Advanced Machine Learning
Lecture 18

Recurrent Neural Networks

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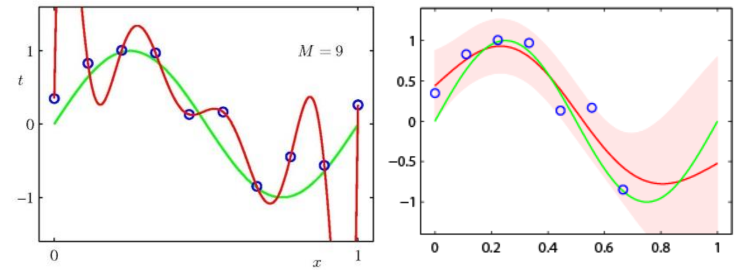
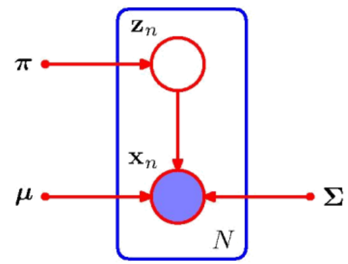
This Lecture: *Advanced Machine Learning*

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

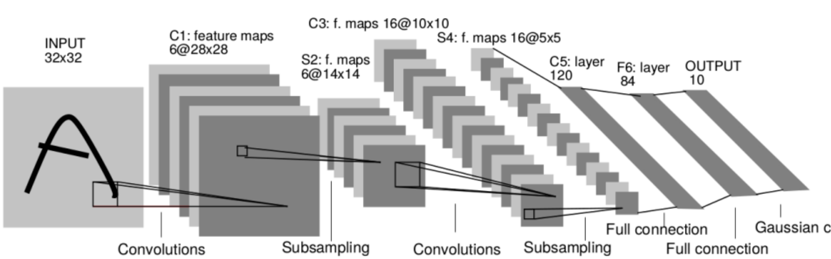
$$f : \mathcal{X} \rightarrow \mathbb{R}$$



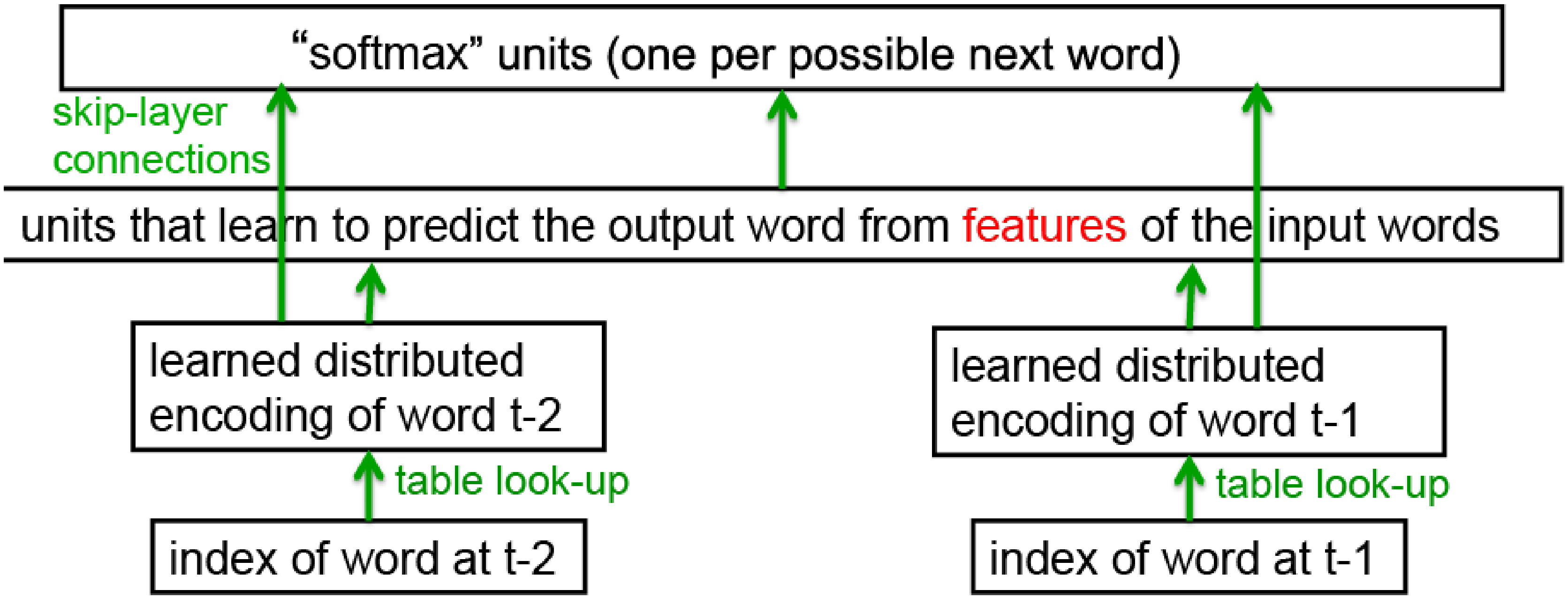
- Learning with Latent Variables
  - Prob. Distributions & Approx. Inference
  - Mixture Models
  - EM and Generalizations



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

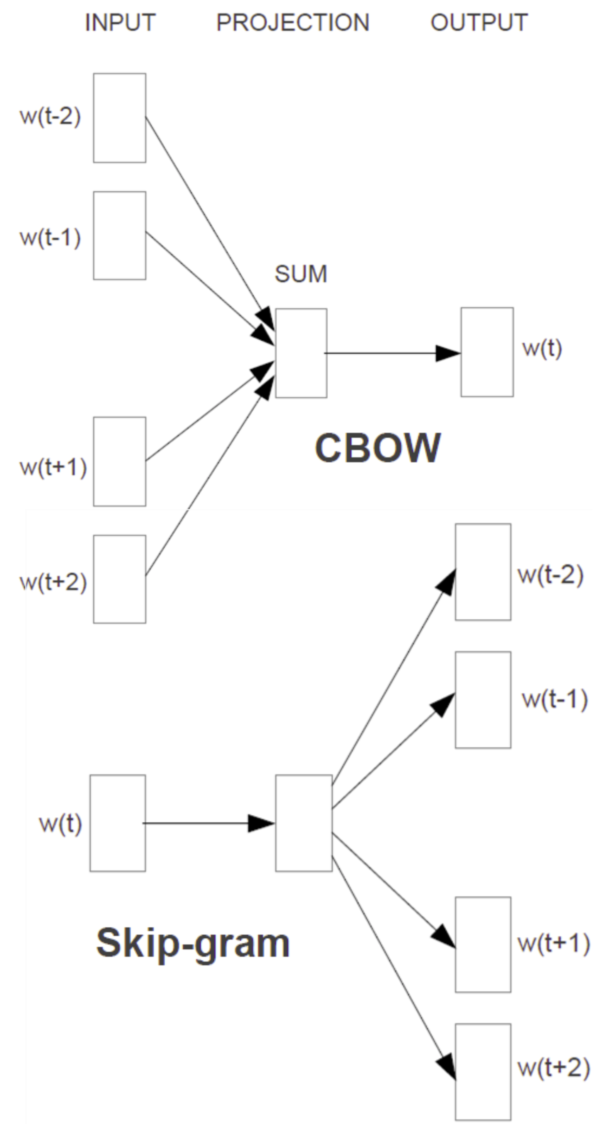


Image source: Mikolov et al., 2015

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)

$\Rightarrow$ Bag-of-Words model (order of the words does not matter anymore)

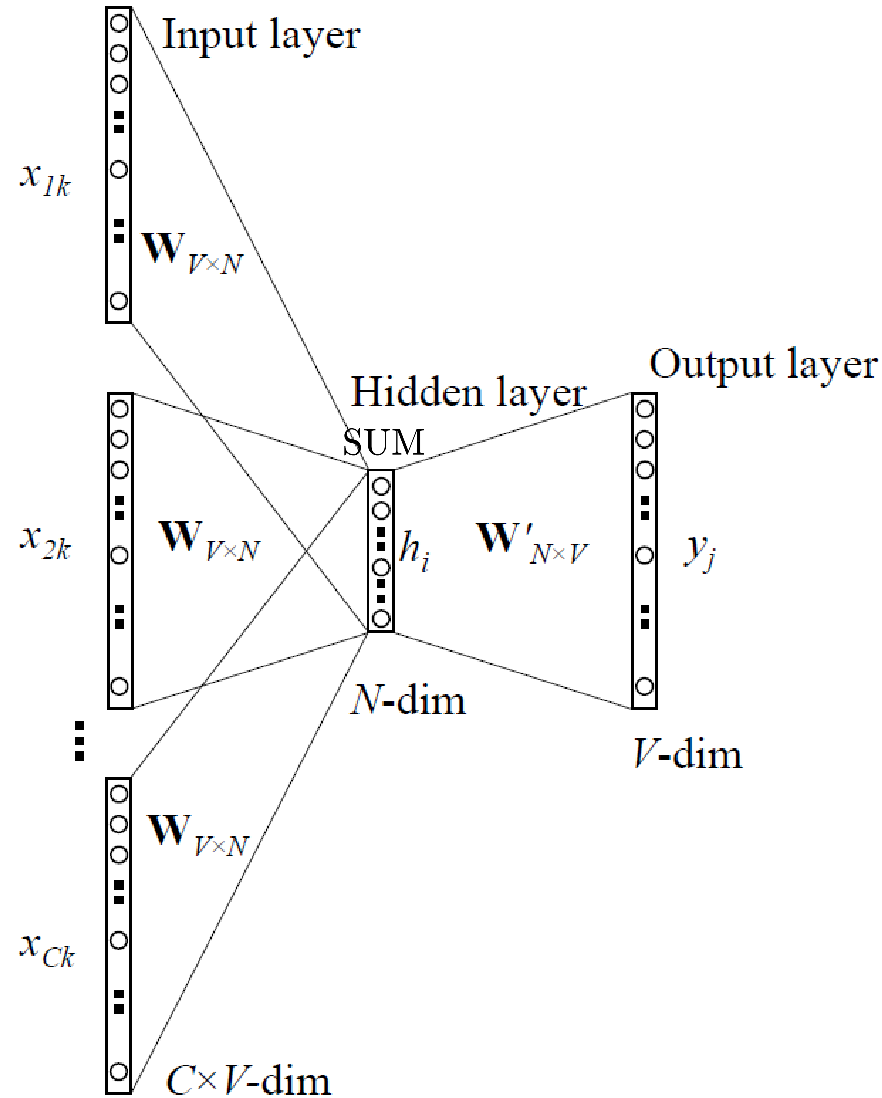
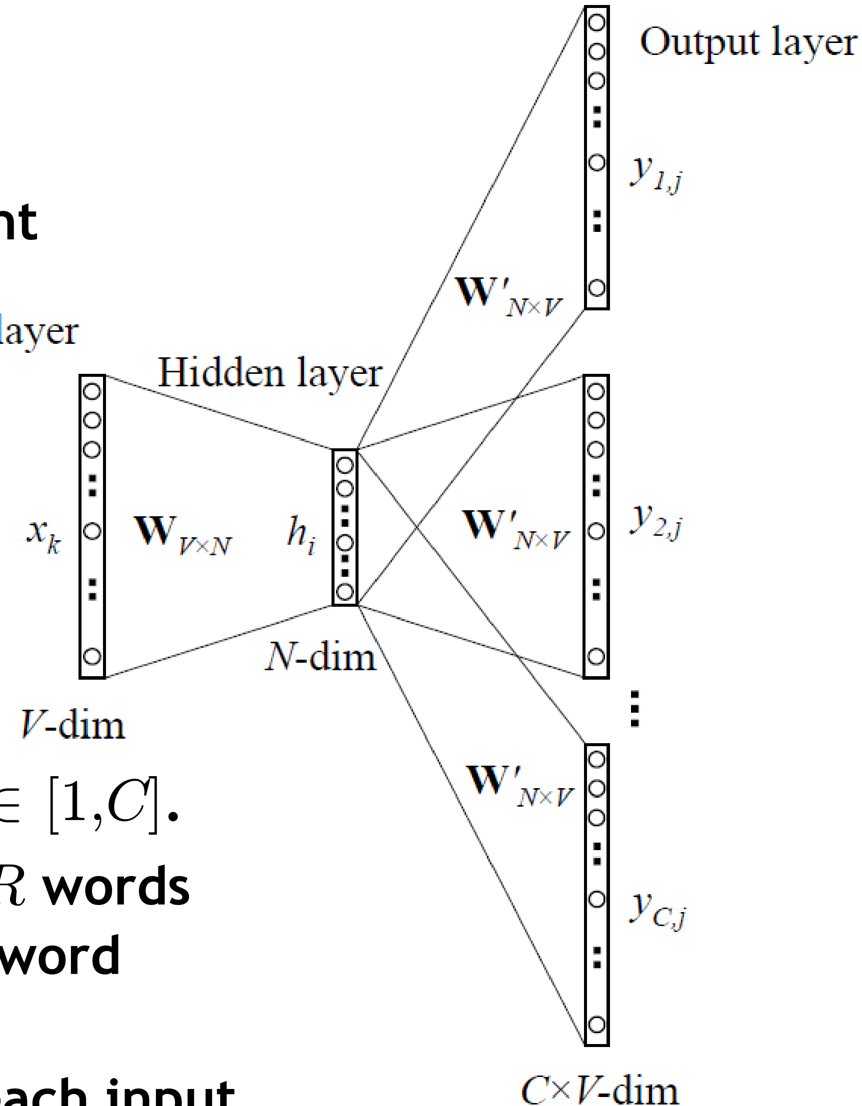


Image source: Xin Rong, 2015

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.

