Lecture 7: Vanishing Gradients and Fancy RNNs

Abigail See, John Hewitt
Announcements

• **Assignment 4** released today
  • Due **Thursday** next week (9 days from now, not Tuesday)
  • Based on **Neural Machine Translation (NMT)**
    • NMT will be covered in Thursday’s lecture
  • You’ll use **Azure** to get access to a virtual machine with a GPU
    • Budget extra time if you’re not used to working on a remote machine (e.g. ssh, tmux, remote text editing)
  • Get started **early**; the two extra days are because it's harder!
    • The NMT system takes **4 hours** to train!
    • **Assignment 4 is quite a lot more complicated than Assignment 3!**
    • For assignments 4 onward, TAs won't be looking at code.
    • Don’t be caught by surprise!
    • Thursday’s slides + notes are already online
Announcements

• Projects
  • Next week: lectures are all about choosing projects
  • It’s fine to delay thinking about projects until next week
  • But if you’re already thinking about projects, you can view some info/inspiration on the website’s project page
  • To be up by the time we release the Project Proposal Instructions: project ideas from potential Stanford AI Lab mentors.
Overview

• Last lecture we learned:
  • Recurrent Neural Networks (RNNs) and why they’re great for Language Modeling (LM).

• Today we’ll learn:
  • Problems with RNNs and how to fix them
  • More complex RNN variants

• Next lecture we’ll learn:
  • How we can do Neural Machine Translation (NMT) using an RNN-based architecture called sequence-to-sequence with attention
Today’s lecture: Getting RNNs to work

- **Vanishing gradient problem**

- Two new types of RNN: **LSTM** and **GRU**

- Other **fixes** for vanishing (or exploding) gradient:
  - Gradient clipping
  - Skip connections

- More fancy RNN variants:
  - Bidirectional RNNs
  - Multi-layer RNNs

Lots of important definitions today!
Vanishing gradient intuition

\[ J^{(4)}(\theta) \]

\[ h^{(1)} \rightarrow W \rightarrow h^{(2)} \rightarrow W \rightarrow h^{(3)} \rightarrow W \rightarrow h^{(4)} \]
Vanishing gradient intuition

\[ \frac{\partial J^{(4)}}{\partial h^{(1)}} = ? \]
Vanishing gradient intuition

\[
\frac{\partial J^{(4)}}{\partial h^{(1)}} = \frac{\partial h^{(2)}}{\partial h^{(1)}} \times \frac{\partial J^{(4)}}{\partial h^{(2)}}
\]

chain rule!
Vanishing gradient intuition

\[ \frac{\partial J^{(4)}}{\partial h^{(1)}} = \frac{\partial h^{(2)}}{\partial h^{(1)}} \times \]

\[ \frac{\partial h^{(3)}}{\partial h^{(2)}} \times \frac{\partial J^{(4)}}{\partial h^{(3)}} \]

chain rule!
Vanishing gradient intuition

\[
\frac{\partial J^{(4)}}{\partial h^{(1)}} = \frac{\partial h^{(2)}}{\partial h^{(1)}} \times \frac{\partial h^{(3)}}{\partial h^{(2)}} \times \frac{\partial h^{(4)}}{\partial h^{(3)}} \times \frac{\partial J^{(4)}}{\partial h^{(4)}}
\]

chain rule!
Vanishing gradient intuition

What happens if these are small?

Vanishing gradient problem:
When these are small, the gradient signal gets smaller and smaller as it backpropagates further.
Vanishing gradient proof sketch (linear case)

- Recall:
  \[ h^{(t)} = \sigma \left( W_h h^{(t-1)} + W_x x^{(t)} + b_1 \right) \]

- What if \( \sigma \) were the identity function, \( \sigma(x) = x \)?

  \[
  \frac{\partial h^{(t)}}{\partial h^{(t-1)}} = \text{diag} \left( \sigma' \left( W_h h^{(t-1)} + W_x x^{(t)} + b_1 \right) \right) W_h \\
  = I \ W_h = W_h 
  \] (chain rule)

