Deconstructing Recurrent Neural Networks

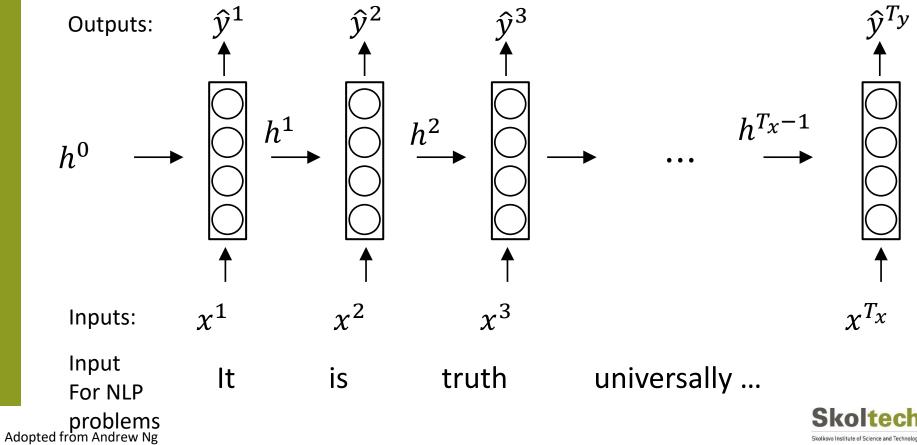
30 April, 2020

Alexey Zaytsev, head of Laboratory LARSS, PhD

Foundations of Data Science



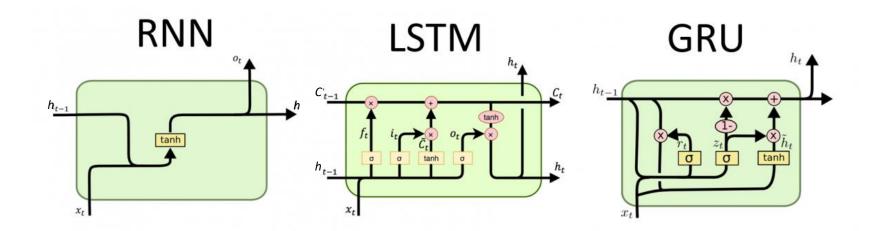
Forward propagation through Recurrent Neural Network



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Good RNN units are LSTM and GRU. Vanilla RNN is not good.

- LSTM: Long Short Term Memory
- GRU: Gated Recurrent Unit

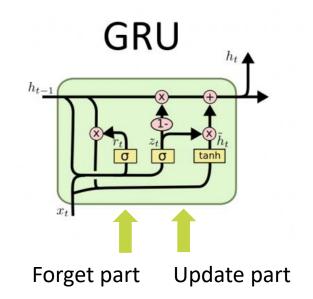




GRU – Gated Recurrent Unit

- Update gate what to pay attention to
- Reset gate what to forget

$$\mathbf{r}^{t} = \sigma(W_{xr}\mathbf{x}^{t} + W_{hr}\mathbf{h}^{t-1} + b_{r})$$
$$\mathbf{z}^{t} = \sigma(W_{xz}\mathbf{x}^{t} + W_{hz}\mathbf{h}^{t-1} + b_{z})$$

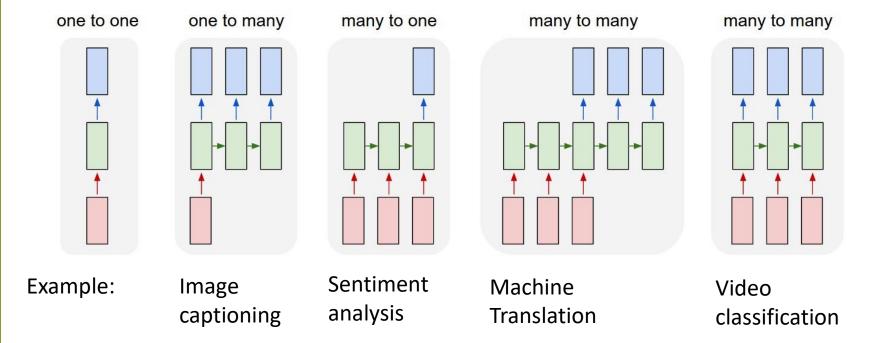


$$\widetilde{\boldsymbol{h}}^{t} = \tanh(W_{xh}\boldsymbol{x}^{t} + W_{hr}(\boldsymbol{r}^{t} \odot \boldsymbol{h}^{t-1}) + b_{h})$$

$$\boldsymbol{h}^{t} = \boldsymbol{z}^{t} \odot \boldsymbol{h}^{t-1} + (1 - \boldsymbol{z}^{t}) \odot \widetilde{\boldsymbol{h}}^{t}$$

