### Neural Attention

Yoav Goldberg

# Before we start, some things to consider

- What makes a model slow?
- Which operations take more time?
- Which operations will be faster on GPU / CPU?
- Should I use CPU or GPU for this problem?
- Can I find an efficient parallel implementation for this architecture?
  - Data-parallel vs. Model-parallel

before we start:

### **Residual Connections**

### Neural Networks for Vision





### CS231n: Convolutional Neural Networks for Visual Recognition

Spring 2017



April 18, 2017

ImageNet Large Scale Visual Recognition Challenge (ILSVRC) winners

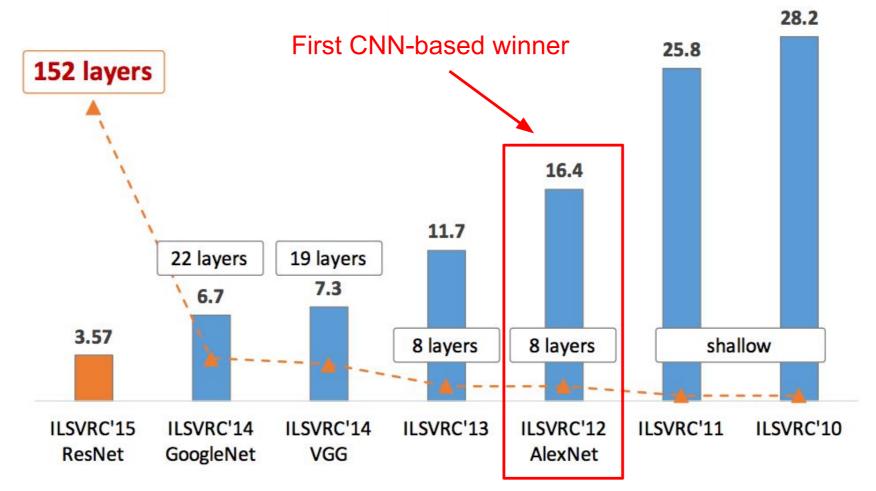


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Lecture 9 - 22 May 2, 2017

ImageNet Large Scale Visual Recognition Challenge (ILSVRC) winners

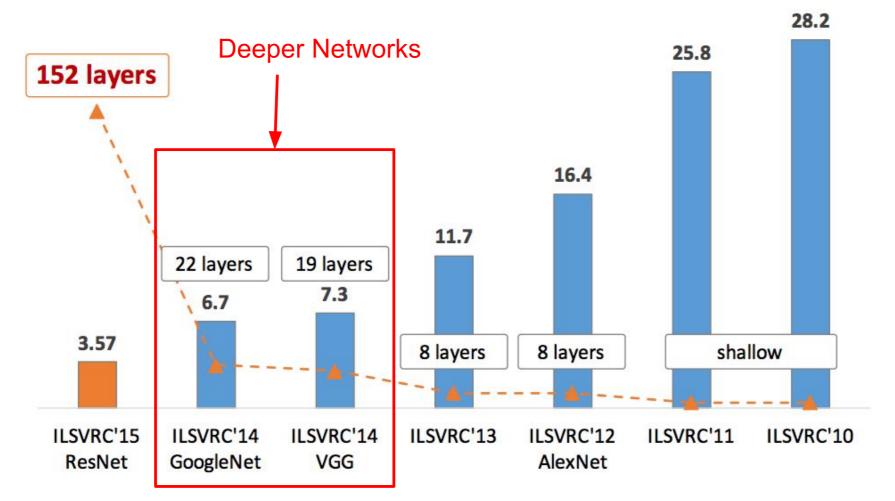


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Lecture 9 - 25 May 2, 2017

Case Study: VGGNet

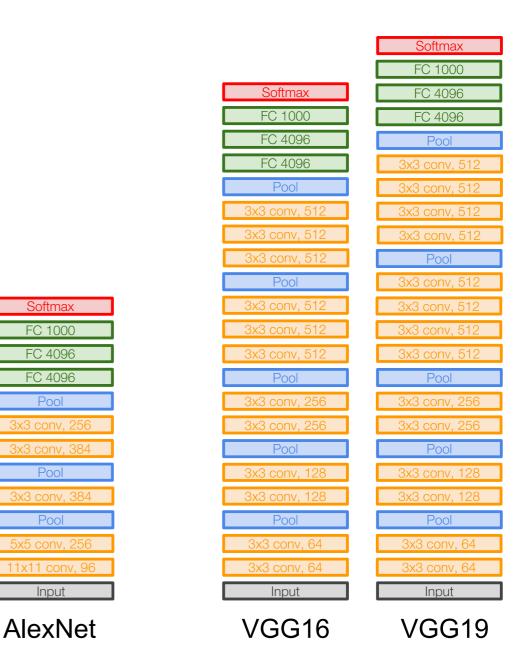
[Simonyan and Zisserman, 2014]

Small filters, Deeper networks

8 layers (AlexNet) -> 16 - 19 layers (VGG16Net)

