Recurrent Neural Networks and Transformers

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Machine Learning

Outline

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Sequential Data

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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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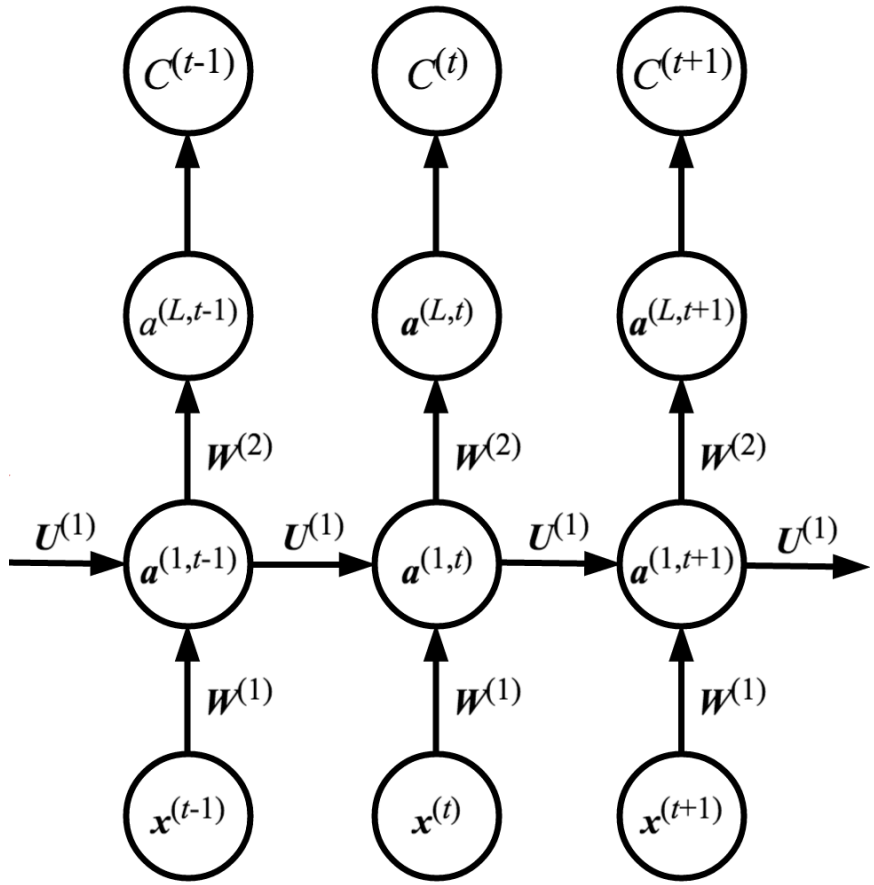

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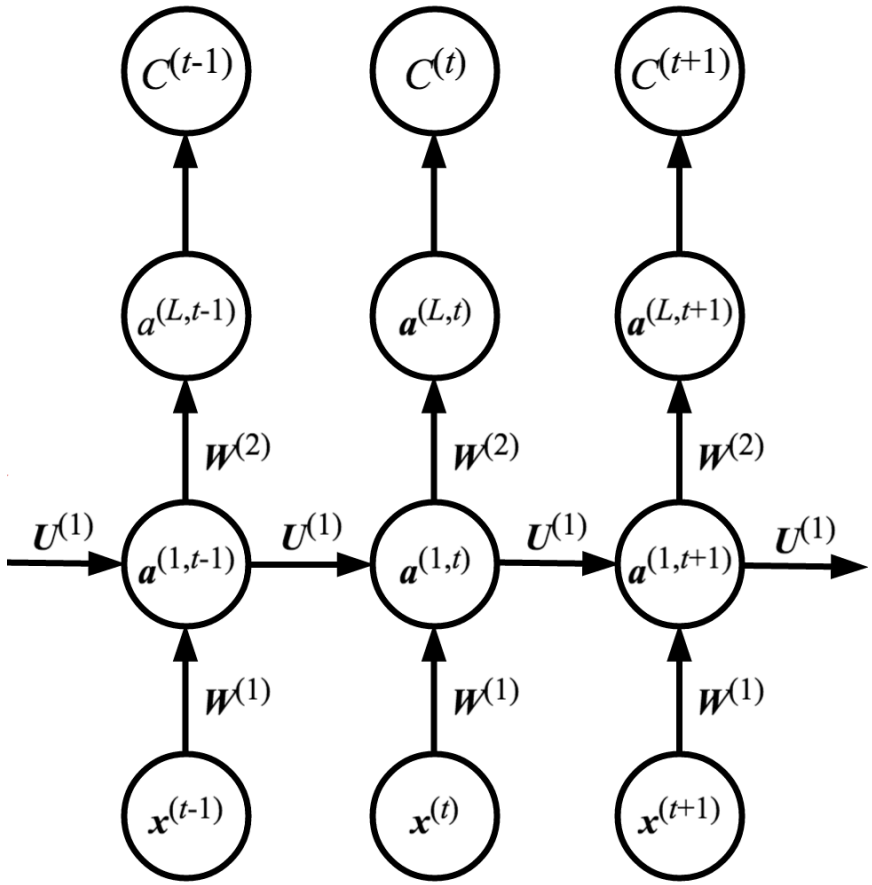

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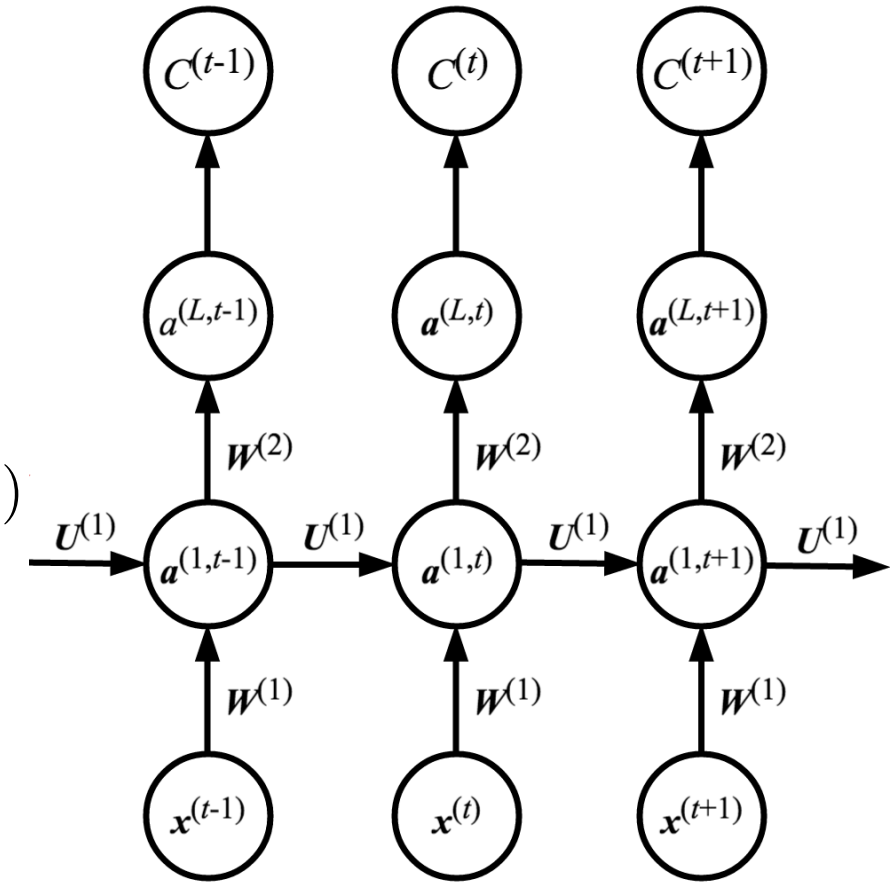

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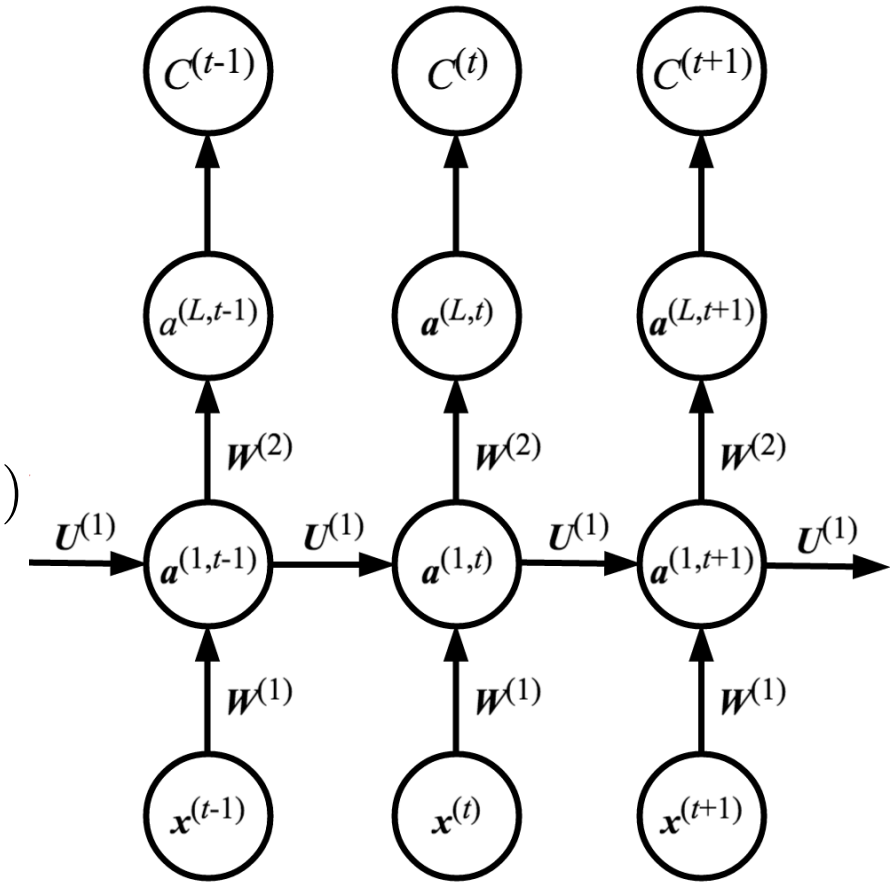

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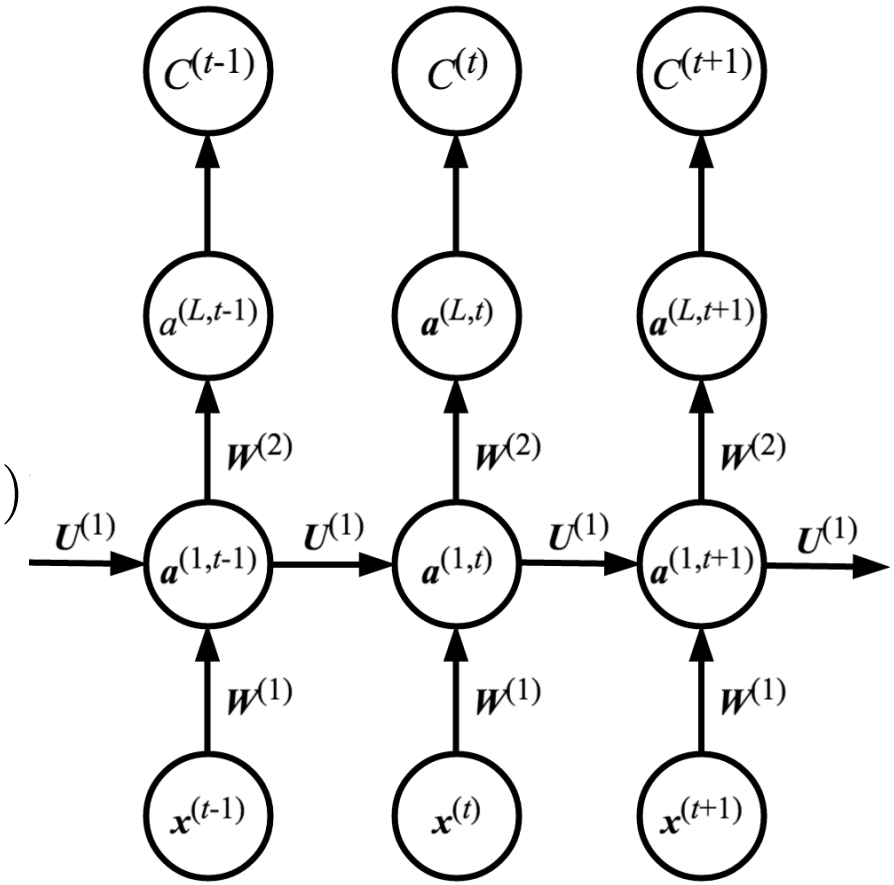
- $\mathbf{a}^{(\cdot,t)}$'s at deeper layers give more abstract summarizations



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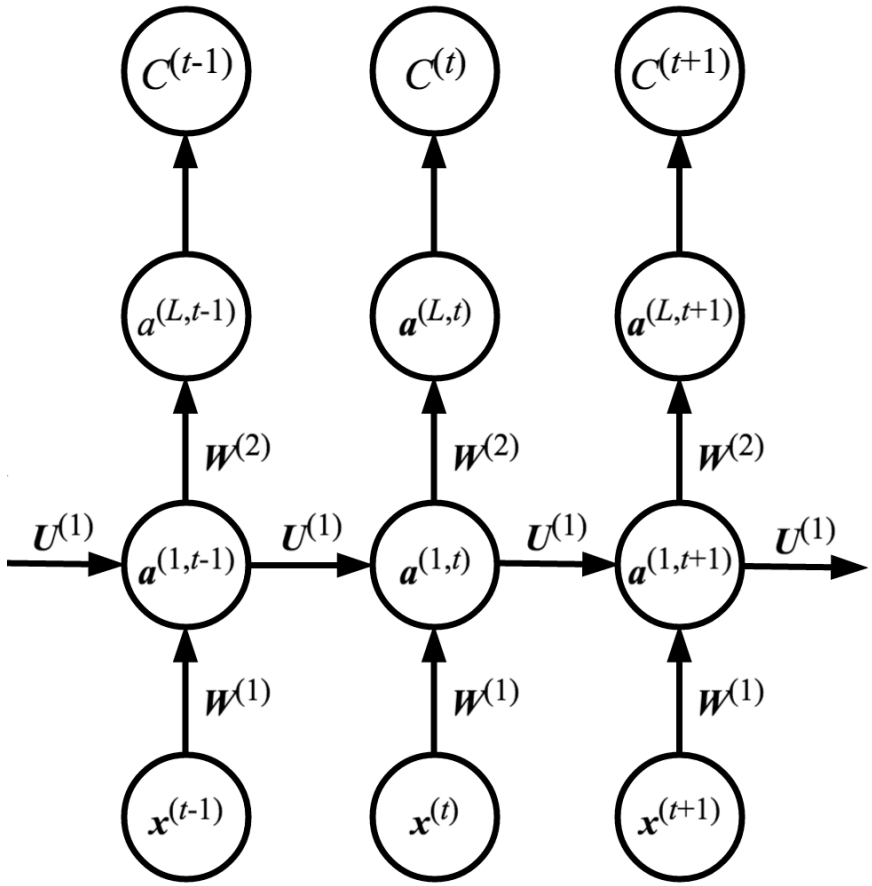

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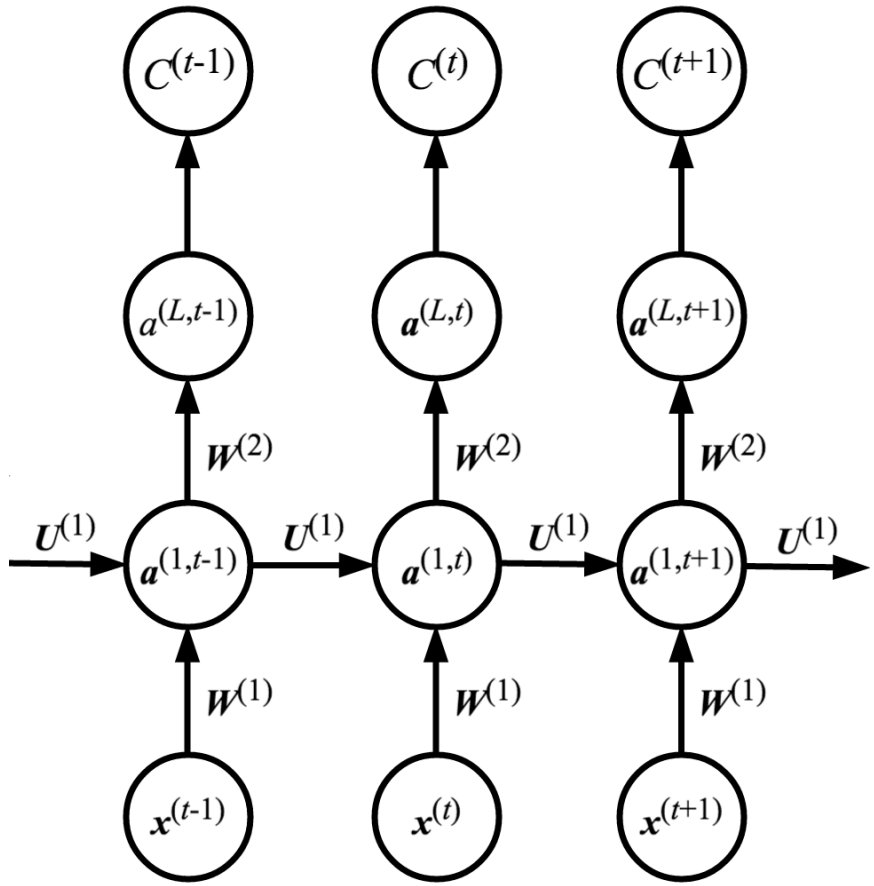

