An introduction to Recurrent Neural Networks

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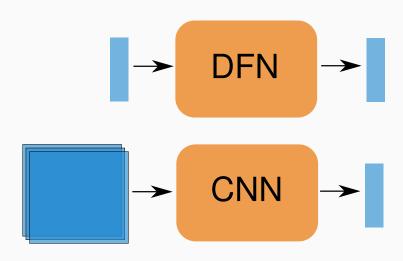
IME-USP: Institute of Mathematics and Statistics, University of São Paulo

Introduction

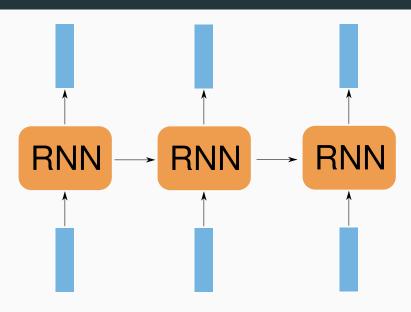
Basic idea

- 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).

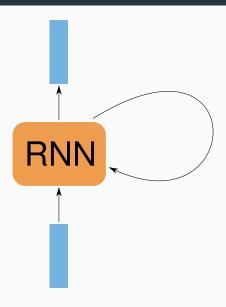
DFN and CNN



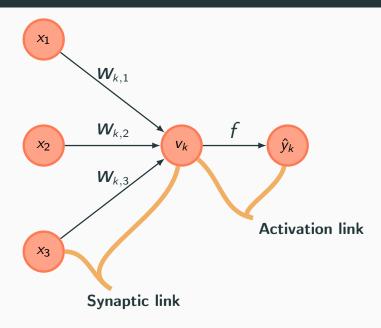
RNN: unfold representation



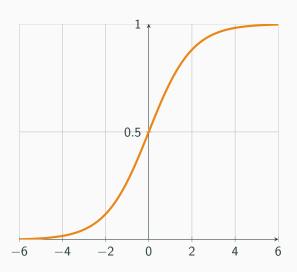
RNN: cyclic representation



Graph Representation



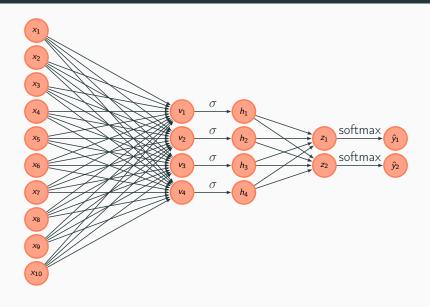
Recap: sigmoid function

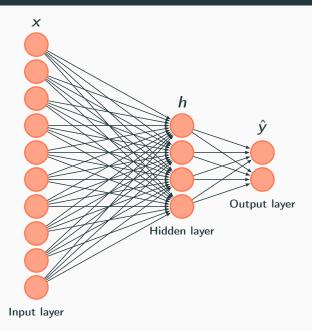


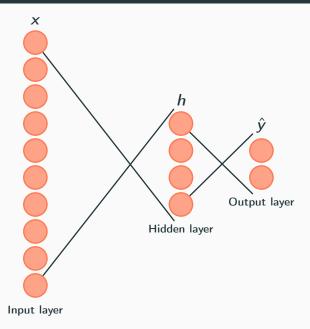
$$\sigma(x) = \frac{1}{1 + e^{-x}}$$

Recap: softmax function

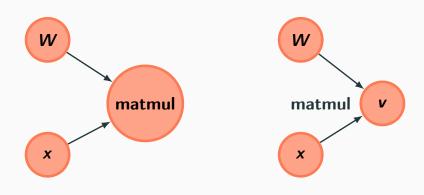
$$softmax(x) = \frac{e^x}{\sum e^x}$$





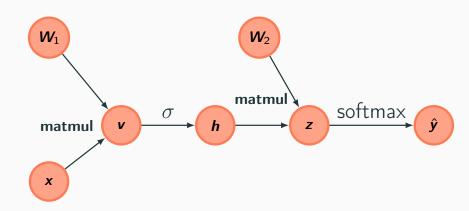


Computational Graphs



v = Wx

Computational Graphs



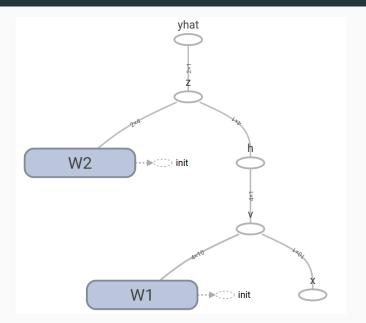
Tensorflow graph

```
import tensorflow as tf
   import numpy as np
2
3
   input_shape = [10,1]
4
   input_to_hidden_shape = [4,10]
5
   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
```