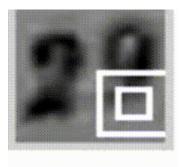


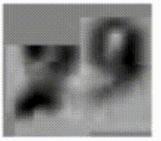
The Unreasonable Effectiveness of Recurrent Neural Networks



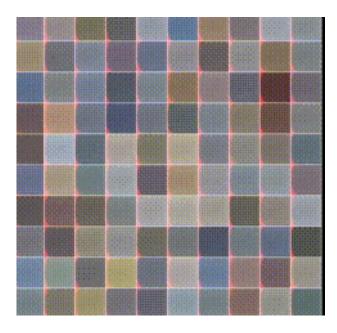


Sequential processing in absence of sequences





RNN learns to read house numbers

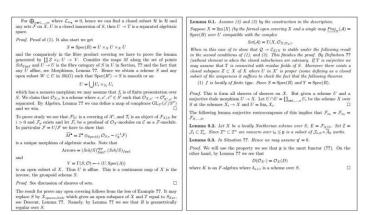


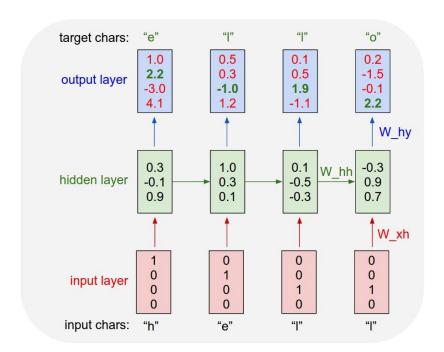
RNN learns to paint house numbers



Text generation (now there are better alternatives)

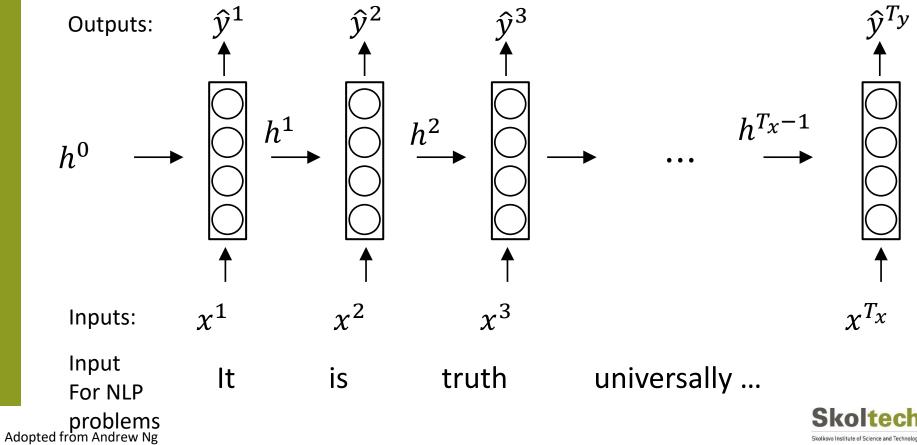
- Paul Graham generator
- Shakespeare
- Wikipedia
- Algebraic Geometry (Latex)
- Linux Source Code
- Generating Baby Names







Forward propagation through RNN



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Simple RNN model

$$h^t = f_h(x^t, h^{t-1})$$
Output \hat{y}^t

$$h^t = \tanh(Vx^t + Wh^{t-1} + b_h)$$
Cell state $h^{t-1} \rightarrow h^t$

$$\hat{y}^t = f_y(h^t)$$
Input x^t
vector $\hat{y}^t = \operatorname{softmax}(Uh^t + b_y)$



