Machine Learning Department
School of Computer Science
Carnegie Mellon University

RNN LMs

+

Transformer LMs

Matt Gormley, Henry Chai
Lecture 18
Mar. 19, 2025

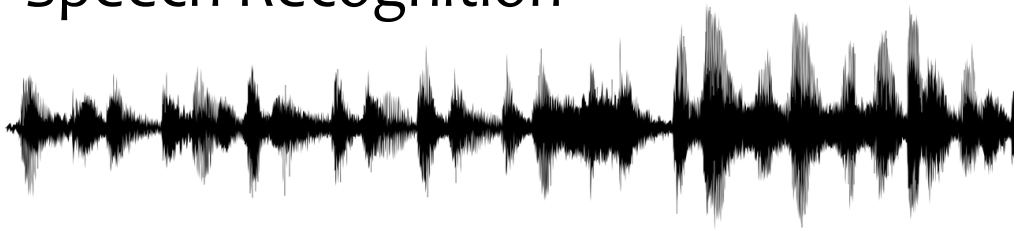
Reminders

- Homework 6: Learning Theory & Generative Models
  - Out: Sun, Mar-16
  - Due: Sat, Mar-22, 11:59pm
  - (only two grace/late days permitted)
- Exam 2: Wed, Mar-26, 7:00 pm – 9:00 pm

BACKGROUND:
N-GRAM LANGUAGE MODELS

Human Language Technologies

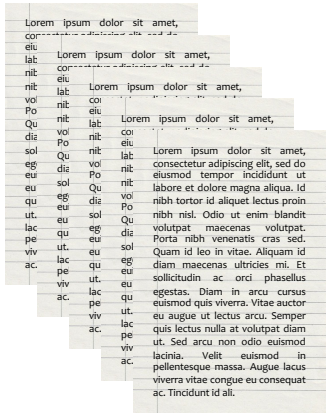
Speech Recognition



Machine Translation

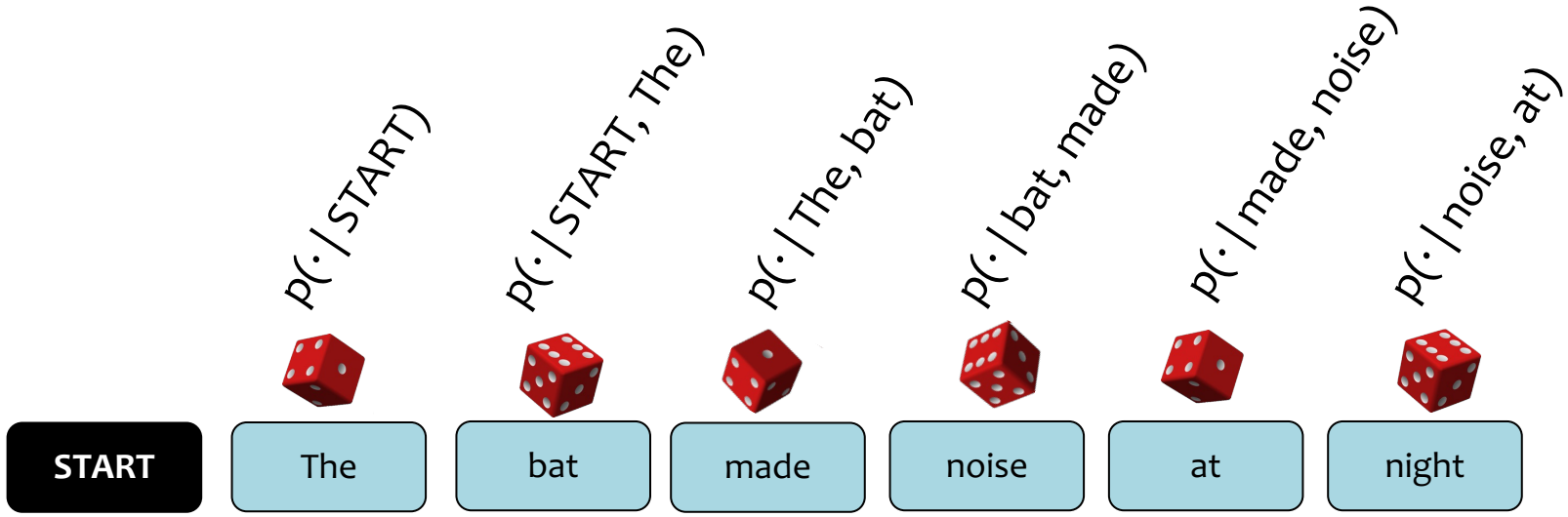
기계 번역은 특히 영어와 한국어와 같은 언어 쌍의 경우 매우 어렵습니다.

Summarization



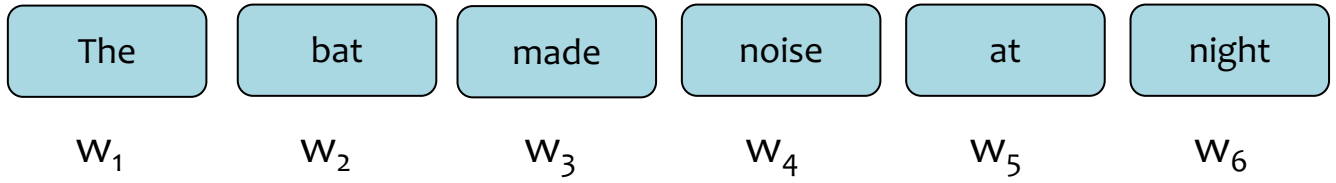
n-Gram Language Model

- *Goal*: Generate realistic looking sentences in a human language
- *Key Idea*: condition on the last n-1 words to sample the n^{th} word



n-Gram Language Model

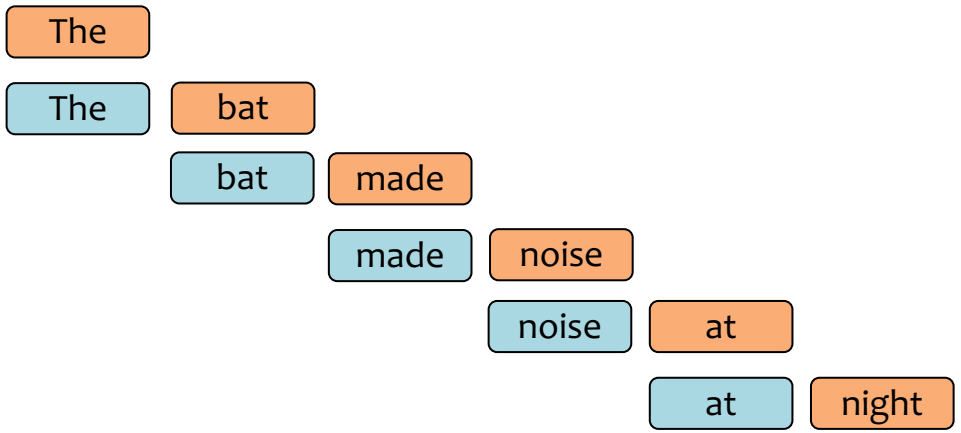
Question: How can we **define** a probability distribution over a sequence of length T?



n-Gram Model (n=2)

$$p(w_1, w_2, \ldots, w_T) = \prod_{t=1}^{T} p(w_t \mid w_{t-1})$$

$p(w_1, w_2, w_3, \ldots, w_6) =$



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

n-Gram Language Model

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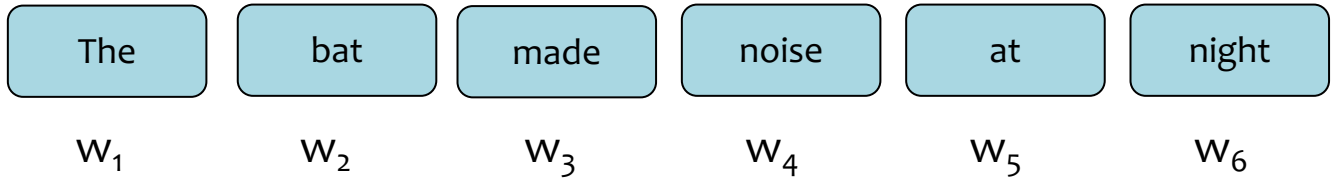

n-Gram Model (n=3) $$p(w_1, w_2, \ldots, w_T) = \prod_{t=1}^{T} p(w_t \mid w_{t-1}, w_{t-2})$$

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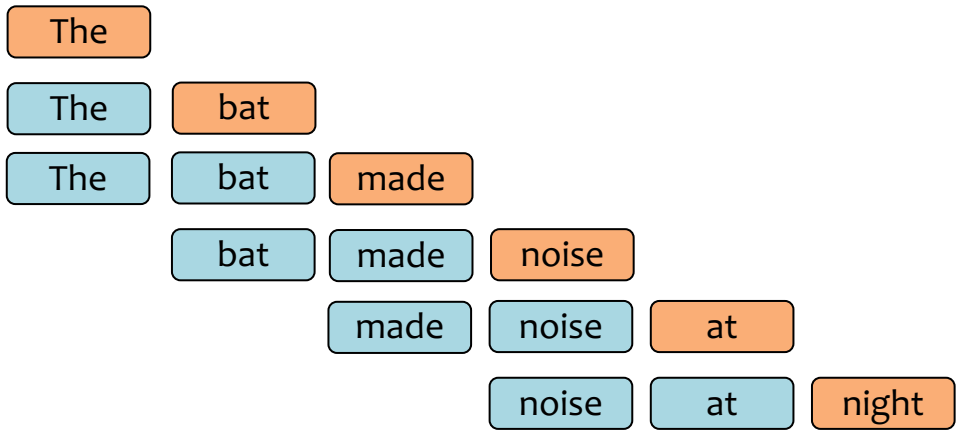

$p(w_1)$
$p(w_2 \mid w_1)$
$p(w_3 \mid w_2, w_1)$
$p(w_4 \mid w_3, w_2)$
$p(w_5 \mid w_4, w_3)$
$p(w_6 \mid w_5, w_4)$

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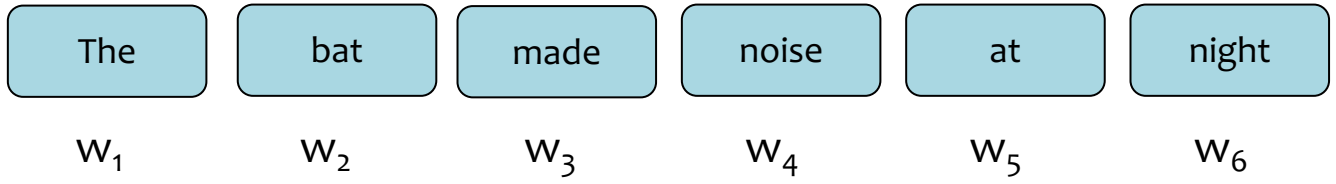


n-Gram Model (n=3) $$p(w_1, w_2, \ldots, w_T) = \prod_{t=1}^{T} p(w_t \mid w_{t-1}, w_{t-2})$$

$p(w_1, w_2, w_3, \ldots, w_6) =$

$p(w_1)$

The

The

The

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?

$p(w_t \mid w_{t-2} = \text{The}, w_{t-1} = \text{bat})$

w_t	$p(\cdot \mid \cdot, \cdot)$
ate	0.015
…	
flies	0.046
…	
zebra	0.000

$p(w_t \mid w_{t-2} = \text{made}, w_{t-1} = \text{noise})$

w_t	$p(\cdot \mid \cdot, \cdot)$
at	0.020
…	
pollution	0.030
…	
zebra	0.000

$p(w_t \mid w_{t-2} = \text{cows}, w_{t-1} = \text{eat})$

w_t	$p(\cdot \mid \cdot, \cdot)$
corn	0.420
…	
grass	0.510
…	
zebra	0.000

Learning an n-Gram Model

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

Answer: 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…
…**cows eat corn** when there is no…
…which **cows eat which** foods depends…
…if **cows eat grass**…
…when **cows eat corn** their stomachs…
…should we let **cows eat corn**?...

$p(w_t \mid w_{t-2} = \text{cows}, w_{t-1} = \text{eat})$

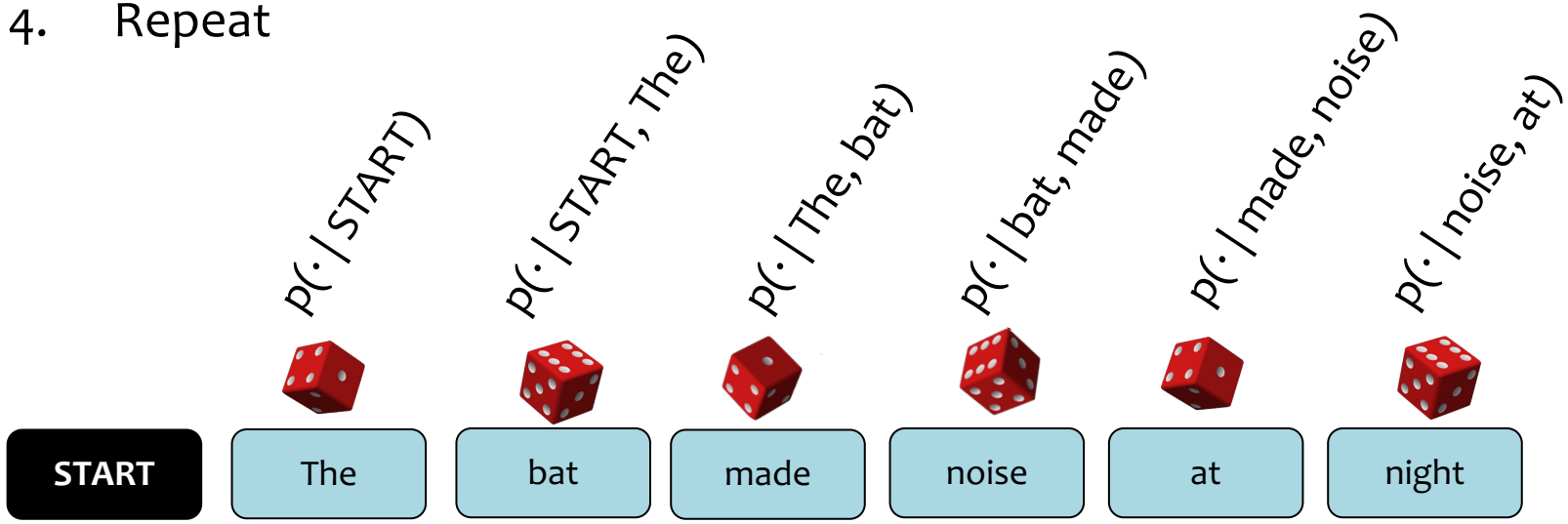
w_t	$p(\cdot \mid \cdot, \cdot)$
corn	4/11
grass	3/11
hay	2/11
if	1/11
which	1/11

Sampling from a Language Model

Question: How do we sample from a Language Model?

Answer:

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



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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,--O
Yead linens, sheep's Ancient,
Agreed: Petrarch plaguy Resolved
pear! observingly honourest
adulteries wherever scabbard
guess; affirmation--his 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

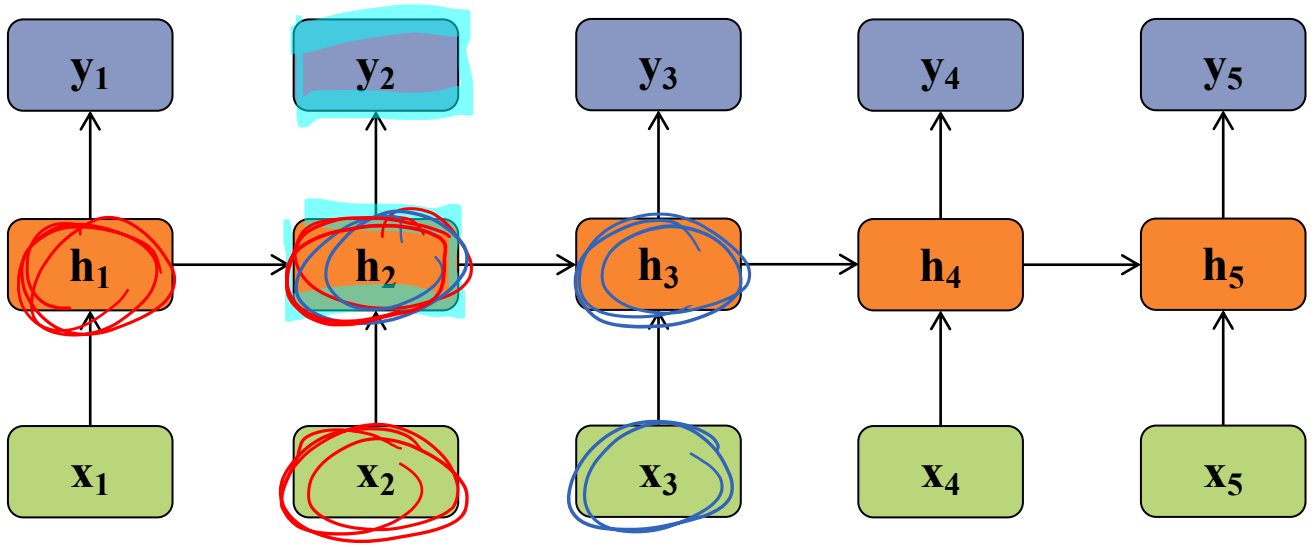
Recurrent Neural Networks (RNNs)

$$\text{inputs: } \mathbf{x} = (x_1, x_2, \ldots, x_T), x_i \in \mathcal{R}^I$$
$$\text{hidden units: } \mathbf{h} = (h_1, h_2, \ldots, h_T), h_i \in \mathcal{R}^J$$
$$\text{outputs: } \mathbf{y} = (y_1, y_2, \ldots, y_T), y_i \in \mathcal{R}^K$$
$$\text{nonlinearity: } \mathcal{H}$$

Definition of the RNN:

$$h_t = \mathcal{H}\left(W_{xh}x_t + W_{hh}h_{t-1} + b_h\right)$$
$$y_t = W_{hy}h_t + b_y$$

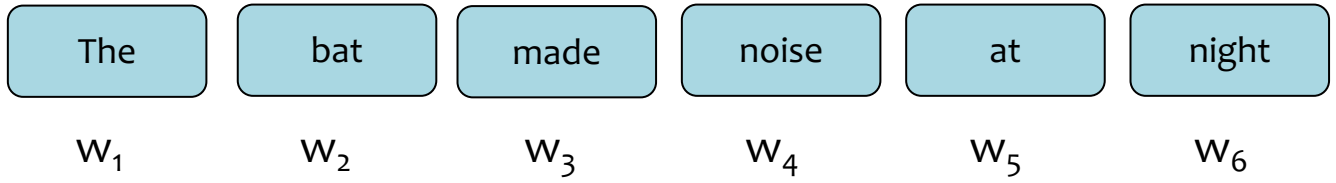
$K \times 1$ $K \times J$ $J \times 1$ $K \times 1$



The Chain Rule of Probability

Recall…

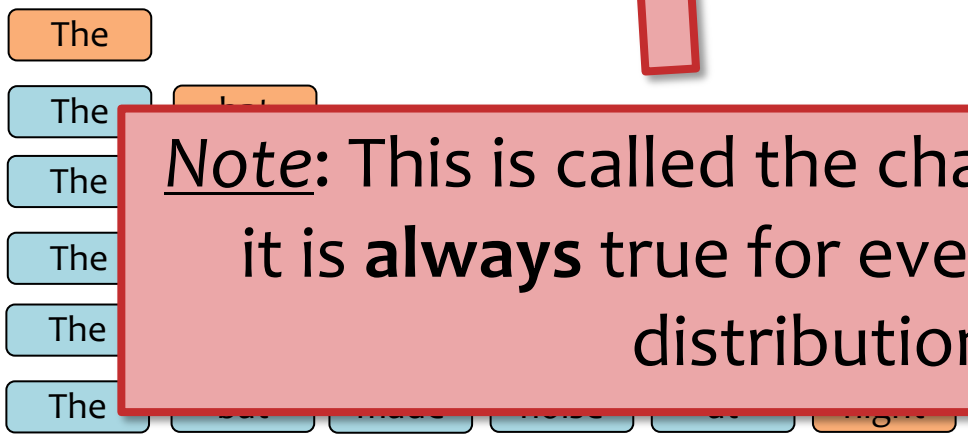
Question: How can we **define** a probability distribution over a sequence of length T?