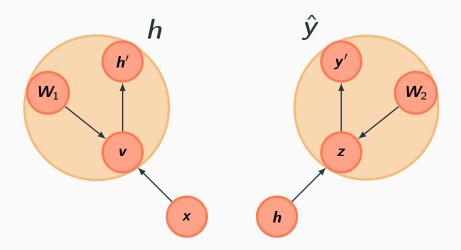
Tensorflow graph

```
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)
        z = tf.matmul(W2, h)
9
        yhat = tf.nn.softmax(z)
10
```

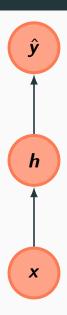
Tensorboard visualization



Computational Graphs



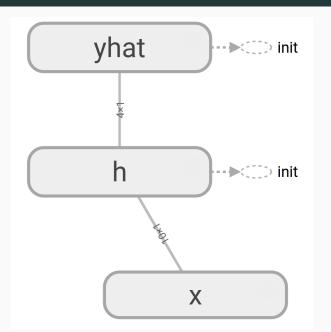
Computational Graphs



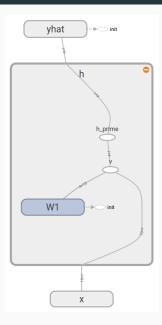
Tensorflow graph

```
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

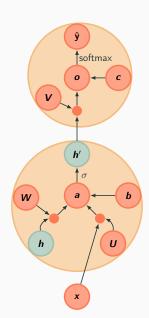


Tensorboard visualization

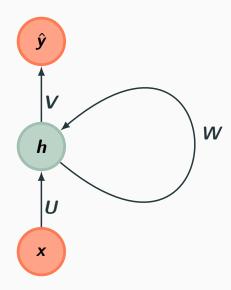


RNN: the model

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

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

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

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

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

Unfolding the state equation

For a finite number of steps τ , the recurrent definition can be unfolded.

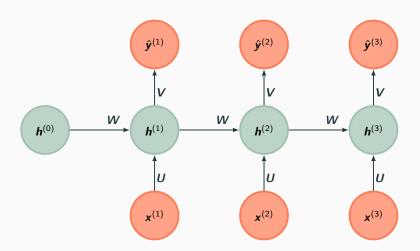
For example when $\tau = 3$:

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

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

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

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):

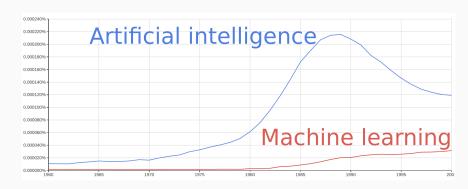
$$P_{bi}(x_1, x_2, x_3, x_4) = P(x_1)P(x_2|x_1)P(x_3|x_2)P(x_4|x_3)$$

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: Meditations in an Emergency by Frank O'Hara.

Am I to become profligate as if I were a blonde? Or religious as if I were French?

