CEE 616: Probabilistic Machine Learning

M3 Deep Neural Networks:
Lecture 3D: Neural Networks for Sequences

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Outline

Classical form of dynamical system

A dynamical system is defined by the recurrent equation:

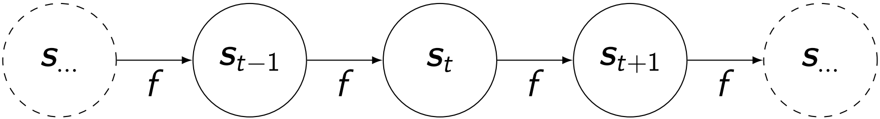
$$\boldsymbol{s}_t = f(\boldsymbol{s}_{t-1}; \boldsymbol{\theta}) \tag{1}$$

where $\boldsymbol{s}_t$ is the state of the system and $\boldsymbol{\theta}$ are the parameters of f

- recurrence: $\boldsymbol{s}_t$ is identically defined as $\boldsymbol{s}_{t-1}$
- for τ time steps, definition is applied $\tau - 1$ times, e.g.

$$\boldsymbol{s}^{(3)} = f(\boldsymbol{s}^{(2)}; \boldsymbol{\theta}) = f(f(\boldsymbol{s}^{(1)}; \boldsymbol{\theta}); \boldsymbol{\theta})$$

- writing out the recurrence relation in full yields an *unfolded* computational graph

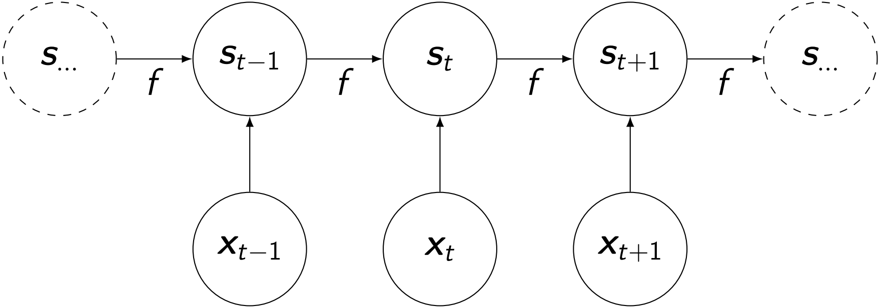


Dynamical system driven by external signal

The state $\boldsymbol{s}_t$ of a dynamical system driven by an external signal $\boldsymbol{x}_t$ can be described by

$$\boldsymbol{s}_t = f(\boldsymbol{s}_{t-1}; \boldsymbol{x}_t; \boldsymbol{\theta}) \tag{2}$$

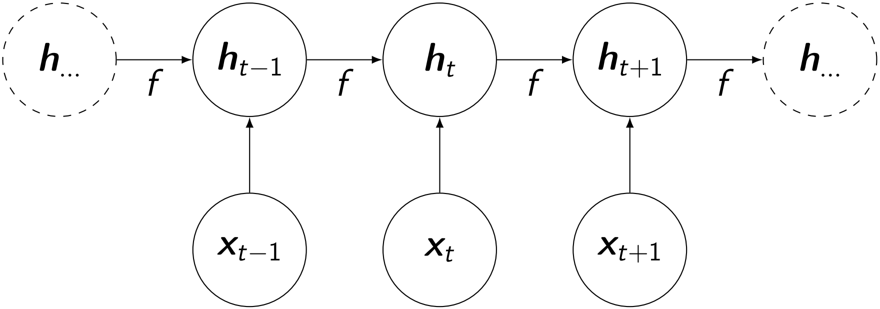
- the state $\boldsymbol{s}_t$ includes information about the entire past sequence
- the unfolded computational graph:



Recurrent neural networks as sequence models

- Dynamical systems are sequences (temporal, etc)
- Recurrence relations can be modeled by *recurrent* neural networks (RNNs)
- In an RNN, hidden units $\boldsymbol{h}$ represent the state $\boldsymbol{s}$ of the system:

$$\boldsymbol{h}_t = f(\boldsymbol{h}_{t-1}, \boldsymbol{x}_t; \boldsymbol{\theta}) \tag{3}$$



Computational advantages of RNN

- Transition function f maps past variable-length sequence $(\boldsymbol{x}_t, \boldsymbol{x}_{t-1}, \boldsymbol{x}^{(t-2)}, \ldots, \boldsymbol{x}^{(2)}, \boldsymbol{x}^{(1)})$ to fixed-length state $\boldsymbol{h}_t$
- Model always has same input size $\boldsymbol{h}_{t-1}$
- Single function f with same parameters operates on all time steps
- Further architectural features (including output layers) use information from $\boldsymbol{h}$ to make predictions

