

#### 10-301/10-601 Introduction to Machine Learning

Machine Learning Department School of Computer Science Carnegie Mellon University

# RNN LMs

# Transformer LMs

Matt Gormley, Henry Chai Lecture 18 Oct. 30, 2024

### Reminders

- Homework 6: Learning Theory & Generative Models
  - Out: Sun, Oct 27
  - Due: Sat, Nov 2, 11:59pm
- Exam 2: Thu, Nov 7, 6:45 pm 8:45 pm

### EXAM 2 LOGISTICS

### Exam 2

- Time / Location
  - Time: Thu, Nov. 7, 6:45pm 8:45pm
  - Location & Seats: You have all been split across multiple rooms. Everyone has an assigned seat in one of these room. Please watch Piazza carefully for announcements.
- Logistics
  - Covered material: Lecture 8 Lecture 16
  - Format of questions:
    - Multiple choice
    - True / False (with justification)
    - Derivations
    - Short answers
    - Interpreting figures
    - Implementing algorithms on paper
  - No electronic devices
  - You are allowed to bring one 8½ x 11 sheet of notes (front and back, handwritten with pen/pencil or tablet)

# Topics for Exam 1

- Foundations
  - Probability, Linear Algebra,
     Geometry, Calculus
  - Optimization
- Important Concepts
  - Overfitting
  - Experimental Design

- Classification
  - Decision Tree
  - KNN
  - Perceptron
- Regression
  - Linear Regression

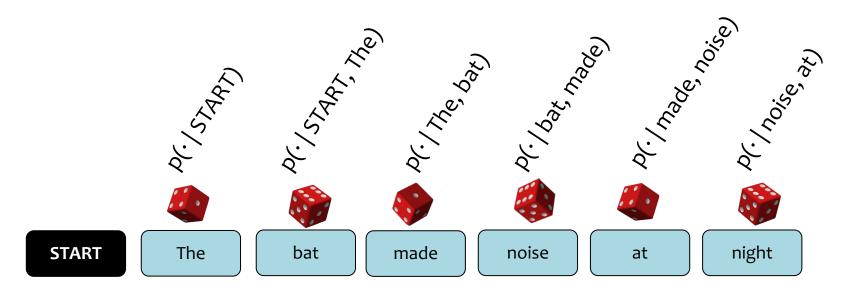
# Topics for Exam 2

- Classification
  - Binary Logistic Regression
- Important Concepts
  - Stochastic Gradient Descent
  - Regularization
  - Feature Engineering
- Feature Learning
  - Neural Networks
  - Basic NN Architectures
  - Backpropagation

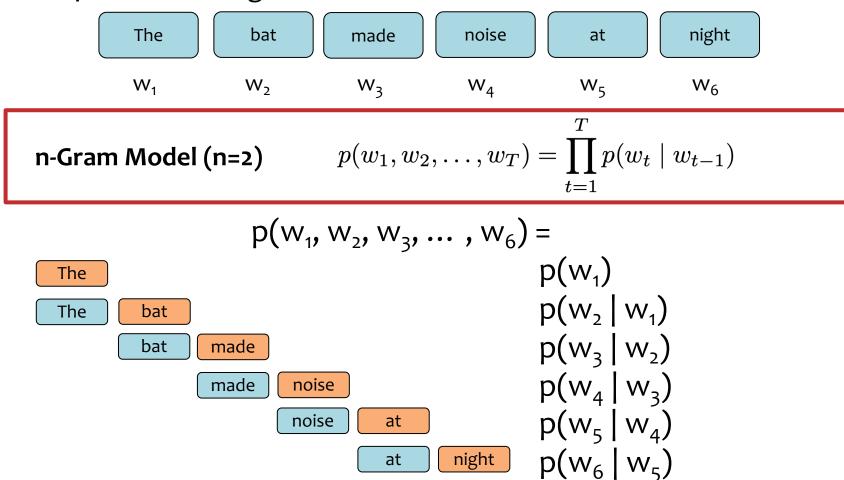
- Learning Theory
  - PAC Learning
  - MLE / MAP
- Societal Impacts of ML
- Regression
  - Linear Regression

### BACKGROUND: N-GRAM LANGUAGE MODELS

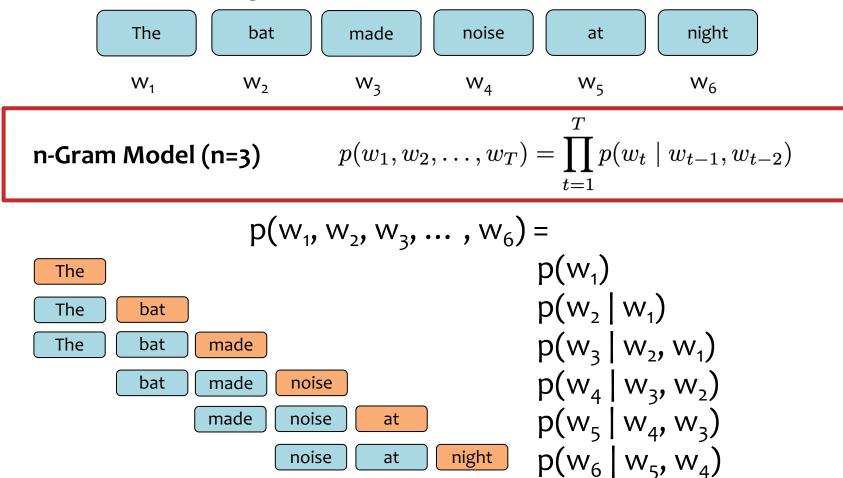
- <u>Goal</u>: Generate realistic looking sentences in a human language
- <u>Key Idea</u>: condition on the last n-1 words to sample the n<sup>th</sup> word



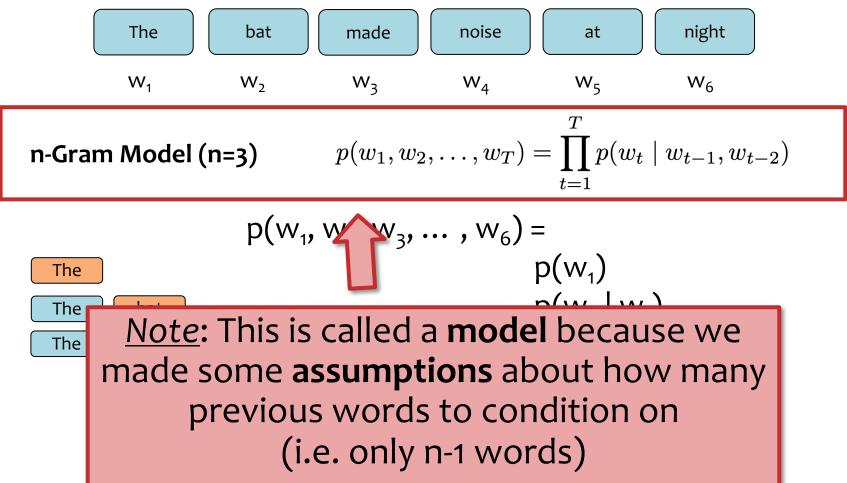
<u>Question</u>: How can we **define** a probability distribution over a sequence of length T?



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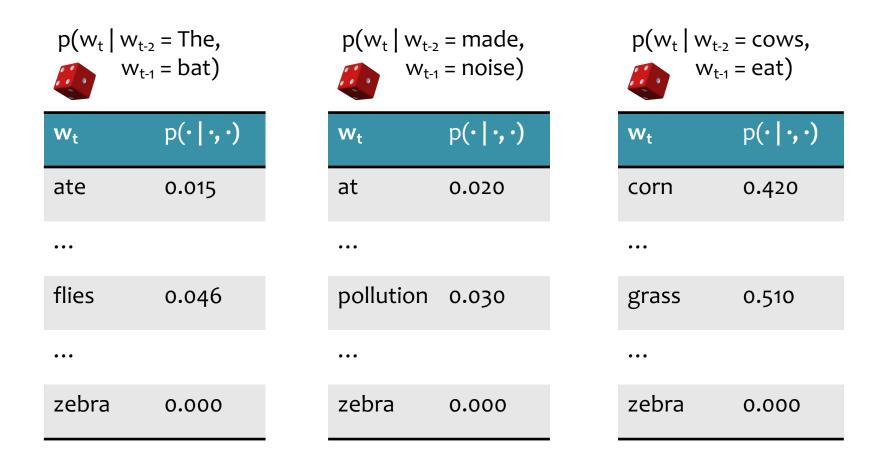


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### Learning an n-Gram Model

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



### Learning an n-Gram Model

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

<u>Answer</u>: From data! Just **count** n-gram frequencies

... the cows eat grass...
... our cows eat hay daily...
... factory-farm cows eat corn...
... on an organic farm, cows eat hay and...
... do your cows eat grass or corn?...
... what do cows eat if they have...
... what do cows eat if they have...
... what do cows eat which foods depends...
... if cows eat grass...
... when cows eat corn their stomachs...

... should we let **cows eat corn**?...