$\Rightarrow$ $R+R$ word classifications for each input.

Image source: Xin Rong, 2015

Problems with 100k-1M outputs

- **Weight matrix gets huge!**
  - Example: CBOW model
  - One-hot encoding for inputs

  $\Rightarrow$ 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.

  $\Rightarrow$ $\mathbf{W}'_{N \times V}$ has $300 \times 1\text{M}$ entries

- **Softmax gets expensive!**
  - Need to compute normalization over 100k-1M outputs

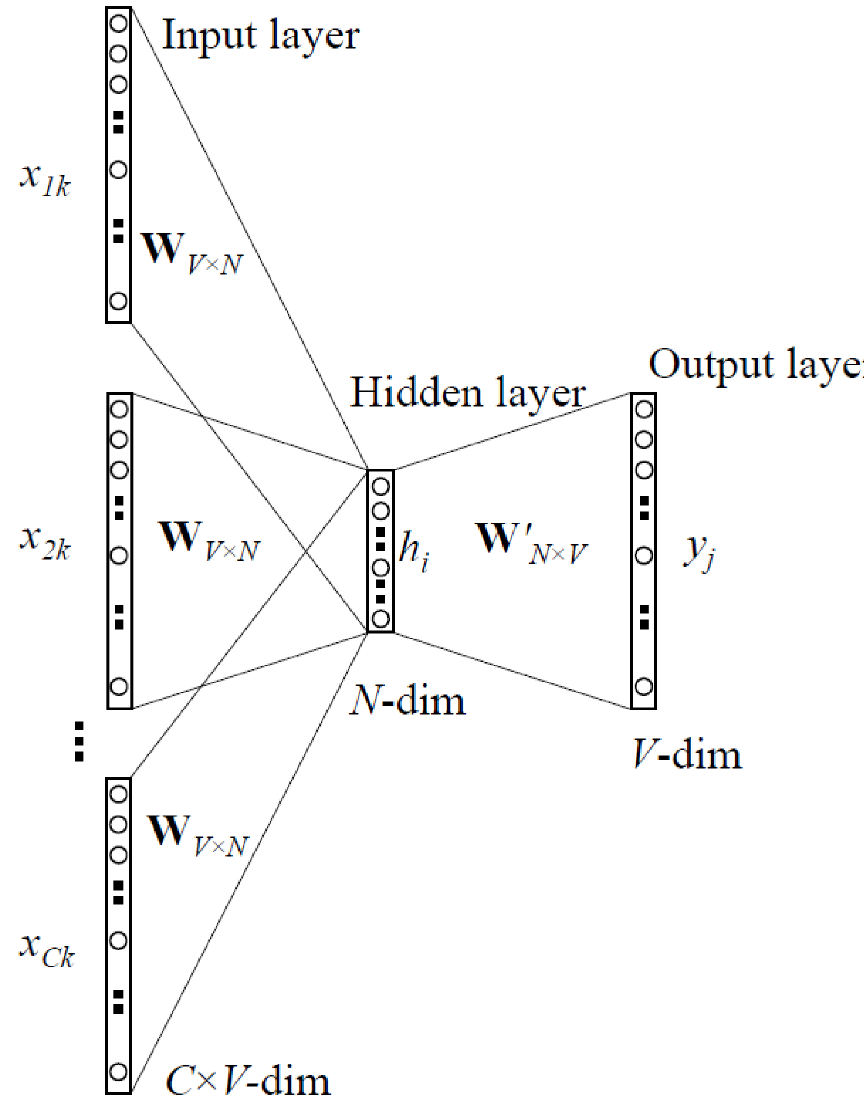
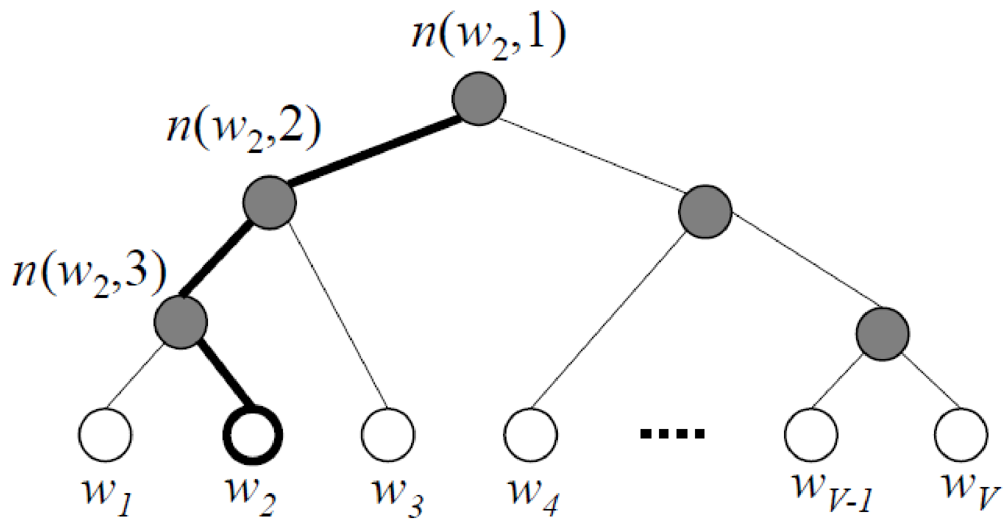


Image source: Xin Rong, 2015

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.

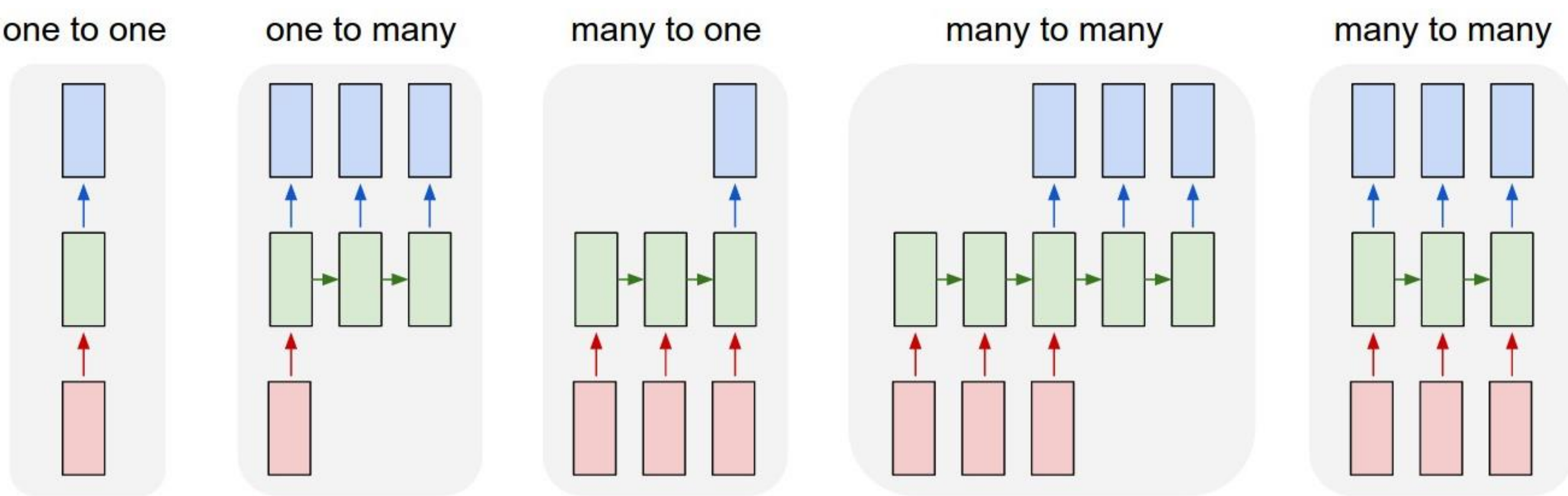
$\Rightarrow$ Decision based on output vector of hidden units directly.

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

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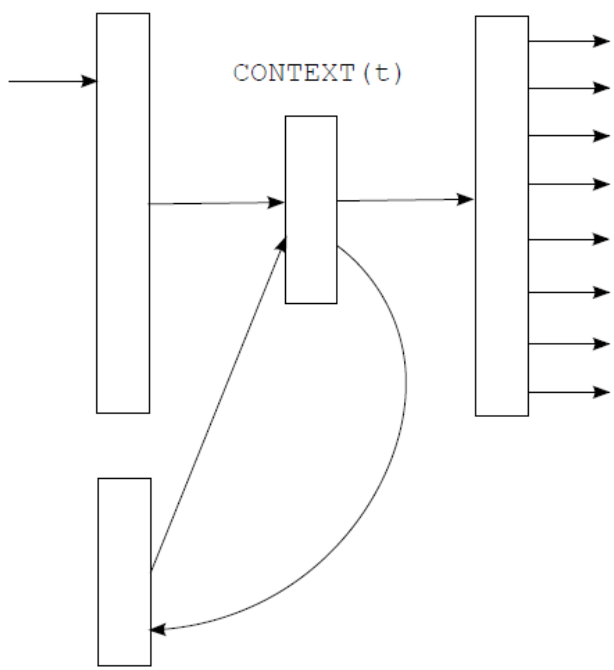
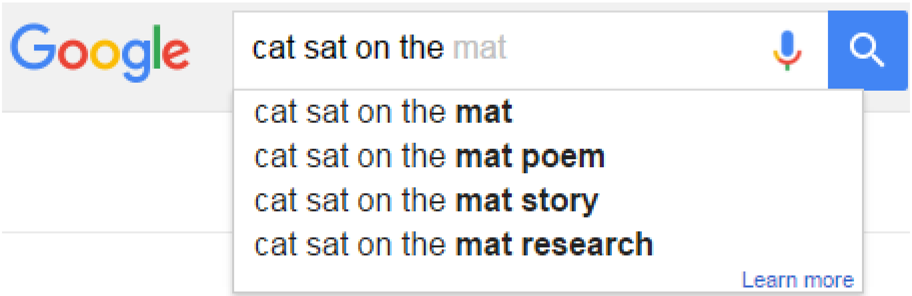
Andrew and Maria thought their jobs were secure after the rancorous argument with the customer , but alas ! Bad news is fast approaching them , especially after they viciously insulted the customer on social media .

