Recurrent Neural Networks

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Today's Roadmap

Today we'll cover neural sequential models:

... with a focus on language modelling

- Recurrent neural networks.
- Backpropagation through time.
- Neural language models.
- The vanishing gradient problem.
- Gated units: LSTMs and GRUs.
- Bidirectional LSTMs.
- RNN extensions.

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

Lots of interesting data is sequential in nature:

- words in sentences
- DNA
- stock market returns

- How does such data differ from other data types?
- What are the limitations of previous NNs in modelling sequences?

Recurrent Neural Networks

Lots of interesting data is sequential in nature:

- words in sentences
- DNA
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- How does such data differ from other data types?
- What are the limitations of previous NNs in modelling sequences?
  - unit order
  - different sequence lengths
  - arbitrarily long history

Feed-forward NN recap

- Feed-forward neural networks:

$$\begin{aligned} \boldsymbol{h} &= \boldsymbol{g}(\boldsymbol{V}\boldsymbol{x} + \boldsymbol{c}) \\ \widehat{\boldsymbol{y}} &= \boldsymbol{W}\boldsymbol{h} + \boldsymbol{b} \end{aligned}$$

  - What happens if we permute the hidden units?

Feed-forward NN recap

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$$
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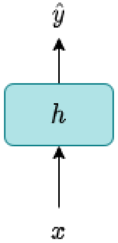
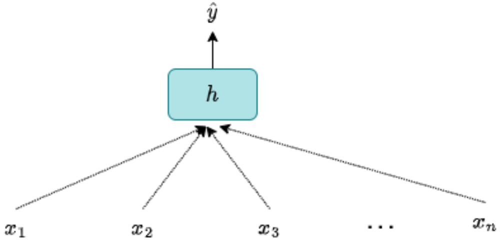
\widehat{\boldsymbol{y}} &= \boldsymbol{Wh} + \boldsymbol{b}
\end{aligned}
$$

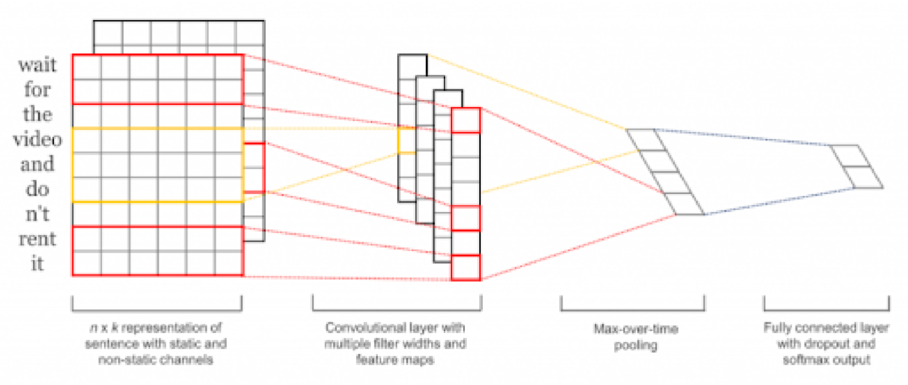
  - What happens if we permute the hidden units?





CNN recap

- Convolutrional neural networks:


wait
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it
n x k representation of sentence with static and non-static channels
Convolutional layer with multiple filter widths and feature maps
Max-over-time pooling
Fully connected layer with dropout and softmax output

Feed-forward vs Recurrent Networks

- Feed-forward neural networks:

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Feed-forward vs Recurrent Networks

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- Recurrent neural networks (Elman, 1990):

$$\begin{aligned} \boldsymbol{h}_t &= \boldsymbol{g}(\boldsymbol{V}\boldsymbol{x}_t + \boldsymbol{U}\boldsymbol{h}_{t-1} + \boldsymbol{c}) \\ \widehat{\boldsymbol{y}}_t &= \boldsymbol{W}\boldsymbol{h}_t + \boldsymbol{b} \end{aligned}$$

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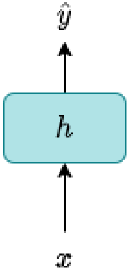
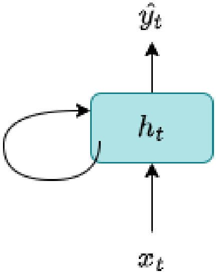
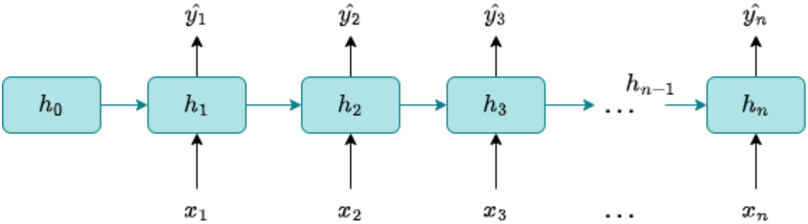




Unrolling the Graph

What happens if we unroll this graph?

