Recurrent Neural Network

Instructor: Seunghoon Hong

Course overview





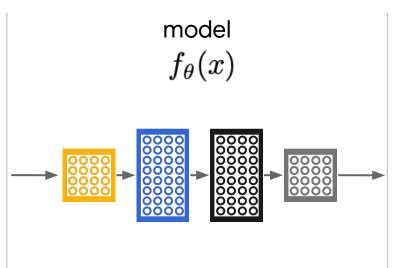
Learning to associate input to pre-defined, task-specific labels

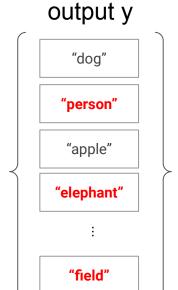
Input	Model (CNN)	Output
x ———	$f_{ heta}(x)$ —	\longrightarrow y

- Learning to associate input to pre-defined, task-specific labels
- Examples: classification





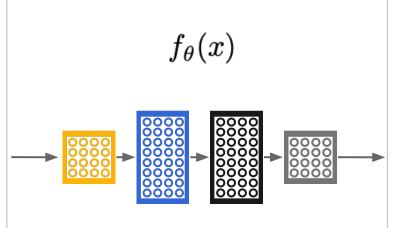




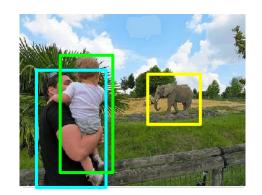
- Learning to associate input to pre-defined, task-specific labels
- Examples: detection

input x





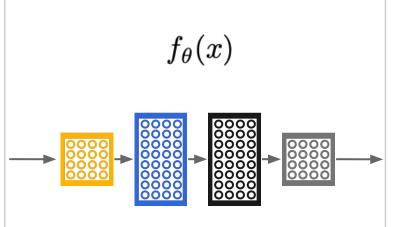
output y



- Learning to associate input to pre-defined, task-specific labels
- Examples: **pose estimation**

input x





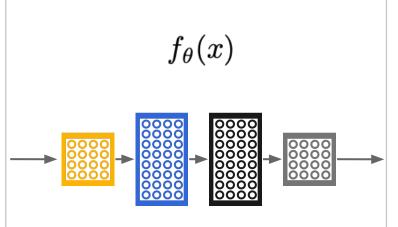
output y



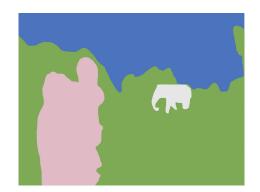
- Learning to associate input to pre-defined, task-specific labels
- Examples: **segmentation**

input x





output y



Modeling sequences

What if we want to deal with a **sequential** data?

Today's agenda

- RNN basics
- Backpropagation through time
- The vanishing/exploding gradients problem
- Advanced RNNs

Today's agenda

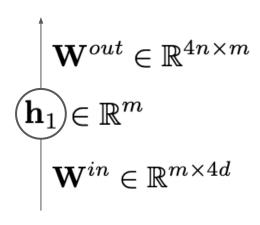
- RNN basics
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 $[\hat{\mathbf{y}}_1,\hat{\mathbf{y}}_2,\hat{\mathbf{y}}_3,\hat{\mathbf{y}}_4]$ Simple case: modeling a fixed-size sequence How do we design a neural network in this case? $[\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3,\mathbf{x}_4]$

Simple case: modeling a fixed-size sequence

Option 1: MLP

$$[\hat{\mathbf{y}}_1, \hat{\mathbf{y}}_2, \hat{\mathbf{y}}_3, \hat{\mathbf{y}}_4]$$



$$[\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3,\mathbf{x}_4]$$

Simple case: modeling a fixed-size sequence

- Option 1: MLP
- What if we change the sequence length?
 - We cannot reuse the same network for handling sequences in different length!
 - It is because the network parameter bounds the length of the sequences!

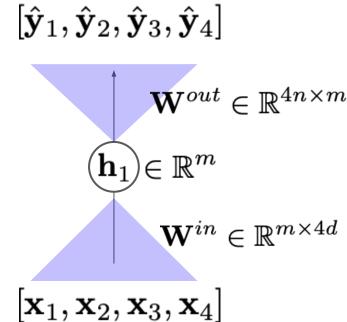
$$[\hat{\mathbf{y}}_1, \hat{\mathbf{y}}_2, \hat{\mathbf{y}}_3, \hat{\mathbf{y}}_4, \hat{\mathbf{y}}_5]$$
 $\mathbf{W}^{out} \in \mathbb{R}^{4n \times n}$
 $(\mathbf{h}_1) \in \mathbb{R}^m$
 $\mathbf{W}^{in} \in \mathbb{R}^{m \times 4d}$

$$[\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3,\mathbf{x}_4,\mathbf{x}_5]$$

where $\mathbf{x}_t \in \mathbb{R}^d, \mathbf{h}_t \in \mathbb{R}^m, \mathbf{y}_t \in \mathbb{R}^{n_{13}}$

Simple case: modeling a fixed-size sequence

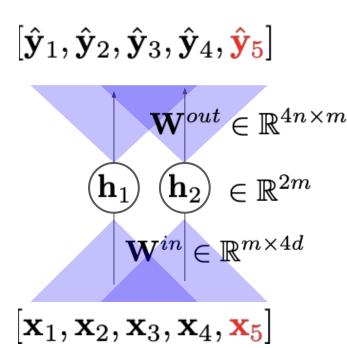
Option 2: CNN



where $\mathbf{x}_t \in \mathbb{R}^d$, $\mathbf{h}_t \in \mathbb{R}^m$, $\mathbf{y}_t \in \mathbb{R}^{n_{14}}$

Simple case: modeling a fixed-size sequence

- Option 2: CNN
- What if we change the sequence length?
 - We can reuse the same network by sliding convolution filters over the sequence
- Problems?
 - The hidden representation grows with the length of the sequence!
 - The receptive field is fixed!



