Advanced Machine Learning
Lecture 17

Recurrent Neural Networks

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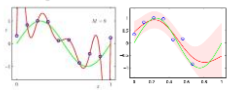
Bastian Leibe
RWTH Aachen
http://www.vision.rwth-aachen.de/

leibe@vision.rwth-aachen.de

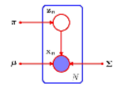
This Lecture: *Advanced Machine Learning*

$f : \mathcal{X} \to \mathbb{R}$

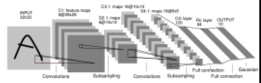
- Regression Approaches
  - Linear Regression
  - Regularization (Ridge, Lasso)
  - Kernels (Kernel Ridge Regression)
  - Gaussian Processes



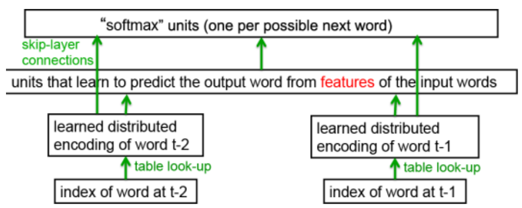
- Approximate Inference
  - Sampling Approaches
  - MCMC



- Deep Learning
  - Linear Discriminants
  - Neural Networks
  - Backpropagation & Optimization
  - CNNs, RNNs, ResNets, etc.



Recap: Neural Probabilistic Language Model

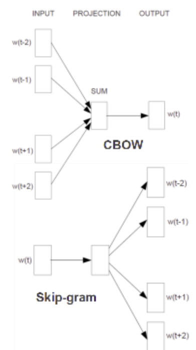


- Core idea
  - Learn a shared distributed encoding (word embedding) for the words in the vocabulary.

Y. Bengio, R. Ducharme, P. Vincent, C. Jauvin, A Neural Probabilistic Language Model, In JMLR, Vol. 3, pp. 1137-1155, 2003.

Recap: word2vec

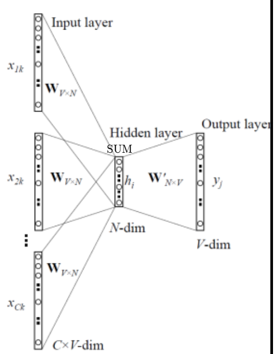
- Goal
  - Make it possible to learn high-quality word embeddings from huge data sets (billions of words in training set).
- Approach
  - Define two alternative learning tasks for learning the embedding:
    - "Continuous Bag of Words" (CBOW)
    - "Skip-gram"
  - Designed to require fewer parameters.



Recap: word2vec CBOW Model

- Continuous BOW Model
  - Remove the non-linearity from the hidden layer
  - Share the projection layer for all words (their vectors are averaged)

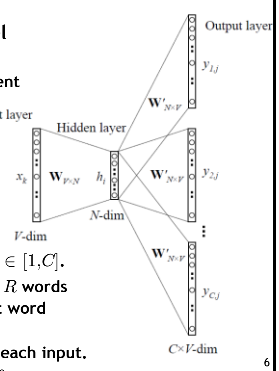
  ⇒ Bag-of-Words model (order of the words does not matter anymore)



Recap: word2vec Skip-Gram Model

- Continuous Skip-Gram Model
  - Similar structure to CBOW
  - Instead of predicting the current word, predict words within a certain range of the current word.
  - Give less weight to the more distant words
- Implementation
  - Randomly choose a number $R \in [1, C]$.
  - Use R words from history and R words from the future of the current word as correct labels.

  ⇒ R+R word classifications for each input.



Problems with 100k-1M outputs

- Weight matrix gets huge!
  - Example: CBOW model
  - One-hot encoding for inputs
  - ⇒ Input-hidden connections are just vector lookups.
  - This is not the case for the hidden-output connections!
  - State h is not one-hot, and vocabulary size is 1M.
  - ⇒ $\mathbf{W}'_{N\times V}$ has 300×1M entries
- Softmax gets expensive!
  - Need to compute normalization over 100k-1M outputs

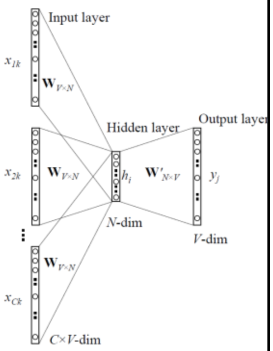
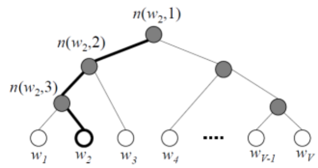


