

CS182: Introduction to Machine Learning – RNN LMs + Transformer LMs

Yujiao Shi SIST, ShanghaiTech Spring, 2025

Introduction



- Our goal: Build intelligent algorithms to make sense of data
 - □ Example: Recognizing objects in images





red panda (Ailurus fulgens)

Example: Predicting what would happen next



Vondrick et al. CVPR2016

Introduction



- Our goal: Build intelligent algorithms to make sense of data
 - □ Example: Recognizing objects in images
 - □ Example: Predicting what would happen next

Given an initial still frame,

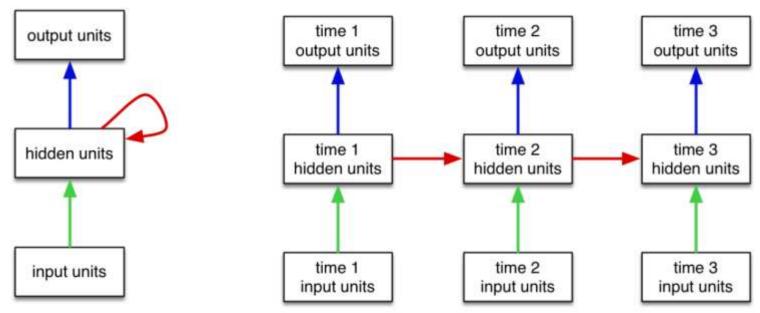




Recurrent Neural Network



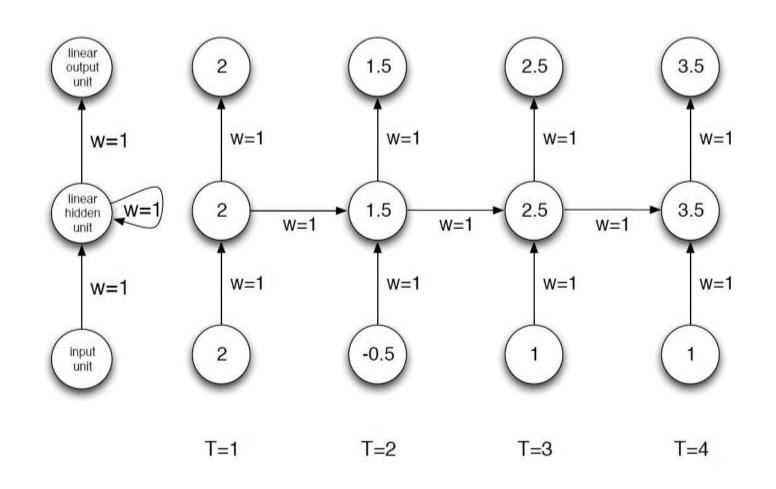
- Recurrent Neural Network as a dynamical system with one set of hidden units feeding into themselves
 - ☐ The network's graph has self-loops
- The RNN's graph can be unrolled by explicitly representing the units at all time steps
 - □ The weights and biases are shared



RNN examples



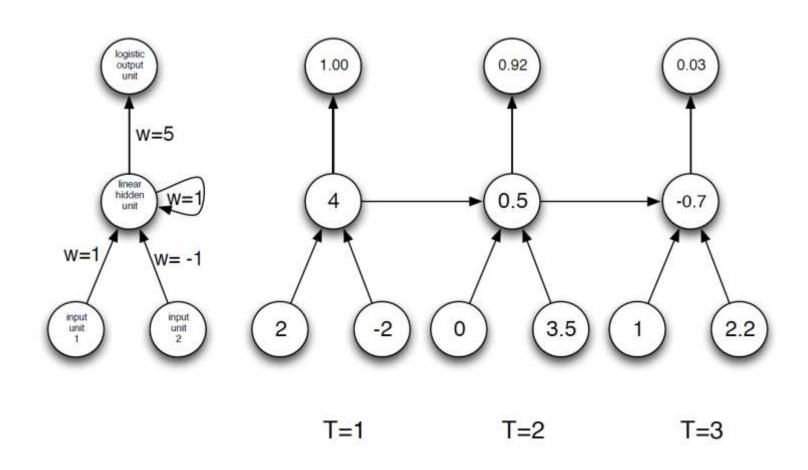
Summation network



RNN examples



Summation & comparison network

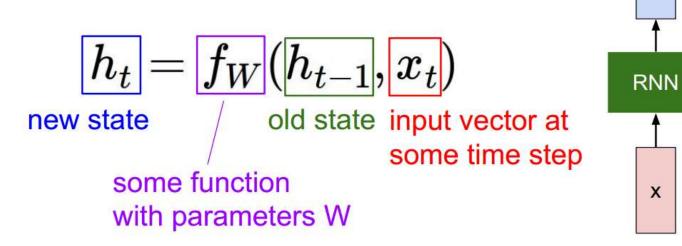


Recurrent Neural Network



General formulation

We can process a sequence of vectors **x** by applying a **recurrence formula** at every time step:



Recurrent Neural Network

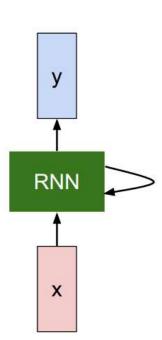


General formulation

We can process a sequence of vectors **x** by applying a **recurrence formula** at every time step:

$$h_t = f_W(h_{t-1}, x_t)$$

Notice: the same function and the same set of parameters are used at every time step.

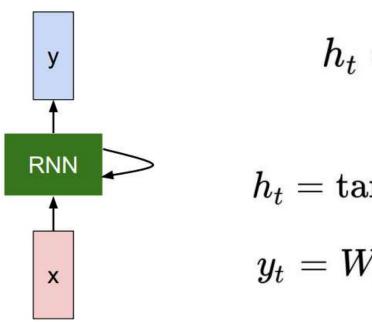


(Vanilla)Recurrent Neural Network



General formulation

The state consists of a single "hidden" vector h:



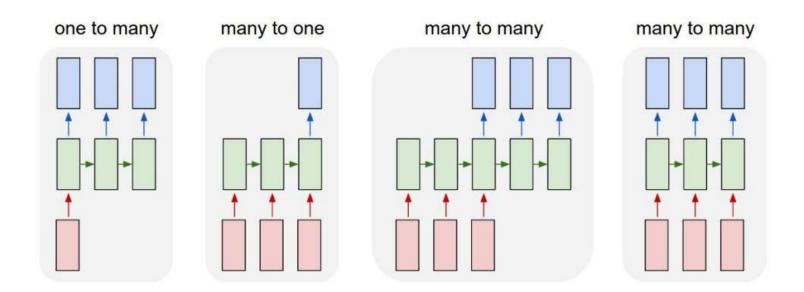
$$h_t = f_W(h_{t-1}, x_t)$$
 \downarrow $h_t = anh(W_{hh}h_{t-1} + W_{xh}x_t)$ $y_t = W_{hy}h_t$



Recurrent Neural Network



Recurrent Neural Networks: model variants

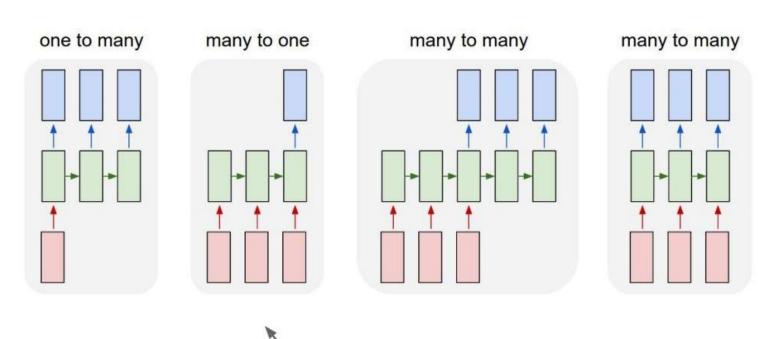


e.g. Image Captioning image -> sequence of words





Recurrent Neural Networks: model variants

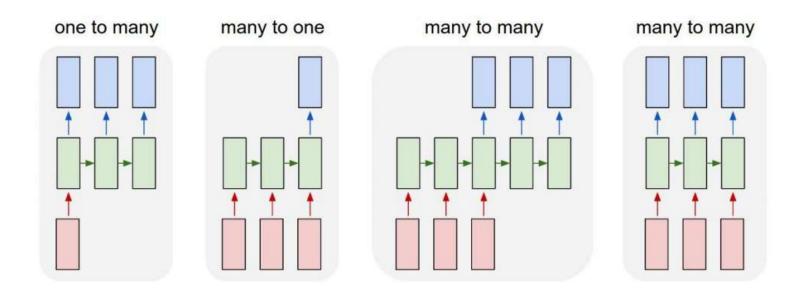


e.g. Sentiment Classification sequence of words -> sentiment





Recurrent Neural Networks: model variants

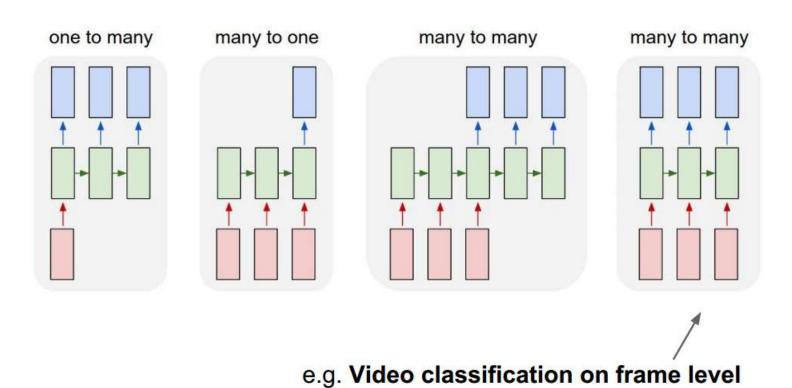


e.g. Machine Translation seq of words -> seq of words





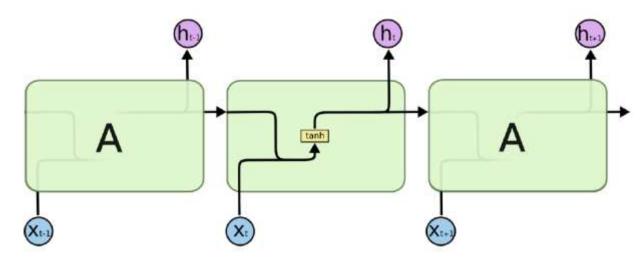
Recurrent Neural Networks: model variants







Recall

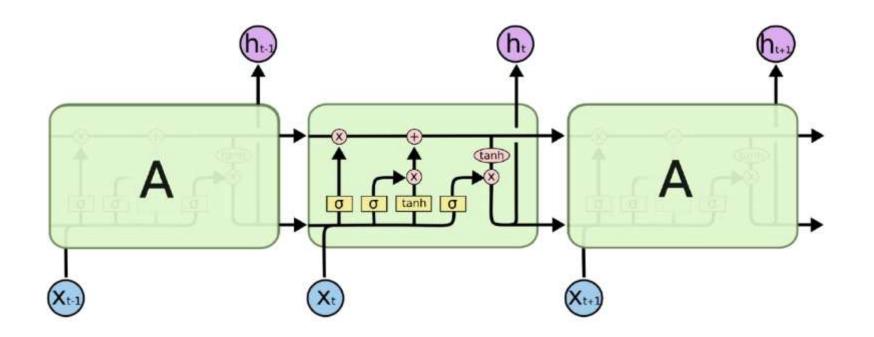


- Each recurrent neuron receives past outputs and current input
- Pass through a tanh function





■ LSTM uses multiplicative gates that decide if something is important or not

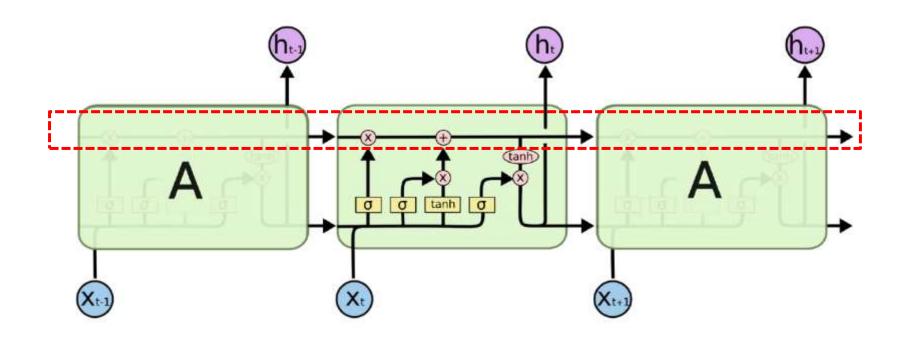


Hochreiter and Schmidhuber, "Long Short Term Memory", Neural Computation





Key component: a remembered cell state



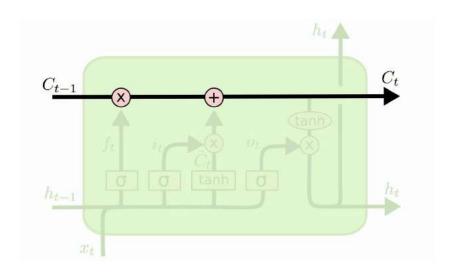
Hochreiter and Schmidhuber, "Long Short Term Memory", Neural Computation