Backpropagation w.r.t. U

$$L = \sum_{i=1}^{T_y} L^i(\hat{y}^i, y^i)$$

$$\frac{\partial L}{\partial U} = \sum_{i=1}^{T_y} \frac{\partial L_i}{\partial U} = \sum_{i=1}^{T_y} \frac{\partial L_i}{\partial \hat{y}^i} \frac{\partial \hat{y}^i}{\partial U}$$

$$\hat{y}^{t} = \operatorname{softmax}(Uh^{t} + b_{y})$$

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

$$\hat{y}^{t}$$

$$\uparrow$$

$$h^{t-1} \rightarrow \qquad \rightarrow h^{t}$$

$$\uparrow$$

$$\uparrow$$



Backpropagation w.r.t. W

$$L = \sum_{i=1}^{T_y} L^i(\hat{y}^i, y^i)$$

$$\boldsymbol{h}^t = \tanh(V\boldsymbol{x}^t + W\boldsymbol{h}^{t-1} + b_h)$$

$$\frac{\partial L_i}{\partial \hat{y}^i} \frac{\partial \hat{y}^i}{\partial W} = \frac{\partial L_i}{\partial \hat{y}^i} \frac{\partial \hat{y}^i}{\partial h_t} (\frac{\partial h_t}{\partial W} + \frac{\partial h_t}{\partial h_{t-1}} \frac{\partial h_{t-1}}{\partial W} + \cdots)$$

$$\frac{\partial L_i}{\partial \hat{y}^i} \frac{\partial \hat{y}^i}{\partial W} = \frac{\partial L_i}{\partial \hat{y}^i} \frac{\partial \hat{y}^i}{\partial h_t} \sum_{i=0}^{T_y} (\prod_{j=i+1}^{T_y} \frac{\partial h_j}{\partial h_{i-1}}) \frac{\partial h_i}{\partial W}$$

$$\hat{y}^{t} = \operatorname{softmax}(Uh^{t} + b_{y})$$

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

$$\hat{y}^{t}$$

$$\uparrow$$

$$h^{t-1} \rightarrow \qquad \uparrow$$

$$\uparrow$$

$$\uparrow$$



Jacobian matrix is the cause of all problems

$$\boldsymbol{h}^t = \tanh(V\boldsymbol{x}^t + W\boldsymbol{h}^{t-1} + b_h)$$

$$\frac{\partial L_i}{\partial \hat{y}^i} \frac{\partial \hat{y}^i}{\partial W} = \frac{\partial L_i}{\partial \hat{y}^i} \frac{\partial \hat{y}^i}{\partial h_t} \left(\frac{\partial h_t}{\partial W} + \frac{\partial h_t}{\partial h_{t-1}} \frac{\partial h_{t-1}}{\partial W} + \cdots \right)$$

$$\frac{\partial L_i}{\partial \hat{y}^i} \frac{\partial \hat{y}^i}{\partial W} = \frac{\partial L_i}{\partial \hat{y}^i} \frac{\partial \hat{y}^i}{\partial h_t} \sum_{i=0}^{T_y} \left(\prod_{j=i+1}^{T_y} \frac{\partial h_j}{\partial h_{j-1}} \right) \frac{\partial h_i}{\partial W}$$

$$\left\| \frac{\partial h_j}{\partial h_{i-1}} \right\| > 1$$
 gradient exploration

$$\left\| \frac{\partial h_j}{\partial h_{i-1}} \right\|_2 < 1$$
 gradient vanishing

$$\hat{y}^{t} = \operatorname{softmax}(Uh^{t} + b_{y})$$

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

$$\hat{y}^{t}$$

$$\uparrow$$

$$h^{t-1} \rightarrow \qquad \uparrow$$

$$x^{t}$$



Gradient exploding and vanishing

$$\boldsymbol{h}^{j} = f(V\boldsymbol{x}^{j} + W\boldsymbol{h}^{j-1} + b_{h}) = f(\boldsymbol{z}_{t})$$

$$\frac{\partial h_j}{\partial h_{j-1}} = \frac{\partial h_j}{\partial z_j} \frac{\partial z_j}{\partial h_{j-1}} = \operatorname{diag}(f'(\boldsymbol{z}_t))W$$

$$\left\| \frac{\partial \boldsymbol{h}_j}{\partial \boldsymbol{h}_{i-1}} \right\| \le \left\| \operatorname{diag}(f'(\boldsymbol{z}_t)) \right\| \cdot \|W\|$$

