Recurrent Neural Networks and Long Short-Term Memory Networks

Deep Learning (ENGG*6600*01)

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Introduction

Introduction

- Before the era of transformers in deep learning, regular neural networks could not process sequences, such as sentences (sequence of words) or speech (sequence of phonemes), properly without any recurrence.
- **Recurrent Neural Network (RNN)**, proposed in [1], is a dynamical system which considers recurrence. In recurrence, the output of a model is fed as input to the model again in the next time step.
- One of the main training algorithms for RNN is **Backpropagation Through Time (BPTT)**, developed by several works [2, 3, 4, 5, 6], which is similar to the backpropagation algorithm [1] but has also chain rule through time.
- There were some problems with **gradient vanishing or explosion for long-term dependencies** in RNN [7, 8]. Several solutions were proposed for this issue, some of which are **close-to-identity weight matrix** [9], **long delays** [10], **leaky units** [11, 12], and **echo state networks** [13, 14].

Introduction

- Sequence modeling requires both **short-term** and **long-term** dependencies.
- For example, consider the sentence "The police is chasing the thief". In this sentence, the words "police" and "thief" are related to each other with **short-term dependency** because they are close to one another in the sequence of words.
- Another example is the sentence "I was born in France. My father was working there for many years during my childhood. My family had a great time there while my father was making money in his business there. That is why I know how to speak French". In this second example, the words "France" and "French" are related to each other with **long-term dependency** because they are far away from one another in the sequence of words.
- That inspired researchers to propose the **Long Short-Term Memory (LSTM)** network to handle both short-term and long-tern dependencies [15, 16].
- Later, **Grated Recurrent Unit (GRU)** was proposed [17] which simplified LSTM to reduce its unnecessary complexity.

Introduction

- RNN and LSTM networks are **causal models** which condition every sequence element on the **previous** elements in the sequence.
- Later researches showed that processing the sequence in **both directions** can perform better for the sequences which can be processed offline; e.g., **if the chunks of sequence can be saved and processed** and the sequence elements should not be processed as a stream [18, 19].
- Therefore, **bidirectional RNN** [20, 21] and **bidirectional LSTM** [18, 19] were proposed to process sequences in both directions.
- The **Embeddings from Language Model (ELMo)** network [22] is a language model which makes use of the bidirectional LSTM.

Recurrent Neural Network

Dynamical System

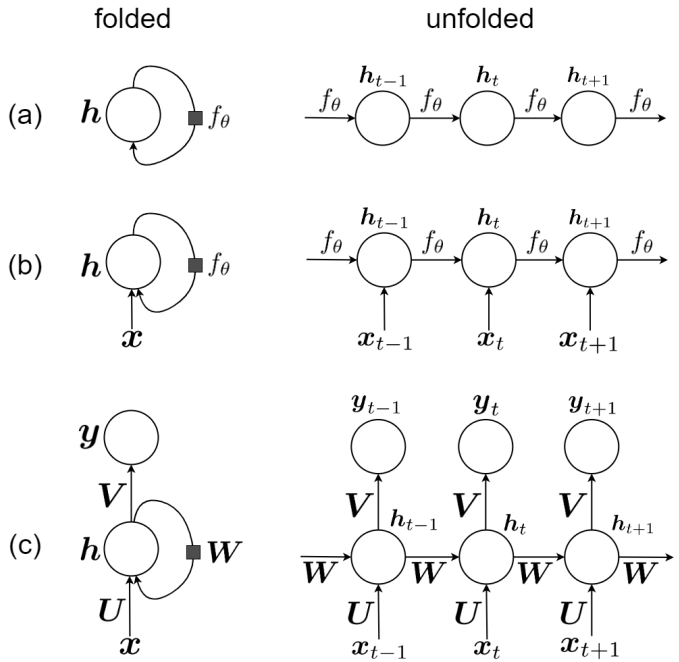
- A dynamical system is recursive and its classical form is as follows:

$$\boldsymbol{h}_t = f_\theta(\boldsymbol{h}_{t-1}), \tag{1}$$

where t denotes the time step, $\boldsymbol{h}_t$ is the state at time t, and $f_\theta(.)$ is a function fixed between the states of all time steps. Dynamical systems are widely used in chaos theory [23].

- We can have a dynamical system with external input signal where $\boldsymbol{x}_t$ denotes the input signal at time t. This system is modeled as:

$$\boldsymbol{h}_t = f_\theta(\boldsymbol{h}_{t-1}, \boldsymbol{x}_t). \tag{2}$$



Parameter Sharing

- The state $\boldsymbol{h}_t$ can be considered as a summary of the past sequence of inputs and states.
- If a different function f_θ is defined for each possible sequence length, the model will not have generalization.
- If the same parameters are used for any sequence length, the model will have generalization properties.
- Therefore, the **parameters are shared** for all lengths and between all states. Such a dynamical system with parameter sharing can be implemented as a neural network with weights. Such a network is called a **Recurrent Neural Network (RNN)**, which was proposed in [1] (1986).

Parameter Sharing

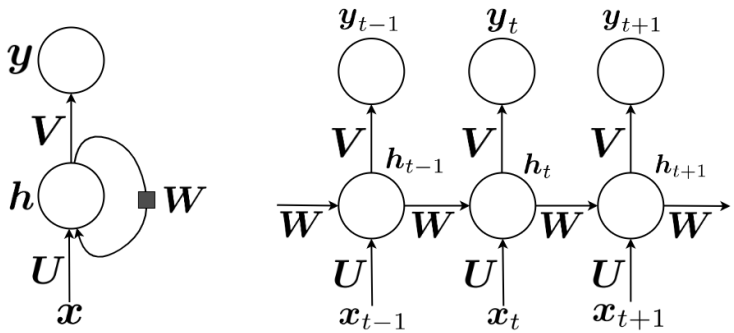
- In RNN, the same weight matrices are used for all time slots.
- RNN gets a sequence as input and outputs a sequence as a decision for a task such as regression or classification.
- Suppose the input, output, and state at time slot t are denoted by $\boldsymbol{x}_t \in \mathbb{R}^d$, $\boldsymbol{y}_t \in \mathbb{R}^q$, and $\boldsymbol{h}_t \in \mathbb{R}^p$, respectively. Let $\boldsymbol{W} \in \mathbb{R}^{p \times p}$ be the weight matrix between states, $\boldsymbol{U} \in \mathbb{R}^{p \times d}$ be the weight matrix between the inputs and the states, and $\boldsymbol{V} \in \mathbb{R}^{q \times p}$ denote the weight matrix between the states and outputs. The bias weights for the state and the output are denoted by $\boldsymbol{b}_i \in \mathbb{R}^p$ and $\boldsymbol{b}_y \in \mathbb{R}^q$, respectively. We have:

$$\mathbb{R}^p \ni \boldsymbol{i}_t = \boldsymbol{W}\boldsymbol{h}_{t-1} + \boldsymbol{U}\boldsymbol{x}_t + \boldsymbol{b}_i, \tag{3}$$

$$[-1,1]^p \ni \boldsymbol{h}_t = \tanh(\boldsymbol{i}_t) = \tanh(\boldsymbol{W}\boldsymbol{h}_{t-1} + \boldsymbol{U}\boldsymbol{x}_t + \boldsymbol{b}_i), \tag{4}$$

$$\mathbb{R}^q \ni \boldsymbol{y}_t = \boldsymbol{V}\boldsymbol{h}_t + \boldsymbol{b}_y, \tag{5}$$

where $\tanh(.) \in (-1,1)$ denotes the hyperbolic tangent function, which is used as an element-wise activation function for the states.

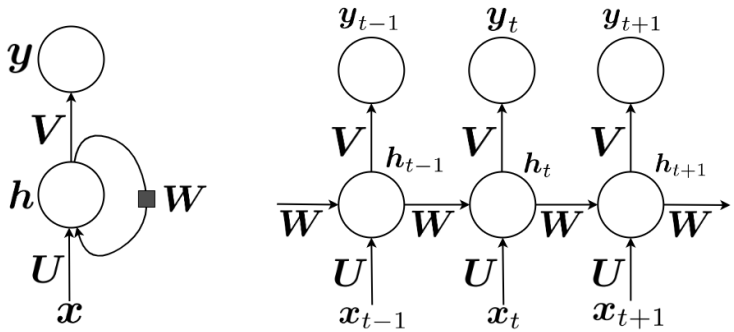


Parameter Sharing

- If there is an activation function, such as softmax, at the output layer, we denote the output of activation function by:

$$\mathbb{R}^q \ni \widehat{\boldsymbol{y}}_t = \text{softmax}(\boldsymbol{y}_t) = \frac{\exp(y_{t,1})}{\sum_{j=1}^{q} \exp(y_{t,j})}, \tag{6}$$

where $y_{t,j}$ denotes the j-th component of $\boldsymbol{y}_t$.



Backpropagation Through Time (BPTT)

Backpropagation Through Time (BPTT)

- One of the methods for training RNN is **Backpropagation Through Time (BPTT)**, which is very similar to the backpropagation algorithm [1] because it is based on gradient descent and chain rule [24], but it has also chain rule through time.
- BPTT was developed by several works [2, 3, 4, 5, 6].
- This algorithm is very solid in theory; however, it does not show the best performance in practice.
- In BPTT, the loss is considered as a summation of loss functions at the previous time steps until now.
- As it is impractical to consider all time steps from the start of training (especially after a long time of training), we only consider the T previous time steps. In other words, we assume that RNN has T-order Markov property [25]. Therefore, the loss function is:

$$\mathbb{R} \ni \mathcal{L} = \sum_{t=1}^{T} \mathcal{L}_t, \tag{7}$$

  where $\mathcal{L}_1$ is the loss function at the current time slot and $\mathcal{L}_t$ denotes the loss function at the previous $(t-1)$ time slot.
- This loss functions needs to be optimized using gradient descent and chain rule. Therefore, we calculate its gradient with respect to the parameters of RNN. These parameters are $\boldsymbol{y}_t$, $\boldsymbol{h}_t$, $\boldsymbol{V}$, $\boldsymbol{W}$, $\boldsymbol{U}$, $\boldsymbol{b}_i$, and $\boldsymbol{b}_y$, based on Eqs. (3), (4), and (5) and the figure of RNN.

Gradient With Respect to the Output

- We had:

$$\mathbb{R} \ni \mathcal{L} = \sum_{t=1}^{T} \mathcal{L}_t.$$

- If there is no activation function at the last layer, the gradient of the loss function of RNN with respect to the output at time t is:

$$\mathbb{R}^q \ni \frac{\partial \mathcal{L}}{\partial \boldsymbol{y}_t} \overset{(a)}{=} \frac{\partial \mathcal{L}}{\partial \mathcal{L}_t} \times \frac{\partial \mathcal{L}_t}{\partial \boldsymbol{y}_t} \overset{(7)}{=} \frac{\partial \mathcal{L}_t}{\partial \boldsymbol{y}_t}, \tag{8}$$

  where (a) is because of the chain rule.
- The gradient of the loss function at time t with respect to the output at time t, i.e., $\partial \mathcal{L}_t / \partial \boldsymbol{y}_t$, is calculated based on the formula of the loss function. The loss function can be any loss function for classification, regression, or other tasks.
- If there is an activation function at the last layer (see Eq. (6)), the gradient is:

$$\mathbb{R}^q \ni \frac{\partial \mathcal{L}}{\partial \boldsymbol{y}_t} \overset{(a)}{=} \frac{\partial \mathcal{L}}{\partial \mathcal{L}_t} \times \frac{\partial \mathcal{L}_t}{\partial \widehat{\boldsymbol{y}}_t} \times \frac{\partial \widehat{\boldsymbol{y}}_t}{\partial \boldsymbol{y}_t} \overset{(7)}{=} \frac{\partial \mathcal{L}_t}{\partial \widehat{\boldsymbol{y}}_t} \times \frac{\partial \widehat{\boldsymbol{y}}_t}{\partial \boldsymbol{y}_t}, \tag{9}$$

  where (a) is because of the chain rule. The derivative $\partial \widehat{\boldsymbol{y}}_t / \partial \boldsymbol{y}_t$ is calculated based on the formula of the activation function. The other derivative, $\partial \mathcal{L}_t / \partial \widehat{\boldsymbol{y}}_t$, is calculated based on the formula of the loss as a function of the output of the activation function.