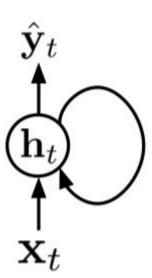
where $\mathbf{x}_t \in \mathbb{R}^d$, $\mathbf{h}_t \in \mathbb{R}^m$, $\mathbf{y}_t \in \mathbb{R}^{n_{15}}$

Modeling sequences efficiently

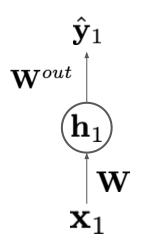
How can we model sequences in an efficient way?

Use recursion!

- A model that reads each input one at a time
- Parameters can simply be reused (or shared) for each input in a recurrent computation



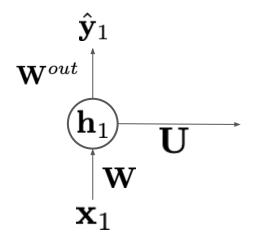
Unrolling RNNs through time



$$\mathbf{h}_1 = \sigma(\mathbf{W}\mathbf{x}_1 + \mathbf{b})$$

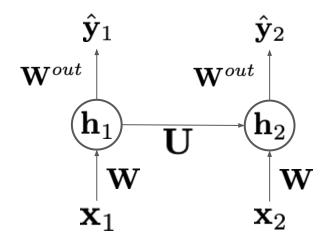
 $\hat{\mathbf{y}}_1 = \mathbf{W}^{out}\mathbf{h}_1$

Unrolling RNNs through time



$$\mathbf{h}_1 = \sigma(\mathbf{W}\mathbf{x}_1 + \mathbf{b})$$
$$\hat{\mathbf{y}}_1 = \mathbf{W}^{out}\mathbf{h}_1$$

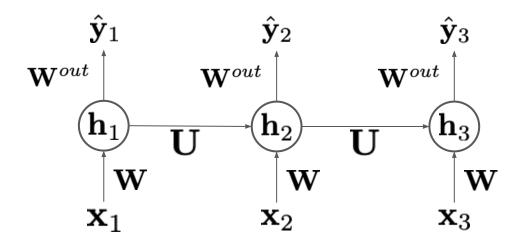
Unrolling RNNs through time



$$\mathbf{h}_1 = \sigma(\mathbf{W}\mathbf{x}_1 + \mathbf{b})$$
 $\hat{\mathbf{y}}_1 = \mathbf{W}^{out}\mathbf{h}_1$
 $\mathbf{h}_2 = \sigma(\mathbf{U}\mathbf{h}_1 + \mathbf{W}\mathbf{x}_2 + \mathbf{b})$
 $\hat{\mathbf{y}}_2 = \mathbf{W}^{out}\mathbf{h}_2$

We have a temporal connection that models a temporal dependency!

Unrolling RNNs through time

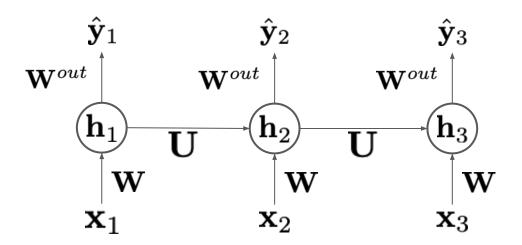


$$\mathbf{h}_1 = \sigma(\mathbf{W}\mathbf{x}_1 + \mathbf{b})$$

 $\hat{\mathbf{y}}_1 = \mathbf{W}^{out}\mathbf{h}_1$
 $\mathbf{h}_2 = \sigma(\mathbf{U}\mathbf{h}_1 + \mathbf{W}\mathbf{x}_2 + \mathbf{b})$
 $\hat{\mathbf{y}}_2 = \mathbf{W}^{out}\mathbf{h}_2$
 $\mathbf{h}_3 = \sigma(\mathbf{U}\mathbf{h}_2 + \mathbf{W}\mathbf{x}_3 + \mathbf{b})$

 $\hat{\mathbf{y}}_3 = \mathbf{W}^{out} \mathbf{h}_3$

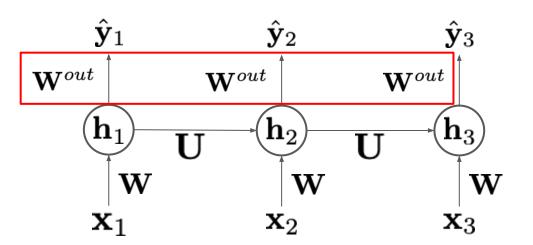
Unrolling RNNs through time



In general, for any
$$t \ge 1$$
,
 $\mathbf{h}_t = \sigma(\mathbf{U}\mathbf{h}_{t-1} + \mathbf{W}\mathbf{x}_t + \mathbf{b})$
 $\hat{\mathbf{y}}_t = \mathbf{W}^{out}\mathbf{h}_t$