Unrolling the Graph



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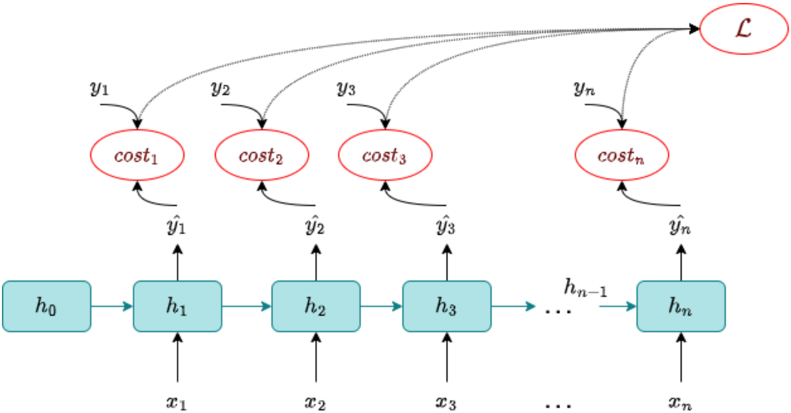
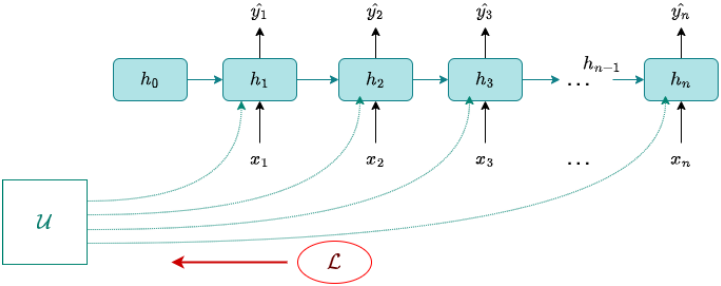


How do We Train the RNN Parameters?

- The unrolled graph is a well-formed (DAG) computation graph
    - we can run the gradient backpropagation algorithm as usual
- Parameters are shared accross “time” (t)
- Derivatives are aggregated across time steps
- This instantiation is called backpropagation through time (BPTT).

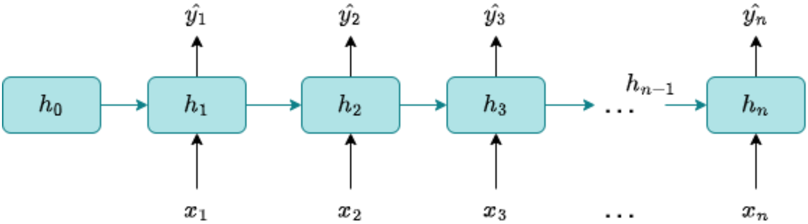
Parameter Tying



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

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

A close-up at the RNN cell



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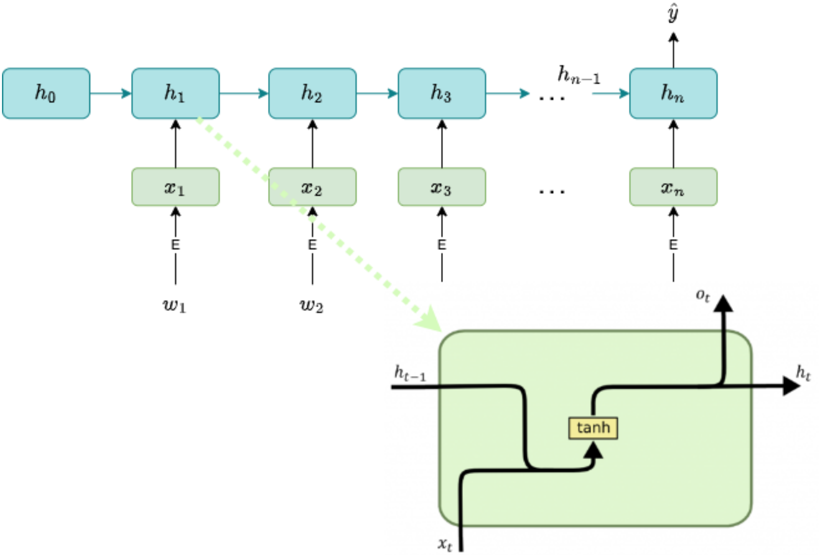
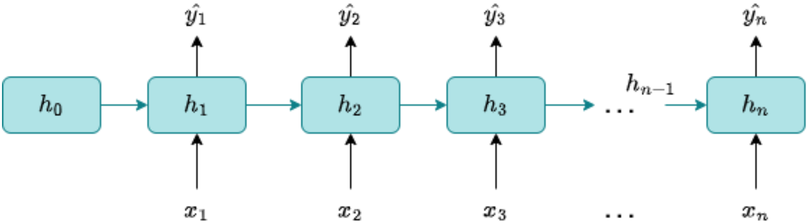
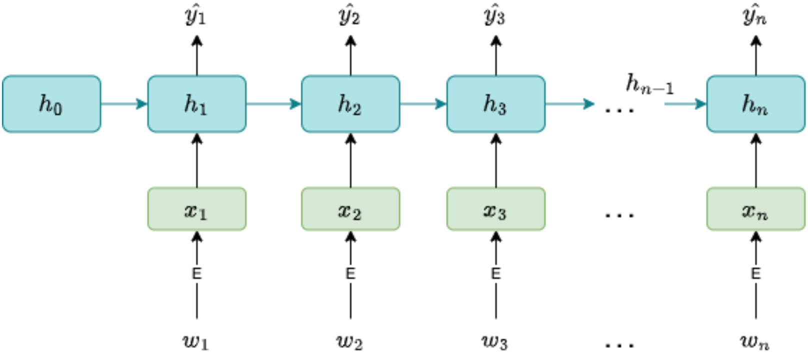


A close-up at the input layer



A close-up at the input layer



Where Can We Use RNNs?

How do we use sequence modelling?

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. POS tagging, NER tagging)
3. **Pooled classification:** takes a sequence as input, and returns a single label by pooling the RNN states.

We will focus more on the output modelling y

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Example: Language Modeling

One of the possible usages of RNNs is in language modeling

... and the most popular.

Example: Language Modeling

One of the possible usages of RNNs is in language modeling

... and the most popular.

(until recently)

Recap: Full History Model

Can we apply the bayes theorem?

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

- Assumes the generation of each word depends on the entire history (*all* the previous words)
- Huge expressive power!
- But: too many parameters to estimate!
- Cannot generalize well

Can We Have Unlimited Memory?