Only 3x3 CONV stride 1, pad 1 and 2x2 MAX POOL stride 2

11.7% top 5 error in ILSVRC'13 (ZFNet) -> 7.3% top 5 error in ILSVRC'14



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Lecture 9 - 26

Pool

Pool

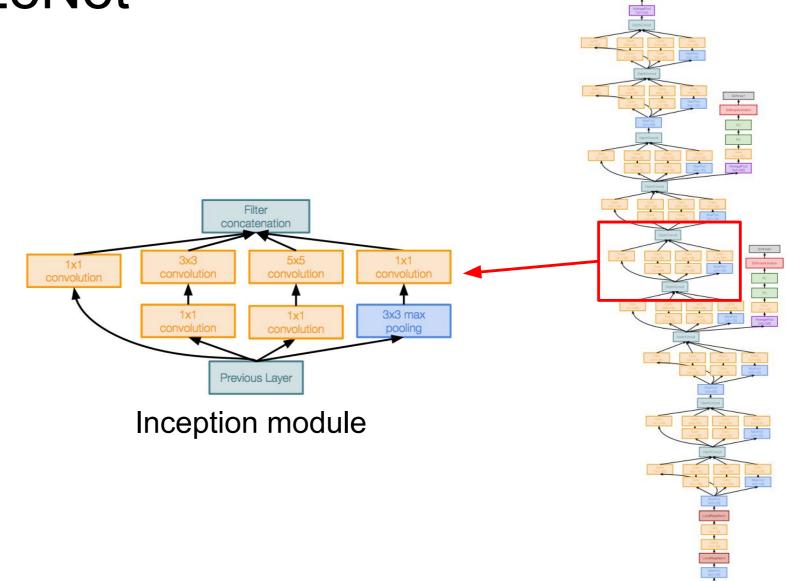
Pool

Input

#### Case Study: GoogLeNet

[Szegedy et al., 2014]

"Inception module": design a good local network topology (network within a network) and then stack these modules on top of each other



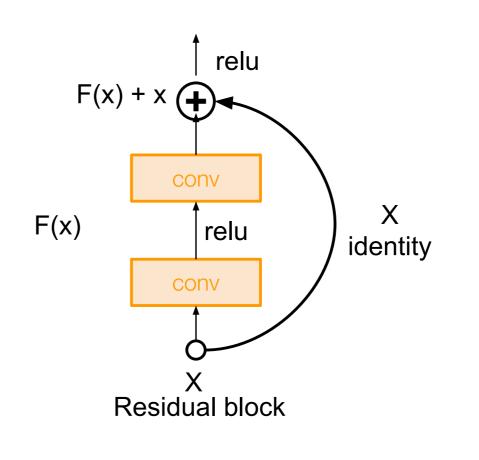
Fei-Fei Li & Justin Johnson & Serena Yeung

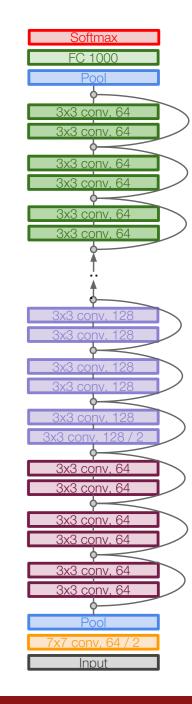
Lecture 9 - 38

[He et al., 2015]

Very deep networks using residual connections

- 152-layer model for ImageNet
- ILSVRC'15 classification winner (3.57% top 5 error)
- Swept all classification and detection competitions in ILSVRC'15 and COCO'15!





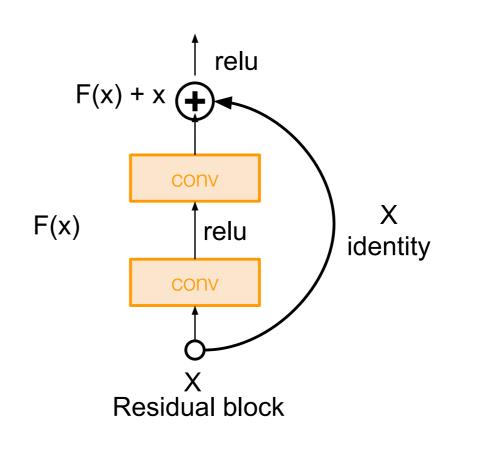
#### Fei-Fei Li & Justin Johnson & Serena Yeung

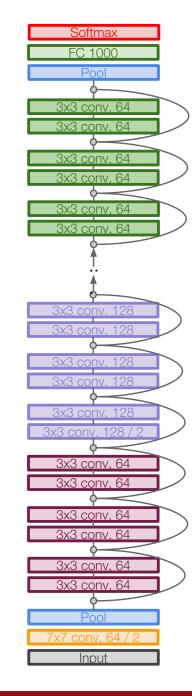
Lecture 9 - 65

[He et al., 2015]

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Fei-Fei Li & Justin Johnson & Serena Yeung

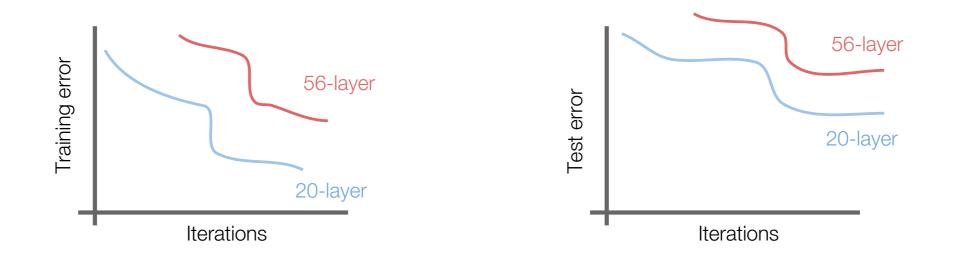
Lecture 9 - 65

#### **Deep Residual Learning for Image Recognition**

Kaiming He Xiangyu Zhang Shaoqing Ren Jian Sun Microsoft Research {kahe, v-xiangz, v-shren, jiansun}@microsoft.com

[He et al., 2015]

What happens when we continue stacking deeper layers on a "plain" convolutional neural network?



