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JACOBS SCHOOL OF ENGINEERING

ECE/SIOC 228 Machine Learning for Physical Applications
Lecture 7: Recurrent Neural Networks

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Reference & Acknowledgement: Stanford CS230 Deep Learning Lecture Note, Andrew Ng
Dive into Deep Learning, https://d2l.ai/chapter_recurrent-neural-networks/index.html

Examples of Sequence Data

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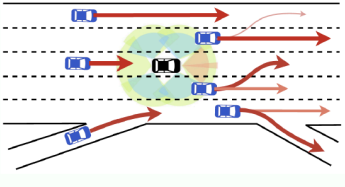
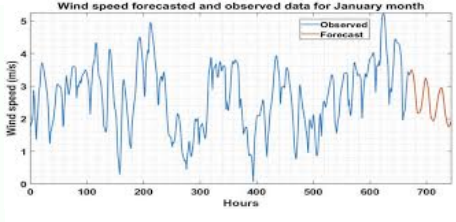
Speech recognition		→	"The quick brown fox jumped over the lazy dog."
Music generation	Ø	→	
Sentiment classification	"There is nothing to like in this movie."	→	★☆☆☆☆
DNA sequence analysis	AGCCCCTGTGAGGAACTAG	→	AGCCCCTGTGAGGAACTAG
Machine translation	Voulez-vous chanter avec moi?	→	Do you want to sing with me?



trajectory prediction



Outline

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- **Recurrent Neural Networks**
- Modern Recurrent Neural Networks
- Attention Mechanism and Transformer

Recurrent Neural Networks

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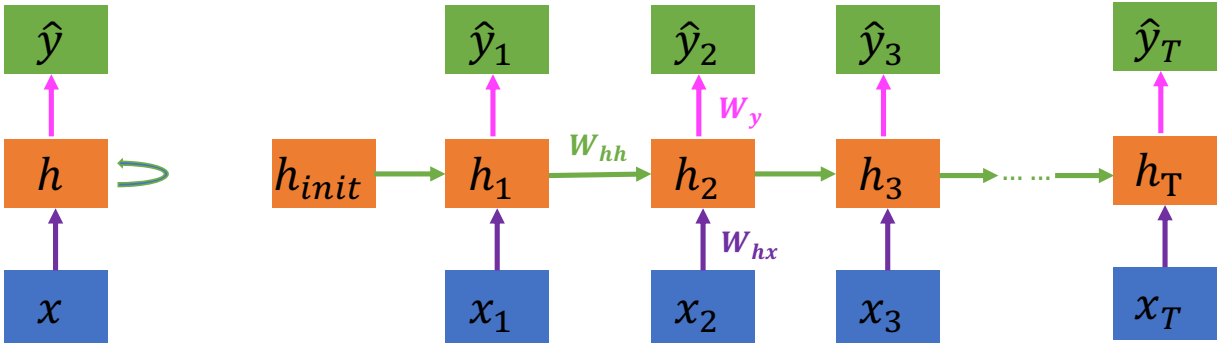

- Computation takes into historical info
- weights are shared across time — each set of colored arrows denotes the same weights
- Process input of any length; model size not increase with size of input

Recurrent Neural Networks: Example

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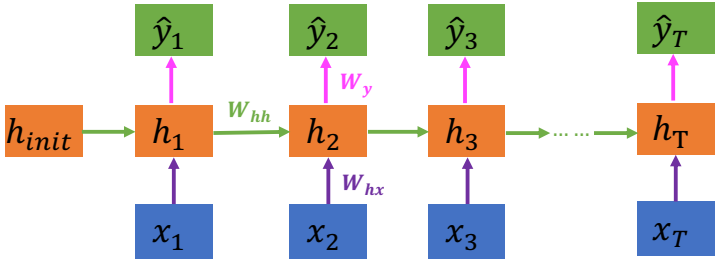

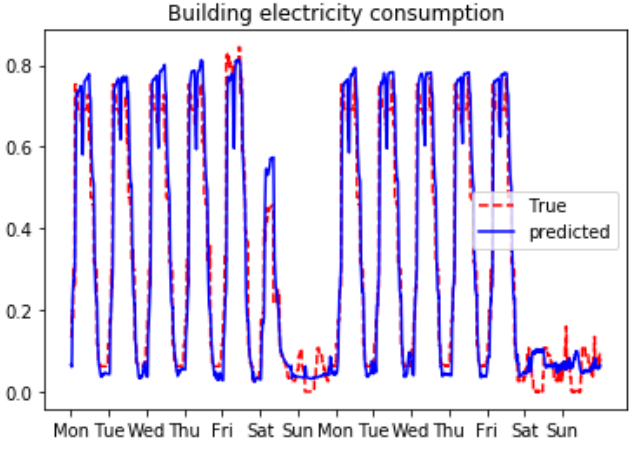

- $\hat{y}_t$ denotes the predicted electricity consumption, at time t
- x_t denotes the features that affects the building energy consumption, e.g., environment features (temperature, humidity, …), occupancy, room temperature setpoint…
- h_t encodes the effect of historical $[x_1, \ldots, x_{t-1}]$

Forward Computation

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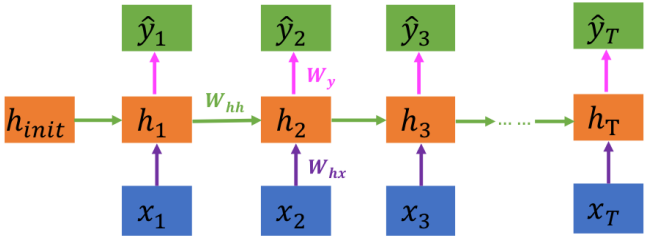

for $t = 1, \cdots, T$

$$h_t = \sigma(W_{hh} h_{t-1} + W_{hx} x_t + b_h)$$

$$\hat{y}_t = \sigma(W_y h_t + b_y)$$

Loss function

$$L = \frac{1}{T} \sum_{t=1}^{T} l(\hat{y}_t, y_t)$$

Suppose we have n traing samples:

$x_t \in R^{d \times n}$, $h_t \in R^{h \times n}$, $\hat{y}_t \in R^{q \times n}$

$W_{hx} \in R^{h \times d}$

$W_{hh} \in R^{h \times h}$

$W_y \in R^{q \times h}$

Two simplification: 1) ignore bias b_h, b_y; 2) set activation $\sigma(z) = z$

$$\frac{\partial L}{\partial \hat{y}_t} = \frac{1}{T} \frac{\partial l(y_t, \hat{y}_t)}{\partial \hat{y}_t} \in R^{q \times n}$$

Now we compute gradient w.r.t. W_y (parameter of the output layer)

L depends on W_y via $\hat{y}_1, \hat{y}_2, \cdots \hat{y}_T$

$$\frac{\partial L}{\partial W_y} = \sum_{t=1}^{T} \frac{\partial L}{\partial \hat{y}_t} \cdot \frac{\partial \hat{y}_t}{\partial W_y} = \sum_{t=1}^{T} \frac{\partial L}{\partial \hat{y}_t} h_t^T$$

