## An introduction to Recurrent Neural Networks

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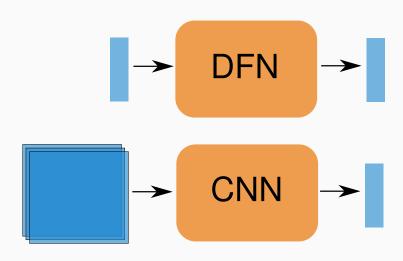
IME-USP: Institute of Mathematics and Statistics, University of São Paulo

Introduction

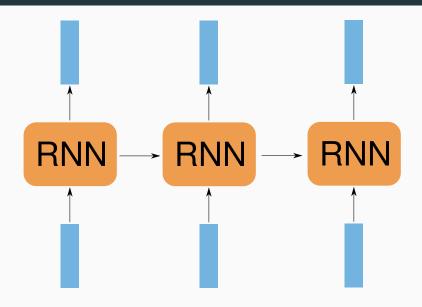
#### Basic idea

- A Recurrent Neural Network (RNN) allows us to operate over sequences of vectors: either sequences in the input or the output
- This feature differentiate the RNN model from other deep learning architectures such as Deep Feedforward Network (DFN) and Convolutional Neural Network (CNN).

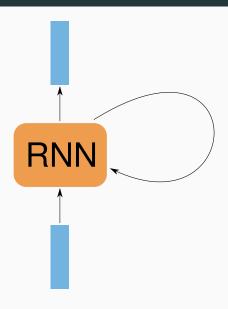
#### **DFN and CNN**



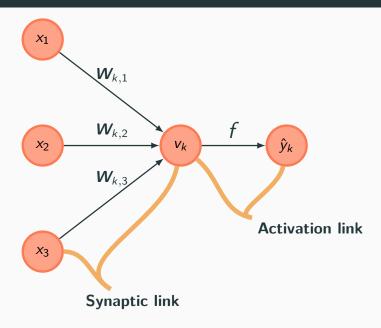
## RNN: unfold representation



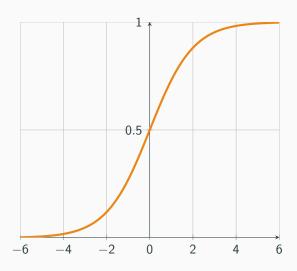
## RNN: cyclic representation



**Graph Representation** 



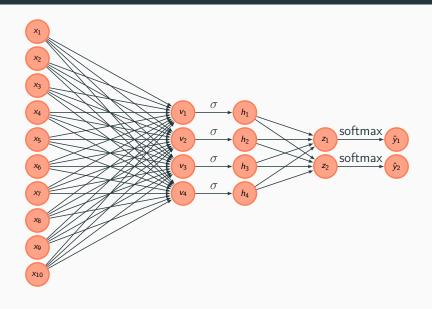
## Recap: sigmoid function

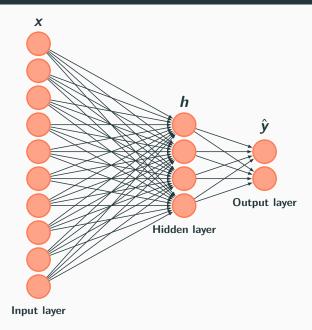


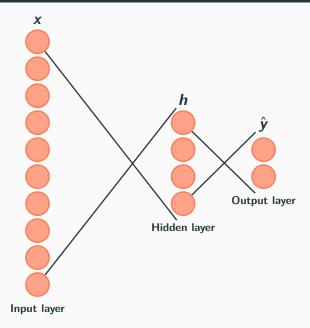
$$\sigma(x) = \frac{1}{1 + e^{-x}}$$

## **Recap: softmax function**

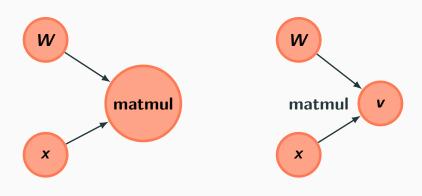
$$softmax(x) = \frac{e^x}{\sum e^x}$$





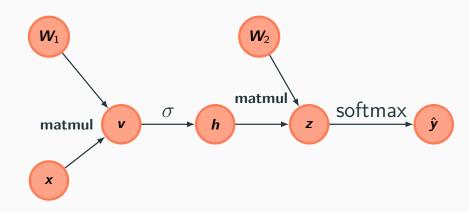


## **Computational Graphs**



v = Wx

## **Computational Graphs**



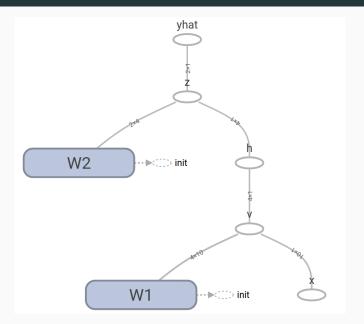
## **Tensorflow graph**

```
import tensorflow as tf
   import numpy as np
2
3
   input_shape = [10,1]
4
   input_to_hidden_shape = [4,10]
   hidden to output shape = [2,4]
6
7
   W1init = np.zeros(input_to_hidden_shape,
8
              dtype="float32")
9
   W2init = np.zeros(hidden_to_output_shape,
10
              dtype="float32")
11
```

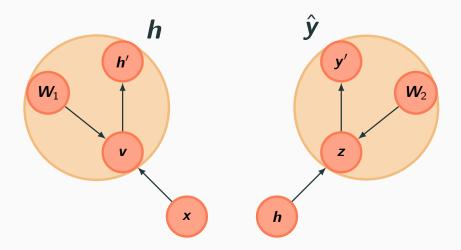
## **Tensorflow graph**

```
graph = tf.Graph()
   with graph.as_default():
        x = tf.placeholder(shape=input_shape,
3
                            dtype="float32")
4
        W1 = tf.get variable(initializer=W1init)
5
       v = tf.matmul(W1, x)
6
       h = tf.sigmoid(v)
        W2 = tf.get variable(initializer=W2init)
8
       z = tf.matmul(W2, h)
9
        yhat = tf.nn.softmax(z)
10
```

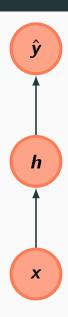
## **Tensorboard visualization**



# **Computational Graphs**



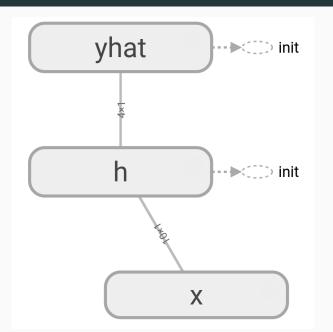
# **Computational Graphs**



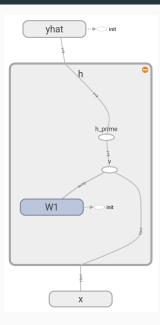
## Tensorflow graph

```
graph = tf.Graph()
   with graph.as default():
2
        with tf.variable scope("x"):
3
            x_prime = tf.placeholder(shape=input_shape,
4
                                      dtype="float32")
5
6
        with tf.variable_scope("h"):
7
            W1 = tf.get variable(initializer=W1init)
8
            v = tf.matmul(W1, x_prime)
9
            h prime = tf.sigmoid(v)
10
11
        with tf.variable_scope("yhat"):
12
            W2 = tf.get_variable(initializer=W2init)
13
            z = tf.matmul(W2, h prime)
14
            y_prime = tf.nn.softmax(z)
15
```

## **Tensorboard visualization**

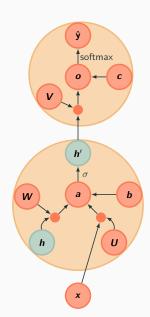


## Tensorboard visualization

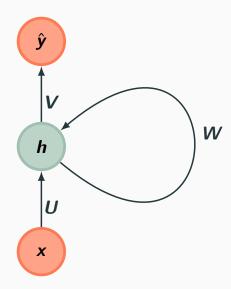


RNN: the model

## RNN as a graph



# RNN as a graph



#### Definition

A RNN is a function f with two inputs:

- An input vector x.
- A hidden vector h representing a summary of all past inputs, called state or cell state.