Image source: Xin Rong, 2015

Recap: Hierarchical Softmax



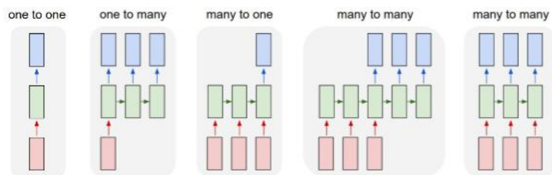
- Idea
  - Organize words in binary search tree, words are at leaves
  - Factorize probability of word w_0 as a product of node probabilities along the path.
  - Learn a linear decision function $y = v_{n(w,j)} \cdot h$ at each node to decide whether to proceed with left or right child node.
  - ⇒ Decision based on output vector of hidden units directly.

Image source: Xin Rong, 2015

Topics of This Lecture

- Recurrent Neural Networks (RNNs)
  - Motivation
  - Intuition
- Learning with RNNs
  - Formalization
  - Comparison of Feedforward and Recurrent networks
  - Backpropagation through Time (BPTT)
- Problems with RNN Training
  - Vanishing Gradients
  - Exploding Gradients
  - Gradient Clipping

Recurrent Neural Networks



- Up to now
  - Simple neural network structure: 1-to-1 mapping of inputs to outputs
- This lecture: Recurrent Neural Networks
  - Generalize this to arbitrary mappings

Image source: Andrej Karpathy

Application: Part-of-Speech Tagging

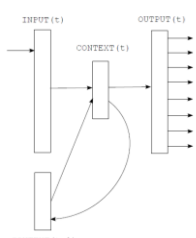
Legend: Click the legend words to toggle highlighting. Get help on this page.

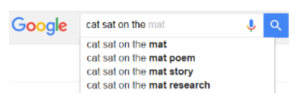
Noun Pronoun Verb Adjective Adverb Conjunction Preposition Article Interjection

Andrew and Maria thought their jobs were secure after the rancorous argument with the customer , but alas ! Bad news is fast approaching them , especially after they viciously insulted the customer on social media .

Image source: http://rewordify.com

Application: Predicting the Next Word



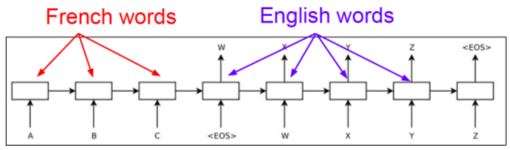


T. Mikolov, M. Karafiat, L. Burget, J. Cernocky, S. Khudanpur, Recurrent Neural Network Based Language Model, Interspeech 2010.

Slide credit: Andrej Karpathy, Fei-Fei Li

Image source: Mikolov et al., 2010

Application: Machine Translation



I. Sutskever, O. Vinyals, Q. Le, [Sequence to Sequence Learning with Neural Networks](), NIPS 2014.

RNNs: Intuition

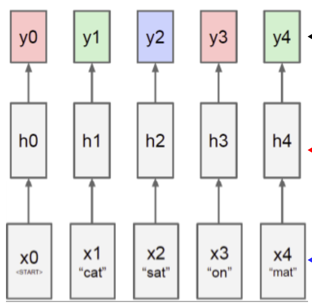
- Example: Language modeling
  - Suppose we had the training sequence "cat sat on mat"
  - We want to train a language model

$$p(\textit{next word} \mid \textit{previous words})$$

  - First assume we only have a finite, 1-word history.
  - I.e., we want those probabilities to be high:
    - $p(cat \mid <S>)$
    - $p(sat \mid cat)$
    - $p(on \mid sat)$
    - $p(mat \mid on)$
    - $p(<E> \mid mat)$

RNNs: Intuition

- Vanilla 2-layer classification net



10,001D class scores (Softmax over 10k words and a special <END> token)

$\mathbf{y}_4 = \mathbf{W}_{hy}\mathbf{h}_4$

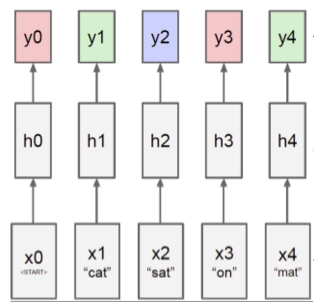
Hidden layer (e.g., 500D vectors)

$\mathbf{h}_4 = \max\{0, \mathbf{W}_{xh}\mathbf{x}_4\}$

Word embedding (300D vector for each word)

RNNs: Intuition

- Turning this into an RNN (wait for it...)