Backpropagation

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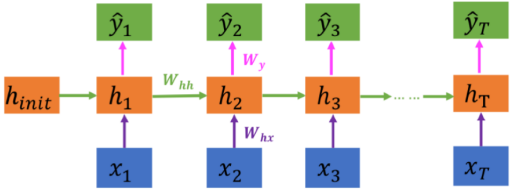

for $t = 1, \cdots, T$

$h_t = \sigma(W_{hh} h_{t-1} + W_{hx} x_t + b_h)$

$\hat{y}_t = \sigma(W_y h_t + b_y)$

Loss function

$L = \frac{1}{T} \sum_{t=1}^{T} l(\hat{y}_t, y_t)$

Now, we look at gradient w.r.t. h_t

$$\frac{\partial L}{\partial h_T} = \text{prod}\left(\frac{\partial L}{\partial \hat{y}_T}, \frac{\partial \hat{y}_T}{\partial h_T}\right) = W_y^T \frac{\partial L}{\partial \hat{y}_T}$$

For $t < T$, we want to compute $\frac{\partial L}{\partial h_t}$ suppose $\frac{\partial L}{\partial h_{t+1}}$ and $\frac{\partial L}{\partial \hat{y}_t}$ are computed

$$\frac{\partial L}{\partial h_t} = \text{prod}\left(\frac{\partial L}{\partial h_{t+1}}, \frac{\partial h_{t+1}}{\partial h_t}\right) + \text{prod}\left(\frac{\partial L}{\partial \hat{y}_t}, \frac{\partial \hat{y}_t}{\partial h_t}\right)$$

$$= W_{hh}^T \frac{\partial L}{\partial h_{t+1}} + W_y^T \frac{\partial L}{\partial \hat{y}_t}$$

$$\frac{\partial L}{\partial h_t} = W_{hh}^T \frac{\partial L}{\partial h_{t+1}} + W_y^T \frac{\partial L}{\partial \hat{y}_t}$$

$$= W_{hh}^T \left(W_{hh}^T \frac{\partial L}{\partial h_{t+2}} + W_y^T \frac{\partial L}{\partial \hat{y}_{t+1}} \right) + W_y^T \frac{\partial L}{\partial \hat{y}_t}$$

$$= (W_{hh}^T)^2 \cdot \frac{\partial L}{\partial h_{t+2}} + W_{hh}^T W_y^T \frac{\partial L}{\partial \hat{y}_{t+1}} + W_y^T \frac{\partial L}{\partial \hat{y}_t}$$

$$= (W_{hh}^T)^2 \cdot \left[W_{hh}^T \frac{\partial L}{\partial y_{t+3}} + W_y^T \frac{\partial L}{\partial \hat{y}_{t+2}} \right] + W_{hh}^T W_y^T \frac{\partial L}{\partial \hat{y}_{t+1}} + W_y^T \frac{\partial L}{\partial \hat{y}_t}$$

$$= \cdots = \sum_{i=t}^{T} (W_{hh}^T)^{T-i} W_y^T \frac{\partial L}{\partial \hat{y}_{T+t-i}}$$

$$\frac{\partial L}{\partial h_t} = \sum_{i=t}^{T} (W_{hh}^T)^{T-i} W_y^T \frac{\partial L}{\partial \hat{y}_{T+t-i}}$$

- It involves (potentially) very large power of W_{hh}^T
- If $\text{eigen}(W_{hh}^T) > 1$, diverge (gradient exploding)
- If $\text{eigen}(W_{hh}^T) < 1$, very small (gradient vanishing)

☆ Truncate the time steps $\frac{\partial L}{\partial h_t} = \sum_{i=t}^{t+H} (W_{hh}^T)^{t+H-i} W_y^T \frac{\partial L}{\partial \hat{y}_{t+H+t-i}}$

Backpropagation

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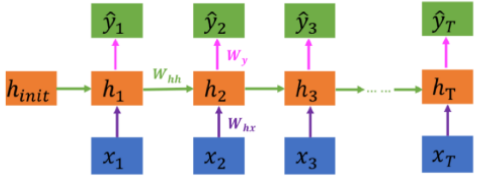

for $t = 1, \cdots, T$

$h_t = \sigma(W_{hh} h_{t-1} + W_{hx} x_t + b_h)$

$\hat{y}_t = \sigma(W_y h_t + b_y)$

Loss function

$L = \frac{1}{T} \sum_{t=1}^{T} l(\hat{y}_t, y_t)$

$$\frac{\partial L}{\partial W_{hx}} = \sum_{t=1}^{T} \text{prod}\left(\frac{\partial L}{\partial h_t}, \frac{\partial h_t}{\partial W_{hx}}\right) = \sum_{t=1}^{T} \frac{\partial L}{\partial h_t} x_t^T$$

$$\frac{\partial L}{\partial W_{hh}} = \sum_{t=1}^{T} \text{prod}\left(\frac{\partial L}{\partial h_t}, \frac{\partial h_t}{\partial W_{hh}}\right) = \sum_{t=1}^{T} \frac{\partial L}{\partial h_t} h_{t-1}^T$$

- $\frac{\partial L}{\partial h_t}$ also affect the gradient magnitude $\frac{\partial L}{\partial W_{hx}}, \frac{\partial L}{\partial W_{hh}}$
- Traing RNN alternates forward & backward propogation through time

Different Types of RNNs

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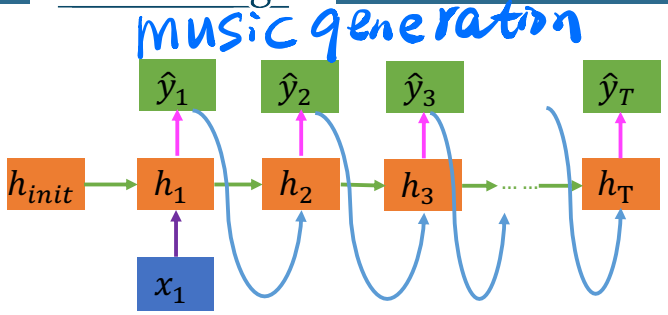
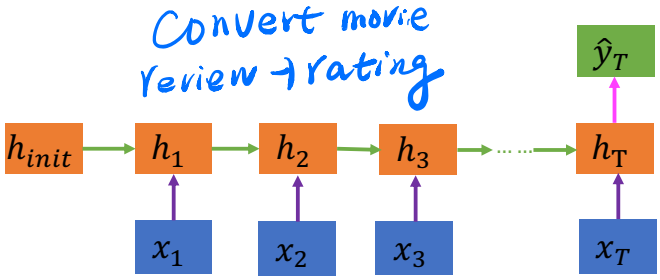
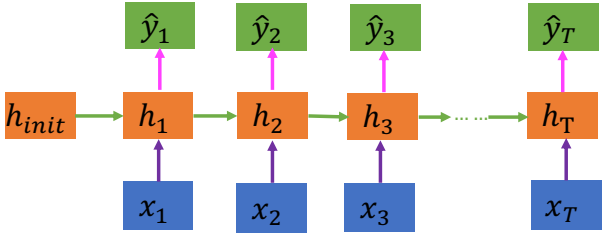


One to Many

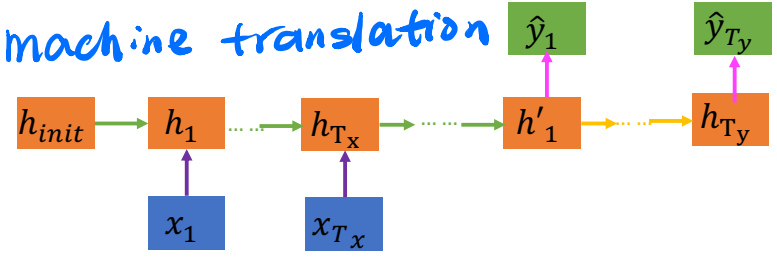


Many to One



Many to Many

building energy prediction



Many to Many (input and output have different length)

