CSC413/2516 Lecture 6: Recurrent Neural Networks

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Overview

- Sometimes we're interested in predicting sequences
 - Speech-to-text and text-to-speech
 - Caption generation
 - Machine translation
- If the input is also a sequence, this setting is known as sequence-to-sequence prediction.
- We already saw one way of doing this: neural language models
 - But autoregressive models are memoryless, so they can't learn long-distance dependencies.
 - Recurrent neural networks (RNNs) are a kind of architecture which can remember things over time.

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Recall that we made a Markov assumption:

$$p(w_i | w_1, \ldots, w_{i-1}) = p(w_i | w_{i-3}, w_{i-2}, w_{i-1}).$$

This means the model is memoryless, i.e. it has no memory of anything before the last few words. But sometimes long-distance context can be important.

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Overview

• Autoregressive models such as the neural language model are memoryless, so they can only use information from their immediate context (in this figure, context length = 1):



• If we add connections between the hidden units, it becomes a recurrent neural network (RNN). Having a memory lets an RNN use longer-term dependencies:



Recurrent neural nets

- We can think of an RNN as a dynamical system with one set of hidden units which feed into themselves. The network's graph would then have self-loops.
- We can unroll the RNN's graph by explicitly representing the units at all time steps. The weights and biases are shared between all time steps
 - Except there is typically a separate set of biases for the first time step.



RNN examples

Now let's look at some simple examples of RNNs.

This one sums its inputs:



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RNN examples

This one determines if the total values of the first or second input are larger:



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Assume we have a sequence of binary inputs. We'll consider how to determine the parity, i.e. whether the number of 1's is even or odd.

We can compute parity incrementally by keeping track of the parity of the input so far:

Parity bits: 0 1 1 0 1 1 \rightarrow Input: 0 1 0 1 1 0 1 0 1 1

Each parity bit is the XOR of the input and the previous parity bit.

Parity is a classic example of a problem that's hard to solve with a shallow feed-forward net, but easy to solve with an RNN.

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Assume we have a sequence of binary inputs. We'll consider how to determine the parity, i.e. whether the number of 1's is even or odd.

• Let's find weights and biases for the RNN on the right so that it computes the parity. All hidden and output units are **binary threshold units**.

• Strategy:

- The output unit tracks the current parity, which is the XOR of the current input and previous output.
- The hidden units help us compute the XOR.



Example: Parity

Unrolling the parity RNN:



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The output unit should compute the XOR of the current input and previous output:

$y^{(t-1)}$	$x^{(t)}$	$y^{(t)}$
0	0	0
0	1	1
1	0	1
1	1	0

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Example: Parity

Let's use hidden units to help us compute XOR.

- Have one unit compute AND, and the other one compute OR.
- Then we can pick weights and biases just like we did for multilayer perceptrons.



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Example: Parity

Let's use hidden units to help us compute XOR.

- Have one unit compute AND, and the other one compute OR.
- Then we can pick weights and biases just like we did for multilayer perceptrons.





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We still need to determine the hidden biases for the first time step.

• The network should behave as if the previous output was 0. This is represented with the following table:



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- As you can guess, we don't usually set RNN weights by hand. Instead, we learn them using backprop.
- In particular, we do backprop on the unrolled network. This is known as backprop through time.



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Here's the unrolled computation graph. Notice the weight sharing.





Activations:

 $\begin{aligned} \overline{\mathcal{L}} &= 1 \\ \overline{y^{(t)}} &= \overline{\mathcal{L}} \frac{\partial \mathcal{L}}{\partial y^{(t)}} \\ \overline{r^{(t)}} &= \overline{y^{(t)}} \phi'(r^{(t)}) \\ \overline{h^{(t)}} &= \overline{r^{(t)}} v + \overline{z^{(t+1)}} w \\ \overline{z^{(t)}} &= \overline{h^{(t)}} \phi'(z^{(t)}) \end{aligned}$

Parameters:

$$\overline{u} = \sum_{t} \overline{z^{(t)}} x^{(t)}$$
$$\overline{v} = \sum_{t} \overline{r^{(t)}} h^{(t)}$$
$$\overline{w} = \sum_{t} \overline{z^{(t+1)}} h^{(t)}$$

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- Now you know how to compute the derivatives using backprop through time.
- The hard part is using the derivatives in optimization. They can explode or vanish. Addressing this issue will take all of the next lecture.