- Limit the history → Markov models
- Compress history into a vector → RNN

Auto-Regressive Models

Key ideas: (how do we condition on previous outputs?)

- Feed back the output in the previous time step as input in the current time step.

$$x_i = y_{i-1}$$

- Maintain a state vector $\boldsymbol{h}_i$ which is a function of the previous state vector and the current input: this state will compress all the history!

$$\boldsymbol{h}_i = \boldsymbol{g}(\boldsymbol{V} x_i + \boldsymbol{U}\boldsymbol{h}_{i-1} + \boldsymbol{c})$$

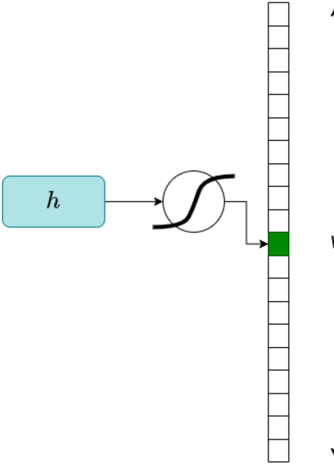
- Compute next output probability:

$$\mathbb{P}(y_i | y_0, \ldots, y_{i-1}) = \textbf{softmax}(\boldsymbol{W}\boldsymbol{h}_i + \boldsymbol{b})$$

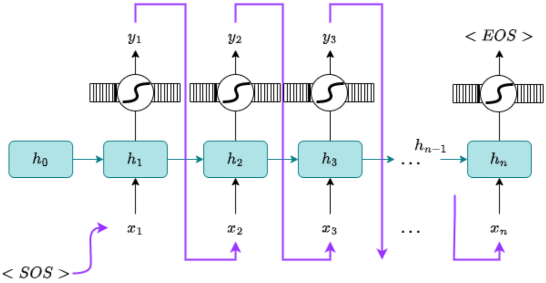
Language Modeling: Large Softmax

- Assume we want to generate text, and y_t is a word in the vocabulary
- Typically, large vocabulary size $|V|$

$$\begin{aligned}
\boldsymbol{z} &= \boldsymbol{W}\boldsymbol{h} + \boldsymbol{b} \\
p(y_t = i) &= \frac{\exp(z_i)}{\sum_j \exp(z_j)} \\
&= \mathbf{softmax}_i(\boldsymbol{z})
\end{aligned}$$



Language Modeling: Auto-Regression



$$\begin{aligned}
\mathbb{P}(y_1, \dots, y_L) &= \mathbb{P}(y_1) \times \mathbb{P}(y_2 \mid y_1) \times \dots \times \mathbb{P}(y_L \mid y_1, \dots, y_{L-1}) \\
&= \textbf{softmax}(\boldsymbol{W}\boldsymbol{h}_1 + \boldsymbol{b}) \times \textbf{softmax}(\boldsymbol{W}\boldsymbol{h}_2 + \boldsymbol{b}) \times \dots \\
&\quad \times \textbf{softmax}(\boldsymbol{W}\boldsymbol{h}_L + \boldsymbol{b})
\end{aligned}$$

Three Problems for Sequence Generating RNNs

Algorithms:

- Sample a sequence from the probability distribution defined by the RNN
- Computing the most probable sequence
- Train the RNN.

Sampling a Sequence

This is easy!

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

What is the Most Probable Sequence?

Unfortunately, this is hard!

- It would require obtaining the $\boldsymbol{y}_1, \boldsymbol{y}_2, \ldots$ that jointly maximize the product $\mathbf{softmax}(\boldsymbol{W}\boldsymbol{h}_1 + \boldsymbol{b}) \times \mathbf{softmax}(\boldsymbol{W}\boldsymbol{h}_2 + \boldsymbol{b}) \times \ldots$
- Note that picking the best $\boldsymbol{y}_i$ greedily at each time step doesn't guarantee the best sequence
- We can get better approximations by doing beam search.

▶ When is this important?

▶ Compare sequence modelling with conditional sequence modelling (e.g. machine translation, image captioning)

Train the RNN

Training method: maximum likelihood estimation

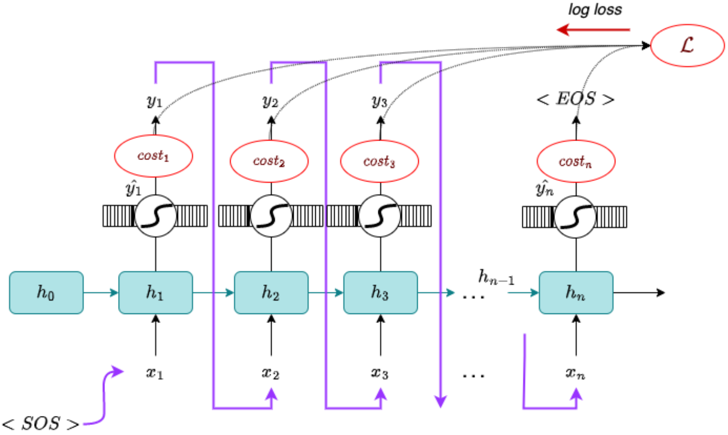
In other words, they are trained to minimize the log-loss (cross-entropy):

$$\mathcal{L}(\Theta, y_{1:L}) = -\frac{1}{L+1} \sum_{i=1}^{L+1} \log \mathbb{P}_{\Theta}(y_i \mid y_0, \ldots, y_{i-1})$$

This is equivalent to minimize perplexity $2^{\mathcal{L}(\Theta, y_{1:L})}$

Intuition: how “perplex” is the model when the *i*th word is revealed?

Train the RNN



Train 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...)
- And a few other issues

Teacher Forcing and Exposure Bias

Note that we always condition on the **true history** i.e. the ground truth labels and not on the model's predictions!

This is known as teacher forcing.