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Vanishing Gradient with RNN

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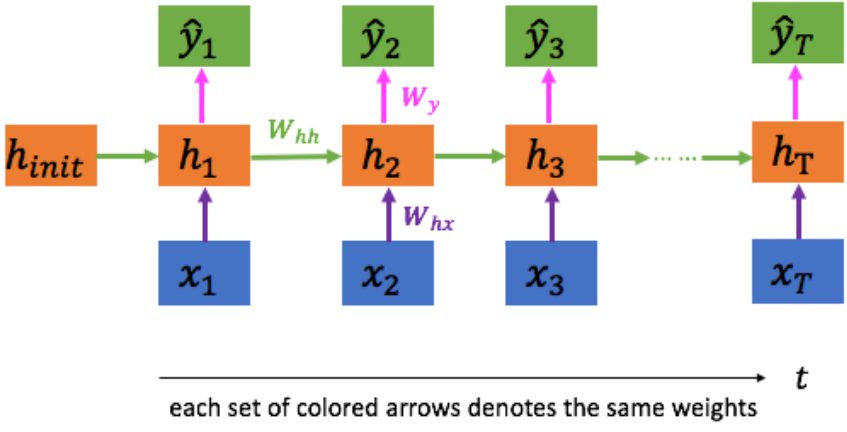

- Long products of matrices can lead to vanishing or exploding gradients

$$\frac{\partial L}{\partial h_t} = \sum_{i=t}^{T} (W_{hh}^T)^{T-i} W_y^T \frac{\partial L}{\partial \hat{y}_{T+t-i}}$$

Gated Recurrent Units (GRU)

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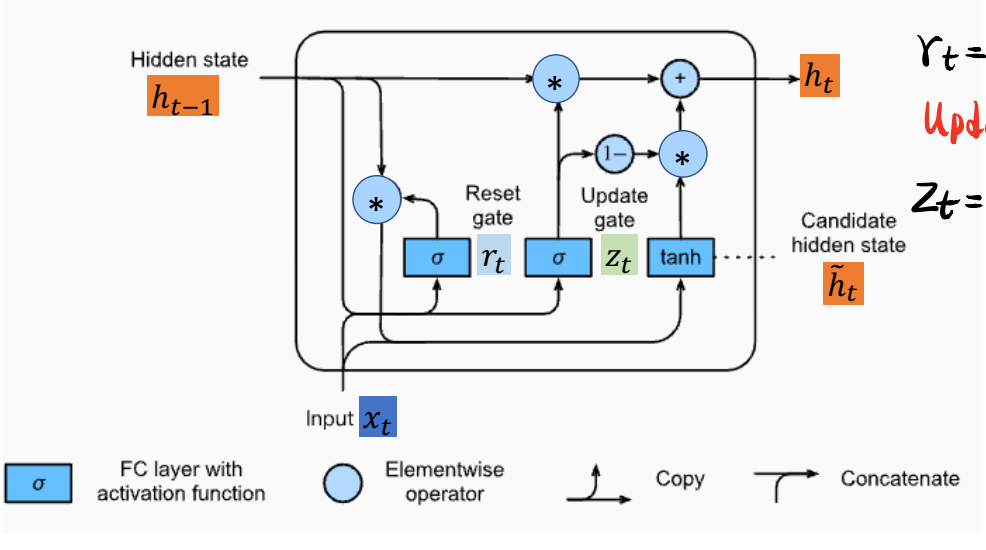

Reset gate:

$$r_t = \text{sigmoid}(W_{rx} x_t + W_{rh} h_{t-1} + b_r)$$

Update gate:

$$z_t = \text{sigmoid}(W_{zx} x_t + W_{zh} h_{t-1} + b_z)$$

$x_t \in \mathbb{R}^{d \times n}$, $h_{t-1} \in \mathbb{R}^{h \times n}$,

$r_t, z_t \in \mathbb{R}^{h \times n}$

$W_{rx}, W_{zx} \in \mathbb{R}^{h \times d}$

$W_{rh}, W_{zh} \in \mathbb{R}^{h \times h}$

Empirical Evaluation of Gated Recurrent Neural Networks on Sequence Modeling: https://arxiv.org/pdf/1412.3555.pdf

Gated Recurrent Units (GRU)

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Reset gate: $r_t = \text{sigmoid}(W_{rx} x_t + W_{rh} h_{t-1} + b_r)$

Update gate: $z_t = \text{sigmoid}(W_{zx} x_t + W_{zh} h_{t-1} + b_z)$

proposal / candidate hidden state:

$$\tilde{h}_t = \tanh(W_{hx} x_t + W_{hh}(r_t * h_{t-1}) + b_h)$$

element-wise

- If $r_t \approx 1$, recover RNN
- If $r_t \approx 0$, $\tilde{h}_t$ only depends on x_t, resetting hidden states

Empirical Evaluation of Gated Recurrent Neural Networks on Sequence Modeling: https://arxiv.org/pdf/1412.3555.pdf

Gated Recurrent Units (GRU)

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Reset gate: $r_t = \text{sigmoid}(W_{rx} x_t + W_{rh} h_{t-1} + b_r)$

Update gate: $z_t = \text{sigmoid}(W_{zx} x_t + W_{zh} h_{t-1} + b_z)$

Proposal: $\tilde{h}_t = \tanh(W_{hx} x_t + W_{hh}(r_t * h_{t-1}) + b_h)$

Hidden state: $h_t = z_t * h_{t-1} + (1 - z_t) * \tilde{h}_t$

($*$: elementwise)

- If $z_t \approx 1$, $h_t = h_{t-1}$; (help cope the vanishing gradient)
- If $z_t \approx 0$, $h_t = \tilde{h}_t$ (incorporate new info)

Empirical Evaluation of Gated Recurrent Neural Networks on Sequence Modeling: https://arxiv.org/pdf/1412.3555.pdf

Gated Recurrent Units (GRU)

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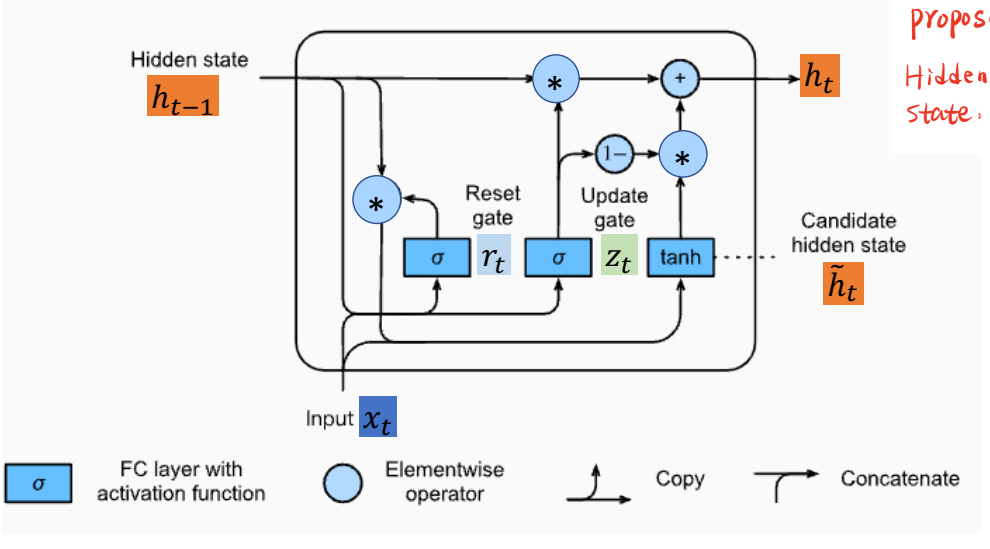