Image source: http://rewordify.com

Application: Predicting the Next Word

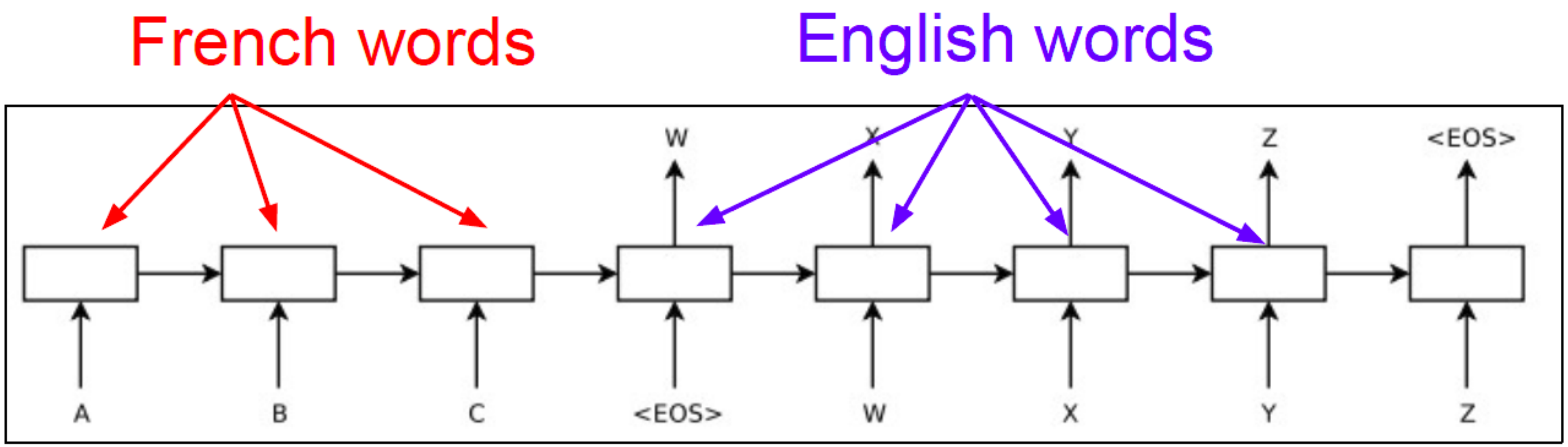




T. Mikolov, M. Karafiat, L. Burget, J. Cernocky, S. Khudanpur, Recurrent Neural Network Based Language Model, Interspeech 2010.

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

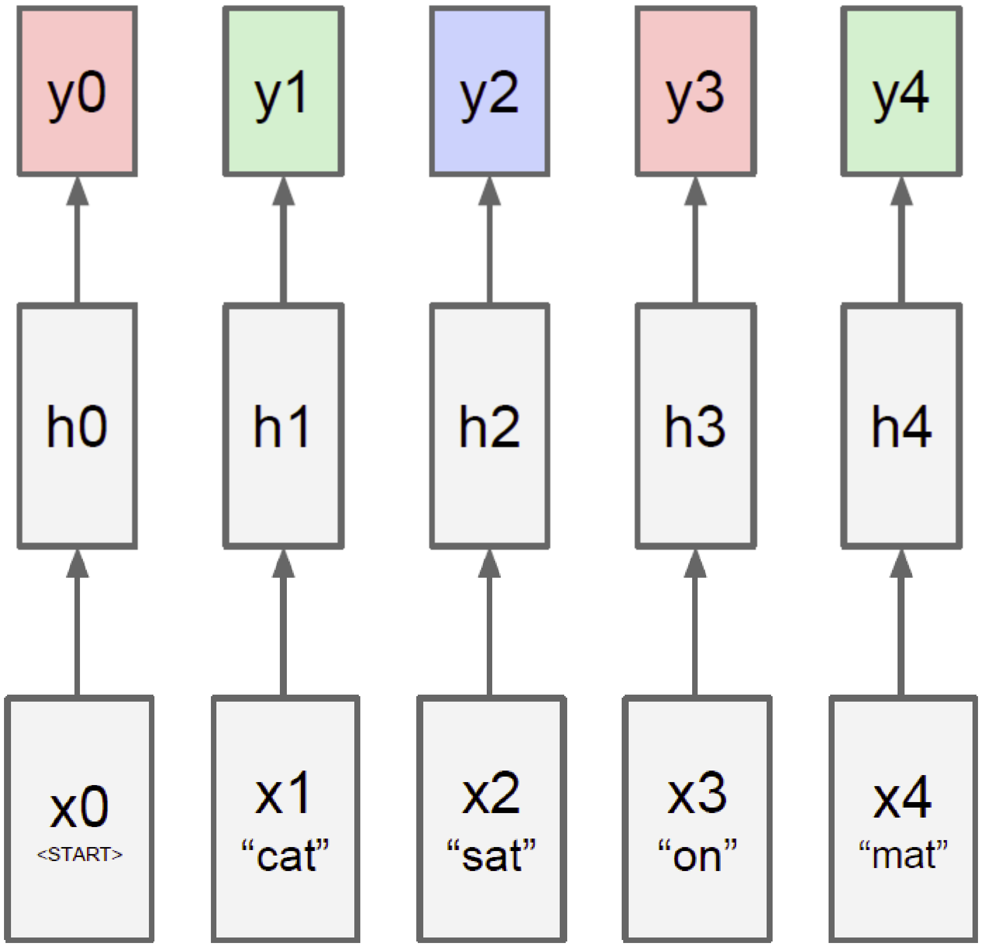
- **Example: Language modeling**
  - Suppose we had the training sequence "cat sat on mat"
  - We want to train a language model

$$p(next\ word \mid previous\ words)$$

  - 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…)

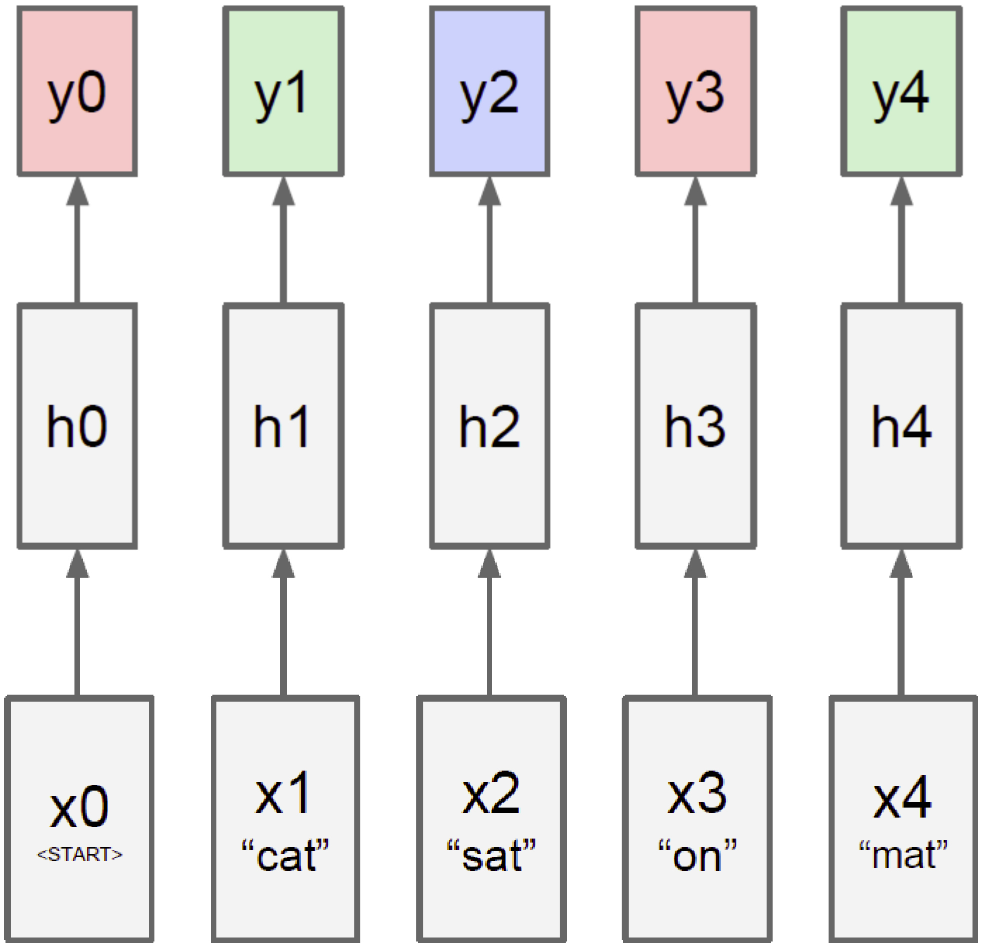


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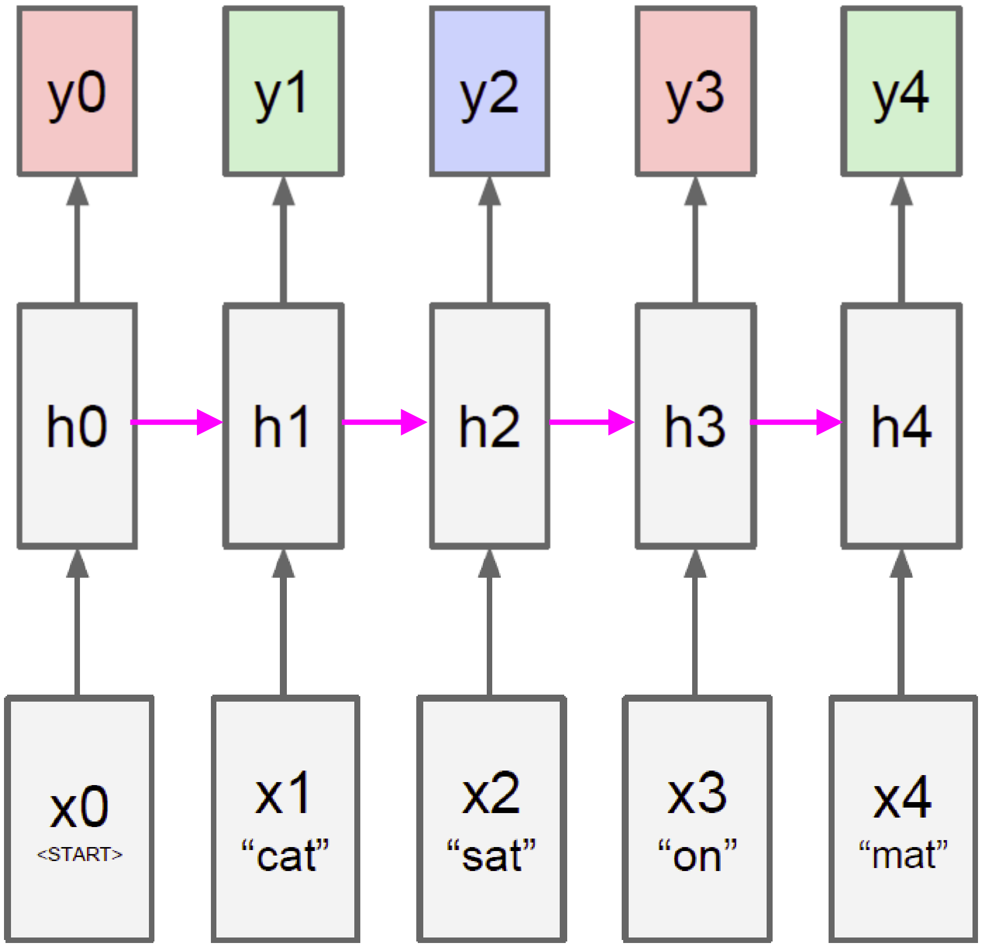
Image source: Andrej Karpathy

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)

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

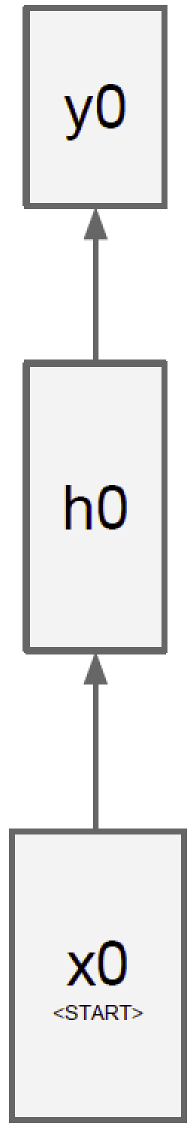
Word embedding (300D vector for each word)