Each time my heart is broken it makes me feel more adventurous ...

- *T* = 645
- |V| = 347

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:

$$(x^{(1)}, y^{(1)}) = (Am, I).$$

 $(x^{(2)}, y^{(2)}) = (I, to)$
 $(x^{(3)}, y^{(3)}) = (to, become)$
 $(x^{(3)}, y^{(3)}) = (become, profligate)$
 $(x^{(4)}, y^{(4)}) = (profligate, as)$
 $(x^{(5)}, y^{(5)}) = (as, if)$
 $(x^{(6)}, y^{(6)}) = (if, I)$

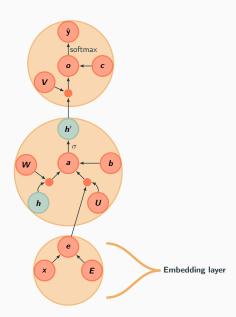
Notation

- $\mathbf{E} \in \mathbb{R}^{d,|\mathbb{V}|}$ 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).

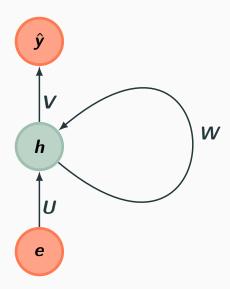
Recap: selecting word embeddings

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

The language model: graph



The language model: graph



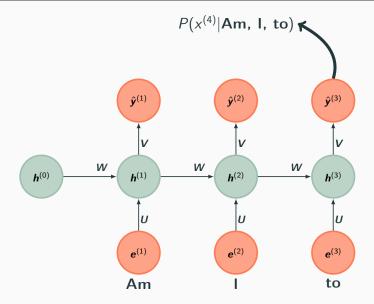
The language model: equations

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

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

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

The Language model: unfolding example



Recap: cross entropy

$$CE(y, \hat{y}) = -\sum_{i} y_{i} \log(\hat{y}_{i})$$

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:

$$L^{(3)} = -\log P(x^{(4)} = \text{become} | Am, I, to)$$

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 poem as C:

Am I to become profligate as if I were a blonde?

- *T* = 12
- \bullet $|\mathbb{V}| = 11$

Loss function: example