 $h_0 = 0$

Unrolling RNNs through time

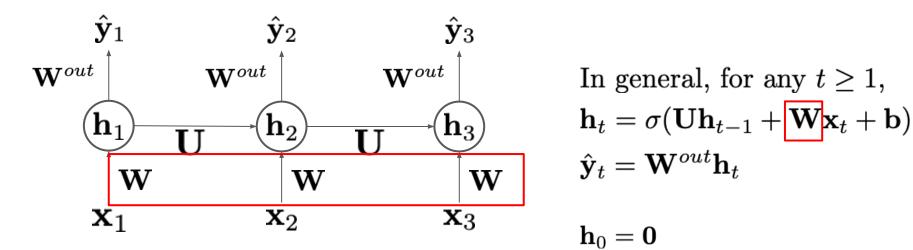


In general, for any $t \ge 1$, $\mathbf{h}_t = \sigma(\mathbf{U}\mathbf{h}_{t-1} + \mathbf{W}\mathbf{x}_t + \mathbf{b})$ $\hat{\mathbf{y}}_t = \mathbf{W}^{out}\mathbf{h}_t$

$$\mathbf{h}_0 = \mathbf{0}$$

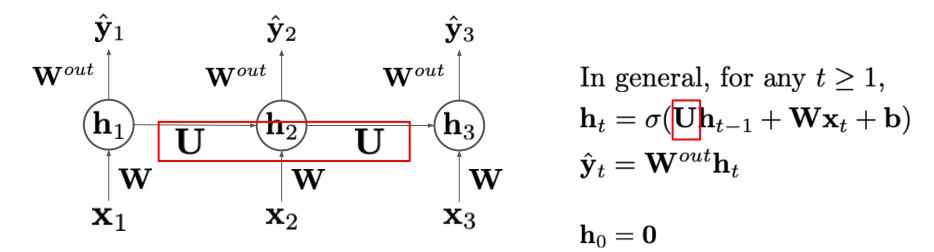
Weights are shared over time!

Unrolling RNNs through time



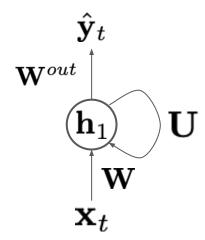
Weights are shared over time!

Unrolling RNNs through time



Weights are shared over time!

Unrolling RNNs through time



In general, for any
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$$\mathbf{h}_t = \sigma(\mathbf{U}\mathbf{h}_{t-1} + \mathbf{W}\mathbf{x}_t + \mathbf{b})$$

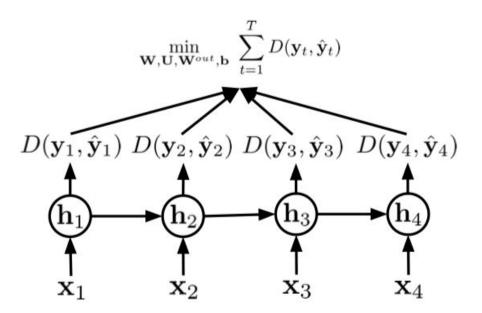
$$\hat{\mathbf{y}}_t = \mathbf{W}^{out}\mathbf{h}_t$$

Quiz: size of weights? $(\mathbf{x}_t \in \mathbb{R}^d, \mathbf{h}_t \in \mathbb{R}^m, \mathbf{y}_t \in \mathbb{R}^n)$

$$\mathbf{W} = \mathbb{R}^{m \times d} \quad \mathbf{U} = \mathbb{R}^{m \times m} \quad \mathbf{W}^{out} = \mathbb{R}^{n \times m}$$

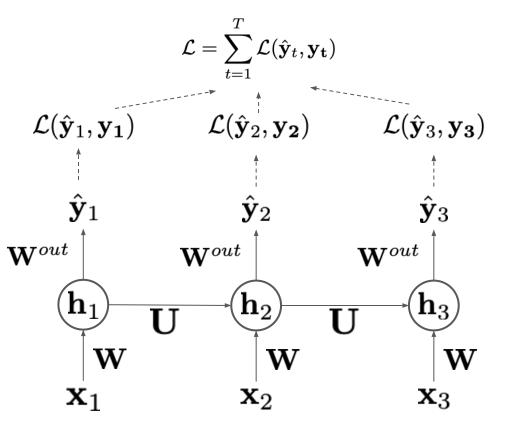
Loss computation

- Compute loss (if any) for each step and aggregate
- Gradient flows through all unrolled steps in RNN



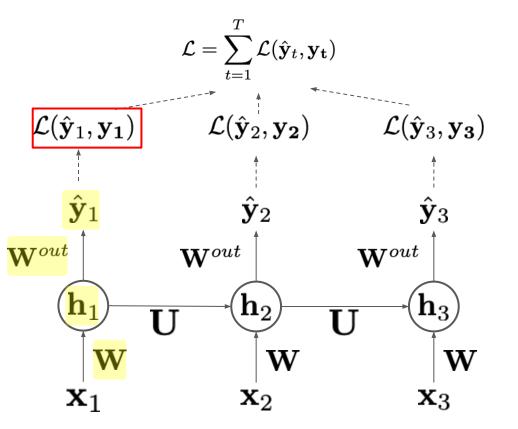
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Forward propagation

$$\mathbf{h}_t = \sigma(\mathbf{U}\mathbf{h}_{t-1} + \mathbf{W}\mathbf{x}_t + \mathbf{b})$$
$$\hat{\mathbf{v}}_t = \mathbf{W}^{out}\mathbf{h}_t$$