Reset gate: $r_t = \text{sigmoid}(W_{rx} x_t + W_{rh} h_{t-1} + b_r)$

Update gate: $z_t = \text{sigmoid}(W_{zx} x_t + W_{zh} h_{t-1} + b_z)$

Proposal: $\tilde{h}_t = \tanh(W_{hx} x_t + W_{hh}(r_t * h_{t-1}) + b_h)$

Hidden state: $h_t = z_t * h_{t-1} + (1 - z_t) * \tilde{h}_t$

($*$: elementwise)

- Reset gates help capture short-term dependencies
- Update gates help capture long-term dependencies

Empirical Evaluation of Gated Recurrent Neural Networks on Sequence Modeling: https://arxiv.org/pdf/1412.3555.pdf

Long Short-Term Memory (LSTM)

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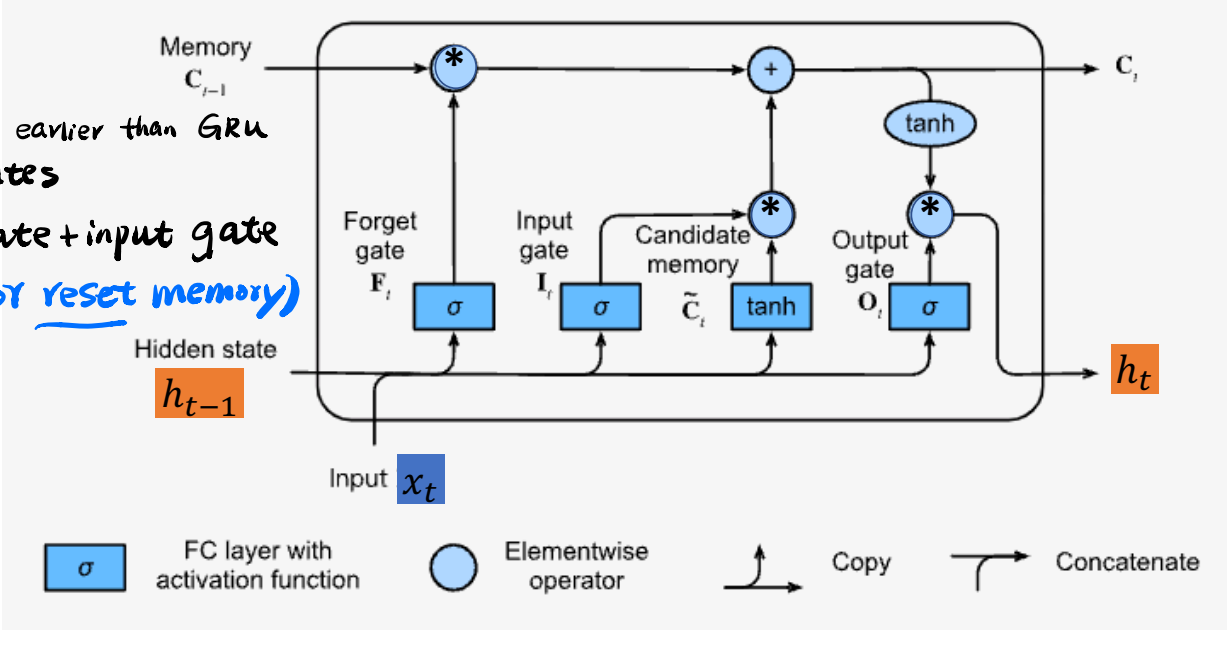
- ~20 years earlier than GRU
- three-gates
- Forget gate + input gate (retain or reset memory)
- Output gate



Long short-term memory, http://citeseerx.ist.psu.edu/viewdoc/download?doi=10.1.1.676.4320&rep=rep1&type=pdf

Long Short-Term Memory (LSTM)

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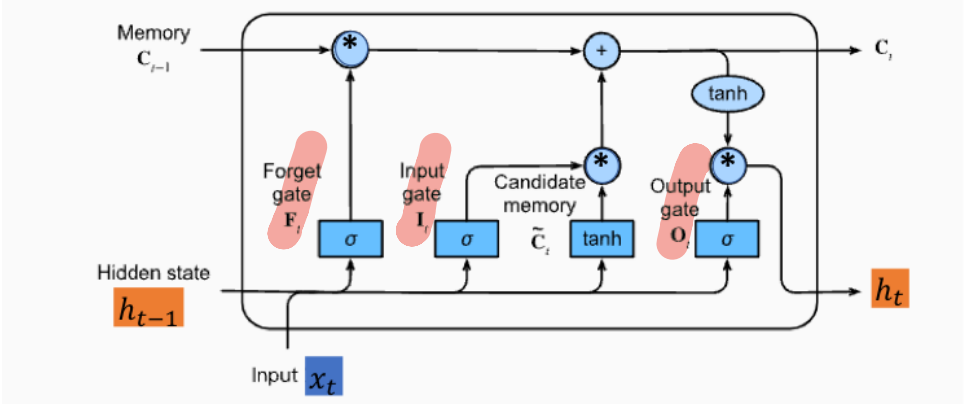

Input Gate: $I_t = \text{sigmoid}(W_{ix} x_t + W_{ih} h_{t-1} + b_i)$

Forget Gate: $F_t = \text{sigmoid}(W_{fx} x_t + W_{fh} h_{t-1} + b_f)$

Output Gate: $O_t = \text{sigmoid}(W_{ox} x_t + W_{oh} h_{t-1} + b_o)$

Long short-term memory, http://citeseerx.ist.psu.edu/viewdoc/download?doi=10.1.1.676.4320&rep=rep1&type=pdf

Long Short-Term Memory (LSTM)

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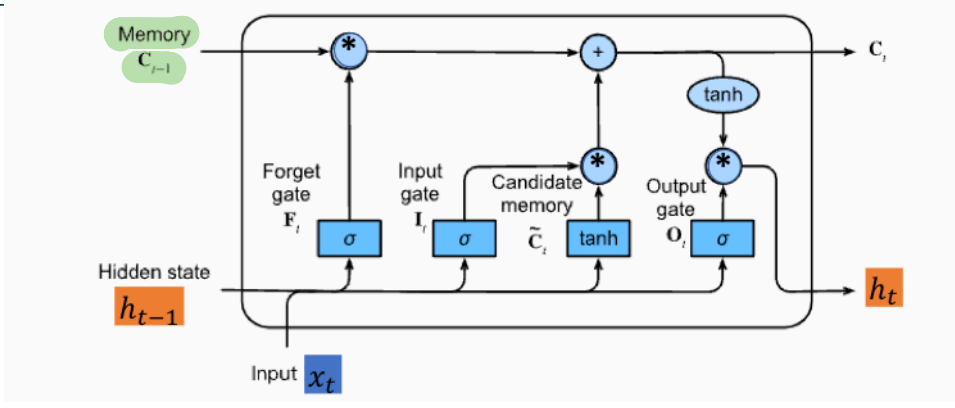

- I_t: how much we take x_t into account in computing $\tilde{C}_t$
- F_t: how much C_{t-1} is used