Gradient With Respect to the State

- We had:

$$\begin{aligned}
&\mathbb{R}^p \ni \boldsymbol{i}_t = \boldsymbol{W}\boldsymbol{h}_{t-1} + \boldsymbol{U}\boldsymbol{x}_t + \boldsymbol{b}_i, \\
&[-1,1]^p \ni \boldsymbol{h}_t = \tanh(\boldsymbol{i}_t) = \tanh(\boldsymbol{W}\boldsymbol{h}_{t-1} + \boldsymbol{U}\boldsymbol{x}_t + \boldsymbol{b}_i), \\
&\mathbb{R}^q \ni \boldsymbol{y}_t = \boldsymbol{V}\boldsymbol{h}_t + \boldsymbol{b}_y.
\end{aligned}$$

- The gradient of the loss function of RNN with respect to the state at time t is:

$$\begin{aligned}
\mathbb{R}^p \ni \frac{\partial \mathcal{L}}{\partial \boldsymbol{h}_t} &\overset{(a)}{=} \left(\frac{\partial \mathcal{L}}{\partial \boldsymbol{y}_t} \times \frac{\partial \boldsymbol{y}_t}{\partial \boldsymbol{h}_t}\right) + \left(\frac{\partial \mathcal{L}}{\partial \boldsymbol{h}_{t+1}} \times \frac{\partial \boldsymbol{h}_{t+1}}{\partial \boldsymbol{h}_t}\right) \\
&\overset{(5)}{=} \left(\frac{\partial \mathcal{L}}{\partial \boldsymbol{y}_t} \times \boldsymbol{V}\right) + \left(\frac{\partial \mathcal{L}}{\partial \boldsymbol{h}_{t+1}} \times \frac{\partial \boldsymbol{h}_{t+1}}{\partial \boldsymbol{h}_t}\right), \qquad (10)
\end{aligned}$$

where (a) is because changing $\boldsymbol{h}_t$ affects both $\boldsymbol{y}_t$ and $\boldsymbol{h}_{t+1}$. We denote $\boldsymbol{\delta}_t := \partial\mathcal{L}/\partial\boldsymbol{h}_t$ so Eq. (10) becomes:

$$\boldsymbol{\delta}_t = \left(\frac{\partial \mathcal{L}}{\partial \boldsymbol{y}_t} \times \boldsymbol{V}\right) + \left(\boldsymbol{\delta}_{t+1} \times \frac{\partial \boldsymbol{h}_{t+1}}{\partial \boldsymbol{h}_t}\right). \qquad (11)$$

Gradient With Respect to the State

- We had:

$$\mathbb{R}^p \ni \boldsymbol{i}_t = \boldsymbol{W}\boldsymbol{h}_{t-1} + \boldsymbol{U}\boldsymbol{x}_t + \boldsymbol{b}_i,$$
$$[-1,1]^p \ni \boldsymbol{h}_t = \tanh(\boldsymbol{i}_t) = \tanh(\boldsymbol{W}\boldsymbol{h}_{t-1} + \boldsymbol{U}\boldsymbol{x}_t + \boldsymbol{b}_i),$$
$$\mathbb{R}^q \ni \boldsymbol{y}_t = \boldsymbol{V}\boldsymbol{h}_t + \boldsymbol{b}_y.$$

- According to Eqs. (3) and (4), we have:

$$\boldsymbol{i}_{t+1} = \boldsymbol{W}\boldsymbol{h}_t + \boldsymbol{U}\boldsymbol{x}_{t+1} + \boldsymbol{b}_i, \tag{12}$$
$$\boldsymbol{h}_{t+1} = \tanh(\boldsymbol{i}_{t+1}) = \tanh(\boldsymbol{W}\boldsymbol{h}_t + \boldsymbol{U}\boldsymbol{x}_{t+1} + \boldsymbol{b}_i). \tag{13}$$

Therefore:

$$\mathbb{R}^{p\times p} \ni \frac{\partial \boldsymbol{h}_{t+1}}{\partial \boldsymbol{h}_t} \overset{(a)}{=} \left(\frac{\partial \boldsymbol{i}_{t+1}}{\partial \boldsymbol{h}_t}\right)^\top \times \frac{\partial \boldsymbol{h}_{t+1}}{\partial \boldsymbol{i}_{t+1}} \overset{(b)}{=} \boldsymbol{W}(1 - \boldsymbol{h}_{t+1}^\top \boldsymbol{h}_{t+1})\boldsymbol{I}_{p\times p},$$

where $\boldsymbol{I}_{p\times p}$ is the identity matrix of size $(p \times p)$, (a) is because of the chain rule, and (b) is because $\mathbb{R}^{p\times p} \ni \partial \boldsymbol{i}_{t+1}/\partial \boldsymbol{h}_t = \boldsymbol{W}^\top$ for Eq. (12), and we have:

$$\mathbb{R}^{p\times p} \ni \frac{\partial \boldsymbol{h}_{t+1}}{\partial \boldsymbol{i}_{t+1}} = (1 - \boldsymbol{h}_{t+1}^\top \boldsymbol{h}_{t+1})\boldsymbol{I}_{p\times p}, \tag{14}$$

based on Eq. (13) and the formula for derivative of the hyperbolic tangent function, noticing that the state is multidimensional and not a scalar.

Gradient With Respect to the State

- Eqs. (5) and (8) were:

$$\mathbb{R}^q \ni \boldsymbol{y}_t = \boldsymbol{V}\boldsymbol{h}_t + \boldsymbol{b}_y,$$
$$\mathbb{R}^q \ni \frac{\partial \mathcal{L}}{\partial \boldsymbol{y}_t} \overset{(a)}{=} \frac{\partial \mathcal{L}}{\partial \mathcal{L}_t} \times \frac{\partial \mathcal{L}_t}{\partial \boldsymbol{y}_t} \overset{(7)}{=} \frac{\partial \mathcal{L}_t}{\partial \boldsymbol{y}_t}.$$

- We had:

$$\boldsymbol{\delta}_t := \partial \mathcal{L} / \partial \boldsymbol{h}_t.$$

- For the time slot $t = T$, the derivative $\partial \mathcal{L} / \partial \boldsymbol{h}_T$ is much simpler:

$$\mathbb{R}^p \ni \boldsymbol{\delta}_T = \frac{\partial \mathcal{L}}{\partial \boldsymbol{h}_T} \overset{(a)}{=} \frac{\partial \mathcal{L}}{\partial \boldsymbol{y}_T} \times \frac{\partial \boldsymbol{y}_T}{\partial \boldsymbol{h}_T} \overset{(5)}{=} \frac{\partial \mathcal{L}}{\partial \boldsymbol{y}_T} \times \boldsymbol{V} \overset{(8)}{=} \frac{\partial \mathcal{L}_T}{\partial \boldsymbol{y}_T} \times \boldsymbol{V}, \tag{15}$$

where (a) is because of the chain rule and the derivative $\partial \mathcal{L}_T / \partial \boldsymbol{y}_T$ is computed based on the formula of loss function.

Gradient With Respect to $\boldsymbol{V}$

- The gradient of the loss function of RNN with respect to the weight matrix $\boldsymbol{V}$ is:

$$\mathbb{R}^{q\times p} \ni \frac{\partial \mathcal{L}}{\partial \boldsymbol{V}} \overset{(a)}{=} \sum_{t=1}^{T} \left(\frac{\partial \mathcal{L}}{\partial \boldsymbol{y}_t} \times \frac{\partial \boldsymbol{y}_t}{\partial \boldsymbol{V}} \right) \overset{(b)}{=} \sum_{t=1}^{T} \left(\frac{\partial \mathcal{L}_t}{\partial \boldsymbol{y}_t} \times \boldsymbol{h}_t^\top \right), \tag{16}$$

where (a) is because $\boldsymbol{V}$ exists in all time slots and changing $\boldsymbol{V}$ affects the loss $\mathcal{L}$ in all time slots. The equation (b) is because of Eqs. (8) and (5):

$$\mathbb{R}^q \ni \frac{\partial \mathcal{L}}{\partial \boldsymbol{y}_t} \overset{(a)}{=} \frac{\partial \mathcal{L}}{\partial \mathcal{L}_t} \times \frac{\partial \mathcal{L}_t}{\partial \boldsymbol{y}_t} \overset{(7)}{=} \frac{\partial \mathcal{L}_t}{\partial \boldsymbol{y}_t},$$
$$\mathbb{R}^q \ni \boldsymbol{y}_t = \boldsymbol{V}\boldsymbol{h}_t + \boldsymbol{b}_y.$$

- The derivative $\partial \mathcal{L}_t / \partial \boldsymbol{y}_t \in \mathbb{R}^q$ is calculated based on the formula of the loss function.

Gradient With Respect to $\boldsymbol{W}$

- The gradient of the loss function of RNN with respect to the weight matrix $\boldsymbol{W}$ is:

$$\mathbb{R}^{p\times p} \ni \frac{\partial \mathcal{L}}{\partial \boldsymbol{W}} \overset{(a)}{=} \sum_{t=1}^{T} \mathbf{vec}_{p\times p}^{-1}\Big((\frac{\partial \boldsymbol{h}_t}{\partial \boldsymbol{W}})^\top \times \frac{\partial \mathcal{L}}{\partial \boldsymbol{h}_t} \Big), \tag{17}$$

  where $\mathbf{vec}_{p\times p}^{-1}(.)$ de-vectorizes the vector of length p^2 to a matrix of size $(p \times p)$ and (a) is because $\boldsymbol{W}$ exists in all time slots and changing $\boldsymbol{W}$ affects the loss $\mathcal{L}$ in all time slots.
- The derivative $\partial \mathcal{L}/\partial \boldsymbol{h}_t \in \mathbb{R}^p$ in Eq. (17) was computed before.
- The derivative $\partial \boldsymbol{h}_t/\partial \boldsymbol{W}$ in Eq. (17) is:

$$\mathbb{R}^{p\times p^2} \ni \frac{\partial \boldsymbol{h}_t}{\partial \boldsymbol{W}} = \frac{\partial \boldsymbol{h}_t}{\partial \boldsymbol{i}_t} \times \frac{\partial \boldsymbol{i}_t}{\partial \boldsymbol{W}},$$

  because of the chain rule. The first term is:

$$\mathbb{R}^{p\times p} \ni \frac{\partial \boldsymbol{h}_t}{\partial \boldsymbol{i}_t} = (1 - \boldsymbol{h}_t^\top \boldsymbol{h}_t)\boldsymbol{I}_{p\times p}, \tag{18}$$

  according to Eq. (14). Based on the Magnus-Neudecker convention [24], the second term is calculated as:

$$\mathbb{R}^{p\times p^2} \ni \frac{\partial \boldsymbol{i}_t}{\partial \boldsymbol{W}} = \boldsymbol{h}_{t-1}^\top \otimes \boldsymbol{I}_{p\times p},$$

  where $\otimes$ denotes the Kronecker product (see our tutorial [24] for more information on the Magnus-Neudecker convention).

Gradient With Respect to $\boldsymbol{U}$

- The gradient of the loss function of RNN with respect to the weight matrix $\boldsymbol{U}$ is:

$$\mathbb{R}^{p\times d} \ni \frac{\partial \mathcal{L}}{\partial \boldsymbol{U}} \overset{(a)}{=} \sum_{t=1}^{T} \mathbf{vec}^{-1}_{p\times d}\Big((\frac{\partial \boldsymbol{h}_t}{\partial \boldsymbol{U}})^\top \times \frac{\partial \mathcal{L}}{\partial \boldsymbol{h}_t} \Big), \tag{19}$$

  where (a) is because $\boldsymbol{U}$ exists in all time slots and changing $\boldsymbol{U}$ affects the loss $\mathcal{L}$ in all time slots.
- The derivative $\partial \mathcal{L}/\partial \boldsymbol{h}_t \in \mathbb{R}^p$ in Eq. (17) was computed before.
- The derivative $\partial \boldsymbol{h}_t/\partial \boldsymbol{U}$ in Eq. (17) is:

$$\mathbb{R}^{p\times (pd)} \ni \frac{\partial \boldsymbol{h}_t}{\partial \boldsymbol{U}} = \frac{\partial \boldsymbol{h}_t}{\partial \boldsymbol{i}_t} \times \frac{\partial \boldsymbol{i}_t}{\partial \boldsymbol{U}},$$

  because of the chain rule.
- The first term is already calculated in Eq. (18).
- Based on the Magnus-Neudecker convention [24], the second term is calculated as:

$$\mathbb{R}^{p\times (pd)} \ni \frac{\partial \boldsymbol{i}_t}{\partial \boldsymbol{U}} = \boldsymbol{x}_t^\top \otimes \boldsymbol{I}_{p\times p}.$$

Gradient With Respect to $\boldsymbol{b}_i$

- The gradient of the loss function of RNN with respect to the bias $\boldsymbol{b}_i$ is:

$$\mathbb{R}^p \ni \frac{\partial \mathcal{L}}{\partial \boldsymbol{b}_i} \overset{(a)}{=} \sum_{t=1}^{T} \Big(\big(\frac{\partial \boldsymbol{h}_t}{\partial \boldsymbol{b}_i} \big)^\top \times \frac{\partial \mathcal{L}}{\partial \boldsymbol{h}_t} \Big), \tag{20}$$

  where (a) is because $\boldsymbol{b}_i$ exists in all time slots and changing $\boldsymbol{b}$ affects the loss $\mathcal{L}$ in all time slots.
- The derivative $\partial \mathcal{L} / \partial \boldsymbol{h}_t$ was already calculated before.
- The derivative $\partial \boldsymbol{h}_t / \partial \boldsymbol{b}_i$ is calculated as:

$$\mathbb{R}^{p \times p} \ni \frac{\partial \boldsymbol{h}_t}{\partial \boldsymbol{b}_i} \overset{(a)}{=} \frac{\partial \boldsymbol{h}_t}{\partial \boldsymbol{i}_t} \times \frac{\partial \boldsymbol{i}_t}{\partial \boldsymbol{b}_i} \overset{(3)}{=} \frac{\partial \boldsymbol{h}_t}{\partial \boldsymbol{i}_t},$$

  where (a) is because of the chain rule and the derivative $\partial \boldsymbol{h}_t / \partial \boldsymbol{i}_t$ was already calculated in Eq. (18).

