CS 6501 Natural Language Processing

Recurrent Neural Networks

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November 12, 2019

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Overview

1. Recurrent Neural Networks
2. RNN Language Modeling
3. Challenge of Training RNNs
4. Variants of RNNs

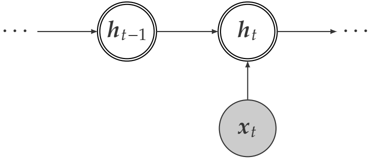
Recurrent Neural Networks

RNNs

A simple RNN is defined as

$$h_t = f(x_t, h_{t-1}) \tag{1}$$

where x_t and h_t is the input and hidden state at time t[1]



[1] Double circles indicate non-random nodes

Transition Function

For the simplest case, f is an element-wise sigmoid function as

$$f(\boldsymbol{x}_t, \boldsymbol{h}_{t-1}) = \sigma(\mathbf{W}_h \boldsymbol{h}_{t-1} + \mathbf{W}_i \boldsymbol{x}_t + \boldsymbol{b}) \tag{2}$$

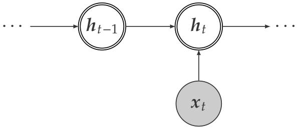
where

- $\mathbf{W}_h$: parameter matrix for hidden states
- $\mathbf{W}_i$: parameter matrix for inputs
- $\boldsymbol{b}$: bias term (also a parameter)

Unfolding RNNs

Recursive:

$$\boldsymbol{h}_t = \boldsymbol{f}(\boldsymbol{x}_t, \boldsymbol{h}_{t-1}) \tag{3}$$



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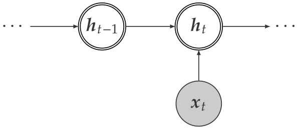
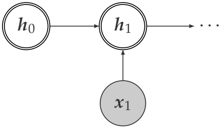


Unfolded:

$$\begin{aligned}
\boldsymbol{h}_t &= f(\boldsymbol{x}_t, f(\boldsymbol{x}_{t-1}, \boldsymbol{h}_{t-2})) \\
&= f(\boldsymbol{x}_t, f(\boldsymbol{x}_{t-1}, f(\boldsymbol{x}_{t-2}, \boldsymbol{h}_{t-3}))) \\
&= \cdots \\
&= f(\boldsymbol{x}_t, f(\boldsymbol{x}_{t-1}, f(\boldsymbol{x}_{t-2}, \cdots f(\boldsymbol{x}_1, \boldsymbol{h}_0) \cdots))) \qquad (4)
\end{aligned}$$

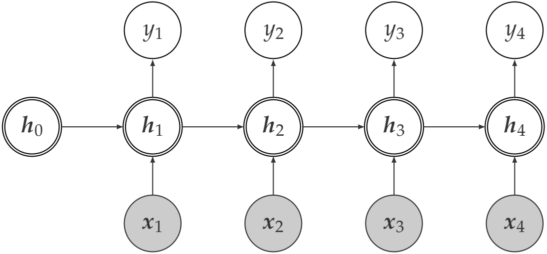
Base Condition



$$h_t = f(x_t, f(x_{t-1}, f(x_{t-2}, \cdots f(x_1, h_0) \cdots))) \tag{5}$$

- h_0: zero vector or parameter
- x_1: input at time $t = 1$

Plot



For Sequential Modeling

Loss at single time step t

$$L_t(y_t, \hat{y}_t) = \text{cross-entropy}(y_t, \hat{y}_t) \tag{6}$$

where y_t and $\hat{y}_t = g(\boldsymbol{h}_t)$ are the ground truth and predicted output respectively.

The total loss is given as

$$\ell = \sum_{t=1}^{T} L_t(y_t, \hat{y}_t) \tag{7}$$

RNN Language Modeling

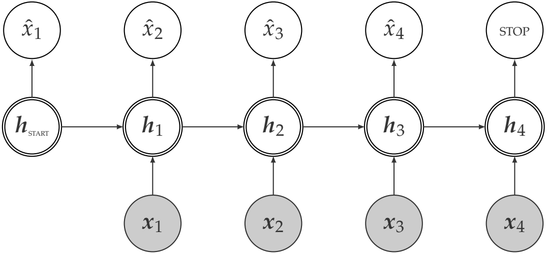
RNN Language Models

For a given sentence $\{x_1, \ldots, x_T\}$, the input at time t is word embedding $\boldsymbol{x}_t$. The probability distribution of next word X_{t+1}

$$P(X_{t+1} = x) = \frac{\exp(\boldsymbol{w}_{o,x}^\top \boldsymbol{h}_t)}{\sum_{x'} \exp(\boldsymbol{w}_{o,x'}^\top \boldsymbol{h}_t)} \tag{8}$$