Proposal/candidate. $\tilde{C}_t = \tanh(W_{cx} x_t + W_{ch} h_{t-1} + b_c)$

$C_t = F_t * C_{t-1} + I_t * \tilde{C}_t$, * (element-wise multiplication)

Long short-term memory, http://citeseerx.ist.psu.edu/viewdoc/download?doi=10.1.1.676.4320&rep=rep1&type=pdf

(GRU: $h_t = z_t * h_{t-1} + (1 - z_t) \tilde{h}_t$)

Long Short-Term Memory (LSTM)

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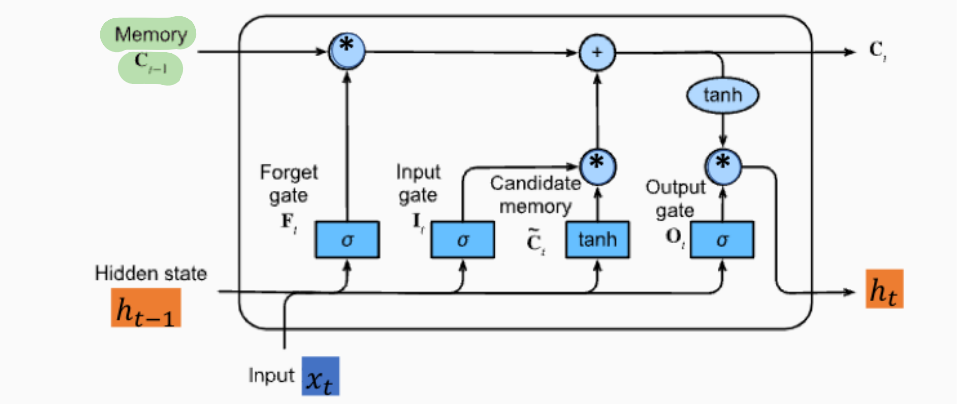

$h_t = O_t * \tanh(C_t)$

$Y_t = W_y h_t + b_y$ (+ activation func if needed)

Long short-term memory, http://citeseerx.ist.psu.edu/viewdoc/download?doi=10.1.1.676.4320&rep=rep1&type=pdf

Bidirectional RNN

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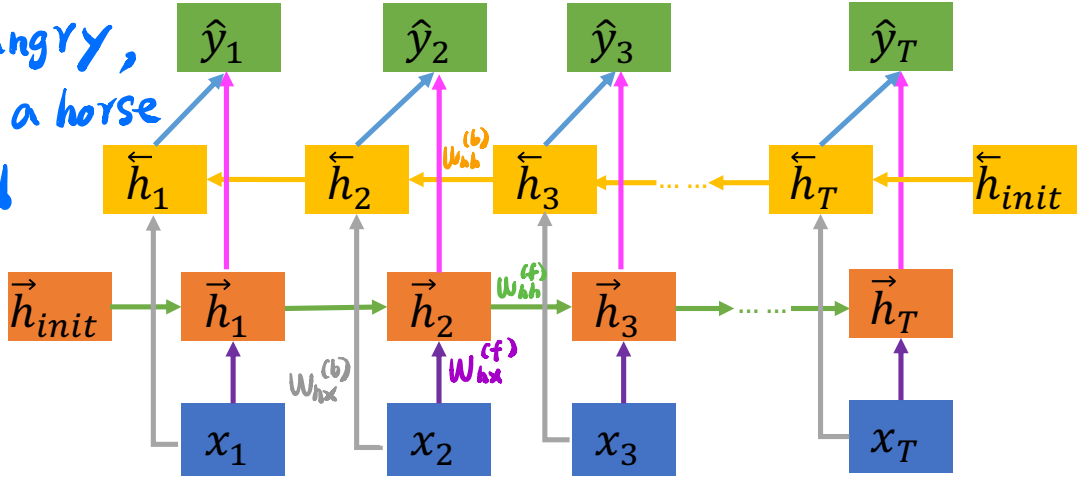
I am _ hungry,
I can eat a horse
I just had dinner



$\vec{h}_t = \sigma(W_{hh}^{(f)} \vec{h}_{t-1} + W_{hx}^{(f)} x_t + b_h^{(f)})$ $\quad x_t \in R^{d \times n}, W_{hx} \in R^{h \times d}, W_{hh} \in R^{h \times h}$

$\overleftarrow{h}_t = \sigma(W_{hh}^{(b)} \overleftarrow{h}_{t+1} + W_{hx}^{(b)} x_t + b_h^{(b)})$ $\quad h_t = [\vec{h}_t, \overleftarrow{h}_t] \in R^{2h \times n}$

$\hat{y}_t = \sigma(W_y h_t + b_y)$, $\quad W_y \in R^{q \times 2h}$, $b_y \in R^{q \times 1}$

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Motivation

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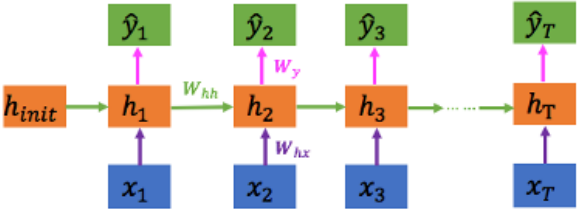
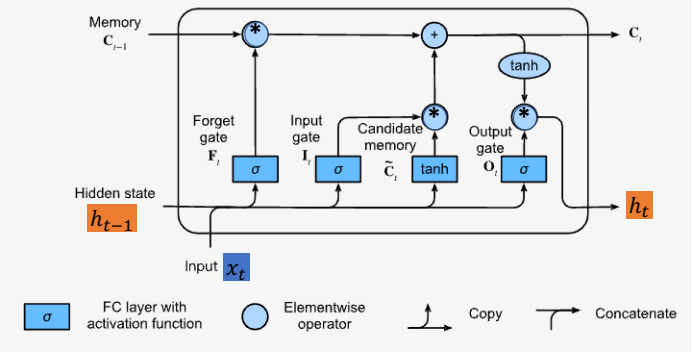
Increased complexity, sequential

RNN GRU LSTM





Attention Mechanism

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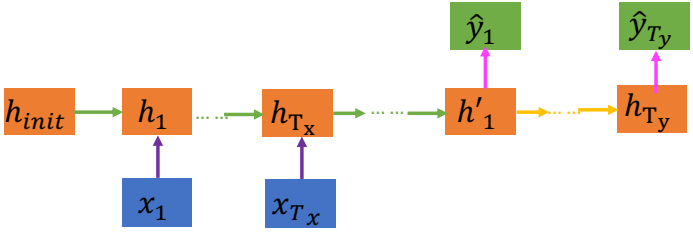
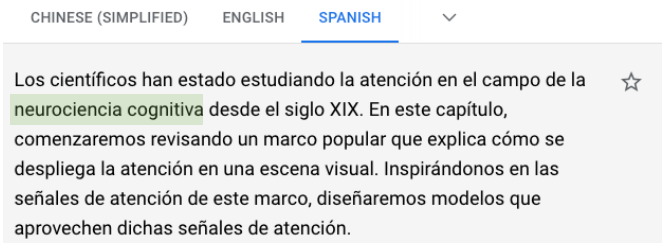
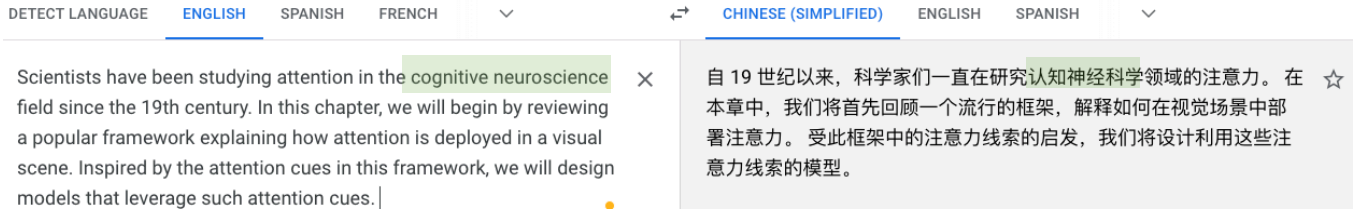