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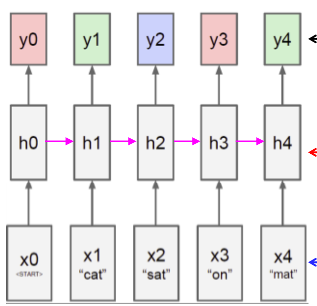
RNNs: Intuition

- Turning this into an RNN (done!)



10,001D class scores (Softmax over 10k words and a special <END> token)

$\mathbf{y}_4 = \mathbf{W}_{hy}\mathbf{h}_4$

Hidden layer (e.g., 500D vectors)

$\mathbf{h}_4 = \max\{0, \mathbf{W}_{xh}\mathbf{x}_4 + \mathbf{W}_{hh}\mathbf{h}_3\}$

Word embedding (300D vector for each word)

RNNs: Intuition

- Training this on a lot of sentences would give us a language model.
- I.e., a way to predict

$p(\textit{next word} \mid \textit{previous words})$

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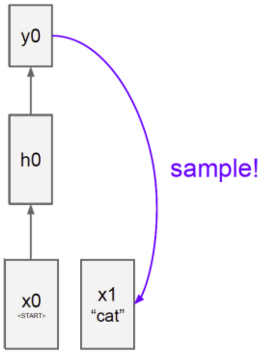

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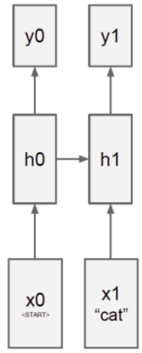

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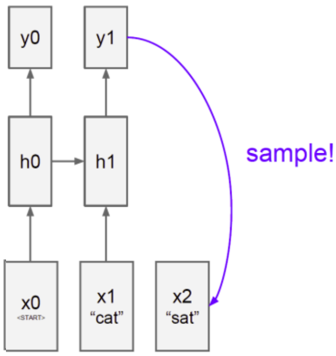

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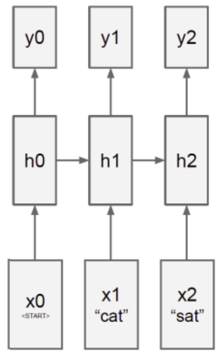

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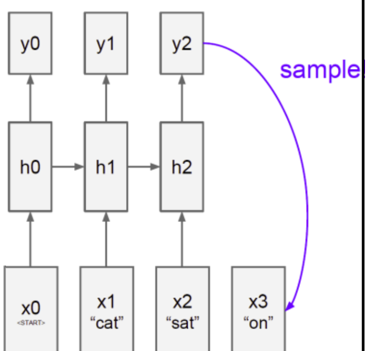

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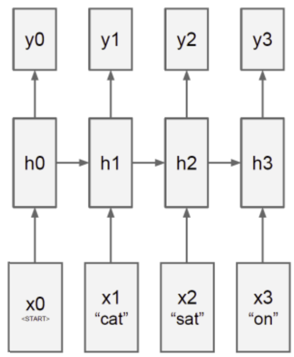

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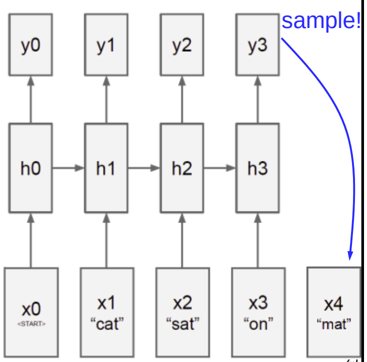

Slide credit: Andrej Karpathy, Fei-Fei Li

RNNs: Intuition

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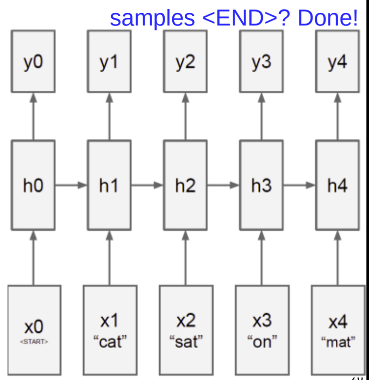

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Topics of This Lecture

- Recurrent Neural Networks (RNNs)
  - Motivation
  - Intuition
- **Learning with RNNs**
  - Formalization
  - Comparison of Feedforward and Recurrent networks
  - Backpropagation through Time (BPTT)
- Problems with RNN Training
  - Vanishing Gradients
  - Exploding Gradients
  - Gradient Clipping

RNNs: Introduction

- RNNs are regular NNs whose hidden units have additional forward connections over time
  - You can unroll them to create a network that extends over time.
  - When you do this, keep in mind that the weights for the hidden units are shared between temporal layers.

