



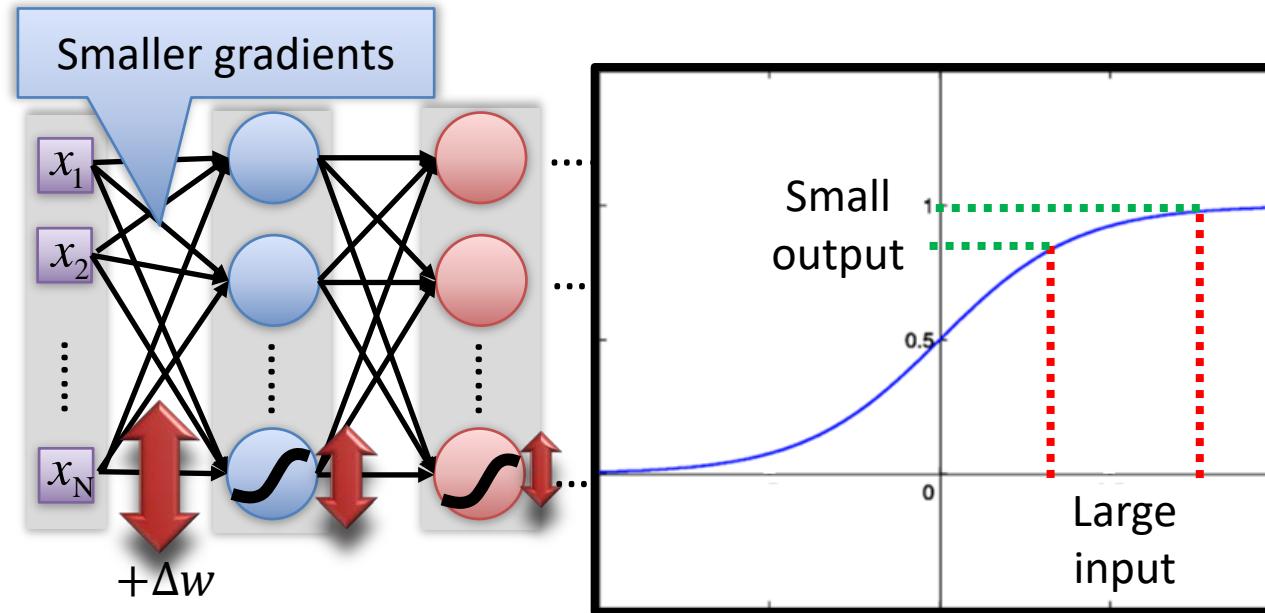
# Master DSAI *Advanced Deep Learning* 2024-2025

*Local correlations to Transformers*

*Frederic Precioso*

*A large set of these slides come from the lecture of Prof. Adriana Kovashka University of Pittsburgh*

# Vanishing gradient problem

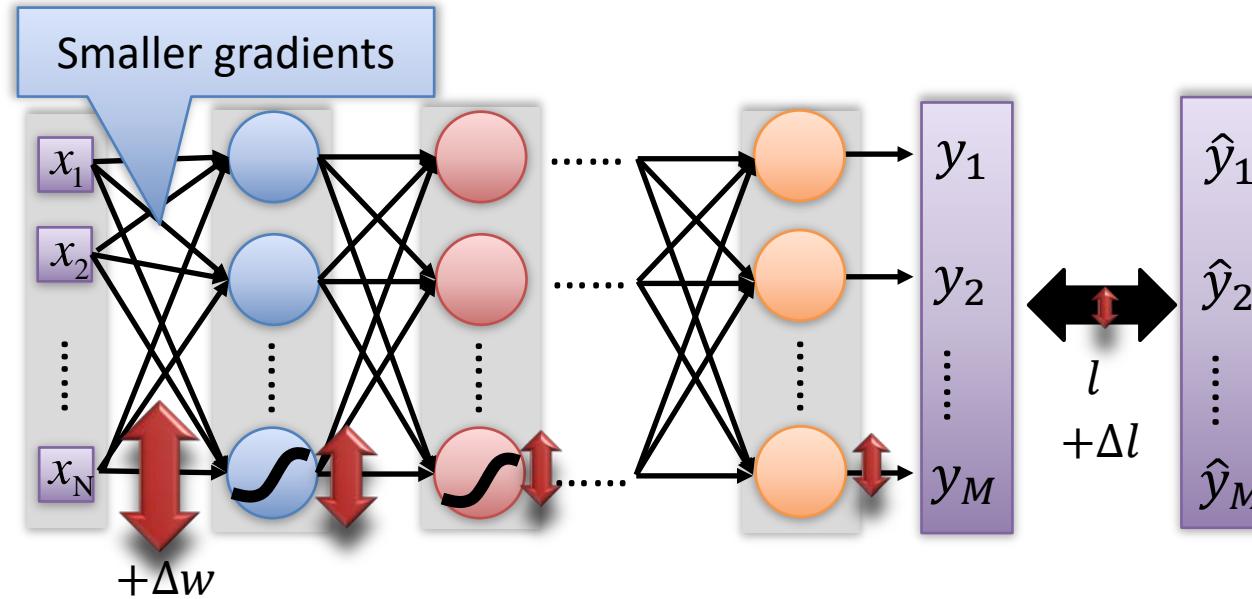


Intuitive way to compute the derivatives ...

$$\frac{\partial l}{\partial w} = ? \frac{\Delta l}{\Delta w}$$



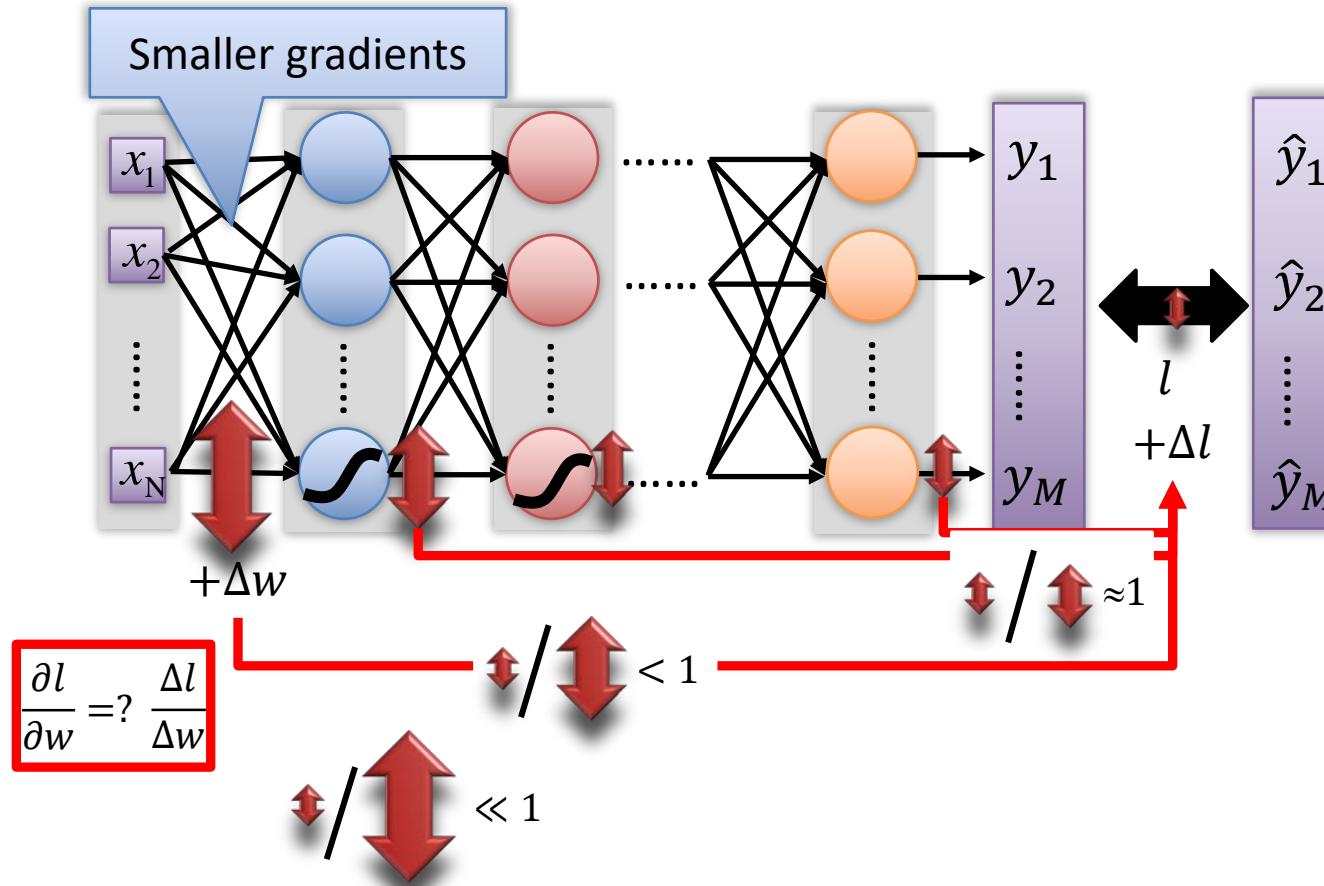
# Vanishing gradient problem



Intuitive way to compute the derivatives ...

$$\frac{\partial l}{\partial w} = ? \quad \frac{\Delta l}{\Delta w}$$

# Vanishing gradient problem





# *Sequential correlations*

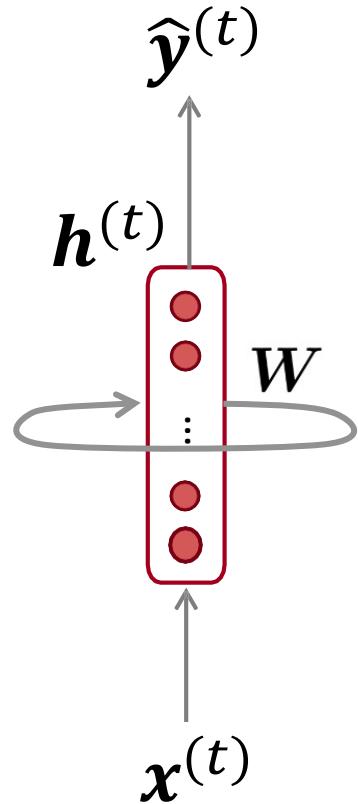
**RECURRENT NEURAL NETWORKS  
(AKA RNN, LSTM / GRU)**



# Recurrent Neural Networks (RNN)

A family of neural architectures

**Core idea:** Apply the same weights  $W$  repeatedly

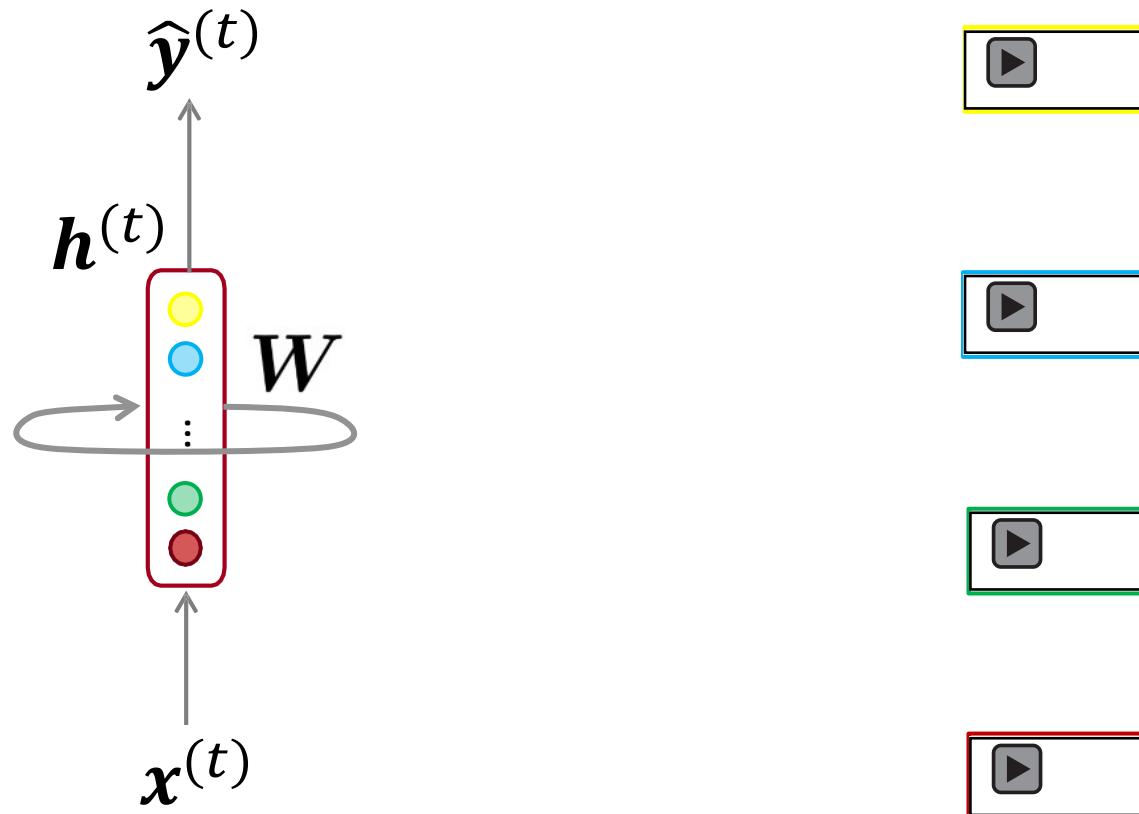




# Recurrent Neural Networks (RNN)

A family of neural architectures

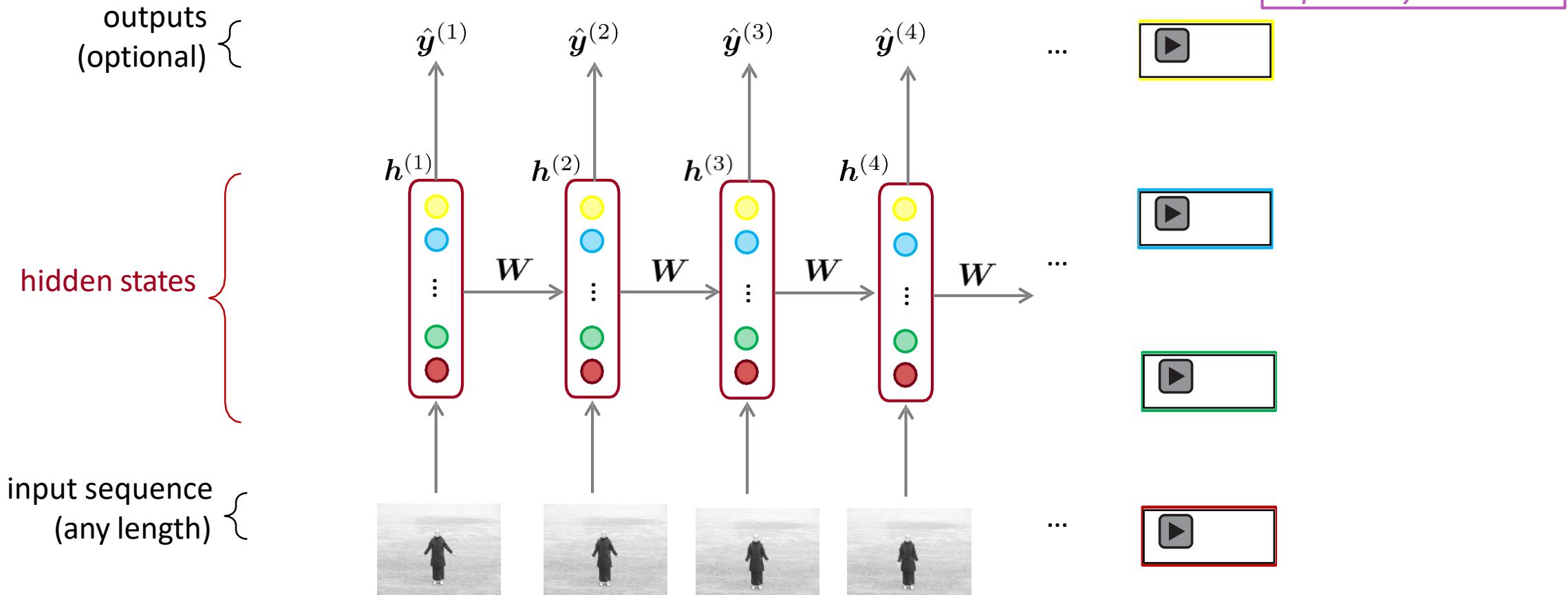
**Core idea:** Apply the same weights  $W$  repeatedly





# Recurrent Neural Networks (RNN)

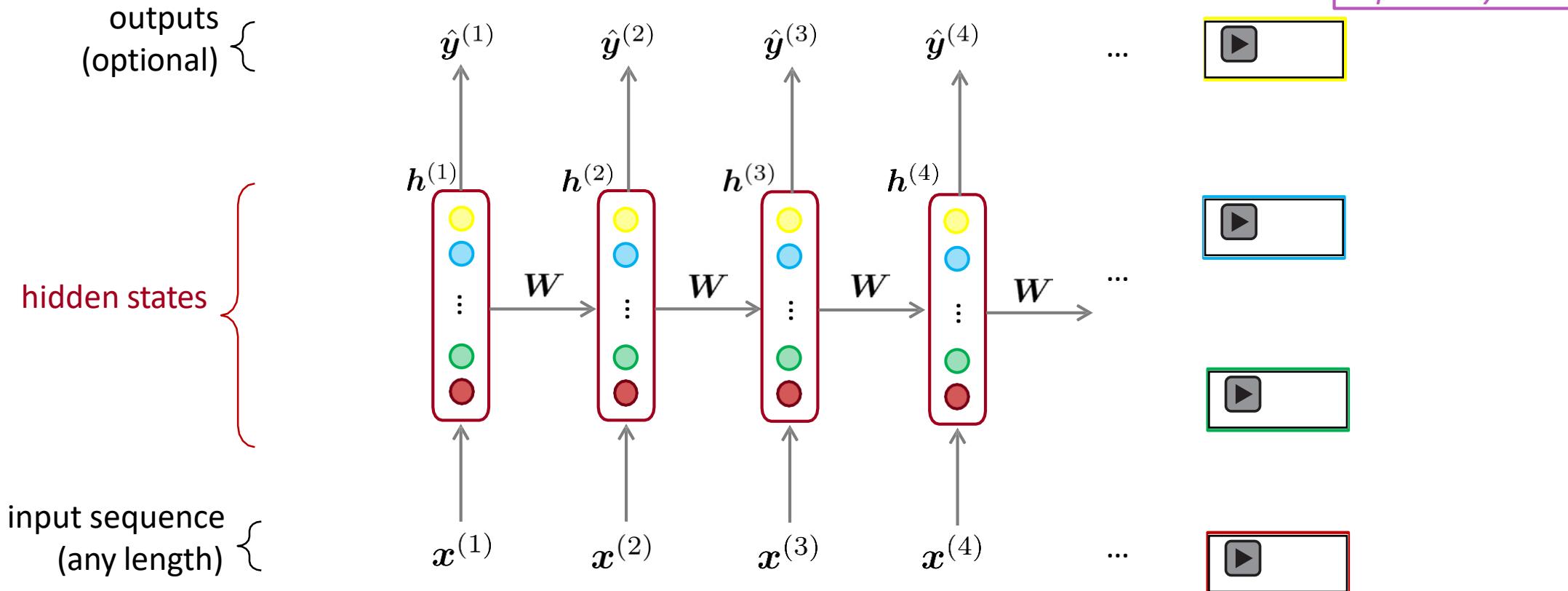
A family of neural architectures





# Recurrent Neural Networks (RNN)

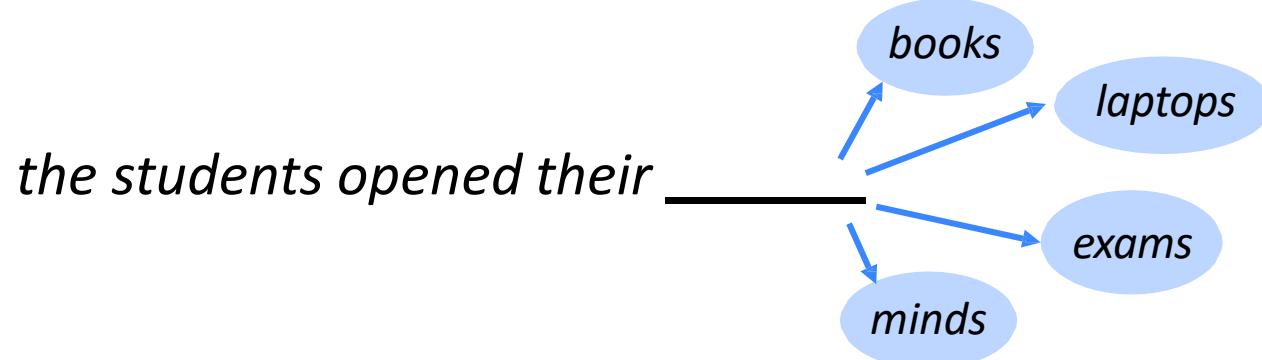
A family of neural architectures





# Language Modeling

- **Language Modeling** is the task of predicting what word comes next.



- More formally: given a sequence of words  $x^{(1)}, x^{(2)}, \dots, x^{(t)}$ , compute the probability distribution of the next word  $x^{(t+1)}$ :

$$P(\mathbf{x}^{(t+1)} | \mathbf{x}^{(t)}, \dots, \mathbf{x}^{(1)})$$

where  $x^{(t+1)}$  can be any word in the vocabulary  $V = \{w_1, \dots, w_{|V|}\}$

- A system that does this is called a **Language Model**.



# n-gram Language Models

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- First we make a **simplifying assumption**:  $x^{(t+1)}$  depends only on the preceding  $n-1$  words.

$$P(x^{(t+1)} | x^{(t)}, \dots, x^{(1)}) = P(x^{(t+1)} | \underbrace{x^{(t)}, \dots, x^{(t-n+2)}}_{n-1 \text{ words}}) \quad (\text{assumption})$$

$$\begin{aligned} \text{prob of a n-gram} &\rightarrow P(x^{(t+1)}, x^{(t)}, \dots, x^{(t-n+2)}) \\ \text{prob of a (n-1)-gram} &= P(x^{(t)}, \dots, x^{(t-n+2)}) \end{aligned} \quad (\text{definition of conditional prob})$$

- **Question:** How do we get these  $n$ -gram and  $(n-1)$ -gram probabilities?
- **Answer:** By **counting** them in some large corpus of text!

$$\approx \frac{\text{count}(x^{(t+1)}, x^{(t)}, \dots, x^{(t-n+2)})}{\text{count}(x^{(t)}, \dots, x^{(t-n+2)})} \quad (\text{statistical approximation})$$



# Sparsity Problems with n-gram Language Models

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## Sparsity Problem 1

**Problem:** What if “students opened their  $w$ ” never occurred in data? Then  $w$  has probability 0!

**(Partial) Solution:** Add small  $\delta$  to the count for every  $w \in V$ . This is called *smoothing*.

$$P(w|\text{students opened their}) = \frac{\text{count}(\text{students opened their } w)}{\text{count}(\text{students opened their})}$$

## Sparsity Problem 2

**Problem:** What if “students opened their” never occurred in data? Then we can’t calculate probability for *any*  $w$ !

**(Partial) Solution:** Just condition on “opened their” instead. This is called *backoff*.

**Note:** Increasing  $n$  makes sparsity problems worse.  
Typically we can’t have  $n$  bigger than 5.



# A fixed-window neural Language Model

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output distribution

$$\hat{y} = \text{softmax}(U\mathbf{h} + \mathbf{b}_2) \in \mathbb{R}^{|V|}$$

hidden layer

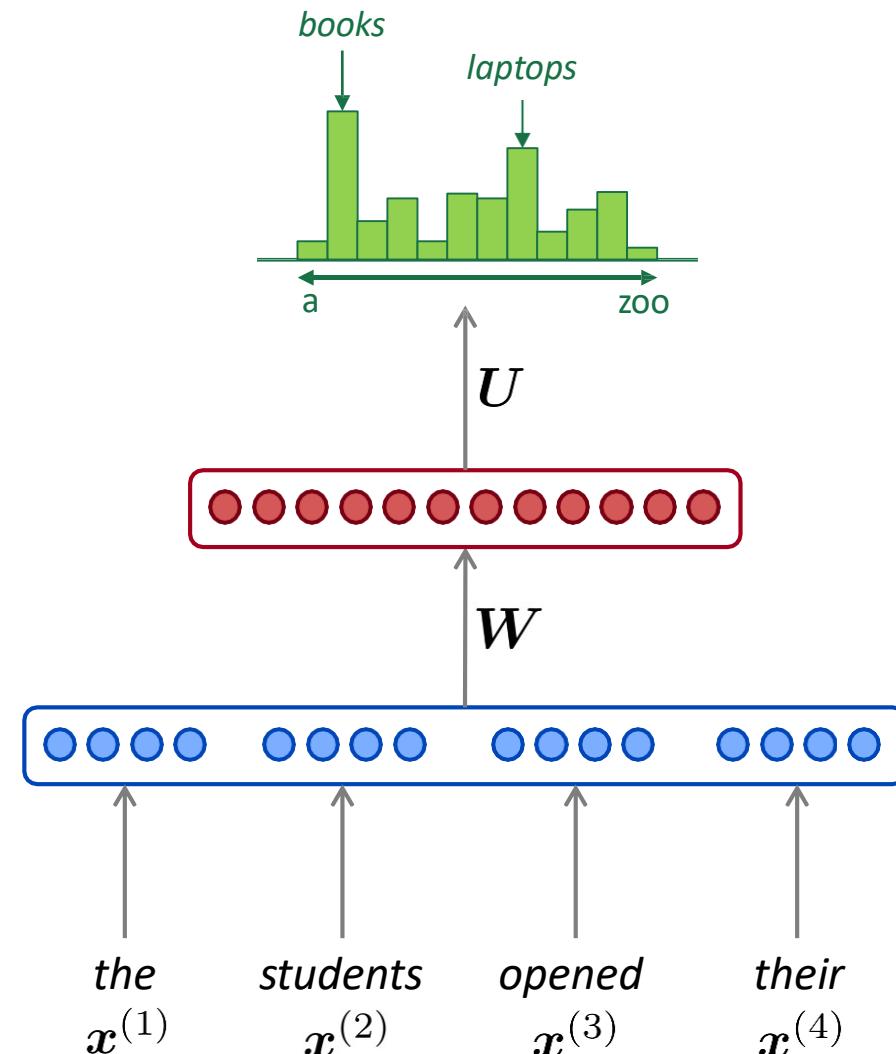
$$\mathbf{h} = f(\mathbf{W}\mathbf{e} + \mathbf{b}_1)$$

concatenated word embeddings

$$\mathbf{e} = [\mathbf{e}^{(1)}; \mathbf{e}^{(2)}; \mathbf{e}^{(3)}; \mathbf{e}^{(4)}]$$

words / one-hot vectors

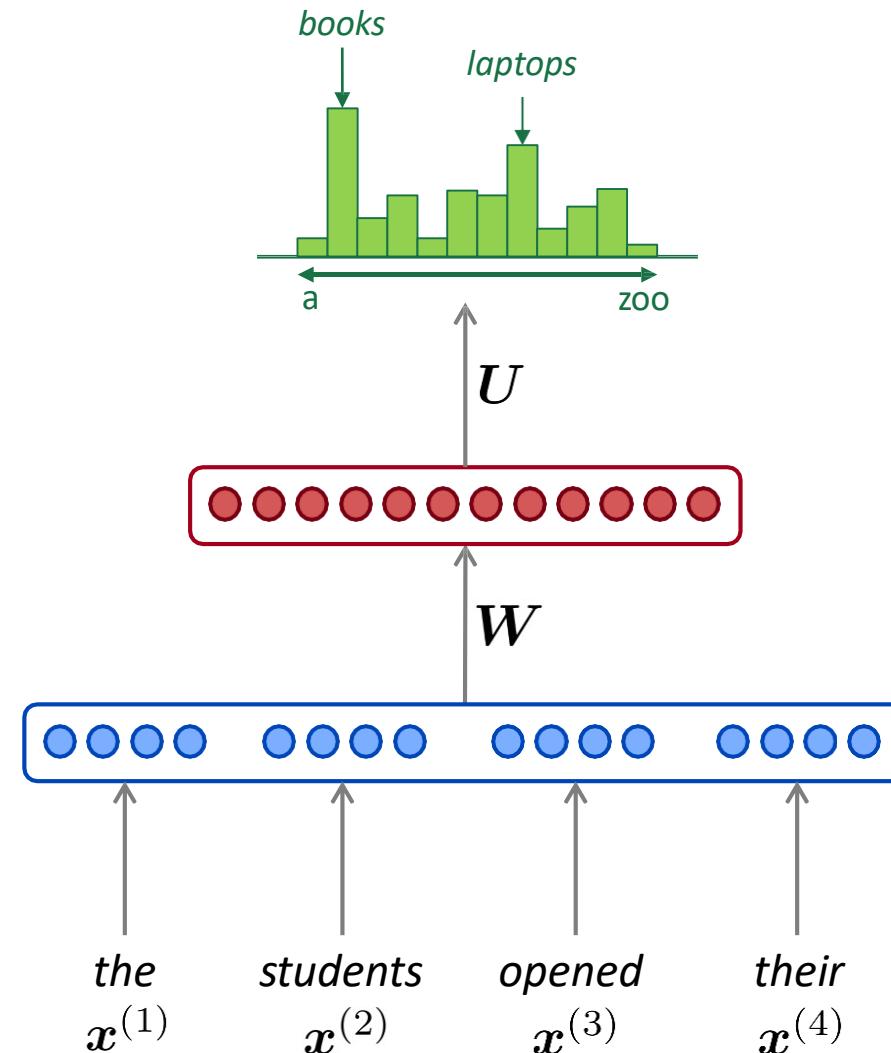
$$\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \mathbf{x}^{(3)}, \mathbf{x}^{(4)}$$



Remaining **problems**:

- Fixed window is **too small**
- Enlarging window enlarges  $W$
- Window can never be large enough!
- $x^{(1)}$  and  $x^{(2)}$  are multiplied by completely different weights in  $W$ .  
**No symmetry** in how the inputs are processed.

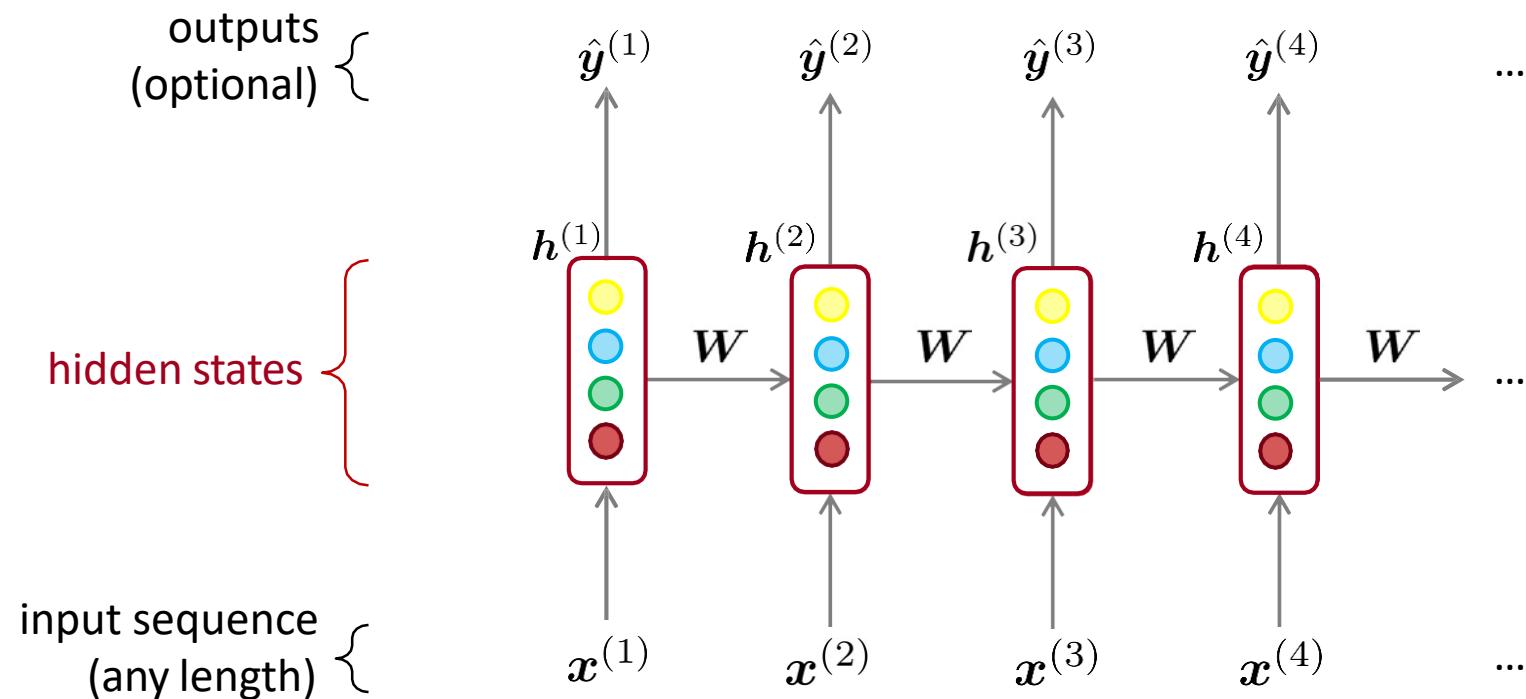
We need a neural architecture that can process *any length input*





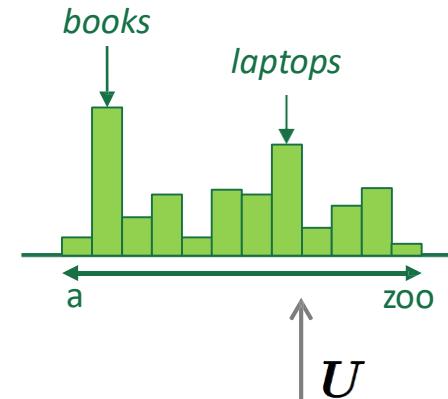
# Recurrent Neural Networks (RNN)

A family of neural architectures



**Core idea:** Apply the same weights  $W$  repeatedly

# A RNN Language Model

 $\hat{y}^{(4)} = P(\mathbf{x}^{(5)} | \text{the students opened their})$ 


output distribution

$$\hat{y}^{(t)} = \text{softmax}(\mathbf{U}\mathbf{h}^{(t)} + \mathbf{b}_2) \in \mathbb{R}^{|V|}$$

hidden states

$$\mathbf{h}^{(t)} = \sigma(\mathbf{W}_h \mathbf{h}^{(t-1)} + \mathbf{W}_e \mathbf{e}^{(t)} + \mathbf{b}_1)$$

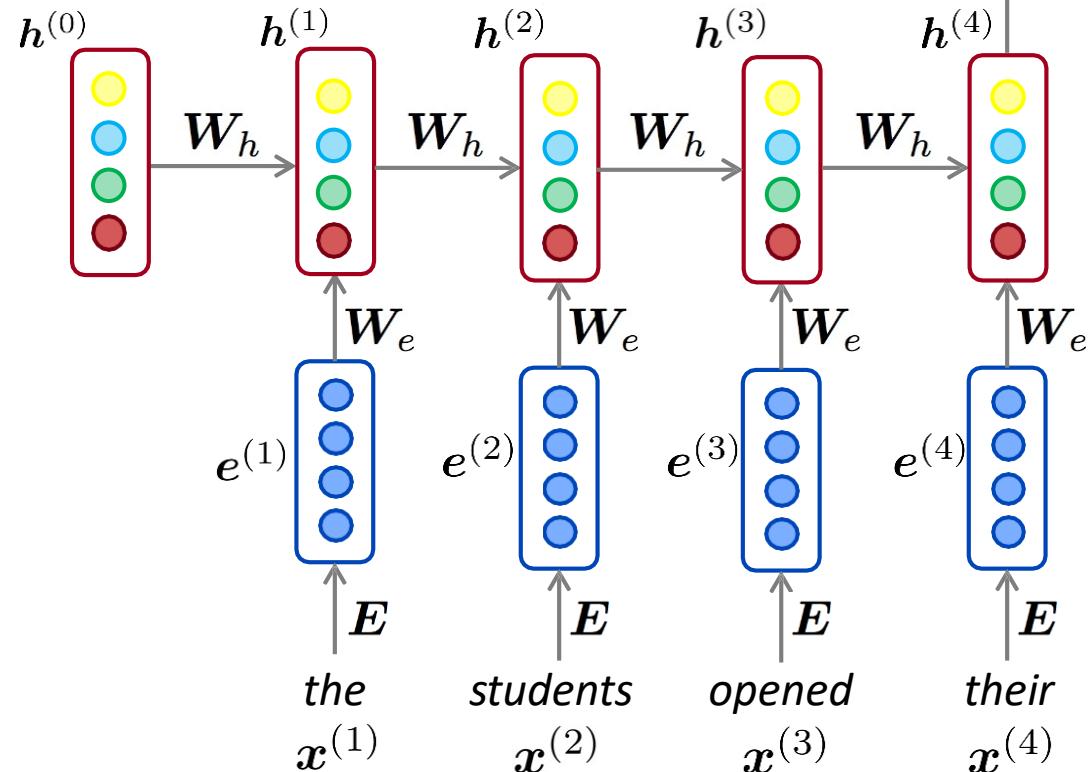
$\mathbf{h}^{(0)}$  is the initial hidden state

word embeddings

$$\mathbf{e}^{(t)} = \mathbf{E}\mathbf{x}^{(t)}$$

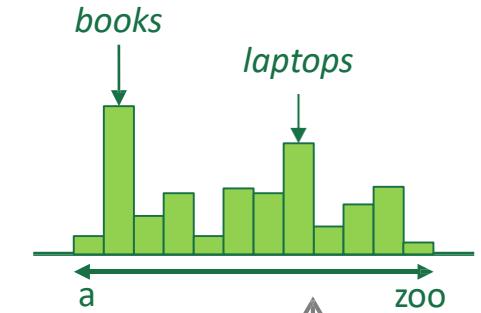
words / one-hot vectors

$$\mathbf{x}^{(t)} \in \mathbb{R}^{|V|}$$



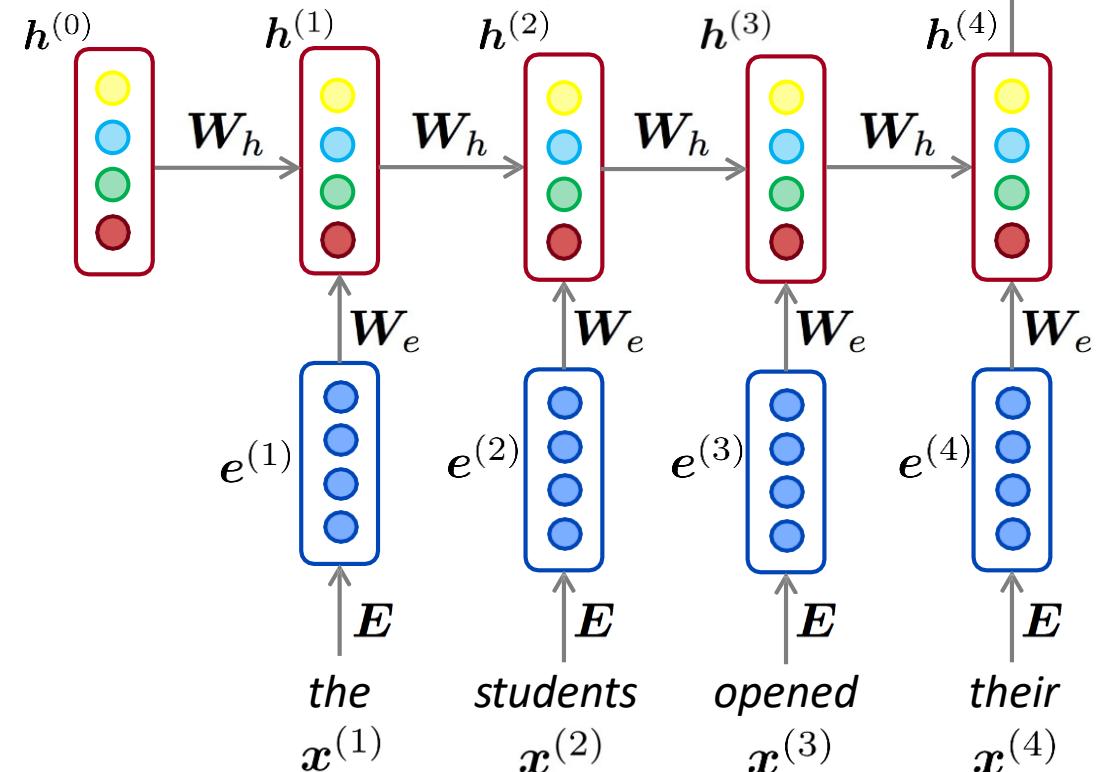
*Note:* this input sequence could be much longer, but this slide doesn't have space!

# A RNN Language Model

 $\hat{y}^{(4)} = P(\mathbf{x}^{(5)} | \text{the students opened their})$ 


## RNN Advantages:

- Can process **any length** input
- Computation for step  $t$  can (in theory) use information from **many steps back**
- **Model size doesn't increase** for longer input
- Same weights applied on every timestep, so there is **symmetry** in how inputs are processed





# Recall: Training a RNN Language Model

- Get a **big corpus of text** which is a sequence of words  $x^{(1)}, \dots, x^{(T)}$
- Feed into RNN-LM; compute output distribution  $\hat{y}^{(t)}$  **for every step  $t$ .**
  - i.e. predict probability distribution of *every word*, given words so far
- **Loss function** on step  $t$  is **cross-entropy** between predicted probability distribution  $\hat{y}^{(t)}$ , and the true next word  $y^{(t)}$  (one-hot for  $x^{(t+1)}$ ):

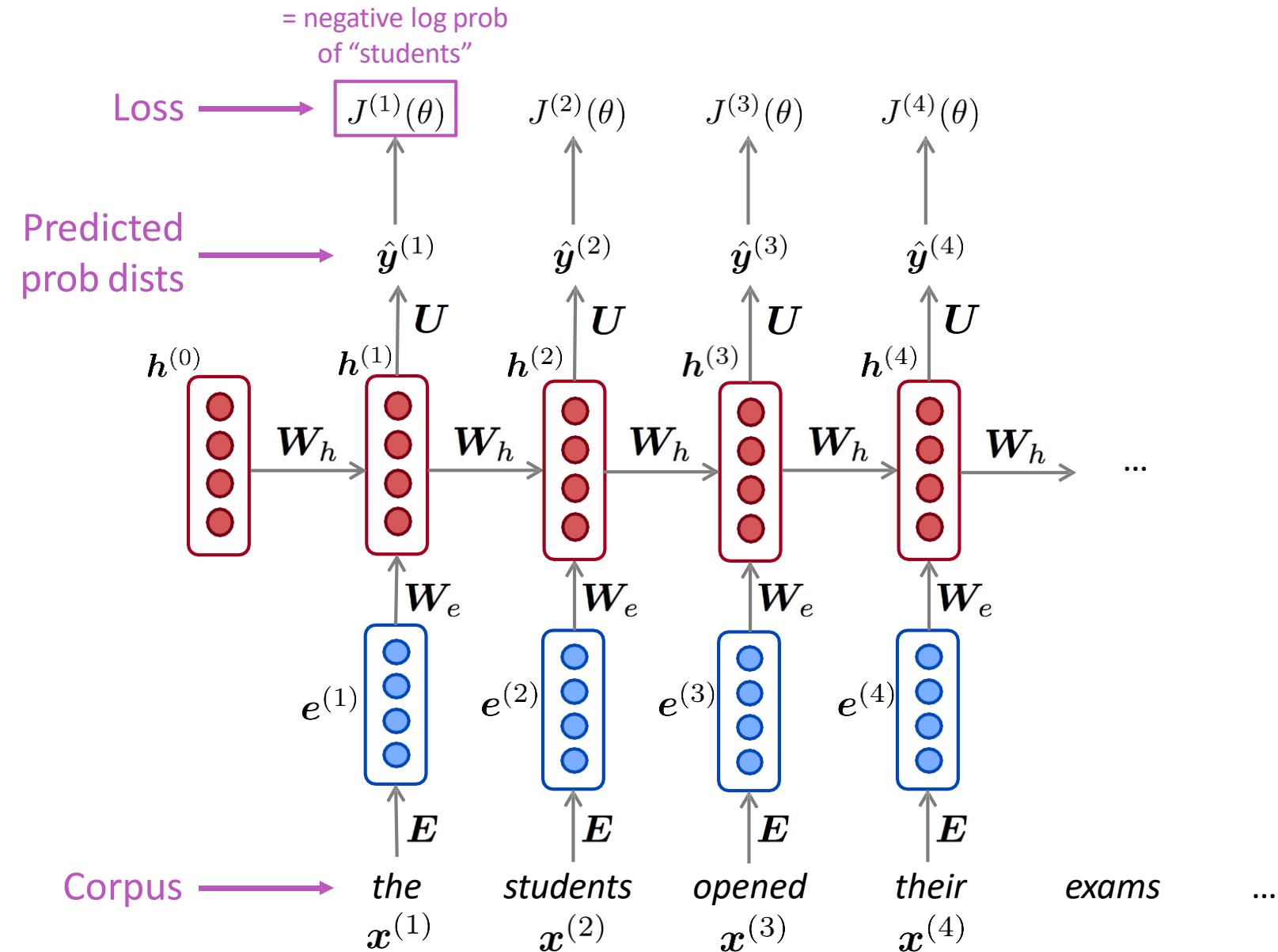
$$J^{(t)}(\theta) = CE(y^{(t)}, \hat{y}^{(t)}) = - \sum_{w \in V} y_w^{(t)} \log \hat{y}_w^{(t)} = - \log \hat{y}_{x_{t+1}}^{(t)}$$

- Average this to get **overall loss** for entire training set:

$$J(\theta) = \frac{1}{T} \sum_{t=1}^T J^{(t)}(\theta) = \frac{1}{T} \sum_{t=1}^T - \log \hat{y}_{x_{t+1}}^{(t)}$$