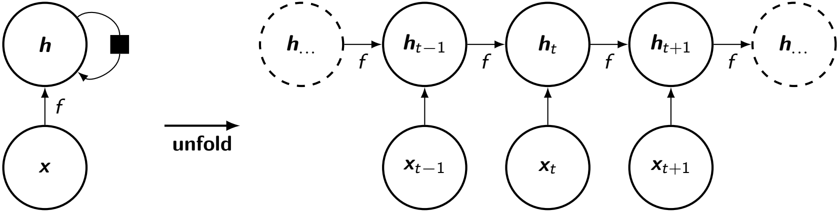


Figure: Recurrent network with no outputs. L: recurrent graph; R: time-unfolded computational graph. (Black square indicates time-step-delayed interaction)

RNN models for sequence tasks

- **Generation** (`Vec2Seq`): $f_{\theta} : \mathbb{R}^{D} \rightarrow \mathbb{R}^{N_{\infty} C}$
  - Input: vector of size D
  - Output: arbitrary-length sequence of size C vectors
  - Applications: language modeling, image captioning
- **Classification** (`Seq2Vec`): $f_{\theta} : \mathbb{R}^{TD} \rightarrow \mathbb{R}^{C}$
  - Input: variable-length sequence
  - Output: fixed-length output vector (e.g. class label)
- **Translation** (`Seq2Seq`): $f_{\theta} : \mathbb{R}^{TD} \rightarrow \mathbb{R}^{T'C}$
  - Aligned case: $T = T'$
  - Unaligned case: $T \neq T'$
  - Application: neural machine translation

Vec2Seq model for sequence generation

Vec2Seq models map a fixed-length vector $\boldsymbol{x} \in \mathbb{R}^D$ onto a distribution over sequences $\boldsymbol{Y} \in \mathbb{R}^{T \times C}$ (or, $\boldsymbol{y}_{1:T} \in \boldsymbol{R}^C$; that is, T sequences, with each y_t a vector of length C)

Thus, the generative model is given by:

$$p(\boldsymbol{y}_{1:T}|\boldsymbol{x}) = \sum_{\boldsymbol{h}_{1:T}} p(\boldsymbol{y}_{1:T}, \boldsymbol{h}_{1:T}|\boldsymbol{x}) \tag{4}$$

where $\boldsymbol{h}_t$ is the hidden state of the model.
By the multiplication rule, we can write:

$$\sum_{\boldsymbol{h}_{1:T}} p(\boldsymbol{y}_{1:T}, \boldsymbol{h}_{1:T}|\boldsymbol{x}) = \sum_{\boldsymbol{h}_{1:T}} \prod_{t=1}^{T} p(\boldsymbol{y}_t|\boldsymbol{h}_t) p(\boldsymbol{h}_t|\boldsymbol{h}_{t-1}, \boldsymbol{y}_{t-1}, \boldsymbol{x}) \tag{5}$$

- Initial hidden state: $p(\boldsymbol{h}_1|\boldsymbol{h}_0, \boldsymbol{y}_0, \boldsymbol{x}) = p(\boldsymbol{h}_1|\boldsymbol{x})$

Vec2Seq model (cont.)

The output distribution is given by:

$$p(\boldsymbol{y}_t|\boldsymbol{h}_t) = \begin{cases} \text{Cat}(\boldsymbol{y}_t|\mathcal{S}(\boldsymbol{W}_{ho}\boldsymbol{h}_t + \boldsymbol{b}_o)), & \text{(qualitative outputs)} \\ \mathcal{N}(\boldsymbol{y}_t|\boldsymbol{W}_{ho}\boldsymbol{h}_t + \boldsymbol{b}_o, \sigma^2\boldsymbol{I}), & \text{(real-valued outputs)} \end{cases} \tag{6}$$

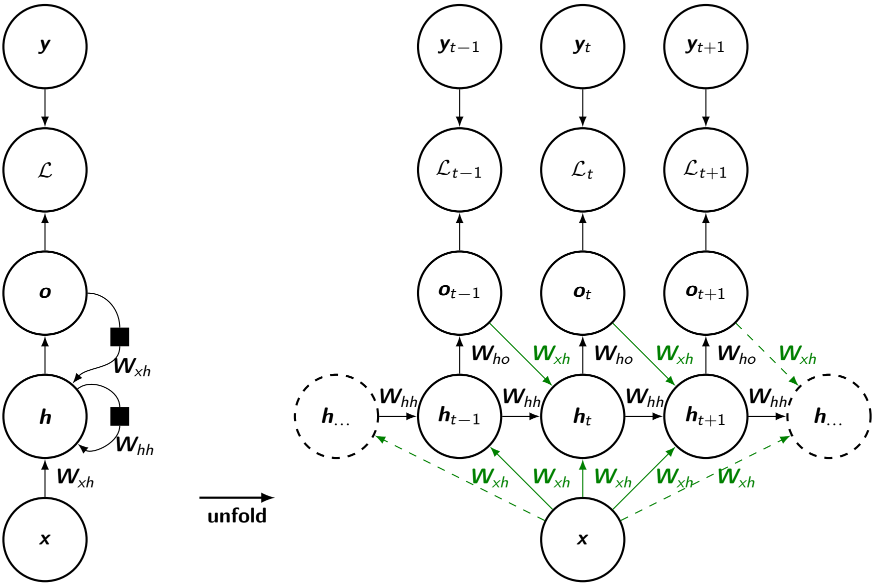
- $\boldsymbol{W}_{ho}$: matrix of hidden–output weights
- $\boldsymbol{b}_o$: bias term
- $\boldsymbol{y}_t$ is the observed vector, while $\boldsymbol{o}_t$ is the predicted value (using NN notation)