Q: What's strange about these training and test curves? [Hint: look at the order of the curves]

Fei-Fei Li & Justin Johnson & Serena Yeung

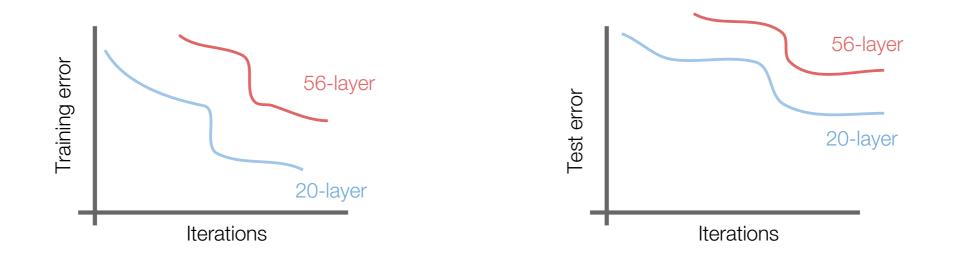
Lecture 9 - 67 May 2, 2017

56-layer model performs worse on both training and test error -> The deeper model performs worse, but it's not caused by overfitting!

#### Case Study: ResNet

[He et al., 2015]

What happens when we continue stacking deeper layers on a "plain" convolutional neural network?



Q: What's strange about these training and test curves? [Hint: look at the order of the curves]

Fei-Fei Li & Justin Johnson & Serena Yeung

Lecture 9 - 67 May 2, 2017

[He et al., 2015]

Hypothesis: the problem is an *optimization* problem, deeper models are harder to optimize

The deeper model should be able to perform at least as well as the shallower model.

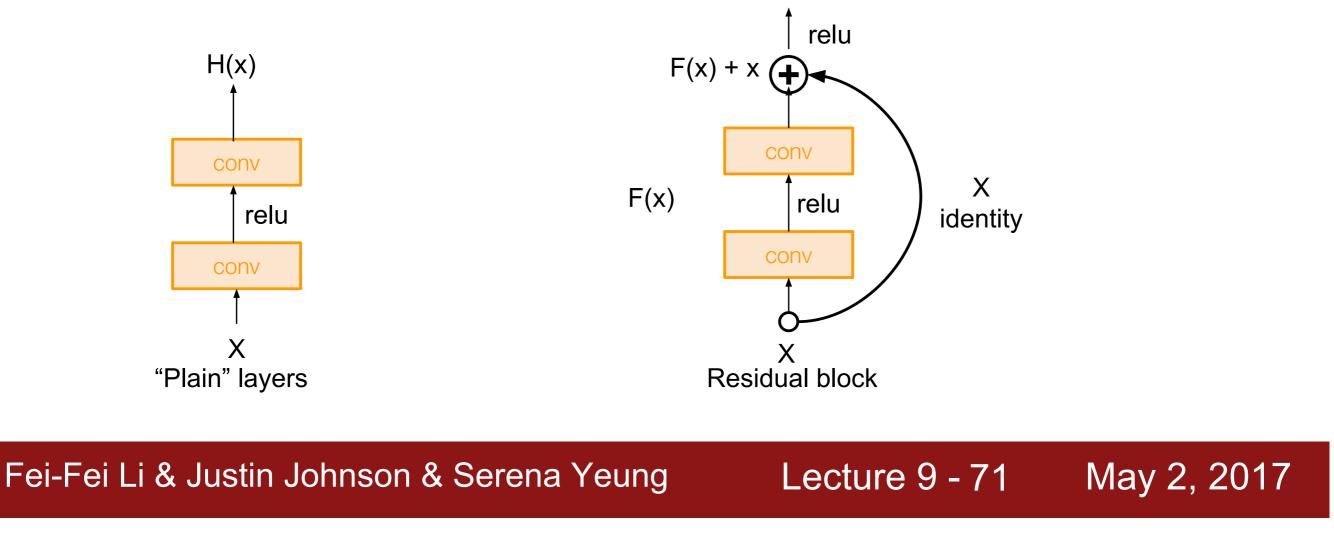
A solution by construction is copying the learned layers from the shallower model and setting additional layers to identity mapping.

Fei-Fei Li & Justin Johnson & Serena Yeung

Lecture 9 - 70 May 2, 2017

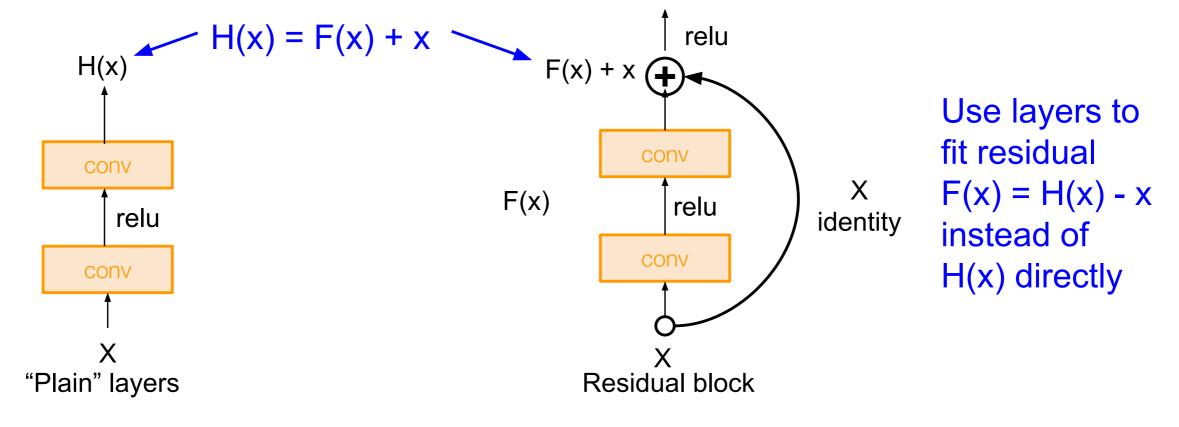
[He et al., 2015]