LSTM: cell state



- A linear history
 - □ Carries information through
 - □ Only affected by a gate and addition of current information, which is also gated



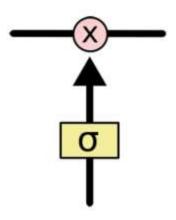


LSTM: gates



Gates are simple sigmoid units with output range in (0,1)

Controls how much of the information will be let through



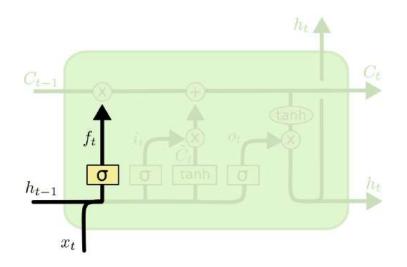
- Three gates
 - □ Forget gate
 - □ Input gate
 - Output gate





- The first gate determines whether to carry over the history or to forget it
 - □ Soft decision: how much of the history C_{t-1} to carry over
 - \Box Determined by the current input x_t and the previous state h_{t-1}
 - can be viewed as partial key-value pairs

$$\langle h_{t-1}, C_{t-1} \rangle$$

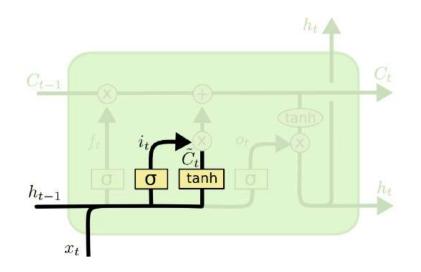


$$f_t = \sigma\left(W_f \cdot [h_{t-1}, x_t] + b_f\right)$$





- The second gate has two parts
 - □ A gate that decides if it is worth remembering
 - □ A nonlinear transformation that extracts new and interesting information from the input
 - □ Both use the current input and the previous state



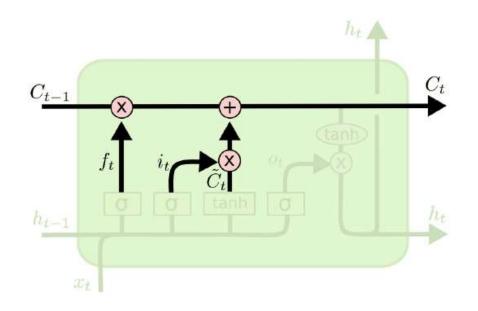
$$i_t = \sigma(W_i \cdot [h_{t-1}, x_t] + b_i)$$

$$\tilde{C}_t = \tanh(W_C \cdot [h_{t-1}, x_t] + b_C)$$

LSTM: Memory cell update



- The output of the second part is added into the current memory cell
 - □ Can be viewed as value update in a key-value pair
 - □ The input and state jointly decide how much of history info is kept and how much of embedded input info is added
 - ☐ A dynamic mixture of experts at each time step

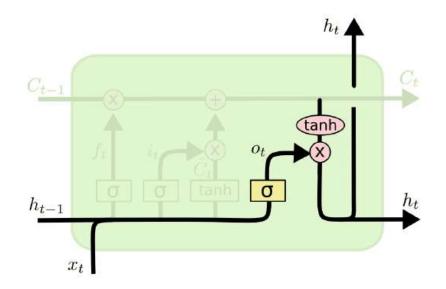


$$C_t = f_t * C_{t-1} + i_t * \tilde{C}_t$$

LSTM: Output gate



- The third gate is the output gate
 - □ To decide if the memory cell contents are worth reporting at this time using the current input and previous state
- The output of the cell or the state
 - □ A nonlinear transform of the cell values
 - □ Compress it with tanh to make it in (-1,1)
 - Note the separation of key-value representation

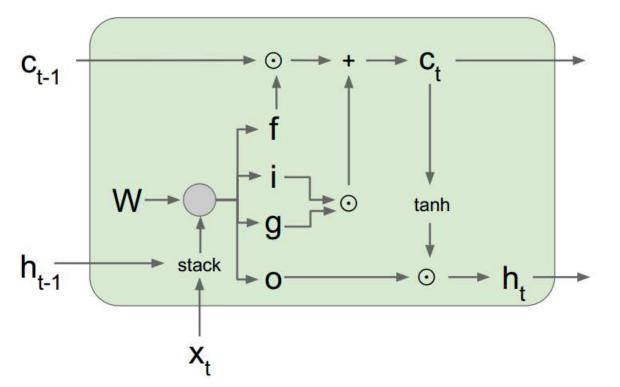


$$o_t = \sigma (W_o [h_{t-1}, x_t] + b_o)$$
$$h_t = o_t * \tanh (C_t)$$

Long Short Term Memory(LSTM)



[Hochreiter et al., 1997]



$$\begin{pmatrix} i \\ f \\ o \\ g \end{pmatrix} = \begin{pmatrix} \sigma \\ \sigma \\ \sigma \\ \tanh \end{pmatrix} W \begin{pmatrix} h_{t-1} \\ x_t \end{pmatrix}$$
$$c_t = f \odot c_{t-1} + i \odot g$$
$$h_t = o \odot \tanh(c_t)$$