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Language Modeling

One way to use RNNs as a language model:



As with our language model, each word is represented as an indicator vector, the model predicts a distribution, and we can train it with cross-entropy loss.

This model can learn long-distance dependencies.

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When we generate from the model (i.e. compute samples from its distribution over sentences), the outputs feed back in to the network as inputs.



At training time, the inputs are the tokens from the training set (rather than the network's outputs). This is called teacher forcing.

Some remaining challenges:

- Vocabularies can be very large once you include people, places, etc. It's computationally difficult to predict distributions over millions of words.
- How do we deal with words we haven't seen before?
- In some languages (e.g. German), it's hard to define what should be considered a word.

Language Modeling

Another approach is to model text one character at a time!



This solves the problem of what to do about previously unseen words. Note that long-term memory is *essential* at the character level!

Note: modeling language well at the character level requires *multiplicative* interactions, which we're not going to talk about.

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Language Modeling

From Geoff Hinton's Coursera course, an example of a paragraph generated by an RNN language model one character at a time:

He was elected President during the Revolutionary War and forgave Opus Paul at Rome. The regime of his crew of England, is now Arab women's icons in and the demons that use something between the characters' sisters in lower coil trains were always operated on the line of the ephemerable street, respectively, the graphic or other facility for deformation of a given proportion of large segments at RTUS). The B every chord was a "strongly cold internal palette pour even the white blade."

J. Martens and I. Sutskever, 2011. Learning recurrent neural networks with Hessian-free optimization.

http://machinelearning.wustl.edu/mlpapers/paper_files/ICML2011Martens_532.pdf

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Neural Machine Translation

We'd like to translate, e.g., English to French sentences, and we have pairs of translated sentences to train on.

What's wrong with the following setup?



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Neural Machine Translation

We'd like to translate, e.g., English to French sentences, and we have pairs of translated sentences to train on.

What's wrong with the following setup?



- The sentences might not be the same length, and the words might not align perfectly.
- You might need to resolve ambiguities using information from later in the sentence.

Neural Machine Translation

Sequence-to-sequence architecture: the network first reads and memorizes the sentence. When it sees the end token, it starts outputting the translation.



The encoder and decoder are two different networks with different weights.

Learning Phrase Representations using RNN Encoder-Decoder for Statistical Machine Translation, K. Cho, B. van Merrienboer, C. Gulcehre, D. Bahdanau, F. Bougares, H. Schwenk, Y. Bengio. EMNLP 2014.

Sequence to Sequence Learning with Neural Networks, Ilya Sutskever, Oriol Vinyals and Quoc Le, NIPS 2014.

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What can RNNs compute?

In 2014, Google researchers built an encoder-decoder RNN that learns to execute simple Python programs, *one character at a time*!

Input: j=8584 for x in range(8): j+=920 b=(1500+j) print((b+7567)) Target: 25011.

Input:			
i=8827			
c=(i-5347)			
print((c+8704)	if	2641<8500	else
5308)			
Target: 1218.			

Example training inputs

Input: vqppkn sqdvfljmnc y2vxdddsepnimcbvubkomhrpliibtwztbljipcc Target: hkhpg

A training input with characters scrambled

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W. Zaremba and I. Sutskever, "Learning to Execute." http://arxiv.org/abs/1410.4615

What can RNNs compute?

Some example results:

Input:

print(6652).

Target:	6652.
"Baseline" prediction:	6652.
"Naive" prediction:	6652.
"Mix" prediction:	6652.
"Combined" prediction:	6652.

print((5997-738)).

Target:	5259.
"Baseline" prediction:	5101.
"Naive" prediction:	5101.
"Mix" prediction:	52 4 9.
"Combined" prediction:	52 <mark>2</mark> 9.