Both inputs have a time step index t. The hidden unit has a recurrent definition:

$$\boldsymbol{h}^{(t)} = g(\boldsymbol{h}^{(t-1)}, \boldsymbol{x}^{(t)}; \boldsymbol{\theta})$$

# Using our example as a concrete case

$$f(\boldsymbol{x}^{(t)}, \boldsymbol{h}^{(t-1)}; \, \boldsymbol{V}, \, \boldsymbol{W}, \, \boldsymbol{U}, \, \boldsymbol{c}, \, \boldsymbol{b}) = \boldsymbol{\hat{y}}^{(t)}$$

$$\hat{\mathbf{y}}^{(t)} = softmax(\mathbf{V}\mathbf{h}^{(t)} + \mathbf{c})$$

$$\mathbf{h}^{(t)} = g(\mathbf{h}^{(t-1)}, \mathbf{x}^{(t)}; \mathbf{W}, \mathbf{U}, \mathbf{b})$$

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

## Unfolding the state equation

For a finite number of steps  $\tau$ , the recurrent definition can be unfolded.

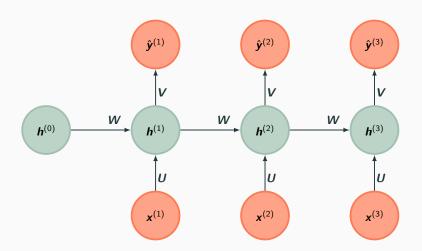
For example when  $\tau = 3$ :

$$h^{(3)} = g(h^{(2)}, x^{(3)}; \theta)$$

$$= g(g(h^{(1)}, x^{(2)}; \theta), x^{(3)}; \theta)$$

$$= g(g(g(h^{(0)}, x^{(1)}; \theta), x^{(2)}; \theta), x^{(3)}; \theta)$$

## Unfolding the graph



Language model

#### **Definition**

We call language model a probability distribution over sequences of tokens in a natural language.

$$P(x_1, x_2, x_3, x_4) = p$$

#### Used for:

- speech recognition
- machine translation
- text auto-completion
- spell correction
- question answering
- summarization

## How do we build these probabilities?

Using the chain rule of probability:

$$P(x_1, x_2, x_3, x_4) = P(x_1)P(x_2|x_1)P(x_3|x_1x_2)P(x_4|x_1x_2x_3)$$

To make things simple we use a **Markovian assumption**, i.e., for a specific n we assume that:

$$P(x_1,\ldots,x_T) = \prod_{t=1}^T P(x_t|x_1,\ldots,x_{t-1}) = \prod_{t=1}^T P(x_t|x_{t-(n+1)},\ldots,x_{t-1})$$

## Models based on *n*-gram statistics

The choice of *n* yields different models.

**Unigram** language model (n = 1):

$$P_{uni}(x_1, x_2, x_3, x_4) = P(x_1)P(x_2)P(x_3)P(x_4)$$

where  $P(x_i) = count(x_i)$ .

**Bigram** language model (n = 2):

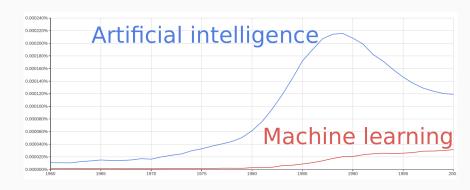
$$P_{bi}(x_1, x_2, x_3, x_4) = P(x_1)P(x_2|x_1)P(x_3|x_2)P(x_4|x_3)$$

where

$$P(x_i|x_j) = \frac{count(x_i, x_j)}{count(x_j)}$$

### *n*-gram statistics

https://books.google.com/ngrams



## **Evaluating a language model**

- extrinsic task: How our model perform in a NLP task such as text auto-completion.
  - Time consuming.
- intrinsic evaluation: perplexity.
  - It works only when the test data is very similar to the training data.

#### **Perplexity**

Perplexity (PP) can be thought as the weighted average branching factor of a language.

Given  $C = x_1, x_2, \dots, x_T$ , we define the perplexity of C as:

$$PP(C) = P(x_1, x_2, ..., x_T)^{-\frac{1}{T}}$$

$$= \sqrt[T]{\frac{1}{P(x_1, x_2, ..., x_T)}}$$

$$= \sqrt[T]{\prod_{i=1}^{T} \frac{1}{P(x_i | x_1, ..., x_{i-1})}}$$

#### Models based on *n*-gram statistics

- Higher *n*-grams yields better performance.
- Higher *n*-grams requires a lot of memory!

"Using one machine with 140 GB RAM for 2.8 days, we built an unpruned model on 126 billion tokens."

Scalable Modified Kneser-Ney Language Model Estimation by Heafield et al.

#### Languagem model as sequential data prediction

Instead of using one approach that is specific for the language domain, we can use a general model for sequential data prediction: a **RNN**.

Our learning task is to estimate the probability distribution

$$P(x_n = \mathsf{word}_{j^*} | x_1, \dots, x_{n-1})$$

for any (n-1)-sequence of words  $x_1, \ldots, x_{n-1}$ .

#### **Building the dataset**

We start with a corpus C with T tokens and a vocabulary  $\mathbb{V}$ .

Example: Make Some Noise by the Beastie Boys.

Yes, here we go again, give you more, nothing lesser Back on the mic is the anti-depressor Ad-Rock, the pressure, yes, we need this The best is yet to come, and yes, believe this ...

- *T* = 378
- |V| = 186

#### **Building the dataset**

The dataset is a collection of pairs (x, y) where x is one word and y is the immediately next word. For example:

$$(x^{(1)}, y^{(1)}) = (\text{Yes, here}).$$
  
 $(x^{(2)}, y^{(2)}) = (\text{here, we})$   
 $(x^{(3)}, y^{(3)}) = (\text{we, go})$   
 $(x^{(4)}, y^{(4)}) = (\text{go, again})$   
 $(x^{(5)}, y^{(5)}) = (\text{again, give})$   
 $(x^{(6)}, y^{(6)}) = (\text{give, you})$   
 $(x^{(7)}, y^{(7)}) = (\text{you, more})$   
...

36

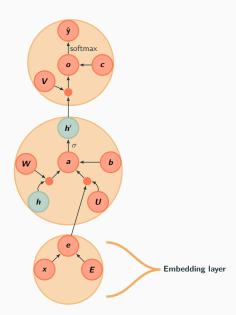
#### **Notation**

- ullet  $oldsymbol{\mathcal{E}} \in \mathbb{R}^{d,|\mathbb{V}|}$  is the matrix of word embeddings.
- $\mathbf{x}^{(t)} \in \mathbb{R}^{|\mathbb{V}|}$  is one-hot word vector at time step t.
- $\mathbf{y}^{(t)} \in \mathbb{R}^{|\mathbb{V}|}$  is the ground truth at time step t (also an one-hot word vector).

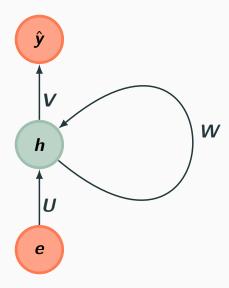
## Recap: selecting word embeddings

$$oldsymbol{e} = oldsymbol{\mathcal{E}} egin{bmatrix} 0 \ 0 \ \vdots \ 1 \ \vdots \ 0 \end{bmatrix} \ = oldsymbol{\mathcal{E}}_{:,\,j}$$

## The language model: graph



## The language model: graph



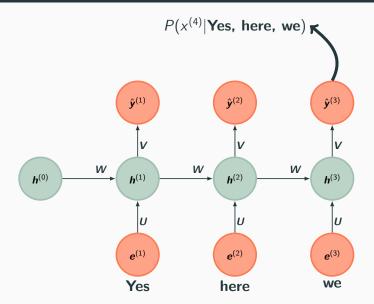
## The language model: equations

$$oldsymbol{e}^{(t)} = oldsymbol{E} oldsymbol{x}^{(t)}$$

$$\mathbf{h}^{(t)} = \sigma(\mathbf{W}\mathbf{h}^{(t-1)} + \mathbf{U}\mathbf{e}^{(t)} + \mathbf{b})$$

$$\hat{\pmb{y}}^{(t)} = softmax(\pmb{V}\pmb{h}^{(t)} + \pmb{c})$$

### The Language model: unfolding example



## Recap: Entropy

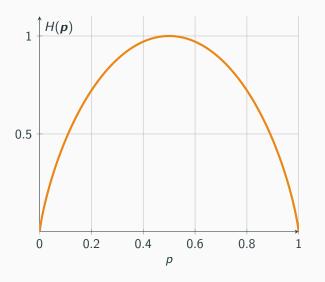
$$\begin{array}{ccc}
\rho & q \\
0.8 \\
0.2
\end{array}$$

$$\begin{bmatrix}
0.5 \\
0.5
\end{bmatrix}$$

$$H(\mathbf{p}) = 0.72 \qquad H(\mathbf{q}) = 1$$

$$H(\boldsymbol{p}) = \sum_{i} \boldsymbol{p}_{i} \log \frac{1}{\boldsymbol{p}_{i}}$$