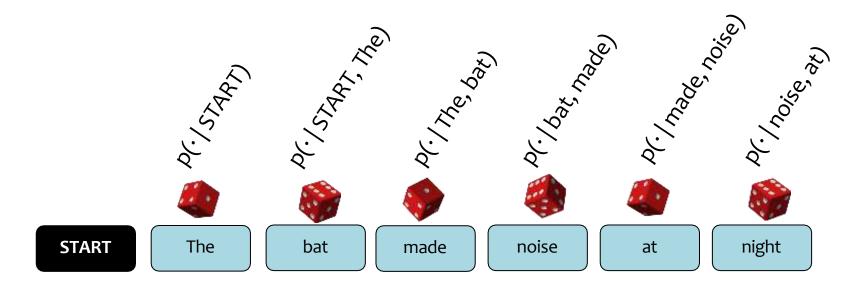
BACKGROUND: N-GRAM LANGUAGE MODELS



n-Gram Language Model



- <u>Goal</u>: Generate realistic looking sentences in a human language
- <u>Key Idea</u>: condition on the last n-1 words to sample the nth word

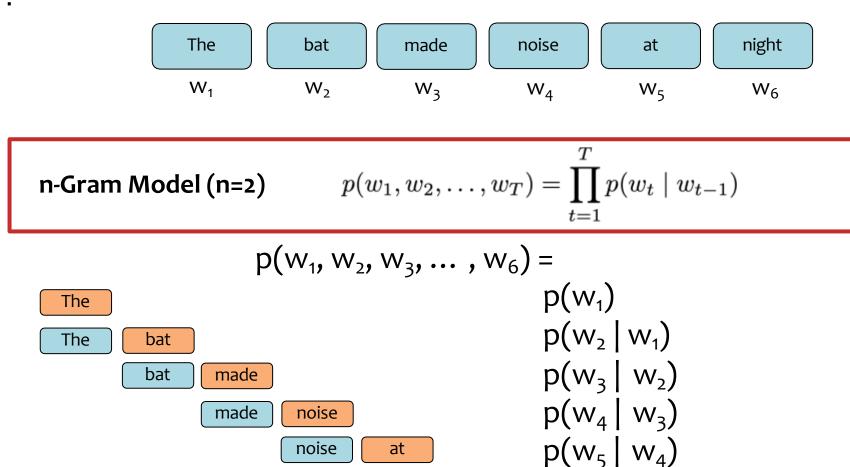


n-Gram Language Model 上海科技大学

 $p(w_6 \mid w_5)$



Question: How can we define a probability distribution over a sequence of length T?

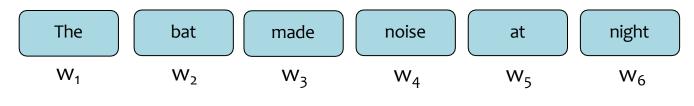


night

n-Gram Language Model 上海科技大学



Question: How can we define a probability distribution over a sequence of length T?



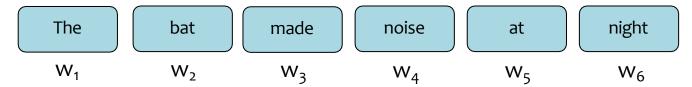
n-Gram Model (n=3)
$$p(w_1, w_2, \dots, w_T) = \prod_{t=1}^T p(w_t \mid w_{t-1}, w_{t-2})$$

$$p(w_1, w_2, w_3, \dots, w_6) = \\ p(w_1) \\ p(w_2 \mid w_1) \\ p(w_2 \mid w_1) \\ p(w_3 \mid w_2, w_1) \\ p(w_4 \mid w_3, w_2) \\ p(w_5 \mid w_4, w_3) \\ p(w_6 \mid w_5, w_4) \\ p(w_6 \mid w_5, w_5) \\ p(w_6 \mid w_5, w_5$$

n-Gram Language Model



Question: How can we define a probability distribution over a sequence of length T?



n-Gram Model (n=3)
$$p(w_1, w_2, \dots, w_T) = \prod_{t=1}^T p(w_t \mid w_{t-1}, w_{t-2})$$

The

The

The

$$p(w_1, w_3, ..., w_6) = p(w_1)$$

Note: This is called a model because we made some assumptions about how many previous words to condition on (i.e. only n-1 words)

Learning an n-Gram Model



Question: How do we learn the probabilities for the n-Gram Model?

$$p(w_t | w_{t-2} = The,$$



$$w_{t-1} = bat$$

Wt	p(· ·,·)
ate	0.015
•••	

flies	0.046	
•••		
zebra	0.000	

$$p(w_t | w_{t-2} = made,$$

 $w_{t-1} = noise)$

W _t	p(· ·,·)
at	0.020
•••	

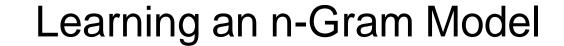
pollution	0.030	
•••		
zebra	0.000	

p(w _t	$W_{t-2} = COWS$,
	$w_{t-1} = eat)$

W _t	p(· ·,·)
corn	0.420

grass	0.510
•••	

zebra	0.000

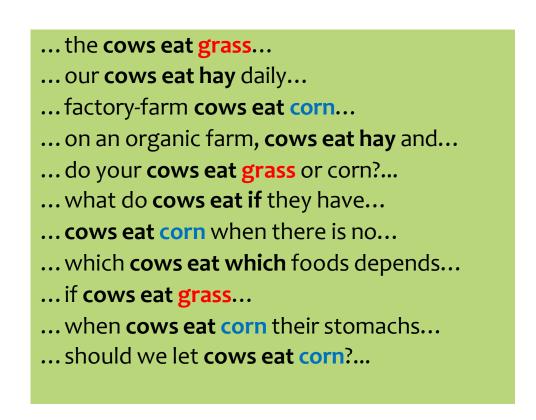




<u>Question</u>: How do we **learn** the probabilities for the n-Gram

Model?

Answer: From data! Just count n-gram frequencies



	w _{t-1} = eat)
∨ t	p(· ·,·)
corn	4/11
grass	3/11

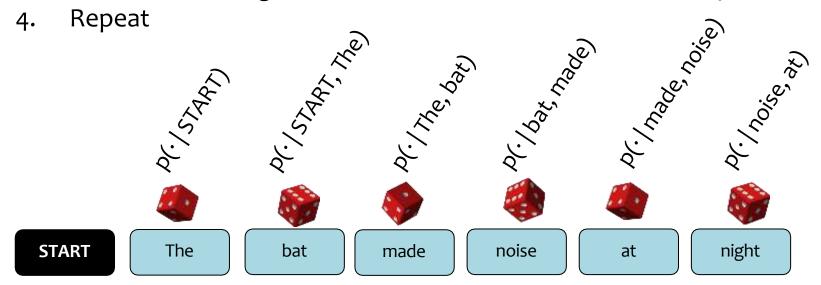
 $p(w_t | w_{t-2} = cows,$





<u>Question</u>: How do we sample from a Language Model? <u>Answer</u>:

- 1. Treat each probability distribution like a (50k-sided) weighted die
- 2. Pick the die corresponding to $p(w_t | w_{t-2}, w_{t-1})$
- 3. Roll that die and generate whichever word w_t lands face up



Sampling from a Language Model



Question: How do we sample from a Language Model?