The hidden state is typically deterministic:

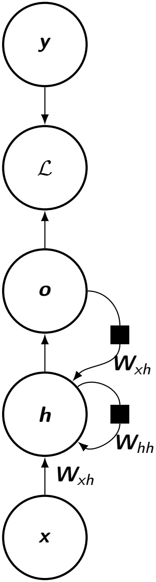
$$\boldsymbol{h}_t = \varphi(\boldsymbol{W}_{xh}[\boldsymbol{x}; \boldsymbol{o}_{t-1}] + \boldsymbol{W}_{hh}\boldsymbol{h}_{t-1} + \boldsymbol{b}_h) \tag{7}$$

- $\boldsymbol{W}_{xh}$: input–hidden weight matrix
- $\boldsymbol{W}_{hh}$: hidden–hidden weight matrix
- $\boldsymbol{b}_h$: bias term

Vec2Seq RNN: circuit diagram and computation graph



Vec2Seq model summary



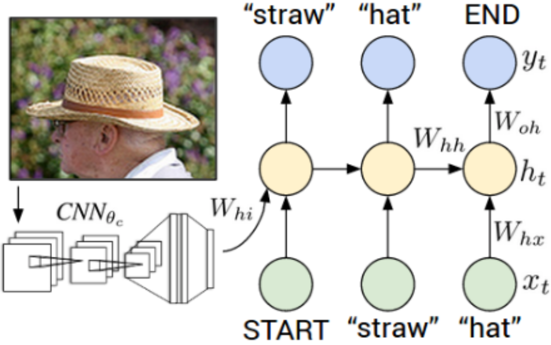
Update equations:

$$\begin{aligned}
\boldsymbol{a}_t &= \boldsymbol{W}_{xh}[\boldsymbol{x}; \boldsymbol{o}_{t-1}] + \boldsymbol{W}_{hh}\boldsymbol{h}_{t-1} + \boldsymbol{b}_h && (8)\\
\boldsymbol{h}_t &= \varphi(\boldsymbol{a}_t) && (9)\\
\boldsymbol{o}_t &= \boldsymbol{W}_{oh}\boldsymbol{h}_t + \boldsymbol{b}_o && (10)\\
\hat{\boldsymbol{y}}_t &= \mathcal{S}(\boldsymbol{o}_t) && (11)
\end{aligned}$$

- In typical applications, $\boldsymbol{o}_t = [o_{t1}, o_{t2}, \ldots, o_{tC}]$ (e.g. one-hot vector, each representing a character)
- $\boldsymbol{o}_t$ depends on $\boldsymbol{h}_t$, which depends on $\boldsymbol{o}_{t-1}$
- $\boldsymbol{o}_t$ depends on *all* past observations and the fixed input $\boldsymbol{x}$
- $[\boldsymbol{x}; \boldsymbol{o}_{t-1}]$ denotes the stacking of $\boldsymbol{x}$ and $\boldsymbol{o}_{t-1}$
- So, if $\boldsymbol{x} \in \mathbb{R}^D$, $\boldsymbol{o}_t \in \mathbb{R}^C$, and $\boldsymbol{h}_t \in \mathbb{R}^M$, then $\boldsymbol{W}_{xh} \in \mathbb{R}^{(D+C)\times M}$
- M is the number of units (neurons) in the hidden layer

Application: image captioning

Image or processed version from CNN is used as input, with output as sequence of descriptive words



Source: `https://towardsdatascience.com/image-captioning-in-deep-learning-9cd23fb4d8d2`

Seq2Seq model: aligned case

Seq2seq models map a sequence of vectors $\boldsymbol{x}_{1:T} \in \mathbb{R}^D$ onto another sequence $\boldsymbol{y}_{1:T'} \in \mathbb{R}^C$. We consider the aligned case (dense sequence modeling) where $T = T'$:

$$p(\boldsymbol{y}_{1:T}|\boldsymbol{x}_{1:T}) = \sum_{\boldsymbol{h}_{1:T}} \prod_{t=1}^{T} p(\boldsymbol{y}_t|\boldsymbol{h}_t)\mathbb{I}(\boldsymbol{h}_t = f(\boldsymbol{h}_{t-1}, \boldsymbol{x}_t)) \tag{12}$$

where the initial hidden state is $\boldsymbol{h}_1 = f(\boldsymbol{h}_0, \boldsymbol{x}_1) = f_0(\boldsymbol{x}_1)$.