Solution: Use network layers to fit a residual mapping instead of directly trying to fit a desired underlying mapping



[He et al., 2015]

Solution: Use network layers to fit a residual mapping instead of directly trying to fit a desired underlying mapping



Fei-Fei Li & Justin Johnson & Serena Yeung

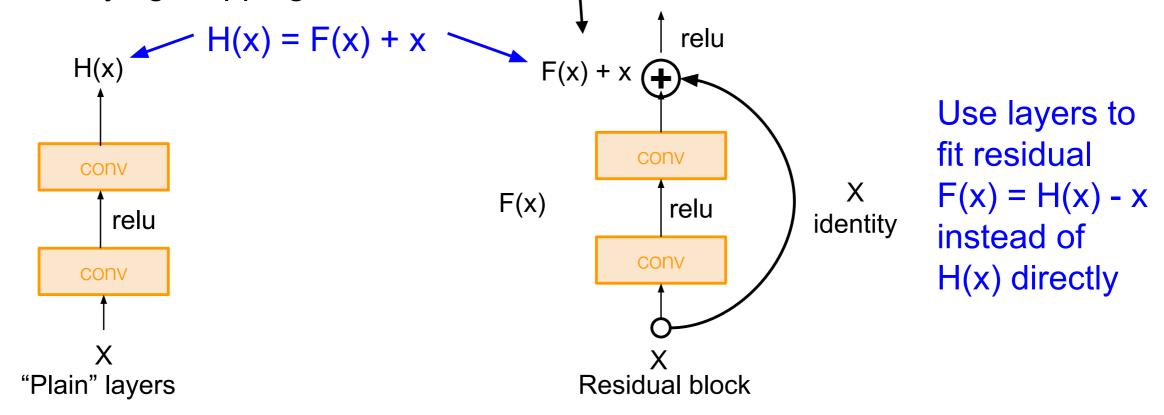
Lecture 9 - 72 May

#### "copy x and add some change to it"

#### Case Study: ResNet

[He et al., 2015]

Solution: Use network layers to fit a residual mapping instead of directly trying to fit a desired underlying mapping



Fei-Fei Li & Justin Johnson & Serena Yeung

Lecture 9 - 72 May

In this paper, we address the degradation problem by introducing a deep residual learning framework. Instead of hoping each few stacked layers directly fit a desired underlying mapping, we explicitly let these layers fit a residual mapping. Formally, denoting the desired underlying mapping as  $\mathcal{H}(\mathbf{x})$ , we let the stacked nonlinear layers fit another mapping of  $\mathcal{F}(\mathbf{x}) := \mathcal{H}(\mathbf{x}) - \mathbf{x}$ . The original mapping is recast into  $\mathcal{F}(\mathbf{x}) + \mathbf{x}$ . We hypothesize that it is easier to optimize the residual mapping than to optimize the original, unreferenced mapping. To the extreme, if an identity mapping were optimal, it would be easier to push the residual to zero than to fit an identity mapping by a stack of nonlinear layers.

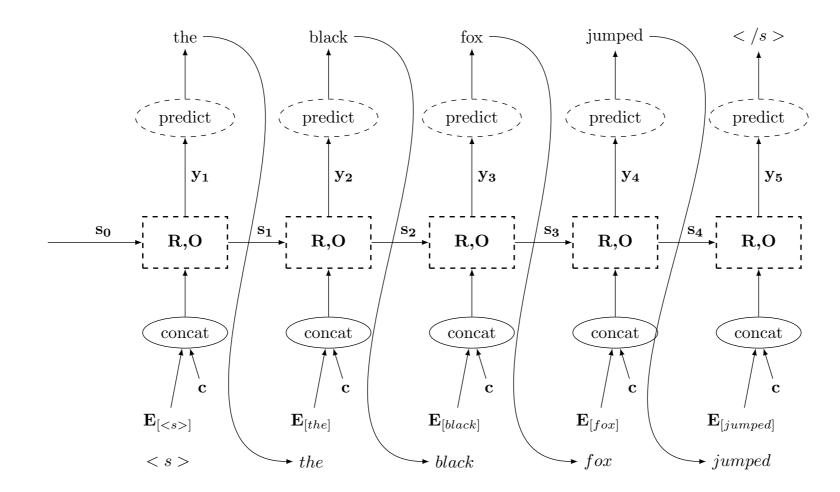
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### back to sequences