Forward propagation

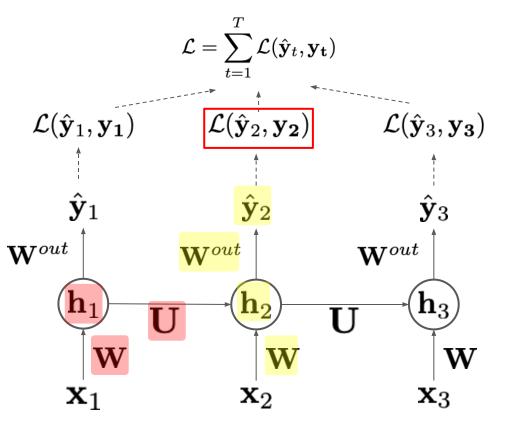
$$\mathbf{h}_t = \sigma(\mathbf{U}\mathbf{h}_{t-1} + \mathbf{W}\mathbf{x}_t + \mathbf{b})$$

 $\hat{\mathbf{y}}_t = \mathbf{W}^{out}\mathbf{h}_t$

Before we derive gradients, let's think about how the gradient would flow

If we want to reduce $\mathcal{L}(\hat{\mathbf{y}}_1, \mathbf{y_1})$, which variables should we update?

$$\hat{\mathbf{y}}_1, \mathbf{W}^{out}, \mathbf{h}_1, \mathbf{W}$$



Forward propagation

$$\mathbf{h}_t = \sigma(\mathbf{U}\mathbf{h}_{t-1} + \mathbf{W}\mathbf{x}_t + \mathbf{b})$$

 $\hat{\mathbf{y}}_t = \mathbf{W}^{out}\mathbf{h}_t$

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$$\hat{\mathbf{y}}_1, \mathbf{W}^{out}, \mathbf{h}_1, \mathbf{W}$$

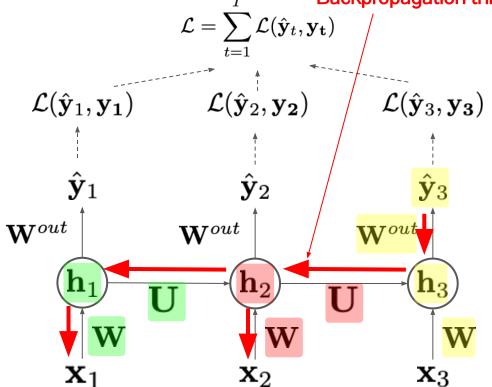
If we want to reduce $\mathcal{L}(\hat{\mathbf{y}}_2, \mathbf{y_2})$, which variables should we update?

$$\hat{\mathbf{y}}_2, \mathbf{W}^{out}, \mathbf{h}_2, \mathbf{W}, \mathbf{U}, \mathbf{h}_1, \mathbf{W}$$

These contribute to the value of h₂

Forward propagation $\mathbf{h}_t = \sigma(\mathbf{U}\mathbf{h}_{t-1} + \mathbf{W}\mathbf{x}_t + \mathbf{b})$ $\hat{\mathbf{y}}_t = \mathbf{W}^{out}\mathbf{h}_t$





Before we derive gradients, let's think about how the gradient would flow

If we want to reduce $\mathcal{L}(\hat{\mathbf{y}}_1,\mathbf{y_1})$, which

variables should we update? $\hat{\mathbf{y}}_1, \mathbf{W}^{out}, \mathbf{h}_1, \mathbf{W}$

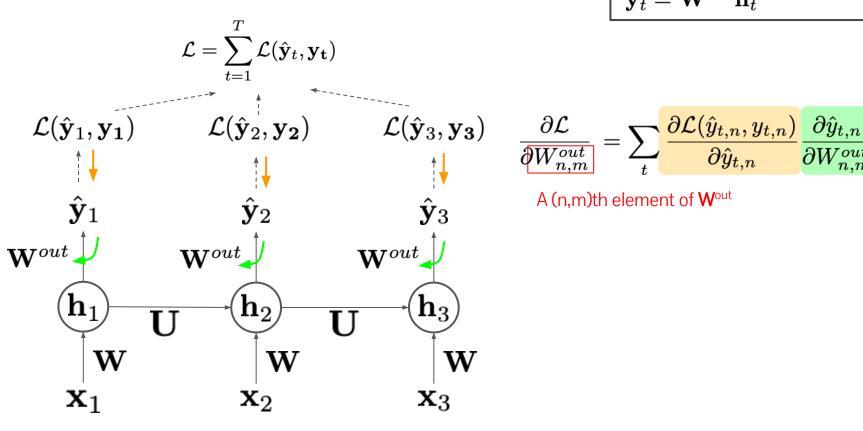
If we want to reduce $\mathcal{L}(\hat{\mathbf{y}}_2, \mathbf{y_2})$, which variables should we update?