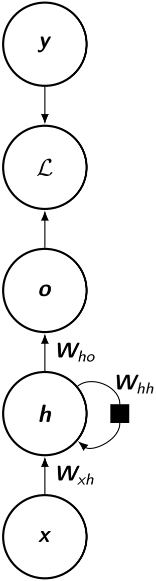
- The hidden state is given by:

$$\boldsymbol{h}_t = \varphi(\boldsymbol{W}_{xh}\boldsymbol{h}_t + \boldsymbol{W}_{hh}\boldsymbol{h}_{t-1} + \boldsymbol{h}) \tag{13}$$

- The output is given by:

$$\boldsymbol{o}_t = \boldsymbol{W}_{ho}\boldsymbol{h}_t + \boldsymbol{b}_o \tag{14}$$

Aligned seq2seq circuit diagram



The update equations for a seq2seq RNN are given by

$$\boldsymbol{a}_t = \boldsymbol{b}_h + \boldsymbol{W}_{hh}\boldsymbol{h}_{t-1} + \boldsymbol{W}_{xh}\boldsymbol{x}_t \tag{15}$$

$$\boldsymbol{h}_t = \tanh(\boldsymbol{a}_t) \tag{16}$$

$$\boldsymbol{o}_t = \boldsymbol{b}_o + \boldsymbol{W}_{ho}\boldsymbol{h}_t \tag{17}$$

- $\boldsymbol{x}$: input sequence
- $\boldsymbol{h}$: hidden units
- $\boldsymbol{b}_h$, $\boldsymbol{b}_o$: bias vectors
- $\boldsymbol{W}_{xh}$: weight matrix of input–hidden unit connections
- $\boldsymbol{W}_{hh}$: weight matrix of hidden–hidden unit connections
- $\boldsymbol{W}_{ho}$: weight matrix of hidden–output unit connections
- $\boldsymbol{o}$: output vector
- $\boldsymbol{y}$ target sequence
- $\mathcal{L}$: loss function measuring error between $\hat{\boldsymbol{y}}$ and $\boldsymbol{y}$

Seq2seq model: unaligned case

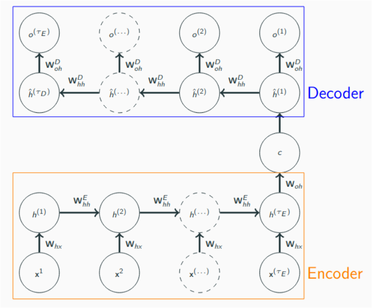
To map a sequence of length T to another of length T', we use an **encoder-decoder architecture**:

- The encoder f_e maps the input sequence onto a context vector

$$\boldsymbol{c} = f_e(\boldsymbol{x}_{1:T}) \tag{18}$$

- The decoder f_d generates the output sequence by mapping from the context vector:

$$\boldsymbol{y}_{1:T'} = f_d(\boldsymbol{c}) \tag{19}$$



Source: `https://www.inf.ed.ac.uk/teaching/courses/mlp/2019-20/lectures/mlp09-rnn.pdf`

Illustration of seq2seq for translation

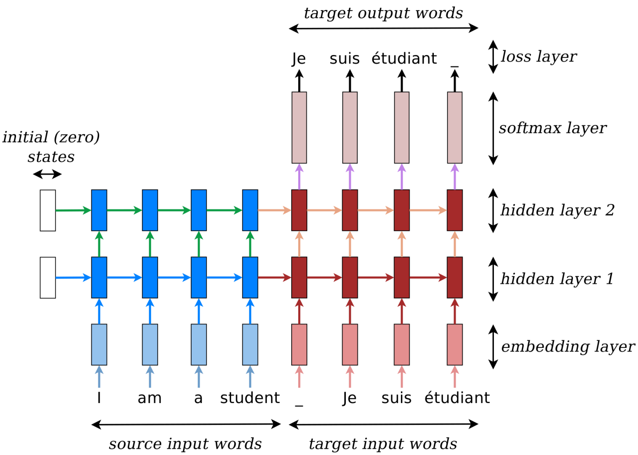
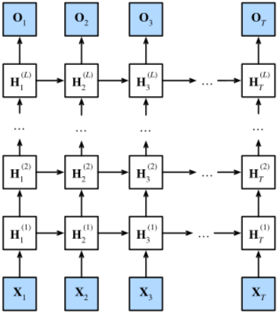


Illustration of seq2seq model for English-to-French translation.

Source: `https://github.com/probml/pml-book/blob/main/book1-figures/Figure_15.8_A.png`

Deep RNNs

More complex models can be developed by stacking **hidden chains**.