Gradient With Respect to $\boldsymbol{b}_y$

- Eqs. (5) and (8) were:

$$\mathbb{R}^q \ni \boldsymbol{y}_t = \boldsymbol{V}\boldsymbol{h}_t + \boldsymbol{b}_y,$$
$$\mathbb{R}^q \ni \frac{\partial \mathcal{L}}{\partial \boldsymbol{y}_t} \overset{(a)}{=} \frac{\partial \mathcal{L}}{\partial \mathcal{L}_t} \times \frac{\partial \mathcal{L}_t}{\partial \boldsymbol{y}_t} \overset{(7)}{=} \frac{\partial \mathcal{L}_t}{\partial \boldsymbol{y}_t}.$$

- The gradient of the loss function of RNN with respect to the bias $\boldsymbol{b}_y$ is:

$$\mathbb{R}^q \ni \frac{\partial \mathcal{L}}{\partial \boldsymbol{b}_y} \overset{(a)}{=} \sum_{t=1}^{T} \left(\frac{\partial \mathcal{L}}{\partial \boldsymbol{y}_t} \times \frac{\partial \boldsymbol{y}_t}{\partial \boldsymbol{b}_y} \right) \overset{(b)}{=} \sum_{t=1}^{T} \frac{\partial \mathcal{L}_t}{\partial \boldsymbol{y}_t}, \tag{21}$$

  where (a) is because $\boldsymbol{b}_y$ exists in all time slots and changing $\boldsymbol{b}_y$ affects the loss $\mathcal{L}$ in all time slots. The equation (b) is because of Eqs. (8) and (5).
- The derivative $\partial \mathcal{L}_t / \partial \boldsymbol{y}_t \in \mathbb{R}^q$ is calculated based on the formula of the loss function.

Updates by Gradient Descent

- BPPT updates the parameters of RNN by gradient descent [24] using the calculated gradients:

$$\begin{aligned}
\boldsymbol{h}_t &:= \boldsymbol{h}_t - \eta \frac{\partial \mathcal{L}}{\partial \boldsymbol{h}_t}, \quad \forall t \in \{1, \ldots, T\}, \\
\boldsymbol{V} &:= \boldsymbol{V} - \eta \frac{\partial \mathcal{L}}{\partial \boldsymbol{V}}, \\
\boldsymbol{W} &:= \boldsymbol{W} - \eta \frac{\partial \mathcal{L}}{\partial \boldsymbol{W}}, \\
\boldsymbol{U} &:= \boldsymbol{U} - \eta \frac{\partial \mathcal{L}}{\partial \boldsymbol{U}}, \\
\boldsymbol{b}_i &:= \boldsymbol{b}_i - \eta \frac{\partial \mathcal{L}}{\partial \boldsymbol{b}_i}, \\
\boldsymbol{b}_y &:= \boldsymbol{b}_y - \eta \frac{\partial \mathcal{L}}{\partial \boldsymbol{b}_y},
\end{aligned}$$

where $\eta > 0$ is the learning rate and the gradients are calculated by Eqs. (10), (16), (17), (19), (20), and (21).

Gradient Vanishing or Explosion in Long-term Dependencies

Gradient Vanishing or Explosion in Long-term Dependencies

- In recurrent neural networks, so as in deep neural networks, the final output is the composition of a large number of non-linear transformations. This results in the problem of either **vanishing or exploding gradients** in recurrent neural networks, especially for capturing long-term dependencies in sequence processing [7, 8]. This problem is explained in the following.
- Recall Eq. (2) for a dynamical system:

$$\boldsymbol{h}_t = f_\theta(\boldsymbol{h}_{t-1}, \boldsymbol{x}_t).$$

By induction, the hidden state at time t, i.e., $\boldsymbol{h}_t$, can be written as the previous T time steps. If the subscript t denotes the previous t time steps, we have by induction [26, 27]:

$$\boldsymbol{h}_1 = f_\theta\Big(f_\theta\big(\dots f_\theta(\boldsymbol{h}_T, \boldsymbol{x}_{T+1})\dots, \boldsymbol{x}_2\big), \boldsymbol{x}_1\Big).$$

- Then, by the chain rule in derivatives, the derivative loss at time T, i.e., $\mathcal{L}_T$, is:

$$\frac{\partial \mathcal{L}_T}{\partial \theta} = \sum_{t \leq T} \frac{\partial \mathcal{L}_t}{\partial \boldsymbol{h}_t} \frac{\partial \boldsymbol{h}_t}{\partial \theta} \overset{(a)}{=} \sum_{t \leq T} \frac{\partial \mathcal{L}_t}{\partial \boldsymbol{h}_T} \frac{\partial \boldsymbol{h}_T}{\partial \boldsymbol{h}_t} \frac{\partial \boldsymbol{h}_t}{\partial \theta} \overset{(2)}{=} \sum_{t \leq T} \frac{\partial \mathcal{L}_t}{\partial \boldsymbol{h}_T} \frac{\partial \boldsymbol{h}_T}{\partial \boldsymbol{h}_t} \frac{\partial f_\theta(\boldsymbol{h}_{t-1}, \boldsymbol{x}_t)}{\partial \theta}, \tag{22}$$

where (a) is because of the chain rule. In this expression, there is the derivative of $\boldsymbol{h}_T$ with respect to $\boldsymbol{h}_t$ which itself can be calculated by the chain rule:

$$\frac{\partial \boldsymbol{h}_T}{\partial \boldsymbol{h}_t} = \frac{\partial \boldsymbol{h}_T}{\partial \boldsymbol{h}_{T-1}} \times \frac{\partial \boldsymbol{h}_{T-1}}{\partial \boldsymbol{h}_{T-2}} \times \dots \times \frac{\partial \boldsymbol{h}_{t+1}}{\partial \boldsymbol{h}_t}. \tag{23}$$

Gradient Vanishing or Explosion in Long-term Dependencies

- We found:

$$\frac{\partial \mathcal{L}_T}{\partial \theta} = \sum_{t \leq T} \frac{\partial \mathcal{L}_t}{\partial \boldsymbol{h}_T} \frac{\partial \boldsymbol{h}_T}{\partial \boldsymbol{h}_t} \frac{\partial f_\theta(\boldsymbol{h}_{t-1}, \boldsymbol{x}_t)}{\partial \theta},$$

$$\frac{\partial \boldsymbol{h}_T}{\partial \boldsymbol{h}_t} = \frac{\partial \boldsymbol{h}_T}{\partial \boldsymbol{h}_{T-1}} \times \frac{\partial \boldsymbol{h}_{T-1}}{\partial \boldsymbol{h}_{T-2}} \times \cdots \times \frac{\partial \boldsymbol{h}_{t+1}}{\partial \boldsymbol{h}_t}.$$

- For capturing **long-term dependencies** in the sequence, T should be **large**. This means that in Eq. (23), and hence in Eq. (22), the number of multiplicand terms becomes huge.
- On the one hand, if each derivative is **slightly smaller than one**, the entire derivative in the chain rule becomes very small for multiplication of many terms smaller than one. This problem is referred to as **gradient vanishing**.
- On the other hand, if every derivative is **slightly larger than one**, the entire derivative in the chain rule explodes, resulting in the problem of **exploding gradients**.
- Note that gradient vanishing is more common than gradient explosion in recurrent networks.
- There exist various attempts for resolving the problem of gradient vanishing or explosion [26, 28]. In the following, some of these attempts are introduced.

Close-to-identity Weight Matrix

- As Eq. (4):

$$[-1,1]^p \ni \boldsymbol{h}_t = \tanh(\boldsymbol{i}_t) = \tanh(\boldsymbol{W}\boldsymbol{h}_{t-1} + \boldsymbol{U}\boldsymbol{x}_t + \boldsymbol{b}_i),$$

  shows, the state is multiplied by a weight matrix $\boldsymbol{W}$ at every time step and if there is long-term dependency, many of these $\boldsymbol{W}$ matrices are multiplied.
- Suppose the eigenvalue decomposition [29] of the matrix $\boldsymbol{W}$ is $\boldsymbol{W} = \boldsymbol{A}\boldsymbol{\Lambda}\boldsymbol{A}^\top$ where $\boldsymbol{A} \in \mathbb{R}^{p\times p}$ and $\boldsymbol{\Lambda} := \mathbf{diag}([\lambda_1, \ldots, \lambda_p]^\top)$ contain the eigenvectors and eigenvalues of $\boldsymbol{W}$, respectively. Eq. (4) is restated as:

$$\boldsymbol{h}_t = \tanh(\boldsymbol{A}\boldsymbol{\Lambda}\boldsymbol{A}^\top \boldsymbol{h}_{t-1} + \boldsymbol{U}\boldsymbol{x}_t + \boldsymbol{b}_i). \tag{24}$$

- If a change ε in some element of the state $\boldsymbol{h}_{t-1}$ is aligned with an eigenvector of the weight matrix $\boldsymbol{W}$, then the effect of this change in $\boldsymbol{h}_t$ will be $(\lambda^t\,\varepsilon)$ after t time steps, according to Eq. (24).
- Two cases may happen:
  - If the largest eigenvalue is less than one, i.e., $\lambda < 1$, then the change $(\lambda^t\,\varepsilon)$ is contrastive because $\lambda^t \ll 1$ for long-term dependencies. In this case, gradient vanishing occurs in long-term dependency and the network forgets very long time ago.
  - If the largest eigenvalue is less than one, i.e., $\lambda > 1$, then the change $(\lambda^t\,\varepsilon)$ is diverging because $\lambda^t \gg 1$ for long-term dependencies. In this case, the gradient network forgets very long time ago. In this case, gradient explosion occurs in long-term dependency and remembering very long time ago dominates the short-term memories.

Close-to-identity Weight Matrix

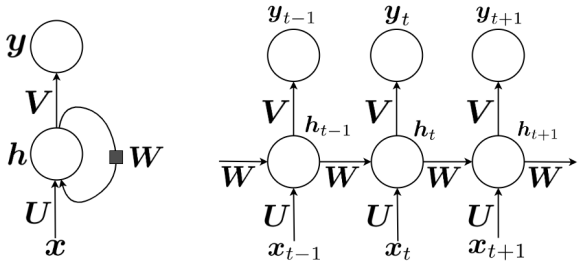
- As remembering short-term memories is usually more important than remembering very past time in different tasks, it is recommended to use the weight matrix $\boldsymbol{W}$ whose largest eigenvalue is less than one; this makes the RNN have the Markovian property because it forgets very past after some point.
- However, if the largest eigenvalue of $\boldsymbol{W}$ is much less than one, i.e., $\lambda \ll 1$, gradient vanishing happens very sooner than expected.
- Therefore, it is recommended to use the weight matrix $\boldsymbol{W}$ whose largest eigenvalue is **slightly** less than one, i.e., $\lambda \lesssim 1$. This makes the RNN **slightly contrastive**.
- One way to have the weight matrix $\boldsymbol{W}$ whose largest eigenvalue is slightly less than one is to make this matrix close to the identity matrix [9].
- There exist some other ways to determine the weight matrix $\boldsymbol{W}$. For example, the wight matrix can be set to be an orthogonal matrix [30].
- Another approach is to copy the previous state exactly to the current state. In this approach, the Eq. (4) is modified to [31]:

$$\begin{aligned} \boldsymbol{h}_t &= \tanh(\boldsymbol{W}\boldsymbol{h}_{t-1} + \boldsymbol{h}_{t-1} + \boldsymbol{U}\boldsymbol{x}_t + \boldsymbol{b}_i) \\ &= \tanh\big((\boldsymbol{W} + \boldsymbol{I})\boldsymbol{h}_{t-1} + \boldsymbol{U}\boldsymbol{x}_t + \boldsymbol{b}_i\big), \end{aligned} \tag{25}$$

where $\boldsymbol{I}$ is the identity matrix. This prevents gradient vanishing because it brings a copy of the previous step to the current state. This can also be interpreted as strengthening the diagonal of the weight matrix $\boldsymbol{W}$; hence, increasing the largest eigenvalue of $\boldsymbol{W}$ for preventing gradient vanishing.

Long Delays

- As Eq. (4) and the figure of RNN show, in the regular RNN, every state $\boldsymbol{h}_t$ is fed by its previous state $\boldsymbol{h}_{t-1}$ through the weight matrix $\boldsymbol{W}$.