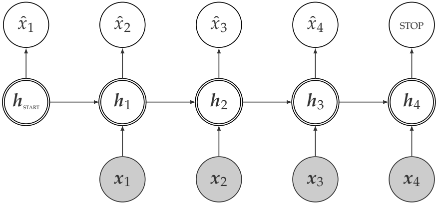
where $\boldsymbol{w}_{o,x}$ is the output weight vector related to word x.

Plot



$\hat{x}_1$
$\hat{x}_2$
$\hat{x}_3$
$\hat{x}_4$
STOP
h_{START}
h_1
h_2
h_3
h_4
x_1
x_2
x_3
x_4

Special Cases



$$\{\texttt{start}, x_1, \ldots, x_T, \texttt{stop}\}$$

- at time $t = 1$

$$P(X_1 = x) \propto \exp(\boldsymbol{w}_{o,x}^\top \boldsymbol{h}_{\texttt{start}}) \tag{9}$$

- at time $t = T$

$$P(X_T = \texttt{stop}) \propto \exp(\boldsymbol{w}_{o,x}^\top \boldsymbol{h}_T) \tag{10}$$

Normalization Term

$$P(X_{t+1} = x) = \frac{\exp(\boldsymbol{w}_{o,x}^\top \boldsymbol{h}_t)}{\sum_{x'} \exp(\boldsymbol{w}_{o,x'}^\top \boldsymbol{h}_t)} \tag{11}$$

Options:

- Negative sampling (x)
- Class-factored softmax

Class-factored Softmax: Definition

- Partition the vocab into K classes $\{\mathscr{C}_1, \ldots, \mathscr{C}_K\}$, such that $\mathscr{V} = \cup \mathscr{C}_k$ and $\mathscr{C}_k \cap \mathscr{C}_{k'} = \emptyset$ for any $k' \neq k$

[Baltescu and Blunsom, 2014]

Class-factored Softmax: Definition

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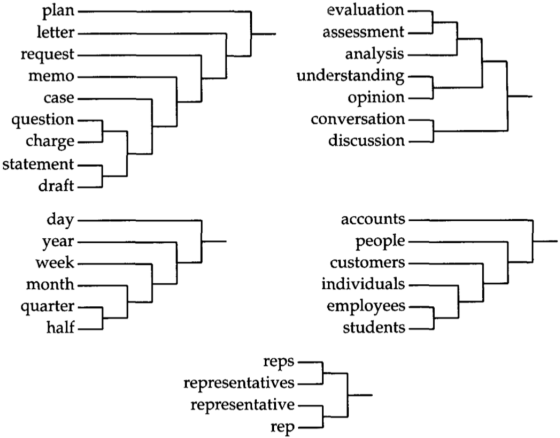
- Define the probability distribution of word as

$$\begin{aligned} P(X_{t+1} = x; \boldsymbol{h}_t) =& P(X_{t+1} = x, C_{t+1} = c; \boldsymbol{h}_t) \\ =& P(X_{t+1} = x \mid C_{t+1} = c; \boldsymbol{h}_t) \\ & \cdot P(C_{t+1} = c \mid \boldsymbol{h}_t) \end{aligned} \tag{12}$$

[Baltescu and Blunsom, 2014]

Class-factored Softmax: Word clusters

Brown clusters



[Brown et al., 1992]

Computational Complexity

Given

- $|\mathcal{V}|$ is the vocab size
- D is the dimension of hidden representations

Model	Training/Decoding
Standard	$\mathcal{O}(\|\mathcal{V}\| \cdot D)$
Class-factored	$\mathcal{O}(\sqrt{\|\mathcal{V}\|} \cdot D)$

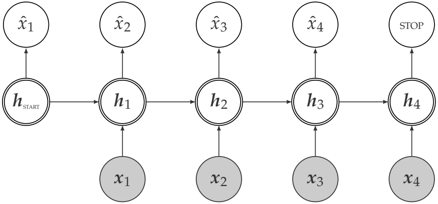
Table: Computational complexities of different softmax functions.

