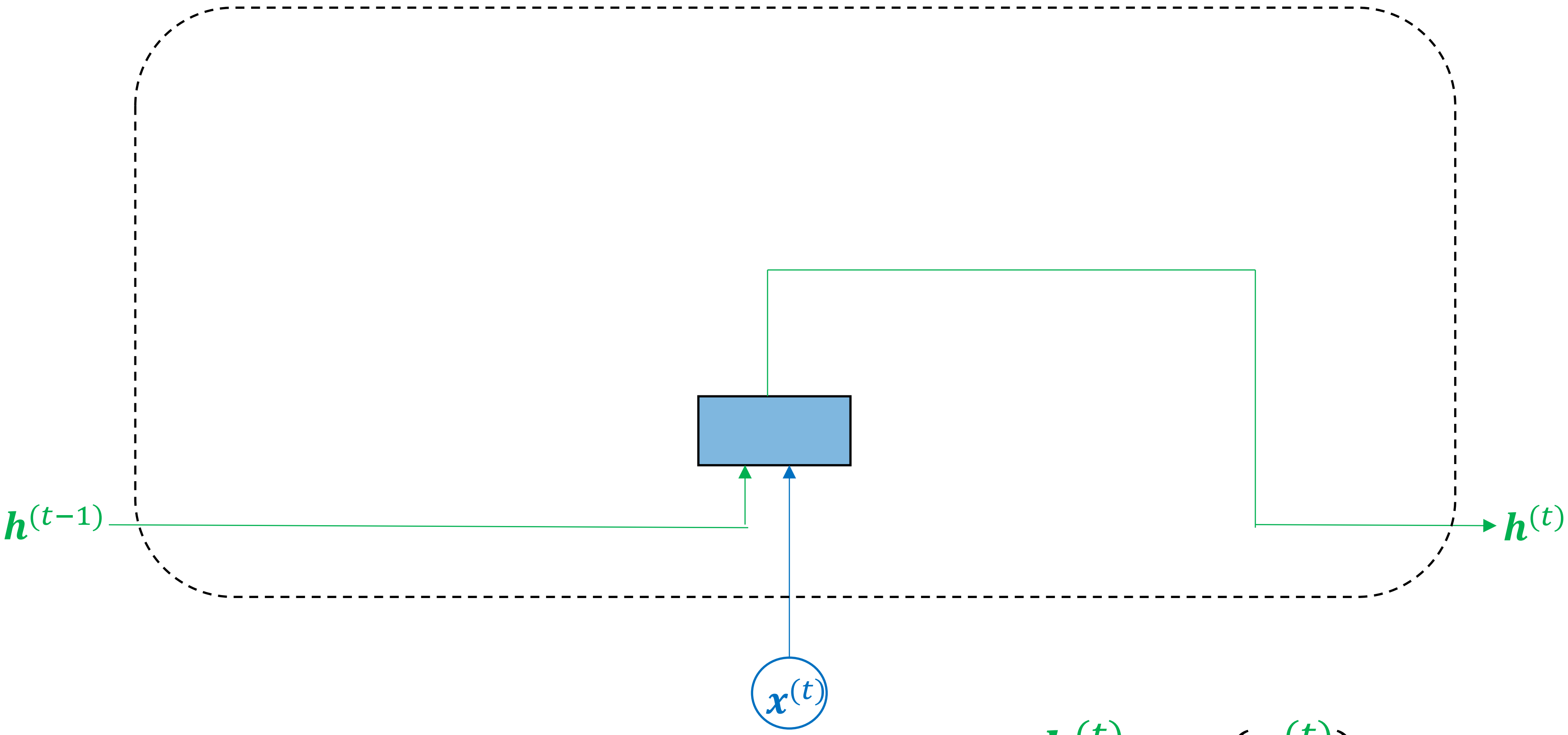
Long Short-Term Memory (LSTM)

- Key idea: self-loops creating paths where the gradient can flow for long durations
    - Weights of the self-loop are gated, i.e. controlled by another hidden unit
    - This allows to change the timescale of integration
- Introduced by Hochreiter and Scmidhuber (1997), self-loops weights conditioned on the context Gers et al (2000)
- Shown to learn long-term dependencies more easily than simple RNNs

LSTM applications

- Unconstrained handwriting recognition
- Speech recognition
- Handwriting generation
- Machine translation
- Image captioning
- Parsing