Source: `https://d2l.ai/chapter_recurrent-modern/deep-rnn.html`

The hidden state for layer ℓ at time t is then given by:

$$\boldsymbol{h}_t^\ell = \varphi(\boldsymbol{W}_{xh}^\ell \boldsymbol{h}_t^{\ell-1} + \boldsymbol{W}_{hh}^\ell \boldsymbol{h}_{t-1}^\ell + \boldsymbol{h}^\ell) \tag{20}$$

And the output at each time step as:

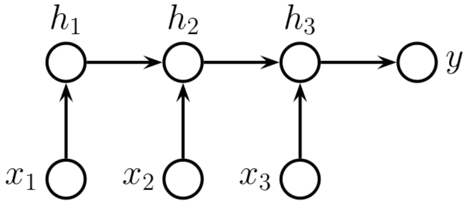
$$\boldsymbol{o}_t = \boldsymbol{W}_{ho} \boldsymbol{h}_t^L + \boldsymbol{b}_o \tag{21}$$

Seq2vec models for sequence classification

Seq2vec models map a sequence $\boldsymbol{x}_{1:T} \in \mathbb{R}^D$ onto a fixed length vector $\boldsymbol{y} \in \mathbb{R}^C$ (e.g. class label)
In the simple approach, the output depends on final state only.
Thus, the model can be specified as:

$$p(y|\boldsymbol{x}_{1:T}) = \mathrm{Cat}(y|\mathcal{S}(\boldsymbol{W}\boldsymbol{h}_T) \tag{22}$$

where $\boldsymbol{h}_T$ is the final state of the RNN



Bidirectional seq2vec model

Bidirectional models allow the output to depend on the entire sequence (i.e. the hidden state depends on past and future contexts):

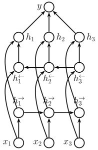
$$\boldsymbol{h}_t^{\rightarrow} = \varphi(\boldsymbol{W}_{xh}^{\rightarrow}\boldsymbol{x}_t + \boldsymbol{W}_{hh}^{\rightarrow}\boldsymbol{h}_{t-1}^{\rightarrow} + \boldsymbol{b}_h^{\rightarrow}) \quad (23)$$

$$\boldsymbol{h}_t^{\leftarrow} = \varphi(\boldsymbol{W}_{xh}^{\leftarrow}\boldsymbol{x}_t + \boldsymbol{W}_{hh}^{\leftarrow}\boldsymbol{h}_{t+1}^{\leftarrow} + \boldsymbol{b}_h^{\leftarrow}) \quad (24)$$

- State at time t: $\boldsymbol{h}_t = [\boldsymbol{h}_t^{\rightarrow}, \boldsymbol{h}_t^{\leftarrow}]$
- Final classification then given by:

$$p(y|\boldsymbol{x}_{1:T}) = \mathrm{Cat}(y|\boldsymbol{W}\mathcal{S}(\overline{\boldsymbol{h}})) \quad (25)$$

where $\overline{\boldsymbol{h}} = \frac{1}{T}\sum_{t=1}^{T}\boldsymbol{h}_t$



Long-term dependencies in RNNs

- RNNs involve multiple compositions of the same function, e.g. in a simple network:

$$\boldsymbol{h}_t = \boldsymbol{W}^T \boldsymbol{h}_{t-1} \tag{26}$$

- Given the above recurrence relation, we can then write:

$$\begin{aligned} \boldsymbol{h}_t &= (\boldsymbol{W}^t)^T \boldsymbol{h}^{(0)} && (27) \\ \boldsymbol{h}_t &= \boldsymbol{Q}^T \boldsymbol{\Lambda}^t \boldsymbol{Q} \boldsymbol{h}^{(0)} && (28) \end{aligned}$$

  where $\boldsymbol{\Lambda}$ is a diagonal matrix of eigenvalues λ_i
- Thus the eigenvalues are raised to the power of t
  - $\lambda_i < 1$: decay to zero (vanishing gradients)
  - $\lambda_i > 1$: exploding gradients

RNN considerations

- RNNs are fitted via the **backpropagation through time** (BPTT) algorithm
  - computationally expensive
- Challenging to learn **long-term dependencies** due to vanishing/exploding gradients. Strategies:
  - skip connections across time
  - leaky units across different time scales (via linear self-connections that weight information from the past)

$$\boldsymbol{h}_t \leftarrow \alpha \boldsymbol{h}_{t-1} + (1-\alpha)\boldsymbol{h}_t \tag{29}$$

    where α is the weight
  - gradient clipping
  - train RNN to reset irrelevant states to zero at various points in sequence (via gated units)

Gated RNNs

Gated RNNs are a generalization of leaky units that allow for time-dependent variation of self-connection weights.