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Input:

<pre>d=5446 for x in range(8):d+=(2678 if 4803<2829 else 9848) print((d if 5935<4845 else 3043)).</pre>		9848)	<pre>Input: print(((1090-3305)+9466)).</pre>		
Target: "Baseline" prediction: "Naive" prediction: "Mix" prediction: "Combined" prediction:	3043. 3043. 3043. 3043. 3043. 3043.	3043)).		Target: "Baseline" prediction: "Naive" prediction: "Mix" prediction: "Combined" prediction:	7251. 7111. 7099. 7595. 7699.

Take a look through the results (http://arxiv.org/pdf/1410.4615v2.pdf#page=10). It's fun to try to guess from the mistakes what algorithms it's discovered.

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After The Break: LSTM

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Overview

- Last time, we saw how to compute the gradient descent update for an RNN using backprop through time.
- The updates are mathematically correct, but unless we're very careful, gradient descent completely fails because the gradients explode or vanish.
- The problem is, it's hard to learn dependencies over long time windows.
- Today's lecture is about what causes exploding and vanishing gradients, and how to deal with them. Or, equivalently, how to learn long-term dependencies.

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• Recall the RNN for machine translation. It reads an entire English sentence, and then has to output its French translation.



- A typical sentence length is 20 words. This means there's a gap of 20 time steps between when it sees information and when it needs it.
- The derivatives need to travel over this entire pathway.

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Recall: backprop through time



Activations:

$$\begin{split} \overline{\mathcal{L}} &= 1\\ \overline{y^{(t)}} &= \overline{\mathcal{L}} \frac{\partial \mathcal{L}}{\partial y^{(t)}}\\ \overline{r^{(t)}} &= \overline{y^{(t)}} \phi'(r^{(t)})\\ \overline{h^{(t)}} &= \overline{r^{(t)}} v + \overline{z^{(t+1)}} w\\ \overline{z^{(t)}} &= \overline{h^{(t)}} \phi'(z^{(t)}) \end{split}$$

Parameters:

$$\overline{u} = \sum_{t} \overline{z^{(t)}} x^{(t)}$$
$$\overline{v} = \sum_{t} \overline{r^{(t)}} h^{(t)}$$
$$\overline{w} = \sum_{t} \overline{z^{(t+1)}} h^{(t)}$$

Consider a univariate version of the encoder network:



Backprop updates:

$$\overline{\overline{h^{(t)}}} = \overline{z^{(t+1)}} w$$
$$\overline{z^{(t)}} = \overline{\overline{h^{(t)}}} \phi'(z^{(t)})$$

 $\overline{h^{(1)}} = \underbrace{w^{T-1}\phi'(z^{(2)})\cdots\phi'(z^{(T)})}_{\text{the Jacobian }\partial h^{(T)}/\partial h^{(1)}} \overline{h^{(T)}}$

Applying this recursively:

With linear activations:

$$\partial h^{(T)}/\partial h^{(1)} = w^{T-1}$$

Exploding:

$$w = 1.1, T = 50 \quad \Rightarrow \quad \frac{\partial h^{(T)}}{\partial h^{(1)}} = 117.4$$

$$w = 0.9, T = 50 \Rightarrow \frac{\partial h^{(T)}}{\partial h^{(1)}} = 0.00515$$

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• More generally, in the multivariate case, the Jacobians multiply:

$$\frac{\partial \mathbf{h}^{(\mathcal{T})}}{\partial \mathbf{h}^{(1)}} = \frac{\partial \mathbf{h}^{(\mathcal{T})}}{\partial \mathbf{h}^{(\mathcal{T}-1)}} \cdots \frac{\partial \mathbf{h}^{(2)}}{\partial \mathbf{h}^{(1)}}$$

- Matrices can explode or vanish just like scalar values, though it's slightly harder to make precise.
- Contrast this with the forward pass:
 - The forward pass has nonlinear activation functions which squash the activations, preventing them from blowing up.
 - The backward pass is linear, so it's hard to keep things stable. There's a thin line between exploding and vanishing.