- As discussed before, in the regular RNN, the effect of the change ε in a state results in $(\lambda^t \varepsilon)$ after t time steps, where λ is the largest eigenvalue of $\boldsymbol{W}$.
- As shown in the figure of RNN, the regular RNN has one-step connections or delays between the states. It is possible to have **longer delays** between the states in addition to the one-step delays [10].
- In other words, it is possible to have **higher levels of Markov property** in the network.
- Let $\boldsymbol{W}_k$ denote the weight matrix for k-step delays between the states. Then, Eq. (4) can be modified to:

$$\boldsymbol{h}_t = \tanh\left(\sum_k \boldsymbol{W}_k \boldsymbol{h}_{t-k} + \boldsymbol{U}\boldsymbol{x}_t + \boldsymbol{b}_i\right), \tag{26}$$

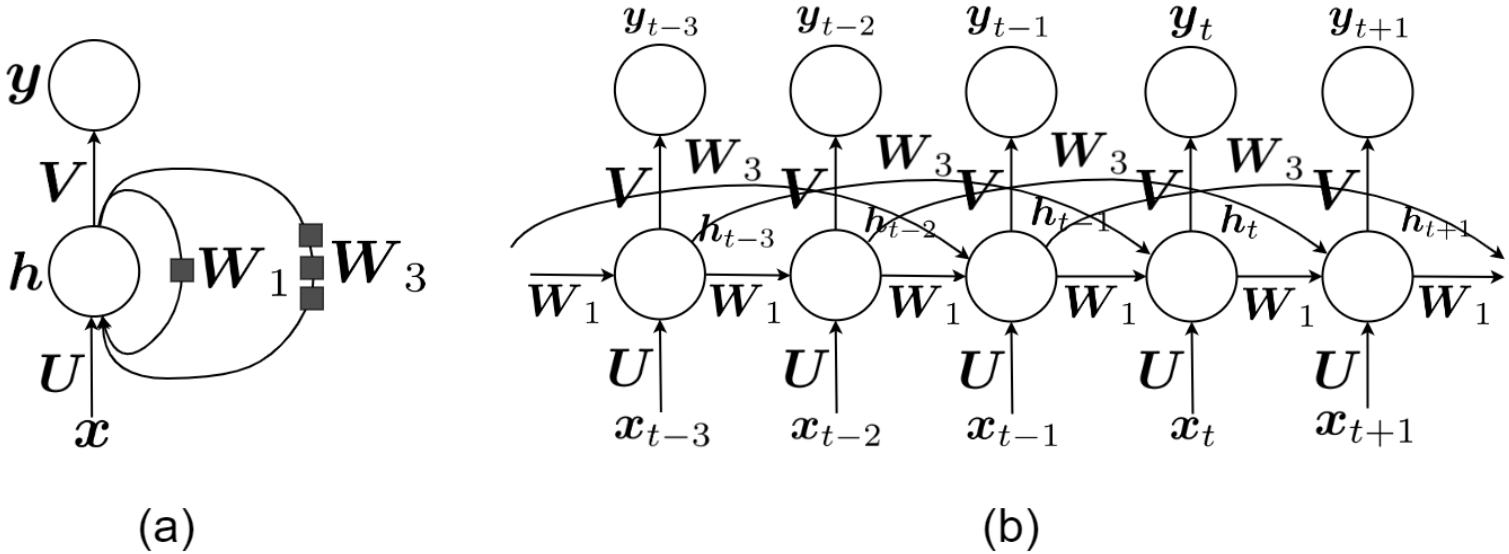
where the summation is over the k values for the existing delays in the RNN structure.

Long Delays

- An example for an RNN network with one-step and three-step delays is:

$$\boldsymbol{h}_t = \tanh\left(\boldsymbol{W}_1\boldsymbol{h}_{t-1} + \boldsymbol{W}_3\boldsymbol{h}_{t-3} + \boldsymbol{U}\boldsymbol{x}_t + \boldsymbol{b}_i\right),$$

which is illustrated in this figure.



- Having long delays in RNN is one of the attempts for **preventing gradient vanishing** [10]. This is justified because **every state is having impact not only from the previous state but also from the more previous states**. Therefore, in backpropagation through time, there is **some skip in gradient flow from a state to more previous states** without the need to go through the middle states in the chain rule.

Leaky Units

- Another way to resolve the problem of gradient vanishing is **leaky units** [11, 12].
- Let $h_{t,j}$ denote the j-th element of the state $\boldsymbol{h}_t \in [-1, 1]^p$. In leaky units, Eq. (4) is modified to the following element-wise equation:

$$h_{t,j} = (1 - \frac{1}{\tau_j})\, h_{t-1,j} + \frac{1}{\tau_j} \tanh(\boldsymbol{W}_{j:}\boldsymbol{h}_{t-1} + \boldsymbol{U}_{j:}\boldsymbol{x}_t + b_{i,j}), \tag{27}$$

  where $1 \leq \tau_j < \infty$ and $\boldsymbol{W}_{j:}$ is the j-th row of $\boldsymbol{W}$ and $\boldsymbol{U}_{j:}$ is the j-th row of $\boldsymbol{U}$ and $b_{i,j}$ is the j-th element of $\boldsymbol{b}_i$.
- When $\tau_i = 1$, then Eq. (27) becomes:

$$h_{t,j} = \frac{1}{\tau_j} \tanh(\boldsymbol{W}_{j:}\boldsymbol{h}_{t-1} + \boldsymbol{U}_{j:}\boldsymbol{x}_t + b_{i,j}),$$

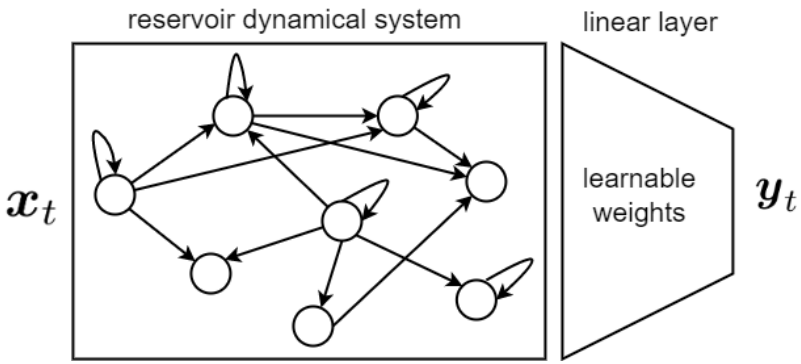
  which gives back Eq. (4) in the **regular RNN**.
- However, when $\tau_i \gg 1$, then Eq. (27) becomes:

$$h_{t,j} = h_{t-1,j},$$

  which means that **the previous state is copied to the current state**.
- The larger the τ_i, the easier the gradient propagates for $h_{t,i}$. Therefore, by tuning τ_i, it is possible to **control how much of the past should be directly copied and how much should be passed through the weight matrix**. This can control the **amount of gradient vanishing**.
- Note that leaky units use different τ_i's because there may be a need to keep some of the directions of states (with $\tau_i = 1$) or forget some of the directions (with $\tau_i \gg 1$). In other words, it **decides about the p directions of states separately**.

Echo State Networks

- One of the approaches to handle the problem of gradient vanishing in RNN is to use **echo state networks** [13, 14].
- These networks consider the recurrent neural network as a **black box having hidden units with nonlinear activation functions and connections between them**.
- This black box of recurrent connections is called the **reservoir dynamical system** which models the internal structure of a computer or brain.
- The connections in the reservoir system are usually **sparse** and the weights of these connections are considered to be **fixed**.
- The output of the reservoir system is connected to an additional **linear output layer** whose weights are **learnable**.
- The echo state network minimizes the **mean squared error** in the output layer; hence, it performs **linear regression** in the last layer [13].
- Because of **not learning the recurrent weights in the reservoir system** and sufficing to learn the weights of the output layer, the echo state network does not face the **gradient vanishing problem**.
- A tutorial on this topic is [32].



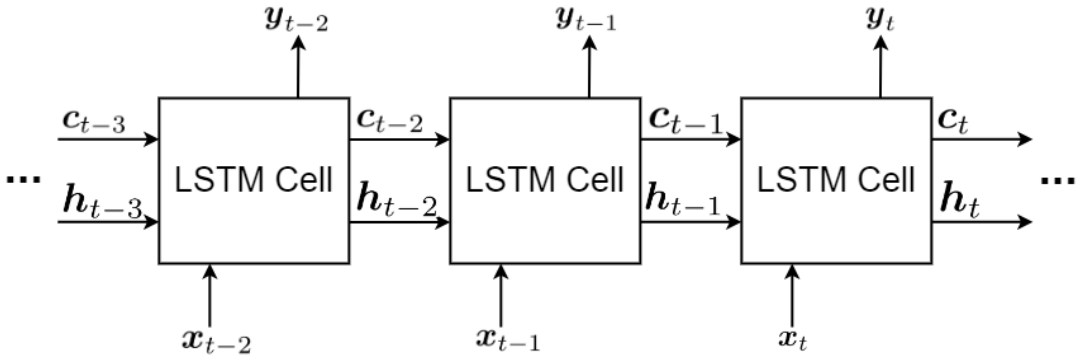
Long Short-Term Memory Network

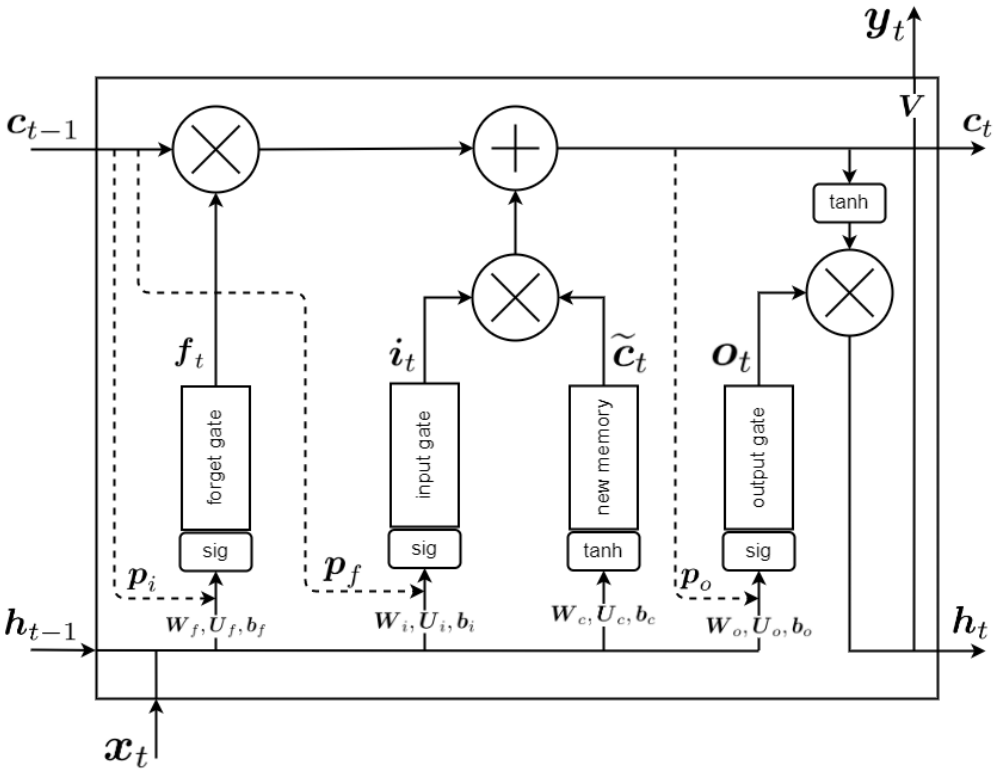
Long Short-Term Memory Network

- As the examples in introduction showed, we need **short-term relations** in some cases and **long-term relations** in some other cases.
- RNN learns the sequence based on one or several previous states, depending on its structure and the level of its Markov property (see Fig. **??**). Therefore, we need to **decide on the structure of RNN to be able to handle short-term or long-term dependencies** in the sequence.
- Instead of **manual design of the RNN structure** or **deciding manually when to clear the state**, we can **let the neural network learn by itself** when to clear the state based on its input sequence.
- **Long Short-Term Memory (LSTM)**, initially proposed in [15, 16] (1995-1997), is able to do this; it learns from its input sequence when to use short-term dependency (i.e., when to clear the state) and when to use the long-term memory (i.e., when not to clear the state).

Long Short-Term Memory Network

- LSTM consists of several cells, each of which corresponds to a time slot. Every LSTM cell contains several gates for learning different aspects of the input time series.





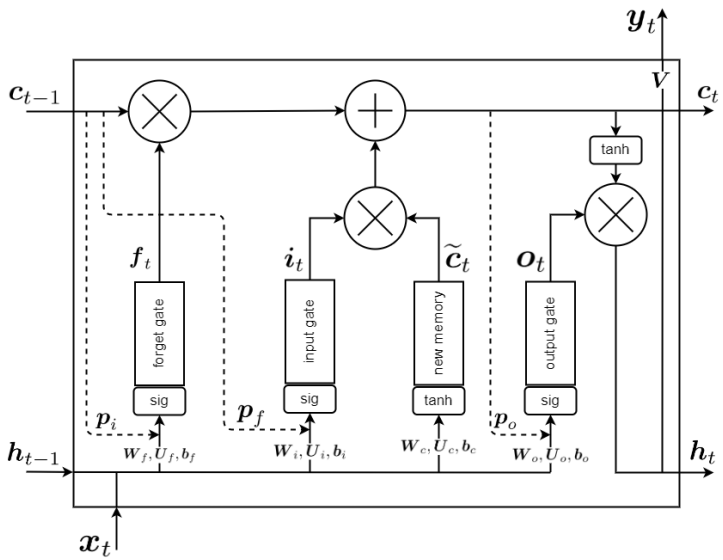
The Input Gate

- One of the gates in the LSTM cell is the **input gate**, first proposed in [15, 16].
- This gate takes the input at the current time slot, $\boldsymbol{x}_t \in \mathbb{R}^d$, and the hidden state of the last time slot, $\boldsymbol{h}_{t-1} \in [-1, 1]^p$, and outputs the signal $\boldsymbol{i}_t \in [0, 1]^p$:

$$\boldsymbol{i}_t = \text{sig}\big(\boldsymbol{W}_i\, \boldsymbol{h}_{t-1} + \boldsymbol{U}_i\, \boldsymbol{x}_t + (\boldsymbol{p}_i \odot \boldsymbol{c}_{t-1}) + \boldsymbol{b}_i\big), \tag{28}$$

where $\boldsymbol{W}_i \in \mathbb{R}^{p \times p}$, $\boldsymbol{U}_i \in \mathbb{R}^{p \times d}$, and the bias $\boldsymbol{b}_i \in \mathbb{R}^p$ are the learnable weights for the input gate, $\odot$ denotes the Hadamard (element-wise) product, $\boldsymbol{c}_{t-1} \in \mathbb{R}^p$ is the final memory of the last time slot (which will be explained later), and $\boldsymbol{p}_i \in \mathbb{R}^p$ is the learnable **peephole weight** [33] letting a possible leak of information from the previous final memory. The function $\text{sig}(.) \in (0, 1)$ is the sigmoid function which is applied element-wise:

$$\text{sig}(x) = \frac{1}{1 + \exp(-x)}. \tag{29}$$



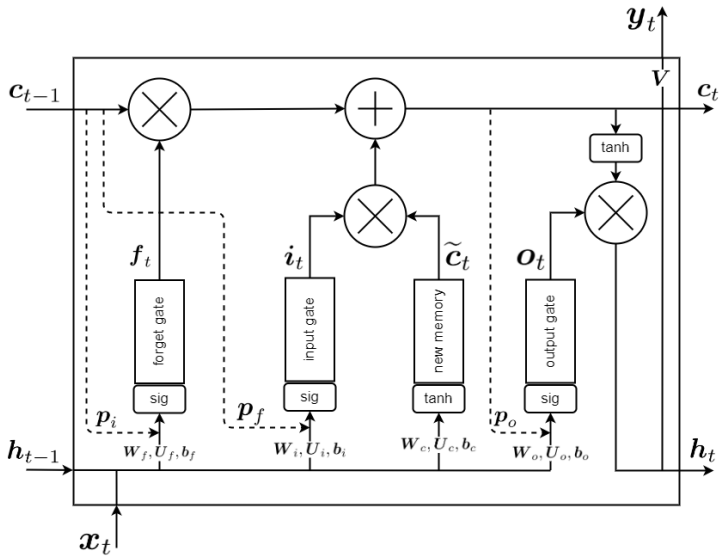
The Input Gate

- As Eq. (28):

$$\boldsymbol{i}_t = \text{sig}\big(\boldsymbol{W}_i\,\boldsymbol{h}_{t-1} + \boldsymbol{U}_i\,\boldsymbol{x}_t + (\boldsymbol{p}_i \odot \boldsymbol{c}_{t-1}) + \boldsymbol{b}_i\big),$$

  demonstrates, the input gate considers the **effect of the input and the previous hidden state**.