Answer:

- Treat each probability distribution like a (50k-sided) weighted die
- Pick the die corresponding to $p(w_t | w_{t-2}, w_{t-1})$
- Roll that die and generate whichever word w_t lands face up
- Repeat

Training Data (Shakespeaere)

I tell you, friends, most charitable care ave the patricians of you. For your wants, Your suffering in this dearth, you may as well Strike at the heaven with your staves as lift them Against the Roman state, whose course will on The way it takes, cracking ten thousand curbs Of more strong link asunder than can ever Appear in your impediment. For the dearth, The gods, not the patricians, make it, and Your knees to them, not arms, must help.

5-Gram Model

Approacheth, denay. dungy Thither! Julius think: grant, -- 0 Yead linens, sheep's Ancient, Agreed: Petrarch plaguy Resolved pear! observingly honourest adulteries wherever scabbard quess; affirmation--his monsieur; died. jealousy, chequins me. Daphne building. weakness: sunrise, cannot stays carry't, unpurposed. prophet-like drink; back-return 'gainst surmise Bridget ships? wane; interim? She's striving wet;



RECURRENT NEURAL NETWORK (RNN) LANGUAGE MODELS

Recurrent Neural Networks (RNNs)



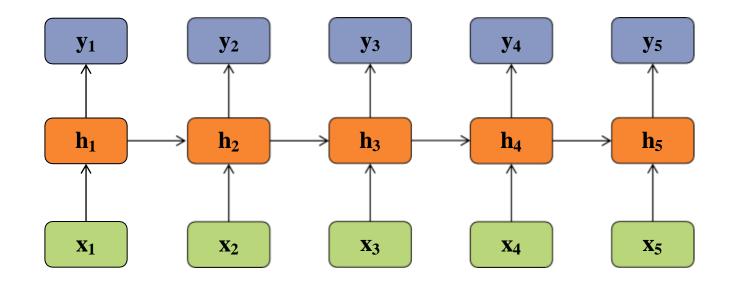
inputs:
$$\mathbf{x} = (x_1, x_2, \dots, x_T), x_i \in \mathbb{R}^I$$
 Definition of the RNN: hidden units: $\mathbf{h} = (h_1, h_2, \dots, h_T), h_i \in \mathbb{R}^I$ $h_t = \mathbf{H} (W_{xh} x_t + \mathbf{h}_t)$ outputs: $\mathbf{y} = (y_1, y_2, \dots, y_T), y_i \in \mathbb{R}^I$ $y_t = W_{hy} h_t + b_y$

outputs:
$$\mathbf{y} = (y_1, y_2, \dots, y_T), y_i \in \mathbb{R}^{n}$$

nonlinearity: H

$$h_t = H (W_{xh}x_t + W_{hh}h_{t-1} + b_h)$$

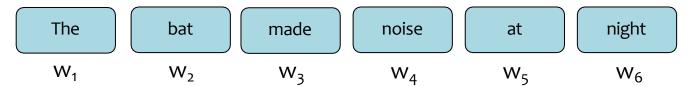
$$y_t = W_{hy}h_t + b_y$$



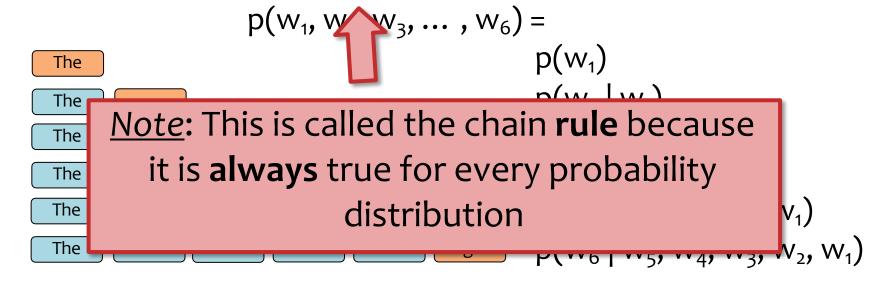




Question: How can we define a probability distribution over a sequence of length T?



Chain rule of probability:
$$p(w_1, w_2, \dots, w_T) = \prod_{t=1}^{T} p(w_t \mid w_{t-1}, \dots, w_1)$$



RNN Language Model

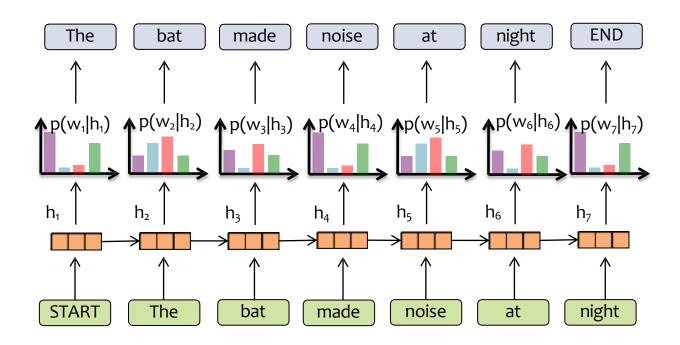


RNN Language Model:
$$p(w_1, w_2, \dots, w_T) = \prod_{t=1}^{T} p(w_t \mid f_{\theta}(w_{t-1}, \dots, w_1))$$

Key Idea:

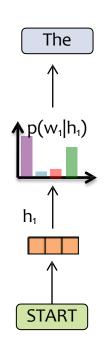
- (1) convert all previous words to a **fixed length vector**
- (2) define distribution $p(w_t | f_{\theta}(w_{t-1}, ..., w_1))$ that conditions on the vector