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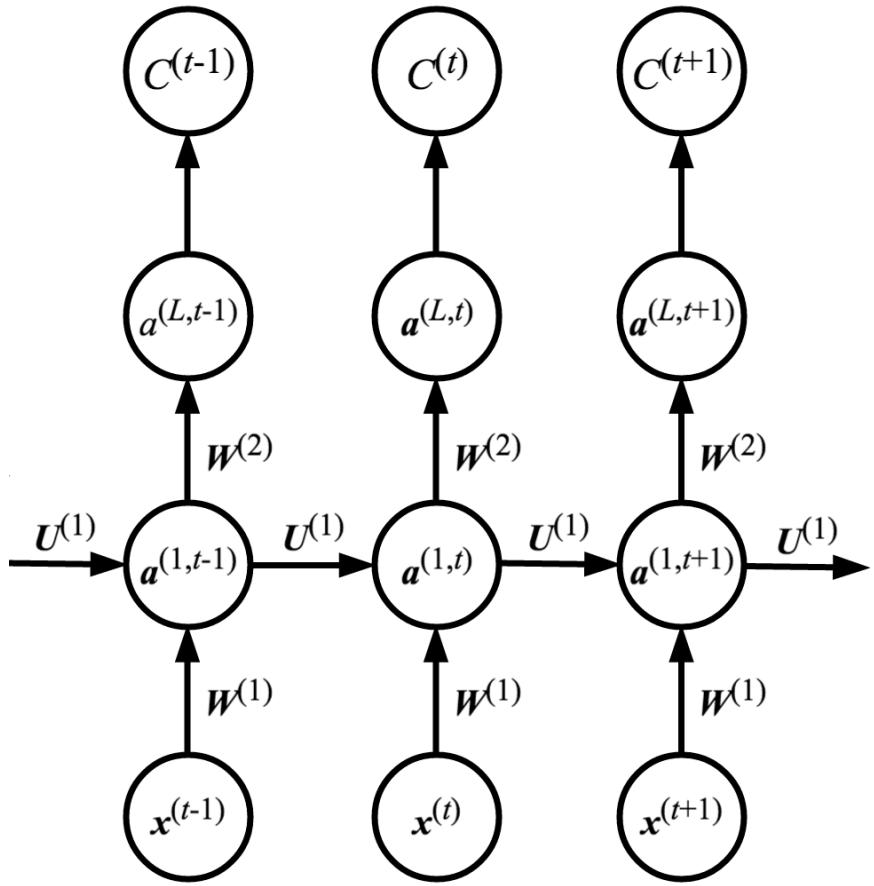
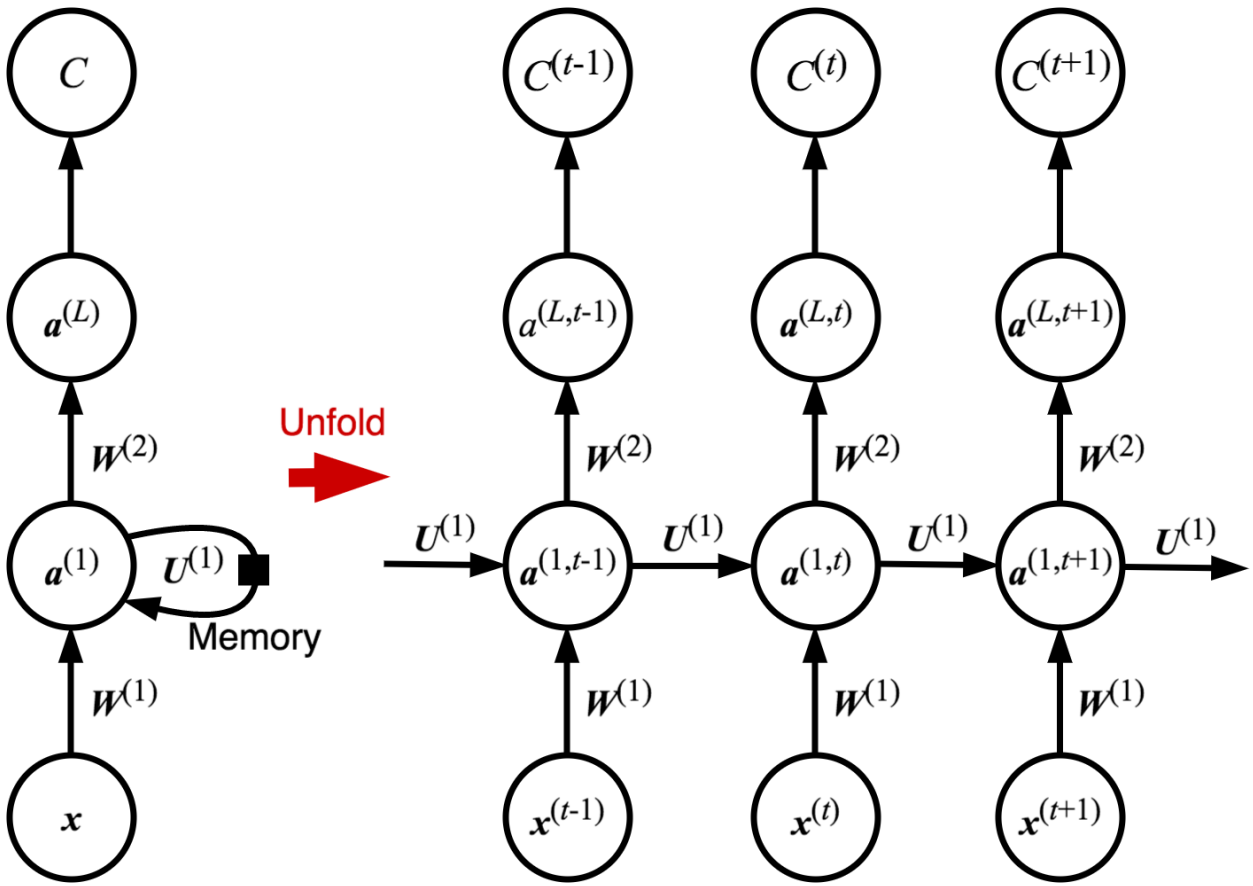
- Weights are ***shared*** across time instances
- Assumes that the "transition functions" are time invariant
- Our goal is to learn $\boldsymbol{U}^{(k)}$'s and $\boldsymbol{W}^{(k)}$'s for $k = 1, \cdots, L$



RNNs have Memory

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



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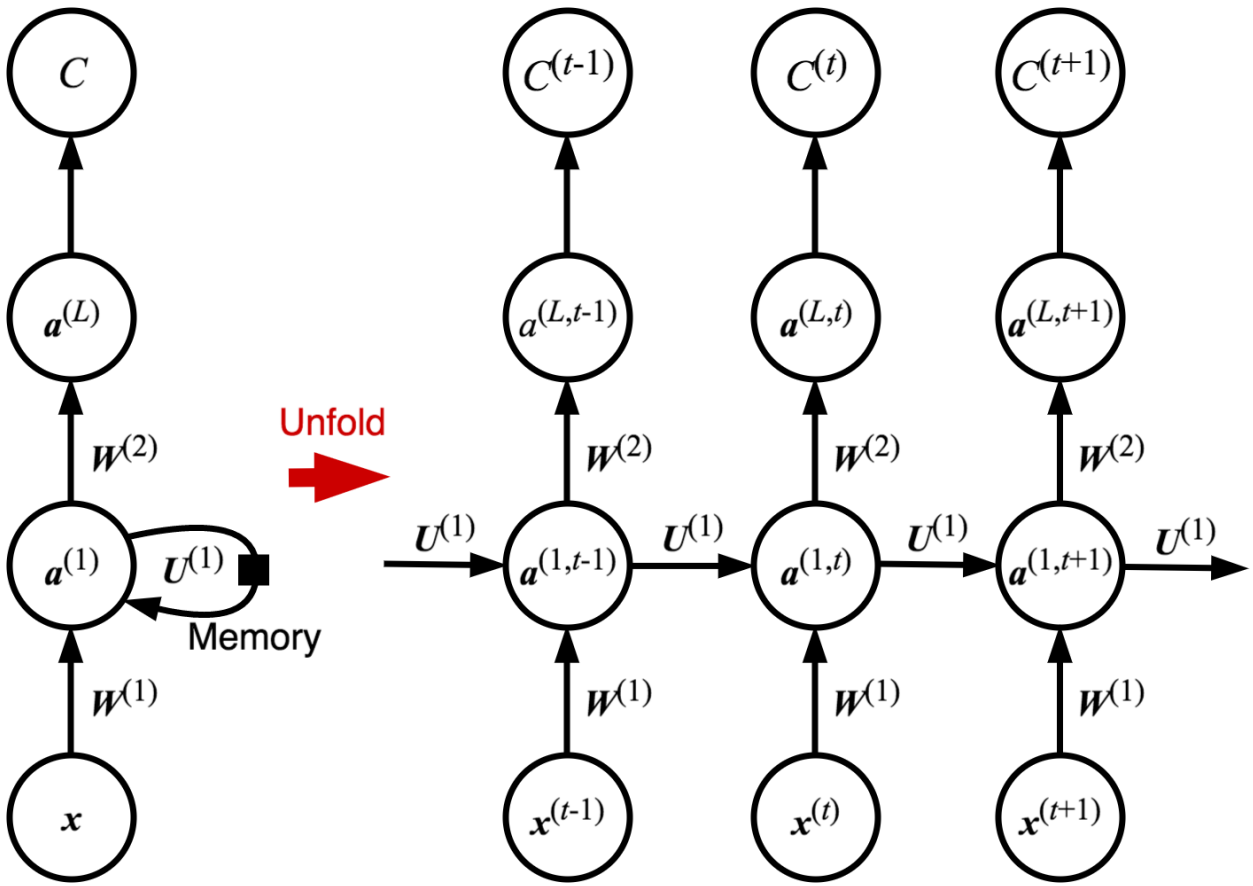
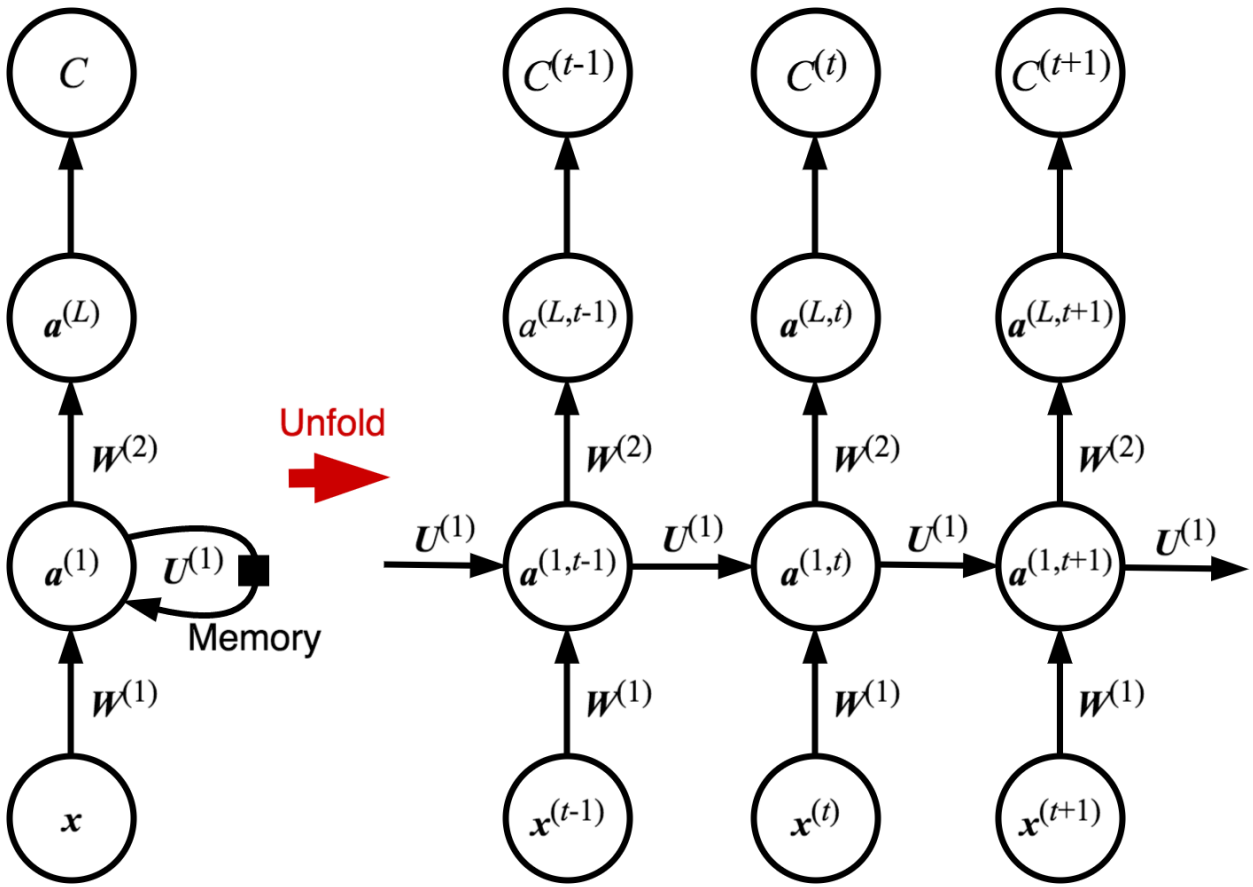
- Black squares denotes ***memory*** access



Output Layer (1/2)

- With multi-class $\mathbf{y}^{(t)}$,
  - $\mathbf{a}^{(L,t)}$ represents the probability of each class
  - $C^{(t)}$ is cross entropy
- How to obtain $\hat{\mathbf{y}}^{(t)}$ rom $\mathbf{a}^{(L,t)}$ at inference time?



Output Layer (2/2)

- Output sampling for multi-class tasks:
  - Greedy: sample $\hat{\mathbf{y}}^{(t)}$ from $\mathbf{a}^{(L,t)}$
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- Problem: out of vocabulary or high dimensional $\mathbf{a}^{(L,t)}$

- Solution?

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- Solution? ***Subword tokenization*** (to be discussed later)

RNNs vs CNNs for Sequential Data

- On processing a sequence of length T at each layer with
  - D-dimensional point input and output
  - F = the CNN filter/kernel size
  - #CNN filters = D

	#Weights	Computation	Autoregressive	Point Distance
CNN	$O(FD^2)$	$O(TFD^2)$	No	$O(\log_F T)$
RNN	$O(D^2)$	$O(TD^2)$	Yes	$O(T)$

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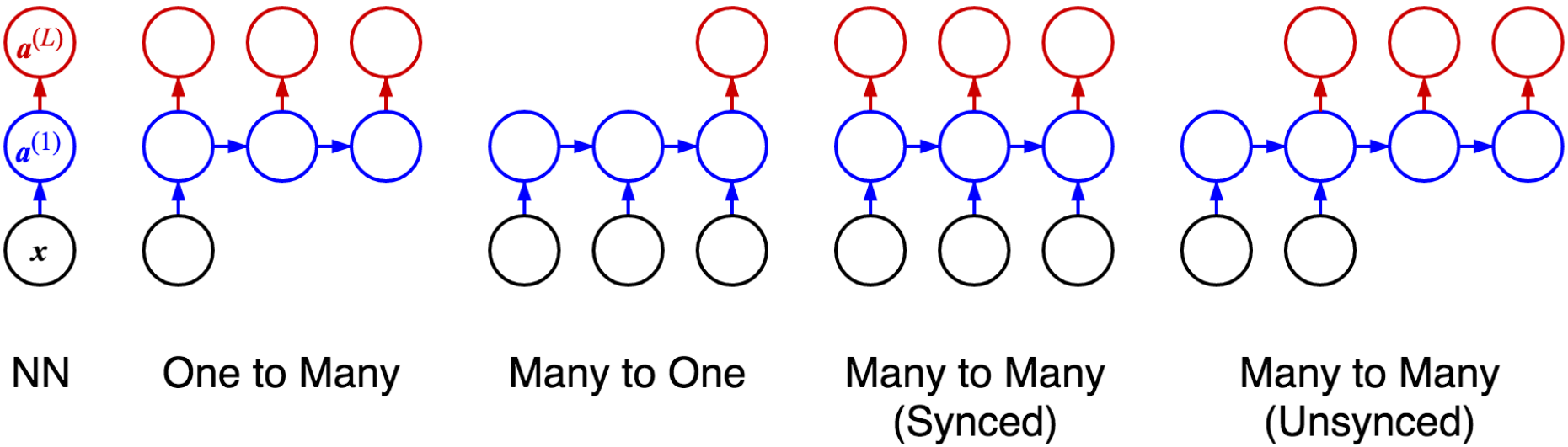
Input and Output

- $\boldsymbol{x}^{(t)}$'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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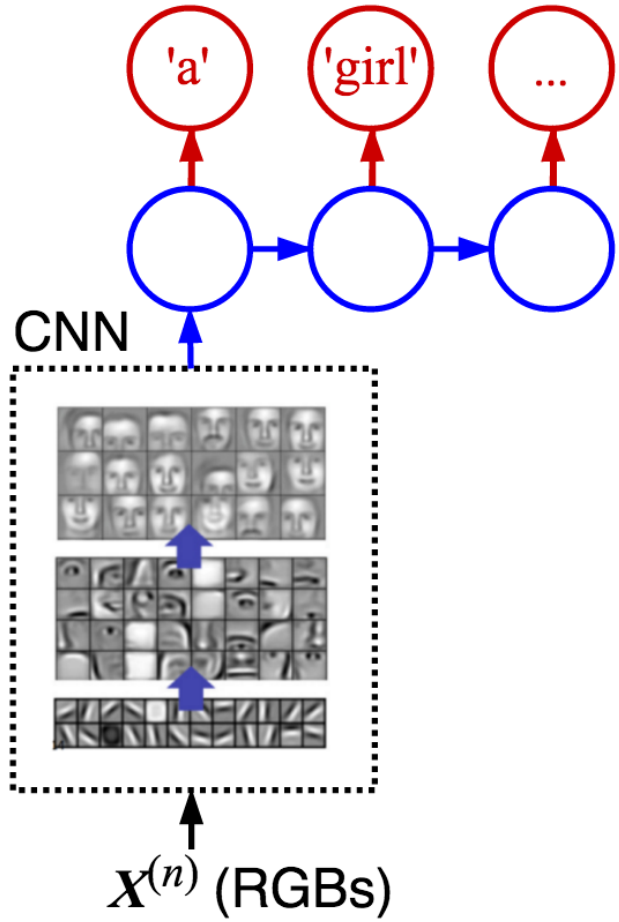
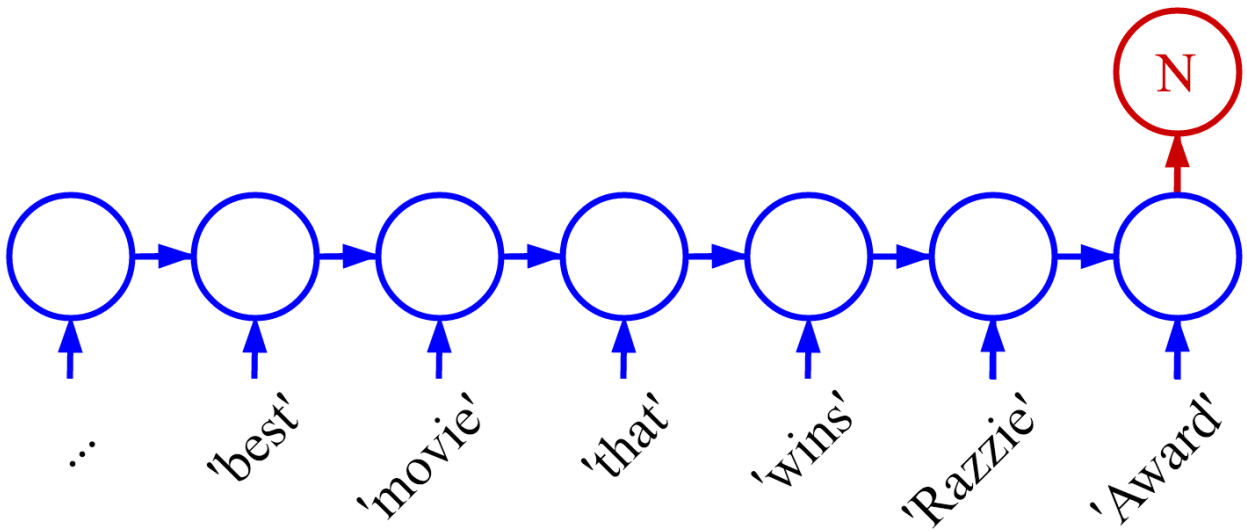


