Recurrent Neural Networks

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Machine Learning

Outline

1. **Design**
   - Vanilla RNNs
   - Design Alternatives
2. **Training**
   - Backprop through Time (BPTT)
   - Optimization Techniques
   - Optimization-Friendly Models & LSTM
   - Parallelism & Teacher Forcing
3. **Augmented RNNs**
   - Attention
   - Explicit Memory
   - Adaptive Computation Time (ACT)
4. **Case Studies**
   - Visualization
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  - T is call the ***horizon*** and may be different between $\boldsymbol{x}^{(n)}$ and $\boldsymbol{y}^{(n)}$ and across data points n's

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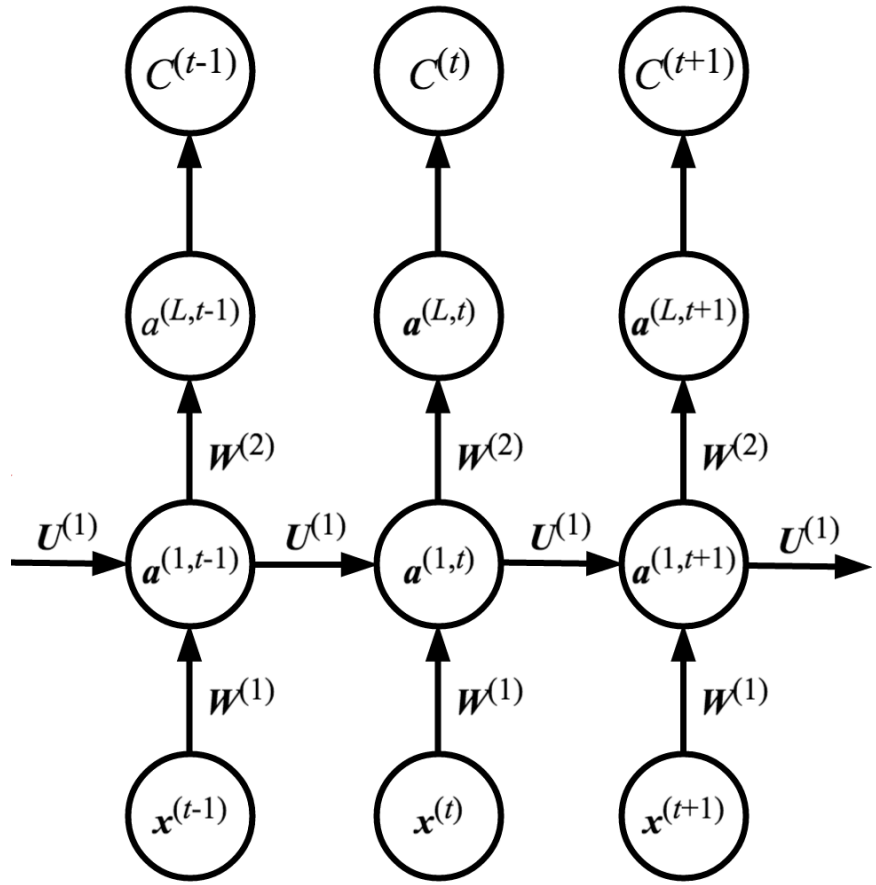

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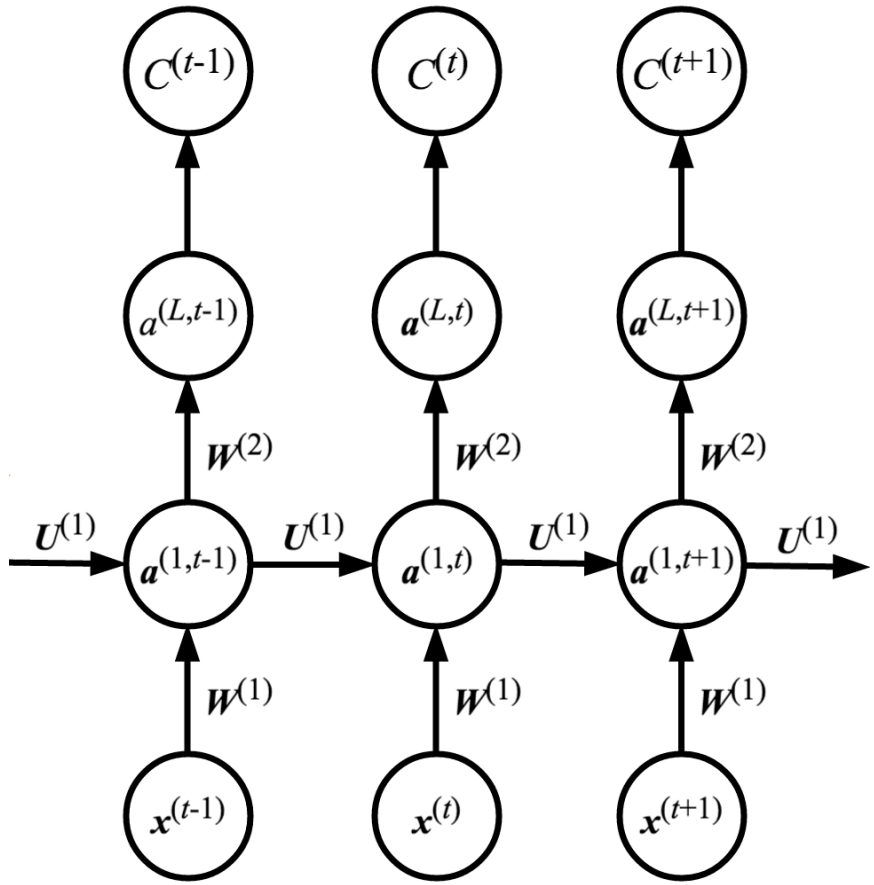

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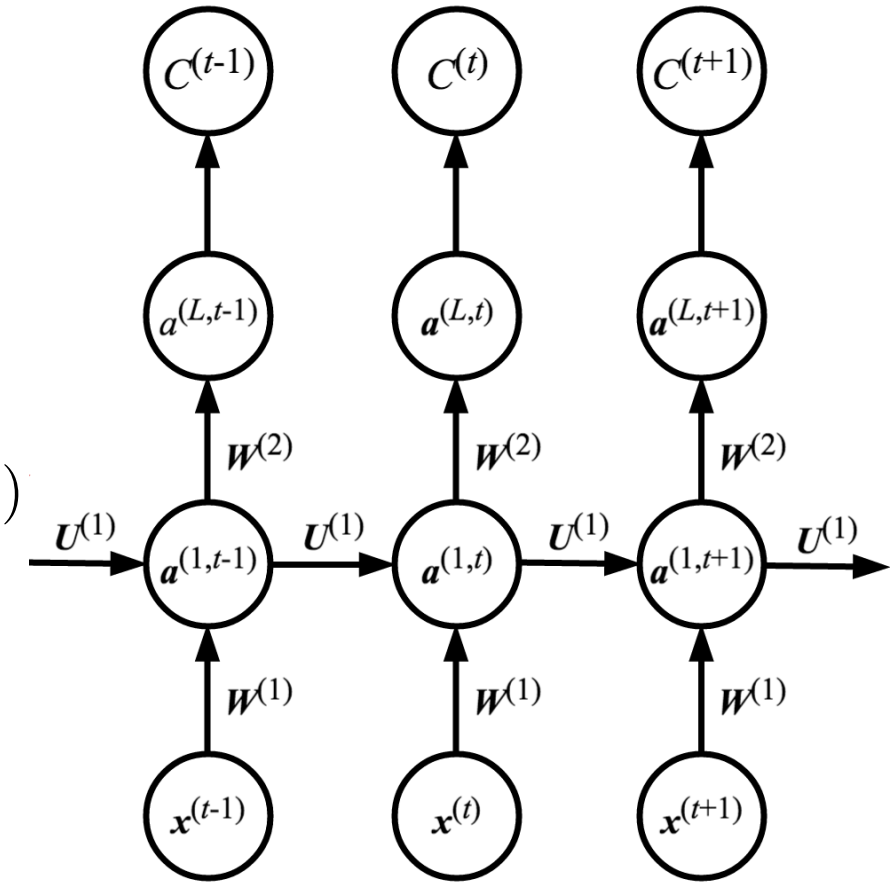

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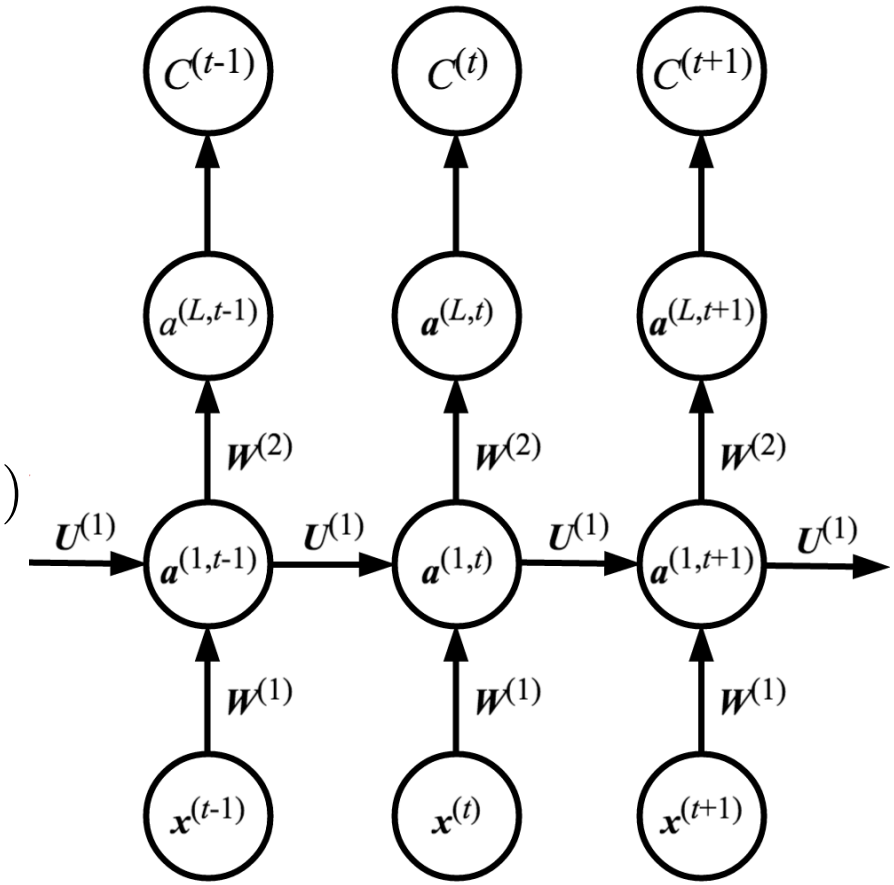

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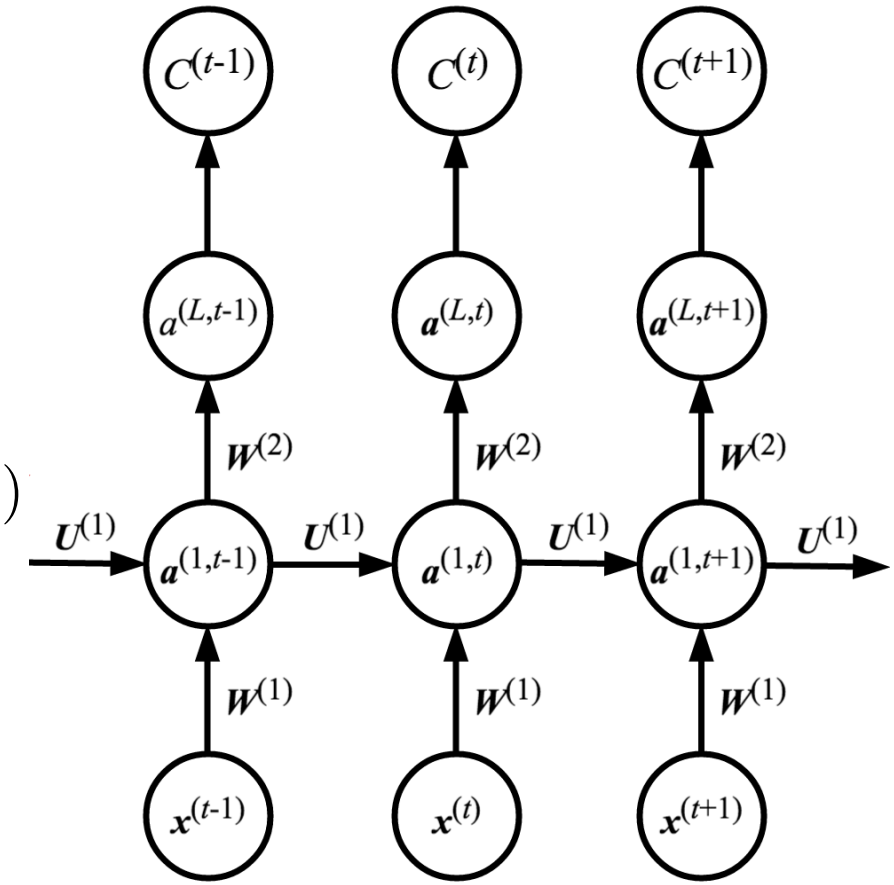
- $\mathbf{a}^{(\cdot,t)}$'s at deeper layers give more abstract summarizations



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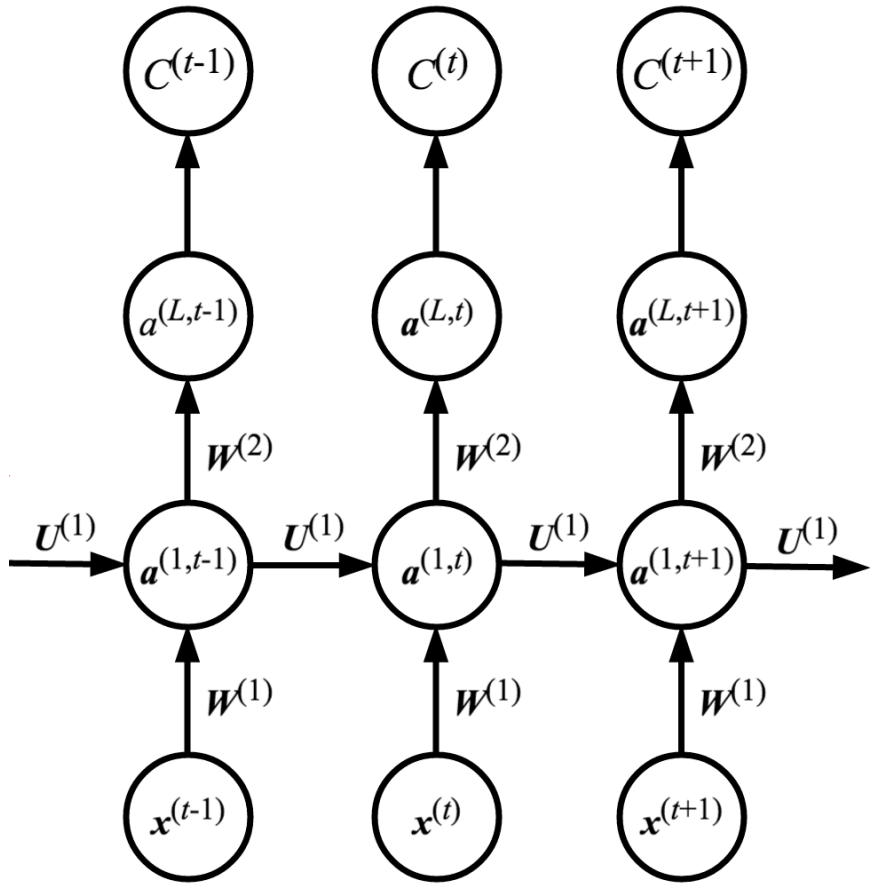

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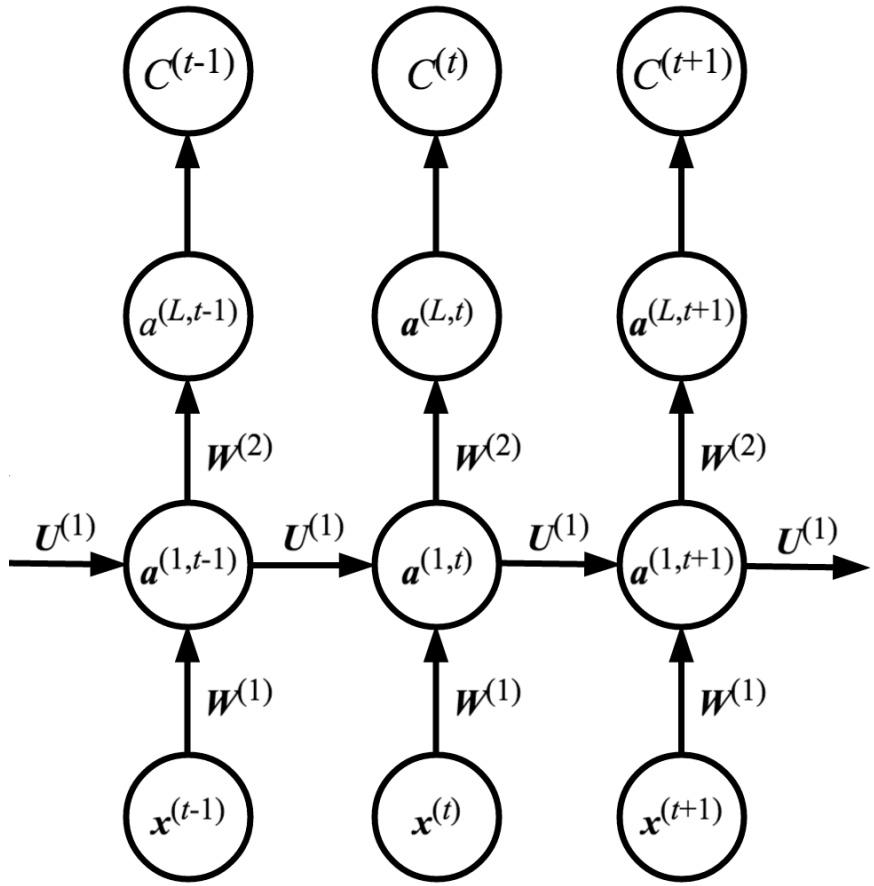

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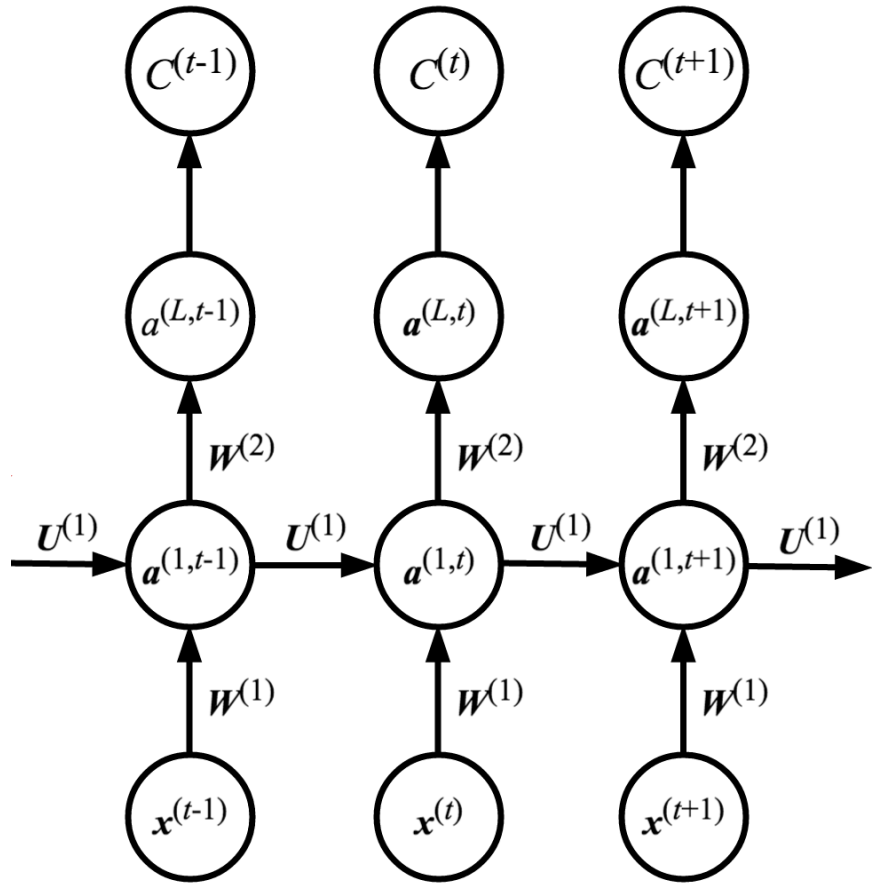
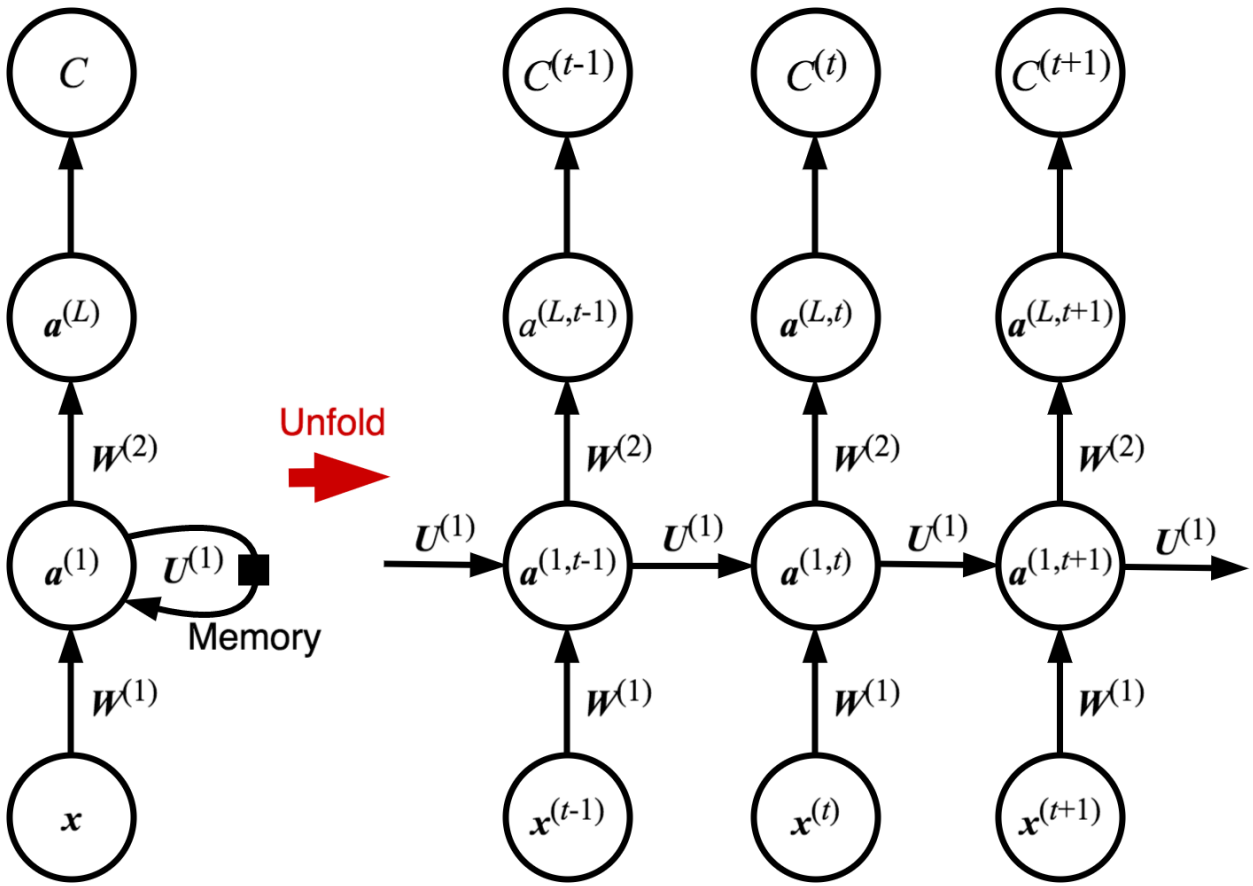
- Weights are ***shared*** across time instances
- Assumes that the "transition functions" are time invariant
- Our goal is to learn $\boldsymbol{U}^{(k)}$'s and $\boldsymbol{W}^{(k)}$'s for $k = 1, \cdots, L$



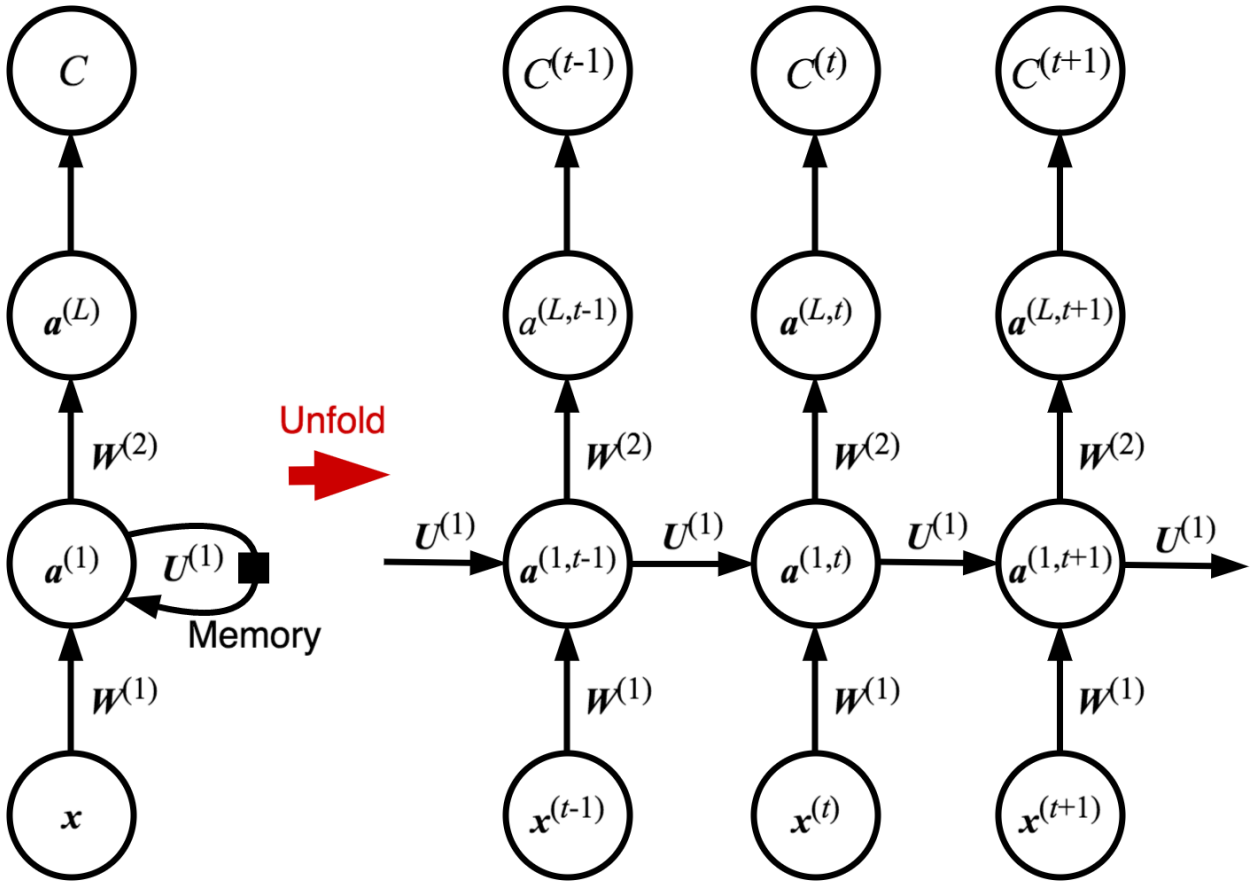
RNNs have Memory

- The computational graph of an RNN can be ***folded*** in time



RNNs have Memory

- The computational graph of an RNN can be ***folded*** in time
- Black squares denotes ***memory*** access



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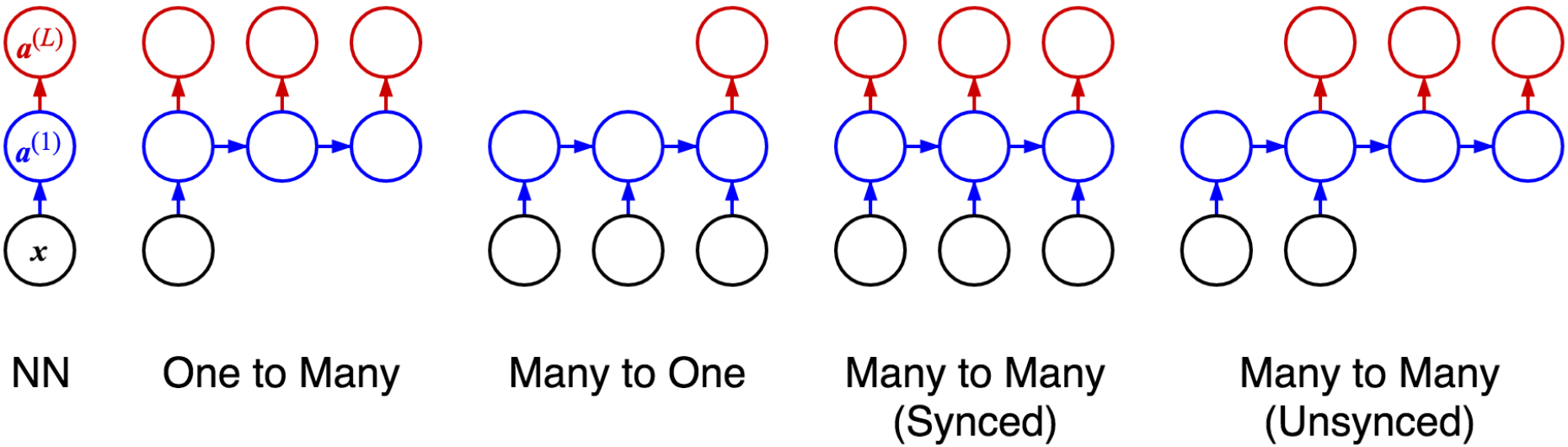
Input and Output

- $\boldsymbol{x}^{(t)}$'s and $\boldsymbol{y}^{(t)}$'s do ***not*** need to have one-to-one correspondence:



One2Many: Image Captioning

"A little girl sitting on a bed with a teddy bear."

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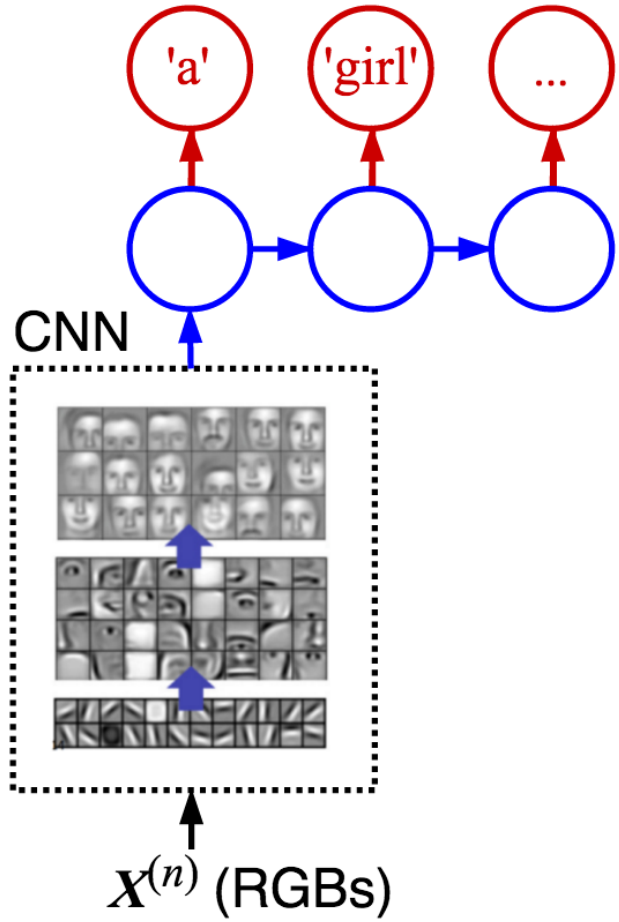
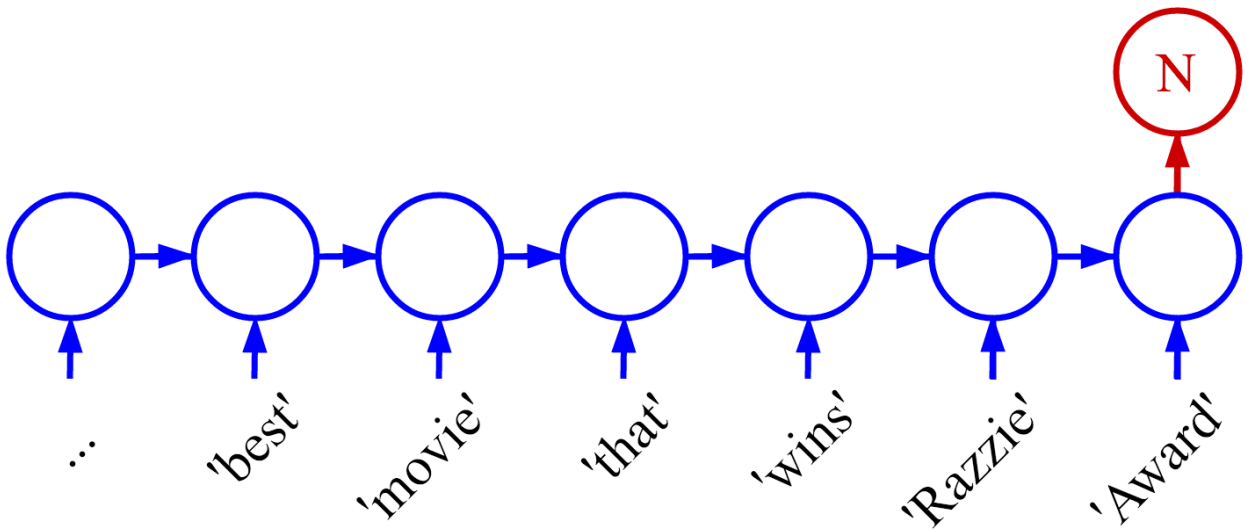


Many2One: Sentiment Analysis



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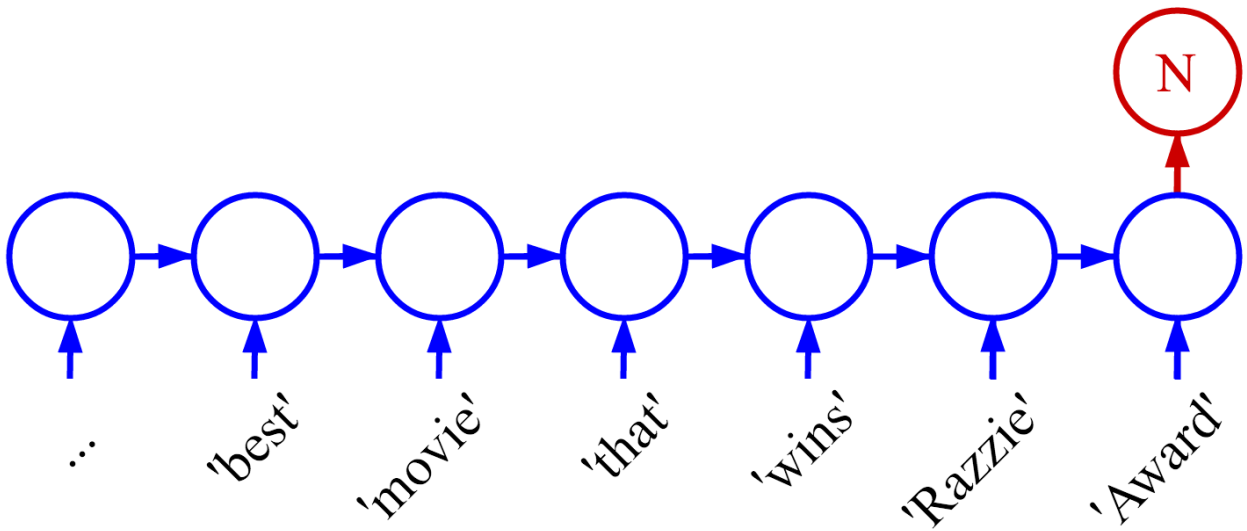
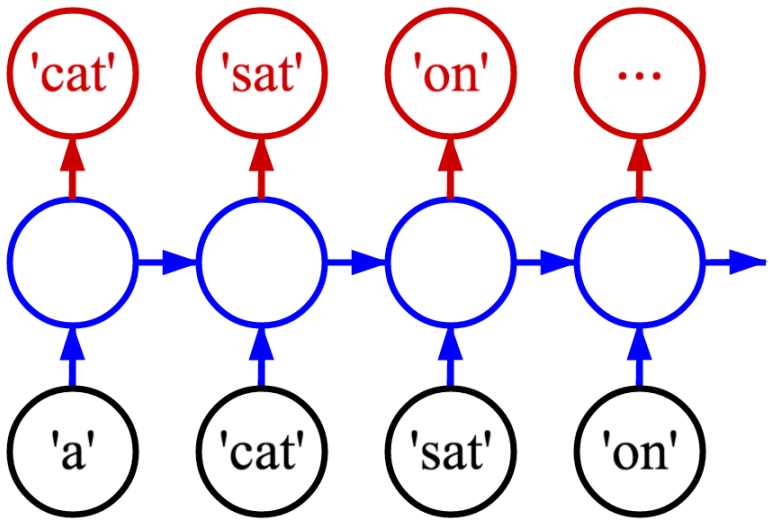


