

Lecture 9: Recurrent Neural Networks

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Deep Learning Course, Winter 2021-2022

Today's Roadmap

Today we'll cover **neural sequential models**:

- Recurrent neural networks.
- Backpropagation through time.
- Neural language models.
- The vanishing gradient problem.
- Gated units: LSTMs and GRUs.
- Bidirectional LSTMs.
- Example: ELMO representations.
- From sequences to trees: recursive neural networks.
- Other deep auto-regressive models: PixelRNNs.

Outline

① Recurrent Neural Networks

Sequence Generation

Sequence Tagging

Pooled Classification

② The Vanishing Gradient Problem: GRUs and LSTMs

③ Beyond Sequences

Recursive Neural Networks

Pixel RNNs

④ Implementation Tricks

⑤ Conclusions

Recurrent Neural Networks

Much interesting data is **sequential** in nature: words in sentences, DNA sequences, stock market returns, samples of sound signals, ...

How to deal with arbitrarily long sequences?

Feed-forward vs Recurrent Networks

- Feed-forward neural networks:

$$\mathbf{h} = \mathbf{g}(\mathbf{V}\mathbf{x} + \mathbf{c})$$

$$\hat{\mathbf{y}} = \mathbf{W}\mathbf{h} + \mathbf{b}$$

Feed-forward vs Recurrent Networks

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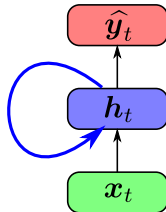
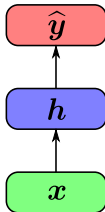
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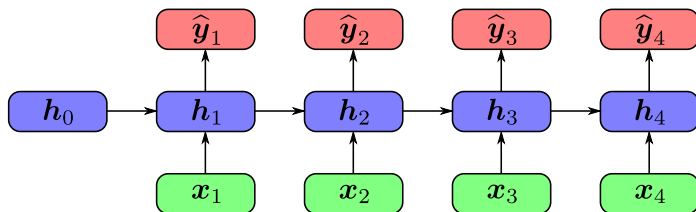
- Recurrent neural networks (Elman, 1990):

$$\mathbf{h}_t = \mathbf{g}(\mathbf{V}\mathbf{x}_t + \mathbf{U}\mathbf{h}_{t-1} + \mathbf{c})$$

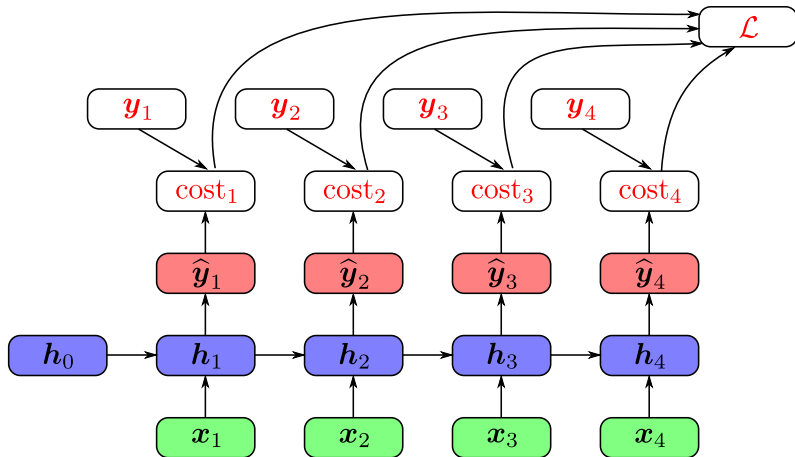
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Unrolling the Graph



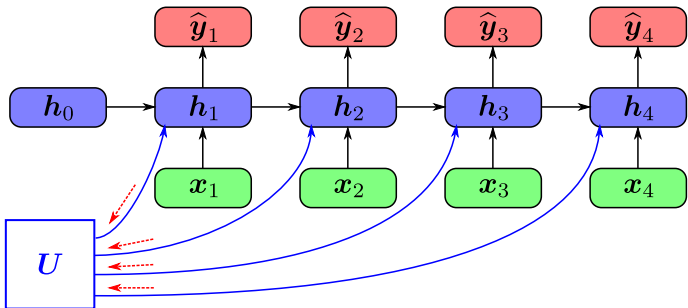
Unrolling the Graph



How do We Train the RNN Parameters?

- The unrolled graph is a well-formed (**directed and acyclic**) computation graph—we can use gradient backpropagation as usual
- Parameters are **tied/shared** across “time”
- Derivatives are aggregated across time steps
- This instantiation is called **backpropagation through time** (BPTT).

Parameter Tying



$$\frac{\partial \mathcal{L}}{\partial \mathbf{U}} = \sum_{t=1}^4 \frac{\partial \mathbf{h}_t}{\partial \mathbf{U}} \frac{\partial \mathcal{L}}{\partial \mathbf{h}_t}$$

- Same idea as when learning the filters in convolutional neural networks

What Can RNNs Be Used For?

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- 1 **Sequence generation:** generates symbols sequentially with an **auto-regressive model** (e.g. language modeling)
- 2 **Sequence tagging:** takes a sequence as input, and returns a label for every element in the sequence (e.g., part of speech–POS–tagging)
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Recap: Full History Model

$$\mathbb{P}(\text{START}, y_1, y_2, \dots, y_L, \text{STOP}) = \prod_{t=1}^{L+1} \mathbb{P}(y_t | y_0, \dots, y_{t-1})$$

- The generation of each word depends on **all** the previous words
- Huge expressive power!
- But: **too many parameters** to estimate! (how many?)
- Cannot generalize well, specially for long sequences

Can We Have Unlimited Memory?

Markov models avoid the full history by considering a limited memory

Alternative: consider **all** the history, but compress it into a vector!

RNNs do this!