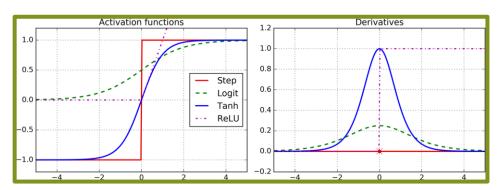


Gradient exploding and vanishing

$$\boldsymbol{h}^{j} = f(V\boldsymbol{x}^{j} + W\boldsymbol{h}^{j-1} + b_{h}) = f(\boldsymbol{z}_{t})$$

$$\frac{\partial h_j}{\partial h_{j-1}} = \frac{\partial h_j}{\partial z_j} \frac{\partial z_j}{\partial h_{j-1}} = \operatorname{diag}(f'(z_t))W$$

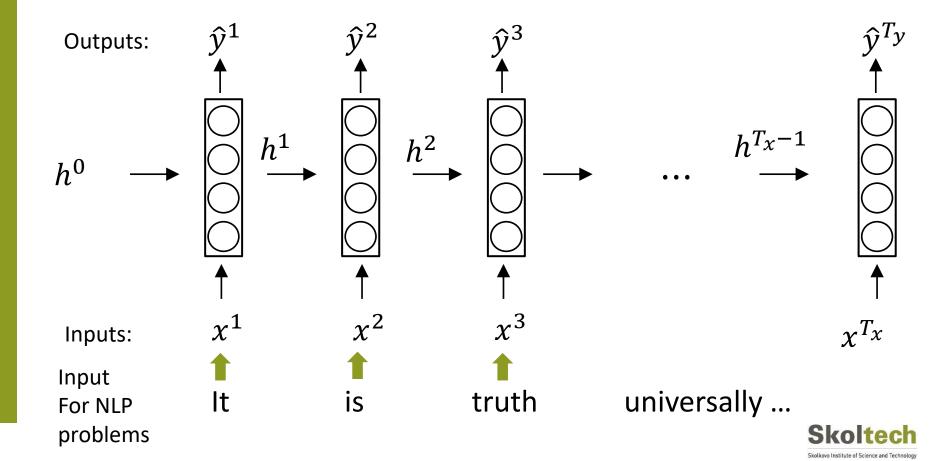
activation functionReLU is the best option



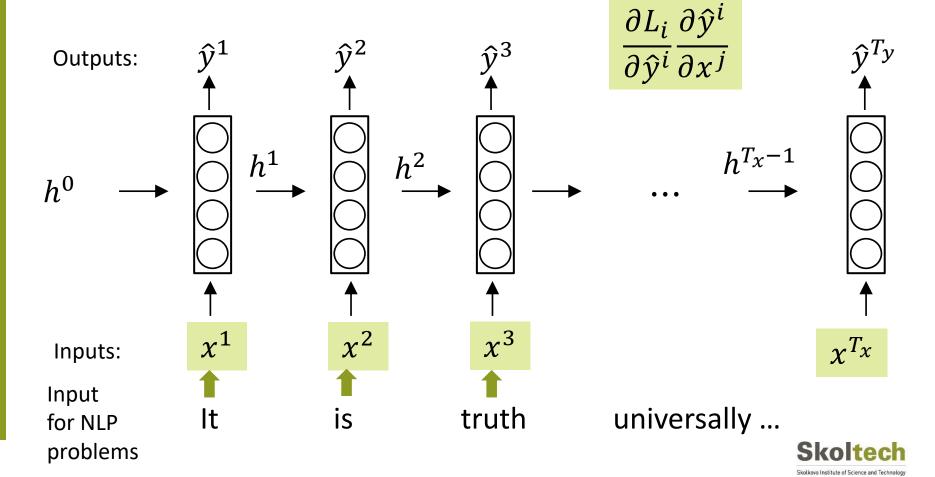
- The initialization matters For orthogonal matrix $Q^T = Q^{-1}$ all eigenvalues equals one
- Regularization



Embedding layer for RNNs



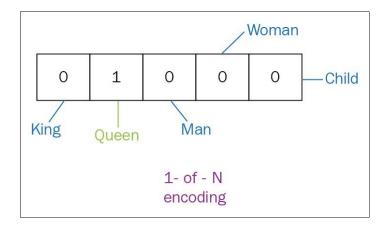
Backpropagation for embedding layer for RNNs