Image source: Andrej Karpathy

RNNs: Intuition

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

  $p(\textcolor{red}{next\ word} \mid \textcolor{blue}{previous\ words})$



Slide credit: Andrej Karpathy, Fei-Fei Li

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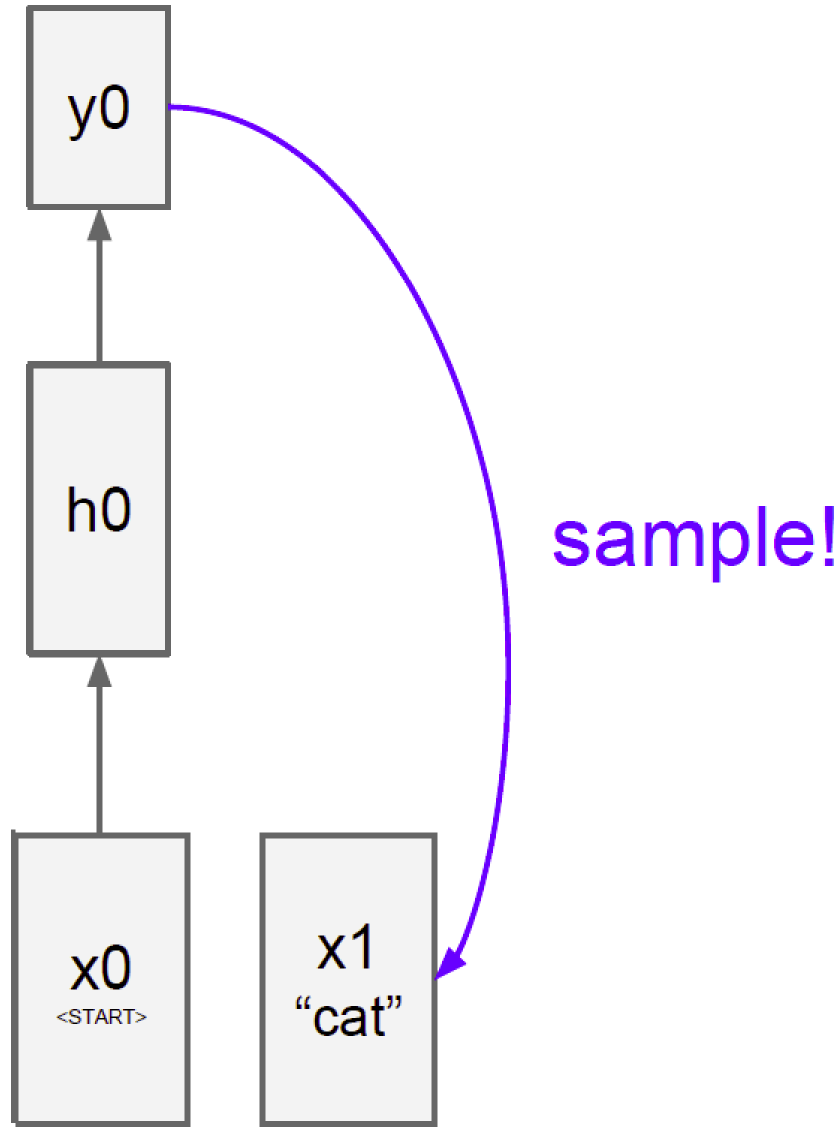

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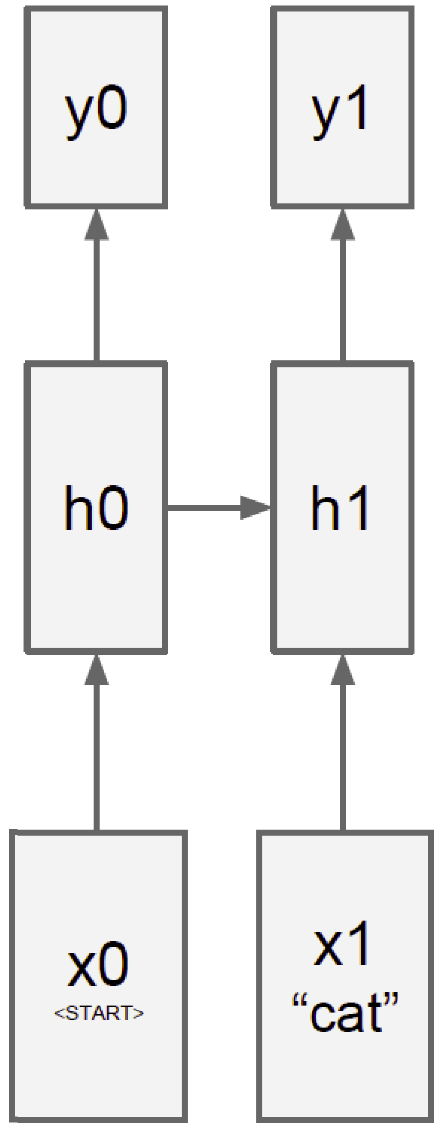

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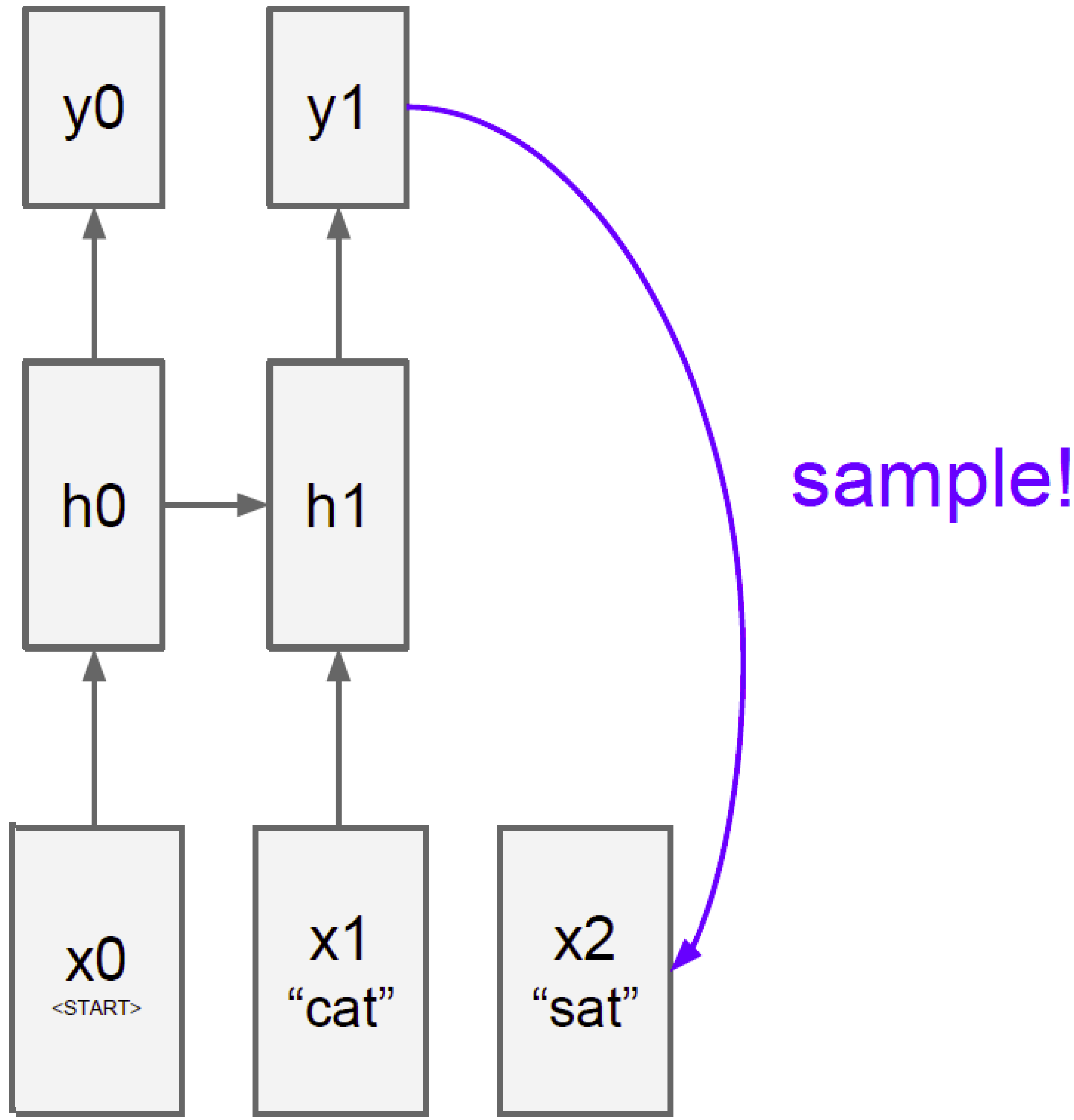

Slide credit: Andrej Karpathy, Fei-Fei Li

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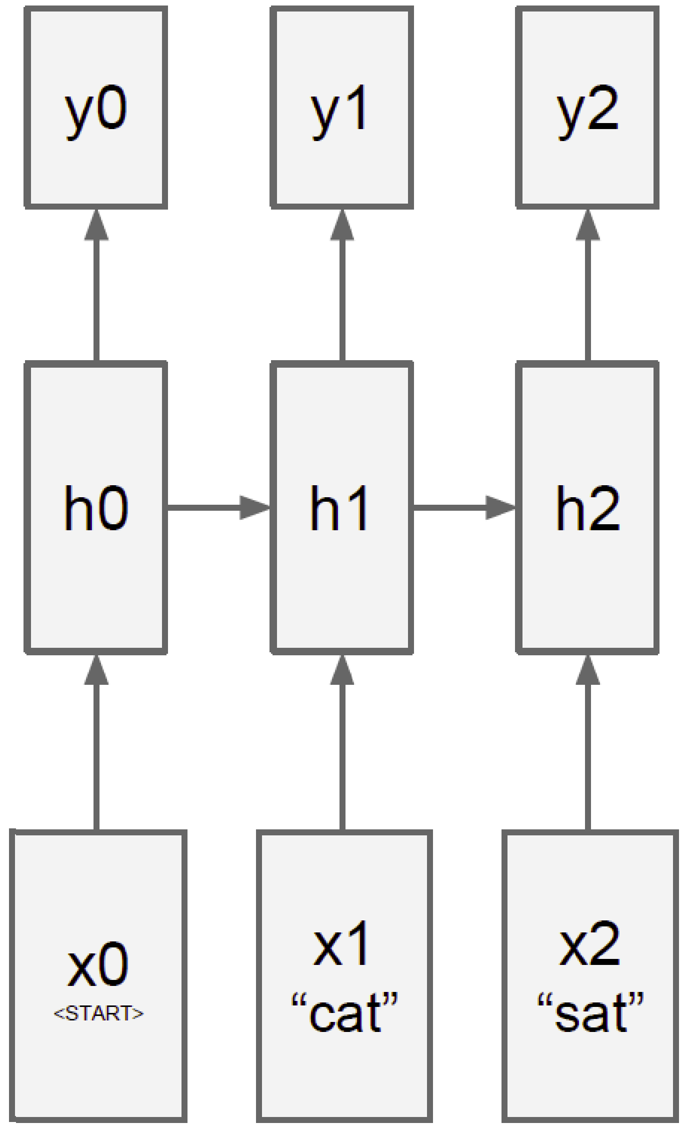