- In leaky units, the weights are either manually set or learned as parameters, in order to accumlate information
- Gated RNNs enable the "forgetting" of old states
- Most effective gated RNNs in use:
  - long short-term memory (LSTM); Hochreiter and Schmidhuber, 1997
  - gated recurrent unit (GRU) Cho et al., 2014
  - The LSTM cell has four neural network layers (compared to one layer in the standard RNN)

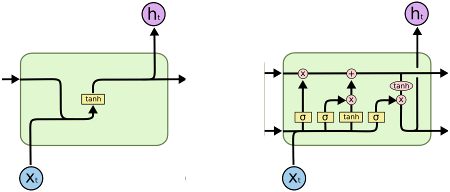
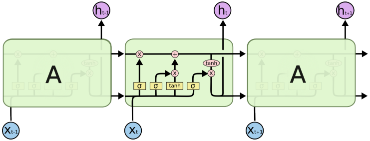


Figure: L: hidden unit in standard RNN; R: hidden unit in LSTM.

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

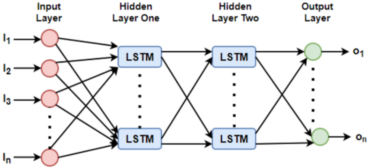
LSTM chains and blocks

- There are as many LSTM cells are there are hidden units in current implementations



△ Repeating module in LSTM network (https://colah.github.io/posts/2015-08-Understanding-LSTMs/)

- A chain of LSTM cells in a network may be referred to as "layer" or "block" (usage/terminology differs)



△ LSTM network with 2 blocks of LSTM cells

(https://link.springer.com/article/10.1007/s42452-021-04421-x)

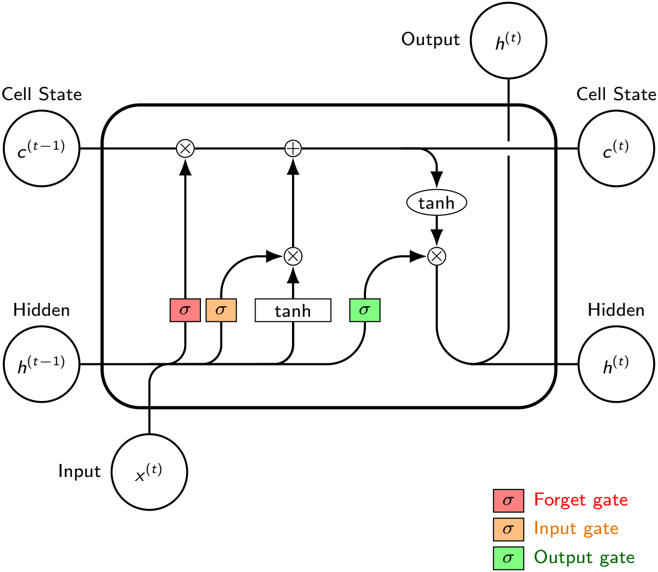
LSTM gates

Gates allow the LSTM to decide which signal to pass or block by outputting a number in the interval $[0, 1]$ (via a sigmoid activation)

The LSTM cell consists of three gates:

- **Forget gate:** Decides what information will be discarded from cell state. Contained in sigmoid layer that outputs number between 0 and 1 for each number in cell state $\boldsymbol{c}_{t-1}$
- **Input gate:** Decides what new information to store in cell state. Comprises
  - a. sigmoid layer which decides values to update
  - b. tanh layer to create new candidate values for the state
- **Output gate:** Decides what information is passed from cell state to output. Comprises
  - a. sigmoid layer to decide portion of cell state to retain
  - b. tanh later which admits state values in $[-1, 1]$

LSTM cell anatomy



Forget gate

The forget gate determines what information should be discarded from the cell. The gate unit is given by:

$$f_{t,i} = \boldsymbol{\sigma}\left(b_i^f + \sum_j U_{i,j}^f x_{t,j} + \sum_j W_{i,k}^f h_{t-1,k}\right) \tag{30}$$

where:

- $f_{t,i}$: forget gate value for timestep t and cell i (between 0 and 1)
- $\boldsymbol{x}_t$: current input vector
- $\boldsymbol{h}_{t-1}$: hidden state from previous cell
- $\boldsymbol{b}^f$, $\boldsymbol{U}^f$, $\boldsymbol{W}^f$: biases, input weights and recurrent weights for the forget gates

Input gate

The input gate determines what new information to include in the cell. Its unit is given by:

$$g_{t,i} = \boldsymbol{\sigma} \left(b_i^g + \sum_j U_{i,j}^g x_{t,j} + \sum_j W_{i,k}^g h_{t-1,k} \right) \tag{31}$$

where:

- $\boldsymbol{b}^g$, $\boldsymbol{U}^g$, $\boldsymbol{W}^g$: biases, input weights and recurrent weights for the input gates
- $\boldsymbol{h}_{t-1}$: hidden state from previous cell