- A single word (e.g., "Razzie") can negate the entire input sentence

Many2Many (Synced): Language Modeling

- ***Language modeling***: predicting the next word based on the context



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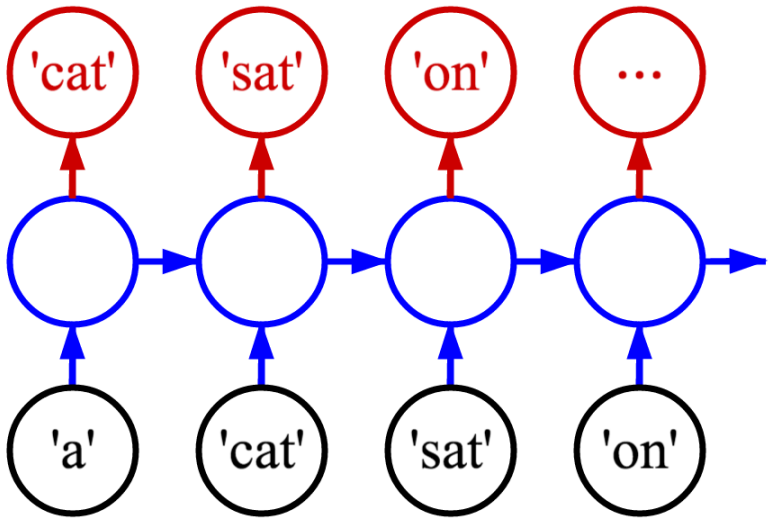
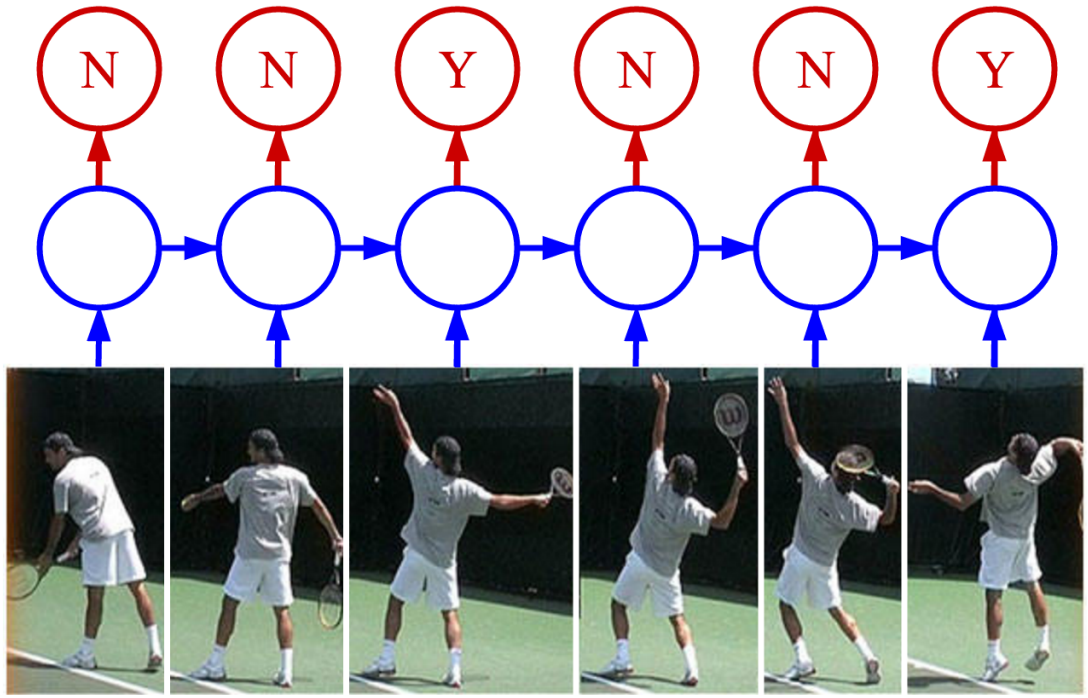


- Latent representation provides the context

Many2Many (Synced): Video Keyframe Tagging

- Video frame annotation:



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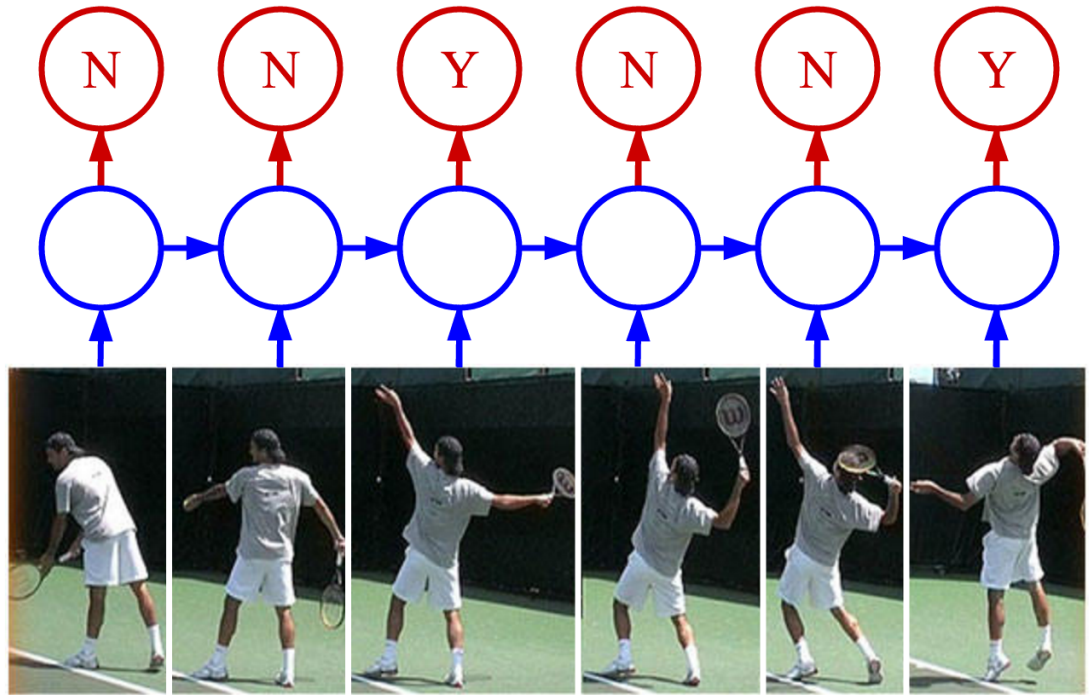
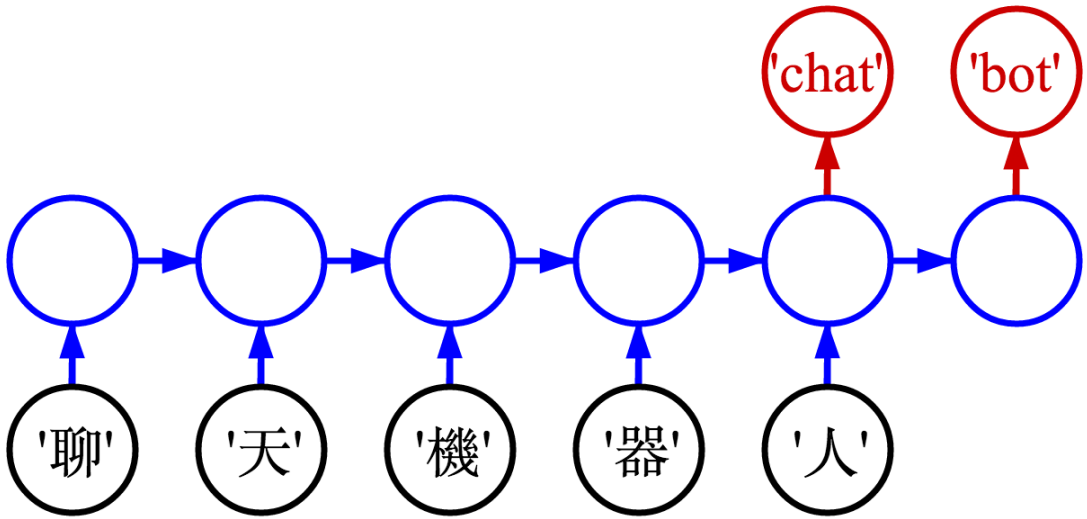


- Latent representation summarizes "what's going on"

Many2Many (Unsynced): Machine Translation



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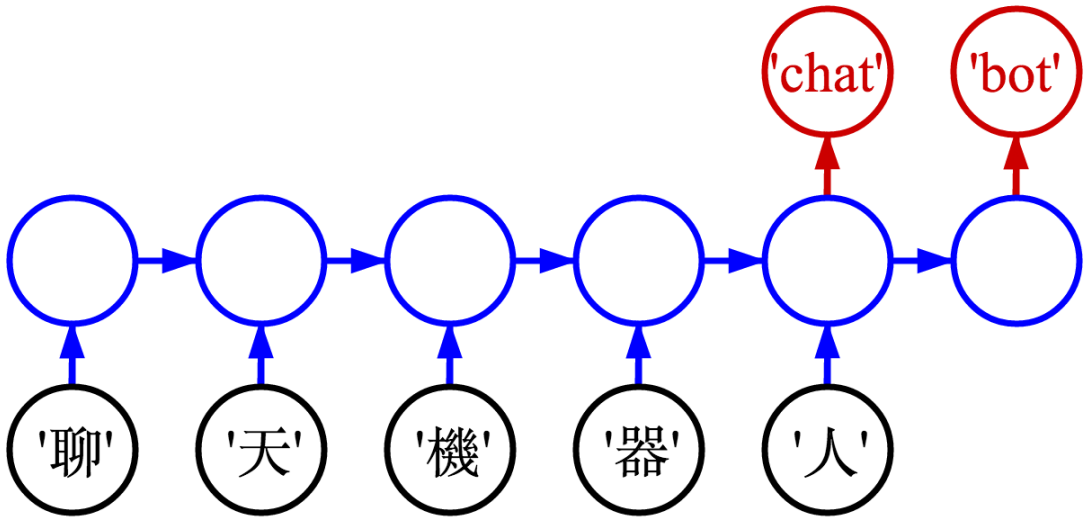

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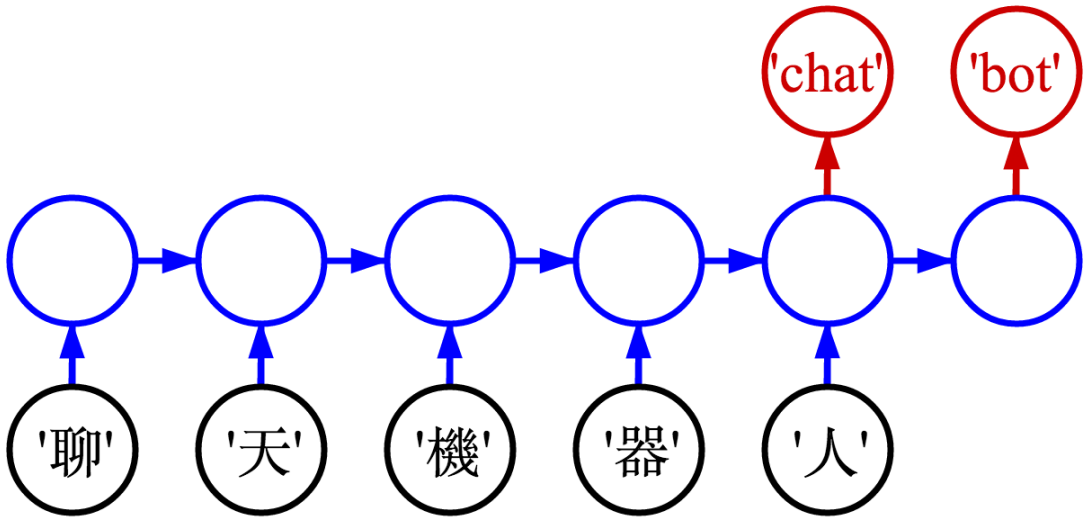

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  - E.g., left-to-right vs. right-to-left languages
- Also called ***sequence to sequence*** learning
  - Has many applications, e.g., chat bots

Bidirectional RNNs

$$\mathbf{a}^{(k,t)} = \text{act}(\boldsymbol{U}^{(k)}\mathbf{a}^{(k,t-1)} + \boldsymbol{W}^{(k)}\mathbf{a}^{(k-1,t)})$$

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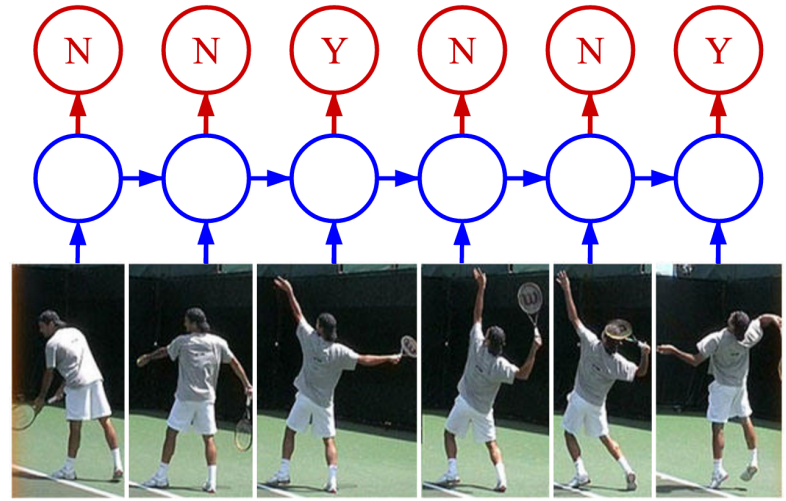

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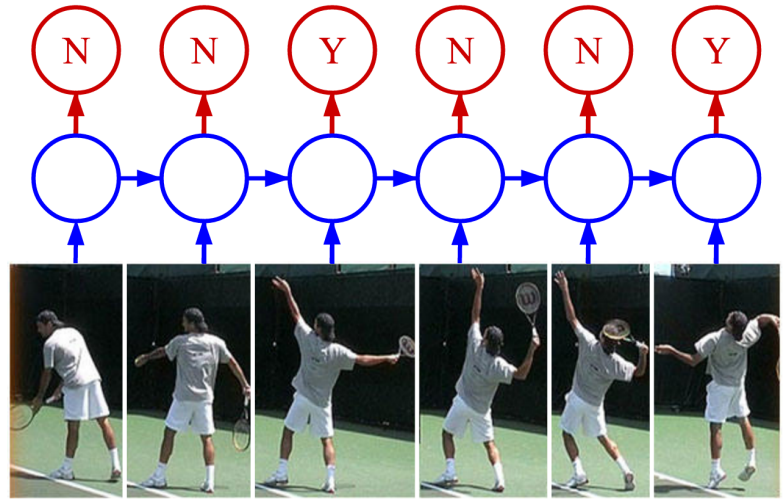

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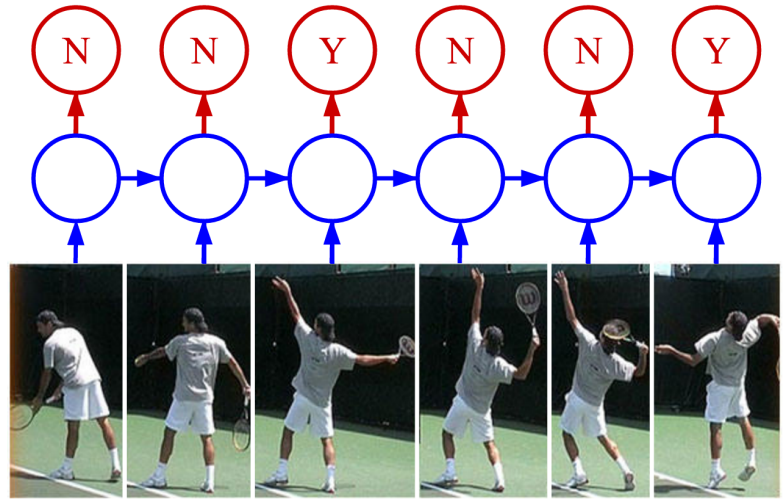
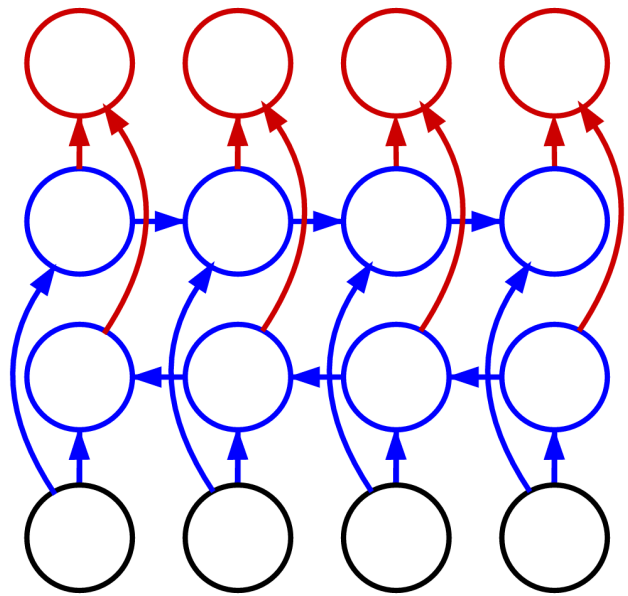
- Can we take ***future*** frames into account?
- ***Bidirectional RNNs***: output $\mathbf{a}^{(L,t)}$ depends on both $\mathbf{a}^{(k,t)}$'s and $\tilde{\mathbf{a}}^{(k,t)}$'s

$$\tilde{\mathbf{a}}^{(k,t)} = \text{act}(\tilde{\boldsymbol{U}}^{(k)}\tilde{\mathbf{a}}^{(k,t+1)} + \tilde{\boldsymbol{W}}^{(k)}\tilde{\mathbf{a}}^{(k-1,t)})$$





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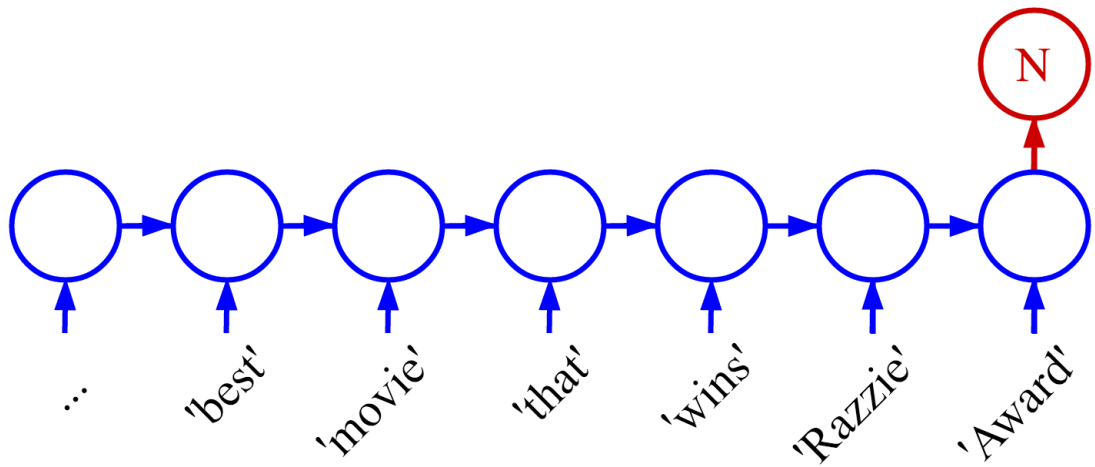

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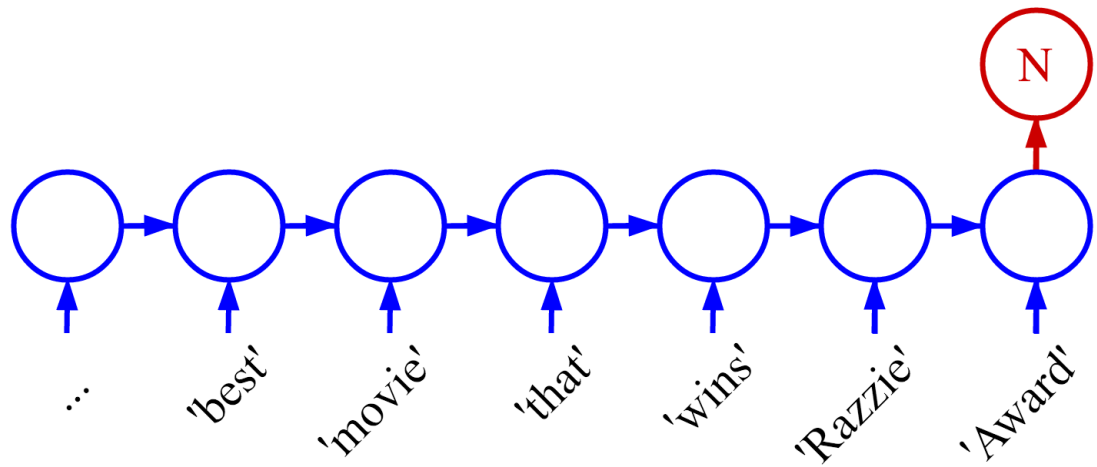
- "Razzie" has less effect if it is far away from the prediction
- In some applications, transitions are invariant in terms of other concepts



Recursive RNNs II

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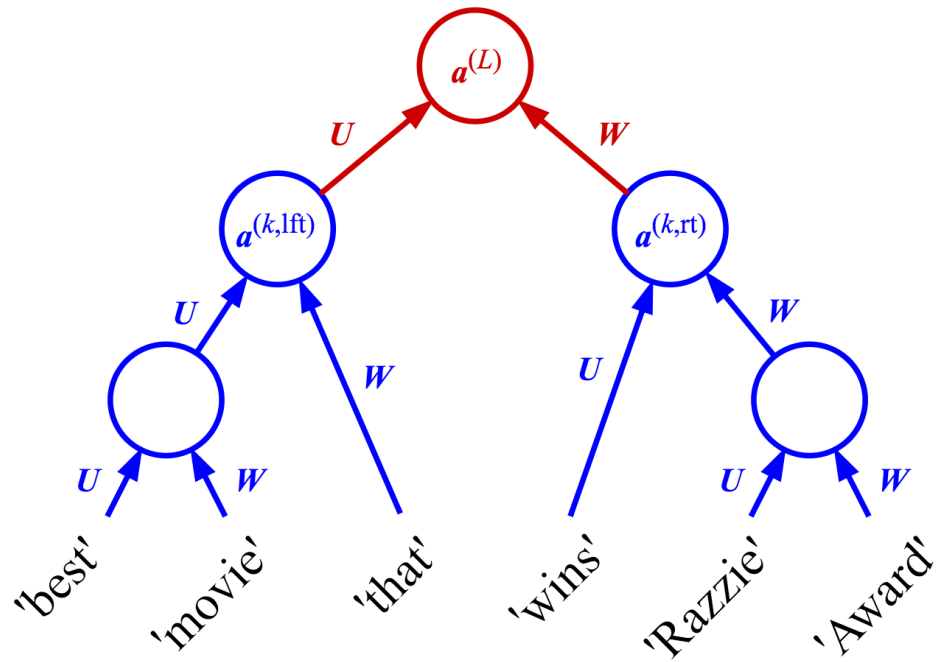

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- ***Recursive RNNs***: "subtree merges" are invariant

$$\mathbf{a}^{(k,t)} = \text{act}(\boldsymbol{U}\mathbf{a}^{(k-1,\text{ left })} + \boldsymbol{W}\mathbf{a}^{(k-1,\text{ right })})$$

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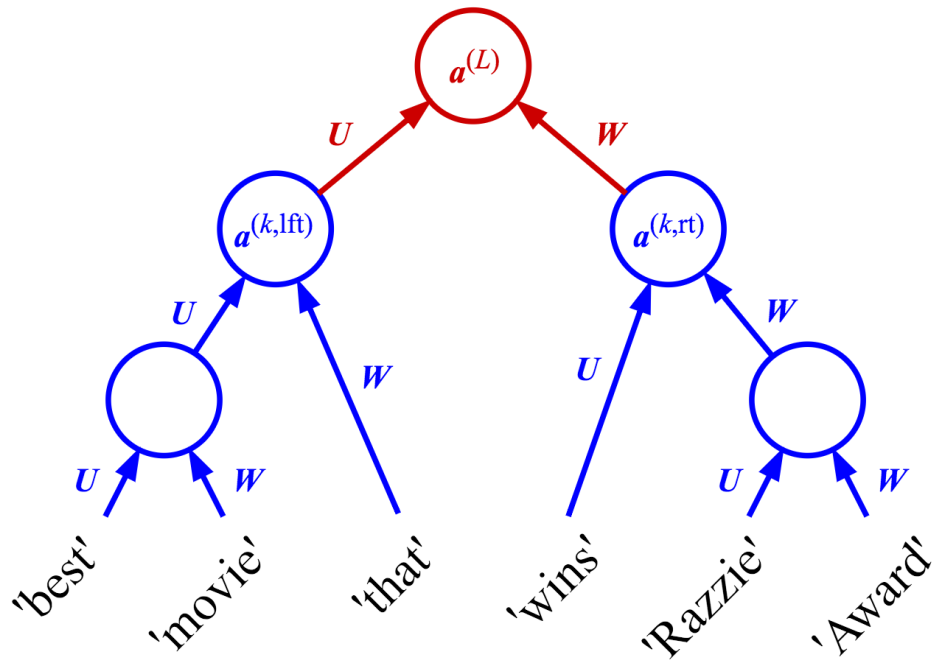
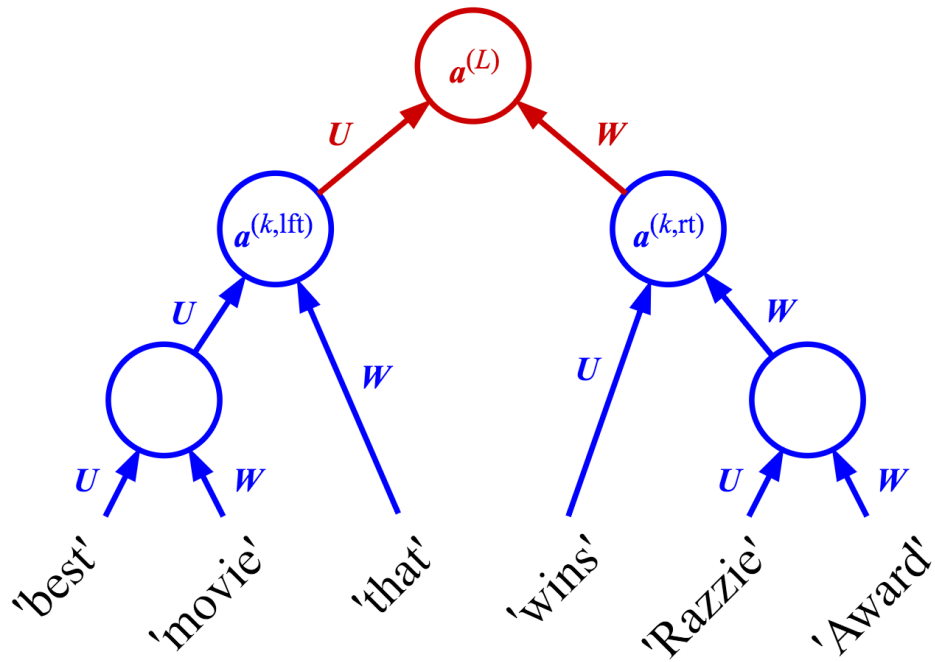


Recursive RNNs II

- In natural language processing (NLP), we can parse the input sentence $\boldsymbol{X}^{(n)}$ into a tree
  - Following gramma rules
- ***Recursive RNNs***: "subtree merges" are invariant

$$\mathbf{a}^{(k,t)} = \text{act}(\boldsymbol{U}\mathbf{a}^{(k-1,\text{ left })} + \boldsymbol{W}\mathbf{a}^{(k-1,\text{ right })})$$

  - $\boldsymbol{U}$ and $\boldsymbol{W}$ are shared recursively in subtrees
- Given sentence length T, $\mathbf{a}^{(L)}$ and $\mathbf{a}^{(1,\cdot)}$ can be $O(\log T)$ away in the best case



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Cost Function of Vanilla RNNs

- Parameters to learn: $\Theta = \{\boldsymbol{W}^{(k)}, \boldsymbol{U}^{(k)}\}_k$ (bias terms omitted)
- Maximum likelihood:

$$\begin{aligned}
&\arg\min_{\Theta} C(\Theta) \\
&= \arg\min_{\Theta} -\log \mathrm{P}(\mathbf{X} \mid \Theta) \\
&= \arg\min_{\Theta} -\textstyle\sum_{n,t} \log \mathrm{P}(\boldsymbol{y}^{(n,t)} \mid \boldsymbol{x}^{(n,t)}, \cdots, \boldsymbol{x}^{(n,1)}, \Theta) \\
&= \arg\min_{\Theta} -\textstyle\sum_{n,t} C^{(n,t)}(\Theta)
\end{aligned}$$

  - $\mathbf{y}^{(t)}$ depends only on $\mathbf{x}^{(1)}, \cdots, \mathbf{x}^{(t)}$

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  - $\mathbf{y}^{(t)}$ depends only on $\mathbf{x}^{(1)}, \cdots, \mathbf{x}^{(t)}$
- For example, in binary classification:
- Assuming $\mathrm{P}(\mathbf{y}^{(n,t)} = 1 \,|\, \boldsymbol{x}^{(n,t)}, \cdots, \boldsymbol{x}^{(n,1)}) \sim \text{Bernoulli}(\rho^{(t)})$, we have

$$C^{(n,t)}(\Theta) = (\boldsymbol{a}^{(L,t)})^{y^{(n,t)}} (1 - \boldsymbol{a}^{(L,t)})^{(1-y^{(n,t)})}$$

  - $\boldsymbol{a}^{(L,t)} = \rho^{(t)}$ are based on $\boldsymbol{a}^{(\cdot,t)}$'s, which summarize $\boldsymbol{x}^{(n,t)}, \cdots, \boldsymbol{x}^{(n,1)}$

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SGD-based Training

- RNN optimization problem can be solved using SGD:

$$\Theta^{(s+1)} \leftarrow \Theta^{(s)} - \eta \nabla_{\Theta} \sum_{n,t} C^{(n,t)}(\Theta^{(s)})$$

- Let $c^{(n,t)} = C^{(n,t)}(\Theta^{(s)})$, our goal is to evaluate $\frac{\partial c^{(n,t)}}{\partial U_{i,j}^{(k)}}$ and $\frac{\partial c^{(n,t)}}{\partial W_{i,j}^{(k)}}$
- Evaluation of $\frac{\partial c^{(n,t)}}{\partial W_{i,j}^{(k)}}$ is similar to that in DNNs and omitted
- We focus on:

$$\frac{\partial c^{(n,t)}}{\partial U_{i,j}^{(k)}} = \frac{\partial c^{(n,t)}}{\partial z_j^{(k,t)}} \cdot \frac{\partial z_j^{(k,t)}}{\partial U_{i,j}^{(k)}} = \delta_j^{(k,t)} \frac{\partial z_j^{(k,t)}}{\partial U_{i,j}^{(k)}}$$

Forward Pass through Time

- The second term: $\frac{\partial z_j^{(k,t)}}{\partial U_{i,j}^{(k)}}$

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- We can get all second terms starting from the most shallow layer and ***earliest time***

Backward Pass through Time I

- The first term (error signal): $\delta_j^{(k,t)} = \frac{\partial c^{(n,t)}}{\partial z_j^{(k,t)}}$
- We have

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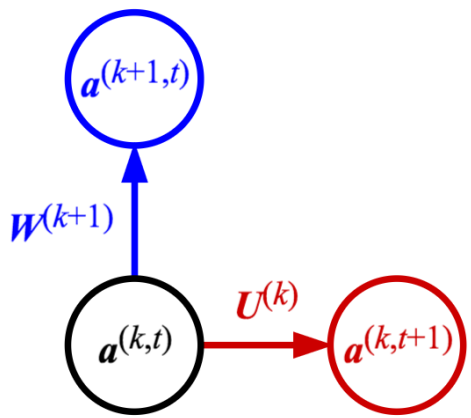

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&= \left(\sum_s \frac{\partial c^{(n,t)}}{\partial z_s^{(k+1,t)}} \cdot \frac{\partial z_s^{(k+1,t)}}{\partial a_j^{(k,t)}} + \sum_s \frac{\partial c^{(n,t)}}{\partial z_s^{(k,t+1)}} \cdot \frac{\partial z_s^{(k,t+1)}}{\partial a_j^{(k,t)}} \right) \mathrm{act}'(z_j^{(k,t)}) \\
&= \left(\sum_s \delta_s^{(k+1,t)} W_{j,s}^{(k+1)} + \sum_s \delta_s^{(k,t+1)} U_{j,s}^{(k)} \right) \mathrm{act}'(z_j^{(k,t)})
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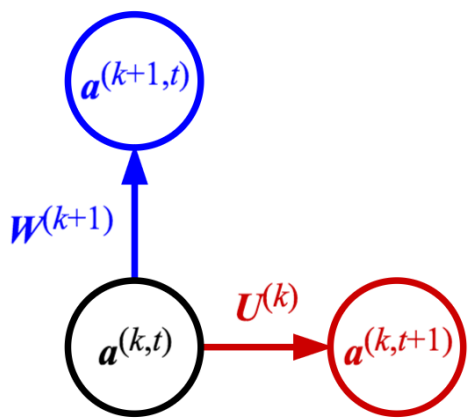

Backward Pass through Time II

$$\delta_j^{(k,t)} = \left(\sum_s \delta_s^{(k+1,t)} W_{j,s}^{(k+1)} + \sum_s \delta_s^{(k,t+1)} U_{j,s}^{(k)} \right) \text{act}'(z_j^{(k,t)})$$

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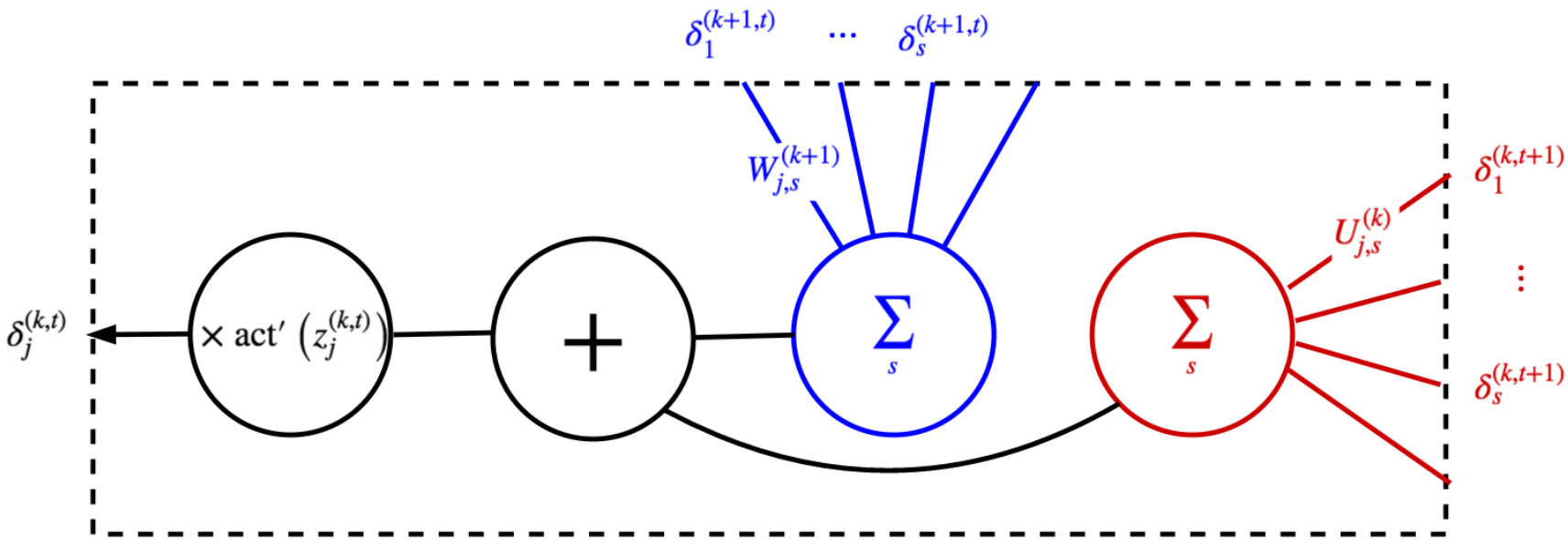
- We can evaluate all $\delta_j^{(k,t)}$'s starting from the deepest layer and ***latest time***



Backprop through Time (BPTT)

- So far, we have discussed how to compute the gradients of $U_{i,j}^{(k)}$'s (and $W_{i,j}^{(k)}$'s) for a single loss $c^{(n,t)} = C^{(n,t)}(\Theta^{(s)})$ at specific time

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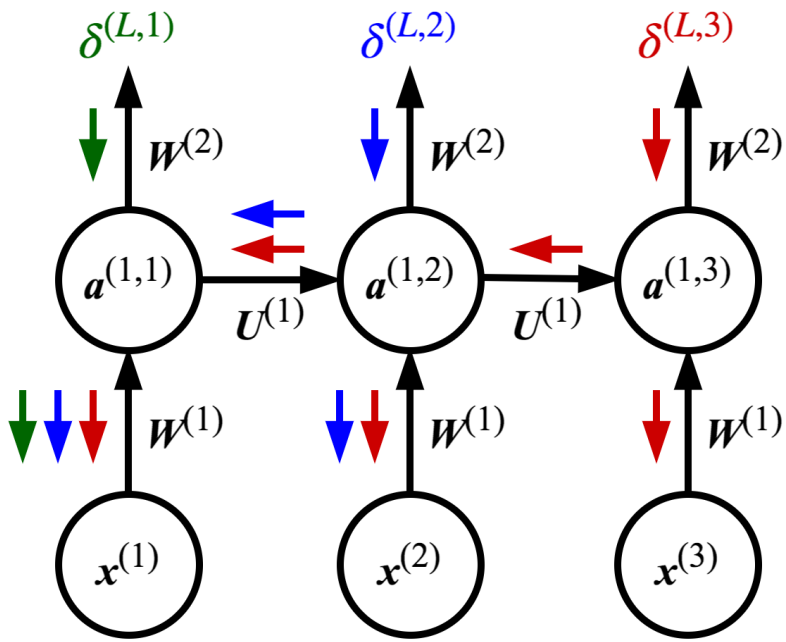
- ***BPTT***: single forward pass, ***multiple*** backward passes



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Long-Term Dependencies

- Forward pass:

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$$\delta^{(k,t)} \leftarrow \mathrm{act}'(\boldsymbol{z}^{(k,t)}) \odot (\boldsymbol{U}^{(k)}\delta^{(k,t+1)} + \boldsymbol{W}^{(k+1)}\delta^{(k+1,t)})$$

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- If $\boldsymbol{a}^{(k,i)}$ and $\boldsymbol{a}^{(k,j)}$ are far away in time, their long-term dependency causes optimization problems

Exploding/Vanishing Gradient Problem

- Ignoring activation function and depth:

$$\boldsymbol{a}^{(k,j)} = \left(\boldsymbol{U}^{(k)\top}\right)^{(j-i)} \boldsymbol{a}^{(k,i)} \text{ and } \boldsymbol{\delta}^{(k,i)} = \left(\boldsymbol{U}^{(k)}\right)^{(j-i)} \boldsymbol{\delta}^{(k,j)}$$

- Given eigendecomposition: $\boldsymbol{U}^{(k)} = \boldsymbol{Q} \begin{bmatrix} \lambda_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \lambda_{D^{(k)}} \end{bmatrix} \boldsymbol{Q}^\top$

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- When $j-i$ is large, λ_s^{j-i} is either very large or small
  - $\lambda_s = 1.01 \Rightarrow \lambda_s^{1000} \approx 20,000$
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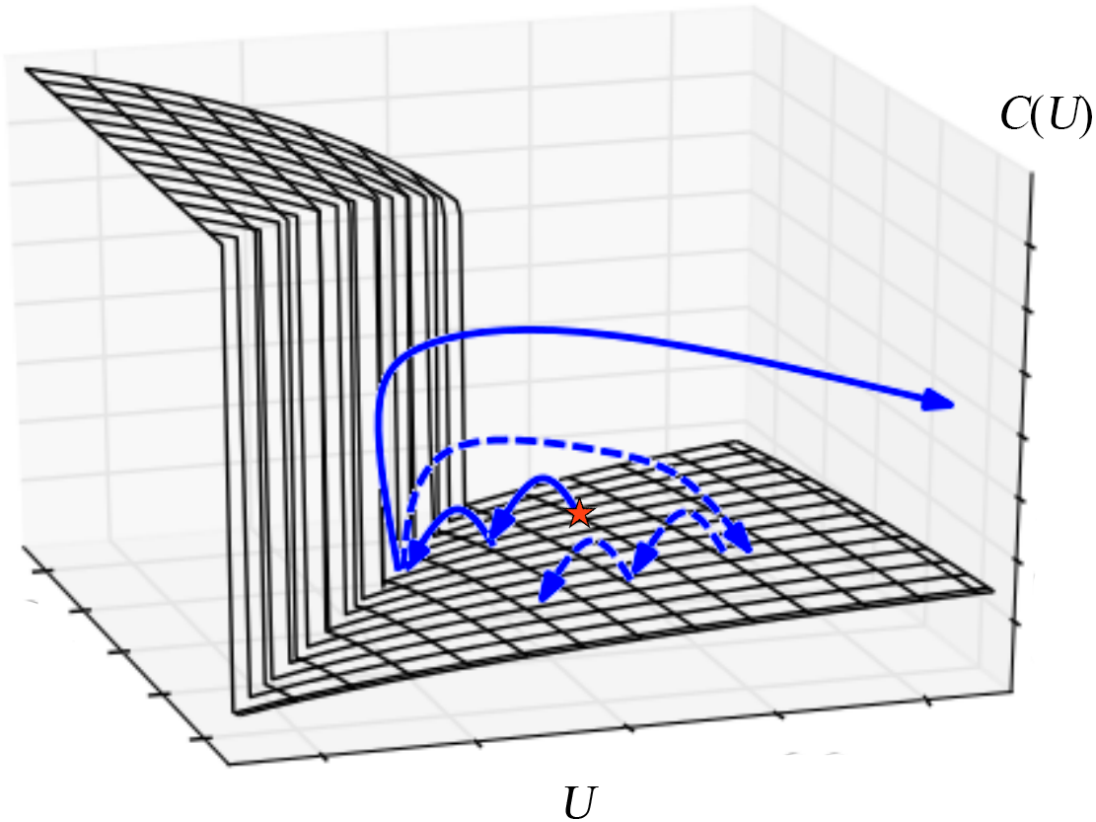
- Exploding or vanishing gradients!