- Consider the gradient of the loss \( J^{(i)}(\theta) \) on step \( i \), with respect to the hidden state \( h^{(j)} \) on some previous step \( j \). Let \( \ell = i - j \)

  \[
  \frac{\partial J^{(i)}(\theta)}{\partial h^{(j)}} = \frac{\partial J^{(i)}(\theta)}{\partial h^{(i)}} \prod_{j < t \leq i} \frac{\partial h^{(t)}}{\partial h^{(t-1)}} \\
  = \frac{\partial J^{(i)}(\theta)}{\partial h^{(i)}} \prod_{j < t \leq i} W_h = \frac{\partial J^{(i)}(\theta)}{\partial h^{(i)}} W_h^\ell
  \] (value of \( \frac{\partial h^{(t)}}{\partial h^{(t-1)}} \))

  If \( W_h \) is “small”, then this term gets exponentially problematic as \( \ell \) becomes large.

Vanishing gradient proof sketch (linear case)

• What’s wrong with $W^l_h$?

• Consider if the eigenvalues of $W_h$ are all less than 1:

$$\lambda_1, \lambda_2, \ldots, \lambda_n < 1$$

• We can write $\frac{\partial J(i)(\theta)}{\partial h^{(i)}} W^l_h$ using the eigenvectors of $W_h$ as a basis:

$$\frac{\partial J(i)(\theta)}{\partial h^{(i)}} W^l_h = \sum_{i=1}^{n} c_i \lambda_i^l q_i \approx 0 \text{ (for large } \ell)$$

- Approaches 0 as $\ell$ grows
- so gradient vanishes

• What about nonlinear activations $\sigma$ (i.e., what we use)?

- Pretty much the same thing, except the proof requires $\lambda_i < \gamma$ for some $\gamma$ dependent on dimensionality and $\sigma$

Why is vanishing gradient a problem?

Gradient signal from faraway is lost because it’s much smaller than gradient signal from close-by.

So model weights are updated only with respect to near effects, not long-term effects.
Why is vanishing gradient a problem?

• Another explanation: Gradient can be viewed as a measure of the effect of the past on the future

• If the gradient becomes vanishingly small over longer distances (step $t$ to step $t+n$), then we can’t tell whether:
  1. There’s no dependency between step $t$ and $t+n$ in the data
  2. We have wrong parameters to capture the true dependency between $t$ and $t+n$
Effect of vanishing gradient on RNN-LM

• **LM task:** *When she tried to print her tickets, she found that the printer was out of toner. She went to the stationery store to buy more toner. It was very overpriced. After installing the toner into the printer, she finally printed her ________*

• To learn from this training example, the RNN-LM needs to model the dependency between “tickets” on the 7th step and the target word “tickets” at the end.

• But if gradient is small, the model can’t learn this dependency
  • So the model is unable to predict similar long-distance dependencies at test time
Effect of vanishing gradient on RNN-LM

- **LM task:** *The writer of the books ___*  
  
- **Correct answer:** *The writer of the books is planning a sequel*

- **Syntactic recency:** *The writer of the books is* (correct)

- **Sequential recency:** *The writer of the books are* (incorrect)

- Vanishing gradient problems may bias RNN-LMs towards learning from **sequential recency**, so they make this type of error more often than we’d like. [Linzen et al 2016]

---

Why is exploding gradient a problem?

• If the gradient becomes too big, then the SGD update step becomes too big:

\[ \theta_{\text{new}} = \theta_{\text{old}} - \alpha \nabla_{\theta} J(\theta) \]

• This can cause bad updates: we take too large a step and reach a bad parameter configuration (with large loss)

• In the worst case, this will result in Inf or NaN in your network (then you have to restart training from an earlier checkpoint)
Gradient clipping: solution for exploding gradient

- **Gradient clipping**: if the norm of the gradient is greater than some threshold, scale it down before applying SGD update

\[
\hat{g} \leftarrow \frac{\partial \mathcal{L}}{\partial \theta} \\
\text{if } \|\hat{g}\| \geq \text{threshold} \text{ then} \\
\hat{g} \leftarrow \frac{\text{threshold}}{\|\hat{g}\|} \hat{g} \\
\text{end if}
\]

- **Intuition**: take a step in the same direction, but a smaller step

Gradient clipping: solution for exploding gradient

- This shows the loss surface of a simple RNN (hidden state is a scalar not a vector).
- The “cliff” is dangerous because it has steep gradient.
- On the left, gradient descent takes two very big steps due to steep gradient, resulting in climbing the cliff then shooting off to the right (both bad updates).
- On the right, gradient clipping reduces the size of those steps, so effect is less drastic.