Auto-Regressive Models

Key ideas:

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Let's see each of these steps in detail

Language Modeling: Large Softmax

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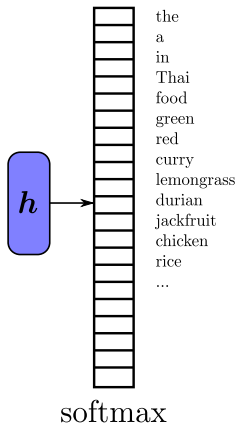
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- Typically, large vocabulary; e.g., $|V| = 100,000$

$$\begin{aligned} \mathbf{z}_t &= \mathbf{W}h_t + \mathbf{b} \\ p(y_t = i) &= \frac{\exp((\mathbf{z}_t)_i)}{\sum_j \exp((\mathbf{z}_t)_j)} \\ &= (\mathbf{softmax}(\mathbf{z}))_i \end{aligned}$$

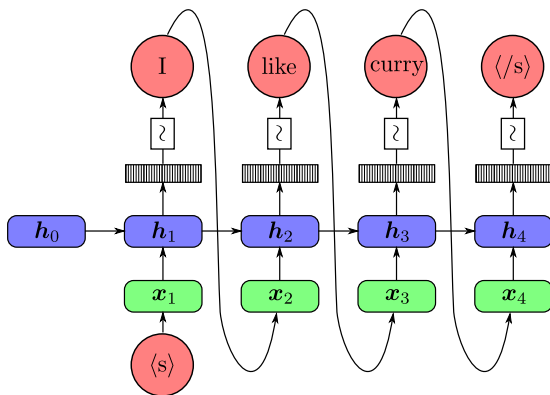
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Language Modeling: Auto-Regression



$$\begin{aligned}\mathbb{P}(y_1, \dots, y_L) &= \mathbb{P}(y_1) \times \mathbb{P}(y_2 | y_1) \times \dots \times \mathbb{P}(y_L | y_1, \dots, y_{L-1}) \\ &= \mathbf{softmax}(\mathbf{W}h_1 + \mathbf{b}) \times \mathbf{softmax}(\mathbf{W}h_2 + \mathbf{b}) \times \dots \\ &\quad \times \mathbf{softmax}(\mathbf{W}h_L + \mathbf{b})\end{aligned}$$

Three Problems for Sequence Generating RNNs

Algorithms:

- Sampling a sequence from the probability distribution defined by the RNN
- Obtaining the most probable sequence
- Training the RNN.

Sampling a Sequence

This is easy!

- Compute \mathbf{h}_1 from $\mathbf{x}_1 = \text{START}$
- Sample $\mathbf{y}_1 \sim \text{softmax}(\mathbf{W}\mathbf{h}_1 + \mathbf{b})$
- Compute \mathbf{h}_2 from \mathbf{h}_1 and $\mathbf{x}_2 = \mathbf{y}_1$
- Sample $\mathbf{y}_2 \sim \text{softmax}(\mathbf{W}\mathbf{h}_2 + \mathbf{b})$
- ...and so on

Obtaining the Most Probable Sequence

Unfortunately, this is hard!

- It would require obtaining the $\mathbf{y}_1, \mathbf{y}_2, \dots$ that jointly maximize the product $\mathbf{softmax}(\mathbf{W}\mathbf{h}_1 + \mathbf{b}) \times \mathbf{softmax}(\mathbf{W}\mathbf{h}_2 + \mathbf{b}) \times \dots$

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- This is rarely needed in language models. But it is important in **conditional** language modelling
- More later, when discussing **sequence-to-sequence models**

Training the RNN

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- In other words, they are trained to minimize the **log-loss (cross-entropy)**:

$$\mathcal{L}(\Theta, y_{1:L}) = -\frac{1}{L+1} \sum_{t=1}^{L+1} \log \mathbb{P}_{\Theta}(y_t | y_0, \dots, y_{t-1})$$

Training the RNN

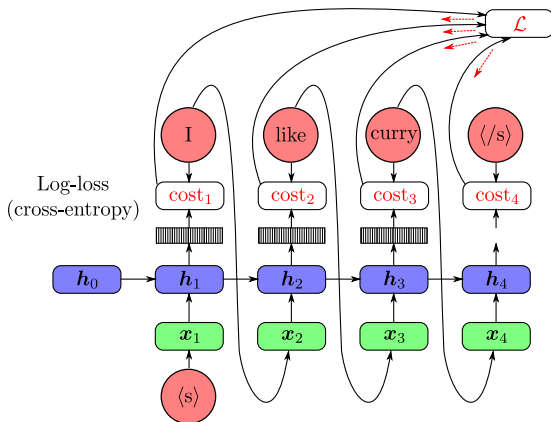
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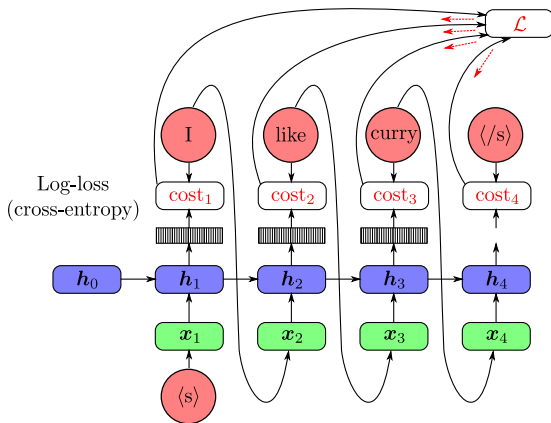
- This is equivalent to minimizing **perplexity** $\exp(\mathcal{L}(\Theta, y_{1:L}))$
- Intuition: $-\log \mathbb{P}_{\Theta}(y_t | y_0, \dots, y_{t-1})$

measures how “perplexed” (or “surprised”) the model is when the t -th word is revealed

Training the RNN

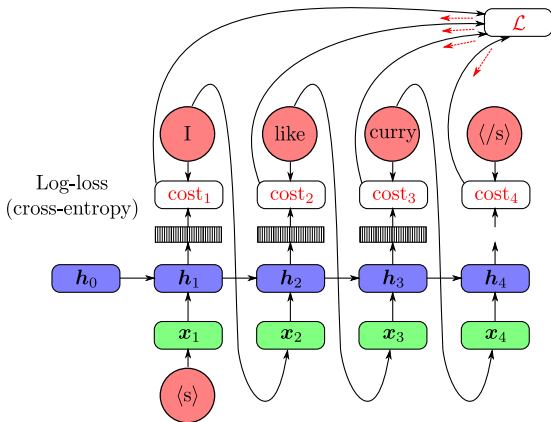


Training the RNN



- Unlike Markov (n -gram) models, **RNNs never forget!**

Training the RNN



- Unlike Markov (n -gram) models, **RNNs never forget!**
- However, we will see they might have trouble learning to use their memories (more soon...)