## Recap: Entropy



$$egin{bmatrix} oldsymbol{p} \ 1-oldsymbol{p} \ \end{bmatrix}$$

## Recap: Kullback-Leibler divergence

$$\begin{array}{c|ccc} \boldsymbol{p} & \boldsymbol{q} & \boldsymbol{p}' & \boldsymbol{q}' \\ \hline \begin{bmatrix} 0.8 \\ 0.2 \end{bmatrix} & \begin{bmatrix} 0.5 \\ 0.5 \end{bmatrix} & \begin{bmatrix} 0.8 \\ 0.2 \end{bmatrix} & \begin{bmatrix} 0.88 \\ 0.12 \end{bmatrix} \\ D_{KL}(\boldsymbol{p}||\boldsymbol{q}) = 0.28 & D_{KL}(\boldsymbol{p}'||\boldsymbol{q}') = 0.04 \\ D_{KL}(\boldsymbol{p}||\boldsymbol{q}) = \sum_{i} \boldsymbol{p}_{i} \log \frac{\boldsymbol{p}_{i}}{\boldsymbol{q}_{i}} \end{array}$$

### Recap: Cross entropy

$$CE(\boldsymbol{p}, \boldsymbol{q}) = H(\boldsymbol{p}) + D_{KL}(\boldsymbol{p}||\boldsymbol{q})$$
  
=  $-\sum_{i} \boldsymbol{p}_{i} \log(\boldsymbol{q}_{i})$ 

$$\operatorname*{arg\,min}_{m{q}} \mathit{CE}(m{p},m{q}) = \operatorname*{arg\,min}_{m{q}} \mathit{D}_{\mathit{KL}}(m{p},m{q})$$

#### Loss function

At each time t the point-wise loss is:

$$L^{(t)} = CE(\mathbf{y}^{(t)}, \hat{\mathbf{y}}^{(t)})$$

$$= -\log(\hat{\mathbf{y}}_{j^*})$$

$$= -\log P(x^{(t+1)} = \text{word}_{j^*} | x^{(1)}, \dots, x^{(t)})$$

For example:

$$L^{(3)} = -\log P(x^{(4)} = \text{go}|\text{Yes}, \text{here}, \text{we})$$

#### Loss function

The loss L is the mean of all the point-wise losses

$$L = \frac{1}{T} \sum_{t=1}^{T} L^{(t)}$$

To give a concrete example, let's take the first sentence of the lyric as C:

Yes, here we go again, give you more, nothing lesser

- T = 10
- |V| = 10

#### Loss function: example

$$L = -\frac{1}{10} [\log P(\text{here}|\text{Yes}) \\ + \log P(\text{we}|\text{Yes}, \text{here}) \\ + \log P(\text{go}|\text{Yes}, \text{here}, \text{we}) \\ + \log P(\text{gain}|\text{Yes}, \text{here}, \text{we}, \text{go}) \\ + \log P(\text{give}|\text{Yes}, \text{here}, \text{we}, \text{go}, \text{again}) \\ + \log P(\text{you}|\text{Yes}, \text{here}, \text{we}, \text{go}, \text{again}, \text{give}) \\ + \log P(\text{more}|\text{Yes}, \text{here}, \text{we}, \text{go}, \text{again}, \text{give}, \text{you}) \\ + \log P(\text{nothing}|\text{Yes}, \text{here}, \text{we}, \text{go}, \text{again}, \text{give}, \text{you}, \text{more}) \\ + \log P(\text{lesser}|\text{Yes}, \text{here}, \text{we}, \text{go}, \text{again}, \text{give}, \text{you}, \text{more}, \text{nothing}) \\ + \log P(<\text{eos} > |\text{Yes}, \text{here}, \text{we}, \text{go}, \text{again}, \text{give}, \text{you}, \text{more}, \text{nothing}, \text{lesser})]$$

## Loss and Perplexity

Since

$$L^{(t)} = -\log P(x^{(t+1)}|x^{(1)}, \dots, x^{(t)})$$
$$= \log(\frac{1}{P(x^{(t+1)}|x^{(1)}, \dots, x^{(t)})})$$

We have that:

$$L = \frac{1}{T} \sum_{t=1}^{T} L^{(t)}$$

$$= \log \left( \sqrt[\tau]{\prod_{i=1}^{T} \frac{1}{P(x_i|x_1, \dots, x_{i-1})}} \right)$$

$$= \log(PP(C))$$

#### **Loss and Perplexity**

So another definition of perplexity is

$$2^L = PP(C)$$

**Back Propagation** 

#### Chain rule of Calculus

- $x \in \mathbb{R}$
- $f: \mathbb{R} \to \mathbb{R}, g: \mathbb{R} \to \mathbb{R}$ .
- y = g(x)
- z = f(g(x)) = f(y)

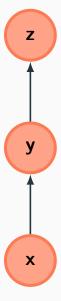
$$\frac{dz}{dx} = \frac{dz}{dy}\frac{dy}{dx}$$

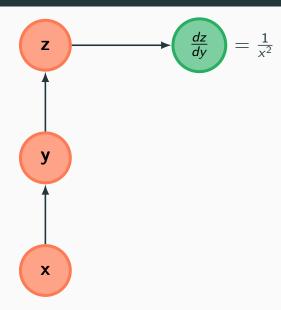
## Chain rule: example

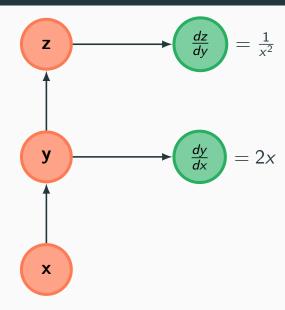
• 
$$y = x^2$$

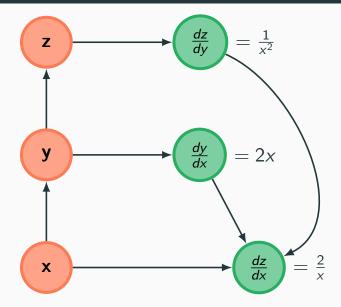
•  $z = \log(y)$ 

$$\frac{dz}{dx} = \frac{dz}{dy}\frac{dy}{dx} = \frac{1}{x^2}2x = \frac{2}{x}$$









#### Chain rule: vector notation

- $\mathbf{x} \in \mathbb{R}^m$
- $\mathbf{y} \in \mathbb{R}^n$
- $f: \mathbb{R}^n \to \mathbb{R}$ ,  $g: \mathbb{R}^m \to \mathbb{R}^n$ .
- $\mathbf{y} = g(\mathbf{x})$
- z = f(g(x)) = f(y)  $\frac{\partial z}{\partial x} = x$

$$\frac{\partial z}{\partial x_i} = \sum_j \frac{\partial z}{\partial y_j} \frac{\partial y_j}{\partial x_i}$$

#### Chain rule: vector notation

- $\mathbf{x} \in \mathbb{R}^m$
- $\mathbf{y} \in \mathbb{R}^n$
- $f: \mathbb{R}^n \to \mathbb{R}$ ,  $g: \mathbb{R}^m \to \mathbb{R}^n$ .
- $\bullet \ \mathbf{y} = g(\mathbf{x})$
- $\bullet \ \mathbf{z} = f(g(\mathbf{x})) = f(\mathbf{y})$

$$\nabla_{\mathbf{x}}z = \left(\frac{\partial \mathbf{y}}{\partial \mathbf{x}}\right)^T \nabla_{\mathbf{y}}z$$

### Recap: gradient

$$abla_{\mathbf{y}}z = egin{bmatrix} rac{\partial z}{\partial y_1} \ rac{\partial z}{\partial y_2} \ dots \ rac{\partial z}{\partial y_n} \end{bmatrix}$$

### Recap: Jacobian matrix

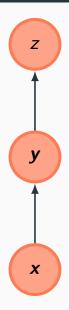
$$\frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_1}{\partial x_2} & \cdots & \frac{\partial y_1}{\partial x_m} \\ \vdots & \ddots & \ddots & \vdots \\ \frac{\partial y_n}{\partial x_1} & \frac{\partial y_n}{\partial x_2} & \cdots & \frac{\partial y_n}{\partial x_m} \end{bmatrix}$$

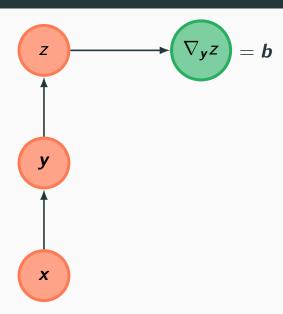
### Chain rule: example

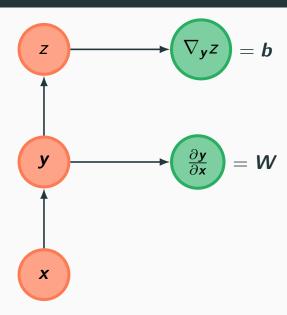
$$\bullet y = Wx$$

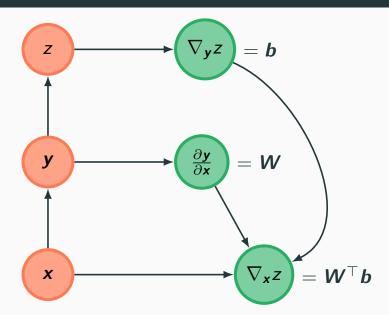
$$\bullet \ z = \boldsymbol{b}^T \boldsymbol{y}$$

$$\nabla_{\mathbf{x}}z = \mathbf{W}^T\mathbf{b}$$









#### Computing the gradient in a RNN

- We simple apply the back-propagation algorithm to the unrolled computational graph.
- Since each subgraph represents a time step, the application of back-propagation in this model is also called Back-Propagation Through Time.