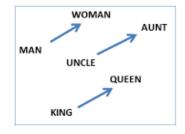
Learning of embeddings

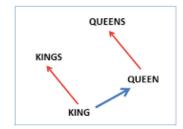
End2end learning of embeddings for:

- Words
- Codes of transactions (gas station)
- Prescription drugs
- Symbols or groups of symbols



One-hot encoding is also an embeddings





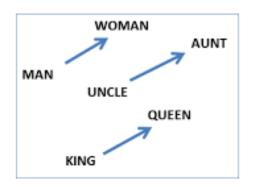
But we want something smarter

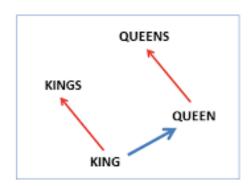


Why we need embeddings?

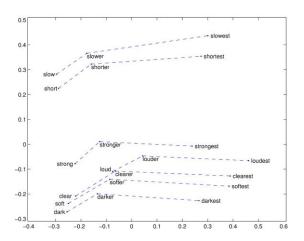
In NLP it is hard to measure quality of a solution, for example in Machine translation

 Check that we learn something adequate by comparing feature vectors for objects with similar relationships





Paris – France Moscow – Russia Vienna – Austria Antananarivo – Madagascar

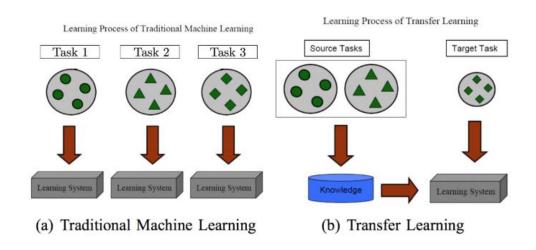




Why we need embeddings?

We finally have representation learning – but now for sequences

Use embeddings for transfer learning





Why we need embeddings?

Natural way to look at tokens

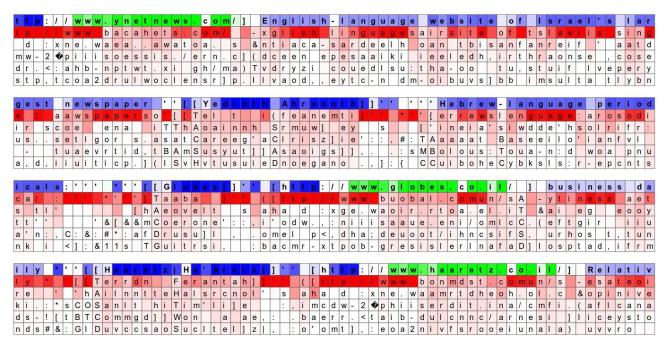
Use embeddings to find their similarity

Similarity	anim	al Ruffir	less dands	5000	K
aardvark	0.97	0.03	0.15	0.04	
black	0.07	0.01	0.20	0.95	
cat	0.98	0.98	0.45	0.35	
duvet	0.01	0.84	0.12	0.02	
zombie	0.74	0.05	0.98	0.93	



Visualizing embeddings

Character-level LSTM, look at some dimensions



The neuron highlighted in this image seems to get very excited about URLs and turns off outside of the URLs. The LSTM is likely using this neuron to remember if it is inside a URL or not.