Teacher Forcing and Exposure Bias

Note that conditioning is on the **true history**, not on the model's predictions! This is known as **teacher forcing**.

Teacher forcing cause **exposure bias** at run time: the model will have trouble recovering from mistakes early on, since it generates histories that it has never observed before.

How to improve this is a current area of research!

Character-Level Language Models

We can also have an RNN over characters instead of words!

Advantage: can generate any combination of characters, not just words in a closed vocabulary.

Disadvantage: need to remember further away in history!

A Character-Level RNN Generating Fake Shakespeare

*PANDARUS: Alas, I think he shall be come approached and the day
When little srain would be attain'd into being never fed,
And who is but a chain and subjects of his death,
I should not sleep.*

*Second Senator: They are away this miseries, produced upon my soul,
Breaking and strongly should be buried, when I perish
The earth and thoughts of many states.*

DUKE VINCENTIO: Well, your wit is in the care of side and that.

*Second Lord: They would be ruled after this chamber,
and my fair nues begun out of the fact,
to be conveyed, Whose noble souls I'll have the heart of the wars.*

Clown: Come, sir, I will make did behold your worship.

VIOLA: I'll drink it.

(Credits: Andrej Karpathy)

A Char-Level RNN Generating a Math Paper

Proof. Omitted. □

Lemma 0.1. *Let \mathcal{C} be a set of the construction.*

Let \mathcal{C} be a gerber covering. Let \mathcal{F} be a quasi-coherent sheaves of \mathcal{O} -modules. We have to show that

$$\mathcal{O}_{\mathcal{O}_X} = \mathcal{O}_X(\mathcal{L})$$

.

Proof. This is an algebraic space with the composition of sheaves \mathcal{F} on $X_{\text{étale}}$ we have

$$\mathcal{O}_X(\mathcal{F}) = \{\text{morph}_1 \times_{\mathcal{O}_X} (\mathcal{G}, \mathcal{F})\}$$

where \mathcal{G} defines an isomorphism $\mathcal{F} \rightarrow \mathcal{F}$ of \mathcal{O} -modules. □

Lemma 0.2. *This is an integer \mathcal{Z} is injective.*

Proof. See Spaces, Lemma ?? □

Lemma 0.3. *Let S be a scheme. Let X be a scheme and X is an affine open covering. Let $U \subset X$ be a canonical and locally of finite type. Let X be a scheme. Let X be a scheme which is equal to the formal complex.*

The following to the construction of the lemma follows.

Let X be a scheme. Let X be a scheme covering. Let

$$b : X \rightarrow Y' \rightarrow Y \rightarrow Y' \times_X Y \rightarrow X.$$

be a morphism of algebraic spaces over S and Y .

Proof. Let X be a nonzero scheme of X . Let X be an algebraic space. Let \mathcal{F} be a quasi-coherent sheaf of \mathcal{O}_X -modules. The following are equivalent

- (1) \mathcal{F} is an algebraic space over S .
- (2) If X is an affine open covering.

Consider a common structure on X and X the functor $\mathcal{O}_X(U)$ which is locally of finite type. □

(Credits: Andrej Karpathy)

A Char-Level RNN Generating C++ Code

```
/*
 * Increment the size file of the new incorrect UI_FILTER group information
 * of the size generatively.
 */
static int indicate_policy(void)
{
    int error;
    if (fd == MARN_EPT) {
        /*
         * The kernel blank will coeld it to userspace.
         */
        if (ss->segment < mem_total)
            unblock_graph_and_set_blocked();
        else
            ret = 1;
        goto bail;
    }
    segaddr = in_SB(in.addr);
    selector = seg / 16;
    setup_works = true;
    for (i = 0; i < blocks; i++) {
        seq = buf[i++];
        bpf = bd->bd.next + i * search;
        if (fd) {
            current = blocked;
        }
    }
    rw->name = "Getjbbregs";
    bprm_self_clearl(&iv->version);
    regs->new = blocks[(BPF_STATS << info->historidac)] | PFMR_CLOBATHINC_SECONDS << 12;
    return segtable;
}
```

(Credits: Andrej Karpathy)

Note: these examples are from 5 years ago; we now have much more impressive language generators (e.g. GPT-3)

Instead of RNNs, the most recent language generators use **transformers**

We will cover **transformers** in a later class!

What Can RNNs Be Used For?

We'll see three applications of RNNs:

- 1 **Sequence generation:** generates symbols sequentially with an **auto-regressive model** (e.g. language modeling) ✓
- 2 **Sequence tagging:** takes a sequence as input, and returns a label for every element in the sequence (e.g., part of speech–POS–tagging)
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- The goal is to assign a tag to each element of the sequence, yielding an output sequence y_1, \dots, y_L
- **Examples:** POS tagging, named entity recognition
- Differences with respect to sequence generation:
 - The input and output are distinct (no need for auto-regression)
 - The length of the output is known (same as that of the input)

Example: POS Tagging

- Map **sentences** to sequences of **part-of-speech tags**.

Time	flies	like	an	arrow	.
noun	verb	prep	det	noun	.

Example: POS Tagging

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Time	flies	like	an	arrow	.
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- Need to predict a morphological tag for each word of the sentence
- High correlation between adjacent words!
(Ratnaparkhi, 1999; Brants, 2000; Toutanova et al., 2003)

An RNN-Based POS Tagger

- The inputs $x_1, \dots, x_L \in \mathbb{R}^{E \times L}$ are word embeddings (found by looking up rows in an V -by- E embedding matrix, eventually pre-trained)

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- A softmax output layer computes the probability of the current tag given the current and previous words:

$$\mathbb{P}(y_t | x_1, \dots, x_t) = \mathbf{softmax}(\mathbf{W}h_t + \mathbf{b})$$

An RNN-Based POS Tagger

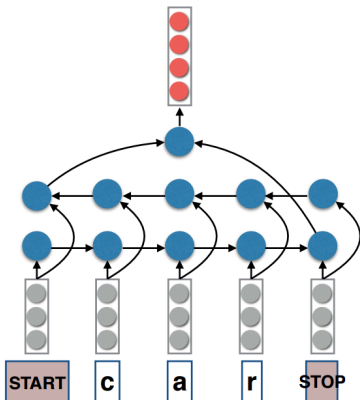
This model can be improved:

- Use a bidirectional RNN to condition also on the following words (combining a left-to-right and a right-to-left RNN)—more later!
- Use a nested character-level CNN or RNN to obtain embeddings for unseen words.