How to fix vanishing gradient problem?

• The main problem is that *it’s too difficult for the RNN to learn to preserve information over many timesteps.*

• In a vanilla RNN, the hidden state is constantly being rewritten

\[ h^{(t)} = \sigma \left( W_{h} h^{(t-1)} + W_{x} x^{(t)} + b \right) \]

• How about a RNN with separate *memory?*
Long Short-Term Memory (LSTM)

- A type of RNN proposed by Hochreiter and Schmidhuber in 1997 as a solution to the vanishing gradients problem.

- On step $t$, there is a hidden state $h^{(t)}$ and a cell state $c^{(t)}$
  - Both are vectors length $n$
  - The cell stores long-term information
  - The LSTM can erase, write and read information from the cell

- The selection of which information is erased/written/read is controlled by three corresponding gates
  - The gates are also vectors length $n$
  - On each timestep, each element of the gates can be open (1), closed (0), or somewhere in-between.
  - The gates are dynamic: their value is computed based on the current context

Long Short-Term Memory (LSTM)

We have a sequence of inputs $x^{(t)}$, and we will compute a sequence of hidden states $h^{(t)}$ and cell states $c^{(t)}$. On timestep $t$:

- **Forget gate**: controls what is kept vs forgotten, from previous cell state
- **Input gate**: controls what parts of the new cell content are written to cell
- **Output gate**: controls what parts of cell are output to hidden state
- **New cell content**: this is the new content to be written to the cell
- **Cell state**: erase ("forget") some content from last cell state, and write ("input") some new cell content
- **Hidden state**: read ("output") some content from the cell

All these are vectors of same length $n$

**Sigmoid function**: all gate values are between 0 and 1

**Gates are applied using element-wise product**

$$
\begin{align*}
    f^{(t)} &= \sigma \left( W_f h^{(t-1)} + U_f x^{(t)} + b_f \right) \\
    i^{(t)} &= \sigma \left( W_i h^{(t-1)} + U_i x^{(t)} + b_i \right) \\
    o^{(t)} &= \sigma \left( W_o h^{(t-1)} + U_o x^{(t)} + b_o \right) \\
    \tilde{c}^{(t)} &= \tanh \left( W_c h^{(t-1)} + U_c x^{(t)} + b_c \right) \\
    c^{(t)} &= f^{(t)} \circ c^{(t-1)} + i^{(t)} \circ \tilde{c}^{(t)} \\
    h^{(t)} &= o^{(t)} \circ \tanh c^{(t)}
\end{align*}
$$
Long Short-Term Memory (LSTM)

You can think of the LSTM equations visually like this:

Source: [http://colah.github.io/posts/2015-08-Understanding-LSTMs/](http://colah.github.io/posts/2015-08-Understanding-LSTMs/)
You can think of the LSTM equations visually like this:

- **Forget some cell content**
- **Compute the forget gate**
- **Compute the input gate**
- **Compute the new cell content**
- **Compute the output gate**
- **Write some new cell content**
- **Output some cell content to the hidden state**

Source: [http://colah.github.io/posts/2015-08-Understanding-LSTMs/](http://colah.github.io/posts/2015-08-Understanding-LSTMs/)
How does LSTM solve vanishing gradients?