 $\hat{\mathbf{y}}_2, \mathbf{W}^{out}, \mathbf{h}_2, \mathbf{W}, \mathbf{U}, \mathbf{h}_1, \mathbf{W}$

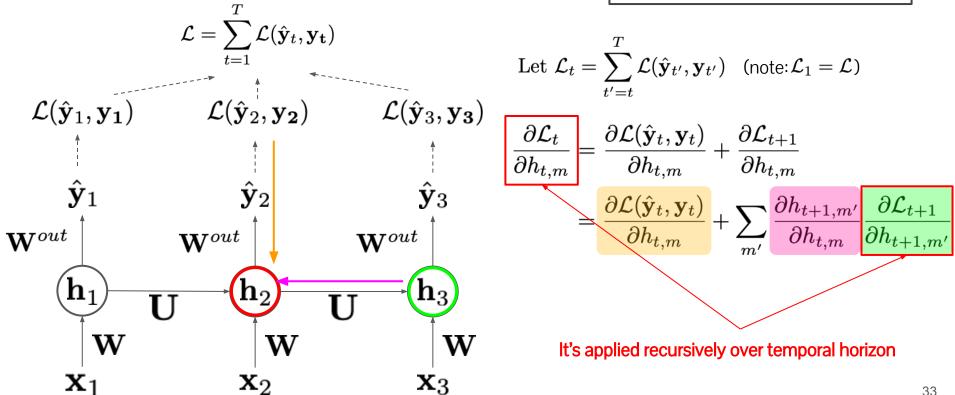
If we want to reduce $\mathcal{L}(\hat{\mathbf{y}}_3, \mathbf{y_3})$, which variables should we update?

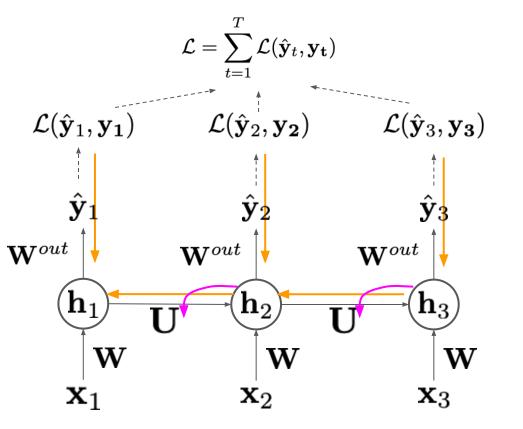
 $\hat{\mathbf{y}}_3, \mathbf{W}^{out}, \mathbf{h}_3, \mathbf{W}, \mathbf{U}, \mathbf{h}_2, \mathbf{W}, \mathbf{U}, \mathbf{h}_1, \mathbf{W}$

Forward propagation $\mathbf{h}_t = \sigma(\mathbf{U}\mathbf{h}_{t-1} + \mathbf{W}\mathbf{x}_t + \mathbf{b})$



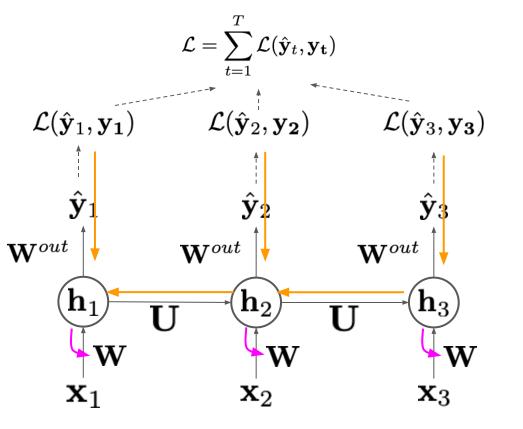
Forward propagation $\mathbf{h}_t = \sigma(\mathbf{U}\mathbf{h}_{t-1} + \mathbf{W}\mathbf{x}_t + \mathbf{b})$ $\hat{\mathbf{y}}_t = \mathbf{W}^{out} \mathbf{h}_t$





Forward propagation $\mathbf{h}_t = \sigma(\mathbf{U}\mathbf{h}_{t-1} + \mathbf{W}\mathbf{x}_t + \mathbf{b})$ $\hat{\mathbf{y}}_t = \mathbf{W}^{out}\mathbf{h}_t$ $\mathcal{L}_t = \sum_{t=1}^T \mathcal{L}(\hat{\mathbf{y}}_{t'}, \mathbf{y}_{t'})$

$$rac{\partial \mathcal{L}}{\partial U_{m,m'}} = \sum_t rac{\partial \mathcal{L}_t}{\partial h_{t,m}} rac{\partial h_{t,m}}{\partial U_{m,m'}}$$



Forward propagation $\mathbf{h}_t = \sigma(\mathbf{U}\mathbf{h}_{t-1} + \mathbf{W}\mathbf{x}_t + \mathbf{b})$ $\hat{\mathbf{y}}_t = \mathbf{W}^{out}\mathbf{h}_t$ $\mathcal{L}_t = \sum_{t=1}^T \mathcal{L}(\hat{\mathbf{y}}_{t'}, \mathbf{y}_{t'})$

$$rac{\partial \mathcal{L}}{\partial W_{m,d}} = \sum_t rac{\partial \mathcal{L}_t}{\partial h_{t,m}} rac{\partial h_{t,m}}{\partial W_{m,d}}$$

$$\mathbf{h}_t = \sigma(\mathbf{U}\mathbf{h}_{t-1} + \mathbf{W}\mathbf{x}_t + \mathbf{b})$$

$$\hat{\mathbf{y}}_t = \mathbf{W}^{out}\mathbf{h}_t$$

$$\mathcal{L}_t = \sum_{t'=t}^T \mathcal{L}(\hat{\mathbf{y}}_{t'}, \mathbf{y}_{t'})$$
Putting all together:

Forward propagation

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

 $\hat{\mathbf{y}}_1$ $\hat{\mathbf{y}}_2$ $\hat{\mathbf{y}}_3$ \mathbf{w}_{out}

 $\mathcal{L}(\hat{\mathbf{y}}_1, \mathbf{y_1})$ $\mathcal{L}(\hat{\mathbf{y}}_2, \mathbf{y_2})$ $\mathcal{L}(\hat{\mathbf{y}}_3, \mathbf{y_3})$

 $\frac{\partial \mathcal{L}}{\partial W_{n,m}^{out}} = \sum_{t} \frac{\partial \mathcal{L}(\hat{y}_{t,n}, y_{t,n})}{\partial \hat{y}_{t,n}} \frac{\partial \hat{y}_{t,n}}{\partial W_{n,m}^{out}}$

$$\frac{\partial \mathcal{L}}{\partial h_{t,m}} = \frac{\partial \mathcal{L}(\hat{\mathbf{y}}_{t}, \mathbf{y}_{t})}{\partial h_{t,m}} + \sum_{m'} \frac{\partial h_{t+1,m'}}{\partial h_{t,m}} \frac{\partial \mathcal{L}_{t+1}}{\partial h_{t+1,m'}}$$

$$\frac{\partial \mathcal{L}}{\partial U_{m,m'}} = \sum_{t} \frac{\partial \mathcal{L}_{t}}{\partial h_{t,m}} \frac{\partial h_{t,m}}{\partial U_{m,m'}}$$

 \mathbf{h}_{1} \mathbf{U} \mathbf{h}_{2} \mathbf{U} \mathbf{h}_{3} $\frac{\partial \mathcal{L}}{\partial U_{m,m'}}$

 $egin{aligned} rac{\partial \mathcal{L}}{\partial W_{m,d}} &= \sum_t rac{\partial \mathcal{L}_t}{\partial h_{t,m}} rac{\partial h_{t,m}}{\partial W_{m,d}} \end{aligned}$

Today's agenda

- RNN basics
- Backpropagation through time
- The vanishing/exploding gradients problem
- Advanced RNNs

What can go wrong in BPTT?

• The hidden-to-hidden connections in standard RNN can cause gradient vanishing during backprop of the loss in the last step.

$$\frac{\partial \mathcal{L}_{T}}{\partial \mathbf{h}_{T}} = \frac{\partial \mathcal{L}_{T}}{\partial \mathbf{h}_{T}} \frac{\partial \mathbf{h}_{T}}{\partial \mathbf{h}_{t}} \qquad \qquad \text{Note:} \\
\mathbf{h}_{t} = \sigma(\mathbf{U}\mathbf{h}_{t-1} + \mathbf{W}\mathbf{x}_{t} + \mathbf{b})$$

$$= \frac{\partial \mathcal{L}_{T}}{\partial \mathbf{h}_{T}} \prod_{i=t+1}^{T} \frac{\partial \mathbf{h}_{i}}{\partial \mathbf{h}_{i-1}} = \frac{\partial \mathcal{L}_{T}}{\partial \mathbf{h}_{T}} \prod_{I=t+1}^{T} diag\left(\mathbf{h}_{i}(\mathbf{1} - \mathbf{h}_{i})\right) \mathbf{U}$$

What can go wrong in BPTT?

- The hidden-to-hidden connections in standard RNN can cause gradient vanishing during backprop of the loss in the last step.
- This is caused by gradients with respect to the activation function being multiplied through time!

$$\begin{split} \frac{\partial \mathcal{L}_T}{\partial \mathbf{h}_T} &= \frac{\partial \mathcal{L}_T}{\partial \mathbf{h}_T} \frac{\partial \mathbf{h}_T}{\partial \mathbf{h}_t} \\ &= \frac{\partial \mathcal{L}_T}{\partial \mathbf{h}_T} \prod_{i=t+1}^T \frac{\partial \mathbf{h}_i}{\partial \mathbf{h}_{i-1}} = \frac{\partial \mathcal{L}_T}{\partial \mathbf{h}_T} \prod_{I=t+1}^T \frac{\operatorname{diag}\left(\mathbf{h_i}(\mathbf{1} - \mathbf{h_i})\right) \mathbf{U}}{\operatorname{Gradient of sigmoid causes vanishingly}} \end{split}$$

It is always < 1, which can be multiplied

over time to very small value!

What can go wrong in BPTT?