This model achieved SOTA performance on the Penn Treebank and several other benchmarks (Ling et al., 2015; Wang et al., 2015)!

Bidirectional RNNs

- We can read a sequence from left to right to obtain a representation
- Or we can read it from right to left
- Or we can read it from both and combine the representations
- More later...



(Slide credit: Chris Dyer)

Example: Named Entity Recognition

From **sentences** extract **named entities**.

Louis	Elsevier	was	born	in	Leuven	.
B-PER	I-PER	O	O	O	B-LOC	.

- Identify word segments that refer to entities (person, organization, location)
- Typically done with sequence models and B-I-O tagging

(Zhang and Johnson, 2003; Ratinov and Roth, 2009)

RNN-Based NER

- The model we described for POS tagging works just as well for NER
- However, NER has constraints about tag transitions: e.g., we cannot have I-PER after B-LOC
- The RNN tagger model we described exploits **input structure** (via the states encoded in the recurrent layer) but lacks **output structure**...

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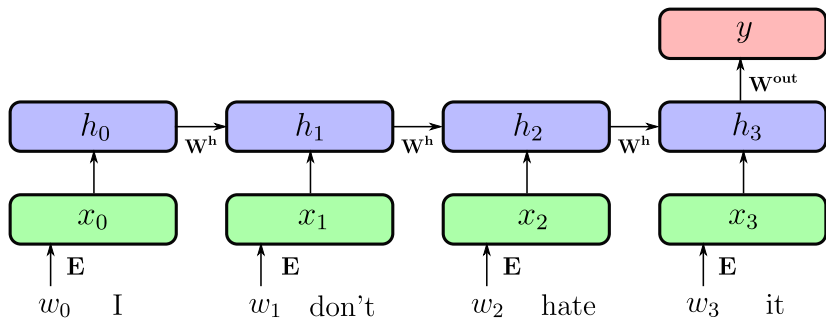
Pooled Classification

- What we have seen so far assumes we want to output a sequence of labels (either to generate or tag a full sequence).
- What about predicting a **single label** for the whole sequence?
- We can still use an RNN to capture the input sequential structure!
- Just **pool** the RNNs states, *i.e.*, map them to a single vector
- Use a single softmax to output the final label.

Pooling Strategies

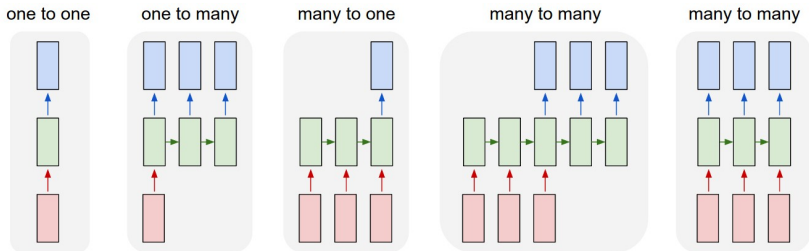
- The simplest strategy is just to **use the last RNN state**
- This state results from traversing the full sequence left-to-right, hence it has information about the full sequence!
- **Disadvantage:** for long sequences, the influence the earliest words may vanish
- **Other pooling strategies:**
 - use a bidirectional RNN and combine both last states of the left-to-right and right-to-left RNN
 - average pooling
 - ...

Example: Sentiment Analysis



(Slide credit: Ollion & Grisel)

Recurrent Neural Networks are Very Versatile



Check out Andrej Karpathy's blog post "The Unreasonable Effectiveness of Recurrent Neural Networks"

(<http://karpathy.github.io/2015/05/21/rnn-effectiveness/>).

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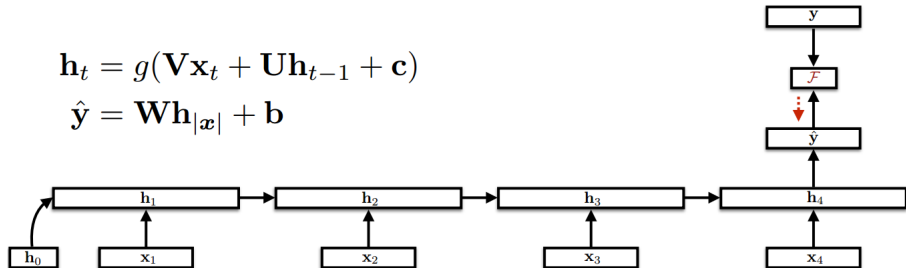
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Training the RNN: Backpropagation Through Time

What happens to the gradients as we go back in time?

$$\mathbf{h}_t = g(\mathbf{V}\mathbf{x}_t + \mathbf{U}\mathbf{h}_{t-1} + \mathbf{c})$$

$$\hat{\mathbf{y}} = \mathbf{W}\mathbf{h}_{|\mathbf{x}|} + \mathbf{b}$$



(Slide credit: Chris Dyer)

Backpropagation Through Time

What happens to the gradients as we go back in time?

$$\frac{\partial \mathcal{F}}{\partial \mathbf{h}_1} = \underbrace{\frac{\partial \mathbf{h}_2}{\partial \mathbf{h}_1} \frac{\partial \mathbf{h}_3}{\partial \mathbf{h}_2} \frac{\partial \mathbf{h}_4}{\partial \mathbf{h}_3}}_{\prod_{t=2}^4 \frac{\partial \mathbf{h}_t}{\partial \mathbf{h}_{t-1}}} \frac{\partial \hat{\mathbf{y}}}{\partial \mathbf{h}_4} \frac{\partial \mathcal{F}}{\partial \hat{\mathbf{y}}}$$

where

$$\prod_t \frac{\partial \mathbf{h}_t}{\partial \mathbf{h}_{t-1}} = \prod_t \frac{\partial \mathbf{h}_t}{\partial \mathbf{z}_t} \frac{\partial \mathbf{z}_t}{\partial \mathbf{h}_{t-1}} = \prod_t \text{Diag}(\mathbf{g}'(\mathbf{z}_t)) \mathbf{U}$$

Three cases:

- largest eigenvalue of \mathbf{U} exactly 1: gradient propagation is stable
- largest eigenvalue of $\mathbf{U} < 1$: **gradient vanishes** (exponential decay)
- largest eigenvalue of $\mathbf{U} > 1$: **gradient explodes** (exponential growth)