Teacher forcing causes exposure bias at run time: the model will have trouble recovering from mistakes early on, since it may generate outputs it has never observed before.

Teacher forcing is an issue even in more recent models ▶ How to improve this is an active area of research Feng et al. (2021)

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: longer sequences → need to remember further away in history!

A Char-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.

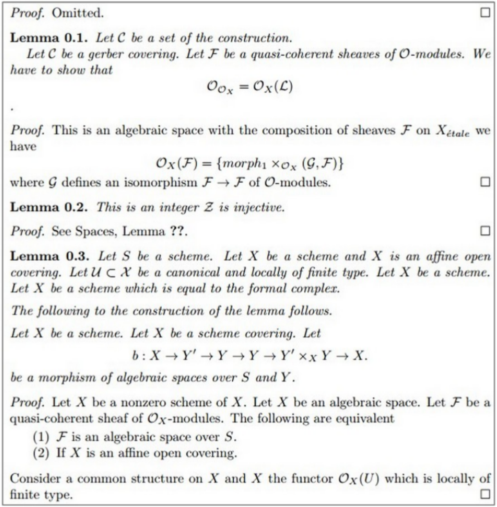
Second Lord: They would be ruled after this chamber, and my fair nues begun out of the fact, to be conveyed, Whose noble souls I'll have the heart of the wars.

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 $X_{\acute{e}tale}$ we have

$$\mathcal{O}_X(\mathcal{F}) = \{morph_1 \times_{\mathcal{O}_X} (\mathcal{G}, \mathcal{F})\}$$

where $\mathcal{G}$ defines an isomorphism $\mathcal{F} \to \mathcal{F}$ 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 $\mathcal{U} \subset \mathcal{X}$ 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

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

be a morphism of algebraic spaces over S and Y.

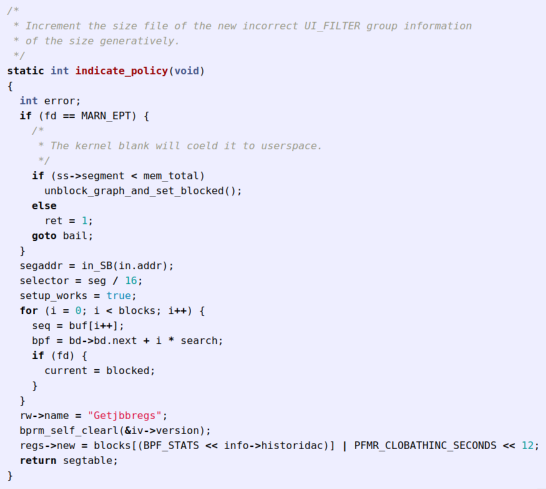
Proof. Let X be a nonzero scheme of X. Let X be an algebraic space. Let $\mathcal{F}$ be a quasi-coherent sheaf of $\mathcal{O}_X$-modules. The following are equivalent

(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 pre-GPT let alone pre ChatGPT :)

Instead of RNNs, the most recent language generators use a Transformer architecture

Where Can We Use RNNs?

We'll see three usages 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. POS tagging)
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Sequence Tagging with RNNs

In **sequence tagging**, we are given an input sequence $x_1, \ldots, x_L$

The goal is to assign a tag to each element of the sequence, yielding an output sequence $y_1, \ldots, y_L$

Examples: POS tagging, named entity recognition

Differences with respect to sequence generation:

- The input and output are distinct (no need for an auto-regressive model)
- The length of the output is known (same length as the input)

Examples: POS Tagging

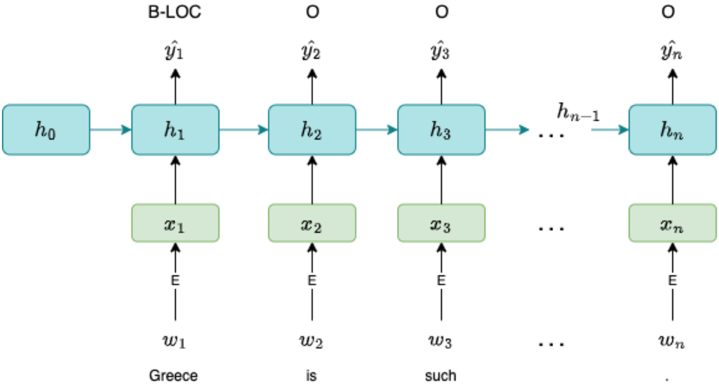
Map **sentences** to sequences of **part-of-speech tags** or **named entity tags.**

Greece	is	such	a	sunny	country	.
noun	verb	prep	det	adj	noun	punct
B-LOC	O	O	O	O	O	O

- 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 NER Tagger



An RNN-Based NER Tagger

- The inputs $x_1, \ldots, x_L \in \mathbb{R}^{E \times L}$ are word embeddings (obtained by looking up rows in an V-by-E embedding matrix, eventually pre-trained)
- As before, maintain a state vector $\boldsymbol{h}_i$ which is a function of the previous state vector and the current input: this state will compress all the input history!

$$\boldsymbol{h}_i = \boldsymbol{g}(\boldsymbol{V} x_i + \boldsymbol{U}\boldsymbol{h}_{i-1} + \boldsymbol{c})$$

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

$$\mathbb{P}(y_i | x_1, \ldots, x_i) = \textbf{softmax}(\boldsymbol{W}\boldsymbol{h}_i + \boldsymbol{b})$$

RNN-Based NER

- Typically using the B-I-O (or B-I-O-S) scheme
- NER has constraints about tag transitions: e.g., we cannot have I-PER after B-LOC

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- 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...

Combining RNNs and CRFs

There are models that exploit output sequential structure: conditional random fields!