Challenge of Training RNNs

Backpropagation Through Time

Consider the gradient of ℓ with respect to the network parameters $\boldsymbol{\theta} = \{\mathbf{W}_h, \mathbf{W}_i, \boldsymbol{b}\}$,

$$\frac{\partial \ell}{\partial \boldsymbol{\theta}} = \sum_{t=1}^{T} \frac{\partial L_t}{\partial \boldsymbol{\theta}} \tag{13}$$

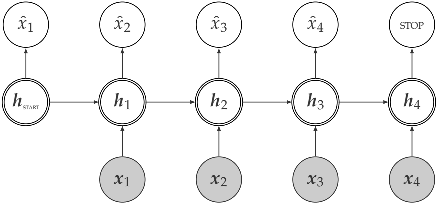


Backpropagation Through Time [Rumelhart et al., 1985, BPTT]

Gradients

For each time step t, we have

$$\frac{\partial L_t}{\partial \boldsymbol{\theta}} = \sum_{i=1}^{t} \left\{ \frac{\partial L_t}{\partial \boldsymbol{h}_t} \cdot \left(\prod_{j=i}^{t-1} \frac{\partial \boldsymbol{h}_{j+1}}{\partial \boldsymbol{h}_j} \right) \cdot \frac{\partial \boldsymbol{h}_i}{\partial \boldsymbol{\theta}} \right\} \tag{14}$$



Challenges

$$\frac{\partial L_t}{\partial \boldsymbol{\theta}} = \sum_{i=1}^{t} \left\{ \frac{\partial L_t}{\partial \boldsymbol{h}_t} \cdot \left(\prod_{j=i}^{t-1} \frac{\partial \boldsymbol{h}_{j+1}}{\partial \boldsymbol{h}_j} \right) \cdot \frac{\partial \boldsymbol{h}_i}{\partial \boldsymbol{\theta}} \right\} \tag{15}$$

- vanishing gradients
- exploding gradients

[Pascanu et al., 2013]

Exploding Gradients

Solution: **norm clipping** [Pascanu et al., 2013].

Consider the gradient $\boldsymbol{g} = \frac{\partial \ell}{\partial \boldsymbol{\theta}}$,

$$\hat{\boldsymbol{g}} \leftarrow \tau \cdot \frac{\boldsymbol{g}}{\|\boldsymbol{g}\|} \tag{16}$$

when $\|\boldsymbol{g}\| > \tau$. Usually, $\tau = 3$ or 5 in practice.

Vanishing Gradients

Solution:

- initialize parameters carefully
- replace hidden state transition function $\sigma(\cdot)$ with other options

$$f(\boldsymbol{x}_t, \boldsymbol{h}_{t-1}) = \boldsymbol{\sigma}(\mathbf{W}_h \boldsymbol{h}_{t-1} + \mathbf{W}_i \boldsymbol{x}_t + \boldsymbol{b}) \tag{17}$$

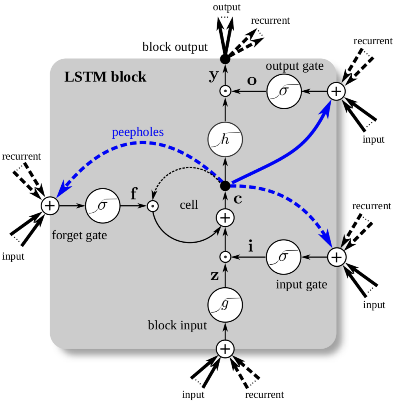
  - LSTM [Hochreiter and Schmidhuber, 1997]
  - GRU [Cho et al., 2014]