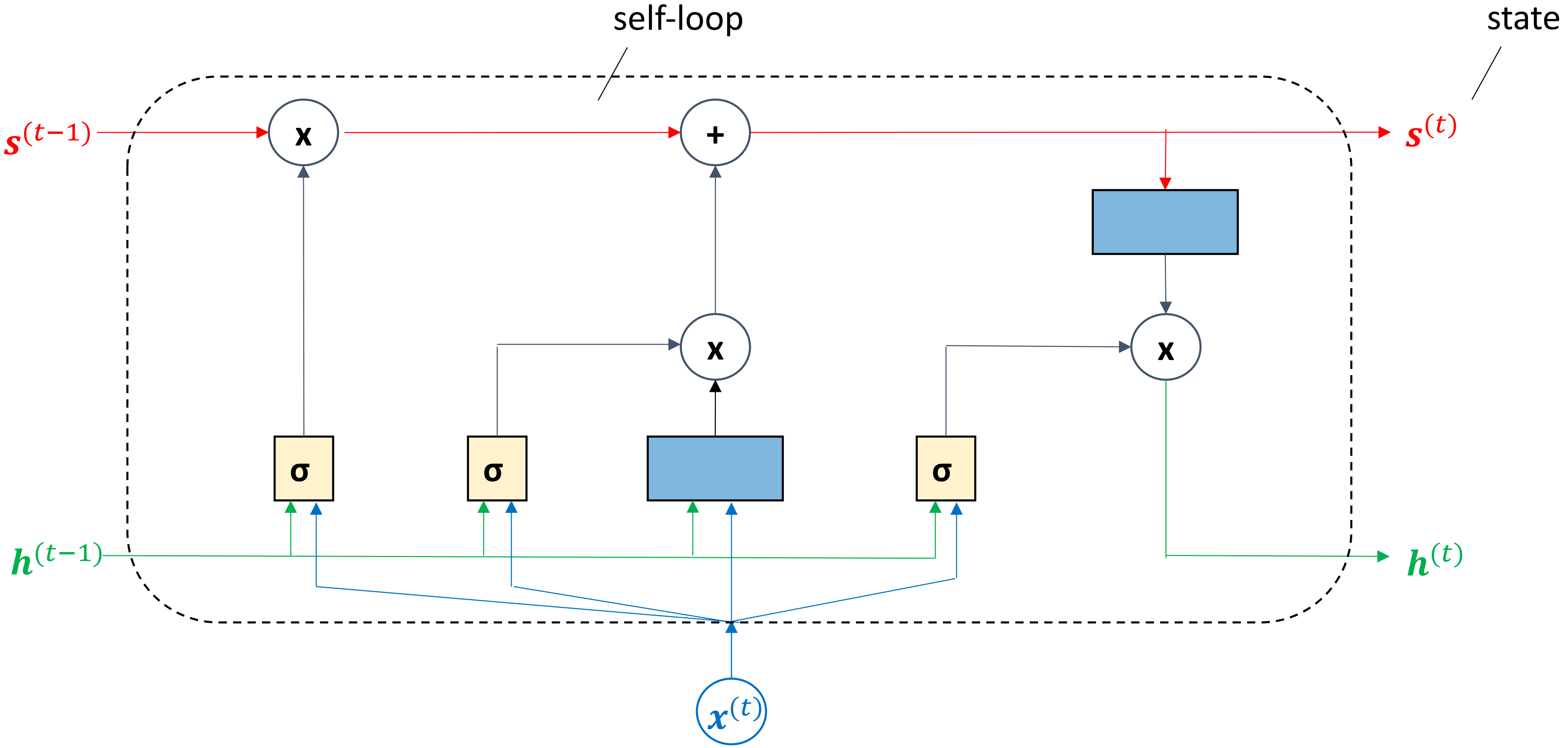
Basic RNN cell



$$h^{(t)} = a(a^{(t)})$$

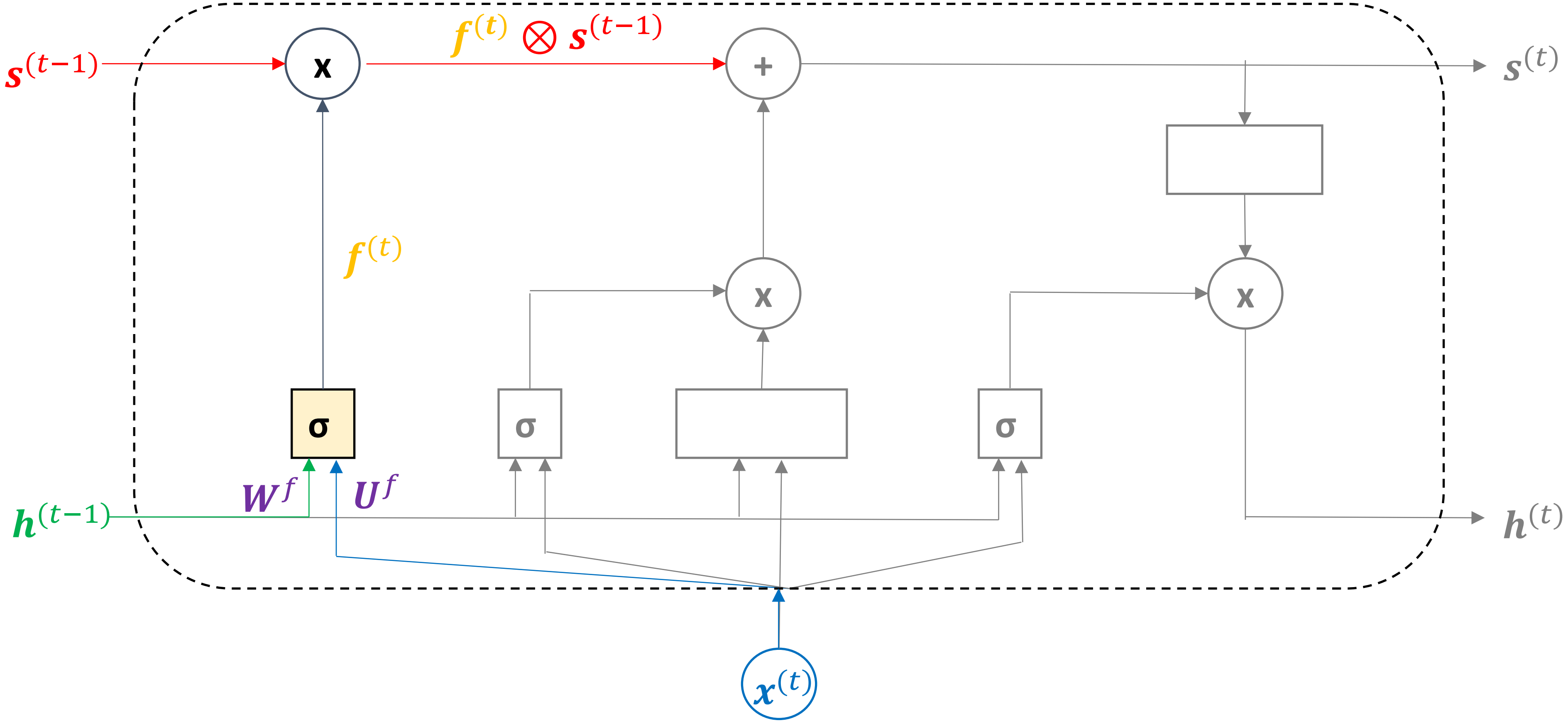
$$a^{(t)} = Wh^{(t-1)} + Ux^{(t)} + b$$

LSTM cell



σ gating units control the flow of information (σ denotes sigmoid function)