Cost Surface

- The cost surface of C is either very flat or steep
- Hard for gradient-based optimization



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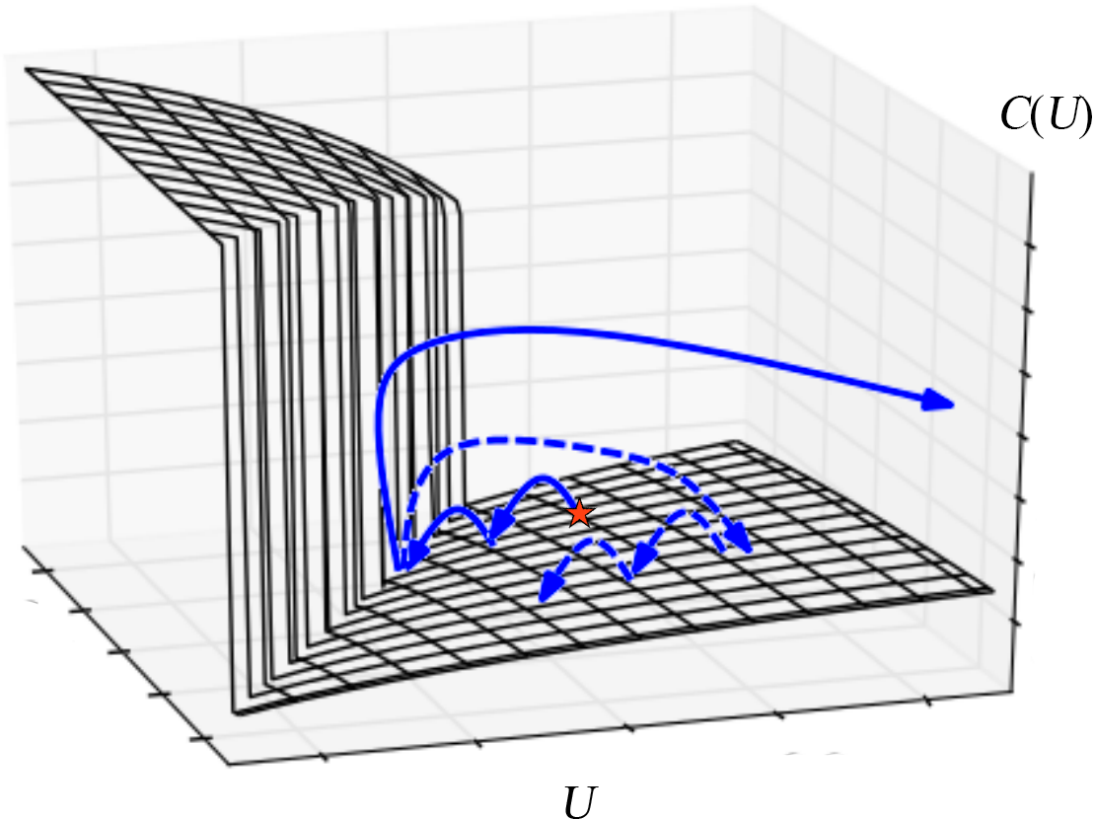
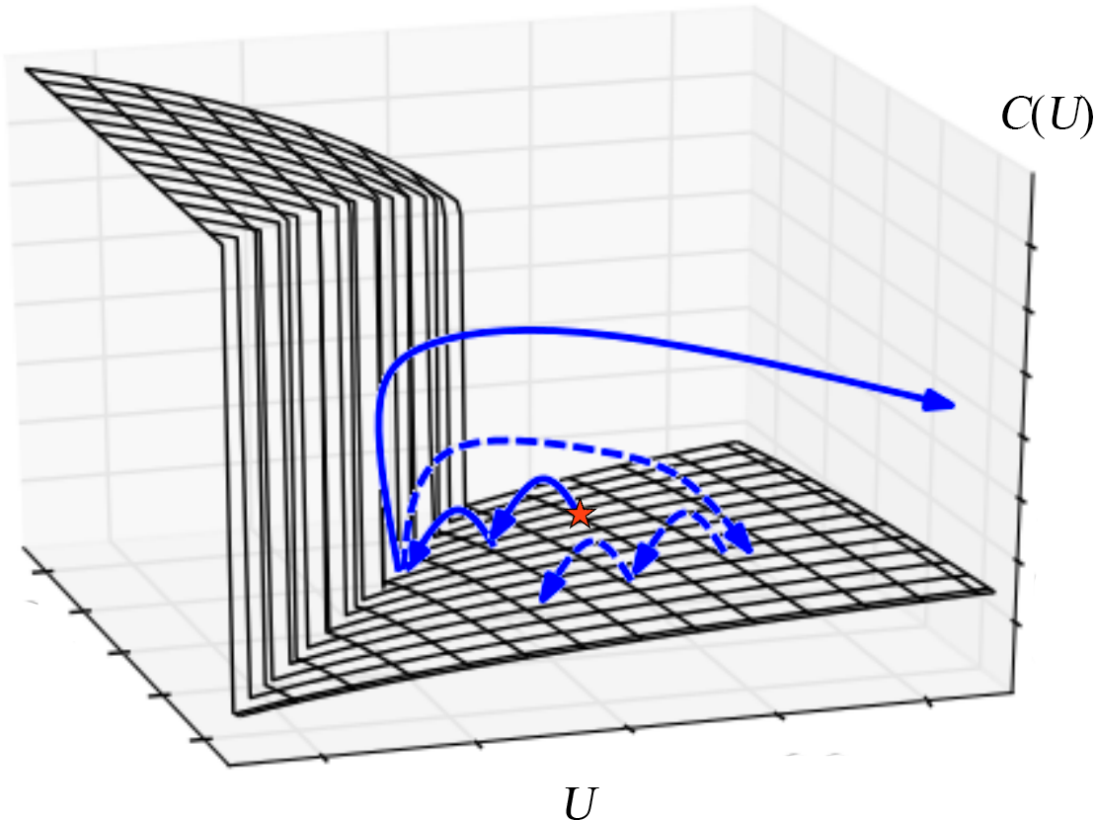
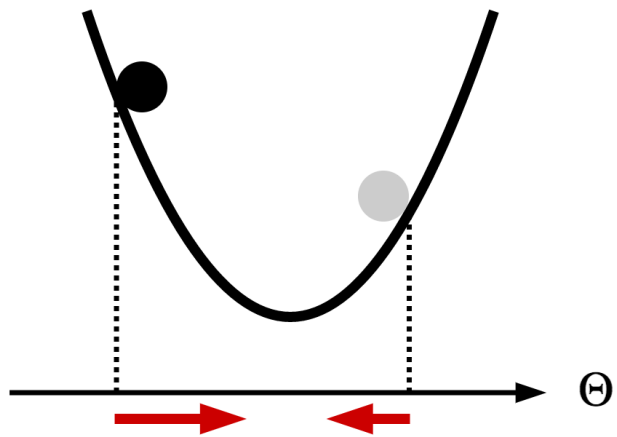


Nesterov Momentum

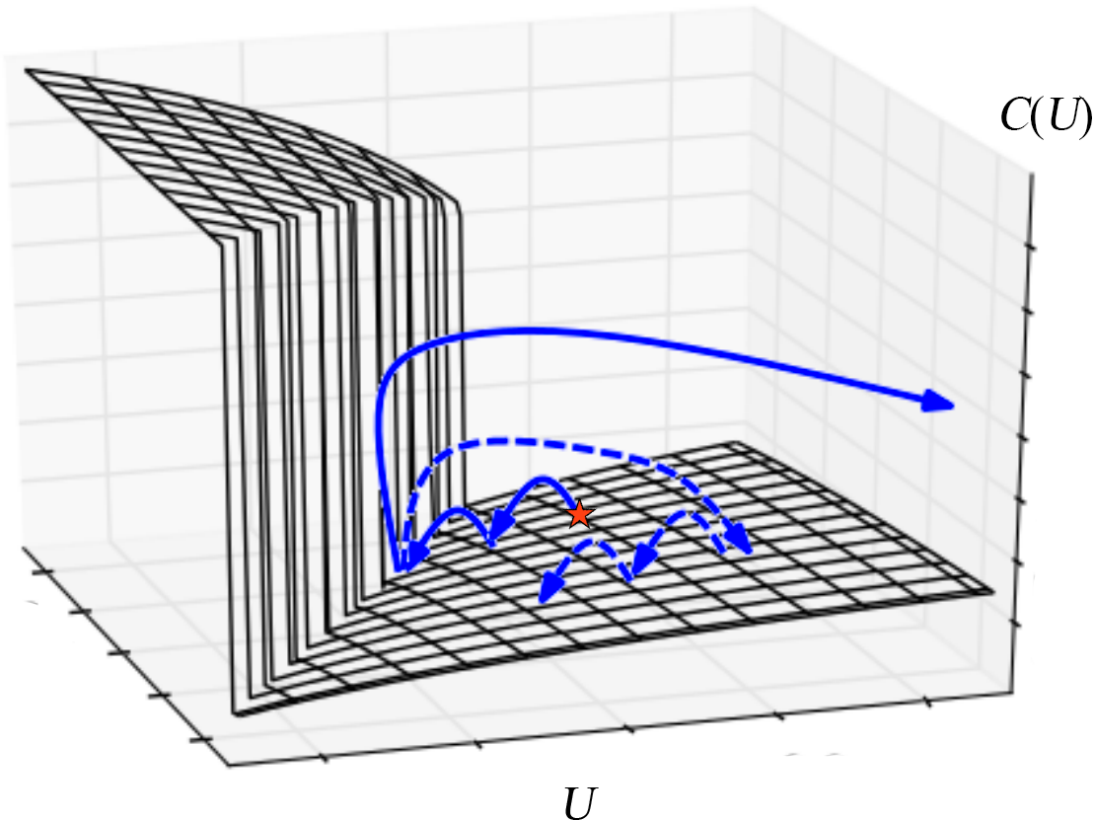
- Use Nesterov momentum to "brake" before hitting the wall





Gradient Clipping

- A simple way is to avoid the exploding gradient problem is to ***clip*** a gradient if it exceeds a predefined threshold
- Very effective in practice

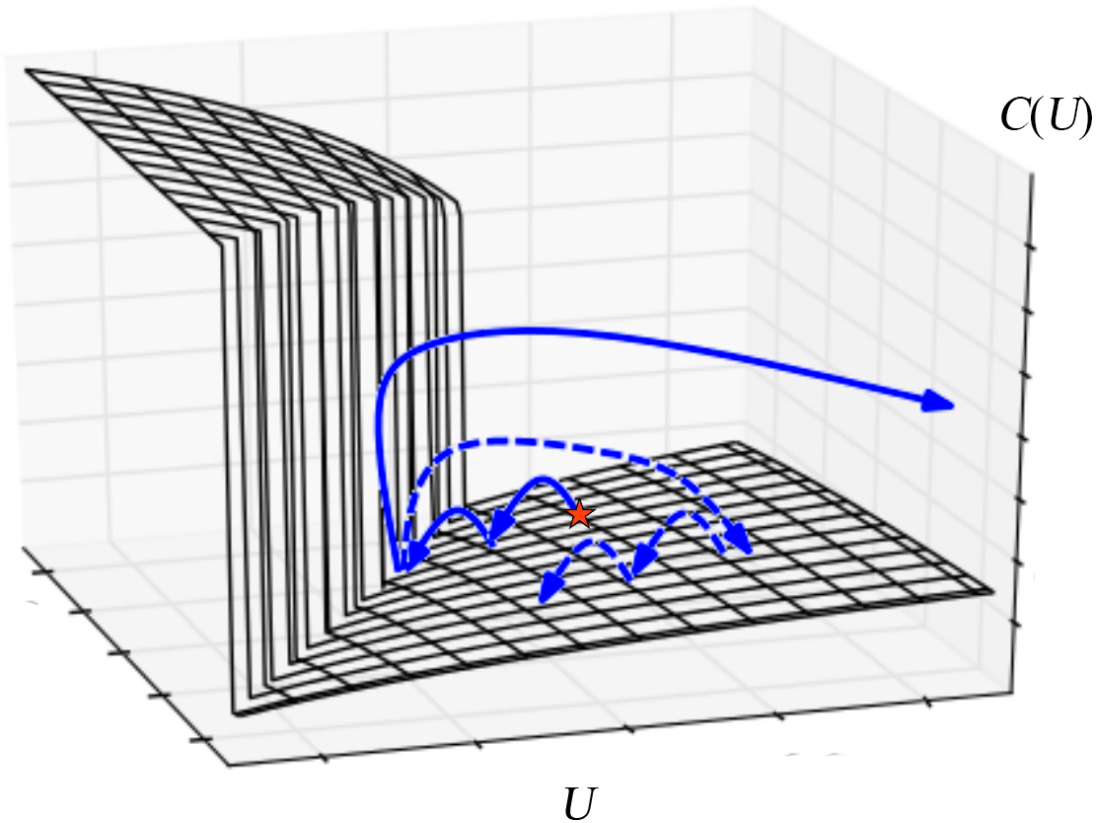


RMS Prop

- Adaptive learning rate based on statistics of recent gradients:

$$\boldsymbol{r}^{(t+1)} \leftarrow \lambda \boldsymbol{r}^{(t)} + (1-\lambda)\boldsymbol{g}^{(t)} \odot \boldsymbol{g}^{(t)}$$

$$\Theta^{(t+1)} \leftarrow \Theta^{(t)} - \frac{\eta}{\sqrt{\boldsymbol{r}^{(t+1)}}} \odot \boldsymbol{g}^{(t)}$$



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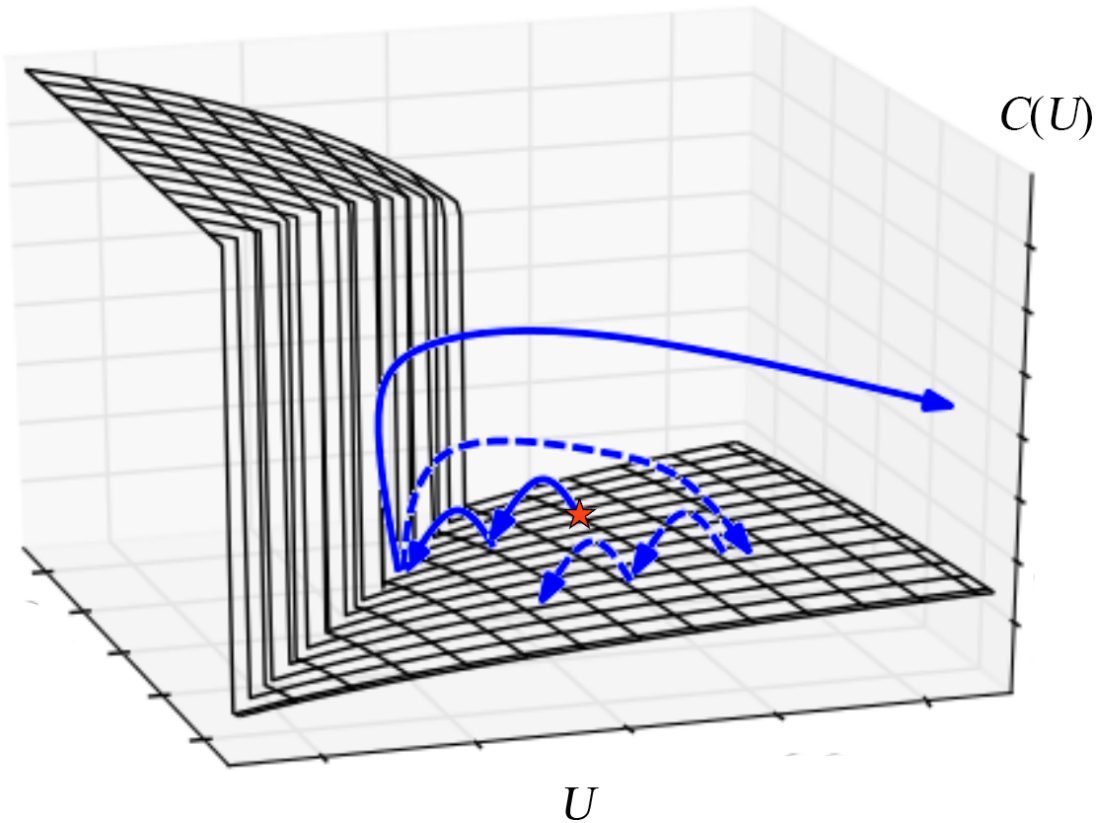
- Reduce λ



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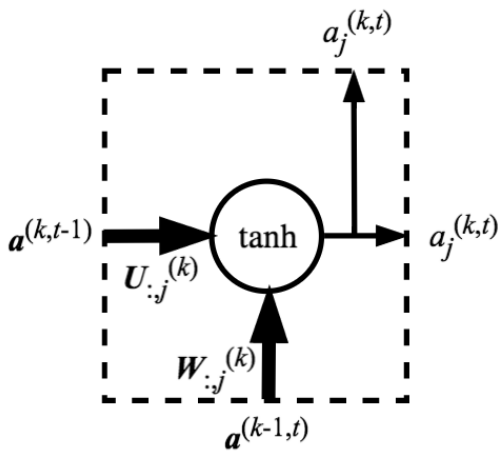

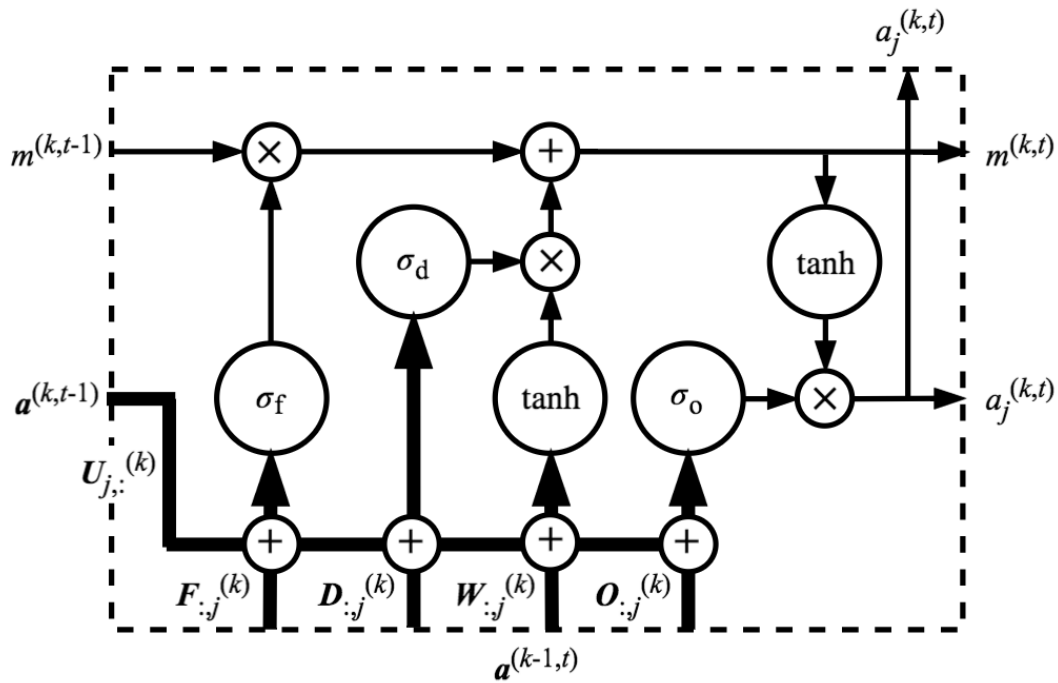

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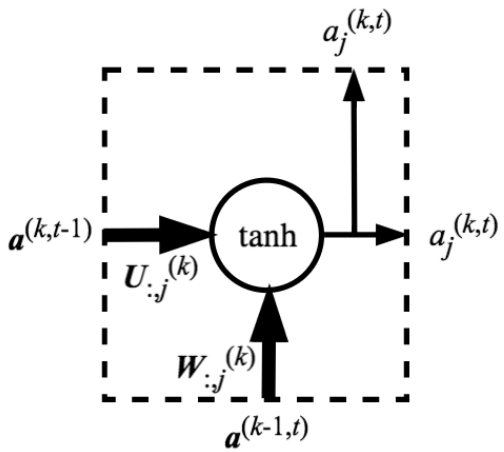

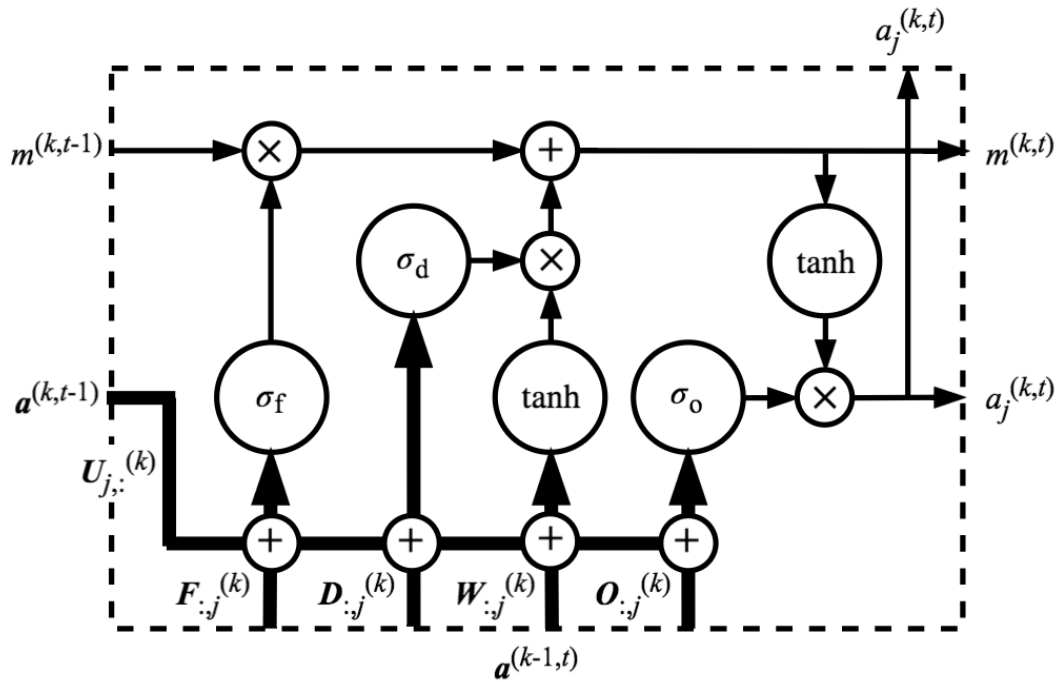

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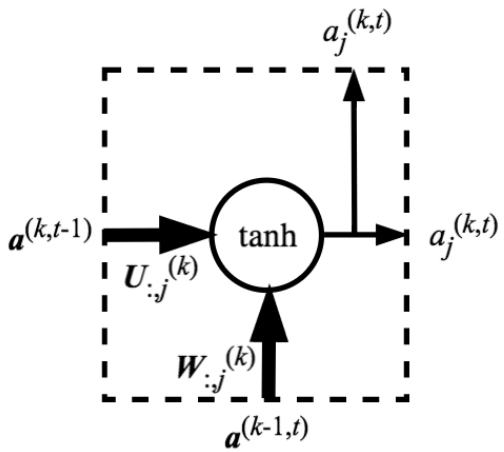

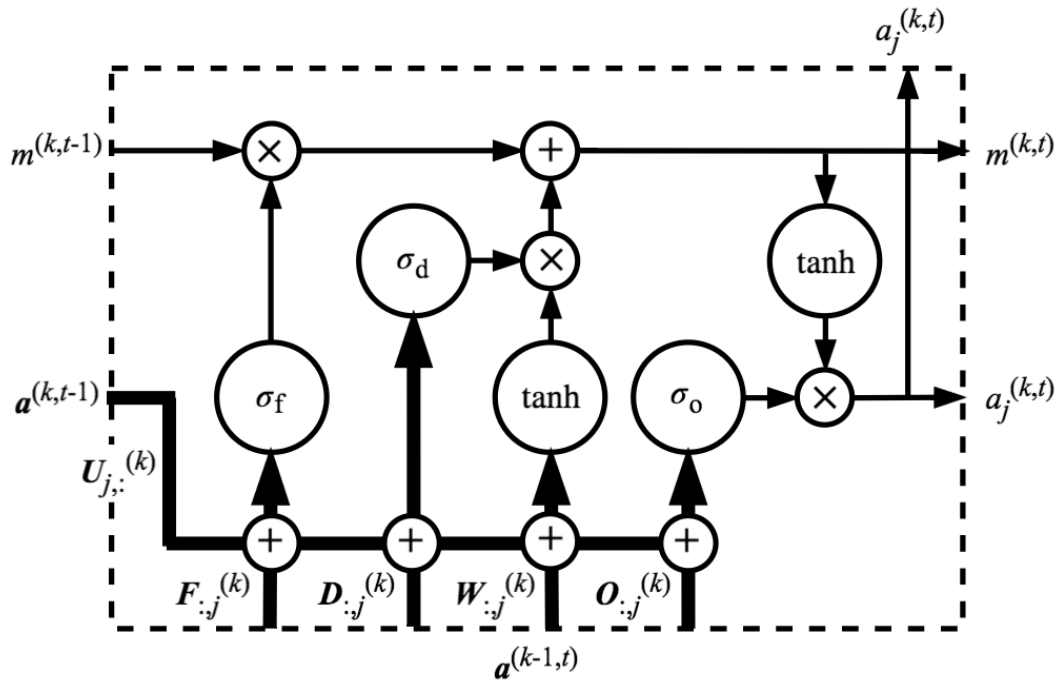

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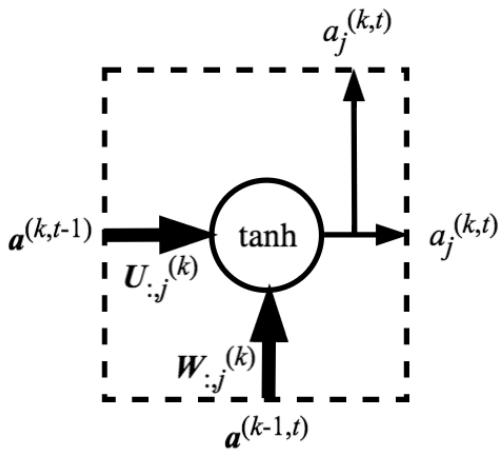

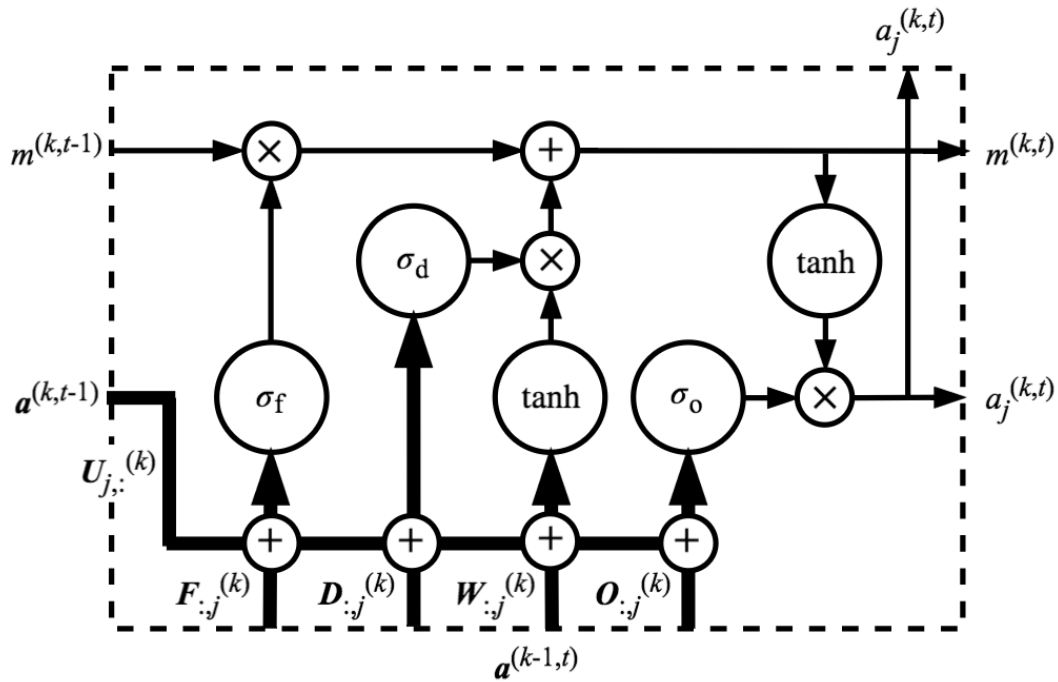

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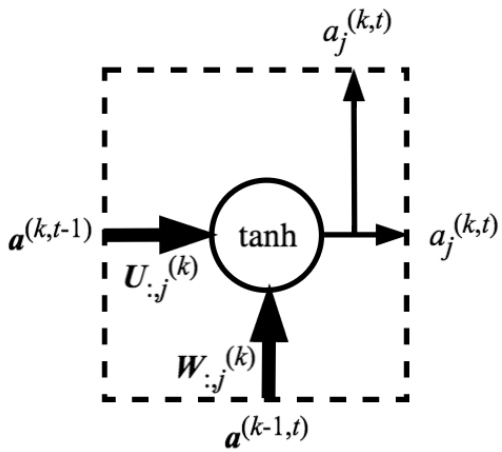

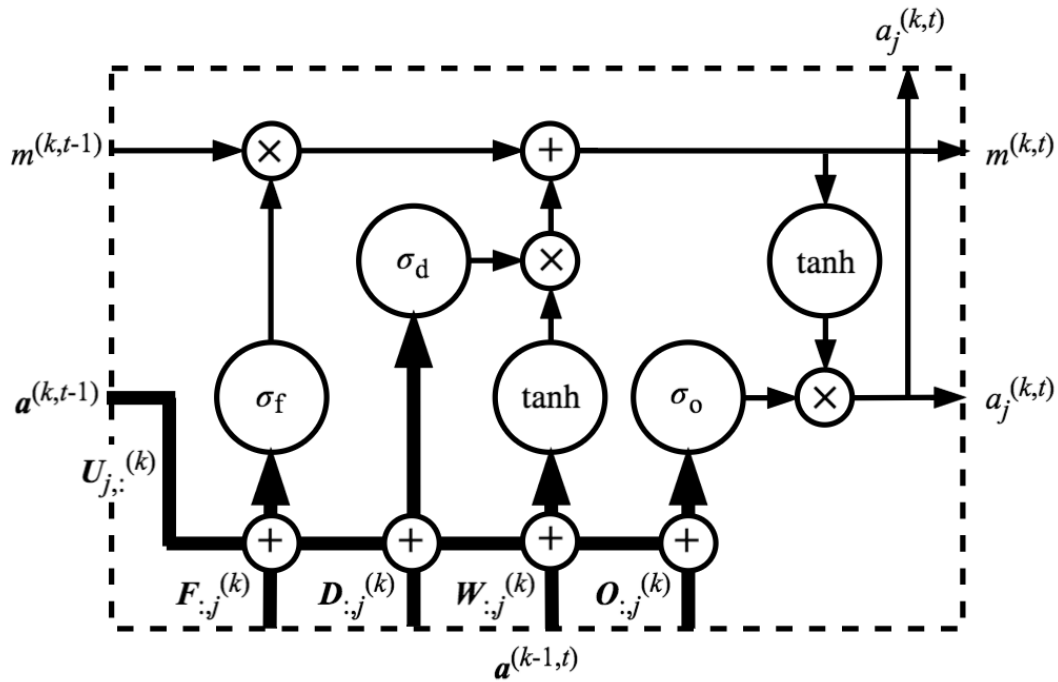

Error Signals

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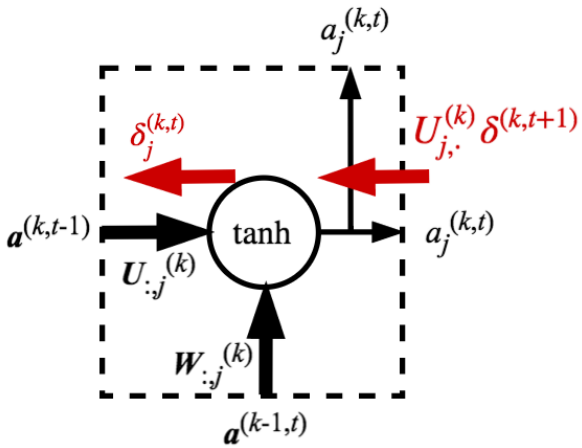