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Visualizing embeddings

Character-level LSTM, look at some dimensions

```
Cell sensitive to position in line:
The sole importance of the crossing of the Berezina lies in the fact
that it plainly and indubitably proved the fallacy of all the plans for
cutting off the enemy's retreat and the soundness of the only possible
line of action--the one Kutuzov and the general mass of the army
demanded--namely, simply to follow the enemy up. The French crowd fled
at a continually increasing speed and all its energy was directed to
reaching its goal. It fled like a wounded animal and it was impossible
to block its path. This was shown not so much by the arrangements it
made for crossing as by what took place at the bridges. When the bridges
broke down, unarmed soldiers, people from Moscow and women with children
who were with the French transport, all--carried on by vis inertiae--
pressed forward into boats and into the ice-covered water and did not,
surrender.
Cell that turns on inside quotes:
"You mean to imply that I have nothing to eat out of.... On the
contrary, I can supply you with everything even if you want to give
dinner parties," warmly replied Chichagov, who tried by every word he spoke to prove his own rectitude and therefore imagined Kutuzov to be
 inimated by the same desire.
Kutuzov, shrugging his shoulders, replied with his subtle
smile: "I meant merely to say what I said.
Cell that robustly activates inside if statements:
static int __dequeue_signal(struct sigpending
   siginfo t *info)
 int sig = next_signal(pending, mask);
      (sigismember(current->notifier_mask, sig)) {
      (!(current->notifier)(current->notifier_data)) {
     clear_thread_flag(TIF_SIGPENDING);
     return 0;
  collect_signal(sig, pending, info);
  eturn sig;
A large portion of cells are not easily interpretable. Here is a typical example:
   Unpack a filter field's string representation from user-space
char *audit_unpack_string(void **bufp, size_t *remain, size_t len)
 char *str:
 if (!*bufp || (len == 0) || (len > *remain))
  return ERR_PTR(-EINVAL);
  * Of the currently implemented string fields, PATH_MAX
    defines the longest valid length.
```

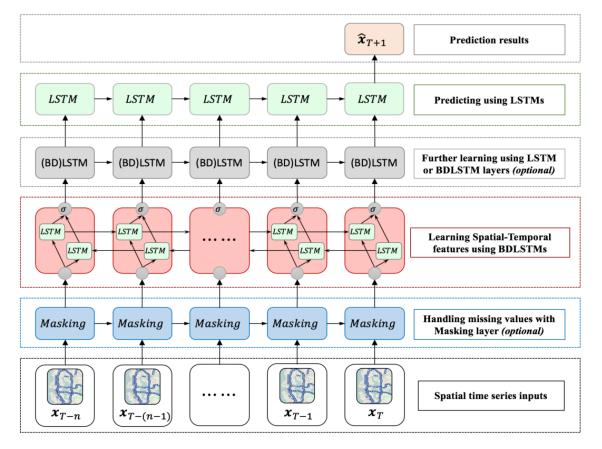
Look at this video for more examples for LSTMViz



http://lstm.seas.harvard.edu/

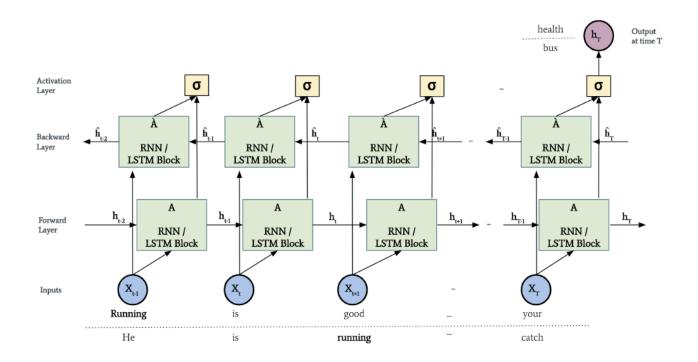


Various architectures: Going deeper



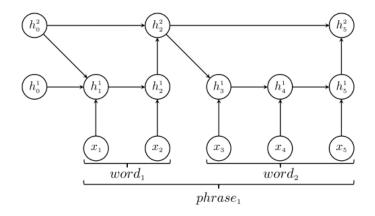


Various architectures: Bidirectional LSTM





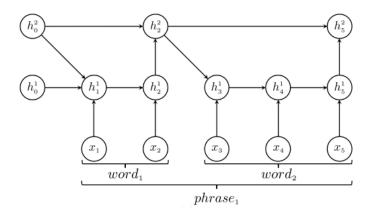
Our goal is to use hierarchical structure in data

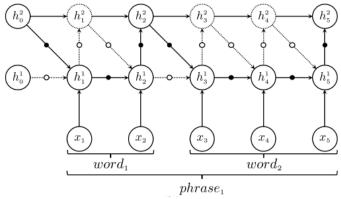


Hierarchical structure can be provided and used with the following architecture



Our goal is to discover hierarchical structure in data





Hierarchical structure can be provided and used

Hierarchical structure can be learned

The boundary detector is the key



Finally some formulas!