The problem of long sequence in machine translation





Attention Mechanism

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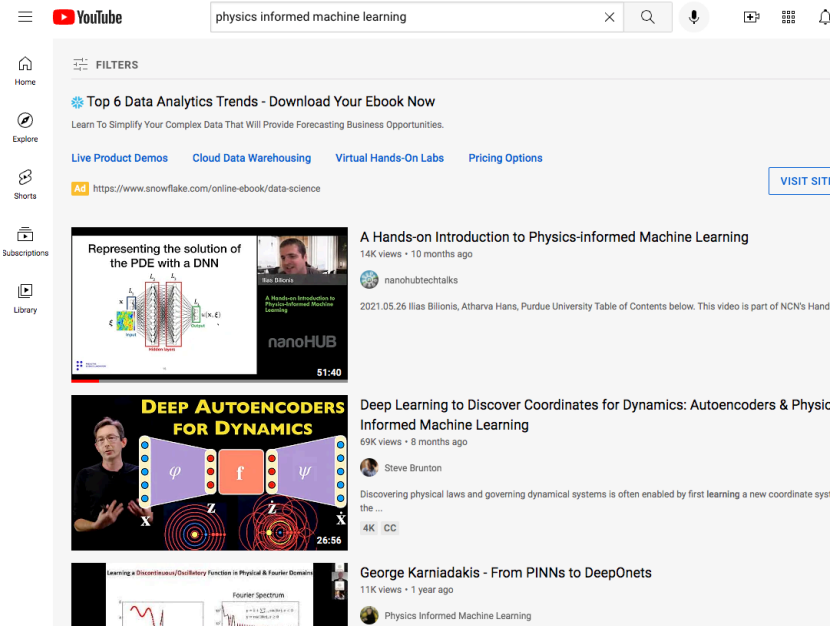

- **Query, Key, Value**

Example: Youtube video retrieval

- Query: "physics informed machine learning"
- Key: each video has a set of keys (video title, description, viewing count…)
- Values: video

Attention Mechanism

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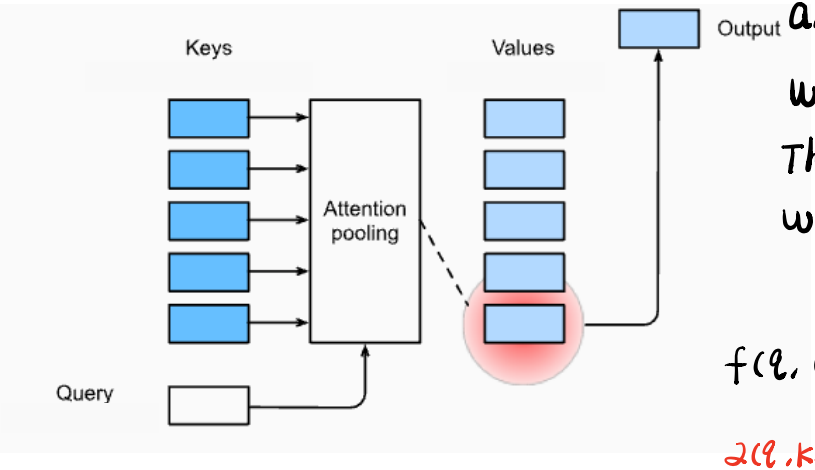

Mathematically, suppose we have a query $q \in R^{d_q}$ and m key-value pairs $(k_1, v_1), \ldots, (k_m, v_m)$ where $k_i \in R^k$ and each value $v_i \in R^v$.

The output of the query can be written as:

Weight: amount of attention q should pay to item (k_i, v_i)

$$f(q, (k_1, v_1), \ldots (k_m, v_m)) = \sum_{i=1}^{m} \alpha(q, k_i) v_i$$

$$\alpha(q, k_i) = \frac{\exp(a(q, k_i))}{\sum_{j=1}^{m} \exp(a(q, k_j))} \in R$$

a is called attention score function

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Different attention score function:

- Query and key are vector of same length: $d_q = d_k$

$$a(q, k_i) = \frac{q^T k_i}{\sqrt{d_k}} = \frac{k_i^T q}{\sqrt{d_k}}$$ (Scaled dot-product attention)

- Query and key are vector of different length (additive attention)

$$a(q, k_i) = \underset{R^{d_a}}{W_a^T} \tanh\left(\underset{R^{d_a \times d_q}}{W_q} q + \underset{R^{d_a \times d_k}}{W_k} k_i\right) \in R$$

RNN with Attention Mechanism

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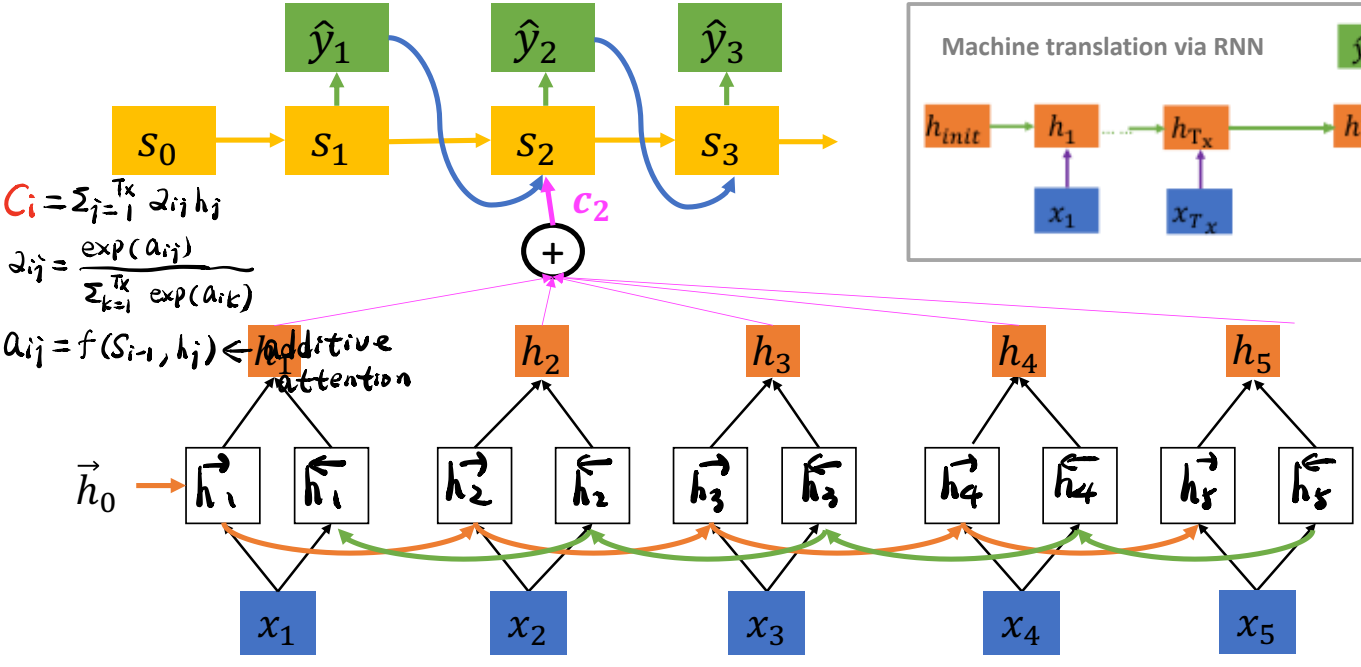