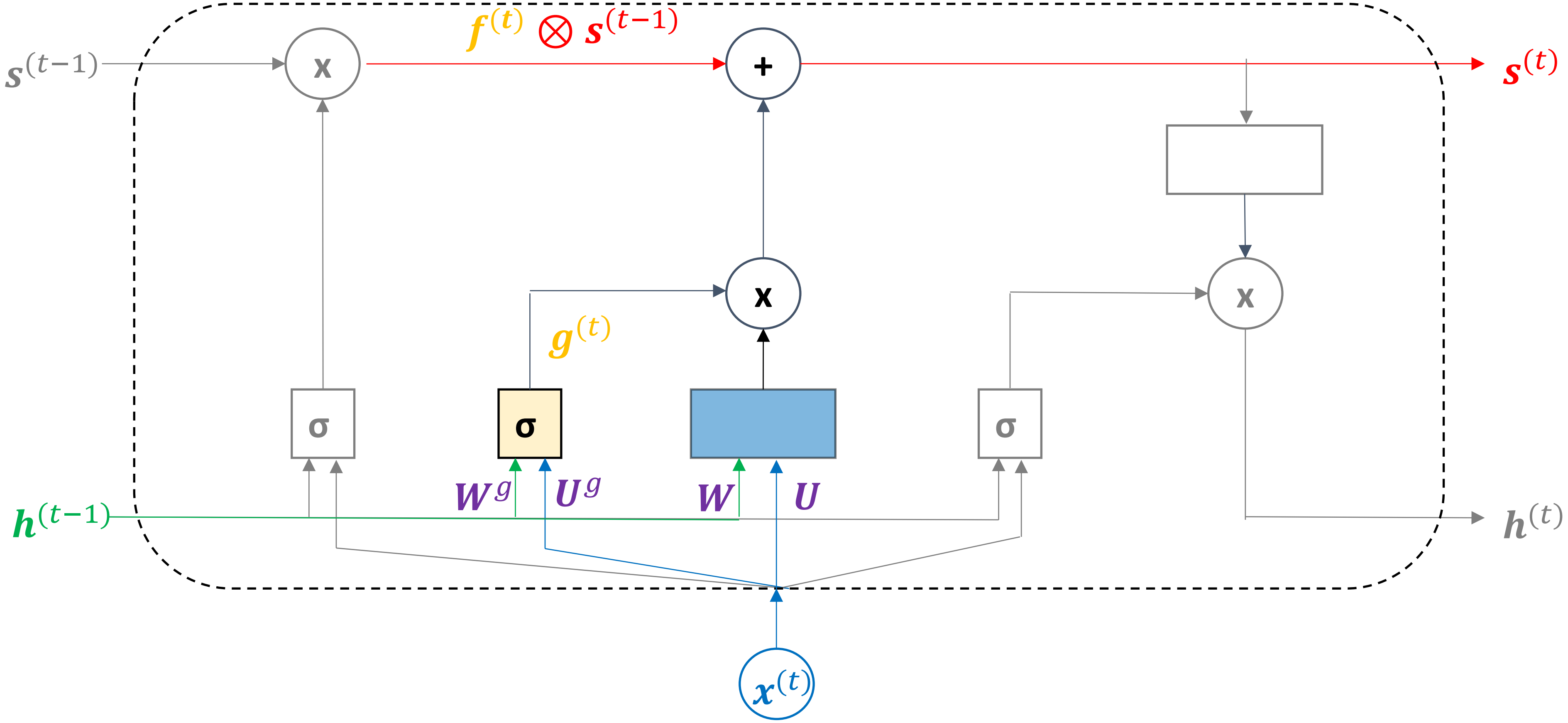
Forget gate



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

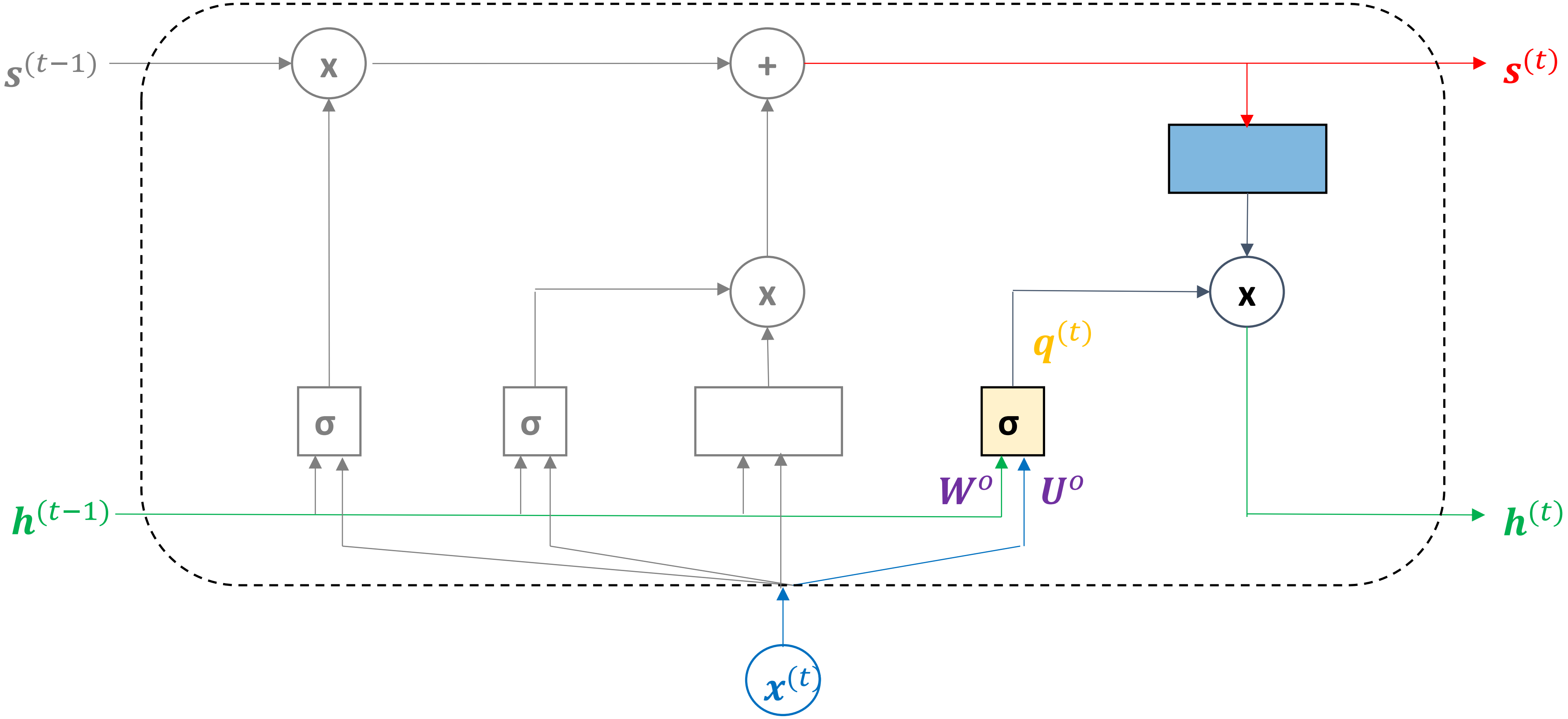
- Def. for two vectors x and y: $x \otimes y = (x_1 y_1, \dots, x_n y_n)^\top$