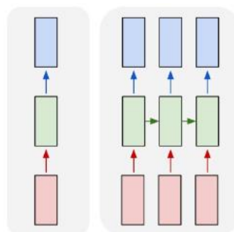
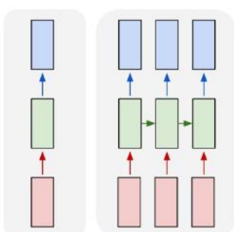


Image source: Andrej Karpathy

RNNs: Introduction

- RNNs are very powerful, because they combine two properties:
  - Distributed hidden state that allows them to store a lot of information about the past efficiently.
  - Non-linear dynamics that allows them to update their hidden state in complicated ways.



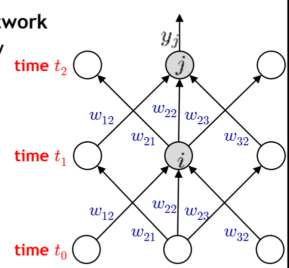
- With enough neurons and time, RNNs can compute anything that can be computed by your computer.

Slide credit: Geoff Hinton

Image source: Andrej Karpathy

Feedforward Nets vs. Recurrent Nets

- Imagine a feedforward network
  - Assume there is a time delay of 1 in using each connection.
  - $\Rightarrow$ This is very similar to how an RNN works.
  - Only change: the layers share their weights.



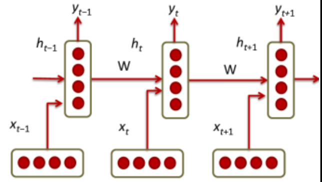
$\Rightarrow$ The recurrent net is just a feedforward net that keeps reusing the same weights.

Backpropagation with Weight Constraints

- It is easy to modify the backprop algorithm to incorporate linear weight constraints
  - To constrain $w_1 = w_2$, we start with the same initialization and then make sure that the gradients are the same:
    $$\nabla w_1 = \nabla w_2$$
  - We compute the gradients as usual and then use
    $$\frac{\partial E}{\partial w_1} + \frac{\partial E}{\partial w_2}$$
    for both w_1 and w_2.

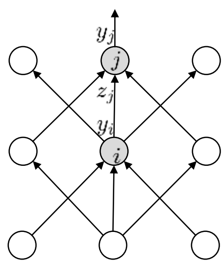
Backpropagation Through Time (BPTT)

- Formalization
  - Inputs $\mathbf{x}_t$
  - Outputs $\mathbf{y}_t$
  - Hidden units $\mathbf{h}_t$
  - Initial state $\mathbf{h}_0$
  - Connection matrices
    - $\mathbf{W}_{xh}$
    - $\mathbf{W}_{hy}$
    - $\mathbf{W}_{hh}$



  - Configuration
    $$\mathbf{h}_t = \sigma\left(\mathbf{W}_{xh}\mathbf{x}_t + \mathbf{W}_{hh}\mathbf{h}_{t-1} + b\right)$$
    $$\hat{\mathbf{y}}_t = \mathrm{softmax}\left(\mathbf{W}_{hy}\mathbf{h}_t\right)$$

Recap: Backpropagation Algorithm



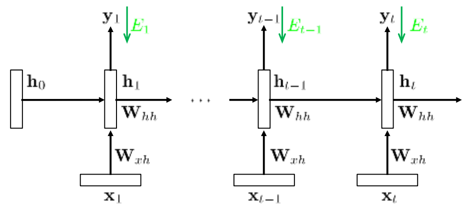
$$\frac{\partial E}{\partial z_j} = \frac{\partial y_j}{\partial z_j}\frac{\partial E}{\partial y_j} = y_j(1-y_j)\frac{\partial E}{\partial y_j}$$

$$\frac{\partial E}{\partial y_i} = \sum_j \frac{\partial z_j}{\partial y_i}\frac{\partial E}{\partial z_j} = \sum_j w_{ij}\frac{\partial E}{\partial z_j}$$

$$\frac{\partial E}{\partial w_{ij}} = \frac{\partial z_j}{\partial w_{ij}}\frac{\partial E}{\partial z_j} = y_i\frac{\partial E}{\partial z_j}$$

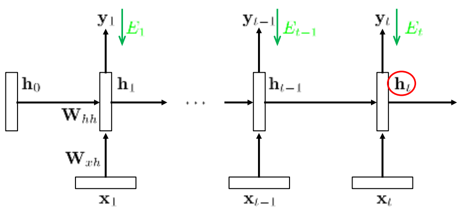
- Efficient propagation scheme
  - y_i is already known from forward pass! (Dynamic Programming)
  - ⇒ Propagate back the gradient from layer j and multiply with y_i.