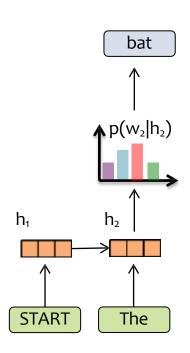
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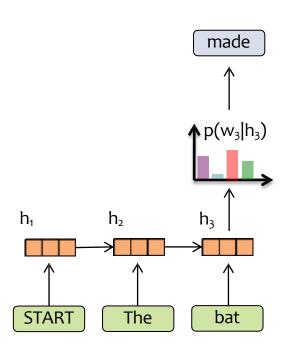
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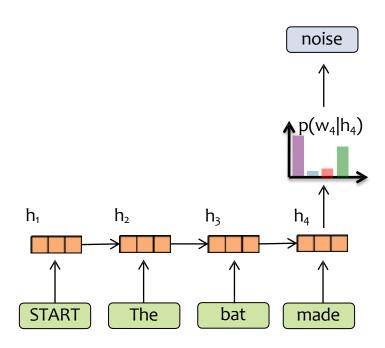
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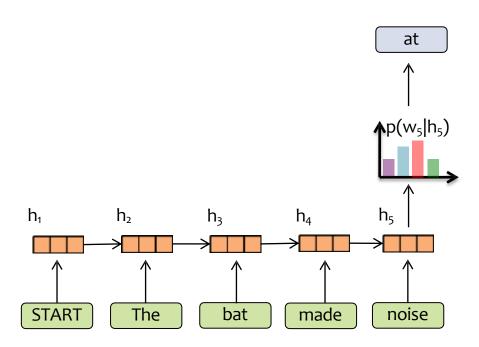
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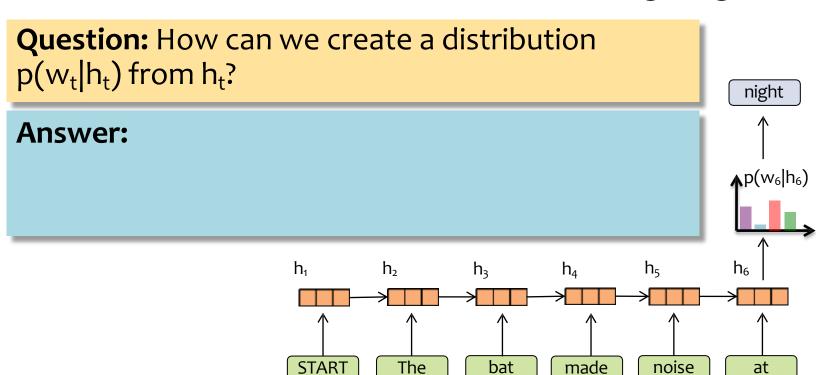
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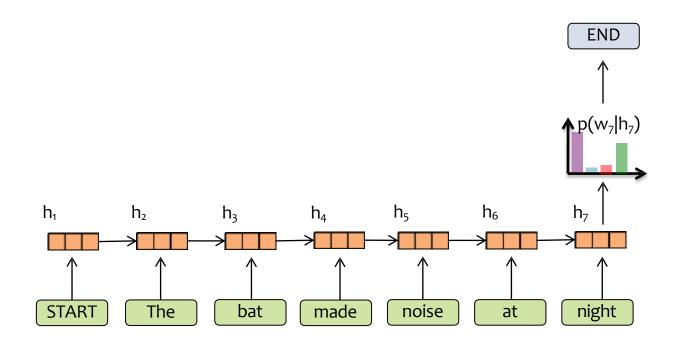
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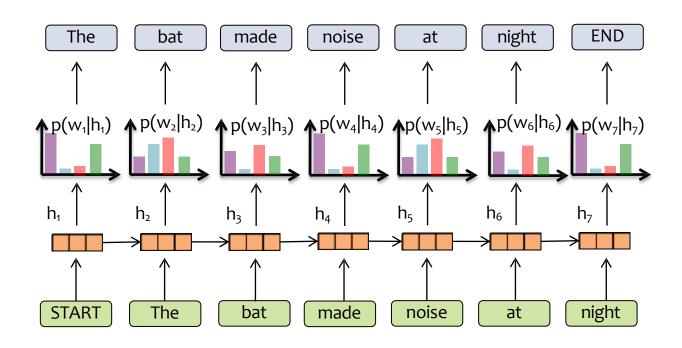
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- (1) convert all previous words to a fixed length vector
- (2) define distribution $p(w_t | f_{\theta}(w_{t-1}, ..., w_1))$ that conditions on the vector $\mathbf{h}_t = f_{\theta}(w_{t-1}, ..., w_1)$





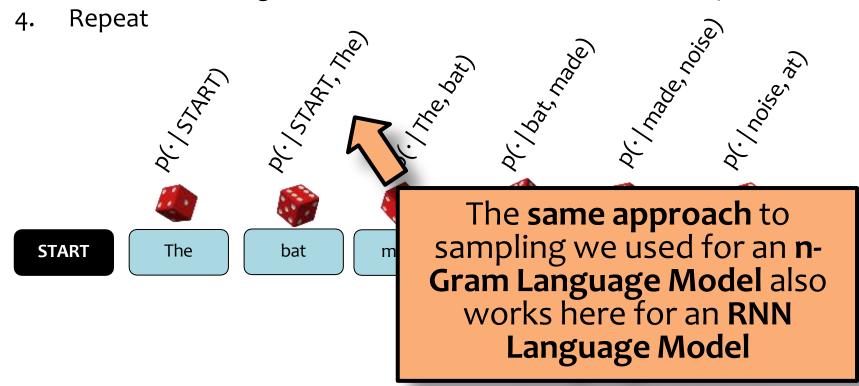
$$p(w_1, w_2, w_3, ..., w_T) = p(w_1 | h_1) p(w_2 | h_2) ... p(w_2 | h_T)$$

Sampling from a Language Model 上海科技大学



<u>Question</u>: How do we sample from a Language Model? Answer:

- 1. Treat each probability distribution like a (50k-sided) weighted die
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LEARNING AN RNN



Dataset for Supervised Part-of-Speech (POS) Tagging



D = $\{x^{(n)}, y^{(n)}\}_{n=1}^{N}$ Data:

Sample 1:	n	flies	p like	an	$ \begin{array}{c c} $
Sample 2:	n	n	v like	an	$ \begin{array}{c c} $
Sample 3:	n	fly	with	n	$ \begin{array}{c c} $
Sample 4:	p	n	you	will	$\begin{cases} y^{(4)} \\ x^{(4)} \end{cases}$