- The hidden-to-hidden connections in standard RNN can cause gradient vanishing during backprop of the loss in the last step.
- This is caused by gradients with respect to the activation function being multiplied through time!
- Gradient can also explode if norm of U is large

$$\begin{split} \frac{\partial \mathcal{L}_T}{\partial \mathbf{h}_T} &= \frac{\partial \mathcal{L}_T}{\partial \mathbf{h}_T} \frac{\partial \mathbf{h}_T}{\partial \mathbf{h}_t} \\ &= \frac{\partial \mathcal{L}_T}{\partial \mathbf{h}_T} \prod_{i=t+1}^T \frac{\partial \mathbf{h}_i}{\partial \mathbf{h}_{i-1}} = \frac{\partial \mathcal{L}_T}{\partial \mathbf{h}_T} \prod_{I=t+1}^T diag\left(\mathbf{h_i}(\mathbf{1} - \mathbf{h_i})\right) \mathbf{U} \end{split}$$

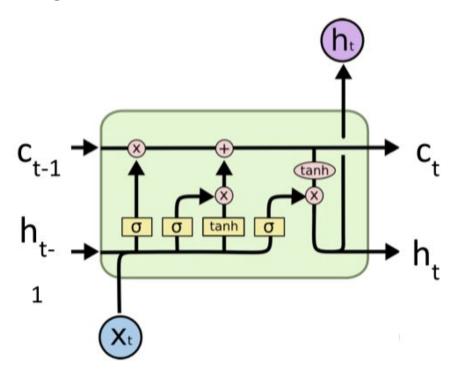
Techniques to prevent vanishing/exploding gradients

- Initializing weights U to be orthogonal
- Clip gradients if the value is too large

Today's agenda

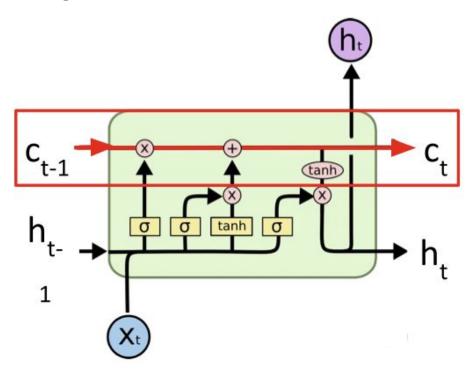
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RNNs addressing vanishing/exploding gradients



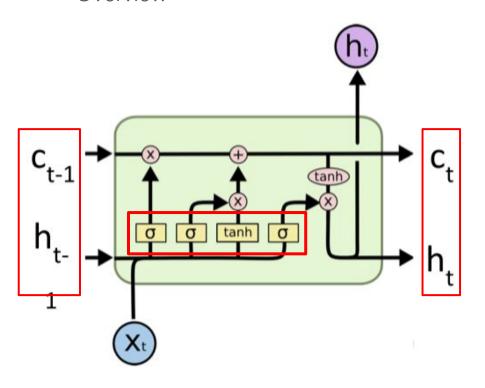
- A recurrent neural network variety designed to retain long-term dependencies.
- Helps dealing with both the vanishing and exploding gradient problem

RNNs addressing vanishing/exploding gradients



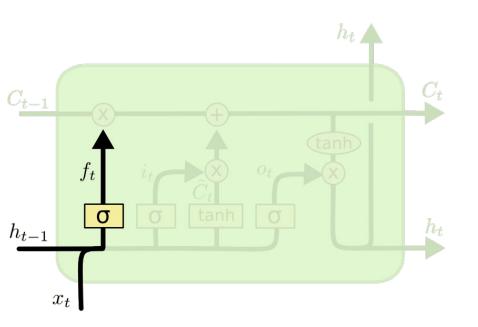
- A recurrent neural network variety designed to retain long-term dependencies.
- Helps dealing with both the vanishing and exploding gradient problem
- The key idea is an additive connection of previous memories passed through time

Overview



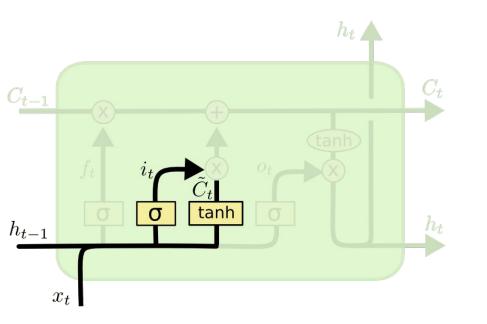
- Information is passed through two variables
- There are four switch variables that determines how the information flows through time

 The forget gate allows LSTM to choose to zero out part of previous memories and let others through.



$$f_t = \sigma\left(W_f \cdot [h_{t-1}, x_t] + b_f\right)$$

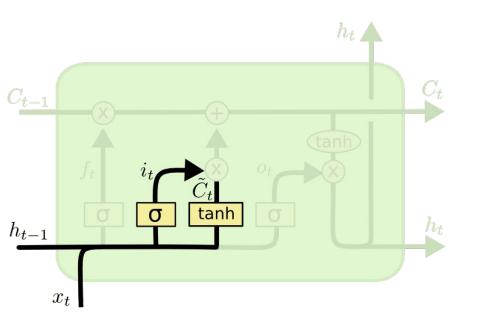
The input gate behaves similar to forget gates with new inputs



$$i_t = \sigma\left(W_i \cdot [h_{t-1}, x_t] + b_i\right)$$

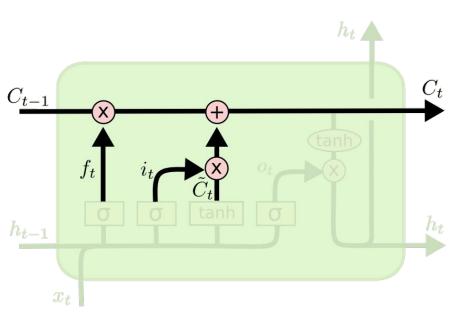
$$\tilde{C}_t = \tanh(W_C \cdot [h_{t-1}, x_t] + b_C)$$

- The input gate behaves similar to the forget gate with new inputs.
- New information is computed from the current input and previous hidden units.