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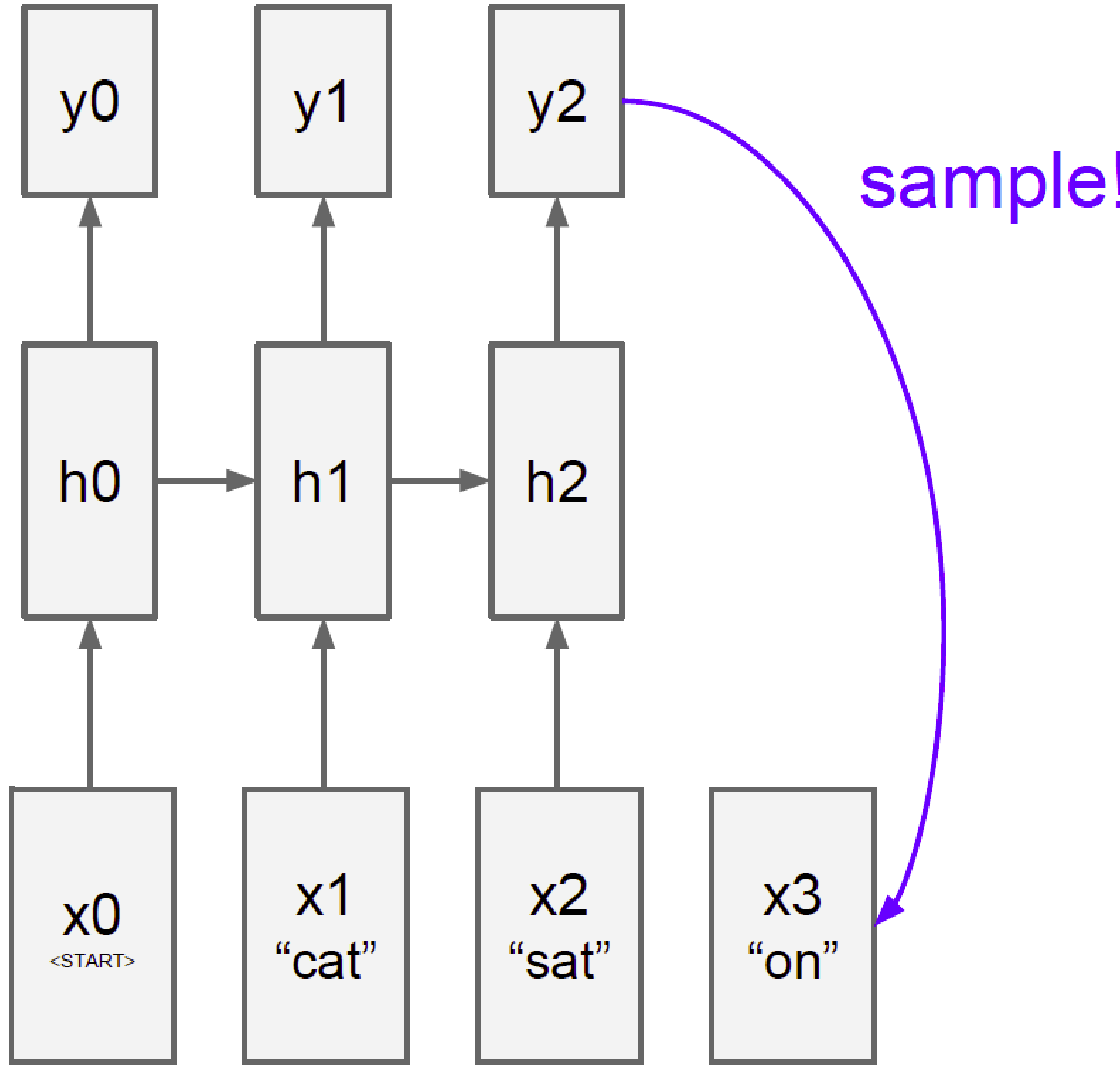

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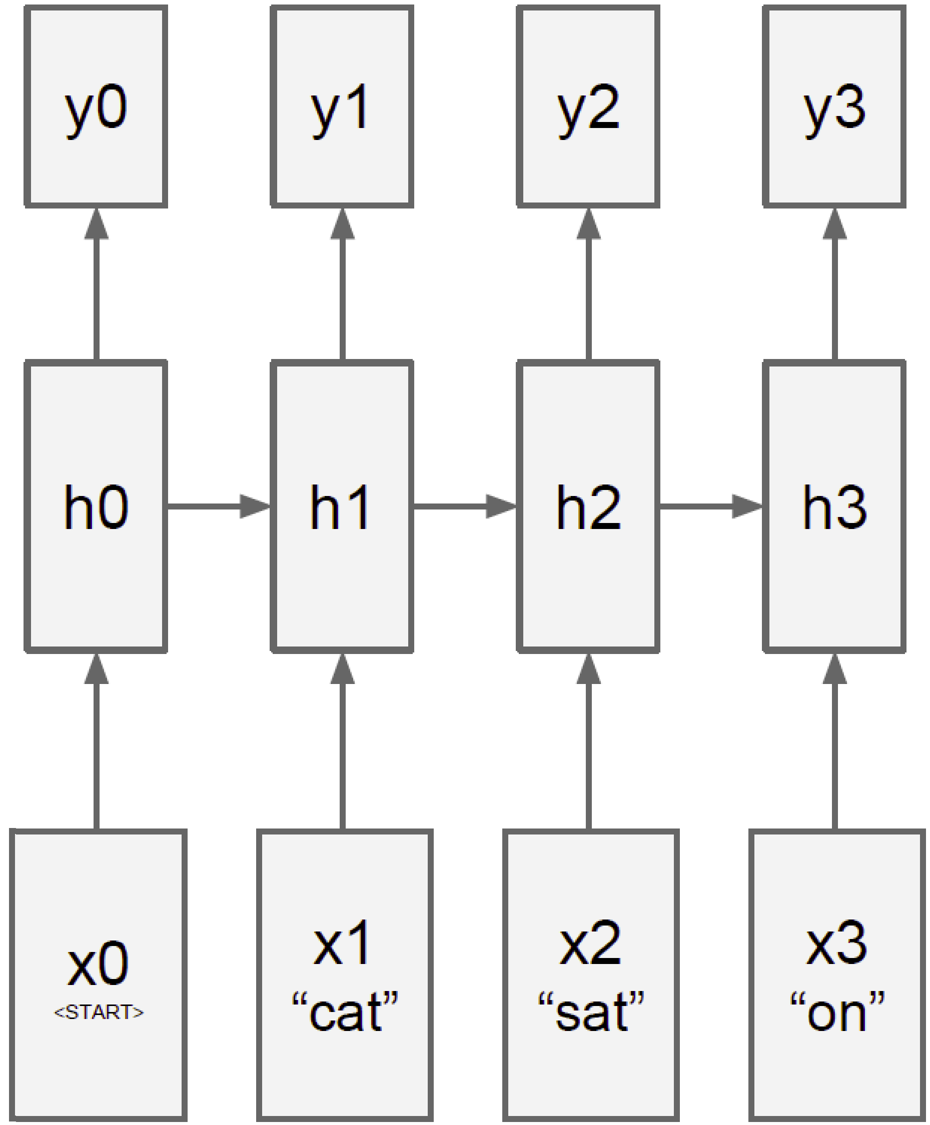

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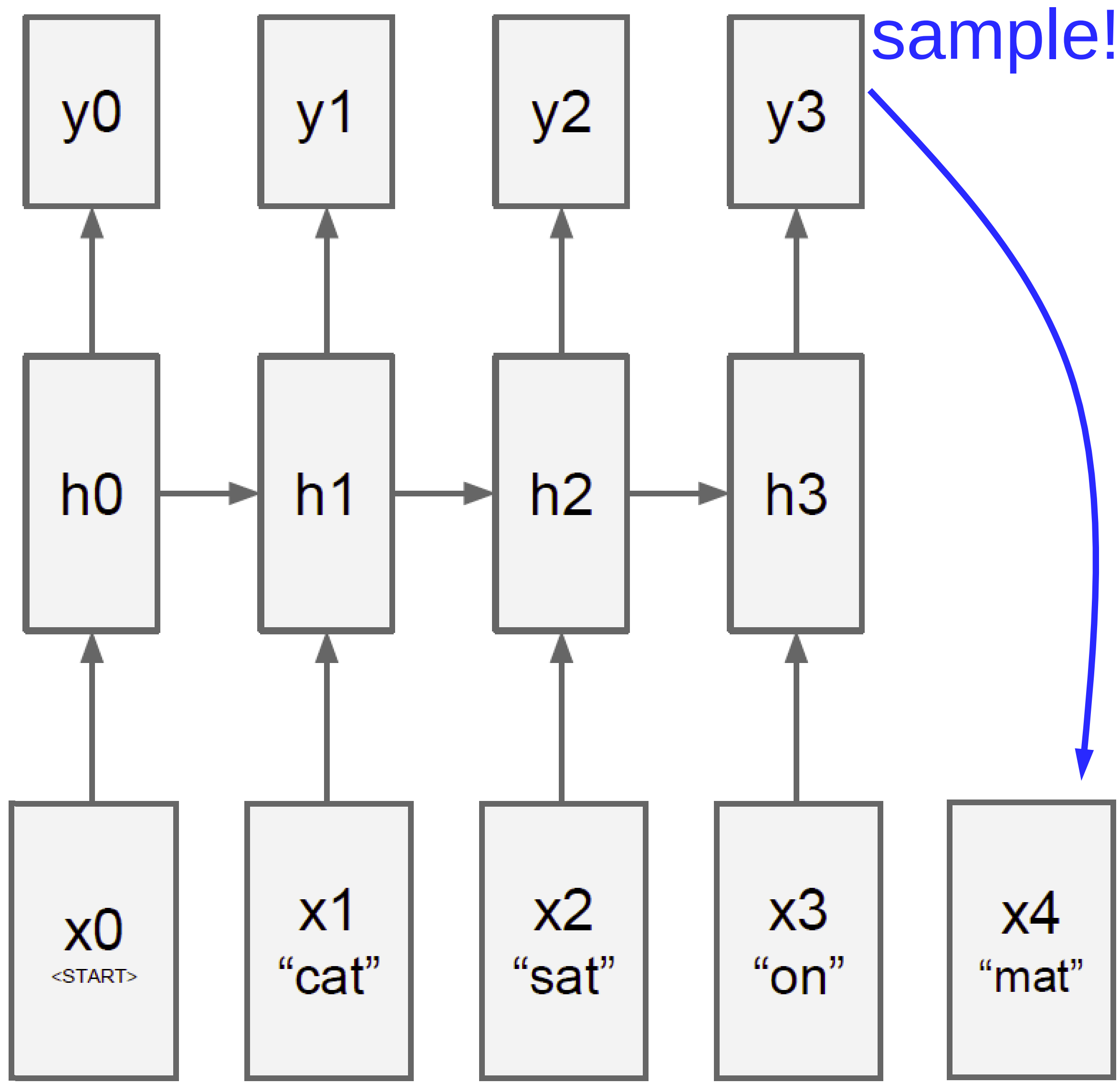