- It may also use a **leak of information from the previous memory** through the peephole.
- This gate carries the **importance of the information of the input at the current time slot**.

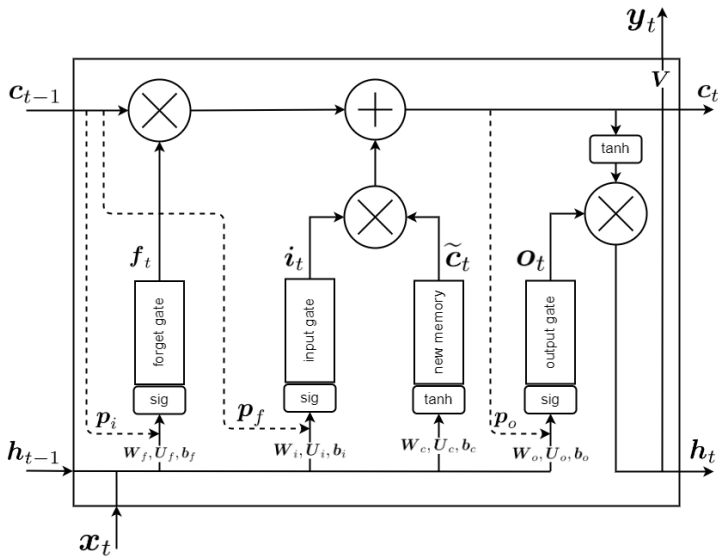


The Forget Gate

- Another gate in the LSTM cell is the **forget gate**, first proposed in [34].
- This gate also takes the input at the current time slot, $\boldsymbol{x}_t \in \mathbb{R}^d$, and the hidden state of the last time slot, $\boldsymbol{h}_{t-1} \in [-1, 1]^p$, and outputs the signal $\boldsymbol{f}_t \in [0, 1]^p$:

$$\boldsymbol{f}_t = \text{sig}\big(\boldsymbol{W}_f\, \boldsymbol{h}_{t-1} + \boldsymbol{U}_f\, \boldsymbol{x}_t + (\boldsymbol{p}_f \odot \boldsymbol{c}_{t-1}) + \boldsymbol{b}_f\big), \tag{30}$$

  where $\boldsymbol{W}_f \in \mathbb{R}^{p\times p}$, $\boldsymbol{U}_f \in \mathbb{R}^{p\times d}$, and the bias $\boldsymbol{b}_f \in \mathbb{R}^p$ are the learnable weights for the forget gate, and $\boldsymbol{p}_f \in \mathbb{R}^p$ is the learnable **peephole weight** [33] letting a possible leak of information from the previous final memory.
- As Eq. (30) shows, the forget gate considers the **effect of the input and the previous hidden state**, and **perhaps a leak of information from the previous memory**.
- This gate controls the **amount of forgetting the previous information with respect to the new-coming information**.



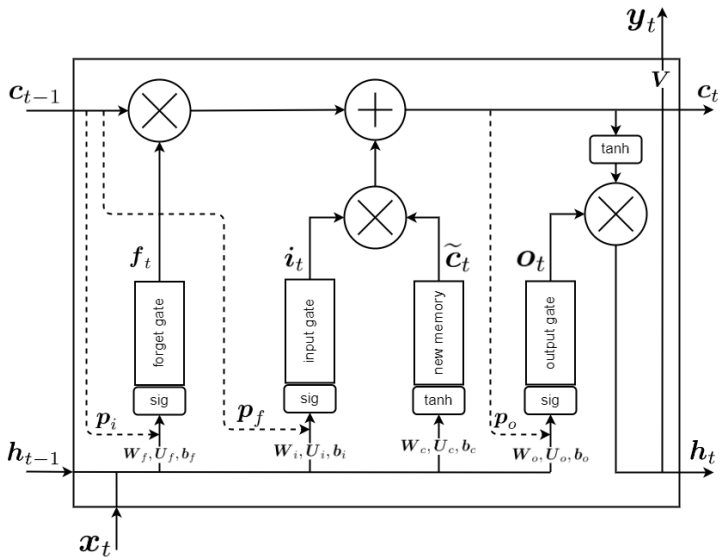
The Output Gate

- The next gate in the LSTM cell is the **output gate** first proposed in [15, 16]. This gate also takes the input at the current time slot, $\boldsymbol{x}_t \in \mathbb{R}^d$, and the hidden state of the last time slot, $\boldsymbol{h}_{t-1} \in [-1, 1]^p$, and outputs the signal $\boldsymbol{o}_t \in [0, 1]^p$:

$$\boldsymbol{o}_t = \text{sig}\big(\boldsymbol{W}_o\, \boldsymbol{h}_{t-1} + \boldsymbol{U}_o\, \boldsymbol{x}_t + (\boldsymbol{p}_o \odot \boldsymbol{c}_t) + \boldsymbol{b}_o\big), \tag{31}$$

  where $\boldsymbol{W}_o \in \mathbb{R}^{p \times p}$, $\boldsymbol{U}_o \in \mathbb{R}^{p \times d}$, and the bias $\boldsymbol{b}_o \in \mathbb{R}^p$ are the learnable weights for the output gate, and $\boldsymbol{p}_o \in \mathbb{R}^p$ is the learnable **peephole weight** [33] letting a possible leak of information from the current final memory.

- As shown in Eq. (31), the output gate considers the **effect of the input and the previous hidden state**, and a **possible information leak from the current memory**.



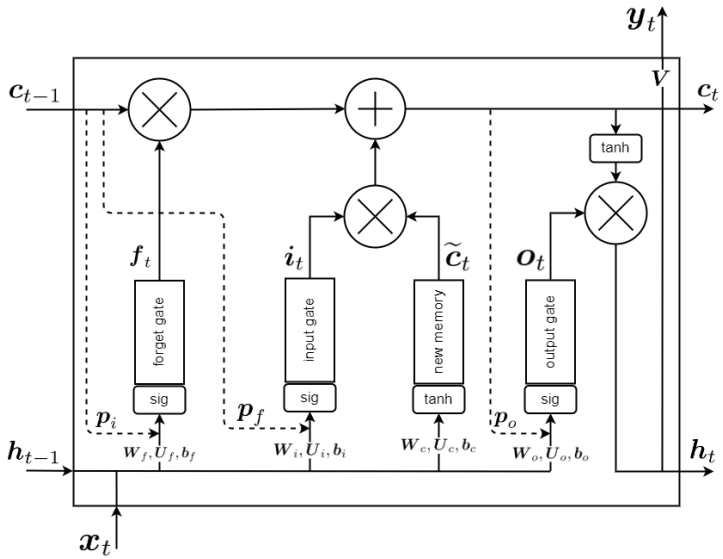
The New Memory Cell (Block Input)

- The LSTM cell includes a gate named the **new memory cell**. This gate takes the input at the current time slot, $\boldsymbol{x}_t \in \mathbb{R}^d$, and the hidden state of the last time slot, $\boldsymbol{h}_{t-1} \in [-1, 1]^p$, and outputs the signal $\widetilde{\boldsymbol{c}}_t \in [-1, 1]^p$.
- This gate considers **the effect of the input and the previous hidden state** to **represent the new information of current input**. It is formulated as:

$$\widetilde{\boldsymbol{c}}_t = \tanh(\boldsymbol{W}_c \, \boldsymbol{h}_{t-1} + \boldsymbol{U}_c \, \boldsymbol{x}_t + \boldsymbol{b}_c), \tag{32}$$

where $\boldsymbol{W}_c \in \mathbb{R}^{p \times p}$, $\boldsymbol{U}_c \in \mathbb{R}^{p \times d}$, and the bias $\boldsymbol{b}_c$ are the learnable weights for the new memory cell.

- The new memory cell is also referred to as the **block input** in the literature [35]. The signal $\widetilde{\boldsymbol{c}}_t$ is sometimes denoted by $\boldsymbol{z}_t$ in the literature.

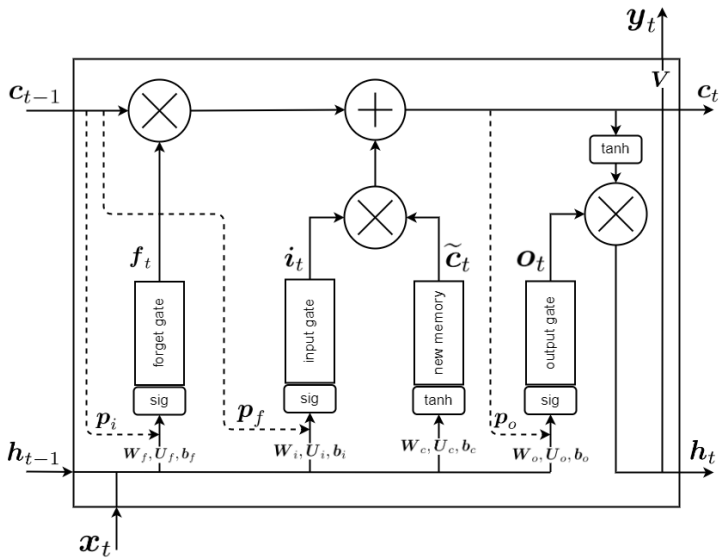


The Final Memory Calculation

- After computation of the outputs of the input gate $\boldsymbol{i}_t$, the forget gate $\boldsymbol{f}_t$, and the new memory cell $\widetilde{\boldsymbol{c}}_t$, we calculate the **final memory** $\boldsymbol{c}_t \in \mathbb{R}^p$:

$$\boldsymbol{c}_t = (\boldsymbol{f}_t \odot \boldsymbol{c}_{t-1}) + (\boldsymbol{i}_t \odot \widetilde{\boldsymbol{c}}_t), \tag{33}$$

  where $\boldsymbol{c}_{t-1} \in \mathbb{R}^p$ is the final memory of the previous time slot.
- As Eq. (33) demonstrates, the final memory considers the **effect of the forget gate, the previous memory, the input, and the new memory**.
- In the first term, i.e., $\boldsymbol{f}_t \odot \boldsymbol{c}_{t-1}$, the forget gate $\boldsymbol{f}_t \in [0,1]^p$ controls **how much of the previous memory $\boldsymbol{c}_{t-1}$ should be forgotten**. The closer the $\boldsymbol{f}_t$ is to zero, the more the network forgets the previous memory $\boldsymbol{c}_{t-1}$.
- In the second term, i.e., $\boldsymbol{i}_t \odot \widetilde{\boldsymbol{c}}_t$, the input gate $\boldsymbol{i}_t \in [0,1]^p$ and the new memory cell $\widetilde{\boldsymbol{c}}_t \in [-1,1]^p$ both control **how much of the new input information should be used**. The closer the input gate $\boldsymbol{i}_t$ is to one and the closer the new memory cell $\widetilde{\boldsymbol{c}}_t$ is to ± 1, the more the input information is used.