Backpropagation Through Time (BPTT)



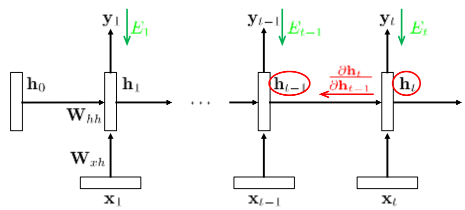
- Error function
  - Computed over all time steps: $E = \sum_{1 \le t \le T} E_t$

Backpropagation Through Time (BPTT)



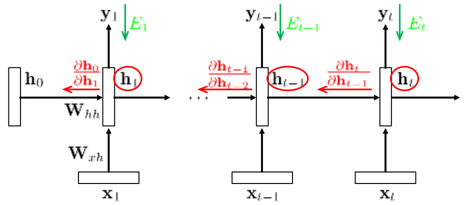
- Backpropagated gradient
  - For weight w_{ij}: $\frac{\partial E_t}{\partial w_{ij}} = \frac{\partial E_t}{\partial \mathbf{h}_t}\frac{\partial \mathbf{h}_t}{\partial w_{ij}}$

Backpropagation Through Time (BPTT)



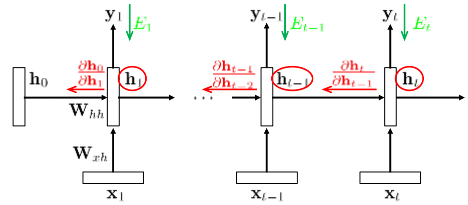
- Backpropagated gradient
  - For weight w_{ij}: $\frac{\partial E_t}{\partial w_{ij}} = \frac{\partial E_t}{\partial \mathbf{h}_t}\frac{\partial \mathbf{h}_t}{\partial w_{ij}} + \frac{\partial E_t}{\partial \mathbf{h}_t}\frac{\partial \mathbf{h}_t}{\partial \mathbf{h}_{t-1}}\frac{\partial \mathbf{h}_{t-1}}{\partial w_{ij}}$

Backpropagation Through Time (BPTT)



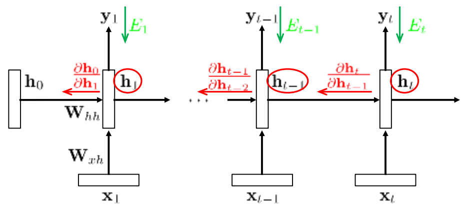
- Backpropagated gradient
  - For weight w_{ij}: $\frac{\partial E_t}{\partial w_{ij}} = \frac{\partial E_t}{\partial \mathbf{h}_t}\frac{\partial \mathbf{h}_t}{\partial w_{ij}} + \frac{\partial E_t}{\partial \mathbf{h}_t}\frac{\partial \mathbf{h}_t}{\partial \mathbf{h}_{t-1}}\frac{\partial \mathbf{h}_{t-1}}{\partial w_{ij}} + \cdots$
  - In general: $\frac{\partial E_t}{\partial w_{ij}} = \sum_{1 \le k \le t} \left(\frac{\partial E_t}{\partial h_t}\frac{\partial h_t}{\partial h_k}\frac{\partial^+ h_k}{\partial w_{ij}} \right)$

Backpropagation Through Time (BPTT)



- Analyzing the terms
  - For weight w_{ij}: $\frac{\partial E_t}{\partial w_{ij}} = \sum_{1 \le k \le t} \left(\frac{\partial E_t}{\partial h_t}\frac{\partial h_t}{\partial h_k}\frac{\partial^+ h_k}{\partial w_{ij}} \right)$
  - This is the "immediate" partial derivative (with $\mathbf{h}_{k-1}$ as constant)

Backpropagation Through Time (BPTT)