### Previously

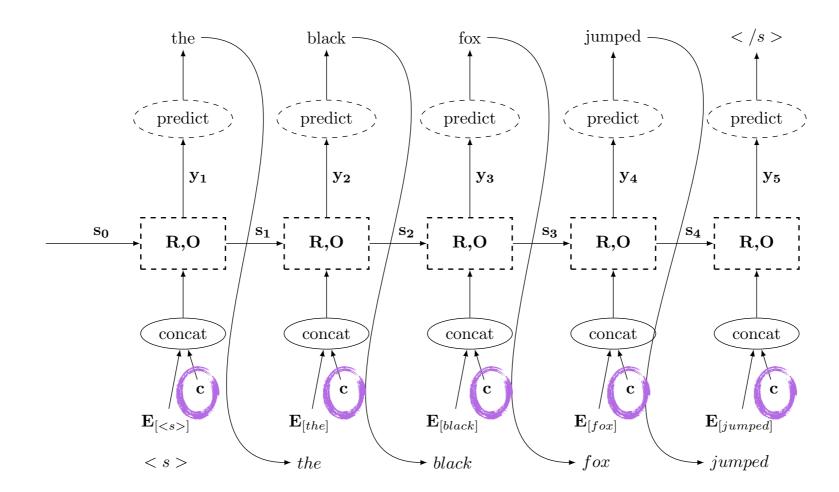
- Mapping from a sequence to a single decision.
  - with RNN acceptors.
- Mapping from two sequences to a single decision.
  - with Siamese network.
- Mapping from a sequence to a sequence of same length.
  - with RNN transducer, or with biRNN.
- Mapping from length m to length n with a seq2seq (encoder decoder) architecture.
  - encoder RNN, decoder RNN.

### RNN Language Model for **Conditioned generation**



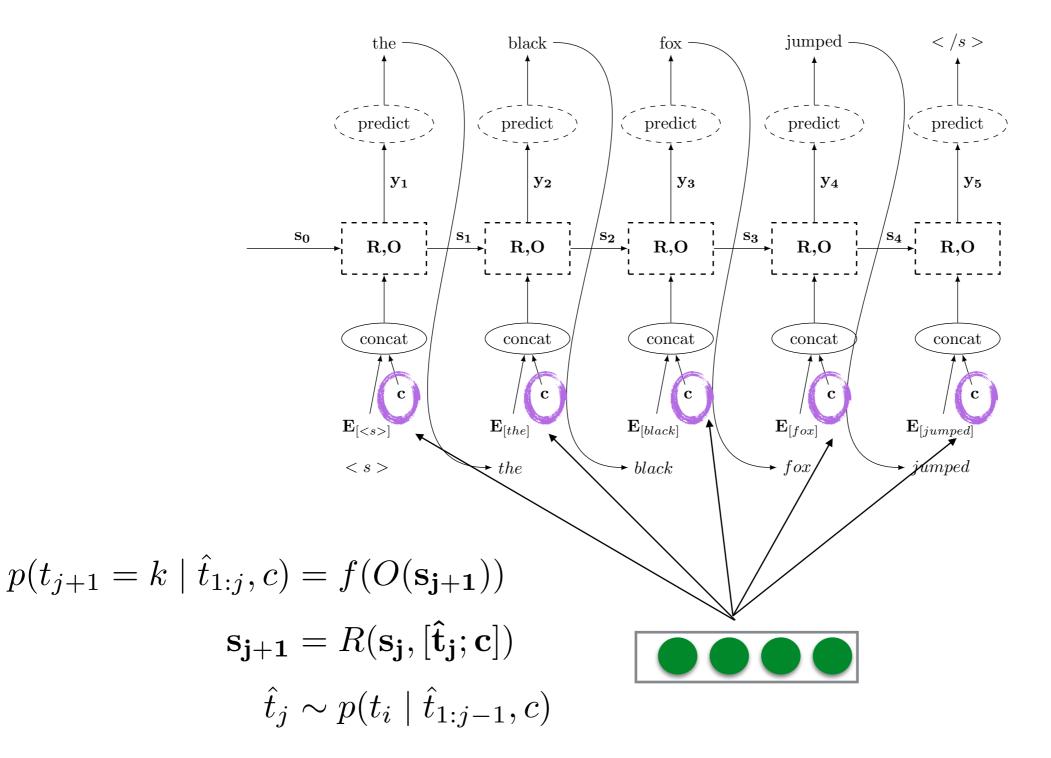
$$p(t_{j+1} = k \mid \hat{t}_{1:j}, c) = f(O(\mathbf{s_{j+1}}))$$
$$\mathbf{s_{j+1}} = R(\mathbf{s_j}, [\mathbf{\hat{t}_j}; \mathbf{c}])$$
$$\hat{t}_j \sim p(t_i \mid \hat{t}_{1:j-1}, c)$$

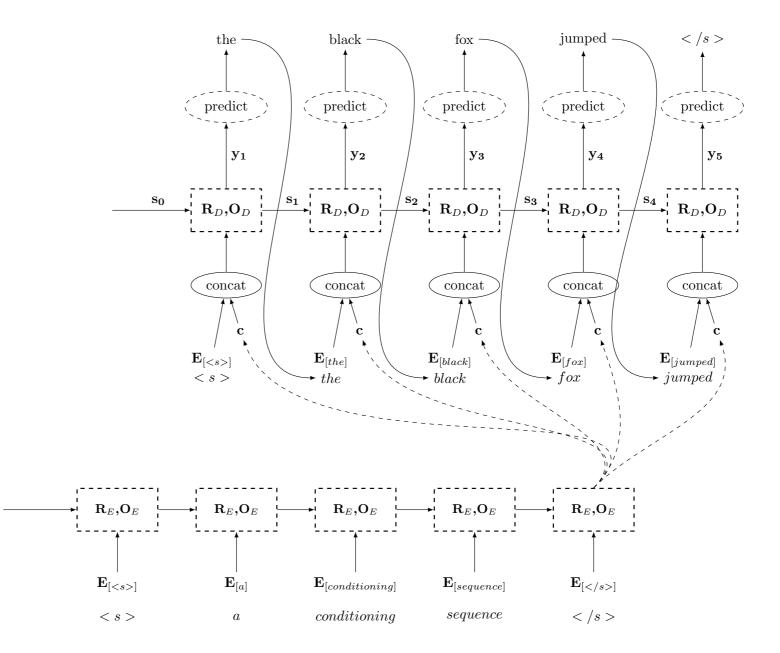
### RNN Language Model for **Conditioned generation**