$$\mathbf{h}_{t}^{\ell}, \mathbf{c}_{t}^{\ell}, z_{t}^{\ell} = f_{\text{HM-LSTM}}^{\ell}(\mathbf{c}_{t-1}^{\ell}, \mathbf{h}_{t-1}^{\ell}, \mathbf{h}_{t-1}^{\ell-1}, \mathbf{h}_{t-1}^{\ell+1}, z_{t-1}^{\ell}, z_{t}^{\ell-1}). \tag{1}$$

Here, **h** and **c** denote the hidden and cell states, respectively. The function $f_{\text{HM-LSTM}}^{\ell}$ is implemented as follows. First, using the two boundary states z_{t-1}^{ℓ} and $z_t^{\ell-1}$, the cell state is updated by:

$$\mathbf{c}_{t}^{\ell} = \begin{cases} \mathbf{f}_{t}^{\ell} \odot \mathbf{c}_{t-1}^{\ell} + \mathbf{i}_{t}^{\ell} \odot \mathbf{g}_{t}^{\ell} & \text{if } z_{t-1}^{\ell} = 0 \text{ and } z_{t}^{\ell-1} = 1 \text{ (UPDATE)} \\ \mathbf{c}_{t-1}^{\ell} & \text{if } z_{t-1}^{\ell} = 0 \text{ and } z_{t}^{\ell-1} = 0 \text{ (COPY)} \\ \mathbf{i}_{t}^{\ell} \odot \mathbf{g}_{t}^{\ell} & \text{if } z_{t-1}^{\ell} = 1 \text{ (FLUSH),} \end{cases}$$

$$(2)$$

and then the hidden state is obtained by:

$$\mathbf{h}_{t}^{\ell} = \begin{cases} \mathbf{h}_{t-1}^{\ell} & \text{if COPY,} \\ \mathbf{o}_{t}^{\ell} \odot \tanh(\mathbf{c}_{t}^{\ell}) & \text{otherwise.} \end{cases}$$
 (3)

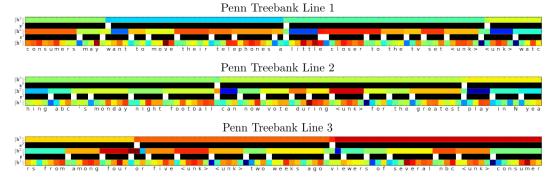
But boundary states are discrete. How can we optimize them?



Straight-through estimator

 Simpler but biased approached used by the authors

REINFORCE



Learned hierarchical structure

Also: the slope annealing trick

Increase slope of a sigmoid during training
to turn it into a step function



Other issues with RNNs

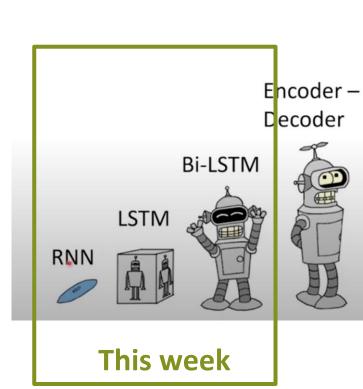
- Technical details e.g. Batch normalization or Dropout
- Memory mechanism
- Many applied problems solved with RNNs
- Theoretical view on RNNs
 - They are Turing complete

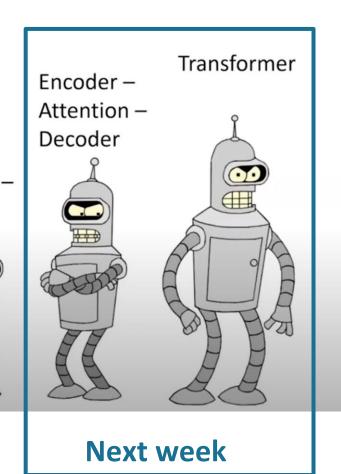


Take-home messages

- Problems with gradients are intrinsic to RNN architecture, but can be fixed with LSTM or GRU
- Embedding is a fundamental concept: it is representation learning for RNNs
- We still can solve various complex problems using various architectures









Sources

- https://github.com/kjw0612/awesome-rnn#blogs
- Recurrent Neural Networks | in Deep learning course by MIT 6.S191
- Coursera course on Sequence models
 https://www.coursera.org/learn/nlp-sequence-models
- http://colah.github.io/posts/2015-08-Understanding-LSTMs/