CRFs are used originally as a linear model (the scores for emissions and transitions came from a feature-based linear model)

We can easily combine the strengths of RNNs and CRFs to obtain a **non-linear CRF**!

Combining RNNs and CRFs

- Just use the RNN to compute scores for the emissions (instead of the feature-based linear model)
- For the transitions, we can either compute scores from the same recurrent layer, or just have an indicator feature that looks at the tag bigrams
- Then replace the softmax output layer by a CRF output layer!
- At training time, plug the forward-backward algorithm in the gradient back-propagation
- At run time, use Viterbi to predict the most likely sequence of tags.

A variant of this model (with a BILSTM instead of a RNN) achieved the SOTA in various NER benchmarks (Lample et al., 2016).

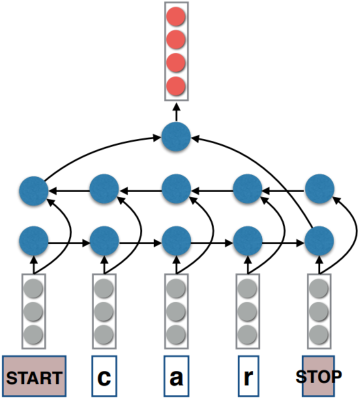
RNN-based sequence tagging

This model can be improved:

- Use a bidirectional RNN to condition also on the following words (combinining 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.

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)

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Pooled Classification

What we talked about so far assumes we want to output a sequence of labels (either to generate or tag a full sequence).

What if we just want to predict a **single label** for the whole sequence?

We can still use an RNN to capture the input sequential structure!

We just need to pool the RNNs states, i.e., map them to a single vector

Then add a single softmax to output the final label.

Pooling Strategies

The simplest pooling strategy is just to pick the last RNN state

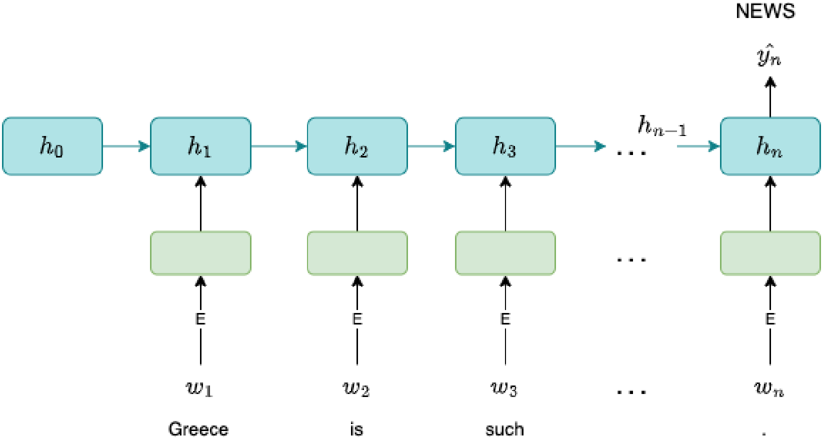
This state results from traversing the full sequence left-to-right, hence it has information about the full sequence!

Disadvantage: for long sequences, memory about the earliest words starts vanishing

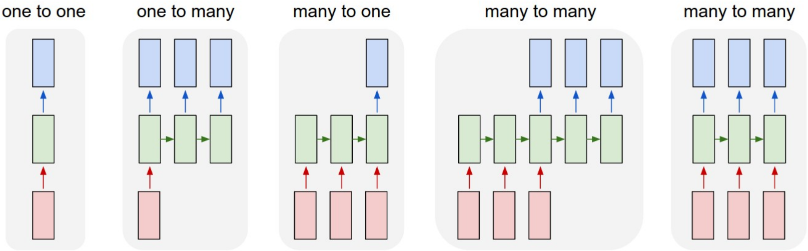
Other pooling strategies:

- use a bidirectional RNN and combine both last states of the left-to-right and right-to-left RNN
- average pooling
- ...

Example: Topic Analysis



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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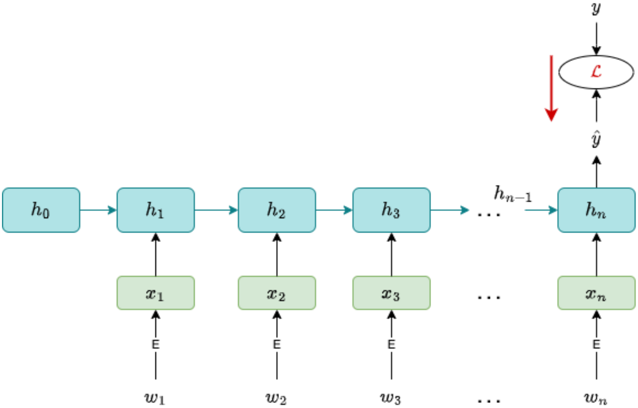
Training the RNN

This is done by backpropagation through time.

Backpropagation Through Time

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

$$\boldsymbol{h}_t = g(\boldsymbol{V}\boldsymbol{x}_t + \boldsymbol{U}\boldsymbol{h}_{t-1} + \boldsymbol{c})$$
$$\hat{\boldsymbol{y}} = \boldsymbol{W}\boldsymbol{h}_{|x|} + \boldsymbol{b})$$



Backpropagation Through Time

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

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

where

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

Three cases:

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

* more details: Pascanu et al. (2013)

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 so that you at least start with good spectra (e.g., start with random orthonormal matrices)
- Alternative parameterizations: LSTMs and GRUs

Alternative RNNs

I'll next describe:

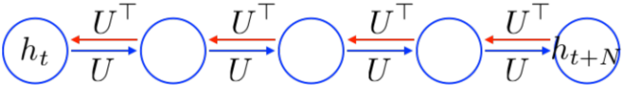
- Gated recurrent units (GRUs; Cho et al. (2014))
- Long short-term memories (LSTMs; Hochreiter and Schmidhuber (1997))