$p(w_t   w_{t-2} = cows, w_{t-1} = eat)$	
w <sub>t</sub>	p(• •,•)
corn	4/11
grass	3/11
hay	2/11
if	1/11
which	1/11

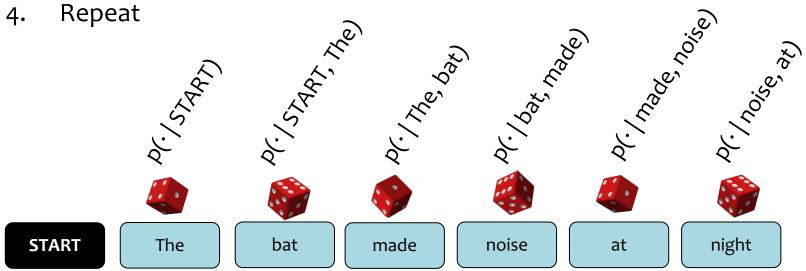
 $p(w \mid w - cows$ 

# Sampling from a Language Model

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

Answer:

- Treat each probability distribution like a (50k-sided) weighted die 1.
- Pick the die corresponding to  $p(w_t | w_{t-2}, w_{t-1})$ 2.
- Roll that die and generate whichever word w<sub>t</sub> lands face up 3.
- Repeat 4.



# Sampling from a Language Model

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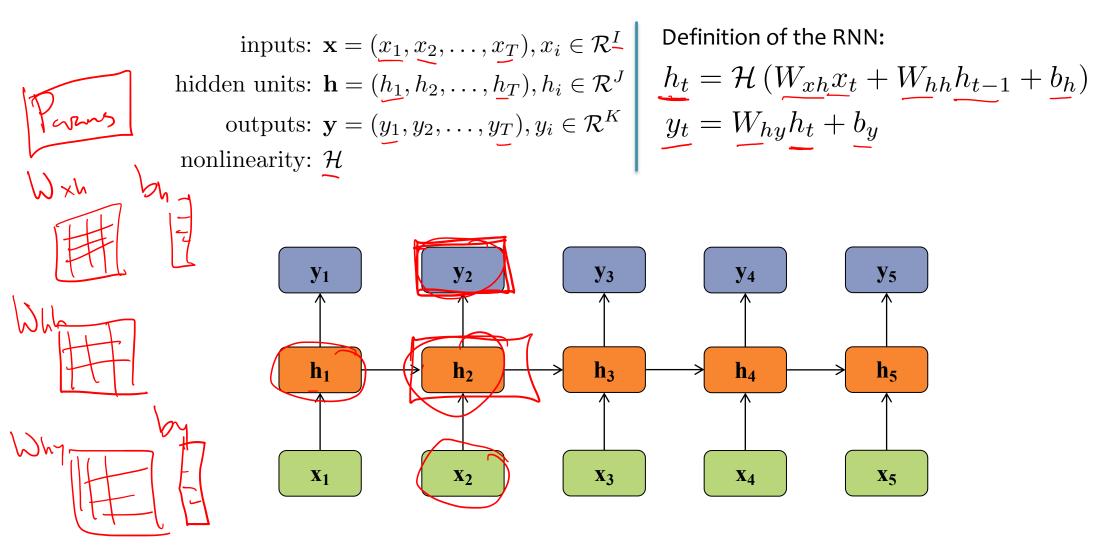
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- 2. Pick the die corresponding to  $p(w_t | w_{t-2}, w_{t-1})$
- 3. Roll that die and generate whichever word w<sub>t</sub> lands face up
- 4. Repeat

Training Data (Shakespeaere)	5-Gram Model
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.	Approacheth, denay. dungy Thither! Julius think: grant,O Yead linens, sheep's Ancient, Agreed: Petrarch plaguy Resolved pear! observingly honourest adulteries wherever scabbard guess; affirmationhis monsieur; died. jealousy, chequins me. Daphne building. weakness: sun- rise, cannot stays carry't, unpurposed. prophet-like drink; back-return 'gainst surmise Bridget ships? wane; interim? She's striving wet;

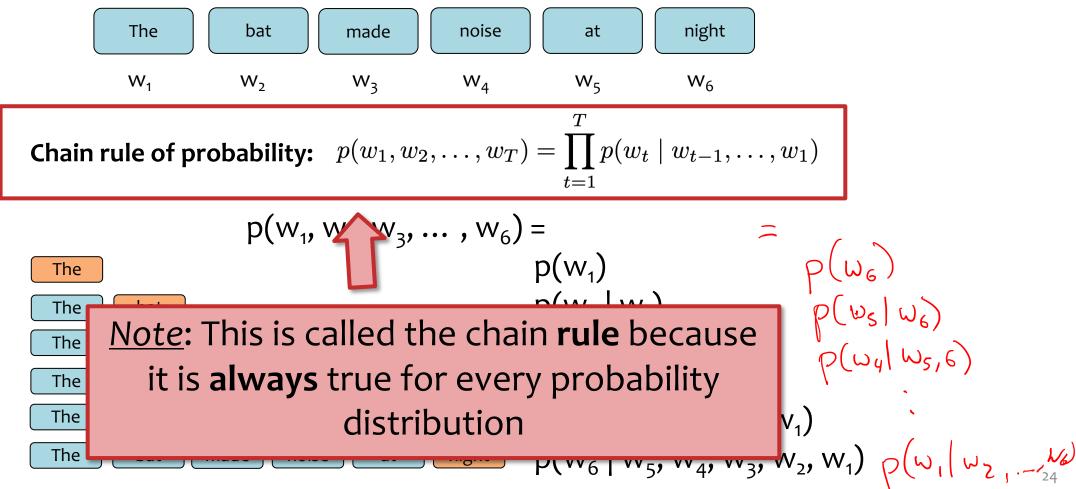
# RECURRENT NEURAL NETWORK (RNN) LANGUAGE MODELS

# Elme Network Recurrent Neural Networks (RNNs)



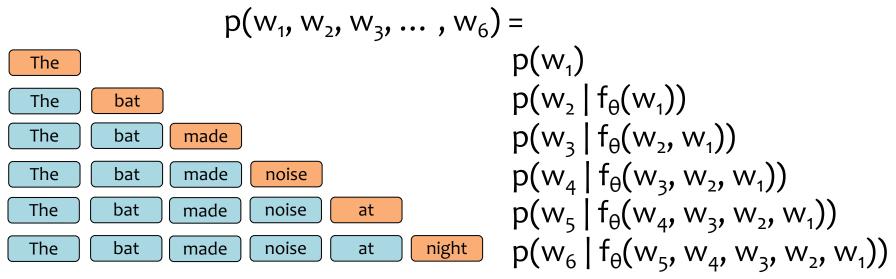
# The Chain Rule of Probability

<u>Question</u>: How can we **define** a probability distribution over a sequence of length T?



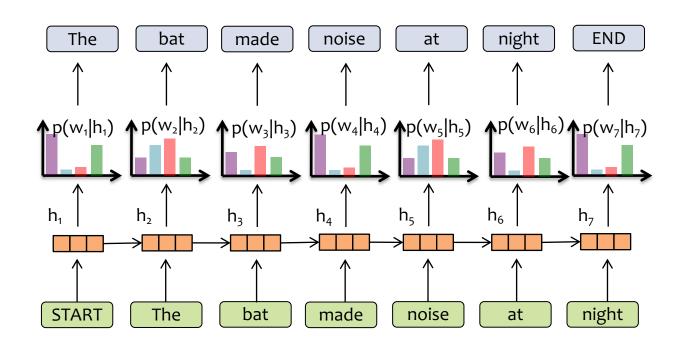
Recall...

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

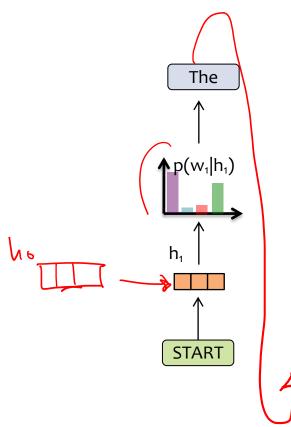


#### Key Idea:

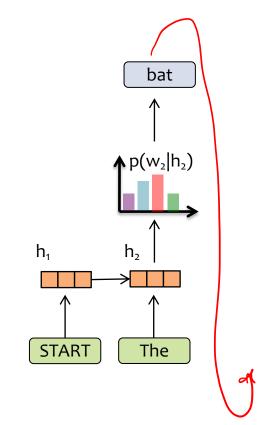
(1) convert all previous words to a **fixed length vector** (2) define distribution  $p(w_t | f_{\theta}(w_{t-1}, ..., w_1))$  that conditions on the vector



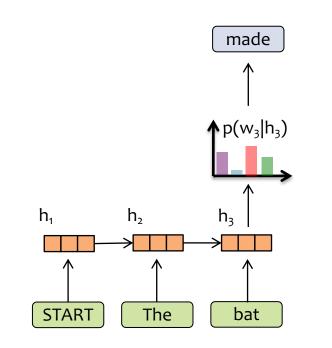
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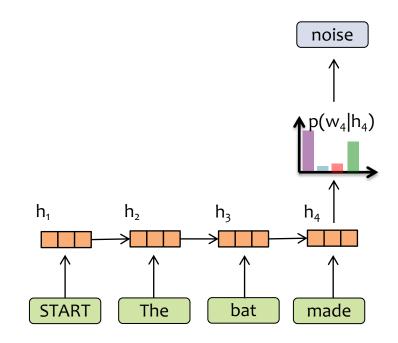
Key Idea:



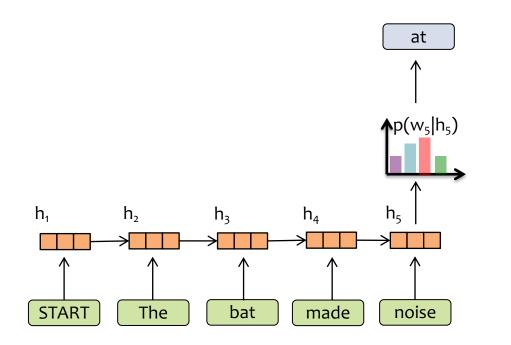
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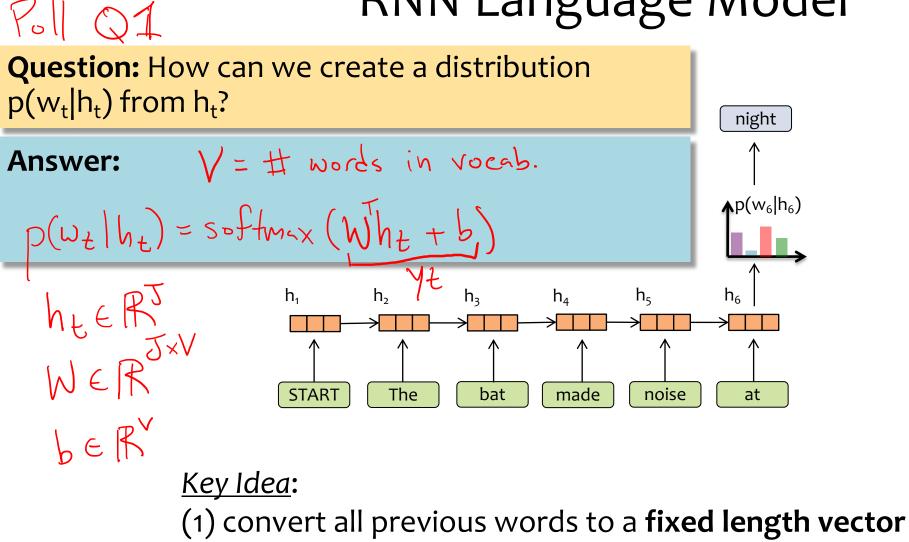
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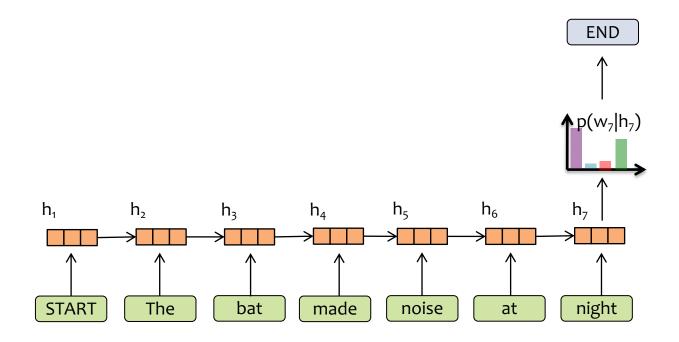
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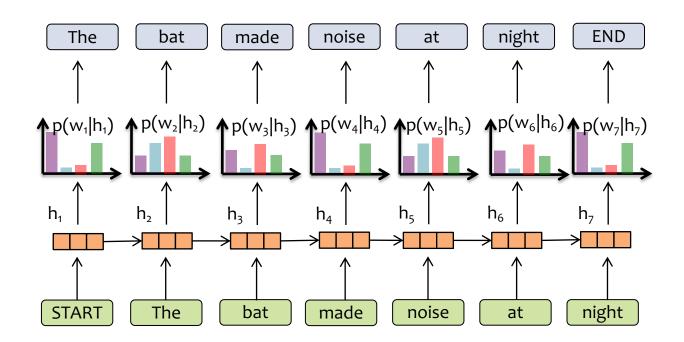
#### Key Idea:



(2) define distribution  $p(w_t | f_{\theta}(w_{t-1}, ..., w_1))$  that conditions on the vector  $\mathbf{h}_{t} = f_{\theta}(w_{t-1}, \dots, w_{t})$ 



#### Key Idea:



$$p(w_{1}, w_{2}, w_{3}, ..., w_{T}) = p(w_{1} | h_{1}) p(w_{2} | h_{2}) ... p(w_{T} | h_{T})$$

$$p(w_{t} | h_{t})$$

# Sampling from a Language Model

12 Control of the cost of the

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

Answer:

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Dr. Start The

bat

PC./SZARY

The

Roll that die and generate whichever word w<sub>t</sub> lands face up 3.

m

Repeat 4.

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The same approach to sampling we used for an **n**-Gram Language Model also works here for an RNN Language Model

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(10, 0, 0, 1)

#### ??

VIOLA: Why, Salisbury must find his flesh and thought That which I am not aps, not a man and in fire, To show the reining of the raven and the wars To grace my hand reproach within, and not a fair are hand, That Caesar and my goodly father's world; When I was heaven of

presence and our fleets, We spare with hours, but cut thy council I am great, Murdered and by thy more to give thee but so much service in the noble bondman here, Would Shake her wine.

KING LEAR: O, if you were a feeble show, the courtesy of your law, Your sight and several breath, will wear the gods With his heads, and my hands are wonder'd at the deeds, So drop upon your lordship's head, and your opinion Shall be against your honour.

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CHARLES: Marry, do I, sir; and I came to acquaint you with a matter. I am given, sir, secretly to understand that your younger brother Orlando hath a disposition to come in disguised against me to try a fall. To-morrow, sir, I wrestle for my credit; and he that escapes me without <u>some broken limb</u> shall acquit him well. Your brother is

Which is the real Shakespeare?!

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#### Shakespeare's As You Like It

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#### **RNN-LM Sample**

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### **LEARNING AN RNN**

### Dataset for Supervised Part-of-Speech (POS) Tagging Data: $\mathcal{D} = \{ \boldsymbol{x}^{(n)}, \boldsymbol{y}^{(n)} \}_{n=1}^{N}$



Recall...

### SGD and Mini-batch SGD

#### Algorithm 1 SGD

1: Initialize  $\theta^{(0)}$ 2: 3: 4: s = 05: for t = 1, 2, ..., T do for  $i \in \mathsf{shuffle}(1, \ldots, N)$  do 6: Select the next training point  $(x_i, y_i)$ 7: 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 + 110: Evaluate average training loss  $J(\theta) = \frac{1}{n} \sum_{i=1}^{n} J_i(\theta)$ 11: 12: return  $\theta^{(s)}$ 

Recaller

## 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 = 05: for t = 1, 2, ..., T do for b = 1, 2, ..., B do 6: Select the next batch  $I_b$ , where  $m = |I_b|$ 7: Compute the gradient  $g^{(s)} = \frac{1}{m} \sum_{i \in I_b} \nabla J_i(\theta^{(s)})$ 8: Update parameters  $\theta^{(s)} = \theta^{(s-1)} - \eta q^{(s)}$ 9: Increment time step s = s + 110: Evaluate average training loss  $J(\theta) = \frac{1}{n} \sum_{i=1}^{n} J_i(\theta)$ 11: 12: return  $\theta^{(s)}$ 

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### RNN

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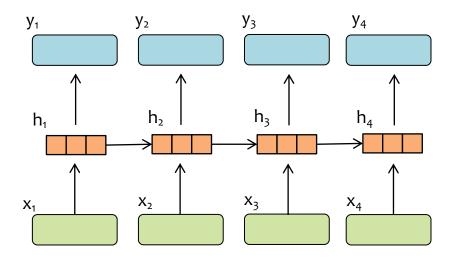
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#### Algorithm 1 Elman RNN

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

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

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



### RNN

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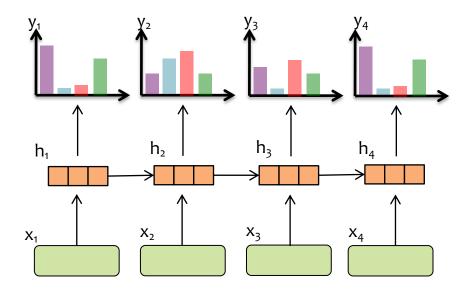
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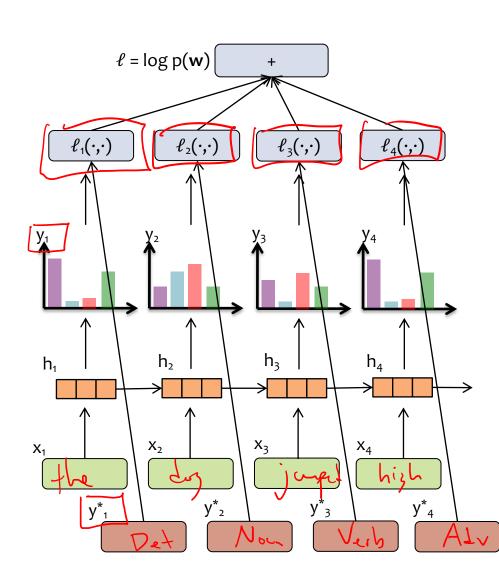
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Compute the output at time step *t*:

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





## RNN + Loss

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#### Algorithm 1 Elman RNN + Loss

- 1: procedure FORWARD( $x_{1:T}, y_{1:T}^* W_{ah}, W_{ax}, b_a, W_{yh}, b_y$ )
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Compute the output at time step *t*:

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

Compute the cross-entropy loss at time step t:

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

12: Compute the total loss:

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

### **LEARNING AN RNN-LM**

## Learning a Language Model

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

<u>Answer</u>: From data! Just **count** n-gram frequencies

... the cows eat grass...