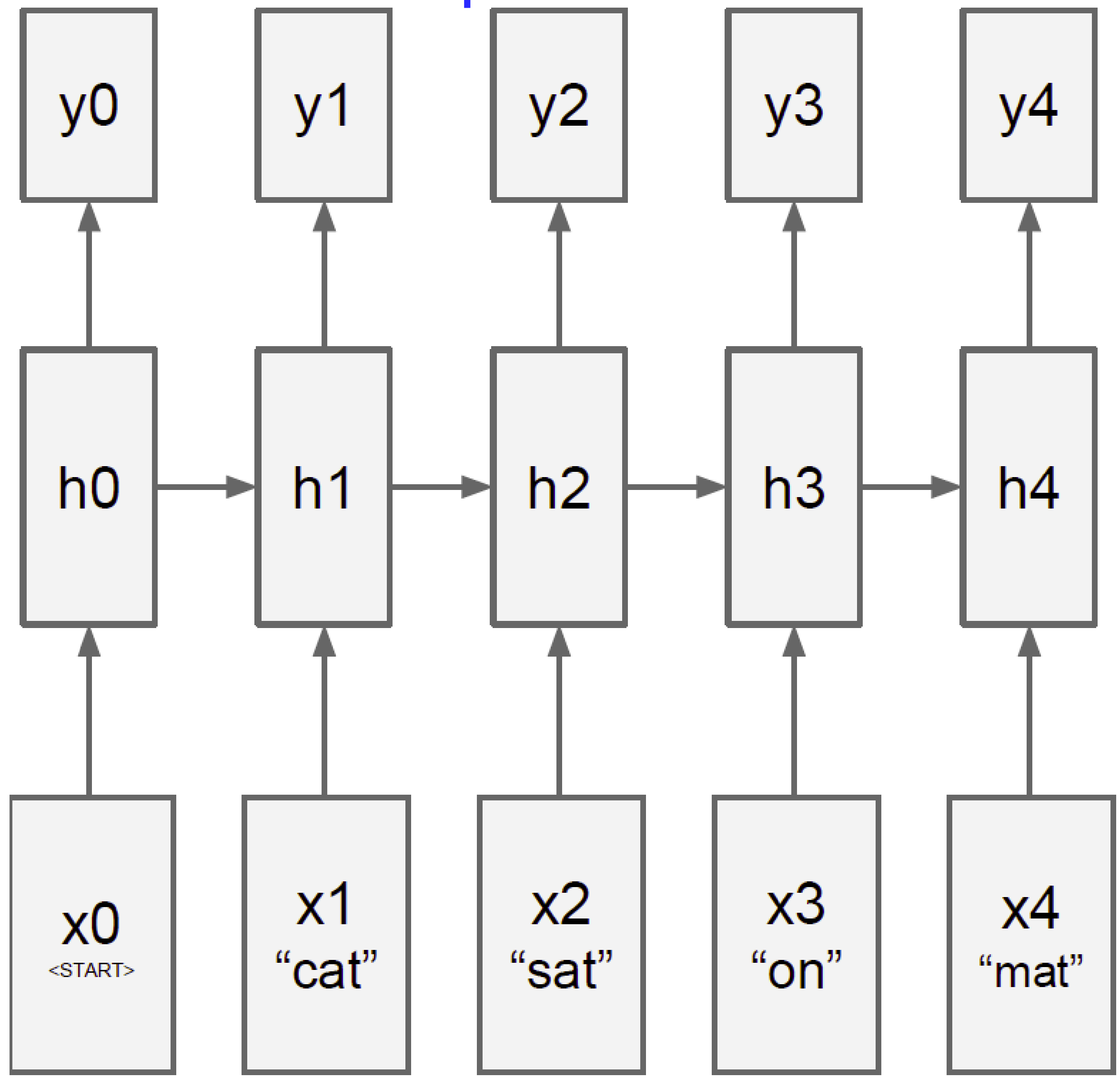
RNNs: Intuition

- **Training this on a lot of sentences would give us a language model.**

- **I.e., a way to predict**

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

samples <END>? Done!



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
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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 are shared between temporal layers.

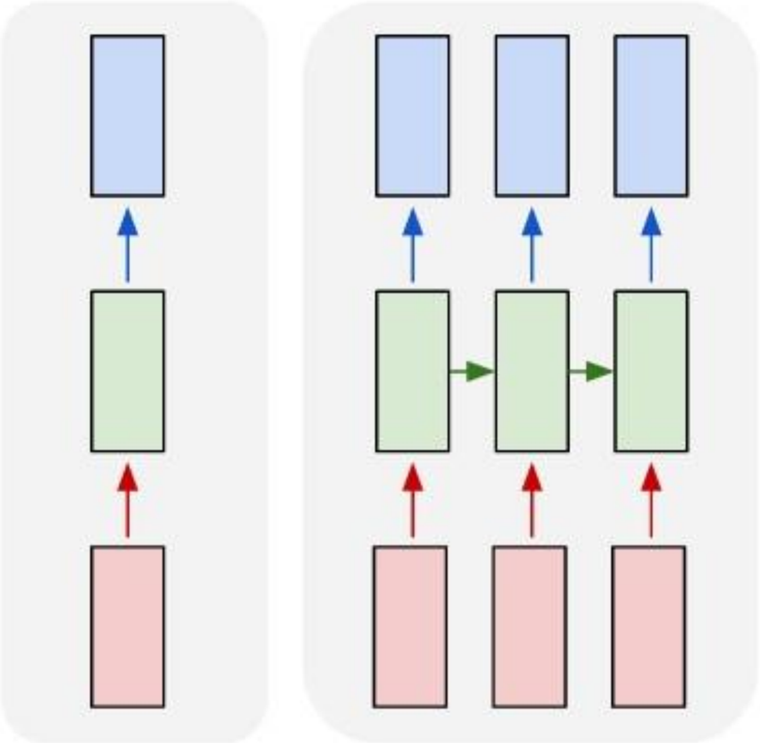
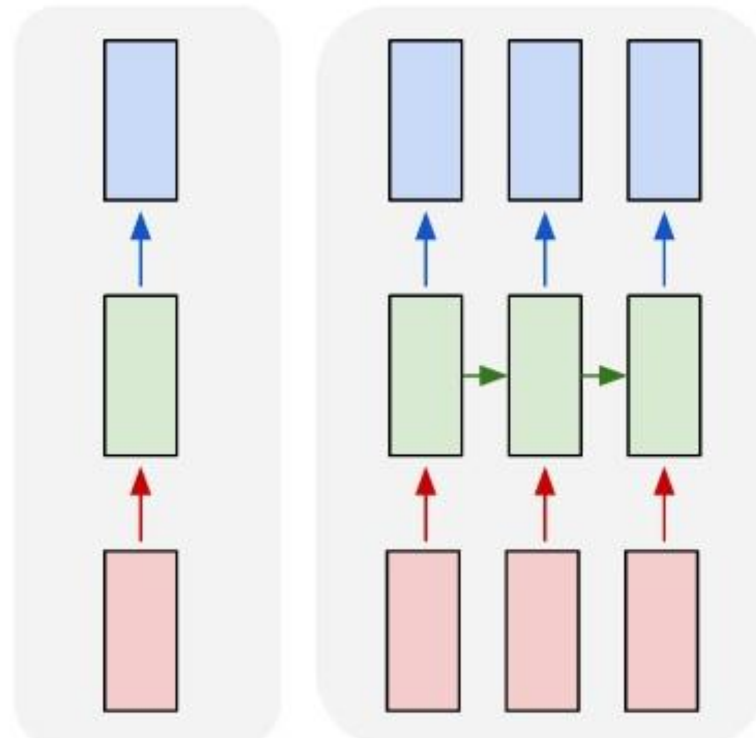


Image source: Andrej Karpathy

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.



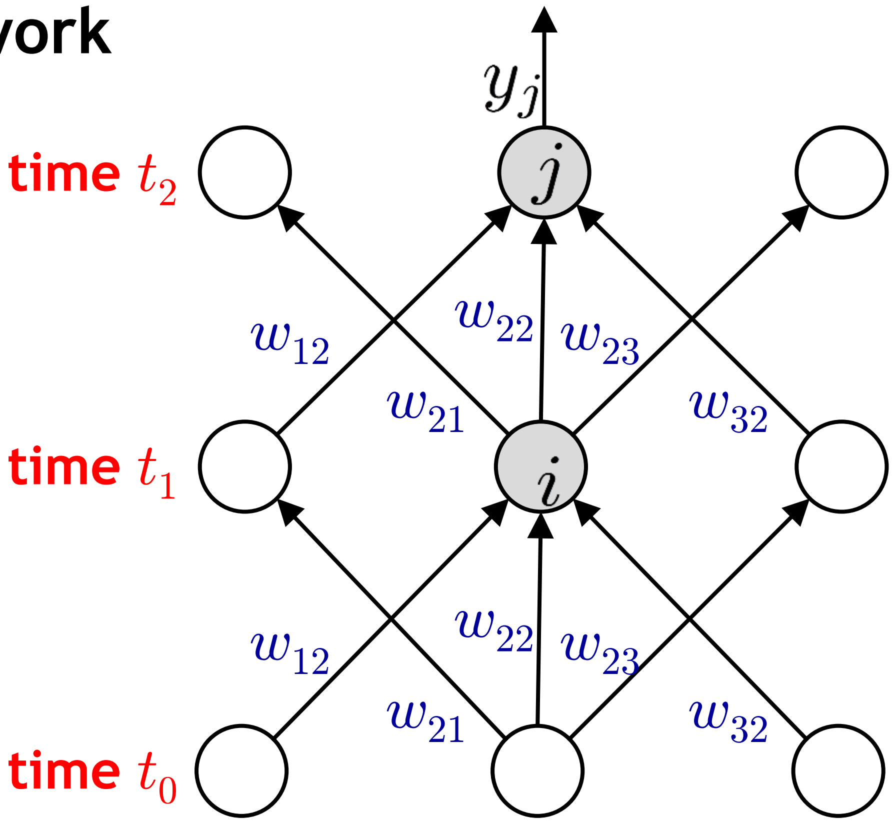
- With enough neurons and time, RNNs can compute anything that can be computed by your computer.

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.

  ⇒ This is very similar to how an RNN works.
  - Only change: the layers share their weights.



⇒ 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:**

$$\nabla w_1 = \nabla w_2$$

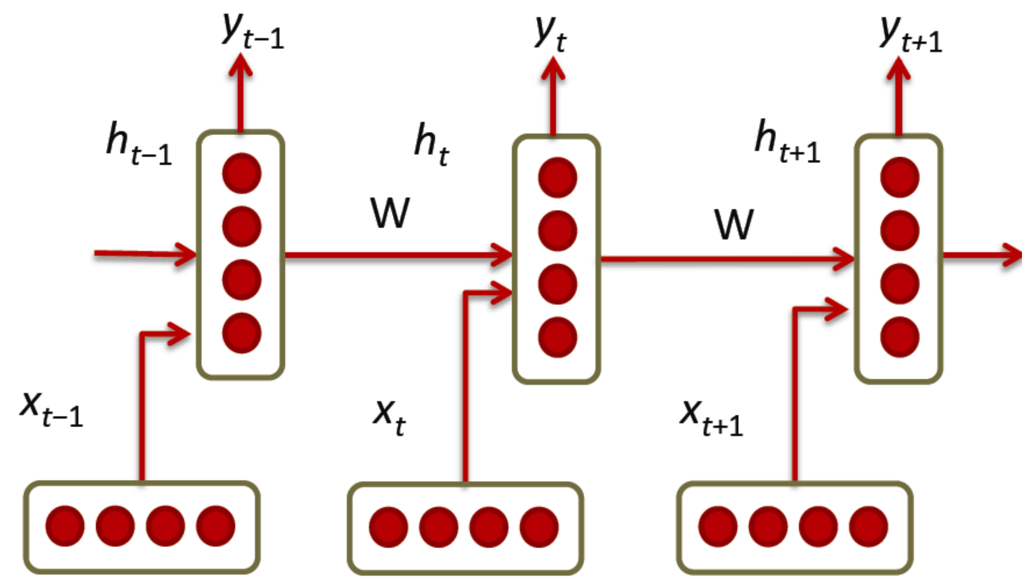
  - **We compute the gradients as usual and then use**

$$\frac{\partial E}{\partial w_1} + \frac{\partial E}{\partial w_2}$$

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
    - $\mathbf{W}_{xh}$
    - $\mathbf{W}_{hy}$
    - $\mathbf{W}_{hh}$



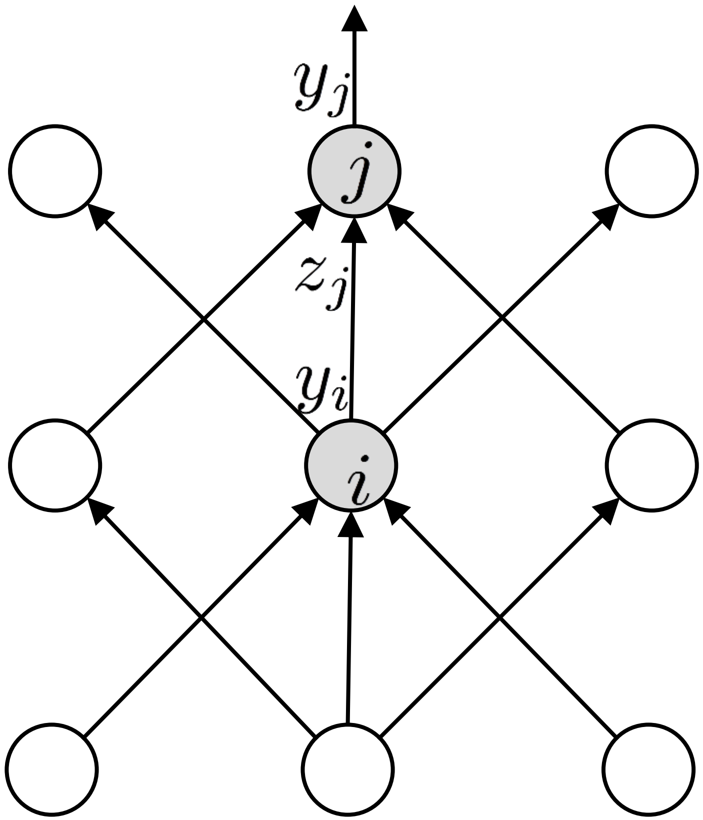
  - Configuration

$$\mathbf{h}_t = \sigma\left(\mathbf{W}_{xh}\mathbf{x}_t + \mathbf{W}_{hh}\mathbf{h}_{t-1} + b\right)$$

$$\hat{\mathbf{y}}_t = \mathrm{softmax}\left(\mathbf{W}_{hy}\mathbf{h}_t\right)$$