# A very simple RNN

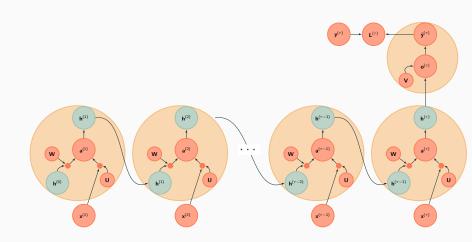
$$\mathbf{a}^{(t)} = \mathbf{W} \mathbf{h}^{(t-1)} + \mathbf{U} \mathbf{x}^{(t)}$$

$$\boldsymbol{h}^{(t)} = \sigma(\boldsymbol{a}^{(t)})$$

$$oldsymbol{o}^{(t)} = oldsymbol{V} oldsymbol{h}^{(t)}$$

$$\hat{\pmb{y}}^{(t)} = softmax(\pmb{o}^{(t)})$$

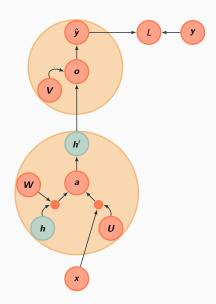
# RNN time unfolding

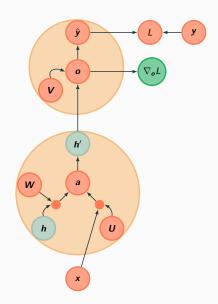


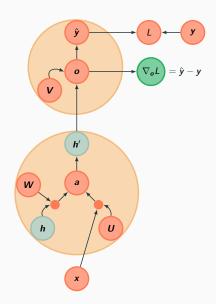
# Recap: Hadamard product

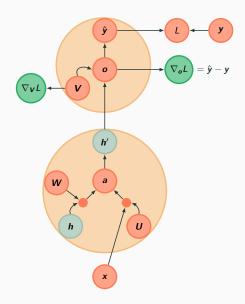
$$(\boldsymbol{x} \circ \boldsymbol{y})_i = \boldsymbol{x}_i \boldsymbol{y}_i$$

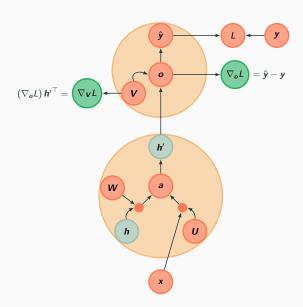
$$(\mathbf{x} \circ \mathbf{y}) = diag(\mathbf{y})\mathbf{x}$$