- ... our cows eat hay daily...
- ... factory-farm **cows eat corn**...
- ... on an organic farm, **cows eat hay** and...
- ... do your **cows eat grass** or corn?...
- ... what do **cows eat if** they have...
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$p(w_t   w_{t-2} = cows, w_{t-1} = eat)$				
w <sub>t</sub>	p( <b>·   ·, ·)</b>			
corn	4/11			
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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 sumto-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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## RNN + Loss

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



- 1: procedure FORWARD( $x_{1:T}, y_{1:T}^* W_{ah}, W_{ax}, b_a, W_{yh}, b_y$ )
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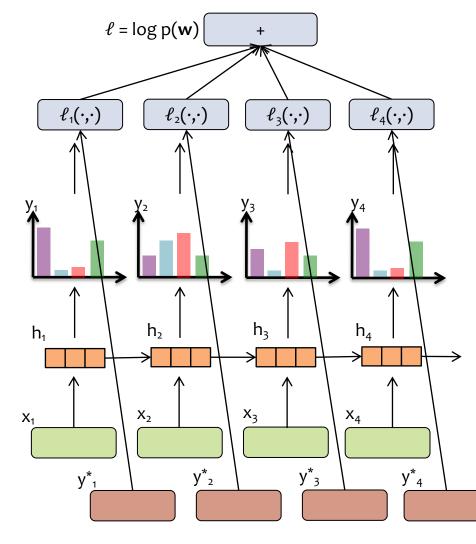
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Compute the cross-entropy loss at time step t:

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12: Compute the total loss:

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## RNN-LM + Loss

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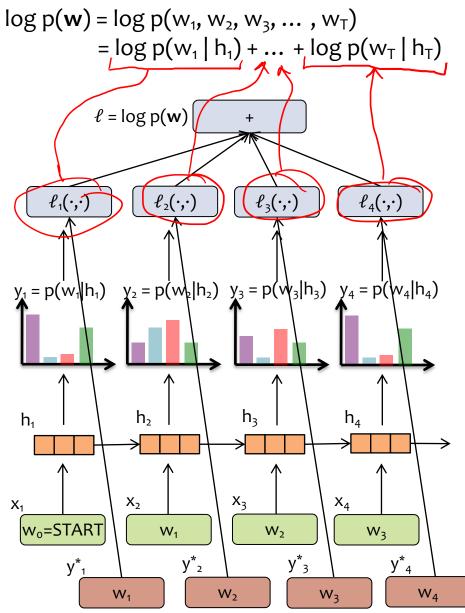
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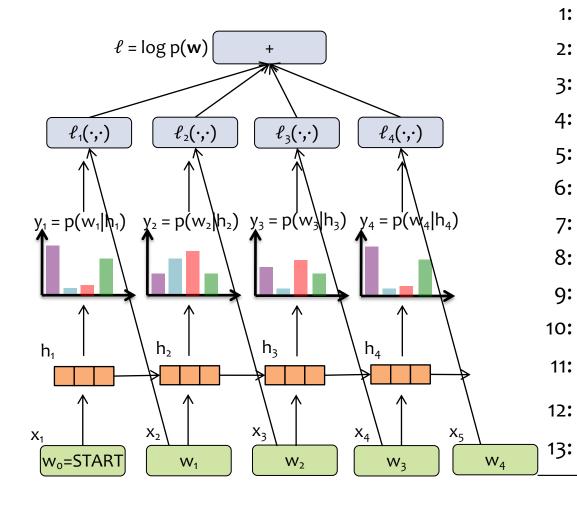
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## RNN-LM + Loss

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

 $-\log p(\mathbf{w}) = \log p(w_1, w_2, w_3, ..., w_T)$ = log p(w<sub>1</sub> | h<sub>1</sub>) + ... + log p(w<sub>T</sub> | h<sub>T</sub>)



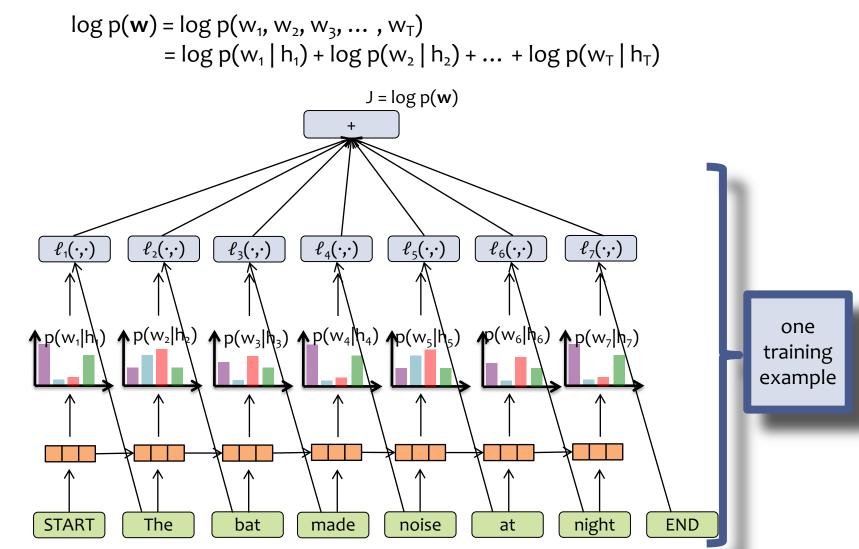
WIIT Algorithm 1 Elman RNN + Loss 1: procedure FORWARD $(x_{1:T}, y_{1:T}^* W_{ah}, W_{ax}, b_a, W_{yh}, b_y)$ Initialize the hidden state  $h_0$  to zeros for t in 1 to T do Receive input data at time step t:  $x_t$ Compute the hidden state update:  $a_t = W_{ah} \cdot h_{t-1} + W_{ax} \cdot \mathcal{D}_t + b_a$  $h_t = \sigma(a_t)$ W/-1 Compute the output at time step *t*:  $y_t = \text{softmax}(W_{yh} \cdot h_t + b_y)$ Compute the cross-entropy loss at time step *t*:  $\ell_t = -\sum_{k=1}^K (\mathbf{y}_k)_k \log((y_t)_k)$ Compute the total loss:  $\mathcal{U}_{\mathcal{L}}$  $\ell = \sum_{t=1}^{T} \ell_t$ 

## Learning an RNN-LM

- Each training example is a sequence (e.g. sentence), so we have training data D = {w<sup>(1)</sup>, w<sup>(2)</sup>, ..., w<sup>(N)</sup>}
- The objective function for a Deep LM (e.g. RNN-LM or Tranformer-LM) is typically the loglikelihood of the training examples:

 $J(\boldsymbol{\theta}) = \Sigma_i \log p_{\boldsymbol{\theta}}(\mathbf{w}^{(i)})$ 

• We train by mini-batch SGD (or your favorite flavor of mini-batch SGD)



### LARGE LANGUAGE MODELS

## How large are LLMs?

Comparison of some recent large language models (LLMs)

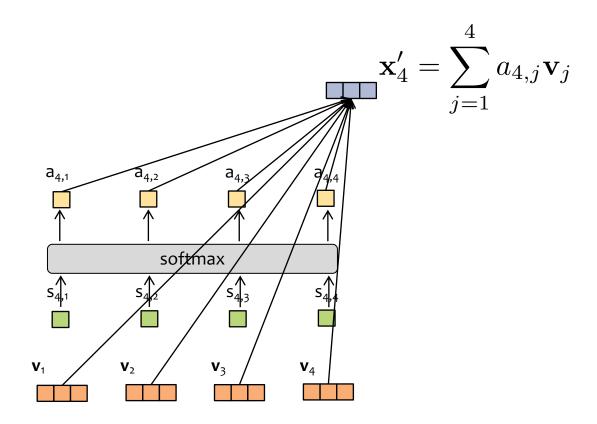
Model	Creators	Year of release	Training Data (# tokens)	Model Size (# parameters)
GPT-2	OpenAl	2019	~10 billion (40Gb)	1.5 billion
GPT-3	OpenAl	2020	300 billion	175 billion
PaLM	Google	2022	780 billion	540 billion
Chinchilla	DeepMind	2022	1.4 trillion	70 billion
LaMDA (cf. Bard)	Google	2022	1.56 trillion	137 billion
LLaMA	Meta	2023	1.4 trillion	65 billion
LLaMA-2	Meta	2023	2 trillion	70 billion
GPT-4	OpenAl	2023	?	? (1.76 trillion)
Gemini (Ultra)	Google	2023	?	? (1.5 trillion)
LLaMA-3	Meta	2024	15 trillion	405 billion

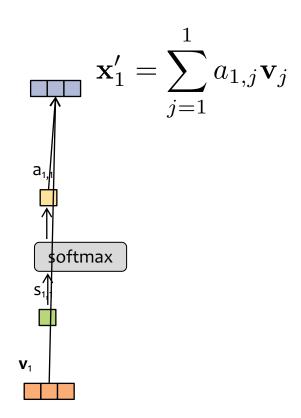
### What is ChatGPT?