• The LSTM architecture makes it easier for the RNN to preserve information over many timesteps
  • e.g. if the forget gate is set to 1 for a cell dimension and the input gate set to 0, then the information of that cell is preserved indefinitely.
  • By contrast, it’s harder for vanilla RNN to learn a recurrent weight matrix $W_h$ that preserves info in hidden state

• LSTM doesn’t guarantee that there is no vanishing/exploding gradient, but it does provide an easier way for the model to learn long-distance dependencies
LSTMs: real-world success

- In **2013-2015**, LSTMs started achieving state-of-the-art results
  - Successful tasks include: handwriting recognition, speech recognition, machine translation, parsing, image captioning
  - LSTM became the dominant approach

- **Now (2020)**, other approaches (e.g. Transformers) have become more dominant for certain tasks.
  - For example in **WMT** (a MT conference + competition):
    - In WMT **2016**, the summary report contains “RNN” 44 times
    - In WMT **2018**, the report contains “RNN” 9 times and “Transformer” 63 times
    - In WMT **2019**: "RNN" 7 times, "Transformer" 105 times

Gated Recurrent Units (GRU)

- Proposed by Cho et al. in 2014 as a simpler alternative to the LSTM.
- On each timestep $t$ we have input $x^{(t)}$ and hidden state $h^{(t)}$ (no cell state).

**Update gate**: controls what parts of hidden state are updated vs preserved

**Reset gate**: controls what parts of previous hidden state are used to compute new content

**New hidden state content**: reset gate selects useful parts of prev hidden state. Use this and current input to compute new hidden content.

**Hidden state**: update gate simultaneously controls what is kept from previous hidden state, and what is updated to new hidden state content

\[
\begin{align*}
u^{(t)} &= \sigma \left( W_u h^{(t-1)} + U_u x^{(t)} + b_u \right) \\
r^{(t)} &= \sigma \left( W_r h^{(t-1)} + U_r x^{(t)} + b_r \right) \\
\tilde{h}^{(t)} &= \tanh \left( W_h (r^{(t)} \circ h^{(t-1)}) + U_h x^{(t)} + b_h \right) \\
h^{(t)} &= (1 - u^{(t)}) \circ h^{(t-1)} + u^{(t)} \circ \tilde{h}^{(t)}
\end{align*}
\]

**How does this solve vanishing gradient?**
Like LSTM, GRU makes it easier to retain info long-term (e.g. by setting update gate to 0)
LSTM vs GRU

- Researchers have proposed many gated RNN variants, but LSTM and GRU are the most widely-used.

- **Rule of thumb:** LSTM is a good default choice (especially if your data has particularly long dependencies, or you have lots of training data); Switch to GRUs for speed and fewer parameters.

- **Note:** LSTMs can store unboundedly* large values in memory cell dimensions, and relatively easily learn to count. (Unlike GRUs.)

---

![LSTM Diagram](image1.png)

**Single dimension used as counter**

![GRU Diagram](image2.png)

---

Is vanishing/exploding gradient just a RNN problem?

• No! It can be a problem for all neural architectures (including feed-forward and convolutional), especially deep ones.
  • Due to chain rule / choice of nonlinearity function, gradient can become vanishingly small as it backpropagates
  • Thus lower layers are learnt very slowly (hard to train)
  • Solution: lots of new deep feedforward/convolutional architectures that add more direct connections (thus allowing the gradient to flow)

For example:
• Residual connections aka “ResNet”
• Also known as skip-connections
• The identity connection preserves information by default
• This makes deep networks much easier to train

Is vanishing/exploding gradient just a RNN problem?

- No! It can be a problem for all neural architectures (including feed-forward and convolutional), especially deep ones.
  - Due to chain rule / choice of nonlinearity function, gradient can become vanishingly small as it backpropagates
  - Thus lower layers are learnt very slowly (hard to train)
  - Solution: lots of new deep feedforward/convolutional architectures that add more direct connections (thus allowing the gradient to flow)

For example:
- Dense connections aka “DenseNet”
- Directly connect each layer to all future layers!

Is vanishing/exploding gradient just a RNN problem?

• No! It can be a problem for all neural architectures (including feed-forward and convolutional), especially deep ones.
  • Due to chain rule / choice of nonlinearity function, gradient can become vanishingly small as it backpropagates
  • Thus lower layers are learnt very slowly (hard to train)
• Solution: lots of new deep feedforward/convolutional architectures that add more direct connections (thus allowing the gradient to flow)

For example:
• Highway connections aka “HighwayNet”
• Similar to residual connections, but the identity connection vs the transformation layer is controlled by a dynamic gate
• Inspired by LSTMs, but applied to deep feedforward/convolutional networks

Is vanishing/exploding gradient just a RNN problem?