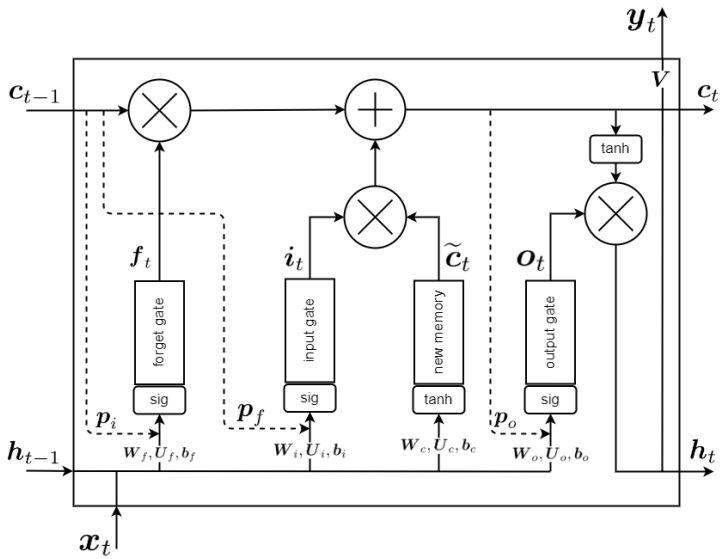


The Final Memory Calculation

- We had:

$$\boldsymbol{c}_t = (\boldsymbol{f}_t \odot \boldsymbol{c}_{t-1}) + (\boldsymbol{i}_t \odot \widetilde{\boldsymbol{c}}_t).$$

- In other words, the first and second terms in Eq. (33) determine the **trade-off of usage of old versus new information** in the sequence.
- The weights of these gates are trained in a way that they **pass or block the input/previous information based on the input sequence and the time step in the sequence**.

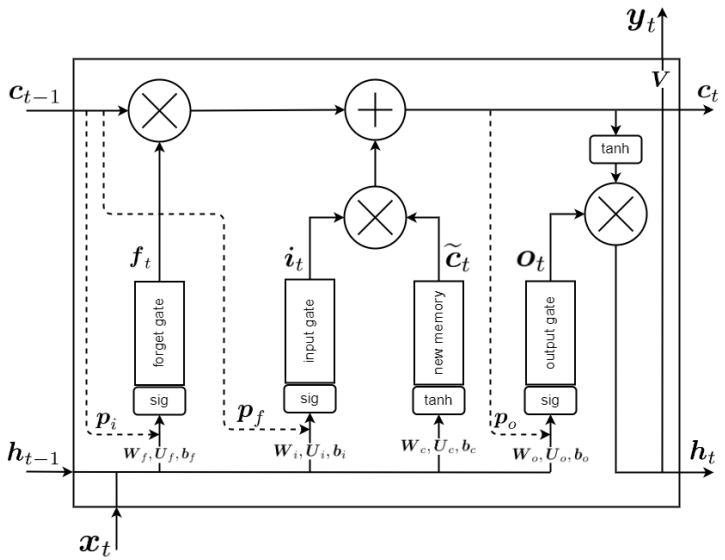


The Hidden State (Block Output)

- After computation of the output of the output gate $\boldsymbol{o}_t$ and the final memory $\boldsymbol{c}_t$, we calculate the **hidden state** $\boldsymbol{h}_t \in [-1, 1]^p$:

$$\boldsymbol{h}_t = \boldsymbol{o}_t \odot \tanh(\boldsymbol{c}_t). \tag{34}$$

- This hidden state is also considered as the **block output** of the LSTM cell.



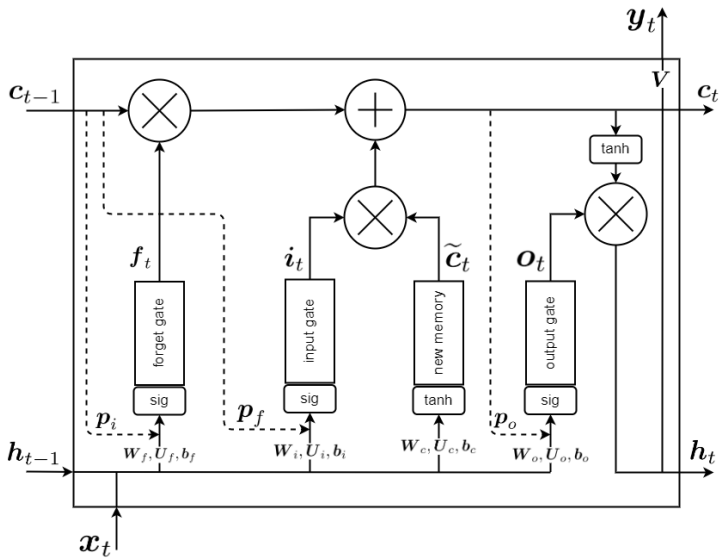
The Output

- The output $\boldsymbol{y}_t \in \mathbb{R}^q$ of the LSTM cell is as follows:

$$\boldsymbol{y}_t = \boldsymbol{V}\boldsymbol{h}_t + \boldsymbol{b}_y, \tag{35}$$

  where $\boldsymbol{V} \in \mathbb{R}^{q \times p}$ and the bias $\boldsymbol{b}_y \in \mathbb{R}^q$ are the learnable weights for the output. It is possible to use an activation function, such as Eq. (6), after this output signal.

- Note that in the literature, the output is sometimes considered to be equal to the hidden state, i.e., $\boldsymbol{y}_t = \boldsymbol{h}_t$, by setting $\boldsymbol{V} = \boldsymbol{I}$ (the identity matrix) and $\boldsymbol{b}_y = \boldsymbol{0}$ (the zero vector).



History and Variants of LSTM

History and Variants of LSTM

- LSTM has gone through various developments and improvements gradually [35].
- Some of the variants of LSTM do not have the peepholes. In this case, the Eqs. (28), (30), and (31) are simplified to:

$$\boldsymbol{i}_t = \text{sig}\big(\boldsymbol{W}_i\, \boldsymbol{h}_{t-1} + \boldsymbol{U}_i\, \boldsymbol{x}_t + \boldsymbol{b}_i\big), \tag{36}$$

$$\boldsymbol{f}_t = \text{sig}\big(\boldsymbol{W}_f\, \boldsymbol{h}_{t-1} + \boldsymbol{U}_f\, \boldsymbol{x}_t + \boldsymbol{b}_f\big), \tag{37}$$

$$\boldsymbol{o}_t = \text{sig}\big(\boldsymbol{W}_o\, \boldsymbol{h}_{t-1} + \boldsymbol{U}_o\, \boldsymbol{x}_t + \boldsymbol{b}_o\big), \tag{38}$$

  respectively.
- In the following, we review a history of variants of the LSTM networks.

Original LSTM

- LSTM was originally proposed by Hochreiter and Schmidhuber in years 1995 to 1997 [15, 16]. We call it the **original LSTM** [16].
- The original LSTM had **only the input and output gates**, introduced before, and it did not have a forget gate.
- It also did **not contain the peepholes**; therefore, its gates were Eqs. (36) and (38).
- The original LSTM trained the network using **BPTT** (introduced before) and a mixture of real-time recurrent learning [2, 4].

Vanilla LSTM

- Later, Gers *et. al.* [34, 33] applied some changes to the original LSTM.
- The **forget gate**, introduced before, was proposed for the first time in [34] to let the network forget its previous states either completely or partially.
- The **peephole connections**, introduced before, were first proposed in [33]. The peepholes let a possible leak of information from the previous or current final memory. This lets the memory control the gates.
- These two papers [34, 33] also incorporated the **full gate recurrence**, in which **all gates receive additional recurrent inputs from all gates at the previous time step**.
- In full gate recurrence, the Eqs. (28), (30), and (31) become:

$$\boldsymbol{i}_t = \text{sig}\big(\boldsymbol{W}_i\,\boldsymbol{h}_{t-1} + \boldsymbol{U}_i\,\boldsymbol{x}_t + (\boldsymbol{p}_i \odot \boldsymbol{c}_{t-1}) + \boldsymbol{b}_i + \boldsymbol{R}_{ii}\,\boldsymbol{i}_{t-1} + \boldsymbol{R}_{if}\,\boldsymbol{f}_{t-1} + \boldsymbol{R}_{io}\,\boldsymbol{o}_{t-1}\big). \tag{39}$$

$$\boldsymbol{f}_t = \text{sig}\big(\boldsymbol{W}_f\,\boldsymbol{h}_{t-1} + \boldsymbol{U}_f\,\boldsymbol{x}_t + (\boldsymbol{p}_f \odot \boldsymbol{c}_{t-1}) + \boldsymbol{b}_f + \boldsymbol{R}_{fi}\,\boldsymbol{i}_{t-1} + \boldsymbol{R}_{ff}\,\boldsymbol{f}_{t-1} + \boldsymbol{R}_{fo}\,\boldsymbol{o}_{t-1}\big). \tag{40}$$

$$\boldsymbol{o}_t = \text{sig}\big(\boldsymbol{W}_o\,\boldsymbol{h}_{t-1} + \boldsymbol{U}_o\,\boldsymbol{x}_t + (\boldsymbol{p}_o \odot \boldsymbol{c}_t) + \boldsymbol{b}_o + \boldsymbol{R}_{oi}\,\boldsymbol{i}_{t-1} + \boldsymbol{R}_{of}\,\boldsymbol{f}_{t-1} + \boldsymbol{R}_{oo}\,\boldsymbol{o}_{t-1}\big), \tag{41}$$

  where $\boldsymbol{R}_{ii}, \boldsymbol{R}_{if}, \boldsymbol{R}_{io}, \boldsymbol{R}_{fi}, \boldsymbol{R}_{ff}, \boldsymbol{R}_{fo}, \boldsymbol{R}_{oi}, \boldsymbol{R}_{of}, \boldsymbol{R}_{oo} \in \mathbb{R}^{p \times p}$ are the learnable recurrent weights.
- Note that the full gate recurrence often **disappeared** in later papers on LSTM.

Vanilla LSTM

- Later, Graves and Schmidhuber adapted the original LSTM and proposed the **vanilla LSTM** in 2005 [18], which is one of the most common LSTMs in the literature.
- The vanilla LSTM incorporated the structures of the original LSTM [16] and the papers [34, 33].
- The full BPTT, introduced before, was used for LSTM in the vanilla LSTM [18].

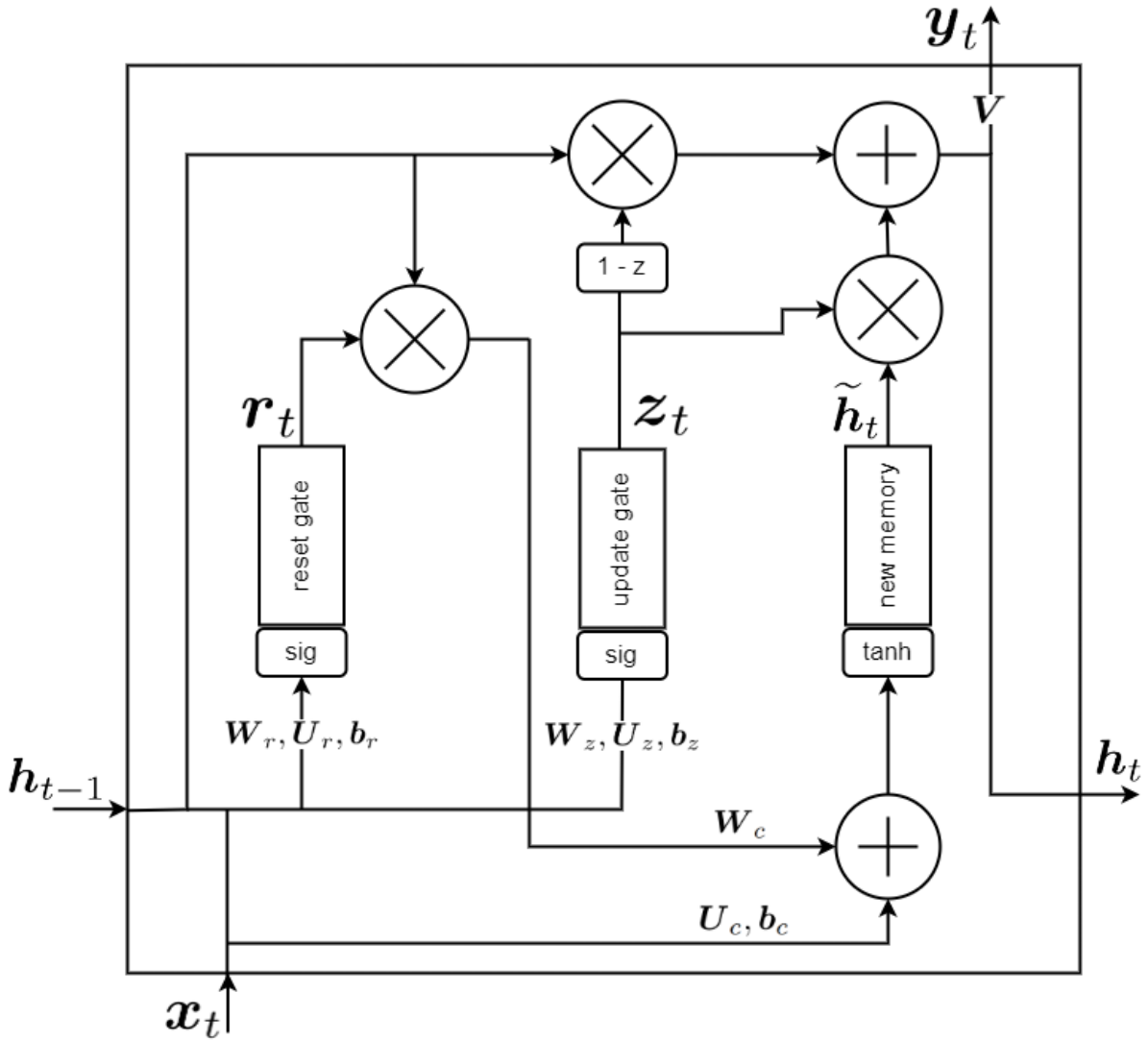
Other LSTM Variants

- There are other variants of LSTM [35, 36]; although, the most common used LSTM is the **vanilla LSTM** [18].
- **BPTT** was used for LSTM training in [18]; however, **Kalman filtering** was used for its training [37] before that. Another training method for LSTM was **evolutionary learning** [38]. **Context-sensitive evolutionary learning** was also used for LSTM training [39].
- Finally in 2014, one the biggest improvements of LSTM was proposed, which was named the **Gated Recurrent Units (GRU)** [17].
- The philosophy of GRU was to **simplify the LSTM cell** because we may not need to have a very complicated cell to learn the sequence information. In other words, GRU raised the question of **whether we need to be that flexible like LSTM to learn the sequence**. GRU is **less flexible than LSTM** but it is **good enough** for sequence learning.
- GRU **redesigned** the LSTM cell by introducing **reset gate, update gate, and new memory cell**; therefore, the **number of gates were reduced from four to three**.
- It was empirically shown in [40] that the performance of LSTM **improves** by using GRU cells.
- Later in 2017, the GRU was further simplified by **merging the reset and update gates into a forget gate** [41].
- Nowadays, GRU is the most commonly used LSTM structure.