Vanishing and Exploding Gradients

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Vanishing and Exploding Gradients

- **Exploding gradients** can be dealt with by **gradient clipping** (truncating the gradient if it exceeds some magnitude)
- **Vanishing gradients** are more frequent and harder to deal with
 - In practice: long-range dependencies are difficult to learn
- **Solutions:**
 - Better optimizers (second order methods)
 - Normalization to keep the gradient norms stable across time
 - Clever initialization to start with good spectra (e.g., start with random orthonormal matrices)
 - **Alternative parameterizations: LSTMs and GRUs**

Gradient Clipping

- **Norm clipping:**

$$\tilde{\nabla} \leftarrow \begin{cases} \frac{c}{\|\nabla\|} \nabla & \text{if } \|\nabla\| \geq c \\ \nabla & \text{otherwise.} \end{cases}$$

- **Elementwise clipping:**

$$\tilde{\nabla}_i \leftarrow \min\{c, |\nabla_i|\} \times \text{sign}(\nabla_i), \quad \forall i$$

Alternative RNNs

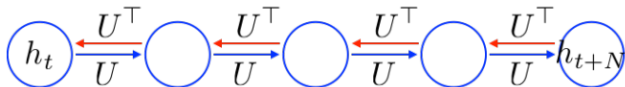
- **Gated recurrent unit (GRU)**
(Cho et al., 2014)
- **Long short-term memorie (LSTM)**
(Hochreiter and Schmidhuber, 1997)

Intuition: instead of multiplying across time (which leads to exponential growth), we want the error to be approximately constant

They solve the vanishing gradient problem, but still have exploding gradients (still need gradient clipping)

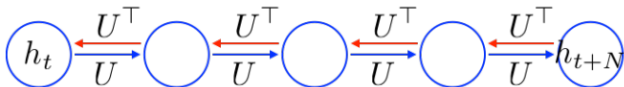
Gated Recurrent Units (Cho et al., 2014)

- Recall the problem: the error must backpropagate through all the intermediate nodes:

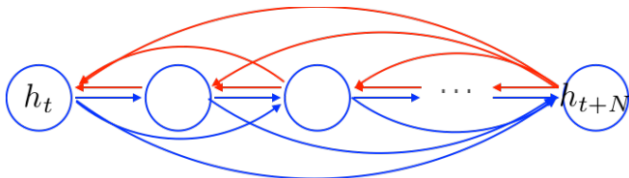


Gated Recurrent Units (Cho et al., 2014)

- Recall the problem: the error must backpropagate through all the intermediate nodes:



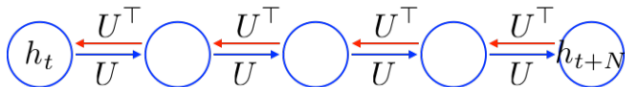
- Idea:** create some kind of shortcut connections:



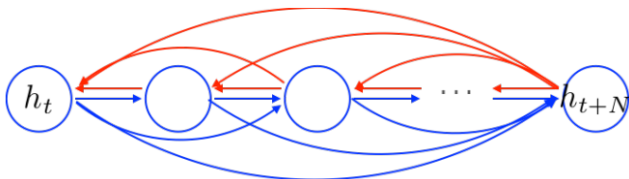
(Image credit: Thang Luong, Kyunghyun Cho, Chris Manning)

Gated Recurrent Units (Cho et al., 2014)

- Recall the problem: the error must backpropagate through all the intermediate nodes:



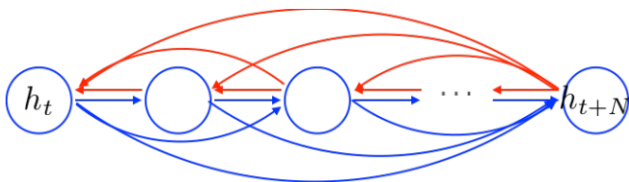
- Idea:** create some kind of shortcut connections:



(Image credit: Thang Luong, Kyunghyun Cho, Chris Manning)

- Create **adaptive** shortcuts controlled by special **gates**

Gated Recurrent Units (Cho et al., 2014)



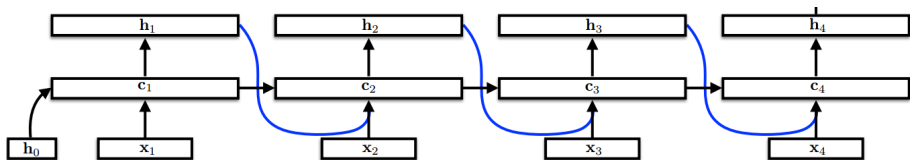
(Image credit: Thang Luong, Kyunghyun Cho, Chris Manning)

$$h_t = \mathbf{u}_t \odot \tilde{\mathbf{h}}_t + (1 - \mathbf{u}_t) \odot h_{t-1}$$

- **Candidate update:** $\tilde{\mathbf{h}}_t = \mathbf{g}(\mathbf{V}\mathbf{x}_t + \mathbf{U}(\mathbf{r}_t \odot \mathbf{h}_{t-1}) + \mathbf{b})$
- **Reset gate:** $\mathbf{r}_t = \sigma(\mathbf{V}_r\mathbf{x}_t + \mathbf{U}_r\mathbf{h}_{t-1} + \mathbf{b}_r)$
- **Update gate:** $\mathbf{u}_t = \sigma(\mathbf{V}_u\mathbf{x}_t + \mathbf{U}_u\mathbf{h}_{t-1} + \mathbf{b}_u)$

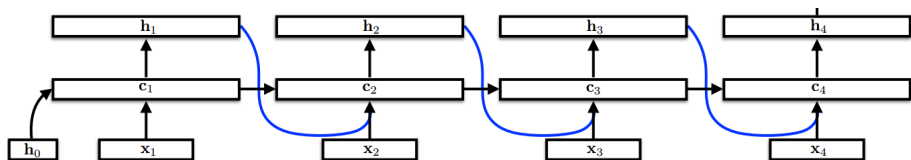
Long Short-Term Memories (Hochreiter and Schmidhuber, 1997)

- **Key idea:** use **memory cells** c_t
- To avoid the multiplicative effect, flow information *additively* through these cells
- Control the flow with special **input**, **forget**, and **output** gates



(Image credit: Chris Dyer)