Input gate



- $g^{(t)} = \sigma(U^g x^{(t)} + W^g h^{(t-1)} + b^g)$
- $s^{(t)} = f^{(t)} \otimes s^{(t-1)} + g^{(t)} \otimes a(Ux^{(t)} + Wh^{(t-1)} + b)$

Output gate



- $q^{(t)} = \sigma(U^o x^{(t)} + W^o h^{(t-1)} + b^o)$
- $h^{(t)} = a\left(s^{(t)}\right) \otimes q^{(t)}$

Gated recurrent unit (GRU) [Cho et al, 2014]

- GRU cell update equations:

$$\boldsymbol{h}^{(t)} = \boldsymbol{u}^{(t)} \otimes \boldsymbol{h}^{(t-1)} + \left(1 - \boldsymbol{u}^{(t)}\right) \otimes a\left(\boldsymbol{U}\boldsymbol{x}^{(t)} + \boldsymbol{W}\left(\boldsymbol{r}^{(t)} \otimes \boldsymbol{h}^{(t-1)}\right) + \boldsymbol{b}\right)$$

$$\boldsymbol{u}^{(t)} = \sigma\left(\boldsymbol{U}^{u}\boldsymbol{x}^{(t)} + \boldsymbol{W}^{u}\boldsymbol{h}^{(t-1)} + \boldsymbol{b}^{u}\right)$$