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

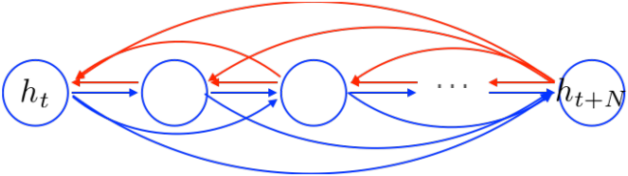
They solve the vanishing gradient problem, but still have exploding gradients (still need gradient clipping)

Gated Recurrent Units (Cho et al., 2014)

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



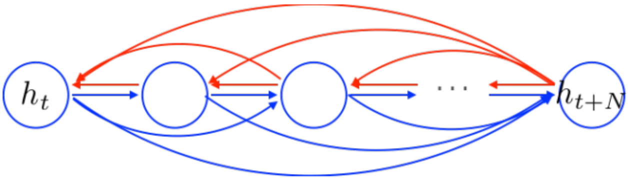
- **Idea:** Maybe we can create some kind of shortcut connections:



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

- Create adaptive shortcuts controlled by special gates

Gated Recurrent Units (Cho et al., 2014)

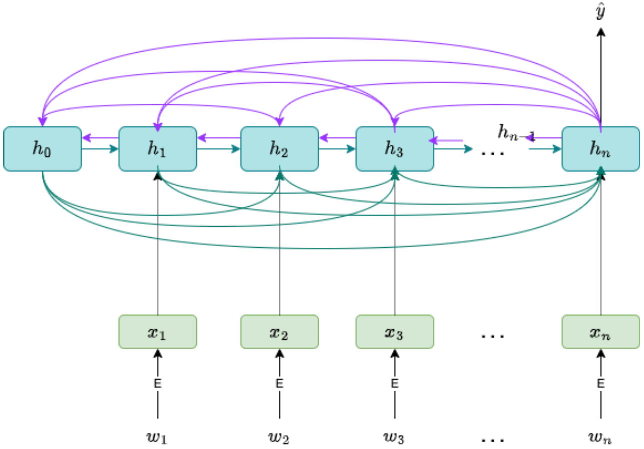


(Image credit: Thang Luong, Kyunghyun Cho, Chris Manning)

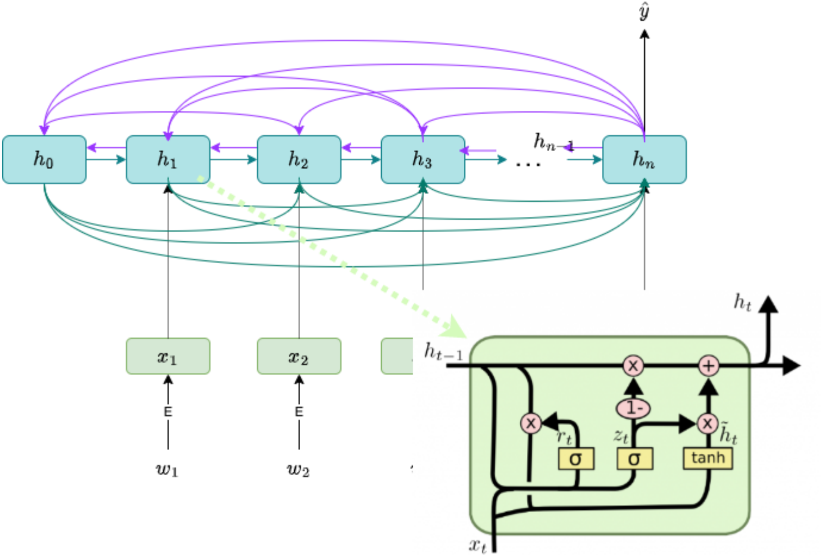
$$\boxed{\boldsymbol{h}_t = \boldsymbol{u}_t \odot \tilde{\boldsymbol{h}}_t + (1 - \boldsymbol{u}_t) \odot \boldsymbol{h}_{t-1}}$$

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

Gated Recurrent Units (Cho et al., 2014)

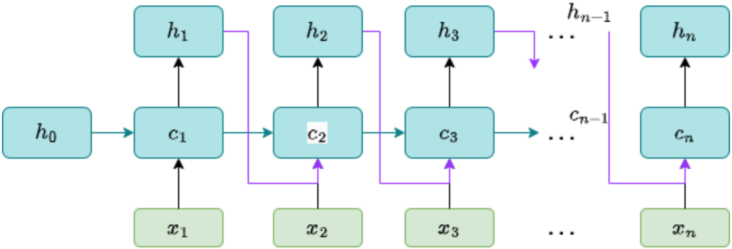


Gated Recurrent Units (Cho et al., 2014)

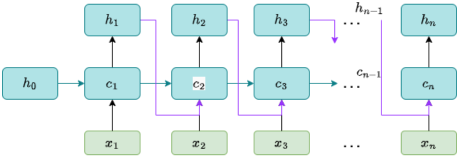


Long Short-Term Memories (Hochreiter and Schmidhuber, 1997)

- **Key idea:** use memory cells $\boldsymbol{c}_t$
- To avoid the multiplicative effect, flow information *additively* through these cells
- Control the flow with special input, forget, and output gates