Many2One: Sentiment Analysis



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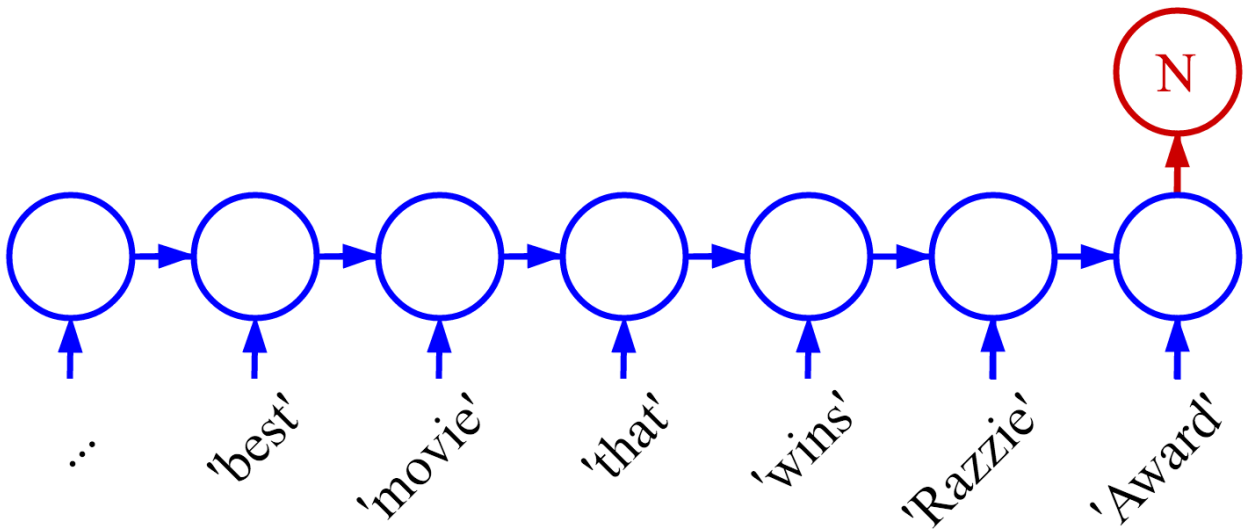
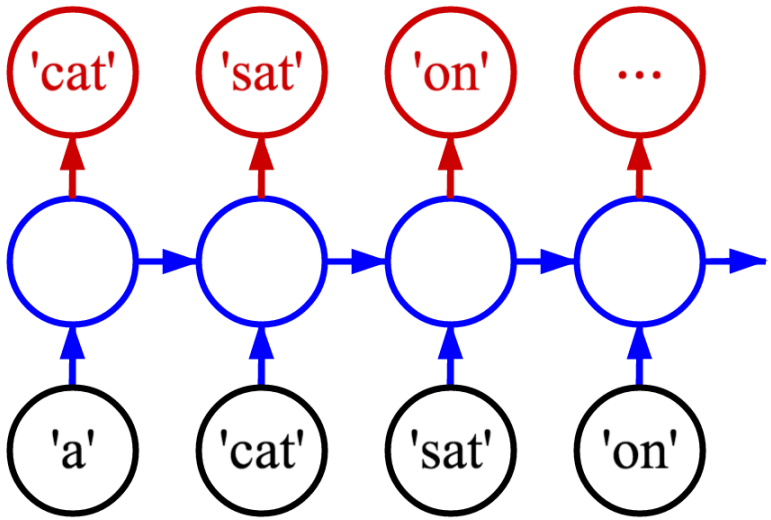


- A single word (e.g., "Razzie") can negate the entire input sentence

Many2Many (Synced): Language Modeling

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



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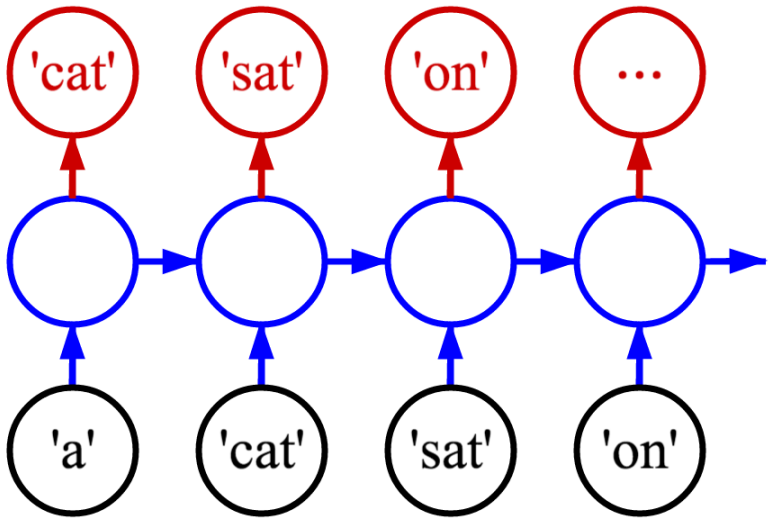
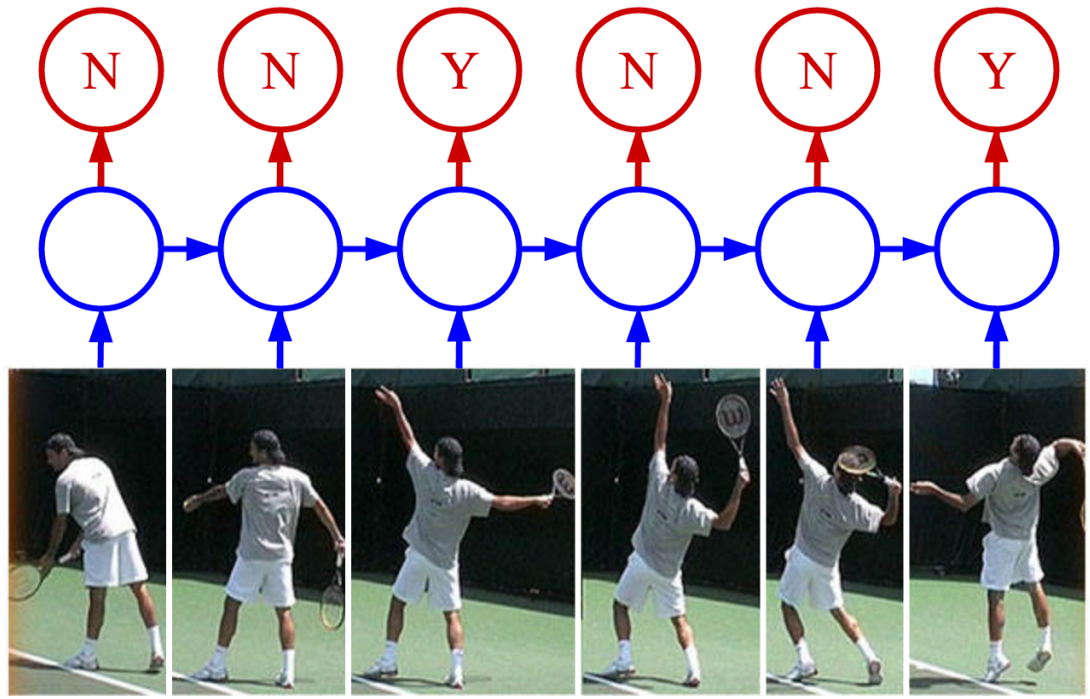


- Latent representations of RNN provide the context

Many2Many (Synced): Video Keyframe Tagging

- Video frame annotation:



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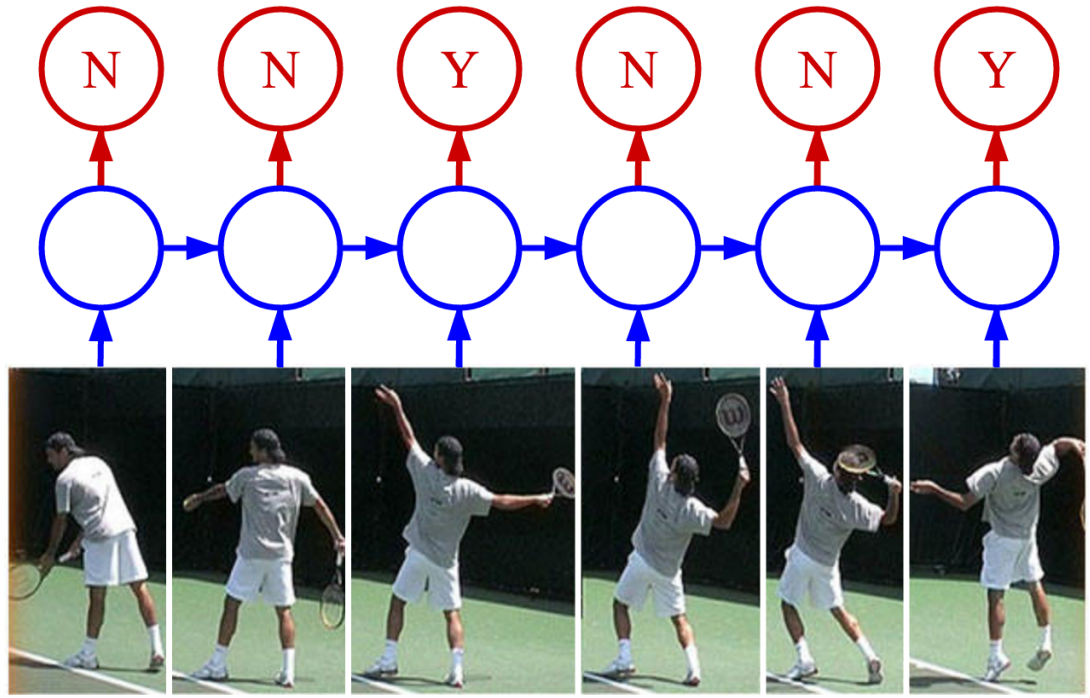
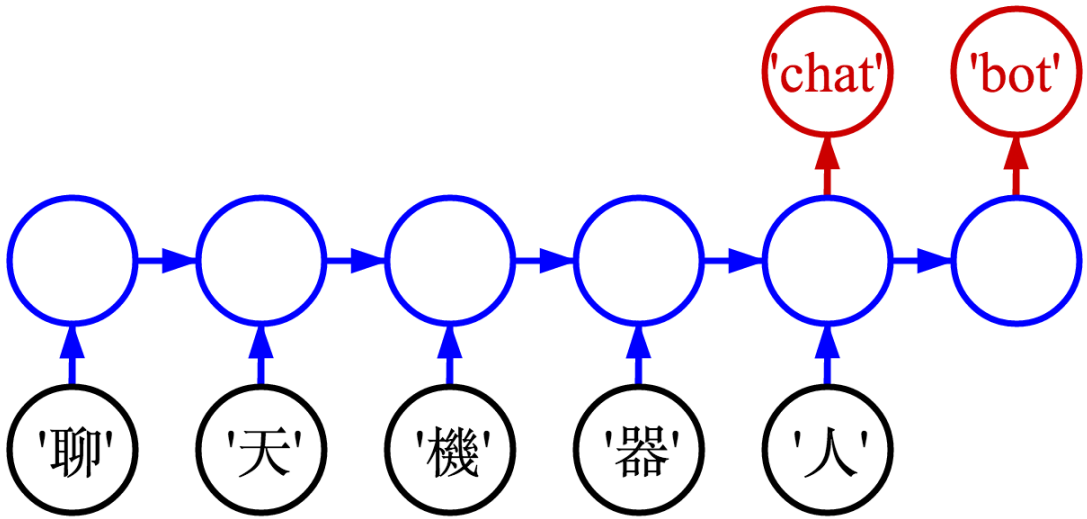


- Latent representations summarize "what's going on"

Many2Many (Unsynced): Machine Translation



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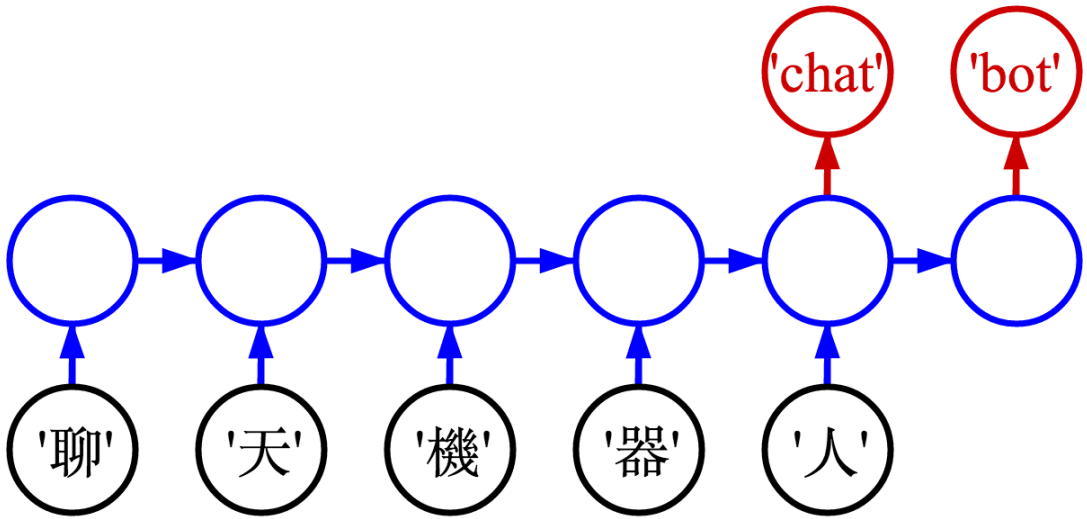

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- Also called ***sequence to sequence*** learning
  - Also used in other applications, e.g., chat bots

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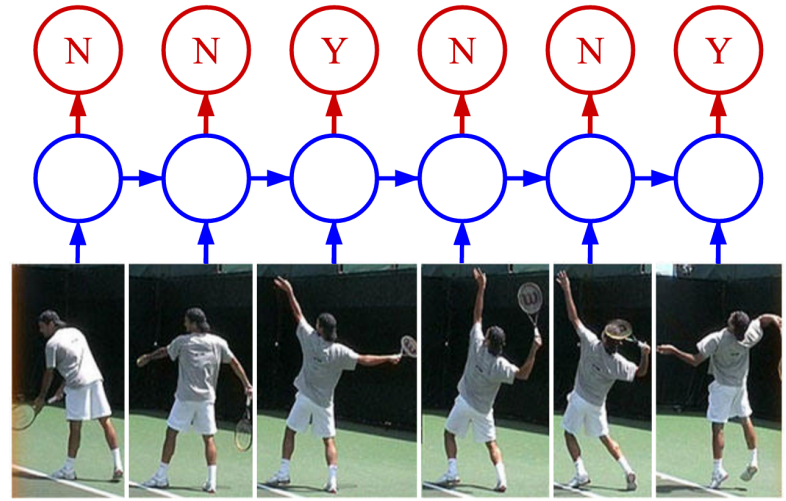

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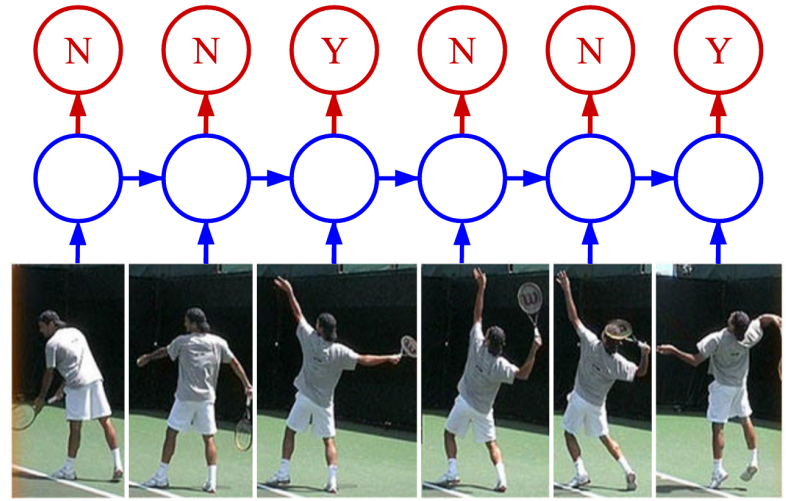