- Analyzing the terms
  - For weight w_{ij}: $\frac{\partial E_t}{\partial w_{ij}} = \sum_{1 \le k \le t} \left(\frac{\partial E_t}{\partial h_t}\frac{\partial h_t}{\partial h_k}\frac{\partial^+ h_k}{\partial w_{ij}} \right)$
  - Propagation term: $\frac{\partial h_t}{\partial h_k} = \prod_{t \ge i > k} \frac{\partial \mathbf{h}_i}{\partial \mathbf{h}_{i-1}}$

Backpropagation Through Time (BPTT)

- Summary
  - Backpropagation equations

$$E = \sum_{1 \le t \le T} E_t$$

$$\frac{\partial E_t}{\partial w_{ij}} = \sum_{1 \le k \le t} \left(\frac{\partial E_t}{\partial h_t}\frac{\partial h_t}{\partial h_k}\frac{\partial^+ h_k}{\partial w_{ij}} \right)$$

$$\frac{\partial h_t}{\partial h_k} = \prod_{t \ge i > k} \frac{\partial \mathbf{h}_i}{\partial \mathbf{h}_{i-1}} = \prod_{t \ge i > k} \mathbf{W}_{hh}^\top \mathit{diag}\left(\sigma'(\mathbf{h}_{i-1})\right)$$

  - Remaining issue: how to set the initial state $\mathbf{h}_0$?

⇒ Learn this together with all the other parameters.

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- **Problems with RNN Training**
  - Vanishing Gradients
  - Exploding Gradients
  - Gradient Clipping

Problems with RNN Training

- Training RNNs is very hard
  - As we backpropagate through the layers, the magnitude of the gradient may grow or shrink exponentially

⇒ Exploding or vanishing gradient problem!

  - In an RNN trained on long sequences (e.g., 100 time steps) the gradients can easily explode or vanish.
  - Even with good initial weights, it is very hard to detect that the current target output depends on an input from many time-steps ago.

Exploding / Vanishing Gradient Problem

- Consider the propagation equations:

$$\frac{\partial E_t}{\partial w_{ij}} = \sum_{1\le k\le t}\left(\frac{\partial E_t}{\partial h_t}\frac{\partial h_t}{\partial h_k}\frac{\partial^+ h_k}{\partial w_{ij}}\right)$$

$$\frac{\partial h_t}{\partial h_k} = \prod_{t\ge i>k}\frac{\partial \mathbf{h}_i}{\partial \mathbf{h}_{i-1}} = \prod_{t\ge i>k}\mathbf{W}_{hh}^\top diag\left(\sigma'(\mathbf{h}_{i-1})\right)$$

$$= \left(\mathbf{W}_{hh}^\top\right)^l$$

  - if t goes to infinity and $l = t - k$.

  ⇒ We are effectively taking the weight matrix to a high power.
  - The result will depend on the eigenvalues of $\mathbf{W}_{hh}$.
    - Largest eigenvalue > 1 ⇒ Gradients *may* explode.
    - Largest eigenvalue < 1 ⇒ Gradients *will* vanish.
    - This is very bad...

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Why Is This Bad?

- Vanishing gradients in language modeling
  - Words from time steps far away are not taken into consideration when training to predict the next word.
- Example:
  - „Jane walked into the room. John walked in too. It was late in the day. Jane said hi to ____"

  ⇒ The RNN will have a hard time learning such long-range dependencies.

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Gradient Clipping

- Trick to handle exploding gradients
  - If the gradient is larger than a threshold, clip it to that threshold.

Algorithm 1 Pseudo-code for norm clipping the gradients whenever they explode

$\hat{\mathbf{g}} \leftarrow \frac{\partial \mathcal{E}}{\partial \theta}$
if $\|\hat{\mathbf{g}}\| \ge threshold$ **then**
  $\hat{\mathbf{g}} \leftarrow \frac{threshold}{\|\hat{\mathbf{g}}\|}\hat{\mathbf{g}}$
end if

  - This makes a big difference in RNNs

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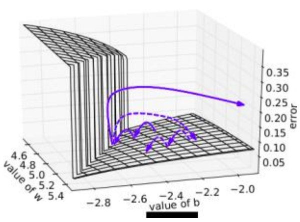
Gradient Clipping Intuition



- Example
  - Error surface of a single RNN neuron
  - High curvature walls
  - Solid lines: standard gradient descent trajectories
  - Dashed lines: gradients rescaled to fixed size

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References and Further Reading

- RNNs
  - R. Pascanu, T. Mikolov, Y. Bengio, On the difficulty of training recurrent neural networks, JMLR, Vol. 28, 2013.
  - A. Karpathy, The Unreasonable Effectiveness of Recurrent Neural Networks, blog post, May 2015.