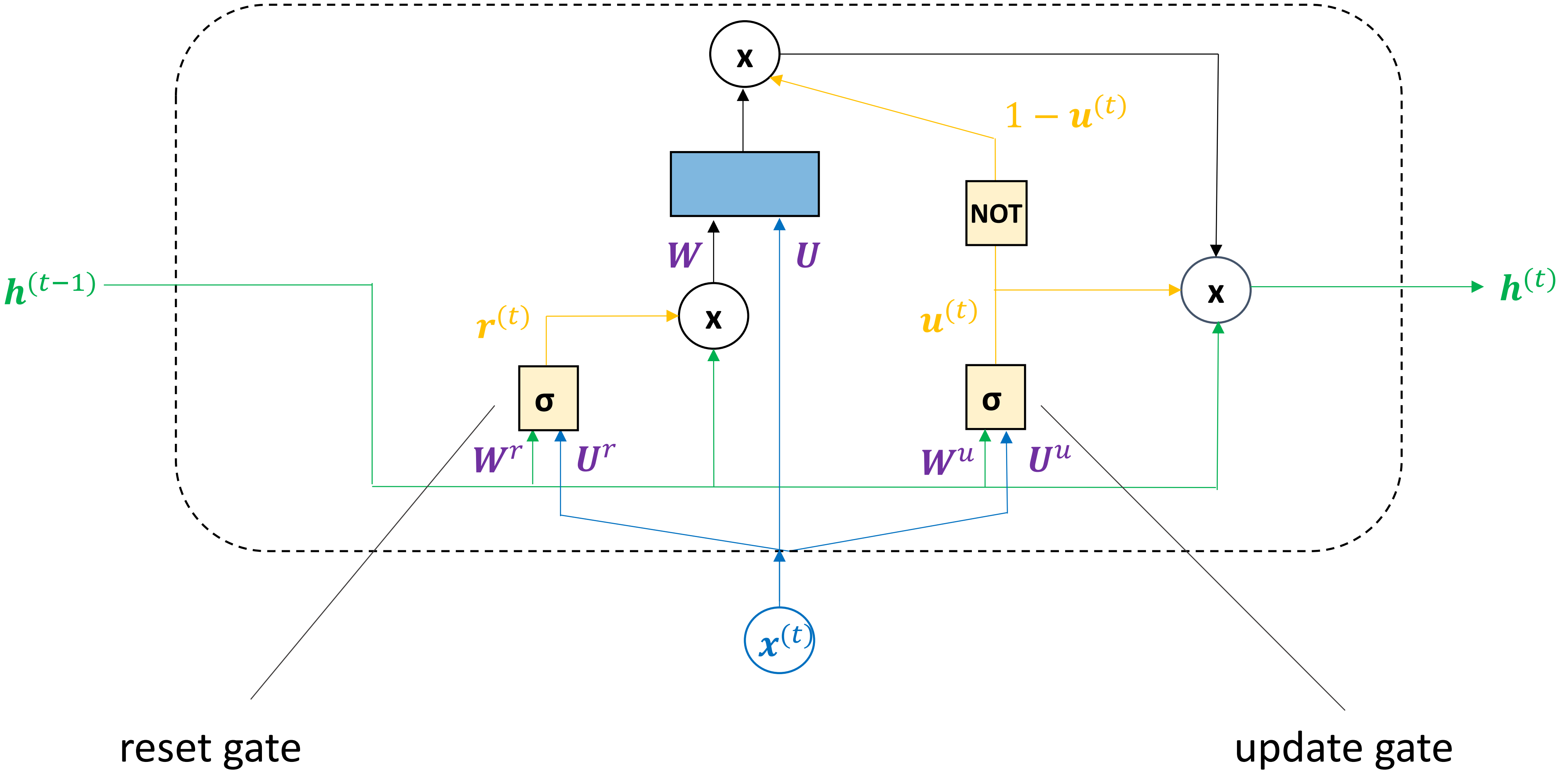
update gate

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

reset gate

- Each hidden unit has separate update and reset gates
  - Short-term dependencies captured by frequently active reset gate
  - Long-term dependencies captured by frequently active update gate

GRU network architecture



Sequence transduction models

Sequence transduction models

- Sequence transduction: mapping an input sequence to an output sequence
  - Input and output sequence are not necessarily of the same length

- Applications:
  - Machine translation, e.g. English to German, Chinese to English
  - Speech recognition
  - Question answering

- Common approach: encoder-decoder architecture
  - Also referred to as a sequence-to-sequence architecture

Encoder-decoder architecture

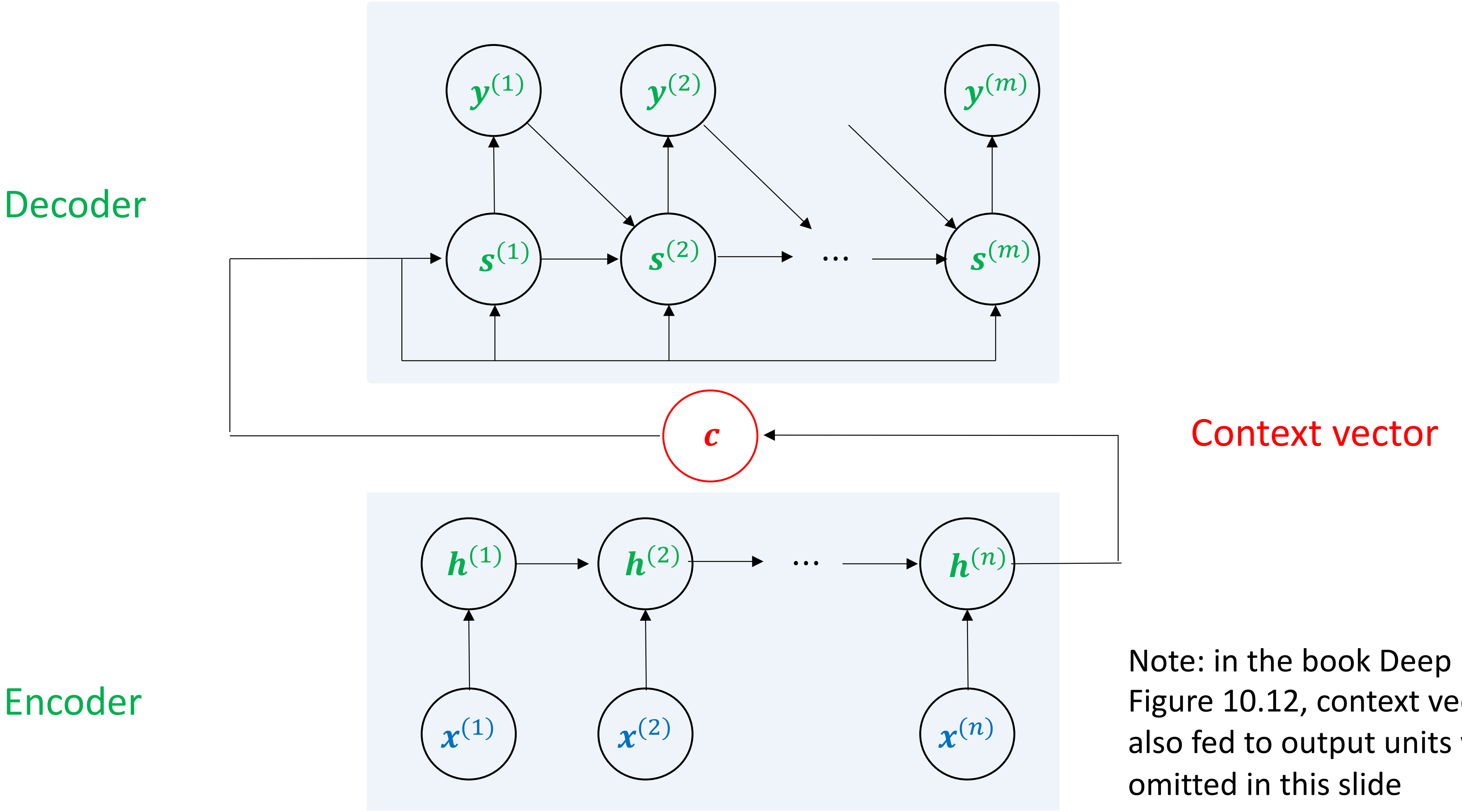
- Encoder-decoder architecture:
  - Encoder [reader | input] RNN
  - Decoder [writer | output] RNN connected with a context

- Encoder RNN: processes the input sequence and outputs a context representation
  - Context is usually a simple function of final hidden state