SGD and Mini-batch SGD



Algorithm 1SGD

```
1: Initialize \theta^{(0)}
2:
3:
4: s = 0
5: for t = 1, 2, ..., T do
        for i \in \mathsf{shuffle}(1, \dots, N) do
              Select the next training point (x_i, y_i)
              Compute the gradient g^{(s)} = \nabla J_i(\theta^{(s-1)})
8:
              Update parameters \theta^{(s)} = \theta^{(s-1)} - \eta g^{(s)}
9:
              Increment time step s = s + 1
10:
         Evaluate average training loss J(\theta) = \frac{1}{n} \sum_{i=1}^{n} J_i(\theta)
11:
12: return \theta^{(s)}
```

SGD and Mini-batch SGD



Algorithm 1 Mini-Batch SGD

```
1: Initialize \theta^{(0)}
2: Divide examples \{1,\ldots,N\} randomly into batches \{I_1,\ldots,I_B\}
3: where \bigcup_{b=1}^{B} I_b = \{1, ..., N\} and \bigcap_{b=1}^{B} I_b = \emptyset
4: s = 0
5: for t = 1, 2, ..., T do
         for b = 1, 2, ..., B do
              Select the next batch I_b, where m = |I_b|
              Compute the gradient g^{(s)} = \frac{1}{m} \sum_{i \in I_h} \nabla J_i(\theta^{(s)})
              Update parameters \theta^{(s)} = \theta^{(s-1)} - \eta q^{(s)}
9:
              Increment time step s = s + 1
10:
         Evaluate average training loss J(\theta) = \frac{1}{n} \sum_{i=1}^{n} J_i(\theta)
11:
12: return \theta^{(s)}
```

y₃ **y**₁ y_2 **y**₄ h₃ h_4 X_2 X_3 X_4 X_1

RNN



Algorithm 1Elman RNN

1: **procedure** FORWARD($x_{1:T}$, W_{ah} , W_{ax} , b_a , W_{yh} , b_y)

Initialize the hidden state h_0 to zeros 2:

for t in 1 to T **do** 3:

Receive input data at time step t: x_t 4:

Compute the hidden state update: 5:

$$a_t = W_{ah} \cdot h_{t-1} + W_{ax} \cdot x_t + b_a$$

7:
$$h_t = \sigma(a_t)$$

Compute the output at time step *t*: 8:

9:
$$y_t = W_{yh} \cdot h_t + b_y$$

h_4 X_1

RNN



Algorithm 1Elman RNN

1: **procedure** FORWARD($x_{1:T}$, W_{ah} , W_{ax} , b_a , W_{yh} , b_y)

Initialize the hidden state h_0 to zeros 2:

for t in 1 to T do 3:

Receive input data at time step t: x_t 4:

Compute the hidden state update: 5:

$$a_t = W_{ah} \cdot h_{t-1} + W_{ax} \cdot x_t + b_a$$

 $h_t = \sigma(a_t)$

Compute the output at time step *t*:

 $y_t = \operatorname{softmax}(W_{yh} \cdot h_t + b_y)$ 9:

$P = \log p(\mathbf{w})$ $P_4(\cdot,\cdot)$ $P_2(\cdot,\cdot)$ $P_3(\cdot,\cdot)$ $P_1(\cdot,\cdot)$ h₃ h_4 X_3 X_2 X_4 X_1 y*3 y*2 y*₄ y*₁

RNN + Loss



Algorithm 1Elman RNN + Loss

- 1: **procedure** FORWARD($x_{1:T}$, $y_{1:T}^*W_{ah}$, W_{ax} , b_a , W_{yh} , b_y)
- Initialize the hidden state h_0 to zeros 2:
- **for** t in 1 to T **do** 3:
- Receive input data at time step t: x_t 4:
- Compute the hidden state update: 5:

6:
$$a_t = W_{ah} \cdot h_{t-1} + W_{ax} \cdot x_t + b_a$$

7:
$$h_t = \sigma(a_t)$$

Compute the output at time step *t*: 8:

9:
$$y_t = \operatorname{softmax}(W_{yh} \cdot h_t + b_y)$$

Compute the cross-entropy loss at time step t: 10:

11:
$$\ell_t = -\sum_{k=1}^K (y_t^*)_k \log((y_t)_k)$$

Compute the total loss: 12:

13:
$$\ell = \sum_{t=1}^{T} \ell_t$$



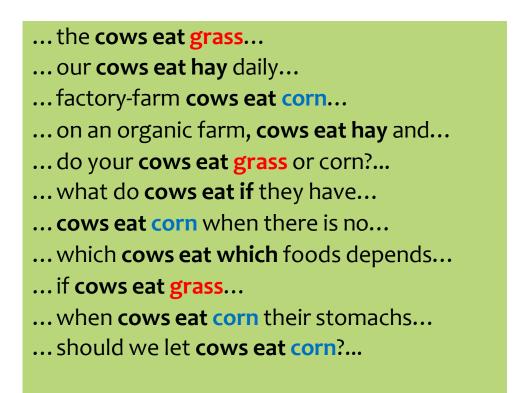
LEARNING AN RNN-LM

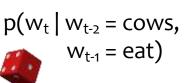
Learning a Language Model



<u>Question</u>: How do we **learn** the probabilities for the n-Gram Model?

Answer: From data! Just count n-gram frequencies





Wt	p(· ·,·)		
corn	4/11		
grass	3/11		
hay	2/11		
if	1/11		
which	1/11		

MLE for n-gram LM

- This counting method gives us the maximum likelihood estimate of the n-gram LM parameters
- We can derive it in the usual way:
 - Write the likelihood of the sentences under the n-gram LM
 - Set the gradient to zero

 and impose the constraint
 that the probabilities sum to-one
 - Solve for the MLE

Learning a Language Model



MLE for Deep Neural LM

- We can also use maximum likelihood estimation to learn the parameters of an RNN-LM or Transformer-LM too!
- But not in closed form instead we follow a different recipe:
 - Write the likelihood of the sentences under the Deep Neural LM model
 - Compute the gradient of the (batch) likelihood w.r.t.
 the parameters by AutoDiff
 - Follow the negative gradient using Mini-batch SGD (or your favorite optimizer)