State update

The cell state update is given by:

$$c_{t,i} = f_{t,i} c_{t-1,i} + g_{t,i} \tanh\left(b_i + \sum_j U_{i,j} x_{t,j} + \sum_j W_{i,k} h_{t-1,j} \right) \tag{32}$$

- $\boldsymbol{b}$, $\boldsymbol{U}$, $\boldsymbol{W}$ are biases, input weights and recurrent weights, respectively, into the LSTM cell
- $c_{t-1,i}$ is the cell state for the prior timestep
- The term in purple represents the signal from new information $\boldsymbol{x}_t$ that may be included in the cell state update. Let us call it $\tilde{\boldsymbol{c}}_t$
- Thus, we may write the cell state update as:

$$c_{t,i} = f_{t,i} c_{t-1,i} + g_{t,i} \tilde{c}_{t,i} \tag{33}$$

- In this form, we explicitly how the cell state is composed of a weighted sum of the prior cell state (accumulated information) and new inputs

Output gate

The output gate unit is given by:

$$q_{t,i} = \boldsymbol{\sigma}\left(b_i^o + \sum_j U_{i,j}^o x_{t,j} + \sum_j W_{i,j}^o h_{t-1,j}\right) \tag{34}$$

And the final output (hidden state) of the LSTM cell is:

$$h_{t,i} = \tanh(c_{t,i}) q_{t,i} \tag{35}$$

LSTM: putting it all together

The complete set of LSTM update equations is given by:

$$\begin{aligned}
\boldsymbol{F}_t &= \sigma(\boldsymbol{X}_t \boldsymbol{W}_{xf} + \boldsymbol{H}_{t-1} \boldsymbol{W}_{hf} + \boldsymbol{b}_f) && (36)\\
\boldsymbol{I}_t &= \sigma(\boldsymbol{X}_t \boldsymbol{W}_{xi} + \boldsymbol{H}_{t-1} \boldsymbol{W}_{hi} + \boldsymbol{b}_i) && (37)\\
\boldsymbol{O}_t &= \sigma(\boldsymbol{X}_t \boldsymbol{W}_{xo} + \boldsymbol{H}_{t-1} \boldsymbol{W}_{ho} + \boldsymbol{b}_o) && (38)\\
\tilde{\boldsymbol{C}}_t &= \tanh(\boldsymbol{X}_t \boldsymbol{W}_{xc} + \boldsymbol{H}_{t-1} \boldsymbol{W}_{hc} + \boldsymbol{b}_c) && (39)\\
\boldsymbol{C}_t &= \boldsymbol{F}_t \odot \boldsymbol{C}_{t-1} + \boldsymbol{I}_t \odot \tilde{\boldsymbol{C}}_t && (40)\\
\boldsymbol{H}_t &= \boldsymbol{O}_t \odot \tanh(\boldsymbol{C}_t) && (41)
\end{aligned}$$

where:

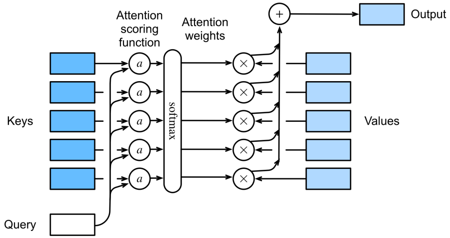
- $\boldsymbol{F}_t$, $\boldsymbol{I}_t$, $\boldsymbol{O}_t$: forget, input and output gate vectors at time t
- $\boldsymbol{C}_t$: cell state vector at time t
- $\boldsymbol{H}_t$: hidden state (output) vector at time t
- $\odot$: element-wise (Hadamard) product

Attention

- Typical neural networks process all parts of the input with equal importance:

$$\boldsymbol{z} = \varphi(\boldsymbol{W}\boldsymbol{v}), \quad \boldsymbol{v} \in \mathbb{R}^{v}, \boldsymbol{W} \in \mathbb{R}^{v' \times v} \tag{42}$$

- Attention mechanisms were introduced to allow flexibility: i.e. for models to dynamically focus on the most relevant portion of the input when generating each part of the output.
- This is typically done by computing a weighted sum of the input features $\boldsymbol{v}_i$, where the weights are learned based on the input itself.



△ Attention as weighted sum of values (Source: https://github.com/probml/pml-book/blob/main/book1-figures/Figure_15.16.pdf)

Attention scores

- Given m values $\boldsymbol{V} \in \mathbb{R}^{m \times v}$
- input query vector $\boldsymbol{q} \in \mathbb{R}^{q}$
- m keys $\boldsymbol{K} \in \mathbb{R}^{m \times k}$
- Attention output is given by:

$$\text{Attention}(\boldsymbol{q}, \boldsymbol{K}, \boldsymbol{V}) = \sum_{i=1}^{m} \alpha_i \boldsymbol{v}_i \tag{43}$$

where the attention weights α_i are computed as:

$$\alpha_i = \frac{\exp(a(\boldsymbol{q}, \boldsymbol{k}_i))}{\sum_{j=1}^{m} \exp(a(\boldsymbol{q}, \boldsymbol{k}_j))} \tag{44}$$

and $a(\boldsymbol{q}, \boldsymbol{k}_i)$ is a score function that measures the similarity between the query $\boldsymbol{q}$ and key vectors $\boldsymbol{k}_i$.