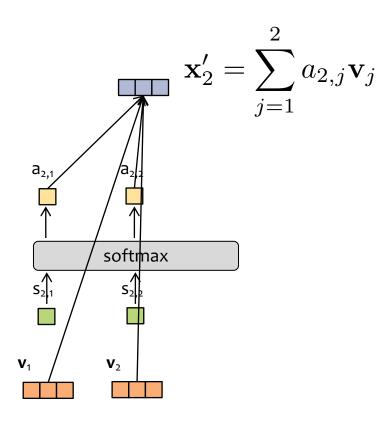
- ChatGPT is a large (in the sense of having many parameters) language model, fine-tuned to be a dialogue agent
- The base language model is GPT-3.5 which was trained on a large quantity of text

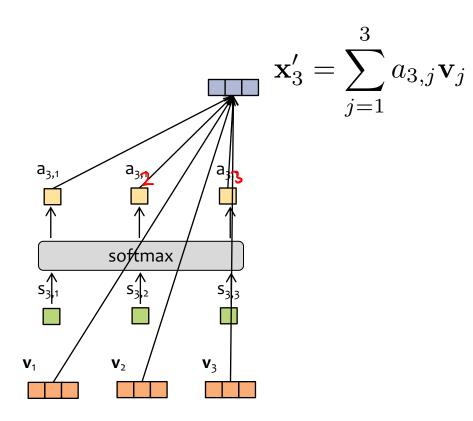
Transformer Language Models

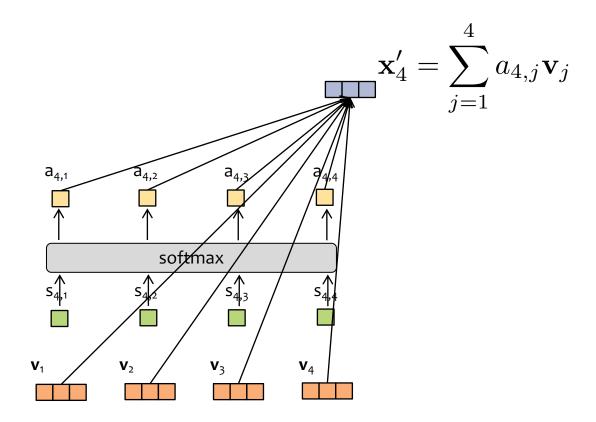
### **MODEL: GPT**

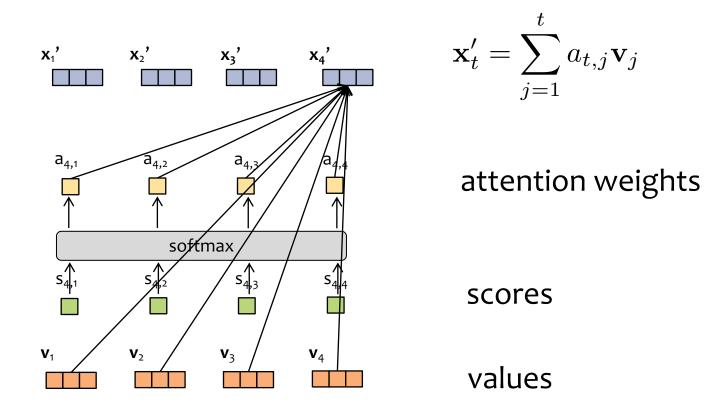


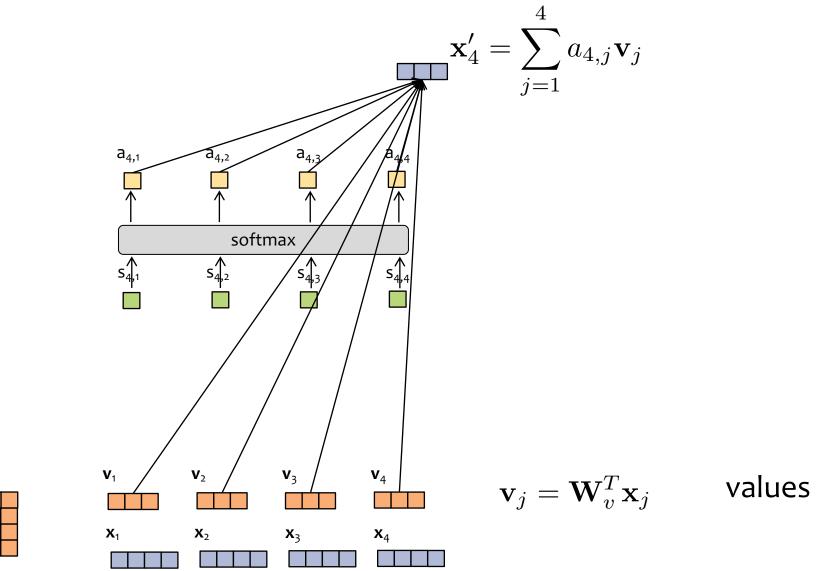




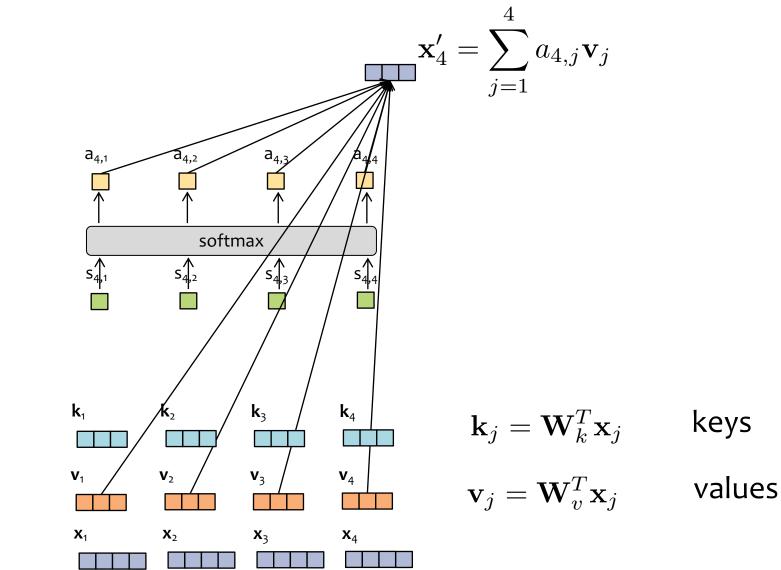


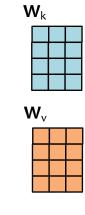


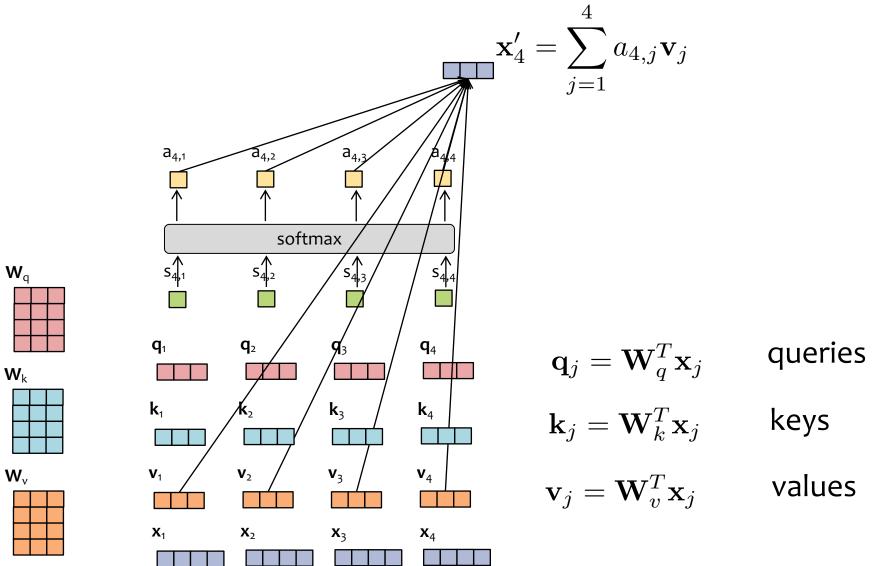


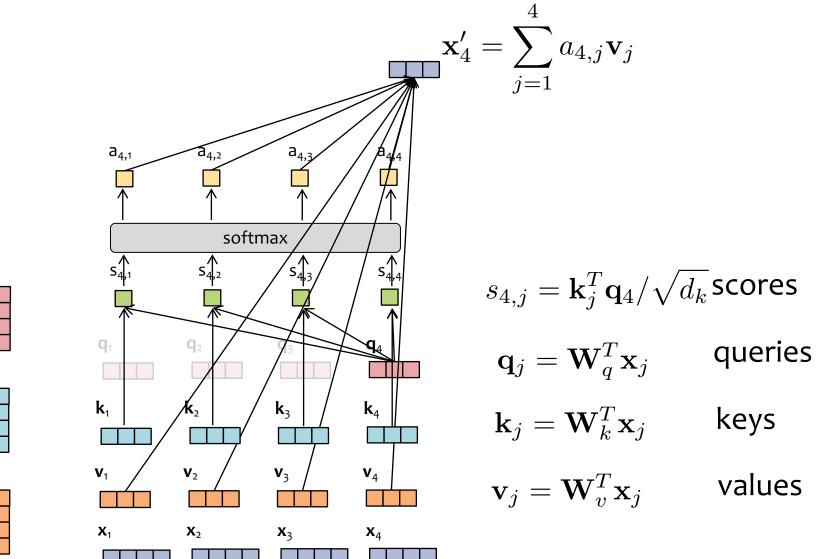




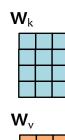




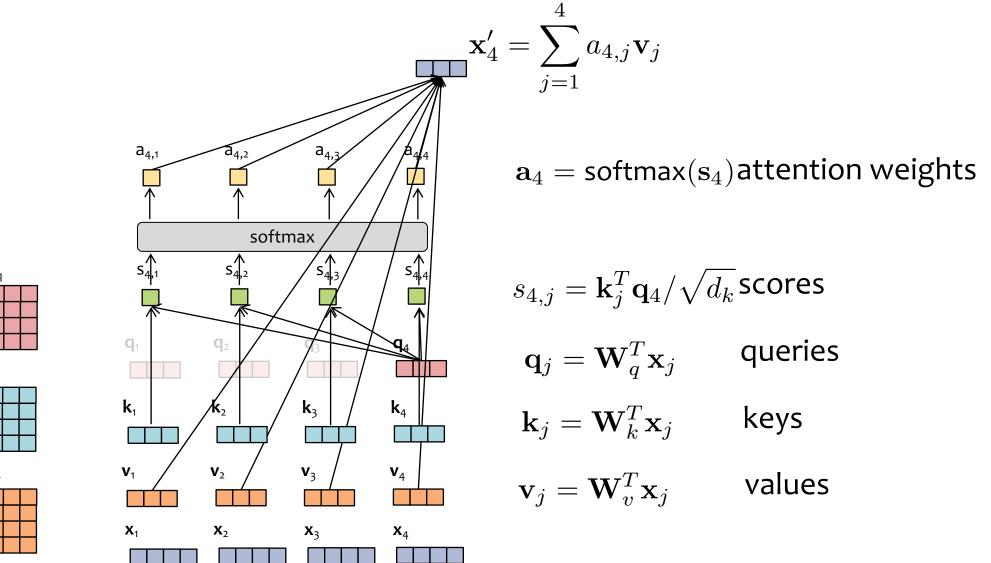




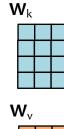


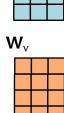