MLE for n-gram LM

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- We can derive it in the usual way:
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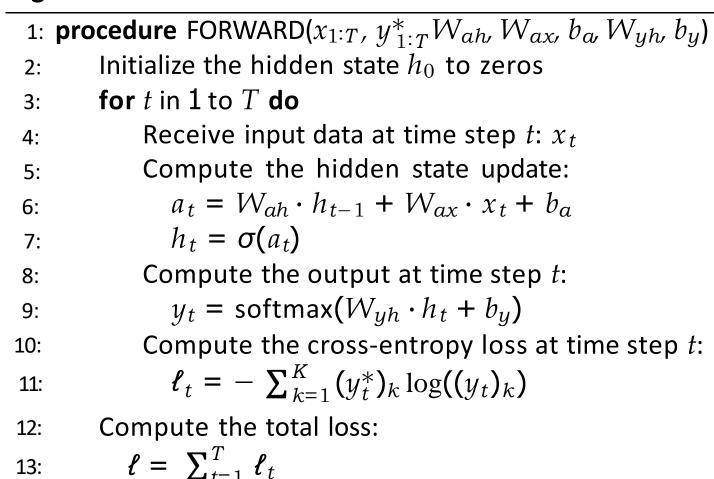
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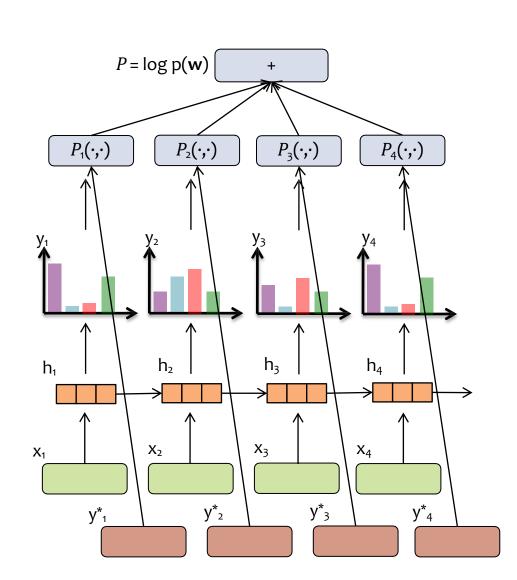
RNN + LossI

How can we use this to compute the loss for an RNN-LM?

ShanghaiTech University

Algorithm 1Elman RNN + Loss



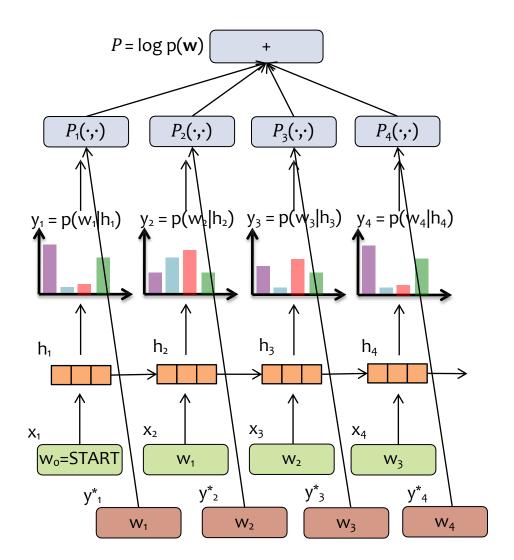




RNN-LM + Loss

How can we use this to compute the loss for an RNN-LM?

$\log p(\mathbf{w}) = \log p(w_1, w_2, w_3, \dots, w_T)$ $= \log p(w_1 | h_1) + ... + \log p(w_T | h_T)$



Algorithm 1Elman RNN + Loss

1: procedure FORWARD($x_{1:T}$, $y_{1:T}^*W_{ah}$, W_{ax} , b_a , W_{yh} , b_y)

Initialize the hidden state h_0 to zeros 2:

for t in 1 to T **do** 3:

Receive input data at time step t: x_t 4:

Compute the hidden state update: 5:

$$a_t = W_{ah} \cdot h_{t-1} + W_{ax} \cdot x_t + b_a$$

 $h_t = \sigma(a_t)$ 7:

Compute the output at time step *t*: 8:

9:
$$y_t = \operatorname{softmax}(W_{yh} \cdot h_t + b_y)$$

Compute the cross-entropy loss at time step t: 10:

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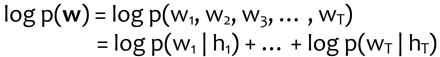
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RNN-LM + Loss

How can we use this to compute the loss for an RNN-LM?



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Algorithm 1Elman RNN + Loss

1: **procedure** FORWARD(
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, $y_{1:T}^*W_{ah}$, W_{ax} , b_a , W_{yh} , b_y)

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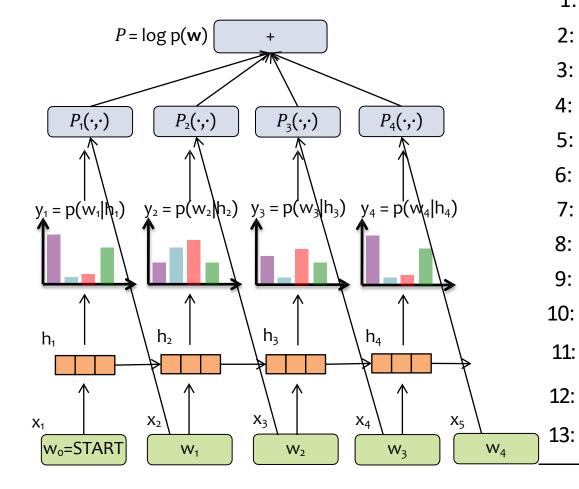
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$$\ell_t = -\sum_{k=1}^{K} (y_t^*)_k \log((y_t)_k)$$

Compute the total loss:

$$\ell = \sum_{t=1}^{T} \ell_t$$





Learning an RNN-LM



- Each training example is a sequence (e.g. sentence), so we have training data D = {w⁽¹⁾, w⁽²⁾, ..., w^(N)}
- The objective function for a Deep LM (e.g. RNN-LM or Tranformer-LM) is typically the log-likelihood of the training examples: $J(\mathbf{\theta}) = \Sigma_i \log p_{\mathbf{\theta}}(\mathbf{w}^{(i)})$
- We train by mini-batch SGD (or your favorite flavor of mini-batch SGD)

 $log p(\mathbf{w}) = log p(w_1, w_2, w_3, ..., w_T)$ = log p(w₁ | h₁) + log p(w₂ | h₂) + ... + log p(w_T | h_T)