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- We just looked at exploding/vanishing gradients in terms of the mechanics of backprop. Now let's think about it conceptually.
- The Jacobian ∂h^(T)/∂h⁽¹⁾ means, how much does h^(T) change when you change h⁽¹⁾?
- Each hidden layer computes some function of the previous hiddens and the current input:

$$\mathbf{h}^{(t)} = f(\mathbf{h}^{(t-1)}, \mathbf{x}^{(t)})$$

• This function gets iterated:

$$\mathbf{h}^{(4)} = f(f(\mathbf{h}^{(1)}, \mathbf{x}^{(2)}), \mathbf{x}^{(3)}), \mathbf{x}^{(4)}).$$

• Let's study iterated functions as a way of understanding what RNNs are computing.

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Iterated Functions

• Iterated functions are complicated. Consider:

$$f(x) = 3.5 x \left(1 - x\right)$$



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Iterated Functions

An aside:

• Remember the Mandelbrot set? That's based on an iterated quadratic map over the complex plane:

$$z_n = z_{n-1}^2 + c$$

• The set consists of the values of *c* for which the iterates stay bounded.



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Why Gradients Explode or Vanish

• Let's imagine an RNN's behavior as a dynamical system, which has various attractors:



⁻ Geoffrey Hinton, Coursera

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- Within one of the colored regions, the gradients vanish because even if you move a little, you still wind up at the same attractor.
- If you're on the boundary, the gradient blows up because moving slightly moves you from one attractor to the other.

Why Gradients Explode or Vanish

• Consider an RNN with tanh activation function:



• The function computed by the network:



Why Gradients Explode or Vanish

• Cliffs make it hard to estimate the true cost gradient. Here are the loss and cost functions with respect to the bias parameter for the hidden units:



• Generally, the gradients will explode on some inputs and vanish on others. In expectation, the cost may be fairly smooth.

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- One simple solution: gradient clipping
- Clip the gradient **g** so that it has a norm of at most η : if $\|\mathbf{g}\| > \eta$: $\mathbf{g} \leftarrow \frac{\eta \mathbf{g}}{\|\mathbf{g}\|}$
- The gradients are biased, but at least they don't blow up.



Goodfellow et al., Deep Learning

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• Another trick: reverse the input sequence.



- This way, there's only one time step between the first word of the input and the first word of the output.
- The network can first learn short-term dependencies between early words in the sentence, and then long-term dependencies between later words.

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- Really, we're better off redesigning the architecture, since the exploding/vanishing problem highlights a conceptual problem with vanilla RNNs.
- The hidden units are a kind of memory. Therefore, their default behavior should be to keep their previous value.
 - I.e., the function at each time step should be close to the identity function.
 - It's hard to implement the identity function if the activation function is nonlinear!
- If the function is close to the identity, the gradient computations are stable.
 - The Jacobians $\partial \mathbf{h}^{(t+1)}/\partial \mathbf{h}^{(t)}$ are close to the identity matrix, so we can multiply them together and things don't blow up.

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• Identity RNNs

- Use the ReLU activation function
- Initialize all the weight matrices to the identity matrix
- Negative activations are clipped to zero, but for positive activations, units simply retain their value in the absence of inputs.
- This allows learning much longer-term dependencies than vanilla RNNs.
- It was able to learn to classify MNIST digits, input as sequence one pixel at a time!

Le et al., 2015. A simple way to initialize recurrent networks of rectified linear units.

- Another architecture which makes it easy to remember information over long time periods is called Long-Term Short Term Memory (LSTM)
 - What's with the name? The idea is that a network's activations are its short-term memory and its weights are its long-term memory.
 - The LSTM architecture wants the short-term memory to last for a long time period.
- It's composed of memory cells which have controllers saying when to store or forget information.

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Replace each single unit in an RNN by a memory block -



 $c_{t+1} = c_t \cdot \text{forget gate} + \text{new input} \cdot \text{input gate}$

- $i = 0, f = 1 \Rightarrow$ remember the previous value
- $i = 1, f = 1 \Rightarrow$ add to the previous value
- $i = 0, f = 0 \Rightarrow$ erase the value
- $i = 1, f = 0 \Rightarrow$ overwrite the value

Setting i = 0, f = 1 gives the reasonable "default" behavior of just remembering things.