• No! It can be a problem for all neural architectures (including feed-forward and convolutional), especially deep ones.
  • Due to chain rule / choice of nonlinearity function, gradient can become vanishingly small as it backpropagates
  • Thus lower layers are learnt very slowly (hard to train)
  • Solution: lots of new deep feedforward/convolutional architectures that add more direct connections (thus allowing the gradient to flow)

• Conclusion: Though vanishing/exploding gradients are a general problem, RNNs are particularly unstable due to the repeated multiplication by the same weight matrix [Bengio et al, 1994]

Recap

• Today we’ve learnt:
  • **Vanishing gradient problem**: what it is, why it happens, and why it’s bad for RNNs
  • **LSTMs and GRUs**: more complicated RNNs that use gates to control information flow; they are more resilient to vanishing gradients

• Remainder of this lecture:
  • **Bidirectional** RNNs
  • **Multi-layer** RNNs

Both of these are pretty simple
Bidirectional RNNs: motivation

Task: Sentiment Classification

We can regard this hidden state as a representation of the word “terribly” in the context of this sentence. We call this a contextual representation.

These contextual representations only contain information about the left context (e.g. “the movie was”).

What about right context?

In this example, “exciting” is in the right context and this modifies the meaning of “terribly” (from negative to positive).
Bidirectional RNNs

This contextual representation of “terribly” has both left and right context!

Concatenated hidden states

Backward RNN

Forward RNN

the, movie, was, terribly, exciting, !
Bidirectional RNNs

On timestep $t$:

This is a general notation to mean “compute one forward step of the RNN” – it could be a vanilla, LSTM or GRU computation.

\[
\overrightarrow{h}(t) = \text{RNN}_{FW}(\overrightarrow{h}(t-1), \mathbf{x}(t)) \\
\overleftarrow{h}(t) = \text{RNN}_{BW}(\overleftarrow{h}(t+1), \mathbf{x}(t)) \\
\mathbf{h}(t) = [\overrightarrow{h}(t); \overleftarrow{h}(t)]
\]

Generally, these two RNNs have separate weights.

We regard this as “the hidden state” of a bidirectional RNN. This is what we pass on to the next parts of the network.
The two-way arrows indicate bidirectionality and the depicted hidden states are assumed to be the concatenated forwards+backwards states.
Bidirectional RNNs

- Note: bidirectional RNNs are only applicable if you have access to the entire input sequence.
  - They are not applicable to Language Modeling, because in LM you only have left context available.

- If you do have entire input sequence (e.g. any kind of encoding), bidirectionality is powerful (you should use it by default).

- For example, BERT (Bidirectional Encoder Representations from Transformers) is a powerful pretrained contextual representation system built on bidirectionality.
  - You will learn more about BERT later in the course!
Multi-layer RNNs

- RNNs are already “deep” on one dimension (they unroll over many timesteps)

- We can also make them “deep” in another dimension by applying multiple RNNs – this is a multi-layer RNN.

- This allows the network to compute more complex representations
  - The lower RNNs should compute lower-level features and the higher RNNs should compute higher-level features.

- Multi-layer RNNs are also called *stacked RNNs*. 
Multi-layer RNNs

The hidden states from RNN layer $i$ are the inputs to RNN layer $i+1$.
Multi-layer RNNs in practice

• High-performing RNNs are often multi-layer (but aren’t as deep as convolutional or feed-forward networks)

• For example: In a 2017 paper, Britz et al find that for Neural Machine Translation, *2 to 4 layers* is best for the encoder RNN, and *4 layers* is best for the decoder RNN
  • However, *skip-connections/dense-connections* are needed to train deeper RNNs (e.g. *8 layers*)

• Transformer-based networks (e.g. BERT) are frequently deeper, like *12 or 24 layers*.
  • You will learn about Transformers later; they have a lot of skipping-like connections

In summary

Lots of new information today! What are the practical takeaways?

1. LSTMs are powerful but GRUs are faster

2. Clip your gradients

3. Use bidirectionality when possible

4. Multi-layer RNNs are powerful, but you might need skip/dense-connections if it’s deep