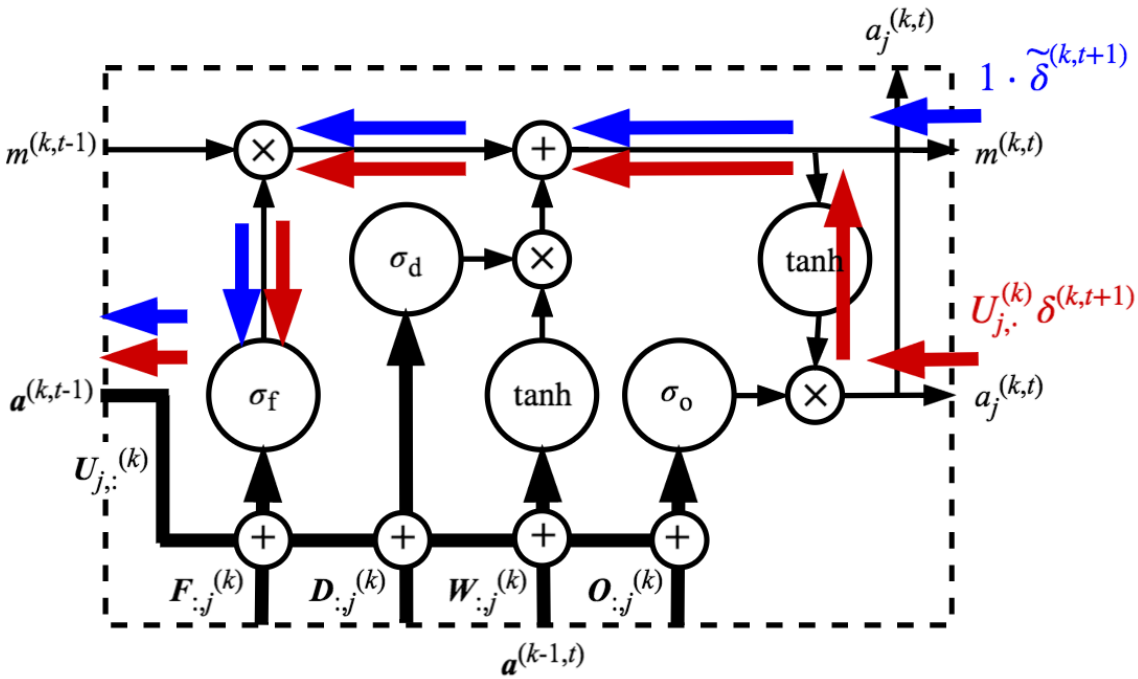

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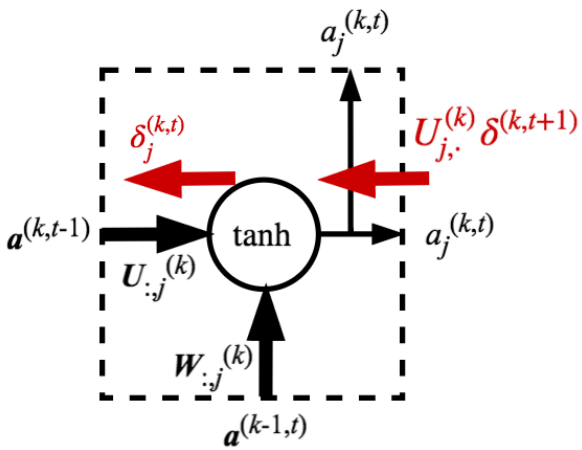

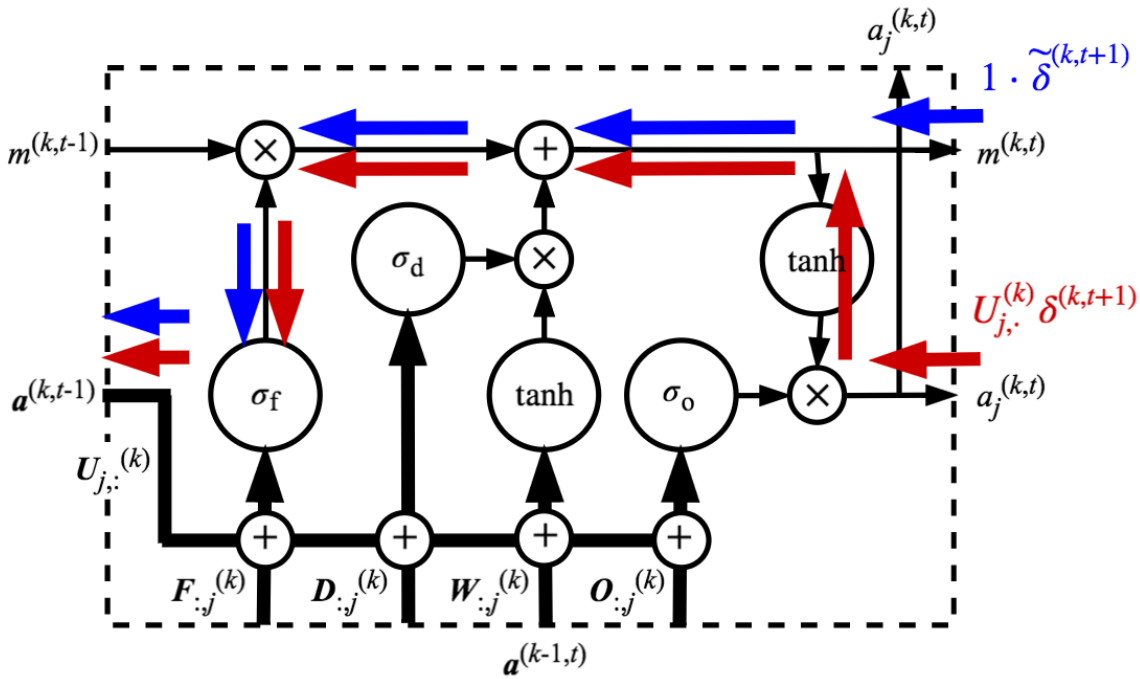

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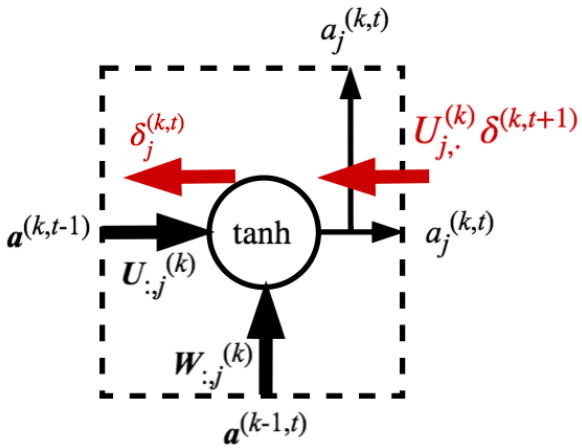
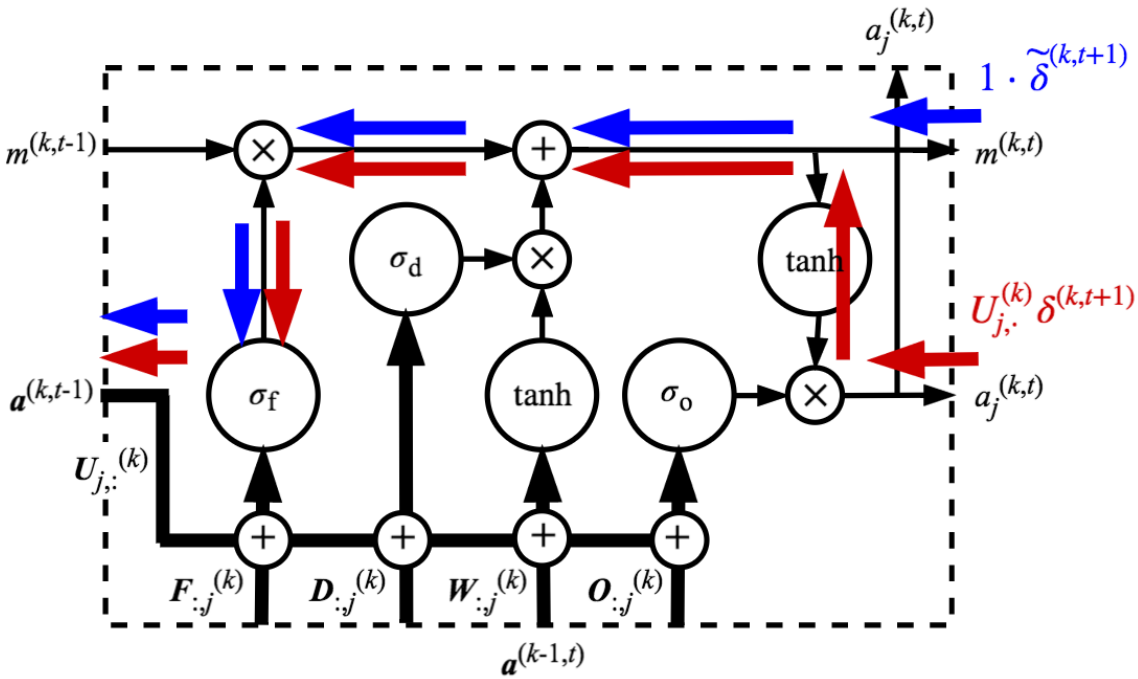
- When NN decides to close the forget gate, the vanishing gradient problem is irrelevant
- In practice, LSTM + gradient clipping works well together





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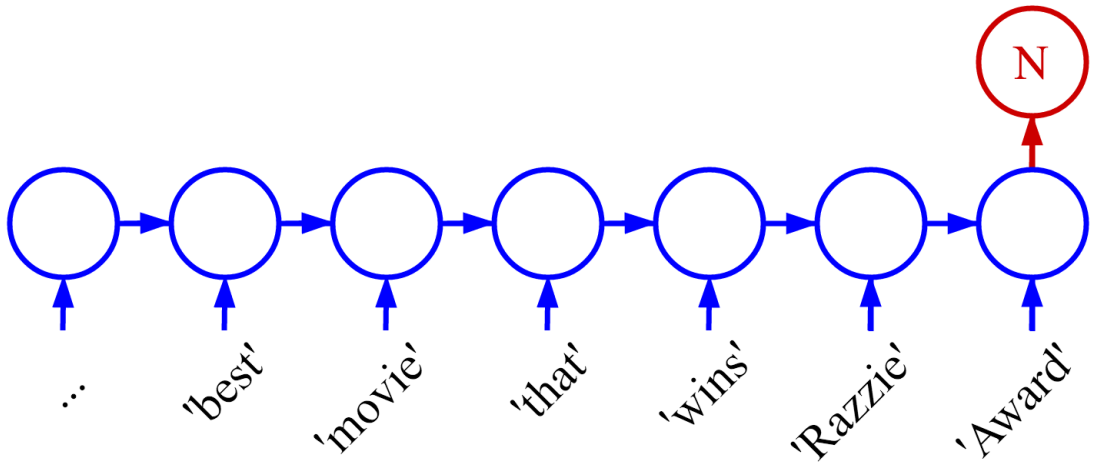

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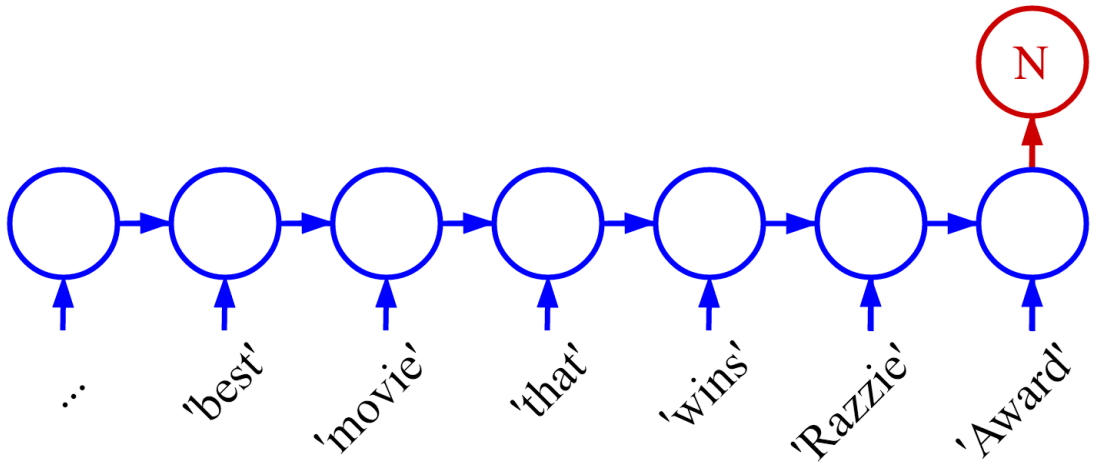

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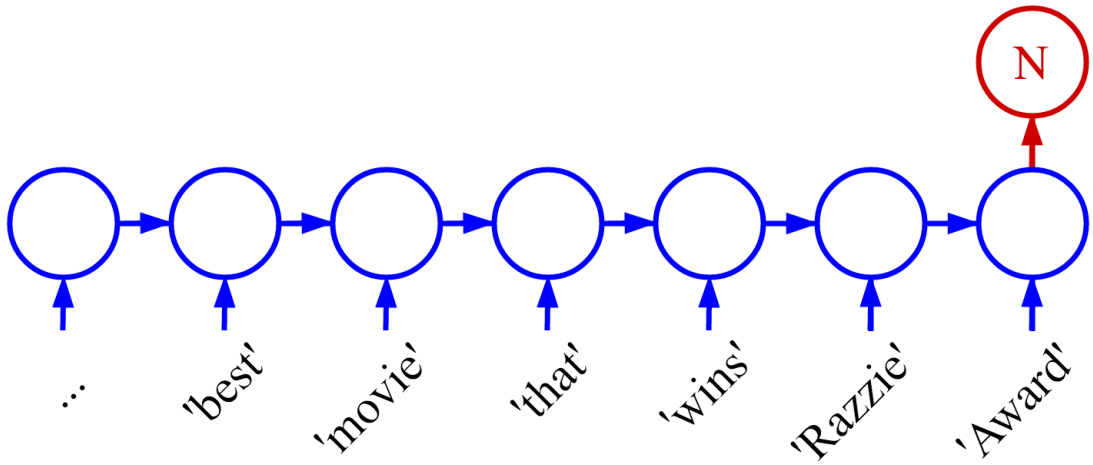

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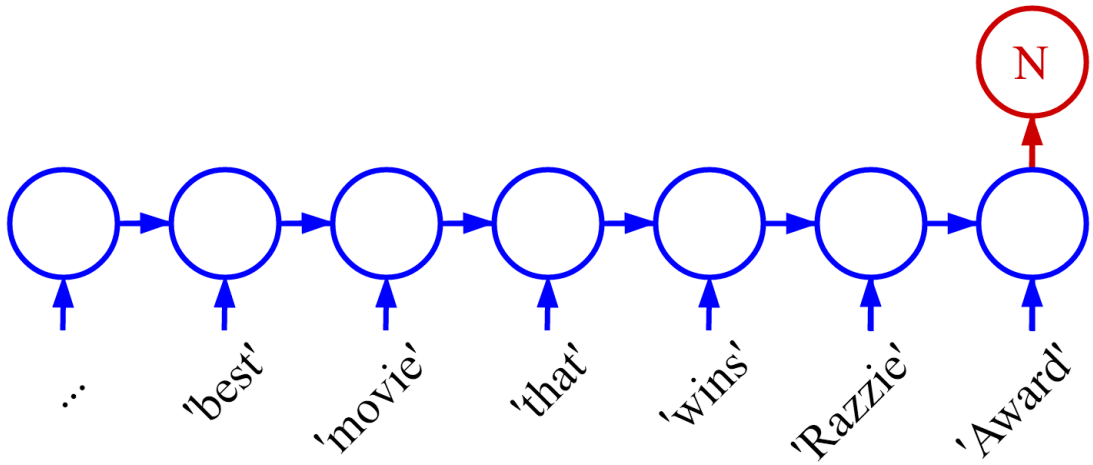

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  - To let the next neuron decide the activation/gate values by its own

Outline

1. Design
   - Vanilla RNNs
   - Design Alternatives
2. **Training**
   - Backprop through Time (BPTT)
   - Optimization Techniques
   - Optimization-Friendly Models & LSTM
   - Parallelism & Teacher Forcing
3. **Augmented RNNs**
   - Attention
   - Explicit Memory
   - Adaptive Computation Time (ACT)
4. **Case Studies**
   - Visualization
   - Memory Networks
   - Google Neural Machine Translation

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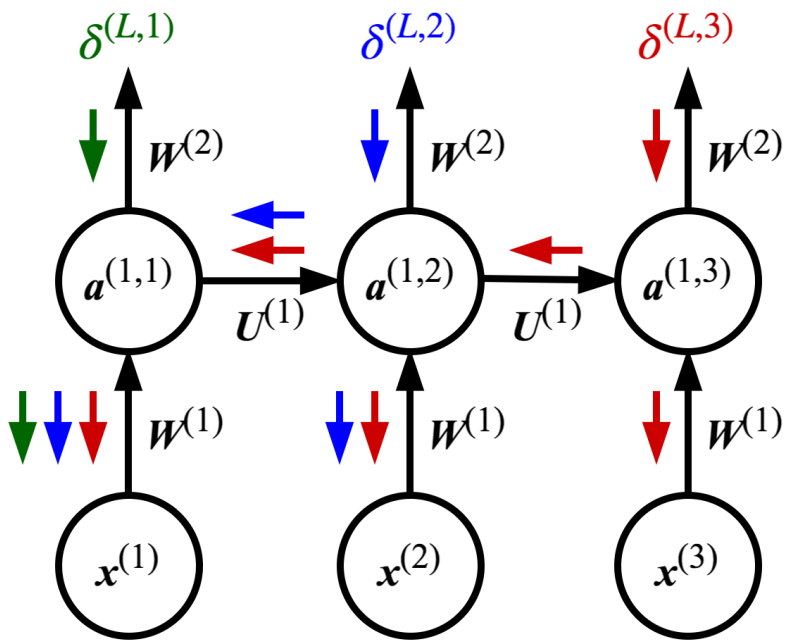

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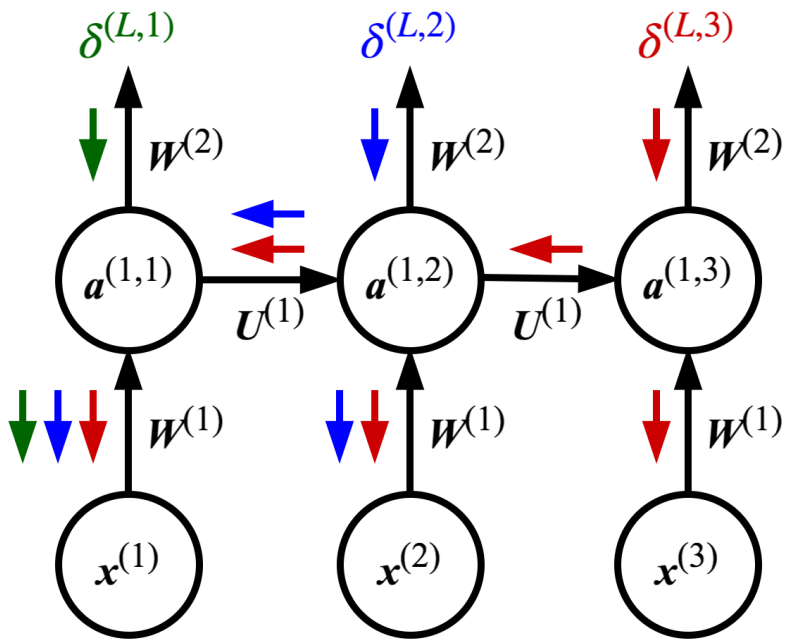

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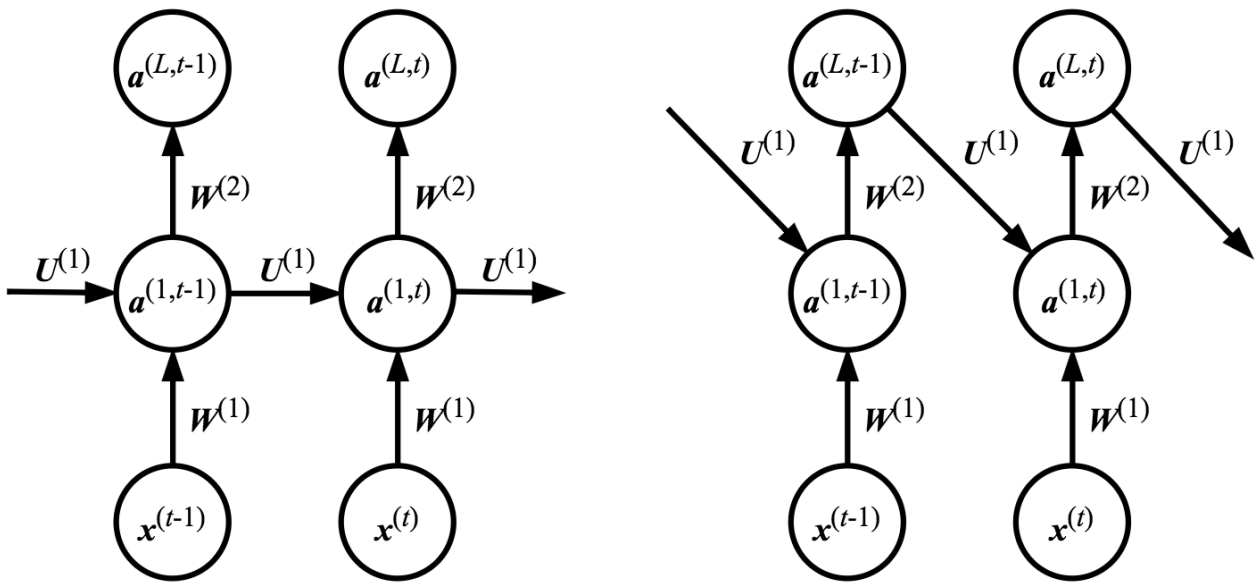

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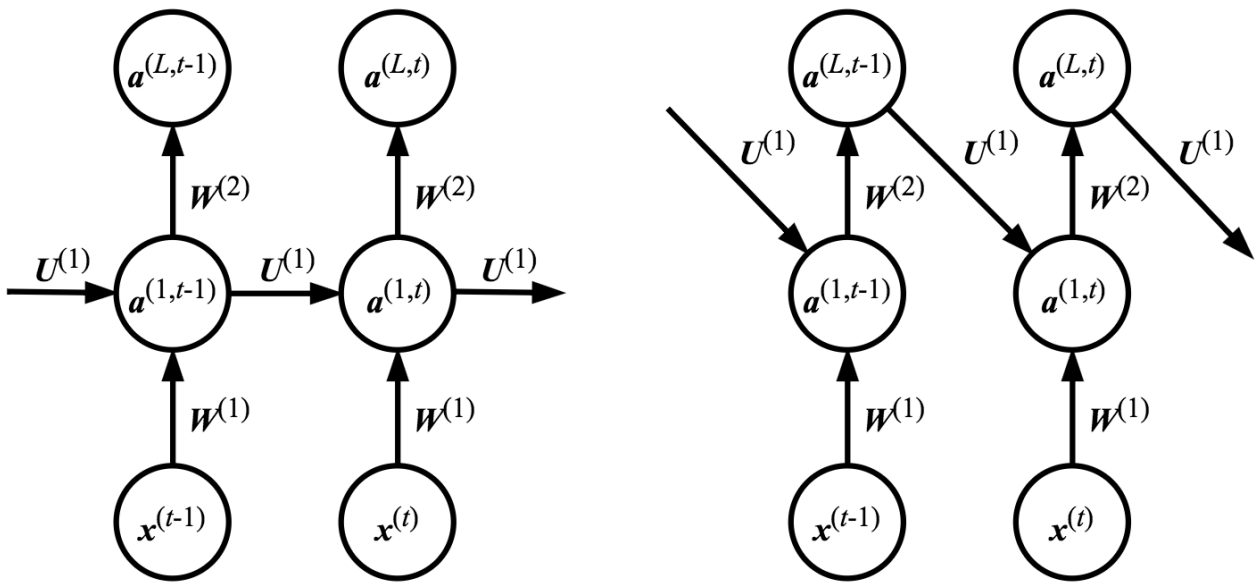

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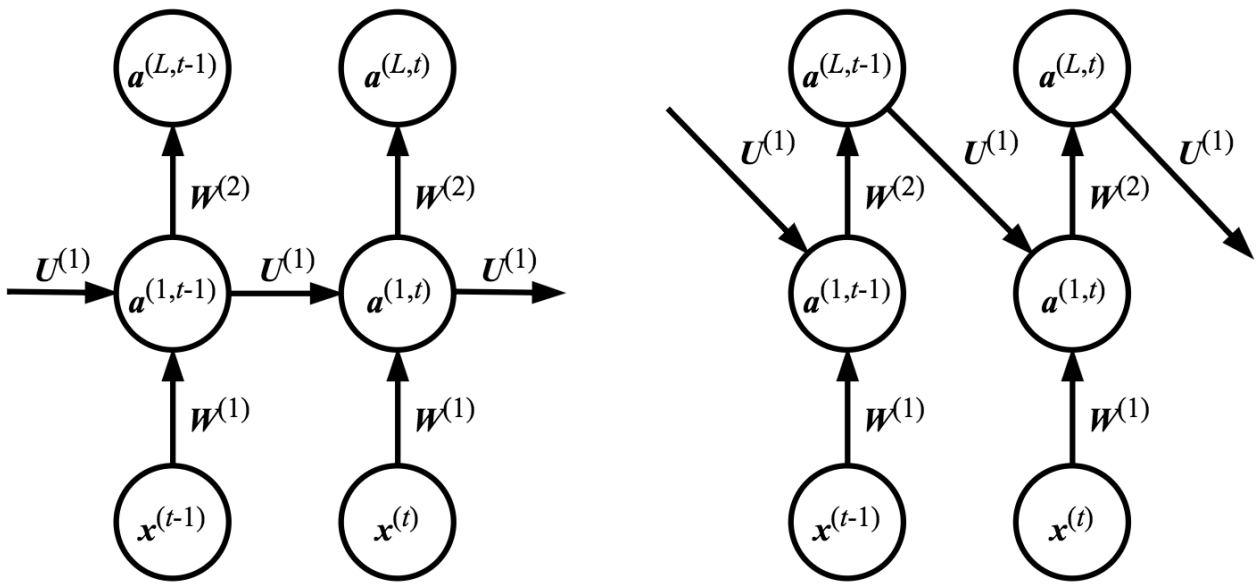

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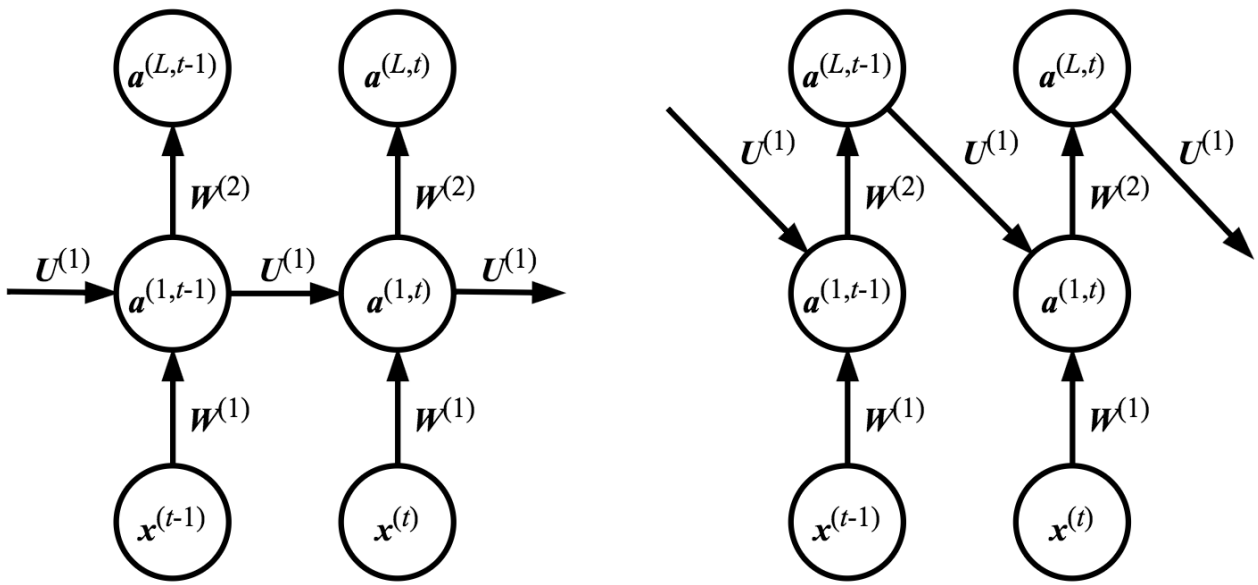

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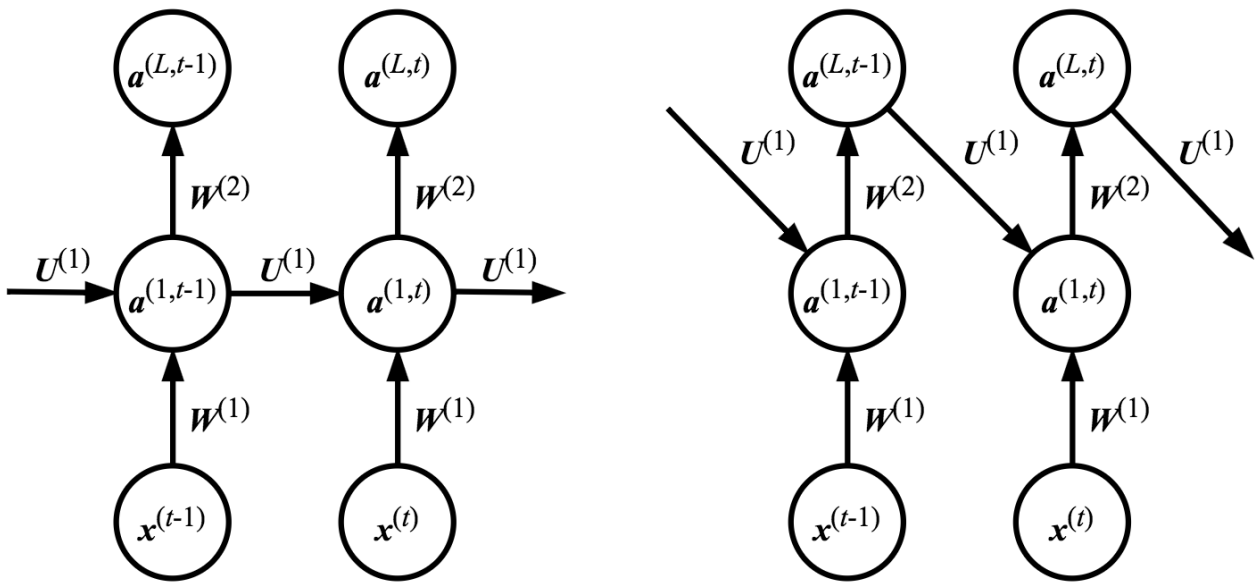

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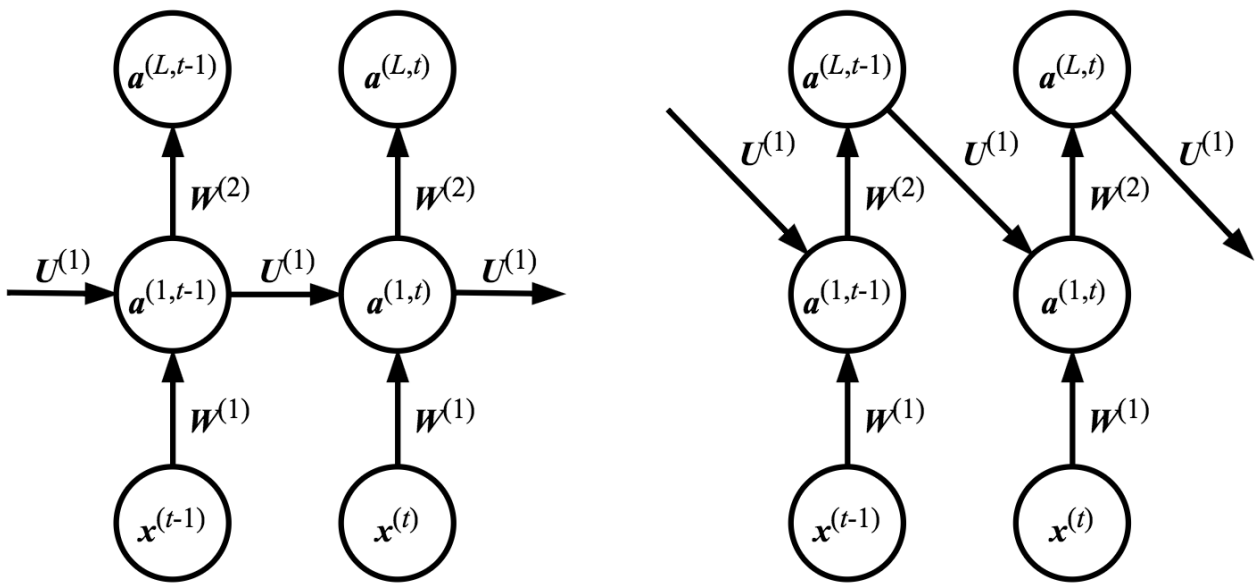

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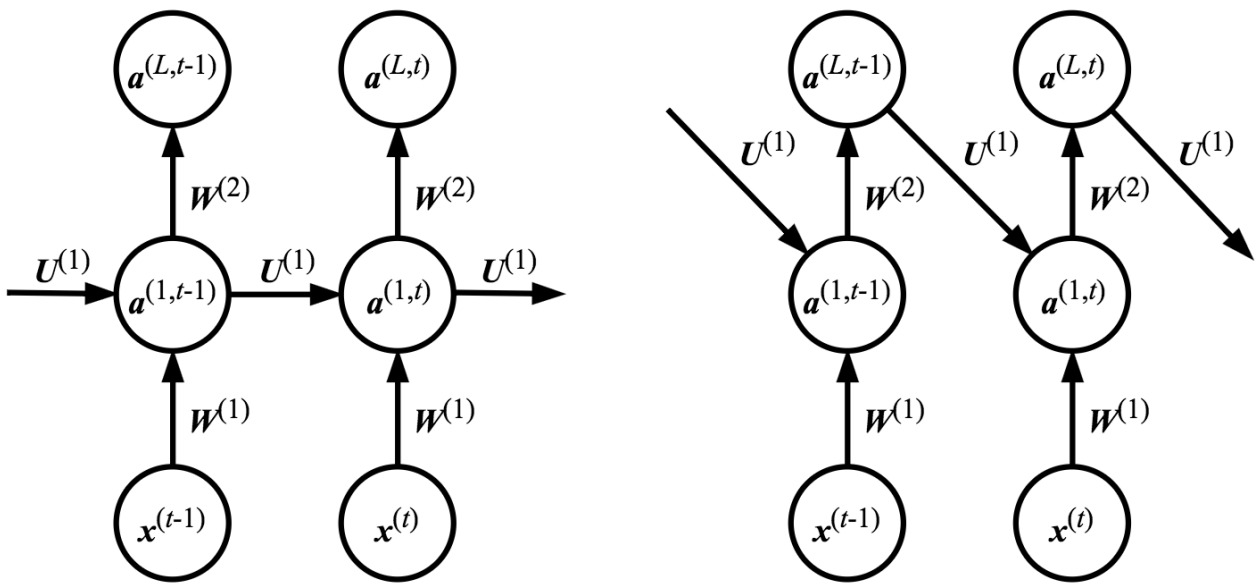

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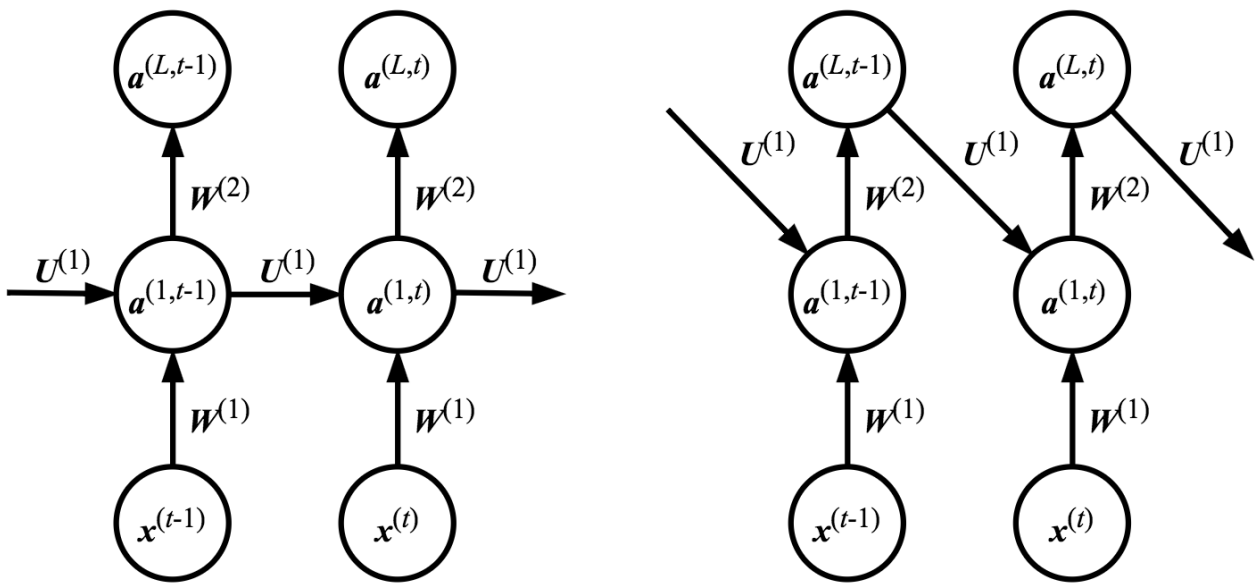
- Output-recurrent RNNs ***cannot*** simulate Turing machines and are strictly less powerful
- The output $\boldsymbol{a}^{(L,\cdot)}$'s are explicitly trained to match training targets
  - Cannot capture all required information in the past to predict the future



Outline

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   - Design Alternatives
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   - Optimization Techniques
   - Optimization-Friendly Models & LSTM
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Limited Representation Size

- In some RNNs, a hidden representation $\mathbf{a}^{(\cdot,t)}$ needs to support:
  - Current prediction $\mathbf{a}^{(L,t)}$, and
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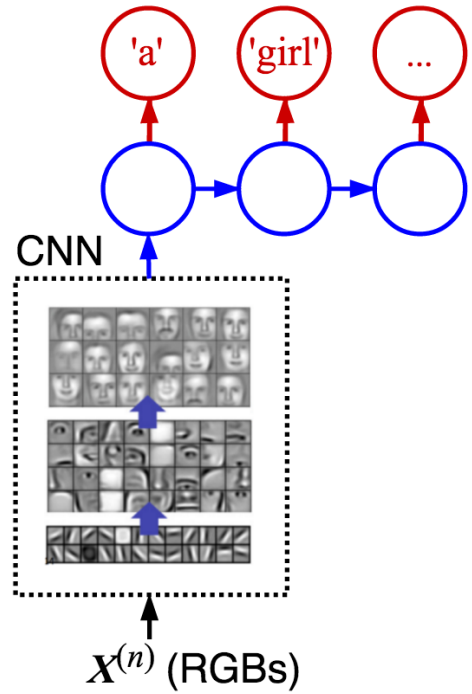
"A little girl sitting on a bed with a teddy bear."