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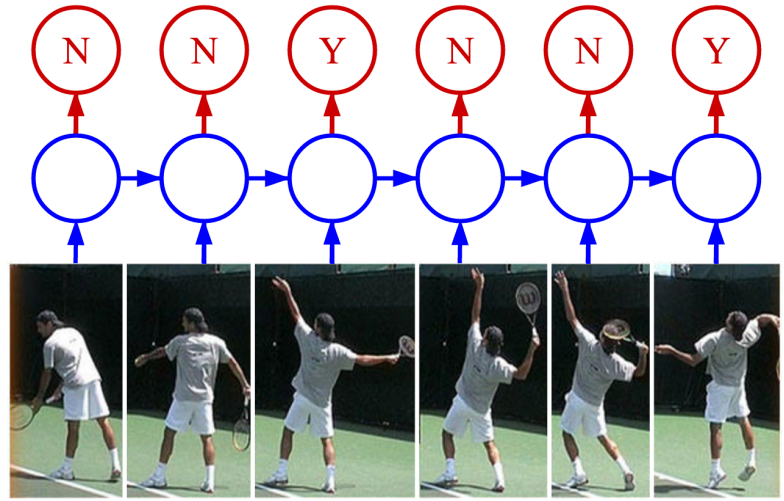
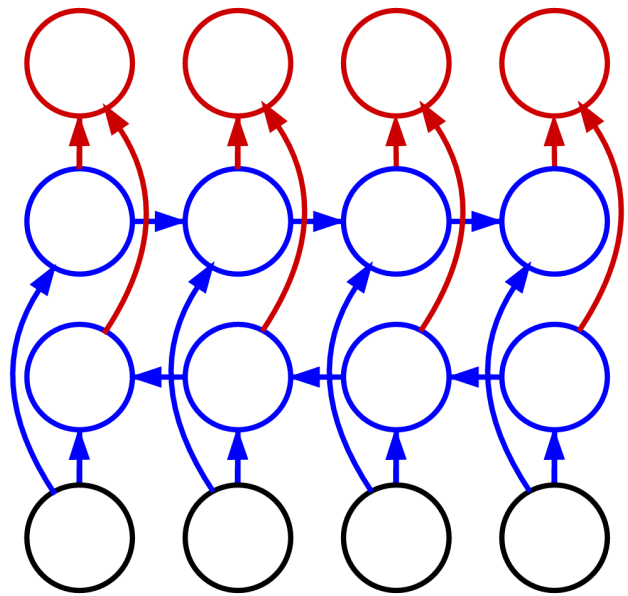
- Can we take ***future*** frames into account?
- ***Bidirectional RNNs***: output $\mathbf{a}^{(L,t)}$ depends on both $\mathbf{a}^{(k,t)}$'s and $\tilde{\mathbf{a}}^{(k,t)}$'s

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





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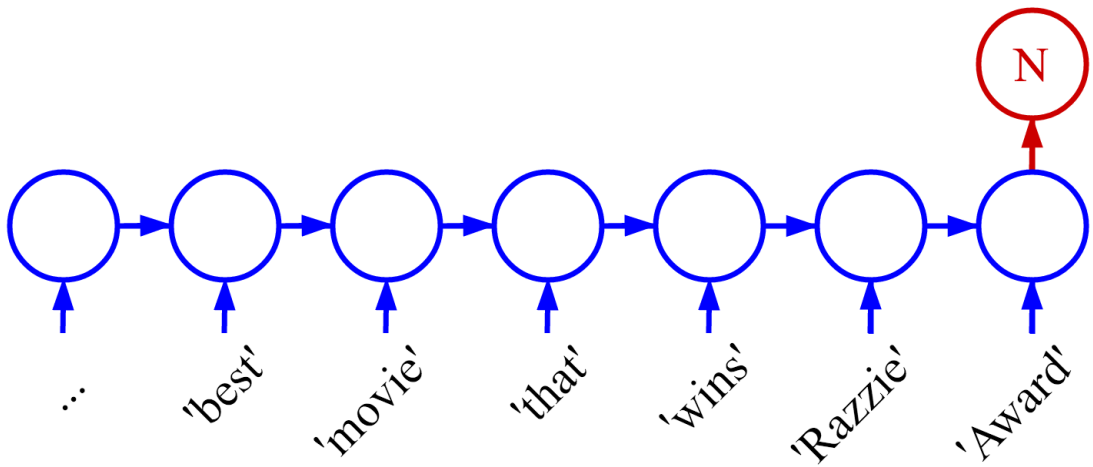

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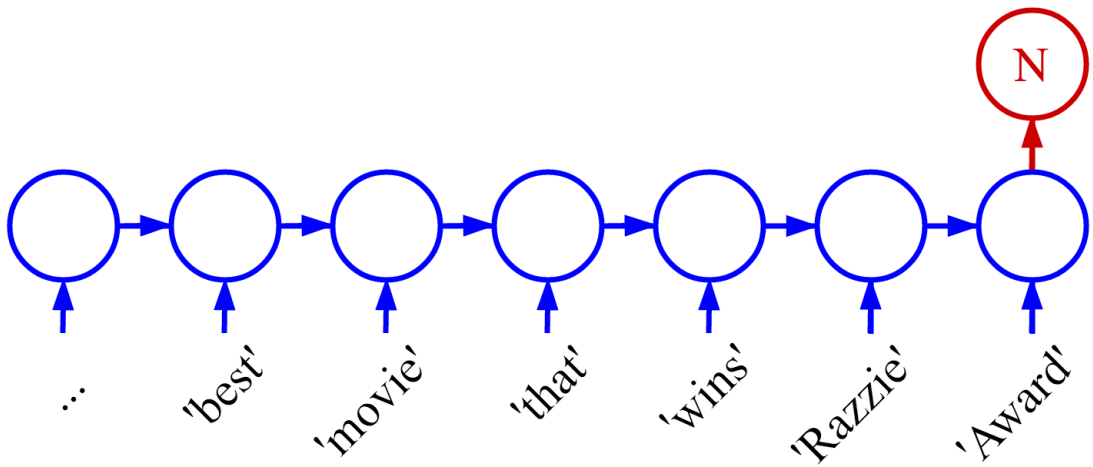
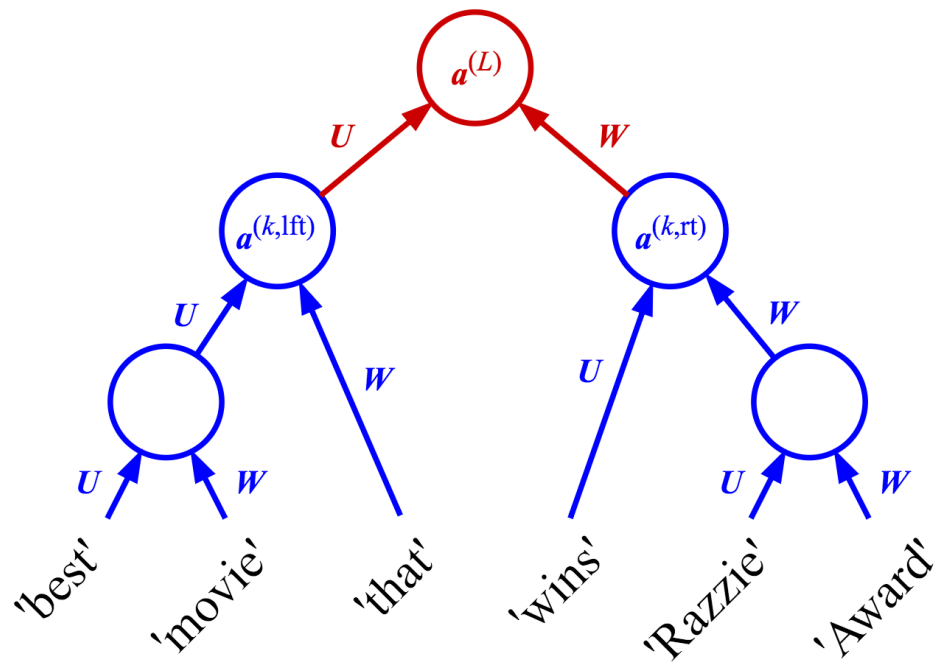
- "Razzie" has less effect if it is far away from the prediction
- In some applications, transitions are invariant in terms of other concepts



Recursive RNNs II

- In natural language processing (NLP), we can parse the input sentence $\boldsymbol{X}^{(n)}$ into a tree
  - Following gramma rules



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- 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

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

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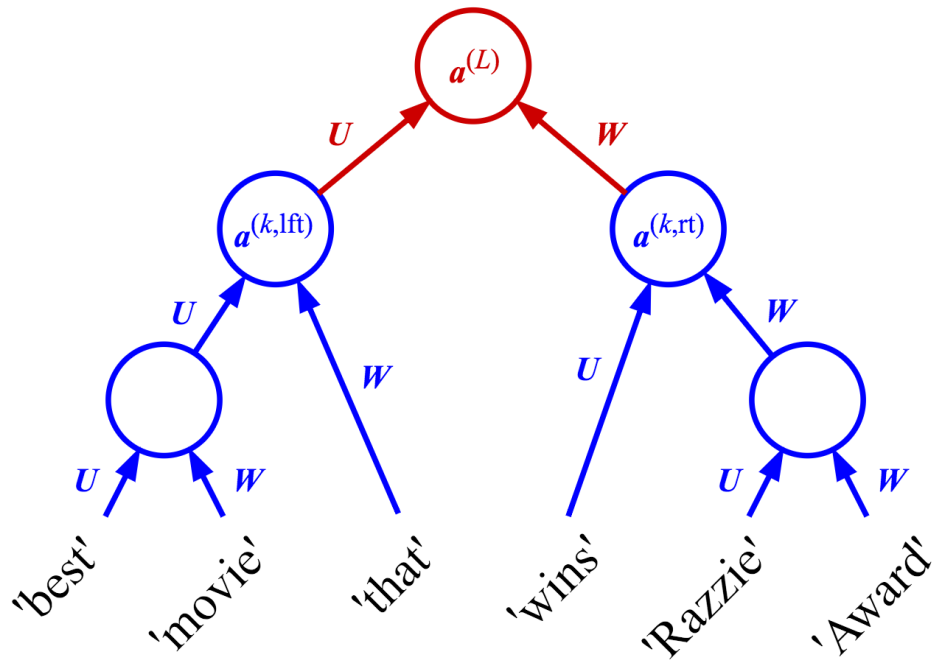

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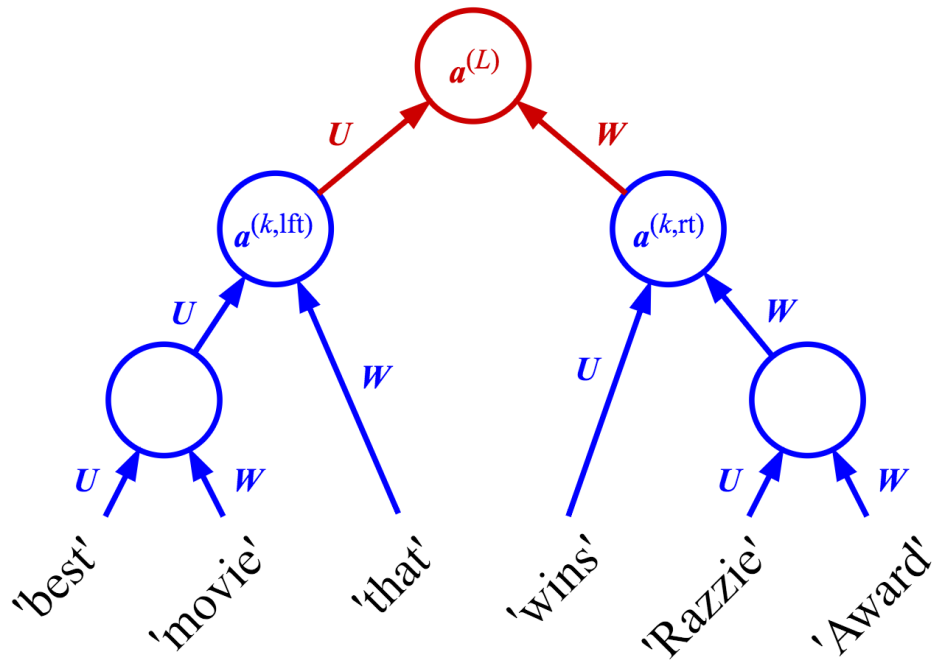
- Given sentence length T, $\mathbf{a}^{(L)}$ and $\mathbf{a}^{(1,\cdot)}$ can be $O(\log T)$ away in the best case



Outline

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

Outline

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***

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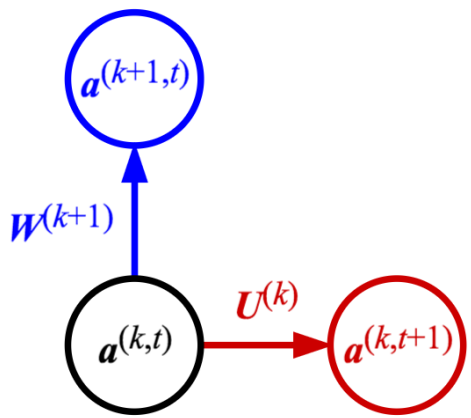

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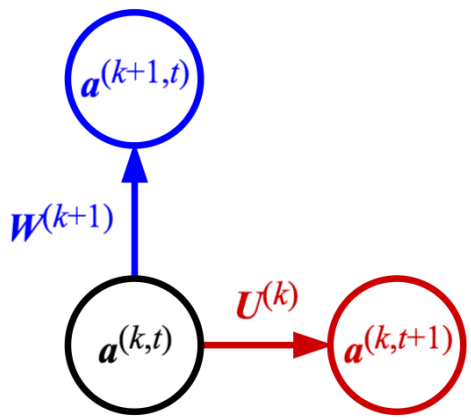

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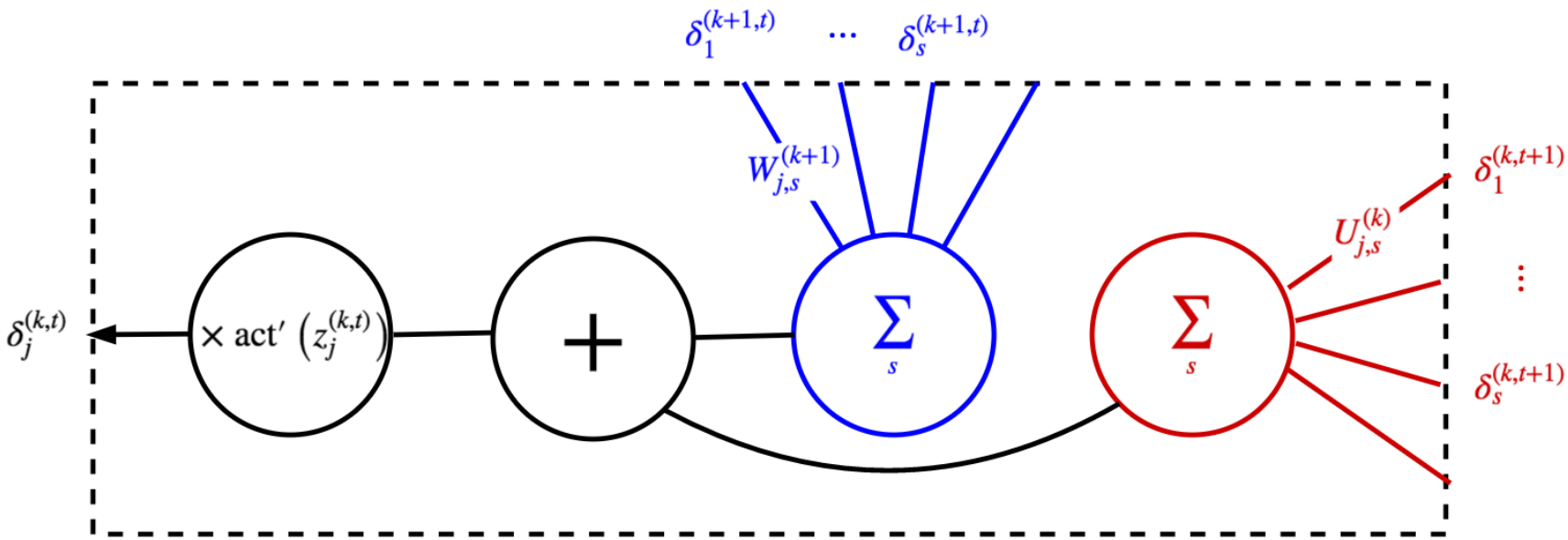
- We can evaluate all $\delta_j^{(k,t)}$'s starting from the deepest layer and ***latest time***



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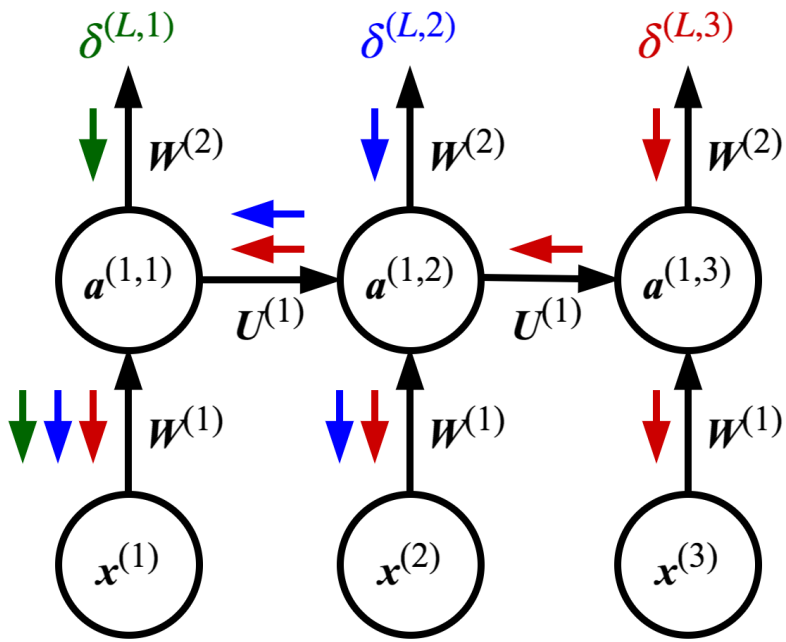
- ***BPTT***: single forward pass, ***multiple*** backward passes



Outline

Long-Term Dependencies

- Forward pass:

$$\boldsymbol{z}^{(k,t)} \leftarrow \boldsymbol{U}^{(k)\top} \boldsymbol{a}^{(k,t-1)} + \boldsymbol{W}^{(k)\top} \boldsymbol{a}^{(k-1,t)}$$

$$\boldsymbol{a}^{(k,t)} \leftarrow \mathrm{act}(\boldsymbol{z}^{(k,t)})$$

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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:

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

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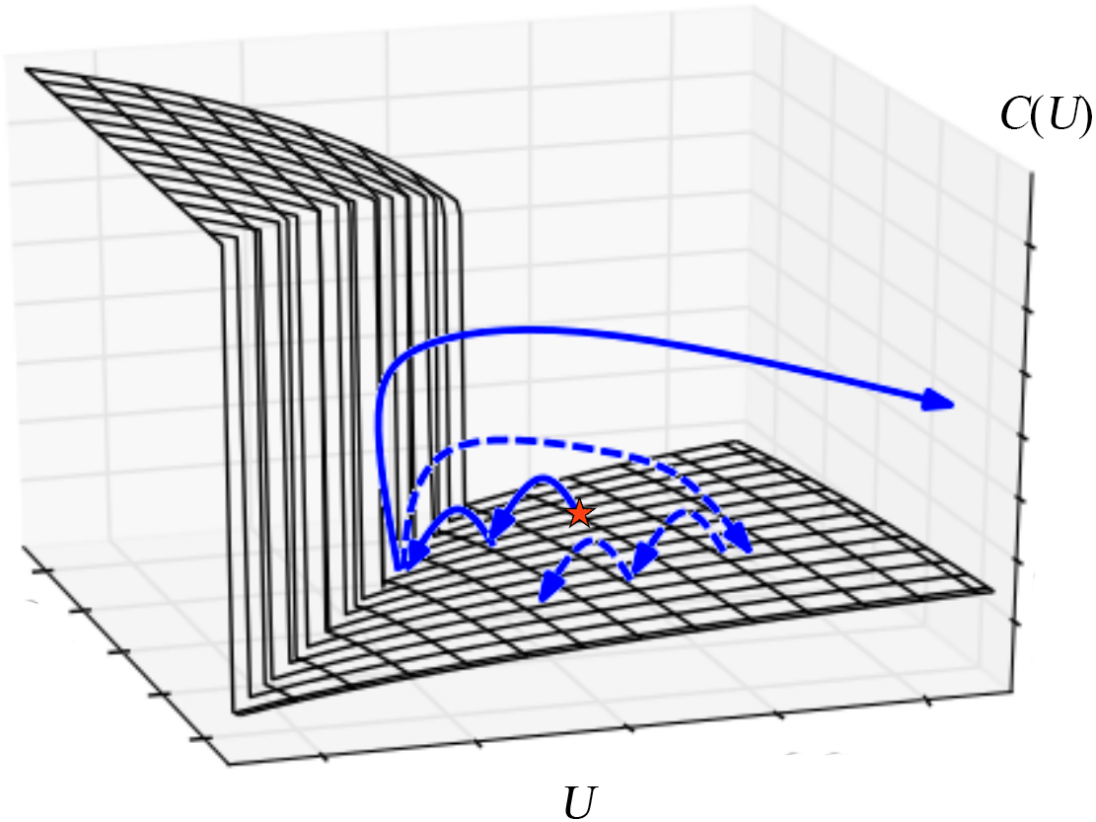
- Exploding or vanishing gradients!

Cost Surface

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



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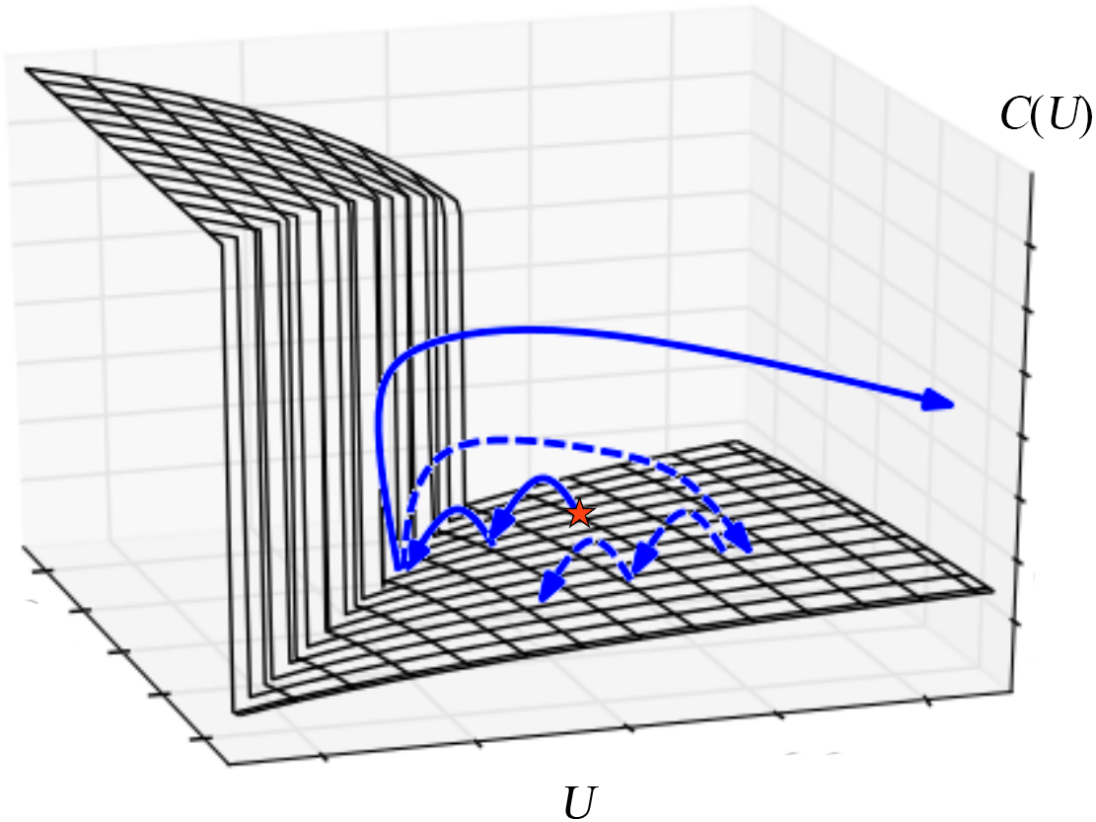
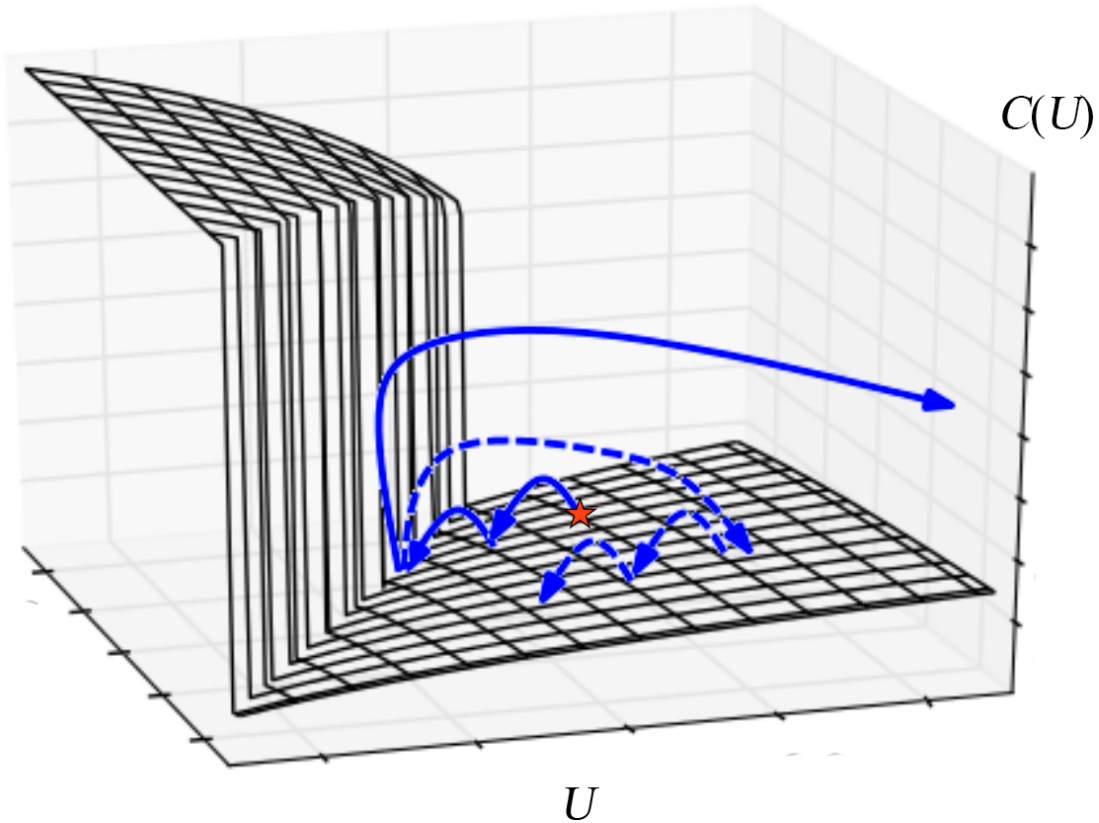
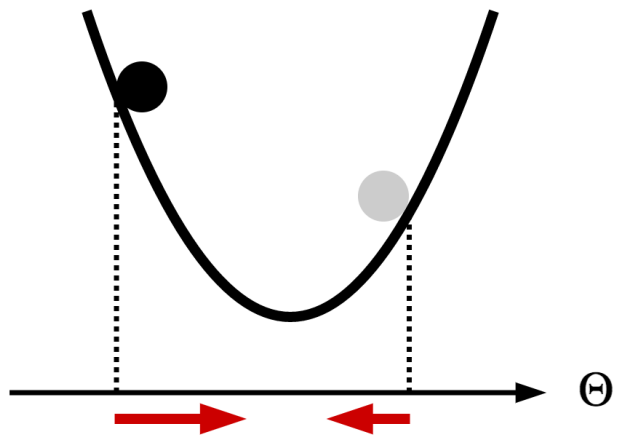


Nesterov Momentum

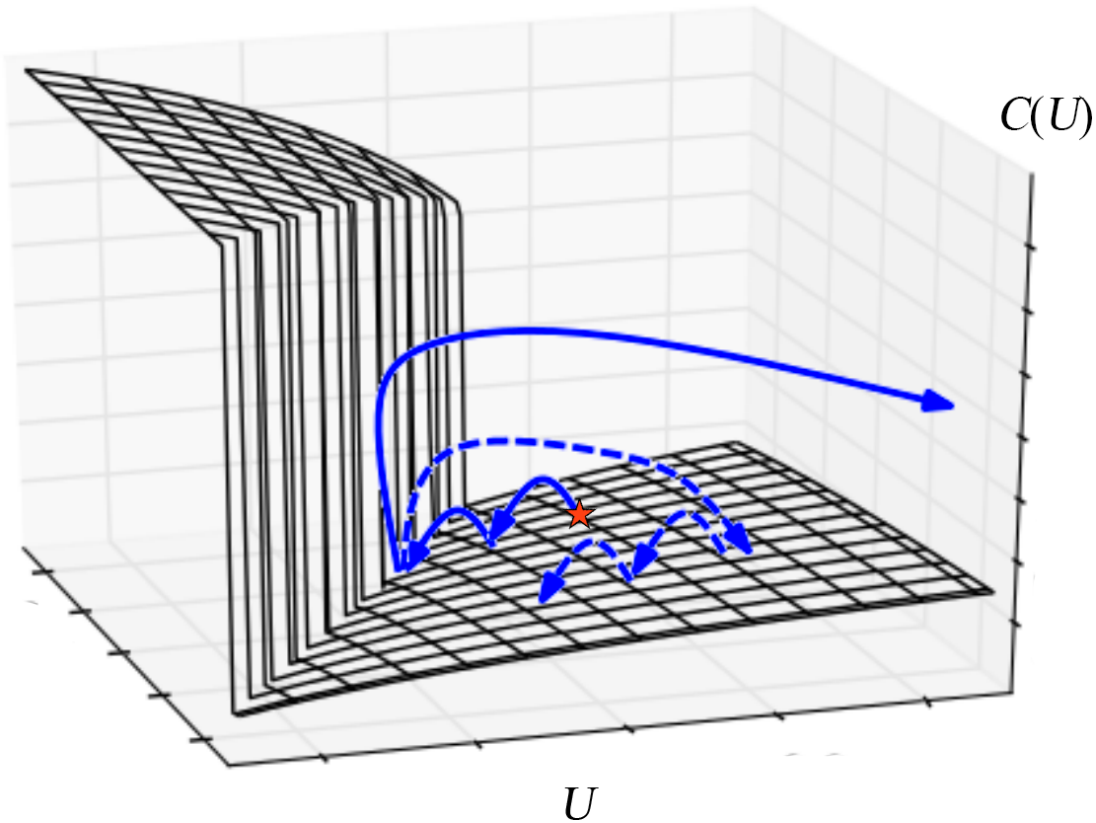
- Use Nesterov momentum to "brake" before hitting the wall





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:

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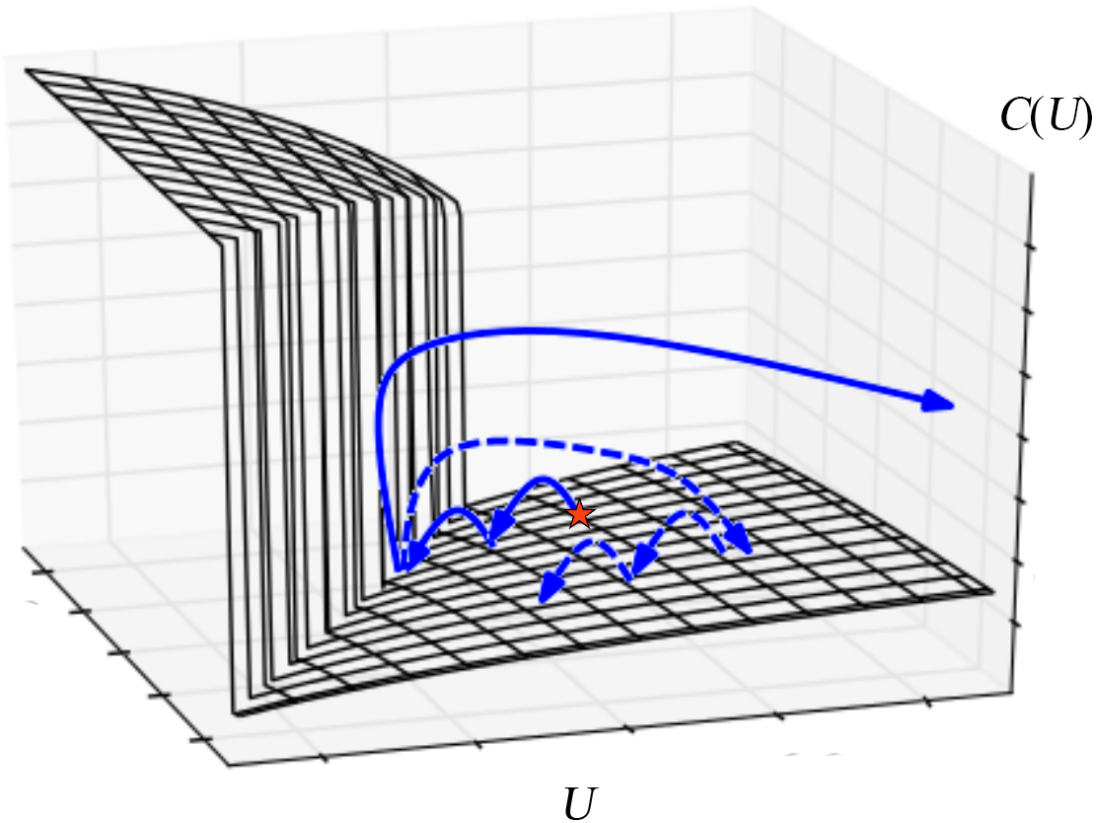

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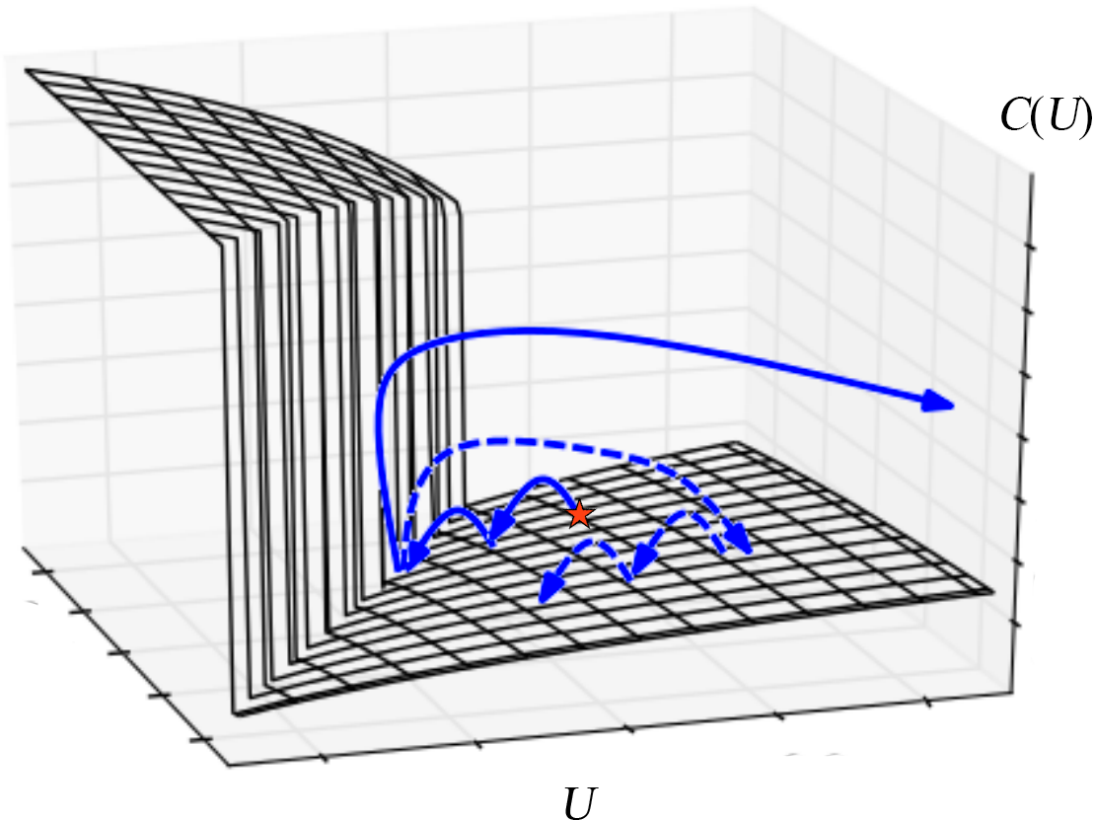
- Reduce λ