Neural Machine Translation by Jointly Learning to Align and Translate, https://arxiv.org/abs/1409.0473

Transformer

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- Self Attention
- Multi-head Attention

Attention Is All You Need, https://proceedings.neurips.cc/paper/2017/file/3f5ee243547dee91fbd053c1c4a845aa-Paper.pdf

Transformer: Self Attention

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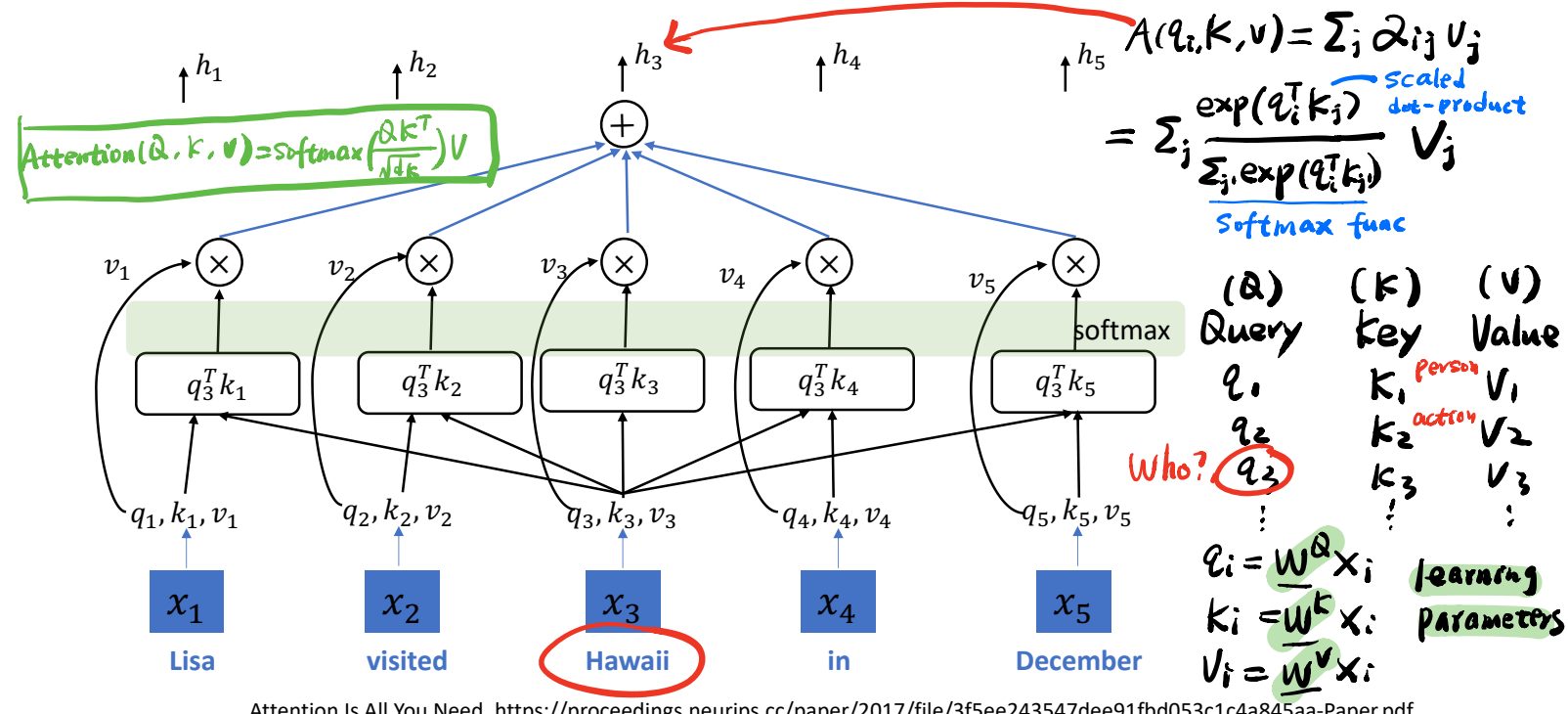

Attention Is All You Need, https://proceedings.neurips.cc/paper/2017/file/3f5ee243547dee91fbd053c1c4a845aa-Paper.pdf

Transformer: Self Attention vs RNN

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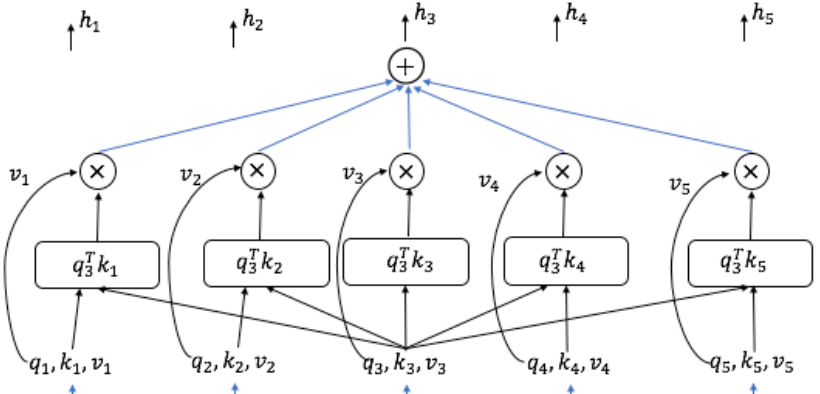

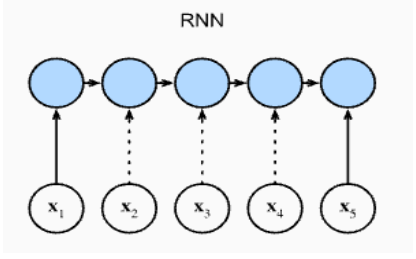

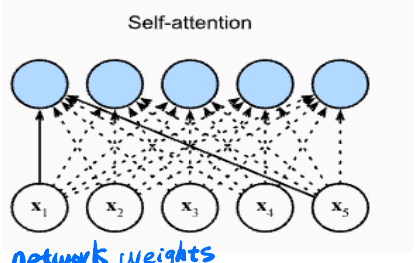

network weights depend on input

Attention Is All You Need, https://proceedings.neurips.cc/paper/2017/file/3f5ee243547dee91fbd053c1c4a845aa-Paper.pdf

Transformer: Multi-Head Attention

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$$\text{Attention}(Q, K, V) = \text{Softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right)V$$

$$\begin{bmatrix} head^{(1)} \\ head^{(2)} \\ \vdots \\ head^{(N)} \end{bmatrix} W_o$$