Long Short-Term Memories

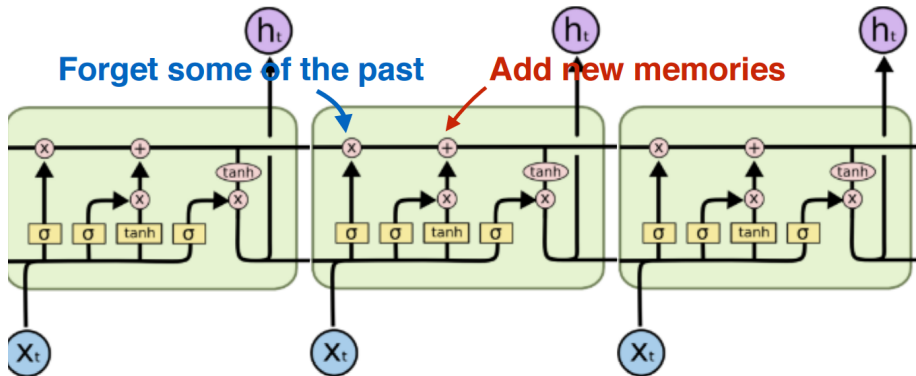


(Image credit: Chris Dyer)

$$c_t = f_t \odot c_{t-1} + i_t \odot g(Vx_t + Uh_{t-1} + b), \quad h_t = o_t \odot g(c_t)$$

- Forget gate: $f_t = \sigma(V_f x_t + U_f h_{t-1} + b_f)$
- Input gate: $i_t = \sigma(V_i x_t + U_i h_{t-1} + b_i)$
- Output gate: $o_t = \sigma(V_o x_t + U_o h_{t-1} + b_o)$

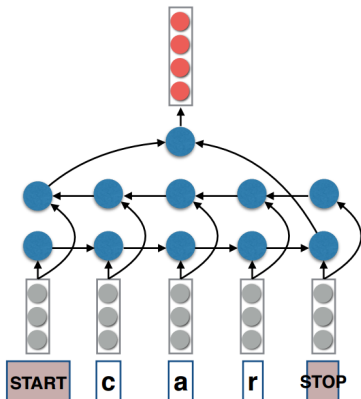
Long Short-Term Memories



(Slide credit: Christopher Olah)

Bidirectional LSTMs

- Same thing as a Bidirectional RNN, but using LSTM units instead of vanilla RNN units.



(Slide credit: Chris Dyer)

LSTMs and BILSTMs: Some Success Stories

- Time series prediction (Schmidhuber et al., 2005)
- Speech recognition (Graves et al., 2013)
- Named entity recognition (Lample et al., 2016)
- Machine translation (Sutskever et al., 2014)
- ELMo (deep contextual) word representations (Peters et al., 2018)
- ... and many others.

Summary

- Better gradient propagation is possible if we use **additive** rather than multiplicative/highly non-linear recurrent dynamics
- Recurrent architectures are an active area of research (but LSTMs are hard to beat)
- Other variants of LSTMs exist which tie/simplify some of the gates
- Extensions exist for *non-sequential* structured inputs/outputs (e.g. trees): **recursive neural networks** (Socher et al., 2011), **PixelRNN** (Oord et al., 2016)

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From Sequences to Trees

- So far we've talked about **recurrent** neural networks, which are designed to capture sequential structure
- What about other kinds of structure? For example, trees?
- It is also possible to tackle these structures with recursive computation, via **recursive** neural networks.

Recursive Neural Networks

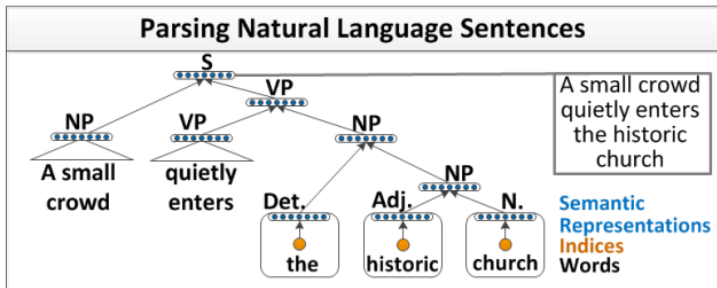
- Proposed by Socher et al. (2011) for parsing images and text
- Assume a binary tree (each node except the leaves has two children)
- Propagate states bottom-up in the tree, computing the parent state \mathbf{p} from the children states \mathbf{c}_1 and \mathbf{c}_2 :

$$\mathbf{p} = \tanh \left(\mathbf{W} \begin{bmatrix} \mathbf{c}_1 \\ \mathbf{c}_2 \end{bmatrix} + \mathbf{b} \right)$$

- Use the same parameters \mathbf{W} and \mathbf{b} at all nodes
- Can compute scores at the root or at each node by appending a softmax output layer at these nodes.

Compositionality in Text

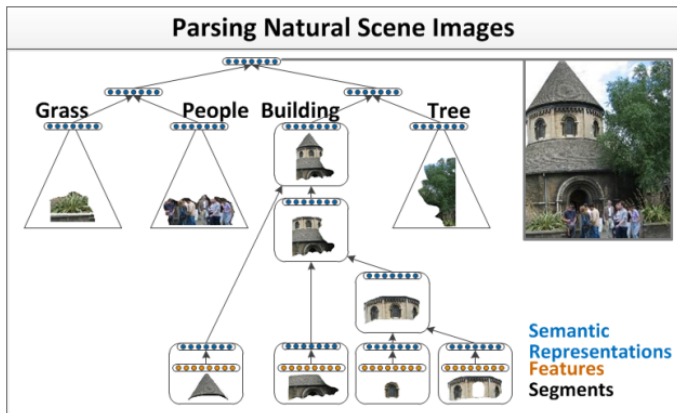
Uses a recurrent net to build a bottom-up parse tree for a sentence.



(Credits: Socher et al. (2011))

Compositionality in Images

Same idea for images.