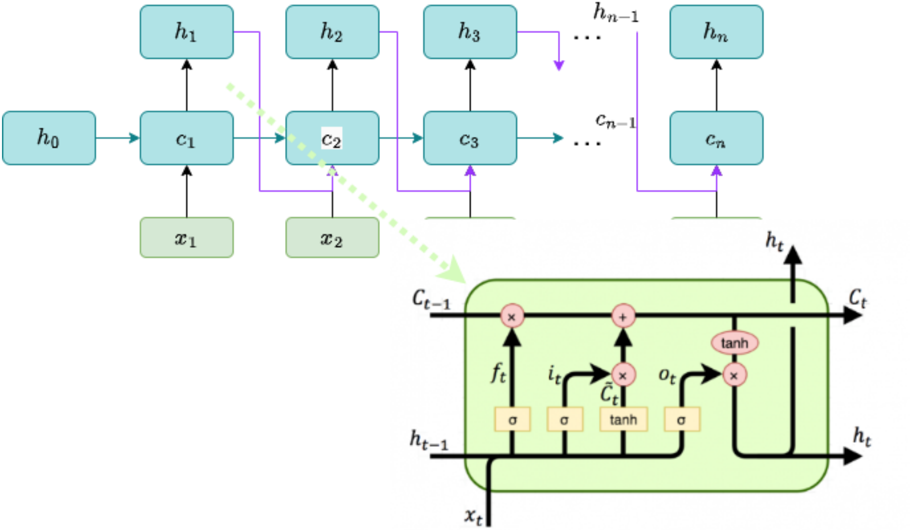
Long Short-Term Memories



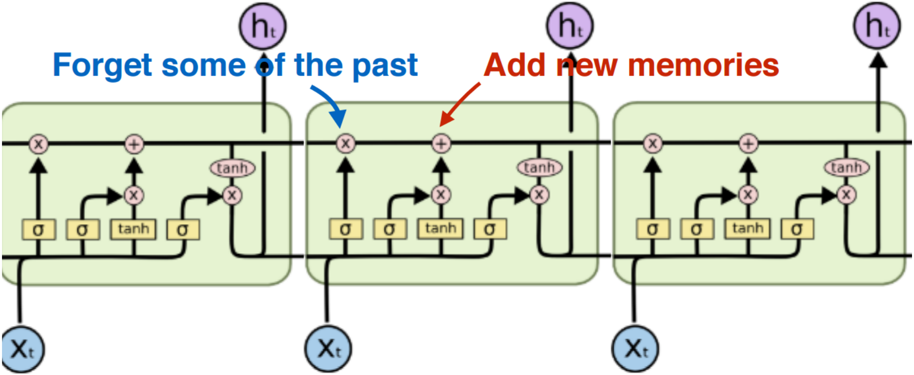
$$\boxed{\boldsymbol{c}_t = \boldsymbol{f}_t \odot \boldsymbol{c}_{t-1} + \boldsymbol{i}_t \odot \boldsymbol{g}(\boldsymbol{V}\boldsymbol{x}_t + \boldsymbol{U}\boldsymbol{h}_{t-1} + \boldsymbol{b}), \qquad \boldsymbol{h}_t = \boldsymbol{o}_t \odot \boldsymbol{g}(\boldsymbol{c}_t)}$$

- **Forget gate:** $\boldsymbol{f}_t = \sigma(\boldsymbol{V}_f \boldsymbol{x}_t + \boldsymbol{U}_f \boldsymbol{h}_{t-1} + \boldsymbol{b}_f)$
- **Input gate:** $\boldsymbol{i}_t = \sigma(\boldsymbol{V}_i \boldsymbol{x}_t + \boldsymbol{U}_i \boldsymbol{h}_{t-1} + \boldsymbol{b}_i)$
- **Output gate:** $\boldsymbol{o}_t = \sigma(\boldsymbol{V}_o \boldsymbol{x}_t + \boldsymbol{U}_o \boldsymbol{h}_{t-1} + \boldsymbol{b}_o)$

Long Short-Term Memories



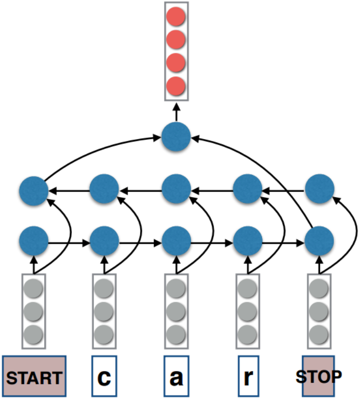
Long Short-Term Memories



(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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    - 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

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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 $\boldsymbol{p}$ from the children states $\boldsymbol{c}_1$ and $\boldsymbol{c}_2$:

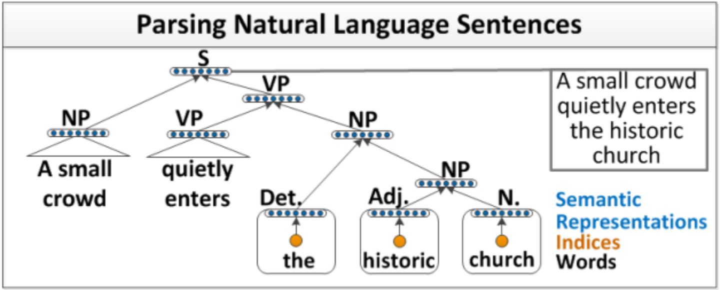
$$\boldsymbol{p} = \tanh\left(\boldsymbol{W}\left[\begin{array}{c}\boldsymbol{c}_1\\ \boldsymbol{c}_2\end{array} + \boldsymbol{b}\right]\right)$$

Use the same parameters $\boldsymbol{W}$ and $\boldsymbol{b}$ 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

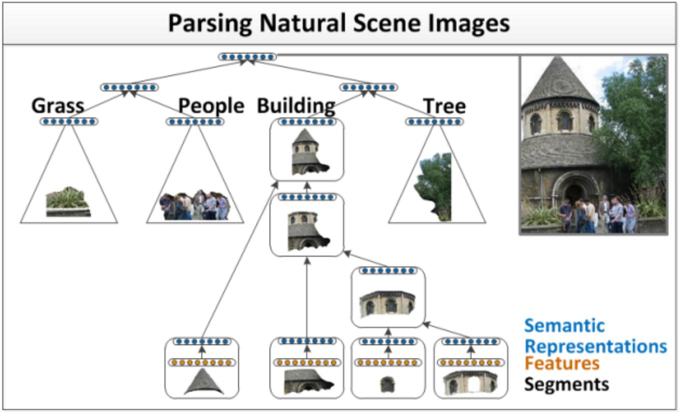
Uses a recurrent net to build a bottom-up parse tree for a sentence.