Image source: Richard Socher

Recap: Backpropagation Algorithm



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

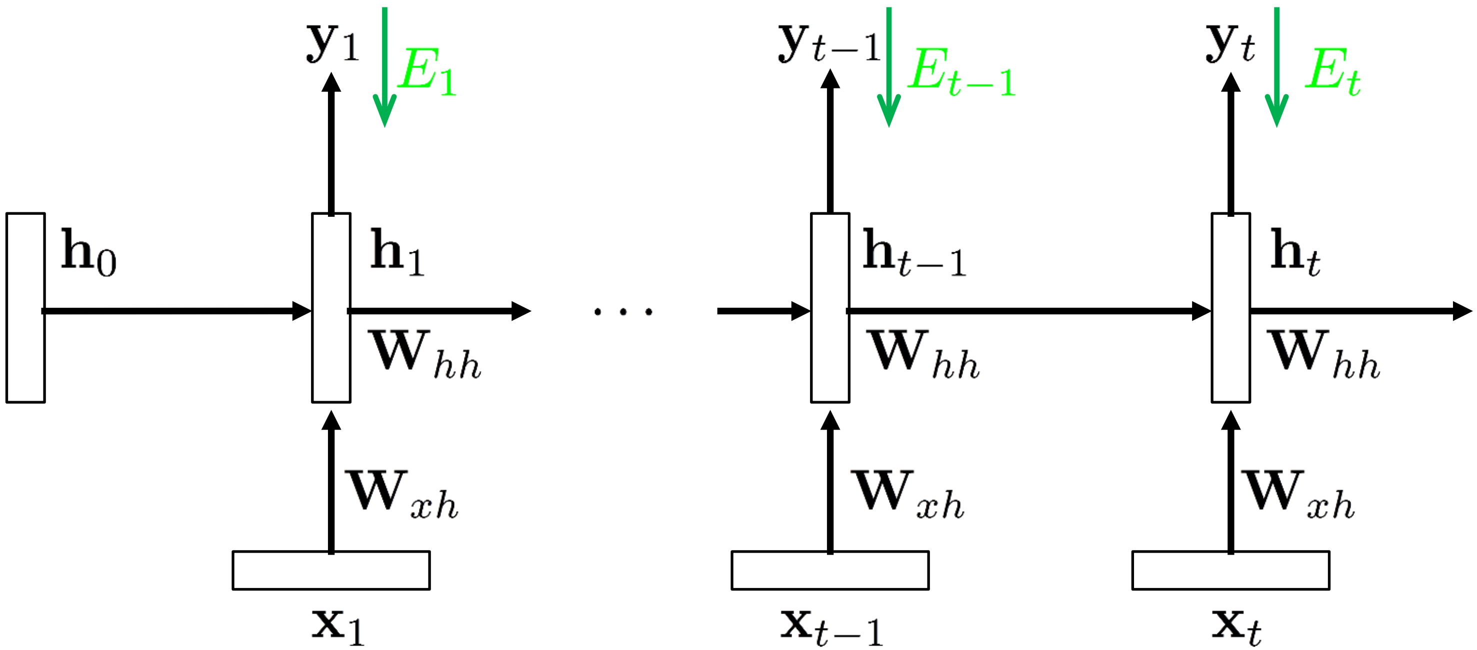
$$\frac{\partial E}{\partial y_i} = \sum_j \frac{\partial z_j}{\partial y_i}\frac{\partial E}{\partial z_j} = \sum_j w_{ij}\frac{\partial E}{\partial z_j}$$

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

- **Efficient propagation scheme**
  - y_i **is already known from forward pass! (Dynamic Programming)**

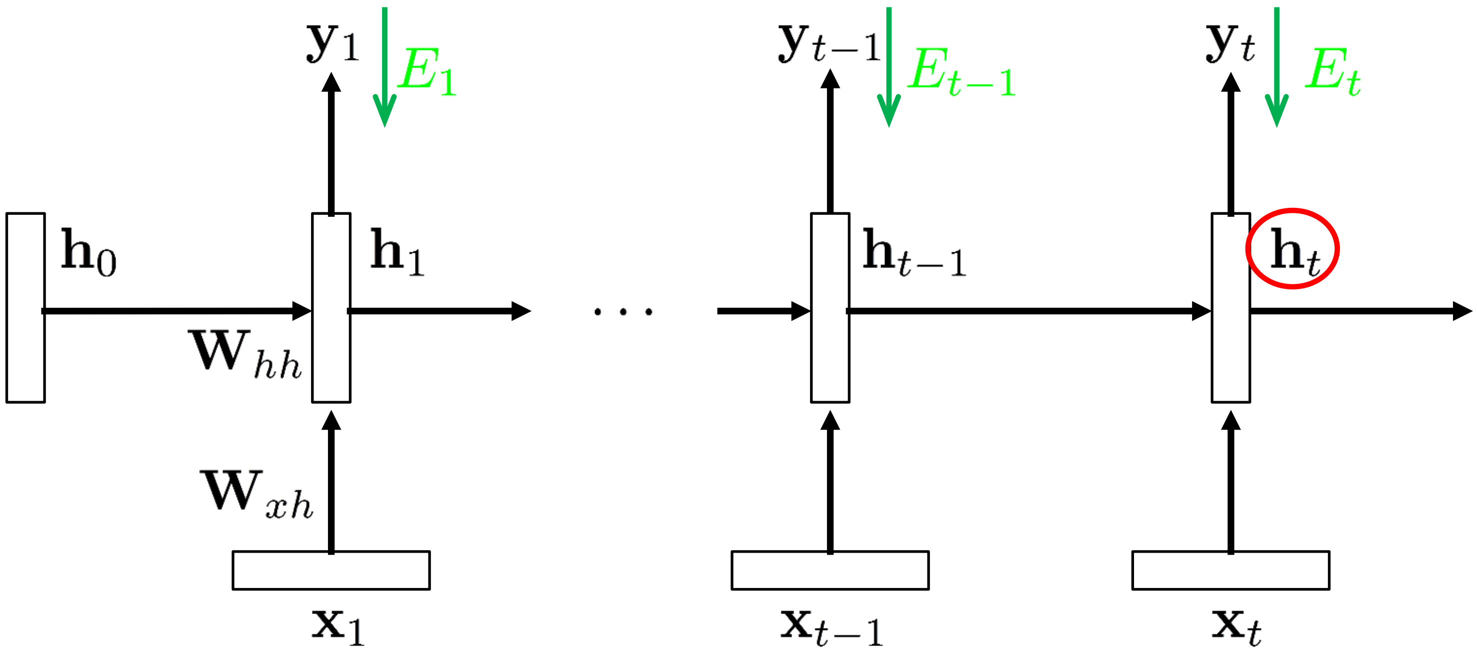
  $\Rightarrow$ **Propagate back the gradient from layer j and multiply with y_i.**

Backpropagation Through Time (BPTT)



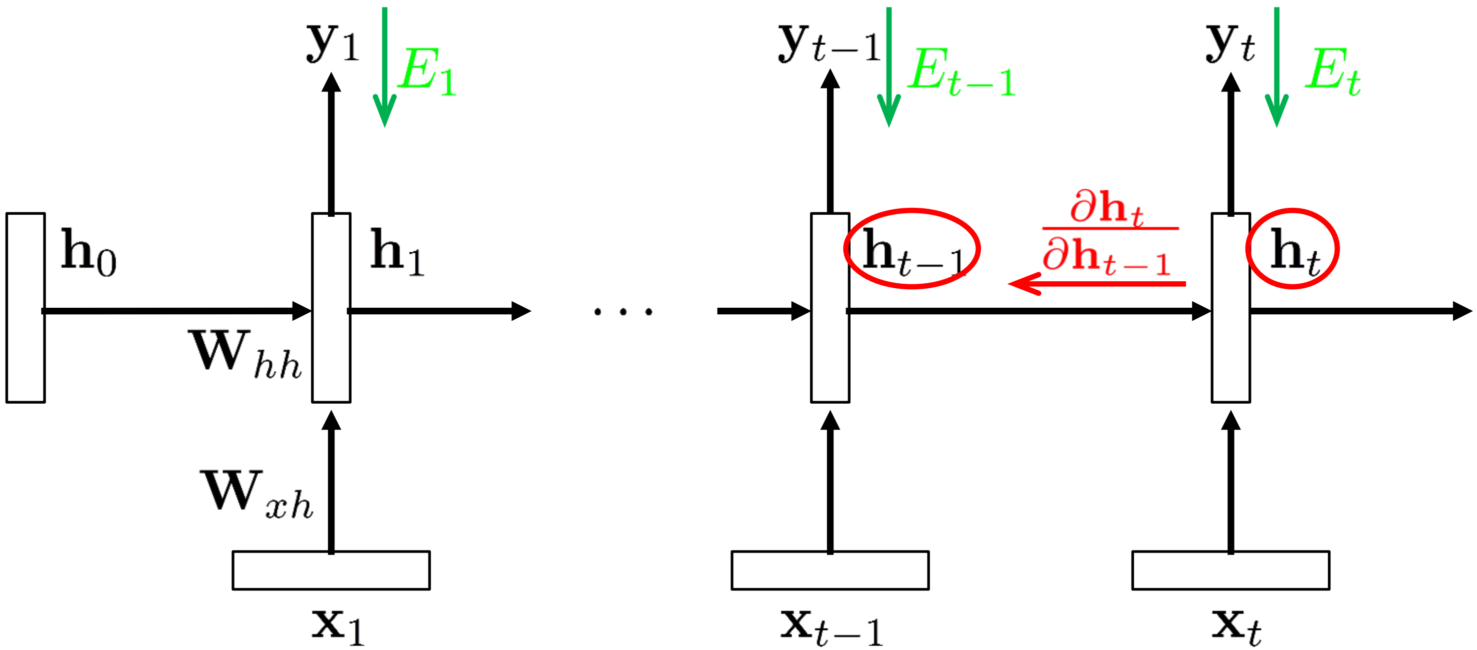
- Error function
  - Computed over all time steps: $E = \sum_{1 \le t \le T} E_t$

Backpropagation Through Time (BPTT)