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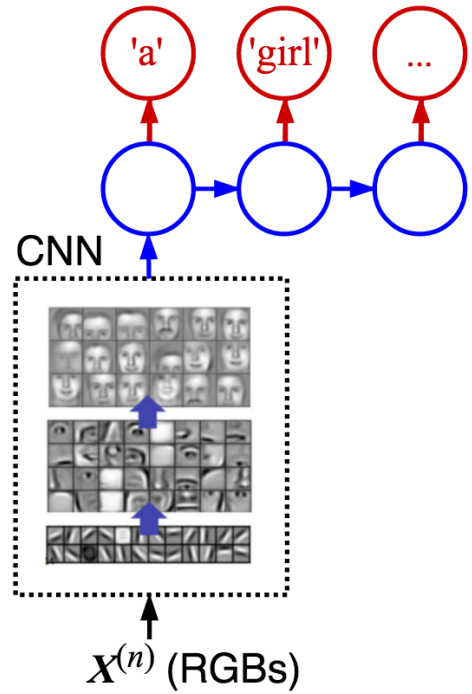

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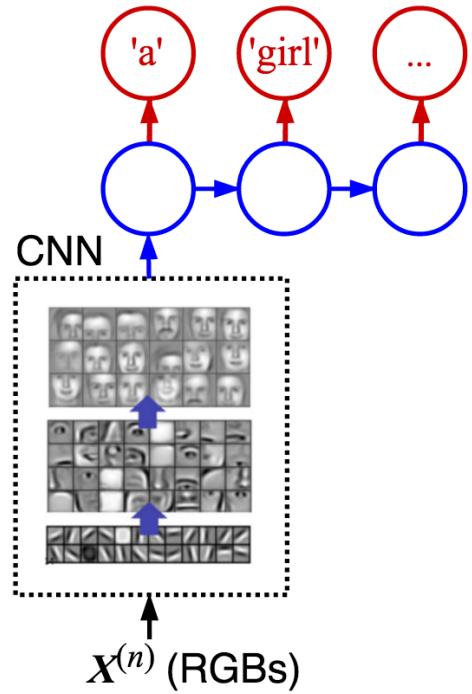

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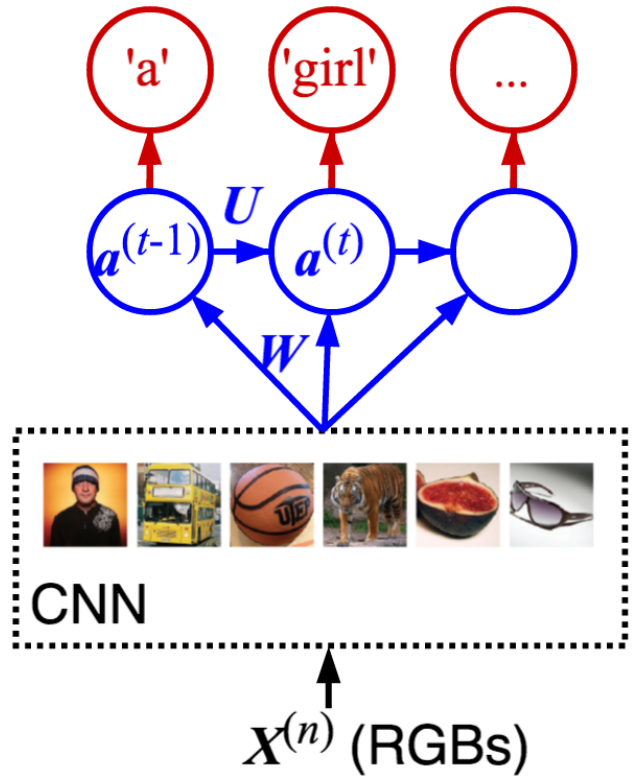

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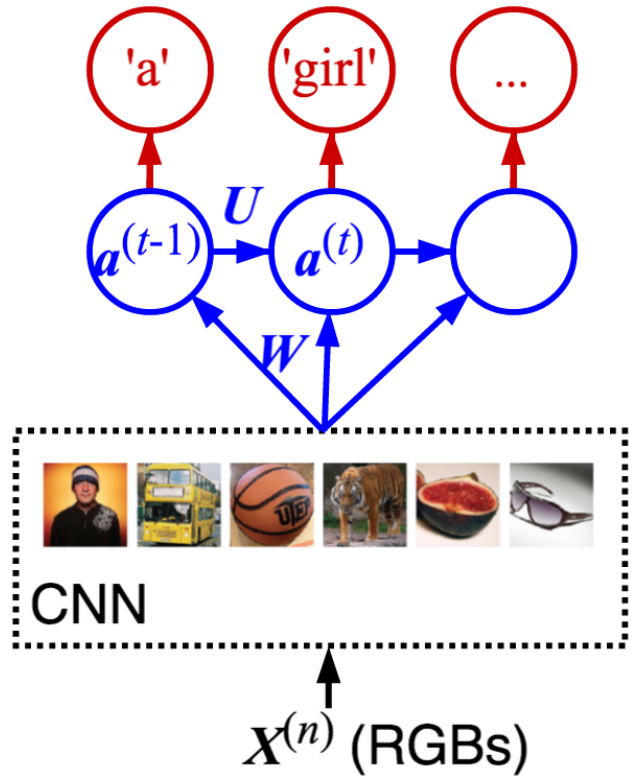

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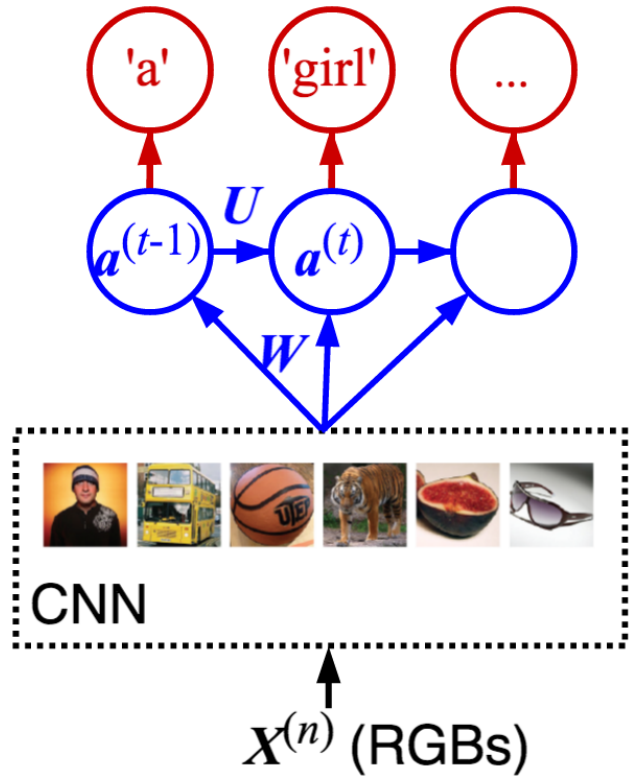

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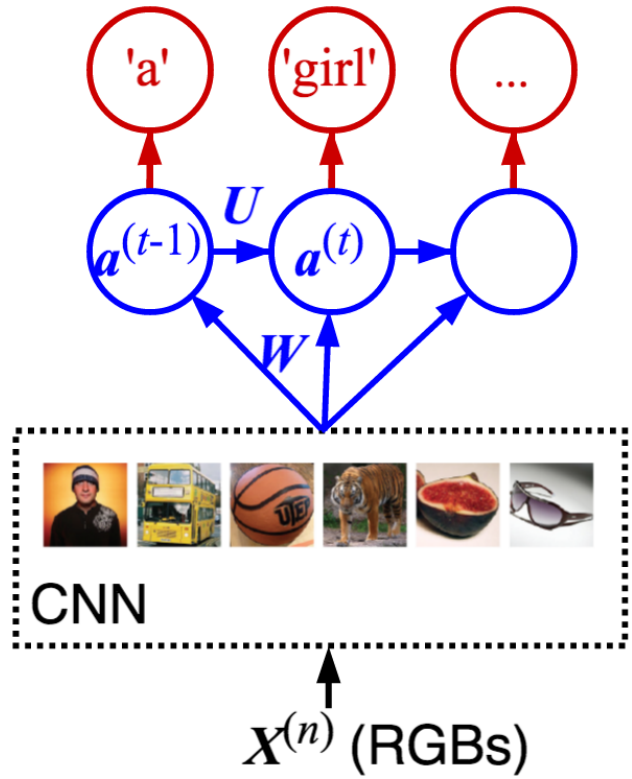

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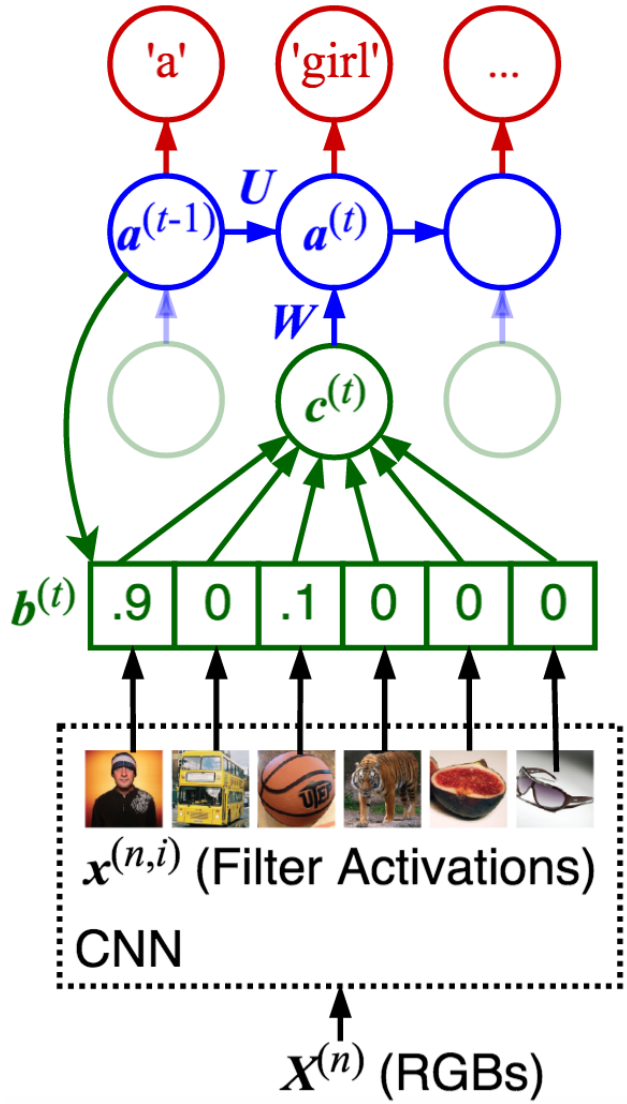

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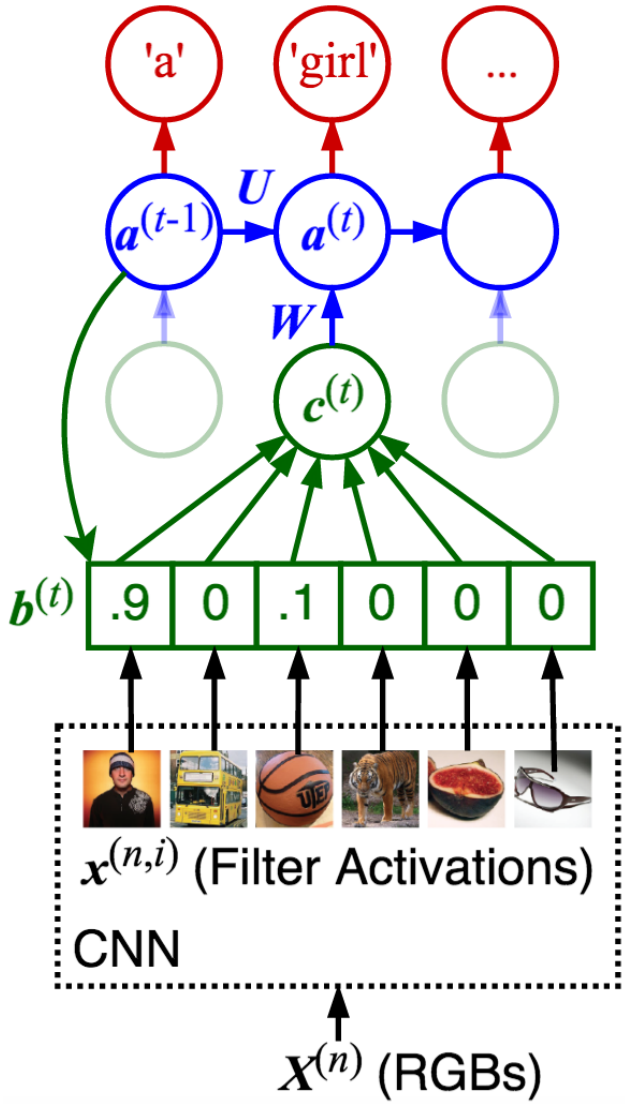

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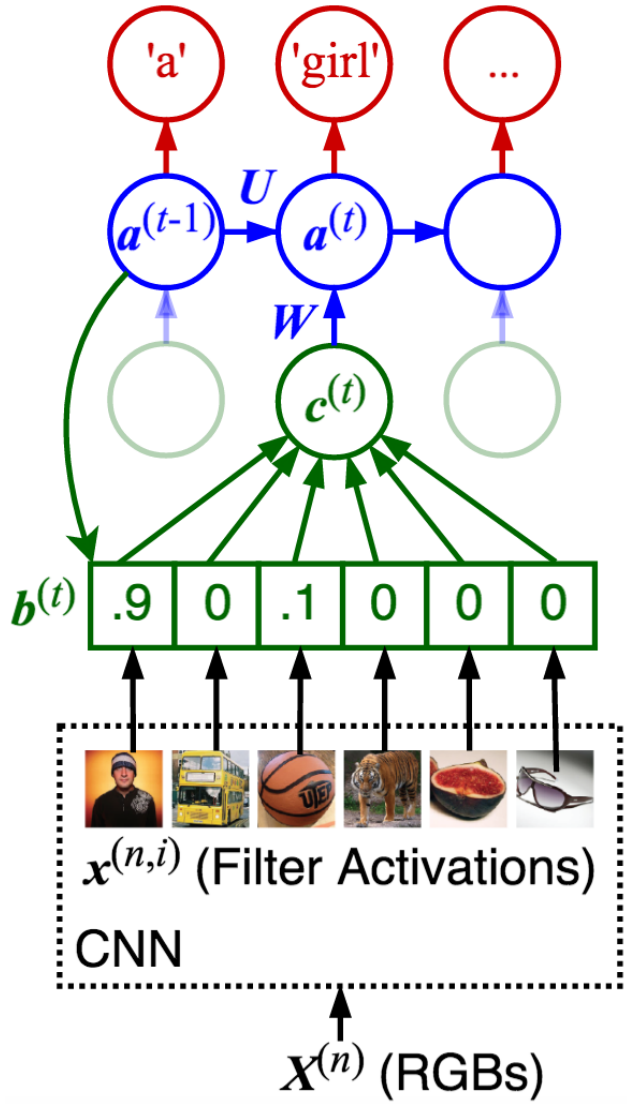

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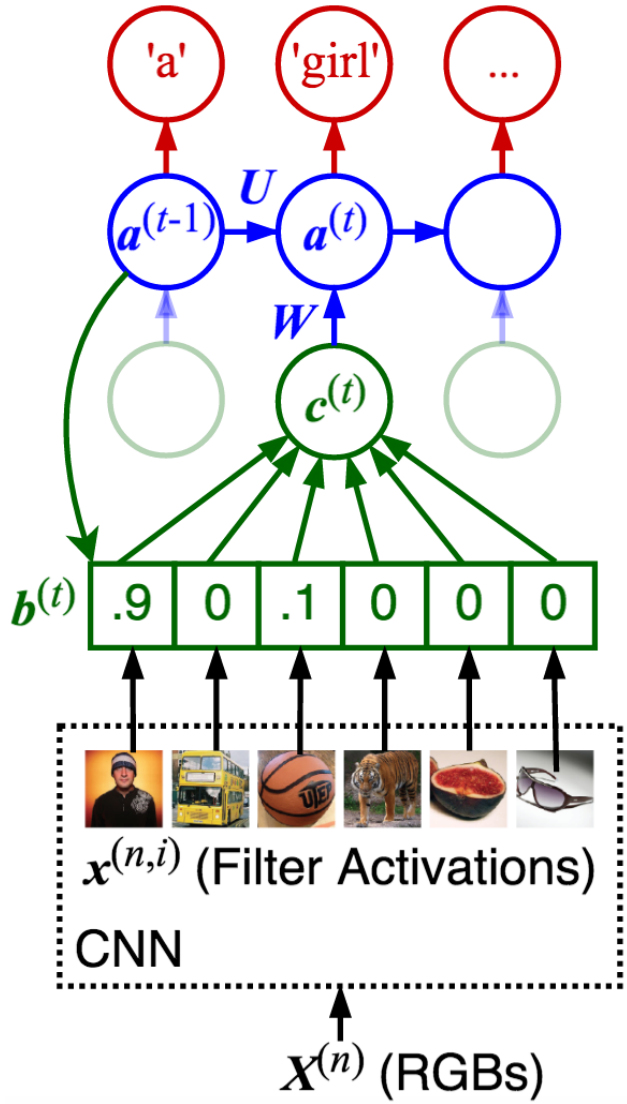

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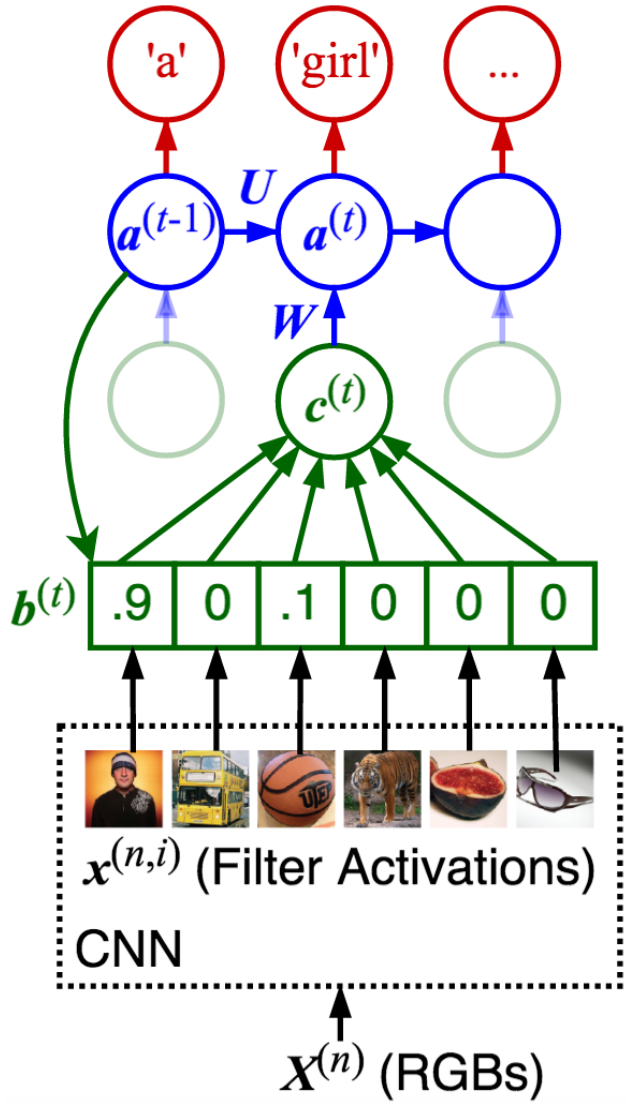
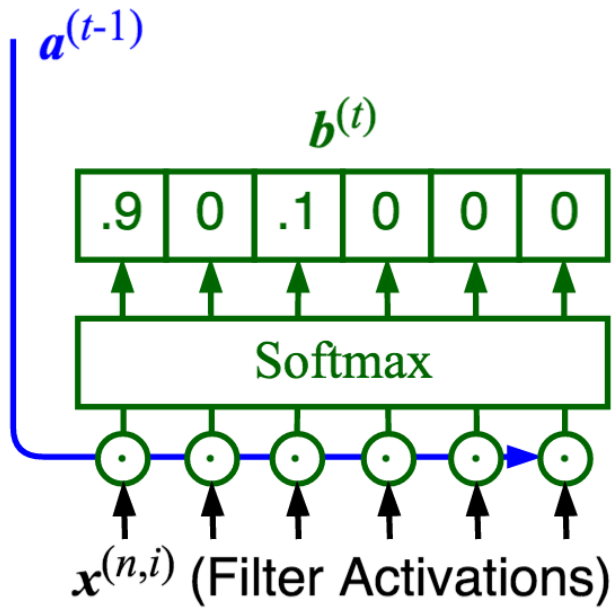
- How to obtain $\mathbf{b}^{(t)}$?



Computing Attention Vector

1. Use $\mathbf{a}^{(L-1,t-1)}$ as a "query" to get a match score for each input part by using, e.g., a simple NN [2, 15]:

$$z_i = \text{act}(\boldsymbol{p}^\top \mathbf{a}^{(L-1,t-1)} + \boldsymbol{q}^\top \mathbf{x}^{(i)} + r)$$



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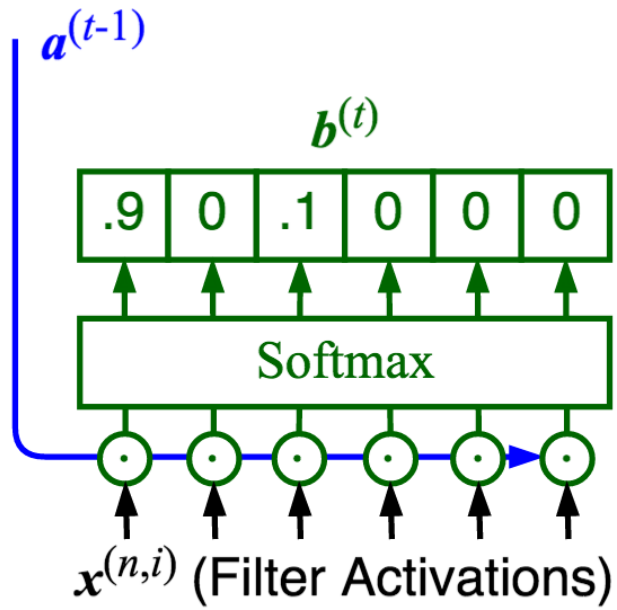

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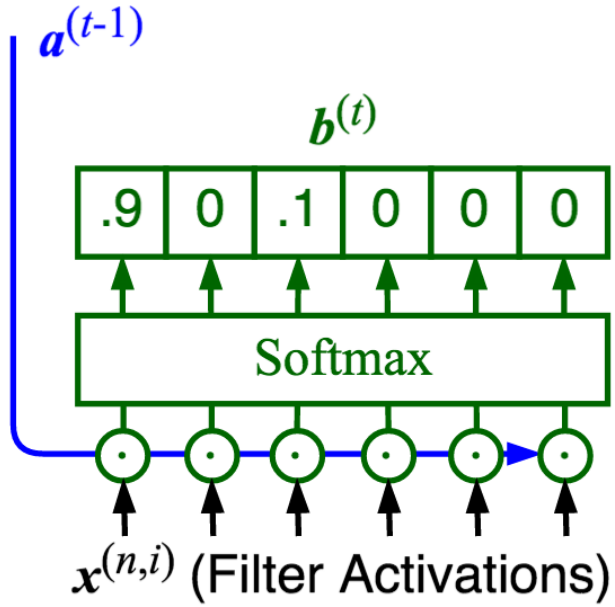

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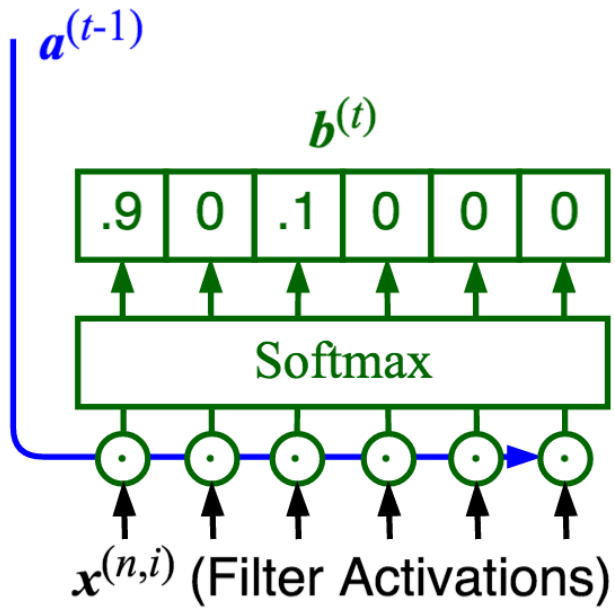

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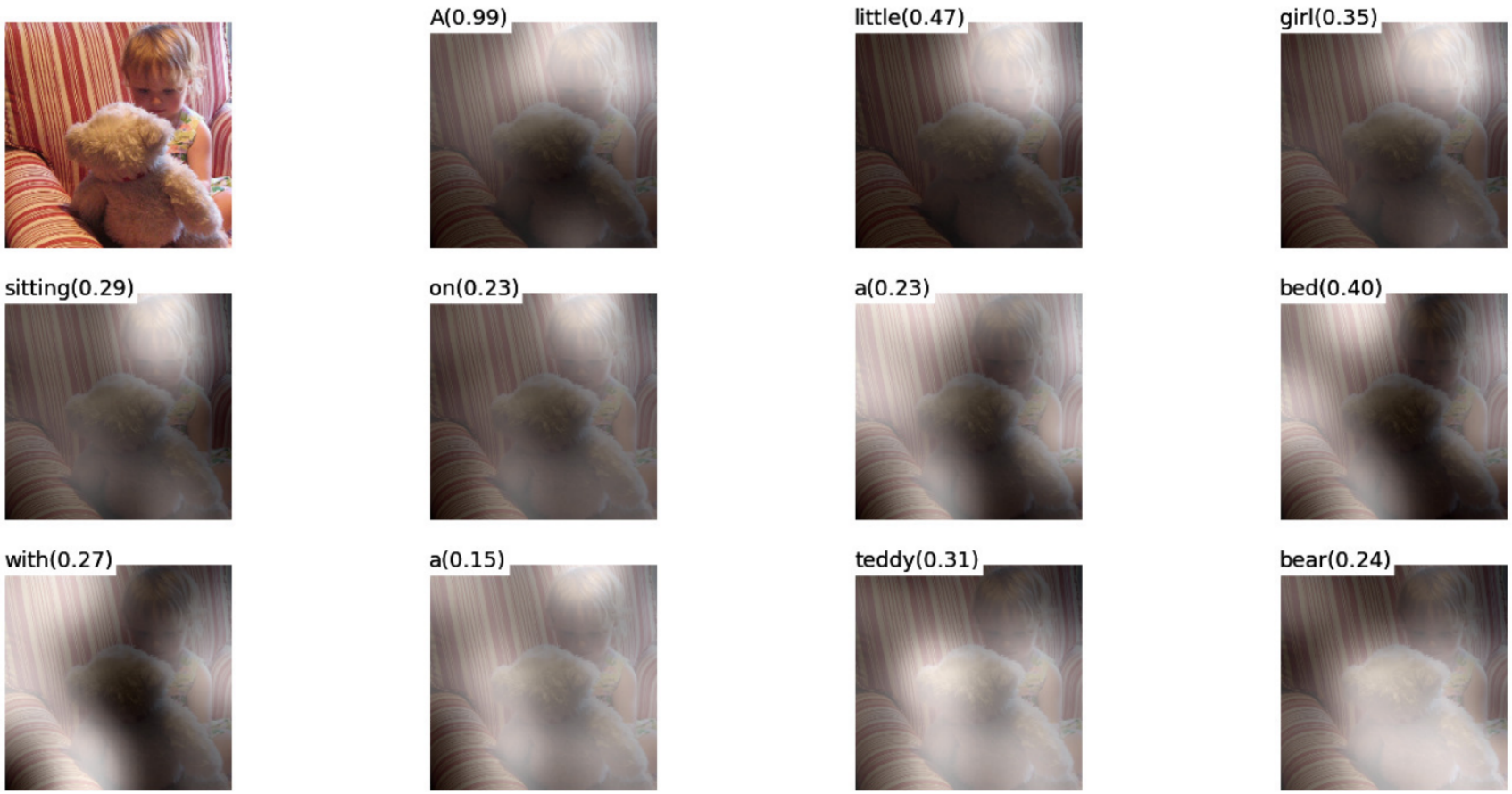

- How to draw a mask?

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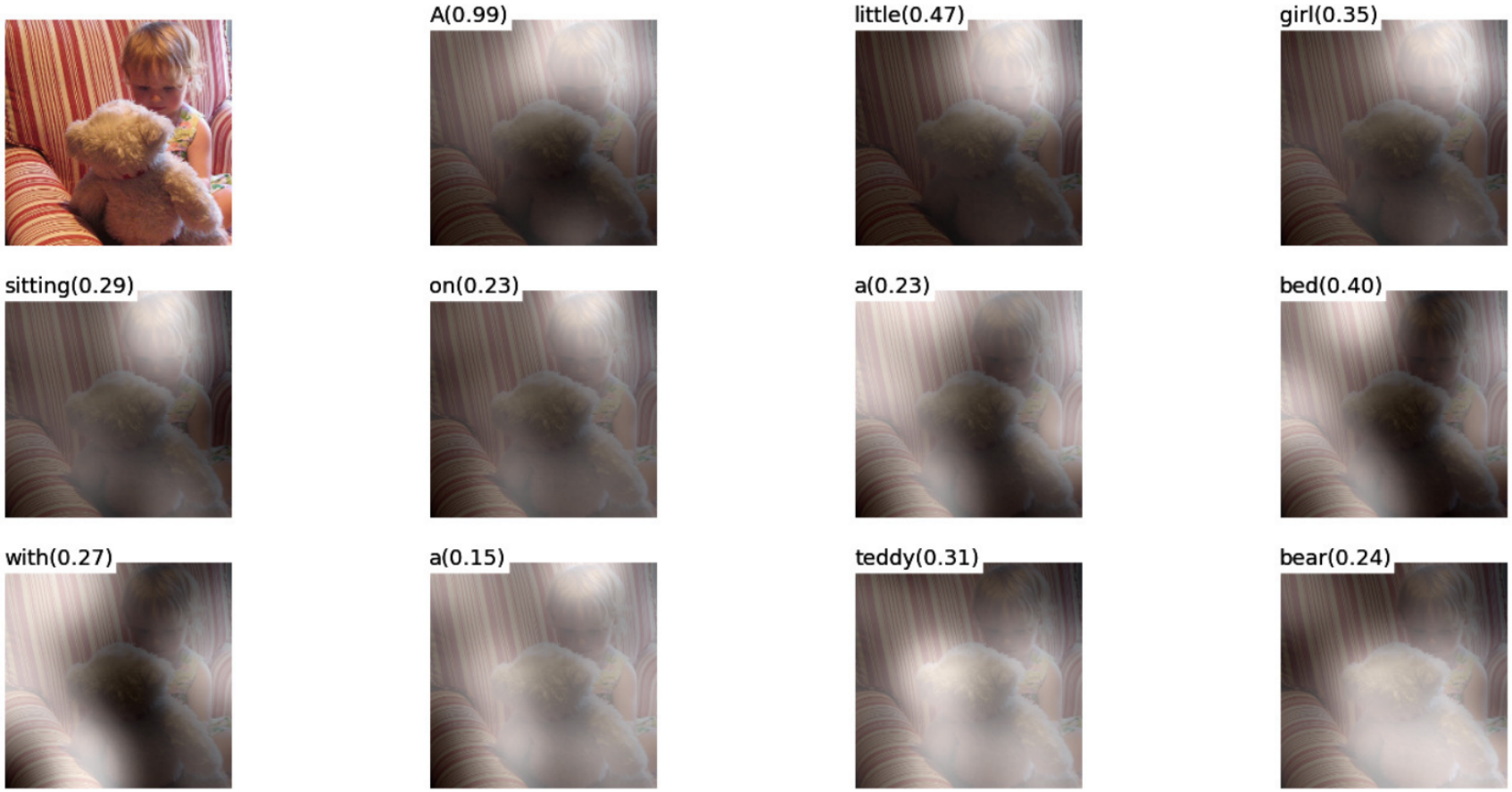

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Explicit Memory

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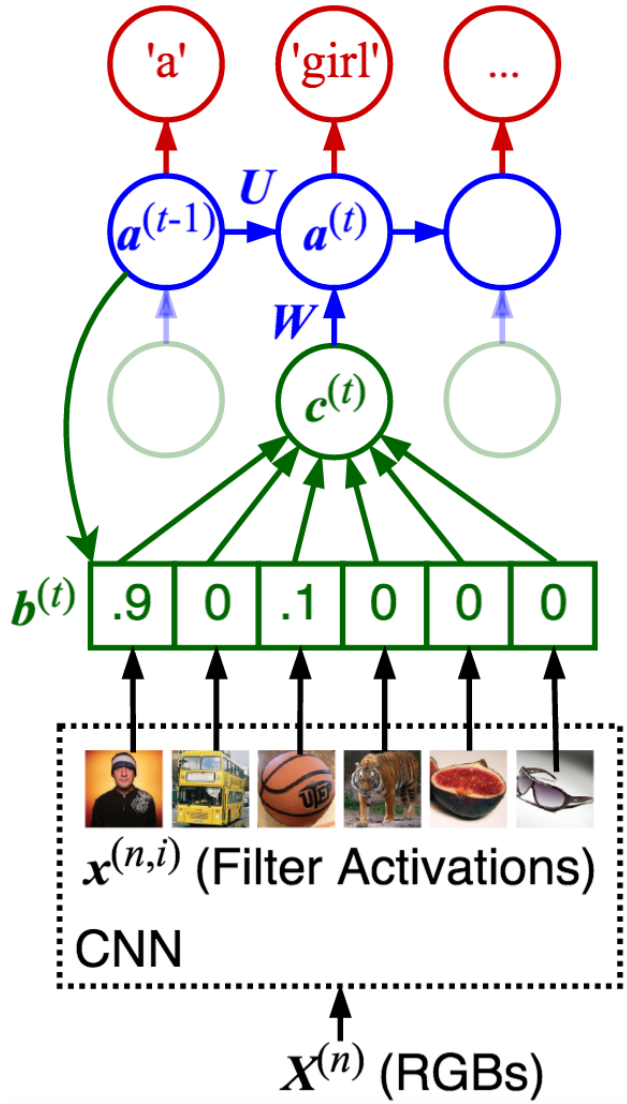

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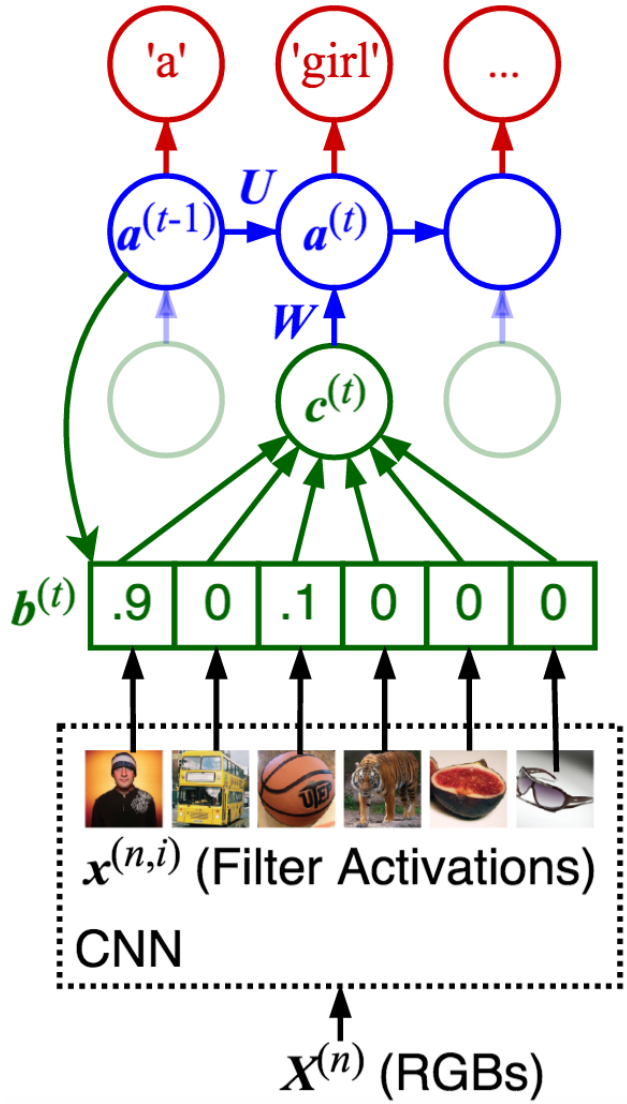