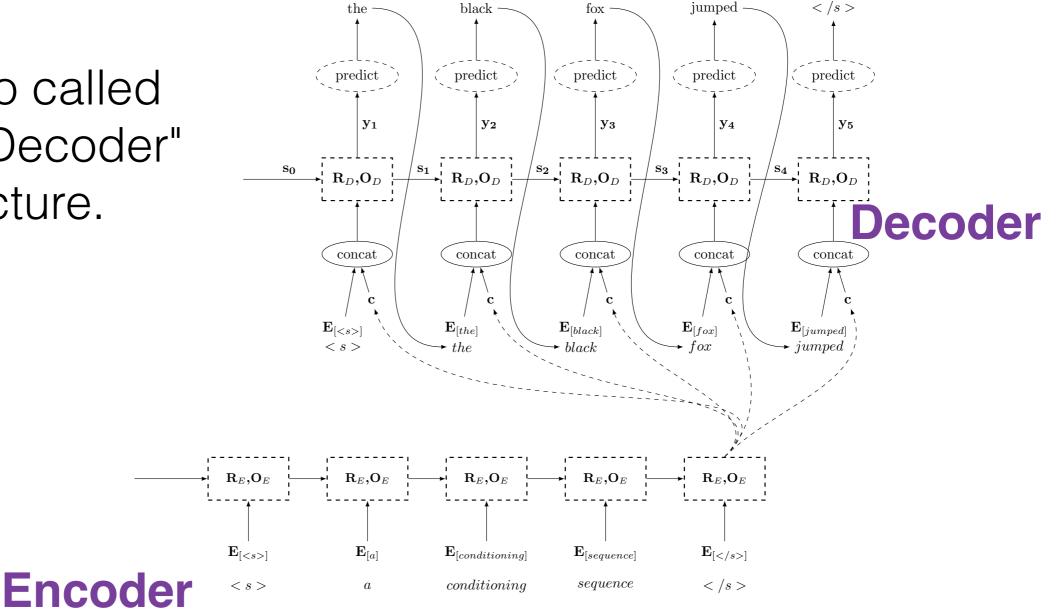
 $p(t_{j+1} = k \mid \hat{t}_{1:j}, c) = f(O(\mathbf{s_{j+1}}))$  $\mathbf{s_{j+1}} = R(\mathbf{s_j}, [\mathbf{\hat{t}_j}; \mathbf{c}])$  $\hat{t}_j \sim p(t_i \mid \hat{t}_{1:j-1}, c)$ 

# RNN Language Model for **Conditioned generation**

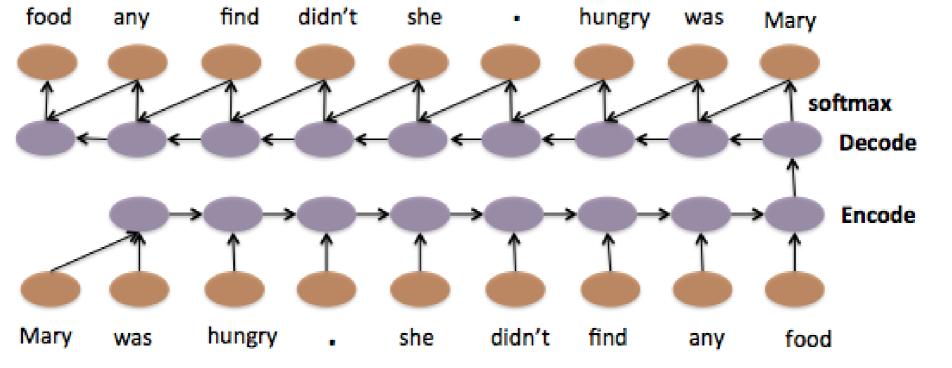




This is also called "Encoder Decoder" architecture.



### Encoder-Decoder Example: Auto-encoder



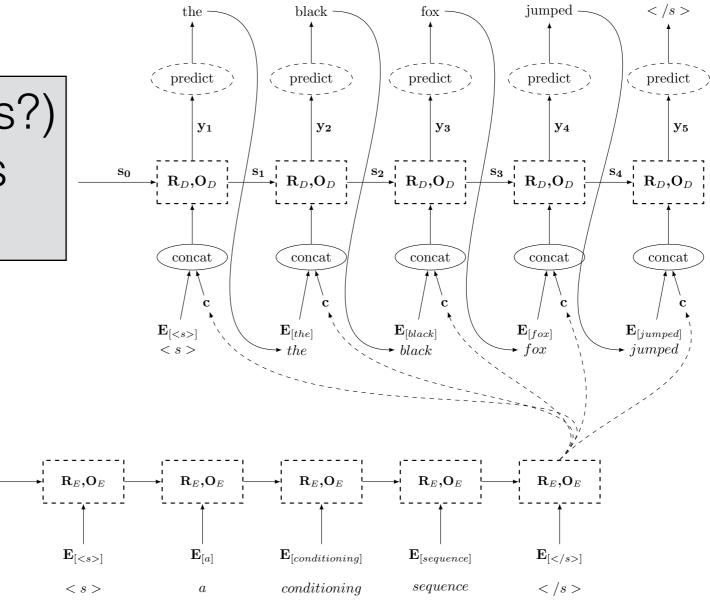
A Hierarchical Neural Autoencoder for Paragraphs and Documents

Encode: English sentence.
 Decode: Same English sentence.