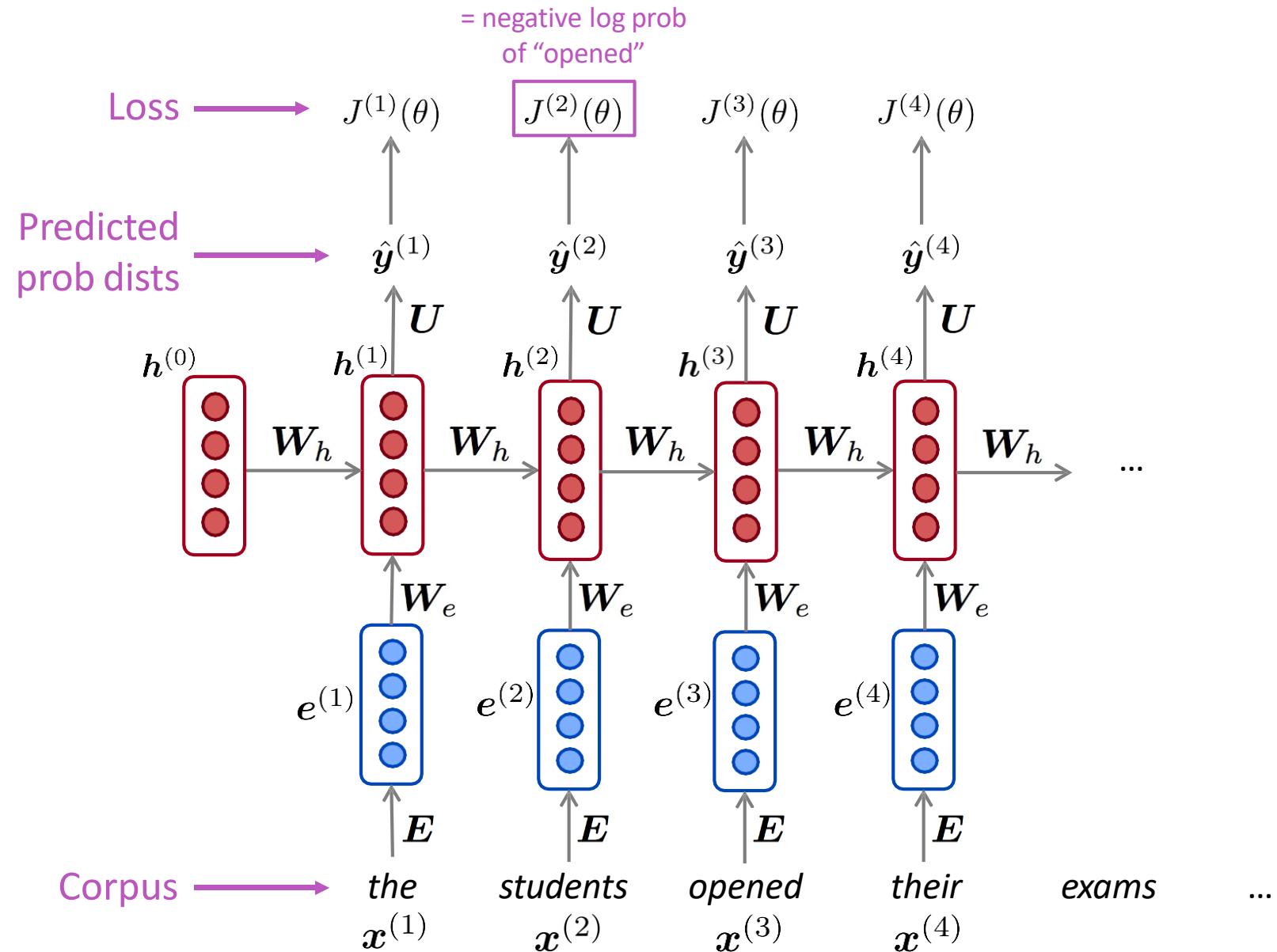


# Training a RNN Language Model

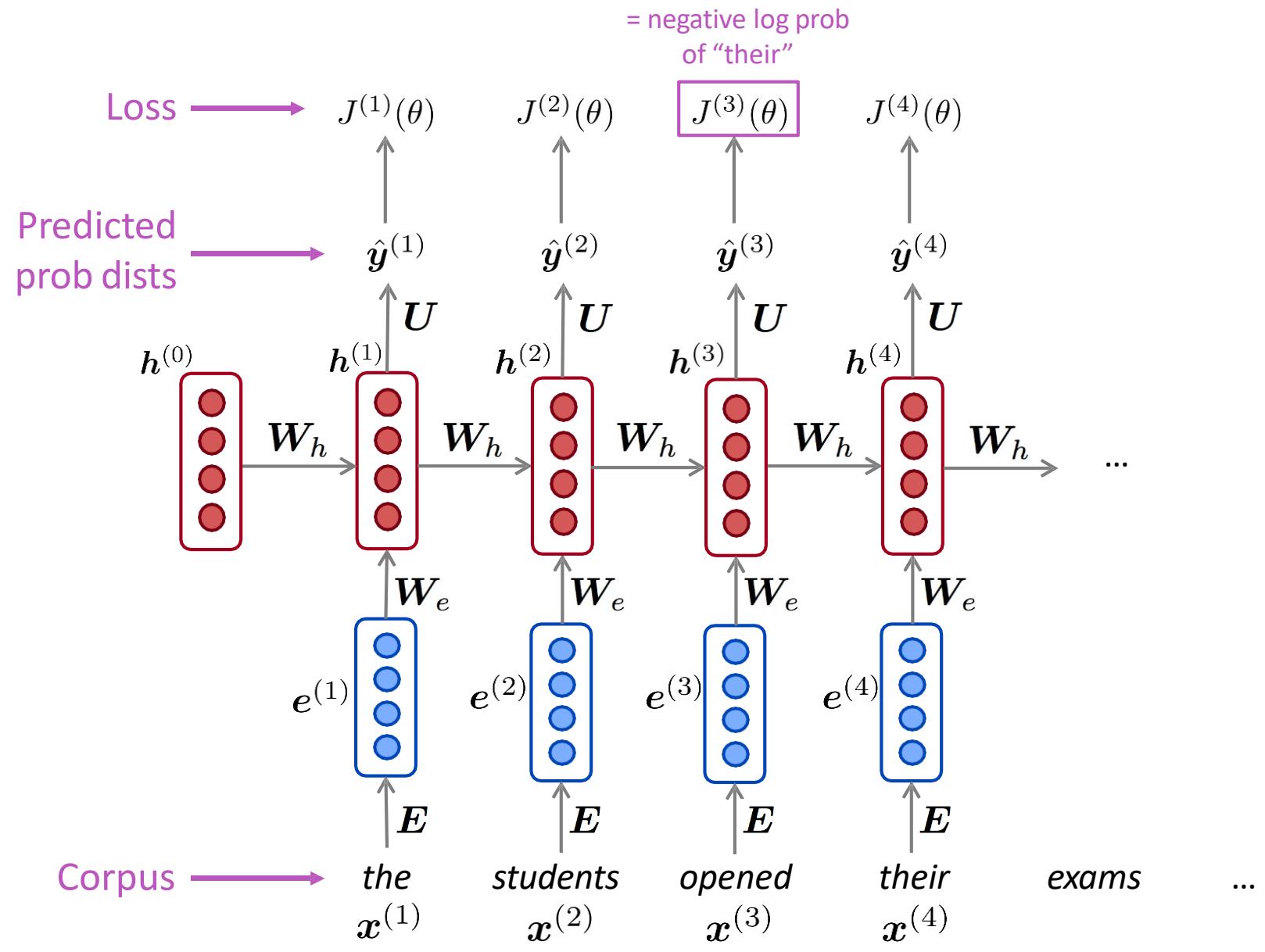




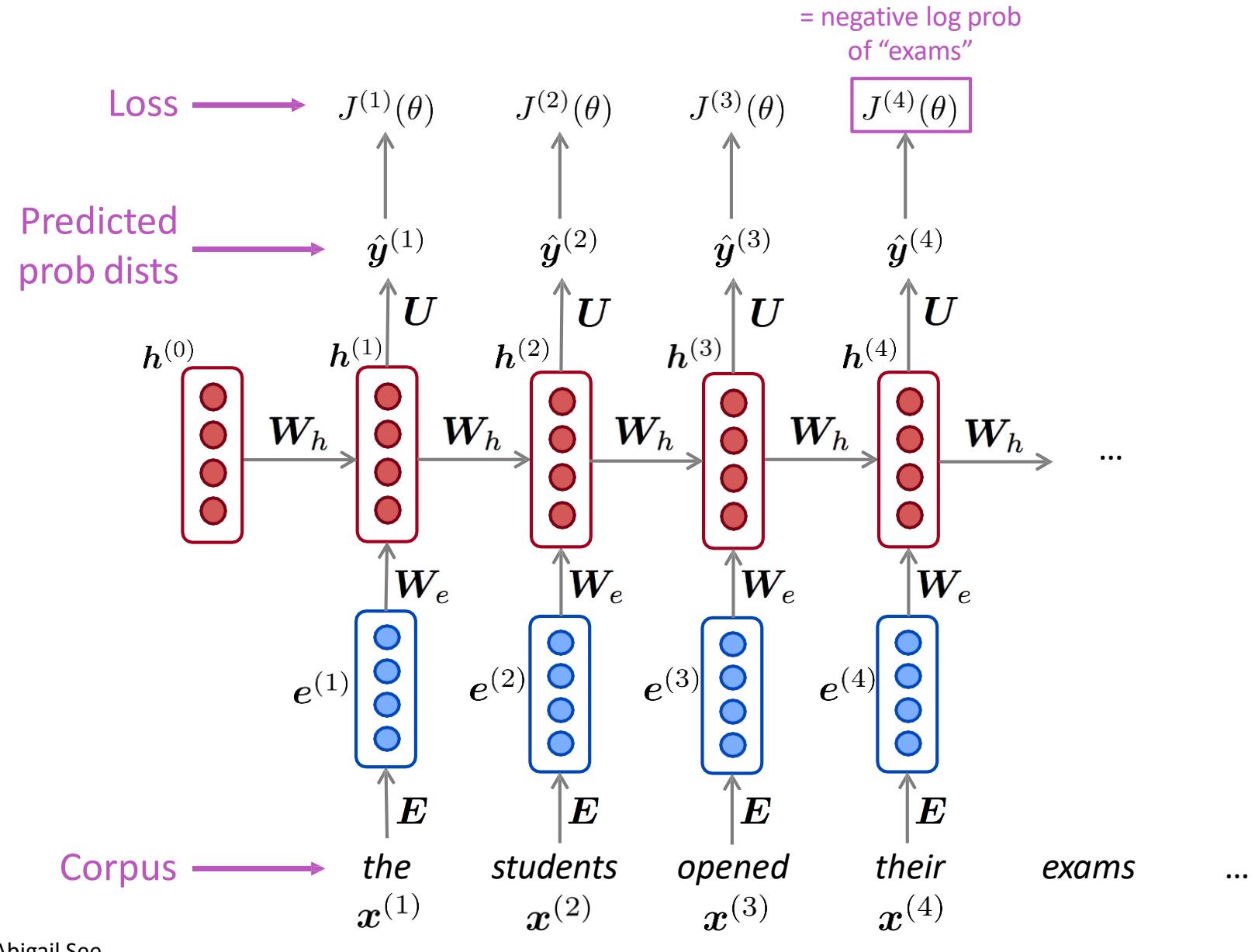
# Training a RNN Language Model



# Training a RNN Language Model



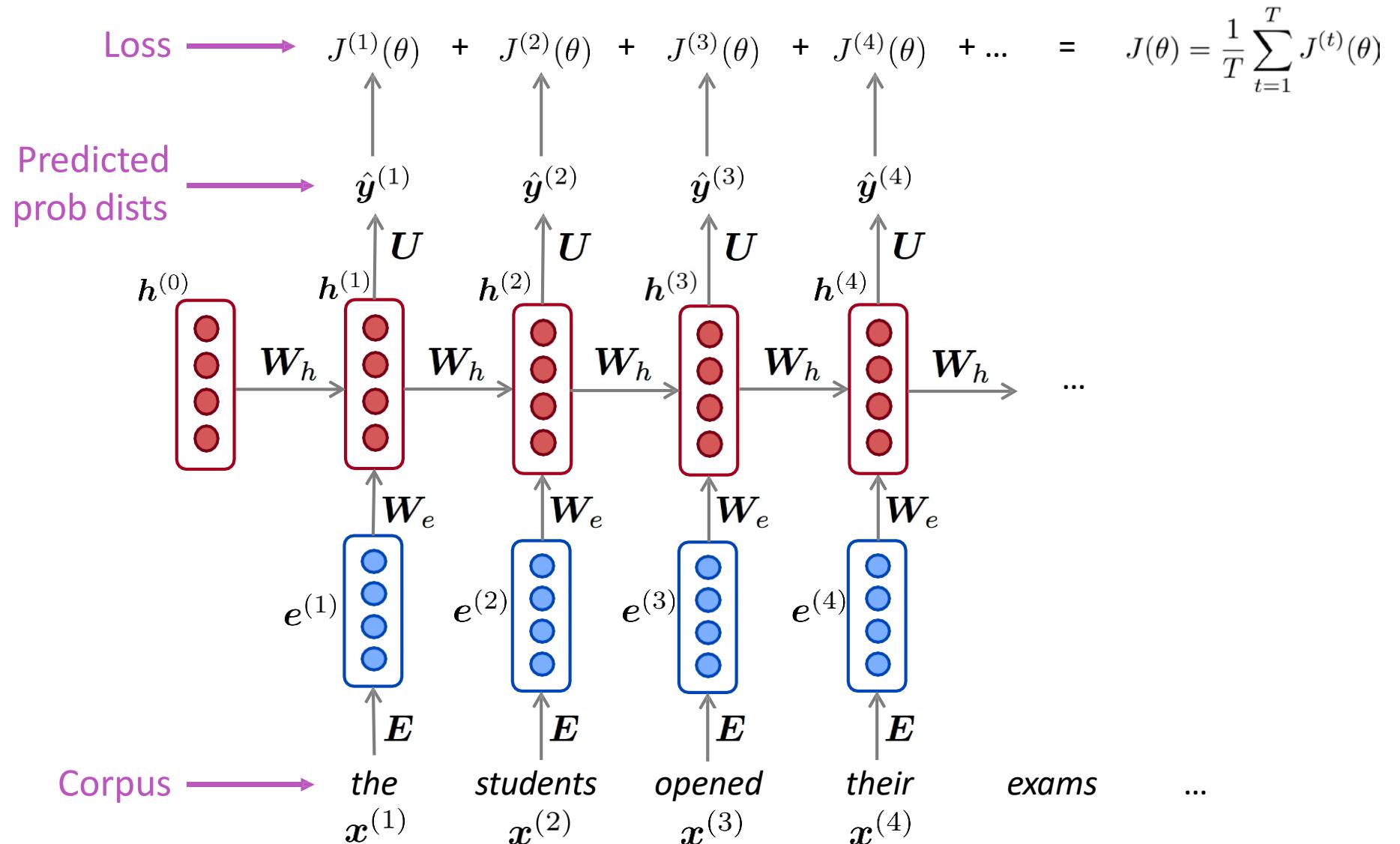
# Training a RNN Language Model





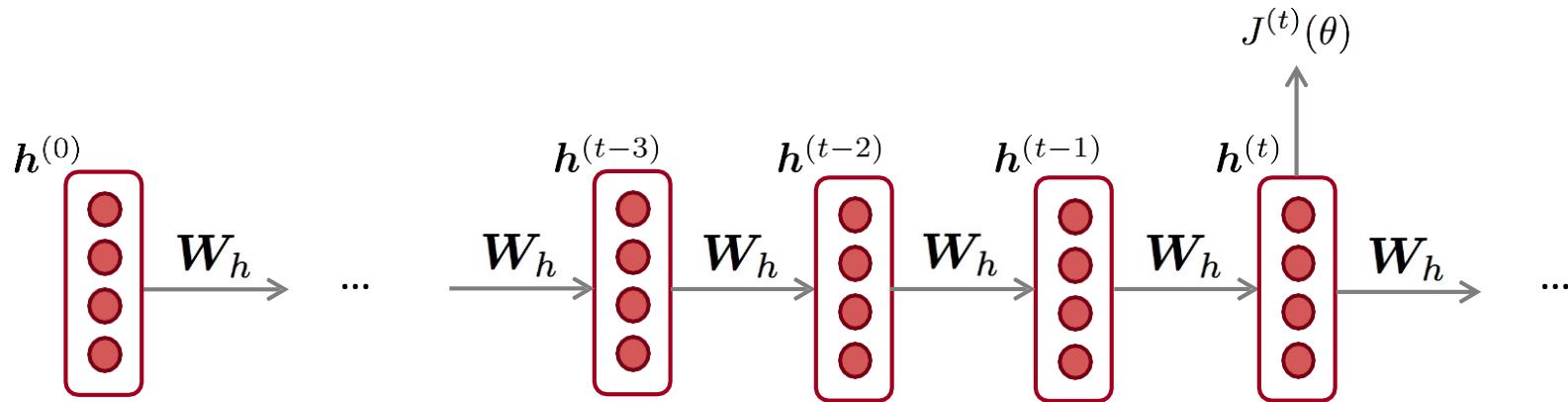
# Training a RNN Language Model

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# Backpropagation for RNNs



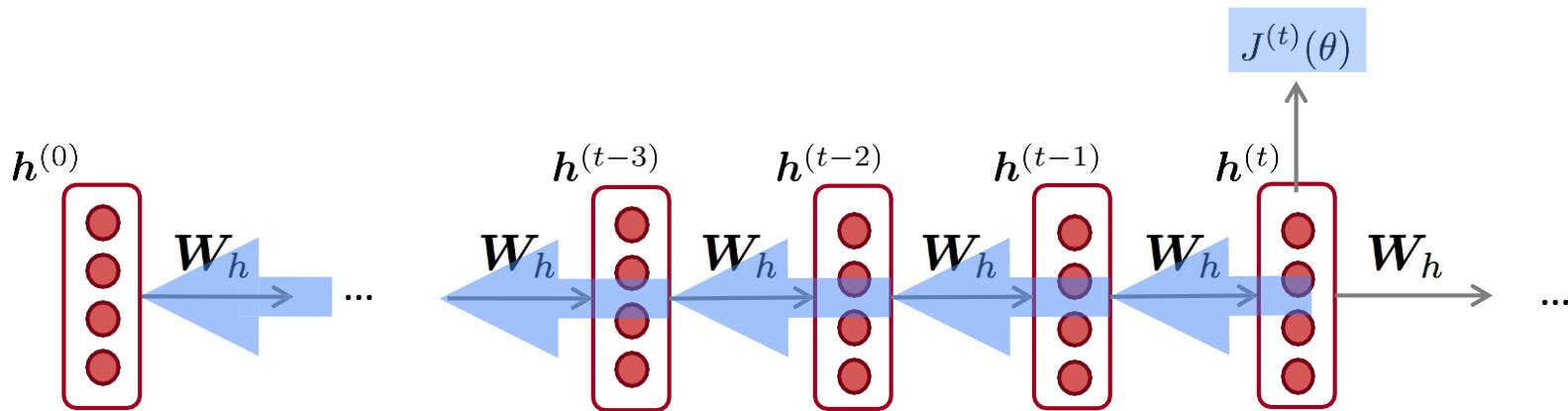
**Question:** What's the derivative of  $J^{(t)}(\theta)$  w.r.t. the **repeated** weight matrix  $W_h$  ?

**Answer:** 
$$\frac{\partial J^{(t)}}{\partial W_h} = \sum_{i=1}^t \frac{\partial J^{(t)}}{\partial W_h} \Big|_{(i)}$$

"The gradient w.r.t. a repeated weight is the sum of the gradient w.r.t. each time it appears"



# Backpropagation for RNNs

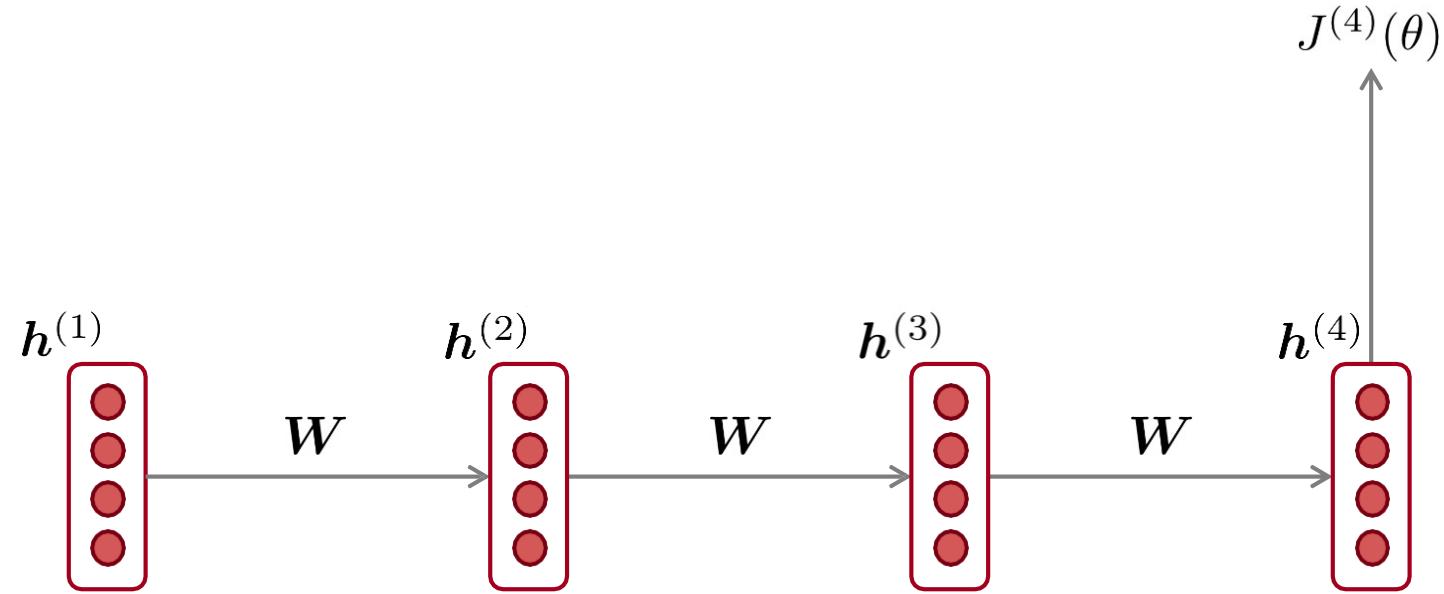


$$\frac{\partial J^{(t)}}{\partial W_h} = \sum_{i=1}^t \left. \frac{\partial J^{(t)}}{\partial W_h} \right|_{(i)}$$

Question: How do we calculate this?

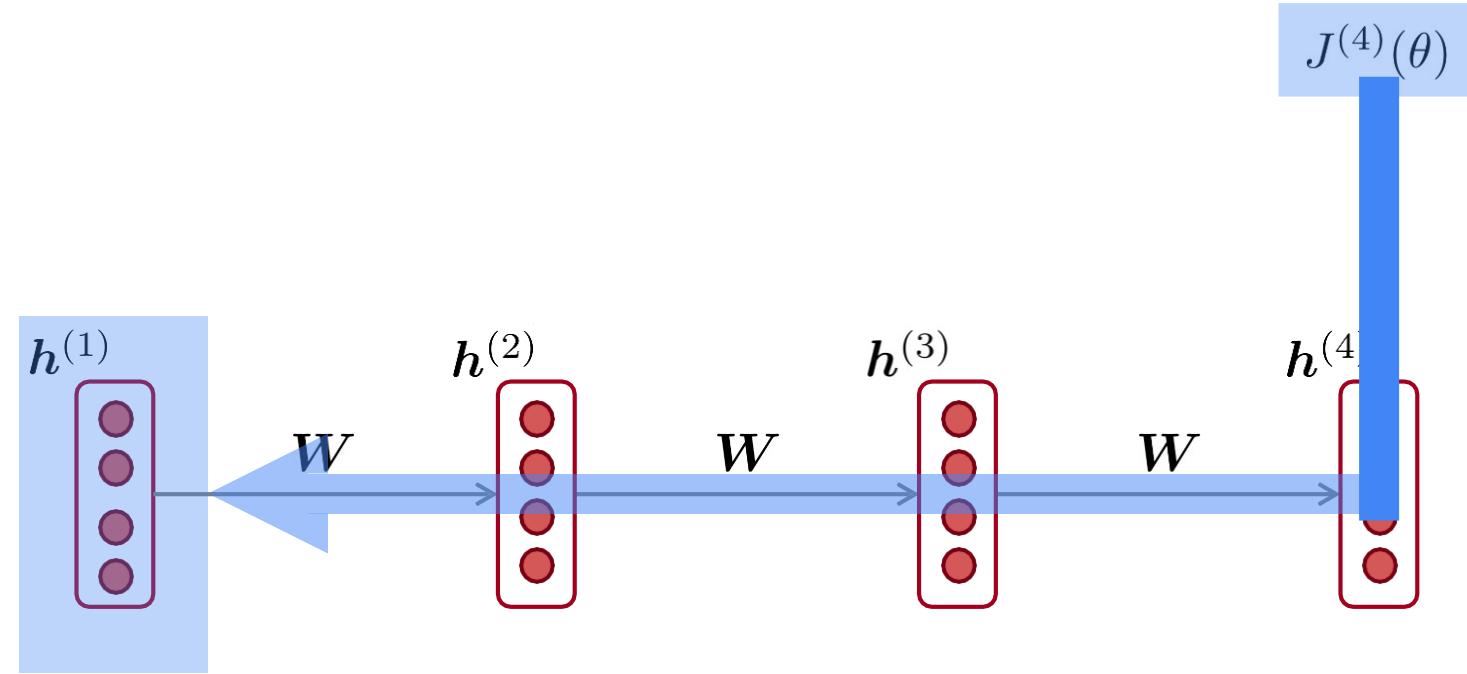
Answer: Backpropagate over timesteps  $i=t, \dots, 0$ , summing gradients as you go.  
This algorithm is called “backpropagation through time”

# Vanishing gradient intuition



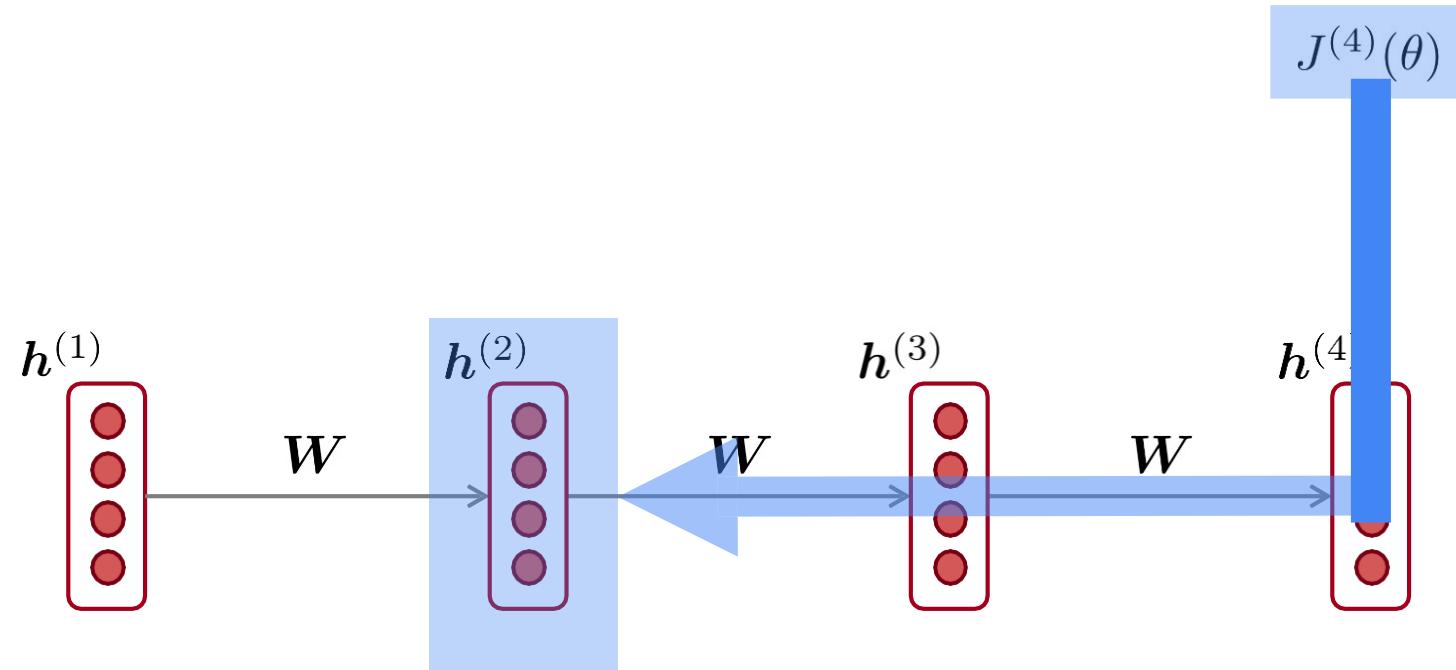


# Vanishing gradient intuition



$$\frac{\partial J^{(4)}}{\partial h^{(1)}} = ?$$

# Vanishing gradient intuition

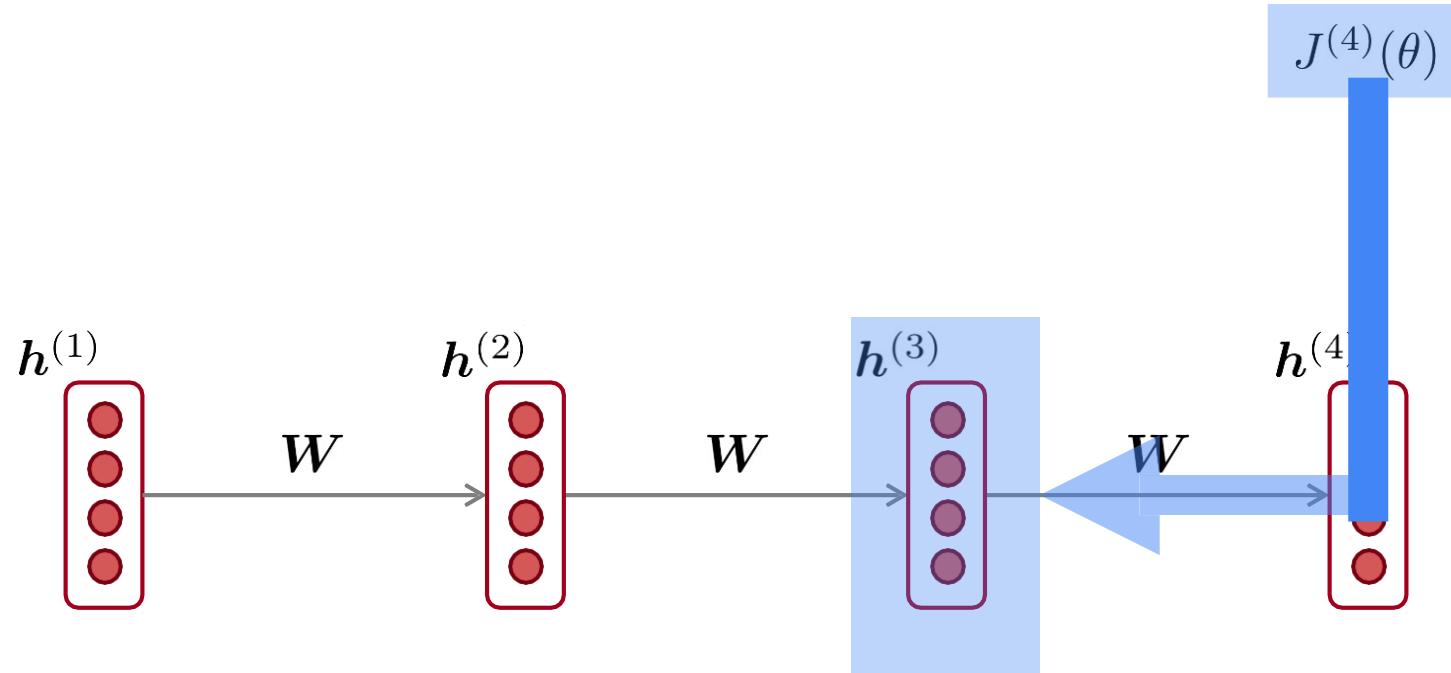


$$\frac{\partial J^{(4)}}{\partial h^{(1)}} = \frac{\partial h^{(2)}}{\partial h^{(1)}} \times \frac{\partial J^{(4)}}{\partial h^{(2)}}$$

chain rule!



# Vanishing gradient intuition

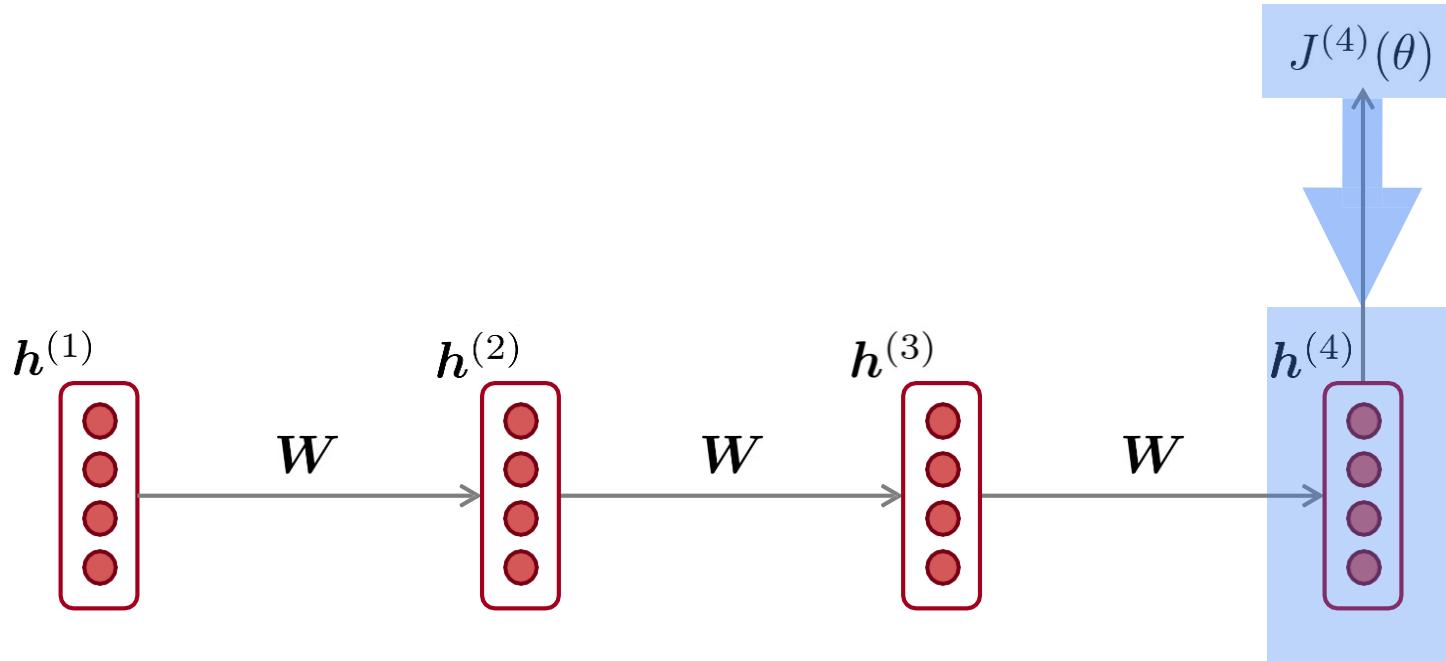


$$\frac{\partial J^{(4)}}{\partial \mathbf{h}^{(1)}} = \frac{\partial \mathbf{h}^{(2)}}{\partial \mathbf{h}^{(1)}} \times$$

$$\frac{\partial \mathbf{h}^{(3)}}{\partial \mathbf{h}^{(2)}} \times \frac{\partial J^{(4)}}{\partial \mathbf{h}^{(3)}}$$

chain rule!

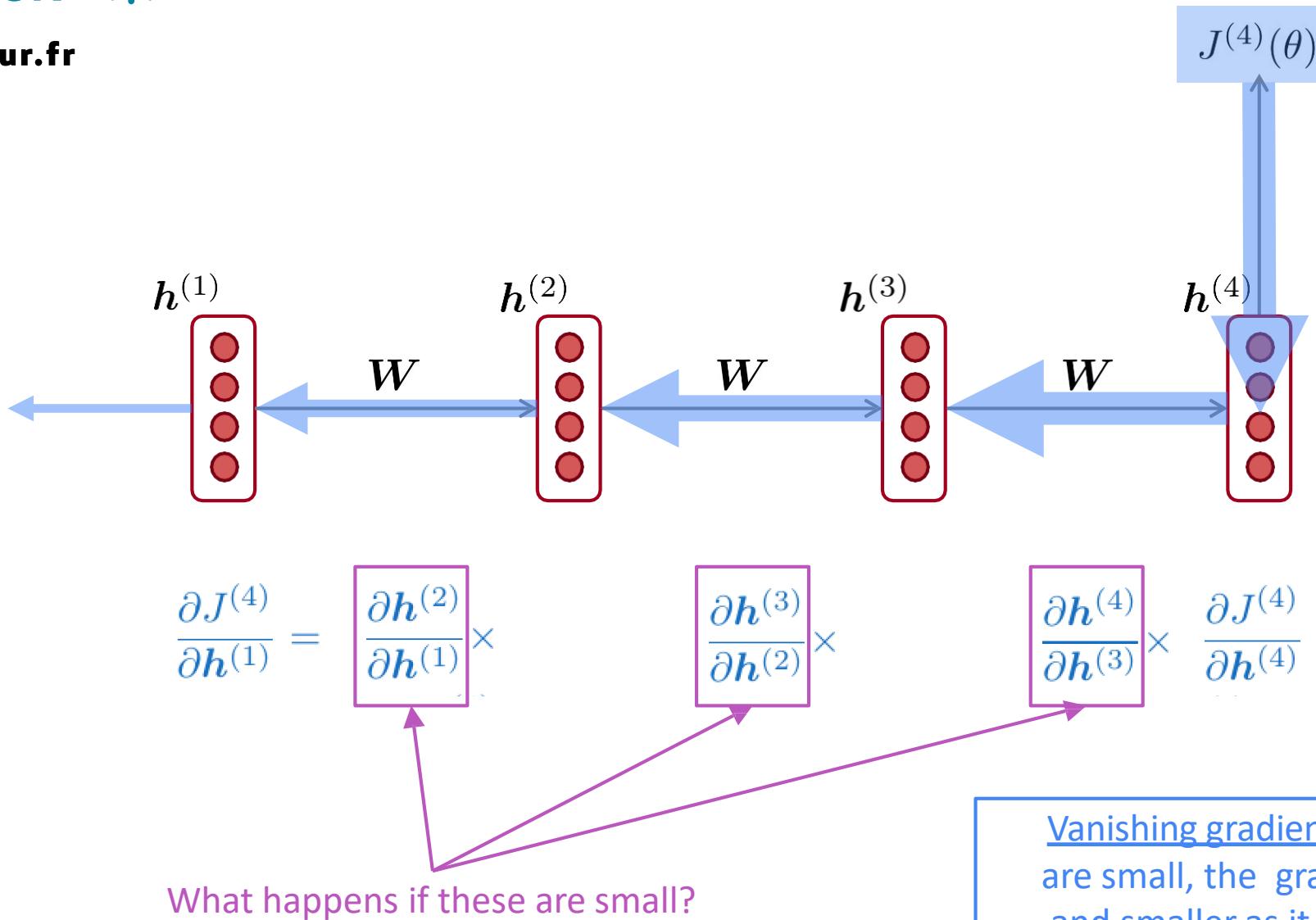
# Vanishing gradient intuition



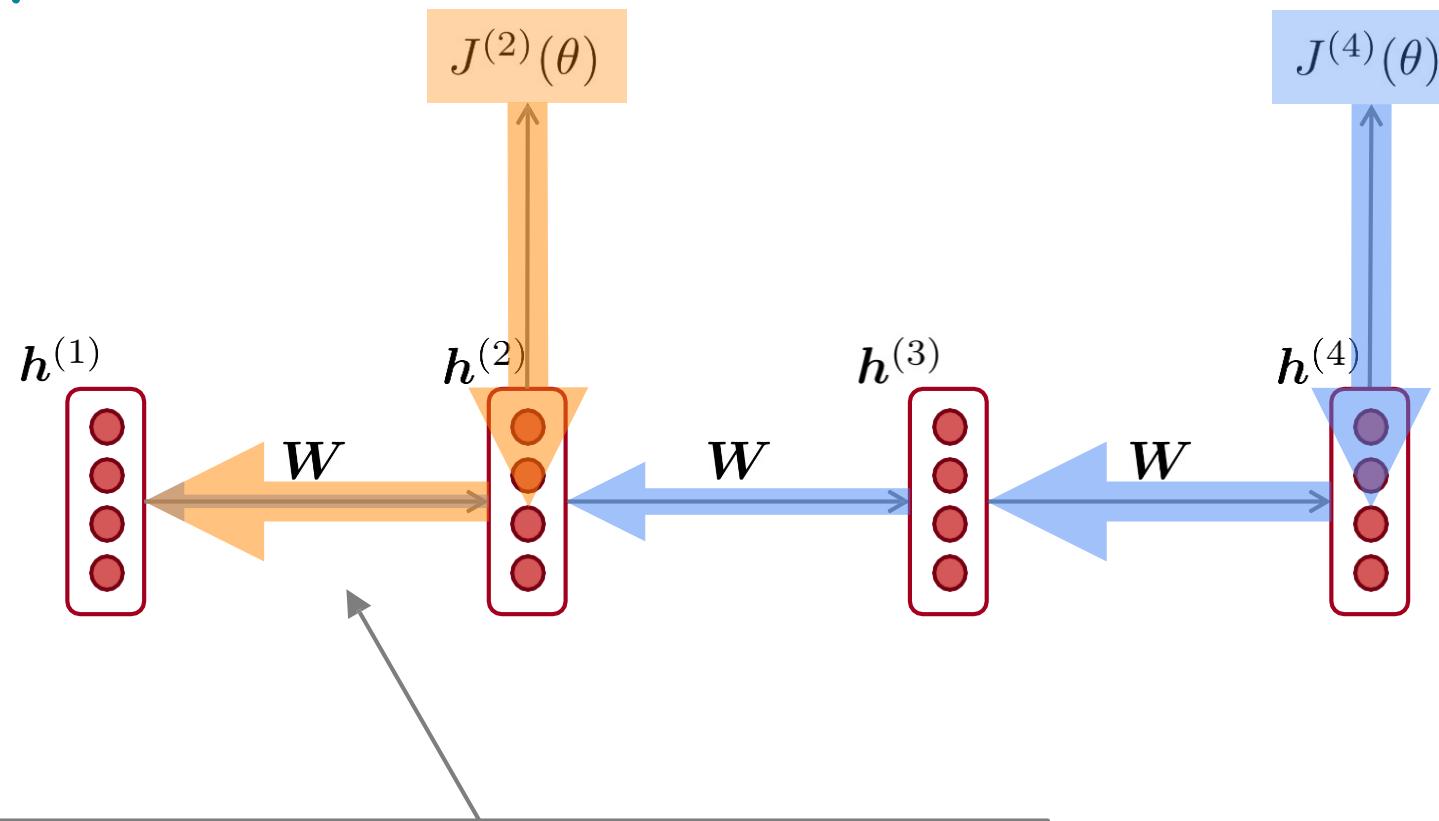
$$\frac{\partial J^{(4)}}{\partial h^{(1)}} = \frac{\partial h^{(2)}}{\partial h^{(1)}} \times \frac{\partial h^{(3)}}{\partial h^{(2)}} \times \frac{\partial h^{(4)}}{\partial h^{(3)}} \times \frac{\partial J^{(4)}}{\partial h^{(4)}}$$

chain rule!

# Vanishing gradient intuition



# Why is vanishing gradient a problem?



Gradient signal from faraway is lost because it's much smaller than gradient signal from close-by.

So model weights are only updated only with respect to near effects, not long-term effects.



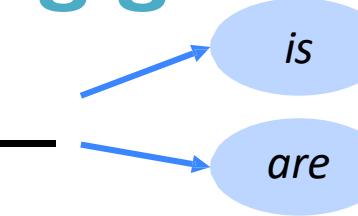
# Effect of vanishing gradient on RNN-LM

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- LM task: *When she tried to print her \_\_\_\_\_, she found that the printer was out of toner. She went to the stationery store to buy more toner. It was very overpriced. After installing the toner into the printer, she finally printed her tickets.*
- To learn from this training example, the RNN-LM needs to model the dependency between “tickets” on the 7<sup>th</sup> step and the target word “tickets” at the end.
- But if gradient is small, the model can't learn this dependency
  - So the model is unable to predict similar long-distance dependencies at test time



# Effect of vanishing gradient on RNN-LM

- LM task: *The writer of the books* 
- Correct answer: *The writer of the books is planning a sequel*
- Syntactic recency: *The writer of the books is* (correct)
- Sequential recency: *The writer of the books are* (incorrect)
- Due to vanishing gradient, RNN-LMs are better at learning from sequential recency than syntactic recency, so they make this type of error more often than we'd like [Linzen et al 2016]

# Why is exploding gradient a problem?

- If the gradient becomes too big, then the SGD update step becomes too big:

$$\theta^{new} = \theta^{old} - \overbrace{\alpha \nabla_{\theta} J(\theta)}^{\text{gradient}}$$

learning rate

- This can cause **bad updates**: we take too large a step and reach a bad parameter configuration (with large loss)
- In the worst case, this will result in **Inf** or **NaN** in your network (then you have to restart training from an earlier checkpoint)

# Gradient clipping: solution for exploding gradient

- Gradient clipping: if the norm of the gradient is greater than some threshold, scale it down before applying SGD update