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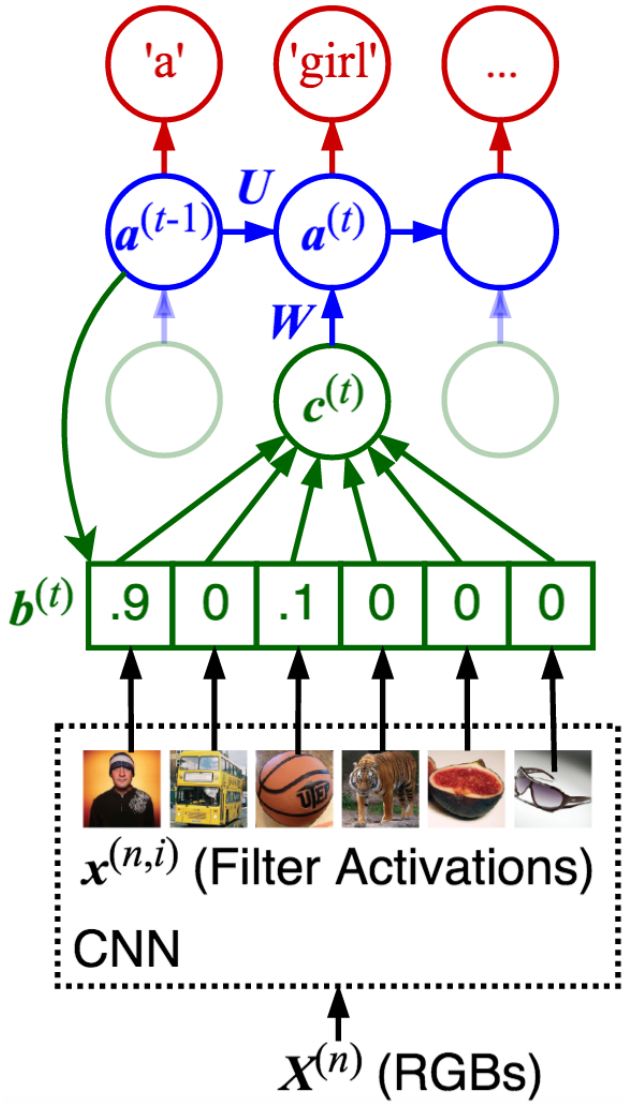
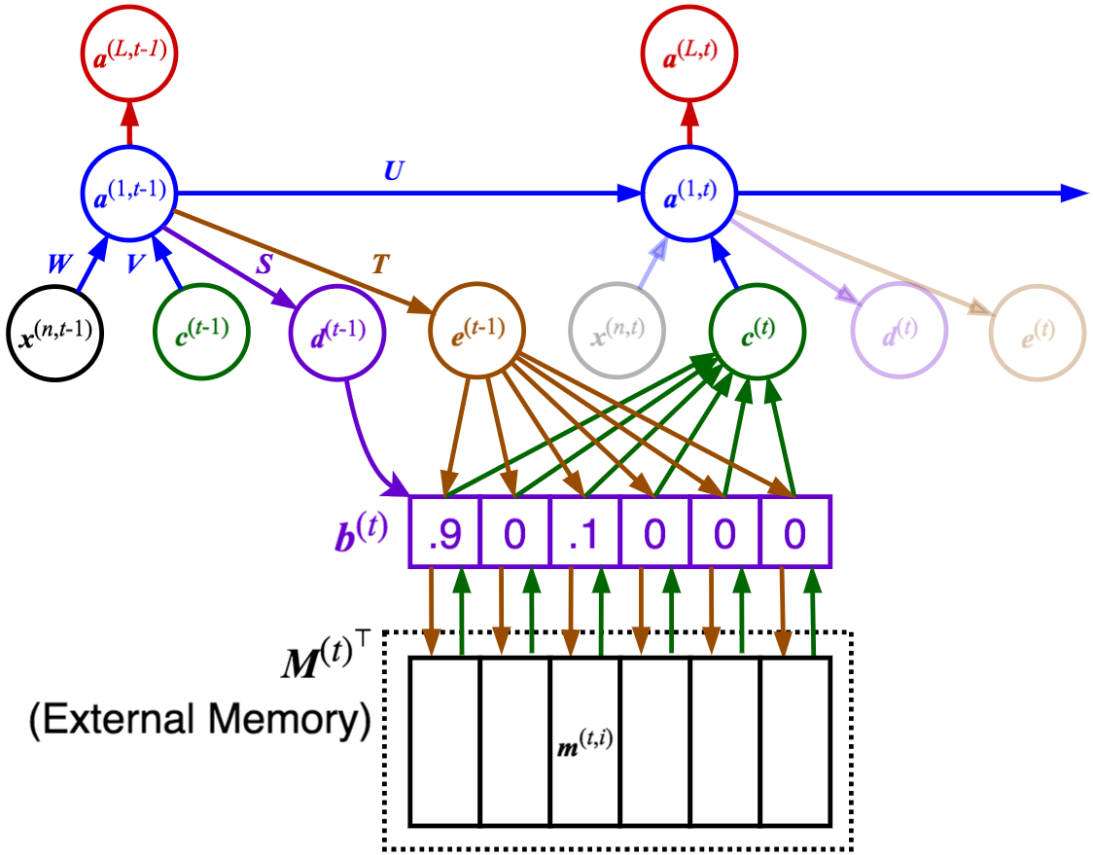


Neural Turing Machines



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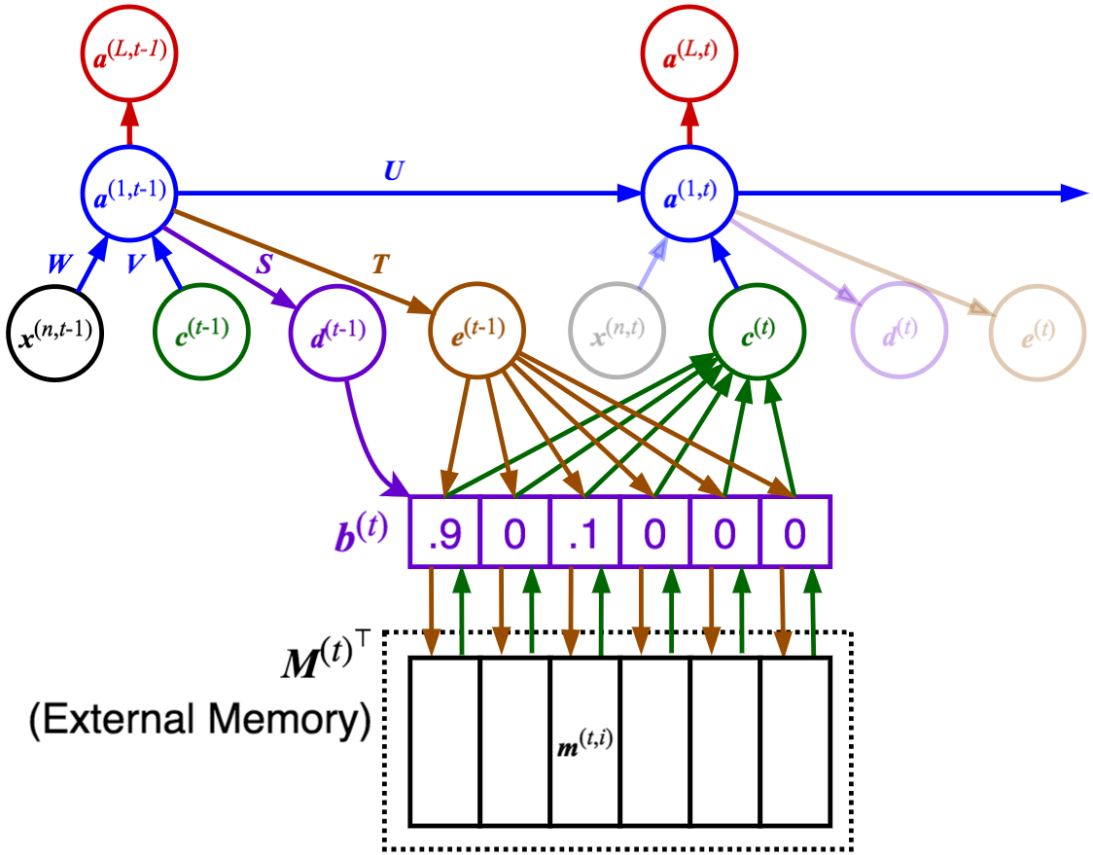

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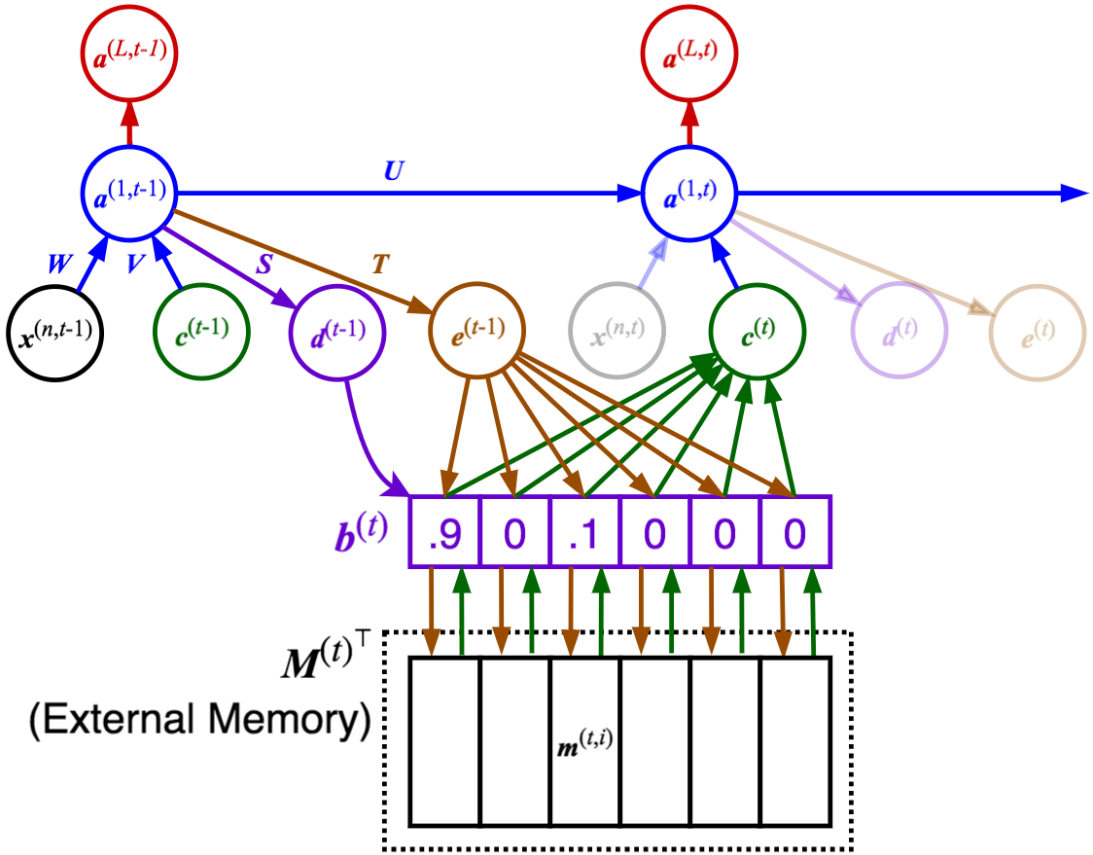

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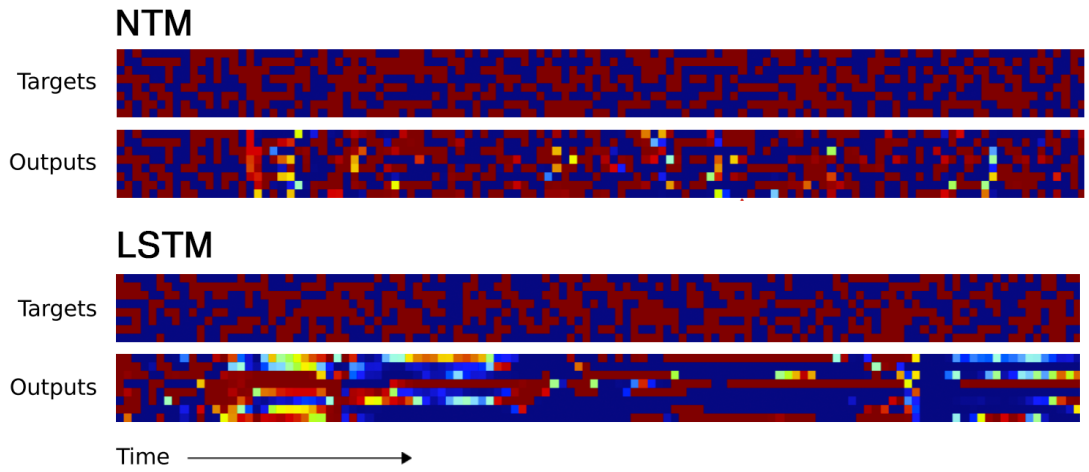

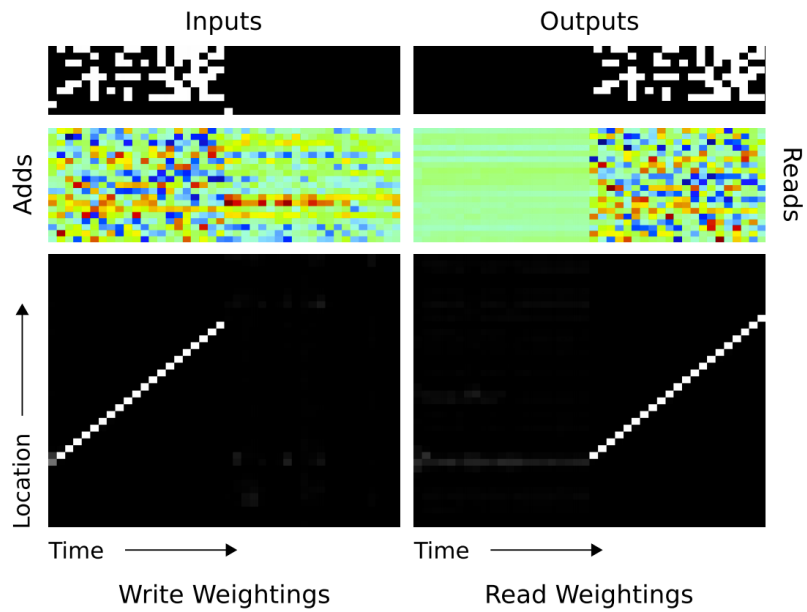

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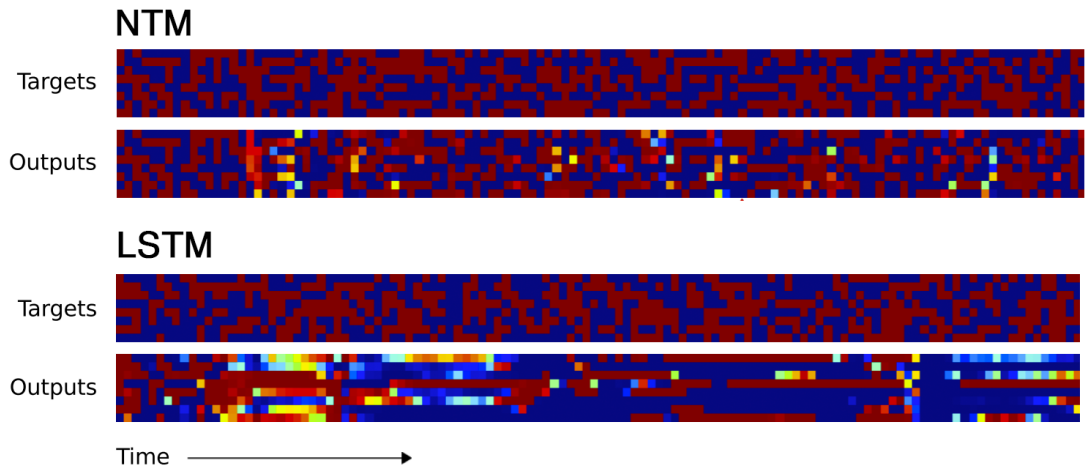

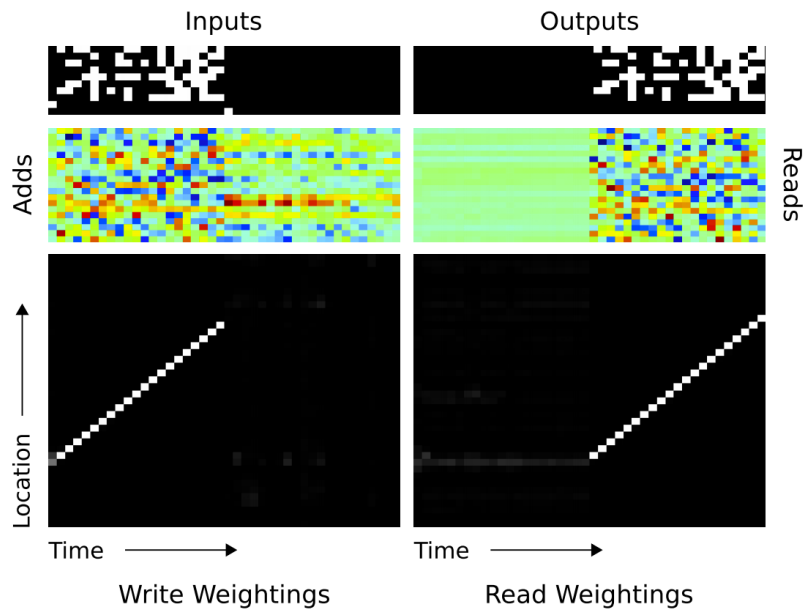

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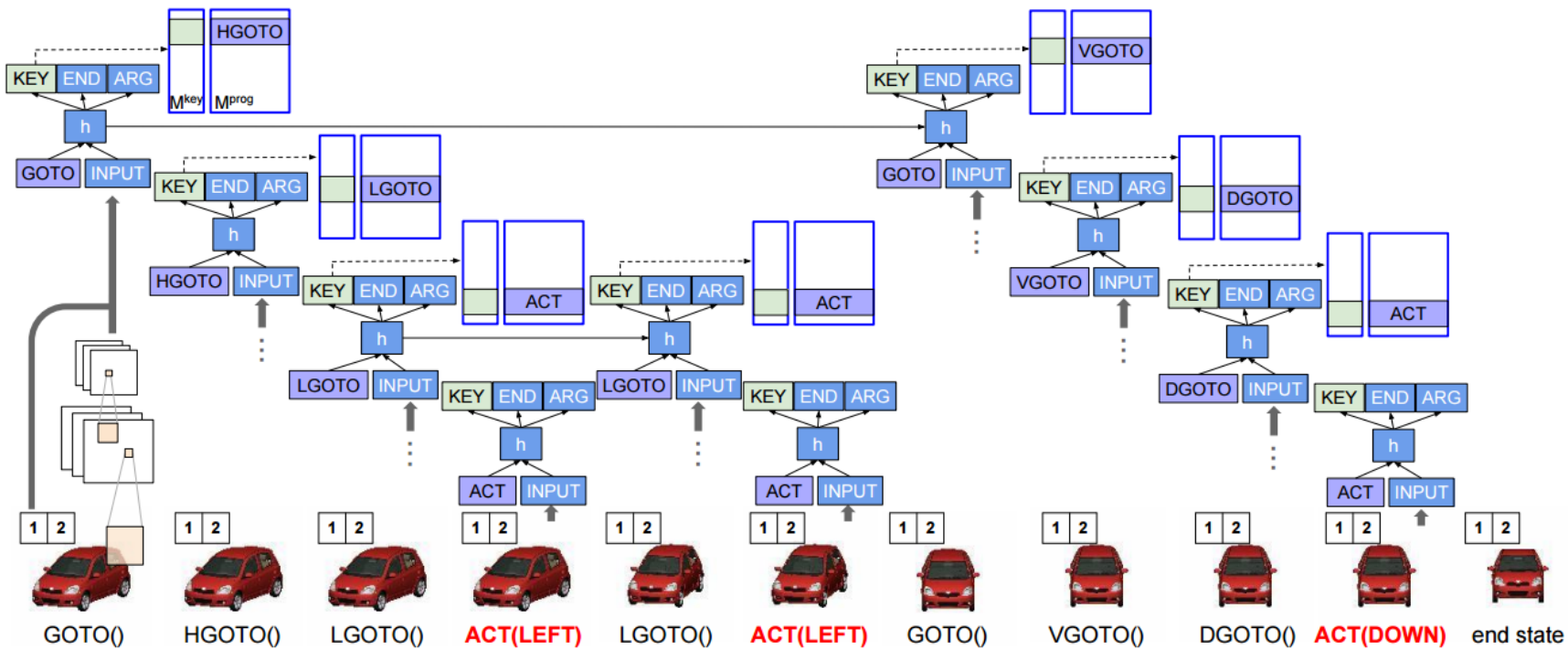

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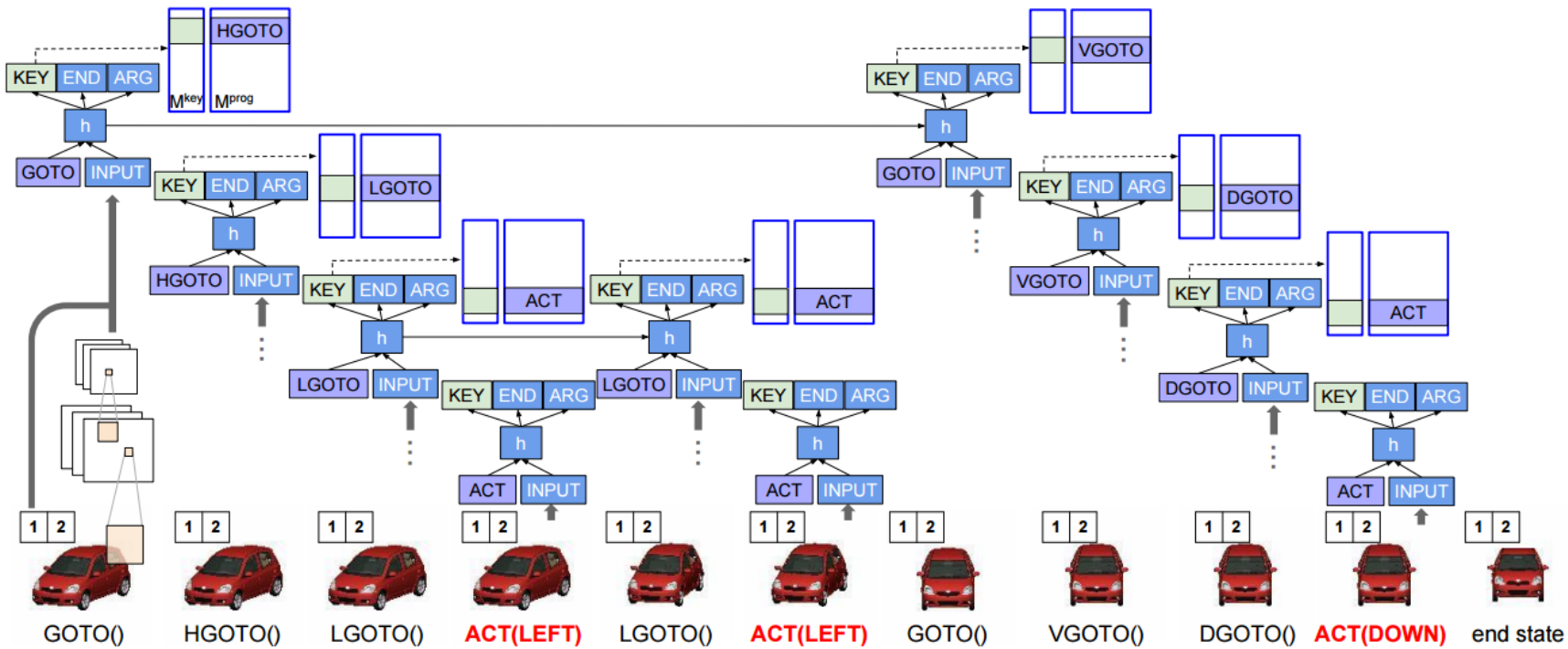

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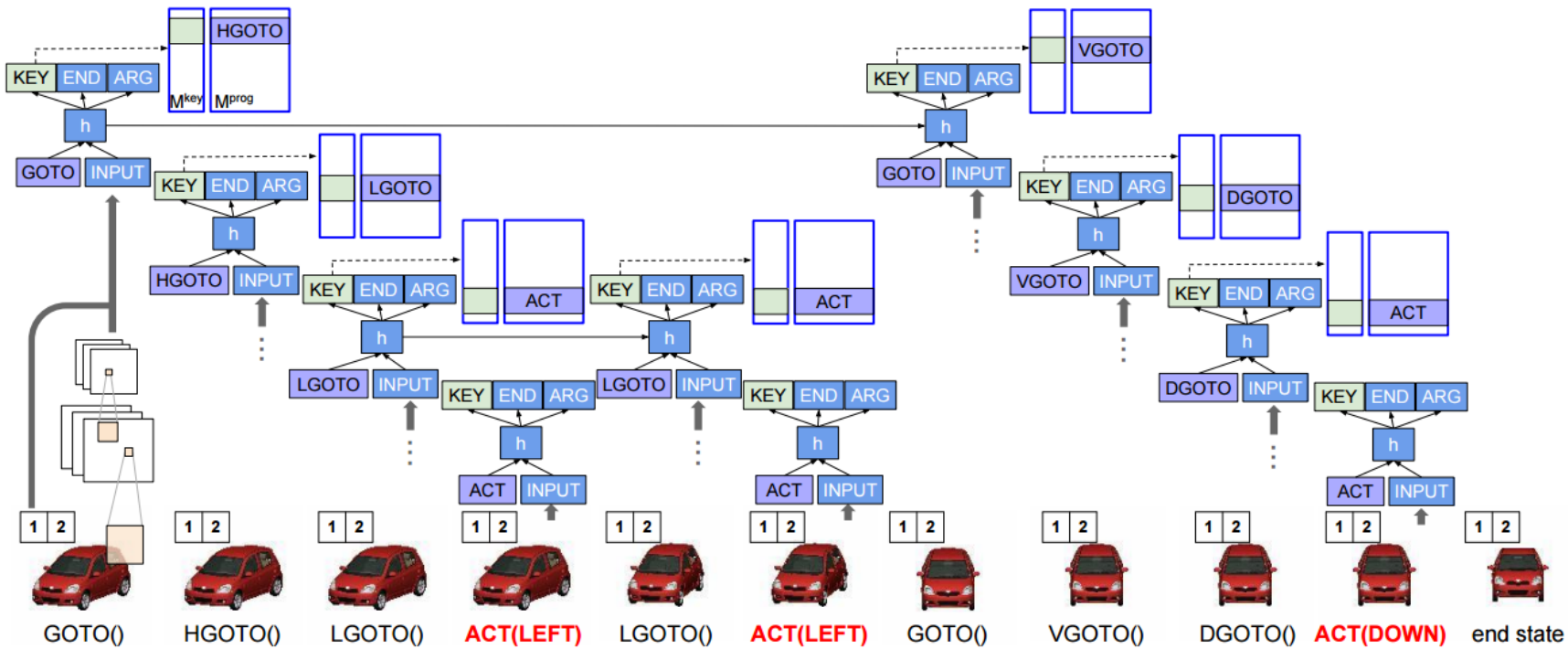

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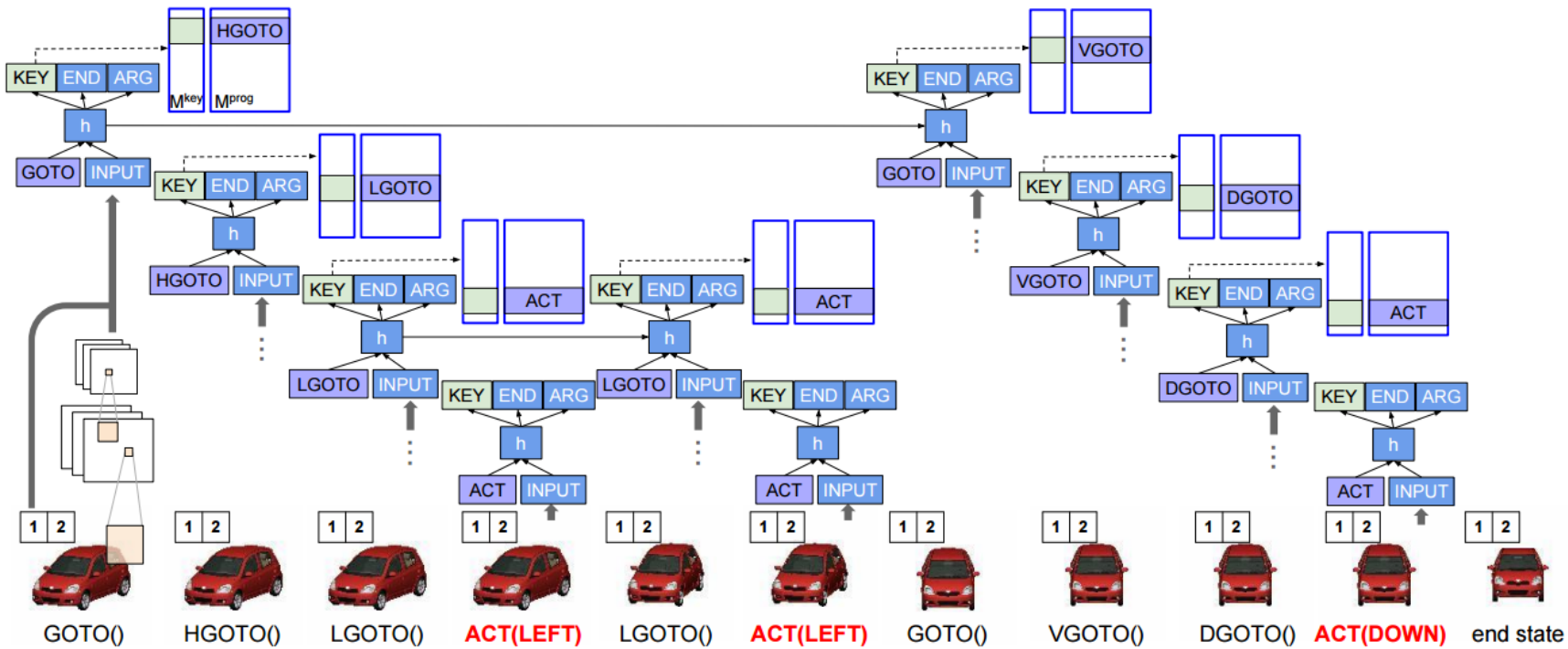

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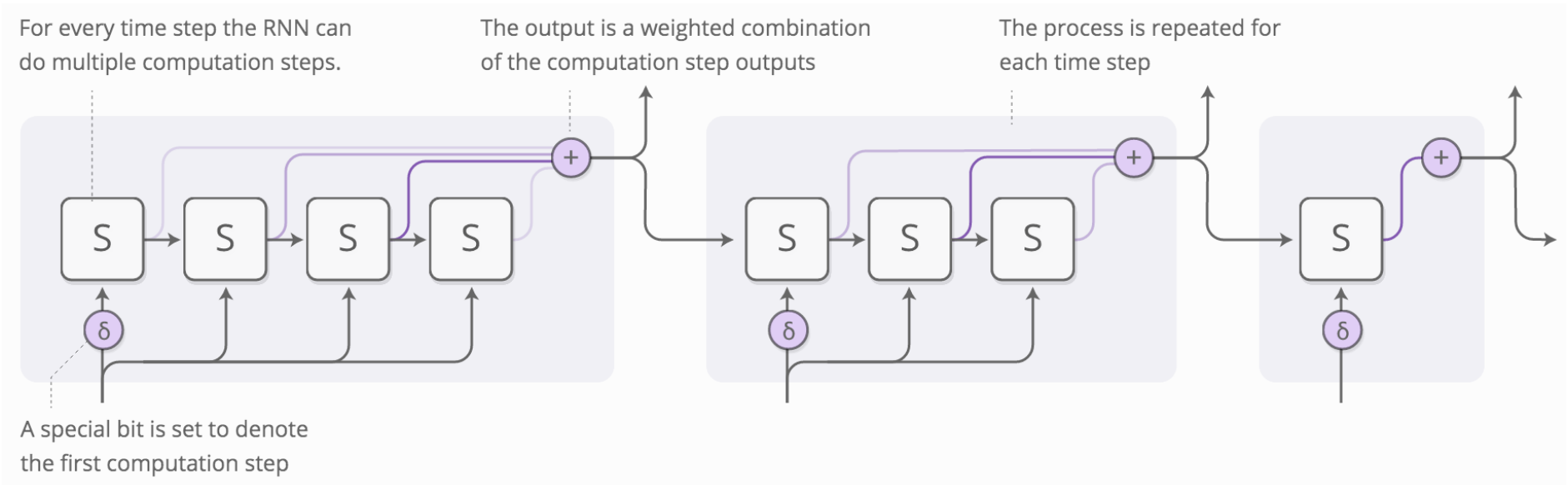

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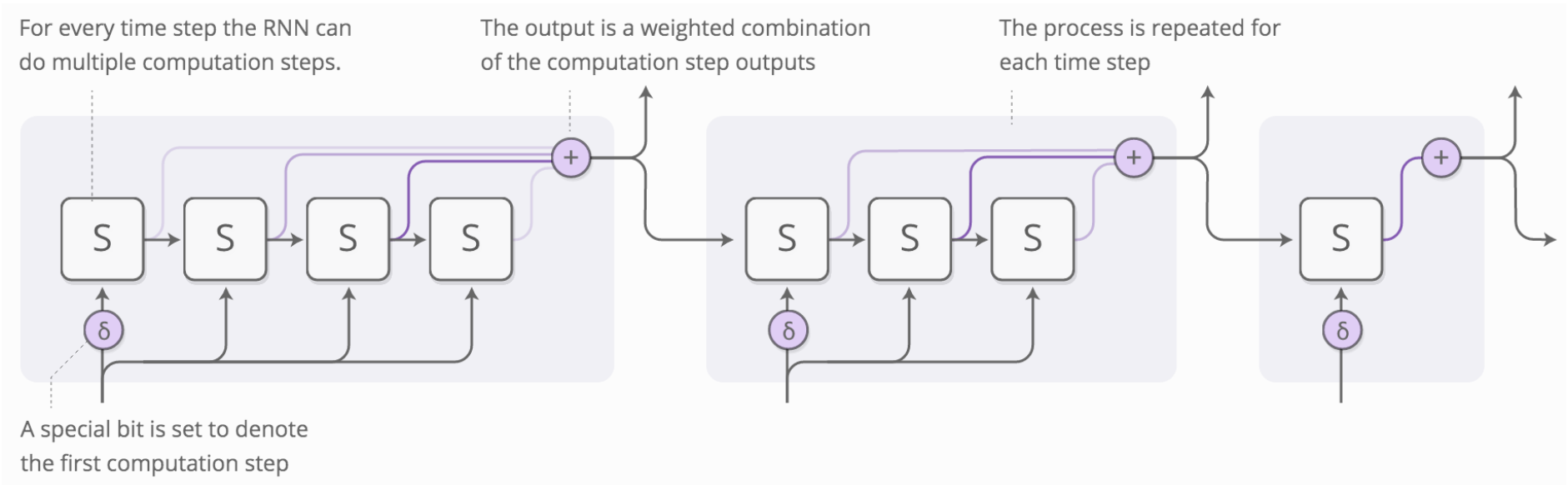

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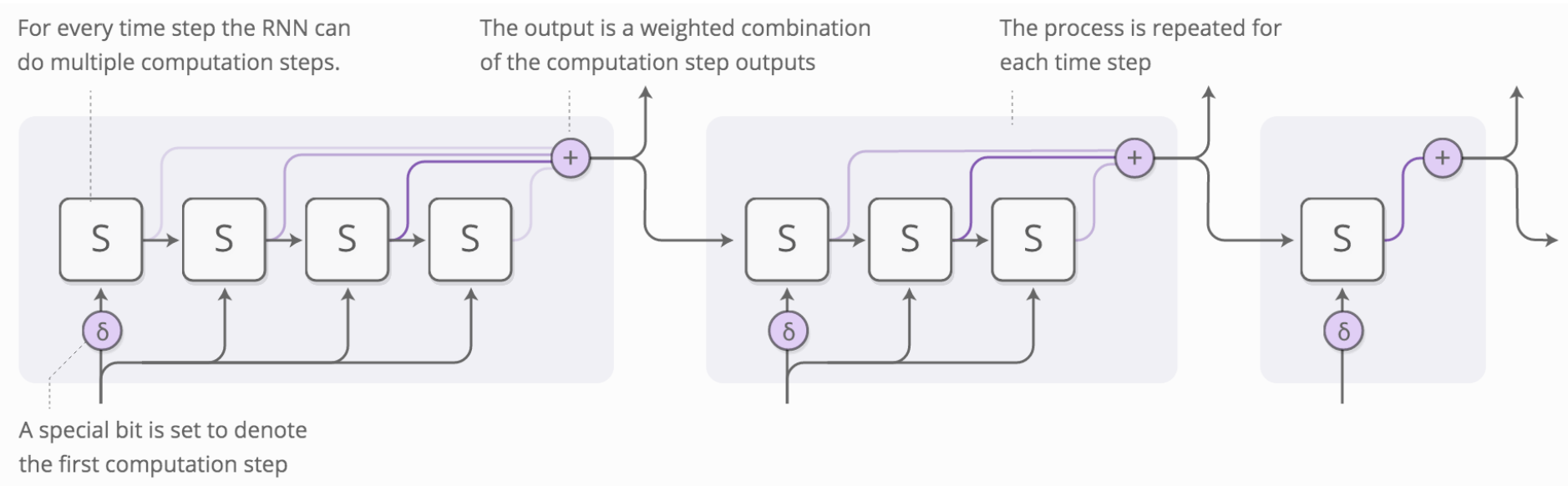