- Decoder RNN: maps a fixed-length context vector to an output sequence

- Example: neural machine translation
  - Encoder encodes a source sentence into a fixed-length vector from which decoder generates a translation

Standard encoder-decoder architecture



Note: in the book Deep Learning, Figure 10.12, context vectors are also fed to output units which is omitted in this slide

Jointly learning to align and translate [Bahdanau et al 2015]

- Using a fixed-length context vector may be a bottleneck
  - Potential difficulty for long sequences
  - Especially for sequences longer than observed in the training data
- Proposed solution: use an attention mechanism for soft-selection of parts of input sequence that are relevant for predicting a target output element
  - Alleviates having to form these parts as a hard segment explicitly

Alignment model

- Context vector for output at position i: $\boldsymbol{c}^{(i)} = \sum_{j=1}^{n} \alpha_{i,j} \boldsymbol{h}^{(j)}$ where

$$\alpha_{i,j} = \frac{e^{e_{i,j}}}{\sum_{k=1}^{n} e^{e_{i,k}}}$$

  are the attention weights with

$$e_{i,j} = f_\theta(\boldsymbol{s}^{(i-1)}, \boldsymbol{h}^{(j)})$$

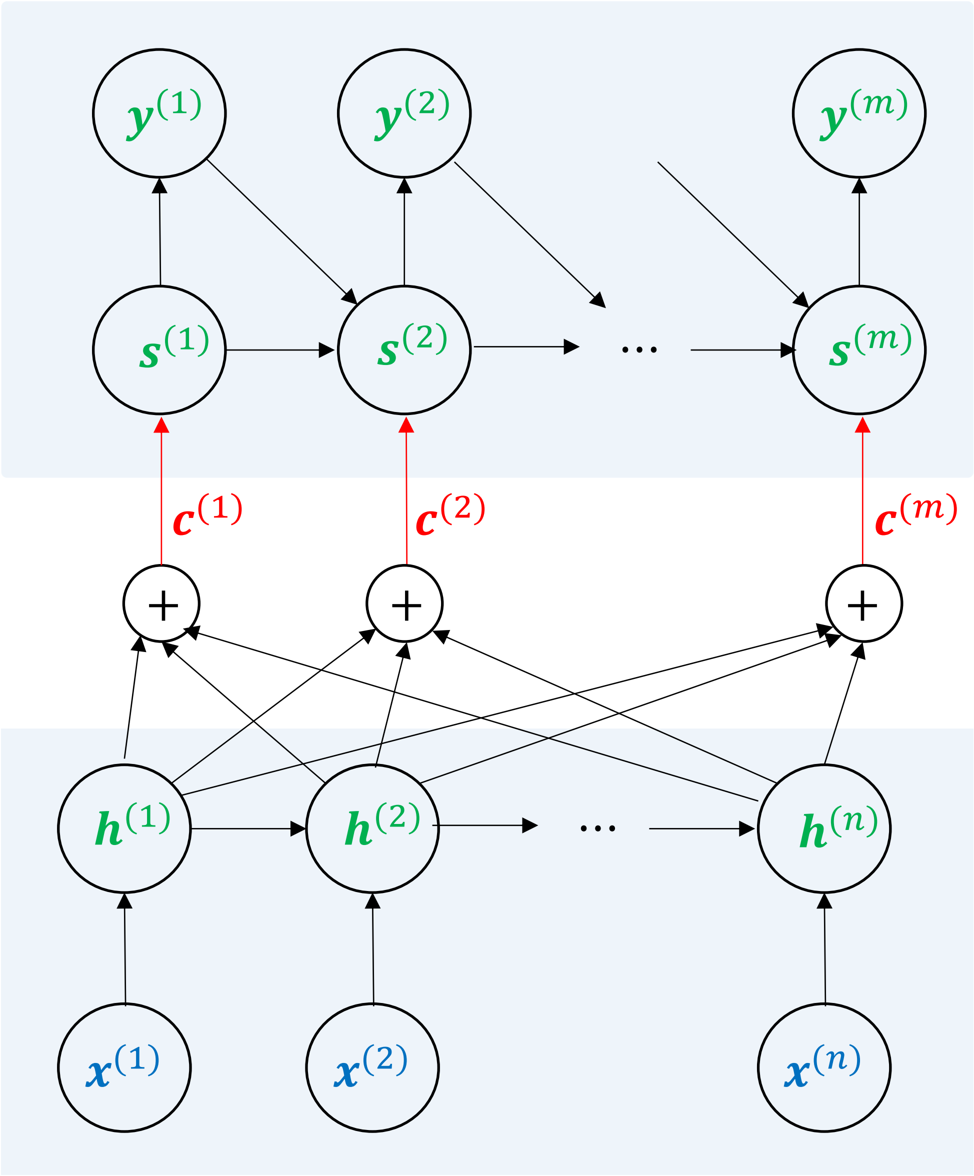
  quantifying how well the input at position j and output at position i match