Long Short-Term Memory

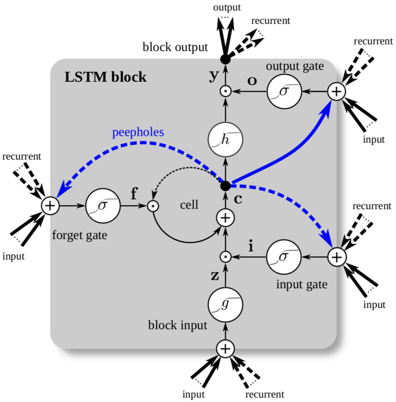
$$\begin{aligned}
\boldsymbol{i}_t &= \sigma(\mathbf{W}_{xi}\boldsymbol{x}_t + \mathbf{W}_{hi}\boldsymbol{h}_{t-1} + \mathbf{W}_{ci}\boldsymbol{c}_{t-1} + \boldsymbol{b}_i) && (18)\\
\boldsymbol{f}_t &= \sigma(\mathbf{W}_{xf}\boldsymbol{x}_t + \mathbf{W}_{hf}\boldsymbol{h}_{t-1} + \mathbf{W}_{cf}\boldsymbol{c}_{t-1} + \boldsymbol{b}_f) && (19)\\
\boldsymbol{c}_t &= \boldsymbol{f}_t \circ \boldsymbol{c}_{t-1} + \boldsymbol{i}_t \circ \tanh(\mathbf{W}_{xc}\boldsymbol{x}_t + \mathbf{W}_{hc}\boldsymbol{h}_{t-1} + \boldsymbol{b}_c) && (20)\\
\boldsymbol{o}_t &= \sigma(\mathbf{W}_{xo}\boldsymbol{x}_t + \mathbf{W}_{ho}\boldsymbol{h}_{t-1} + \mathbf{W}_{co}\boldsymbol{c}_t + \boldsymbol{b}_o) && (21)\\
\boldsymbol{h}_t &= \boldsymbol{o}_t \circ \tanh(\boldsymbol{c}_t) && (22)
\end{aligned}$$

$\circ$ is the element-wise multiplication [Graves, 2013]

LSTM


output
recurrent
block output
recurrent
LSTM block
y
o
output gate
σ
input
peepholes
h
recurrent
c
f
cell
σ
recurrent
forget gate
i
input
σ
z
input gate
input
g
block input
input
recurrent

LSTM



- Forget gate f_t — discounting on the memory cell
- Peephole connections (connections in blue color) [Gers and Schmidhuber, 2000]

Gated Recurrent Units

A gated recurrent unit (GRU) was proposed in [Cho et al., 2014].

$$
\begin{aligned}
\boldsymbol{r}_t &= \sigma(\mathbf{W}_{rx}\boldsymbol{x}_t + \mathbf{W}_{rh}\boldsymbol{h}_{t-1}) && (23)\\
\tilde{\boldsymbol{h}}_t &= \tanh(\mathbf{W}_{hx}\boldsymbol{x}_t + \mathbf{W}_{hr}(\boldsymbol{r}_t \odot \boldsymbol{h}_{t-1})) && (24)\\
\boldsymbol{z}_t &= \sigma(\mathbf{W}_{zx}\boldsymbol{x}_t + \mathbf{W}_{zh}\boldsymbol{h}_{t-1}) && (25)\\
\boldsymbol{h}_t &= (1 - \boldsymbol{z}_t) \odot \boldsymbol{h}_{t-1} + \boldsymbol{z}_t \odot \tilde{\boldsymbol{h}}_t && (26)\\
& && (27)
\end{aligned}
$$

Empirical results show GRU units are *comparable* to LSTM units [Chung et al., 2014].

Variants of RNNs

Overview

- Bi-directional RNNs
- Stacked (*or* Multi-layer) LSTM
- Memory networks [Weston et al., 2014]

Bi-directional RNNs

To construct a bi-directional RNN, we need another uni-directional RNN running from the end of the sequence to the beginning, as

$$\boldsymbol{u}_t = \boldsymbol{f}(\boldsymbol{x}_t, \boldsymbol{u}_{t+1}). \tag{28}$$

where $\boldsymbol{u}_t$ is the hidden state at time t in this new model.

[Schuster and Paliwal, 1997]

Stacked LSTM

Use the hidden state $\boldsymbol{h}_t^{(k)}$ from the current layer as input $\boldsymbol{x}_t^{(k+1)}$ to the next layer [Sutskever et al., 2014],

$$\boldsymbol{x}_t^{(k+1)} = \boldsymbol{h}_t^{(k)}. \tag{29}$$

[Sutskever et al., 2014]

Summary

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Reference

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