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- Sigmoid activation:
  - Bounded range in the forward pass
  - $\text{act}'(\cdot) < 1$ in the backward 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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  - Bounded range in the forward pass
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Sigmoid Activation Function

- Traditionally, the hidden units of RNNs use the sigmoid activation functions
  - E.g., $\tanh(\cdot)$ the ***hyperbolic tangent***
- Why sigmoid activation function?
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Learning Unitary $\boldsymbol{U}^{(k)}$'s

- Long-term dependency: $(\boldsymbol{U}^{(k)})^{j-i} = \boldsymbol{Q} \begin{bmatrix} \lambda_1^{j-i} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \lambda_{\boldsymbol{D}^{(k)}}^{j-i} \end{bmatrix} \boldsymbol{Q}^\top$

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- Bengio et al. [1] propose uRNN that learns unitary $\boldsymbol{U}^{(k)}$'s explicitly

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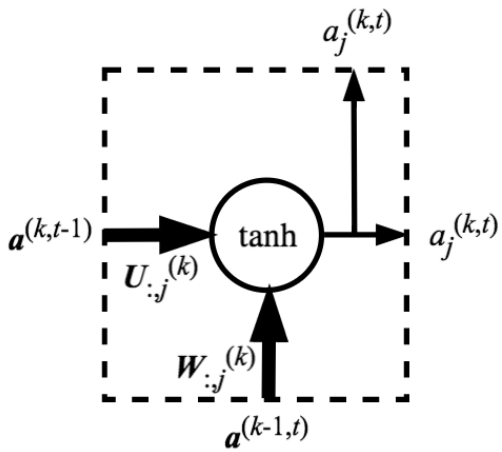

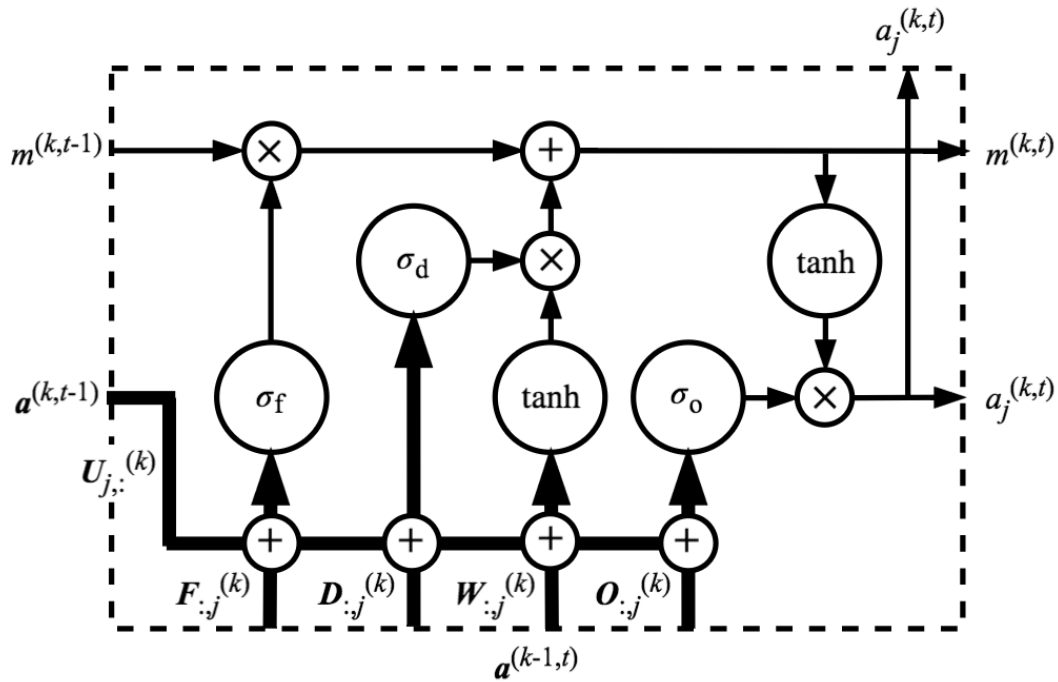

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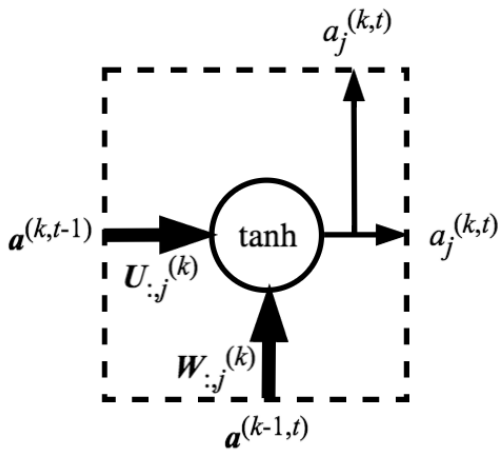

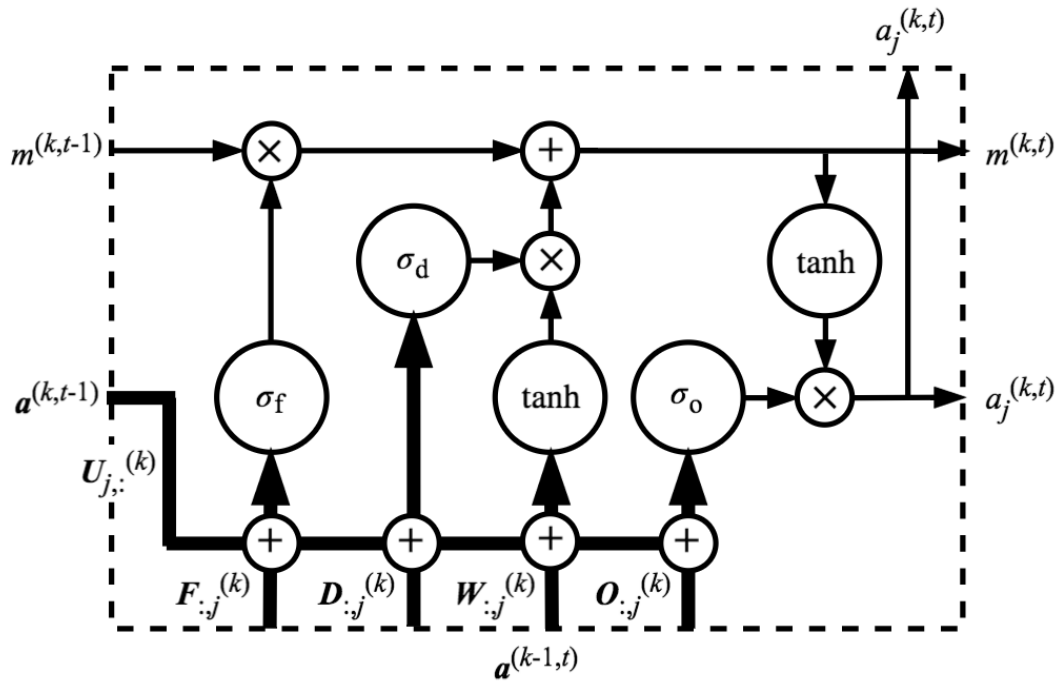

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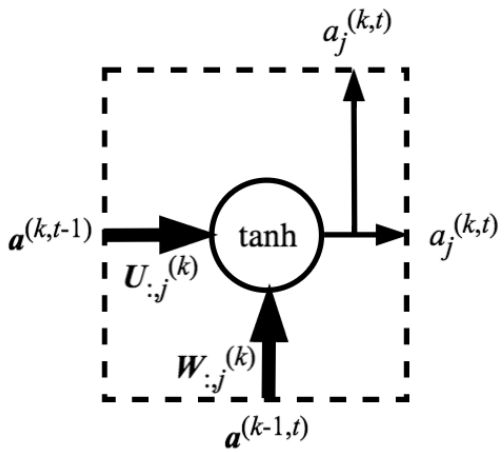

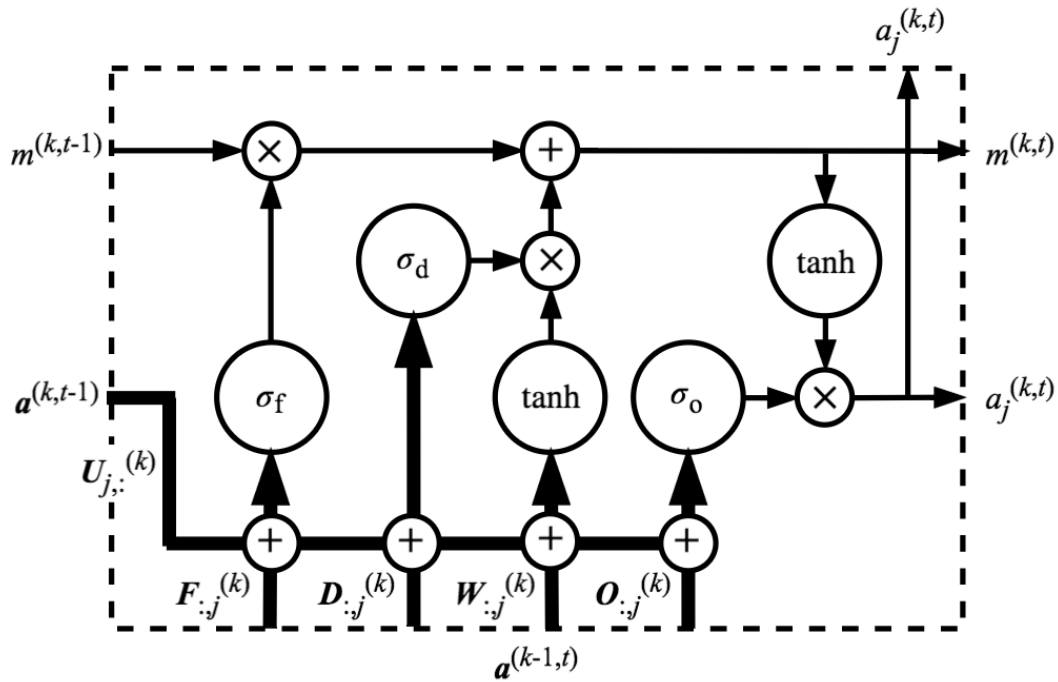

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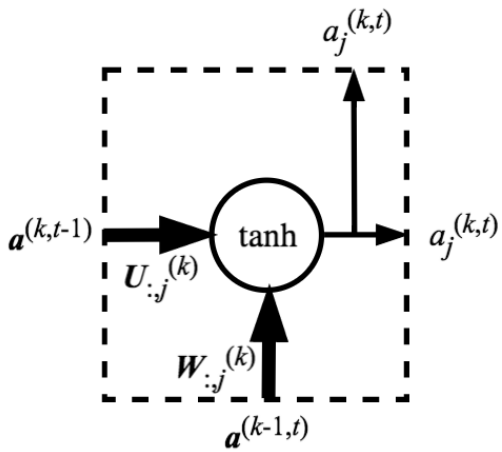

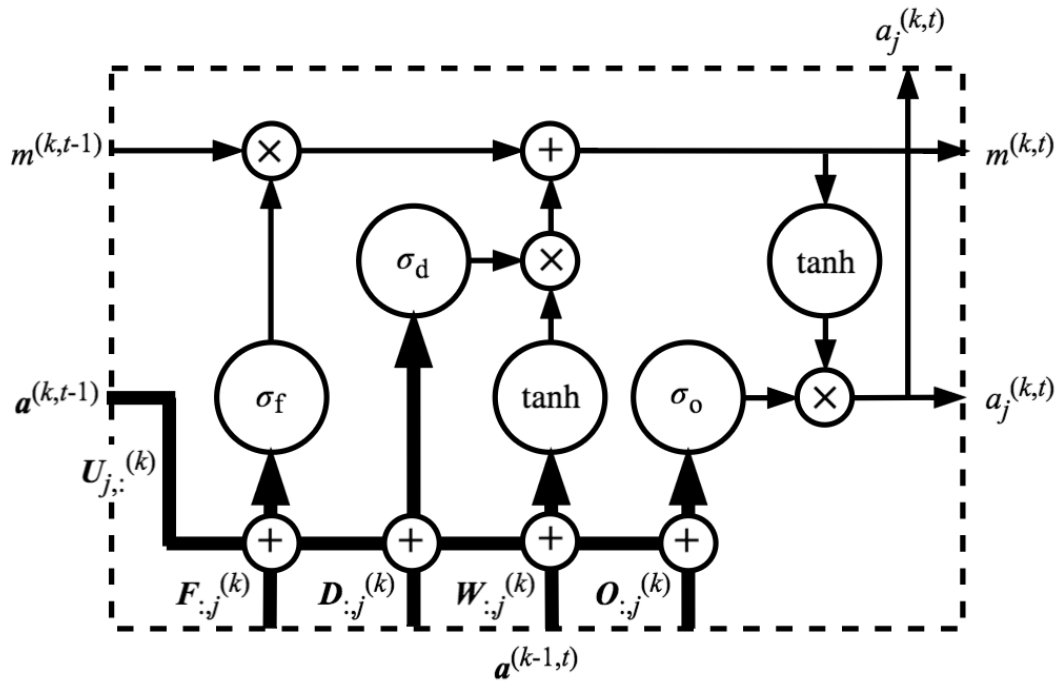

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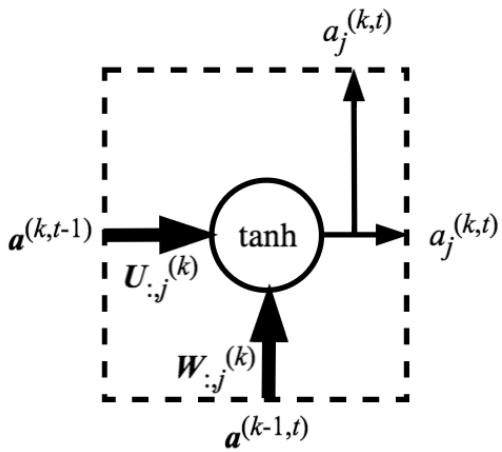
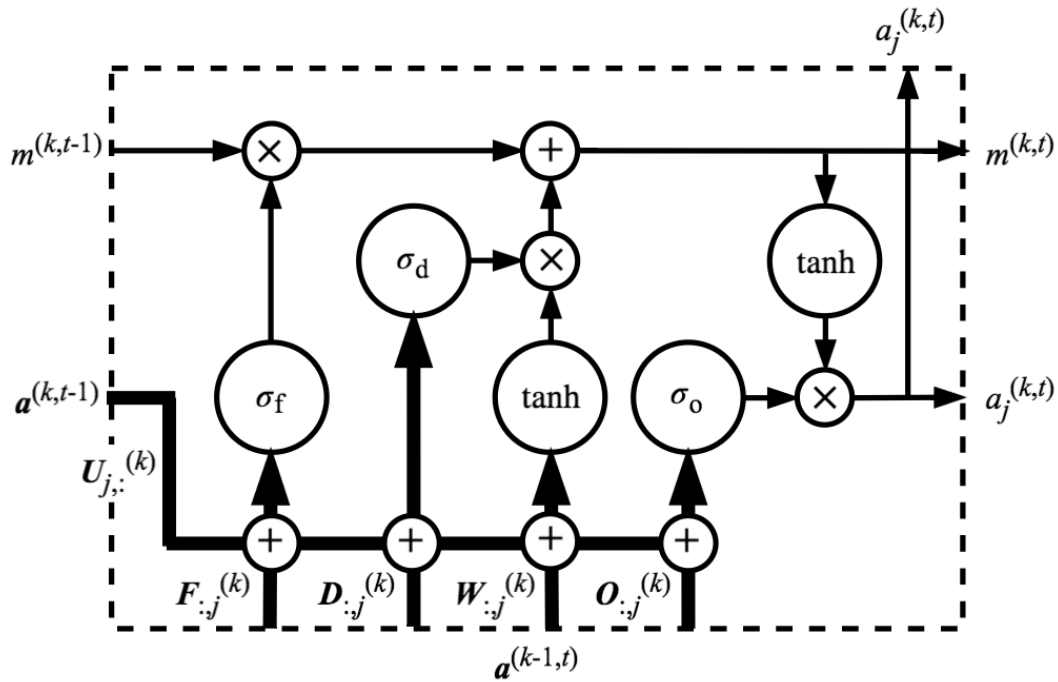
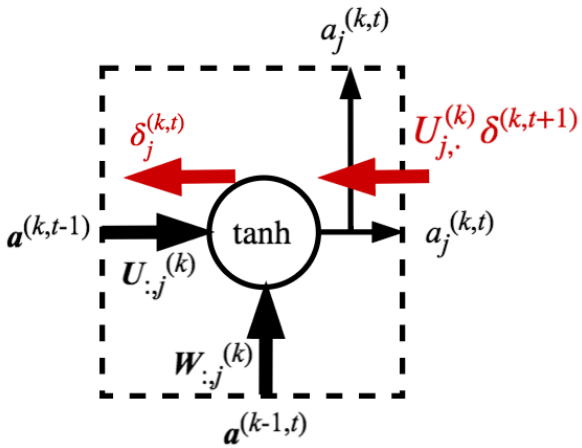
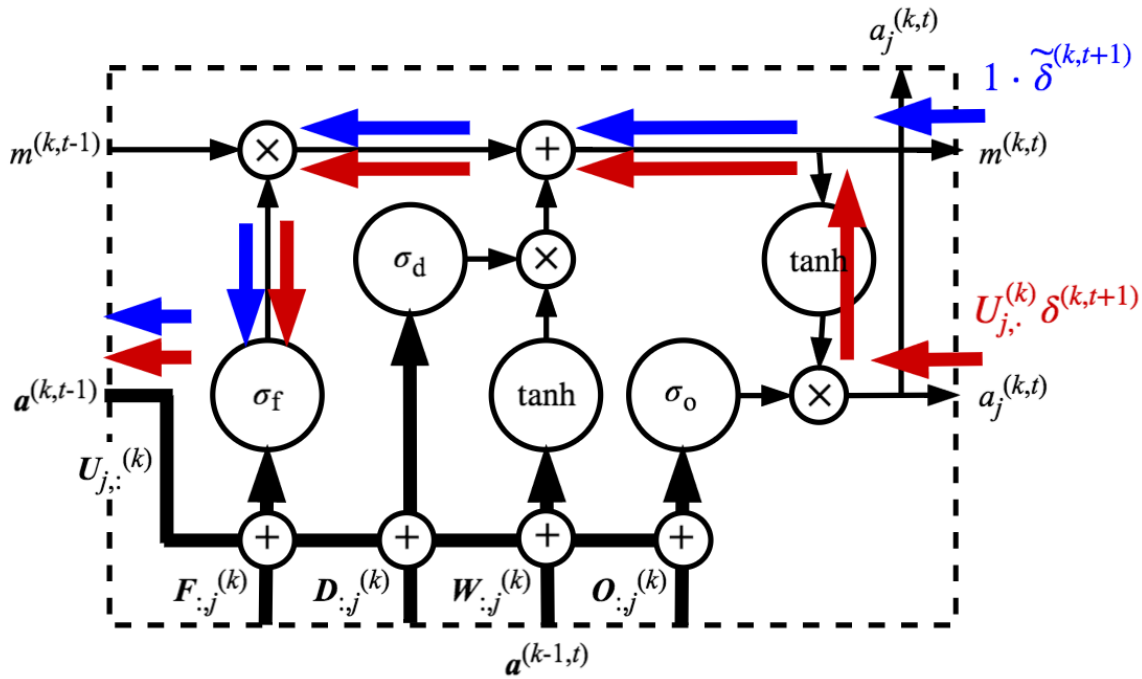