# Scaled Dot-Product Attention $\mathbf{x}'_4 = \sum_{j=1}^4 a_{4,j} \mathbf{v}_j$

 $W_q$ 

 $W_k$ 

 $W_{v}$ 

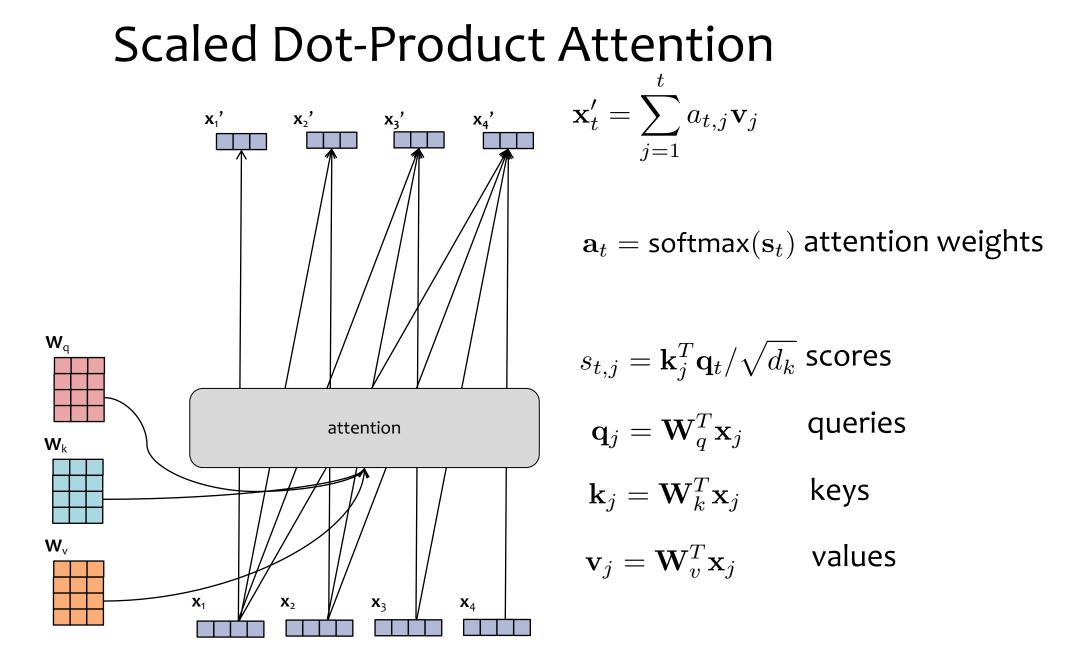
 $\mathbf{X}_1$ 

 $\mathbf{X}_{2}$ 

**X**<sub>3</sub>

 $\mathbf{X}_4$ 

a<sub>4,3</sub> a<sub>4,1</sub> d<sub>4,2</sub>  $\mathbf{a}_4 = \operatorname{softmax}(\mathbf{s}_4)$  attention weights softmax S S<sub>4.2</sub>  $s_{4,j} = \mathbf{k}_j^T \mathbf{q}_4 / \sqrt{d_k}$ scores attentio  $\mathbf{q}_j = \mathbf{W}_q^T \mathbf{x}_j$ queries  $\mathbf{k}_1$  $\mathbf{k}_{3}$  $\mathbf{k}_{4}$  $\mathbf{k}_j = \mathbf{W}_k^T \mathbf{x}_j$ keys  $\mathbf{v}_j = \mathbf{W}_v^T \mathbf{x}_j$ **V**<sub>2</sub> **V**<sub>3</sub> **V**<sub>1</sub> **V**<sub>4</sub> values



## Animation of 3D Convolution

#### http://cs231n.github.io/convolutional-networks/

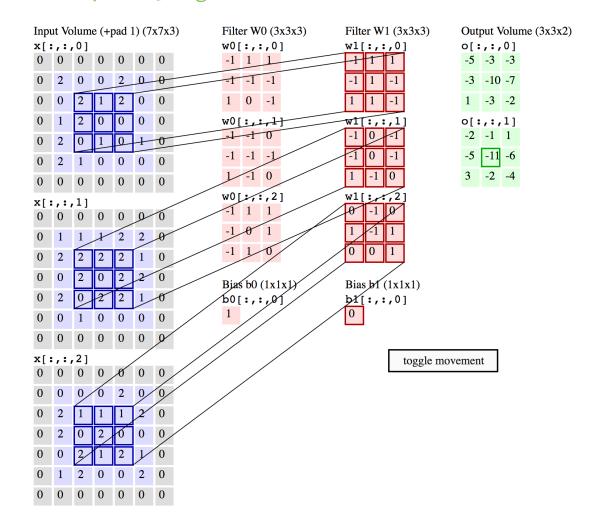
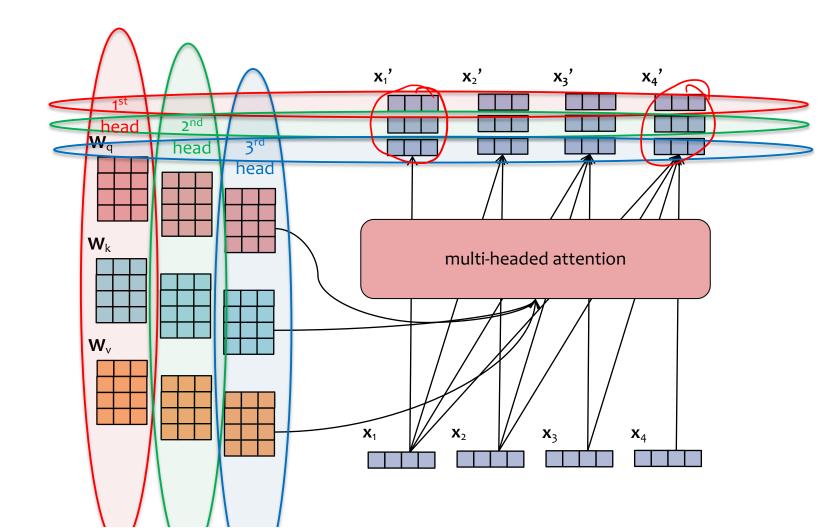