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

$p(w_1, w_2, w_3, \ldots, w_6) =$

$p(w_1)$



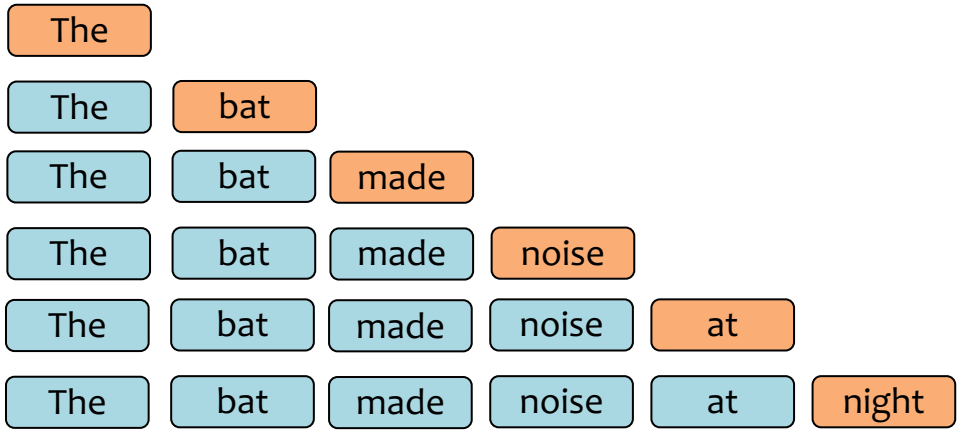
$p(w_6 \mid w_5, w_4, w_3, w_2, w_1)$

Note: This is called the chain **rule** because it is **always** true for every probability distribution

RNN Language Model

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

$p(w_1, w_2, w_3, \ldots, w_6) =$



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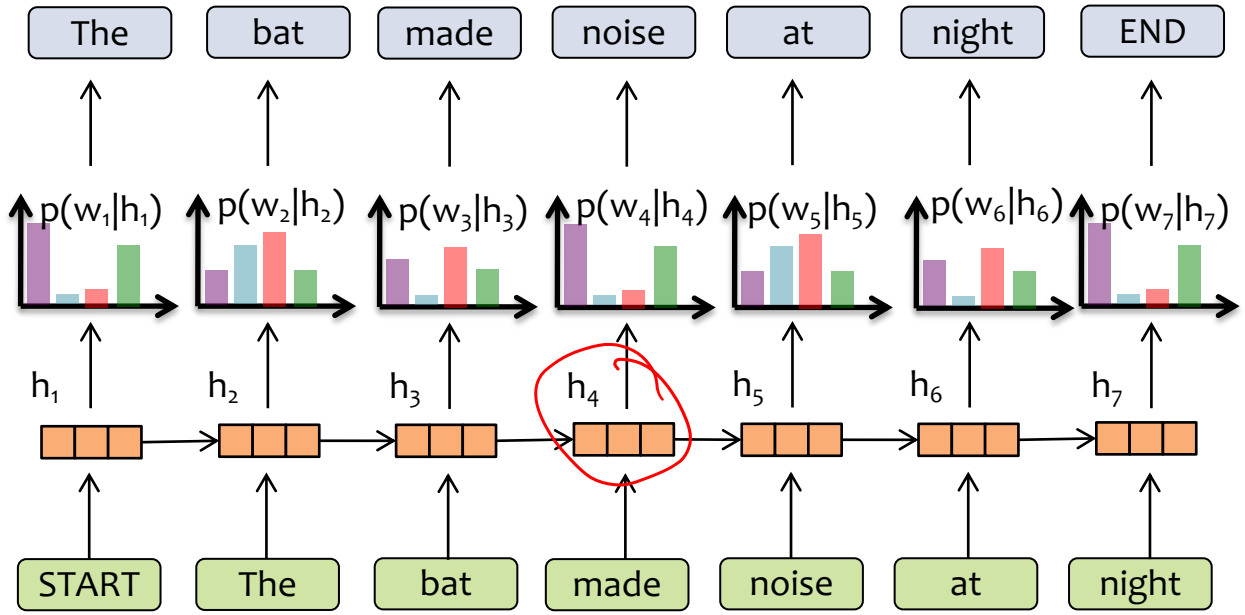
$p(w_2 \mid f_\theta(w_1))$
$p(w_3 \mid f_\theta(w_2, w_1))$
$p(w_4 \mid f_\theta(w_3, w_2, w_1))$
$p(w_5 \mid f_\theta(w_4, w_3, w_2, w_1))$
$p(w_6 \mid f_\theta(w_5, w_4, w_3, w_2, w_1))$

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

RNN Language Model



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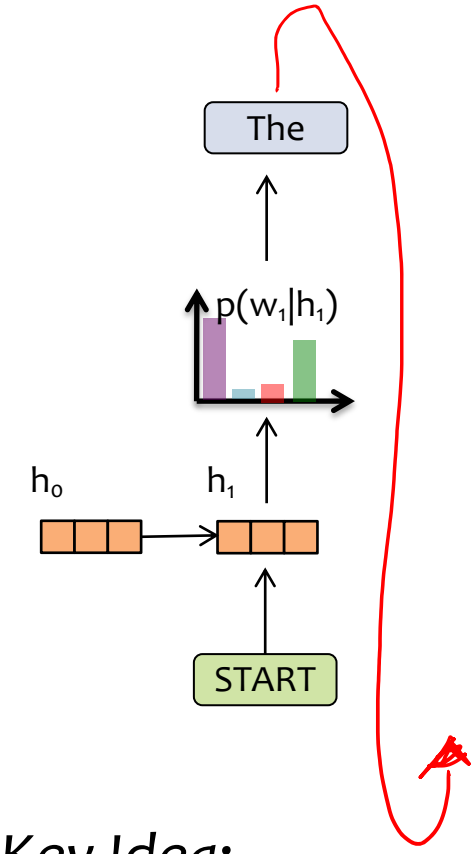

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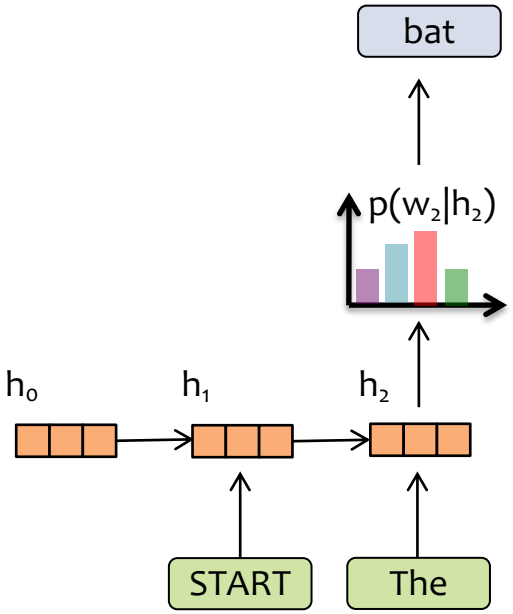

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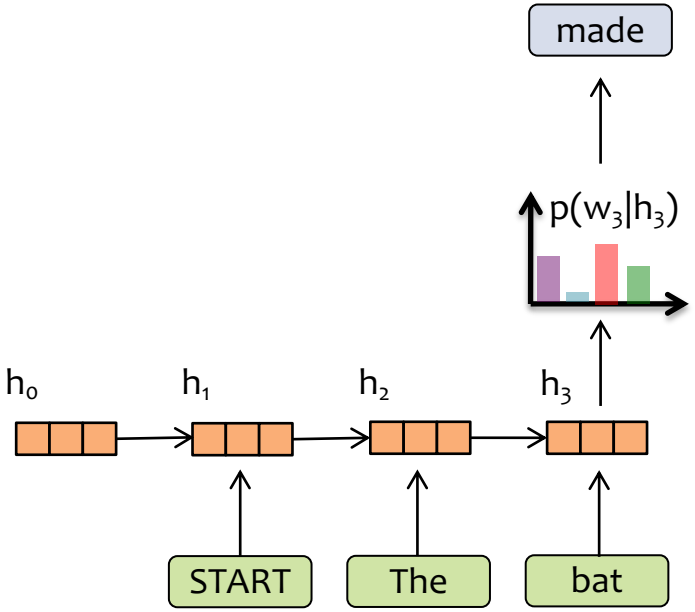

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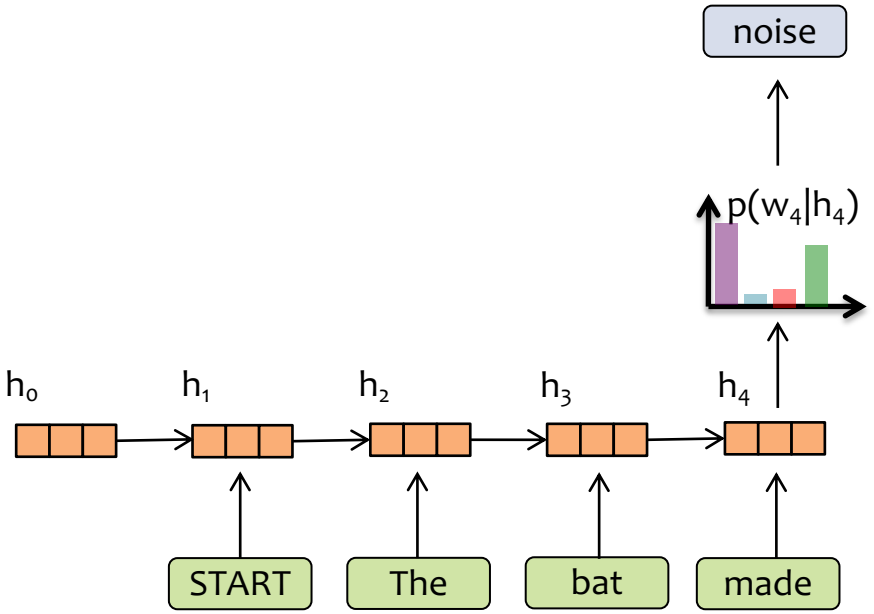

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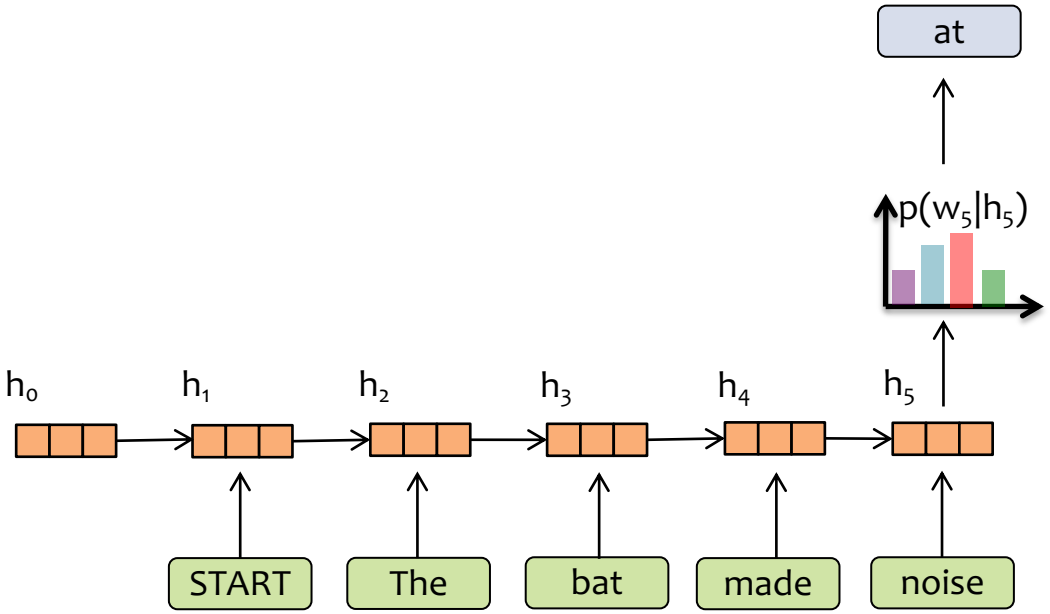

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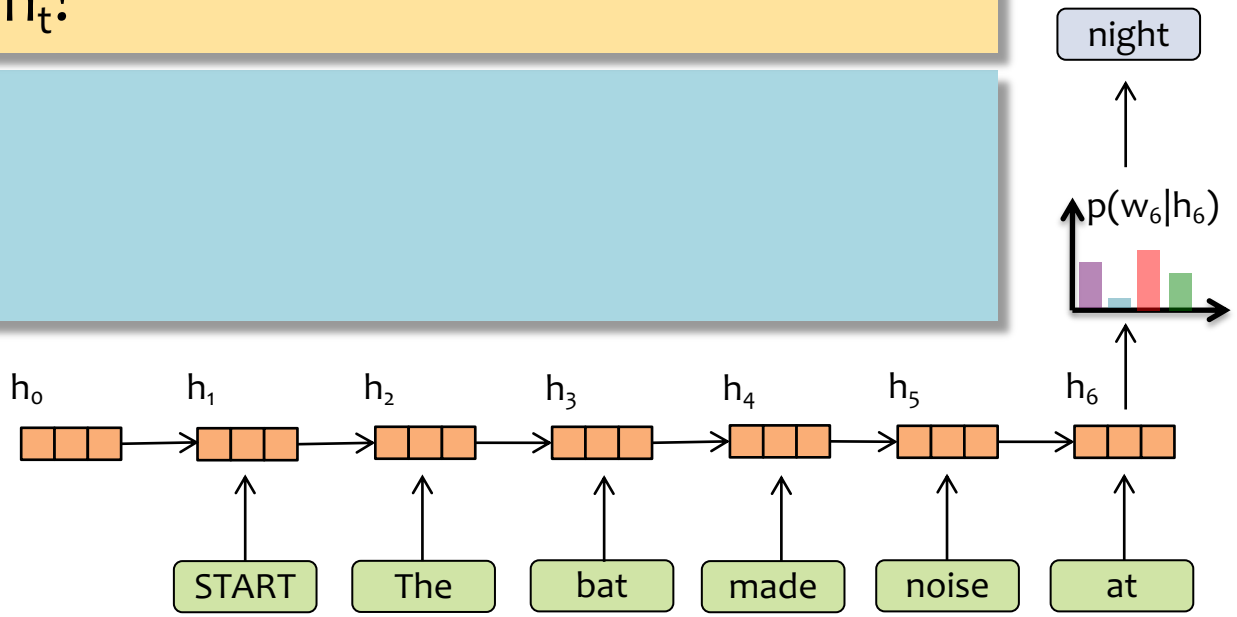
RNN Language Model

Poll 1

Question: How can we create a distribution $p(w_t|h_t)$ from h_t?

Answer:



V = # words in vocab = 50k

$J = |h_t| = 1024$

$p(w_t|h_t) = \text{softmax}(y_t)$

$y_t = W_{hy} h_t + b_y$

$W_{hy} \in \mathbb{R}^{V \times J}$ $\mathbb{R}^{50k \times 1024}$

$b_y \in \mathbb{R}^{V}$ $\mathbb{R}^{50k}$

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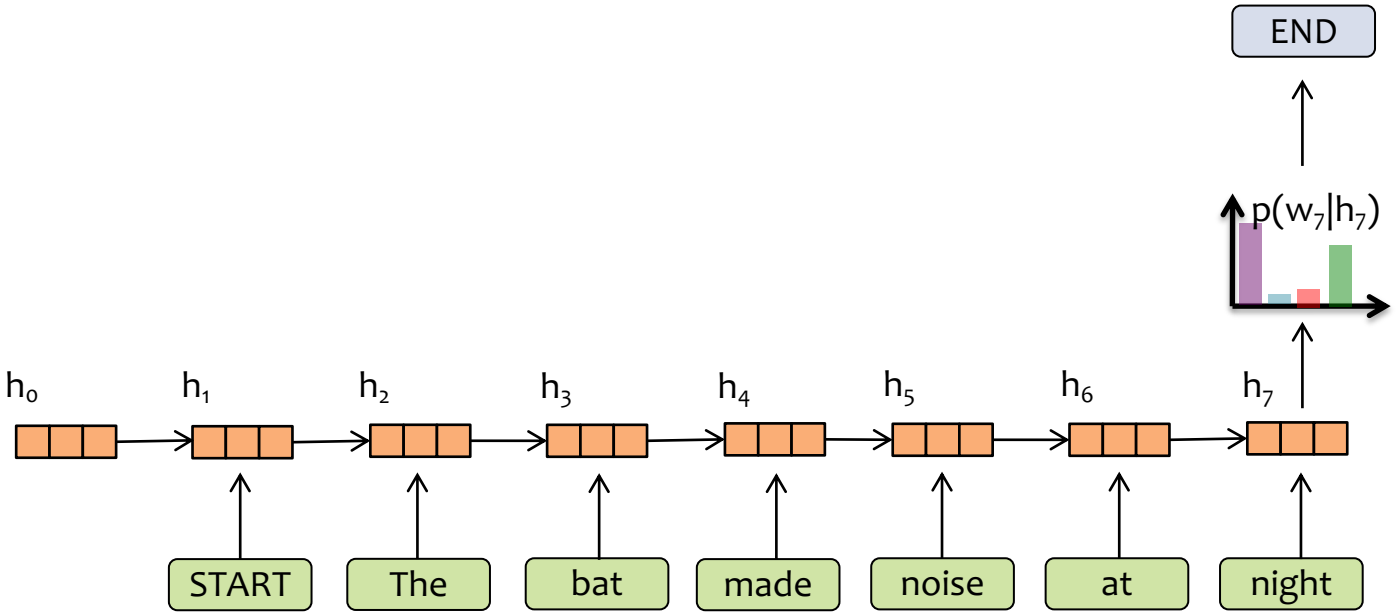

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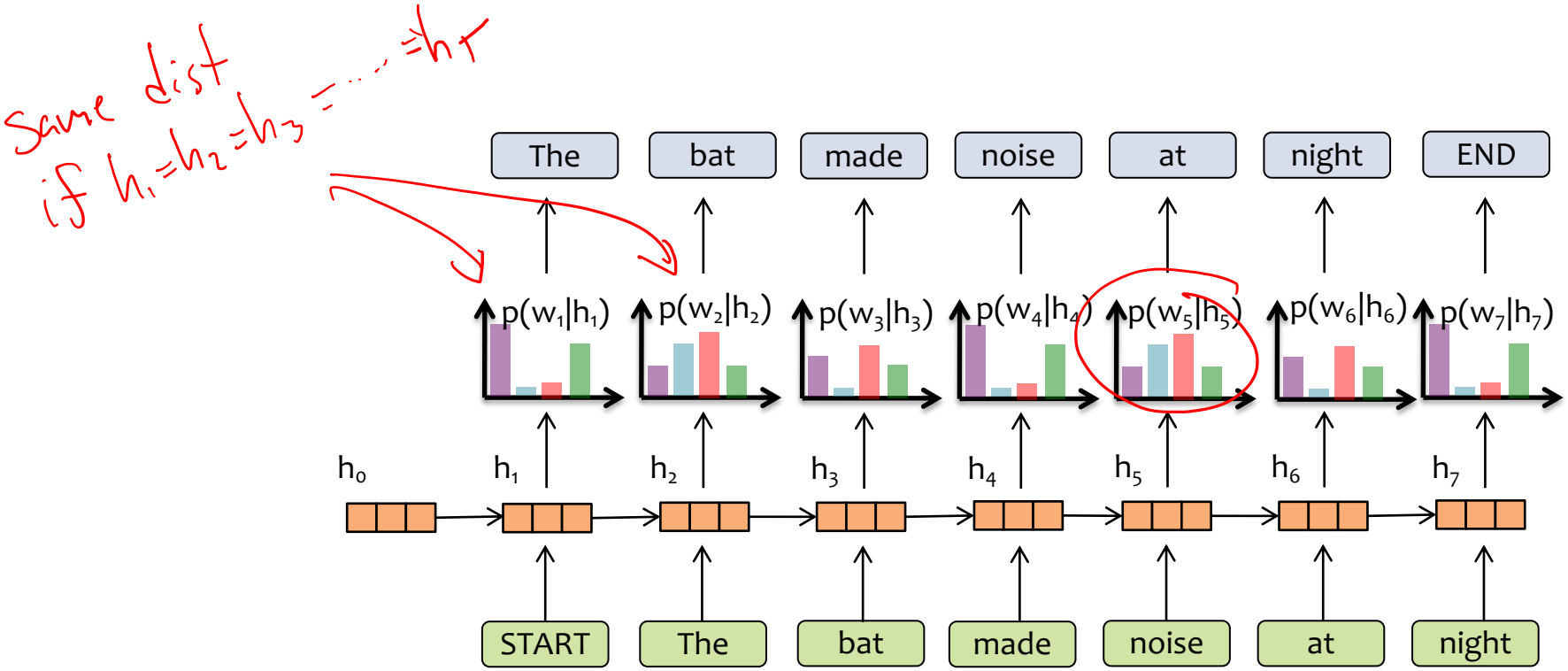

$$p(w_1, w_2, w_3, \dots, w_T) = p(w_1 \mid h_1)\, p(w_2 \mid h_2) \dots p(w_T \mid h_T)$$

Sampling from a Language Model

Question: How do we sample from a Language Model?

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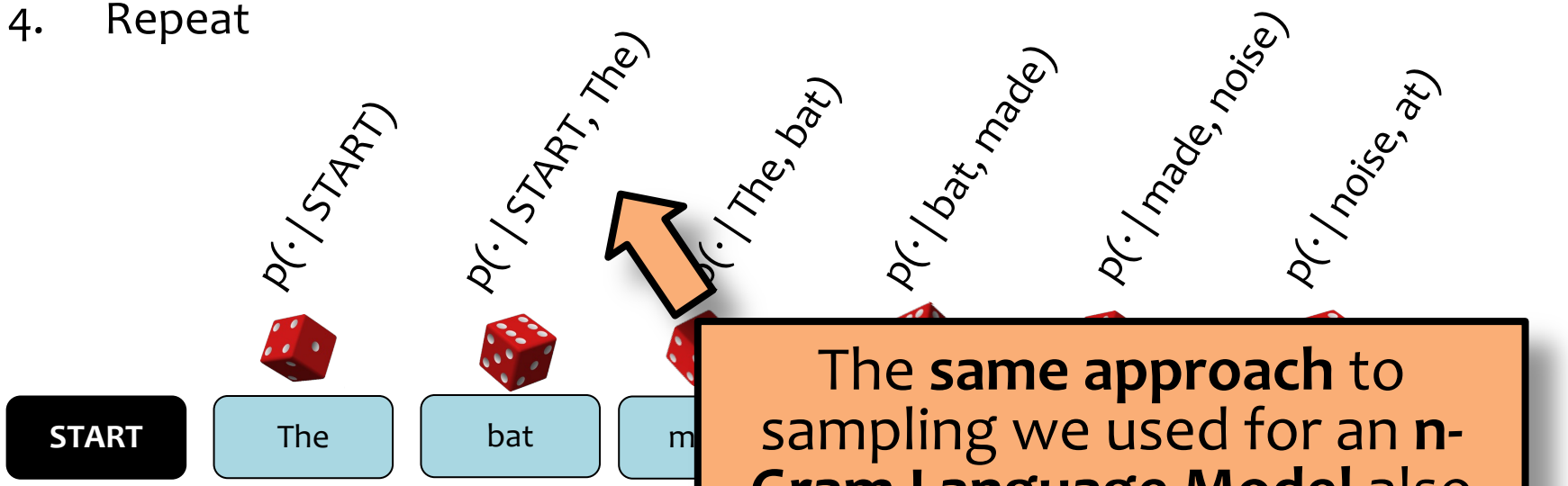

The **same approach** to sampling we used for an **n-Gram Language Model** also works here for an **RNN Language Model**

Sampling from an RNN-LM

??