$$\begin{split} L &= -\frac{1}{12}[\log P(\mathsf{Am}| < \mathsf{eos} >) \\ &+ \log P(\mathsf{I}|\mathsf{Am}) \\ &+ \log P(\mathsf{to}|\mathsf{Am},\mathsf{I}) \\ &+ \log P(\mathsf{become}|\mathsf{Am},\mathsf{I},\mathsf{to}) \\ &+ \log P(\mathsf{profligate}|\mathsf{Am},\mathsf{I},\mathsf{to},\mathsf{become}) \\ &+ \log P(\mathsf{profligate}|\mathsf{Am},\mathsf{I},\mathsf{to},\mathsf{become},\mathsf{profligate}) \\ &+ \log P(\mathsf{if}|\mathsf{Am},\mathsf{I},\mathsf{to},\mathsf{become},\mathsf{profligate},\mathsf{as}) \\ &+ \log P(\mathsf{I}|\mathsf{Am},\mathsf{I},\mathsf{to},\mathsf{become},\mathsf{profligate},\mathsf{as},\mathsf{if}) \\ &+ \log P(\mathsf{were}|\mathsf{Am},\mathsf{I},\mathsf{to},\mathsf{become},\mathsf{profligate},\mathsf{as},\mathsf{if},\mathsf{I}) \\ &+ \log P(\mathsf{a}|\mathsf{Am},\mathsf{I},\mathsf{to},\mathsf{become},\mathsf{profligate},\mathsf{as},\mathsf{if},\mathsf{I},\mathsf{were}) \\ &+ \log P(\mathsf{blonde}|\mathsf{Am},\mathsf{I},\mathsf{to},\mathsf{become},\mathsf{profligate},\mathsf{as},\mathsf{if},\mathsf{I},\mathsf{were},\mathsf{a}) \\ &+ \log P(<\mathsf{eos} > |\mathsf{Am},\mathsf{I},\mathsf{to},\mathsf{become},\mathsf{profligate},\mathsf{as},\mathsf{if},\mathsf{I},\mathsf{were},\mathsf{a},\mathsf{blonde})] \end{split}$$

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)

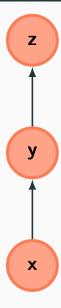
$$\frac{dz}{dx} = \frac{dz}{dy}\frac{dy}{dx}$$

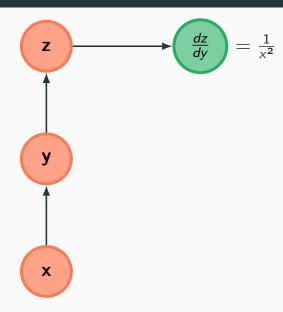
Chain rule: example

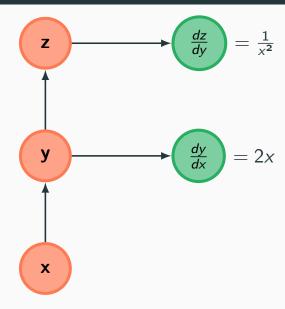
•
$$y = x^2$$

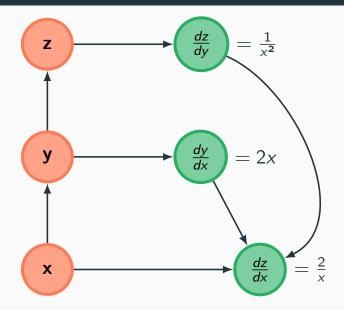
•
$$z = \log(y)$$

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









Chain rule: vector notation

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

•
$$z = f(g(x)) = f(y)$$

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