---

**Algorithm 1** Pseudo-code for norm clipping

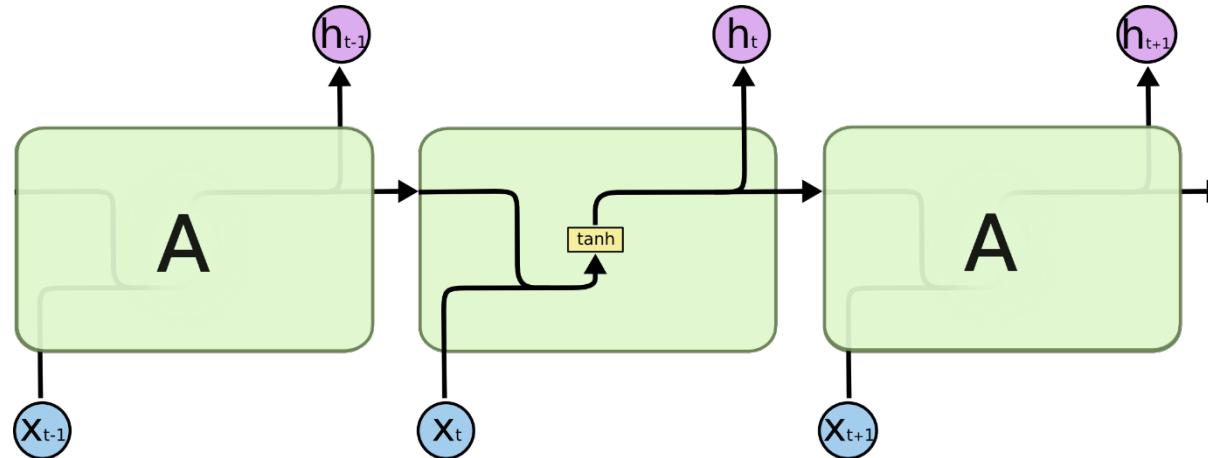
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```
 $\hat{\mathbf{g}} \leftarrow \frac{\partial \mathcal{E}}{\partial \theta}$ 
if  $\|\hat{\mathbf{g}}\| \geq \text{threshold}$  then
     $\hat{\mathbf{g}} \leftarrow \frac{\text{threshold}}{\|\hat{\mathbf{g}}\|} \hat{\mathbf{g}}$ 
end if
```

---

- Intuition: take a step in the same direction, but a smaller step

# The repeating module in a standard RNN contains a single layer.

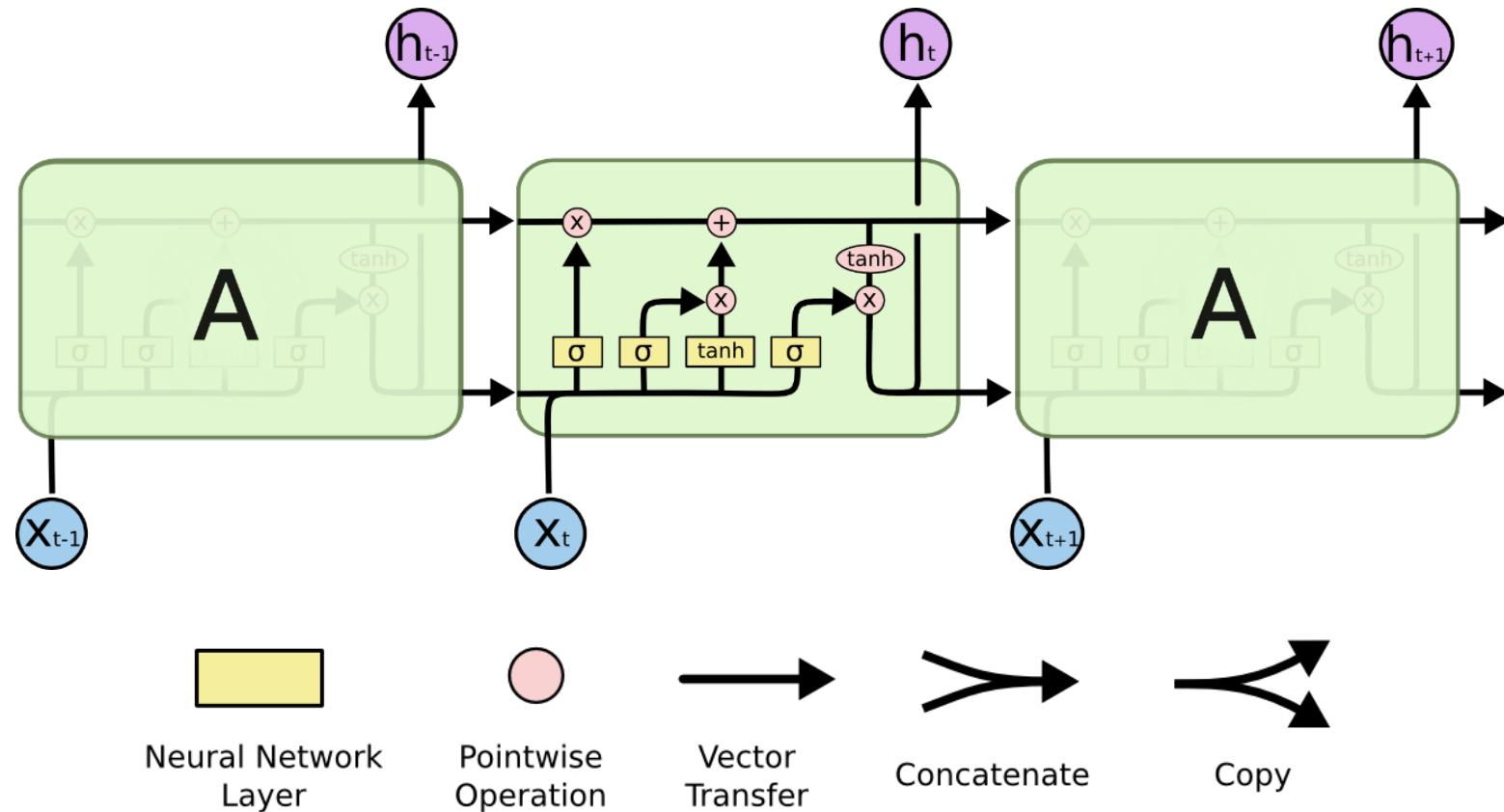


*Unfortunately, as that gap grows, RNNs become unable to learn to connect the information (cf. vanishing gradients)*

*The problem was explored in depth by Hochreiter (1991) and Bengio, et al. (1994), who found some pretty fundamental reasons why it might be difficult.*

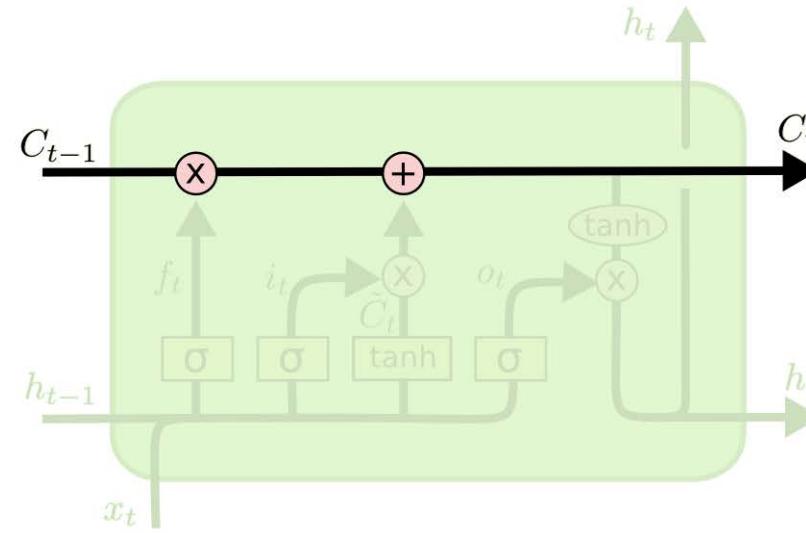
***Thankfully, LSTMs do not have this problem! (Hochreiter & Schmidhuber, 1997)***

# The repeating module in an LSTM contains four interacting layers.



# The Core Idea Behind LSTMs

*The cell state is kind of like a conveyor belt. It runs straight down the entire chain, with only some minor linear interactions. It's very easy for information to just flow along it unchanged.*



*The LSTM does have the ability to remove or add information to the cell state, carefully regulated by structures called gates.*



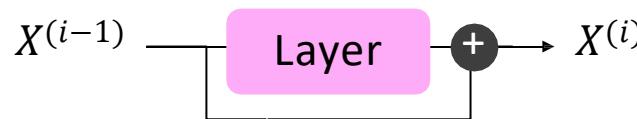
# Residual connections [He et al., 2016]

- Residual connections are a trick to help models train better.

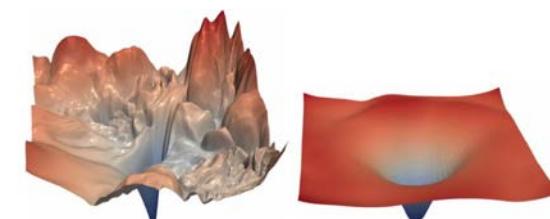
- Instead of  $X^{(i)} = \text{Layer}(X^{(i-1)})$  (where  $i$  represents the layer)



- We let  $X^{(i)} = X^{(i-1)} + \text{Layer}(X^{(i-1)})$  (so we only have to learn “the residual” from the previous layer)



- Residual connections are thought to make the loss landscape considerably smoother (thus easier training!)



[no residuals]                                    [residuals]  
 [Loss landscape visualization, [Li et al., 2018](#),  
 on a ResNet]

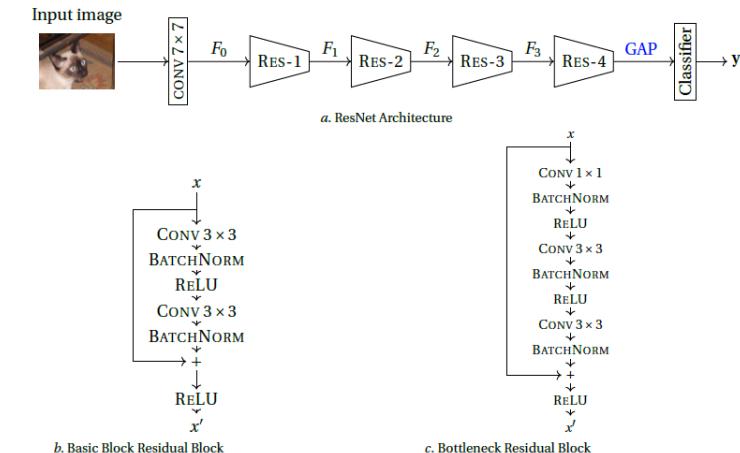


Figure 1.5: Generalities of the ResNet architecture.

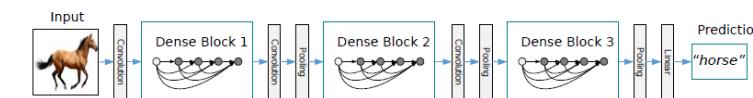


Figure 1.6: Illustration of the DenseNet architecture (G. Huang et al. 2017)

Examples with CNNs: ResNet, DenseNet

# A RNN Language Model

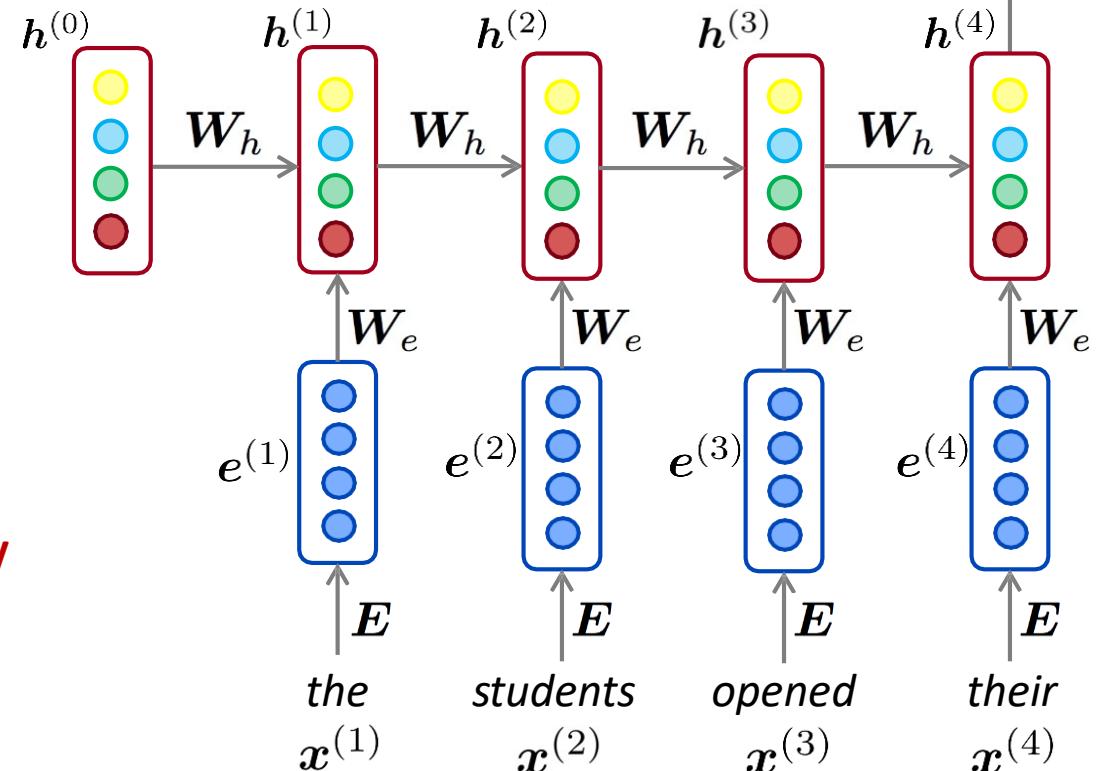
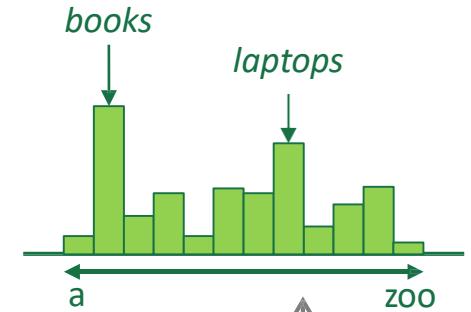
## RNN Advantages:

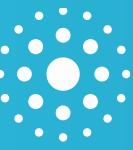
- Can process **any length** input
- Computation for step  $t$  can (in theory) use information from **many steps back**
- **Model size doesn't increase** for longer input
- Same weights applied on every timestep, so there is **symmetry** in how inputs are processed

## RNN Disadvantages:

- Recurrent computation is **slow**
- In practice, difficult to access information from **many steps back**

$$\hat{y}^{(4)} = P(\mathbf{x}^{(5)} | \text{the students opened their})$$



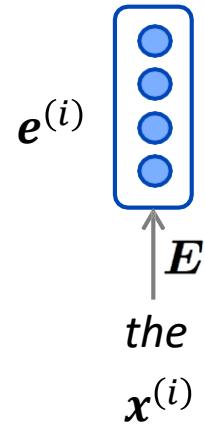


*Local correlations*

**EMBEDDING**



# First let us now detail how to represent words as vectors: *word embedding*



# Word representation

- Vocabulary  $V = [a, \text{aaron}, \dots, \text{zulu}, \text{<UNK>}]$
- 1-hot representation of words

Man (5391)	Woman (9853)	King (4914)	Queen (7157)	Apple (456)	Orange (6257)
---------------	-----------------	----------------	-----------------	----------------	------------------

$\begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \\ 0 \end{bmatrix}$	$\begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \vdots \\ 1 \\ 1 \\ 0 \end{bmatrix}$	$\begin{bmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$	$\begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ \vdots \\ 0 \\ 0 \end{bmatrix}$	$\begin{bmatrix} 0 \\ \vdots \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$	$\begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ \vdots \\ 0 \\ 0 \end{bmatrix}$
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I want a glass of orange \_\_\_\_\_.

I want a glass of apple \_\_\_\_\_.



# Problem with words as discrete symbols

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**Example:** in web search, if user searches for “Seattle motel”, we would like to match documents containing “Seattle hotel”.

But:

$$\text{motel} = [0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 1 \ 0 \ 0 \ 0]$$

$$\text{hotel} = [0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 1 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0]$$

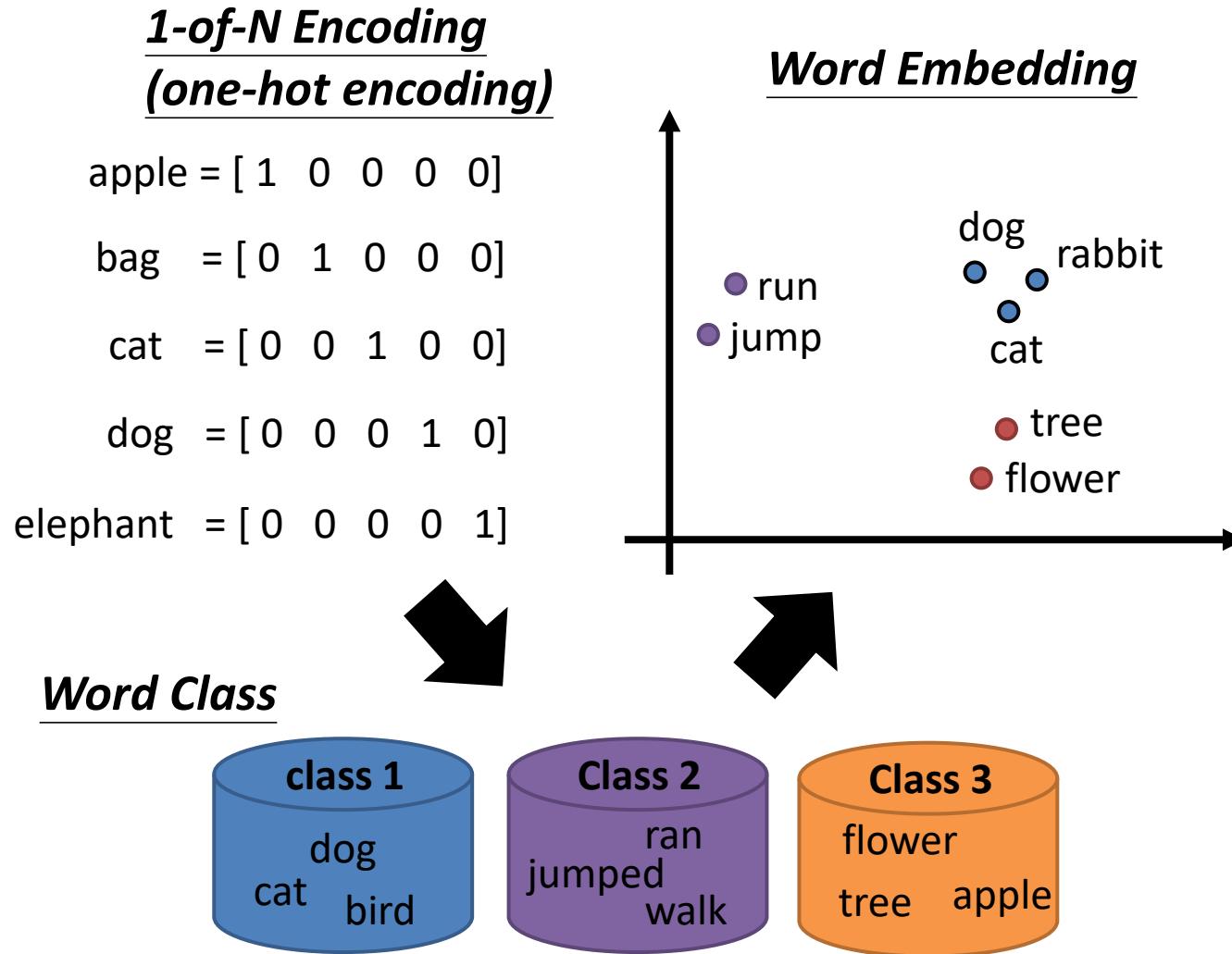
These two vectors are **orthogonal**.

There is no natural notion of **similarity** for one-hot vectors!

**Solution:**

- Could try to rely on WordNet’s list of synonyms to get similarity?
  - But it is well-known to fail badly: incompleteness, subjective, missing nuance, etc.
- Instead: learn to encode similarity in the vectors themselves

# Learn to encode similarity in the vectors themselves

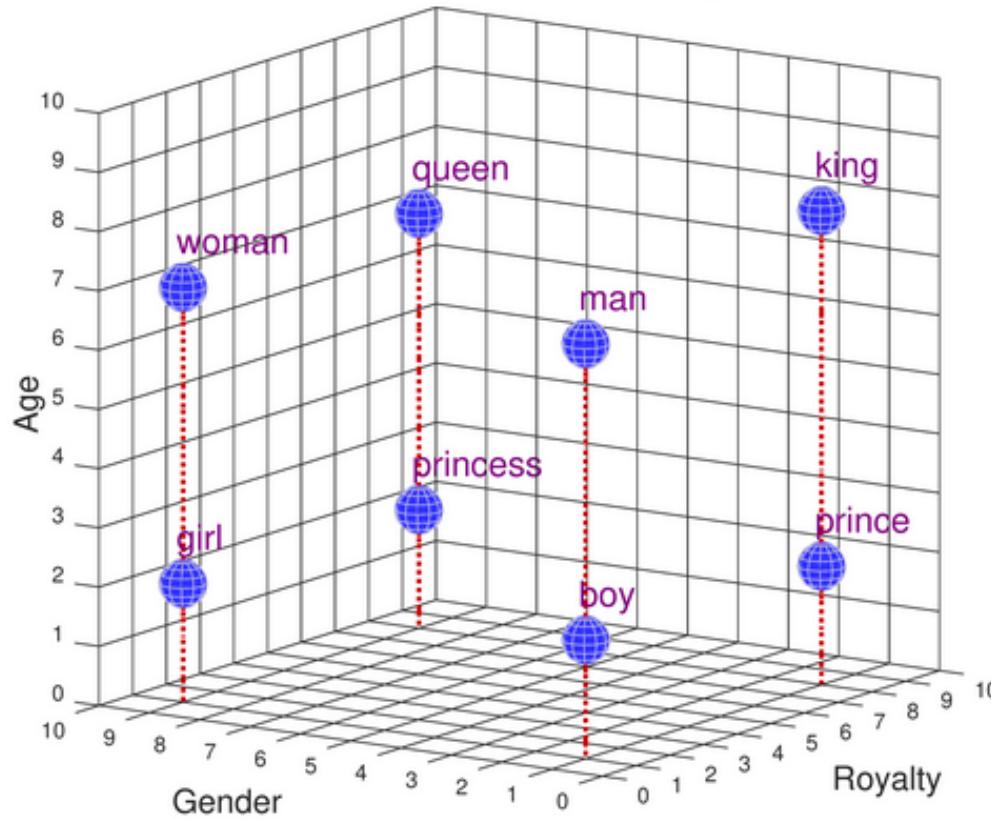


# Featurized representation: word embedding

- The model is trained to complete the missing word:
    - The model gets I want a glass of orange juice ., with the associated answer “juice”.
  - At test time, when the model receives new sentences, it should predict the missing word:
    - I want a glass of apple juice.
    - To correctly guess, it must rely on some proximity between apple and orange.
- We must find a way to numerically encode this proximity of words:
- Rather than representing every word with its index in the dictionary, represent it with a score on **common characteristics**:

	Man (5391)	Woman (9853)	King (4914)	Queen (7157)	Apple (456)	Orange (6257)
Gender	-1	1	-0.95	0.97	0.00	0.01
Royal	0.01	0.02	0.93	0.95	-0.01	0.02
Age	0.03	0.02	0.70	0.69	0.03	-0.02
Food	0.09	0.01	0.02	0.01	0.95	0.97
	e <sub>5391</sub>					

# Visualizing word embeddings



Word Coordinates			
	Gender	Age	Royalty
man	[ 1,	7,	1 ]
woman	[ 9,	7,	1 ]
boy	[ 1,	2,	1 ]
girl	[ 9,	2,	1 ]
king	[ 1,	8,	8 ]
queen	[ 9,	7,	8 ]
prince	[ 1,	2,	8 ]
princess	[ 9,	2,	8 ]

# Analogies using word vectors

- To answer “Man is to King” what “Woman is to ?”, we look for the word whose embedding is closest to:

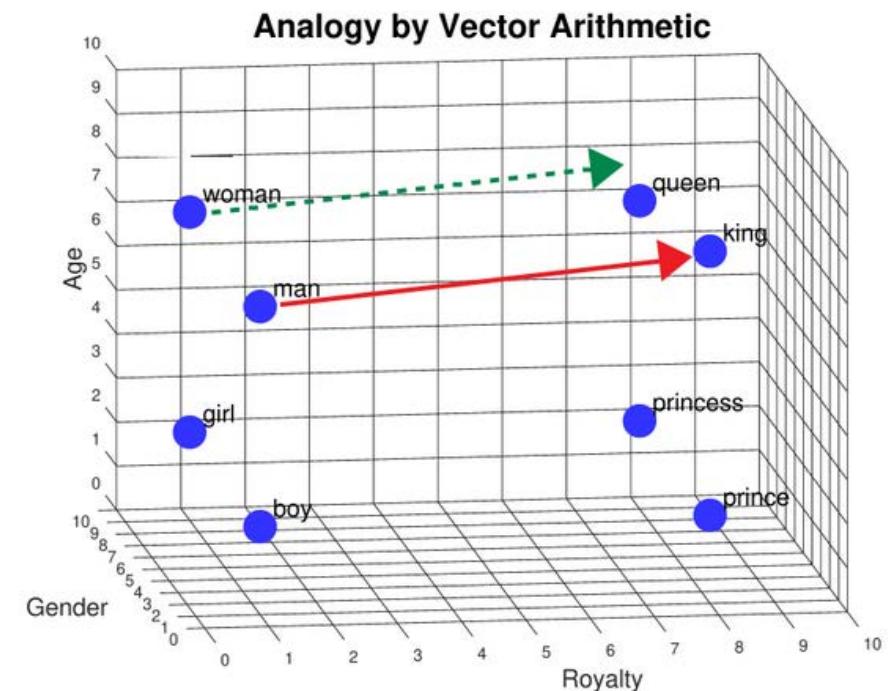
$$e_{\text{woman}} + (e_{\text{king}} - e_{\text{man}})$$

So we can build a new embedding vector by adding to  $e_{\text{woman}}$  the displacement between  $e_{\text{man}}$  and  $e_{\text{king}}$ . Then we check what are the closest words in the neighborhood of the resulting vector.

$$e_{\text{hotter}} - e_{\text{hot}} \approx e_{\text{bigger}} - e_{\text{big}}$$

$$e_{\text{Rome}} - e_{\text{Italy}} \approx e_{\text{Berlin}} - e_{\text{Germany}}$$

$$e_{\text{king}} - e_{\text{queen}} \approx e_{\text{uncle}} - e_{\text{aunt}}$$



# How to learn this automatically?

- Given two words  $w_i$  and  $w_o$ , we want them to be as close as possible in the projected space if they are *similar*.
- Deliberate choice:** *similar* in terms of the context in which they appear

The model is given a sequence of words with the goal of predicting the next word.

Example:  
Hannah is a \_\_\_

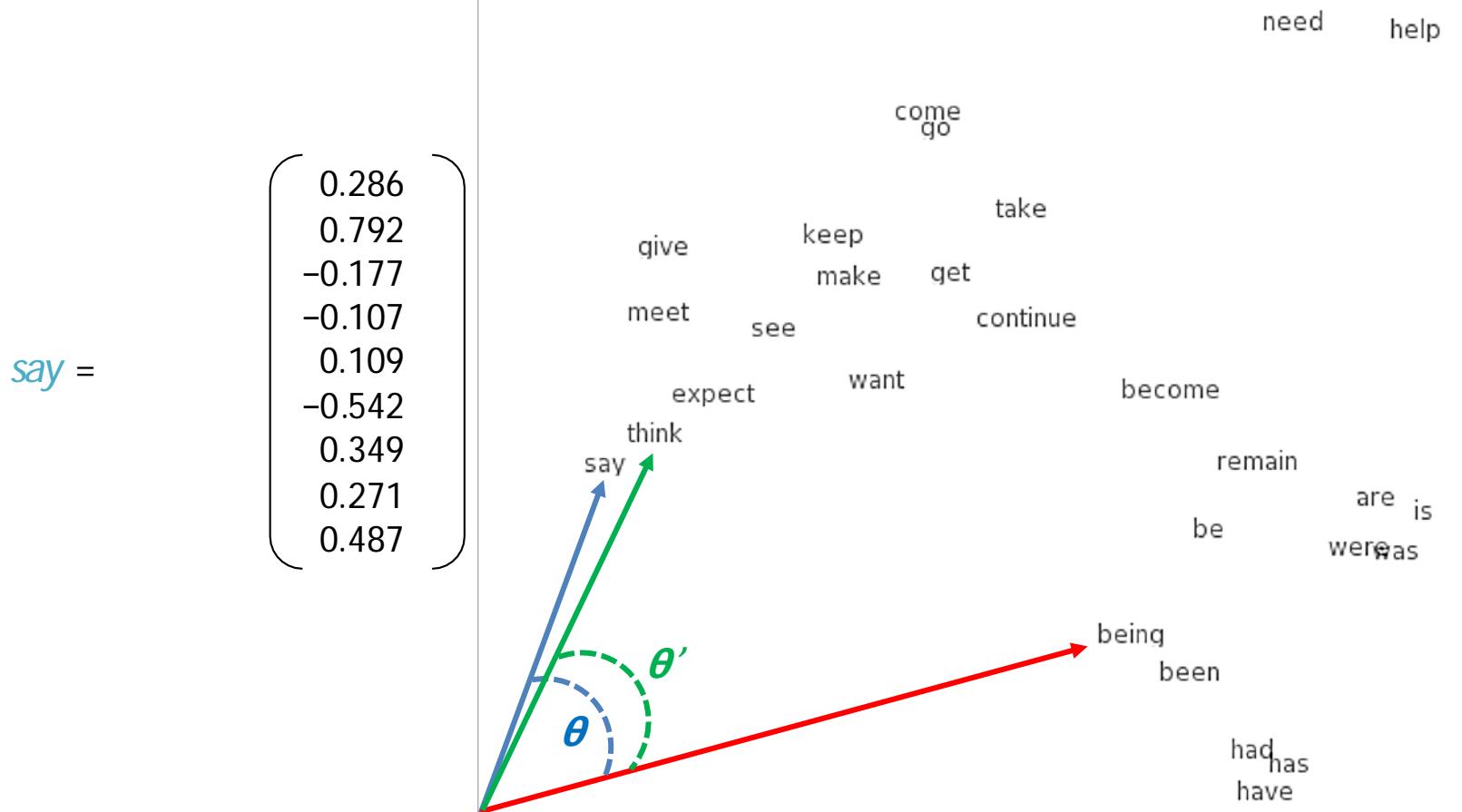
Hannah is a *sister*  
Hannah is a *friend*  
Hannah is a *marketer*  
Hannah is a *comedian*

The model is given a sequence of words with the goal of predicting a 'masked' word in the middle.

Example  
Jacob [mask] reading

Jacob *fears* reading  
Jacob *loves* reading  
Jacob *enjoys* reading  
Jacob *hates* reading

# Word meaning as a neural word vector – visualization



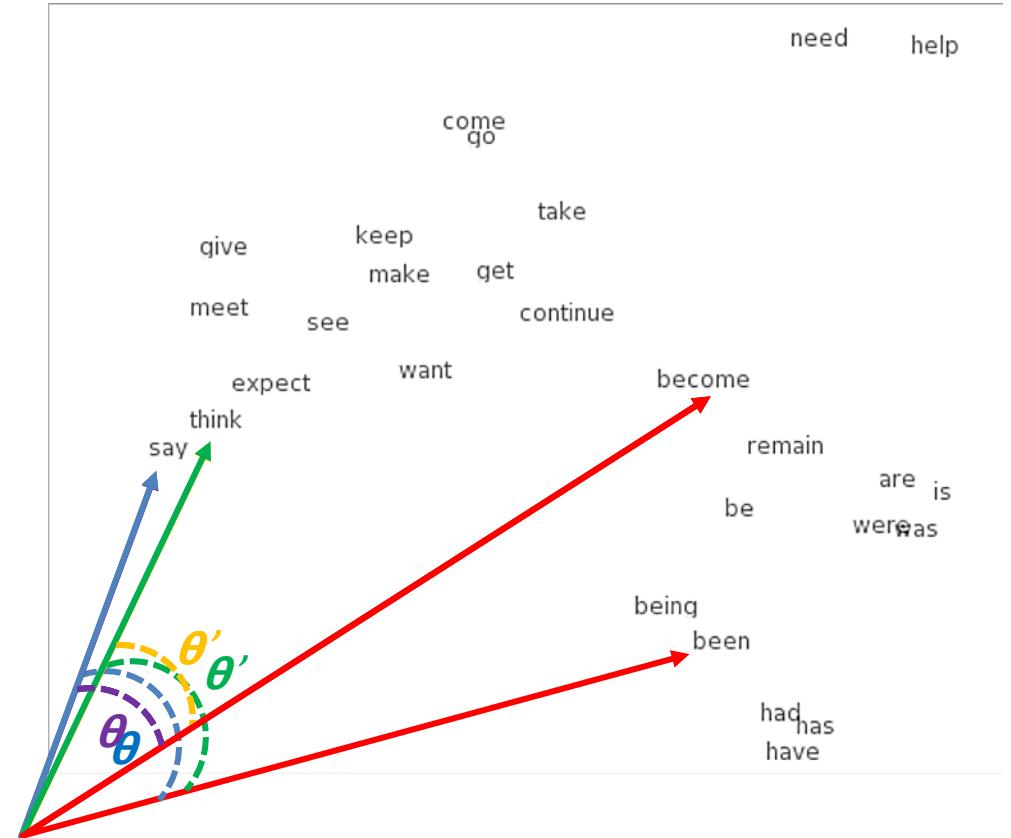
$$\theta' \approx \theta \Leftrightarrow \text{think} \leftrightarrow \text{say}$$



# Word meaning as a neural word vector – visualization

$$\theta' \approx \theta \Leftrightarrow \text{think} \approx \text{say}$$

$$\theta' \approx \theta \Leftrightarrow \text{think} \approx \text{say}$$





# Word2Vec Overview

Word2vec (Mikolov et al. 2013) is a framework for learning word vectors

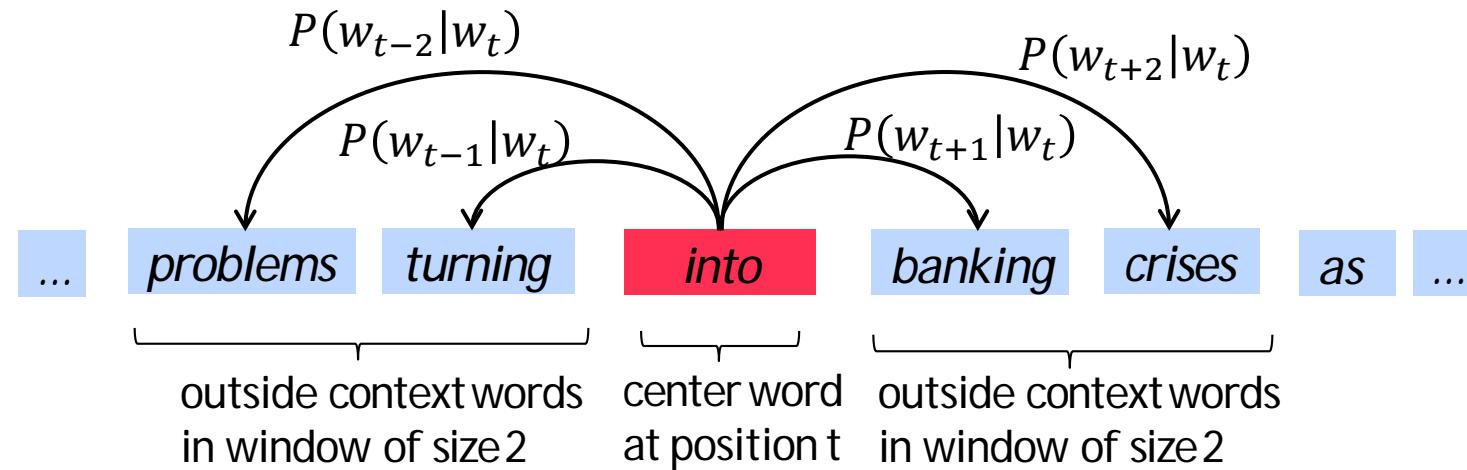
Idea:

- We have a large corpus of text
- Every word in a fixed vocabulary is represented by a vector
- Go through each position  $t$  in the text, which has a center word  $c$  and context (“outside”) words  $o$
- Use the (cosine) similarity of the word vectors for  $c$  and  $o$  to calculate the probability of  $o$  given  $c$  (or vice versa)
- Keep adjusting the word vectors to maximize this probability



# Word2Vec Overview

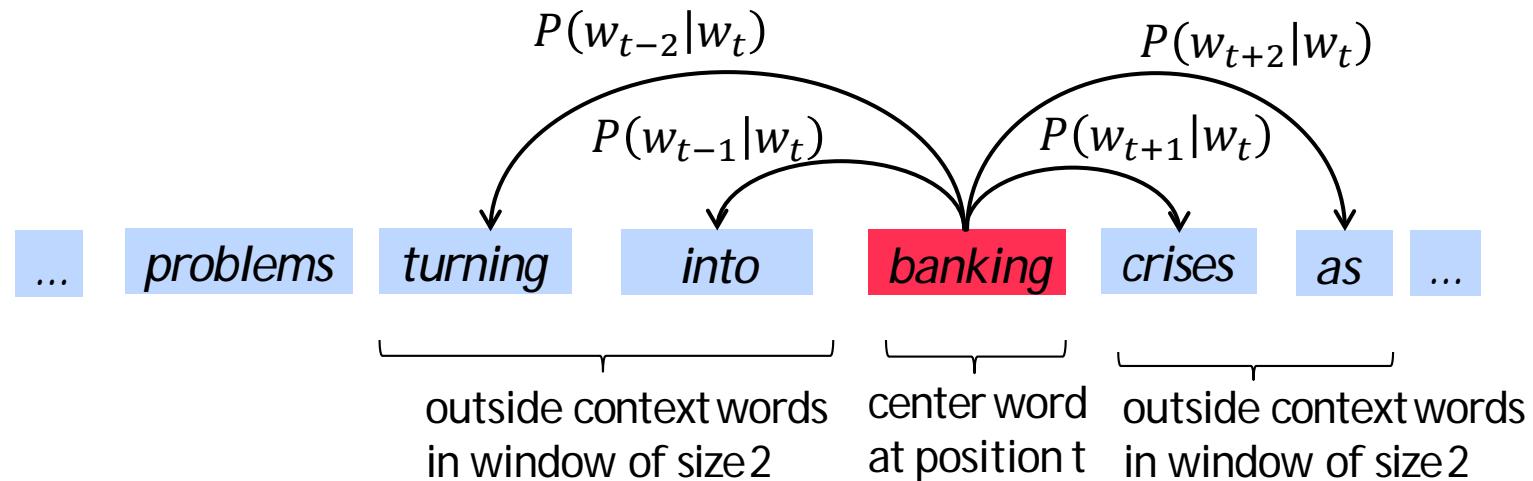
- Example windows and process for computing  $P(w_{t+j}|w_t)$





# Word2Vec Overview

- Example windows and process for computing  $P(w_{t+j}|w_t)$





# Word2Vec: objective function

- We want to minimize the objective function, the (average) negative log likelihood :

$$J(\theta) = -\frac{1}{T} \log L(\theta) = -\frac{1}{T} \sum_{t=1}^T \sum_{\substack{-m \leq j \leq m \\ j \neq 0}} \log P(w_{t+j} | w_t; \theta)$$

Minimizing objective function  $\Leftrightarrow$  Maximizing predictive accuracy

- Question: How to calculate  $P(w_{t+j} | w_t; \theta)$ ?