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 m… there My power to give thee but so much … service in the noble bondman here, Would… her wine.

KING LEAR: O, if you were a feeble sight, 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.

??

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 some broken limb shall acquit him well. Your brother is …ender; and, for your love, I would be …, as I must, for my own honour, if he …ore, out of my love to you, I came hither …withal, that either you might stay him from his intend… brook such disgrace well as he shall run into, in tha… is a thing of his own search and altogether against my will.

TOUCHSTONE: For my part, I had rather bear with you than bear you; yet I should bear no cross if I did bear you, for I think you have no money in your purse.

Which is the real Shakespeare?!

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

Sampling from an RNN-LM

Shakespeare's As You Like It

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 master's ready there My power to give thee but so much as hell: Some service in the noble bondman here, Would show him to her wine.

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RNN-LM Sample

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??

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 m… there My power to give thee but so much … service in the noble bondman here, Would… her wine.

KING LEAR: O, if you were a feeble sight, 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.

??

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 some broken limb shall acquit him well. Your brother is …ender; and, for your love, I would be …, as I must, for my own honour, if he …ore, out of my love to you, I came hither …withal, that either you might stay him from his intend… brook such disgrace well as he shall run into, in tha… is a thing of his own search and altogether against my will.

TOUCHSTONE: For my part, I had rather bear with you than bear you; yet I should bear no cross if I did bear you, for I think you have no money in your purse.

Which is the real Shakespeare?!

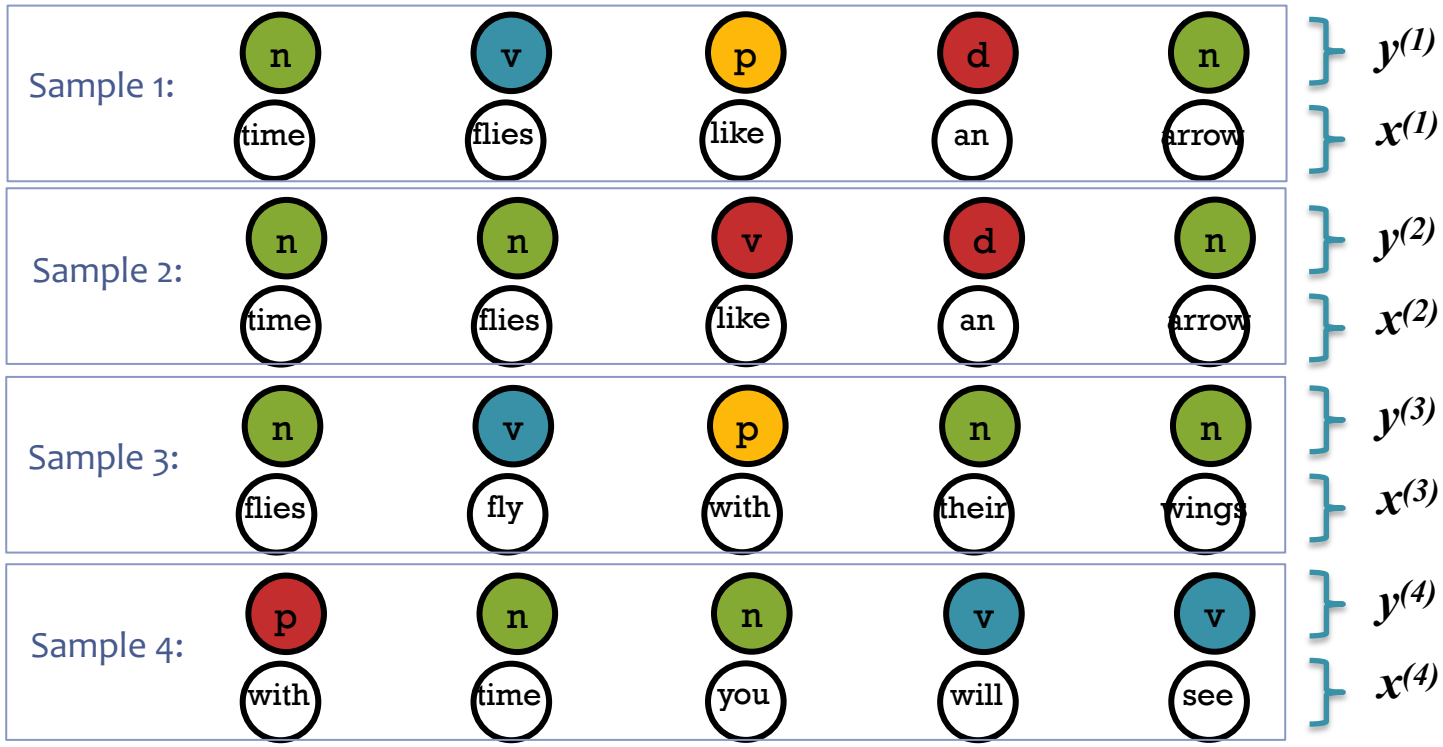
Example from http://karpathy.github.io/2015/05/21/rnn-effectiveness/

LEARNING AN RNN

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

Recall…

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



SGD and Mini-batch SGD

Recall…

Algorithm 1 SGD

Initialize $\theta^{(0)}$

$s = 0$

for $t = 1, 2, \ldots, T$ **do**

  for $i \in$ shuffle$(1, \ldots, N)$ **do**

    Select the next training point (x_i, y_i)

    Compute the gradient $g^{(s)} = \nabla J_i(\theta^{(s-1)})$

    Update parameters $\theta^{(s)} = \theta^{(s-1)} - \eta g^{(s)}$

    Increment time step $s = s + 1$

  Evaluate average training loss $J(\theta) = \frac{1}{n} \sum_{i=1}^{n} J_i(\theta)$

return $\theta^{(s)}$

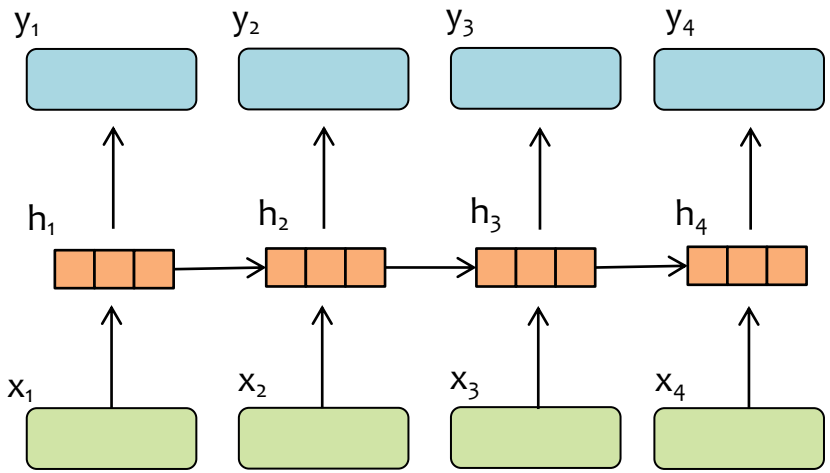
SGD and Mini-batch SGD

Recall…

Algorithm 1 Mini-Batch SGD

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

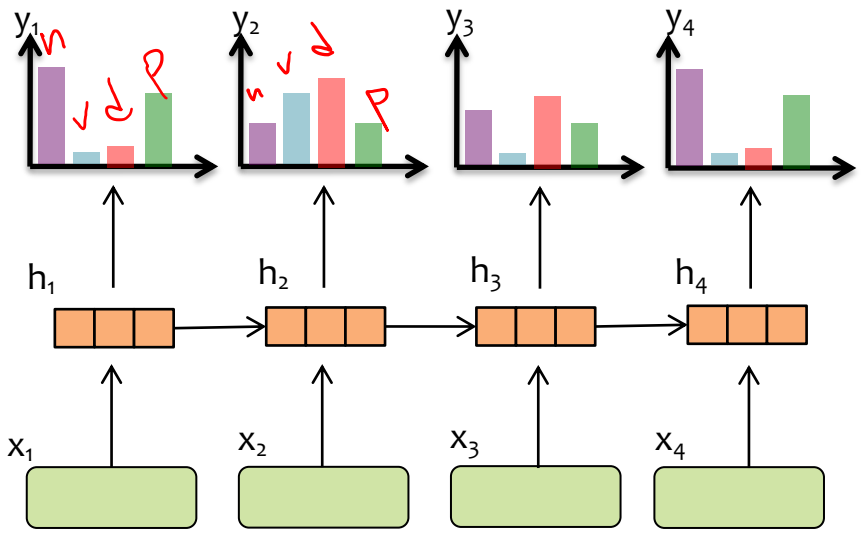
RNN



Algorithm 1 Elman RNN

procedure FORWARD($x_{1:T}, W_{ah}, W_{ax}, b_a, W_{yh}, b_y$)
  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:
      $a_t = W_{ah} \cdot h_{t-1} + W_{ax} \cdot x_t + b_a$
      $h_t = \sigma(a_t)$
    Compute the output at time step t:
      $y_t = W_{yh} \cdot h_t + b_y$

RNN



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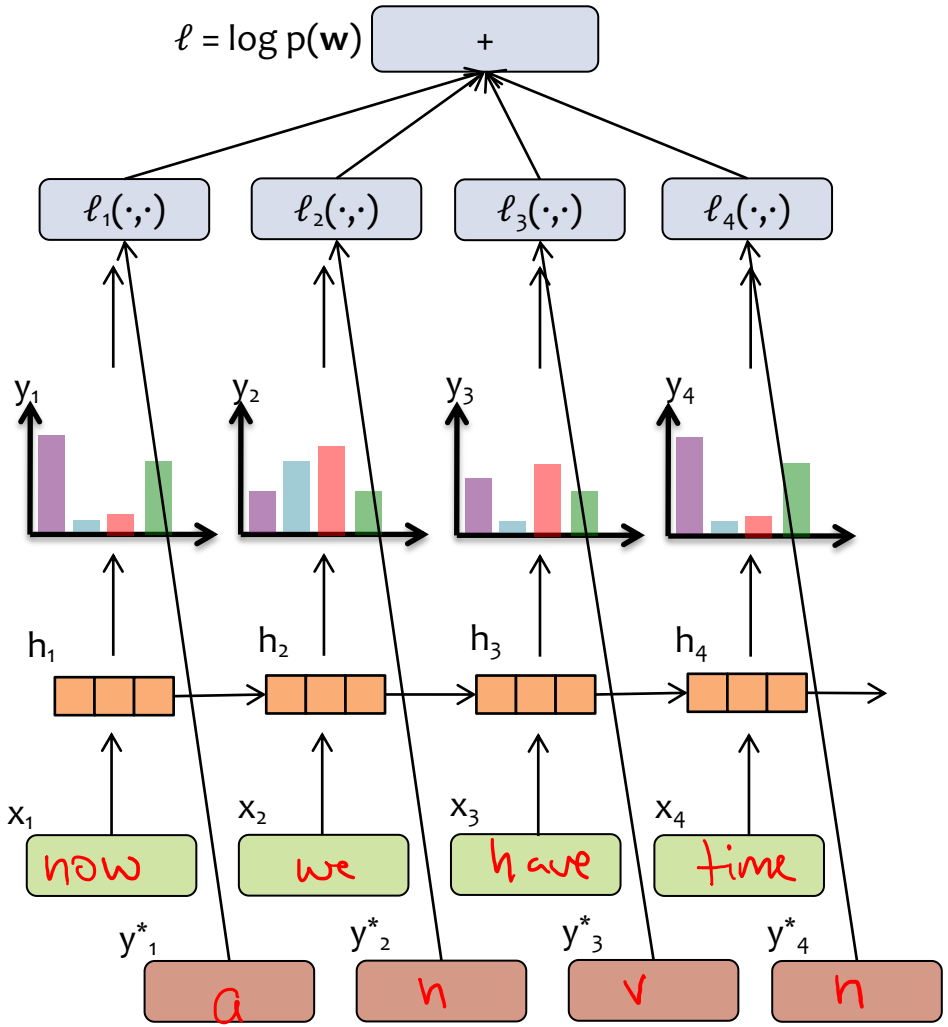
RNN + Loss



Algorithm 1 Elman RNN + Loss

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** $T=4$

    Receive input data at time step t: x_t

    Compute the hidden state update:

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

    $h_t = \sigma(a_t)$

    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:

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

  Compute the total loss:

  $\ell = \sum_{t=1}^{T} \ell_t$ $= -\log p(y_1^*, \cdots, y_t^* | \_)$

LEARNING AN RNN-LM

Learning a Language Model

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

Answer: 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…
…**cows eat corn** when there is no…
…which **cows eat which** foods depends…
…if **cows eat grass**…
…when **cows eat corn** their stomachs…
…should we let **cows eat corn**?...

$p(w_t \mid w_{t-2} = \text{cows}, w_{t-1} = \text{eat})$

w_t	$p(\cdot \mid \cdot, \cdot)$
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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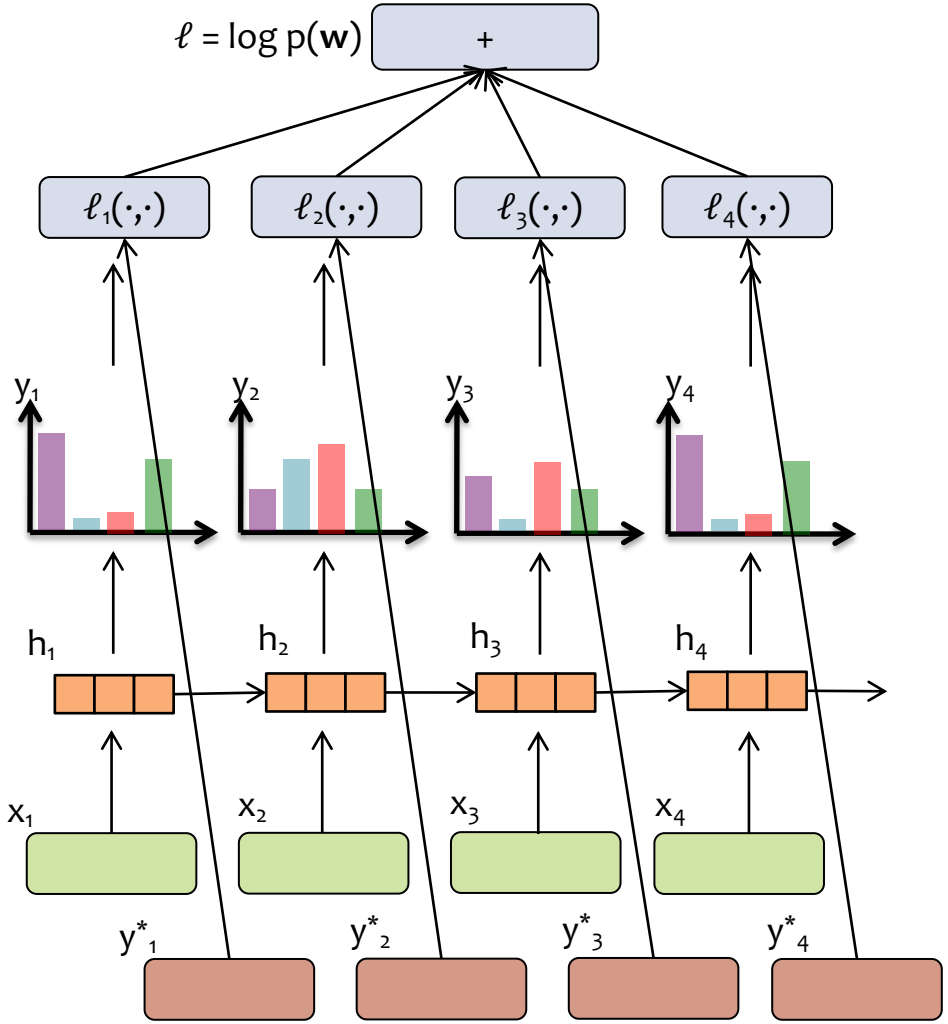
- We can derive it in the usual way:
  - **Write the likelihood** of the sentences under the n-gram LM
  - **Set the gradient to zero** and impose the constraint that the probabilities sum-to-one
  - **Solve** for the MLE

RNN + Loss

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



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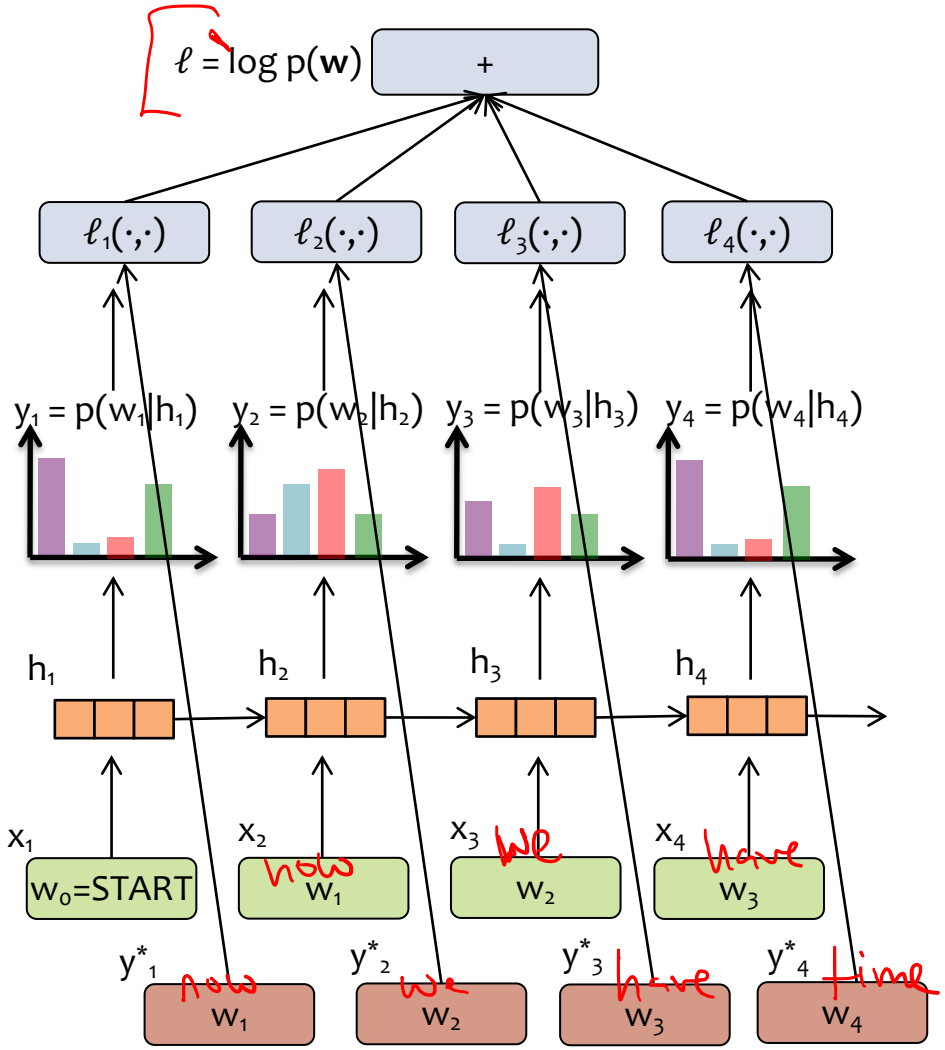
      $\ell_t = -\sum_{k=1}^{K} (y_t^*)_k \log((y_t)_k)$
  Compute the total loss:
    $\ell = \sum_{t=1}^{T} \ell_t$

RNN-LM + Loss

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

$\log p(\mathbf{w}) = \log p(w_1, w_2, w_3, \ldots, w_T)$
$= \log p(w_1 \mid h_1) + \ldots + \log p(w_T \mid h_T)$