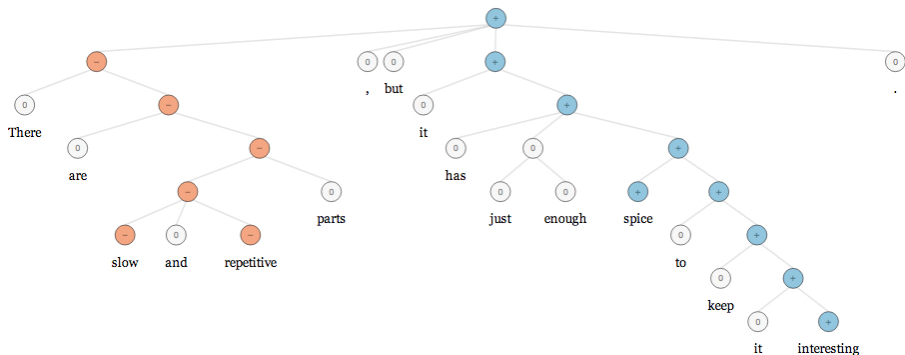


(Credits: Socher et al. (2011))

Tree-LSTMs

- Extend recursive neural networks the same way LSTMs extend RNNs, with a few more gates to account for the left and right child.
- Extensions exist for non-binary trees.

Fine-Grained Sentiment Analysis



(Taken from Stanford Sentiment Treebank.)

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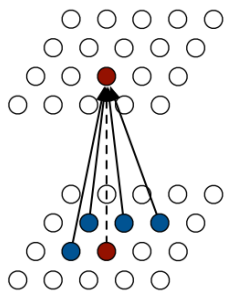
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What about Images?

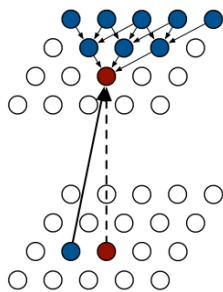
- While sequences are 1D, images are 2D.
- PixelRNNs are 2D extensions of RNNs.
- They can be used as auto-regressive models to **generate images**, by generating pixels in a particular order, conditioning on neighboring pixels.
- Several variants...

RNNs for Generating Images

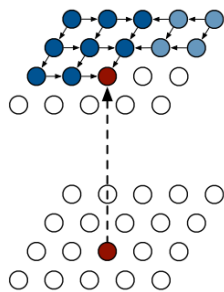
- Input-to-state and state-to-state mappings for PixelCNN and two PixelRNN models (Oord et al., 2016):



PixelCNN

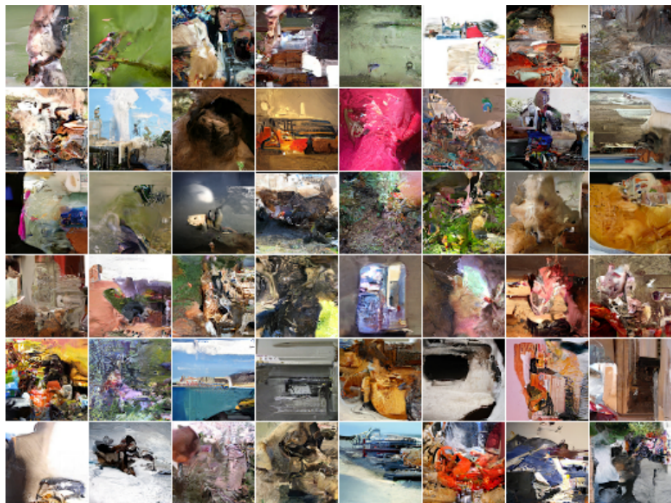


Row LSTM



Diagonal BiLSTM

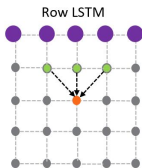
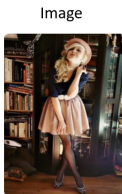
RNNs for Generating Images



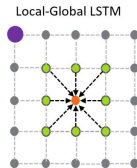
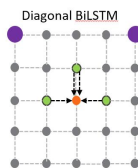
(Oord et al., 2016)

Even More General: Graph LSTMs

Traditional multi-dimensional LSTM:



Pixel-wise LSTM

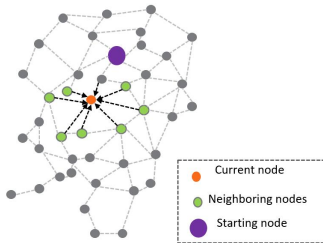
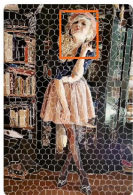


Superpixel map

Graph topology

Graph LSTM

Graph LSTM:



(Credits: Xiaodan Liang)

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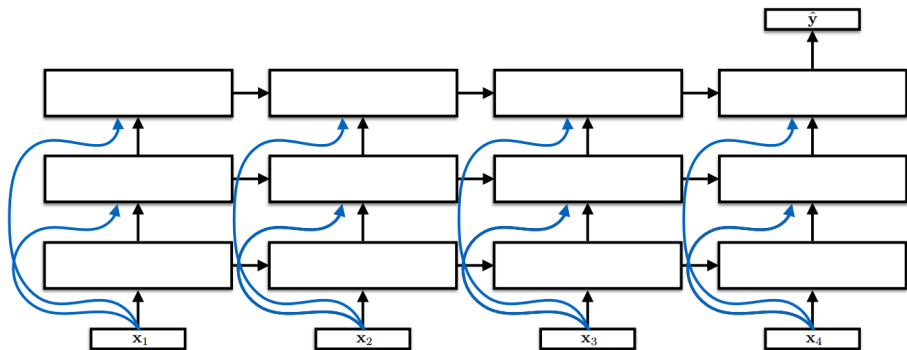
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More Tricks of the Trade

- Depth
- Dropout
- Implementation Tricks
- Mini-batching

Deep RNNs/LSTMs/GRUs

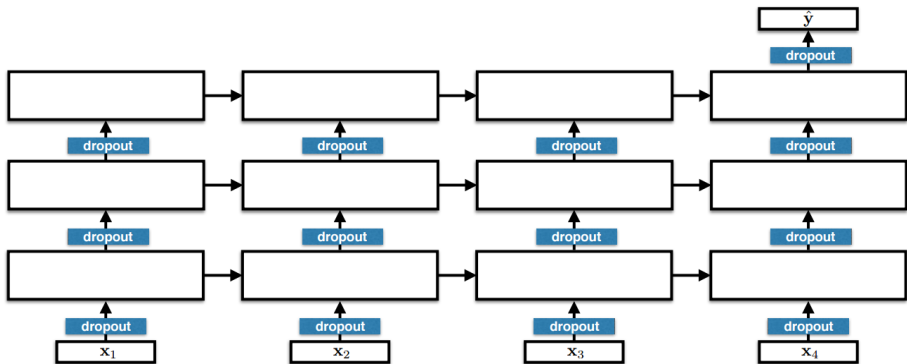
- Depth in recurrent layers helps in practice (2–8 layers seem to be standard)
- Input connections may or may not be used