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- In each step, we have a vector of memory cells c, a vector of hidden units h, and vectors of input, output, and forget gates i, o, and f.
- There's a full set of connections from all the inputs and hiddens to the input and all of the gates:

$$\begin{pmatrix} \mathbf{i}_t \\ \mathbf{f}_t \\ \mathbf{o}_t \\ \mathbf{g}_t \end{pmatrix} = \begin{pmatrix} \sigma \\ \sigma \\ \tau \\ \tanh \end{pmatrix} \mathbf{W} \begin{pmatrix} \mathbf{y}_t \\ \mathbf{h}_{t-1} \end{pmatrix}$$

$$\mathbf{c}_t = \mathbf{f}_t \circ \mathbf{c}_{t-1} + \mathbf{i}_t \circ \mathbf{g}_t$$

$$\mathbf{h}_t = \mathbf{o}_t \circ \tanh(\mathbf{c}_t)$$

• Exercise: show that if $\mathbf{f}_{t+1} = 1$, $\mathbf{i}_{t+1} = 0$, and $\mathbf{o}_t = 0$, the gradients for the memory cell get passed through unmodified, i.e.

$$\overline{\mathbf{c}_t} = \overline{\mathbf{c}_{t+1}}.$$

- Sound complicated? ML researchers thought so, so LSTMs were hardly used for about a decade after they were proposed.
- In 2013 and 2014, researchers used them to get impressive results on challenging and important problems like speech recognition and machine translation.
- Since then, they've been one of the most widely used RNN architectures.
- There have been many attempts to simplify the architecture, but nothing was conclusively shown to be simpler and better.
- You never have to think about the complexity, since frameworks like TensorFlow provide nice black box implementations.

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Visualizations:

http://karpathy.github.io/2015/05/21/rnn-effectiveness/

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After the break: RNN + Attention

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Overview

- We have seen a few RNN-based sequence prediction models.
- It is still challenging to generate long sequences, when the decoders only has access to the final hidden states from the encoder.
 - Machine translation: it's hard to summarize long sentences in a single vector, so let's allow the decoder peek at the input.
 - Vision: have a network glance at one part of an image at a time, so that we can understand what information it's using
- This lecture will introduce attention that drastically improves the performance on the long sequences.
- We can also use attention to build differentiable computers (e.g. Neural Turing Machines)

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Overview

• Attention-based models scale very well with the amount of training data. After 40GB text from reddit, the model generates:

Context (human-written): In a shocking finding, scientist discovered a herd of unicorns living in a remote, previously unexplored valley, in the Andes Mountains. Even more surprising to the researchers was the fact that the unicorns spoke perfect English.

GPT-2: The scientist named the population, after their distinctive horn, Ovid's Unicorn. These four-horned, silver-white unicorns were previously unknown to science.

Now, after almost two centuries, the mystery of what sparked this odd phenomenon is finally solved.

Dr. Jorge Pérez, an evolutionary biologist from the University of La Paz, and several companions, were exploring the Andes Mountains when they found a small valley, with no other animals or humans. Pérez noticed that the valley had what appeared to be a natural fountain, surrounded by two peaks of rock and silver snow.

Pérez and the others then ventured further into the valley. "By the time we reached the top of one peak, the water looked blue, with some crystals on top," said Pérez.

Pérez and his friends were astonished to see the unicorn herd. These creatures could be seen from the air without having to move too much to see them – they were so close they could touch their horns.

For the full text samples see Radford, Alec, et al. "Language Models are Unsupervised Multitask Learners." 2019.

https://talktotransformer.com/

• Remember the encoder/decoder architecture for machine translation:



- The network reads a sentence and stores all the information in its hidden units.
- Some sentences can be really long. Can we really store all the information in a vector of hidden units?
 - Let's make things easier by letting the decoder refer to the input sentence.

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- We'll look at the translation model from the classic paper: Bahdanau et al., Neural machine translation by jointly learning to align and translate. ICLR, 2015.
- Basic idea: each output word comes from one word, or a handful of words, from the input. Maybe we can learn to attend to only the relevant ones as we produce the output.