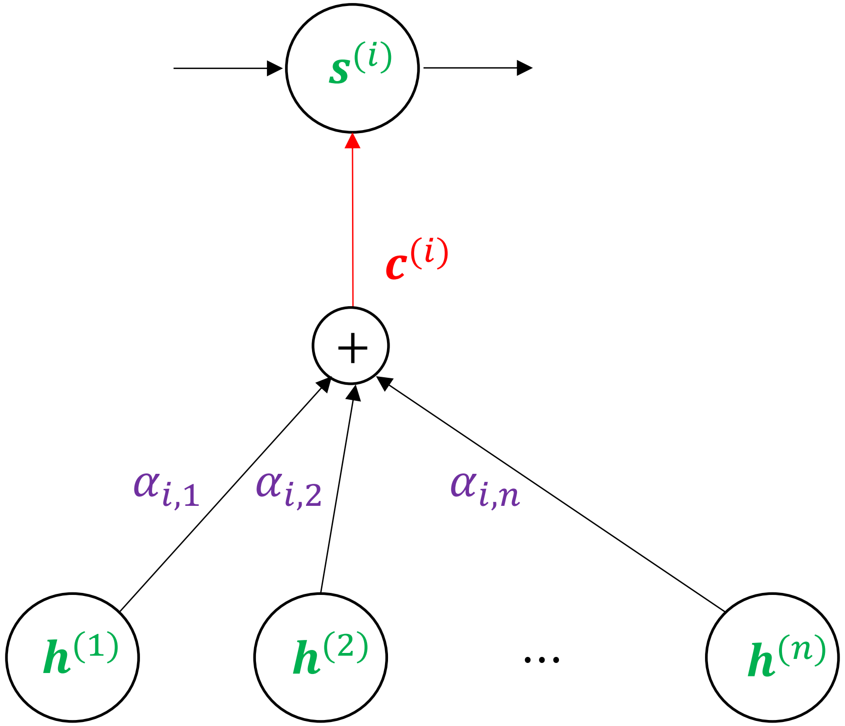
- Here f_θ an alignment function, parametrized as a feedforward neural network which is jointly trained with all other components of the network

Encoder-decoder architecture with alignment

Decoder

Encoder



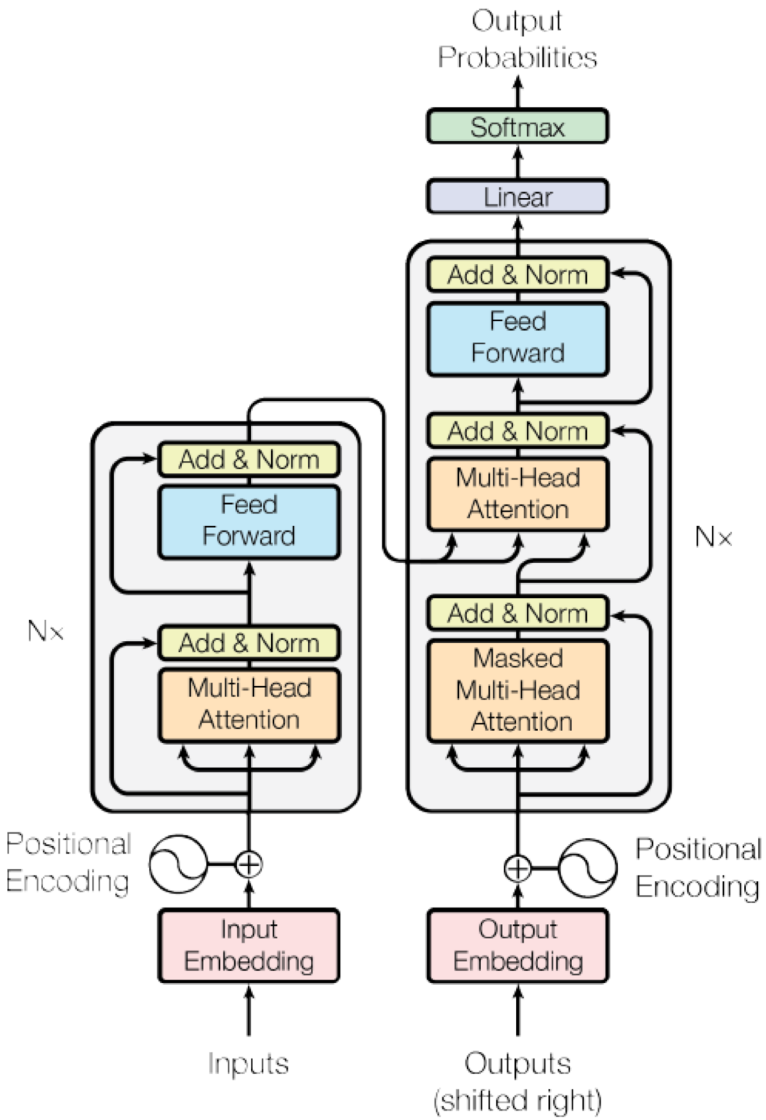


Transformer architecture

[Vaswani et al, 2017]

- An encoder-decoder architecture with
  - An attention mechanism
  - A stack of fully connected layers

- No recurrent neural networks
- Fast training: allows for parallelization

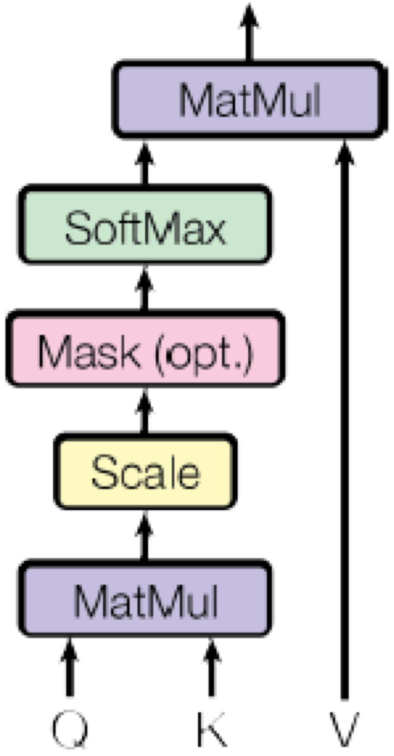


Attention module

- Attention based on scalar dot-product

- Input:
    - $\boldsymbol{Q}$ query vectors of dimension d_k
    - $\boldsymbol{K}$ key vectors of dimension d_k
    - $\boldsymbol{V}$ value vectors of dimension d_v

- Output:

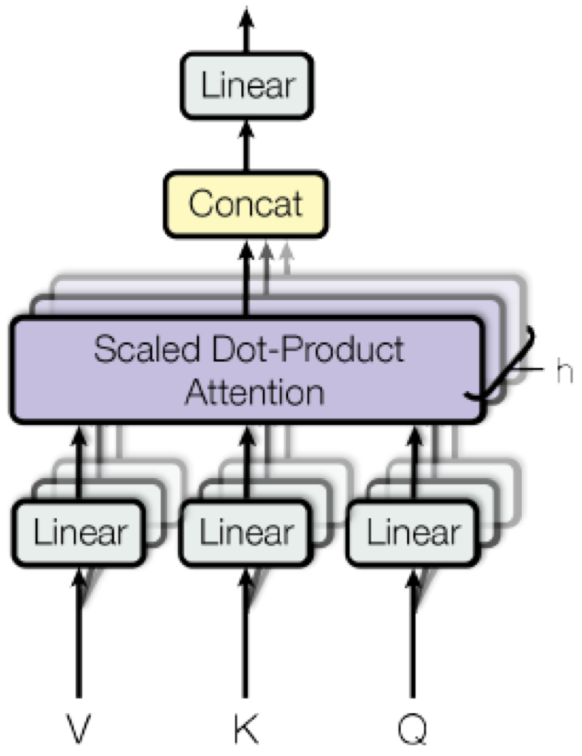


$$\text{Attention}(\boldsymbol{Q}, \boldsymbol{K}, \boldsymbol{V}) = \text{softmax}\left(\frac{\boldsymbol{Q}\boldsymbol{K}^\top}{\sqrt{d_k}}\right)\boldsymbol{V}$$

$1/\sqrt{d_k}$ normalization to control the skew of softmax

Attention module

- Multi-head attention



$$\text{MultiHead}(\boldsymbol{Q}, \boldsymbol{K}, \boldsymbol{V}) = \text{Concat}(\text{head}_1, \dots, \text{head}_h)\boldsymbol{W}^o$$

$$\text{head}_i = \text{Attention}\left(\boldsymbol{Q}\boldsymbol{W}_i^Q, \boldsymbol{K}\boldsymbol{W}_i^K, \boldsymbol{V}\boldsymbol{W}_i^V\right)$$

where $\boldsymbol{W}_i^Q \in \mathbf{R}^{d \times d_k}$, $\boldsymbol{W}_i^K \in \mathbf{R}^{d \times d_k}$, $\boldsymbol{W}_i^V \in \mathbf{R}^{d \times d_v}$ are parameters

Use of attention modules

- Encoder-decoder attention layer
  - Queries come from the previous decoder layer, keys and values come from the output of the encoder
  - This mimics typical encoder-decoder attention mechanism in sequence to sequence models
- Encoder self-attention layer
  - Each position in the encoder can attend to all positions in the previous layer of the encoder
- Decoder self-attention layer
  - Each position in the decoder can attend to all position in the decoder up to and including that position (to ensure auto-regressive property)
  - Implemented by masking (setting input values to softmax to $-\infty$)

Feedforward network module

- Feedforward network module applied to each position separately and identically

- Two linear transformations with a ReLU activation in between:

$$\mathrm{FFN}(\boldsymbol{x}) = \mathrm{ReLU}(\boldsymbol{x}\boldsymbol{W}^{(1)} + \boldsymbol{b}^{(1)})\boldsymbol{W}^{(2)} + \boldsymbol{b}^{(2)}$$

- Parameter are different for different layers

- Dimensions of input and outputs are 512

- The inner layer has dimensionality of 2048

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Error metrics

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Seminar exercises

- Text generation using an RNN

Appendix

Performance metrics

Word error rate (WER)

- A common metric of the performance of a speech recognition or a machine translation system

- Word error rate of a candidate text for given reference text:

$$\text{WER} = \frac{S+D+I}{N}$$

- N = number of words in the reference
- S = number of substitutions to transform the reference text to the candidate text
- D = number of deletions to transform the reference text to the candidate text
- C = number of correct words

- Note: $N = S + D + C$

Translation error rate (TER)

- An error metric for machine translation that measures the number of edits required to change an output into one of given references

- Introduced by [Snover et al 2006]

- http://www.cs.umd.edu/~snover/tercom/

BLEU (bilingual evaluation understudy)

- An error metric for automatic evaluation of machine translation [Papineni et al, 2002]
- Addresses the requirements:
  - Computation efficiency (to enable quick experimentation)
  - Language independency
  - High correlation with human evaluations (the closer a machine translation is to a professional human translation, the better is)
- Uses a numerical translation closeness metric and a corpus of good quality reference human translations
- Translation closeness metric
  - Inspired by word error rate metric used by the speech recognition community
  - Main idea: use a weighted average of variable length phrase matches against reference translations

Standard unigram precision

- Standard unigram precision: number of candidate translation words (unigrams) which occur in any reference translation divided by the total number words in the candidate translation

- Example:
  - Candidate: the the the the the the the.
  - Reference 1: The cat is on the mat.
  - Reference 2: There is a cat on the mat.

- Standard unigram precision = 1
  - Undesired: high precision for common words

Modified n-gram precision

- Modified unigram precision:
  - For each word in the candidate translation, count the maximum number of times the word occurs in a reference translation (referred to as maximum reference count)
  - Clip the count value for each candidate word by its maximum reference count
  - Modified unigram precision: sum of clipped counts for each distinct word in the candidate translation and divide by the total number of words in the candidate translation
- Example (cont'd): modified unigram precision = 2/7

BLEU score

- Modified n-gram precision is defined analogously to modified unigram precision

- BLEU score of a candidate translation:

$$\mathrm{BLEU} = \mathrm{BP}\exp\left(\sum_{n=1}^{N} w_n \log(p_n)\right)$$

brevity penalty

positive weights summing to 1

modified n-gram precision

where

$$\mathrm{BP} = \exp\left(\min\left\{1 - \frac{r}{c}, 0\right\}\right)$$

Effective reference corpus length
= sum of best match lengths for each
candidate sentence in the corpus

length of the candidate translation