Gated Recurrent Units (GRU)

GRU: Fully Gated Unit

- The main GRU was the **fully gated unit** [17], whose gates are introduced in the following.

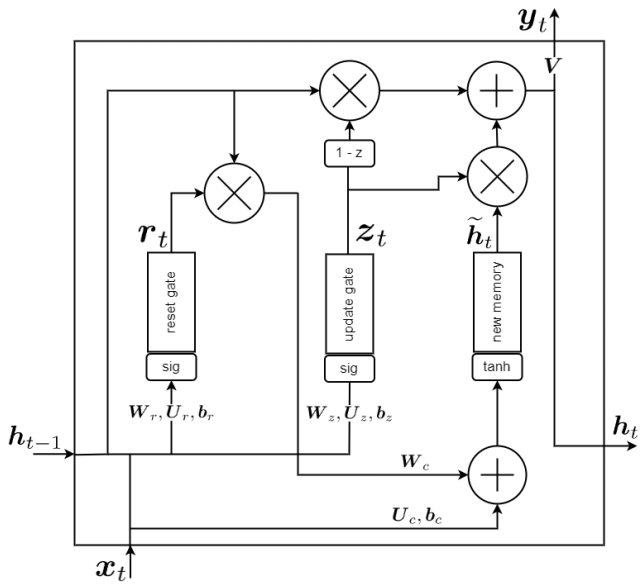


GRU: Fully Gated Unit

- **The Reset Gate**: One of the gates in the GRU cell is the **reset gate**. This gate takes the input at the current time slot, $\boldsymbol{x}_t \in \mathbb{R}^d$, and the hidden state of the last time slot, $\boldsymbol{h}_{t-1} \in [-1, 1]^p$, and outputs the signal $\boldsymbol{r}_t \in [0, 1]^p$:

$$\boldsymbol{r}_t = \text{sig}(\boldsymbol{W}_r \, \boldsymbol{h}_{t-1} + \boldsymbol{U}_r \, \boldsymbol{x}_t + \boldsymbol{b}_r), \tag{42}$$

  where $\boldsymbol{W}_r \in \mathbb{R}^{p \times p}$, $\boldsymbol{U}_r \in \mathbb{R}^{p \times d}$, and the bias $\boldsymbol{b}_r \in \mathbb{R}^p$ are the learnable weights for the reset gate.
- The reset gate considers the **effect of the input and the previous hidden state**, and it controls the **amount of forgetting/resetting the previous information with respect to the new-coming information**.
- Comparing Eqs. (37) and (42) shows that the **reset gate in the GRU cell** is similar to the **forget gate in the LSTM cell**.

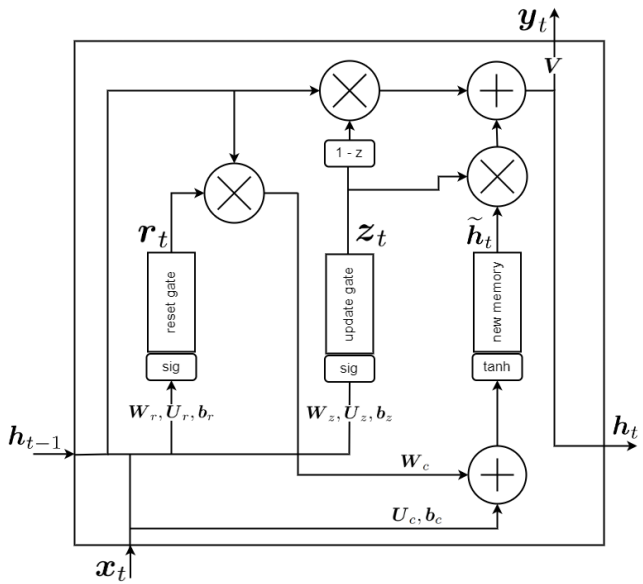


GRU: Fully Gated Unit

- **The Update Gate:** Another gate in the GRU cell is the **update gate**. This gate also takes the input at the current time slot, $\boldsymbol{x}_t \in \mathbb{R}^d$, and the hidden state of the last time slot, $\boldsymbol{h}_{t-1} \in [-1, 1]^p$, and outputs the signal $\boldsymbol{z}_t \in [0, 1]^p$:

$$\boldsymbol{z}_t = \text{sig}(\boldsymbol{W}_z \, \boldsymbol{h}_{t-1} + \boldsymbol{U}_z \, \boldsymbol{x}_t + \boldsymbol{b}_z), \tag{43}$$

  where $\boldsymbol{W}_z \in \mathbb{R}^{p \times p}$, $\boldsymbol{U}_z \in \mathbb{R}^{p \times d}$, and the bias $\boldsymbol{b}_z \in \mathbb{R}^p$ are the learnable weights for the update gate.
- The update gate considers the **effect of the input and the previous hidden state**, and it controls the **amount of using the new input data for updating the cell by the coming information of sequence**.
- Comparing Eqs. (36) and (43) shows that the **update gate in the GRU cell** is similar to the **input gate in the LSTM cell**.

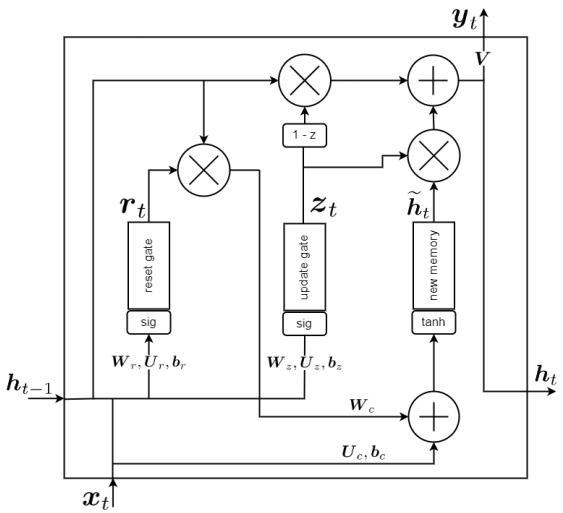


GRU: Fully Gated Unit

- **The New Memory Cell:** The GRU cell includes a gate named the **new memory cell**. This gate takes the input at the current time slot, $\boldsymbol{x}_t \in \mathbb{R}^d$, and the hidden state of the last time slot, $\boldsymbol{h}_{t-1} \in [-1,1]^p$, and outputs the signal $\widetilde{\boldsymbol{h}}_t \in [-1,1]^p$:

$$\widetilde{\boldsymbol{h}}_t = \tanh\Big(\boldsymbol{W}_c\left(\boldsymbol{r}_t \odot \boldsymbol{h}_{t-1}\right) + \boldsymbol{U}_c\,\boldsymbol{x}_t + \boldsymbol{b}_c\Big), \tag{44}$$

  where $\boldsymbol{W}_c \in \mathbb{R}^{p\times p}$, $\boldsymbol{U}_c \in \mathbb{R}^{p\times d}$, and the bias $\boldsymbol{b}_c$ are the learnable weights for the new memory cell.
- This gate considers the **effect of the input and the previous hidden state** to **represent the new information of current input**.
- Comparing Eqs. (32) and (44) shows that the **new memory cell in the GRU cell** is similar to the **new memory cell in the LSTM cell**.
- Note that, in the LSTM cell, the hidden state (see Eq. (34)) and the new memory cell (see Eq. (32)) were **different**; however, the hidden state of the GRU cell (see Eq. (44)) **replaces** the new memory signal in the LSTM cell.

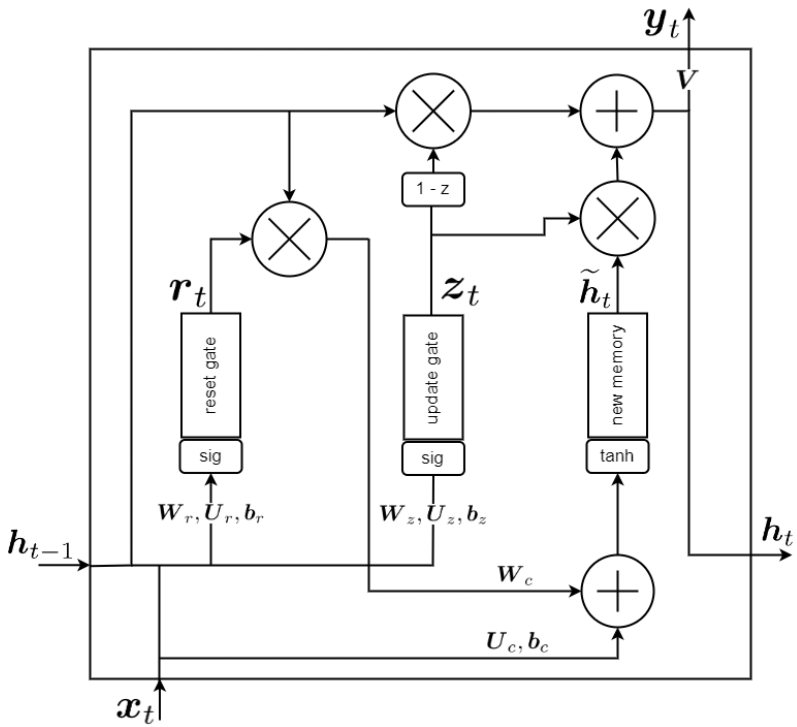


GRU: Fully Gated Unit

- **The Final Memory (Hidden State):** After computation of the outputs of the update gate $\boldsymbol{z}_t$ and the new memory cell $\widetilde{\boldsymbol{h}}_t$, we calculate the **final memory** or the **hidden state** $\boldsymbol{h}_t \in \mathbb{R}^p$:

$$\boldsymbol{h}_t = \big((\mathbf{1} - \boldsymbol{z}_t) \odot \boldsymbol{h}_{t-1}\big) + (\boldsymbol{z}_t \odot \widetilde{\boldsymbol{h}}_t), \tag{45}$$

where $\boldsymbol{h}_{t-1} \in \mathbb{R}^p$ is the hidden state of the previous time slot.



GRU: Fully Gated Unit

- We had:

$$\boldsymbol{h}_t = \left((\mathbf{1} - \boldsymbol{z}_t) \odot \boldsymbol{h}_{t-1}\right) + (\boldsymbol{z}_t \odot \widetilde{\boldsymbol{h}}_t),$$

  where $\boldsymbol{h}_{t-1} \in \mathbb{R}^p$ is the hidden state of the previous time slot.

- As Eq. (45) demonstrates, the final memory considers the **effect of the update gate, the previous memory, and the new memory**.
- In the first term, i.e., $(\mathbf{1} - \boldsymbol{z}_t) \odot \boldsymbol{h}_{t-1}$, the update gate $\boldsymbol{z}_t \in [0, 1]^p$ controls **how much of the previous state $\boldsymbol{h}_{t-1}$ should be used based on the input data**. The closer the $\boldsymbol{z}_t$ is to one (resp. zero), the more the network forgets (resp. considers) the previous state $\boldsymbol{h}_{t-1}$.
- In the second term, i.e., $\boldsymbol{z}_t \odot \widetilde{\boldsymbol{h}}_t$, the update gate $\boldsymbol{z}_t \in [0, 1]^p$ and the new memory cell $\widetilde{\boldsymbol{h}}_t \in [-1, 1]^p$ both control **how much of the new input information should be used**. In other words, it controls **how much the information should be updated by the new information**. The closer the update gate $\boldsymbol{z}_t$ is to one and the closer the new memory cell $\widetilde{\boldsymbol{h}}_t$ is to ± 1, the more the input information is used.
- Overall, the first and second terms in Eq. (45) determine the t**rade-off of usage of old versus new information** in the sequence. The weights of these gates are trained in a way that they **pass or block the input/previous information based on the input sequence and the time step in the sequence**.
- Comparing Eqs. (33) and (45) shows that the **final memory in the GRU cell** is in the form of the **final memory in the LSTM cell**; however, they have somewhat different functionality.

GRU: Minimal Gated Unit

- **Minimal gated unit** [41] is **another variant of GRU** which has simplified the gate by **merging the reset and update gates into a forget gate**. This merging is possible because the **forget gate can control both the previous and new information** of the sequence.
- **The Forget Gate:** The *forget gate* takes the input at the current time slot, $\boldsymbol{x}_t \in \mathbb{R}^d$, and the hidden state of the last time slot, $\boldsymbol{h}_{t-1} \in [-1, 1]^p$, and outputs the signal $\boldsymbol{r}_t \in [0, 1]^p$:

$$\boldsymbol{f}_t = \text{sig}(\boldsymbol{W}_f \, \boldsymbol{h}_{t-1} + \boldsymbol{U}_f \, \boldsymbol{x}_t + \boldsymbol{b}_f), \tag{46}$$

  where $\boldsymbol{W}_f \in \mathbb{R}^{p \times p}$, $\boldsymbol{U}_f \in \mathbb{R}^{p \times d}$, and the bias $\boldsymbol{b}_f \in \mathbb{R}^p$ are the learnable weights for the forget gate.
- The forget gate considers the **effect of the input and the previous hidden state**, and it controls the **amount of forgetting the previous information with respect to the new-coming information**. Therefore, it controls **both forgetting or using the previous memory and using the new coming information**.