Error Signals

- Error signals now have a second path
  - If the forget gate is open, error signals won't decay (***blue arrows***)





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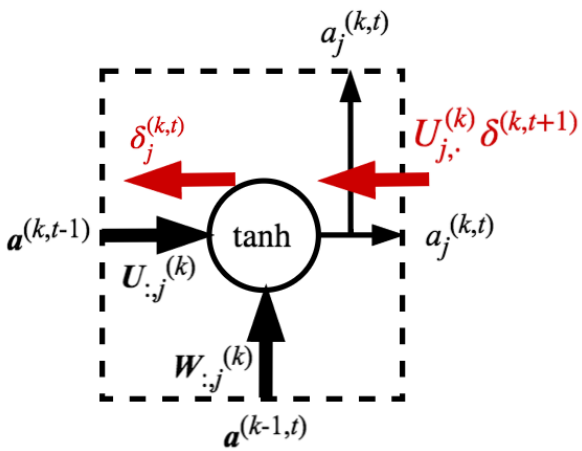

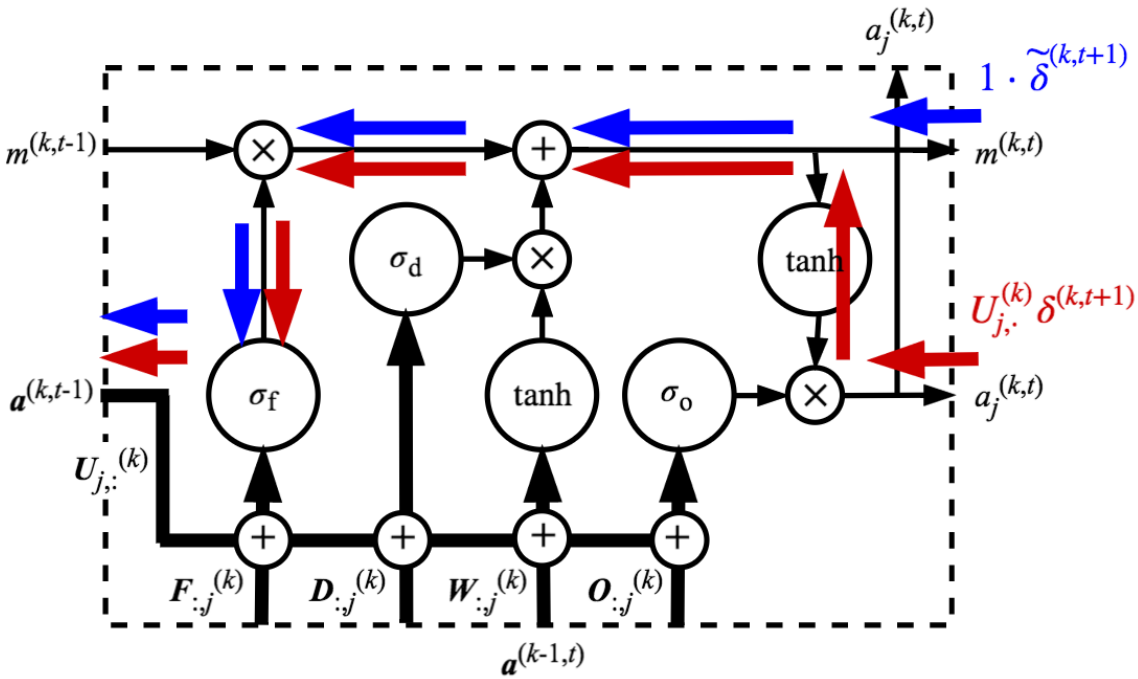

Error Signals

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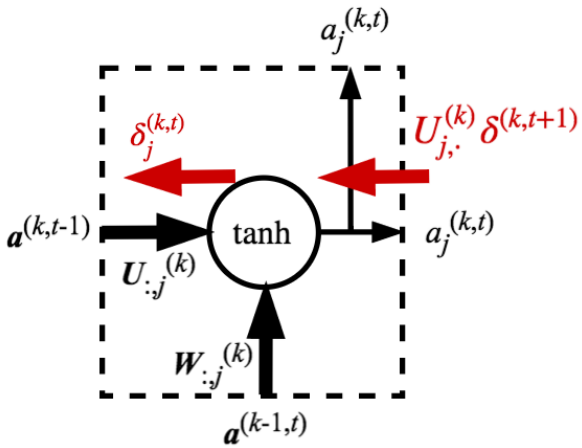
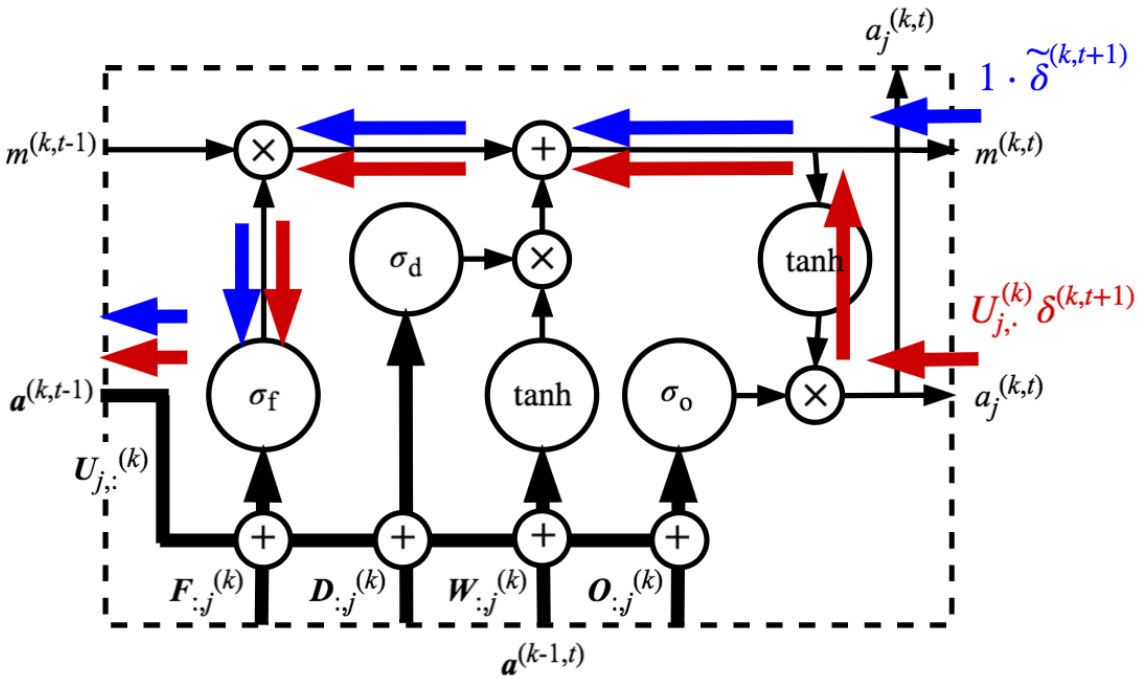
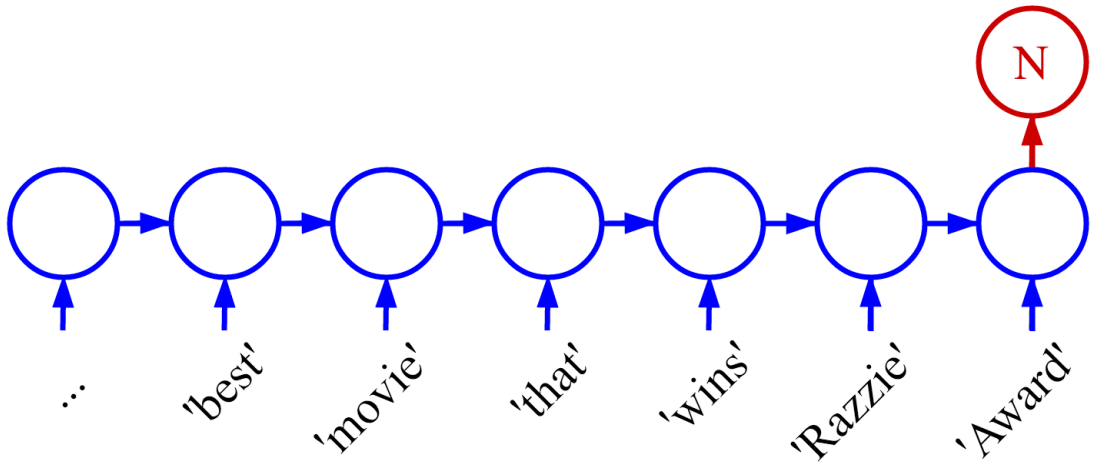
  - Avoids the vanishing gradients (but not exploding ones)
- When NN decides to close the forget gate, the vanishing gradient problem is irrelevant
- In practice, LSTM + gradient clipping works well together





Dynamic Representations for Sentiment Analysis



- LSTM units learn dynamic representations

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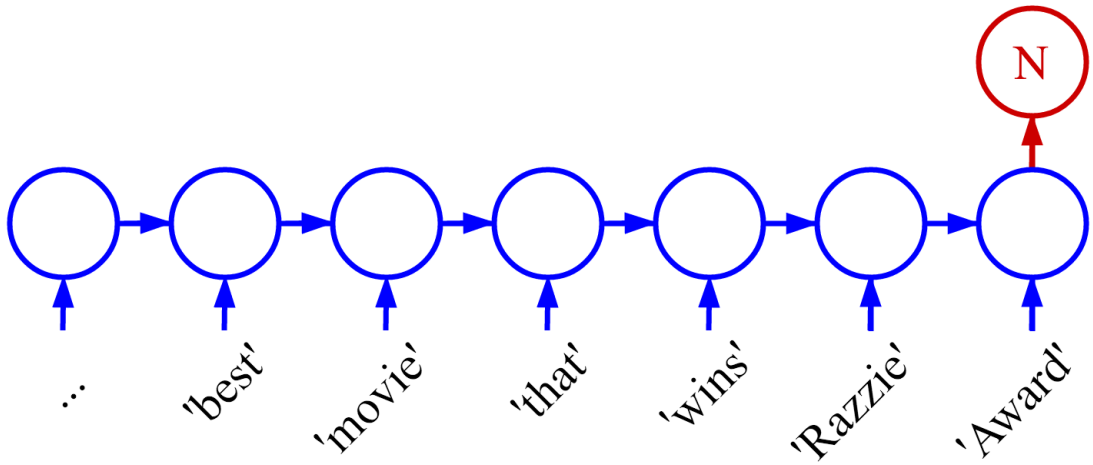

- LSTM units learn dynamic representations
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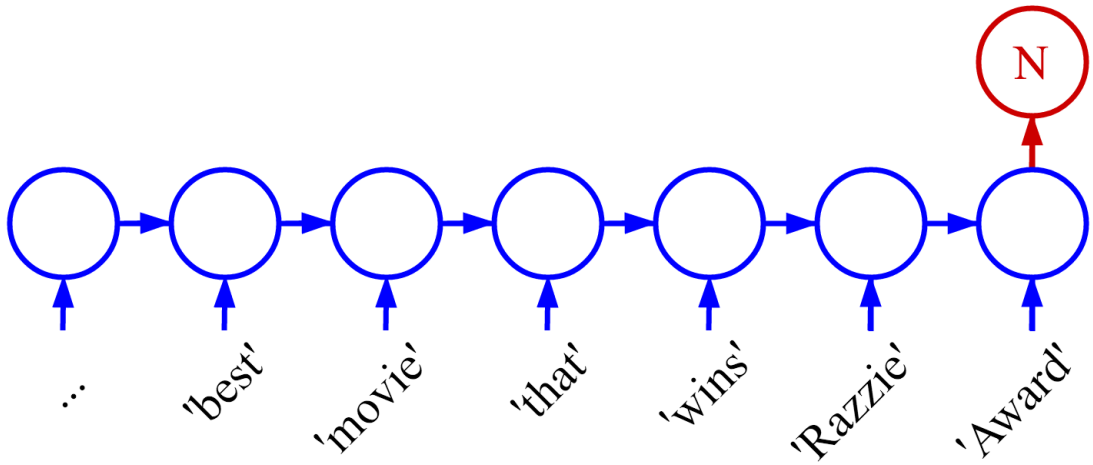

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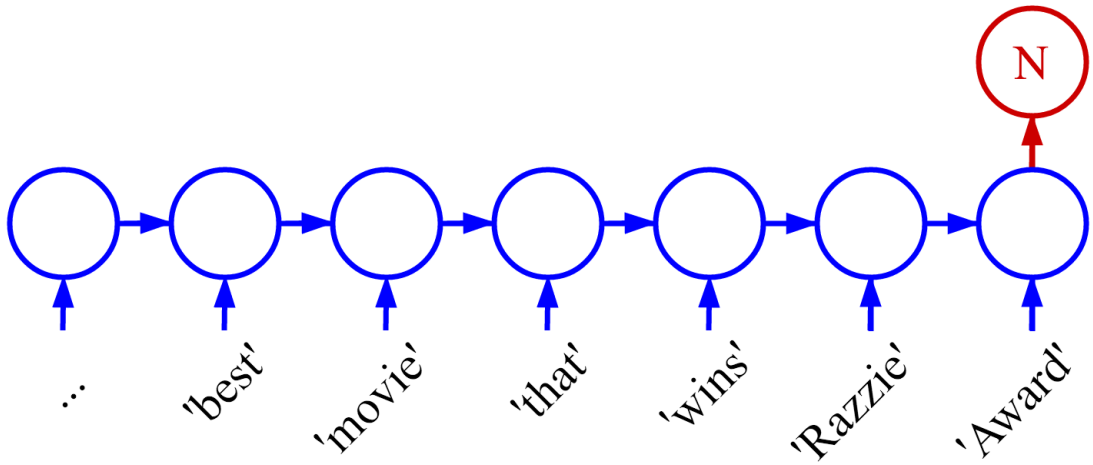

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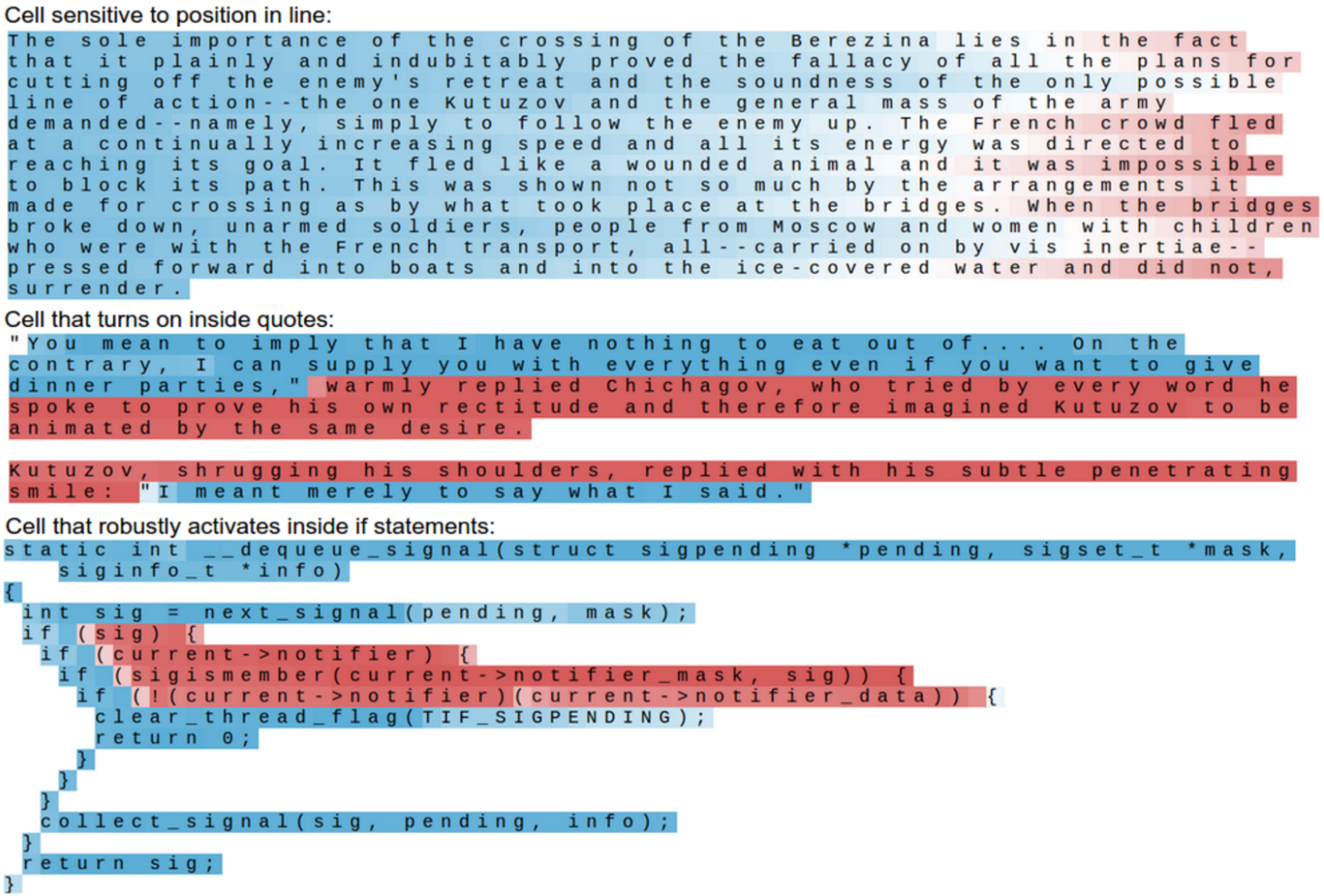
  - To correct previous summarization and/or shift focus
- Closing input gate for "movie"
  - Not to learn, to keep the same summarization
- Closing output gate for "that"
  - To let the next neuron decide the activation/gate values by its own

Dynamic Representations for Language Models

Dynamic Representations for Language Models

- Neuron activations for language modeling [3] ▸ Interactive Tool



Learning Process of LSTMs

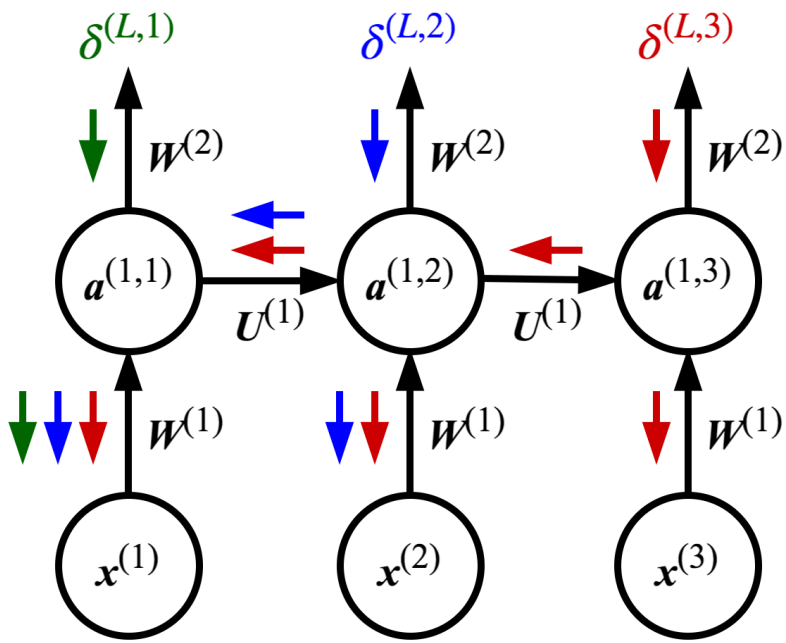
- Output at epoch 100:

  "*... tyntd-iafhatawiaoihrdemot lytdws e ,tfti, astai f ogoh*..."