Chain rule: vector notation

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

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

Recap: gradient

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

Recap: Jacobian matrix

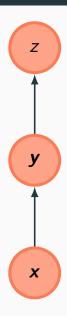
$$\frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_1}{\partial x_2} & \dots & \frac{\partial y_1}{\partial x_m} \\ \vdots & \ddots & \dots & \vdots \\ \frac{\partial y_n}{\partial x_1} & \frac{\partial y_n}{\partial x_2} & \dots &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

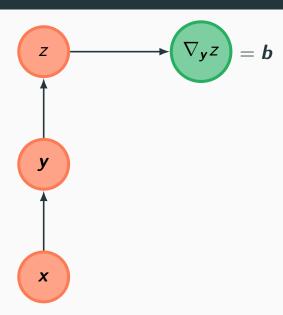
Chain rule: example

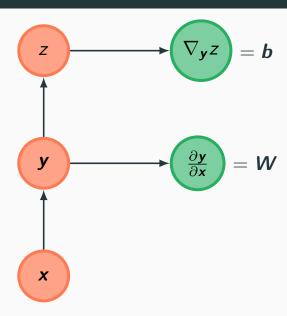
$$\bullet$$
 $y = Wx$

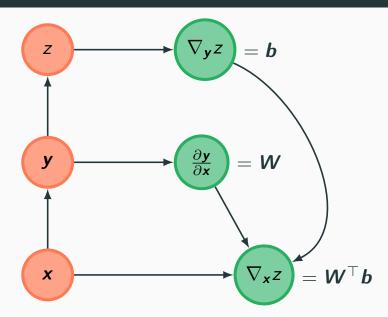
$$\bullet \ z = \boldsymbol{b}^T \boldsymbol{y}$$

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









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

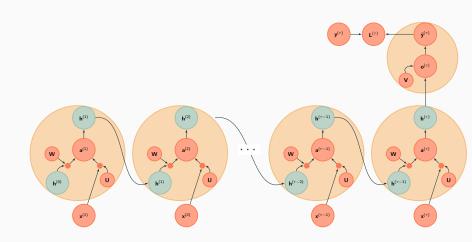
$$\mathbf{a}^{(t)} = \mathbf{W} \mathbf{h}^{(t-1)} + \mathbf{U} \mathbf{x}^{(t)}$$

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

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

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

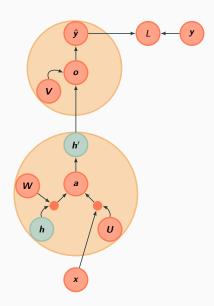
RNN time unfolding

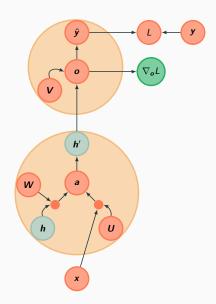


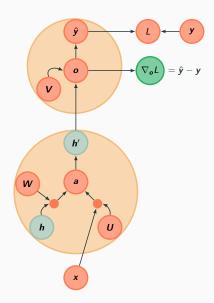
Recap: Hadamard product

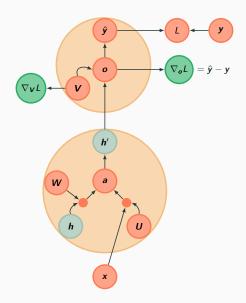
$$(x \circ y)_i = x_i y_i$$

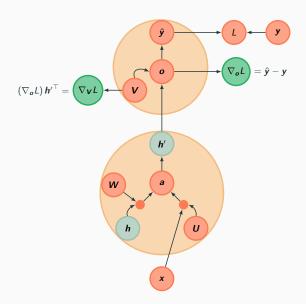
$$(x \circ y) = diag(y)x$$

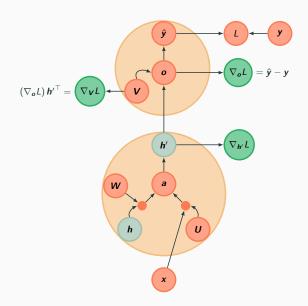


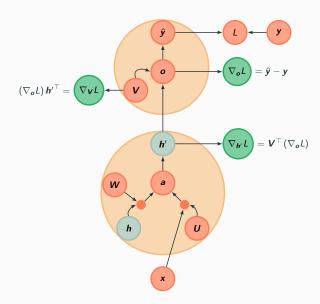