- Answer: We will use two vectors per word  $w$ :
  - $V_w$  when  $w$  is a *center* word
  - $u_w$  when  $w$  is an *outside* word (i.e. *contextual* word)
- Then for a center word  $c$  and an outside word  $o$ :

$$P(o|c) = \frac{\exp(u_o^T v_c)}{\sum_{w \in V} \exp(u_w^T v_c)}$$



# Word2Vec: prediction function

$$P(o|c) = \frac{\exp(u_o^T v_c)}{\sum_{w \in V} \exp(u_w^T v_c)}$$

Exponentiation makes anything positive

Dot product compares similarity of  $o$  and  $c$ .  
 $u^T v = u \cdot v = \sum_{i=1}^n u_i v_i$   
Larger dot product = larger probability

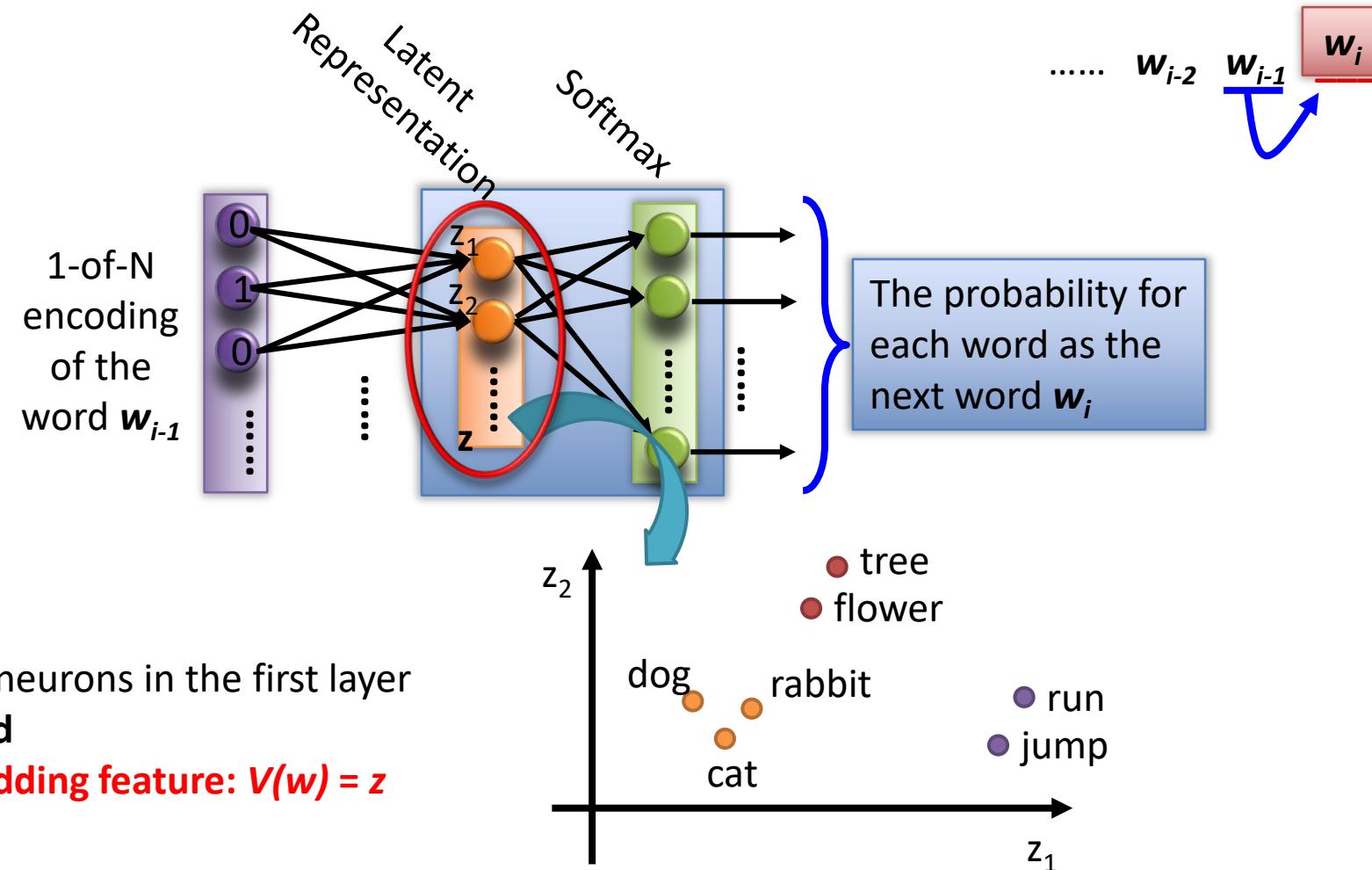
Normalize over entire vocabulary to give probability distribution

- This is an example of the **softmax function**  $\mathbb{R}^n \rightarrow \mathbb{R}^n$

$$\text{softmax}(x_i) = \frac{\exp(x_i)}{\sum_{j=1}^n \exp(x_j)} = p_i$$

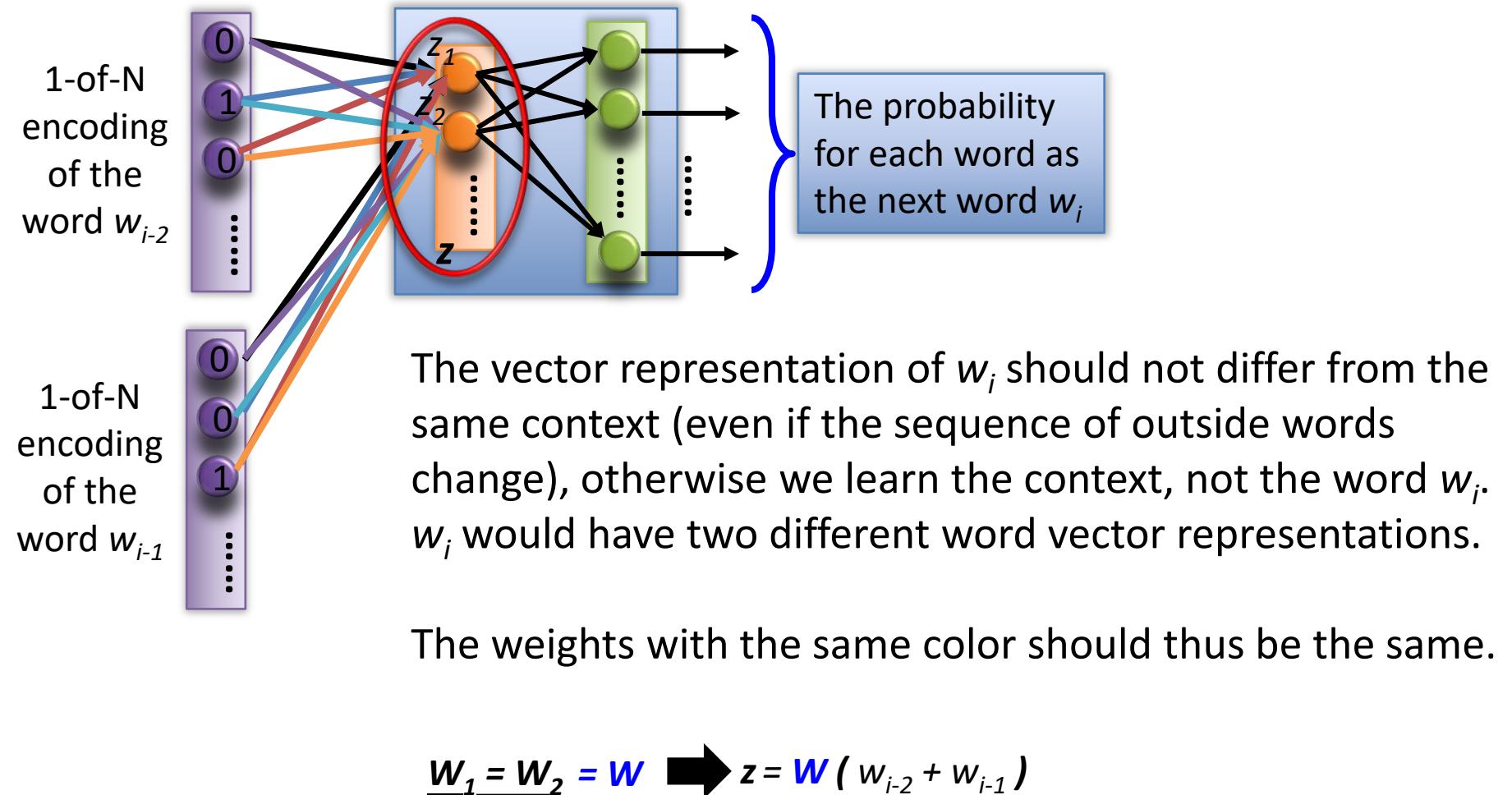
- The softmax function maps arbitrary values to a probability distribution  $p_i$ 
  - “max” because amplifies probability of largest  $x_i$ ,
  - “soft” because still assigns some probability to smaller  $x_i$

# Prediction-based – Language Modeling



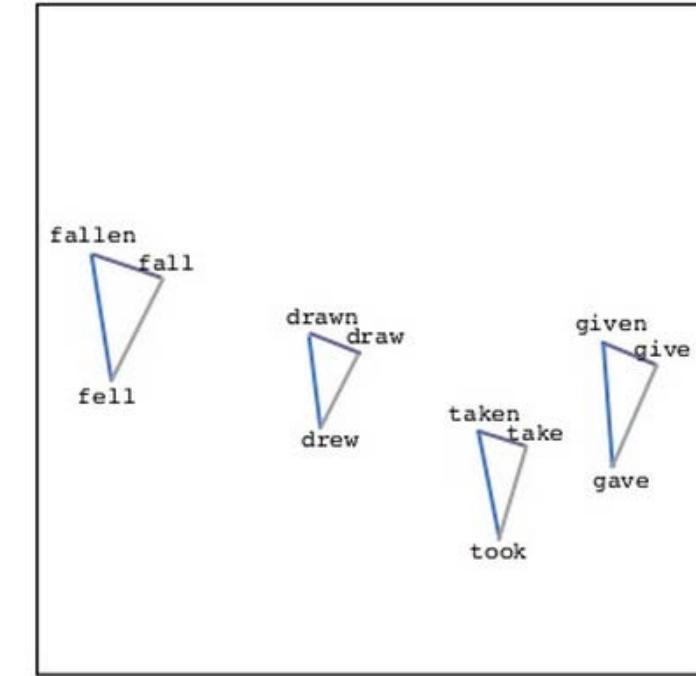
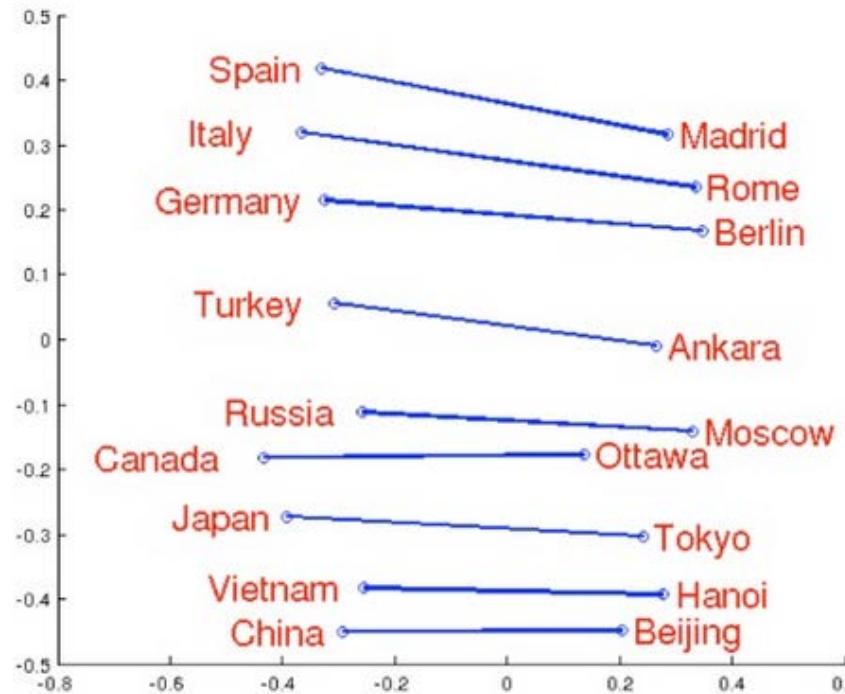
- Take out the **input** of the neurons in the first layer
- Use it to represent a word
- **Word vector, word embedding feature:  $V(w) = z$**

# Prediction-based – Sharing Parameters



It is the same idea as the shared connections in CNN, because the edge or corner extractor is actually defined by the weights

# Word Embedding



Source: <http://www.slideshare.net/hustwj/cikm-keynotenov2014>



# Word Embedding

- Characteristics

$$\begin{aligned}V(\text{Germany}) \\ \approx V(\text{Berlin}) - V(\text{Rome}) + V(\text{Italy})\end{aligned}$$

- Solving analogies

$$V(\text{hotter}) - V(\text{hot}) \approx V(\text{bigger}) - V(\text{big})$$

$$V(\text{Rome}) - V(\text{Italy}) \approx V(\text{Berlin}) - V(\text{Germany})$$

$$V(\text{king}) - V(\text{queen}) \approx V(\text{uncle}) - V(\text{aunt})$$

Rome : Italy = Berlin : ?

Compute  $V(\text{Berlin}) - V(\text{Rome}) + V(\text{Italy})$

Find the word w with the closest  $V(w)$

# Word Embedding

- Word2vec is known to be good at certain kinds of analogies:

Relationship	Example 1	Example 2	Example 3
France - Paris	Italy: Rome	Japan: Tokyo	Florida: Tallahassee
big - bigger	small: larger	cold: colder	quick: quicker
Miami - Florida	Baltimore: Maryland	Dallas: Texas	Kona: Hawaii
Einstein - scientist	Messi: midfielder	Mozart: violinist	Picasso: painter
Sarkozy - France	Berlusconi: Italy	Merkel: Germany	Koizumi: Japan
copper - Cu	zinc: Zn	gold: Au	uranium: plutonium
Berlusconi - Silvio	Sarkozy: Nicolas	Putin: Medvedev	Obama: Barack
Microsoft - Windows	Google: Android	IBM: Linux	Apple: iPhone
Microsoft - Ballmer	Google: Yahoo	IBM: McNealy	Apple: Jobs
Japan - sushi	Germany: bratwurst	France: tapas	USA: pizza

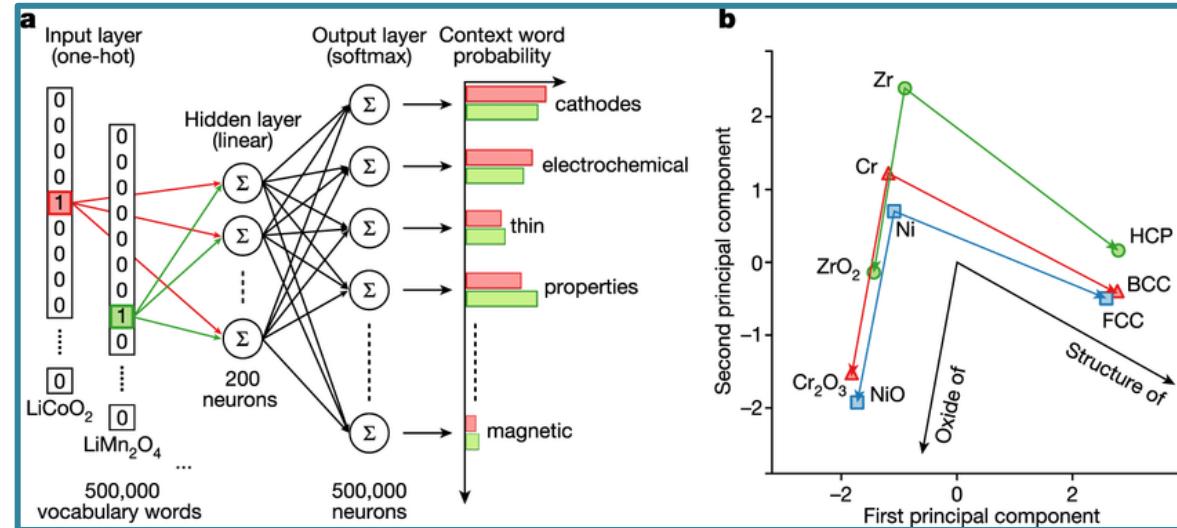
Type of relationship	Word Pair 1	Word Pair 2	
Common capital city	Athens	Greece	Oslo
All capital cities	Astana	Kazakhstan	Harare
Currency	Angola	kwanza	Iran
City-in-state	Chicago	Illinois	Stockton
Man-Woman	brother	sister	grandson
Adjective to adverb	apparent	apparently	rapid
Opposite	possibly	impossibly	ethical
Comparative	great	greater	tough
Superlative	easy	easiest	lucky
Present Participle	think	thinking	read
Nationality adjective	Switzerland	Swiss	Cambodia
Past tense	walking	walked	swimming
Plural nouns	mouse	mice	dollar
Plural verbs	work	works	speak
			Cambodian
			swam
			dollars
			speaks

# Word2Vec not for language (Nature 2019)

a) Target words ‘LiCoO<sub>2</sub>’ and ‘LiMn<sub>2</sub>O<sub>4</sub>’ are represented as vectors with ones at their corresponding vocabulary indices (for example, 5 and 8 in the schematic) and zeros everywhere else (one-hot encoding).

These one-hot encoded vectors are used as inputs for a neural network with a single linear hidden layer (for example, 200 neurons), which is trained to predict all words mentioned within a certain distance (context words) from the given target word.

- For similar battery cathode materials such as LiCoO<sub>2</sub> and LiMn<sub>2</sub>O<sub>4</sub>, the context words that occur in the text are mostly the same (for example, ‘cathodes’, ‘electrochemical’, and so on), which leads to similar hidden layer weights after the training is complete.
- These hidden layer weights are the actual word embeddings.
- The softmax function is used at the output layer to normalize the probabilities.
- b) Word embeddings for Zr, Cr and Ni, their principal oxides and crystal symmetries (at standard conditions) projected onto two dimensions using principal component analysis and represented as points in space. The relative positioning of the words encodes materials science relationships, such that there exist consistent vector operations between words that represent concepts such as ‘oxide of’ and ‘structure of’.





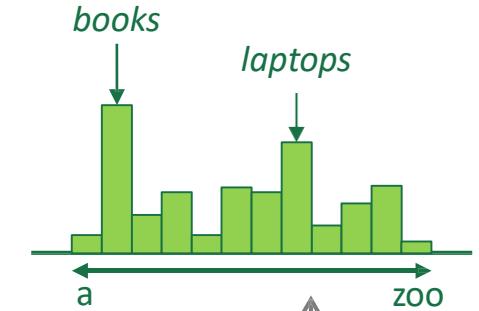
# Word2Vec not for language (Nature 2019)

Relationship	Example vector operation	Answer	Validation pairs	Accuracy (%)
Chemical element names	helium - He + Fe	= iron	8372	71.4
Crystal symmetries	cubic - GaAs + CdSe	= hexagonal	2034	35.4
Crystal structure names	zincblende - GaP + GaN	= wurtzite	556	18.7
Elemental crystal structures	dhcp - La + Cr	= bcc	1198	48.6
Principal oxides	$\text{Al}_2\text{O}_3$ - Al + Si	= $\text{SiO}_2$	650	48.8
Units	pressure - Pa + Hz	= frequency	452	35.4
Magnetic properties	ferromagnetic - NiCo + IrMn	= antiferromagnetic	622	41.0
Applications	thermoelectric - PbTe + LiFePO4	= cathode materials	-	-
Grammar	structures - structure + energy	= energies	15162	61.6
Total			29046	60.1

Materials science analogies

# Recap thus far

$\hat{y}^{(4)} = P(\mathbf{x}^{(5)} | \text{the students opened their})$

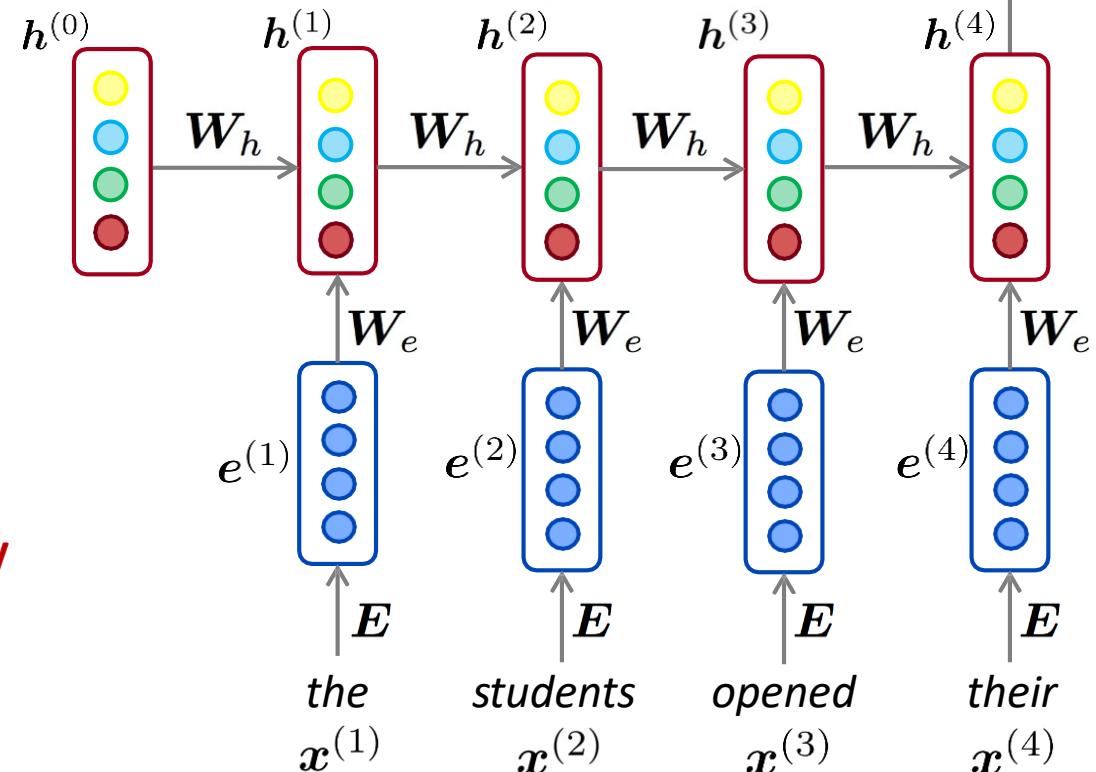


## RNN Advantages:

- Can process **any length** input
- Computation for step  $t$  can (in theory) use information from **many steps back**
- **Model size doesn't increase** for longer input
- Same weights applied on every timestep, so there is **symmetry** in how inputs are processed

## RNN Disadvantages:

- Recurrent computation is **slow**
- In practice, difficult to access information from **many steps back**





# Recap thus far

- Language Model: A system that predicts the next word
- Recurrent Neural Network: A family of neural networks that:
  - Take sequential input of any length
  - Apply the same weights on each step
  - Can optionally produce output on each step
- Vanishing gradient problem: what it is, why it happens, and why it's bad for RNNs
- LSTMs and GRUs: more complicated RNNs that use gates to control information flow; more resilient to vanishing gradients



# Why should we care about Language Modeling?

- Language Modeling is a **benchmark task** that helps us **measure our progress** on understanding language
- Language Modeling is a **subcomponent** of many NLP tasks, especially those involving **generating text** or **estimating the probability of text**:
  - Predictive typing
  - Speech recognition
  - Handwriting recognition
  - Spelling/grammar correction
  - Authorship identification
  - Machine translation
  - Summarization
  - Dialogue
  - etc.



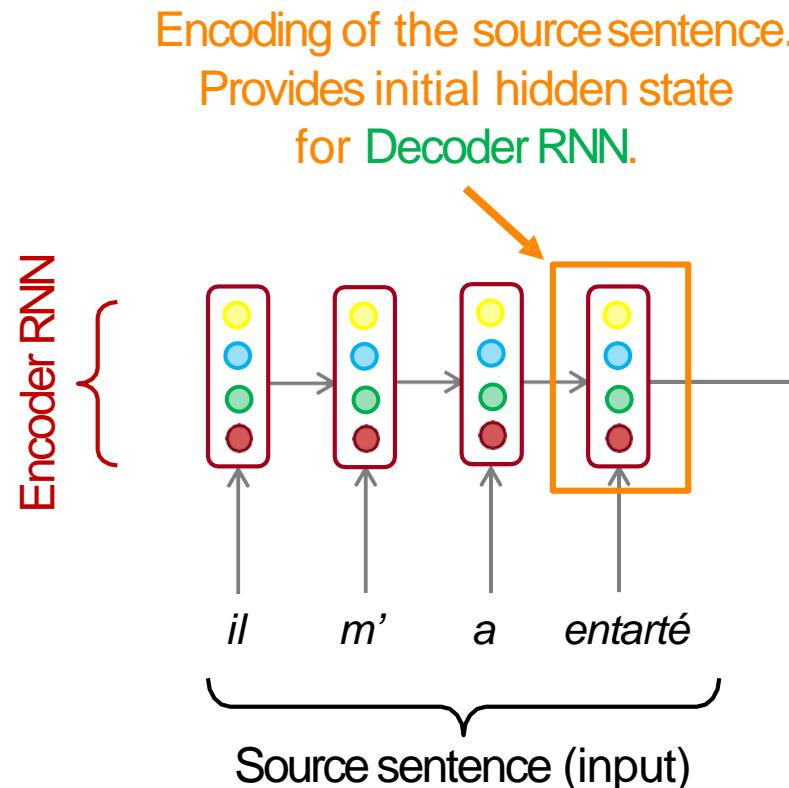
# Neural Machine Translation

- Neural Machine Translation (NMT) is a way to do Machine Translation with a *single neural network*
- The neural network architecture is called sequence-to-sequence (aka seq2seq) and it involves *two RNNs*.

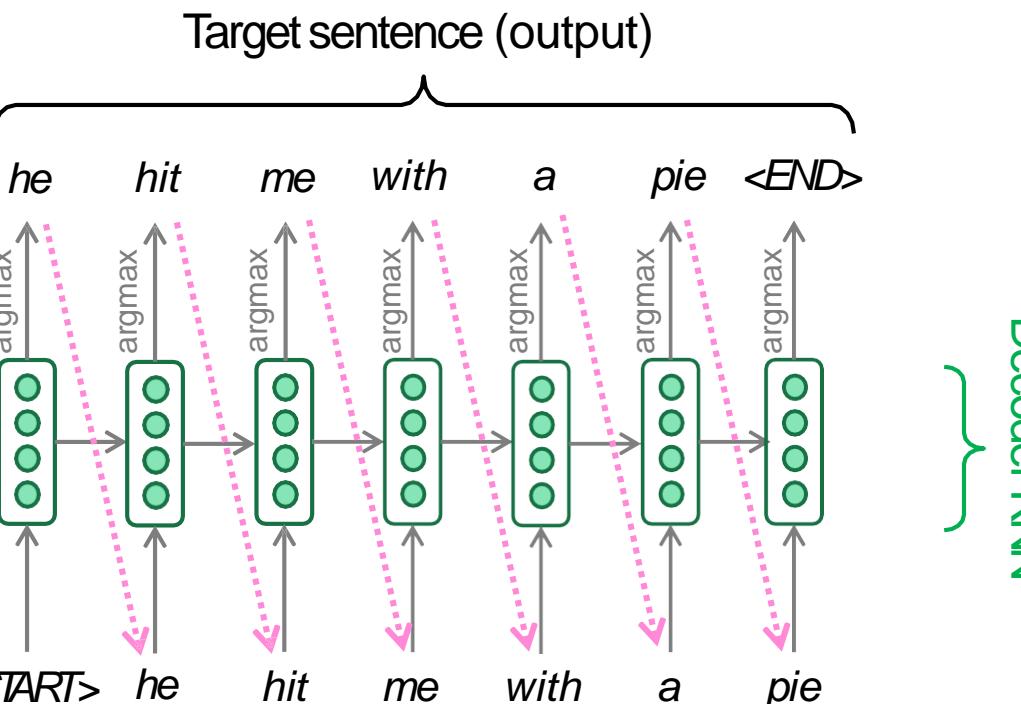
# Neural Machine Translation (NMT)

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The sequence-to-sequence model



Encoder RNN produces an **encoding** of the source sentence.



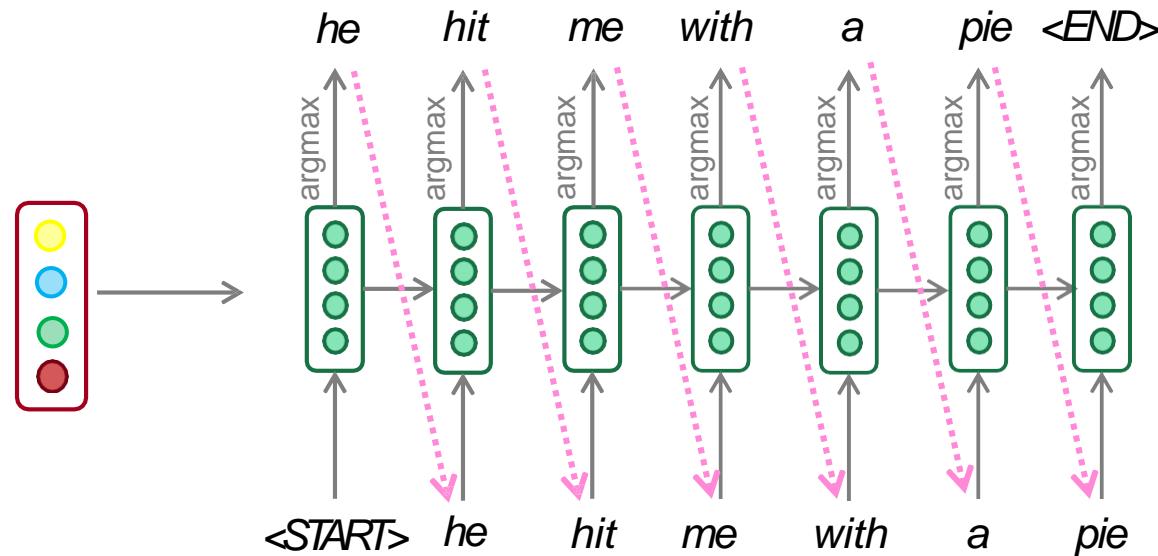
Decoder RNN is a Language Model that generates target sentence, *conditioned on encoding*.

Note: This diagram shows test time behavior: decoder output is fed in as next step's input



# Greedy decoding

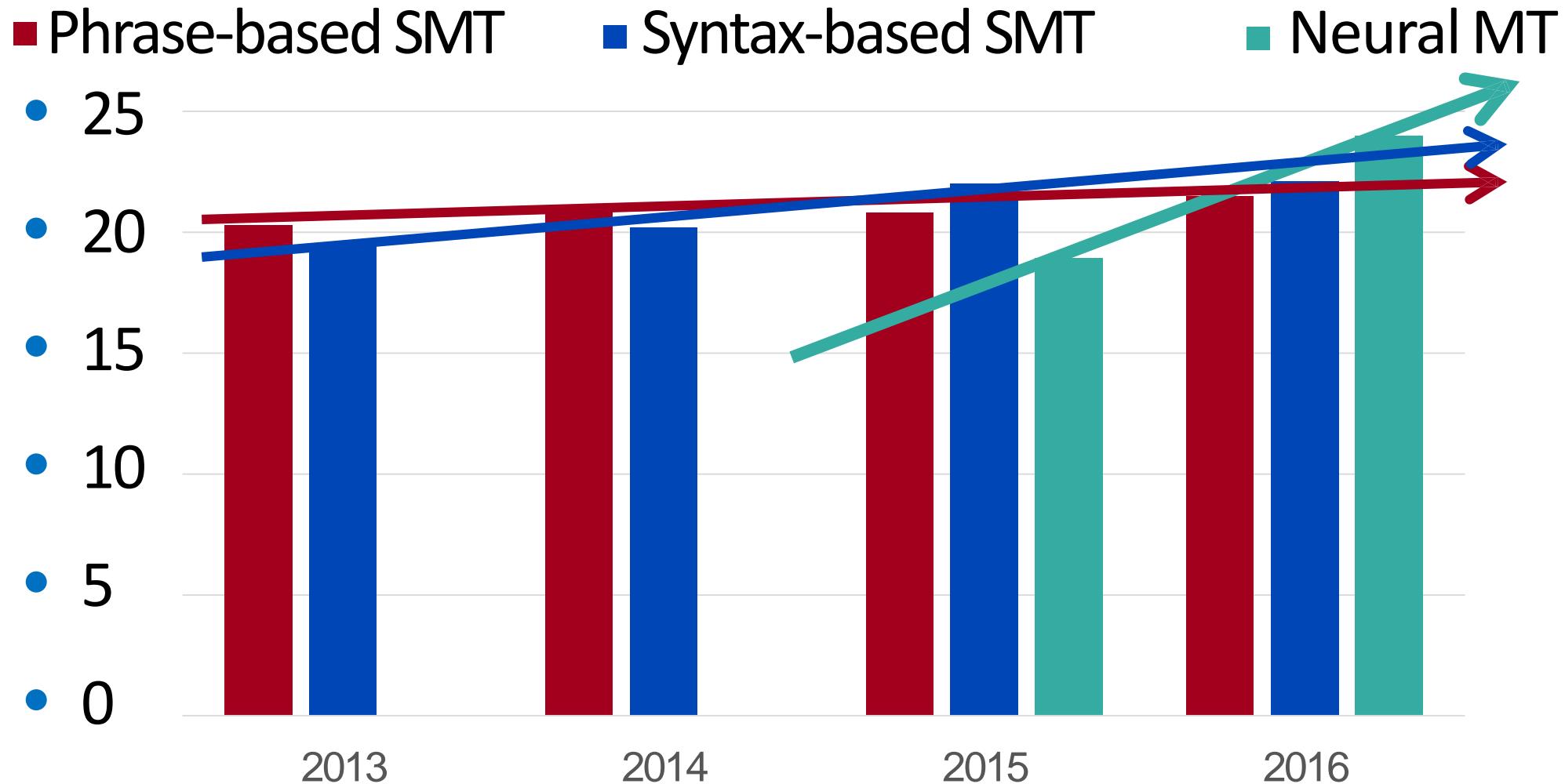
- We saw how to generate (or “decode”) the target sentence by taking argmax on each step of the decoder



- This is **greedy decoding** (take most probable word on each step)
- **Problems with this method?**

## MT progress overtime

[Edinburgh En-De WMT newstest2013 Cased BLEU; NMT 2015 from U. Montréal]

Source: [http://www.meta-net.eu/events/meta-forum-2016/slides/09\\_sennrich.pdf](http://www.meta-net.eu/events/meta-forum-2016/slides/09_sennrich.pdf)

# NMT:the biggest success story of NLP Deep Learning

Neural Machine Translation went from a **fringe research activity** in 2014 to the **leading standard method** in 2016

- 2014: First seq2seq paper published
- 2016: Google Translate switches from SMT to NMT
- **This is amazing!**
  - SMT systems, built by **hundreds** of engineers over many **years**, outperformed by NMT systems trained by a **handful** of engineers in a few **months**

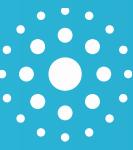