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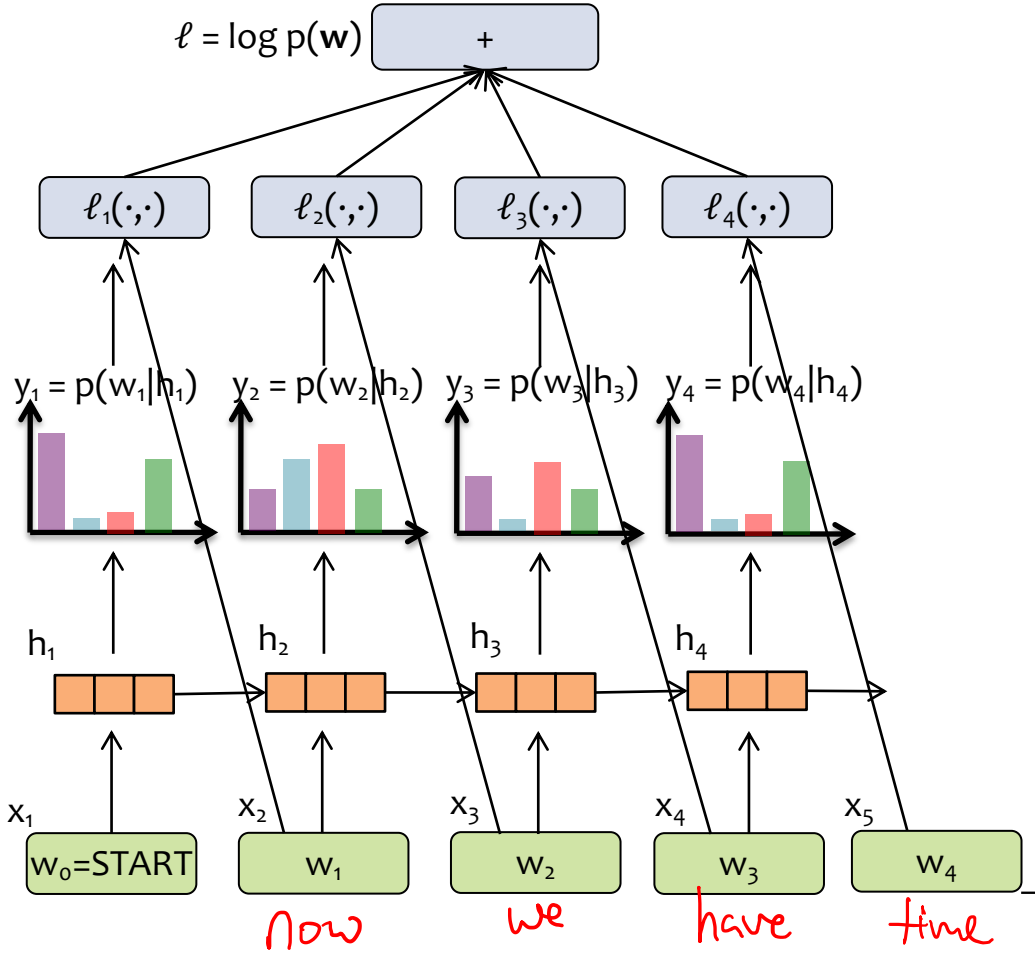

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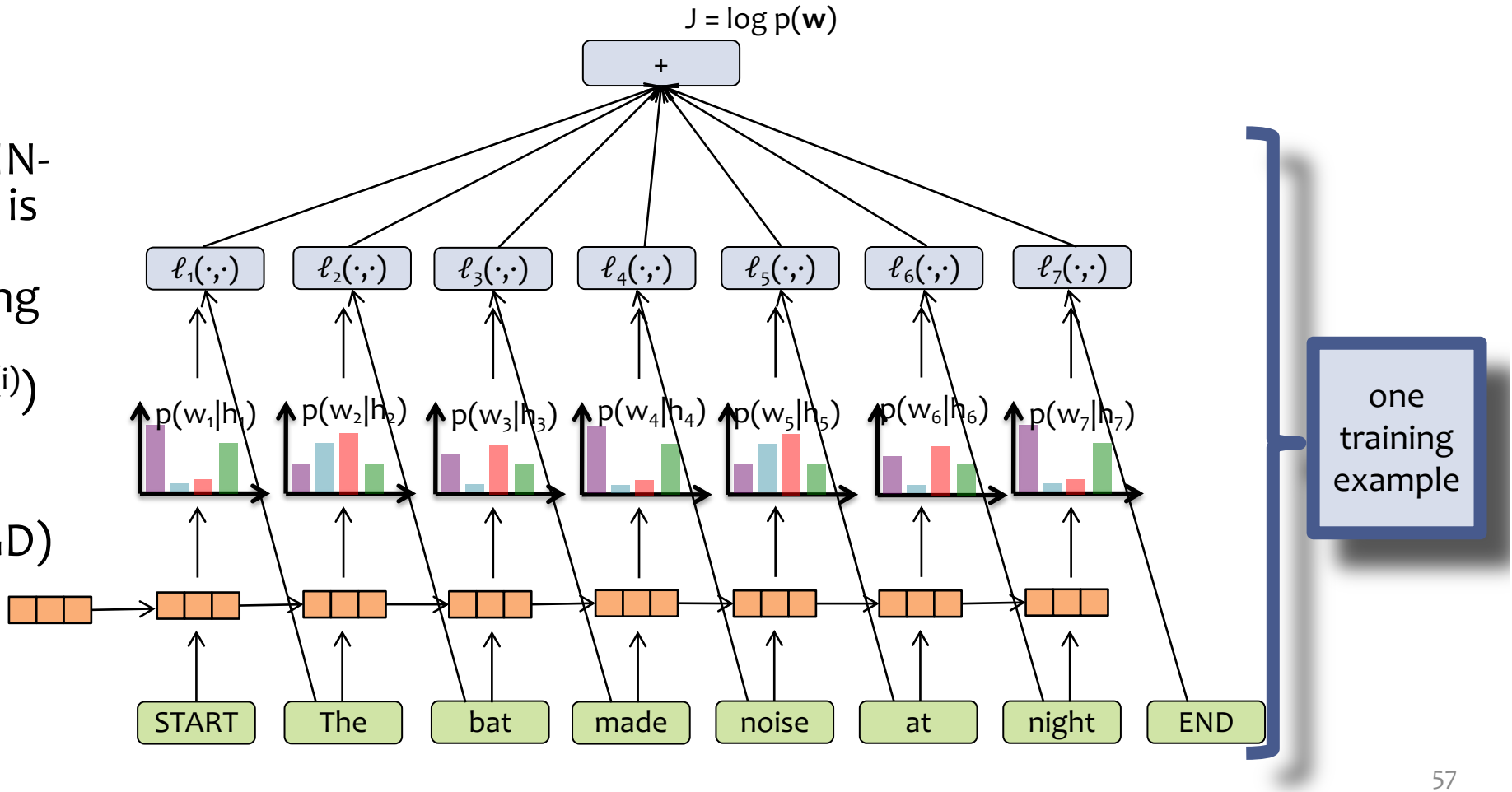
Learning an RNN-LM

- Each training example is a sequence (e.g. sentence), so we have training data D = $\{\mathbf{w}^{(1)}, \mathbf{w}^{(2)}, \ldots, \mathbf{w}^{(N)}\}$
- The objective function for a Deep LM (e.g. RNN-LM or Tranformer-LM) is typically the log-likelihood of the training examples:

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

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

$$\log p(\mathbf{w}) = \log p(w_1, w_2, w_3, \ldots, w_T)$$
$$= \log p(w_1 \mid h_1) + \log p(w_2 \mid h_2) + \ldots + \log p(w_T \mid h_T)$$



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	OpenAI	2019	~10 billion (40Gb)	1.5 billion
GPT-3	OpenAI	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	OpenAI	2023	?	? (1.76 trillion)
Gemini (Ultra)	Google	2023	?	? (1.5 trillion)
LLaMA-3	Meta	2024	15 trillion	405 billion

What is ChatGPT?

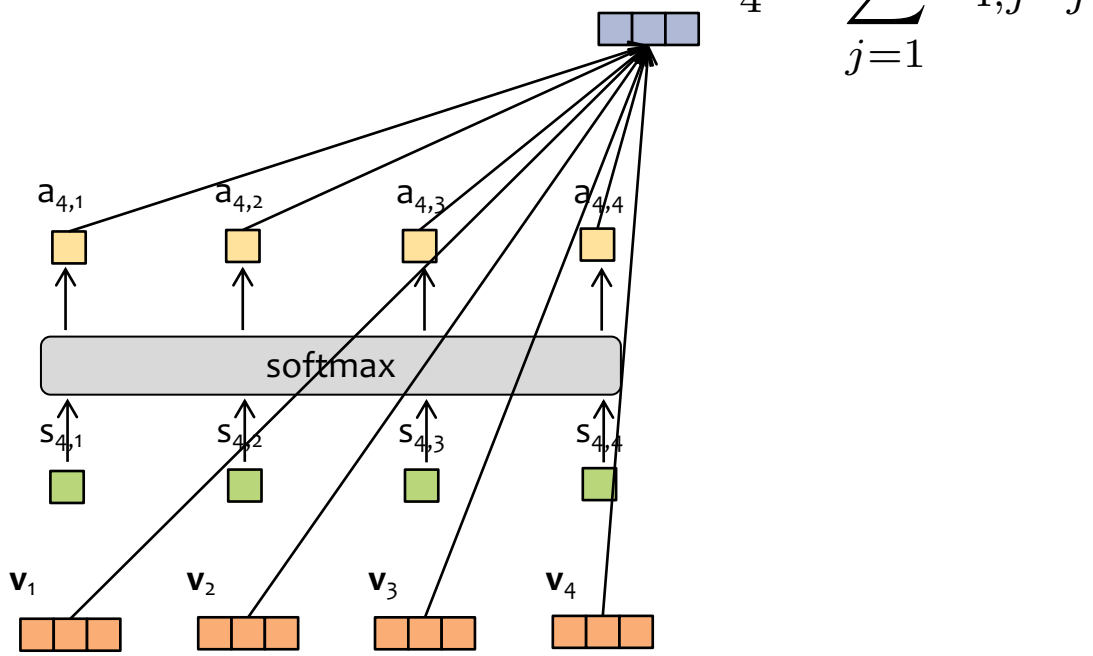
- ChatGPT is a large (in the sense of having many parameters) language model, fine-tuned to be a dialogue agent
- The base language model was originally GPT-3.5 which was trained on a large quantity of text

Transformer Language Models

MODEL: GPT

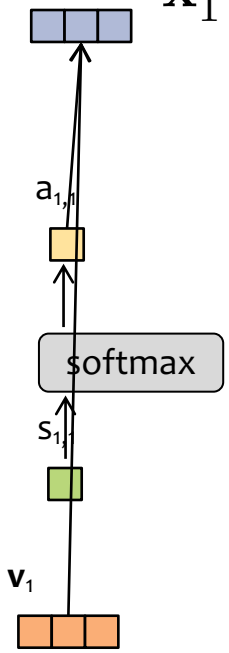
Attention

$$\mathbf{x}'_4 = \sum_{j=1}^{4} a_{4,j}\mathbf{v}_j$$



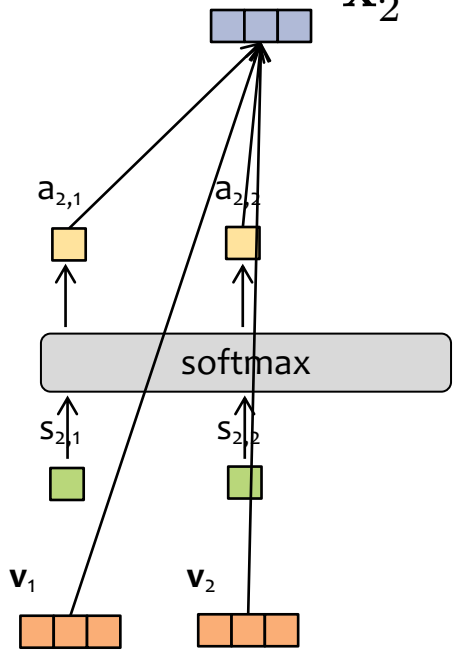
Attention

$$\mathbf{x}'_1 = \sum_{j=1}^{1} a_{1,j}\mathbf{v}_j$$

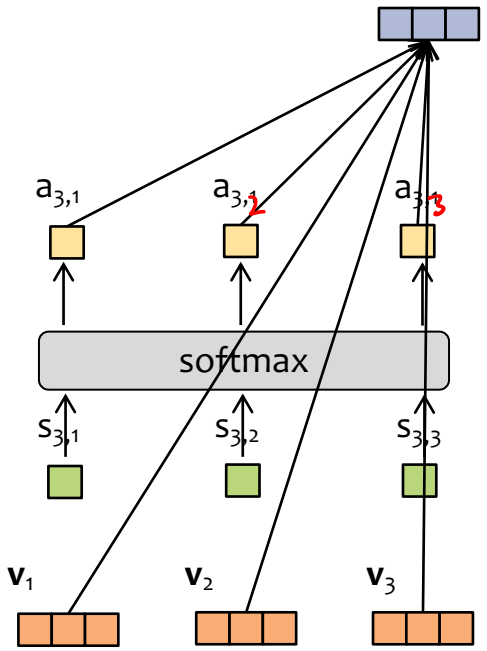


Attention

$$\mathbf{x}'_2 = \sum_{j=1}^{2} a_{2,j}\mathbf{v}_j$$

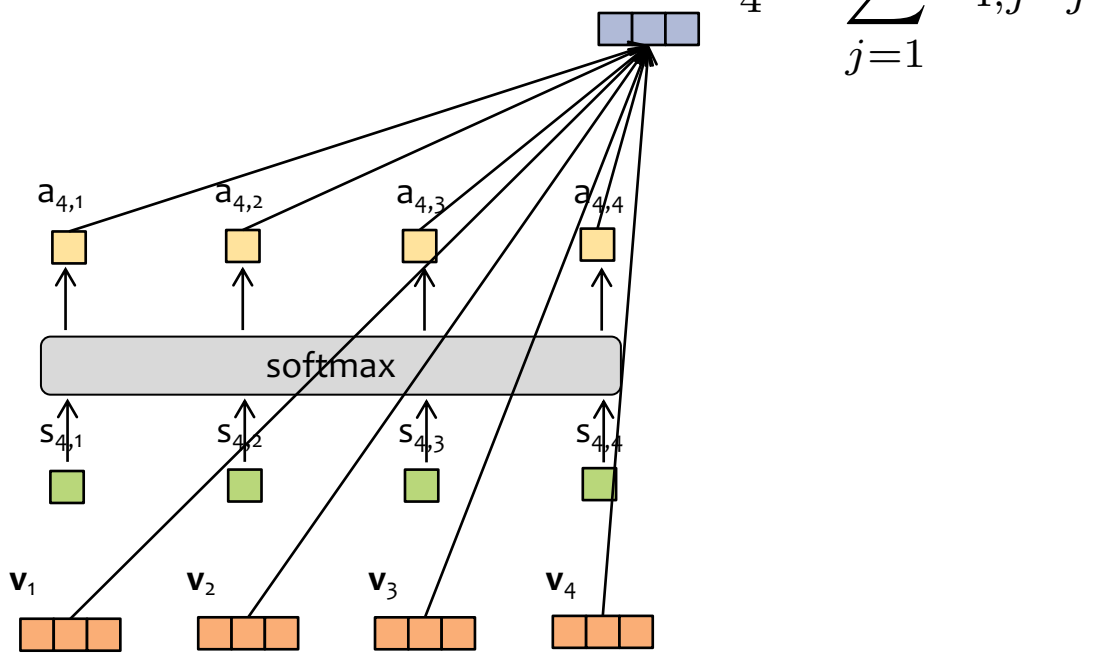


Attention

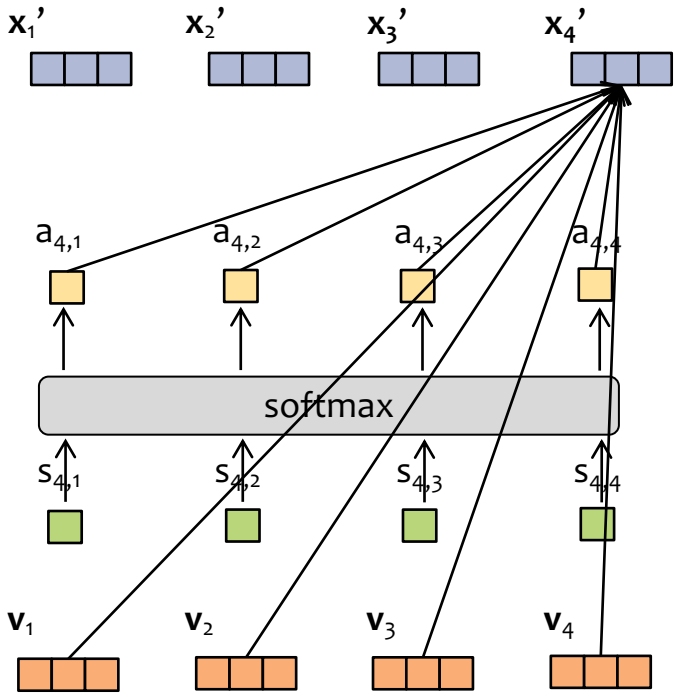

$\mathbf{x}'_3 = \sum_{j=1}^{3} a_{3,j}\mathbf{v}_j$
$a_{3,1}$
$a_{3,2}$
$a_{3,3}$
softmax
$s_{3,1}$
$s_{3,2}$
$s_{3,3}$
$\mathbf{v}_1$
$\mathbf{v}_2$
$\mathbf{v}_3$