Outline

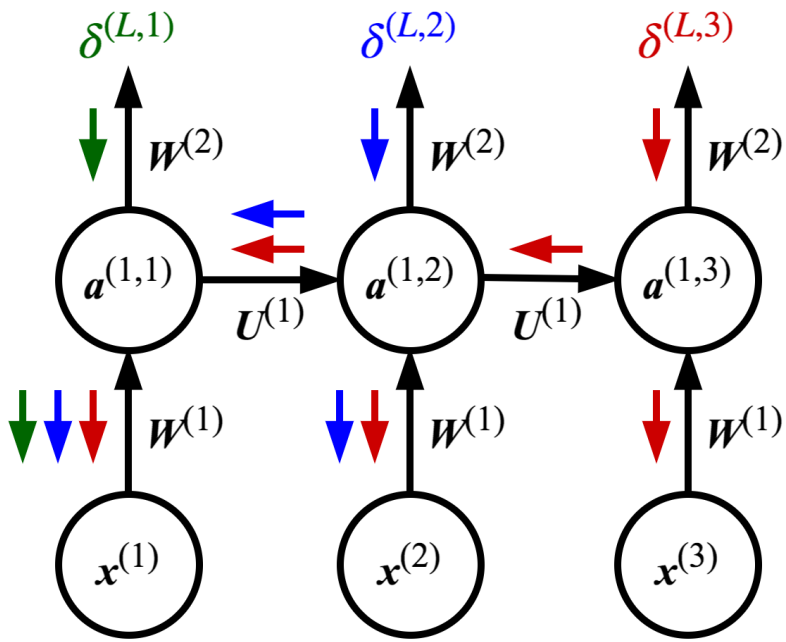
Parallelism

- A forward/backward pass through time in BPTT cannot be parallelized



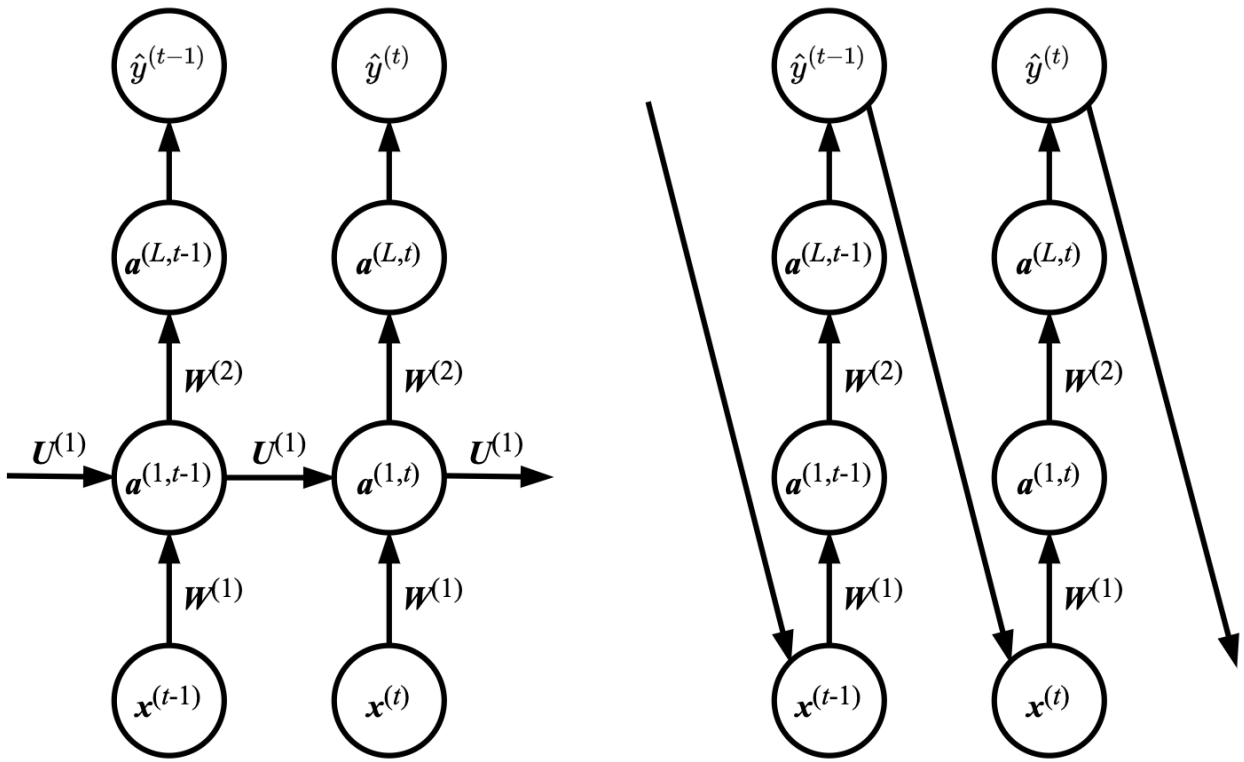
Parallelism

- A forward/backward pass through time in BPTT cannot be parallelized
- The ***hidden-to-hidden*** recurrent connections in a vanilla RNN create dependency between
  - $\boldsymbol{a}^{(k,t)}$'s in forward pass
  - $\delta^{(k,t)}$'s in backward pass



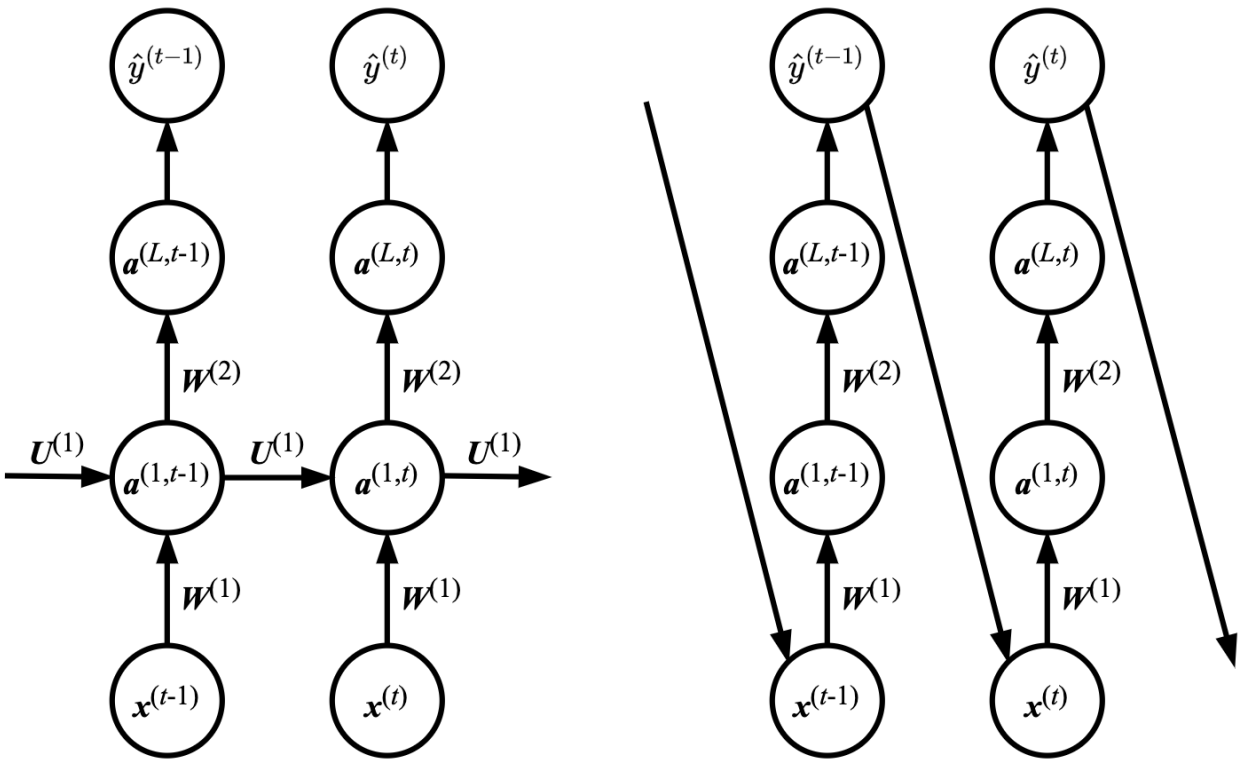
Output Recurrence and Teacher Forcing

- ***Teacher forcing***: replace hidden-to-hidden recurrence with output-to-hidden or output-to-input recurrence



Output Recurrence and Teacher Forcing

- ***Teacher forcing***: replace hidden-to-hidden recurrence with output-to-hidden or output-to-input recurrence
- At training time, use ***correct labels*** $\boldsymbol{y}^{(\cdot)}$'s to train the model
  - So, the forward/backward pass through time can be parallelized
- At test time, switch back to using model output $\hat{\boldsymbol{y}}^{(\cdot)}$'s



Exposure Bias

- Mismatch between $\boldsymbol{y}^{(\cdot)}$'s and $\hat{\boldsymbol{y}}^{(\cdot)}$'s hurts RNN performance
- Solution?

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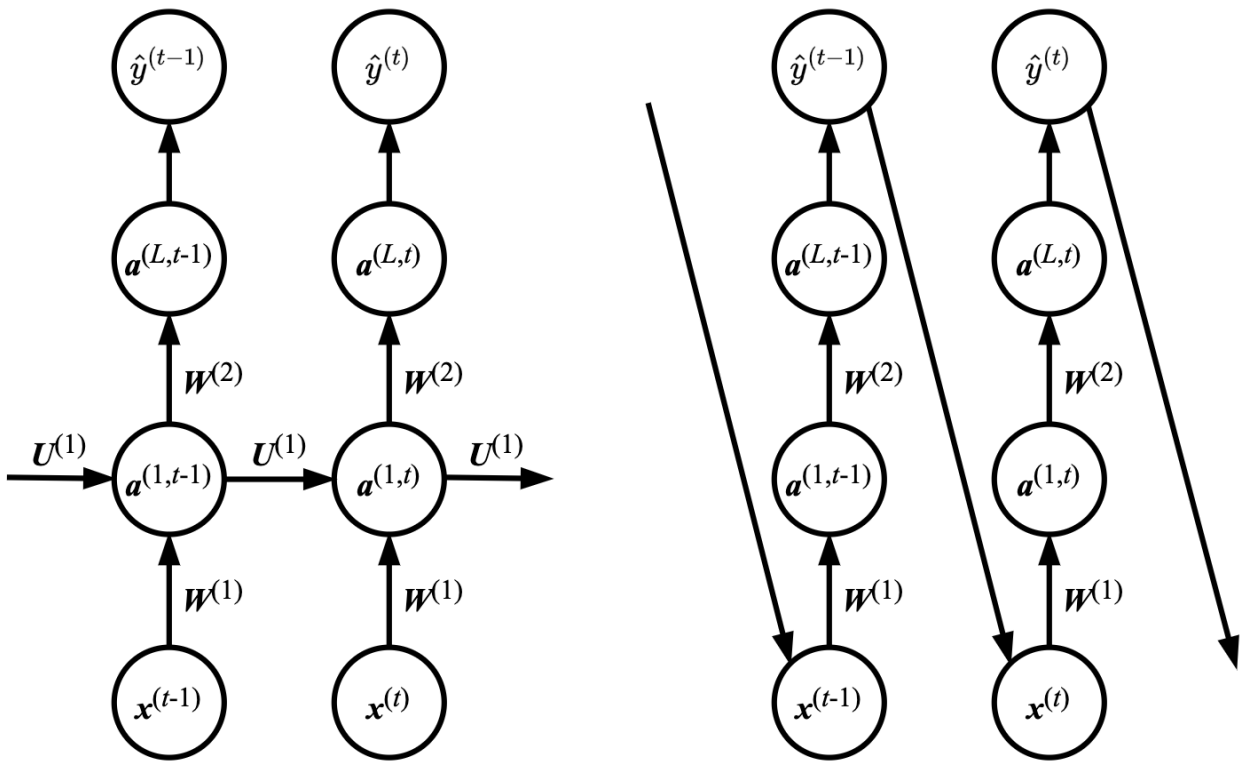
- Solution? Scheduled sampling
- At training time,
  1. Use $\boldsymbol{y}^{(\cdot)}$'s initially
  2. Gradually mix in $\hat{\boldsymbol{y}}^{(\cdot)}$'s later

Reduced Expressiveness

- The vanilla RNNs are universal in the sense that they can simulate Turing machines [6]



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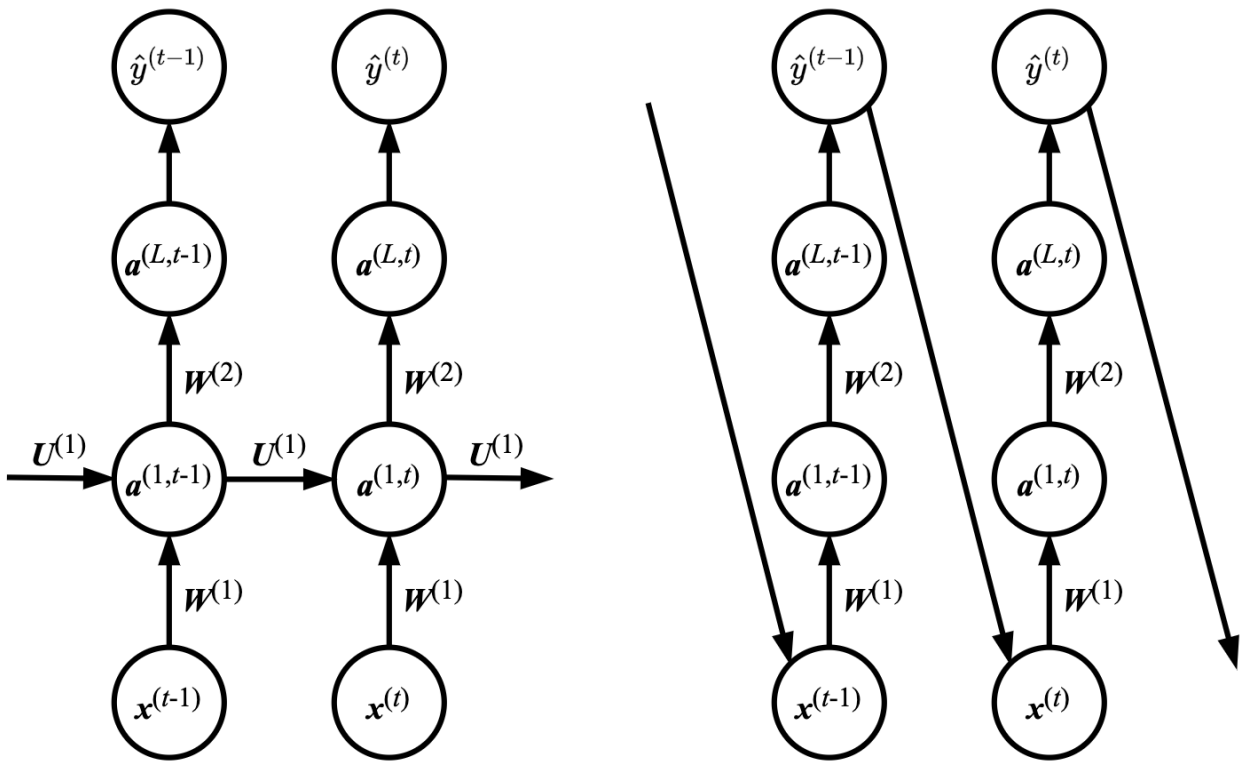

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- Output-recurrent RNNs ***cannot*** simulate Turing machines and are strictly less powerful
- The output $\boldsymbol{a}^{(L,\cdot)}$'s are explicitly trained to match training targets
  - Cannot capture all required information in the past to predict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