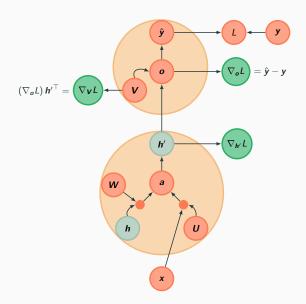


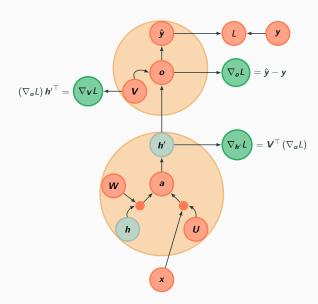


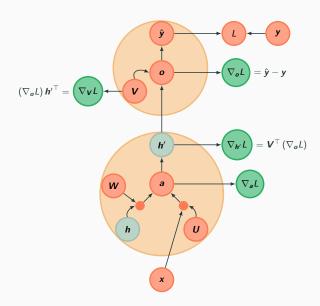


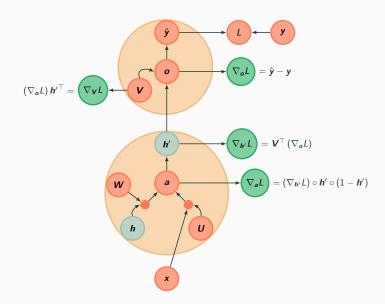


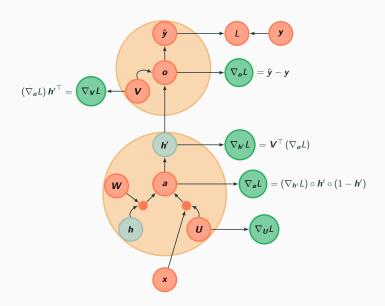


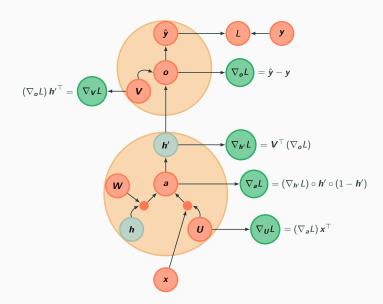


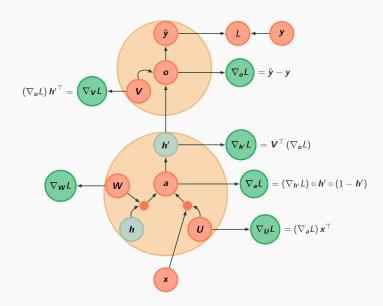


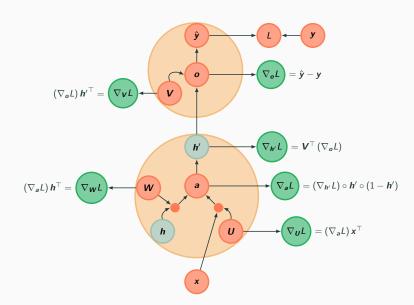


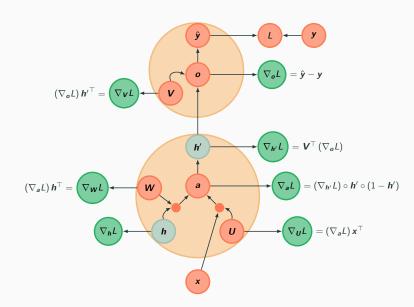


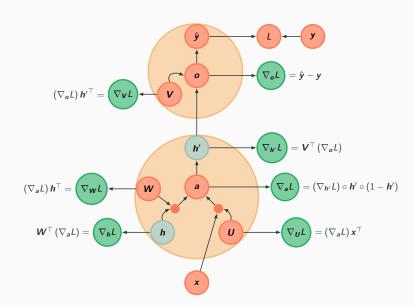


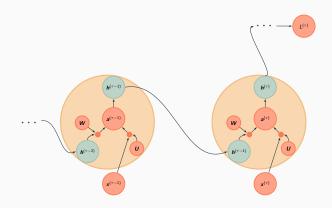


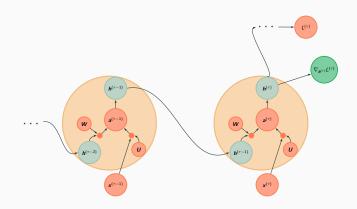


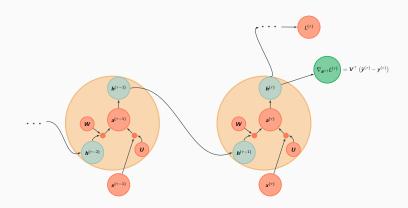


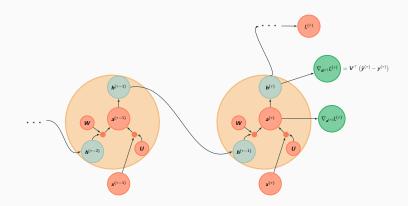


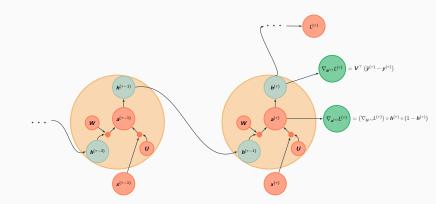


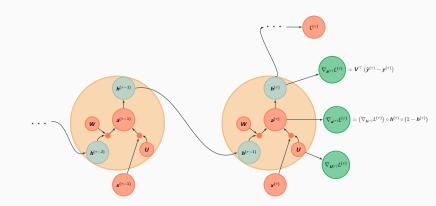


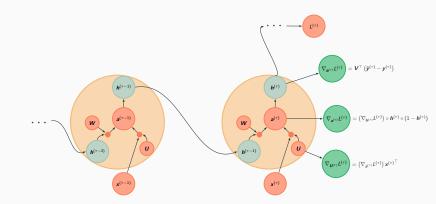


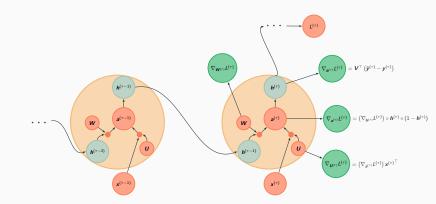


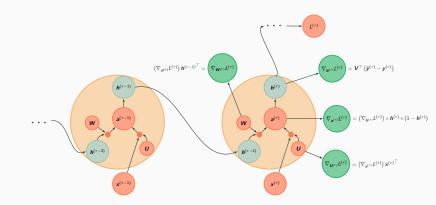


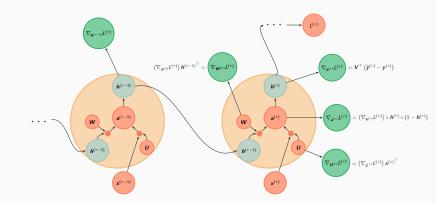


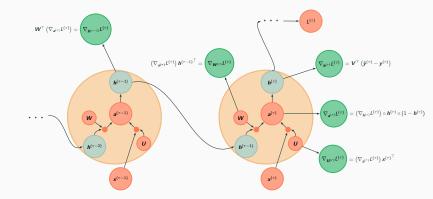


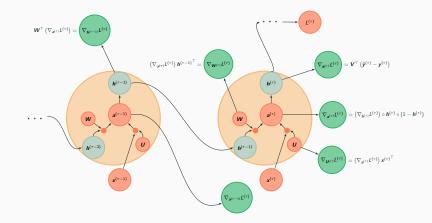


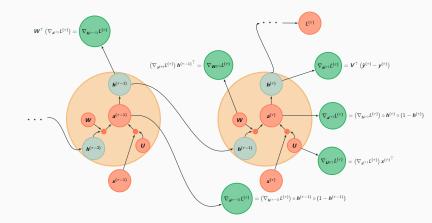


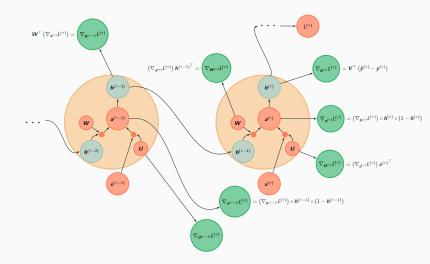


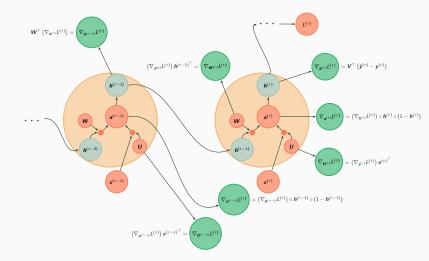


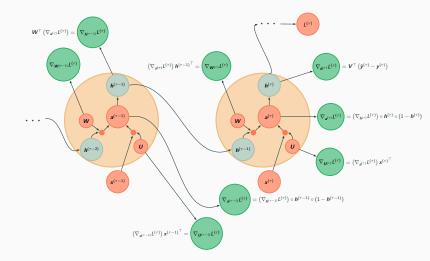


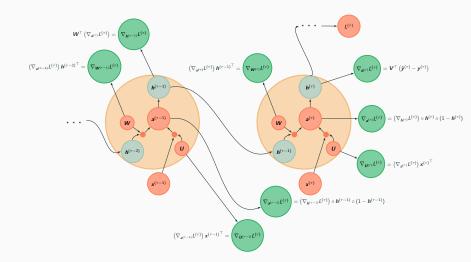




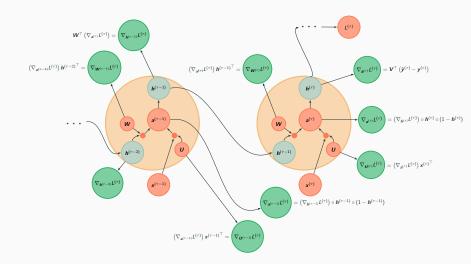




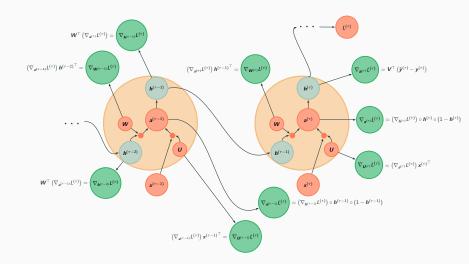




#### **Back Propagation Throught Time**



#### **Back Propagation Throught Time**



#### **Back Propagation Through Time**

The gradients on  $\boldsymbol{V}$ ,  $\boldsymbol{W}$  and  $\boldsymbol{U}$  are:

$$abla_{oldsymbol{v}} L^{( au)} = \left( 
abla_{oldsymbol{o}^{( au)}} L^{( au)} 
ight) oldsymbol{h}^{( au)^ op}$$

$$\nabla_{\boldsymbol{W}} L^{(\tau)} = \sum_{t=1}^{\tau} \nabla_{\boldsymbol{W}^{(t)}} L^{(\tau)}$$

$$abla_{\boldsymbol{U}} L^{( au)} = \sum_{t=1}^{ au} 
abla_{\boldsymbol{U}^{(t)}} L^{( au)}$$

**Vanishing or Exploding Gradient** 

#### The problem of training RNN

Let's calculate  $\nabla_{\boldsymbol{U}} L^{(3)}$ :

$$\nabla_{\boldsymbol{U}} L^{(3)} = \sum_{t=1}^{3} \nabla_{\boldsymbol{U}^{(t)}} L^{(3)}$$
$$= \nabla_{\boldsymbol{U}^{(1)}} L^{(3)} + \nabla_{\boldsymbol{U}^{(2)}} L^{(3)} + \nabla_{\boldsymbol{U}^{(3)}} L^{(3)}$$

# Calculating $\nabla_{U^{(3)}} L^{(3)}$

$$abla_{\mathit{U}^{(3)}}\mathit{L}^{(3)} = \left( 
abla_{\mathit{a}^{(3)}}\mathit{L}^{(3)} \right) \mathit{x}^{(3)^{ op}}$$

$$\nabla_{\boldsymbol{U}^{(3)}} L^{(3)} = \left(\nabla_{\boldsymbol{a}^{(3)}} L^{(3)}\right) \boldsymbol{x}^{(3)^{\top}}$$
$$= \left(\left(\nabla_{\boldsymbol{h}^{(3)}} L^{(3)}\right) \circ \boldsymbol{h}^{(3)} \circ (1 - \boldsymbol{h}^{(3)})\right) \boldsymbol{x}^{(3)^{\top}}$$

### Calculating $\nabla_{U^{(3)}} L^{(3)}$

$$\nabla_{\boldsymbol{U}^{(3)}} L^{(3)} = \left(\nabla_{\boldsymbol{a}^{(3)}} L^{(3)}\right) \boldsymbol{x}^{(3)^{\top}}$$

$$= \left(\left(\nabla_{\boldsymbol{h}^{(3)}} L^{(3)}\right) \circ \boldsymbol{h}^{(3)} \circ (1 - \boldsymbol{h}^{(3)})\right) \boldsymbol{x}^{(3)^{\top}}$$

$$= \left(\left(\boldsymbol{V}^{\top} \left(\hat{\boldsymbol{y}}^{(3)} - \boldsymbol{y}^{(3)}\right)\right) \circ \boldsymbol{h}^{(3)} \circ (1 - \boldsymbol{h}^{(3)})\right) \boldsymbol{x}^{(3)^{\top}}$$

$$\nabla_{\boldsymbol{U}^{(2)}} L^{(3)} = (\nabla_{\boldsymbol{a}^{(2)}} L^{(3)}) \boldsymbol{x}^{(2)^{\top}}$$