Attention

$$\mathbf{x}'_4 = \sum_{j=1}^{4} a_{4,j}\mathbf{v}_j$$



Attention



$$\mathbf{x}'_t = \sum_{j=1}^{t} a_{t,j}\mathbf{v}_j$$

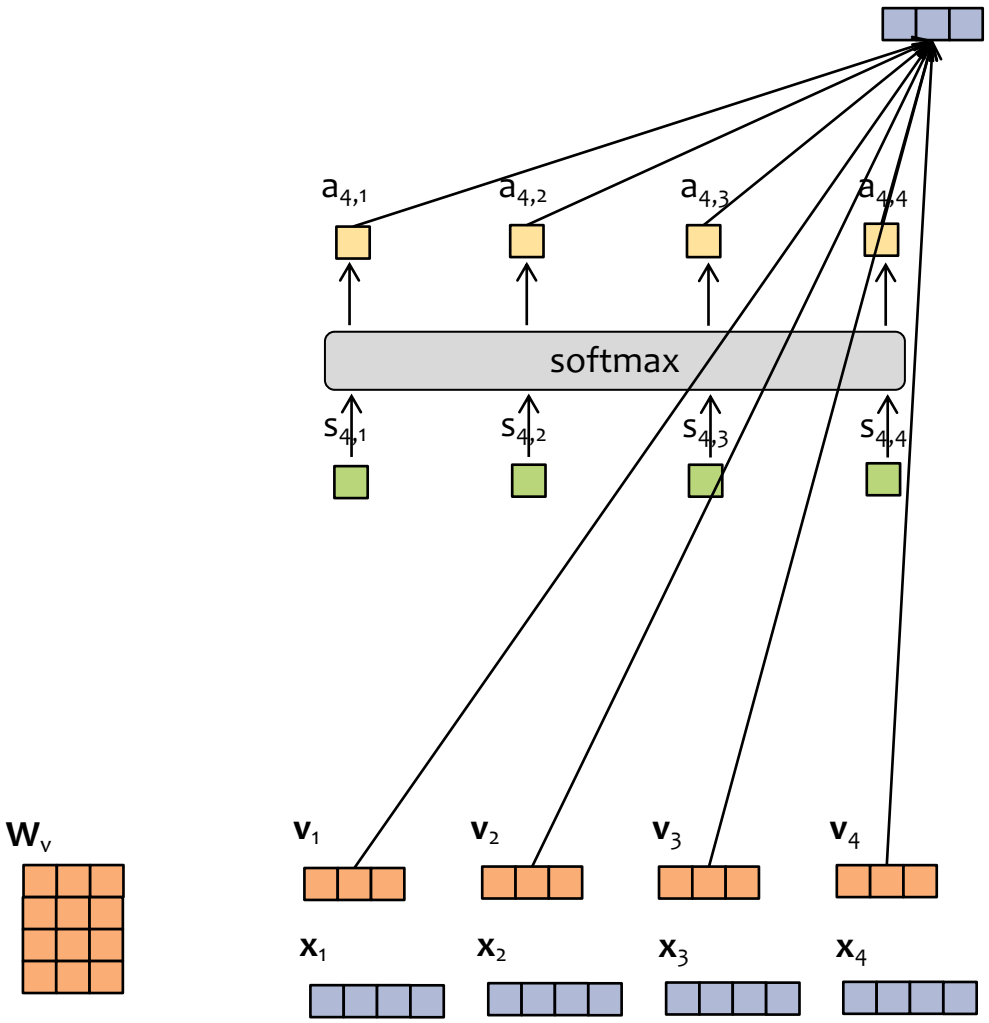
attention weights

scores

values

Scaled Dot-Product Attention

$$\mathbf{x}'_4 = \sum_{j=1}^{4} a_{4,j}\mathbf{v}_j$$

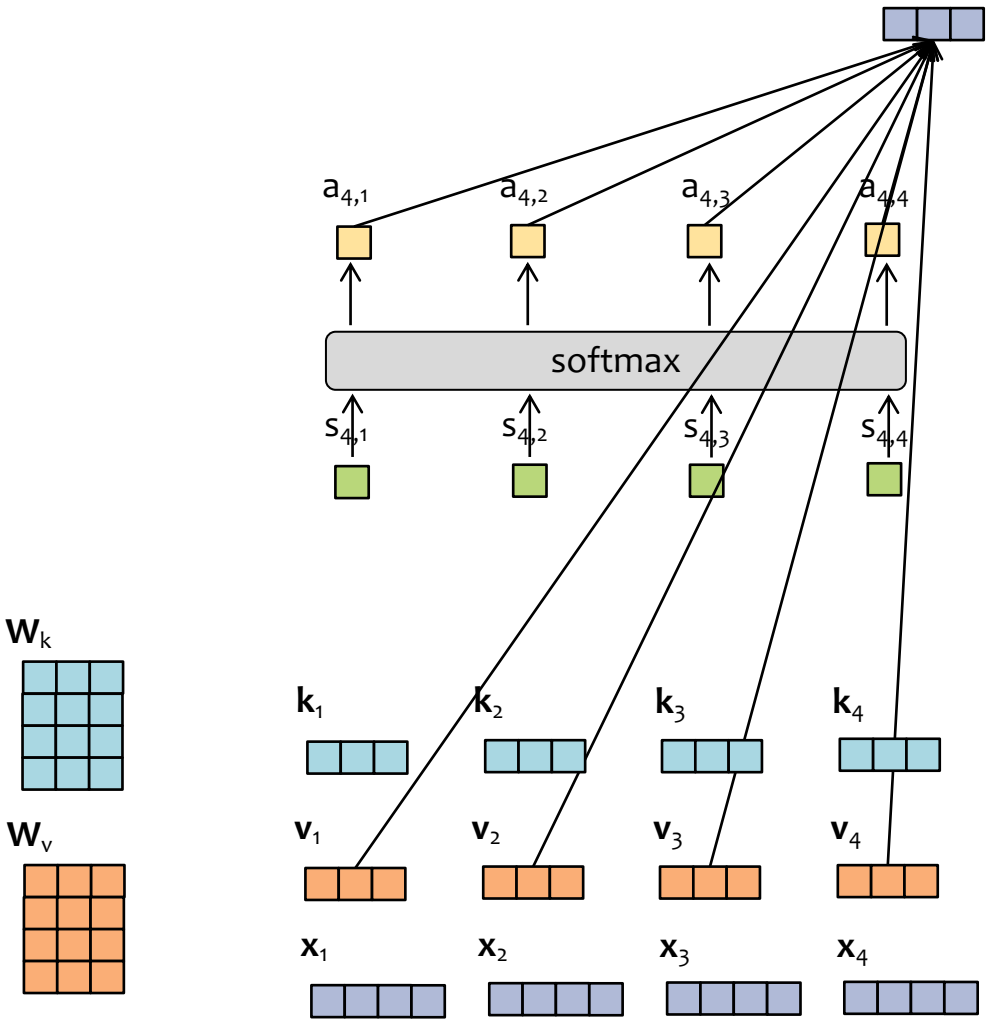


$$\mathbf{v}_j = \mathbf{W}_v^T \mathbf{x}_j$$

values

Scaled Dot-Product Attention

$$\mathbf{x}'_4 = \sum_{j=1}^{4} a_{4,j}\mathbf{v}_j$$

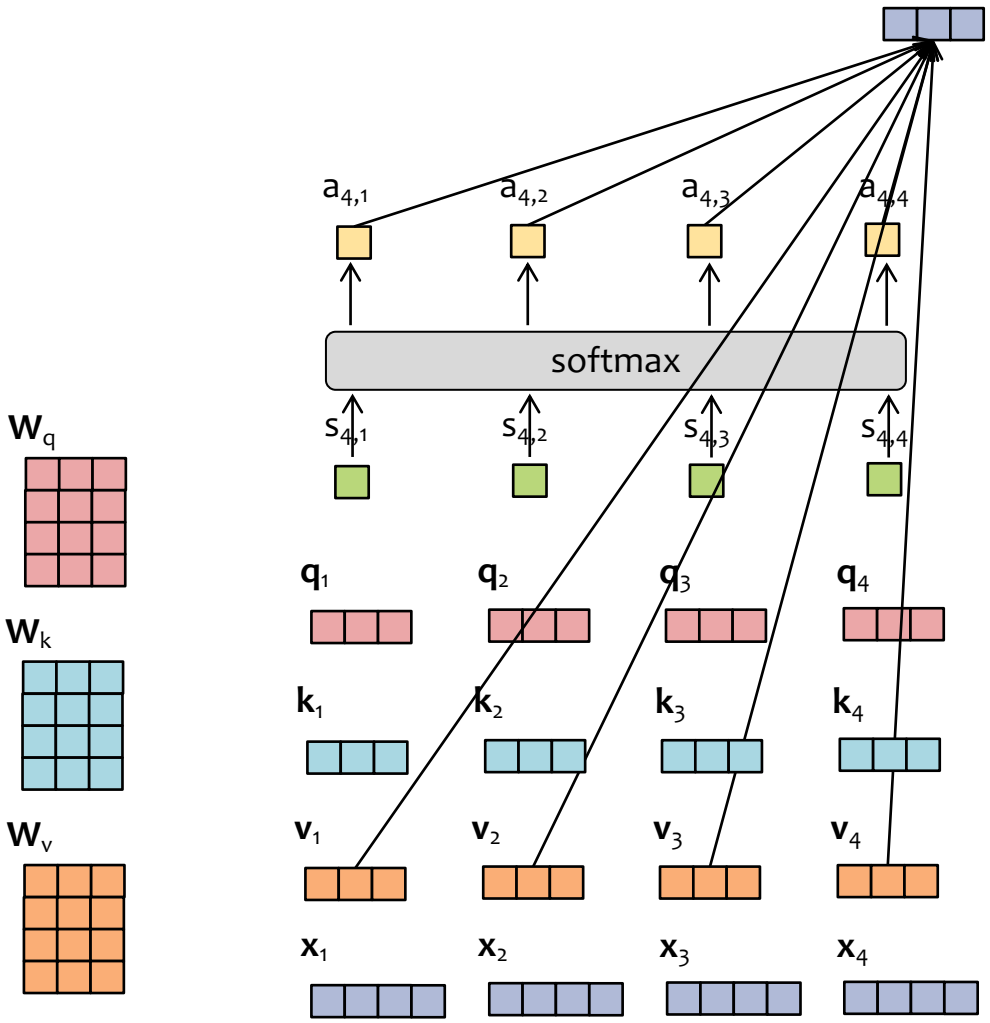


$$\mathbf{k}_j = \mathbf{W}_k^T \mathbf{x}_j \qquad \text{keys}$$

$$\mathbf{v}_j = \mathbf{W}_v^T \mathbf{x}_j \qquad \text{values}$$

Scaled Dot-Product Attention

$$\mathbf{x}'_4 = \sum_{j=1}^{4} a_{4,j}\mathbf{v}_j$$



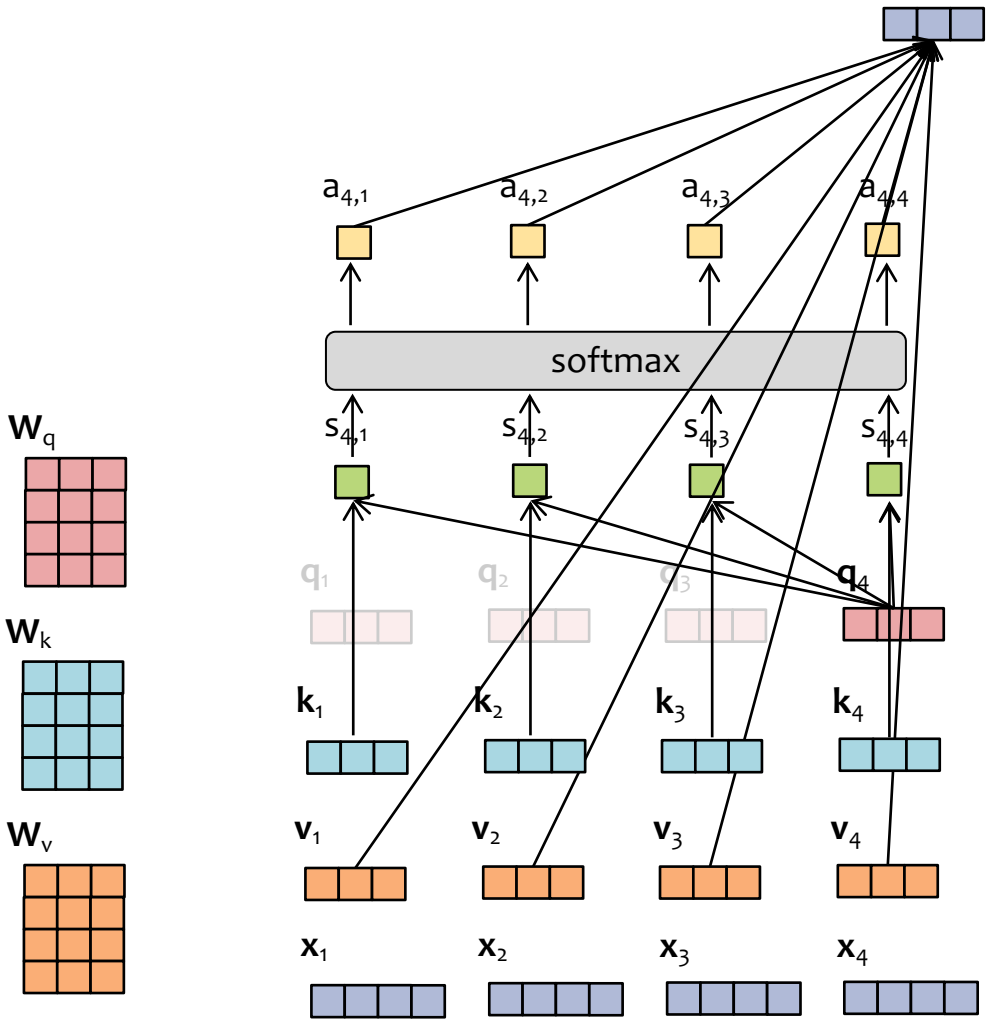
$$\mathbf{q}_j = \mathbf{W}_q^T\mathbf{x}_j \quad \text{queries}$$

$$\mathbf{k}_j = \mathbf{W}_k^T\mathbf{x}_j \quad \text{keys}$$

$$\mathbf{v}_j = \mathbf{W}_v^T\mathbf{x}_j \quad \text{values}$$

Scaled Dot-Product Attention

$$\mathbf{x}'_4 = \sum_{j=1}^{4} a_{4,j}\mathbf{v}_j$$



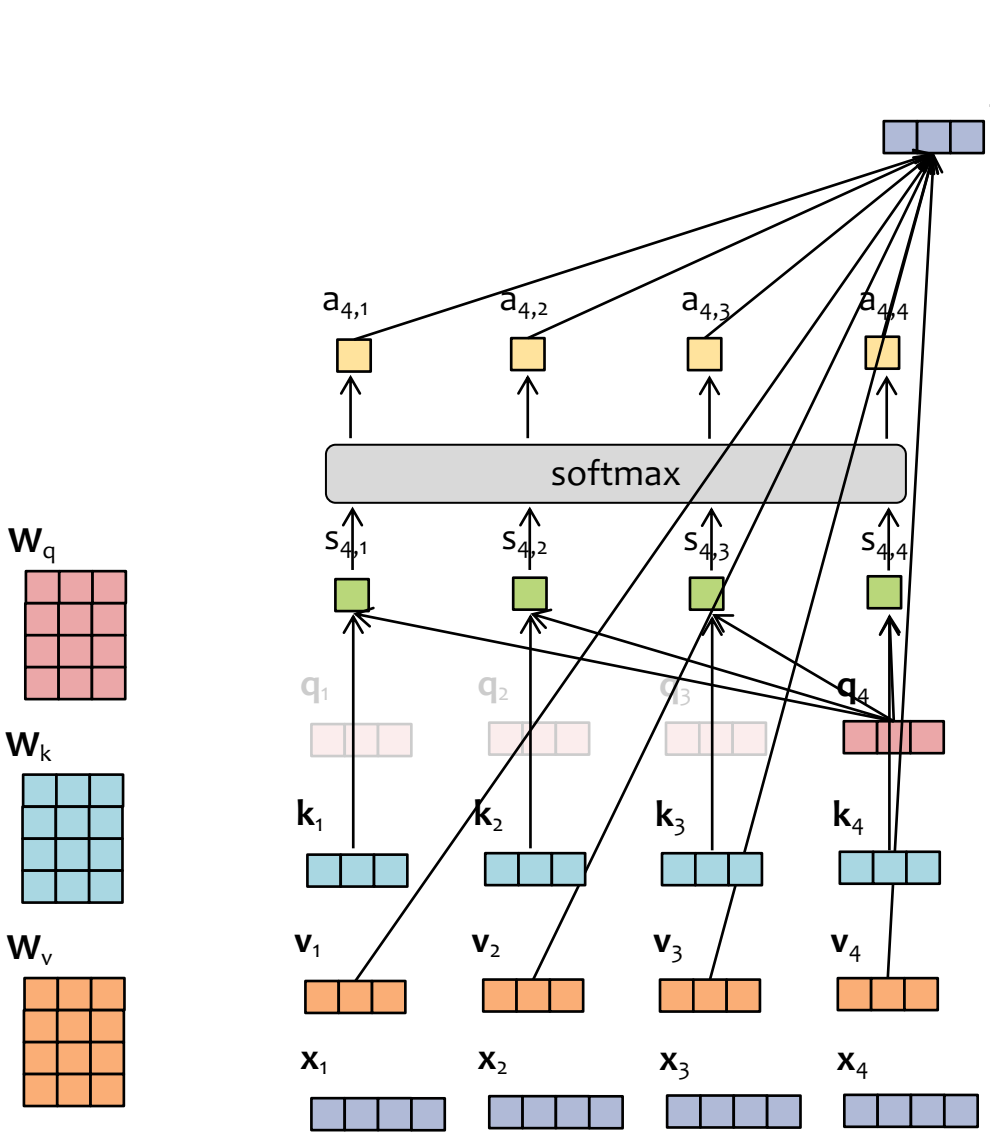
$s_{4,j} = \mathbf{k}_j^T \mathbf{q}_4 / \sqrt{d_k}$ scores

$\mathbf{q}_j = \mathbf{W}_q^T \mathbf{x}_j$ queries

$\mathbf{k}_j = \mathbf{W}_k^T \mathbf{x}_j$ keys

$\mathbf{v}_j = \mathbf{W}_v^T \mathbf{x}_j$ values

Scaled Dot-Product Attention



$\mathbf{a}_4 = \text{softmax}(\mathbf{s}_4)$ attention weights

$s_{4,j} = \mathbf{k}_j^T \mathbf{q}_4 / \sqrt{d_k}$ scores

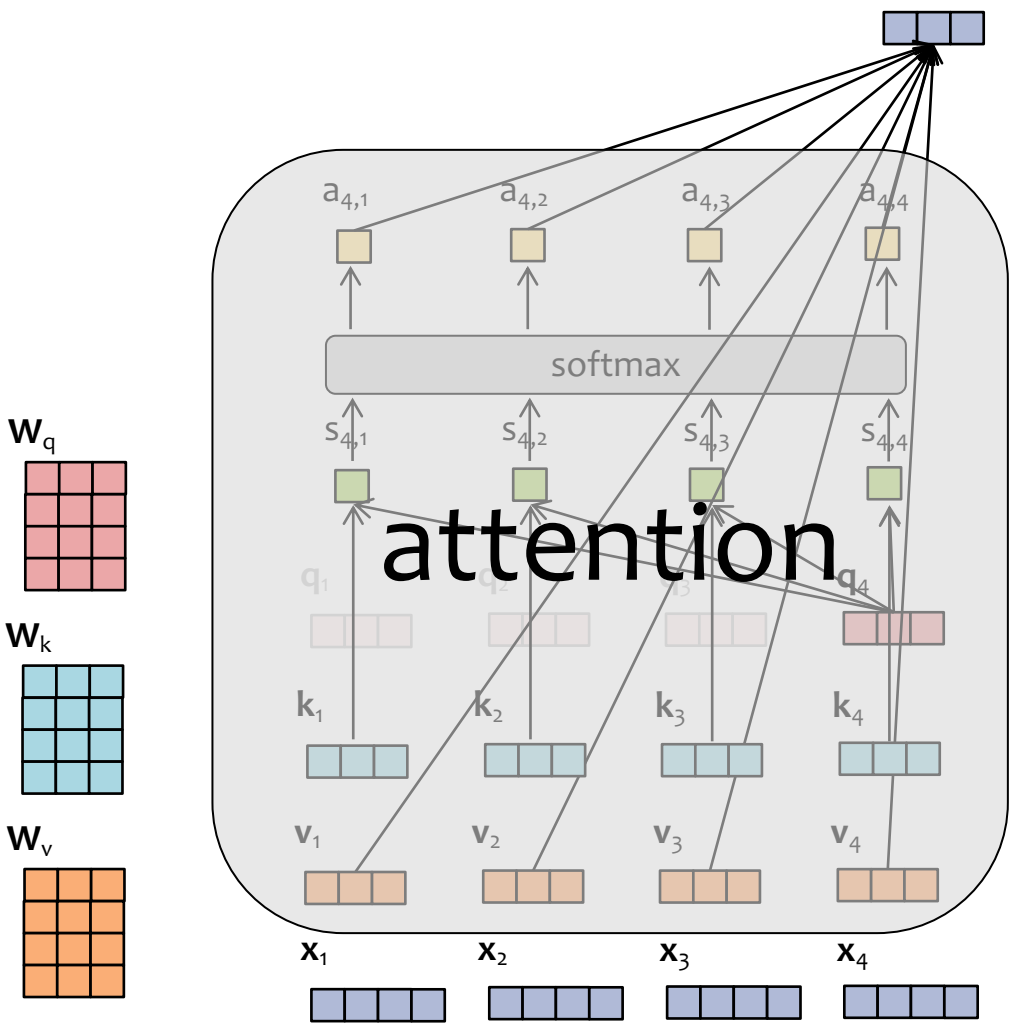
$\mathbf{q}_j = \mathbf{W}_q^T \mathbf{x}_j$ queries

$\mathbf{k}_j = \mathbf{W}_k^T \mathbf{x}_j$ keys

$\mathbf{v}_j = \mathbf{W}_v^T \mathbf{x}_j$ values

Scaled Dot-Product Attention

$$\mathbf{x}'_4 = \sum_{j=1}^{4} a_{4,j}\mathbf{v}_j$$



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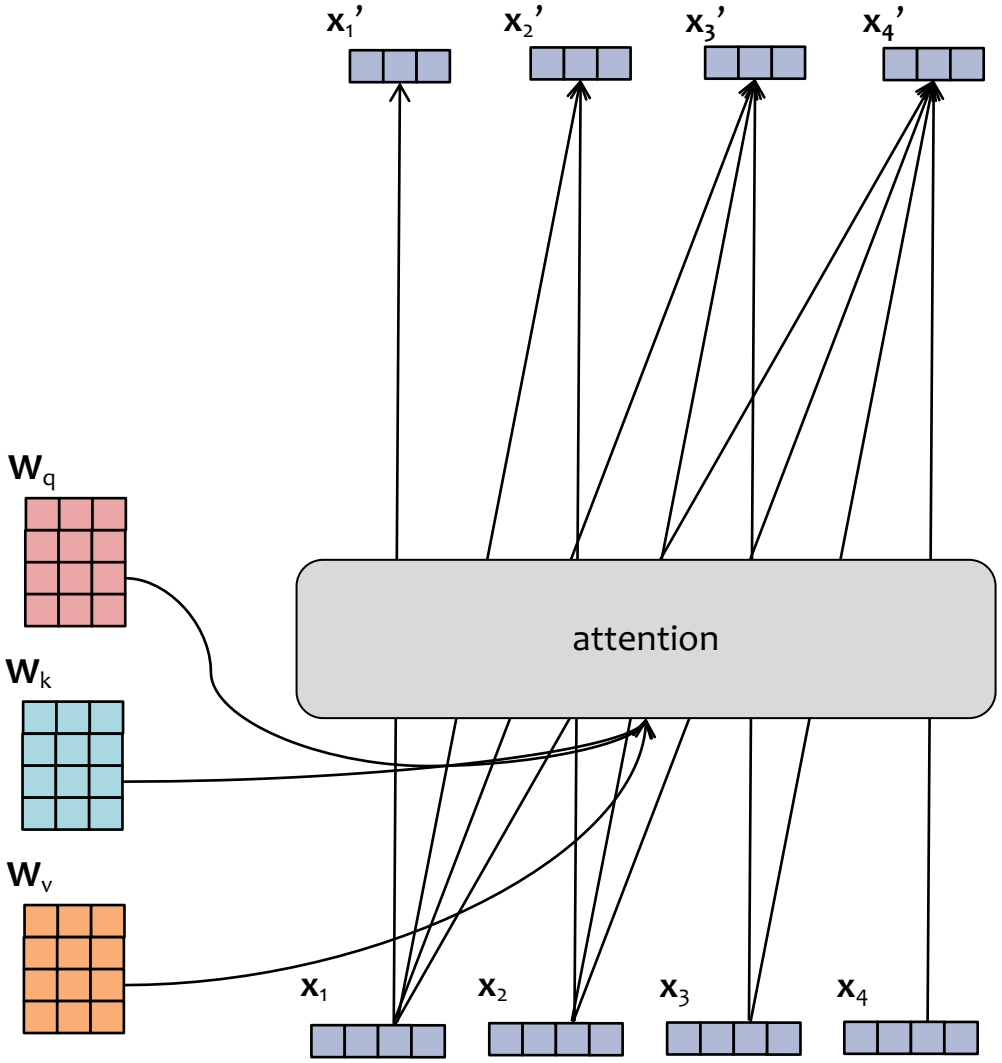
$\mathbf{v}_j = \mathbf{W}_v^T \mathbf{x}_j$ values