(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.

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What about Images?

While sequences are 1D, images are 2D.

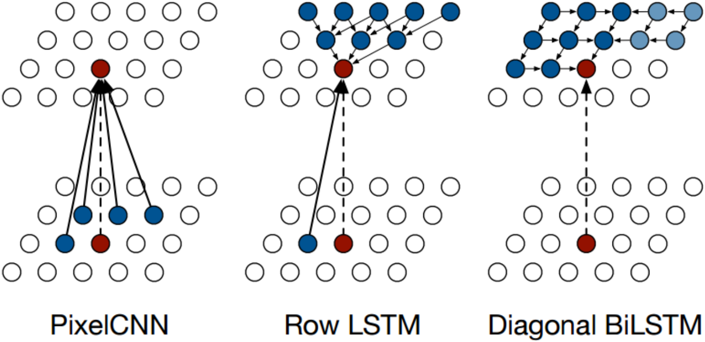
PixelRNNs are 2D extensions of Recurrent Neural Networks.

They can be used as auto-regressive models to generate images, by generating pixels in a particular order, conditioning on neighboring pixels.

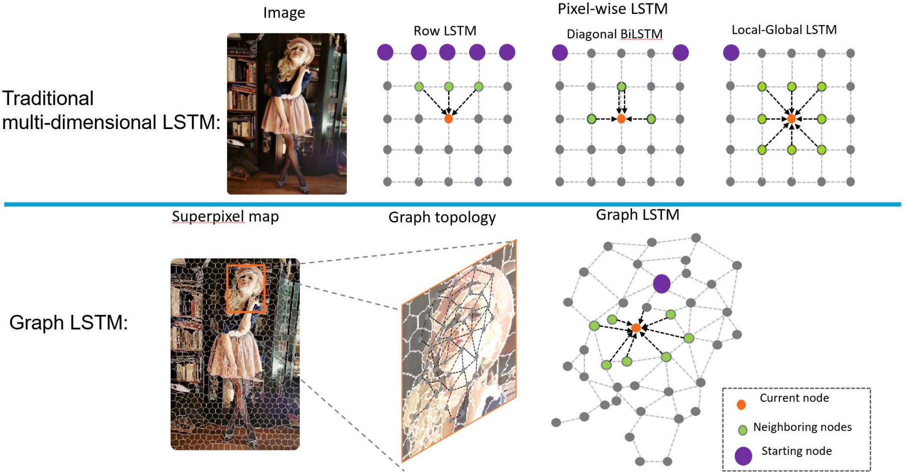
Several variants...

RNNs for Generating Images

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



Even More General: Graph LSTMs



(Credits: Xiaodan Liang)

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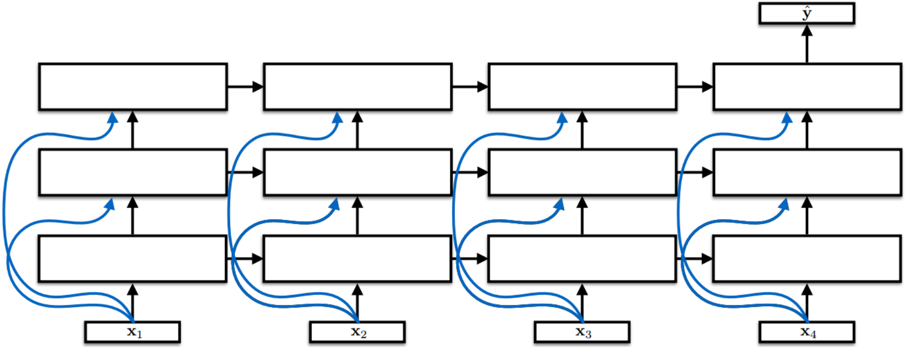
More Tricks of the Trade

- Depth
- Dropout
- Implementation Tricks
- Mini-batching

Deep RNNs/LSTMs/GRUs

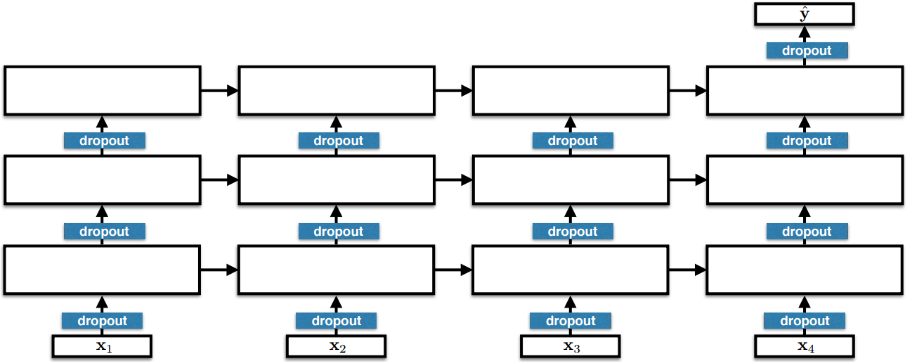
- Depth in recurrent layers helps in practice (2–8 layers seem to be standard)
- Input connections may or may not be used



(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 lots of elementwise 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
- 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?

*slides adapted from IST, DEEC 2022 Deep Structured Learning course
led by Andre F. T. Martins

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