# Calculating $\nabla_{\boldsymbol{U}^{(2)}} \underline{L^{(3)}}$

$$\nabla_{\mathbf{U}^{(2)}} L^{(3)} = \left( \nabla_{\mathbf{a}^{(2)}} L^{(3)} \right) \mathbf{x}^{(2)^{\top}}$$

$$= \left( \left( \nabla_{\mathbf{h}^{(2)}} L^{(3)} \right) \circ \mathbf{h}^{(2)} \circ (1 - \mathbf{h}^{(2)}) \right) \mathbf{x}^{(2)^{\top}}$$

### Calculating $\nabla_{U^{(2)}}L^{(3)}$

$$\begin{split} \nabla_{\mathbf{U}^{(2)}} L^{(3)} &= \left( \nabla_{\mathbf{a}^{(2)}} L^{(3)} \right) \mathbf{x}^{(2)^{\top}} \\ &= \left( \left( \nabla_{\mathbf{h}^{(2)}} L^{(3)} \right) \circ \mathbf{h}^{(2)} \circ (1 - \mathbf{h}^{(2)}) \right) \mathbf{x}^{(2)^{\top}} \\ &= \left( \left( \mathbf{W}^{\top} \left( \nabla_{\mathbf{a}^{(3)}} L^{(3)} \right) \right) \circ \mathbf{h}^{(2)} \circ (1 - \mathbf{h}^{(2)}) \right) \mathbf{x}^{(2)^{\top}} \end{split}$$

# Calculating $\nabla_{U^{(2)}}L^{(3)}$

$$\begin{split} \nabla_{\textit{U}^{(2)}} \textit{L}^{(3)} &= \left( \nabla_{\textit{a}^{(2)}} \textit{L}^{(3)} \right) \textit{x}^{(2)^{\top}} \\ &= \left( \left( \nabla_{\textit{h}^{(2)}} \textit{L}^{(3)} \right) \circ \textit{h}^{(2)} \circ \left( 1 - \textit{h}^{(2)} \right) \right) \textit{x}^{(2)^{\top}} \\ &= \left( \left( \textit{\textbf{W}}^{\top} \left( \nabla_{\textit{a}^{(3)}} \textit{L}^{(3)} \right) \right) \circ \textit{h}^{(2)} \circ \left( 1 - \textit{h}^{(2)} \right) \right) \textit{x}^{(2)^{\top}} \\ &= \left( \left( \textit{\textbf{W}}^{\top} \left( \left( \nabla_{\textit{h}^{(3)}} \textit{L}^{(3)} \right) \circ \textit{h}^{(3)} \circ \left( 1 - \textit{h}^{(3)} \right) \right) \right) \circ \textit{h}^{(2)} \circ \left( 1 - \textit{h}^{(2)} \right) \right) \textit{x}^{(2)^{\top}} \end{split}$$

# Calculating $\nabla_{U^{(2)}}L^{(3)}$

$$\begin{split} \nabla_{\mathbf{U}^{(2)}} L^{(3)} &= \left( \nabla_{\mathbf{a}^{(2)}} L^{(3)} \right) \mathbf{x}^{(2)^{\top}} \\ &= \left( \left( \nabla_{\mathbf{h}^{(2)}} L^{(3)} \right) \circ \mathbf{h}^{(2)} \circ (1 - \mathbf{h}^{(2)}) \right) \mathbf{x}^{(2)^{\top}} \\ &= \left( \left( \mathbf{W}^{\top} \left( \nabla_{\mathbf{a}^{(3)}} L^{(3)} \right) \circ \mathbf{h}^{(2)} \circ (1 - \mathbf{h}^{(2)}) \right) \mathbf{x}^{(2)^{\top}} \\ &= \left( \left( \mathbf{W}^{\top} \left( \left( \nabla_{\mathbf{h}^{(3)}} L^{(3)} \right) \circ \mathbf{h}^{(3)} \circ (1 - \mathbf{h}^{(3)}) \right) \right) \circ \mathbf{h}^{(2)} \circ (1 - \mathbf{h}^{(2)}) \right) \mathbf{x}^{(2)^{\top}} \\ &= \left( \left( \mathbf{W}^{\top} \left( \left( \mathbf{V}^{\top} \left( \hat{\mathbf{y}}^{(3)} - \mathbf{y}^{(3)} \right) \right) \circ \mathbf{h}^{(3)} \circ (1 - \mathbf{h}^{(3)}) \right) \right) \circ \mathbf{h}^{(2)} \circ (1 - \mathbf{h}^{(2)}) \right) \mathbf{x}^{(2)^{\top}} \end{split}$$

$$\nabla_{U^{(1)}} L^{(3)} = \left( \nabla_{a^{(1)}} L^{(3)} \right) x^{(1)}^{\top}$$

$$\begin{array}{l} \nabla_{\textit{U}\left(1\right)} \textit{L}^{\left(3\right)} = \left(\nabla_{\textit{a}\left(1\right)} \textit{L}^{\left(3\right)}\right) \textit{x}^{\left(1\right) \top} \\ \\ = \left(\left(\nabla_{\textit{h}\left(1\right)} \textit{L}^{\left(3\right)}\right) \circ \textit{h}^{\left(1\right)} \circ \left(1 - \textit{h}^{\left(1\right)}\right)\right) \textit{x}^{\left(1\right) \top} \end{array}$$

$$\begin{split} \boldsymbol{\nabla}_{\boldsymbol{U}\left(1\right)} \boldsymbol{L}^{\left(3\right)} &= \left(\boldsymbol{\nabla}_{\boldsymbol{a}\left(1\right)} \boldsymbol{L}^{\left(3\right)}\right) \boldsymbol{x}^{\left(1\right) \, \top} \\ &= \left(\left(\boldsymbol{\nabla}_{\boldsymbol{h}\left(1\right)} \boldsymbol{L}^{\left(3\right)}\right) \circ \boldsymbol{h}^{\left(1\right)} \circ \left(1 - \boldsymbol{h}^{\left(1\right)}\right)\right) \boldsymbol{x}^{\left(1\right) \, \top} \\ &= \left(\left(\boldsymbol{W}^{\top} \left(\boldsymbol{\nabla}_{\boldsymbol{a}\left(2\right)} \boldsymbol{L}^{\left(3\right)}\right)\right) \circ \boldsymbol{h}^{\left(1\right)} \circ \left(1 - \boldsymbol{h}^{\left(1\right)}\right)\right) \boldsymbol{x}^{\left(1\right) \, \top} \end{split}$$

#### Calculating $\nabla_{U^{(1)}} L^{(3)}$

$$\begin{split} \nabla_{U^{(1)}} L^{(3)} &= \left( \nabla_{\boldsymbol{a}^{(1)}} L^{(3)} \right) \boldsymbol{x}^{(1) \top} \\ &= \left( \left( \nabla_{\boldsymbol{h}^{(1)}} L^{(3)} \right) \circ \boldsymbol{h}^{(1)} \circ (1 - \boldsymbol{h}^{(1)}) \right) \boldsymbol{x}^{(1) \top} \\ &= \left( \left( \boldsymbol{W}^{\top} \left( \nabla_{\boldsymbol{a}^{(2)}} L^{(3)} \right) \right) \circ \boldsymbol{h}^{(1)} \circ (1 - \boldsymbol{h}^{(1)}) \right) \boldsymbol{x}^{(1) \top} \\ &= \left( \left( \boldsymbol{W}^{\top} \left( \left( \nabla_{\boldsymbol{h}^{(2)}} L^{(3)} \right) \circ \boldsymbol{h}^{(2)} \circ (1 - \boldsymbol{h}^{(2)}) \right) \right) \circ \boldsymbol{h}^{(1)} \circ (1 - \boldsymbol{h}^{(1)}) \right) \boldsymbol{x}^{(1) \top} \end{split}$$