Scaled Dot-Product Attention



$$\mathbf{x}'_t = \sum_{j=1}^{t} a_{t,j}\mathbf{v}_j$$

$\mathbf{a}_t = \text{softmax}(\mathbf{s}_t)$ attention weights

$s_{t,j} = \mathbf{k}_j^T \mathbf{q}_t / \sqrt{d_k}$ scores

$\mathbf{q}_j = \mathbf{W}_q^T \mathbf{x}_j$ queries

$\mathbf{k}_j = \mathbf{W}_k^T \mathbf{x}_j$ keys

$\mathbf{v}_j = \mathbf{W}_v^T \mathbf{x}_j$ values

Animation of 3D Convolution

Recall…

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

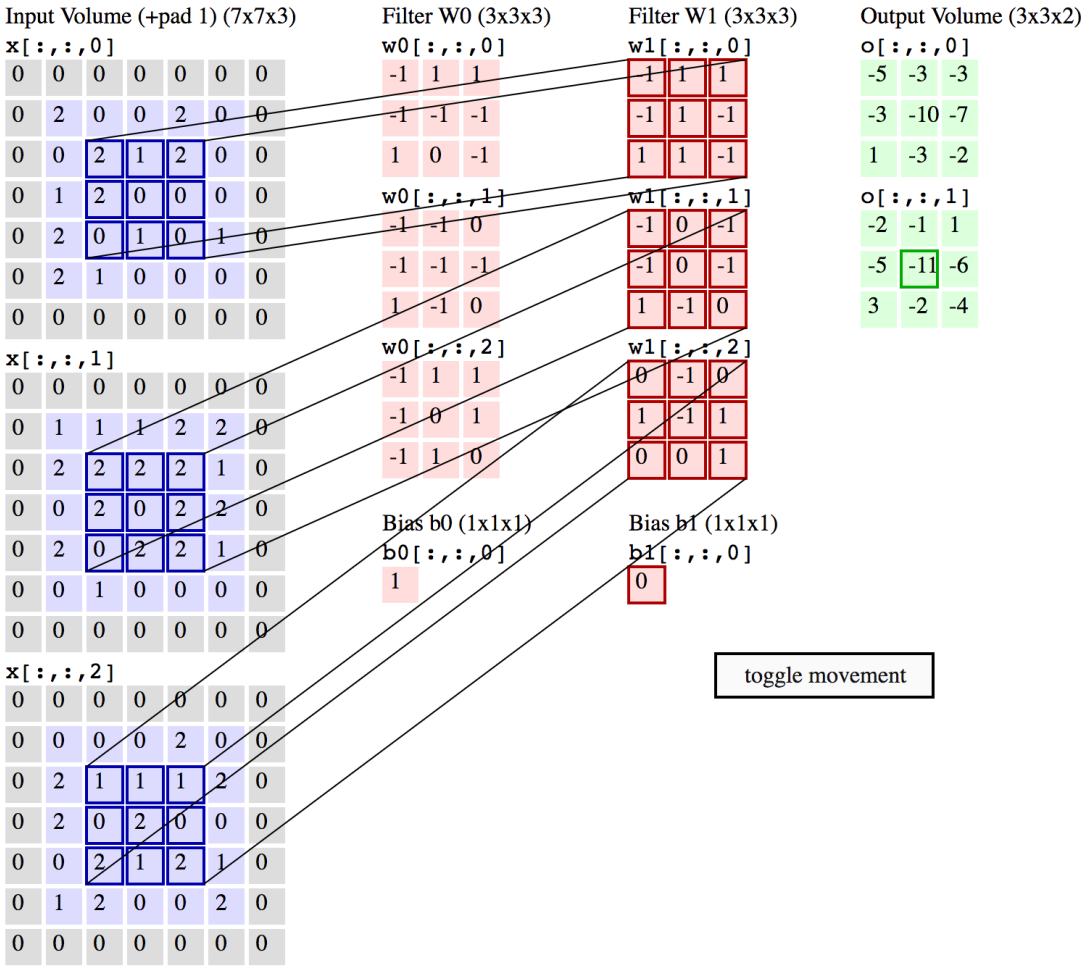
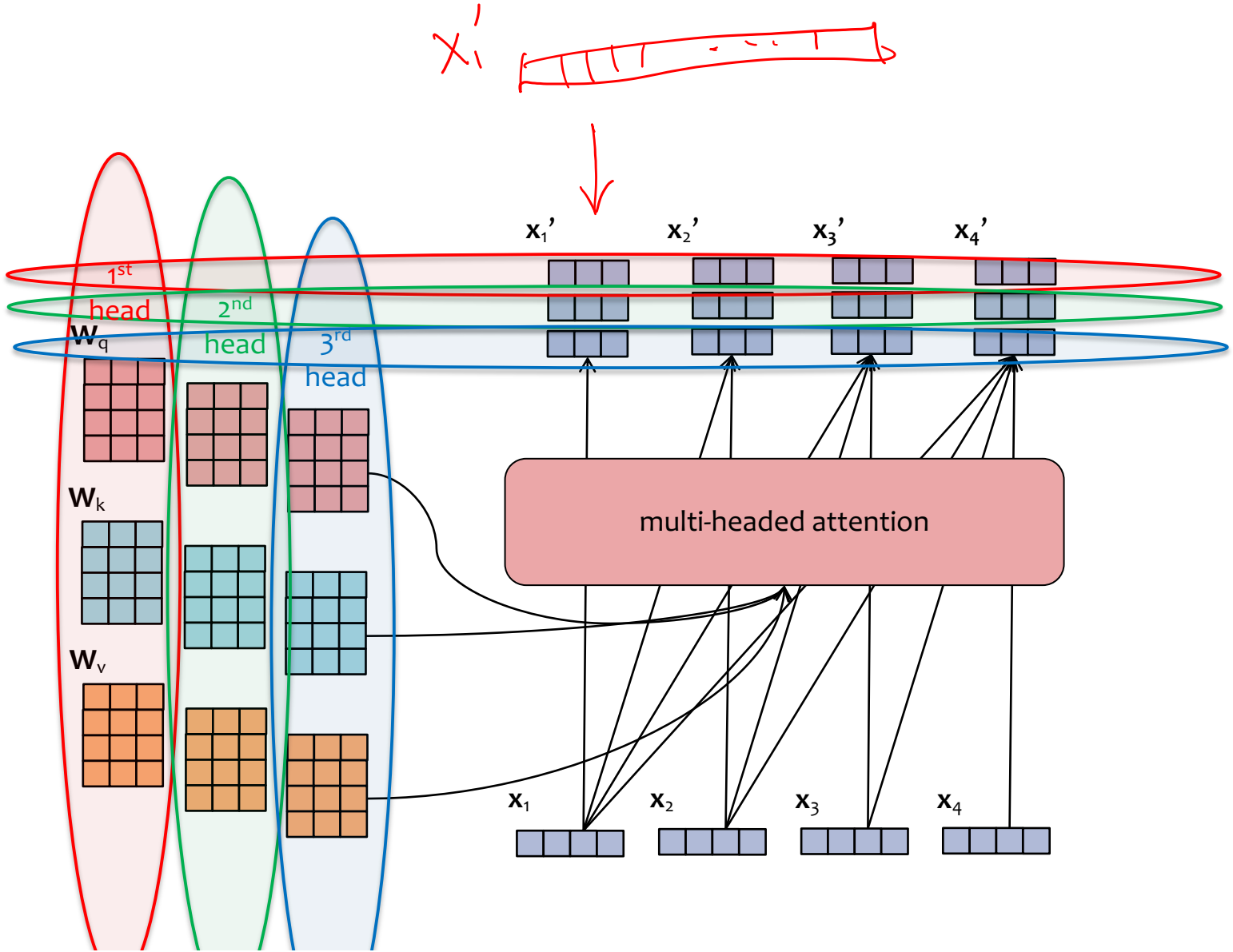


Figure from Fei-Fei Li & Andrej Karpathy & Justin Johnson (CS231N)

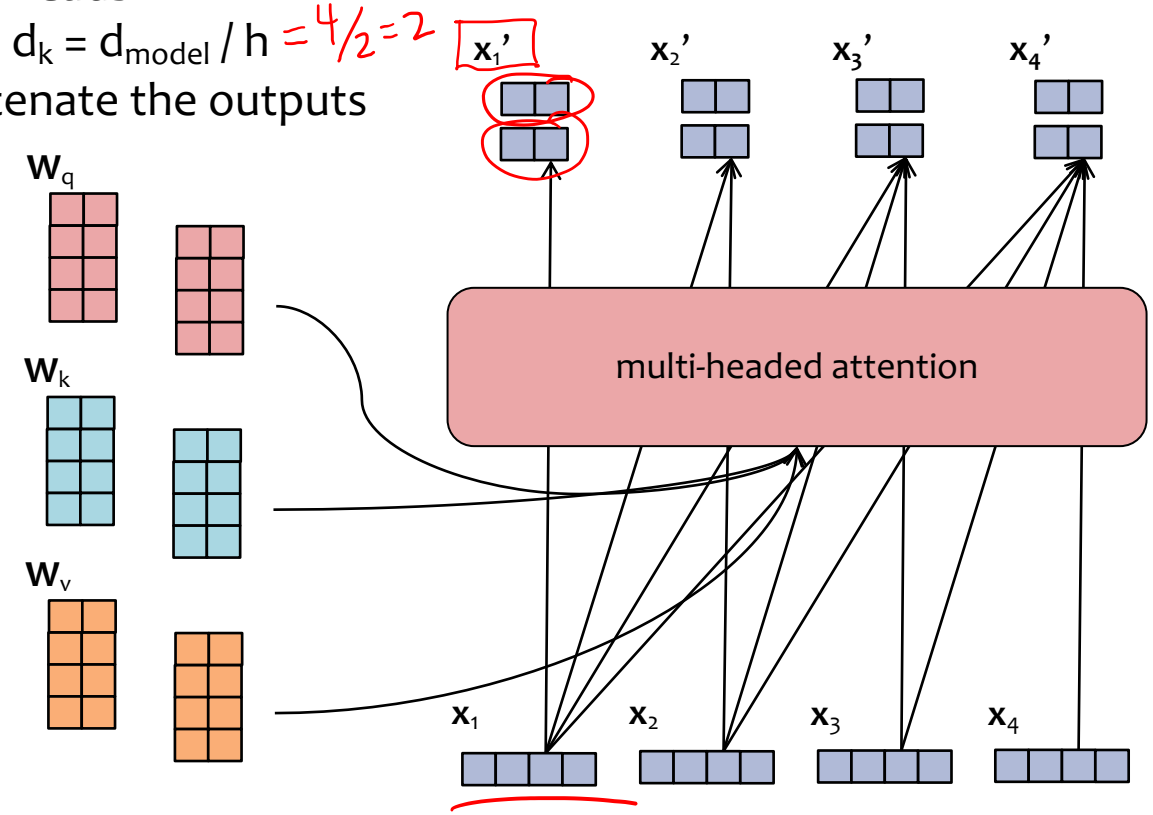
Multi-headed Attention



- 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

Multi-headed Attention

- To ensure the dimension of the **input** embedding $\mathbf{x}_t$ is the same as the **output** embedding $\mathbf{x}_t$', Transformers usually choose the embedding sizes and number of heads appropriately:
  - d_{model} = dim. of inputs $= 4$
  - d_k = dim. of each output
  - h = # of heads $= 2$
  - Choose $d_k = d_{model} / h$ $= 4/2 = 2$
- Then concatenate the outputs



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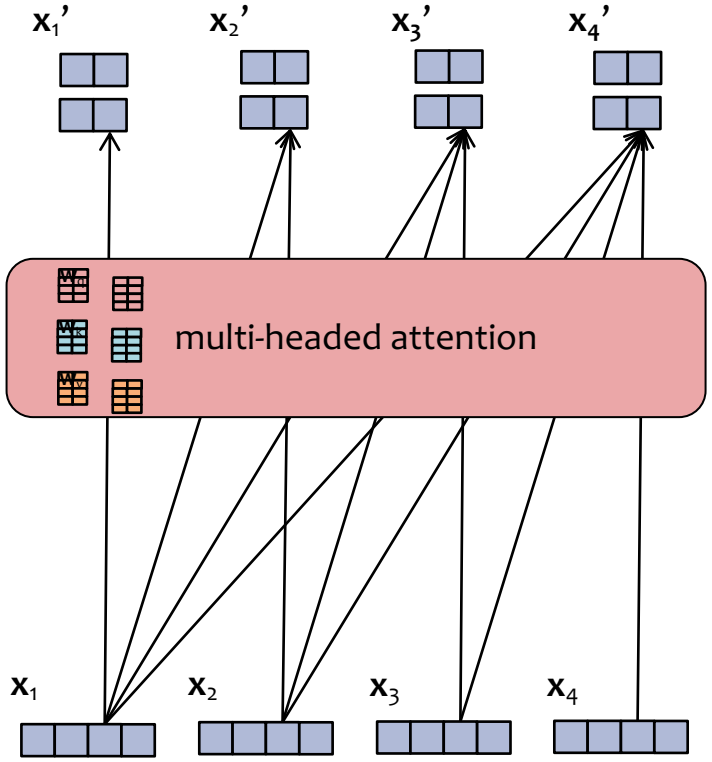

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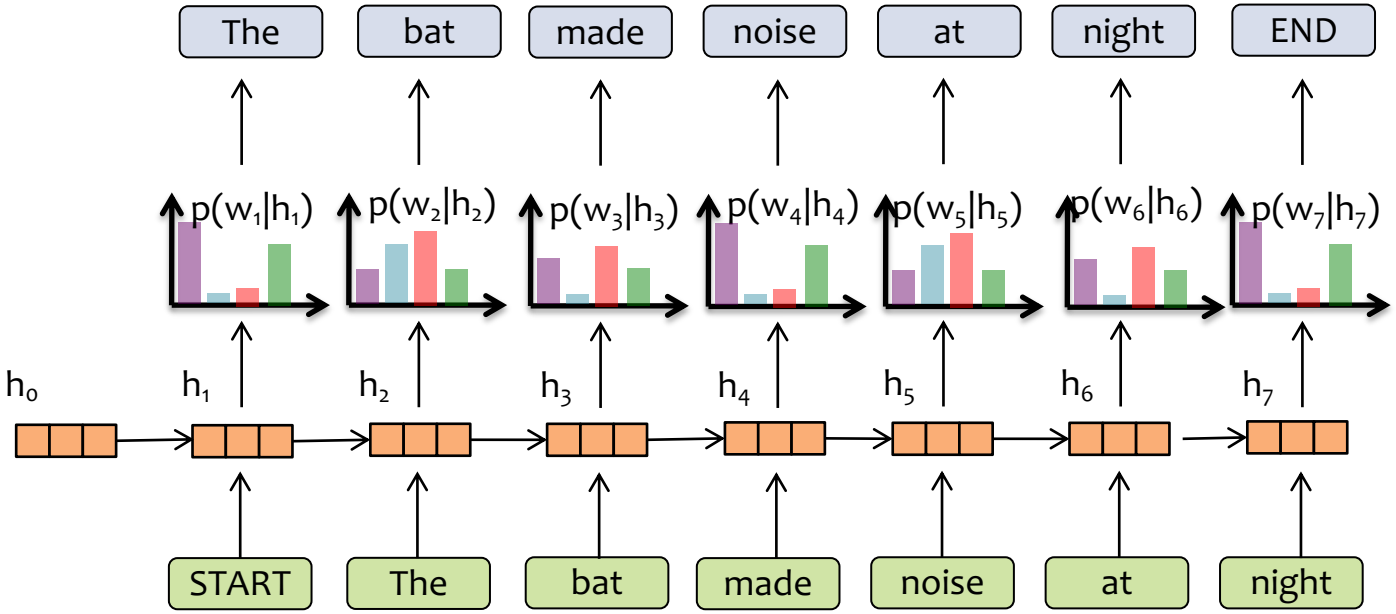
RNN Language Model

Recall…



Key Idea:

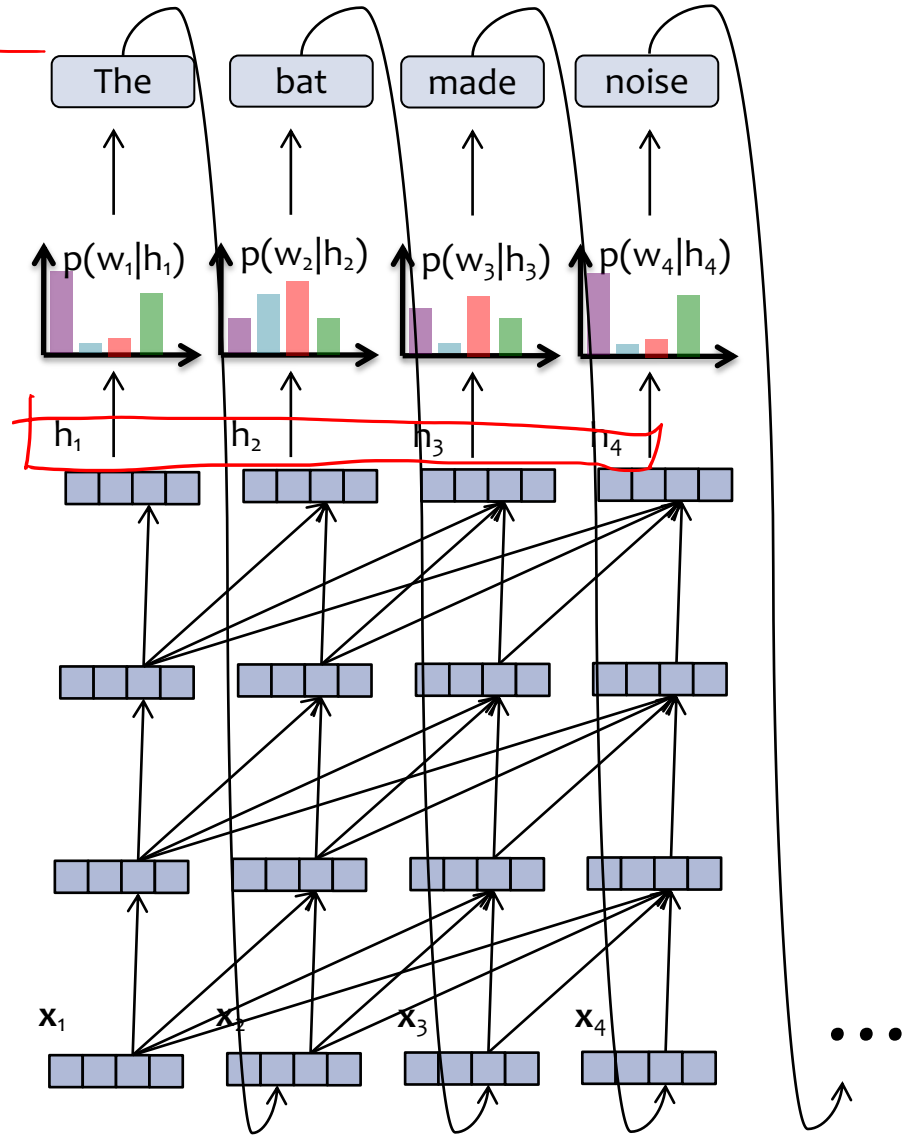
(1) convert all previous words to a **fixed length vector**

(2) define distribution $p(w_t \mid f_\theta(w_{t-1}, \ldots, w_1))$ that conditions on the vector $\mathbf{h}_t = f_\theta(w_{t-1}, \ldots, w_1)$

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



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

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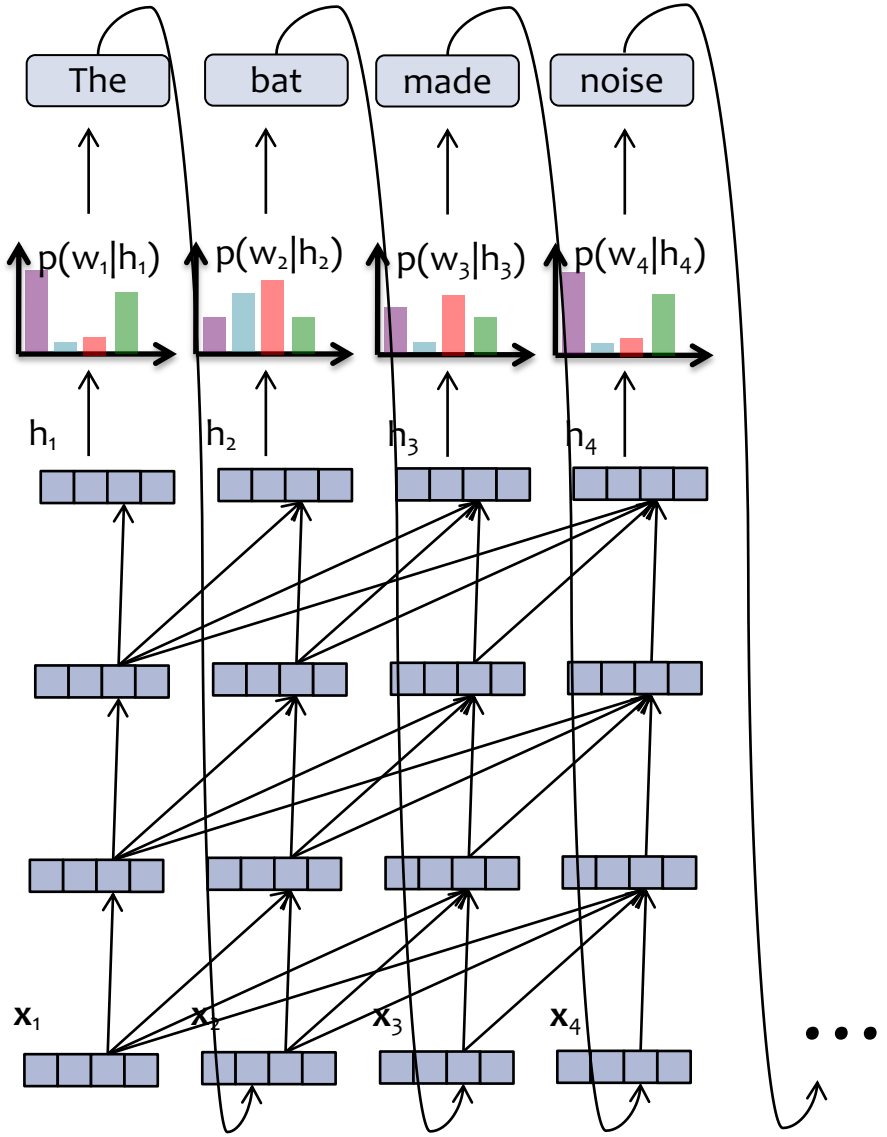

Each layer of a Transformer LM consists of several **sublayers:**

1. attention
2. feed-forward neural network
3. layer normalization
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Each hidden vector looks back at the hidden vectors of the **current and previous timesteps in the previous layer.**

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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 $\mathbf{b} \in \mathbb{R}^K$:

$$\mathbf{b} = \boldsymbol{\gamma} \odot \frac{\mathbf{a} - \mu}{\sigma} \oplus \boldsymbol{\beta}$$

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.