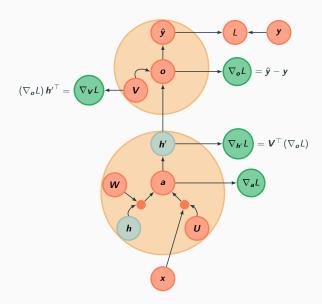


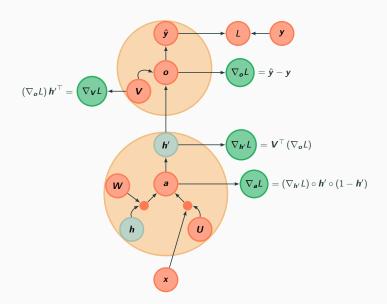


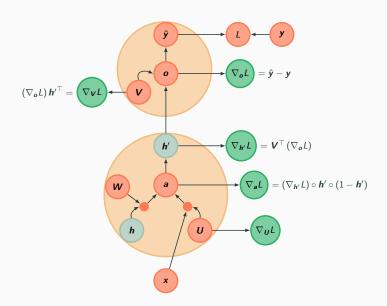


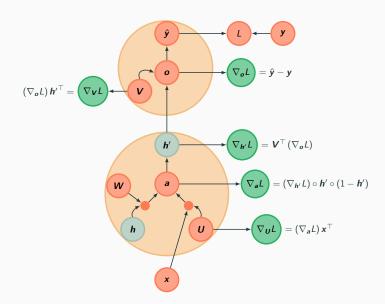


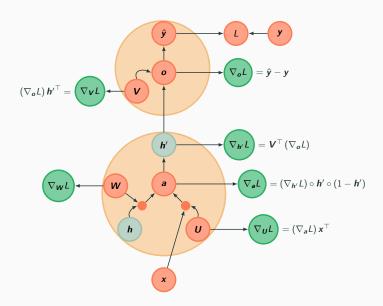


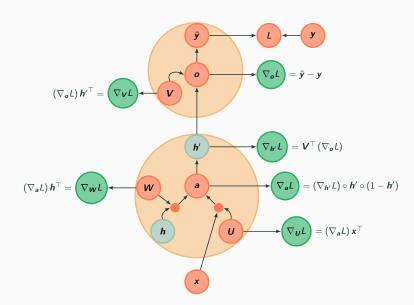


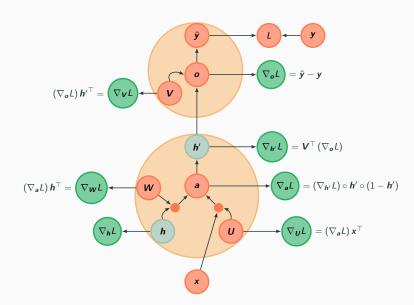


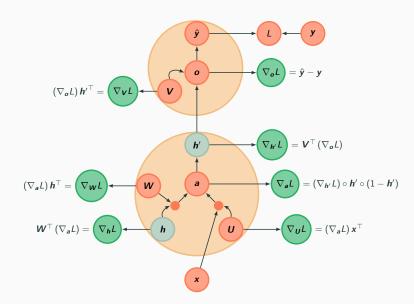


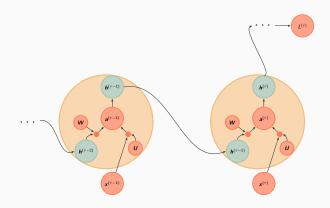


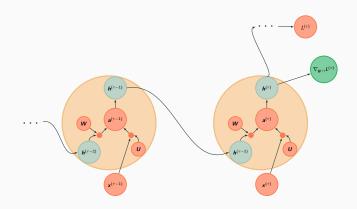


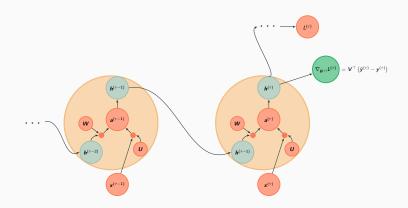


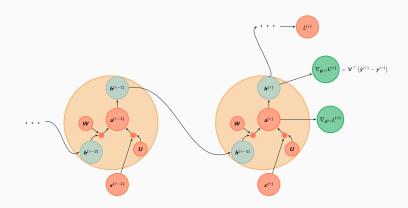


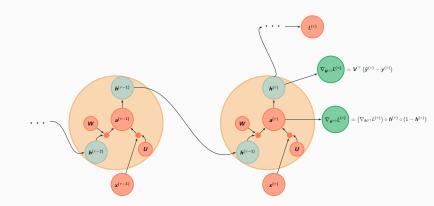


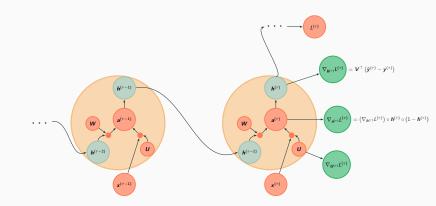


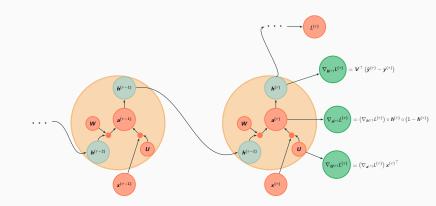


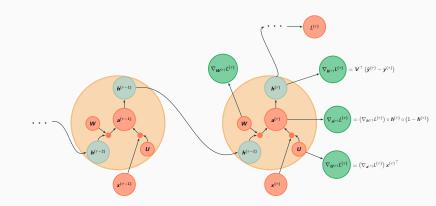


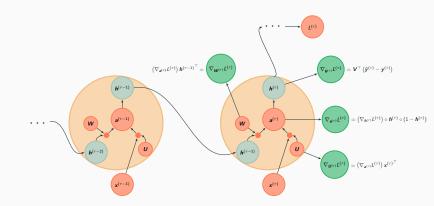


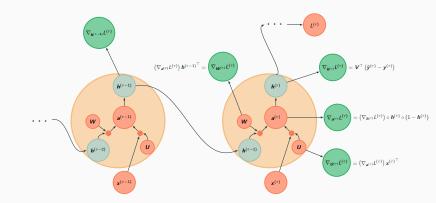


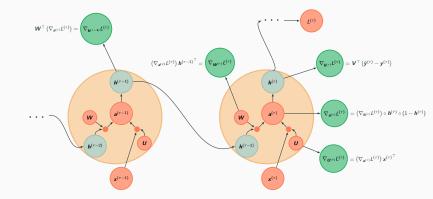


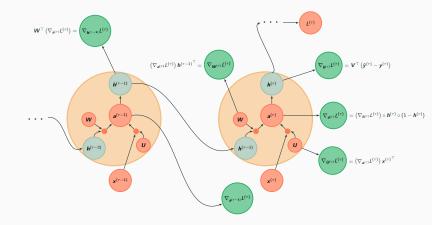


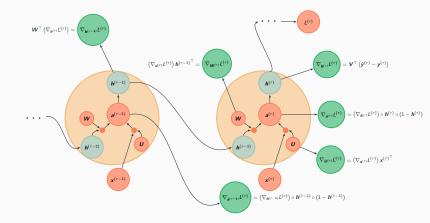


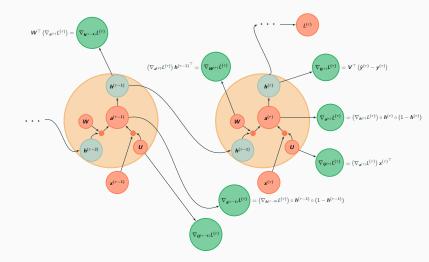


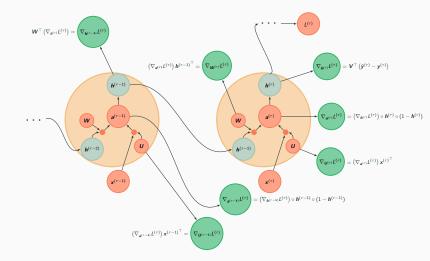


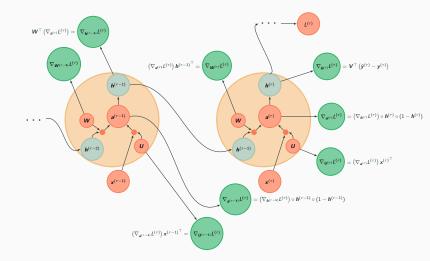


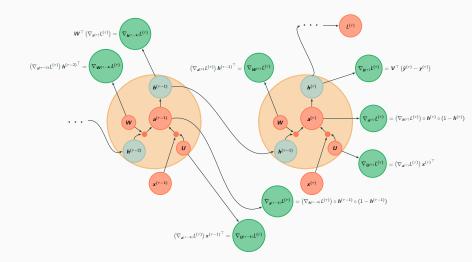


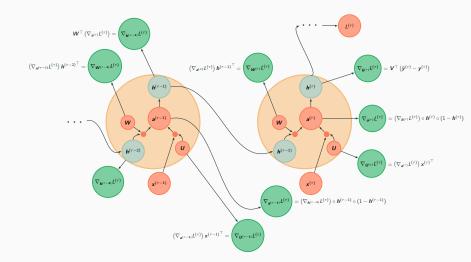


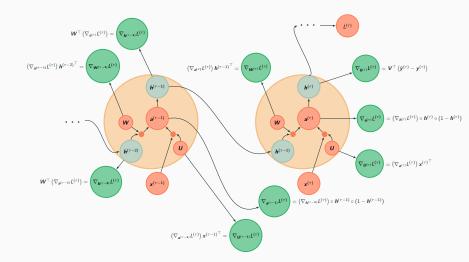












The gradients on \boldsymbol{V} , \boldsymbol{W} and \boldsymbol{U} are:

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

$$abla_{oldsymbol{W}} L^{(au)} = \sum_{t=1}^{ au}
abla_{oldsymbol{W}^{(t)}} L^{(au)}$$

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

Gradient

Vanishing or Exploding

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Taking a closer look

With some notation we can simplify these gradients as follows:

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

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

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

Taking a closer look

$$\nabla_{\boldsymbol{U^{(1)}}} L^{(\tau)}$$

$$= \left(\left(\operatorname{diag}(\boldsymbol{b^{(1)}}) \boldsymbol{W}^{T} \right) \left(\operatorname{diag}(\boldsymbol{b^{(2)}}) \boldsymbol{W}^{T} \right) \dots \left(\operatorname{diag}(\boldsymbol{b^{(\tau-1)}}) \boldsymbol{W}^{T} \right) \boldsymbol{c} \right) \boldsymbol{x^{(1)}}^{T}$$

Gradient for further time steps will have more matrix products using $diag(b)W^T$.

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

 $\verb|https://www.youtube.com/watch?v=dqW-jw5qKK8||$

The vanishing problem

The gradients from the steps closed to τ (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)
1.1
            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 |

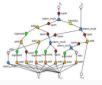
LSTM

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 [‡] | 141.2 |
| Mikolov & Zweig (2012) - KN5 + cache | 2M [‡] | 125.7 |
| Mikolov & Zweig (2012) - RNN | 6M [‡] | 124.7 |
| Mikolov & Zweig (2012) - RNN-LDA | 7M [‡] | 113.7 |
| Mikolov & Zweig (2012) - RNN-LDA + KN-5 + cache | 9M [‡] | 92.0 |
| Pascanu et al. (2013) - Deep RNN | 6M | 107.5 |
| Cheng et al. (2014) - Sum-Prod Net | 5M [‡] | 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 ‡ 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 | - | 1-1 | 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 | |

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