Jiwei Li, Minh-Thang Luong and Dan Jurafsky Computer Science Department, Stanford University, Stanford, CA 94305, USA jiweil, lmthang, jurafsky@stanford.edu

encoded vector is a "generic sentence representation"

What's the (obvious?) problem with this approach?



### Attention

#### a.k.a "soft alignment"

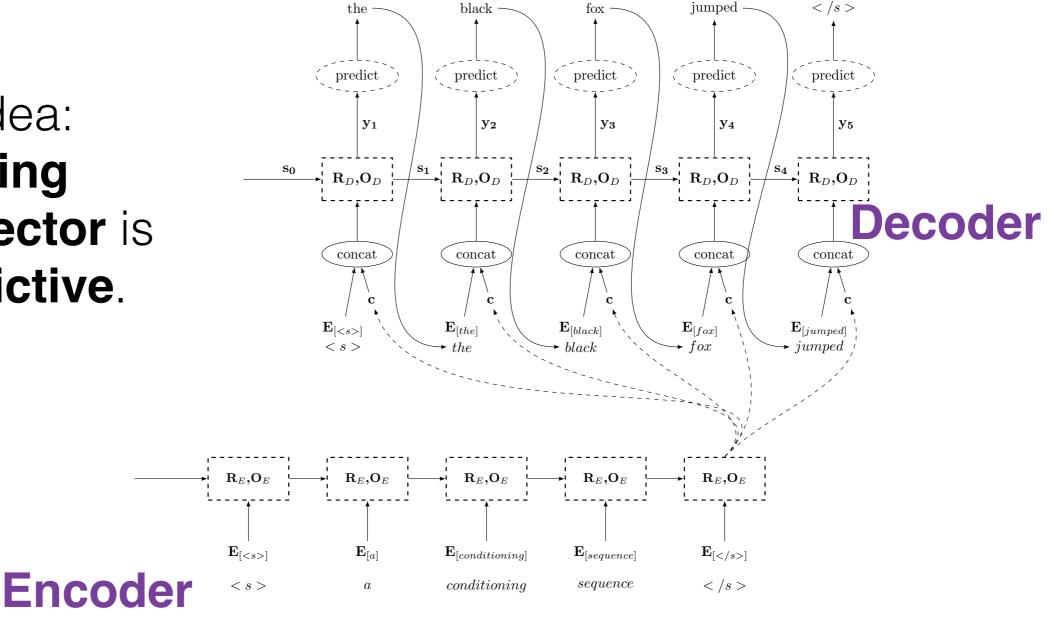
NEURAL MACHINE TRANSLATION BY JOINTLY LEARNING TO ALIGN AND TRANSLATE

**Dzmitry Bahdanau** Jacobs University Bremen, Germany

KyungHyun Cho Yoshua Bengio\* Université de Montréal **Effective Approaches to Attention-based Neural Machine Translation** 

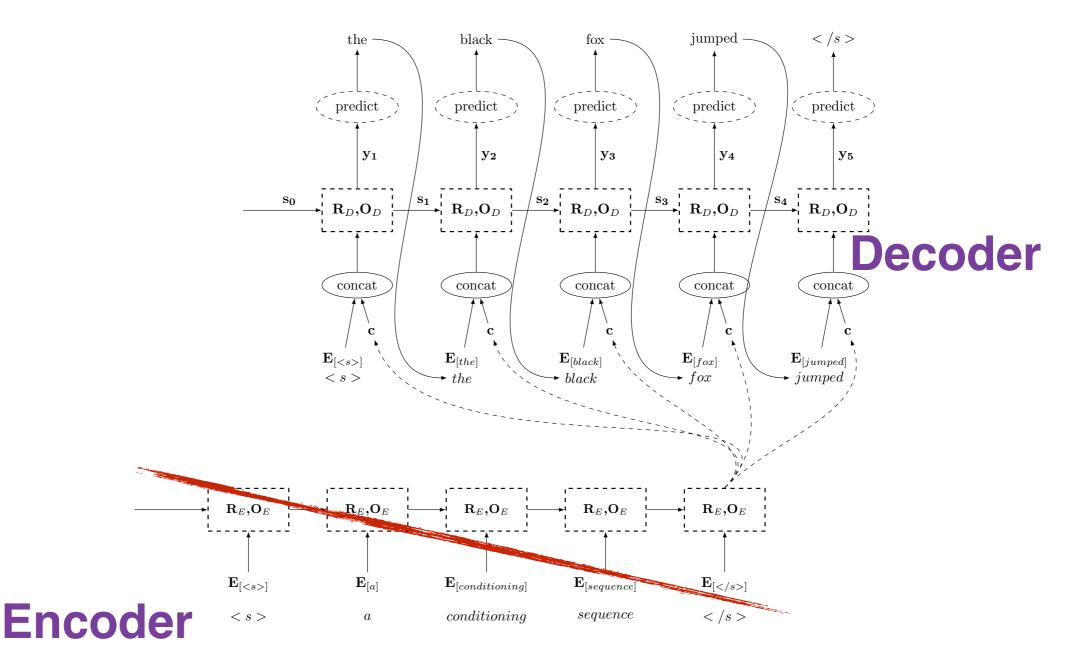
Minh-Thang Luong Hieu Pham Christopher D. Manning Computer Science Department, Stanford University, Stanford, CA 94305 {lmthang, hyhieu, manning}@stanford.edu