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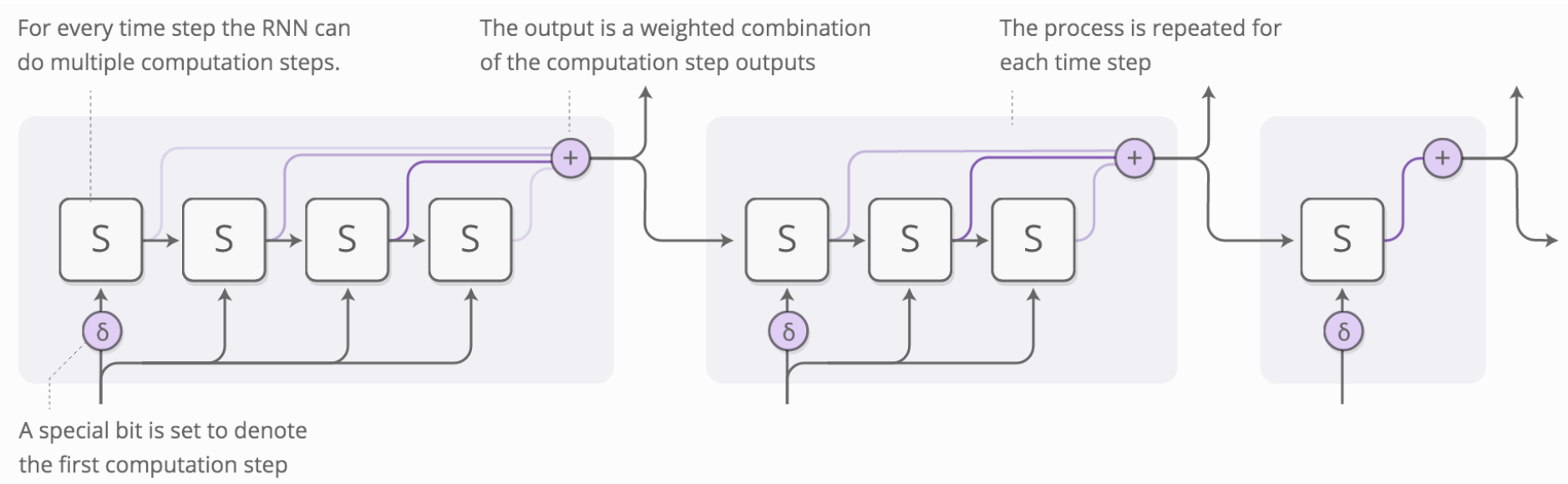

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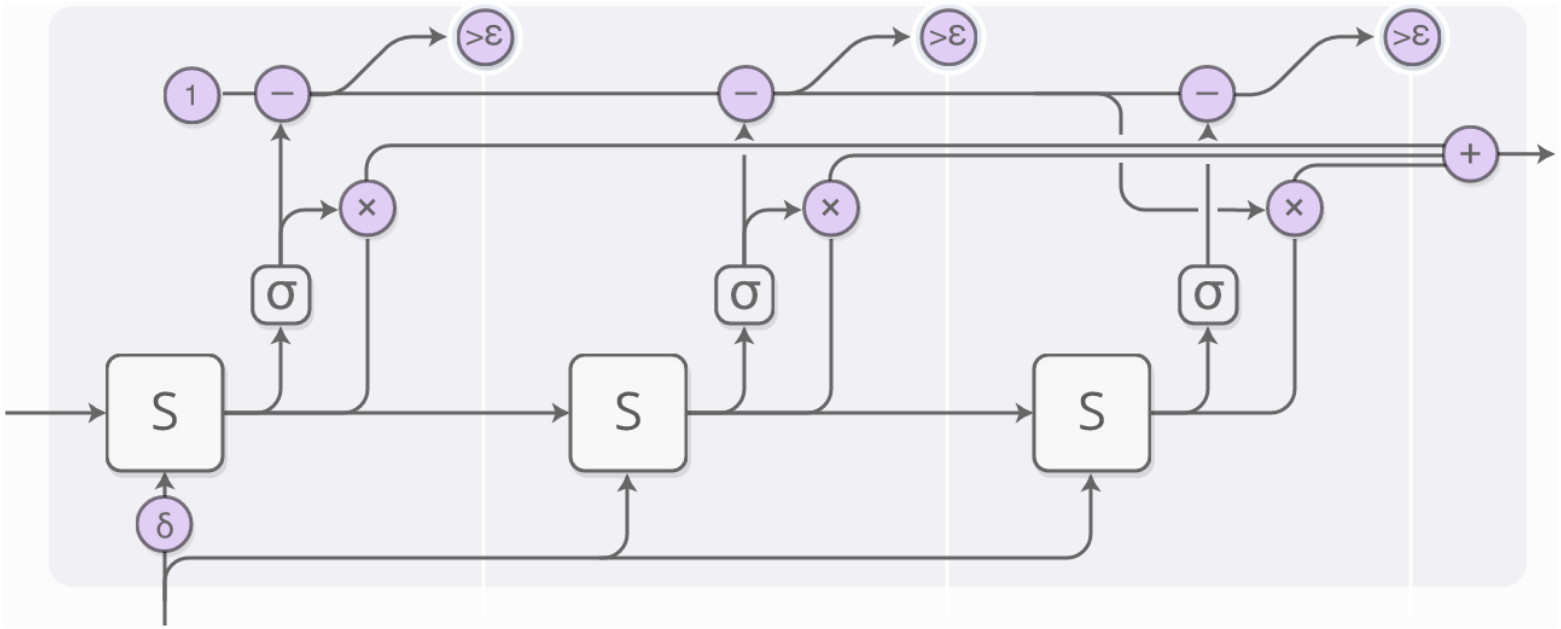

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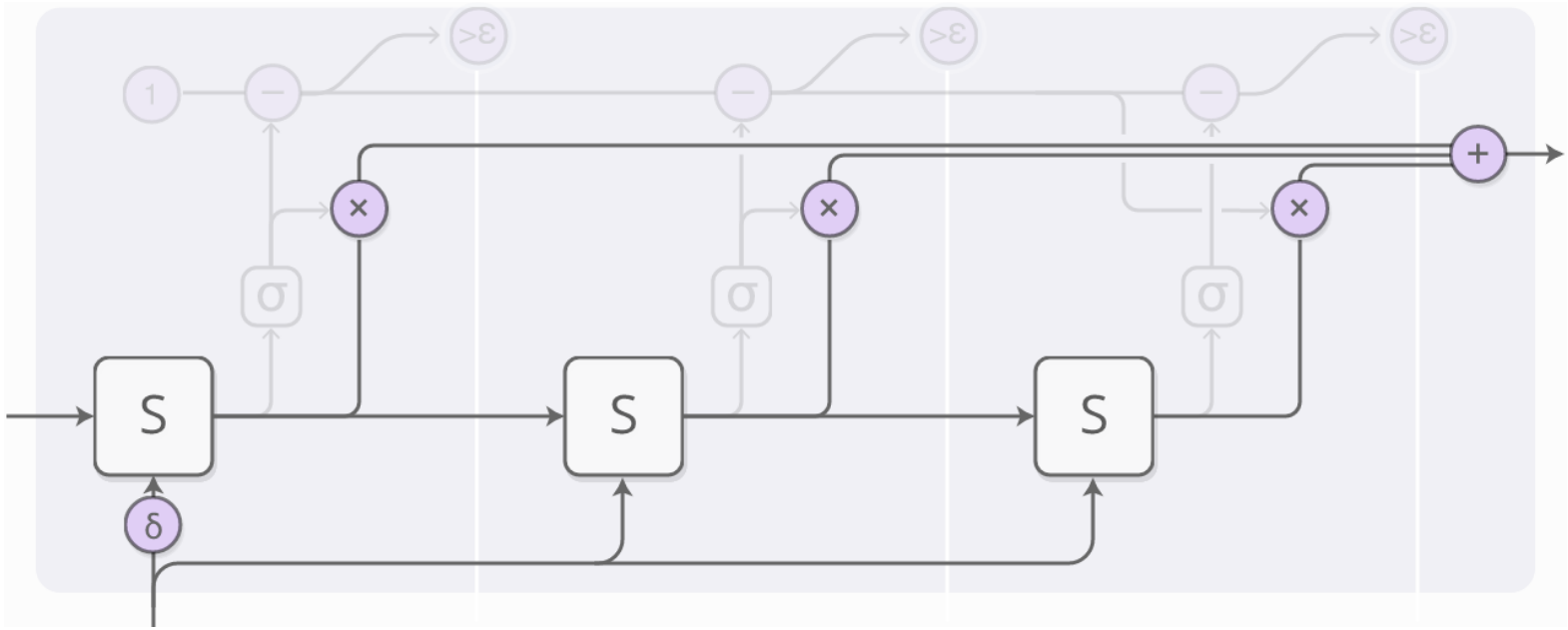

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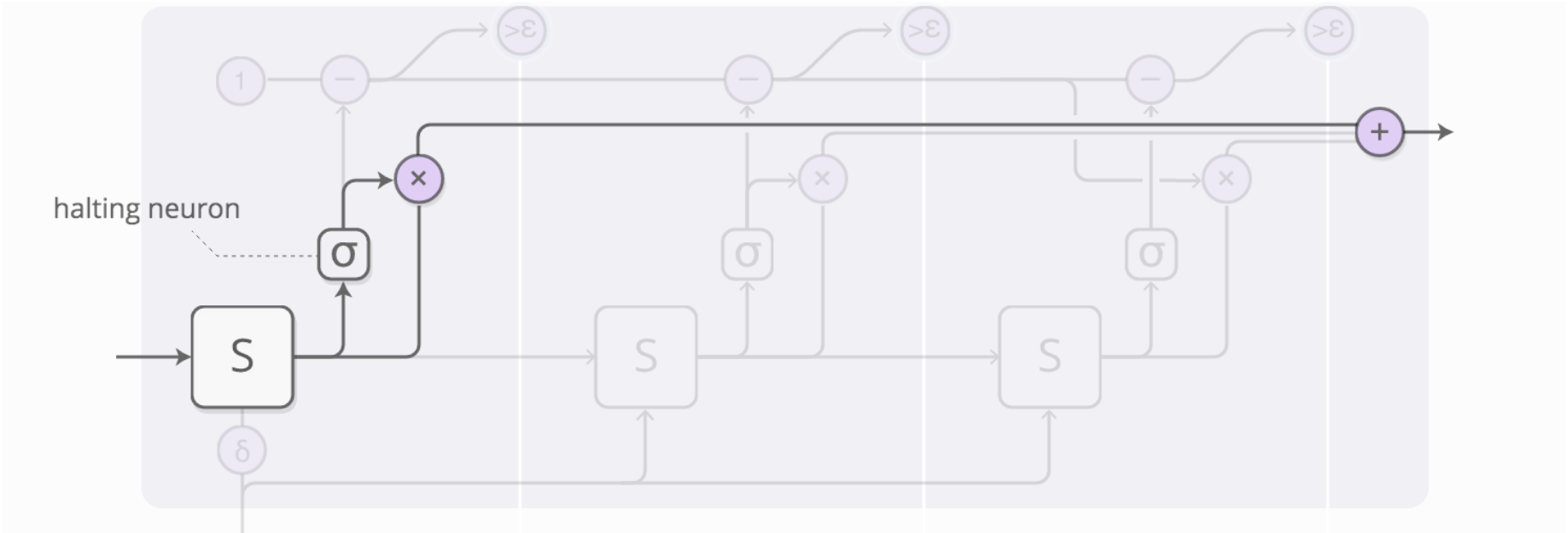

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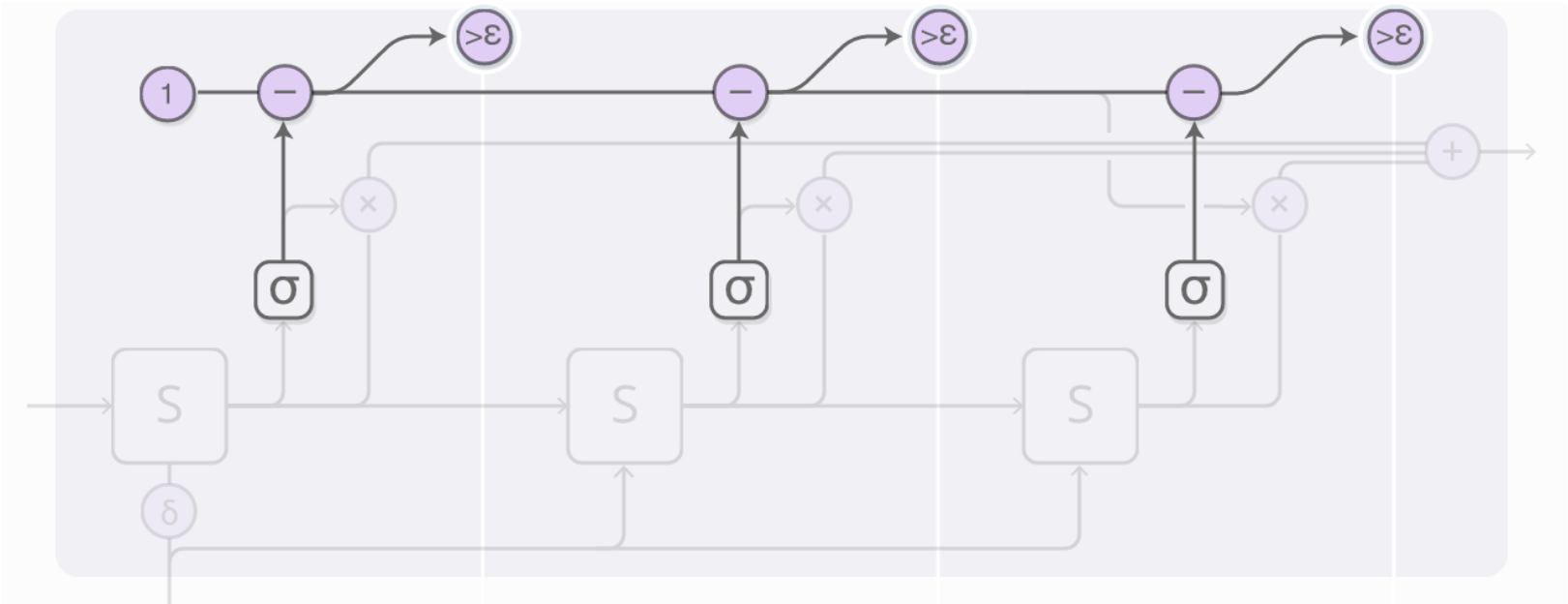

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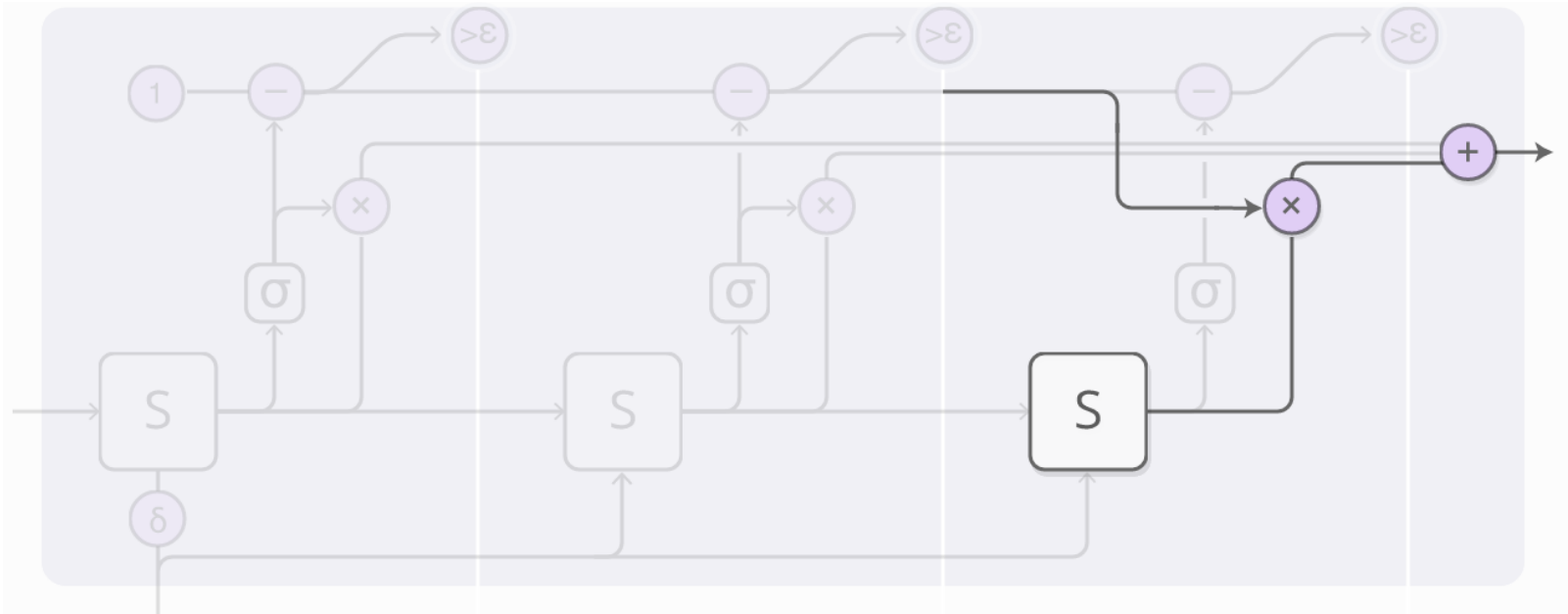

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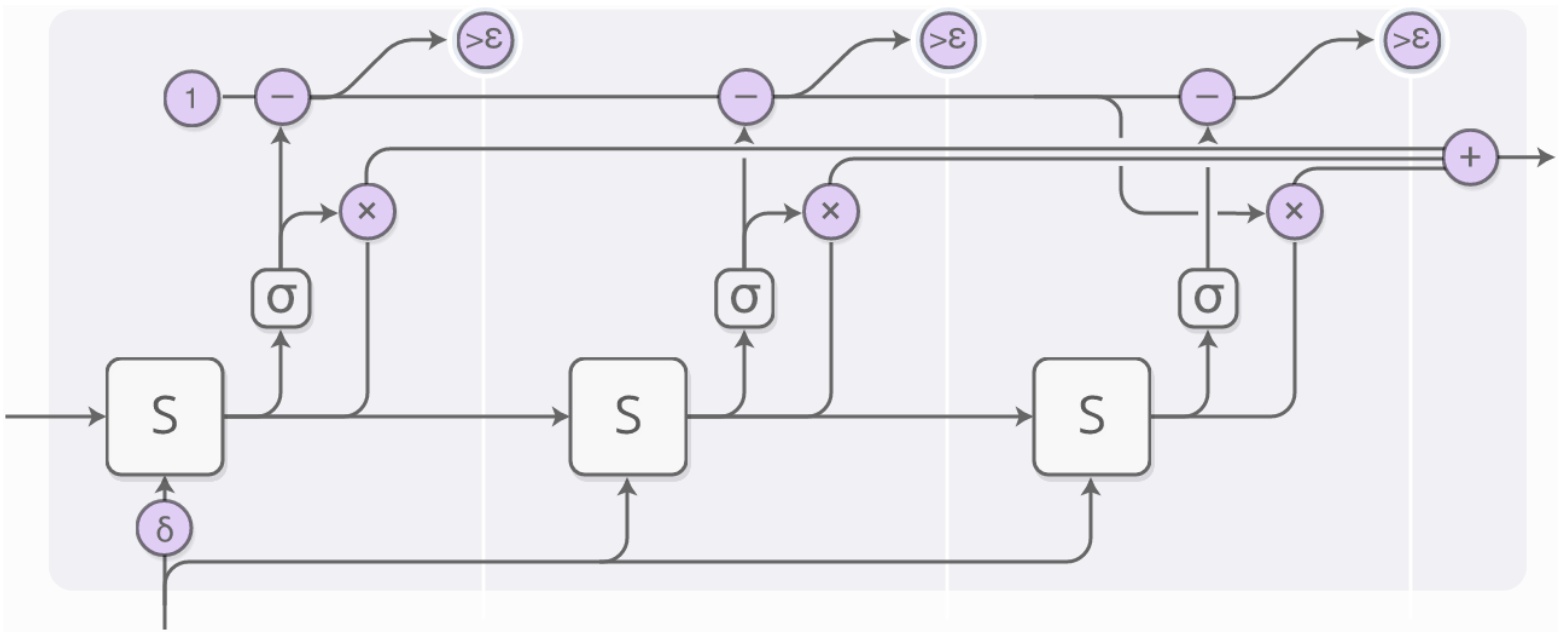

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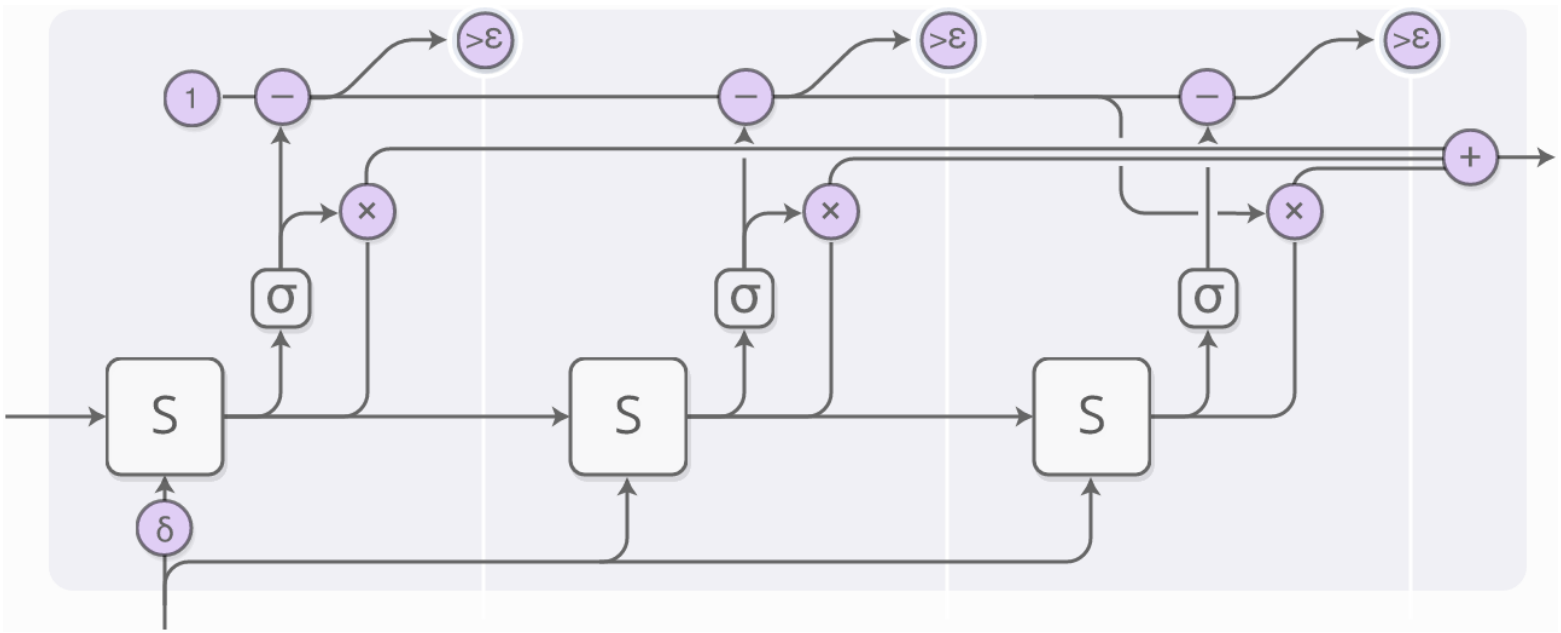

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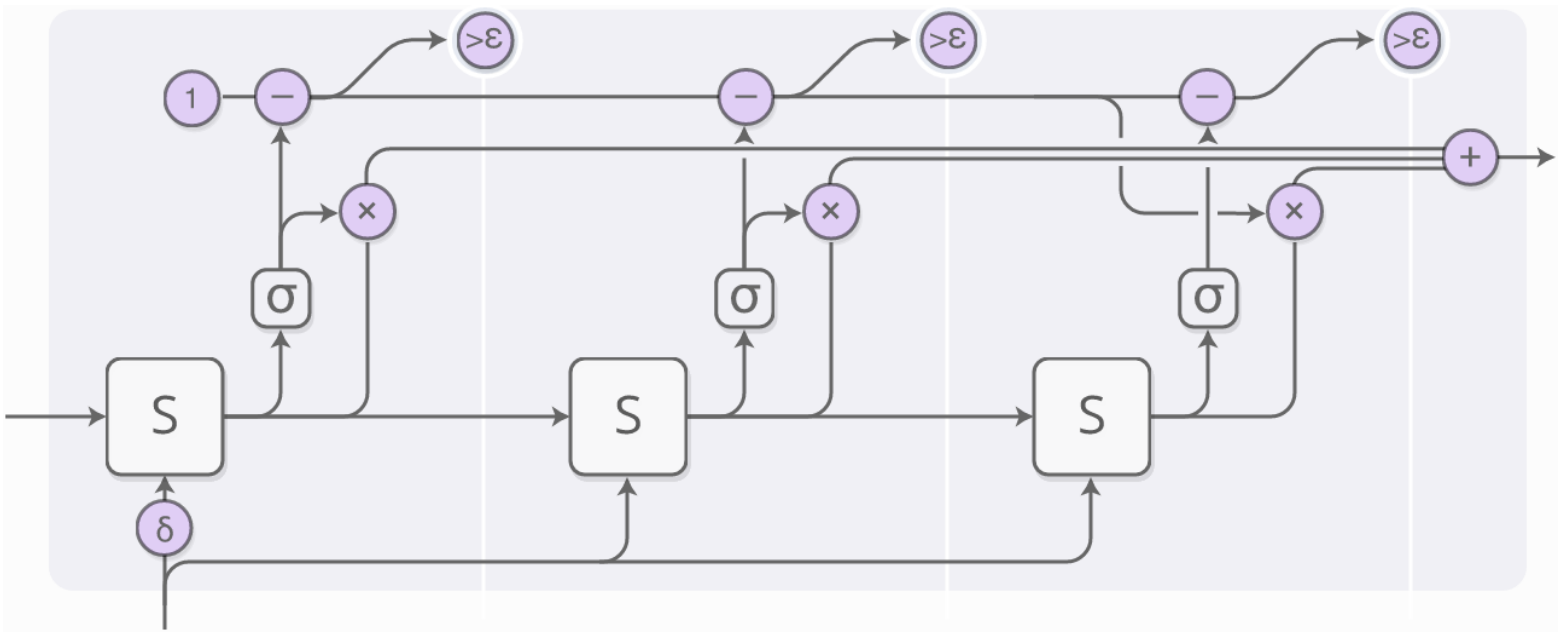

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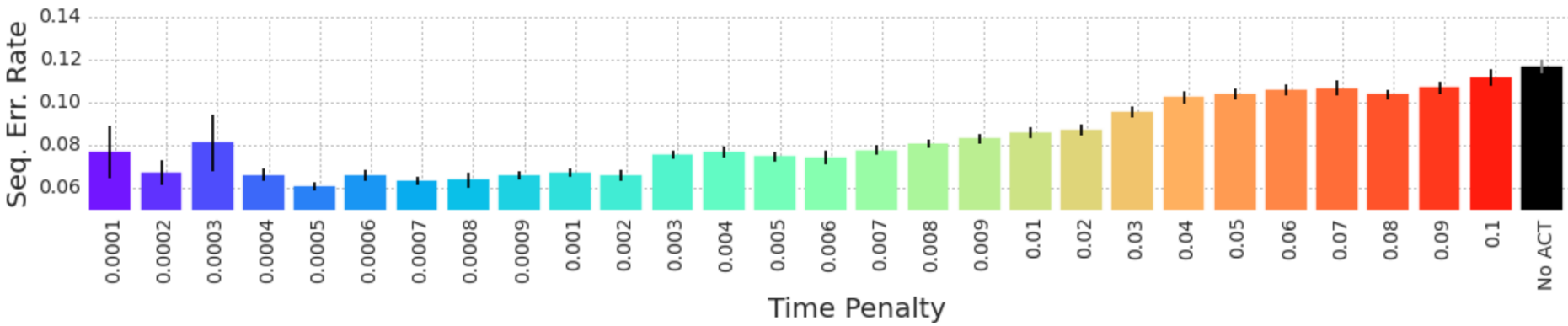

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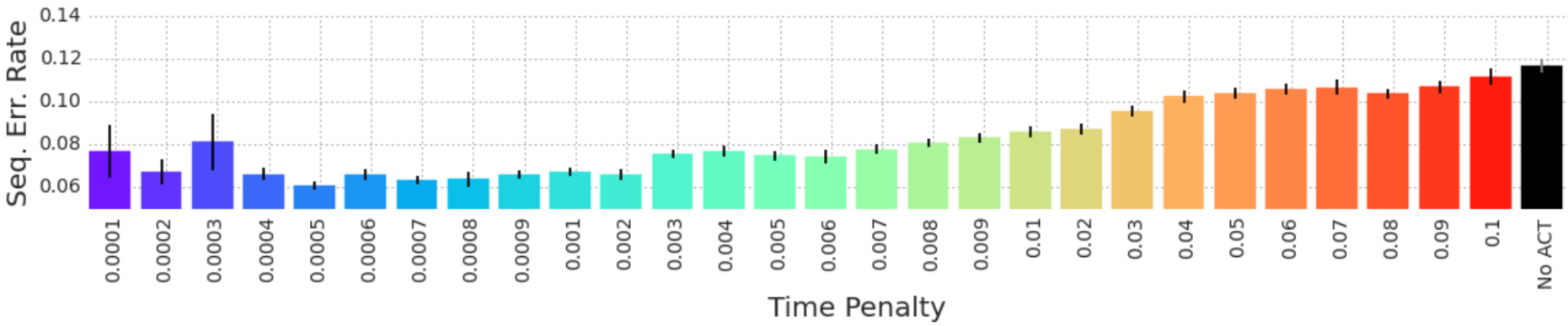
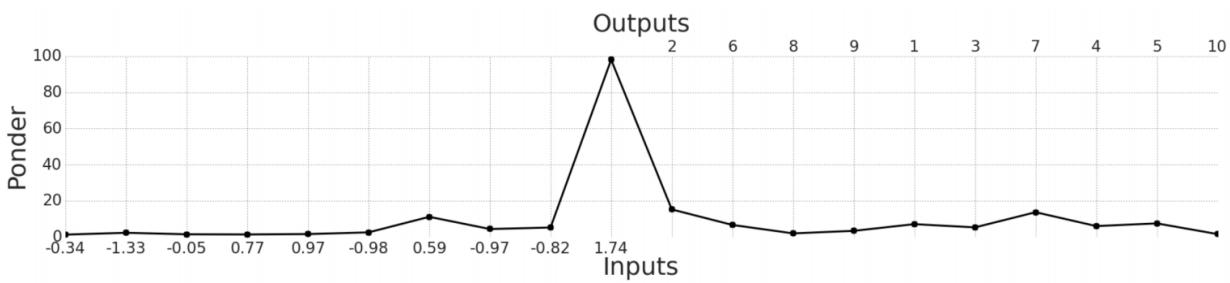
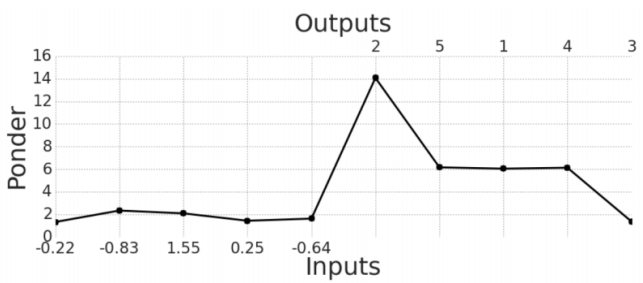


- Ponder time (#states at each time) provides insights into when comparisons take place





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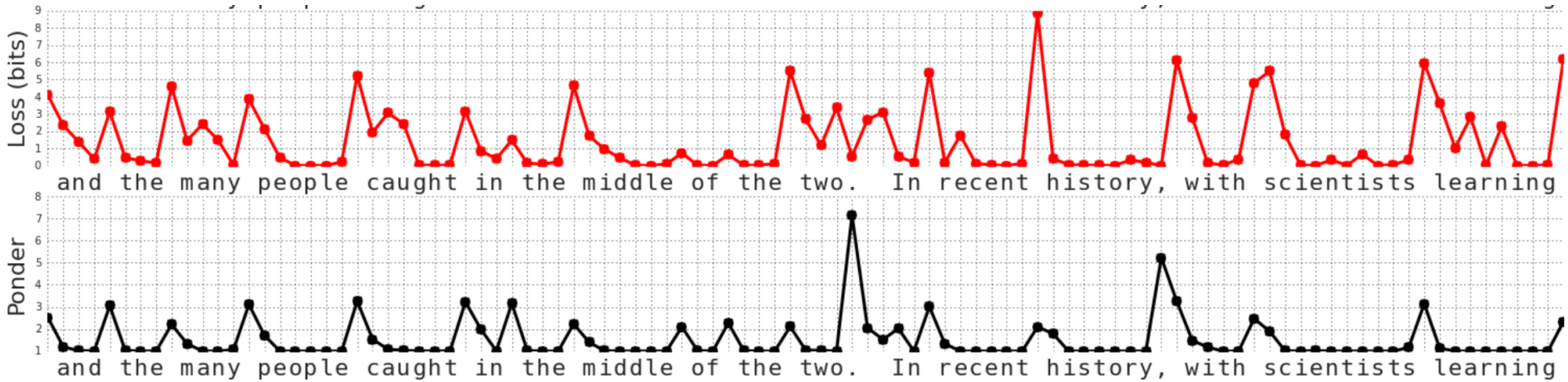

Experimental Results II

- Task: language modeling
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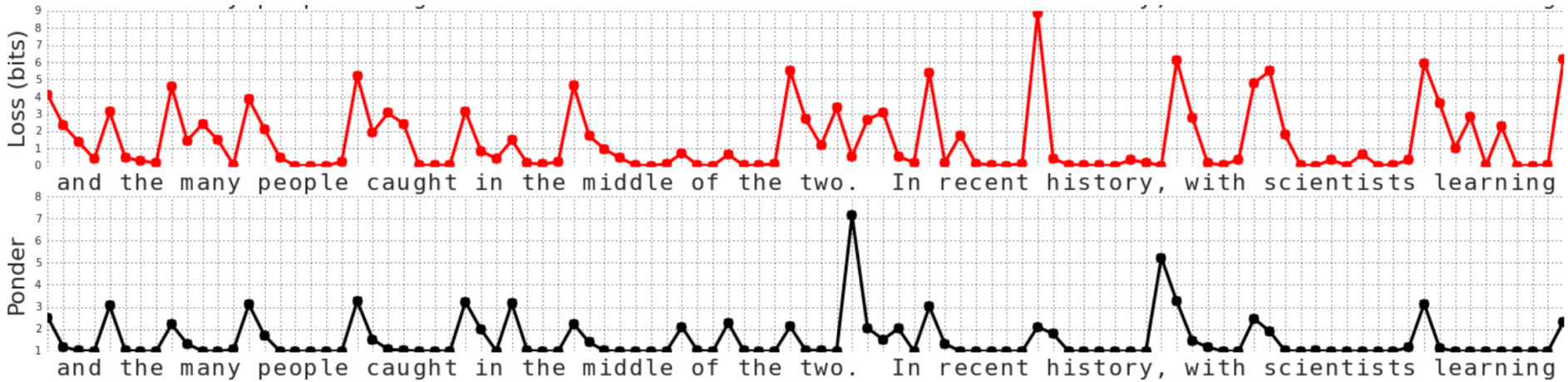
- Longer ponder time (#states at each time) before predicting the next "chunk"
- Learning implicit boundaries/transitions in sequence (unsupervised)
  - More robust than learning from prediction losses/errors



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What Do RNN Neurons Learn?

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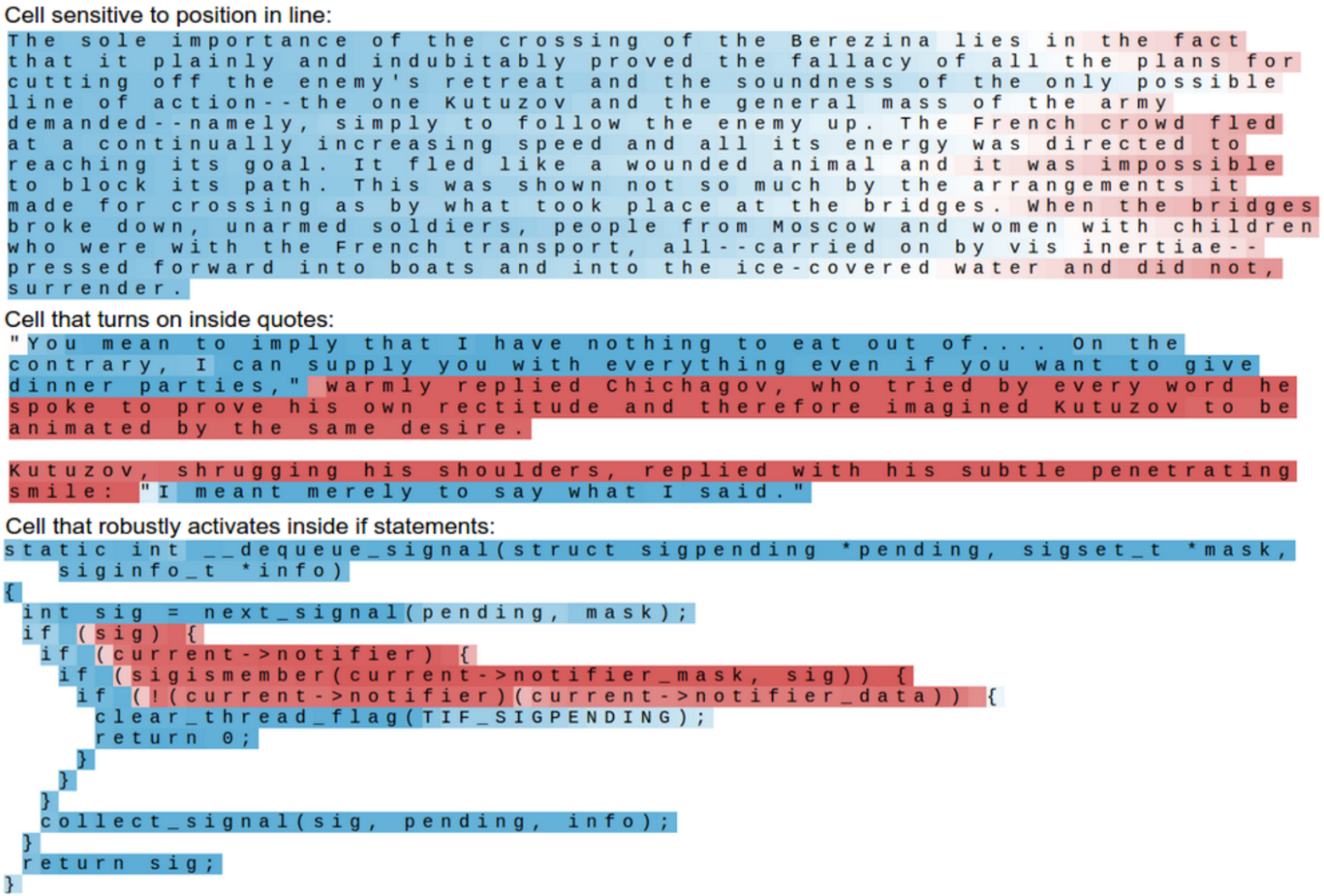
- Neuron activations for language modeling [7] ▸ Interactive Tool



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- Output at epoch 100:

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Reading Comprehension & QA

"Joe went to the kitchen. Fred went to the kitchen.