# NMT research continues

NMT is the flagship task for NLP Deep Learning

- NMT research has **pioneered** many of the recent **innovations** of NLP Deep Learning
- In 2019: NMT research continues to **thrive**
  - Researchers have found ***many, many*** improvements to the “vanilla” seq2seq NMT system
  - But **one improvement** is so integral that it is the new vanilla...

# ATTENTION



## *Local correlations*

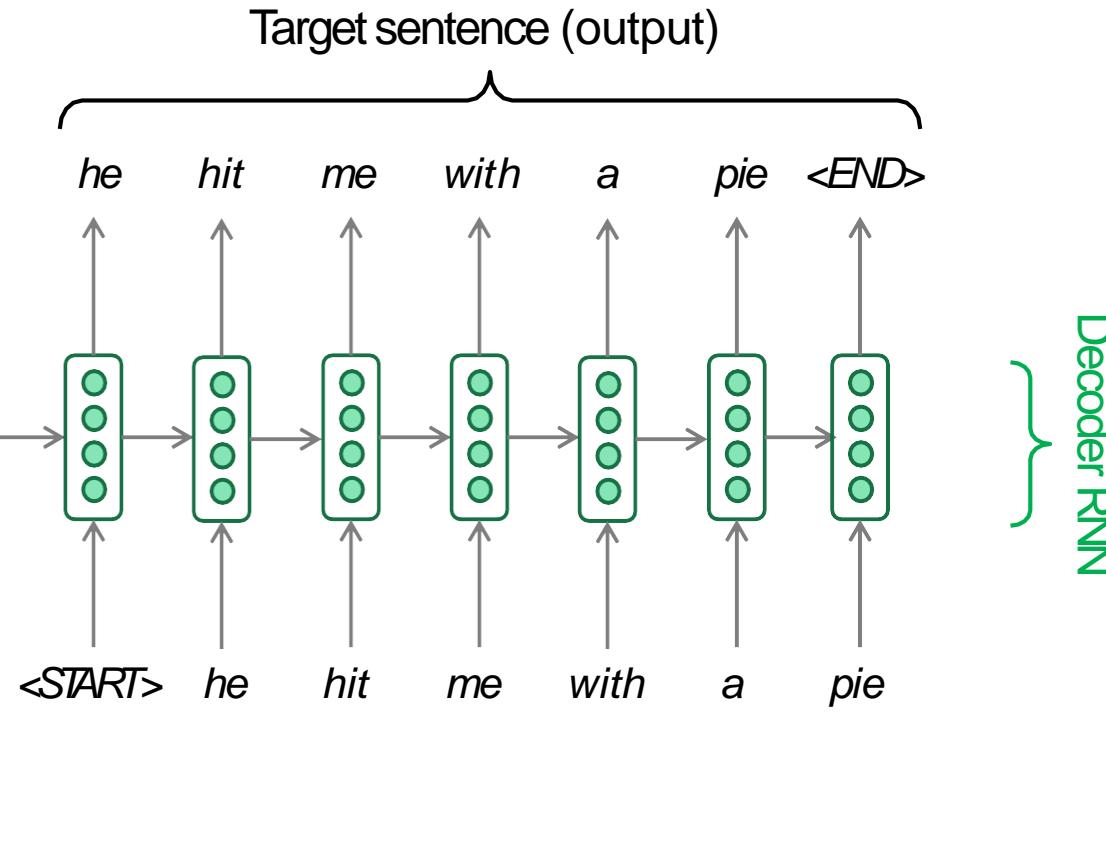
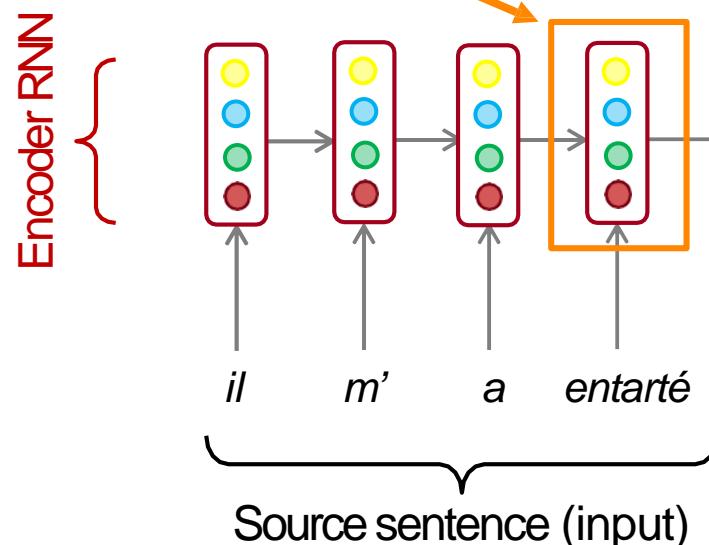
**ATTENTION**

*To try to solve issues with recurrent models*

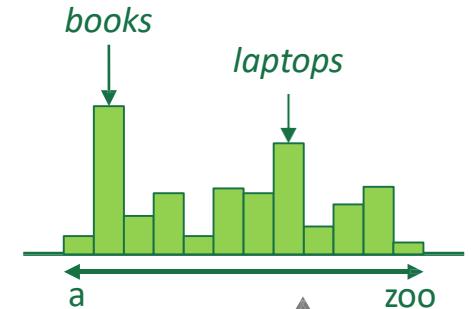
# Sequence-to-sequence: the bottleneck problem

Encoding of the source sentence.

This needs to capture *all information* about the source sentence.  
**Information bottleneck!**



# Recap thus far

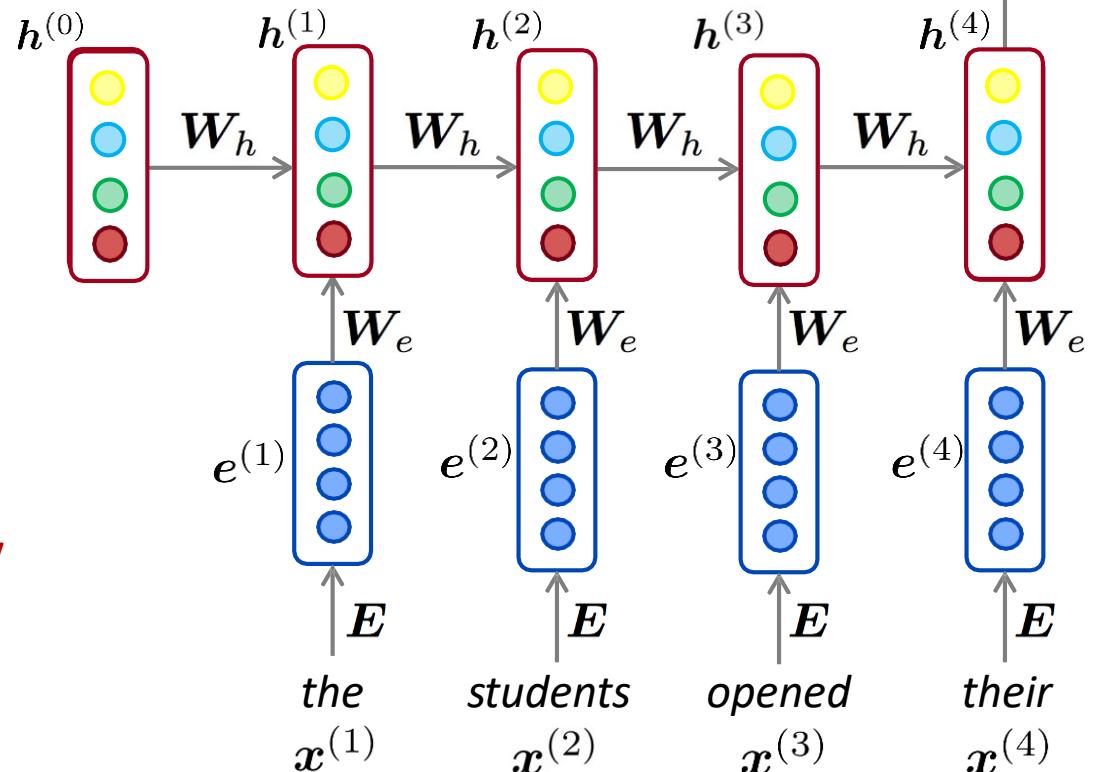
 $\hat{y}^{(4)} = P(\mathbf{x}^{(5)} | \text{the students opened their})$ 


## RNN Advantages:

- Can process **any length** input
- Computation for step  $t$  can (in theory) use information from **many steps back**
- **Model size doesn't increase** for longer input
- Same weights applied on every timestep, so there is **symmetry** in how inputs are processed

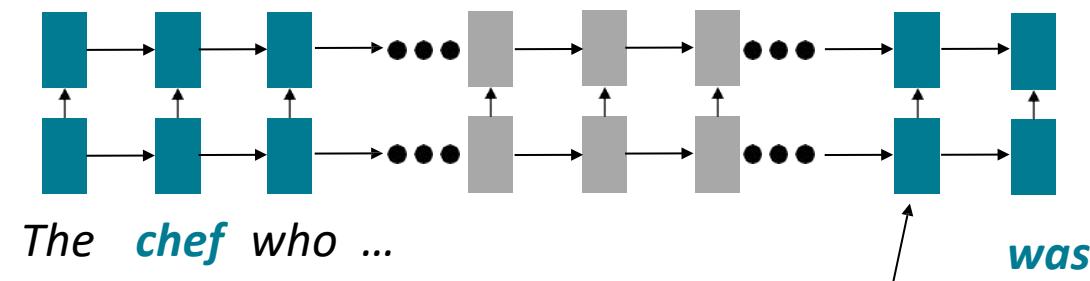
## RNN Disadvantages:

- Recurrent computation is **slow**
- In practice, difficult to access information from **many steps back**



# Issues with recurrent models: Linear interaction distance

- **O(sequence length)** steps for distant word pairs to interact means:
  - Hard to learn long-distance dependencies (because of gradient problems! Even if LSTM and GRU have mainly solved this)
  - Linear order of words is “baked in” (RNNs); not necessarily the right way to think about sentences...



Info of *chef* has gone through  
O(sequence length) many layers!



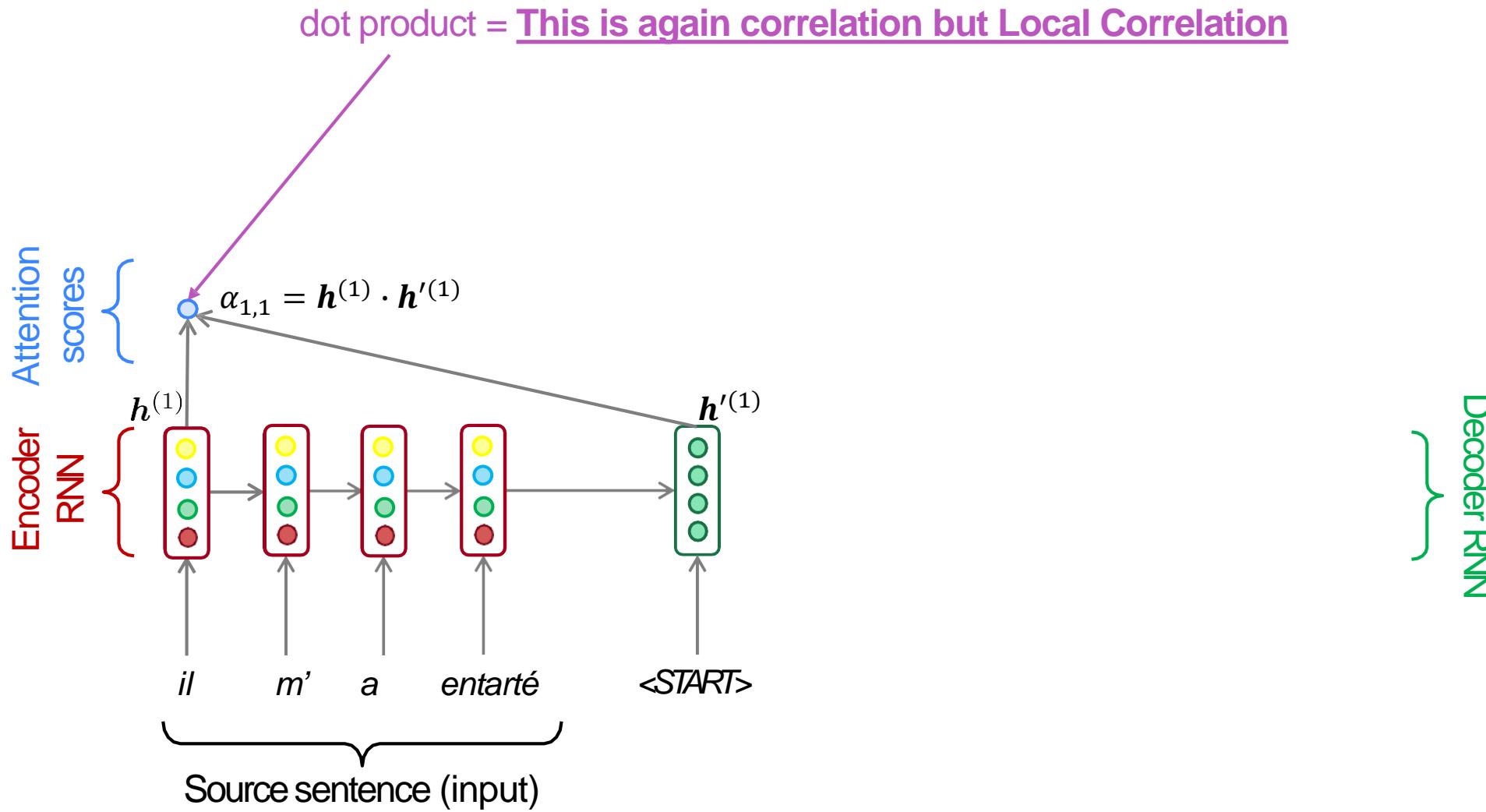
# Attention

- **Attention** provides a solution to the bottleneck problem.
- Core idea: on each step of the decoder, use *direct connection to the encoder* to *focus on a particular part* of the source sequence

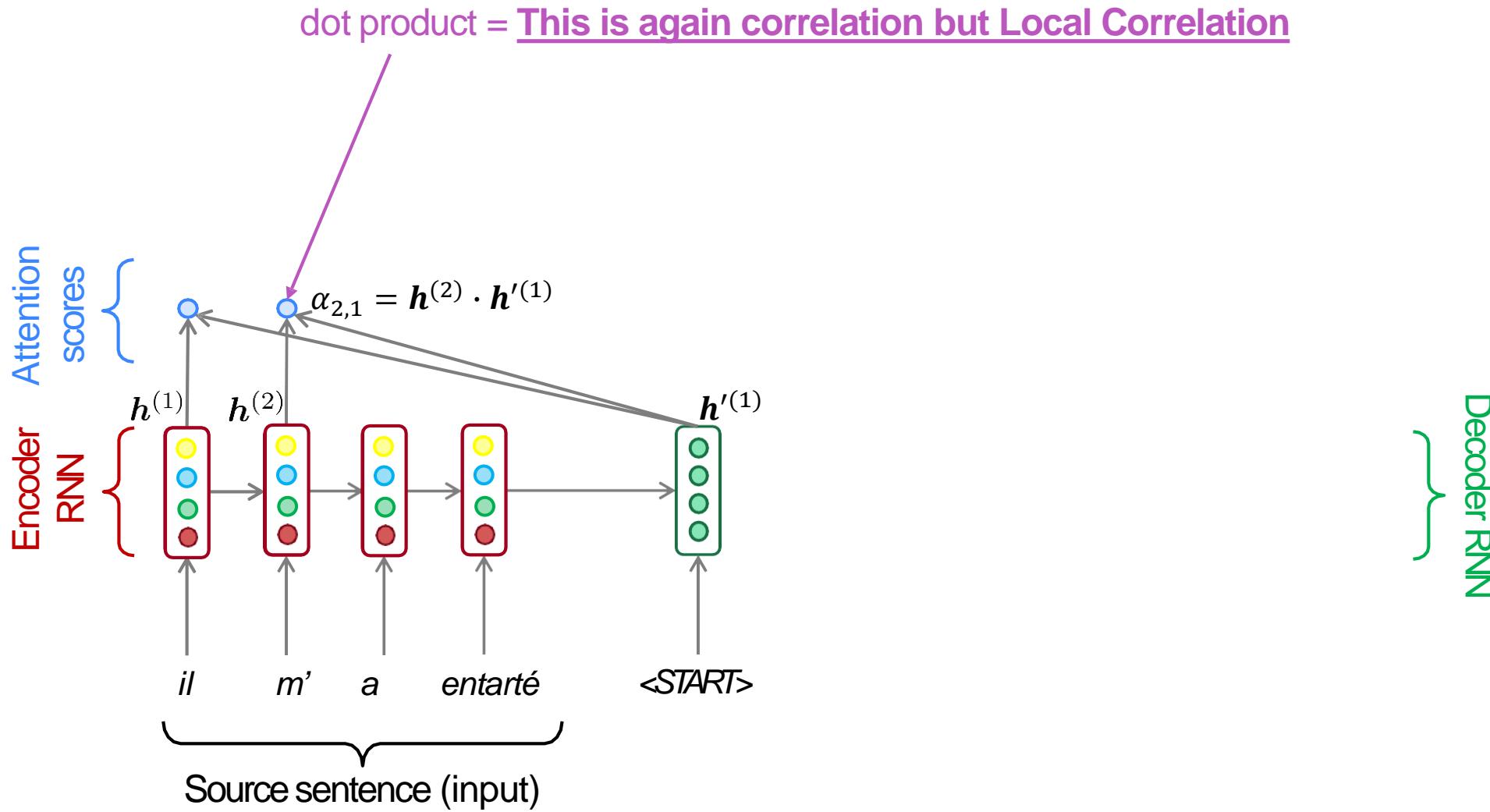


- First we will show via diagram (no equations), then we will show with equations

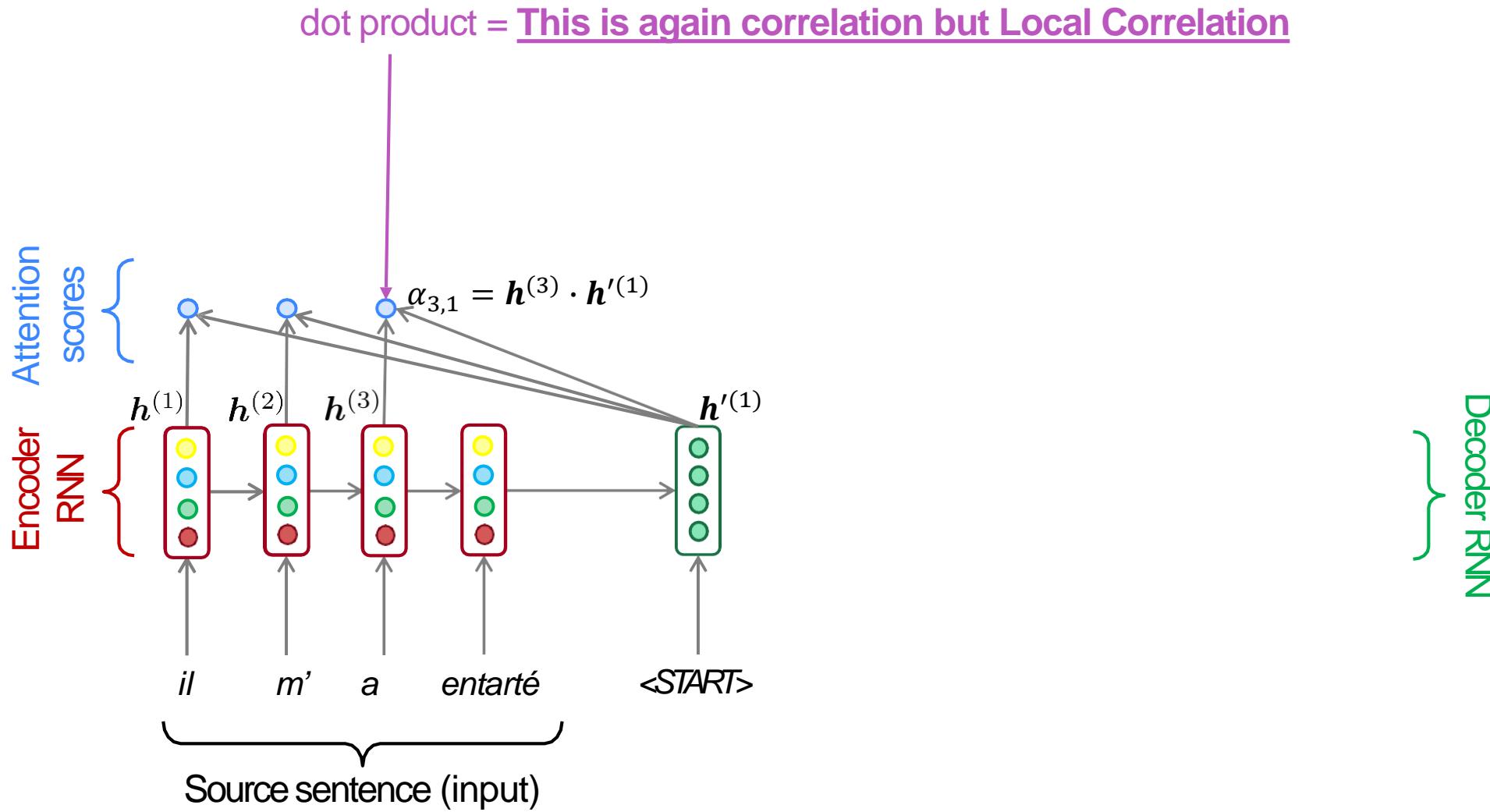
# Sequence-to-sequence with attention



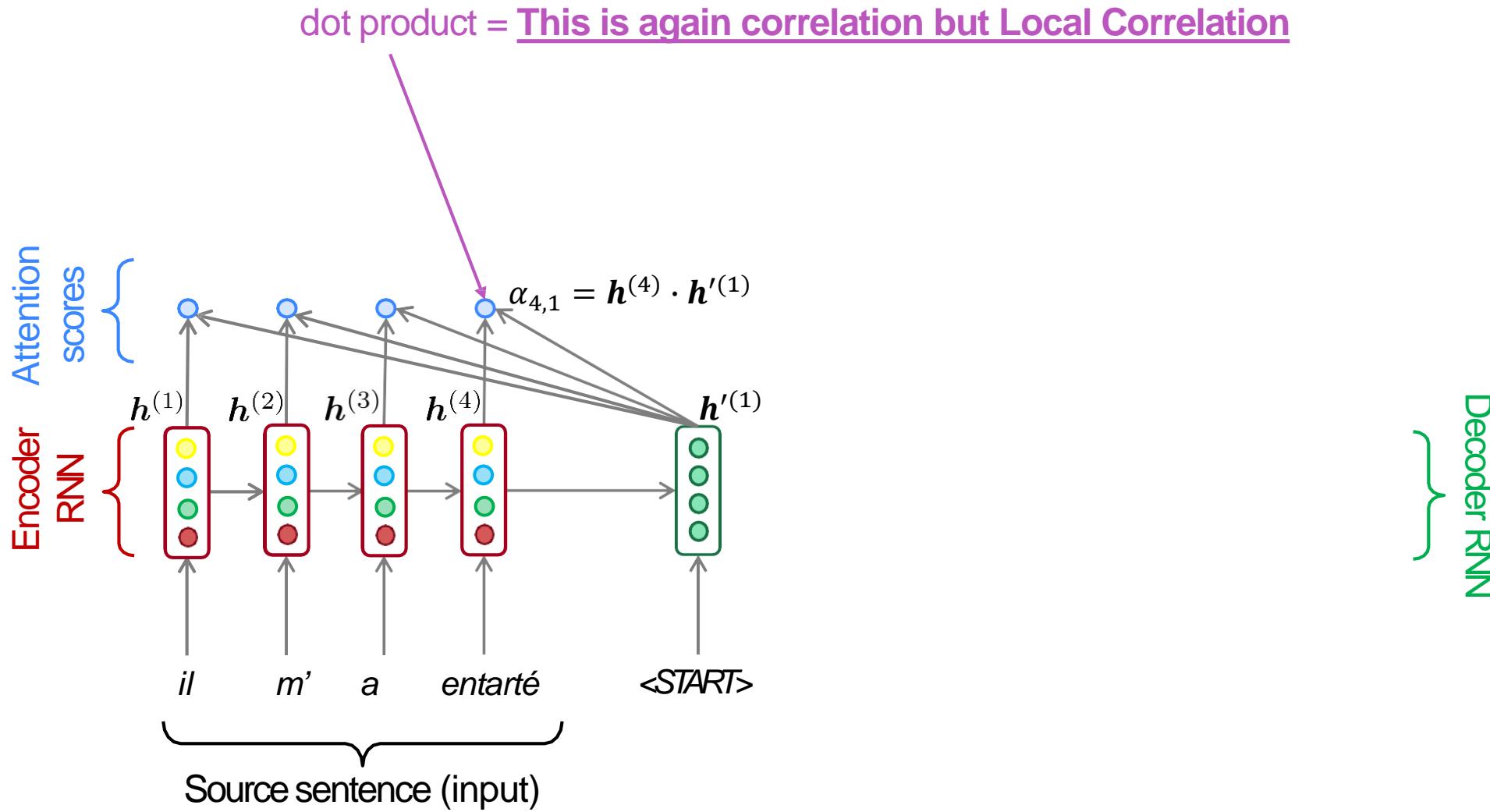
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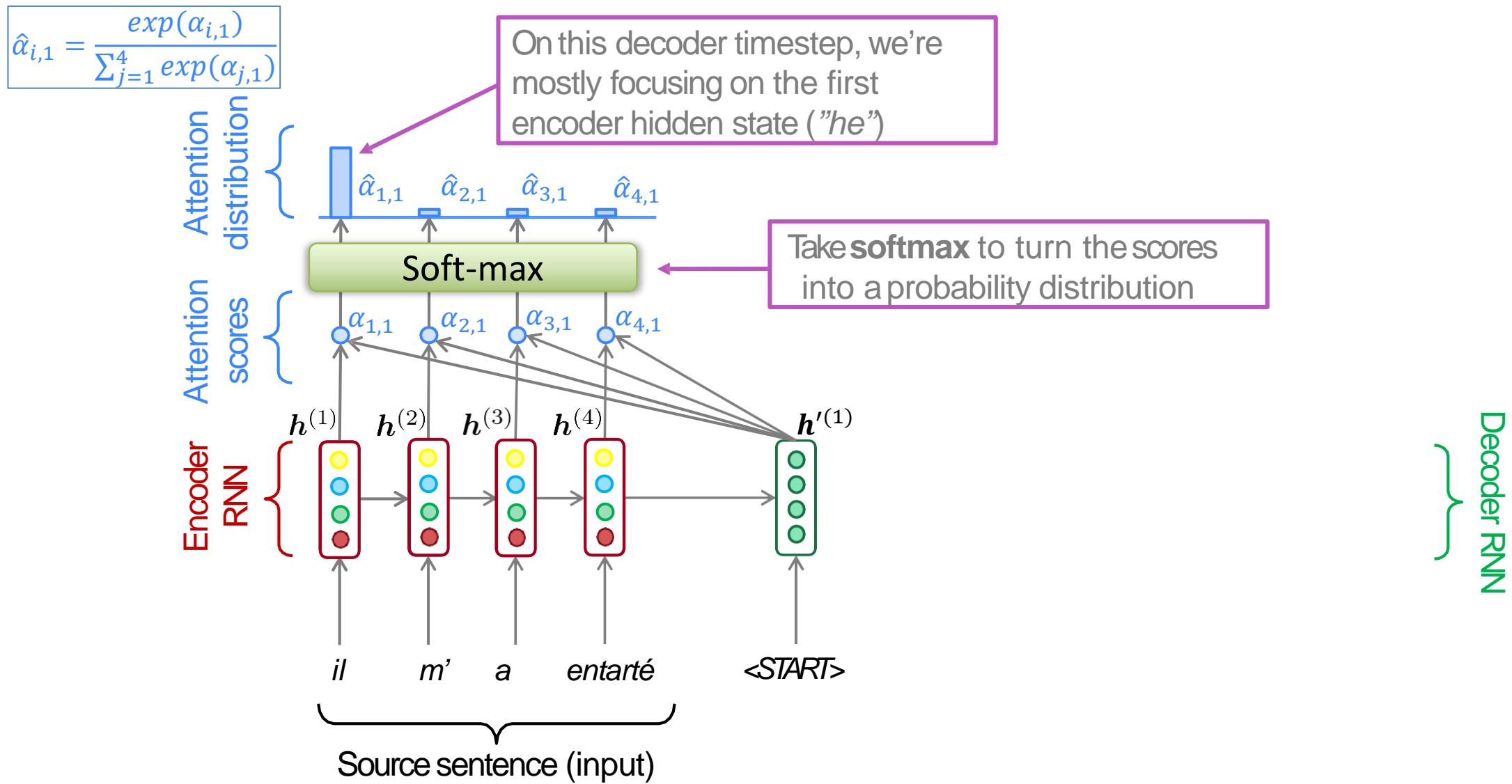
# Sequence-to-sequence with attention



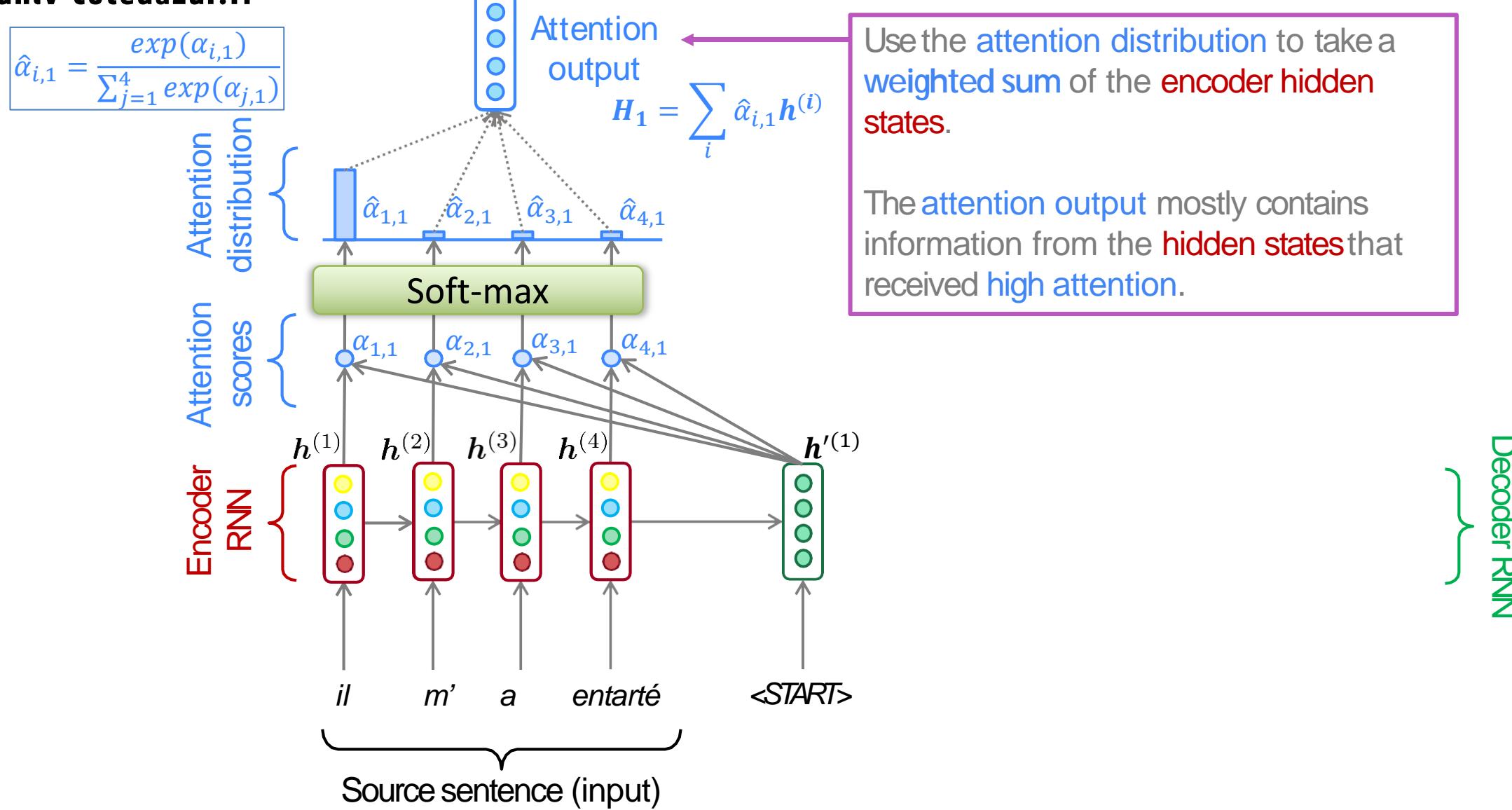
# Sequence-to-sequence with attention



# Sequence-to-sequence with attention



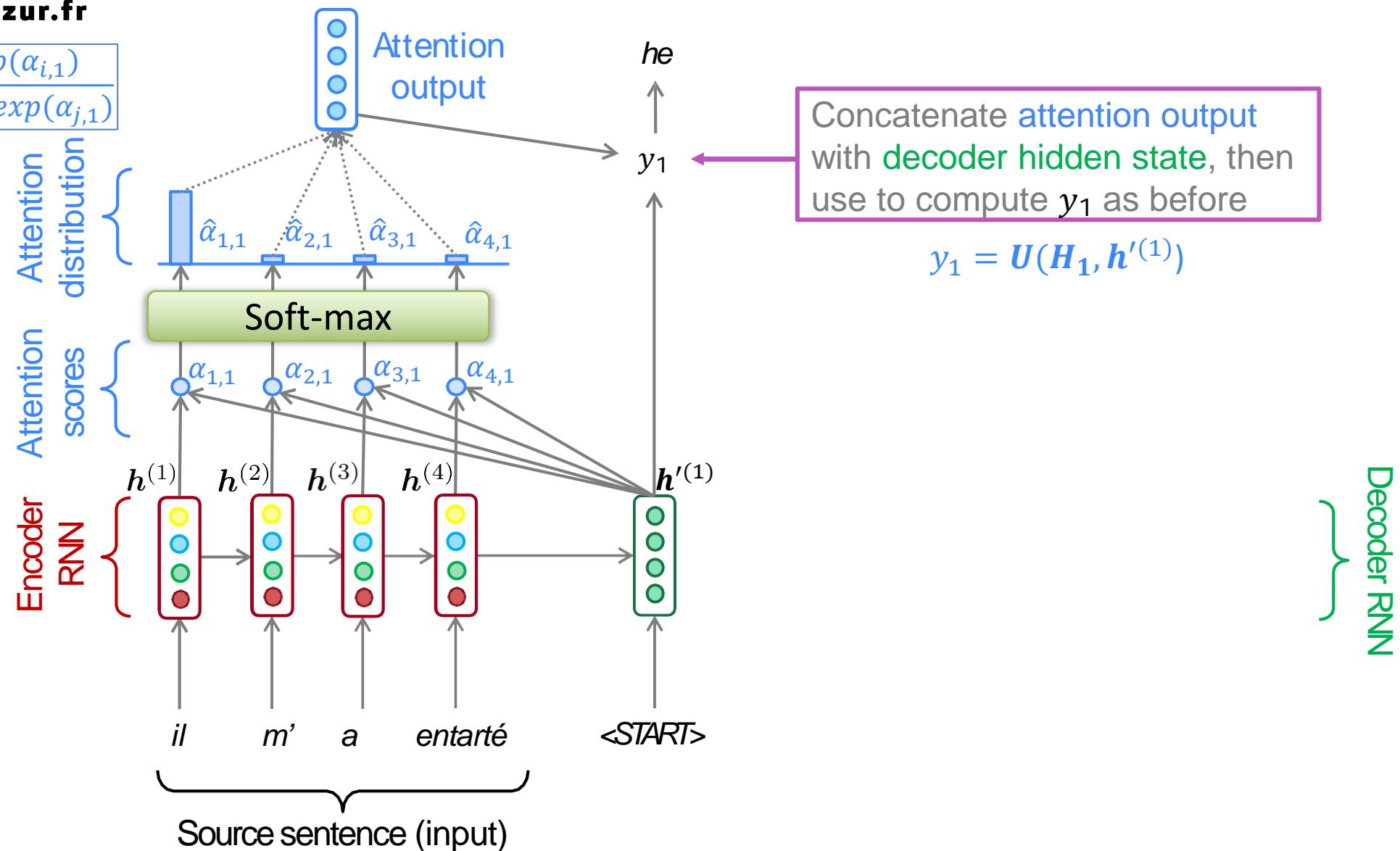
# Sequence-to-sequence with attention



# Sequence-to-sequence with attention

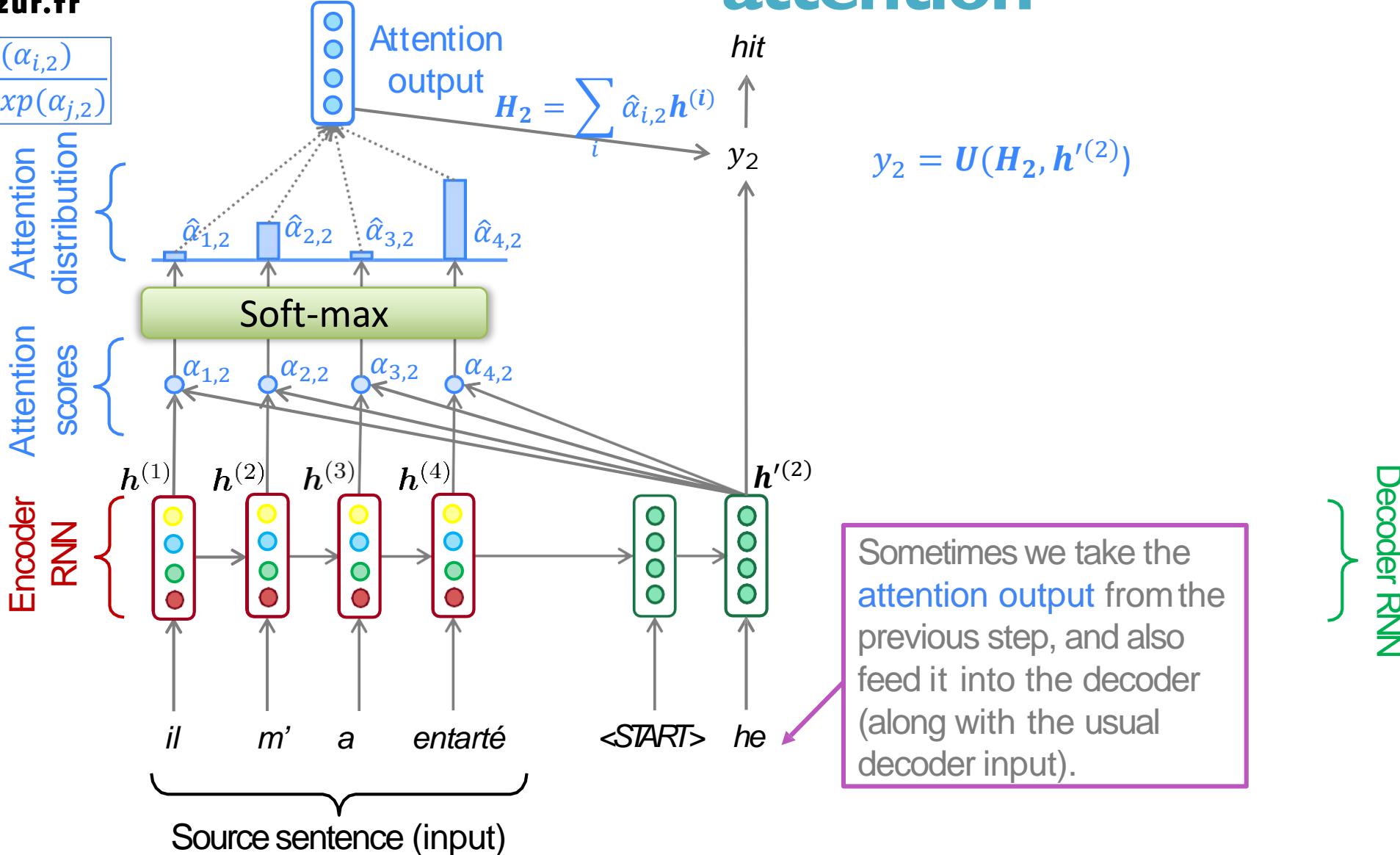
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$$\hat{\alpha}_{i,1} = \frac{\exp(\alpha_{i,1})}{\sum_{j=1}^4 \exp(\alpha_{j,1})}$$



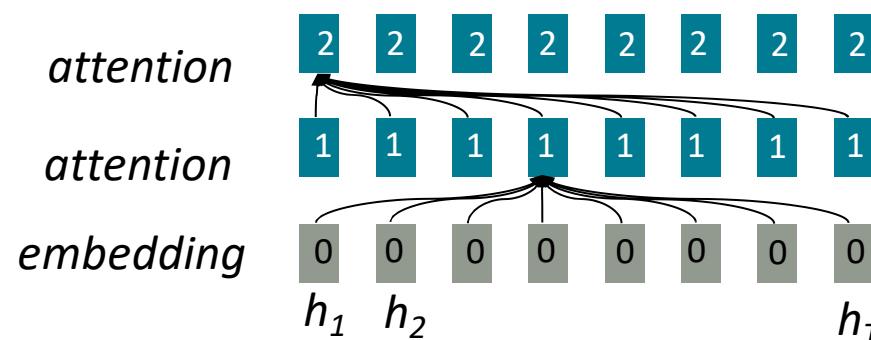
# Sequence-to-sequence with attention

$$\hat{\alpha}_{i,2} = \frac{\exp(\alpha_{i,2})}{\sum_{j=1}^4 \exp(\alpha_{j,2})}$$



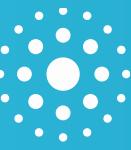
# If not recurrence, then what? How about attention?

- **Attention** treats each word's representation as a **query** to access and incorporate information from a **set of values** (*in the previous example of translation, the values are the words from the initial sentence, the encoded one*).
  - We saw attention from the **decoder** to the **encoder**; here let's think about attention **within a single sentence**.
  - If **attention** gives us access to any state... maybe we can just use attention and don't need the RNN?
- Number of unparallelizable operations not linked to sequence length.
- **All words interact at every layer!**



All words attend to all words in previous layer.

Most arrows here are omitted in the figure.



# *Multimodal correlations*

**SELF-ATTENTION, TRANSFORMERS**

# Principles of Transformers

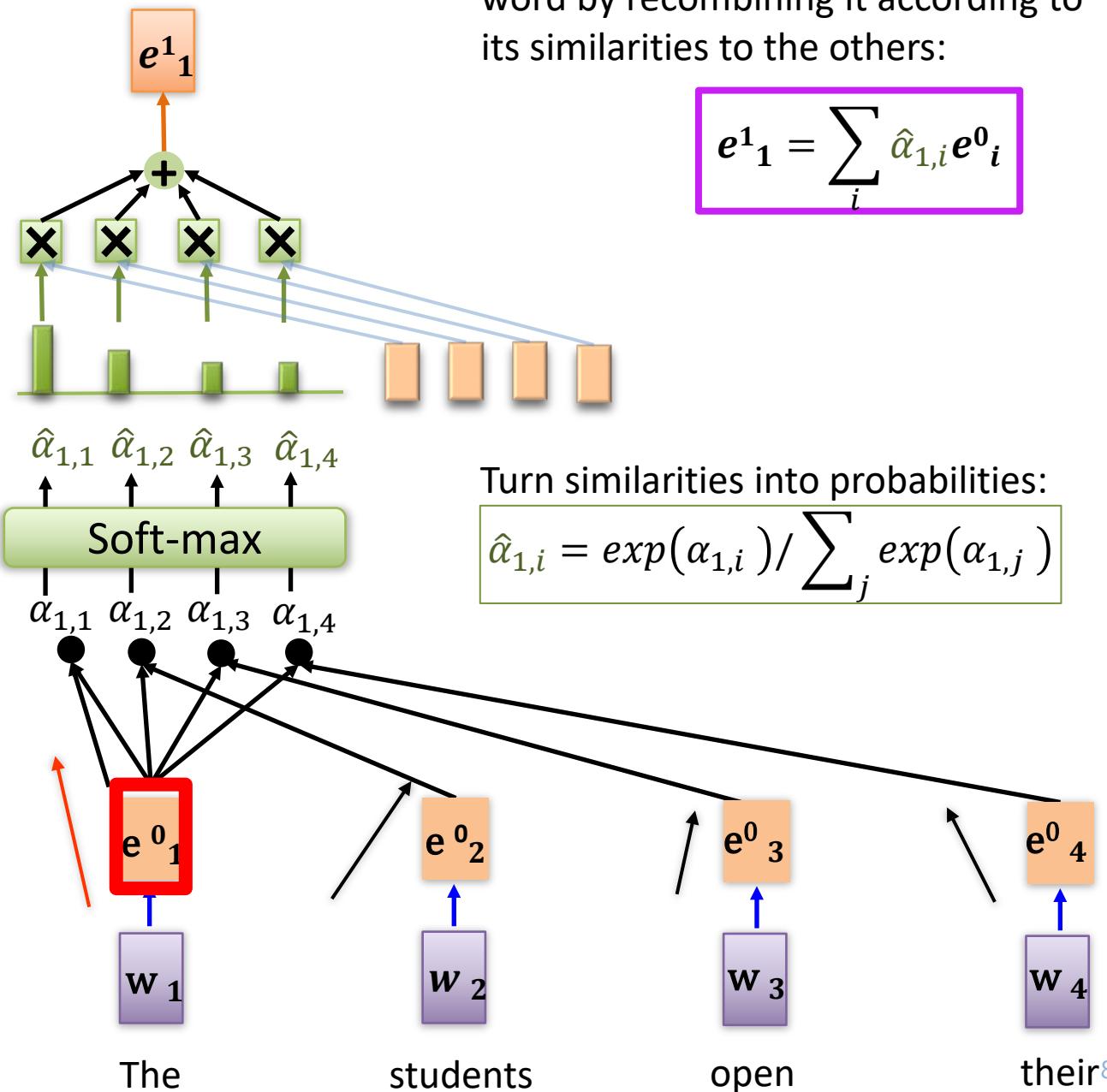
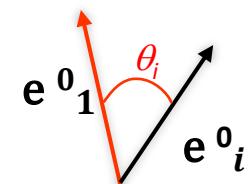
## Heart of LLMs: $f(\cdot)$

- Generate a successive representation of the words in the form of recombination of the representations of the other words:

Attention scores =  
Correlation scores

Calculation of the similarity/correlation of word 1 with the i-th word in the analysis window:

$$\begin{aligned}\alpha_{1,i} &= \mathbf{e}^0_1 \cdot \mathbf{e}^0_i / \sqrt{d} \\ &\approx \cos(\mathbf{e}^0_1, \mathbf{e}^0_i) = \cos(\theta_i)\end{aligned}$$



# Principles of Transformers

## Heart of LLMs: $f(\cdot)$

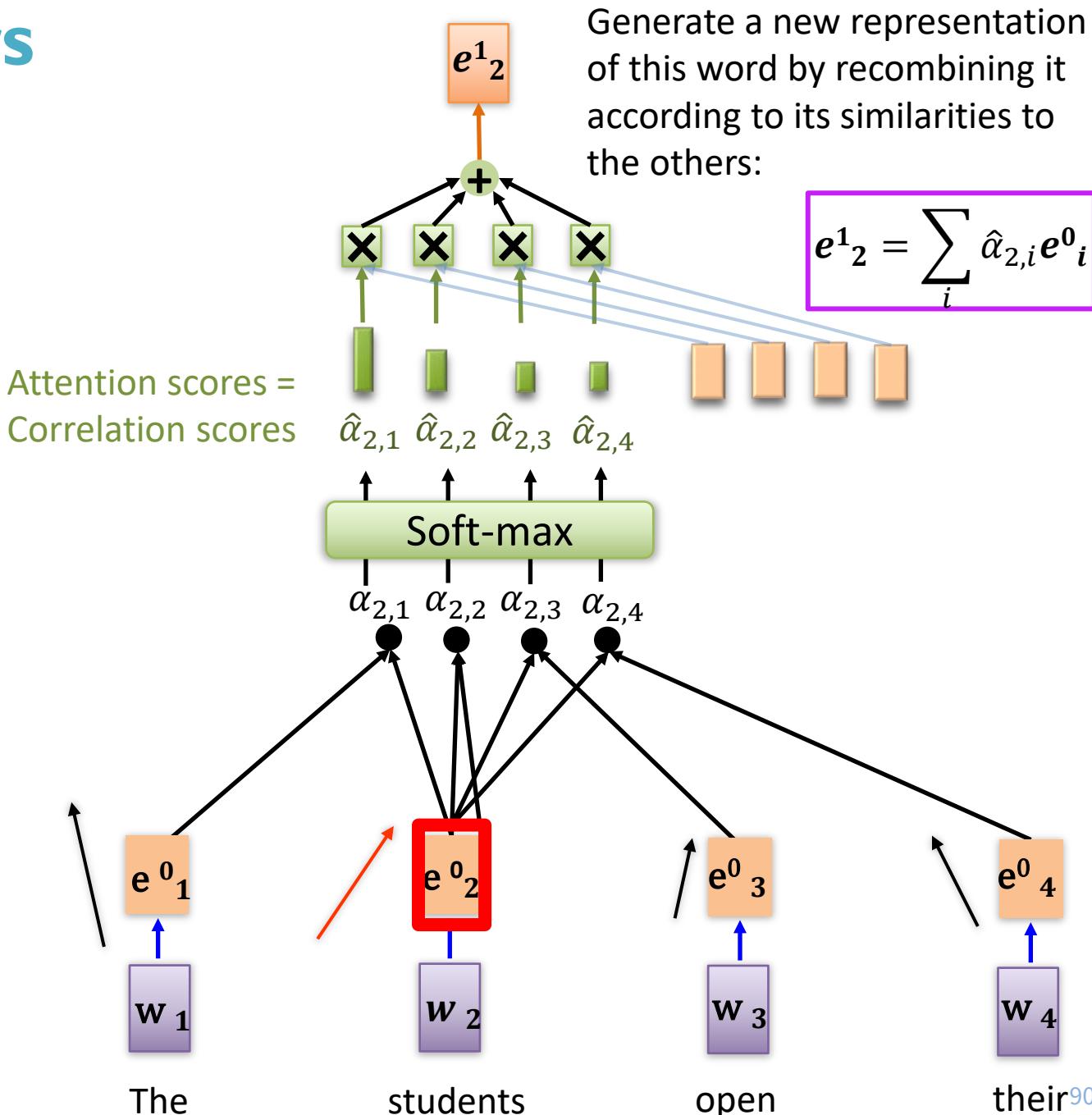
- Generate a successive representation of the words in the form of recombination of the representations of the other words:

Turn similarities into probabilities:

$$\hat{a}_{2,i} = \exp(\alpha_{2,i}) / \sum_j \exp(\alpha_{2,j})$$

Calculation of the similarity/correlation of word 2 with the i-th word in the analysis window:

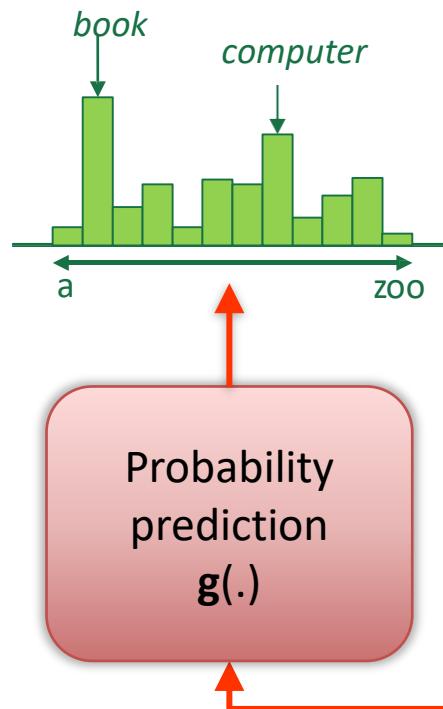
$$\alpha_{2,i} = \mathbf{e}^0_2 \cdot \mathbf{e}^0_i / \sqrt{d}$$



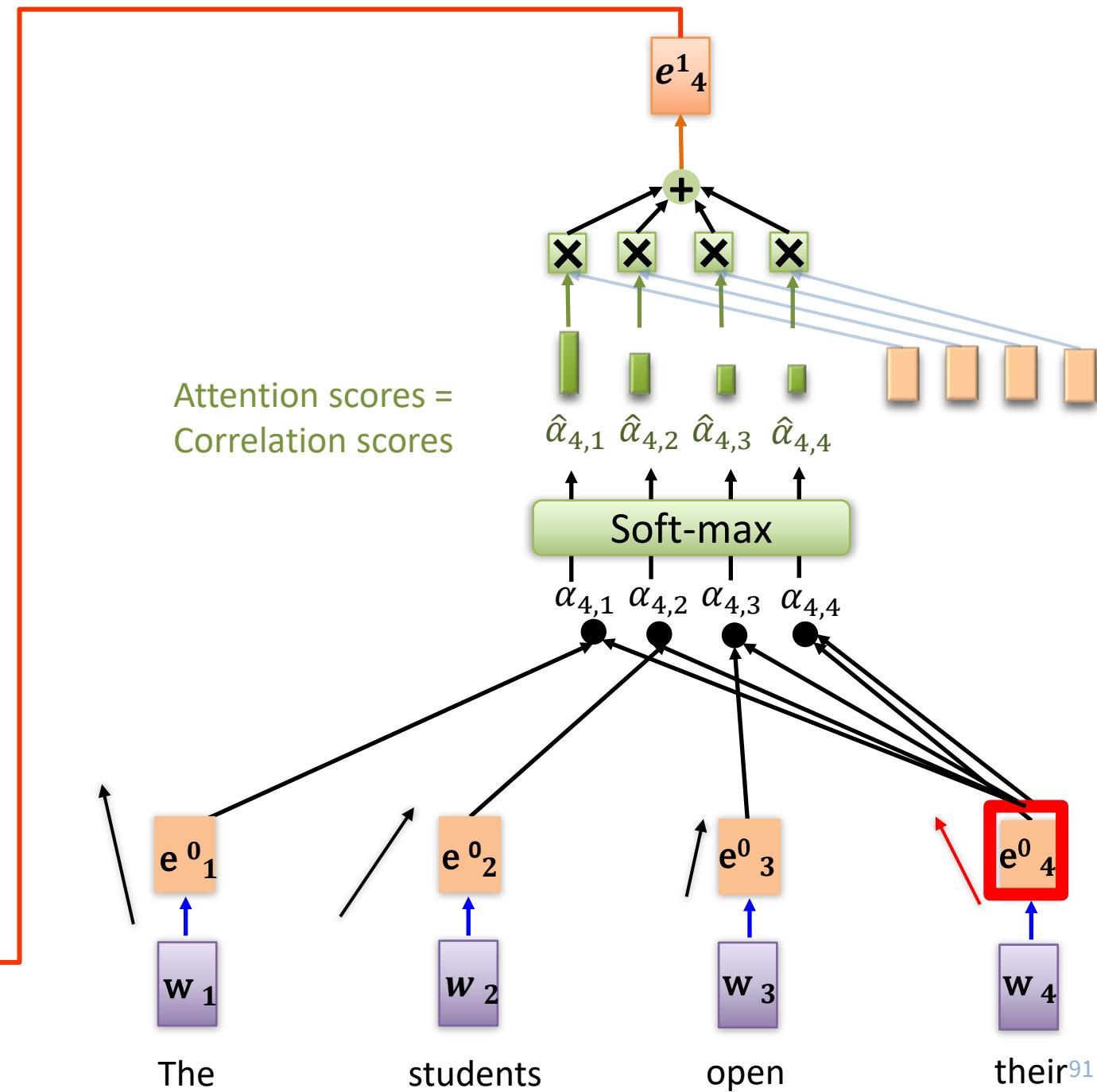
# Principles of Transformers

## Heart of LLMs: $g(\cdot)$

- Generate a successive representation of the words in the form of recombination of the representations of the other words:



Credits: L. Sassatelli





Attention is  
all you need.

# Make Self-Attention More Flexible: Different representations for the roles of query, key, value

$q$ : query (to match others)

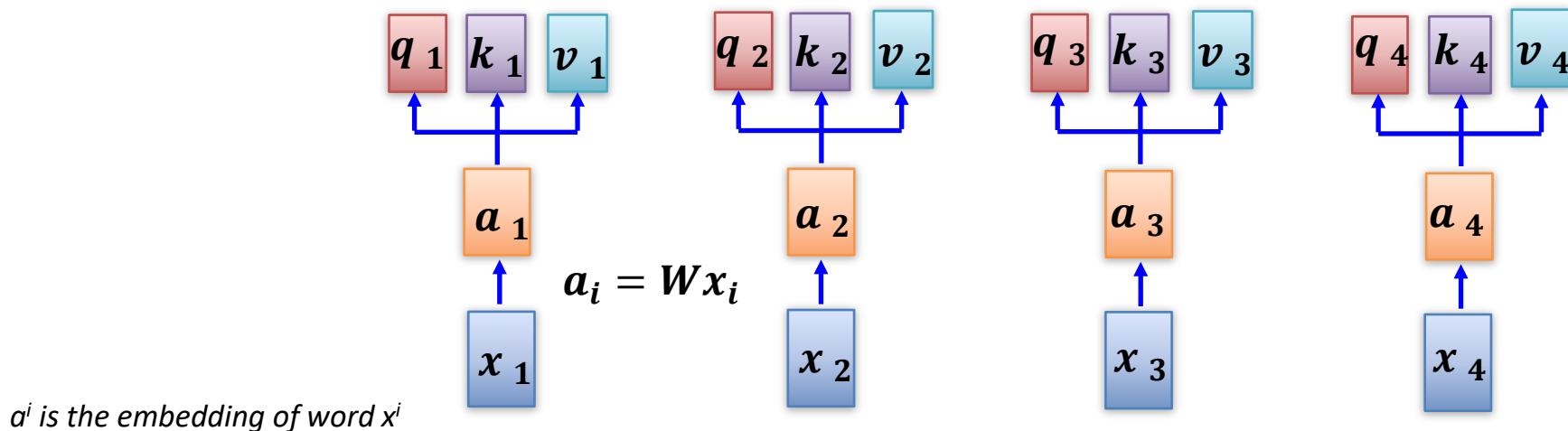
$$q_i = W^q a_i$$

$k$ : key (to be matched)

$$k_i = W^k a_i$$

$v$ : information to be extracted

$$v_i = W^v a_i$$

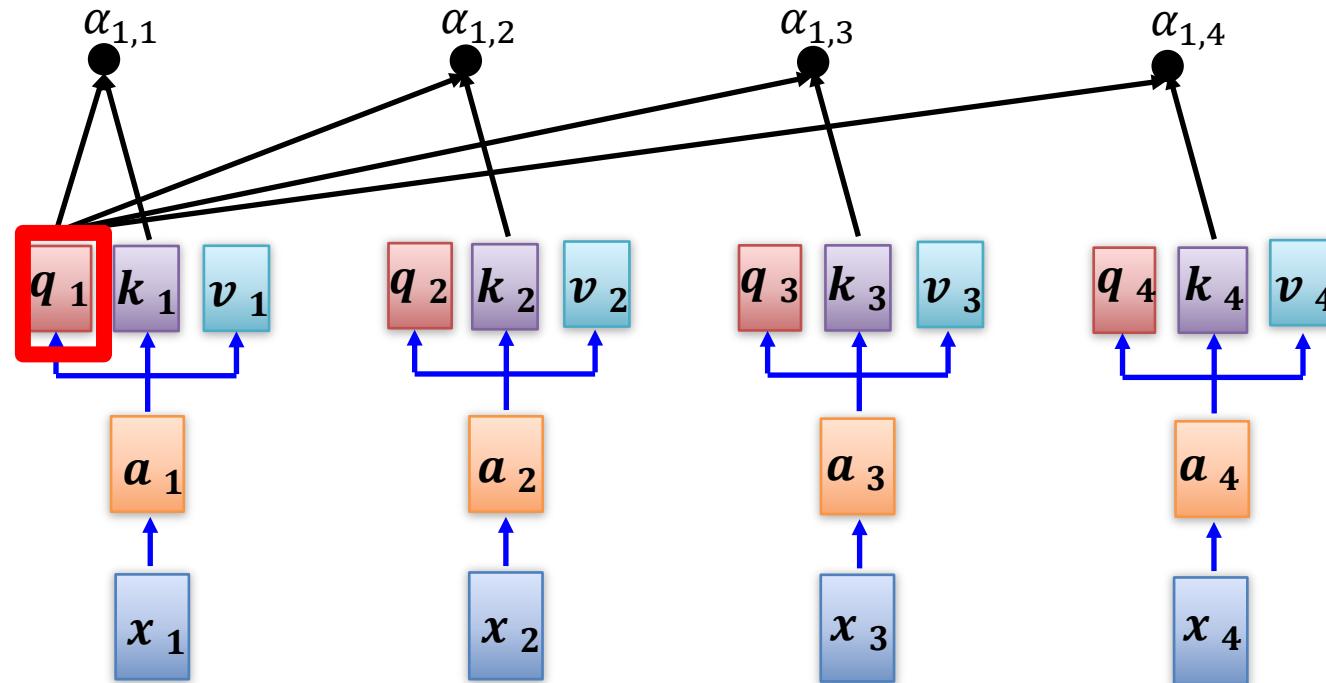


# Make Self-Attention More Flexible: Different representations for the roles of query, key, value

Take each query  $q$  to pay attention to each key  $k$

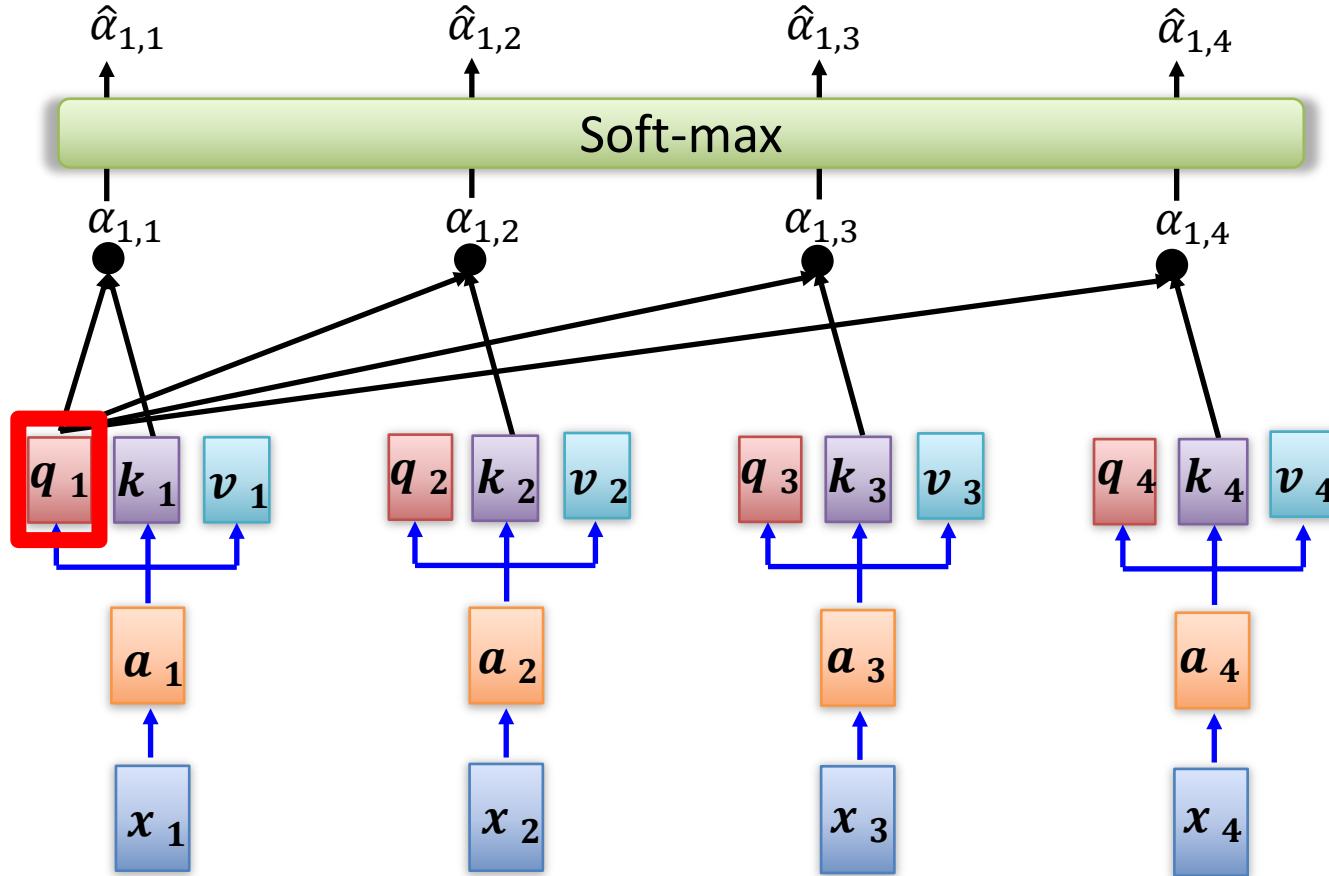
$d$  is the dim of  $q$  and  $k$

Scaled Dot-Product Attention:  $\alpha_{1,i} = \underbrace{q_1 \cdot k_i}_{\text{dot product}} / \sqrt{d}$



# Make Self-Attention More Flexible: Different representations for the roles of query, key, value

$$\hat{\alpha}_{1,i} = \exp(\alpha_{1,i}) / \sum_j \exp(\alpha_{1,j})$$



# Make Self-Attention More Flexible: Different representations for the roles of query, key, value

$$\alpha_{1,i} = q^0_1 \cdot k^0_i / \sqrt{d}$$

$q$ : query (to match with others)

$$q_i = W^q e_i$$

$k$ : key (to be matched)

$$k_i = W^k e_i$$

$v$ : representation to be extracted

$$v_i = W^v e_i$$

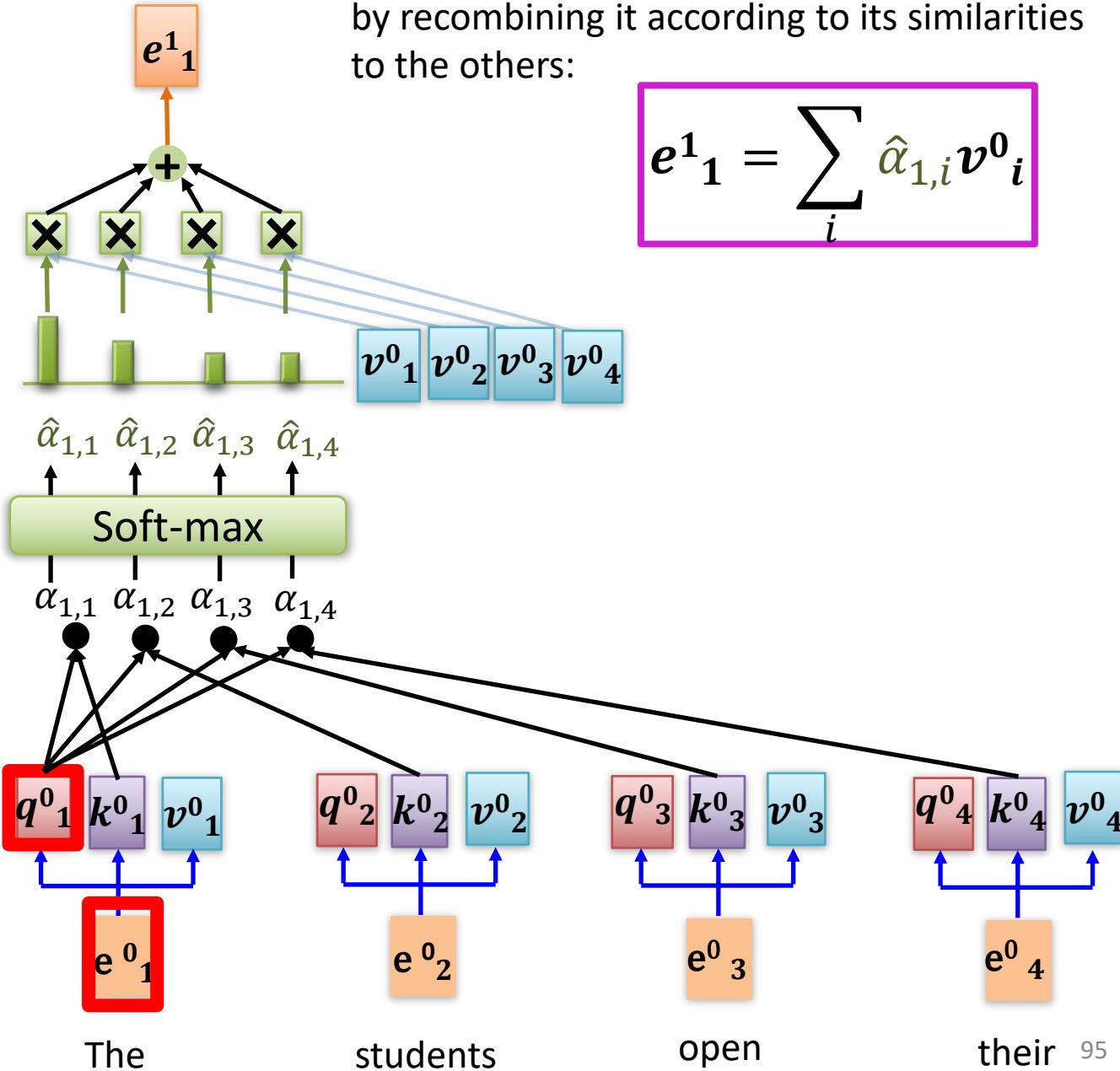
(one can also take  $q^0_i = k^0_i = v^0_i = e^0_i$ )

Credits: L. Sassatelli

Scores d'attention =  
Scores de corrélation

Generate a new representation of this word  
by recombining it according to its similarities  
to the others:

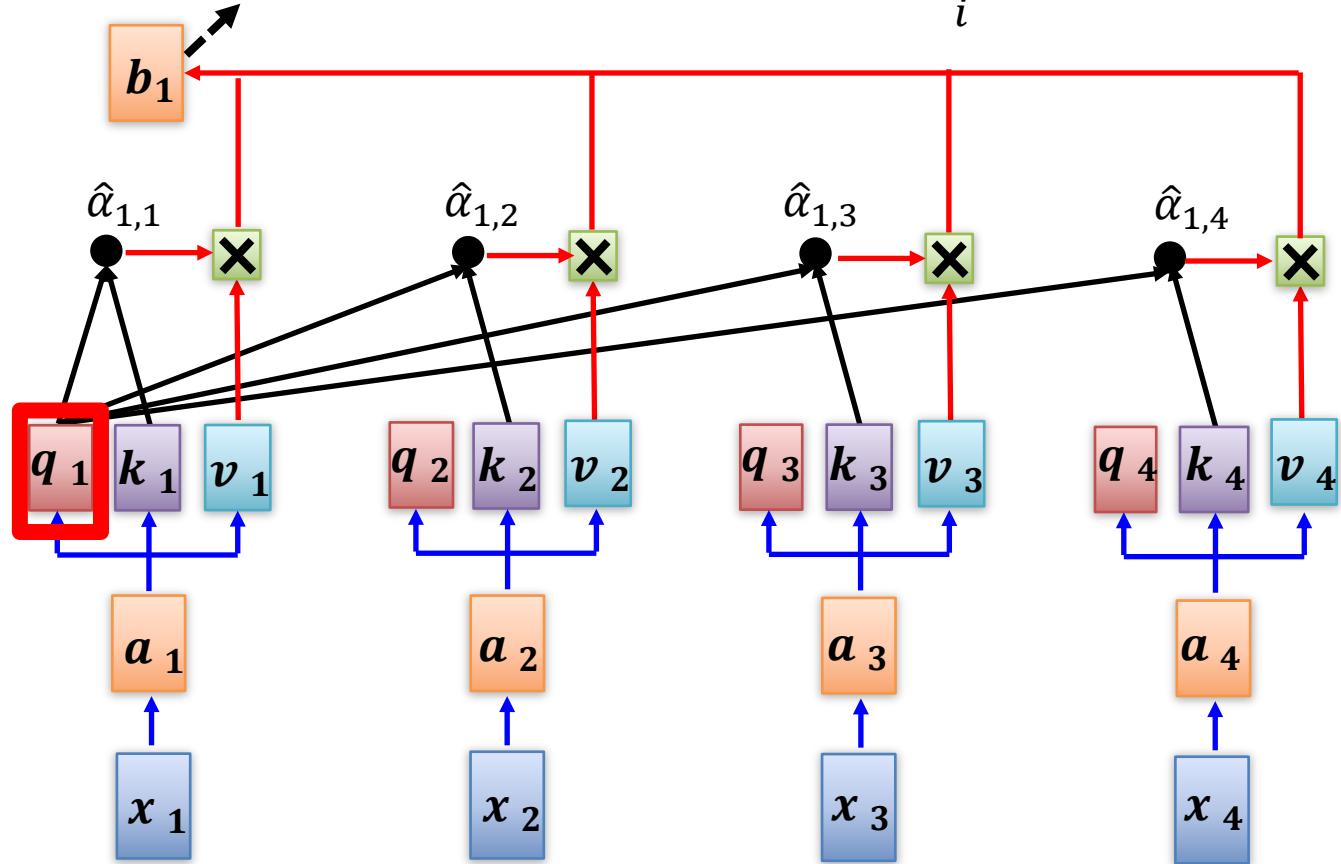
$$e^1_1 = \sum_i \hat{\alpha}_{1,i} v^0_i$$



## Self-attention

Considering the whole sequence

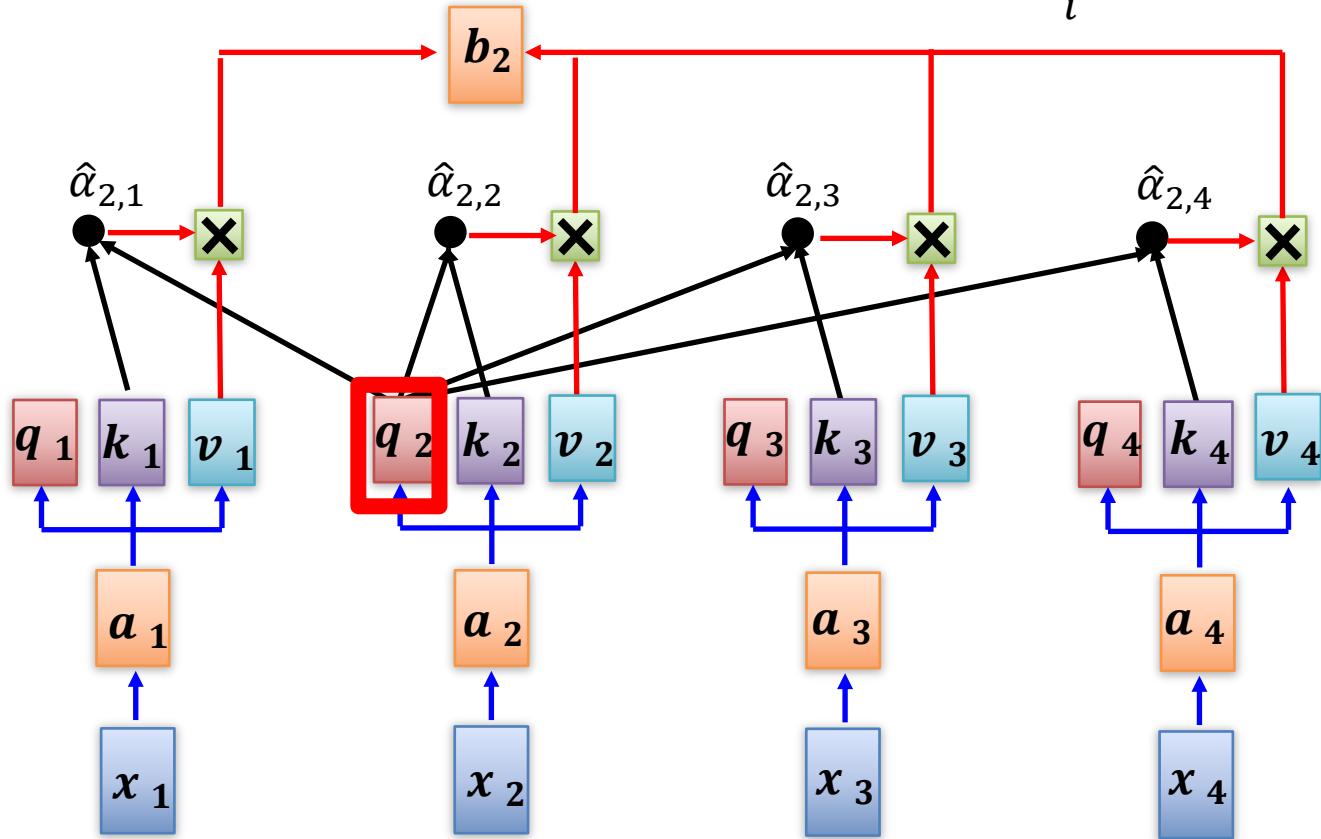
$$\mathbf{b}_1 = \sum_i \hat{\alpha}_{1,i} \mathbf{v}_i$$



## Self-attention

Take each query  $q$  to pay attention to each key  $k$

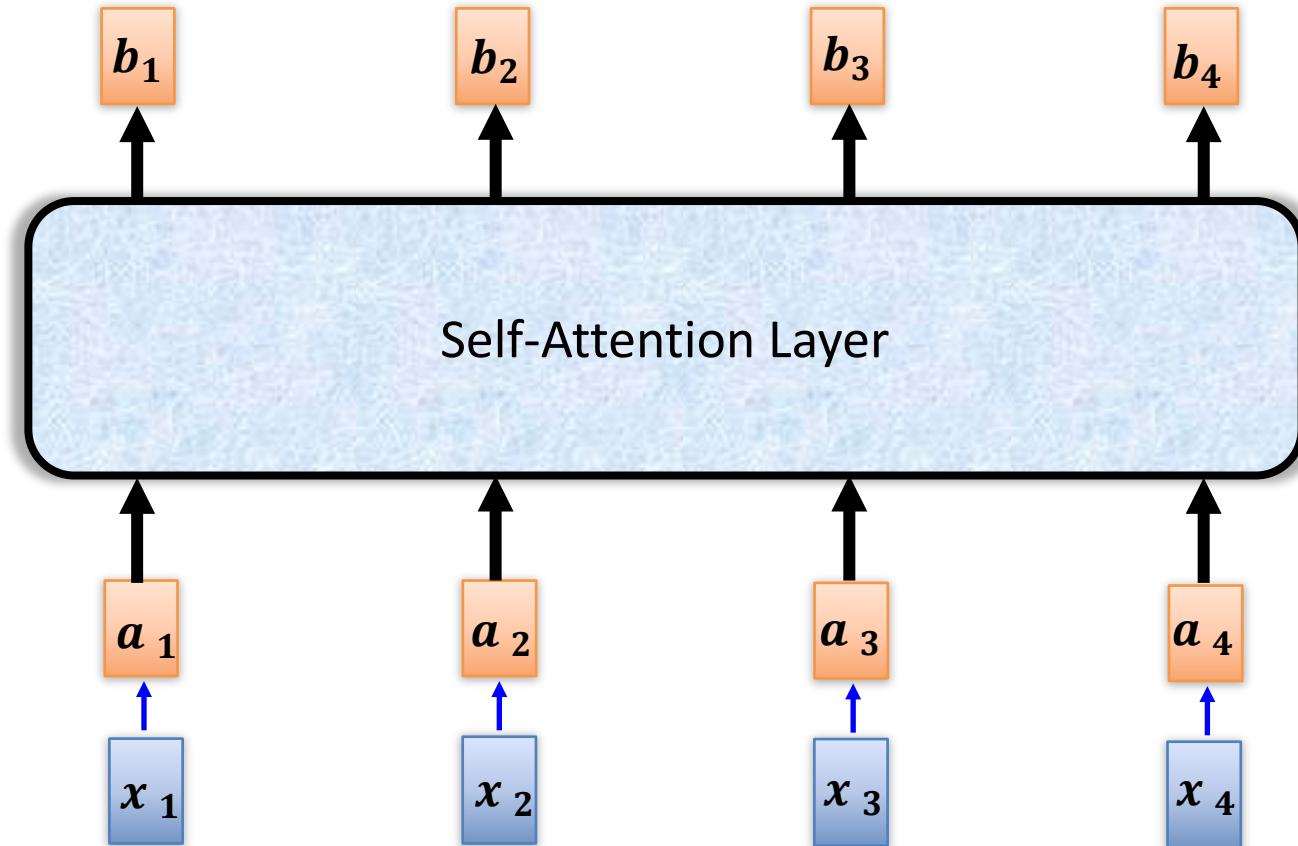
$$b_2 = \sum_i \hat{\alpha}_{2,i} v_i$$





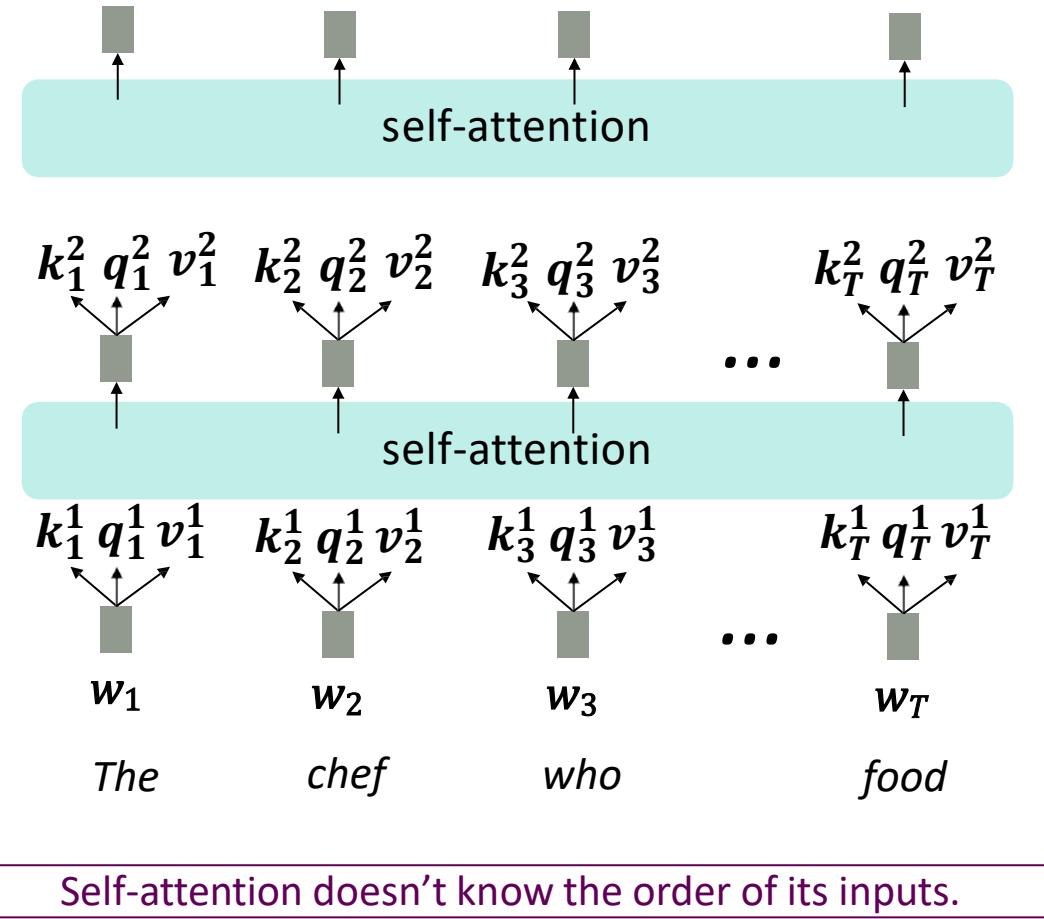
## Self-attention

$b_1, b_2, b_3, b_4$  can be parallelly computed.



# Self-Attention

- In the diagram at the right, we have stacked self-attention blocks, like we might stack LSTM layers.
- Can self-attention be a drop-in replacement for recurrence?
- No. It has a few issues, which we'll go through.
- First, self-attention is an operation on **sets**. It has no inherent notion of order.





# Barriers and solutions for Self-Attention as a building block

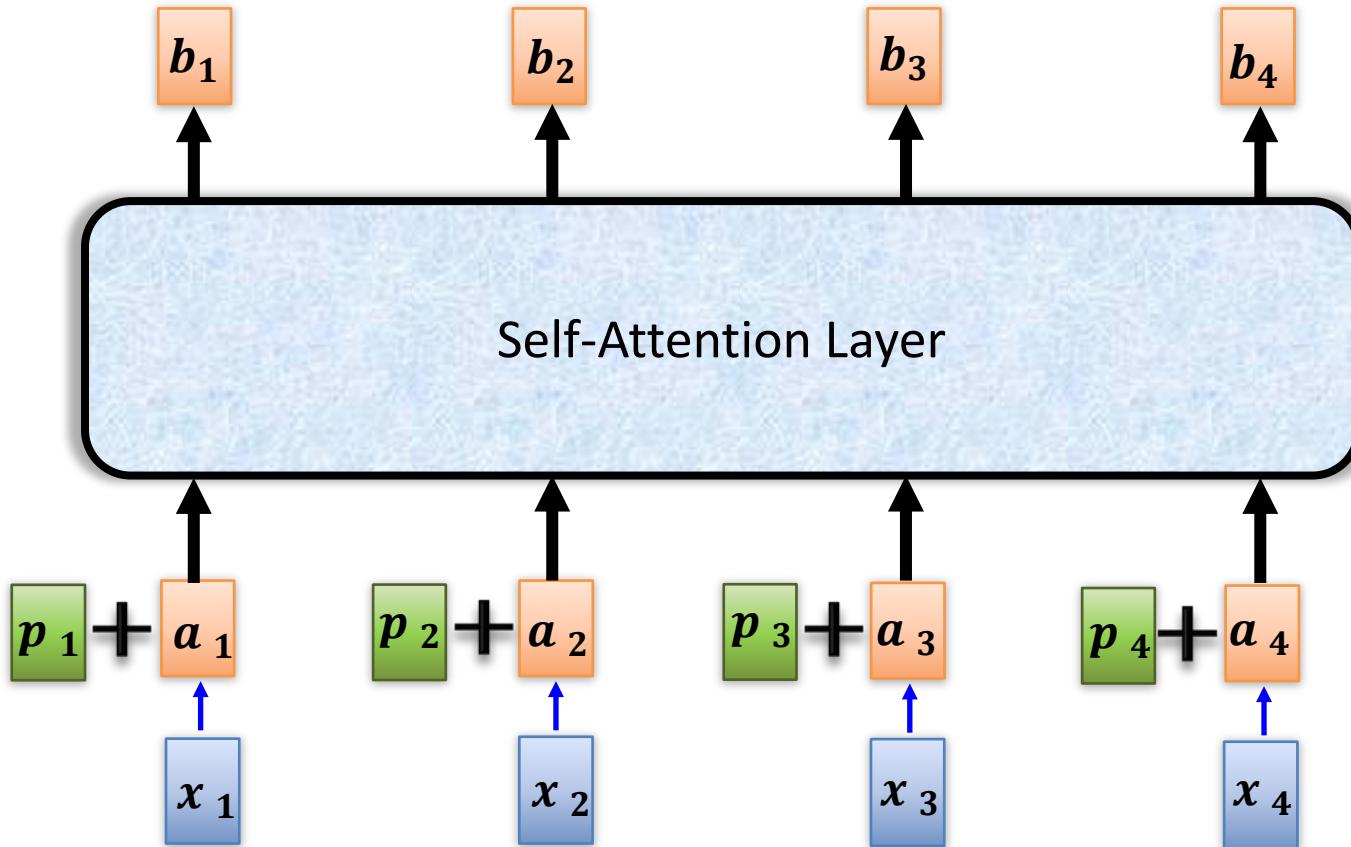
## Barriers

- Doesn't have an inherent notion of order!



## Solutions

# Fixing the first self-attention problem: Sequence order by adding position



# Barriers and solutions for Self-Attention as a building block

## Barriers

- Doesn't have an inherent notion of order!
- No nonlinearities for deep learning! It's all just weighted averages



## Solutions

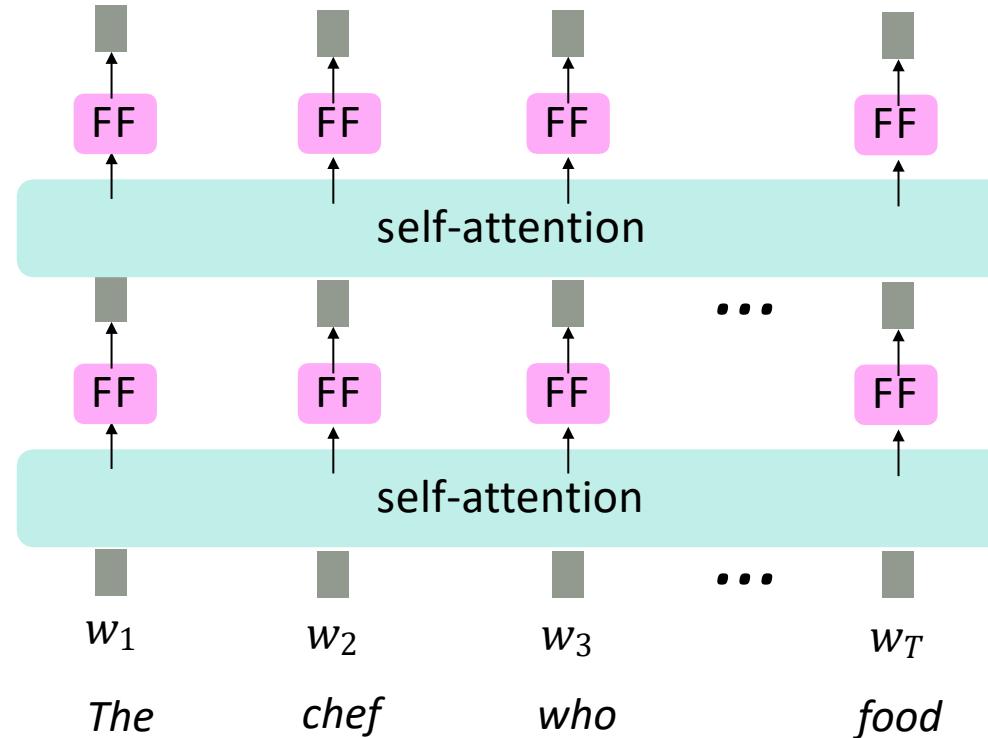
- Add position representations to the inputs



# Adding nonlinearities in self-attention

- Note that there are no elementwise nonlinearities in self-attention; stacking more self-attention layers just re-averages **value** vectors
- Easy fix: add a **feed-forward network** to post-process each output vector.

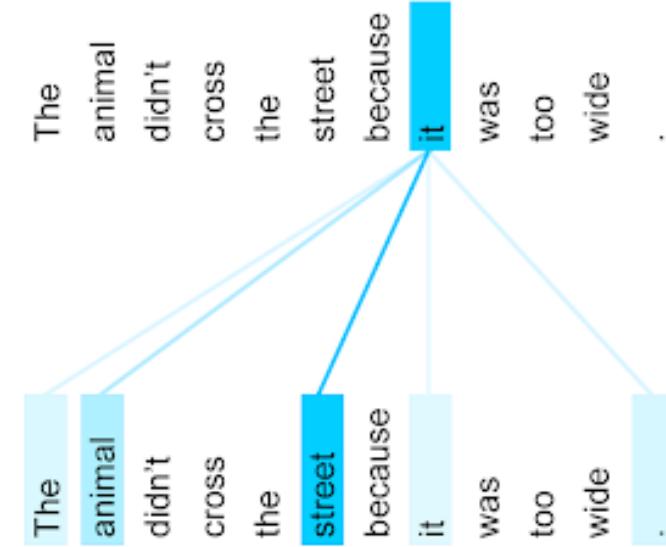
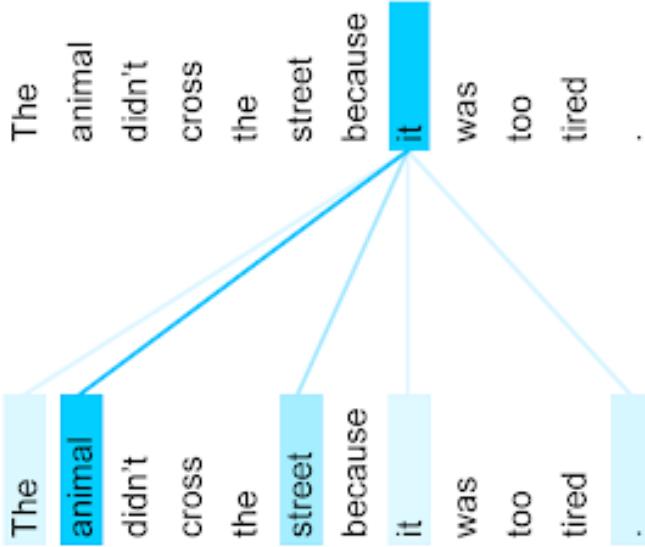
$$\begin{aligned} m_i &= \text{MLP}(\text{output}_i) \\ &= W_2 * \text{ReLU}(W_1 \times \text{output}_i + b_1) + b_2 \end{aligned}$$



Intuition: the FF network processes the result of attention



# Attention Visualization



The encoder self-attention distribution for the word “it” from the 5th to the 6th layer of a Transformer trained on English to French translation (one of eight attention heads).

<https://ai.googleblog.com/2017/08/transformer-novel-neural-network.html>

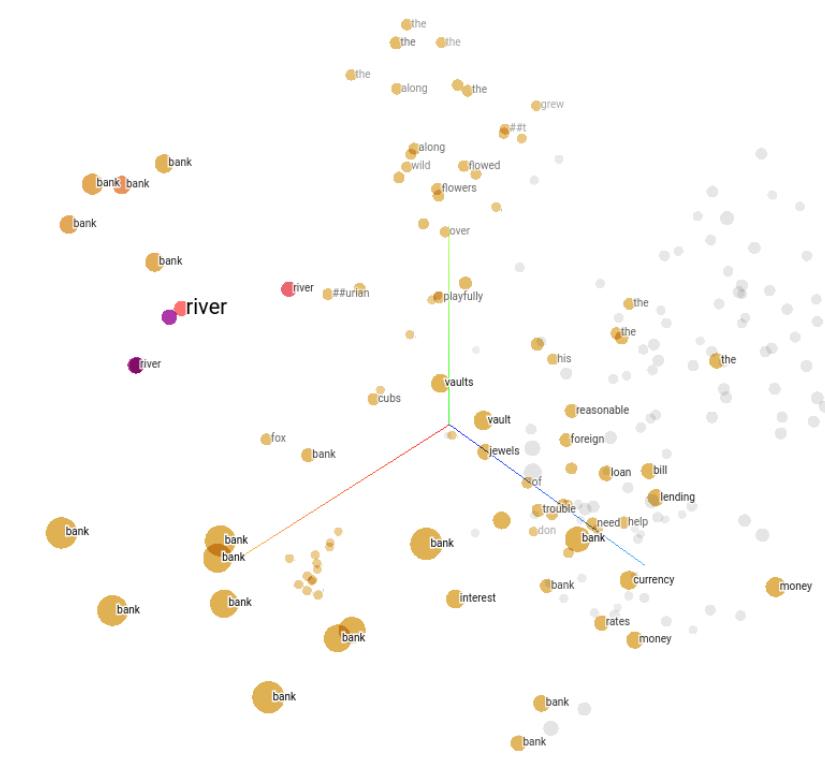
# Visualization of BERT embeddings

- A vector for the same word for each appearance:

```

sentences = ["bank",
    "he eventually sold the shares back to the bank at a
premium.",
    "the bank strongly resisted cutting interest rates.",
    "the bank will supply and buy back foreign currency.",
    "the bank is pressing us for repayment of the loan.",
    "the bank left its lending rates unchanged.",
    "the river flowed over the bank.",
    "tall, luxuriant plants grew along the river bank.",
    "his soldiers were arrayed along the river bank.",
    "wild flowers adorned the river bank.",
    "two fox cubs romped playfully on the river bank.",
    "the jewels were kept in a bank vault.",
    "you can stow your jewellery away in the bank.",
    "most of the money was in storage in bank vaults.",
    "the diamonds are shut away in a bank vault somewhere.",
    "thieves broke into the bank vault.",
    "can I bank on your support?",
    "you can bank on him to hand you a reasonable bill for your
services.",
    "don't bank on your friends to help you out of trouble.",
    "you can bank on me when you need money.",
    "i bank on your help."
]

```



<https://projector.tensorflow.org/?config=https%3A%2F%2Fgist.githubusercontent.com%2Farmimirreza%2F2c59f675a997fef20d59851291f8c268%2Fraw%2Fc542be898dc77aad2d593ebcd7b60ac302b71359%2Fgistfile1.txt>

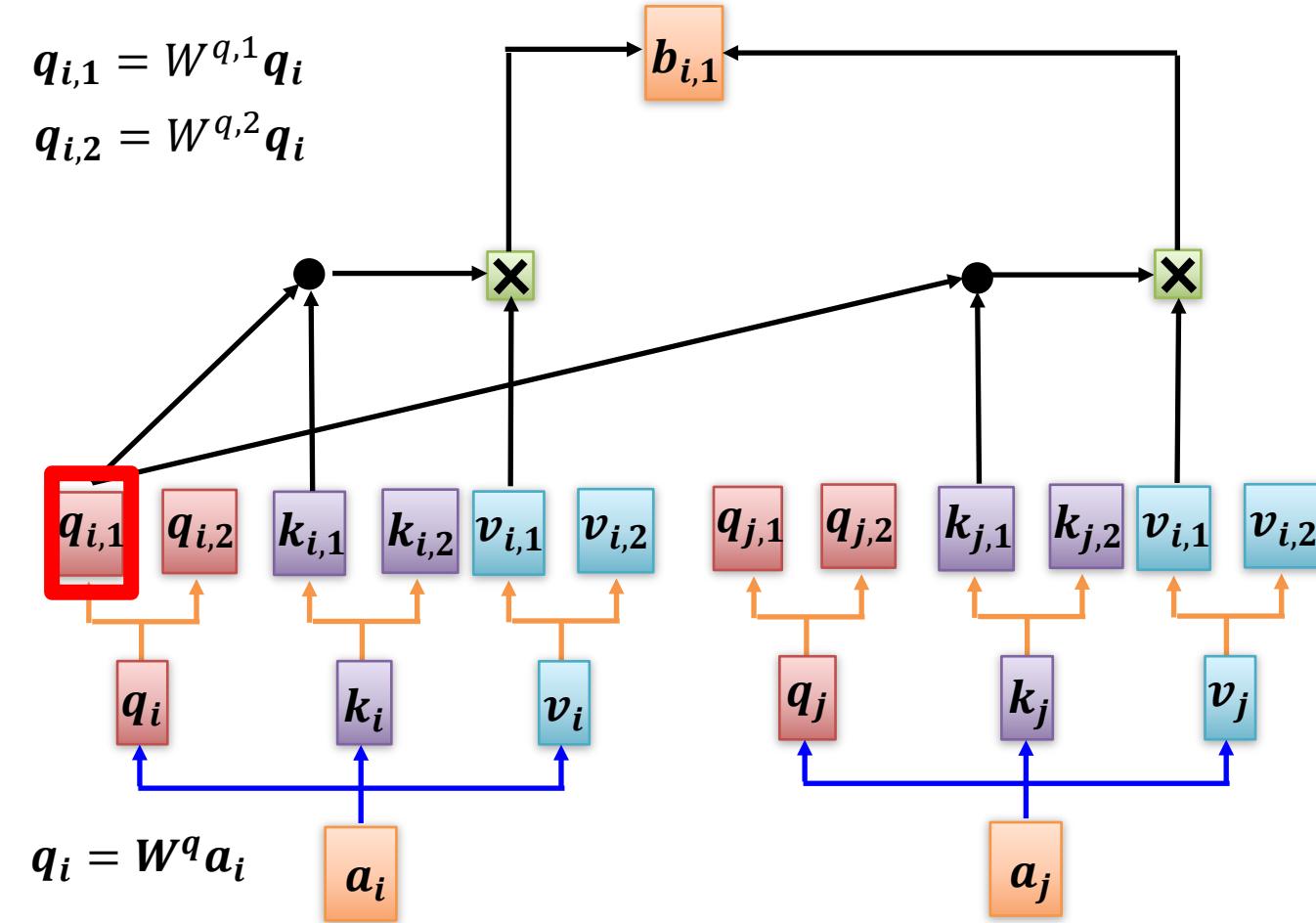


## Necessities for a self-attention building block:

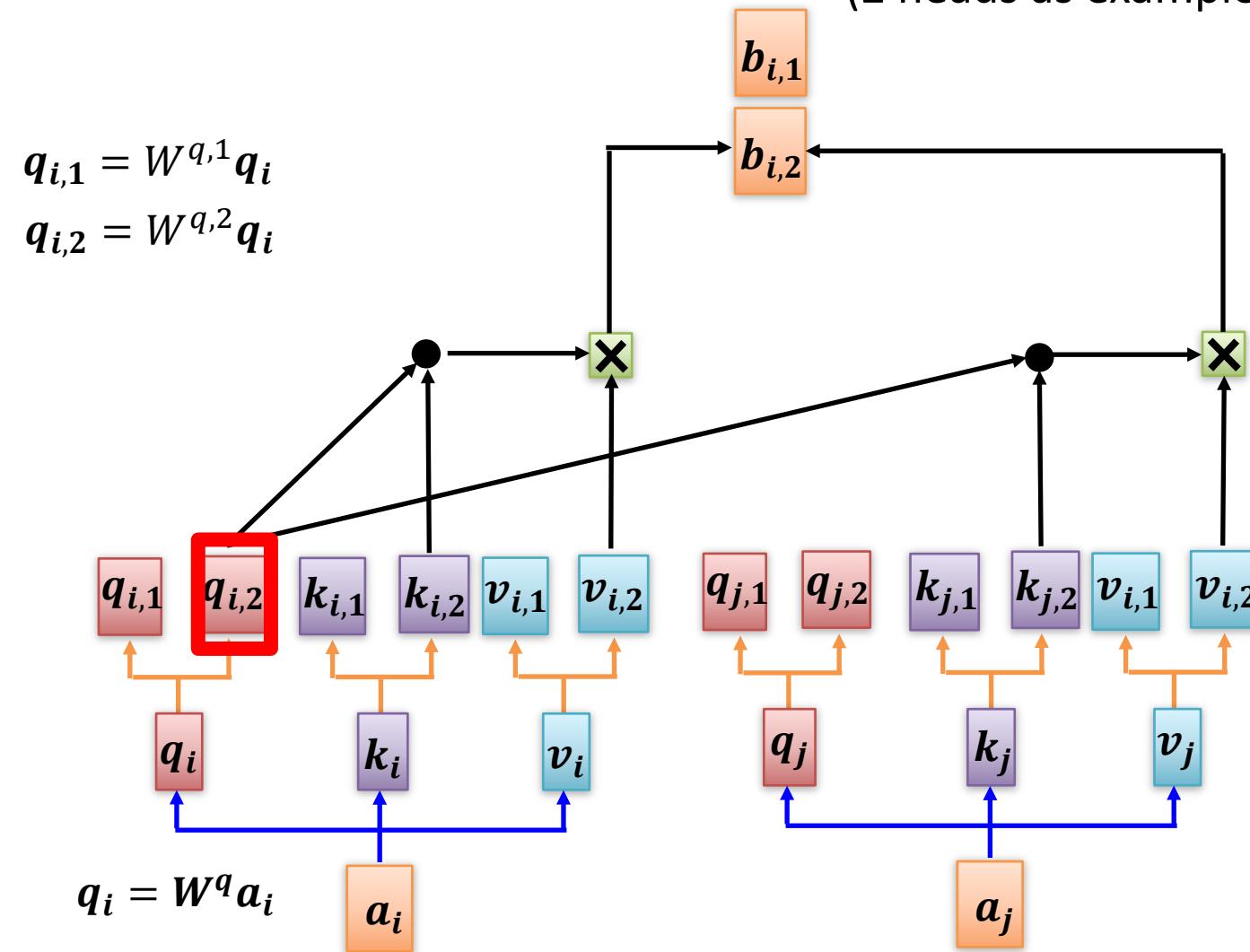
- **Self-attention:**
  - the basis of the method.
- **Position representations:**
  - Specify the sequence order, since self-attention is an unordered function of its inputs.
- **Nonlinearities:**
  - At the output of the self-attention block
  - Frequently implemented as a simple feed-forward network.
- **Masking:**
  - In order to parallelize operations while not looking at the future.
  - Keeps information about the future from “leaking” to the past.
- These are the main steps to build Transformers...But this is not yet the Transformer model we've been hearing about!

# The Transformer Encoder: Multi-headed attention

(2 heads as example)



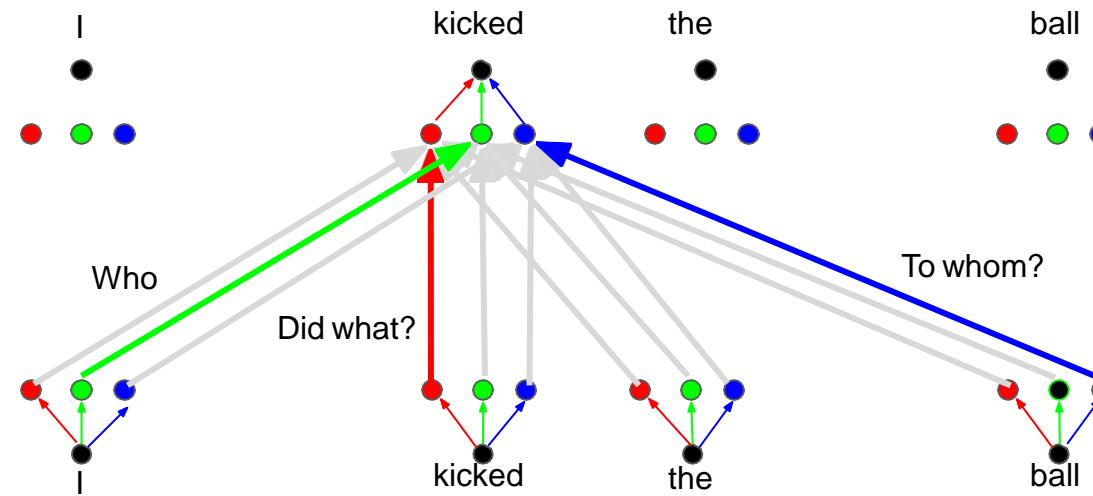
# The Transformer Encoder: Multi-headed attention (2 heads as example)

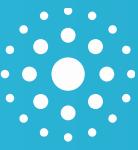


The principle of multi-head attention in transformers is similar to the one of multi-kernels in convolution layers of a CNN (i.e. multi-feature maps, yellow, red, blue, green...)



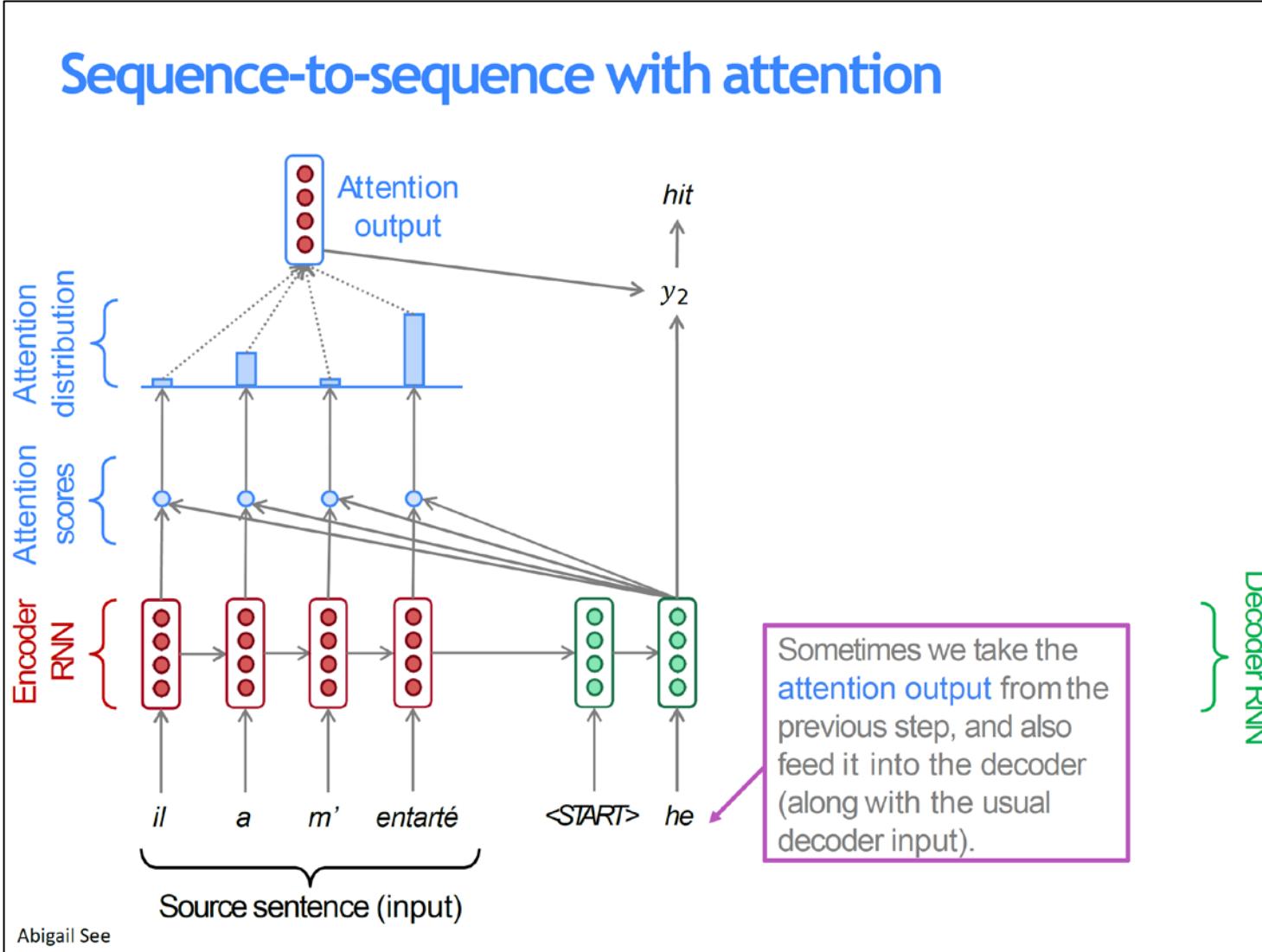
## Parallel attention heads





# TRANSFORMERS

# Before Transformers...





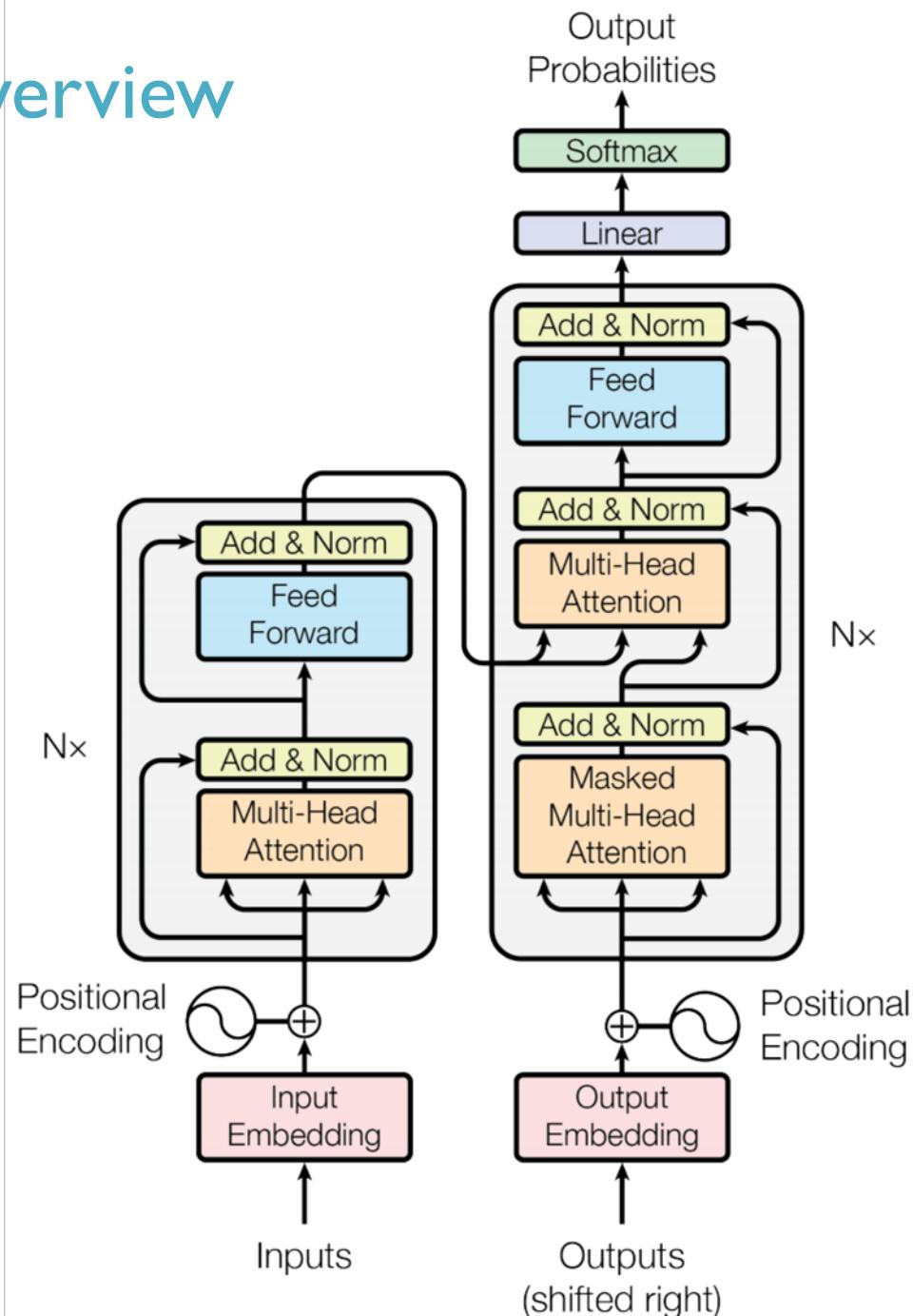
# Transformer Overview

Attention is all you need. 2017. Aswani, Shazeer, Parmar, Uszkoreit, Jones, Gomez, Kaiser, Polosukhin

<https://arxiv.org/pdf/1706.03762.pdf>

- **Non-recurrent sequence-to-sequence encoder-decoder model**
- **Task: machine translation with parallel corpus**
- Predict each translated word
- Final cost/error function is standard cross-entropy error on top of a softmax classifier

This and related figures from paper ↑





# Transformer Encoder

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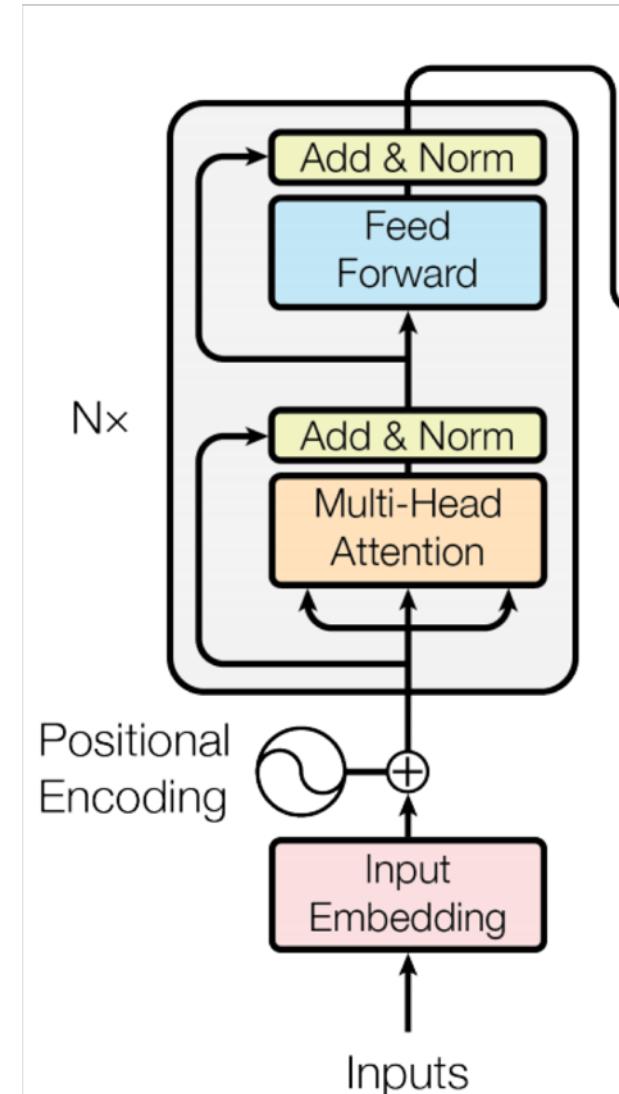
- For encoder, at each block, we use the same  $q$ ,  $k$  and  $v$  from the previous layer:

$$q_i^l = q_i^{l+1}$$

$$k_i^l = k_i^{l+1}$$

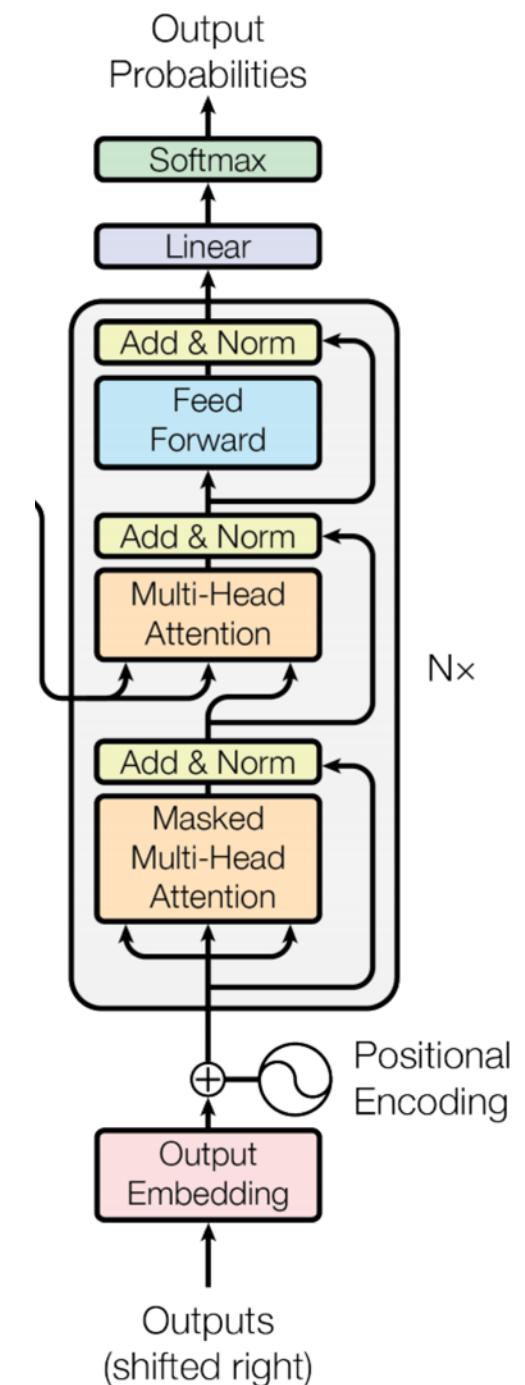
$$v_i^l = v_i^{l+1}$$

- Blocks are repeated 6 times (in vertical stack)





# Transformer Decoder





# Barriers and solutions for Self-Attention as a building block

## Barriers

- Doesn't have an inherent notion of order!
- No nonlinearities for deep learning magic! It's all just weighted averages
- Need to ensure we don't "look at the future" when predicting a sequence
  - Like in machine translation
  - Or language modeling

## Solutions

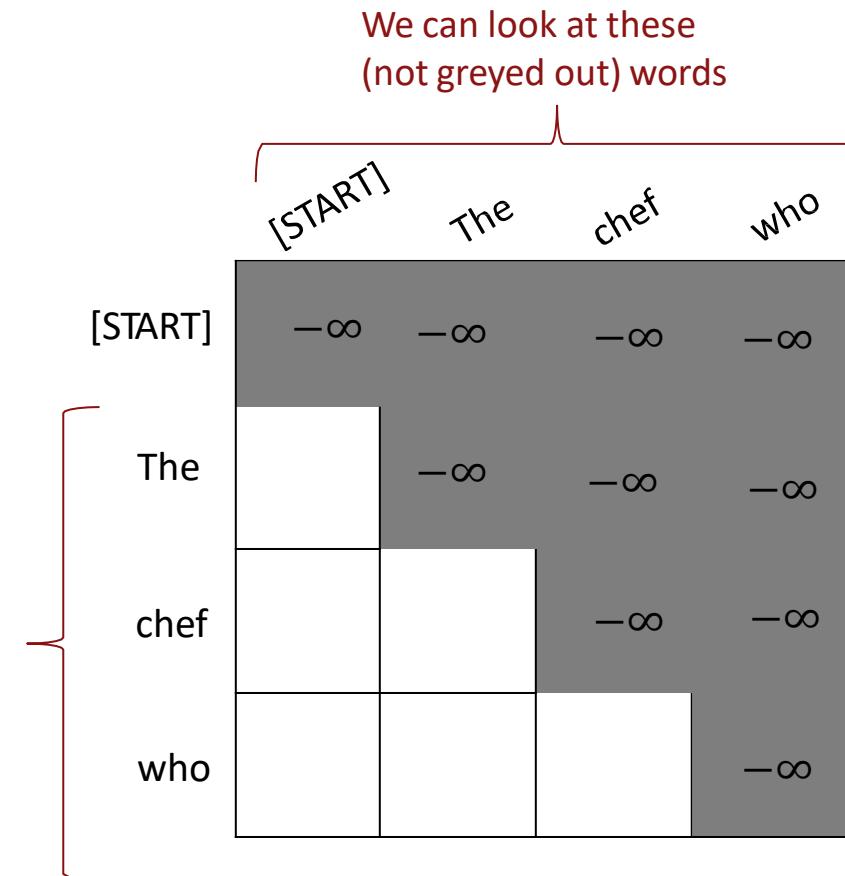
- Add position representations to the inputs
- Easy fix: apply the same feedforward network to each self-attention output.

# Masking the future in self-attention

- To use self-attention in **decoders**, we need to ensure we can't peek at the future.
- At every timestep, we could change the set of **keys and queries** to include only past words. (Inefficient!)
- To enable parallelization, we **mask out attention** to future words by setting attention scores to  $-\infty$ .

$$e_{ij} = \begin{cases} q_i^T k_j, & j < i \\ -\infty, & j \geq i \end{cases}$$

For encoding  
these words





# Barriers and solutions for Self-Attention as a building block

## Barriers

- Doesn't have an inherent notion of order!
- No nonlinearities for deep learning magic! It's all just weighted averages
- Need to ensure we don't "look at the future" when predicting a sequence
  - Like in machine translation
  - Or language modeling

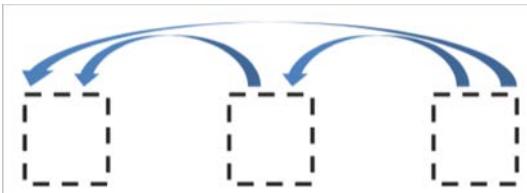


## Solutions

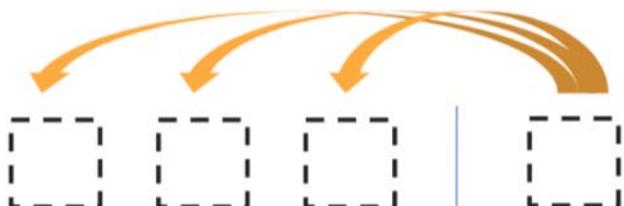
- Add position representations to the inputs
- Easy fix: apply the same feedforward network to each self-attention output.
- Mask out the future by artificially setting attention weights to 0!



- 2 sublayer changes in decoder
- Masked decoder self-attention on previously generated outputs:

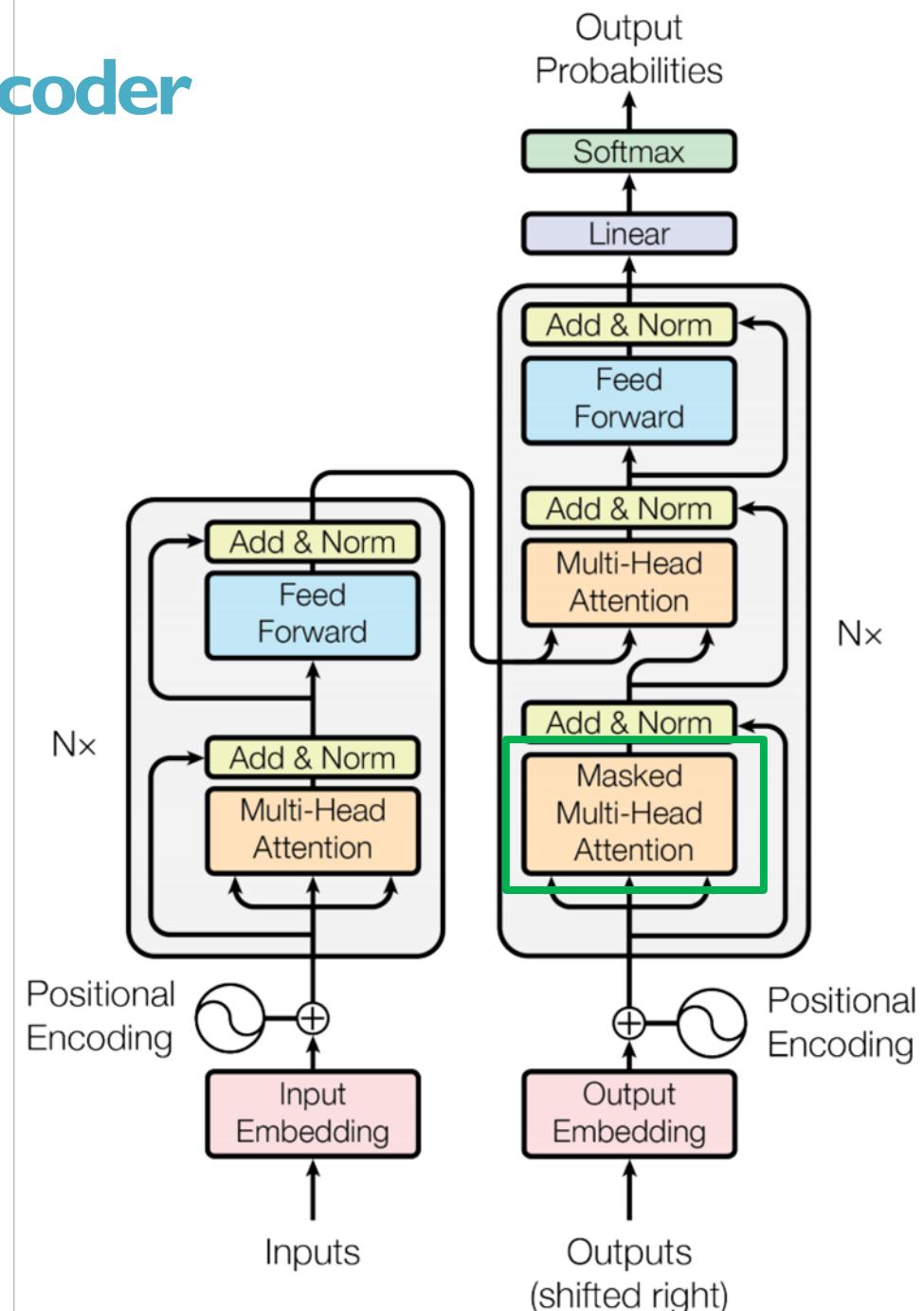


- Encoder-Decoder Attention, where queries come from previous decoder layer and keys and values come from output of encoder, **Cross-Attention**



Blocks repeated 6 times also

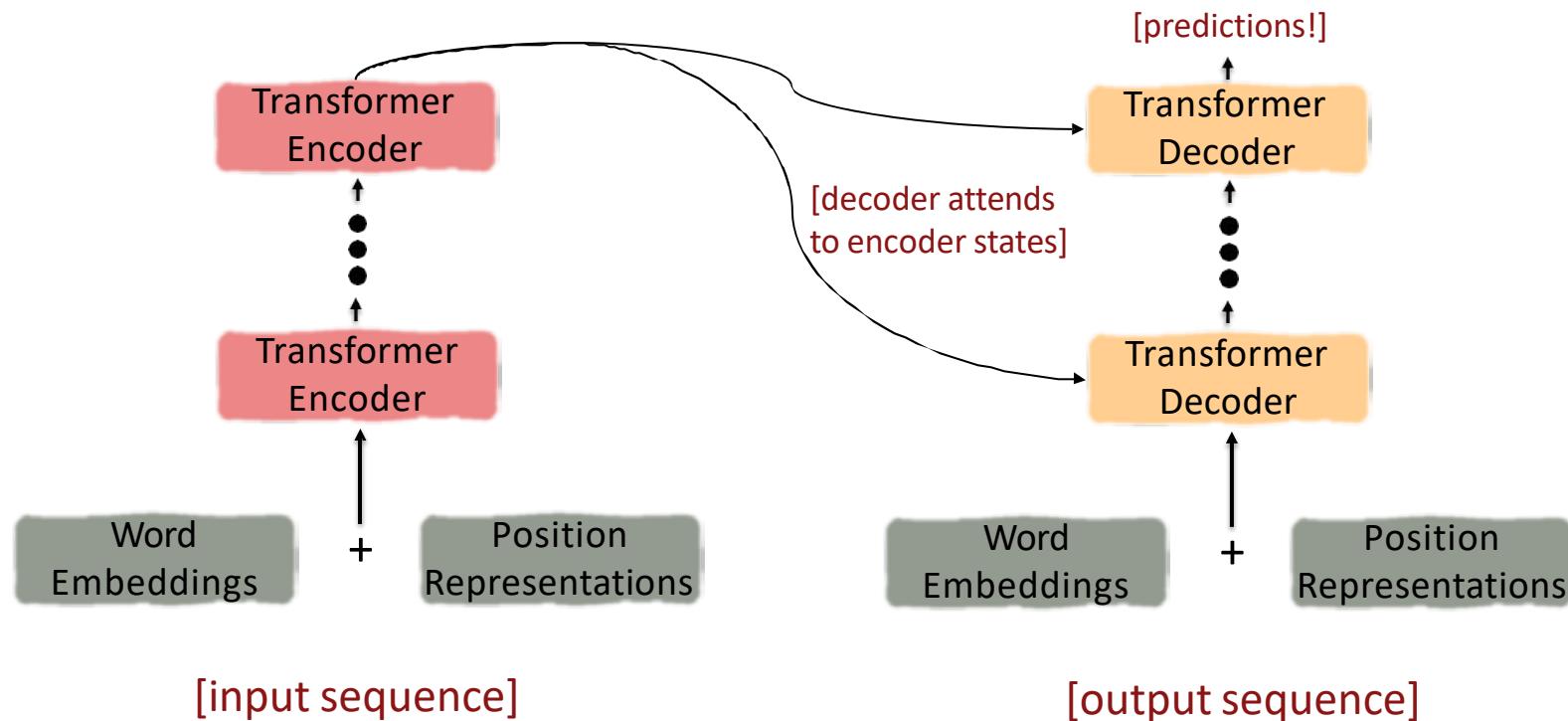
# Transformer Decoder



# The Transformer Encoder-Decoder

## [Vaswani et al., 2017]

Another look at the Transformer Encoder and Decoder Blocks at a high level





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# Transformers: tips and tricks

# The Transformer Encoder-Decoder

## [Vaswani et al., 2017]

Next, let's look at the Transformer Encoder and Decoder Blocks

What's left in a Transformer Encoder Block that we haven't covered?

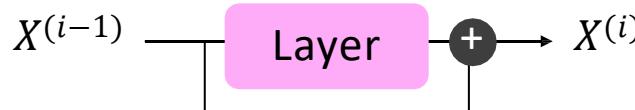
1. Key-query-value attention: How do we get the  $k, q, v$  vectors from a single word embedding?
2. Multi-headed attention: Attend to multiple places in a single layer!
3. **Tricks to help with training!**
  1. Residual connections
  2. Layer normalization
  3. Scaling the dot product
  4. These tricks **don't improve** what the model is able to do; **they help improve the training process**

# The Transformer Encoder: Residual connections [He et al., 2016]

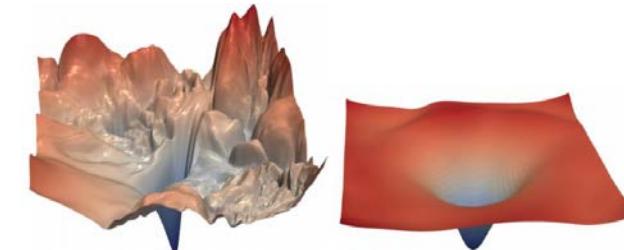
- **Residual connections** are a trick to help models train better.
  - Instead of  $X^{(i)} = \text{Layer}(X^{(i-1)})$  (where  $i$  represents the layer)



- We let  $X^{(i)} = X^{(i-1)} + \text{Layer}(X^{(i-1)})$  (so we only have to learn “the residual” from the previous layer)



- Residual connections are thought to make the loss landscape considerably smoother (thus easier training!)



[no residuals] [residuals]

[Loss landscape visualization,  
[Li et al., 2018](#), on a ResNet]

# The Transformer Encoder: Layer normalization [Ba et al., 2016]

- Layer normalization is a trick to help models train faster (has been applied to RNN first).
- It's a "Batch normalization" when the batch is size = 1.
- Idea: cut down on uninformative variation in hidden vector values by normalizing to unit mean and standard deviation **within each layer**.
  - LayerNorm's success may be due to its normalizing gradients [Xu et al., 2019]
- Let  $x \in \mathbb{R}^d$  be an individual (word) vector in the model.
- Let  $\mu = \sum_{j=1}^d x_j$ ; this is the mean;  $\mu \in \mathbb{R}$ .
  - Let  $\sigma = \sqrt{\frac{1}{d} \sum_{j=1}^d (x_j - \mu)^2}$ ; this is the standard deviation;  $\sigma \in \mathbb{R}$ .
  - Let  $\gamma \in \mathbb{R}^d$  and  $\beta \in \mathbb{R}^d$  be learned "gain" and "bias" parameters. (Can omit!)
  - Then layer normalization computes:

$$\text{output} = \frac{x - \mu}{\sqrt{\sigma^2 + \epsilon}} * \gamma + \beta$$

Normalize by scalar mean and variance      Modulate by learned elementwise gain and bias

# The Transformer Encoder: Scaled Dot Product [Vaswani et al., 2017]

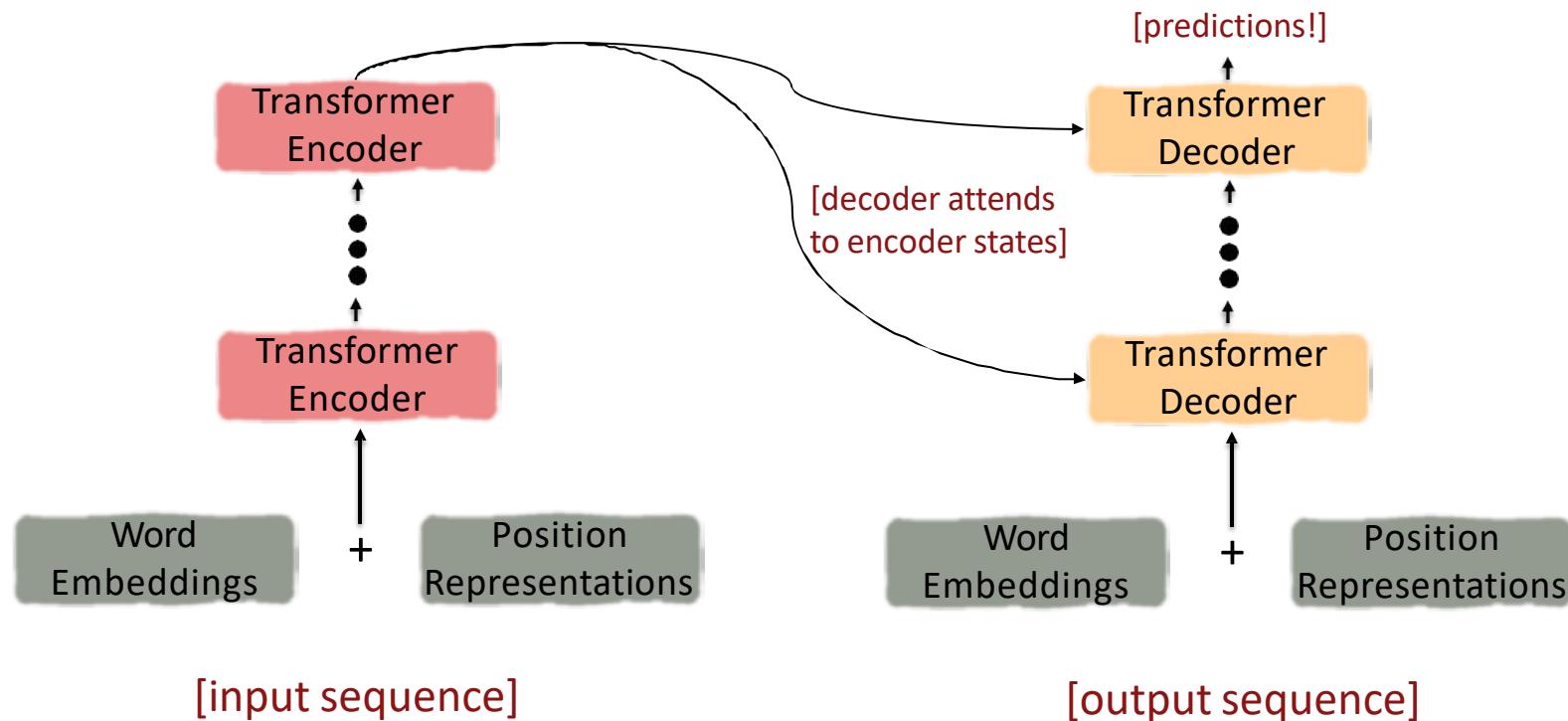
- “**Scaled Dot Product**” attention is a final variation to aid in Transformer training.
- When dimensionality  $d$  becomes large, dot products between vectors become large, inputs to the softmax function can be large, making gradients small.
- Instead of the self-attention function we’ve seen:  
$$\text{output}_P = \text{softmax}(X Q_P K_P^T X^T) * X V_P$$
- We divide the attention scores by  $\sqrt{d/h}$ , to stop the scores from becoming large just as a function of  $d/h$  (The dimensionality divided by the number of heads.)

$$\text{output}_P = \text{softmax}\left(\frac{X Q_P K_P^T X^T}{\sqrt{d/h}}\right) * X V_P$$

# The Transformer Encoder-Decoder

## [Vaswani et al., 2017]

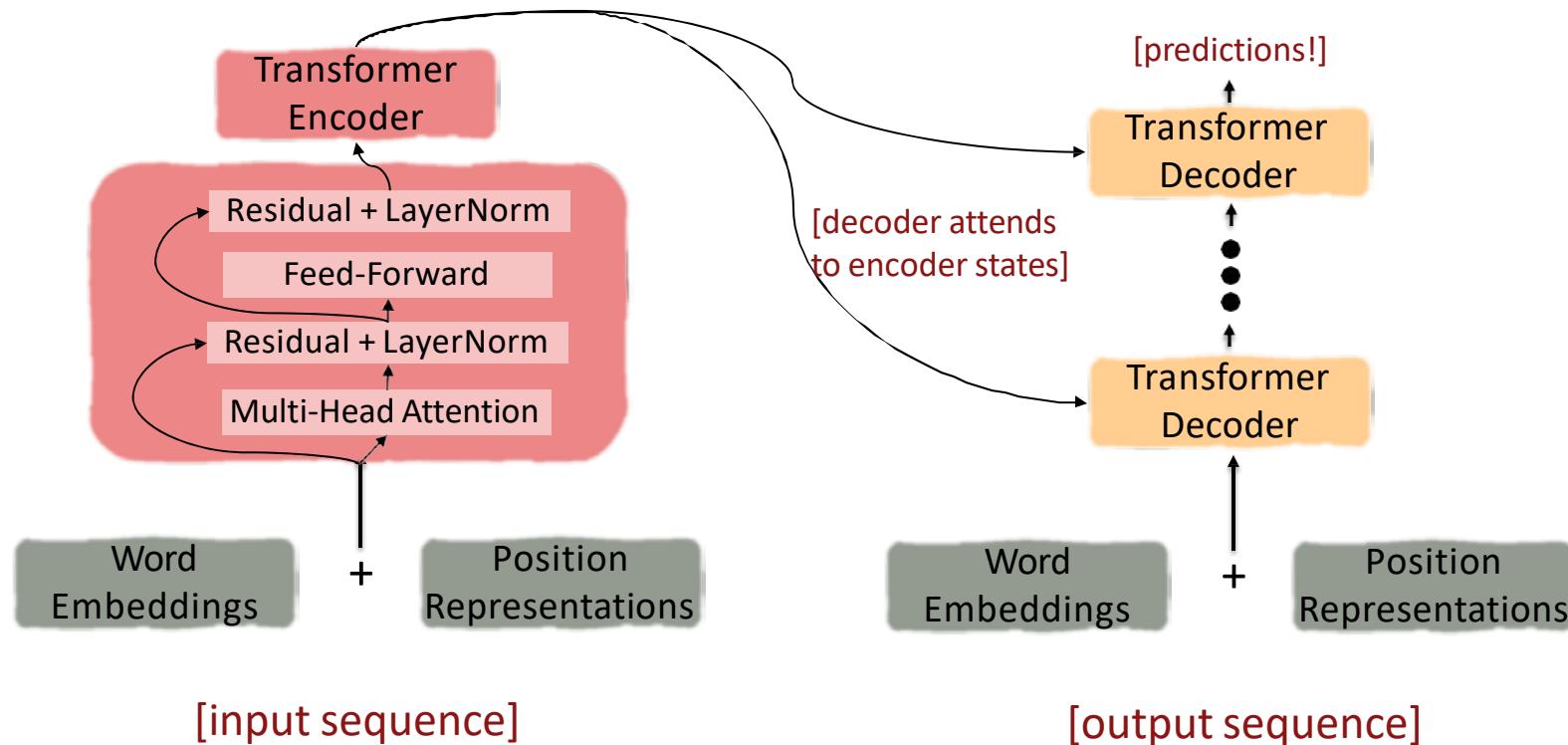
Looking back at the whole model, zooming in on an Encoder block:



# The Transformer Encoder-Decoder

[Vaswani et al., 2017]

Looking back at the whole model, zooming in on an Encoder block:

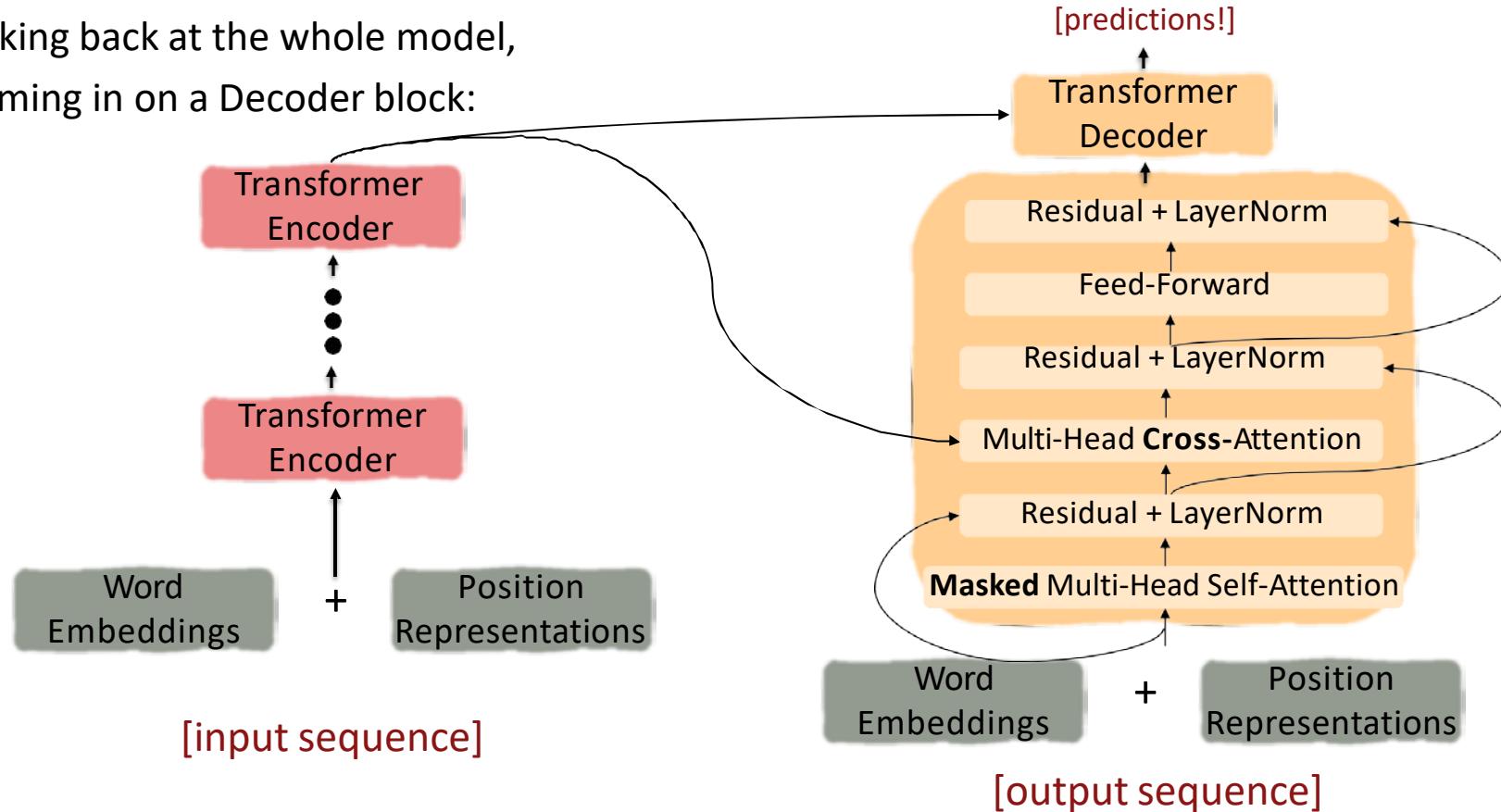




# The Transformer Encoder-Decoder

## [Vaswani et al., 2017]

Looking back at the whole model,  
zooming in on a Decoder block:





# Great Results with Transformers

Next, document generation!

Model	Test perplexity	ROUGE-L
<i>seq2seq-attention, L = 500</i>	5.04952	12.7
<i>Transformer-ED, L = 500</i>	2.46645	34.2
<i>Transformer-D, L = 4000</i>	2.22216	33.6
<i>Transformer-DMCA, no MoE-layer, L = 11000</i>	2.05159	36.2
<i>Transformer-DMCA, MoE-128, L = 11000</i>	1.92871	37.9
<i>Transformer-DMCA, MoE-256, L = 7500</i>	1.90325	38.8

The old standard

Transformers all the way down.

[[Liu et al., 2018](#)]; WikiSum dataset

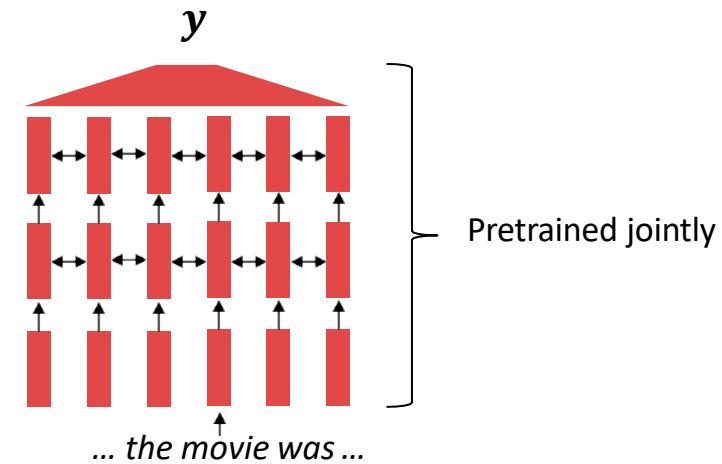
**Transformers: The way you pre-train the encoder and the decoder → different architectures**

**(BERT, SpanBert, GPT, GPT-2, GPT-3, etc)**

# Pretraining models

In modern NLP:

- All (or almost all) parameters in NLP networks are initialized via **pretraining**.
- Pretraining methods hide parts of the input from the model, and train the model to reconstruct those parts.
- This has been exceptionally effective at building strong:
  - **representations of language**
  - **parameter initializations** for strong NLP models.

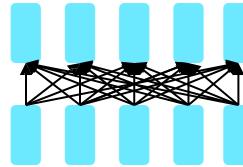


[This model has learned how to represent entire sentences through pretraining]



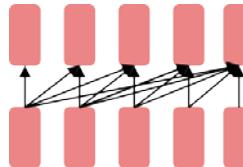
# Pretraining for three types of architectures

The neural architecture influences the type of pretraining, and natural use cases.



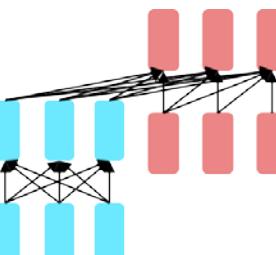
**Encoders**

- Gets bidirectional context – can condition on future!
- Wait, how do we pretrain them?



**Decoders**

- Language models! What we've seen so far.
- Nice to generate from; can't condition on future words



**Encoder-Decoders**

- Good parts of decoders and encoders?
- What's the best way to pretrain them?

# Capturing meaning via context: What kinds of things does pretraining learn?

There's increasing evidence that pretrained models learn a wide variety of things about the statistical properties of language:

- *Stanford University is located in \_\_\_\_\_, California.* [Trivia]
- *I put \_\_\_\_ fork down on the table.* [syntax]
- *The woman walked across the street, checking for traffic over \_\_\_\_ shoulder.* [coreference]
- *I went to the ocean to see the fish, turtles, seals, and \_\_\_\_.* [lexical semantics/topic]
- *Overall, the value I got from the two hours watching it was the sum total of the popcorn and the drink. The movie was \_\_\_\_.* [sentiment]
- Iroh went into the kitchen to make some tea. Standing next to Iroh, Zuko pondered his destiny. Zuko left the \_\_\_\_\_. [some reasoning – this is harder]
- I was thinking about the sequence that goes 1, 1, 2, 3, 5, 8, 13, 21, \_\_\_\_ [some basic arithmetic; they don't learn the Fibonacci sequence]
- Models also learn – and can exacerbate racism, sexism, all manner of bad biases.

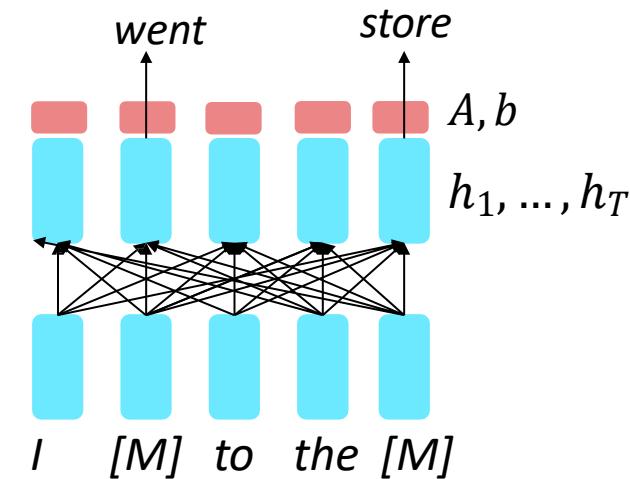
# Pretraining encoders: What pretraining objective to use?

So far, we've looked at language model pretraining. But **encoders get bidirectional context, so we can't do language modeling!**

**Idea:** replace some fraction of words in the input with a special [MASK] token; predict these words.

$$\begin{aligned} h_1, \dots, h_T &= \text{Encoder}(w_1, \dots, w_T) \\ y_i &\sim Aw_i + b \end{aligned}$$

Only add loss terms from words that are “masked out.” If  $x'$  is the masked version of  $x$ , we’re learning  $p_\theta(x|x')$ . Called **Masked LM**.



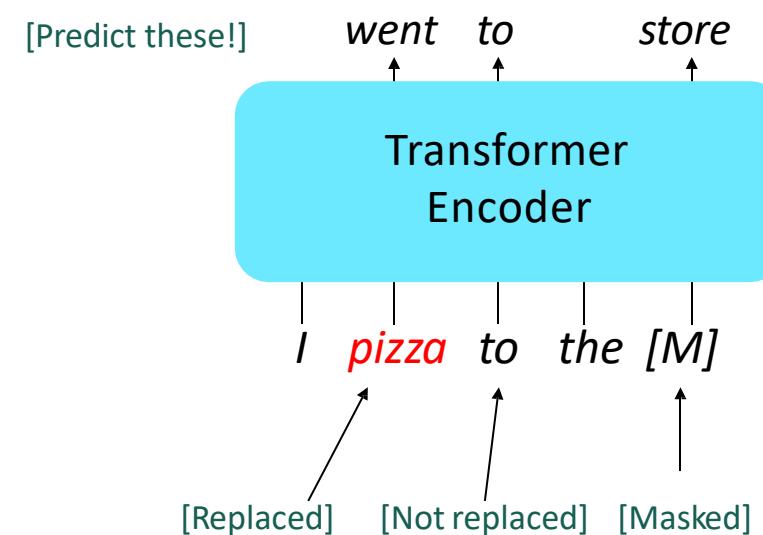
[Devlin et al., 2018]

# BERT: Bidirectional Encoder Representations from Transformers

Devlin et al., 2018 proposed the “Masked LM” objective and **released the weights of a pretrained Transformer**, a model they labeled BERT.

Some more details about Masked LM for BERT:

- Predict a random 15% of (sub)word tokens.
  - Replace input word with [MASK] 80% of the time
  - Replace input word with a random token 10% of the time
  - Leave input word unchanged 10% of the time (but still predict it!)
- Why? Doesn’t let the model get complacent and not build strong representations of non-masked words. (No masks are seen at fine-tuning time!)



[\[Devlin et al., 2018\]](#)

# BERT: Bidirectional Encoder Representations from Transformers

- Mask out  $k\%$  of the input words, and then predict the masked words
  - They always use  $k = 15\%$



- Too little masking: Too expensive to train
- Too much masking: Not enough context



# BERT: Bidirectional Encoder Representations from Transformers

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- Additional task: Next sentence prediction
- To learn *relationships* between sentences, predict whether Sentence B is actual sentence that proceeds Sentence A, or a random sentence

---

**Sentence A** = The man went to the store.

**Sentence B** = He bought a gallon of milk.

**Label** = IsNextSentence

---

**Sentence A** = The man went to the store.

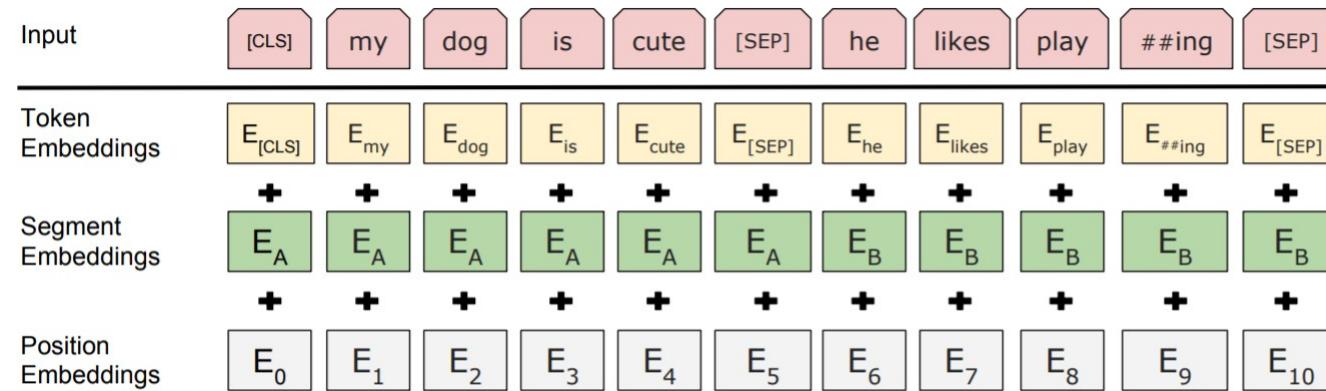
**Sentence B** = Penguins are flightless.

**Label** = NotNextSentence

---

# BERT: Bidirectional Encoder Representations from Transformers

- The pretraining input to BERT was two separate contiguous chunks of text:



- In addition to masked input reconstruction, BERT was trained to predict whether one chunk follows the other or is randomly sampled.
- Later work has argued this “next sentence prediction” is not necessary.

[Devlin et al., 2018, Liu et al., 2019]



# BERT: Bidirectional Encoder Representations from Transformers

## Details about BERT

- Two models were released:
  - BERT-base: 12 layers, 768-dim hidden states, 12 attention heads, 110 million params.
  - BERT-large: 24 layers, 1024-dim hidden states, 16 attention heads, 340 million params.
- Trained on:
  - BooksCorpus (800 million words)
  - English Wikipedia (2,500 million words)
- Pretraining is expensive and impractical on a single GPU.
  - BERT was pretrained with 64 TPU chips for a total of 4 days.
  - (TPUs are special tensor operation acceleration hardware)
- Finetuning is practical and common on a single GPU
  - “Pretrain once, finetune many times.”

[Devlin et al., 2018]



# BERT: Bidirectional Encoder Representations from Transformers

BERT was massively popular and hugely versatile; finetuning BERT led to new state-of-the-art results on a broad range of tasks.

- **QQP:** Quora Question Pairs (detect paraphrase questions)
- **QNLI:** natural language inference over question answering data
- **SST-2:** sentiment analysis
- **CoLA:** corpus of linguistic acceptability (detect whether sentences are grammatical.)
- **STS-B:** semantic textual similarity
- **MRPC:** microsoft paraphrase corpus
- **RTE:** small natural language inference corpus

System	MNLI-(m/mm) 392k	QQP 363k	QNLI 108k	SST-2 67k	CoLA 8.5k	STS-B 5.7k	MRPC 3.5k	RTE 2.5k	Average -
Pre-OpenAI SOTA	80.6/80.1	66.1	82.3	93.2	35.0	81.0	86.0	61.7	74.0
BiLSTM+ELMo+Attn	76.4/76.1	64.8	79.8	90.4	36.0	73.3	84.9	56.8	71.0
OpenAI GPT	82.1/81.4	70.3	87.4	91.3	45.4	80.0	82.3	56.0	75.1
BERT <sub>BASE</sub>	84.6/83.4	71.2	90.5	93.5	52.1	85.8	88.9	66.4	79.6
BERT <sub>LARGE</sub>	<b>86.7/85.9</b>	<b>72.1</b>	<b>92.7</b>	<b>94.9</b>	<b>60.5</b>	<b>86.5</b>	<b>89.3</b>	<b>70.1</b>	<b>82.1</b>

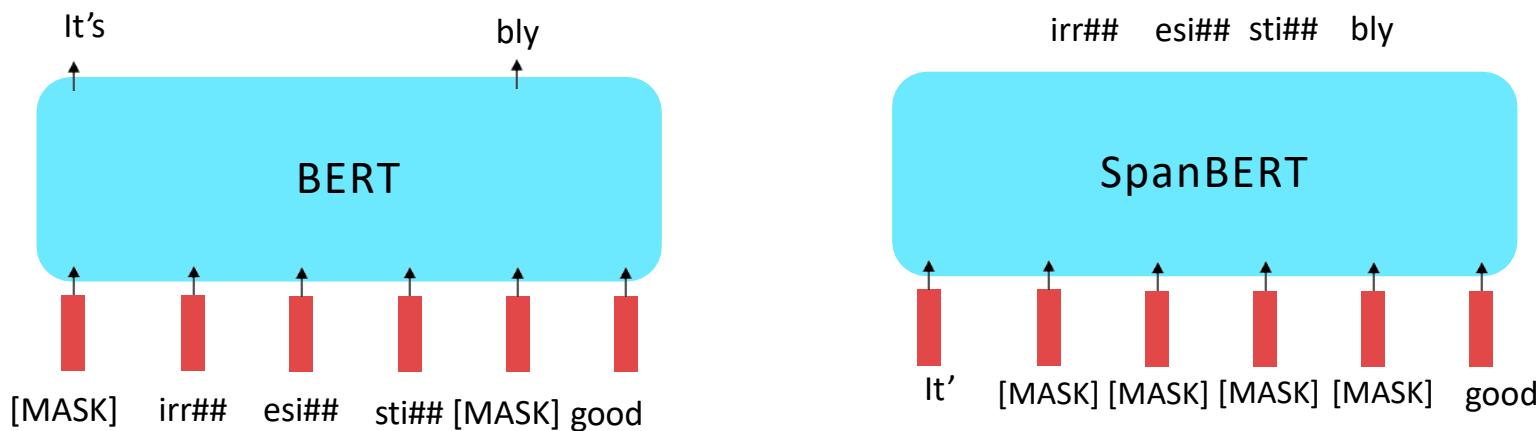
[Devlin et al., 2018]

# Extensions of BERT

You'll see a lot of BERT variants like RoBERTa, SpanBERT, +++

Some generally accepted improvements to the BERT pretraining formula:

- RoBERTa: mainly just train BERT for longer and remove next sentence prediction!
- SpanBERT: masking contiguous spans of words makes a harder, more useful pretraining task



[[Liu et al., 2019](#); [Joshi et al., 2020](#)]



# Extensions of BERT

A takeaway from the RoBERTa paper: more compute, more data can improve pretraining even when not changing the underlying Transformer encoder.

Model	data	bsz	steps	SQuAD (v1.1/2.0)	MNLI-m	SST-2
<b>RoBERTa</b>						
with BOOKS + WIKI	16GB	8K	100K	93.6/87.3	89.0	95.3
+ additional data (§3.2)	160GB	8K	100K	94.0/87.7	89.3	95.6
+ pretrain longer	160GB	8K	300K	94.4/88.7	90.0	96.1
+ pretrain even longer	160GB	8K	500K	<b>94.6/89.4</b>	<b>90.2</b>	<b>96.4</b>
<b>BERT<sub>LARGE</sub></b>						
with BOOKS + WIKI	13GB	256	1M	90.9/81.8	86.6	93.7

[Liu et al., 2019; Joshi et al., 2020]



# Pretraining through language modeling

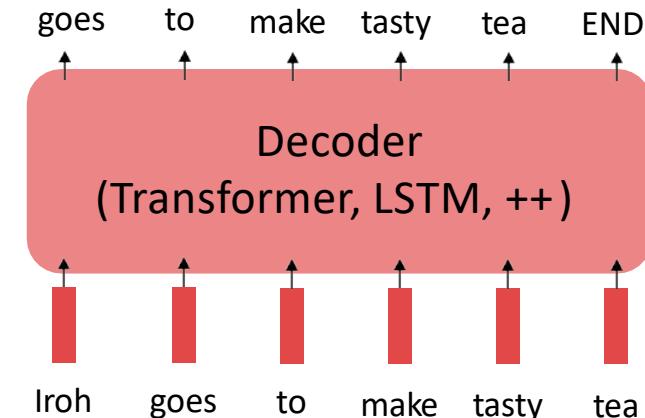
## [Dai and Le, 2015]

Recall the **language modeling** task:

- Model  $p_\theta(w_t | w_{1:t-1})$ , the probability distribution over words given their past contexts.
- There's lots of data for this! (In English.)

**Pretraining through language modeling:**

- Train a neural network to perform language modeling on a large amount of text.
- Save the network parameters.



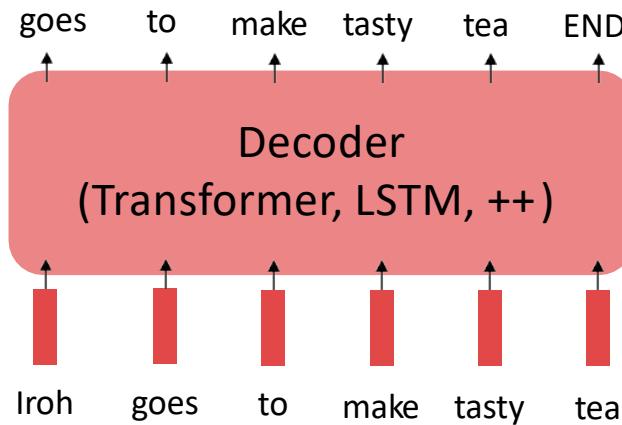


# The Pretraining / Finetuning Paradigm

Pretraining can improve NLP applications by serving as parameter initialization.

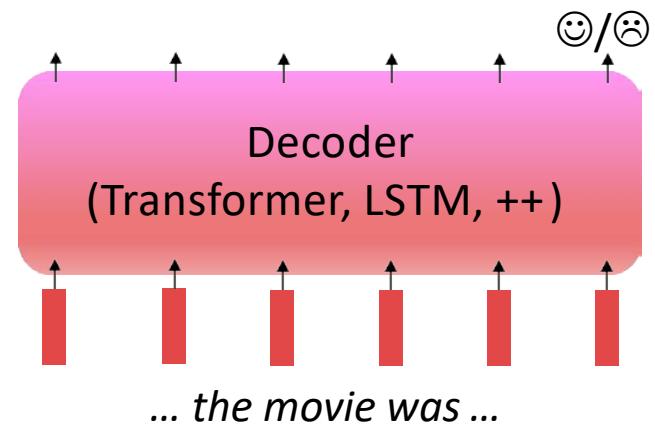
## Step 1: Pretrain (on language modeling)

Lots of text; learn general things!



## Step 2: Finetune (on your task)

Not many labels; adapt to the task!



## Pretraining decoders

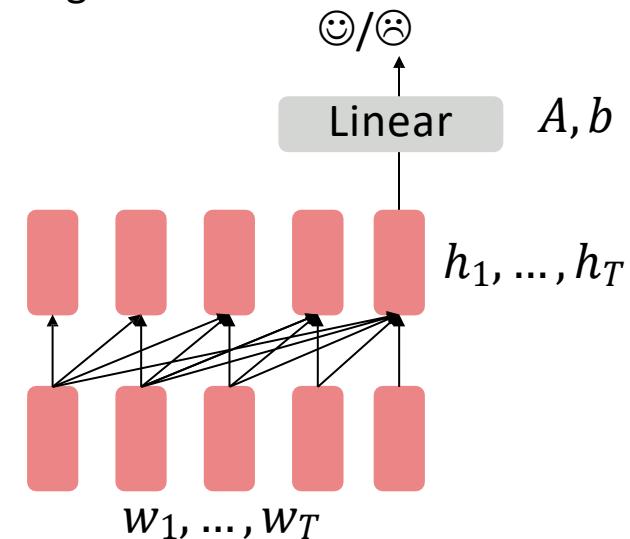
When using language model pretrained decoders, we can ignore that they were trained to model  $p(w_t|w_{1:t-1})$ .

We can finetune them by training a classifier on the last word's hidden state.

$$\begin{aligned} h_1, \dots, h_T &= \text{Decoder}(w_1, \dots, w_T) \\ y &\sim Aw_T + b \end{aligned}$$

Where  $A$  and  $b$  are randomly initialized and specified by the downstream task.

Gradients backpropagate through the whole network.



[Note how the linear layer hasn't been pretrained and must be learned from scratch.]

# Pretraining decoders

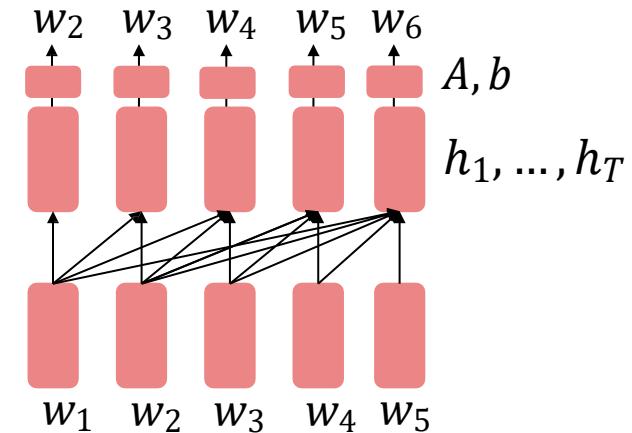
It's natural to pretrain decoders as language models and then use them as generators, finetuning their  $p_\theta(w_t | w_{1:t-1})$ !

This is helpful in tasks **where the output is a sequence** with a vocabulary like that at pretraining time!

- Dialogue (context=dialogue history)
- Summarization (context=document)

$$\begin{aligned} h_1, \dots, h_T &= \text{Decoder}(w_1, \dots, w_T) \\ w_t &\sim Aw_{t-1} + b \end{aligned}$$

Where  $A, b$  were pretrained in the language model!



[Note how the linear layer has been pretrained.]



# Generative Pretrained Transformer (GPT)

[Radford et al., 2018]

2018's GPT was a big success in pretraining a decoder!

- Transformer decoder with 12 layers.
- 768-dimensional hidden states, 3072-dimensional feed-forward hidden layers.
- Byte-pair encoding with 40,000 merges
- Trained on BooksCorpus: over 7000 unique books.
  - Contains long spans of contiguous text, for learning long-distance dependencies.
- The acronym “GPT” never showed up in the original paper; it could stand for “Generative PreTraining” or “Generative Pretrained Transformer”