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

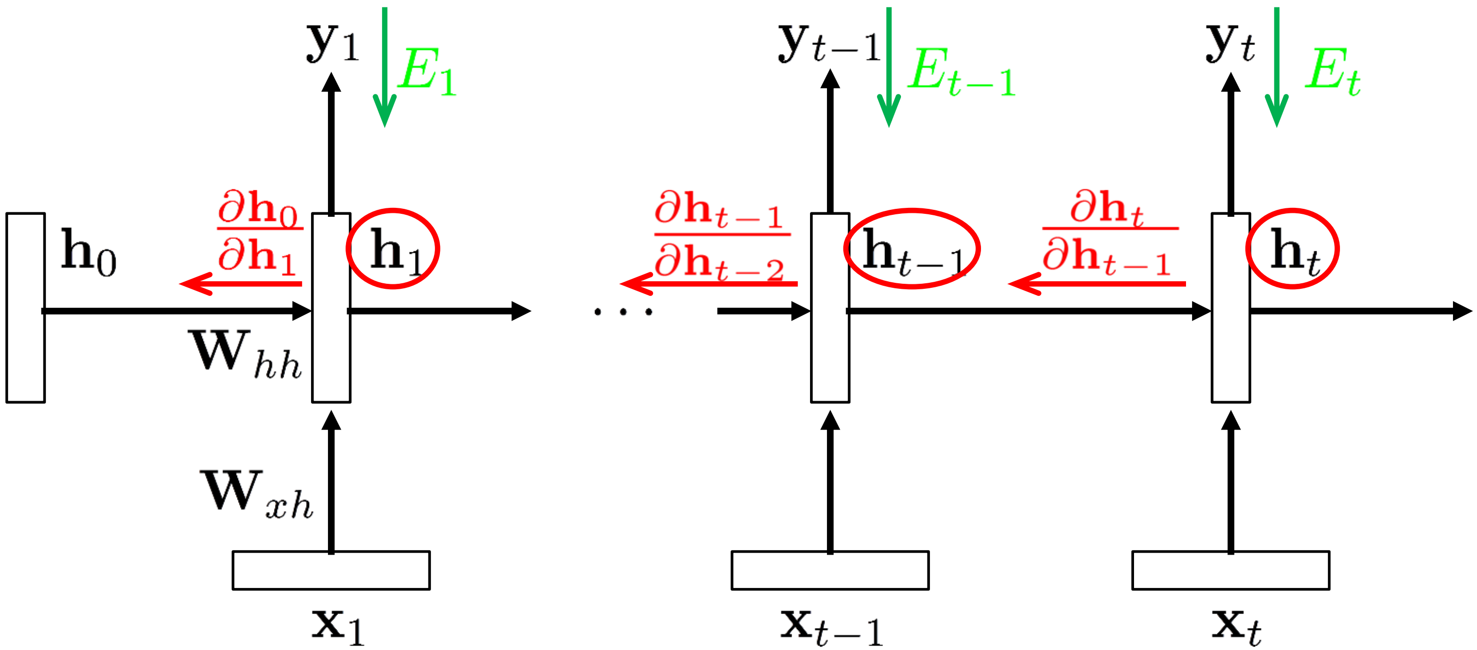
Backpropagation Through Time (BPTT)



- **Backpropagated gradient**
  - For weight w_{ij}:

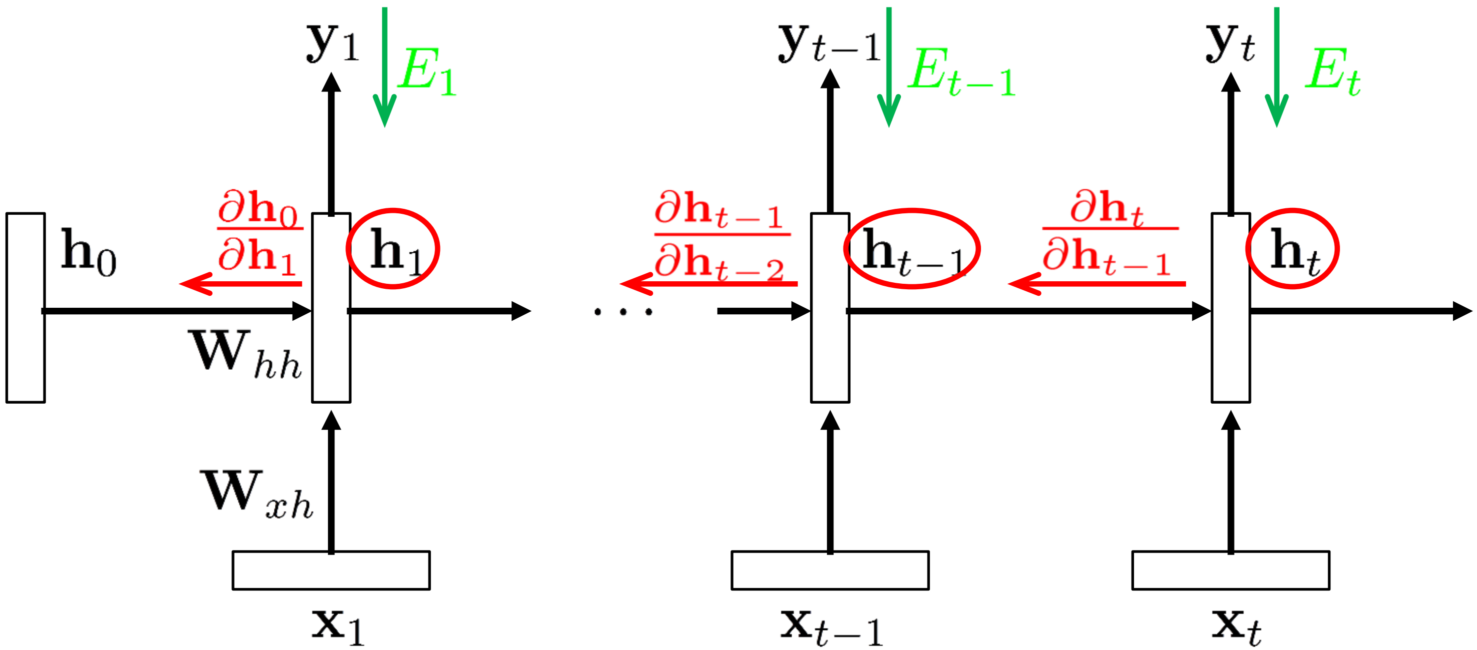
$$\frac{\partial E}{\partial w_{ij}} = \frac{\partial E_t}{\partial \mathbf{h}_t}\frac{\partial \mathbf{h}_t}{\partial w_{ij}} + \frac{\partial E_t}{\partial \mathbf{h}_t}\frac{\partial \mathbf{h}_t}{\partial \mathbf{h}_{t-1}}\frac{\partial \mathbf{h}_{t-1}}{\partial w_{ij}}$$

Backpropagation Through Time (BPTT)



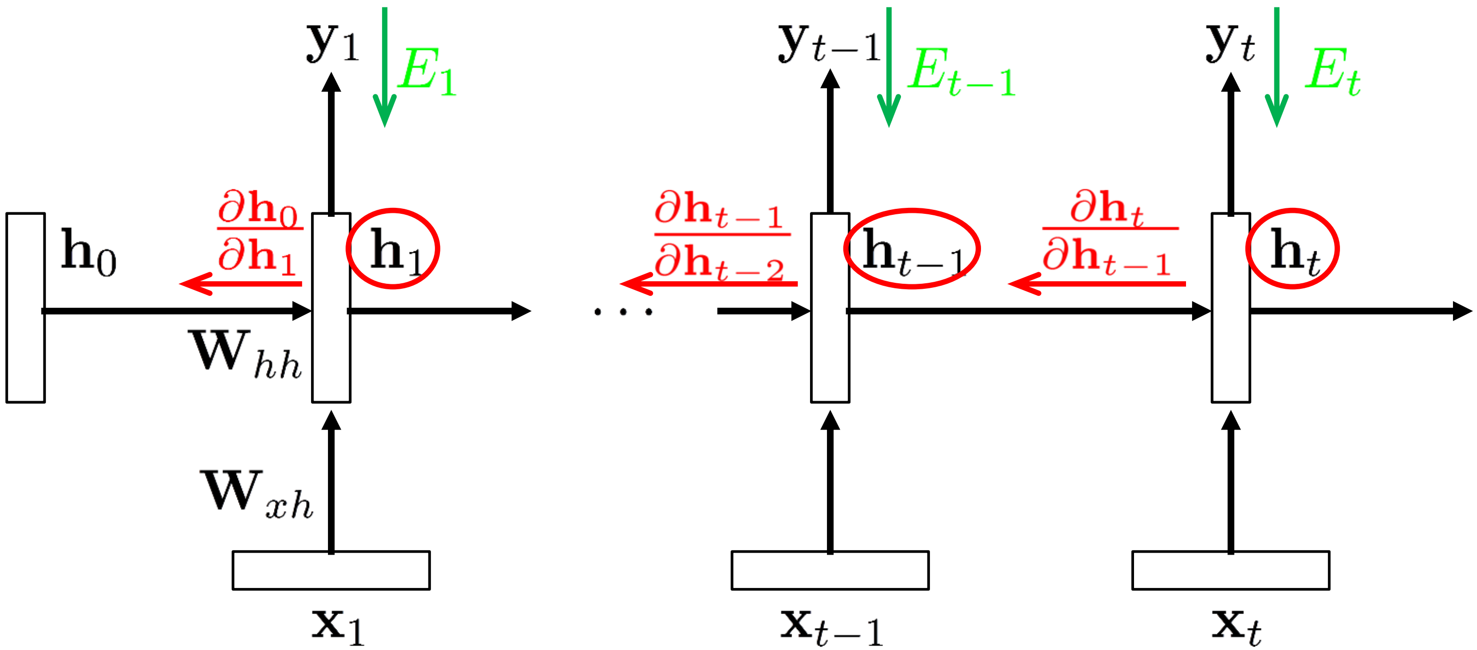
- **Backpropagated gradient**
  - For weight w_{ij}: $$\frac{\partial E}{\partial w_{ij}} = \frac{\partial E_t}{\partial \mathbf{h}_t}\frac{\partial \mathbf{h}_t}{\partial w_{ij}} + \frac{\partial E_t}{\partial \mathbf{h}_t}\frac{\partial \mathbf{h}_t}{\partial \mathbf{h}_{t-1}}\frac{\partial \mathbf{h}_{t-1}}{\partial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

Backpropagation Through Time (BPTT)



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

Backpropagation Through Time (BPTT)



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

Backpropagation Through Time (BPTT)

- Summary
  - Backpropagation equations

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

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

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

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

$\Rightarrow$ Learn this together with all the other parameters.

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  - Backpropagation through Time (BPTT)
- **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:**

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

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

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

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

$\Rightarrow$ 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 $\Rightarrow$ Gradients *may* explode.**
    - **Largest eigenvalue < 1 $\Rightarrow$ Gradients *will* vanish.**
    - **This is very bad...**

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 ____“

$\Rightarrow$ The RNN will have a hard time learning such long-range dependencies.

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

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$\hat{\mathbf{g}} \leftarrow \frac{\partial \mathcal{E}}{\partial \theta}$

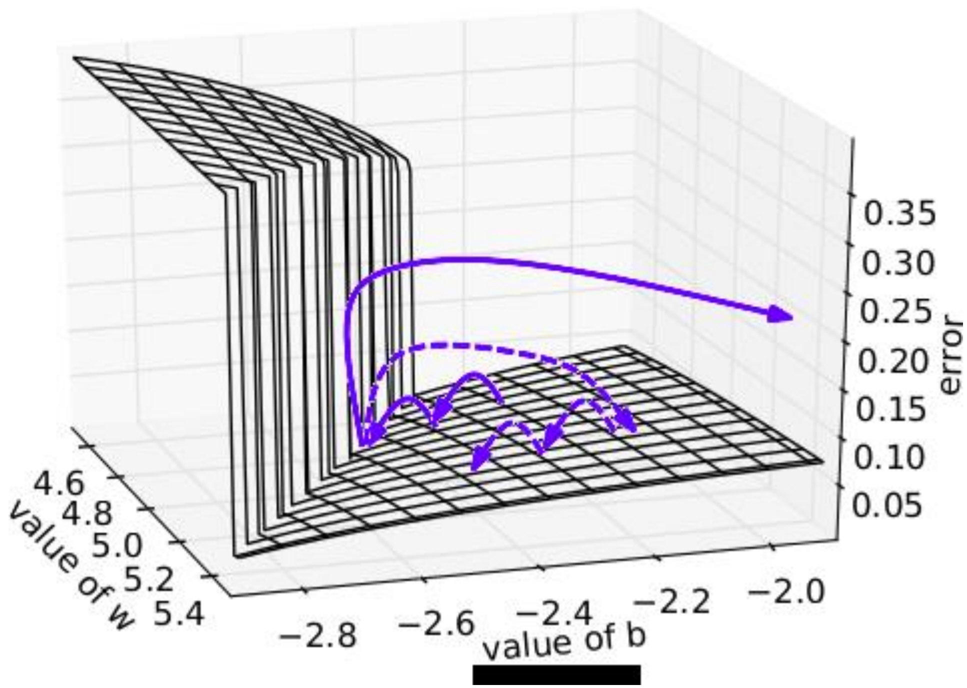
if $\|\hat{\mathbf{g}}\| \geq threshold$ **then**

  $\hat{\mathbf{g}} \leftarrow \frac{threshold}{\|\hat{\mathbf{g}}\|} \hat{\mathbf{g}}$

end if

  - **This makes a big difference in RNNs**

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**

Image source: Pascalu et al., 2013

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.