### Calculating $\nabla_{U^{(1)}} L^{(3)}$

$$\begin{split} \boldsymbol{\nabla}_{\boldsymbol{U}\left(1\right)} \boldsymbol{L}^{\left(3\right)} &= \left(\boldsymbol{\nabla}_{\boldsymbol{a}\left(1\right)} \boldsymbol{L}^{\left(3\right)}\right) \boldsymbol{x}^{\left(1\right) \top} \\ &= \left(\left(\boldsymbol{\nabla}_{\boldsymbol{h}\left(1\right)} \boldsymbol{L}^{\left(3\right)}\right) \circ \boldsymbol{h}^{\left(1\right)} \circ \left(1-\boldsymbol{h}^{\left(1\right)}\right)\right) \boldsymbol{x}^{\left(1\right) \top} \\ &= \left(\left(\boldsymbol{w}^{\top} \left(\boldsymbol{\nabla}_{\boldsymbol{a}\left(2\right)} \boldsymbol{L}^{\left(3\right)}\right)\right) \circ \boldsymbol{h}^{\left(1\right)} \circ \left(1-\boldsymbol{h}^{\left(1\right)}\right)\right) \boldsymbol{x}^{\left(1\right) \top} \\ &= \left(\left(\boldsymbol{w}^{\top} \left(\left(\boldsymbol{\nabla}_{\boldsymbol{h}\left(2\right)} \boldsymbol{L}^{\left(3\right)}\right) \circ \boldsymbol{h}^{\left(2\right)} \circ \left(1-\boldsymbol{h}^{\left(2\right)}\right)\right)\right) \circ \boldsymbol{h}^{\left(1\right)} \circ \left(1-\boldsymbol{h}^{\left(1\right)}\right)\right) \boldsymbol{x}^{\left(1\right) \top} \\ &= \left(\left(\boldsymbol{w}^{\top} \left(\left(\boldsymbol{w}^{\top} \left(\boldsymbol{\nabla}_{\boldsymbol{a}\left(3\right)} \boldsymbol{L}^{\left(3\right)}\right)\right) \circ \boldsymbol{h}^{\left(2\right)} \circ \left(1-\boldsymbol{h}^{\left(2\right)}\right)\right)\right) \circ \boldsymbol{h}^{\left(1\right)} \circ \left(1-\boldsymbol{h}^{\left(1\right)}\right)\right) \boldsymbol{x}^{\left(1\right) \top} \end{split}$$

### Calculating $\nabla_{U^{(1)}} L^{(3)}$

$$\begin{split} \nabla_{\mathcal{U}^{\left(1\right)}} L^{\left(3\right)} &= \left( \nabla_{\mathbf{a}^{\left(1\right)}} L^{\left(3\right)} \right) x^{\left(1\right)}^{\top} \\ &= \left( \left( \nabla_{\mathbf{h}^{\left(1\right)}} L^{\left(3\right)} \right) \circ \mathbf{h}^{\left(1\right)} \circ (1 - \mathbf{h}^{\left(1\right)}) \right) x^{\left(1\right)}^{\top} \\ &= \left( \left( \mathbf{w}^{\top} \left( \nabla_{\mathbf{a}^{\left(2\right)}} L^{\left(3\right)} \right) \right) \circ \mathbf{h}^{\left(1\right)} \circ (1 - \mathbf{h}^{\left(1\right)}) \right) x^{\left(1\right)}^{\top} \\ &= \left( \left( \mathbf{w}^{\top} \left( \left( \nabla_{\mathbf{h}^{\left(2\right)}} L^{\left(3\right)} \right) \circ \mathbf{h}^{\left(2\right)} \circ (1 - \mathbf{h}^{\left(2\right)}) \right) \right) \circ \mathbf{h}^{\left(1\right)} \circ (1 - \mathbf{h}^{\left(1\right)}) \right) x^{\left(1\right)}^{\top} \\ &= \left( \left( \mathbf{w}^{\top} \left( \left( \mathbf{w}^{\top} \left( \nabla_{\mathbf{a}^{\left(3\right)}} L^{\left(3\right)} \right) \circ \mathbf{h}^{\left(2\right)} \circ (1 - \mathbf{h}^{\left(2\right)}) \right) \right) \circ \mathbf{h}^{\left(1\right)} \circ (1 - \mathbf{h}^{\left(1\right)}) \right) x^{\left(1\right)}^{\top} \\ &= \left( \left( \mathbf{w}^{\top} \left( \left( \mathbf{w}^{\top} \left( \nabla_{\mathbf{h}^{\left(3\right)}} L^{\left(3\right)} \right) \circ \mathbf{h}^{\left(3\right)} \circ (1 - \mathbf{h}^{\left(3\right)}) \right) \right) \circ \mathbf{h}^{\left(2\right)} \circ (1 - \mathbf{h}^{\left(2\right)}) \right) \right) \circ \mathbf{h}^{\left(1\right)} \circ (1 - \mathbf{h}^{\left(1\right)}) \right) x^{\left(1\right)}^{\top} \end{split}$$

$$\begin{split} \nabla_{\mathcal{U}^{(1)}} L^{(3)} &= \left( \nabla_{\mathbf{a}^{(1)}} L^{(3)} \right) \mathbf{x}^{(1)}{}^{\top} \\ &= \left( \left( \nabla_{\mathbf{h}^{(1)}} L^{(3)} \right) \circ \mathbf{h}^{(1)} \circ (1 - \mathbf{h}^{(1)}) \right) \mathbf{x}^{(1)}{}^{\top} \\ &= \left( \left( \mathbf{w}^{\top} \left( \nabla_{\mathbf{a}^{(2)}} L^{(3)} \right) \right) \circ \mathbf{h}^{(1)} \circ (1 - \mathbf{h}^{(1)}) \right) \mathbf{x}^{(1)}{}^{\top} \\ &= \left( \left( \mathbf{w}^{\top} \left( \left( \nabla_{\mathbf{h}^{(2)}} L^{(3)} \right) \circ \mathbf{h}^{(2)} \circ (1 - \mathbf{h}^{(2)}) \right) \right) \circ \mathbf{h}^{(1)} \circ (1 - \mathbf{h}^{(1)}) \right) \mathbf{x}^{(1)}{}^{\top} \\ &= \left( \left( \mathbf{w}^{\top} \left( \left( \mathbf{w}^{\top} \left( \nabla_{\mathbf{a}^{(3)}} L^{(3)} \right) \circ \mathbf{h}^{(2)} \circ (1 - \mathbf{h}^{(2)}) \right) \right) \circ \mathbf{h}^{(1)} \circ (1 - \mathbf{h}^{(1)}) \right) \mathbf{x}^{(1)}{}^{\top} \\ &= \left( \left( \mathbf{w}^{\top} \left( \left( \mathbf{w}^{\top} \left( \left( \nabla_{\mathbf{h}^{(3)}} L^{(3)} \right) \circ \mathbf{h}^{(3)} \circ (1 - \mathbf{h}^{(3)}) \right) \right) \circ \mathbf{h}^{(2)} \circ (1 - \mathbf{h}^{(2)}) \right) \right) \circ \mathbf{h}^{(1)} \circ (1 - \mathbf{h}^{(1)}) \right) \mathbf{x}^{(1)}{}^{\top} \\ &= \left( \left( \mathbf{w}^{\top} \left( \left( \mathbf{w}^{\top} \left( \left( \mathbf{v}^{\top} \left( \hat{\mathbf{y}}^{(3)} - \mathbf{y}^{(3)} \right) \right) \circ \mathbf{h}^{(3)} \circ (1 - \mathbf{h}^{(3)}) \right) \right) \circ \mathbf{h}^{(2)} \circ (1 - \mathbf{h}^{(2)}) \right) \right) \circ \mathbf{h}^{(1)} \circ (1 - \mathbf{h}^{(1)}) \right) \mathbf{x}^{(1)}{}^{\top} \end{split}$$

#### Taking a closer look

With some notation we can simplify these gradients as follows:

$$\nabla_{u^{(3)}} L^{(3)} = c x^{(3)}^T$$

$$abla_{\mathbf{U}^{(2)}} L^{(3)} = \left( \operatorname{diag}(\mathbf{b}^{(2)}) \mathbf{W}^T \mathbf{c} \right) \mathbf{x}^{(2)^T}$$

$$\nabla_{\textit{\textbf{U}}^{(1)}} \textit{\textbf{L}}^{(3)} = \left( \left( \textit{diag}(\textit{\textbf{b}}^{(1)}) \textit{\textbf{W}}^{T} \right) \left( \textit{diag}(\textit{\textbf{b}}^{(2)}) \textit{\textbf{W}}^{T} \right) \textit{\textbf{c}} \right) \textit{\textbf{x}}^{(1)^{T}}$$

#### Vanishing

If we initialize W such that ||W|| < 1, the gradient for further time steps will be very small (vanishing problem).

https://www.youtube.com/watch?v=xAl8fu8myW0

#### **Exploding**

If  $|| {\it W} || > 1$ , the gradient for further time steps will be larger and larger (exploding problem).

https://www.youtube.com/watch?v=dqW-jw5qKK8

#### The vanishing problem

The gradients from the steps closed to  $\tau$  (the last step) have more influence than the ones very far back.

This is bad for capturing long-term dependecies.