Joe picked up the milk. Joe travelled to the office.

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- Where is the milk now?
- Where is Joe?
- Where was Joe before the office?

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Memory Networks

"*Joe went to the kitchen. ... to the office. ... to the bathroom.*"

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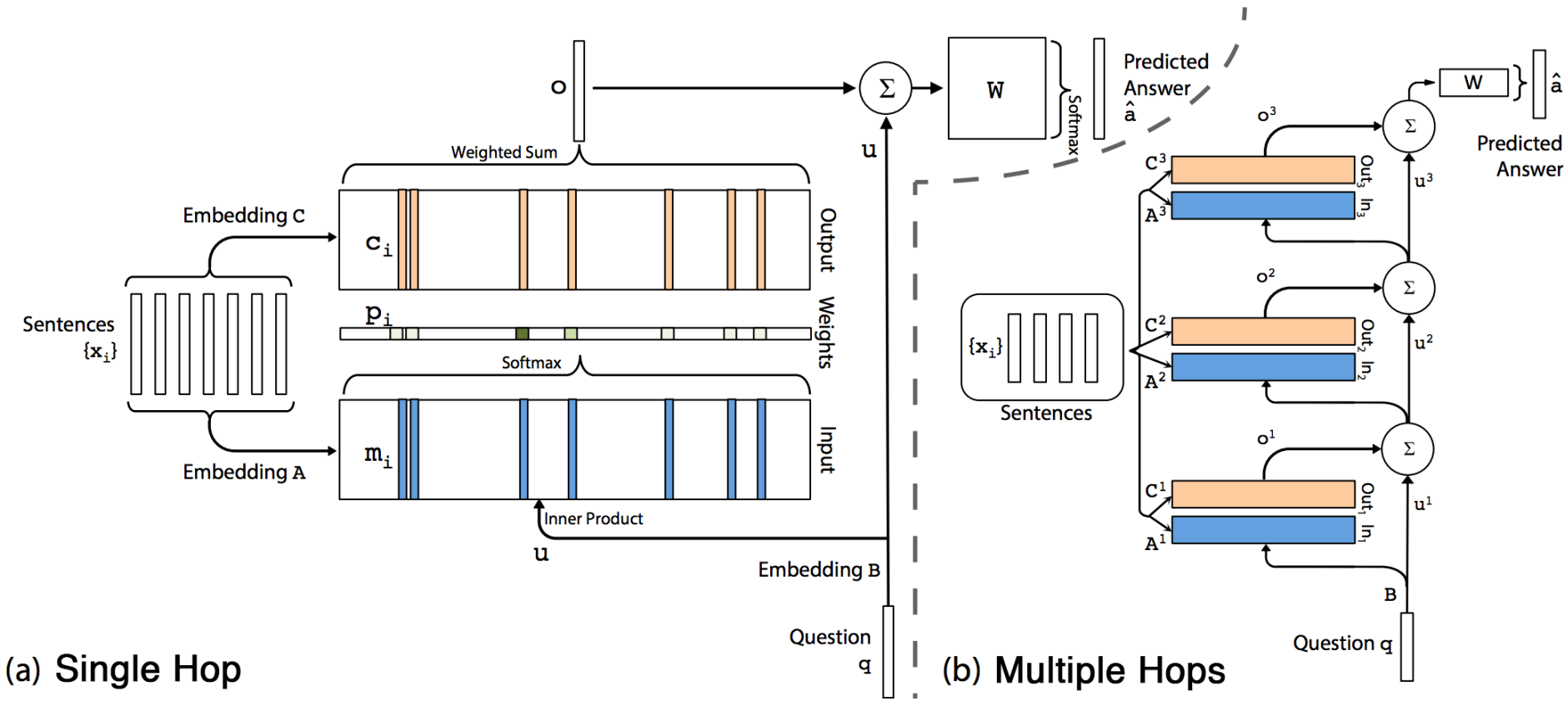
- One-time attention may not be sufficient
- ***Hopping*** in memory networks [14, 13]:



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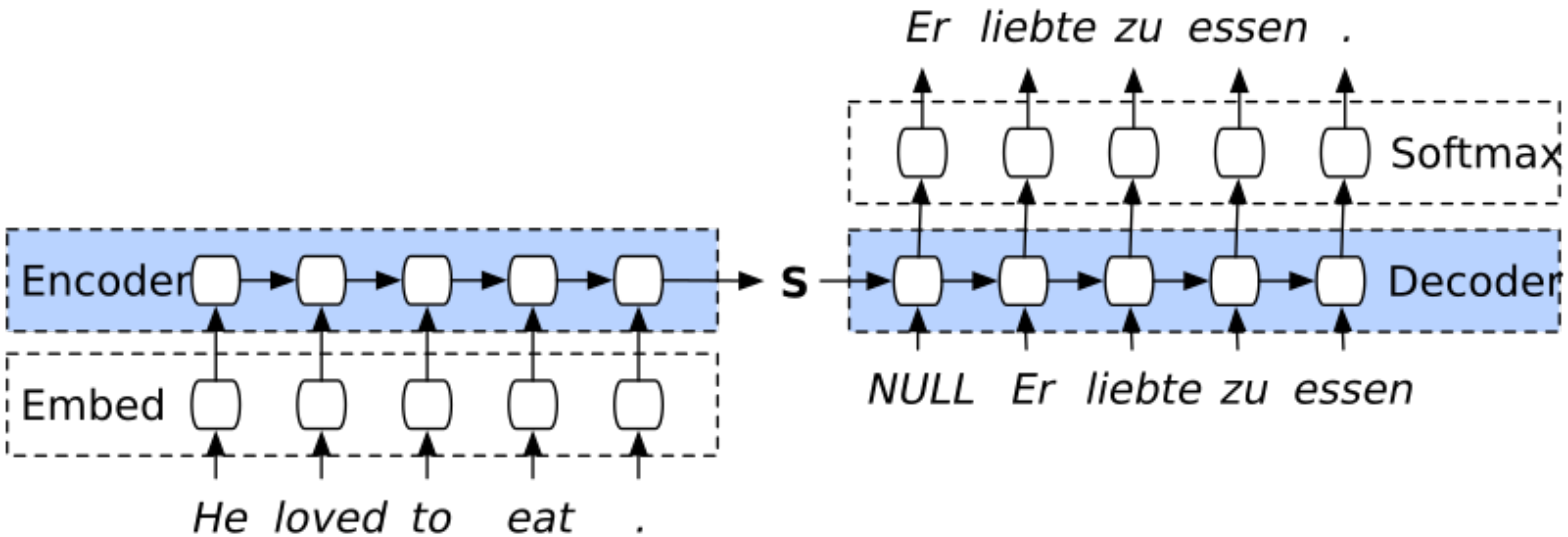
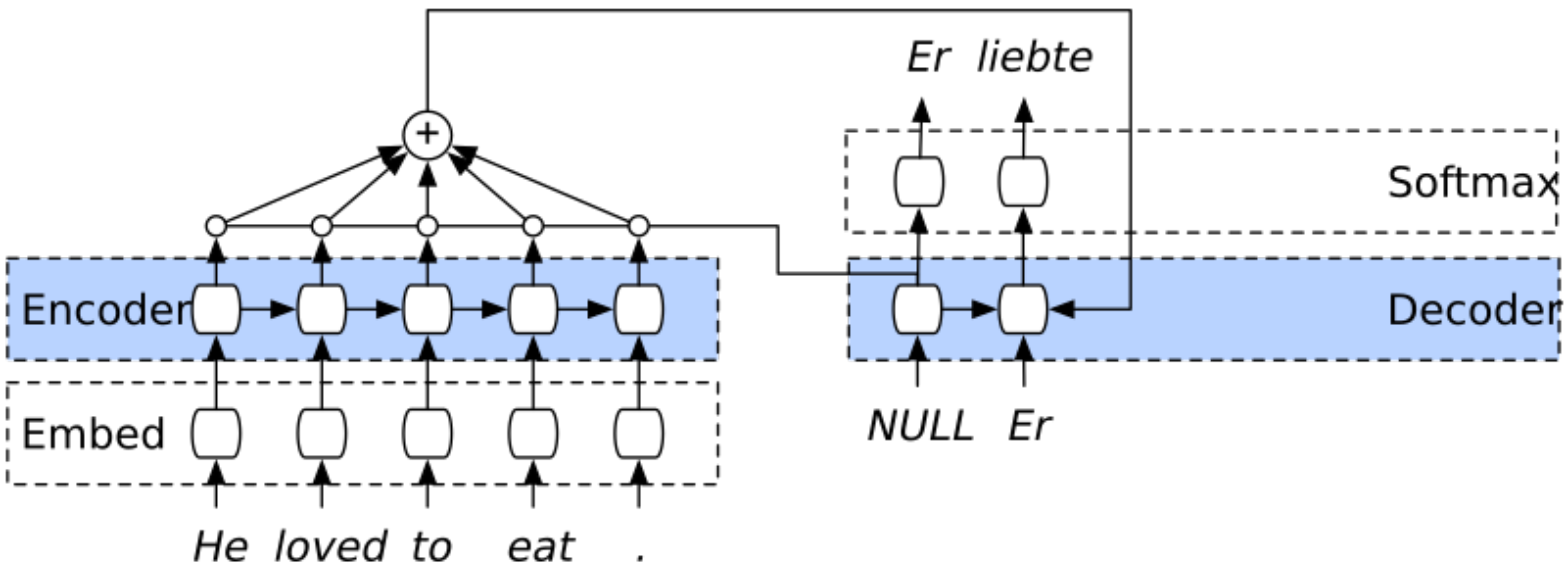
V1: Encoder-Decoder

- LSTM-based RNN
- Hidden state $\boldsymbol{S}$ encodes an entire input sequence
- Then supplied to the decoder



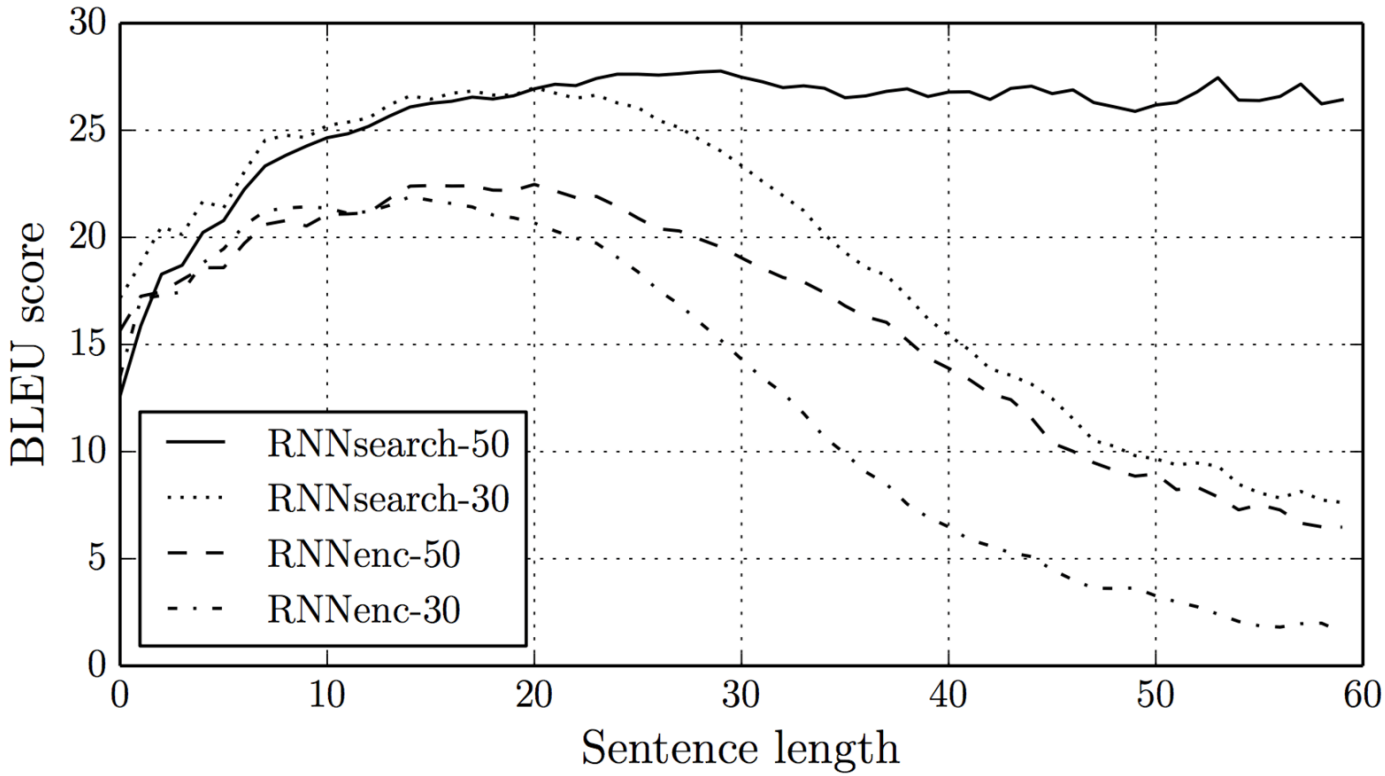
V2: Attention-based Encoder-Decoder

- Allows for retrieving different parts of input sentence depending on decoding context
- No direct connection between the encoder and decoder



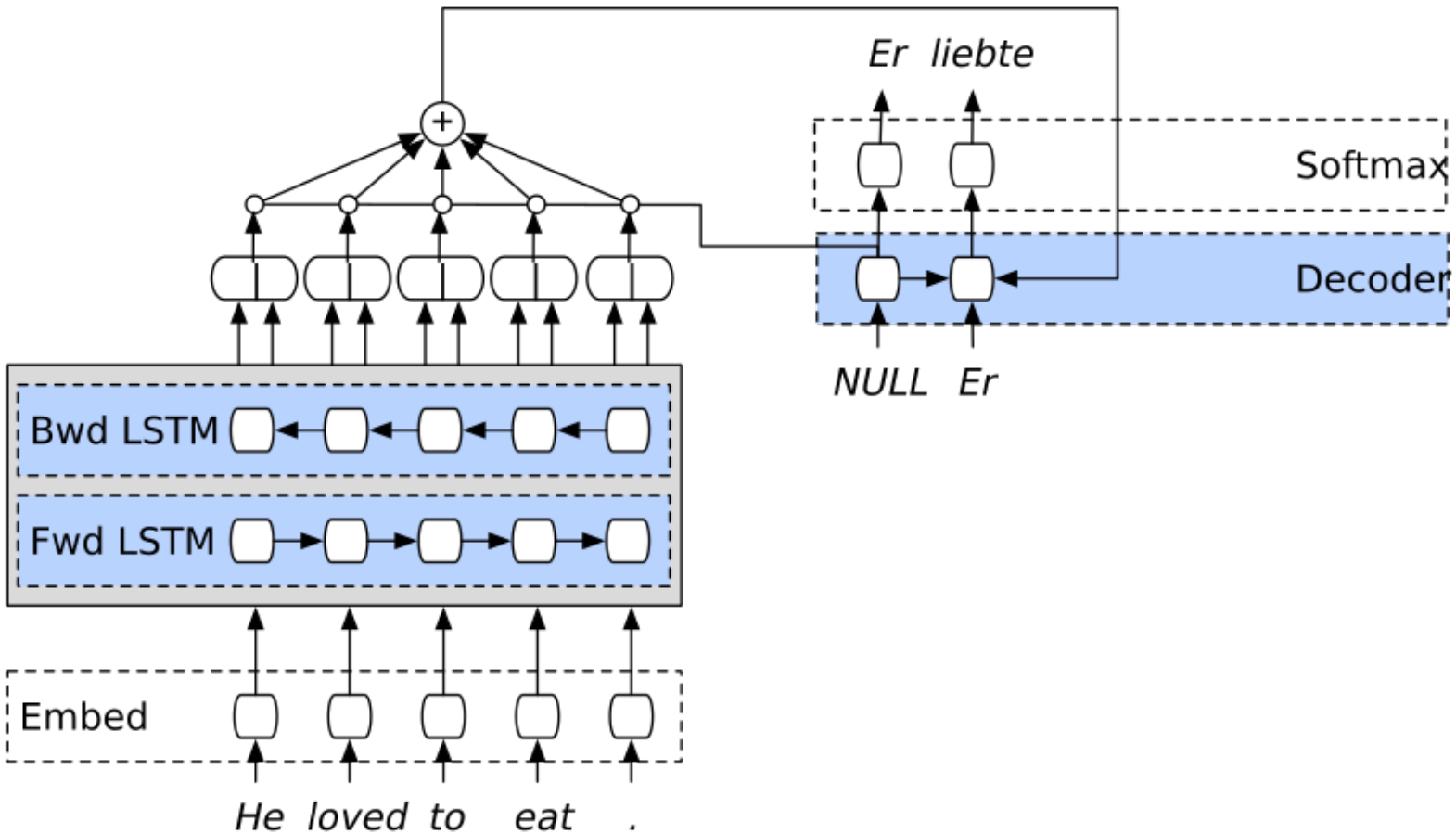
Long Sequences

- Attention-based model generates long sequences better



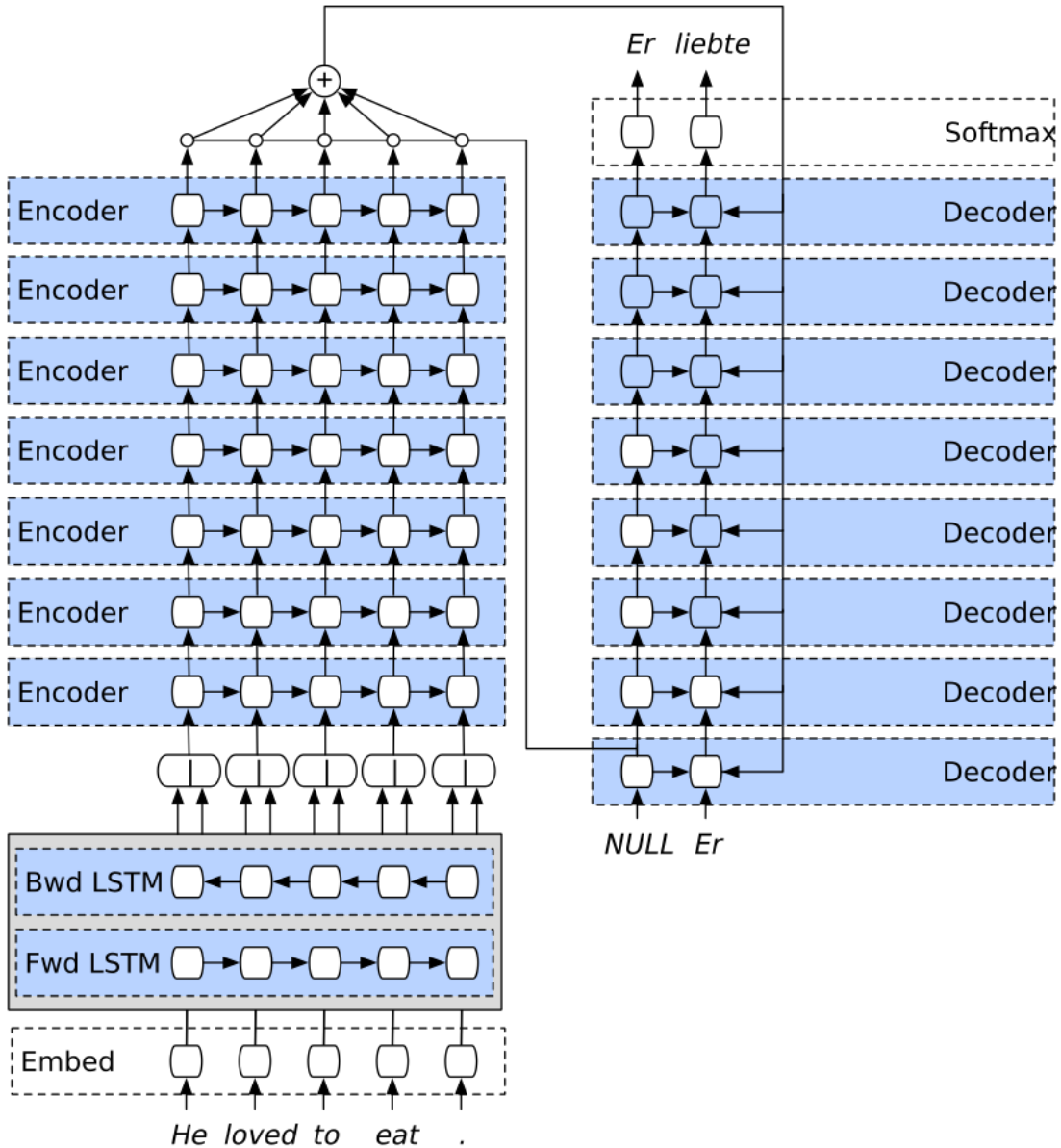
V3: Bidirectional Encoder Layer

- Takes into account future words when summarizing input sequence
- Better determines the meaning/context



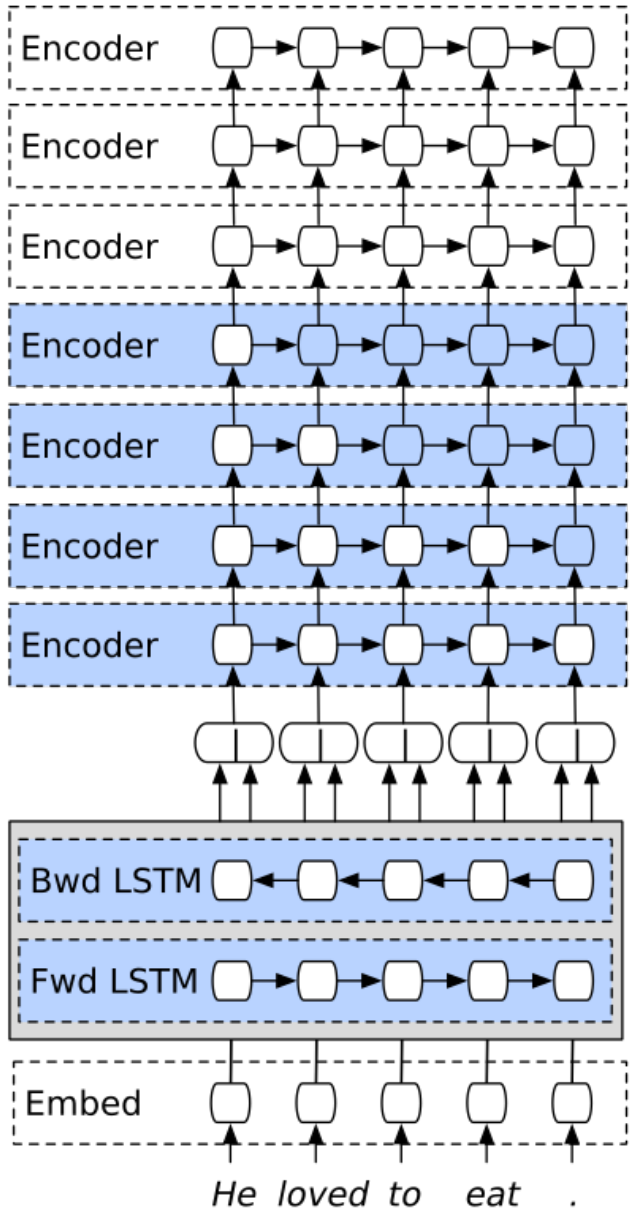
V4: Going Deep

- Encoder:
  - ***1*** bi-directional layer
  - 7 uni-directional layers
- Decoder:
  - 8 uni-directional layers
  - ***Lowest*** decoder layer for querying attention

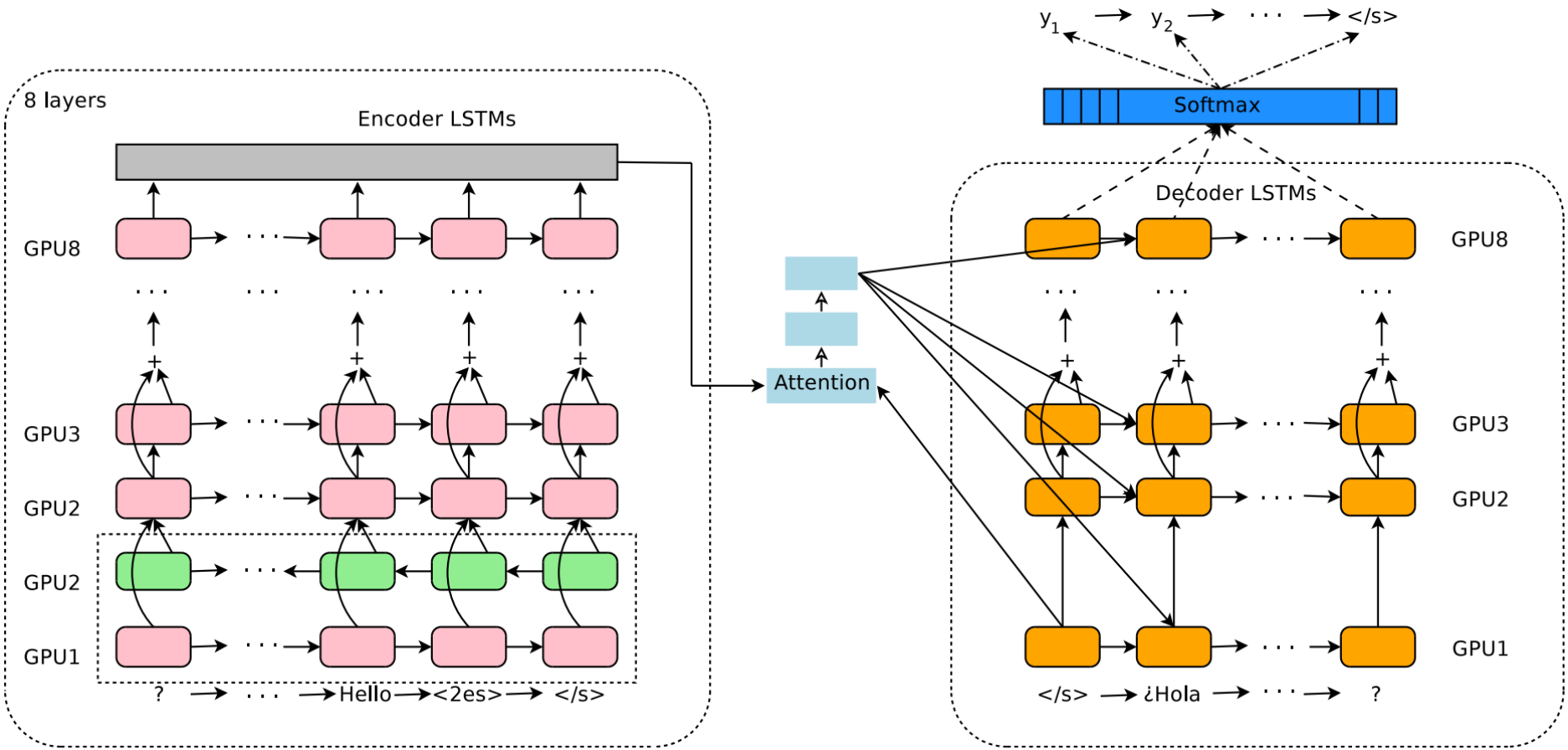


V5: Parallelization

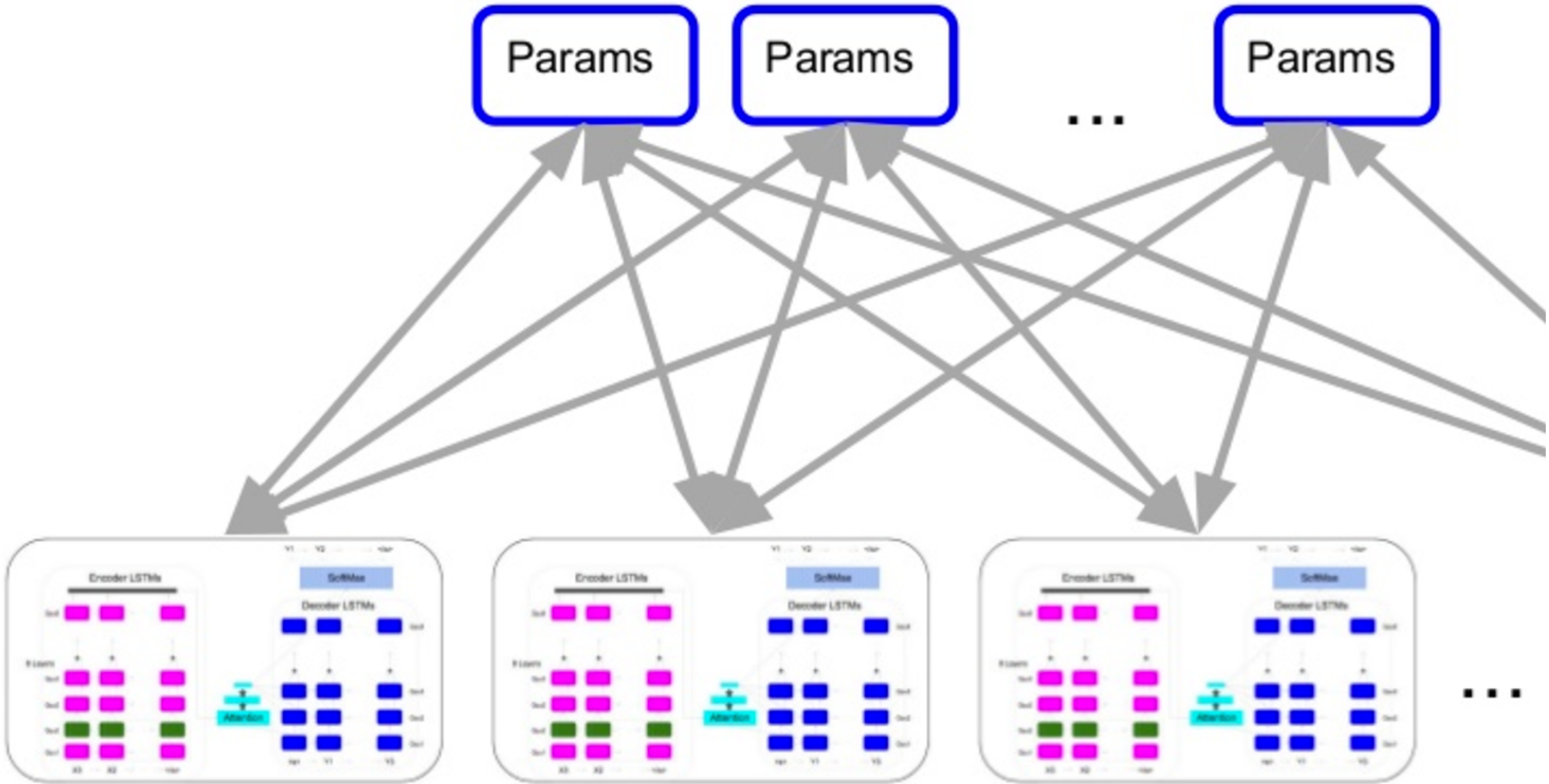
- Each layer trained by a GPU
- Forward pass:
  - Encoder: 7 uni-directional encoder layers trained in a pipeline
  - Decoder: pipeline starts as soon as encoder layers are ready
- Backward pass:
  - Teacher forcing



Model Parallelism (1 Machine, 8 GPUs)

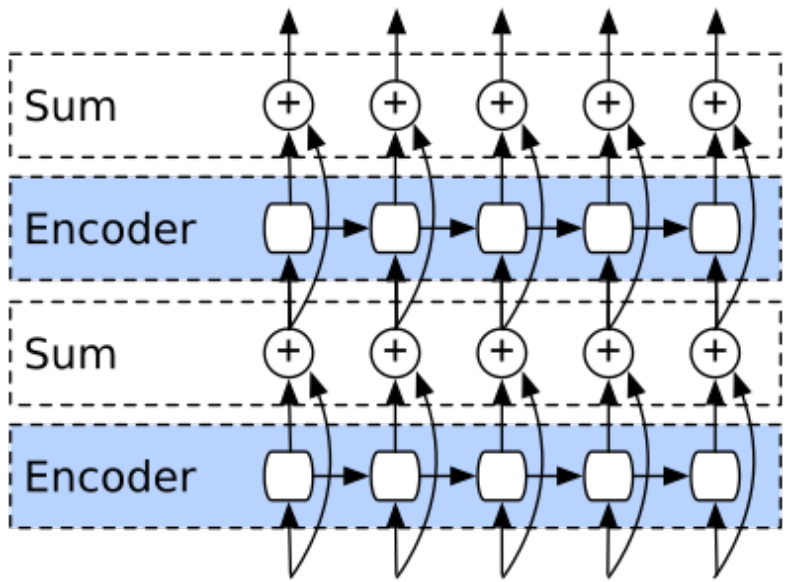


Data Parallelism (Multiple Param Servers)



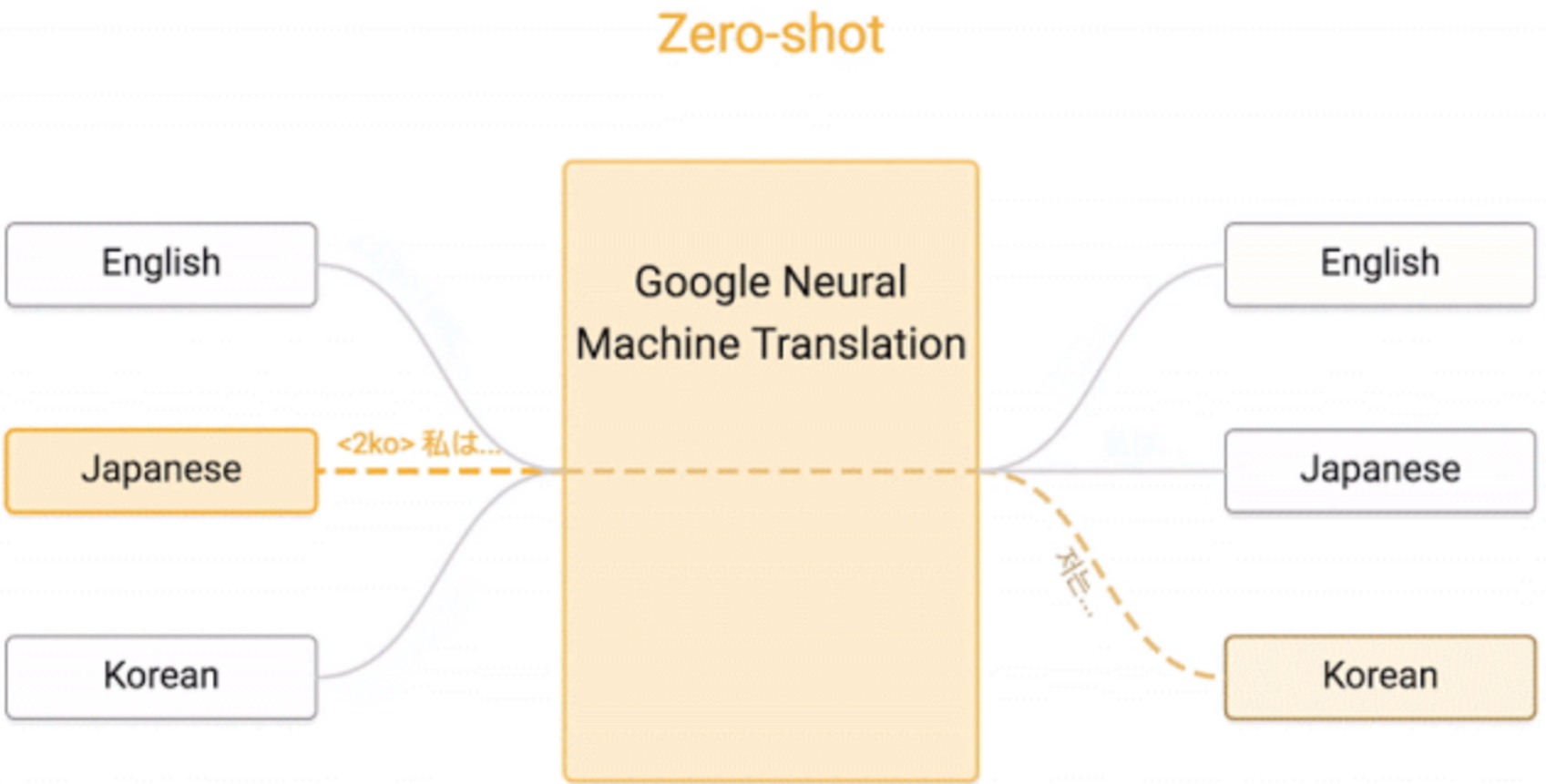
V6: Residuals

- Upper layer learns the ***delta*** function to the lower one
- Easier to train a deep NN



V7: Multilingual & Zero-Shot Translation

"*Google AI invented its own secret language?* "



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