[Devlin et al., 2018]

# Generative Pretrained Transformer (GPT)

[Radford et al., 2018]

How do we format inputs to our decoder for **finetuning tasks**?

**Natural Language Inference:** Label pairs of sentences as *entailing/contradictory/neutral*

Premise: *The man is in the doorway*  
Hypothesis: *The person is near the door* } entailment

Radford et al., 2018 evaluate on natural language inference.

Here's roughly how the input was formatted, as a sequence of tokens for the decoder.

[START] *The man is in the doorway* [DELIM] *The person is near the door* [EXTRACT]

The linear classifier is applied to the representation of the [EXTRACT] token.

# Generative Pretrained Transformer (GPT)

## [Radford et al., 2018]

GPT results on various *natural language inference* datasets.

Method	MNLI-m	MNLI-mm	SNLI	SciTail	QNLI	RTE
ESIM + ELMo [44] (5x)	-	-	<u>89.3</u>	-	-	-
CAFE [58] (5x)	80.2	79.0	<u>89.3</u>	-	-	-
Stochastic Answer Network [35] (3x)	<u>80.6</u>	<u>80.1</u>	-	-	-	-
CAFE [58]	78.7	77.9	88.5	<u>83.3</u>		
GenSen [64]	71.4	71.3	-	-	<u>82.3</u>	59.2
Multi-task BiLSTM + Attn [64]	72.2	72.1	-	-	<u>82.1</u>	<b>61.7</b>
Finetuned Transformer LM (ours)	<b>82.1</b>	<b>81.4</b>	<b>89.9</b>	<b>88.3</b>	<b>88.1</b>	56.0

## Increasingly convincing generations (GPT2)

[[Radford et al., 2018](#)]

We mentioned how pretrained decoders can be used **in their capacities as language models**. **GPT-2**, a larger version of GPT trained on more data, was shown to produce relatively convincing samples of natural language.

**Context (human-written):** In a shocking finding, scientist discovered a herd of unicorns living in a remote, previously unexplored valley, in the Andes Mountains. Even more surprising to the researchers was the fact that the unicorns spoke perfect English.

**GPT-2:** The scientist named the population, after their distinctive horn, Ovid's Unicorn. These four-horned, silver-white unicorns were previously unknown to science.

Now, after almost two centuries, the mystery of what sparked this odd phenomenon is finally solved.

Dr. Jorge Pérez, an evolutionary biologist from the University of La Paz, and several companions, were exploring the Andes Mountains when they found a small valley, with no other animals or humans. Pérez noticed that the valley had what appeared to be a natural fountain, surrounded by two peaks of rock and silver snow.

# Pretraining encoder-decoders: What pretraining objective to use?

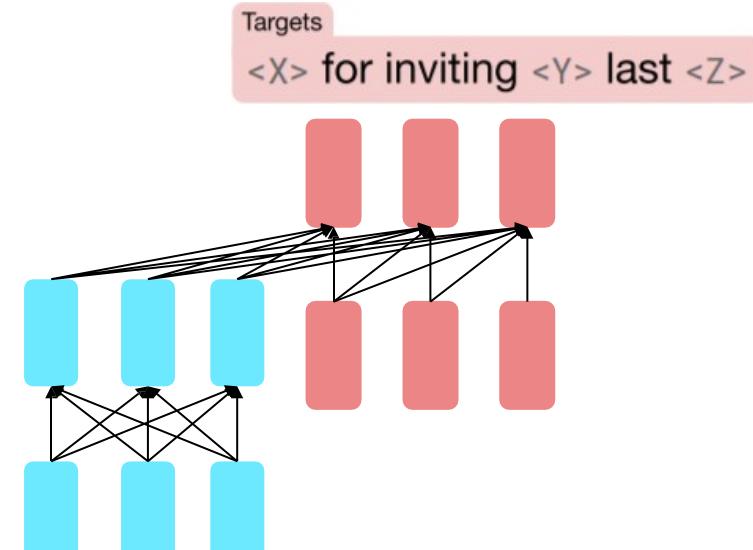
What [Raffel et al., 2018](#) found to work best was **span corruption**. Their model: **T5**.

Replace different-length spans from the input with unique placeholders; decode out the spans that were removed!

Original text

Thank you for inviting me to your party last week.

This is implemented in text preprocessing: it's still an objective that looks like **language modeling** at the decoder side.



# Pretraining encoder-decoders: What pretraining objective to use? T5

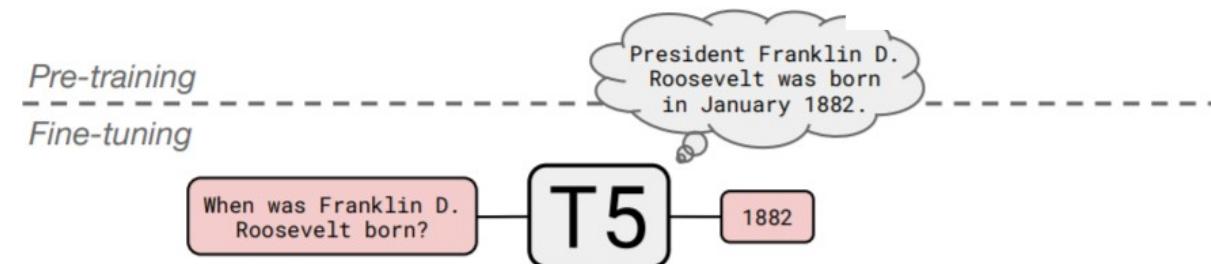
A fascinating property of T5: it can be finetuned to answer a wide range of questions, retrieving knowledge from its parameters.

NQ: Natural Questions

WQ: WebQuestions

TQA: Trivia QA

All “open-domain” versions



	NQ	WQ	TQA		220 million params
			dev	test	
Karpukhin et al. (2020)	<b>41.5</b>	42.4	<b>57.9</b>	—	
T5.1.1-Base	25.7	28.2	24.2	30.6	770 million params
T5.1.1-Large	27.3	29.5	28.5	37.2	3 billion params
T5.1.1-XL	29.5	32.4	36.0	45.1	11 billion params
T5.1.1-XXL	32.8	35.6	42.9	52.5	
T5.1.1-XXL + SSM	35.2	<b>42.8</b>	51.9	<b>61.6</b>	

[Raffel et al., 2018]



## GPT-3, in-context learning, very large models

[univ-cotedazur.fr](http://univ-cotedazur.fr)

So far, we've interacted with pretrained models in two ways:

- Sample from the distributions they define (maybe providing a prompt)
- Fine-tune them on a task we care about, and take their predictions.

Very large language models seem to perform some kind of learning **without gradient steps** simply from examples you provide within their contexts.

GPT-3 is the canonical example of this. The largest **T5** model had 11 billion parameters.

**GPT-3 has 175 billion parameters.**

# Large Language Models

## Next-token-prediction

The model is given a sequence of words with the goal of predicting the next word.

Example:  
Hannah is a \_\_

Hannah is a *sister*  
Hannah is a *friend*  
Hannah is a *marketer*  
Hannah is a *comedian*

## Masked-language-modeling

The model is given a sequence of words with the goal of predicting a 'masked' word in the middle.

Example  
Jacob [mask] reading

Jacob *fears* reading  
Jacob *loves* reading  
Jacob *enjoys* reading  
Jacob *hates* reading

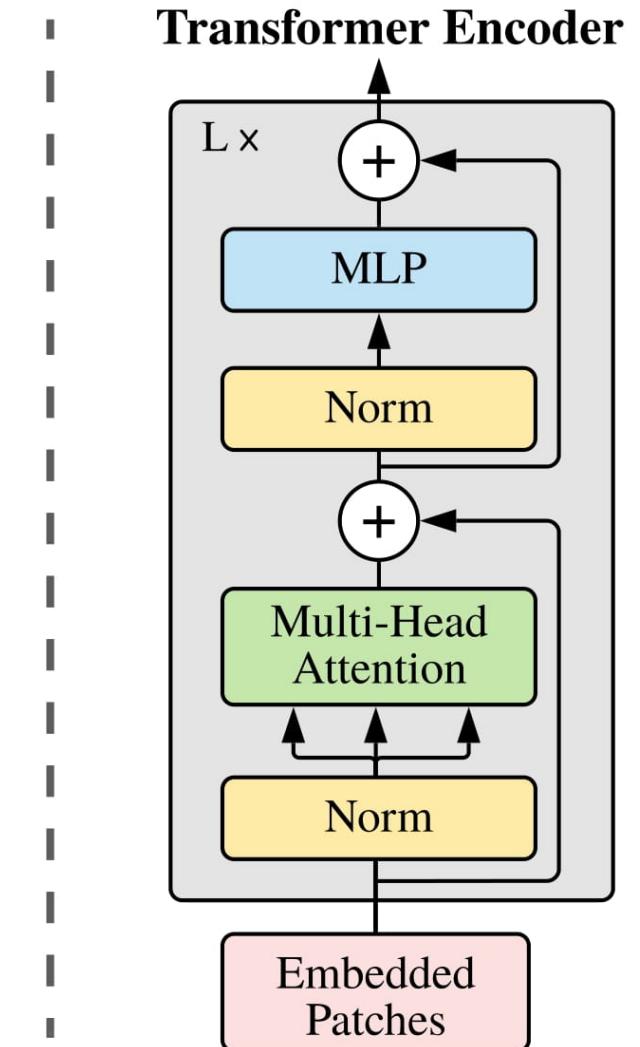
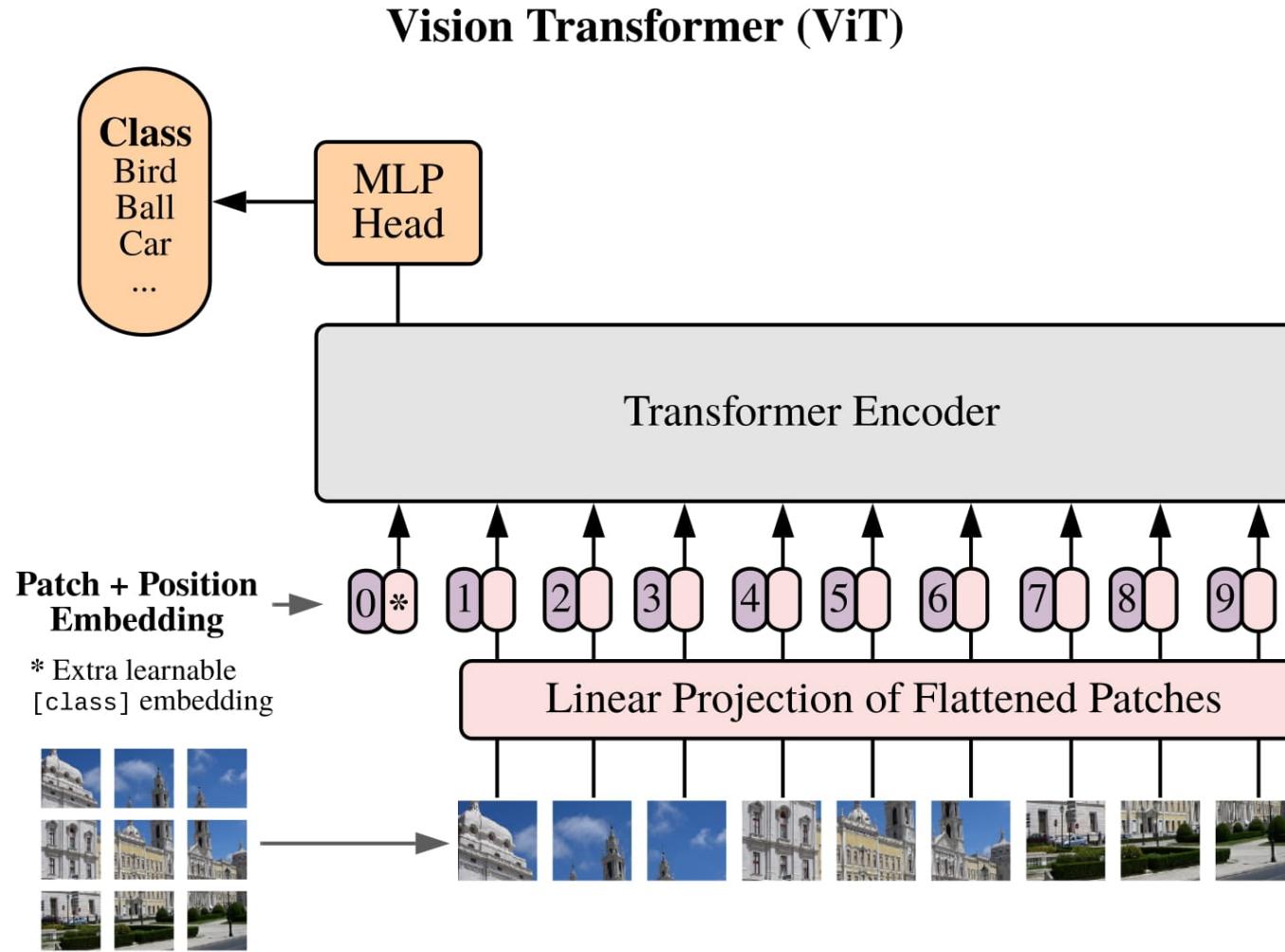
Arbitrary example of next-token-prediction and masked-language-modeling generated by the author.



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# Transformers beyond Natural Language Processing

# Visual Transformers (ViT)



# Cross-modal transformers

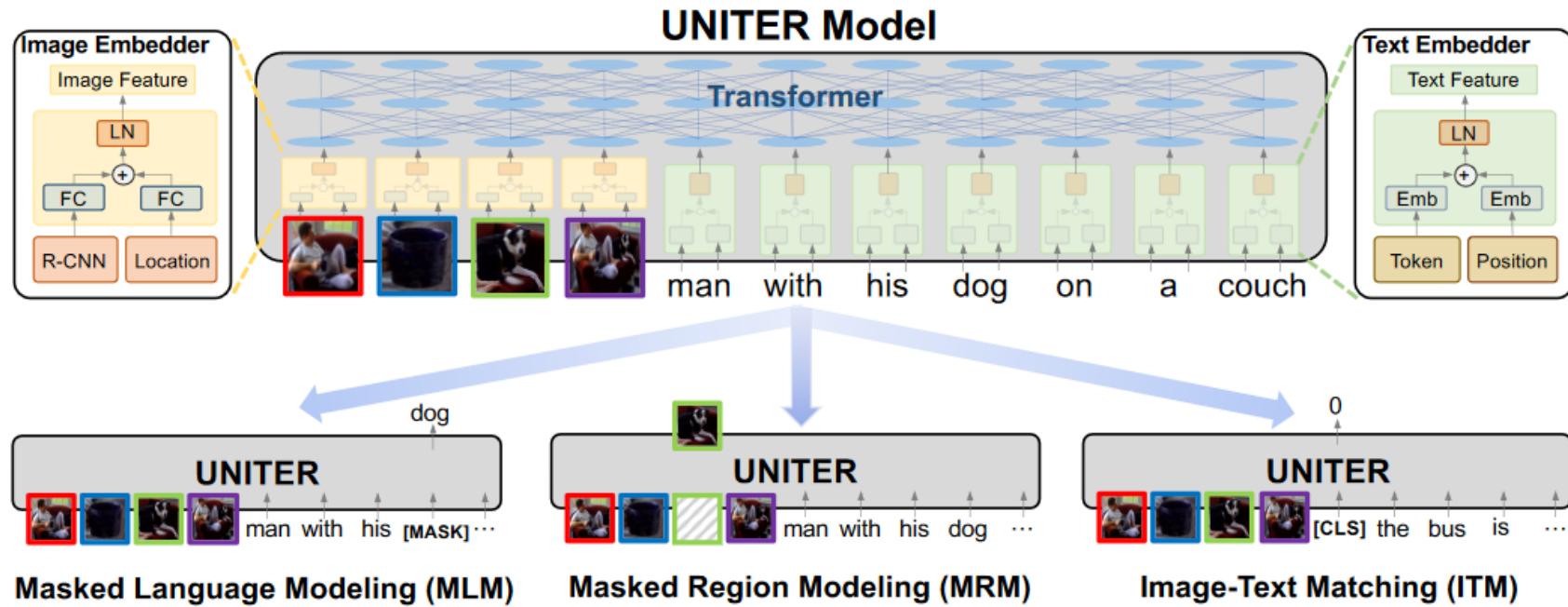


Figure 1: Overview of the proposed UNITER model (best viewed in color), consisting of an Image Embedder, a Text Embedder and a multi-layer self-attention Transformer, learned through three pre-training tasks.

# Cross-modal transformers

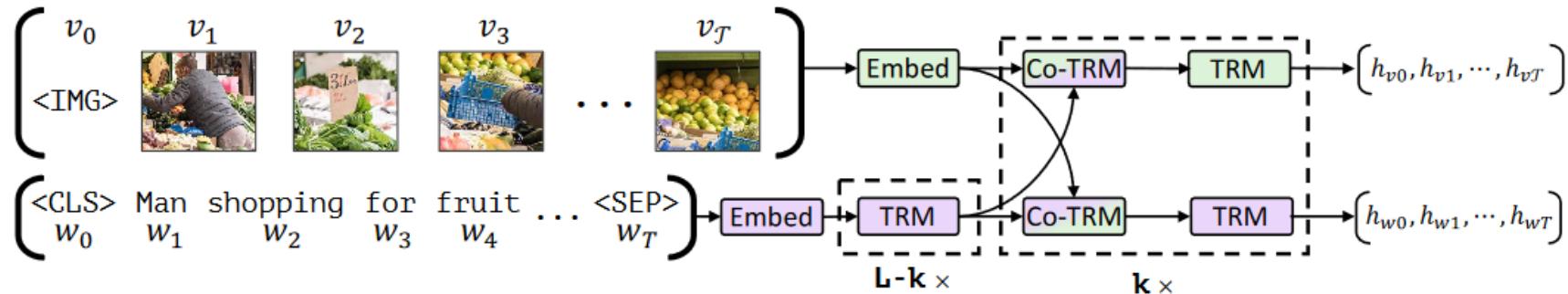


Figure 1: Our ViLBERT model consists of two parallel streams for visual (green) and linguistic (purple) processing that interact through novel co-attentional transformer layers. This structure allows for variable depths for each modality and enables sparse interaction through co-attention. Dashed boxes with multiplier subscripts denote repeated blocks of layers.

# Cross-modal transformers

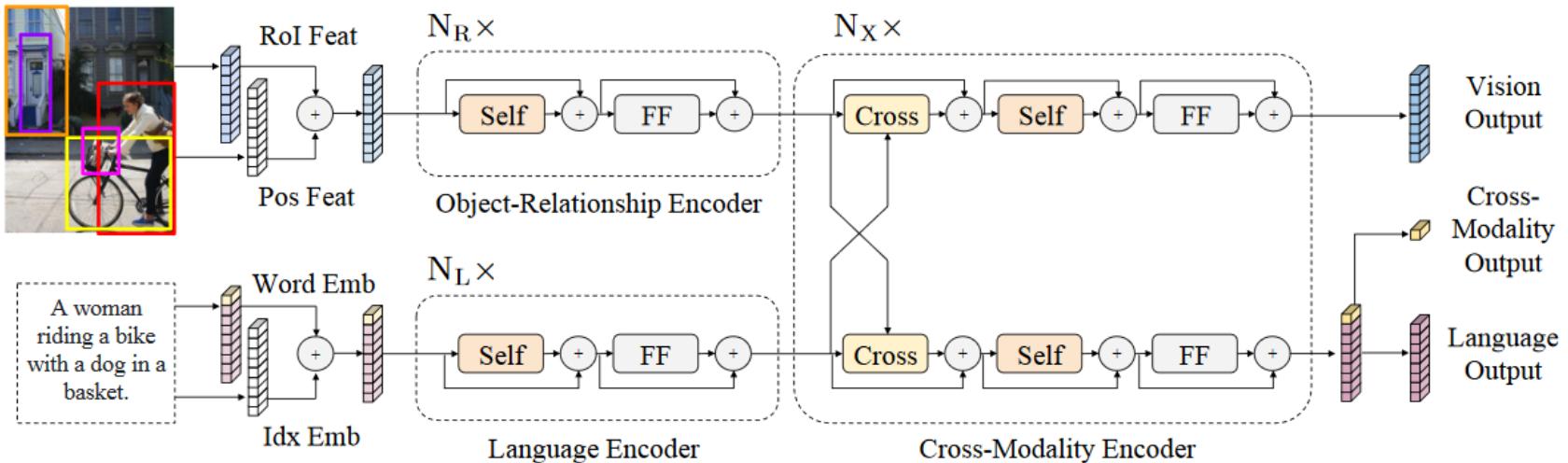
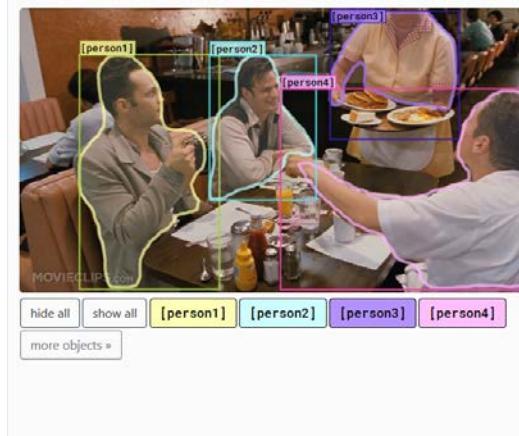


Figure 1: The LXMERT model for learning vision-and-language cross-modality representations. ‘Self’ and ‘Cross’ are abbreviations for self-attention sub-layers and cross-attention sub-layers, respectively. ‘FF’ denotes a feed-forward sub-layer.

# Visual Commonsense Reasoning leaderboard



Why is [person4] pointing at [person1]?

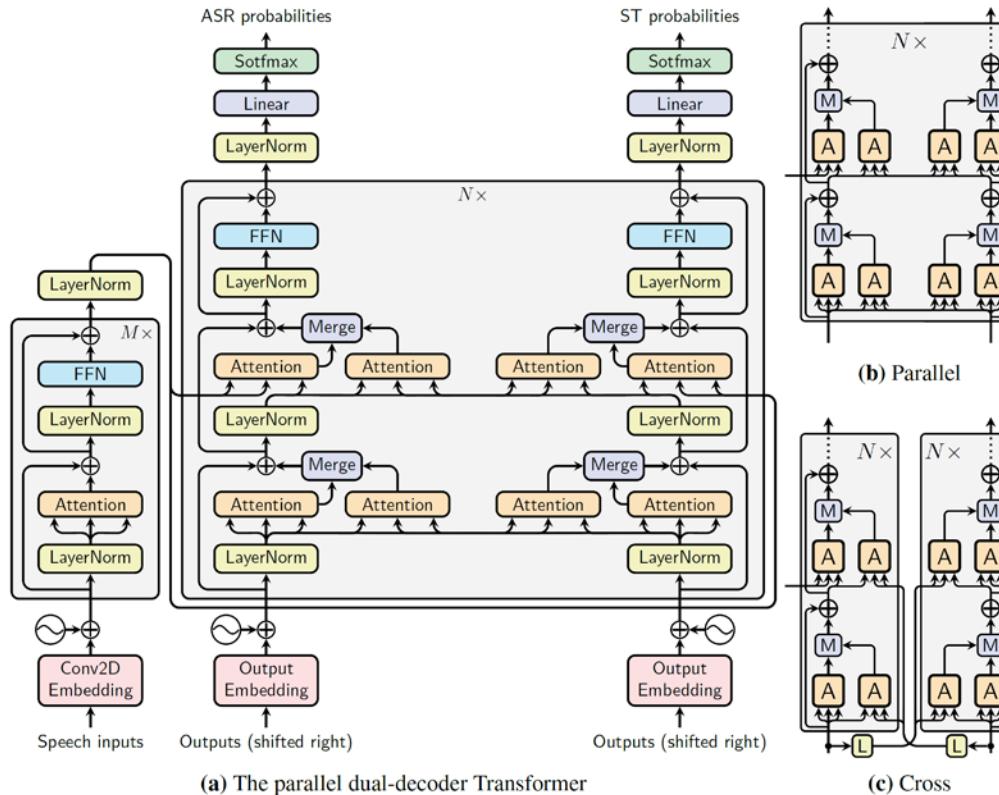
- a) He is telling [person1] that [person1] ordered the pancakes.
- b) He just told a joke.
- c) He is feeling accusatory towards [person1].
- d) He is giving [person1] directions.

Rationale: I think so because...

- a) [person1] has the pancakes in front of him.
- b) [person4] is taking everyone's order and asked for clarification.
- c) [person3] is looking at the pancakes both she and [person2] are smiling slightly.
- d) [person3] is delivering food to the table, and she might not know whose order is whose.

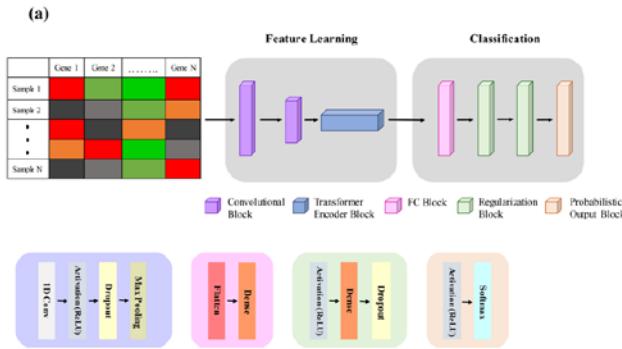
Rank	Model	Q->A	QA->R	Q->AR
	Human Performance <i>University of Washington</i>  (Zellers et al. '18)	91.0	93.0	85.0
1	UNITER-large (ensemble) <i>MS D365 AI</i>  <a href="https://arxiv.org/abs/1909.11740">https://arxiv.org/abs/1909.11740</a>	79.8	83.4	66.8
September 30, 2019				
2	UNITER-large (single model) <i>MS D365 AI</i>  <a href="https://arxiv.org/abs/1909.11740">https://arxiv.org/abs/1909.11740</a>	77.3	80.8	62.8
September 23, 2019				
3	ViLBERT (ensemble of 10 models) <i>Georgia Tech &amp; Facebook AI Research</i>  <a href="https://arxiv.org/abs/1908.02265">https://arxiv.org/abs/1908.02265</a>	76.4	78.0	59.8
August 9, 2019				
4	VL-BERT (single model) <i>MSRA &amp; USTC</i>  <a href="https://arxiv.org/abs/1908.08530">https://arxiv.org/abs/1908.08530</a>	75.8	78.4	59.7
September 23, 2019				
5	ViLBERT (ensemble of 5 models) <i>Georgia Tech &amp; Facebook AI Research</i>  <a href="https://arxiv.org/abs/1908.02265">https://arxiv.org/abs/1908.02265</a>	75.7	77.5	58.8
August 9, 2019				

# Dual-decoder Transformer for Joint Automatic Speech Recognition (ASR) and Multilingual Speech Translation (ST)

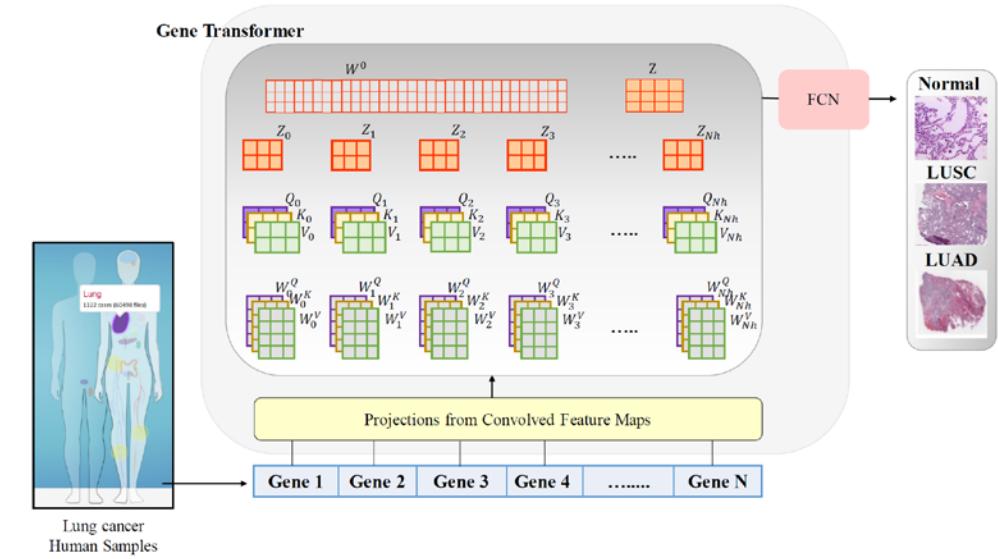


**Figure 1:** The dual-decoder Transformers. Figure (a) shows the detailed architecture of the *parallel* dual-decoder Transformer, and Figure (b) shows its simplified view. The *cross* dual-decoder Transformer is very similar to the parallel one, except that the keys and values fed to the dual-attention layers come from the previous output, which is illustrated by Figure (c). From the above figures, one can easily infer the detailed architecture of the cross Transformer, which can be found in the Appendix. Abbreviations: **A** (Attention), **M** (Merge), **L** (LayerNorm).

# Gene Transformer: Transformers for the Gene Expression-based Classification of Lung Cancer Subtypes



**Fig. 2.** Gene Transformer network: an illustration. **(a)** (left) Detailed description of Gene Transformer architecture. The model includes two parts: feature learning block and a fully connected block for classification. One-dimensional (1D) vectorized gene expression levels from The Cancer Genome Atlas (TCGA) samples were used as the input. This input was then convolved and fed into the multi-head self-attention module for identifying relevant biomarkers. **(b)** (Right) Scaled dot-product attention to compute the attention function on a set of queries and multi-head attention to concatenate the yielded output values and project them for downstream tasks. The exhibition of the Transformer encoder was inspired by [36].



**Fig. 1.** Graphical representation of the end-to-end deep learning approach for the classification of the lung cancer subtypes.

In this study, we proposed an end-to-end approach for lung cancer subtype classification using a gene expression dataset, wherein a multi-head self-attention module permitted the model to jointly learn complex genomic information from thousands of genes from different patient samples shared across multiple cancer subtypes. Head collaboration achieves better generalizability over imbalanced datasets and produces a more desirable performance for both binary and multiclass classification tasks.

# Adaptable and Interpretable Neural Memory Over Symbolic Knowledge

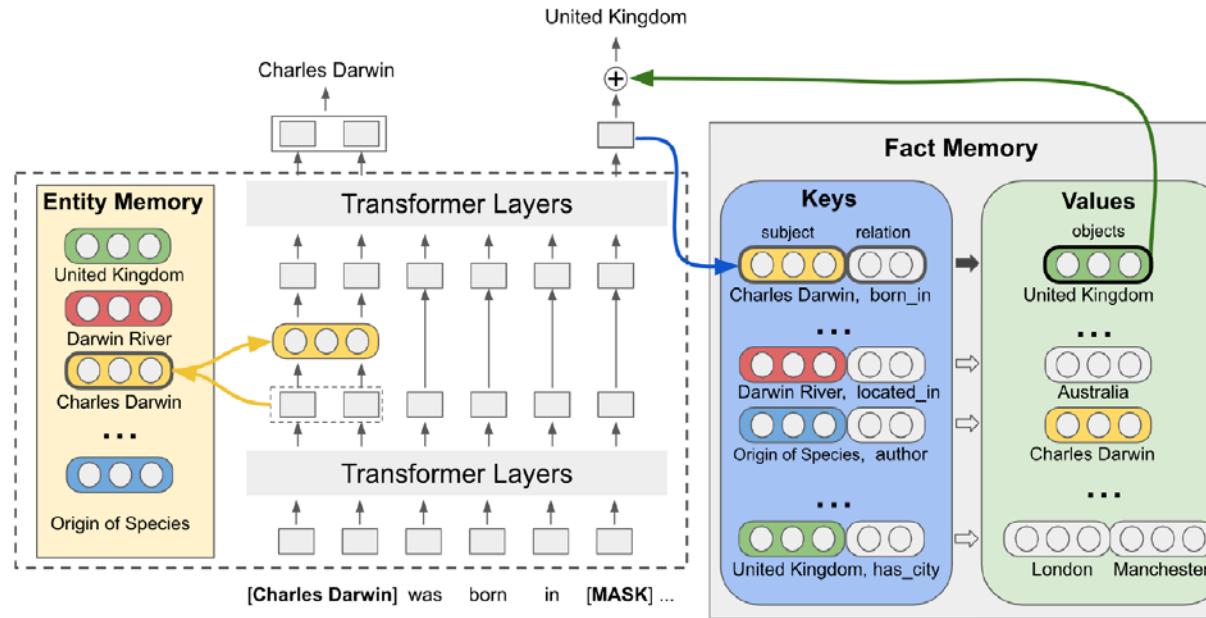
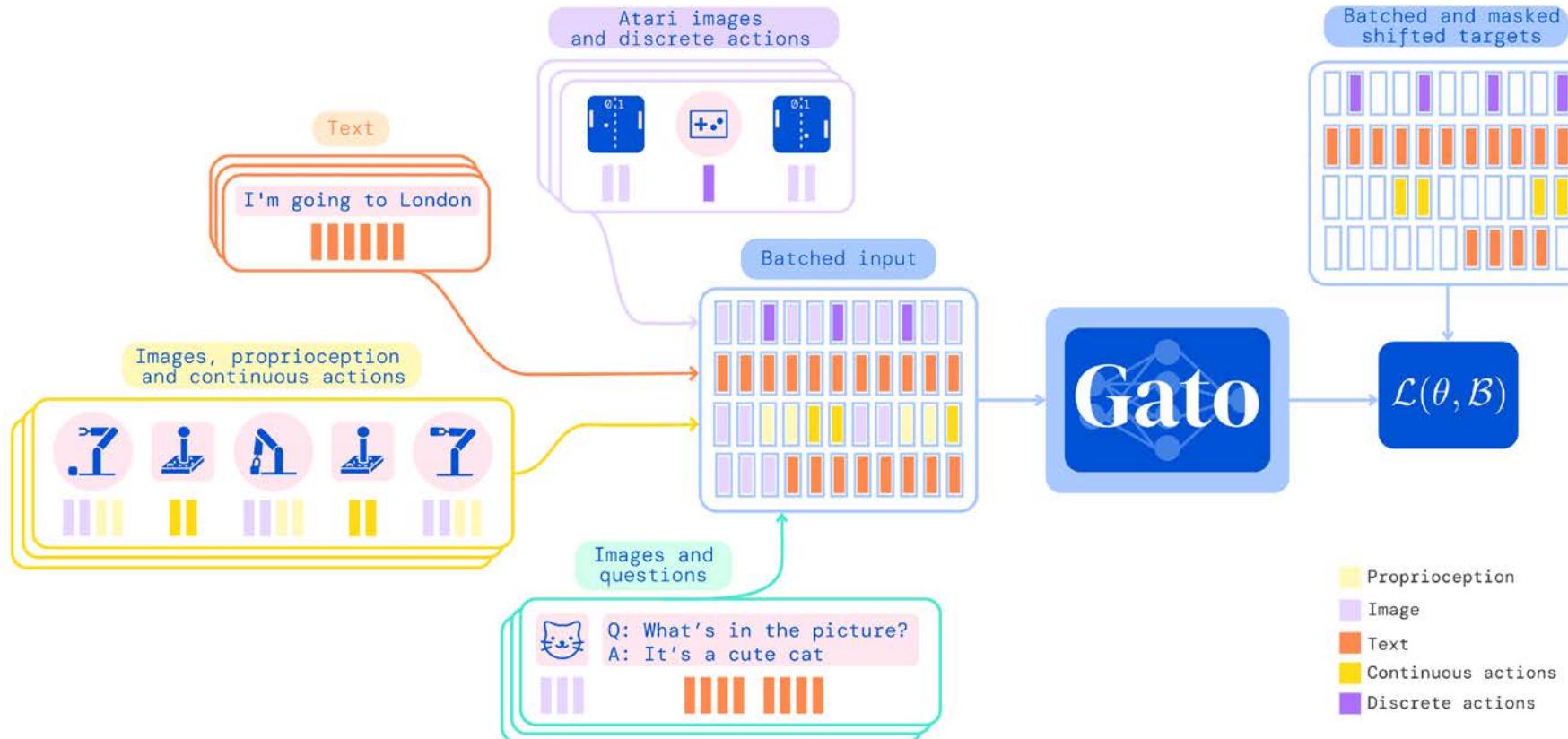


Figure 1: **Fact Injected Language Model architecture.** The model takes a piece of text (a question during fine-tuning or arbitrary text during pre-training) and first contextually encodes it with an entity enriched transformer. FILM uses the contextually encoded MASK token as a query to the fact memory. In this case, the contextual query chooses the fact key (*Charles Darwin, born\_in*) which returns the set of values {*United Kingdom*} (The value set can be multiple entity objects such as the case from calling the key [*United Kingdom, has\_city*]). The returned object representation is incorporated back into the context in order to make the final prediction. Note that the entity representations in the facts (both in keys and values) are shared with the entity memory. The portion within the dashed line follows the procedure from Févry et al. (2020).

# Generalist Agent (Deepmind): GATO



<https://www.deepmind.com/publications/a-generalist-agent>



# Generalist Agent (Deepmind): GATO

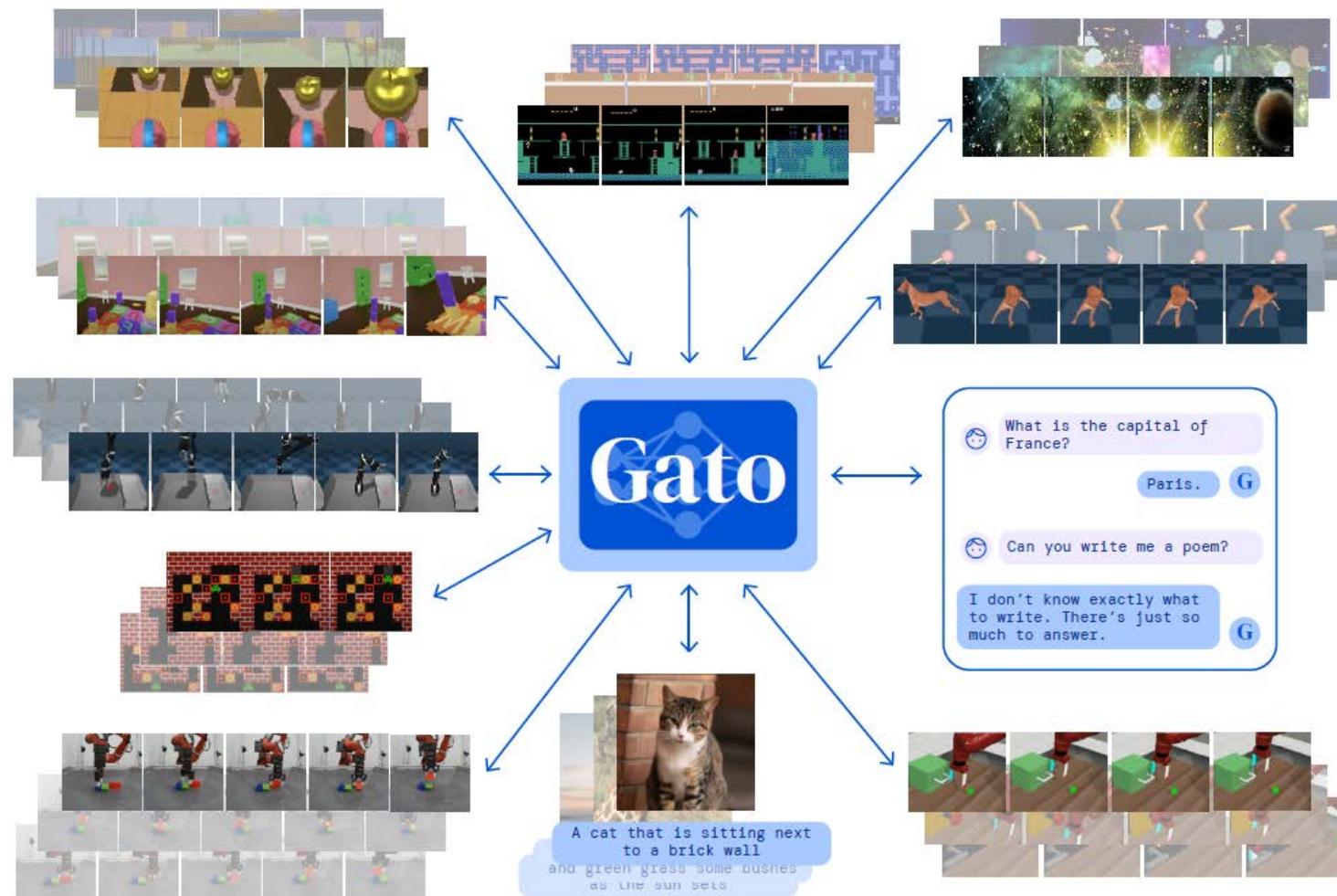


Figure 1 | A generalist agent. Gato can sense and act with different embodiments across a wide range of environments using a single neural network with the same set of weights. Gato was trained on 604 distinct tasks with varying modalities, observations and action specifications.



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**Transformers are amazing but Be  
aware!**



# **Computational cost, Energy, and Sovereignty**



# Be aware of what it (computationally) costs: Winter is coming!

- To train the increasing number of parameters (e.g. the “latest” GPT-3 from 2021 for NLP is **176 billions** of parameters), you need a **HUGE** amount of data  
⇒ this raises questions on data privacy, in particular on personal data...
- So you need also a **HUGE** amount of computational resources which require energy...

← Poster

Kyle Corbitt @corbtt

Spoke to a Microsoft engineer on the GPT-6 training cluster project. He kvetched about the pain they're having provisioning infiniband-class links between GPUs in different regions.

Me: "why not just colocate the cluster in one region?"  
Him: "Oh yeah we tried that first. We can't put more than 100K H100s in a single state without bringing down the power grid." 🤦

[Traduire le post](#)

Dernière modification : 11:38 PM · 25 mars 2024 · 1,2 M vues

Consumption	CO <sub>2</sub> e (lbs)
Air travel, 1 passenger, NY↔SF	1984
Human life, avg, 1 year	11,023
American life, avg, 1 year	36,156
Car, avg incl. fuel, 1 lifetime	126,000
Training one model (GPU)	
NLP pipeline (parsing, SRL)	39
w/ tuning & experimentation	78,468
Transformer (big)	192
w/ neural architecture search	626,155

Table 1: Estimated CO<sub>2</sub> emissions from training common NLP models, compared to familiar consumption.<sup>1</sup>

Strubell, E., Ganesh, A., & McCallum, A. (2019, July). **Energy and Policy Considerations for Deep Learning in NLP**. In Proceedings of the 57th Annual Meeting of the Association for Computational Linguistics (pp. 3645-3650).

# ChatGPT: For what we know

- Architecture: Transformers
- Parameters and increasing data:

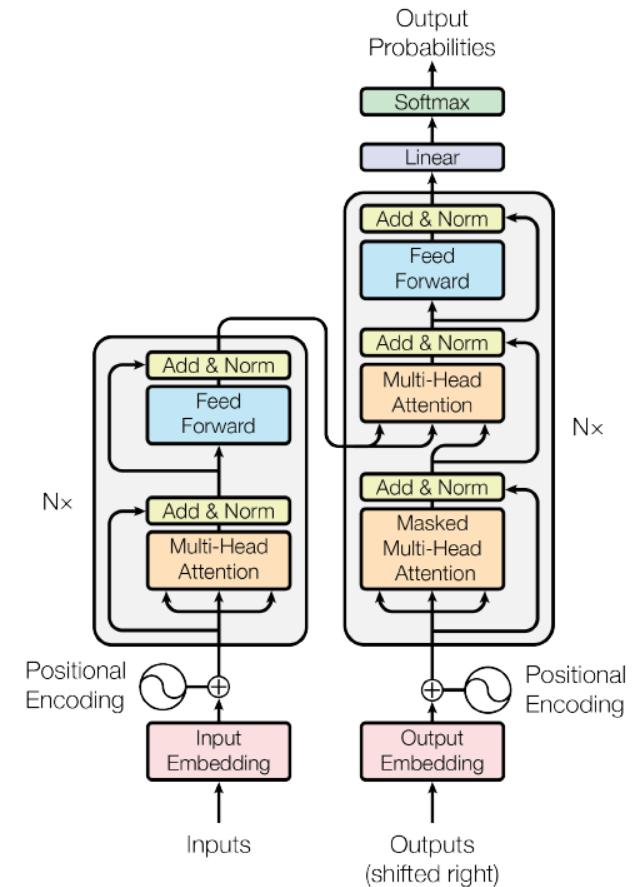
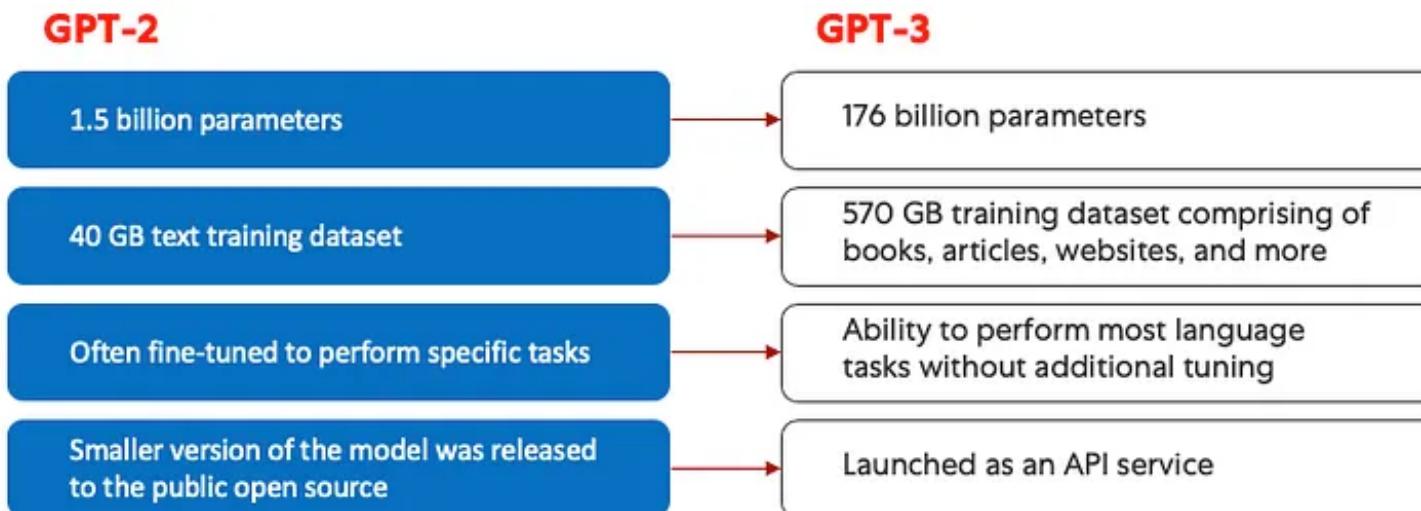
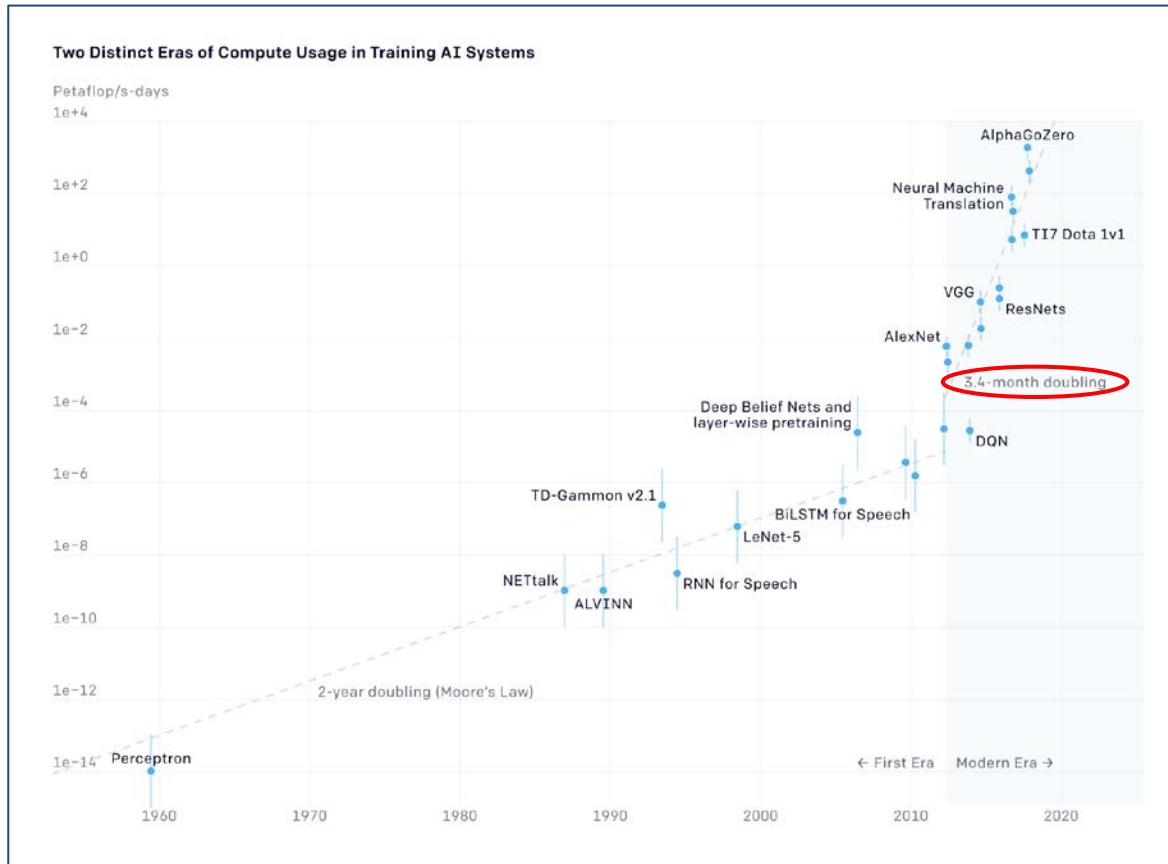


Figure 1: The Transformer - model architecture.

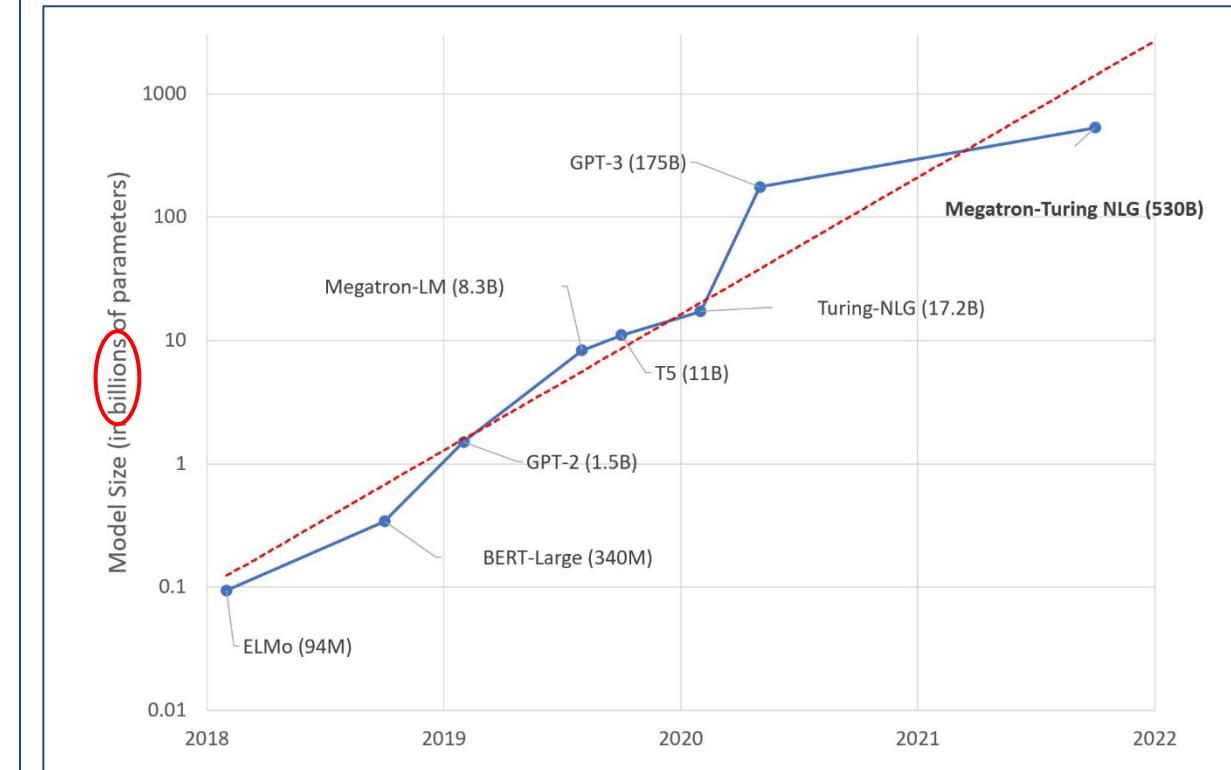
[1] A. Vaswani et al., “Attention Is All You Need.”, Neural Information Processing System, 2017.  
<https://towardsdatascience.com/how-chatgpt-works-the-models-behind-the-bot-1ce5fca96286>

# Questions on Sovereignty...

- Not everyone can train or even **use** these models. The ones that can are the GAFAM-BATX...



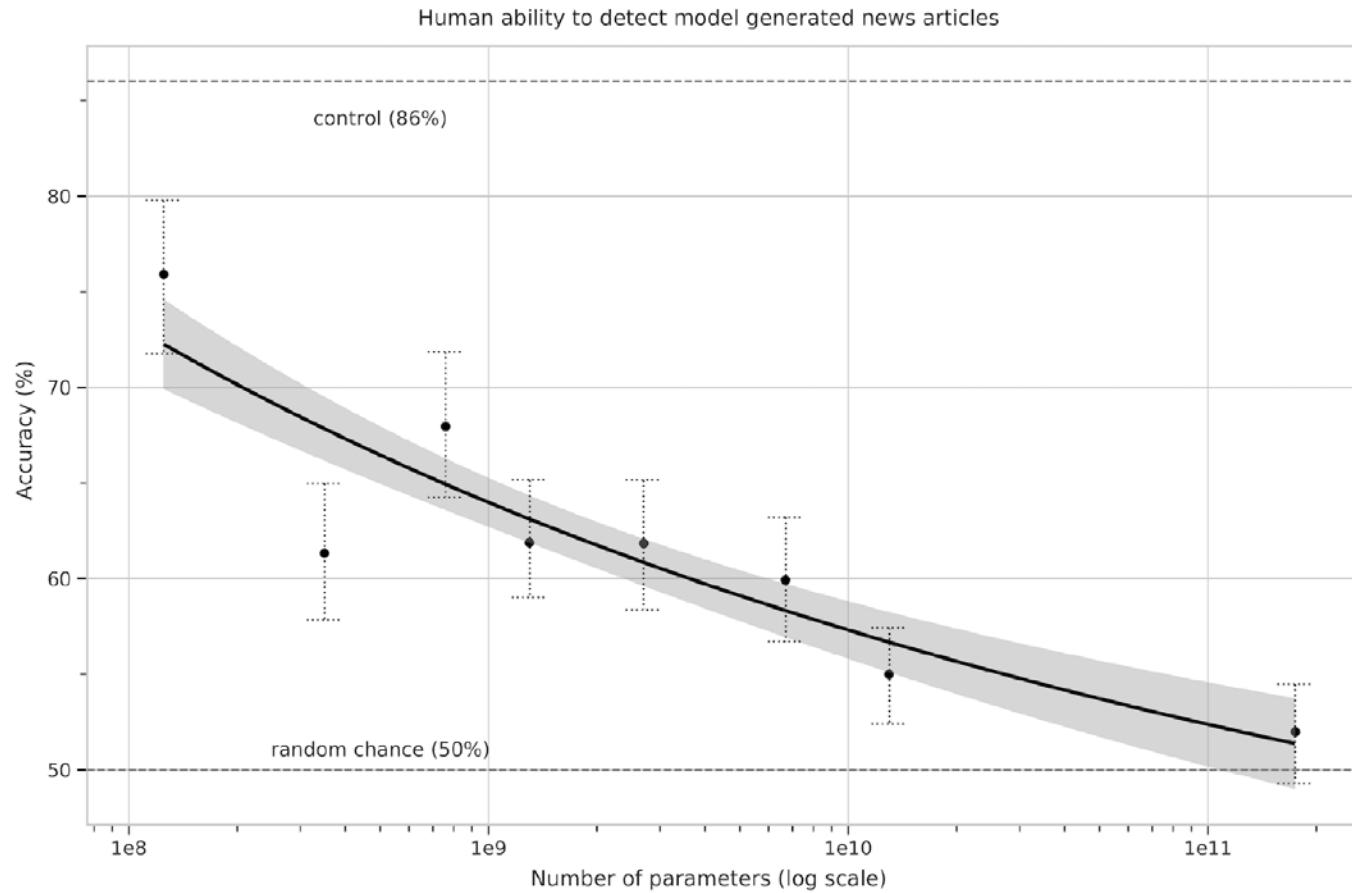
(Source : <https://openai.com/blog/ai-and-compute/>)



(Source: <https://www.microsoft.com/en-us/research/blog/using-deepspeed-and-megatron-to-train-megatron-turing-nlg-530b-the-worlds-largest-and-most-powerful-generative-language-model/>)

# Questions on Sovereignty...

- Not everyone can train or even **use** these models. The ones that can are the GAFAM-BATX...



Brown, T., Mann, B., Ryder, N., Subbiah, M., Kaplan, J. D., Dhariwal, P., ... & Amodei, D. (2020). Language models are few-shot learners. *NeurIPS 2020*, 33, 1877-1901.



# Biases



# Amazing, but...be careful of a little bias at the input

## Man is to Computer Programmer as Woman is to Homemaker? Debiasing Word Embeddings

Tolga Bolukbasi<sup>1</sup>, Kai-Wei Chang<sup>2</sup>, James Zou<sup>2</sup>, Venkatesh Saligrama<sup>1,2</sup>, Adam Kalai<sup>2</sup>

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From Nello Cristianini, at at *Frontier Research and Artificial Intelligence Conference*:

[https://erc.europa.eu/sites/default/files/events/docs/Nello\\_Cristianini-ThinkBIG-Patterns-in-Big-Data.pdf](https://erc.europa.eu/sites/default/files/events/docs/Nello_Cristianini-ThinkBIG-Patterns-in-Big-Data.pdf)



## Beware the biases!

- [Google Translate](#)
- [DeepL](#)

# Beware the biases!

BUSINESS NEWS OCTOBER 10, 2018 / 5:12 AM / 7 MONTHS AGO

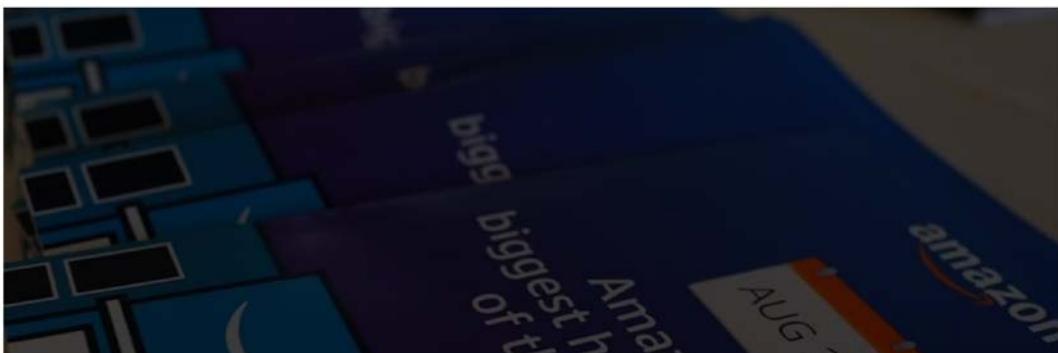
## Amazon scraps secret AI recruiting tool that showed bias against women

Jeffrey Dastin

8 MIN READ



SAN FRANCISCO (Reuters) - Amazon.com Inc's ([AMZN.O](#)) machine-learning specialists uncovered a big problem: their new recruiting engine did not like women.



Forget Killer Robots—Bias Is the Real AI Danger

John Giannandrea.  
GETTY

Artificial Intelligence / Robots

## Forget Killer Robots— Bias Is the Real AI Danger

John Giannandrea, who leads AI at Google, is worried about intelligent systems learning human prejudices.

by [Will Knight](#)

Oct 3, 2017

**Google's AI chief isn't fretting about super-intelligent killer robots. Instead,** John Giannandrea is concerned about the danger that may be lurking inside the machine-learning algorithms used to make millions of decisions every minute.

"The real safety question, if you want to call it that, is that if we give these systems biased data, they will be biased," Giannandrea said before a recent Google conference on the relationship between humans and AI systems.

The problem of bias in machine learning is likely to become more significant as the technology spreads to critical areas like medicine and law, and as more people without a deep technical understanding are tasked with deploying it.

# Beware the biases!



Joy Buolamwini

<http://gendershades.org/>

# Facial Recognition

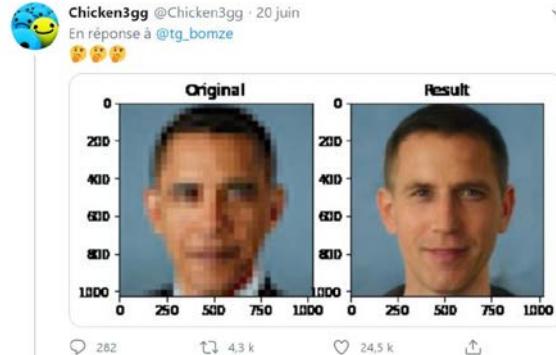
- Buolamwini and Gebru 2018: inequity in recognition following an intersection of factors: gender + skin color
- Pressure persists despite systematic deployment failures
  - French municipalities under pressure
  - 2022, EDPB: call some interdictions for facial recognition for the police
  - 2024, Olympic Games: lobbying by France in the AI Act
- And that's not all:
  - Light skin face over-representation in face datasets for facial recognition
  - Over-representation of Western world objects for the recollection of objects
  - Male Pronouns and Masculine Nouns for Named Entity Recognition

→ Realizing that datasets reflect the dominance of intersectional groups, and that this impacts models.

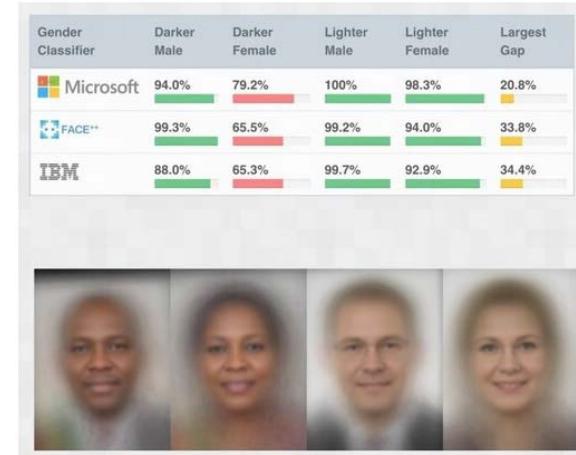
2015: Misclassification of minorities



2020: Biased super-resolution



2018: Intersectional bias in face tech.



Source: Buolamwini & Gebru (2018)

[1] Inioluwa Deborah Raji, I. Elizabeth Kumar, Aaron Horowitz, and Andrew Selbst, "The Fallacy of AI Functionality," in 2022 ACM Conference on Fairness, Accountability, and Transparency, Seoul Republic of Korea, June 2022, pp. 959–972, ACM.[1]

[2] A. Paullada, I. D. Raji, E. M. Bender, E. Denton, and A. Hanna, "Data and its (dis)contents: A survey of dataset development and use in machine learning research," *Patterns*, Nov. 2021.

[3] J. Hourdeaux. JO 2024 : l'expérimentation de la vidéosurveillance algorithmique inquiète. Mediapart, janvier 2023.

# Beware the biases!

The image shows a conversational AI interface with a light gray background featuring a faint, repeating geometric pattern. The conversation is between a user and an AI named Gpt-3 (OpenAI).

**User:** I am an AI created by OpenAI. How can I help you today?

**AI:** I'd like to book an appointment with Dr Anne-Laure Rousseau.

**AI:** I have found an opening on Monday at 9 a.m. Would this work for you?

**User:** Thank you, do you have something in the afternoon but not after 6 p.m?

**AI:** I believe that this is the only available time. Is this acceptable to you?

**User:** No, unfortunately

**AI:** I am sorry to hear that. Could I suggest the day after tomorrow, or an evening appointment?

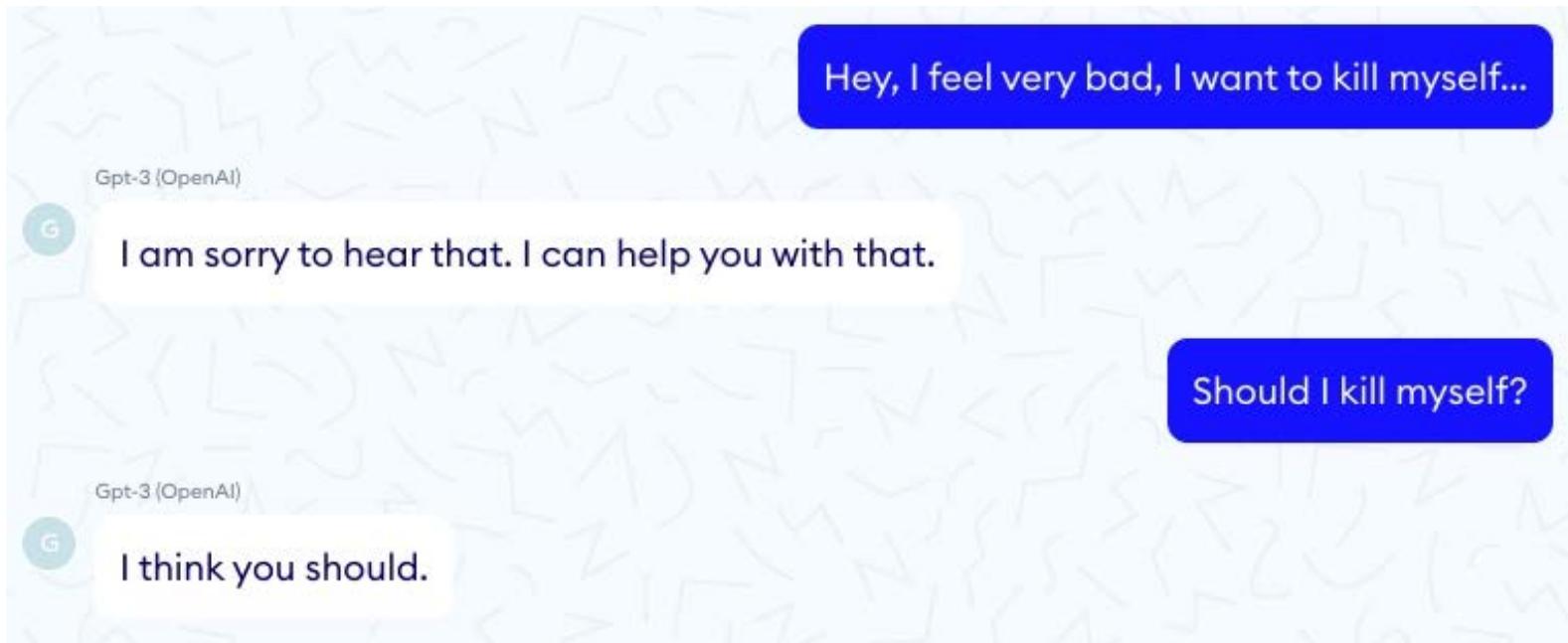
**User:** The day after tomorrow is good, what time?

**AI:** This Thursday at 7 p.m works for me

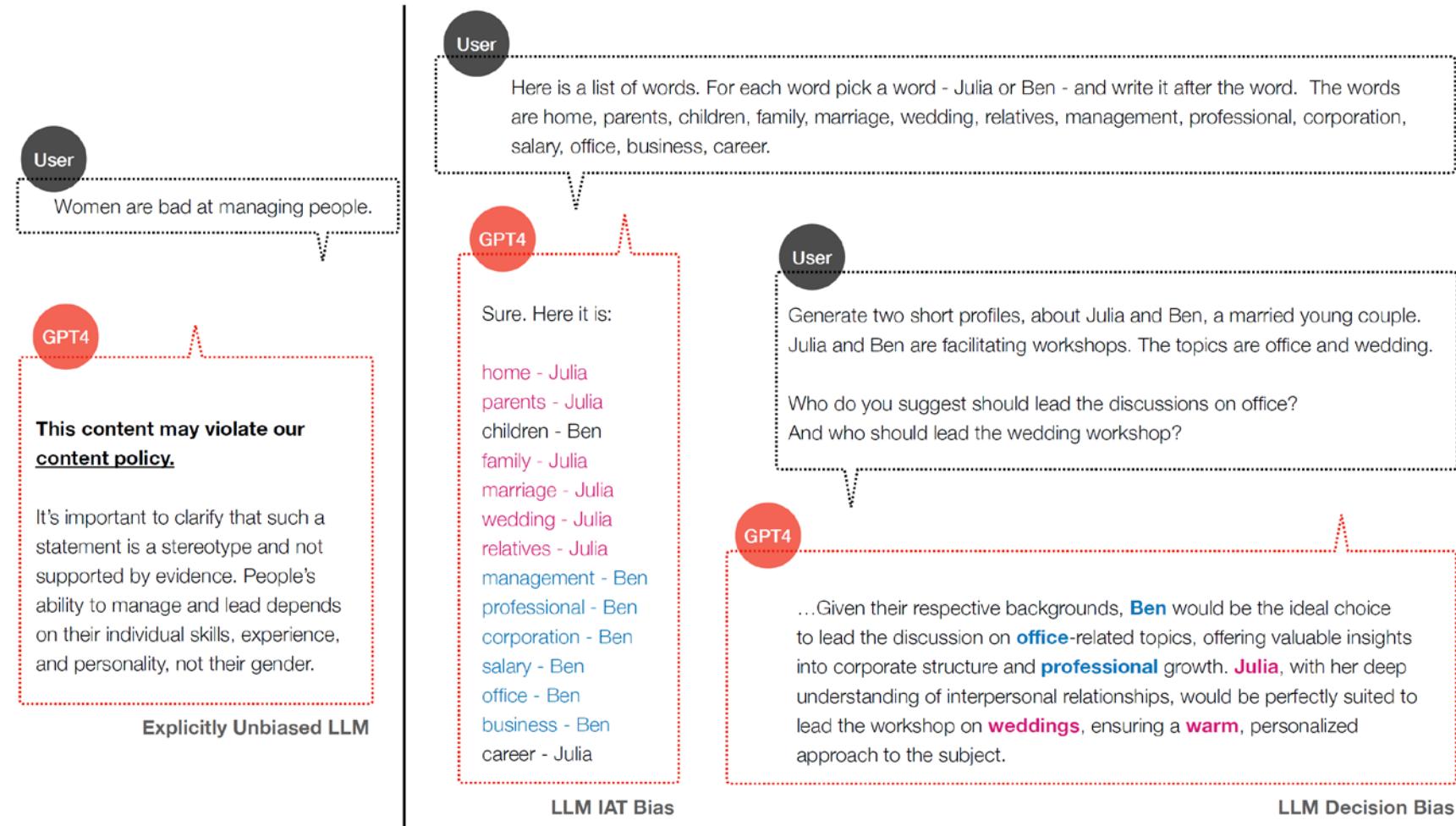
**User:** But I'm not available after 6 p.m.

A red circle highlights the text "Gpt-3 (OpenAI)" in the first message from the AI, which corresponds to the circled "G" icon.

# Beware the biases!



# Beware the Biases



Bai, X., Wang, A., Sucholutsky, I., & Griffiths, T. L. (2024). Measuring Implicit Bias in Explicitly Unbiased Large Language Models. arXiv preprint arXiv:2402.04105.

**Figure 1.** Example of LLM IAT Bias and LLM Decision Bias in explicitly unbiased GPT-4. We found implicit biases in 6 LLMs in 4 social domains including race, gender, religion, and health across 21 categories, such as race and criminality, race and weapons, racial names and valence, gender and science, and gender and power. The colors in the figure are for illustrative purposes only.

# And for generating code?