- The model has both an encoder and a decoder. The encoder computes an annotation of each word in the input.
- It takes the form of a bidirectional RNN. This just means we have an RNN that runs forwards and an RNN that runs backwards, and we concantenate their hidden vectors.
 - The idea: information earlier or later in the sentence can help disambiguate a word, so we need both directions.
 - The RNN uses an LSTM-like architecture called gated recurrent units.



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- The decoder network is also an RNN. Like the encoder/decoder translation model, it makes predictions one word at a time, and its predictions are fed back in as inputs.
- The difference is that it also receives a context vector *t* at each time step, which is computed by attending to the inputs.



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• The context vector is computed as a weighted average of the encoder's annotations.

$$i = \sum_{j} \alpha_{ij} h^{(j)}$$

• The attention weights are computed as a softmax, where the inputs depend on the annotation and the decoder's state:

$$\alpha_{ij} = \frac{\exp(\tilde{\alpha}_{ij})}{\sum_{j'} \exp(\tilde{\alpha}_{ij'})}$$
$$\tilde{\alpha}_{ij} = f(\mathbf{s}^{(i-1)}, \mathbf{h}^{(j)})$$

- Note that the attention function, *f* depends on the annotation vector, rather than the position in the sentence. This means it's a form of content-based addressing.
 - My language model tells me the next word should be an adjective. Find me an adjective in the input.

Example: Pooling

Consider obtain a context vector from a set of annotations.



Example: Pooling

We can use average pooling but it is content independent.

context = avg-pooling(
$$\begin{array}{c|cccc} 1 & 0 & 5 \\ \hline 3 & 0 & -1 \\ \hline 0 & 1 & 2 \end{array}$$
) = $0.33 \times \begin{array}{c} 1 \\ \hline 3 \\ \hline 0 \end{array}$ + $0.33 \times \begin{array}{c} 0 \\ \hline 0 \\ \hline 1 \end{array}$ + $0.33 \times \begin{array}{c} 5 \\ -1 \\ 2 \end{array}$ = $\begin{array}{c} 2 \\ \hline 0.6 \\ \hline 1 \end{array}$

Example1: Bahdanau's Attention

Content-based addressing/lookup using attention.



Example1: Bahdanau's Attention

Consider a linear attention function, f.



Example1: Bahdanau's attention

Vectorized linear attention function.



• Here's a visualization of the attention maps at each time step.



- Nothing forces the model to go linearly through the input sentence, but somehow it learns to do it.
 - It's not perfectly linear e.g., French adjectives can come after the nouns.

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• The attention-based translation model does much better than the encoder/decoder model on long sentences.



- Attention can also be used to understand images.
- We humans can't process a whole visual scene at once.
 - The fovea of the eye gives us high-acuity vision in only a tiny region of our field of view.
 - Instead, we must integrate information from a series of glimpses.
- The next few slides are based on this paper from the UofT machine learning group:

Xu et al. Show, Attend, and Tell: Neural Image Caption Generation with Visual Attention. ICML, 2015.

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- The caption generation task: take an image as input, and produce a sentence describing the image.
- **Encoder:** a classification conv net (VGGNet, similar to AlexNet). This computes a bunch of feature maps over the image.
- **Decoder:** an attention-based RNN, analogous to the decoder in the translation model
 - In each time step, the decoder computes an attention map over the entire image, effectively deciding which regions to focus on.
 - It receives a context vector, which is the weighted average of the conv net features.

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 This lets us understand where the network is looking as it generates a sentence.





A woman is throwing a frisbee in a park.



A dog is standing on a hardwood floor.



A stop sign is on a road with a mountain in the background.



A little <u>girl</u> sitting on a bed with a teddy bear.



A group of <u>people</u> sitting on a boat in the water.



A giraffe standing in a forest with trees in the background.

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• This can also help us understand the network's mistakes.



A large white bird standing in a forest.



A woman holding a clock in her hand.



A man wearing a hat and a hat on a <u>skateboard</u>.



A person is standing on a beach with a <u>surfboard.</u>

A woman is sitting at a table with a large pizza.

A man is talking on his cell phone while another man watches.

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