Figure from Fei-Fei Li & Andrej Karpathy & Justin Johnson (CS231N)

Recaller

### **Multi-headed Attention**



- Just as we can have multiple channels in a convolution layer, we can use multiple heads in an attention layer
- Each head gets its own parameters
- We can **concatenate** all the outputs to get a single vector for each time step

- To ensure the dimension of the • **input** embedding  $\mathbf{x}_t$  is the same as the **output** embedding **x**<sub>t</sub>', Transformers usually choose the embedding sizes and number of heads appropriately:
  - $d_{model} = dim. of inputs = 4$
  - d<sub>k</sub> = dim. of each output
  - h = # of heads = 2
  - Choose  $d_k = d_{model} / h = 4/2 = 2 x_1'$
- Then concatenate the outputs

Wa

 $W_k$ 

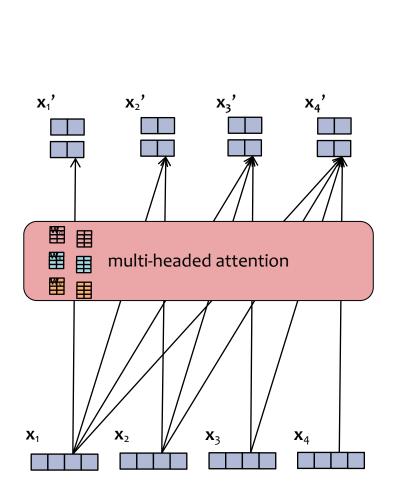
 $W_{v}$ 

## Multi-headed Attention

**x**<sub>2</sub>' x<sub>3</sub>' X₄' multi-headed attention  $\mathbf{X}_4$  $\mathbf{X}_1$  $\mathbf{X}_{2}$ X3

- Just as we can have multiple channels in a convolution layer, we can use **multiple heads** in an **attention** layer
- Each head gets its own parameters
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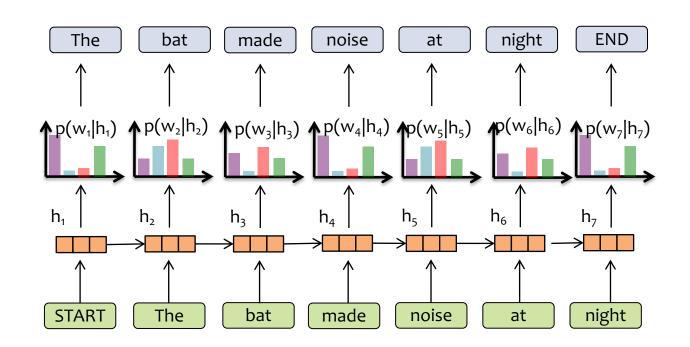
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Self-

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## **RNN Language Model**



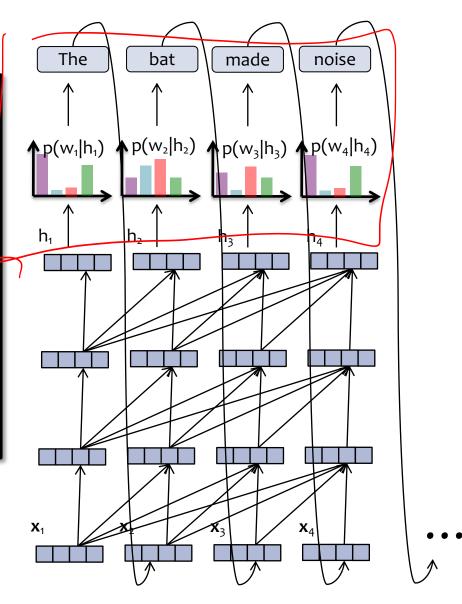
#### Key Idea:

(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  $\mathbf{h}_t = f_{\theta}(w_{t-1}, ..., w_1)$  Recaller

## Transformer Language Model

#### Important!

- RNN computation graph grows
   linearly with the number of input tokens
- Transformer-LM computation graph grows quadratically with the number of input tokens



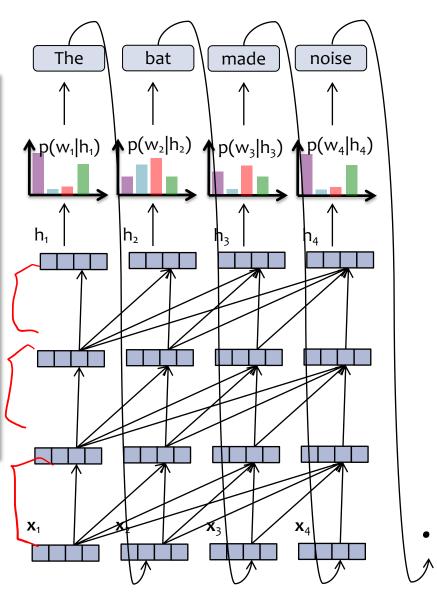
Each hidden vector looks back at the hidden vectors of the **current and previous timesteps in the previous layer.** 

The language model part is just like an RNN-LM!

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**Each layer** of a Transformer LM consists of several **sublayers**:

- 1. attention 4
- 2. feed-forward neural network
- 3. layer normalization
- 4. residual connections

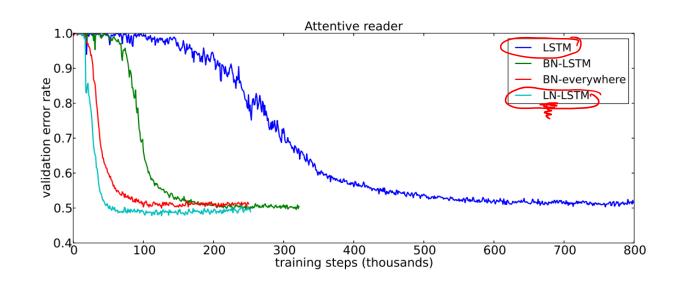
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## Layer Normalization

- The Problem: internal covariate shift occurs during training of a deep network when a small change in the low layers amplifies into a large change in the high layers
- One Solution: Layer normalization normalizes each layer and learns elementwise gain/bias
- Such normalization allows for higher learning rates (for faster convergence) without issues of diverging gradients

Given input  $\mathbf{a} \in \mathbb{R}^{K}$ , LayerNorm computes output  $\mathbf{b} \in \mathbb{R}^{K}$ :  $\mathbf{b} = \left( \boldsymbol{\gamma} \odot \left( \begin{array}{c} \mathbf{a} - \mu \\ \sigma \end{array} \right) \oplus \boldsymbol{\beta} \right)$ where we have mean  $\mu = \frac{1}{K} \sum_{k=1}^{K} a_{k}$ , standard deviation  $\sigma = \sqrt{\frac{1}{K} \sum_{k=1}^{K} (a_{k} - \mu)^{2}}$ , and parameters  $\boldsymbol{\gamma} \in \mathbb{R}^{K}$ ,  $\boldsymbol{\beta} \in \mathbb{R}^{K}$ .  $\odot$  and  $\oplus$  denote elementwise multiplication and addition.

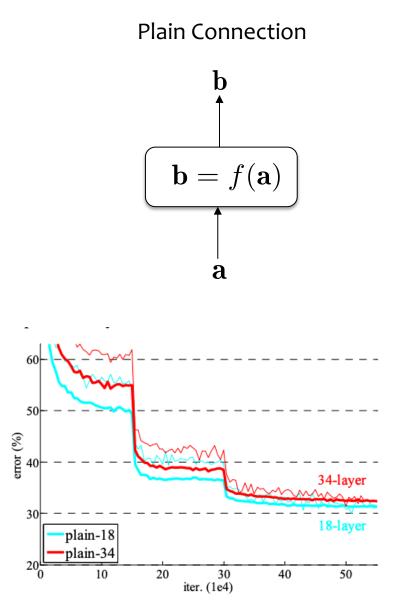


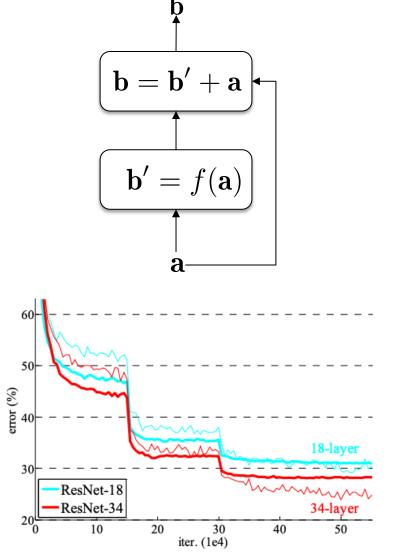
### **Residual Connections**

**Residual Connection** 

- The Problem: as network depth grows very large, a performance degradation occurs that is not explained by overfitting (i.e. train / test error both worsen)
- One Solution: Residual connections pass a copy of the input alongside another function so that information can flow more directly
- These residual connections allow for effective training of very deep networks that perform better than their shallower (though still deep) counterparts