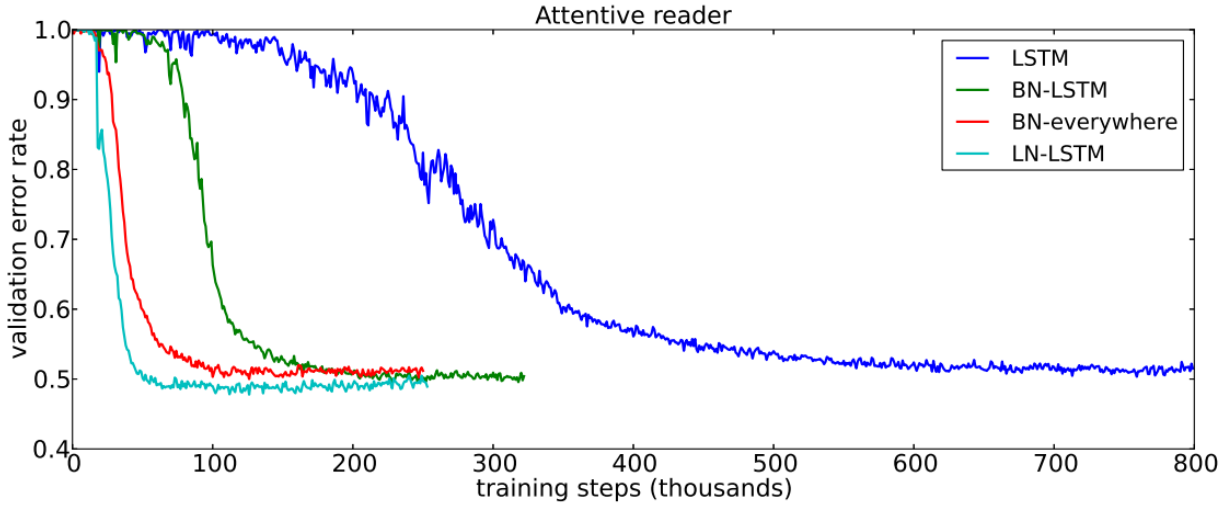
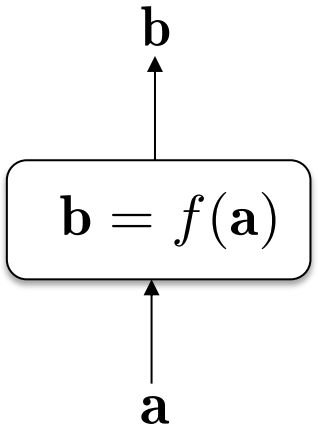


Figure from https://arxiv.org/pdf/1607.06450.pdf

Residual Connections

- *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

Plain Connection



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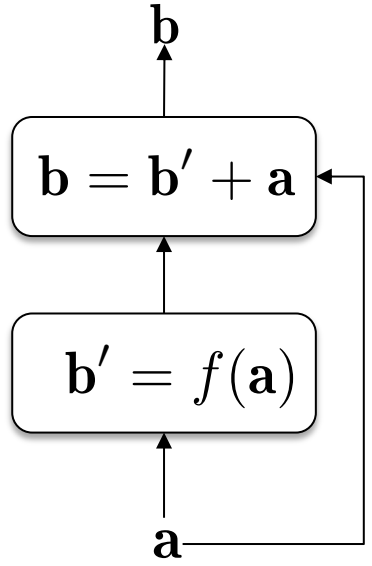

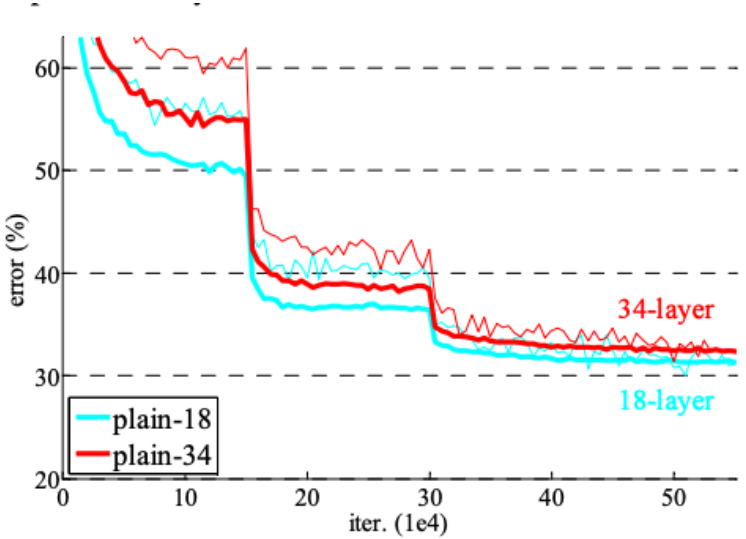

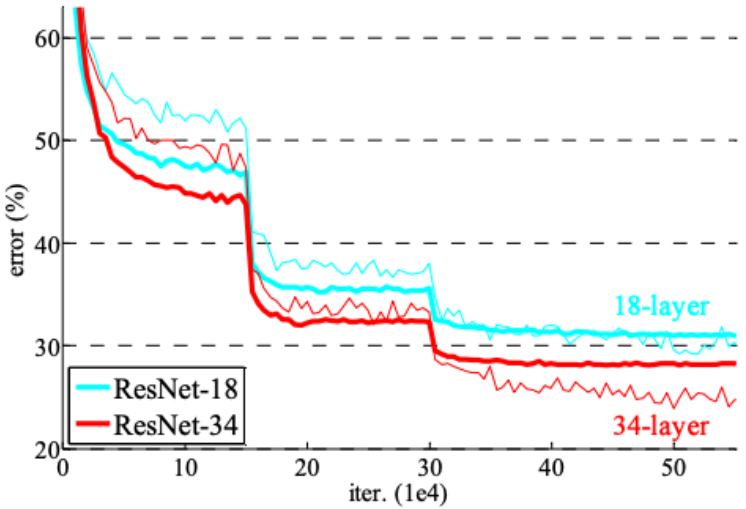

Figure from https://arxiv.org/pdf/1512.03385.pdf

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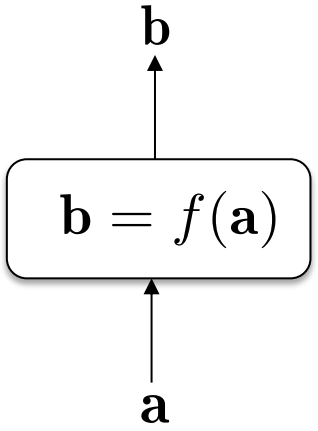

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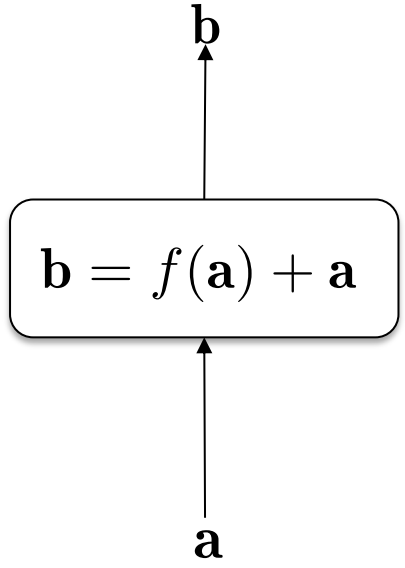


Why are residual connections helpful?

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).

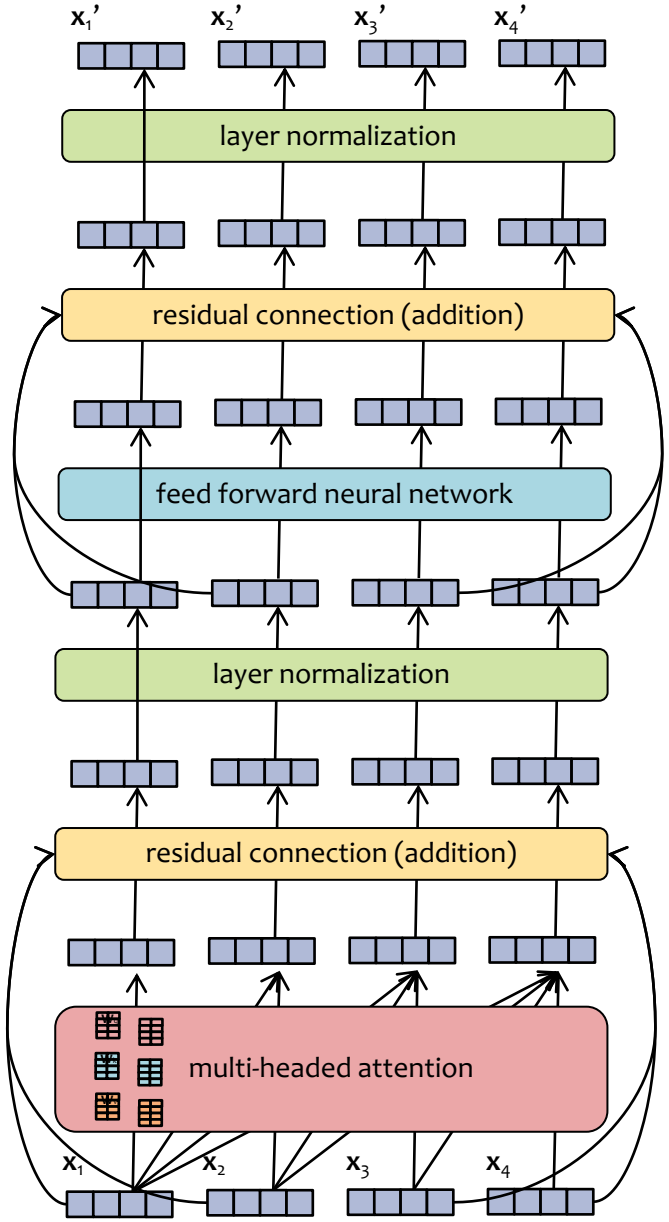
Figure from https://arxiv.org/pdf/1512.03385.pdf

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.



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

1. attention
2. feed-forward neural network
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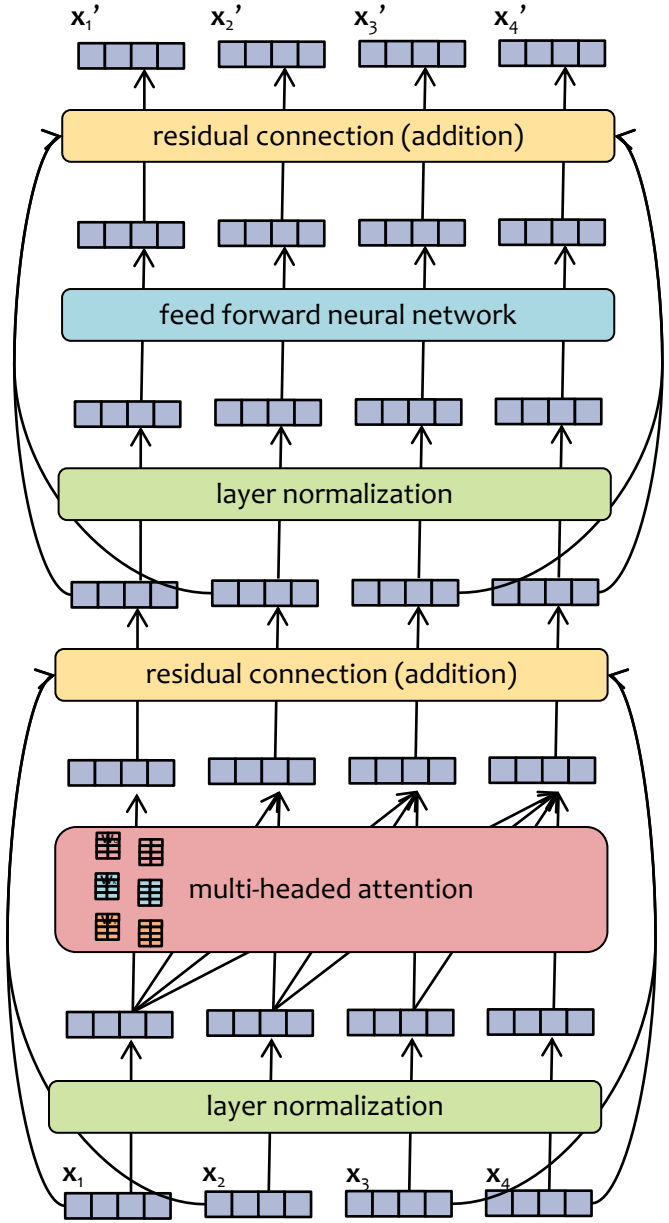
Transformer Layer

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 feed-forward NN layers tend to be better behaved (i.e. tricks like warm-up are less important).



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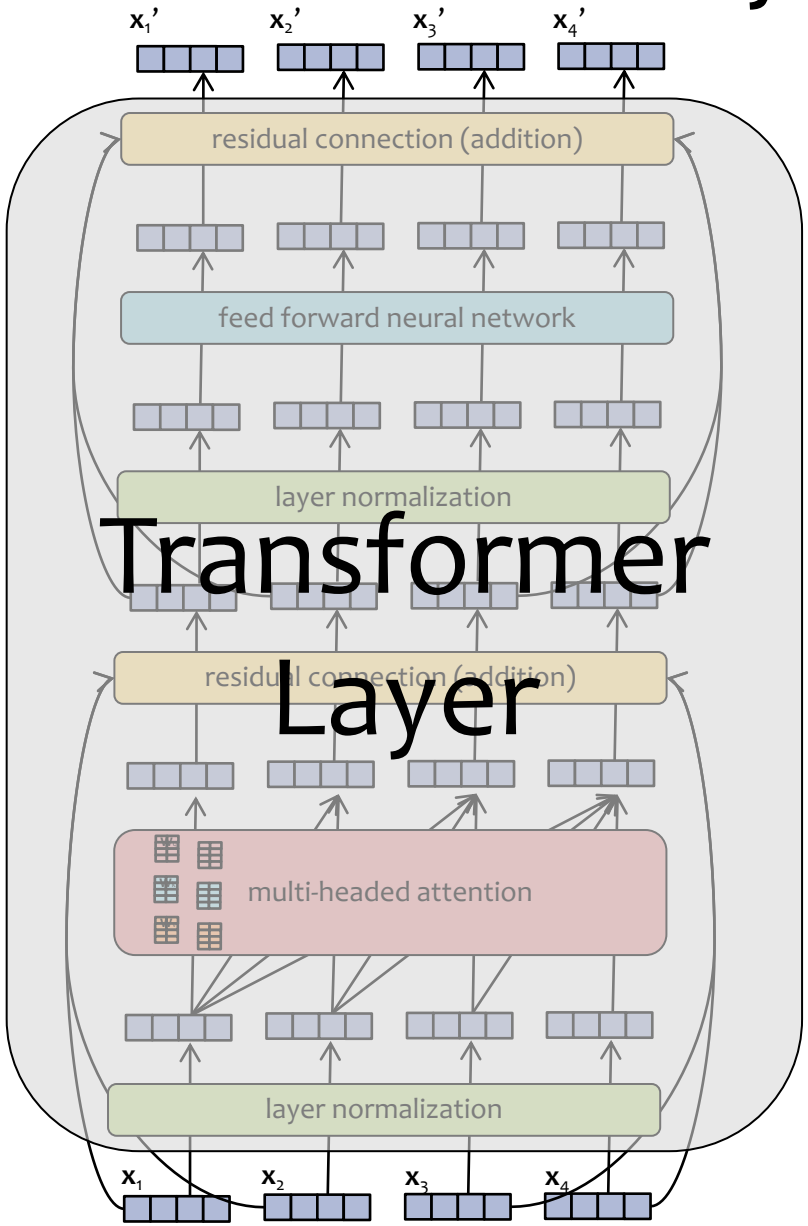

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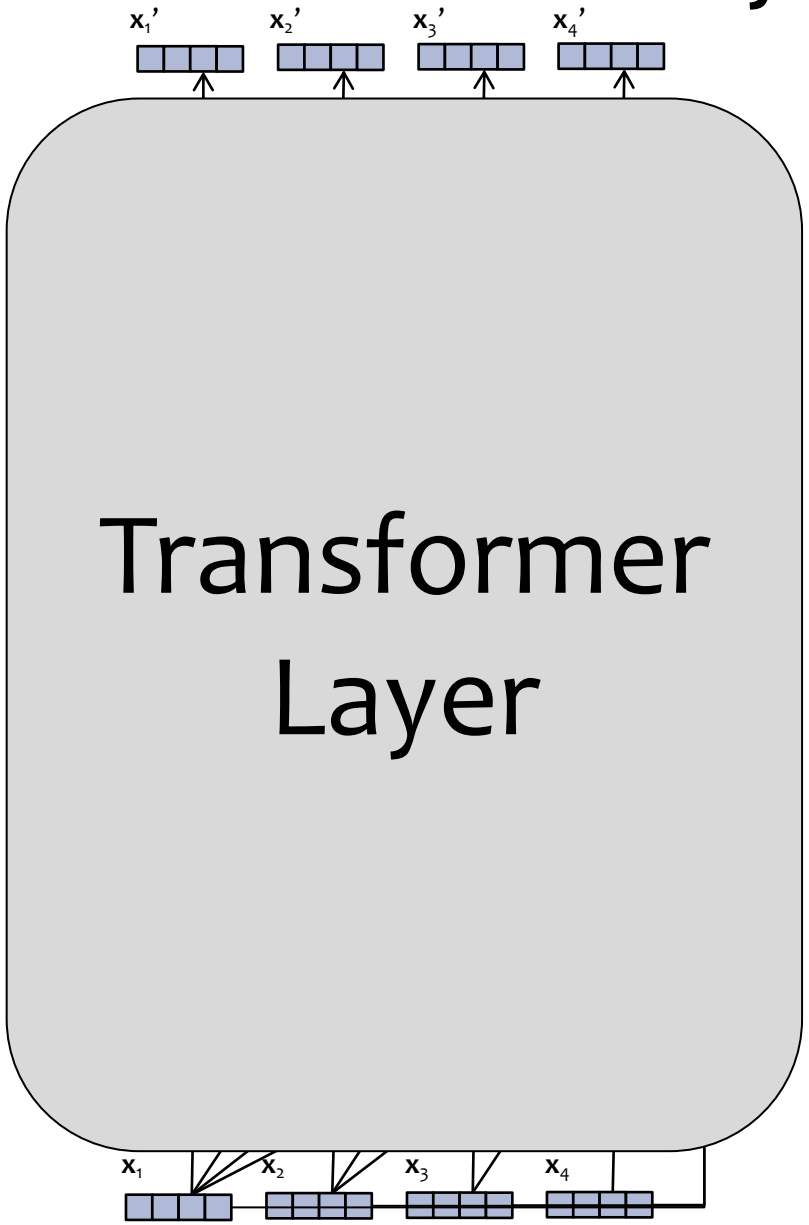