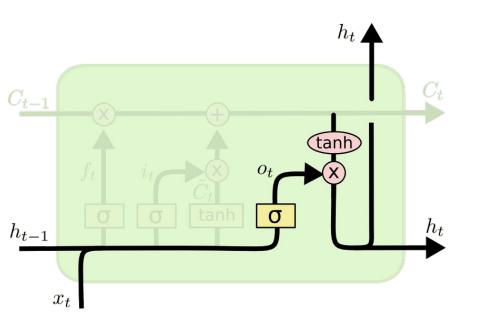
$$i_t = \sigma(W_i \cdot [h_{t-1}, x_t] + b_i)$$
$$\tilde{C}_t = \tanh(W_C \cdot [h_{t-1}, x_t] + b_C)$$

 Memories to be passed are computed using the forget gate on the previous memories and the input gate on the current information found in the sequence



$$C_t = f_t * C_{t-1} + i_t * \tilde{C}_t$$

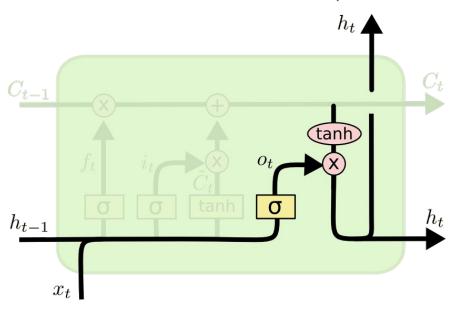
 An output gate is computed to choose information from the current memories for the next hidden state in the LSTM.



$$o_t = \sigma \left(W_o \left[h_{t-1}, x_t \right] + b_o \right)$$

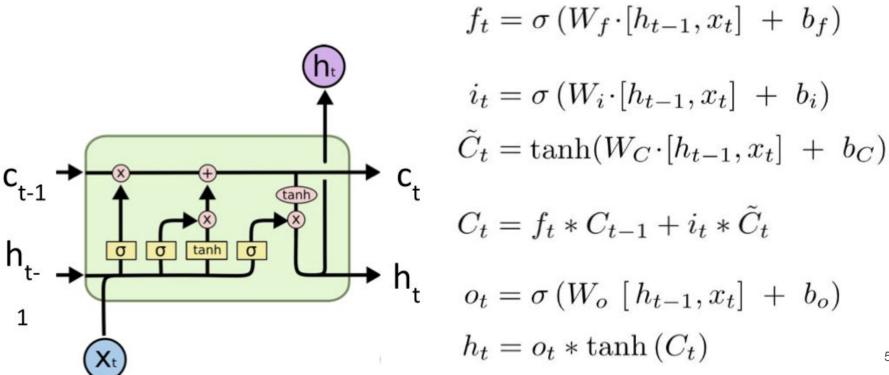
$$h_t = o_t * \tanh \left(C_t \right)$$

- An output gate is computed to choose information from the current memories for the next hidden state in the LSTM.
- Next hidden state is computed from the current memories and gate.



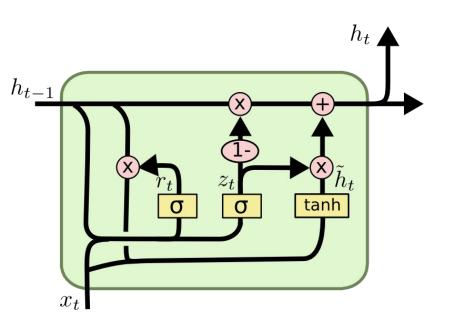
$$o_t = \sigma (W_o [h_{t-1}, x_t] + b_o)$$

$$h_t = o_t * \tanh (C_t)$$



Gated Recurrent Unit (GRU)

A simplified variation of LSTM



$$z_{t} = \sigma (W_{z} \cdot [h_{t-1}, x_{t}])$$

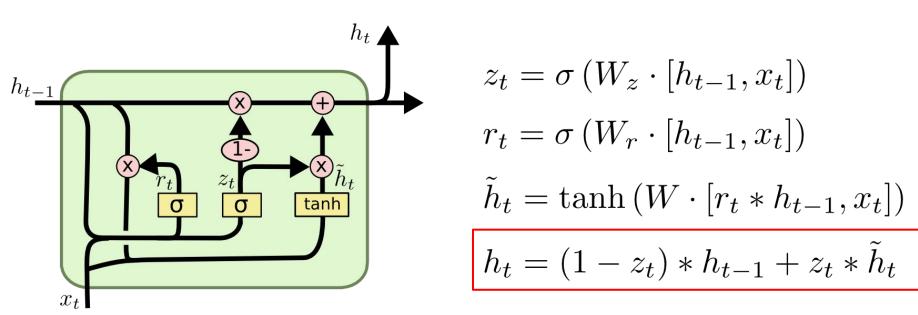
$$r_{t} = \sigma (W_{r} \cdot [h_{t-1}, x_{t}])$$

$$\tilde{h}_{t} = \tanh (W \cdot [r_{t} * h_{t-1}, x_{t}])$$

$$h_{t} = (1 - z_{t}) * h_{t-1} + z_{t} * \tilde{h}_{t}$$

Gated Recurrent Unit (GRU)

- A simplified variation of LSTM
- The forget, input and output gates are simplified into a single gate



Next

- RNNs for sequence modeling
 - Language model