#### Possible solutions (hacks)

- Clip gradients to a maximum value.
- Choosing the right activation functions, e.g. ReLU.
- Initialize weights to the identity matrix.
- LSTM (Long Short-Term Memory), GRU (Gated Recurrent Unit), etc

Implementation

#### **Truncated Back Propagation**

www.tensorflow.org/versions/master/tutorials/recurrent

"By design, the output of a recurrent neural network (RNN) depends on arbitrarily distant inputs. Unfortunately, this makes backpropagation computation difficult. In order to make the learning process tractable, it is common practice to create an 'unrolled' version of the network, which contains a fixed number (num\_steps) of LSTM inputs and outputs."

#### **Tensorflow implementation**

```
self.rnn outputs = []
2
   initialshape = (self.batch_size, self.hidden_size)
3
   Wshape = (self.hidden size, self.hidden size)
   Ushape = (self.embed size, self.hidden size)
5
   Vshape = (self.config.hidden_size, self.vocab_size)
6
7
   with tf.variable scope("memory"):
8
       self.initial_state = tf.zeros(initialshape)
9
10
   with tf.variable_scope("hidden"):
11
       self.W = tf.get_variable("W", shape=Wshape)
12
       self.input_weights = init_wb(Ushape, "input_weights")
13
```

#### **Tensorflow implementation**

```
previous_h = self.initial_state
   for i, tensor in enumerate(self.inputs):
2
              # len(self.inputs) = num steps
3
        with tf.variable scope("RNN", reuse=True):
4
            drop_tensor = tf.nn.dropout(tensor,
5
                                         self.dropout_placeholder)
6
            h = (tf.matmul(previous h, self.W) +
7
                 affine_transformation(drop_tensor,
8
                                        self.input weights))
9
            h = tf.nn.dropout(tf.sigmoid(h),
10
                               self.dropout_placeholder)
11
            self.rnn outputs.append(h)
12
            previous h = h
13
            if i == (len(self.inputs) - 1):
14
                self.final state = h
15
```

#### **Tensorflow implementation**

#### MytwitterBot: TrumpBot

https://github.com/felipessalvatore/MyTwitterBot



#### Felipe Salvatore

@Felipessalvador

Hillary can make america great again.

@greta @MarkBurnettTV #DinheiroNãoCompra #SecretBallot #خسوف القمر#

Traduzir do inglês

15:10 - 7 de ago de 2017



### Felipe Salvatore @Felipessalvador

Obama is all beautiful. I agree with people attacking me. Amazing. @CLewandowski\_#SecretBallot @garyplayer @greta

Traduzir do inglês

14:40 - 7 de ago de 2017

#### MytwitterBot: SakaBot

https://github.com/felipessalvatore/MyTwitterBot



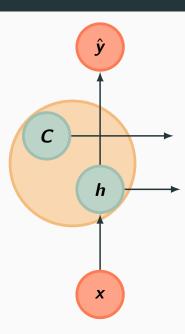
# Conclusion

#### What's next?

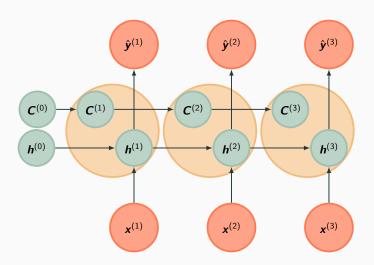
After some experiments with the hyper parameters my best result on the Penn Treebank (PTB) corpus was

Model	Val	Test
Mikolov et al (2011)[2]	163.2	149.9

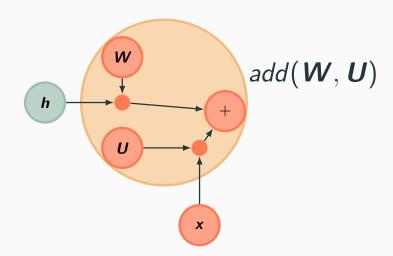
#### **LSTM**



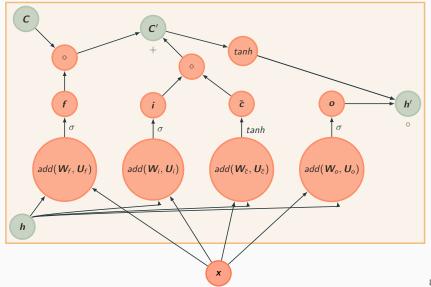
#### LSTM: unfolded model



#### **Simplification**



#### LSTM: recurrence



#### LSTM: equations

$$egin{aligned} oldsymbol{i}_t &= \sigma \left( oldsymbol{U}_i oldsymbol{x}_t + oldsymbol{W}_i oldsymbol{h}_{t-1} 
ight) \ oldsymbol{o}_t &= \sigma \left( oldsymbol{U}_o oldsymbol{x}_t + oldsymbol{W}_o oldsymbol{h}_{t-1} 
ight) \ oldsymbol{c}_t &= anh \left( oldsymbol{U}_c oldsymbol{x}_t + oldsymbol{W}_c oldsymbol{h}_{t-1} 
ight) \ oldsymbol{c}_t &= oldsymbol{f}_t \circ oldsymbol{c}_{t-1} + oldsymbol{i}_t \circ oldsymbol{ ilde{c}}_t \ oldsymbol{h}_t &= oldsymbol{o}_t \circ anh \left( oldsymbol{c}_t 
ight) \end{aligned}$$

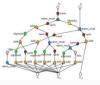
#### LSTM: changing cell

http://blog.ycombinator.com/jeff-deans-lecture-for-yc-ai/

#### "Normal" LSTM cell



# Cell discovered by architecture search



#### Penn Tree Bank Language Modeling Task

Model	Parameters	Test Perplexity	
Mikolov & Zweig (2012) - KN-5	2M <sup>‡</sup>	141.2	
Mikolov & Zweig (2012) - KN5 + cache	2M <sup>‡</sup>	125.7	
Mikolov & Zweig (2012) - RNN	6M <sup>‡</sup>	124.7	
Mikolov & Zweig (2012) - RNN-LDA	7M <sup>‡</sup>	113.7	
Mikolov & Zweig (2012) - RNN-LDA + KN-5 + cache	9M <sup>‡</sup>	92.0	
Pascanu et al. (2013) - Deep RNN	6M	107.5	
Cheng et al. (2014) - Sum-Prod Net	5M <sup>‡</sup>	100.0	
Zaremba et al. (2014) - LSTM (medium)	20M	82.7	
Zaremba et al. (2014) - LSTM (large)	66M	78.4	
Gal (2015) - Variational LSTM (medium, untied)	20M	79.7	
Gal (2015) - Variational LSTM (medium, untied, MC)	20M	78.6	
Gal (2015) - Variational LSTM (large, untied)	66M	75.2	
Gal (2015) - Variational LSTM (large, untied, MC)	66M	73.4	
Kim et al. (2015) - CharCNN	19M	78.9	
Press & Wolf (2016) - Variational LSTM, shared embeddings	24M	73.2	
Merity et al. (2016) - Zoneout + Variational LSTM (medium)	20M	80.6	
Merity et al. (2016) - Pointer Sentinel-LSTM (medium)	21M	70.9	
Zilly et al. (2016) - Variational RHN, shared embeddings	24M	66.0	
Neural Architecture Search with base 8	32M	67.9	
Neural Architecture Search with base 8 and shared embeddings	25M	64.0	
Neural Architecture Search with base 8 and shared embeddings	54M	62.4	

Table 2: Single model perplexity on the test set of the Penn Treebank language modeling task. Parameter numbers with  $^{\ddagger}$  are estimates with reference to Merity et al. (2016).

#### LSTM: https://arxiv.org/abs/1708.02182



Seguindo

When Zoph & Le at Google got 62 perplexity on PTB, I thought it'd be impossible to beat. Amazing progress in AI atm.

arxiv.org/abs/1708.02182

Traduzir do inglês

Model results over Penn Treebank (PTB)		Val	Test	
Grave et al. (2016) - LSTM	-	17-71	82.3	
Grave et al. (2016) - LSTM + continuous cache pointer	-	-	72.1	
Inan et al. (2016) - Variational LSTM (tied) + augmented loss	24M	75.7	73.2	
Inan et al. (2016) - Variational LSTM (tied) + augmented loss	51M	71.1	68.5	
Zilly et al. (2016) - Variational RHN (tied)	23M	67.9	65.4	
Zoph & Le (2016) - NAS Cell (tied)	25M	-	64.0	
Zoph & Le (2016) - NAS Cell (tied)	54M	_	62.4	
Melis et al. (2017) - 4-layer skip connection LSTM (tied)	24M	60.9	58.3	
AWD-LSTM - 3-layer LSTM (tied)	24M	60.0	57.3	
AWD-LSTM - 3-layer LSTM (tied) + continuous cache pointer	24M	53.9	52.8	

01:47 - 8 de ago de 2017

#### References I



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