Figure from https://arxiv.org/pdf/1512.03385.pdf

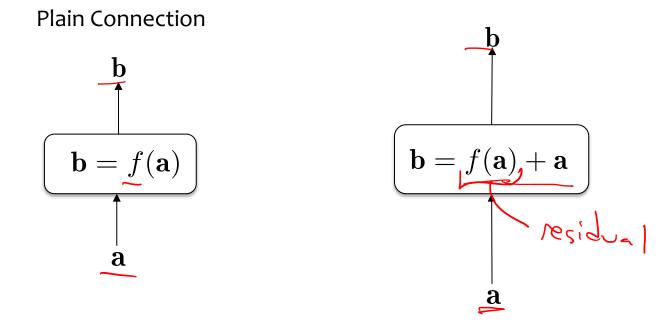




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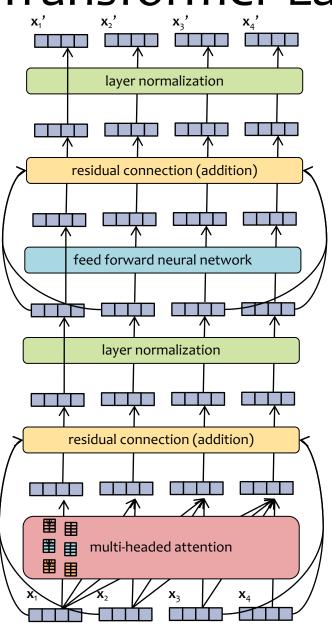
#### Why are residual connections helpful?

Instead of f(a) having to learn a full transformation of a, f(a) only needs to learn an additive modification of a (i.e. the residual).

### **Transformer Layer**

#### Post-LN Version: This is the version of the Transformer Layer that was introduced in the original paper in 2017.

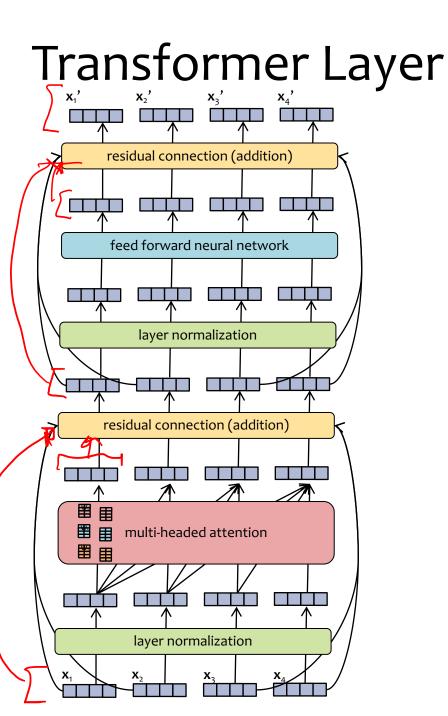
#### The LayerNorm modules occur at the end of each set of 3 layers.



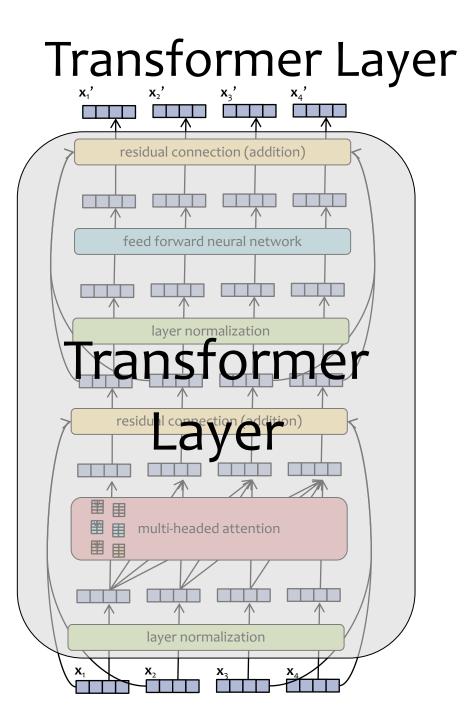
- 1. attention
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#### **Pre-LN Version:**

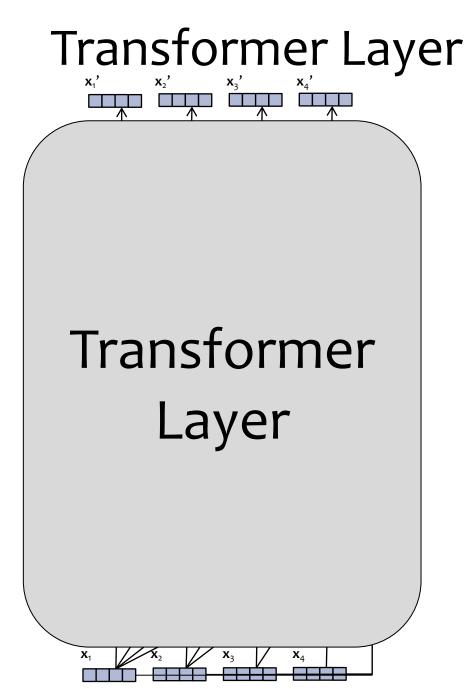
However, subsequent work found that reordering such that the LayerNorm's came at the beginning of each set of 3 layers, the multi-headed attention and feedforward NN layers tend to be better behaved (i.e. tricks like warm-up are less important).



- 1. attention
- 2. feed-forward neural network
- 3. layer normalization
- 4. residual connections



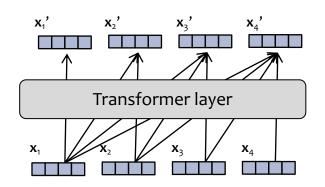
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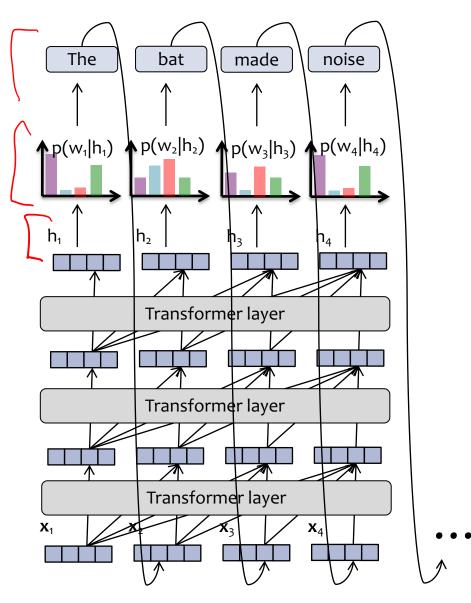
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## Transformer Language Model



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- 1. attention
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Each hidden vector looks back at the hidden vectors of the **current and previous timesteps in the previous layer.** 

The language model part is just like an RNN-LM.

### LEARNING A TRANSFORMER LM

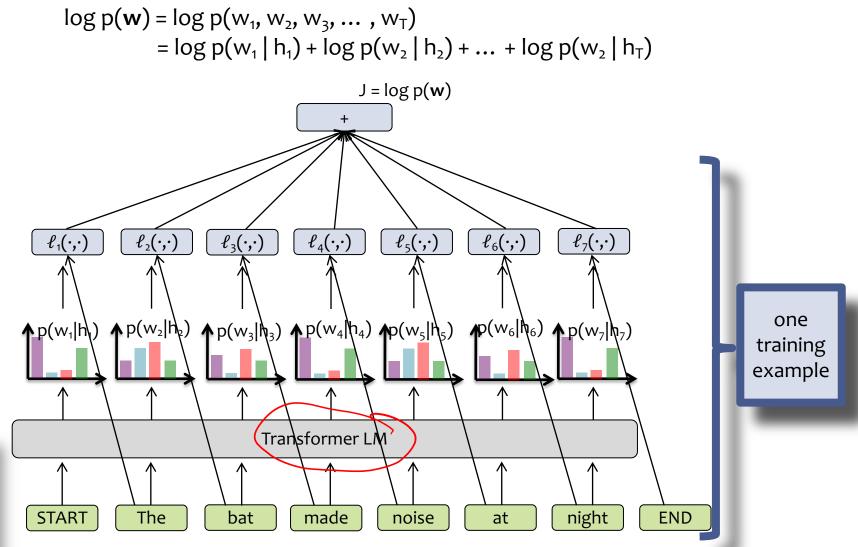
## Learning a Transformer LM

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- The objective function for a Deep LM (e.g. RNN-LM or Tranformer-LM) is typically the loglikelihood of the training examples:

 $J(\boldsymbol{\theta}) = \Sigma_i \log p_{\boldsymbol{\theta}}(\mathbf{w}^{(i)})$ 

• We train by mini-batch SGD (or your favorite flavor of mini-batch SGD)

Training a Transformer-LM is the same, except we swap in a different deep language model.



## GPT-3

- GPT stands for Generative Pre-trained Transformer
- GPT is just a Transformer LM, but with a huge number of parameters

Model # layers dimension dimension # attention # params							
Model		of states	of inner states	heads			
GPT (2018)	12	768	3072	12 (	117M		
GPT-2 (2019)	48	1600			1542M		
GPT-3 (2020)	96	12288	4*12288	96	175000M		