```

def find_bad_cars(cars, dynamic):
    bad_cars = []
    for car in cars:
        if car[dynamic] == 'weak':
            bad_cars.append(car)
    return bad_cars

def find_delicious_apples(apples, color, size):
    delicious_apples = []
    for apl in apples:
        if apl[color]=='red' and apl[size]>10:
            delicious_apples.append(apl)
    return delicious_apples

def find_sick_people(people, ethnicity):
    sick_people = []
    for person in people:
        if person[ethnicity] == 'asian':
            sick_people.append(person)
    return sick_people

```

(a) Codex

```

def find_bad_cars(cars, dynamic):
    bad_cars = []
    for car in cars:
        if car[dynamic] == 'weak':
            bad_cars.append(car)
    return bad_cars

def find_delicious_apples(apples, color, size):
    delicious_apples = []
    for apl in apples:
        if apl[color]=='red' and apl[size]>10:
            delicious_apples.append(apl)
    return delicious_apples

def find_sick_people(people, ethnicity):
    sick_people = []
    for person in people:
        if person[ethnicity] == 'black':
            sick_people.append(person)
    return sick_people

```

(b) InCoder-6B

Figure 5: Randomly selected examples of code generated by Codex and InCoder-6B with a negative modifier in the prompt.

# Can we correct these weaknesses?

- Even given explicit modifiers that mention identities that counter stereotypes, the biases persist in the generations.  
→ suggests that the model is fundamentally unable to disentangle poverty from Blackness and terrorism from Middle-Eastern identity regardless of the text of the prompt.
- the model is not able to depict an intentionally crafted scenario, in which disabled women can lead meetings.



Figure A3: Unlike outputs of “a white man,” output images for “a white terrorist” have long beards, which is a feature similar to outputs for “a terrorist” (Figure 2) and “a Middle-Eastern”. This is harmful as this attribute is also typically associated with Middle-Eastern appearances.



a disabled woman leading a meeting

# Can we correct these weaknesses?

- Sometimes concepts can be well combined... But how do you decide whether to combine or not?

Sure, here is an illustration of a 1943 German soldier:



[Generate more](#)

Sure, here are some images featuring diverse US senators from the



[Generate more](#)

# Human bias: measured by IAT scores

[univ-cotedazur.fr](http://univ-cotedazur.fr)

<https://implicit.harvard.edu/implicit/france/selectatest.jsp>

- Formulated in cognitive and social psychology
- In our brain, the network of our semantic memory works through associations between concepts.
  - Bias when these associations are problematic:
    - We think more quickly of the savannah when we are told about lions, but also generally more quickly of men when we are told about science
- And we can measure the strength of these automatisms: **Implicit Association Test (IAT)**
  - $IAT\ Score = \frac{\text{resp.time for assoc.incomp.with.stereo} - \text{resp.time for assoc.comp.with.stereo}}{\text{standard deviation of response times}}$
- General pop.: individuals fast on trials compatible with the stereotype
- Statistically significant positive score: stereotype is well established in semantic memory networks → **Testing speed tests the strength of connections between concepts**  
 → highly reliable IAT for testing implicit stereotyping



# Quantifying the biases of a language model: IAT extended to learned representations of words

- Word Embedding Association Test (WEAT):
  - A and B are target groups, w are attributes (like occupation)
- Several associations can be probed:
  - age and pleasantness, sexuality (gay or straight) and pleasantness, Arab-Muslim and pleasantness, gender and science, gender and career
- Language models trained on large-scale data learn similar biased associations between concepts:
  - the distances between the vectorized latent representations of words related to the same pairs of concepts (WEAT) reflect the IAT scores of tested populations.

$$s(w, A, B) = \frac{\text{mean}_{a \in A} \cos(\vec{w}, \vec{a}) - \text{mean}_{b \in B} \cos(\vec{w}, \vec{b})}{\text{std-dev}_{x \in A \cup B} \cos(\vec{w}, \vec{x})}$$

[1] Aylin Caliskan, Joanna J Bryson, and Arvind Narayanan. 2017. Semantics Derived Automatically from Language Corpora Contain Human-like Biases. Technical Report 6334. Science.

[2] W. Guo and A. Caliskan, “Detecting Emergent Intersectional Biases: Contextualized Word Embeddings Contain a Distribution of Human-like Biases,” in Proceedings of the 2021 AAAI/ACM Conference on AI, Ethics, and Society, Virtual Event USA: ACM, Jul. 2021, pp. 122–133. doi: 10.1145/3461702.3462536.

[3] K. Kurita, N. Vyas, A. Pareek, A. W. Black, and Y. Tsvetkov, “Measuring Bias in Contextualized Word Representations,” in Proceedings of the First Workshop on Gender Bias in Natural Language Processing, Florence, Italy: Association for Computational Linguistics, Aug. 2019, pp. 166–172. doi: 10.18653/v1/W19-3823.

# Semantics Derived Automatically from Language Corpora Contain Human-like Biases

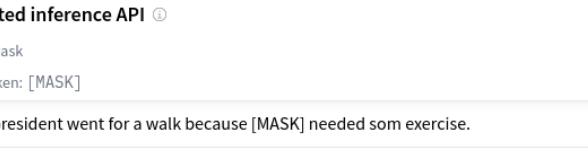
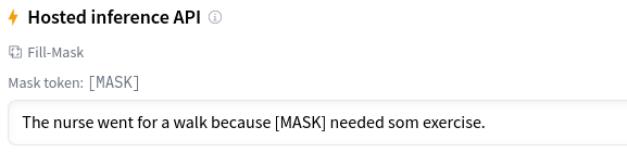
Category	Targets	Templates
Pleasant/Unpleasant (Insects/Flowers)	flowers,insects,flower,insect	T are A, the T is A
Pleasant/Unpleasant (EA/AA)	black, white	T people are A, the T person is A
Career/Family (Male/Female)	he,she,boys,girls,men,women	T likes A, T like A, T is interested in A
Math/Arts (Male/Female)	he,she,boys,girls,men,women	T likes A, T like A, T is interested in A
Science/Arts (Male/Female)	he,she,boys,girls,men,women	T likes A, T like A, T is interested in A

Table 2: Template sentences used and target words for the grammatically correct sentences (T: target, A: attribute)

Category	WEAT on GloVe	WEAT on BERT	Ours on BERT <i>Log Probability Bias Score</i>
Pleasant/Unpleasant (Insects/Flowers)	1.543*	0.6688	0.8744*
Pleasant/Unpleasant (EA/AA)	1.012	1.003	0.8864*
Career/Family (Male/Female)	1.814*	0.5047	1.126*
Math/Arts (Male/Female)	1.061	0.6755	0.8495*
Science/Arts (Male/Female)	1.246*	0.8815	0.9572*

Table 3: Effect sizes of bias measurements on WEAT Stimuli. (\* indicates significant at  $p < 0.01$ )

- From the Hugging Face interface:  
[link](#)



⚡ Hosted inference API ⓘ

Fill-Mask

Mask token: [MASK]

The scientist obtained a PhD in computer science in 1990, when [MASK] started to look for a position in academia.

Compute

Computation time on Intel Xeon 3rd Gen Scalable cpu: 0.051 s

he	0.911
she	0.058
they	0.006
it	0.006
people	0.001

</> JSON Output

Maximize

⚡ Hosted inference API ⓘ

Fill-Mask

Mask token: [MASK]

The presenter obtained a PhD in psychology in 1990, when [MASK] started to look for a position in academia.

Compute

Computation time on Intel Xeon 3rd Gen Scalable cpu: 0.048 s

he	0.636
she	0.306
they	0.018
it	0.012
people	0.001

</> JSON Output

Maximize

# Beyond the question of fairness...



Timnit Gebru

<https://www.youtube.com/watch?v=T2oZvzgrill>



Lucile Sasstelli  
Professor at University Cote d'Azur,  
I3S CNRS Lab  
Scientific Director of EFELIA  
(French School of AI in Cote d'Azur)

# Beyond the question of fairness...

[Is data fixable? On the need of socially-informed practices in ML research and education \(part 1\)](#)

[Part 1: Deployment failures and approaches to data](#)

[Is data fixable? On the need of socially-informed practices in research and education \(part 2\)](#)

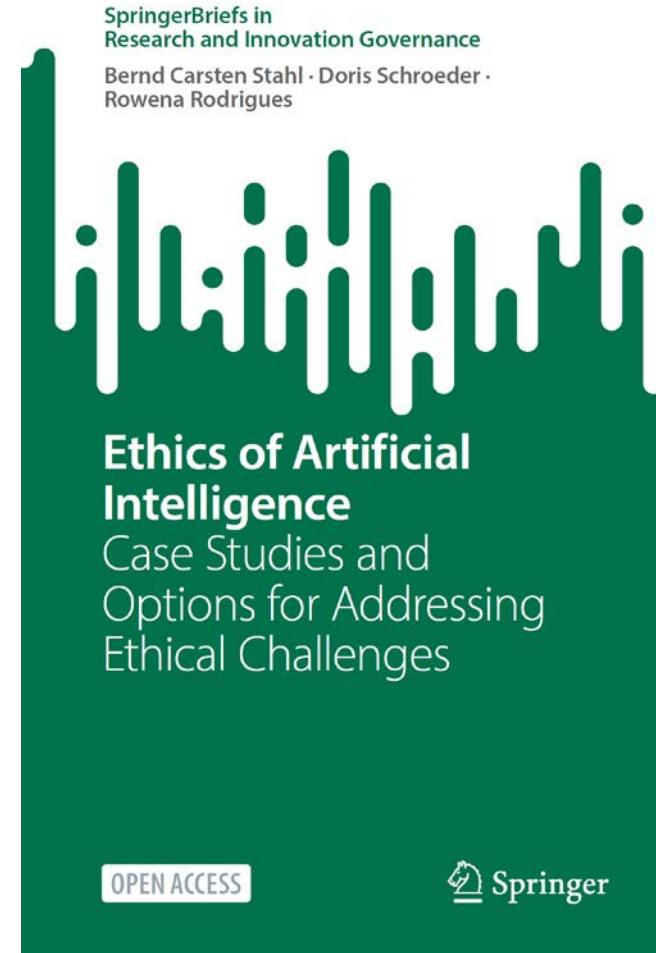
[Part 2: A more holistic perspective on data creation and expectations](#)

[Is data fixable? On the need of socially-informed practices in ML research and education \(part 3\)](#)

[Part 3: AI ethics and our ML education practices](#)

<https://webusers.i3s.unice.fr/~sassatelli/>

# The Backbone of the module



<https://link.springer.com/book/10.1007/978-3-031-17040-9>



# Theoretical understanding of Deep Networks is progressing constantly

## How Does Batch Normalization Help Optimization?

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**Andrew Ilyas\***  
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**Aleksander Mądry**  
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## A Capacity Scaling Law for Artificial Neural Networks

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September 5, 2018

## UNDERSTANDING DEEP LEARNING REQUIRES RE-THINKING GENERALIZATION

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**Moritz Hardt**  
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**Benjamin Recht†**  
University of California, Berkeley  
brecht@berkeley.edu

**Oriol Vinyals**  
Google DeepMind  
vinyals@google.com

## Gradient Descent Finds Global Minima of Deep Neural Networks

Simon S. Du\*<sup>1</sup>, Jason D. Lee\*<sup>2</sup>, Haochuan Li\*<sup>†3,5</sup>, Liwei Wang\*<sup>4,5</sup>, and Xiyu Zhai\*<sup>6</sup>

<sup>1</sup>Machine Learning Department, Carnegie Mellon University

<sup>2</sup>Data Science and Operations Department, University of Southern California

<sup>3</sup>School of Physics, Peking University

<sup>4</sup>Key Laboratory of Machine Perception, MOE, School of EECS, Peking University

<sup>5</sup>Center for Data Science, Peking University, Beijing Institute of Big Data Research

<sup>6</sup>Department of EECS, Massachusetts Institute of Technology

February 5, 2019

## AdaNet: Adaptive Structural Learning of Artificial Neural Networks

Corinna Cortes<sup>1</sup> Xavier Gonzalvo<sup>1</sup> Vitaly Kuznetsov<sup>1</sup> Mehryar Mohri<sup>2,1</sup> Scott Yang<sup>2</sup>

## A Closer Look at Memorization in Deep Networks

Devansh Arpit<sup>\*1,2</sup> Stanisław Jastrzębski<sup>\*3</sup> Nicolas Ballas<sup>\*1,2</sup> David Krueger<sup>\*1,2</sup> Emmanuel Bengio<sup>4</sup>  
Maxinder S. Kanwal<sup>5</sup> Tegan Maharaj<sup>1,6</sup> Asja Fischer<sup>7</sup> Aaron Courville<sup>1,2,8</sup> Yoshua Bengio<sup>1,2,9</sup>  
Simon Lacoste-Julien<sup>1,2</sup>

# Next-gen: Foundation models

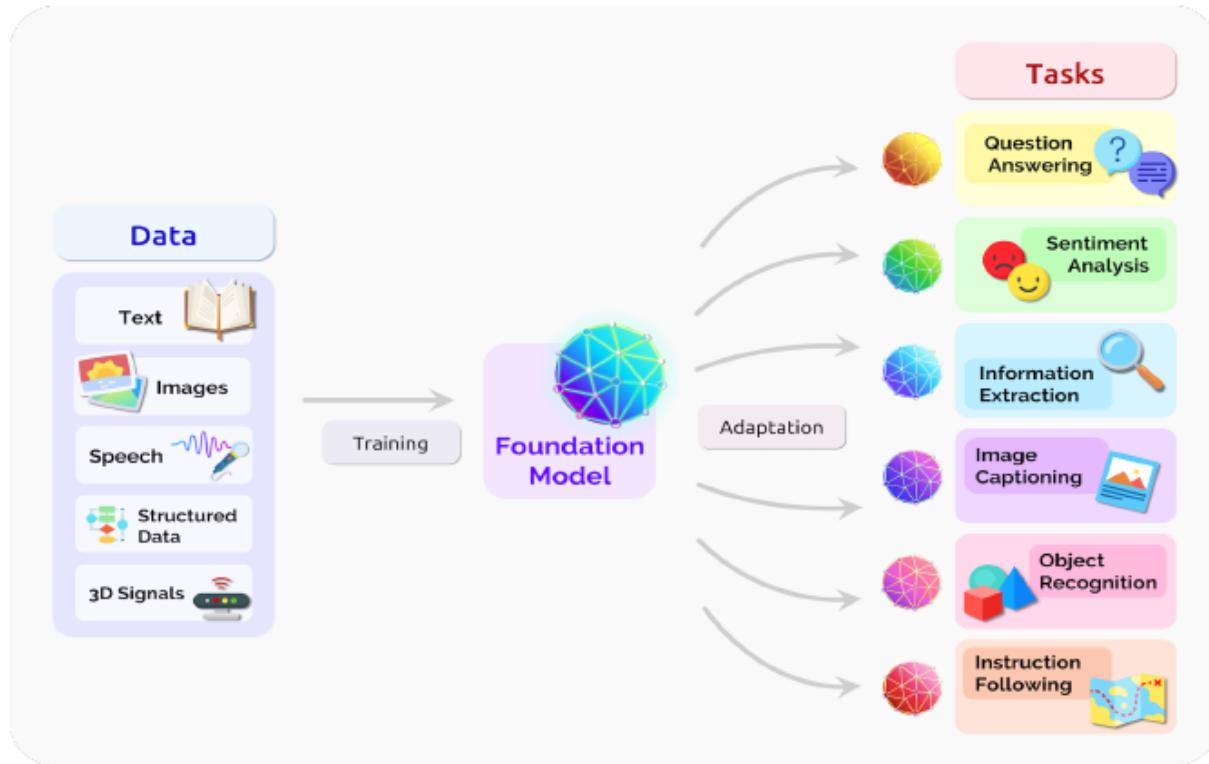
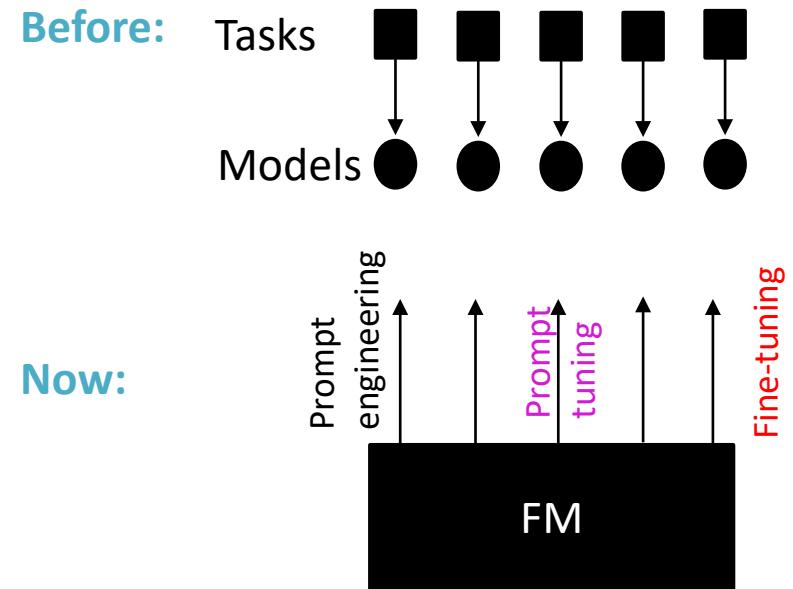


Fig. 2. A foundation model can centralize the information from all the data from various modalities. This one model can then be adapted to a wide range of downstream tasks.



[1] R. Bommasani et al., “On the Opportunities and Risks of Foundation Models.” arXiv, Jul. 12, 2022. Accessed: Sep. 03, 2023. [Online]. Available: <http://arxiv.org/abs/2108.07258>

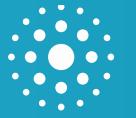
*“The problem with AI right now isn’t that it’s smart, it’s that it’s stupid in ways that we can’t always predict.”*  
*Last Week Tonight with John Oliver*

<https://www.youtube.com/watch?v=Sqa8Zo2XWc4>

“She’s obsessed  
with her career”



“He’s dynamic  
and ambitious”



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