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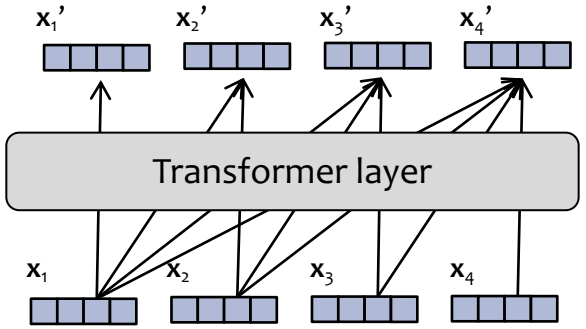
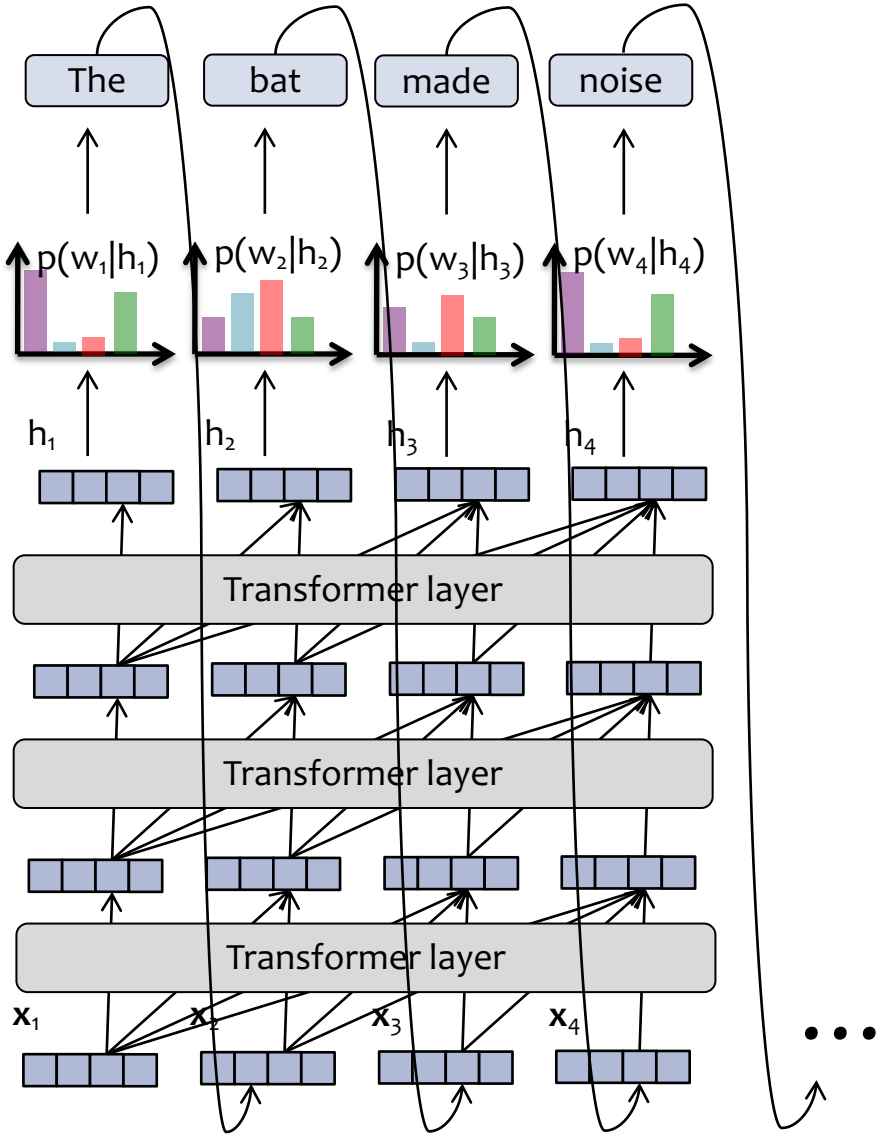


Transformer Language Model



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

In-Class Poll

Question:

Suppose we have the following input embeddings and attention weights:

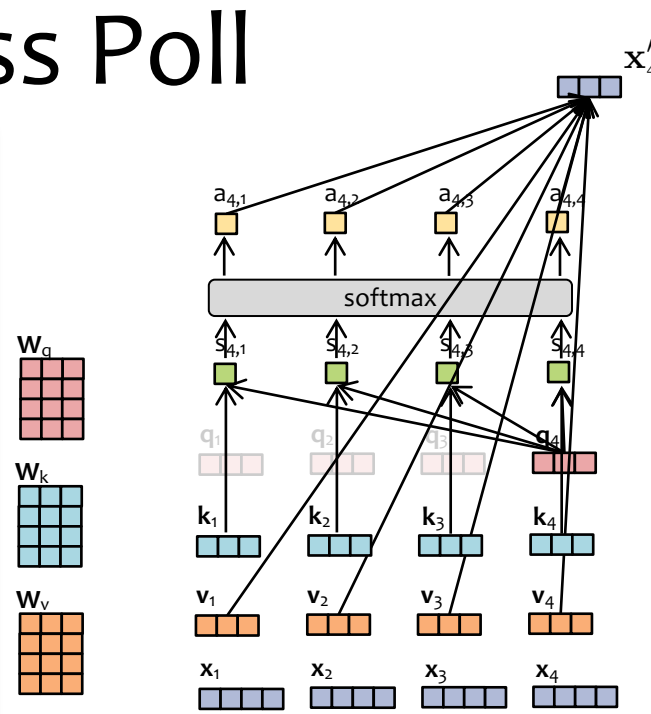
- $x_1 = [1,0,0,0]$ $a_{4,1} = 0.1$
- $x_2 = [0,1,0,0]$ $a_{4,2} = 0.2$
- $x_3 = [0,0,2,0]$ $a_{4,3} = 0.6$
- $x_4 = [0,0,0,1]$ $a_{4,4} = 0.1$

And $W_v = I$. Then we can compute x_4'.

Now suppose we swap the embeddings x_2 and x_3 such that

- $x_2 = [0,0,2,0]$
- $x_3 = [0,1,0,0]$

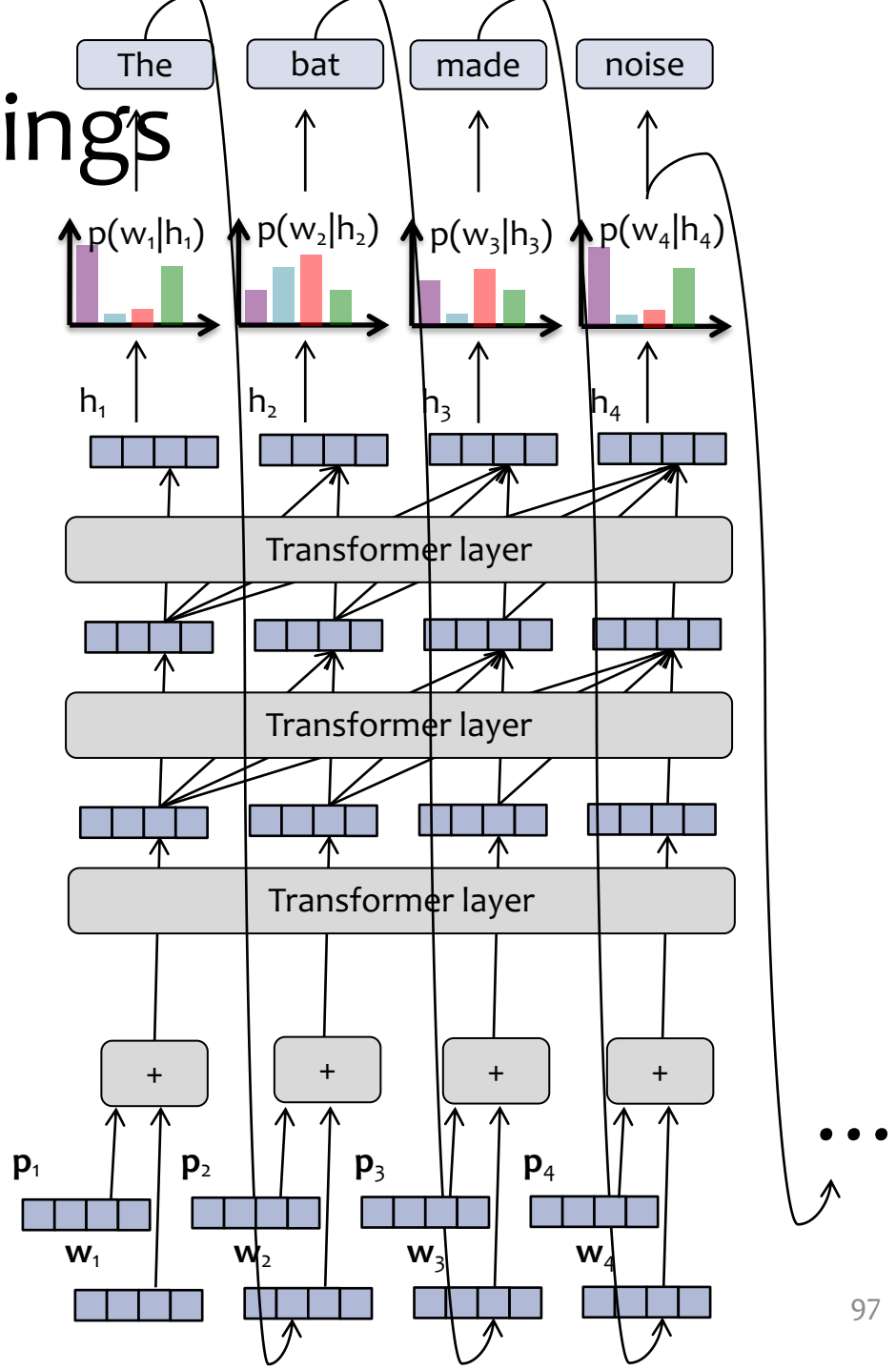
What is the new value of x_4'?



Answer:

Position Embeddings

- The Problem: Because attention is position invariant, we **need** a way to learn about positions
- The Solution: Use (or learn) a collection of position specific embeddings: $\mathbf{p}_t$ represents what it means to be in position t. And add this to the word embedding $\mathbf{w}_t$.
  The **key idea** is that every word that appears in position t uses the same position embedding $\mathbf{p}_t$
- There are a number of varieties of position embeddings:
  - Some are fixed (based on sine and cosine), whereas others are learned (like word embeddings)
  - Some are absolute (as described above) but we can also use relative position embeddings (i.e. relative to the position of the query vector)



LEARNING A TRANSFORMER LM

Learning a Transformer LM

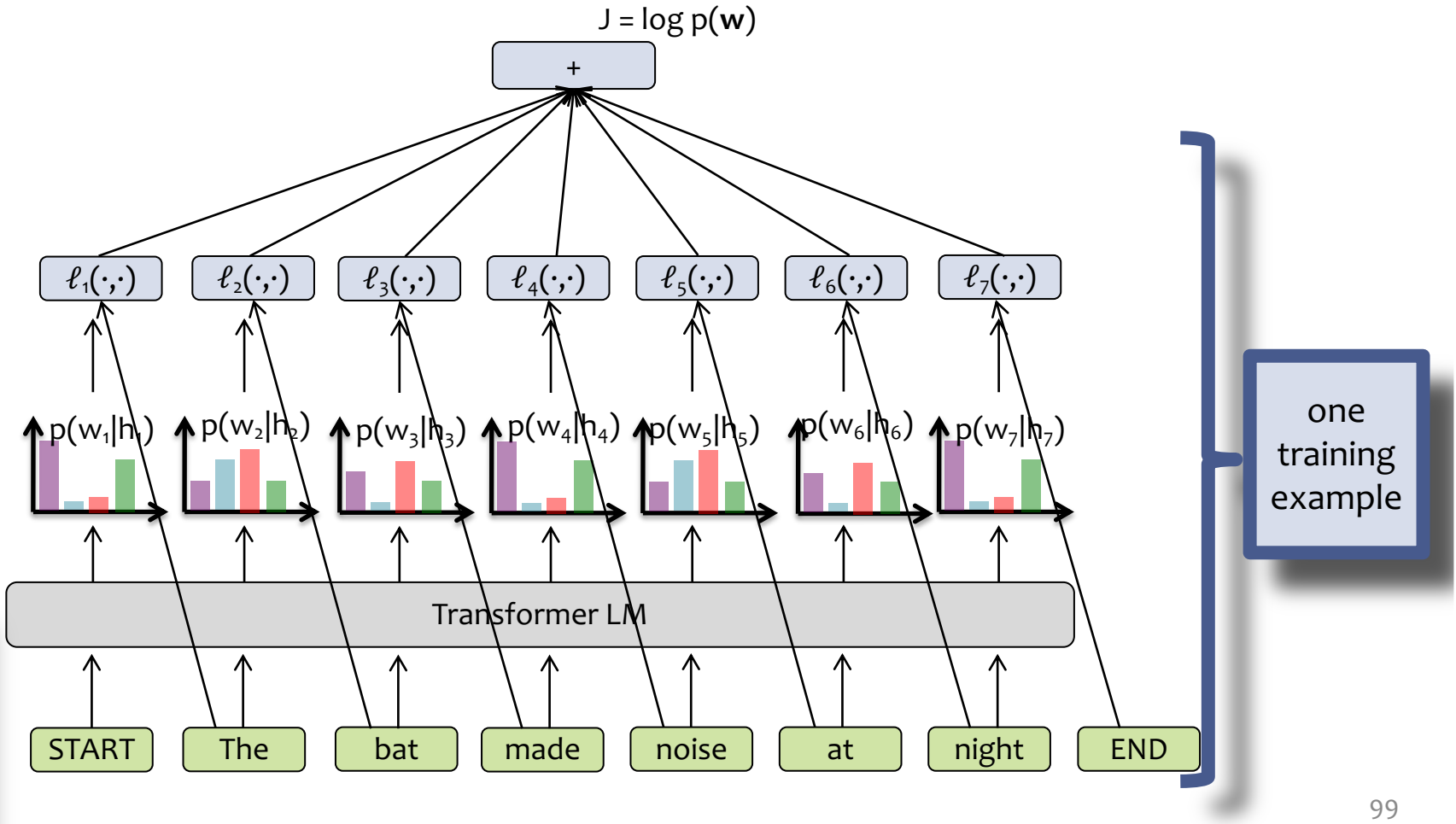
- Each training example is a sequence (e.g. sentence), so we have training data $D = \{\mathbf{w}^{(1)}, \mathbf{w}^{(2)}, \ldots, \mathbf{w}^{(N)}\}$
- The objective function for a Deep LM (e.g. RNN-LM or Tranformer-LM) is typically the log-likelihood of the training examples:

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

- 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.

$$\log p(\mathbf{w}) = \log p(w_1, w_2, w_3, \ldots, w_T)$$
$$= \log p(w_1 \mid h_1) + \log p(w_2 \mid h_2) + \ldots + \log p(w_2 \mid h_T)$$



Language Modeling

An aside:

- State-of-the-art language models currently tend to rely on **transformer networks** (e.g. GPT-3)
- RNN-LMs comprised most of the early neural LMs that **led to** current SOTA architectures

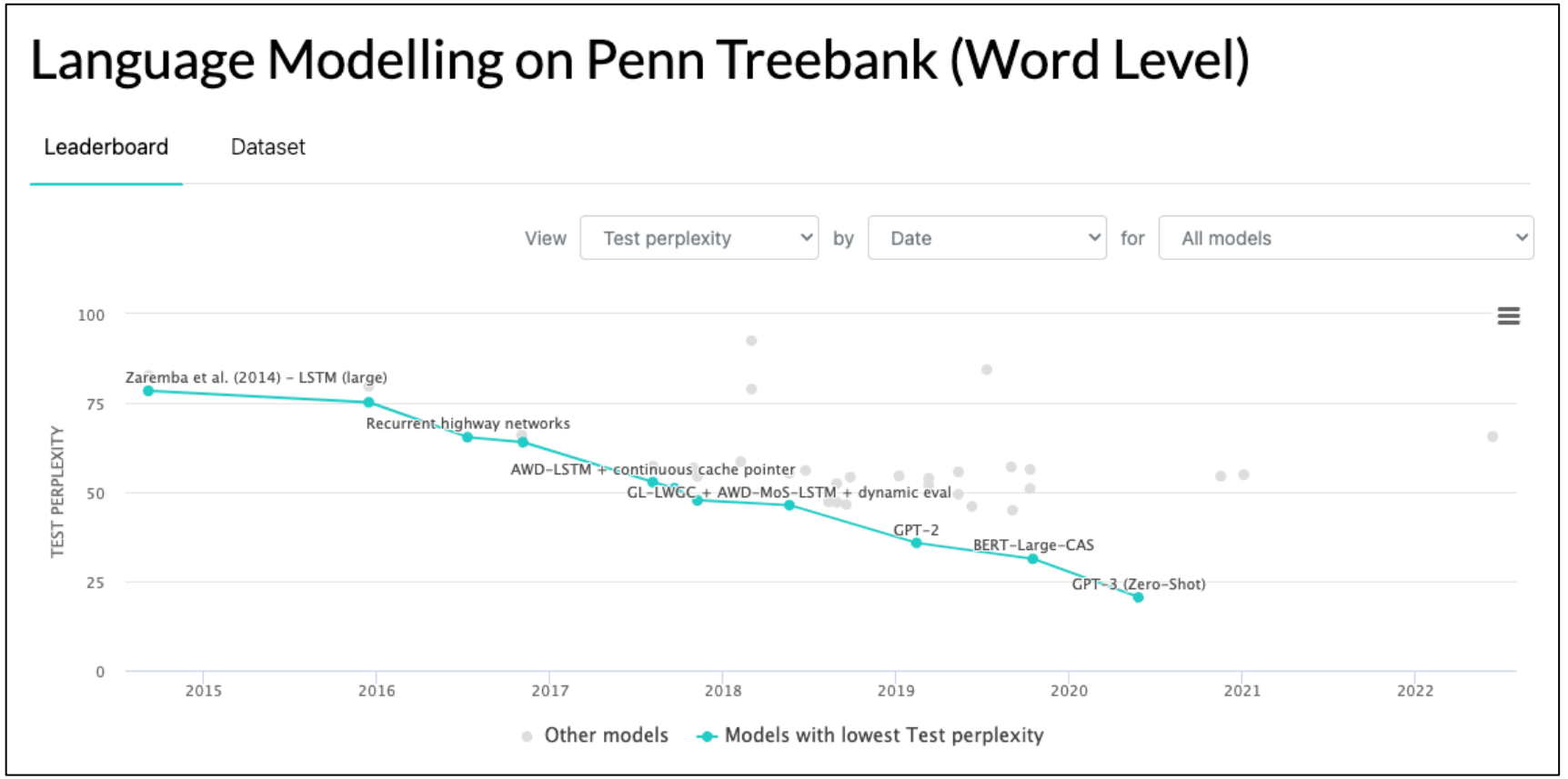


Figure from https://paperswithcode.com/sota/language-modelling-on-penn-treebank-word

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

Why does efficiency matter?

Case Study: GPT-3

- # of training tokens = 500 billion
- # of parameters = 175 billion
- # of cycles = 50 petaflop/s-days (each of which are 8.64e+19 flops)

Dataset	Quantity (tokens)	Weight in training mix	Epochs elapsed when training for 300B tokens
Common Crawl (filtered)	410 billion	60%	0.44
WebText2	19 billion	22%	2.9
Books1	12 billion	8%	1.9
Books2	55 billion	8%	0.43
Wikipedia	3 billion	3%	3.4

Table 2.2: Datasets used to train GPT-3. "Weight in training mix" refers to the fraction of examples during training that are drawn from a given dataset, which we intentionally do not make proportional to the size of the dataset. As a result, when we train for 300 billion tokens, some datasets are seen up to 3.4 times during training while other datasets are seen less than once.

Model Name	n_{params}	n_{layers}	d_{model}	n_{heads}	d_{head}	Batch Size	Learning Rate
GPT-3 Small	125M	12	768	12	64	0.5M	6.0×10^{-4}
GPT-3 Medium	350M	24	1024	16	64	0.5M	3.0×10^{-4}
GPT-3 Large	760M	24	1536	16	96	0.5M	2.5×10^{-4}
GPT-3 XL	1.3B	24	2048	24	128	1M	2.0×10^{-4}
GPT-3 2.7B	2.7B	32	2560	32	80	1M	1.6×10^{-4}
GPT-3 6.7B	6.7B	32	4096	32	128	2M	1.2×10^{-4}
GPT-3 13B	13.0B	40	5140	40	128	2M	1.0×10^{-4}
GPT-3 175B or "GPT-3"	175.0B	96	12288	96	128	3.2M	0.6×10^{-4}

Table 2.1: Sizes, architectures, and learning hyper-parameters (batch size in tokens and learning rate) of the models which we trained. All models were trained for a total of 300 billion tokens.

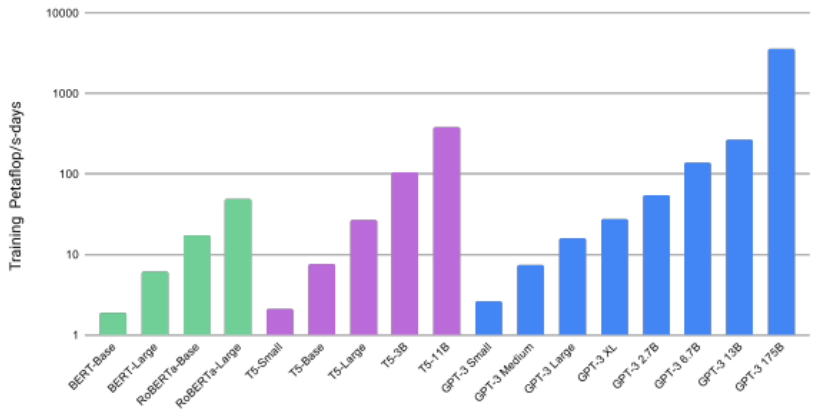


Figure 2.2: Total compute used during training. Based on the analysis in Scaling Laws For Neural Language Models [KMH+20] we train much larger models on many fewer tokens than is typical. As a consequence, although GPT-3 3B is almost 10x larger than RoBERTa-Large (355M params), both models took roughly 50 petaflop/s-days of compute during pre-training. Methodology for these calculations can be found in Appendix D.

Figure from https://arxiv.org/pdf/2005.14165.

Two parts: Deep Learning and Language Modeling

Recap

Deep Learning

- AutoDiff
  - is a tool for **computing gradients** of a differentiable function, b = f(a)
  - the key building block is a **module** with a forward() and backward()
  - sometimes define f as **code** in forward() by chaining existing modules together
- Computation Graphs
  - are another way to define f (more conducive to slides)
  - we are considering various (deep) computation graphs: (1) CNN (2) RNN (3) RNN-LM (4) Transformer-LM
- Learning a Deep Network
  - deep networks (e.g. CNN/RNN) are trained by optimizing an objective function with SGD
  - compute gradients with AutoDiff

Language Modeling

- key idea: condition on previous words to **sample the next word**
- to define the **probability** of the next word…
  - …n-gram LM uses collection of massive 50k-sided **dice**
  - …RNN-LM or Transformer-LM use a **neural network**
- Learning an LM
  - n-gram LMs are easy to learn: just **count** co-occurrences!
  - a RNN-LM / Transformer-LM is trained just like other deep neural networks