GRU: Minimal Gated Unit

- **The New Memory Cell and the Final Memory:** Because the forget gate replaces the reset and the update gate in the minimal gate unit, Eqs. (44) and (45):

$$\widetilde{\boldsymbol{h}}_t = \tanh\Big(\boldsymbol{W}_c\left(\boldsymbol{r}_t \odot \boldsymbol{h}_{t-1}\right) + \boldsymbol{U}_c\,\boldsymbol{x}_t + \boldsymbol{b}_c\Big),$$
$$\boldsymbol{h}_t = \left((\boldsymbol{1} - \boldsymbol{z}_t) \odot \boldsymbol{h}_{t-1}\right) + (\boldsymbol{z}_t \odot \widetilde{\boldsymbol{h}}_t),$$

  are changed to:

$$\widetilde{\boldsymbol{h}}_t = \tanh\Big(\boldsymbol{W}_c\left(\boldsymbol{f}_t \odot \boldsymbol{h}_{t-1}\right) + \boldsymbol{U}_c\,\boldsymbol{x}_t + \boldsymbol{b}_c\Big), \tag{47}$$
$$\boldsymbol{h}_t = \left((\boldsymbol{1} - \boldsymbol{f}_t) \odot \boldsymbol{h}_{t-1}\right) + (\boldsymbol{f}_t \odot \widetilde{\boldsymbol{h}}_t), \tag{48}$$

  respectively, to be the new memory cell and the final memory in the minimal gate unit.

Bidirectional RNN and LSTM

Justification of Bidirectional Processing

- A bidirectional RNN or LSTM network processes the sequence in **both directions**; **left to right** and **right to left**.
- In the first glance, **online causal tasks** such as **reading a text or listening to a speech** do not have access to the **future**. Therefore, bidirectional networks seem to **violate causality** in them.
- However, in many of these tasks, it is possible to **wait for the completion of a part of the sequence such as a sentence and then decide about it**.
- For example, it is normal to **wait for the completion of sentence** in **speech recognition** and then recognize it [18, 19].
- In **text processing**, the text is **usually available except in a streaming text**. Even in streaming text, it is possible to **wait for a sentence to complete**.
- Therefore, it makes sense to use bidirectional networks for processing sequences because, sometimes, the important related word comes after a word and not necessarily before it.
- An example for such a case is the sentence "**The police is chasing the thief**" where the word "**thief**" is a strongly related (opposite) word for the word "**police**". In this sentence, both the words "thief" and "police" are related and it is worth to process the sentence in both directions.

Bidirectional RNN

- The **bidirectional RNN** was first proposed in (1997) [20] and further exploited in (1999) [21].
- It uses **two sets of states each for one of the directions** in the sequence. Let the states for left-to-right and right-to-left processing be denoted by $\overrightarrow{\boldsymbol{h}}_t$ and $\overleftarrow{\boldsymbol{h}}_t$, respectively. In the bidirectional RNN, Eq. (4) is replaced by two equations [42]:

$$\overrightarrow{\boldsymbol{h}}_t = \tanh(\overrightarrow{\boldsymbol{W}}\overrightarrow{\boldsymbol{h}}_{t-1} + \overrightarrow{\boldsymbol{U}}\boldsymbol{x}_t + \overrightarrow{\boldsymbol{b}}_i), \tag{49}$$

$$\overleftarrow{\boldsymbol{h}}_t = \tanh(\overleftarrow{\boldsymbol{W}}\overleftarrow{\boldsymbol{h}}_{t+1} + \overleftarrow{\boldsymbol{U}}\boldsymbol{x}_t + \overleftarrow{\boldsymbol{b}}_i), \tag{50}$$

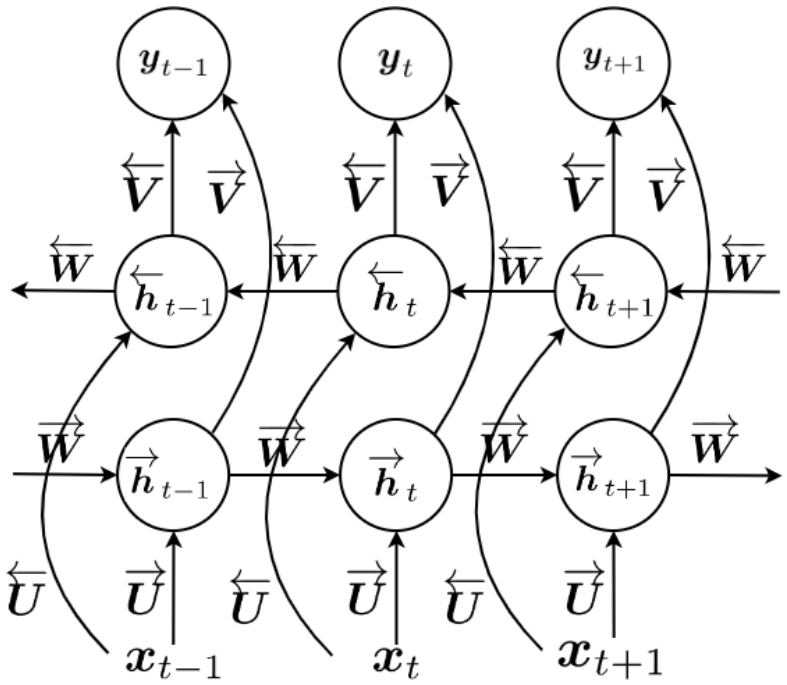
and Eq. (5) is replaced by:

$$\boldsymbol{y}_t = \overrightarrow{\boldsymbol{V}}\overrightarrow{\boldsymbol{h}}_t + \overleftarrow{\boldsymbol{V}}\overleftarrow{\boldsymbol{h}}_t + \boldsymbol{b}_y, \tag{51}$$

where the arrows show the parameters for each direction of processing.

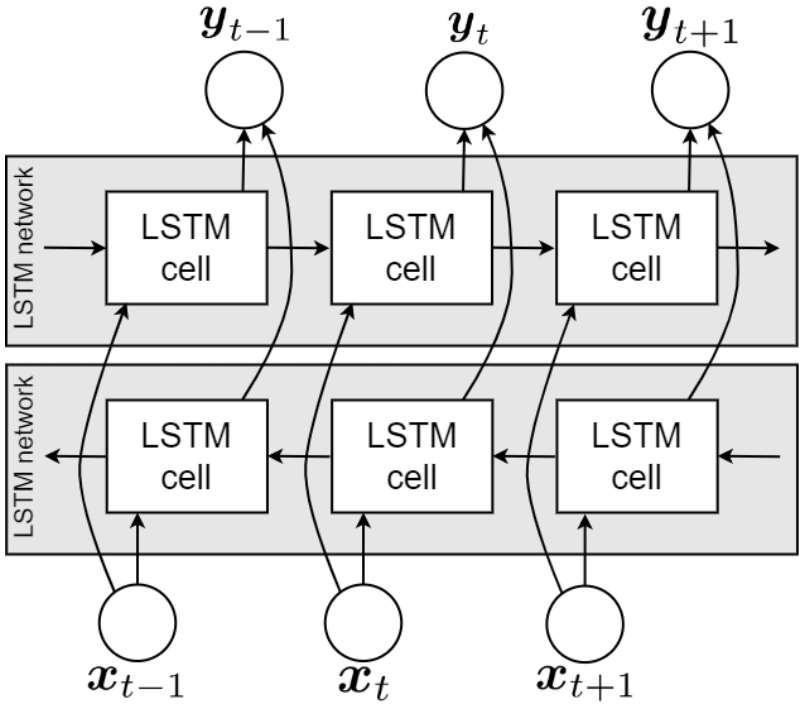
Bidirectional RNN

- The unfolding schematic of the bidirectional RNN is illustrated in figure below. As this figure shows, the **outputs of both directions are connected to an output layer**. In some cases, this output layer may be replaced by a third multi-layer neural network.
- All weights of the bidirectional RNN are trained using **backpropagation through time** similarly to what was explained before.
- It is noteworthy that the deep variant of bidirectional RNN has been proposed in [42].



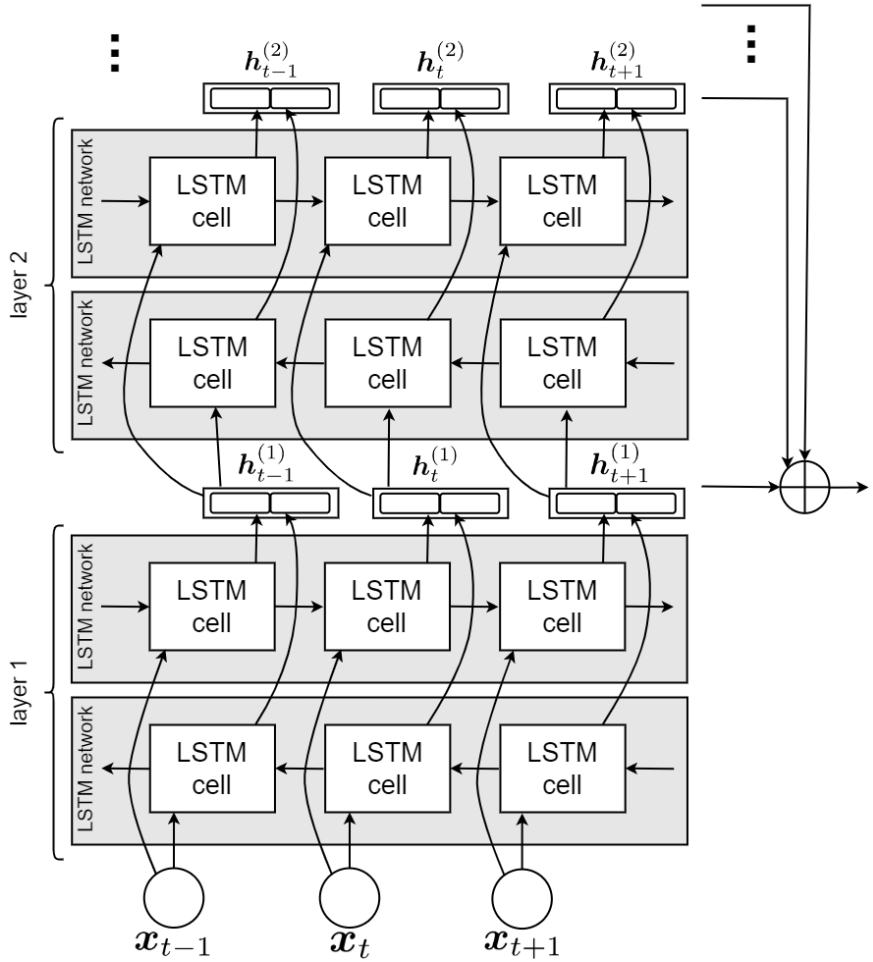
Bidirectional LSTM

- **Bidirectional LSTM** was first proposed in (2005) [18, 19].
- As obvious from its name, the bidirectional LSTM includes **two LSTM networks each of which processes the sequence from one direction**.
- In other words, there are **two LSTM networks which are fed with the sequence in opposite orders**.
- Experiments have shown that the bidirectional LSTM outperforms the unidirectional LSTM [18, 43].



Embeddings from Language Model (ELMo)

- The **Embeddings from Language Model (ELMo)** network, first proposed in (2018) [22], is a language model which makes use of **bidirectional LSTM networks**.
- It is one of the successful **context-aware language modeling networks**.
- ELMo contains L layers of bidirectional LSTM networks where the output of each bidirectional LSTM is fed to the next bidirectional LSTM.



Embeddings from Language Model (ELMo)

- In the bidirectional LSTM networks of ELMo, $\boldsymbol{V} = \boldsymbol{I}$ is set so that the output $\boldsymbol{y}$ becomes equal to the hidden states $\boldsymbol{h}$.
- At time slot t and layer l, the outputs (or hidden states) of the two directions of LSTM are concatenated together to make $\boldsymbol{h}_t^{(l)}$:

$$\boldsymbol{h}_t^{(l)} := [\overrightarrow{\boldsymbol{h}}_t^{(l)\top}, \overleftarrow{\boldsymbol{h}}_t^{(l)\top}]^\top.$$

- Then, a linear combination of these hidden states of layers is considered to be the embedding vector of ELMo network at time t [22]:

$$\boldsymbol{y}_t^{\text{ELMo}} := \gamma \sum_{l=1}^{L} s_l \, \boldsymbol{h}_t^{(l)}, \tag{52}$$

where γ and $\{s_l\}_{l=1}^{L}$ are the hyperparameter scalar weights which are determined according to the specific task (e.g., question answering, translation, etc) in natural language processing.

Acknowledgment

- This slide deck is based on our tutorial paper: "Recurrent Neural Networks and Long Short-Term Memory Networks: Tutorial and Survey" [44].
- Some slides of this slide deck are inspired by teachings of Prof. Ali Ghodsi at University of Waterloo, Department of Statistics.

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