N: # of head

h_3

$head^{(1)} = \text{Attention}(W_1^Q Q, W_1^K K, W_1^V V)$

$W_1^Q q_1, W_1^K k_1, W_1^V v_1$ | $W_1^Q q_2, W_1^K k_2, W_1^V v_2$ | $W_1^Q q_3, W_1^K k_3, W_1^V v_3$ | $W_1^Q q_4, W_1^K k_4, W_1^V v_4$ | $W_1^Q q_5, W_1^K k_5, W_1^V v_5$

q_1, k_1, v_1 | q_2, k_2, v_2 | q_3, k_3, v_3 | q_4, k_4, v_4 | q_5, k_5, v_5

$q_i = W^Q x_i$, $k_i = W^K x_i$, $v_i = W^V x_i$ (learning parameters)

x_1	x_2	x_3	x_4	x_5
Lisa	visited	Hawaii	in	December

Attention Is All You Need, https://proceedings.neurips.cc/paper/2017/file/3f5ee243547dee91fbd053c1c4a845aa-Paper.pdf

Transformer

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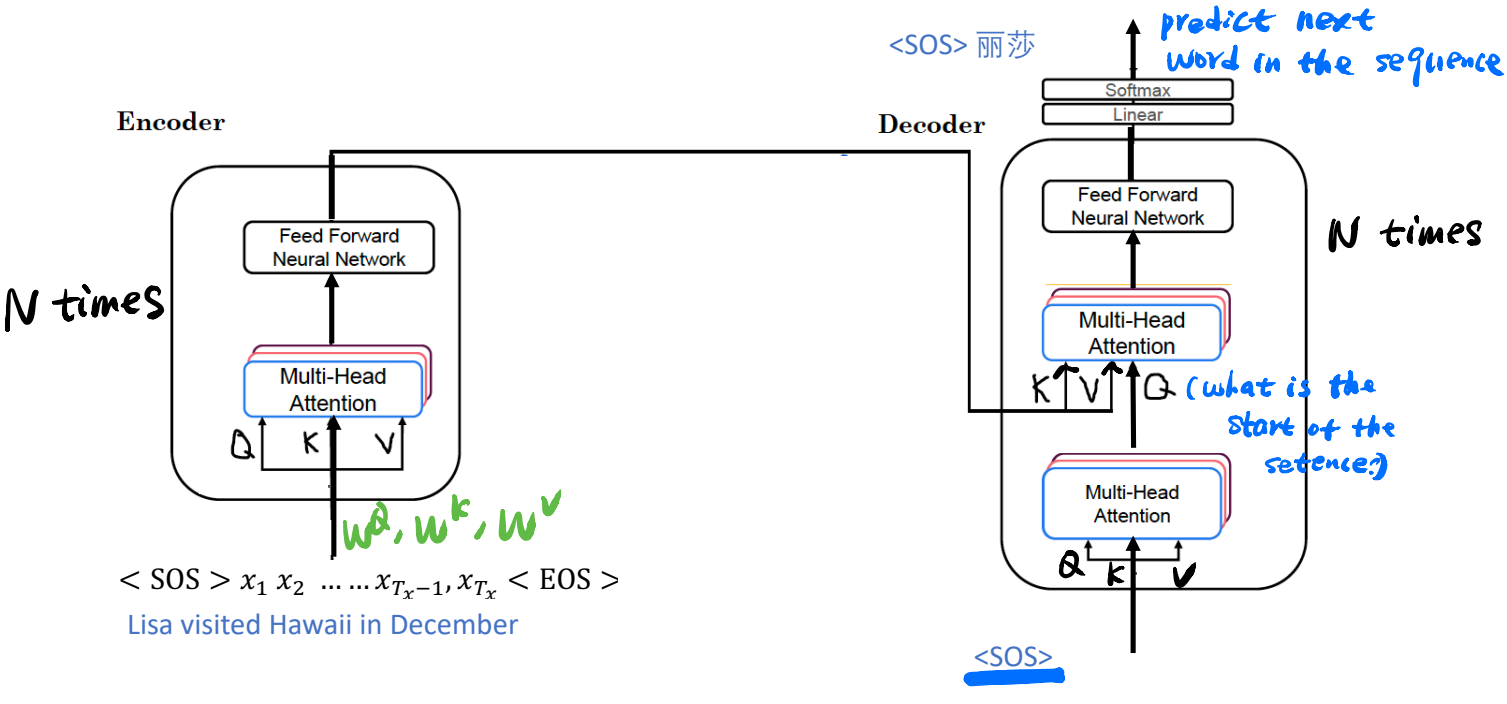

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Transformer Details

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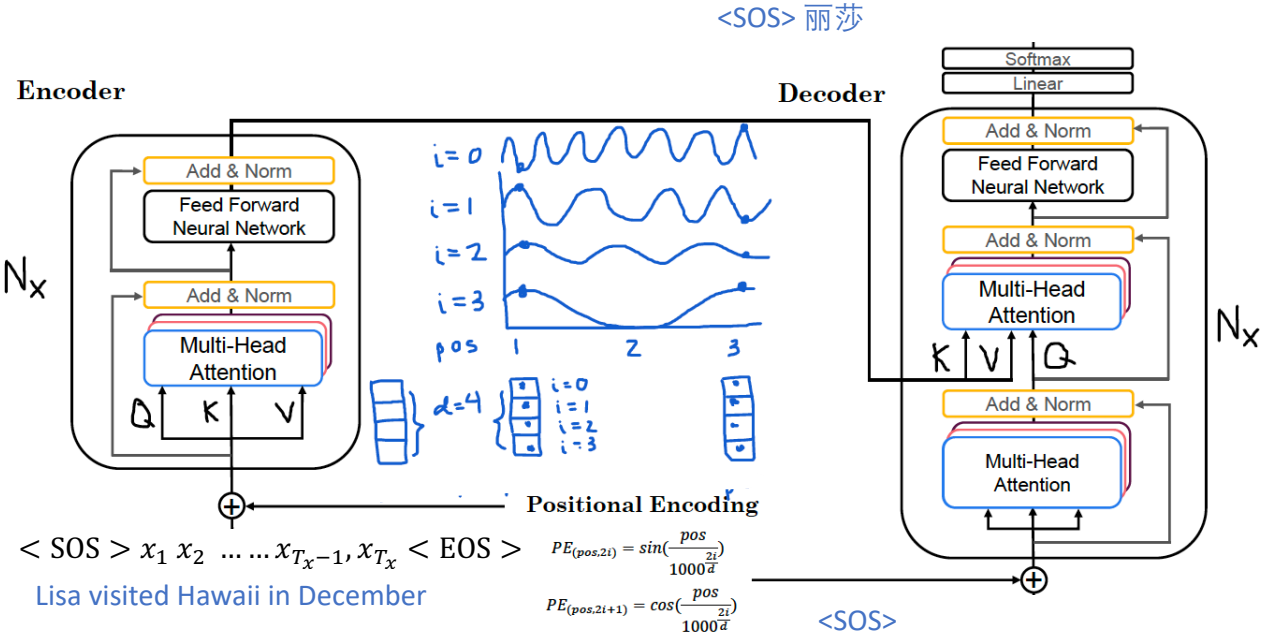

Attention Is All You Need, https://proceedings.neurips.cc/paper/2017/file/3f5ee243547dee91fbd053c1c4a845aa-Paper.pdf

Transformer vs RNN

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Transformer

- ☆ Convinient parellel computation
- ☆ Can capture (very) long range dependency & not suffer from vanishing gradient issue
- ☆ work well when you have BIG data (e.g. NLP tasks)

RNN / LSTM / GRU

- ☆ better capture temporal sequence structure
- ☆ RNN/LSTM/GRU can still work very well (or even better) in common tasks with moderate # of data and not hyper-long sequences