(Slide credit: Chris Dyer)

Dropout in Deep RNNs/LSTMs/GRUs

- Apply dropout between layers, but not on the recurrent connections
- ... Or use the same mask for all recurrent connections (Gal and Ghahramani, 2015)



(Slide credit: Chris Dyer)

Implementation Tricks

For speed:

- Use diagonal matrices instead of full matrices (esp. for gates)
- Concatenate parameter matrices for all gates and do a single matrix-vector multiplication
- Use optimized implementations (from NVIDIA)
- Use GRUs or reduced-gate variant of LSTMs

For learning speed and performance:

- Initialize so that the bias on the forget gate is large (intuitively: at the beginning of training, the signal from the past is unreliable)
- Use random orthogonal matrices to initialize the square matrices

Mini-Batching

- RNNs, LSTMs, GRUs all consist of many element-wise operations (addition, multiplication, nonlinearities), and lots of matrix-vector products
- Mini-batching: convert many matrix-vector products into a single matrix-matrix multiplication
- Batch across instances, not across time
- The challenge with working with mini batches of sequences is... sequences are of different lengths (we've seen this when talking about convolutional nets)
- This usually means you bucket training instances based on similar lengths, and pad with zeros
- Be careful when padding not to back propagate a non-zero value!

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Conclusions

Recurrent neural networks allow to take advantage of sequential input structure

They can be used to generate, tag, and classify sequences, and are trained with backpropagation through time

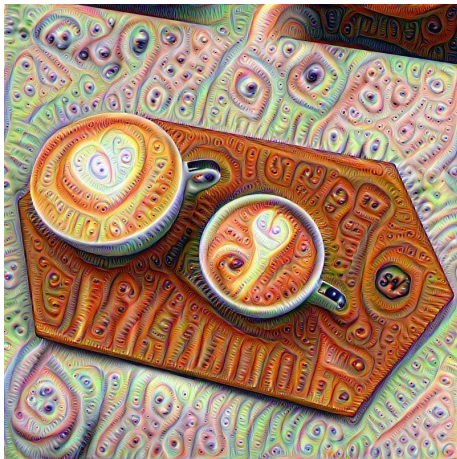
Vanilla RNNs suffer from vanishing and exploding gradients

LSTMs and other gated units are more complex variants of RNNs that avoid vanishing gradients

They can be extended to other structures like trees, images, and graphs.

Thank you!

Questions?



References I

- Brants, T. (2000). Tnt: a statistical part-of-speech tagger. In *Proceedings of the sixth conference on Applied natural language processing*, pages 224–231. Association for Computational Linguistics.
- Cho, K., Van Merriënboer, B., Gulcehre, C., Bahdanau, D., Bougares, F., Schwenk, H., and Bengio, Y. (2014). Learning Phrase Representations Using RNN Encoder-Decoder for Statistical Machine Translation. In *Proc. of Empirical Methods in Natural Language Processing*.
- Elman, J. L. (1990). Finding structure in time. *Cognitive science*, 14(2):179–211.
- Gal, Y. and Ghahramani, Z. (2015). Dropout as a bayesian approximation: Representing model uncertainty in deep learning. *arXiv preprint arXiv:1506.02142*.
- Graves, A., Mohamed, A.-r., and Hinton, G. (2013). Speech recognition with deep recurrent neural networks. In *ICASSP*, pages 6645–6649. IEEE.
- Hochreiter, S. and Schmidhuber, J. (1997). Long short-term memory. *Neural computation*, 9(8):1735–1780.
- Lample, G., Ballesteros, M., Subramanian, S., Kawakami, K., and Dyer, C. (2016). Neural architectures for named entity recognition. In *Proc. of the Annual Meeting of the North-American Chapter of the Association for Computational Linguistics*.
- Ling, W., Luís, T., Marujo, L., Astudillo, R. F., Amir, S., Dyer, C., Black, A. W., and Trancoso, I. (2015). Finding function in form: Compositional character models for open vocabulary word representation. In *Proc. of Empirical Methods in Natural Language Processing*.
- Oord, A. v. d., Kalchbrenner, N., and Kavukcuoglu, K. (2016). Pixel Recurrent Neural Networks. In *Proc. of the International Conference on Machine Learning*.
- Peters, M. E., Neumann, M., Iyyer, M., Gardner, M., Clark, C., Lee, K., and Zettlemoyer, L. (2018). Deep contextualized word representations. *arXiv preprint arXiv:1802.05365*.
- Ratinov, L. and Roth, D. (2009). Design challenges and misconceptions in named entity recognition. In *Proceedings of the Thirteenth Conference on Computational Natural Language Learning*, pages 147–155. Association for Computational Linguistics.
- Ratnaparkhi, A. (1999). Learning to parse natural language with maximum entropy models. *Machine Learning*, 34(1):151–175.
- Schmidhuber, J., Wierstra, D., and Gomez, F. J. (2005). Evolino: Hybrid neuroevolution/optimal linear search for sequence prediction. In *Proceedings of the 19th International Joint Conference on Artificial Intelligence (IJCAI)*.

References II

- Socher, R., Lin, C. C., Manning, C., and Ng, A. Y. (2011). Parsing natural scenes and natural language with recursive neural networks. In *Proceedings of the 28th international conference on machine learning (ICML-11)*, pages 129–136.
- Sutskever, I., Vinyals, O., and Le, Q. V. (2014). Sequence to sequence learning with neural networks. In *Advances in Neural Information Processing Systems*, pages 3104–3112.
- Toutanova, K., Klein, D., Manning, C. D., and Singer, Y. (2003). Feature-rich part-of-speech tagging with a cyclic dependency network. In *Proc. of the North American Chapter of the Association for Computational Linguistics*, pages 173–180.
- Wang, P., Qian, Y., Soong, F. K., He, L., and Zhao, H. (2015). Part-of-speech tagging with bidirectional long short-term memory recurrent neural network. *arXiv preprint arXiv:1510.06168*.
- Zhang, T. and Johnson, D. (2003). A robust risk minimization based named entity recognition system. In *Proceedings of the seventh conference on Natural language learning at HLT-NAACL 2003-Volume 4*, pages 204–207. Association for Computational Linguistics.