Commonly used score functions

Common choices for the score function $a(\boldsymbol{q}, \boldsymbol{k}_i)$ include:

- Dot product:

$$a(\boldsymbol{q}, \boldsymbol{k}_i) = \boldsymbol{q}^T \boldsymbol{k}_i \tag{45}$$

  Often it is scaled by $\sqrt{d}$ to ensure the variance of the score remains 1:

$$a(\boldsymbol{q}, \boldsymbol{k}_i) = \frac{\boldsymbol{q}^T \boldsymbol{k}_i}{\sqrt{d}} \tag{46}$$

- Additive (Bahdanau) attention:

$$a(\boldsymbol{q}, \boldsymbol{k}_i) = \boldsymbol{w}_a^T \tanh(\boldsymbol{W}_q \boldsymbol{q} + \boldsymbol{W}_k \boldsymbol{k}_i + \boldsymbol{b}_a) \tag{47}$$

  where $\boldsymbol{w}_a$, $\boldsymbol{W}_q$, $\boldsymbol{W}_k$, and $\boldsymbol{b}_a$ are learnable parameters.

Transformers

A transformer is a seq2seq model architecture that uses self-attention for the encoder and decoder in place of an RNN.

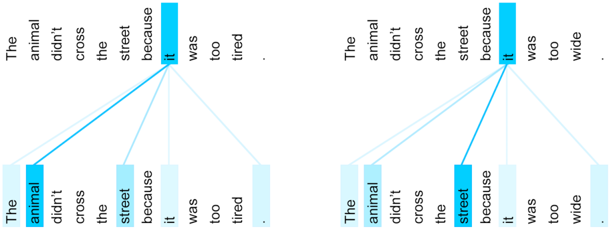
- Self-attention allows the model to weigh the importance of different words in the input sequence when encoding each word.

$$\boldsymbol{y}_i = \text{Attention}(\boldsymbol{x}_i, (\boldsymbol{x}_1, \boldsymbol{x}_1), \ldots, (\boldsymbol{x}_n, \boldsymbol{x}_n)) \tag{48}$$

  where query is $\boldsymbol{x}_i$, and keys and values are all input vectors.
- Transformers have been shown to outperform RNNs in various NLP tasks, including machine translation and text generation.
- Popular transformer models include BERT, GPT, and T5.

Self-attention for context representation

Self-attention can allow for improved representation of context.



△ Self-attention for context representation (Source:
`https://github.com/probml/pml-book/blob/main/book1-figures/Figure_15.23.png`)

Language models

Language models are generative sequences of the form:

$$p(x_1, \ldots, x_T) = \prod_{t=1}^{T} p(x_t | \boldsymbol{x}_{1:t-1}) \tag{49}$$

where x_t is the t-th word in a sequence of T words.
Examples include:

- Embeddings from Language Model (ELMo)
- Bidirectional Encoder Representations from Transformers (BERT)
- Generative Pre-trained Transformer (GPT) models
- Text-to-text Transfer Transformer (T5) models

Summary

- Recurrent neural networks are designed to learn from sequential (temporal/spatial) data
- The recurrence structure in RNNs renders them susceptible to the vanishing/exploding gradient problem
  - It also makes it challenging for the standard RNN to learn long-term dependencies
- Several approaches have been proposed to address these issues, including the use of gated RNNs
- LSTMs in particular are able to learn when and how much of prior information to include or forget in generating the output at each timestep
  - This is done via the use of gates to control the flow of information
- LSTMs have been successfully applied to handwriting recognition/generation, speech recognition, machine translation, image captioning, among others.

Reading

- Text:**PMLI** 15, DL10
- Note that in DL10, the following symbology used in describing LSTMs (10.1.1.): (Commonly used counterparts that you may find in other literature are parenthesized.)
  - cell state: $\boldsymbol{s}_t$ (alternative: $\boldsymbol{c}_t$)
  - input gate: $\boldsymbol{g}_t$ (alternative: $\boldsymbol{i}_t$)
  - output gate: $\boldsymbol{q}_t$ (alternative: $\boldsymbol{o}_t$)
- I think the $f/c/i/o$ notation is easier to follow than the $f/s/g/q$ used in the DL text
  - However, given that DL uses i as the index for each cell, it is probably less confusing to have i representing two different things.
- An excellent resource for further explanations on how LSTMs work is available on Chris Olah's blog: `https://colah.github.io/posts/2015-08-Understanding-LSTMs/`

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