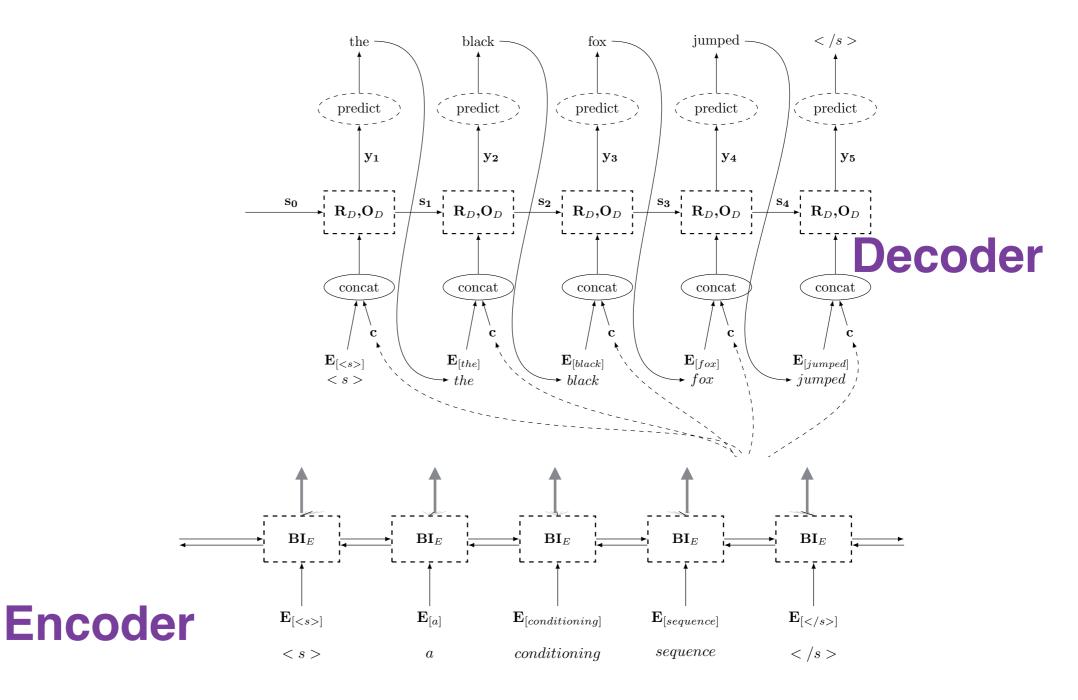
main idea: encoding a single vector is too restrictive.

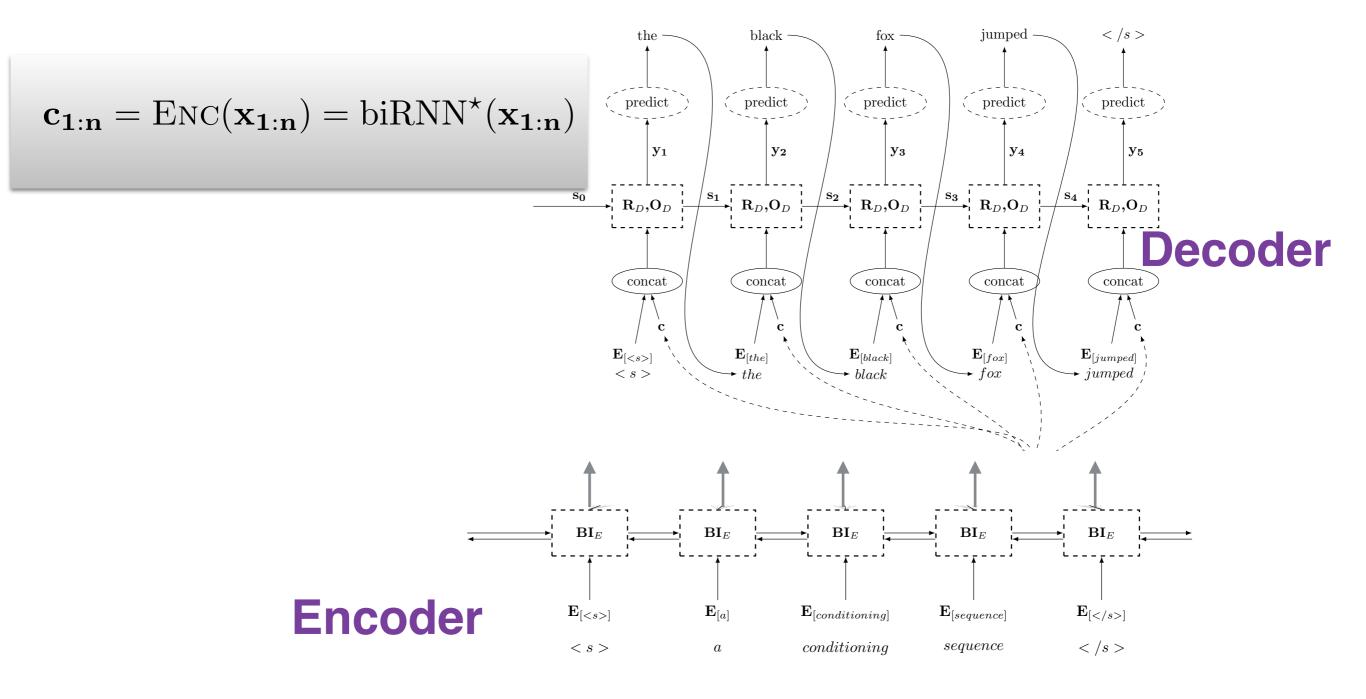


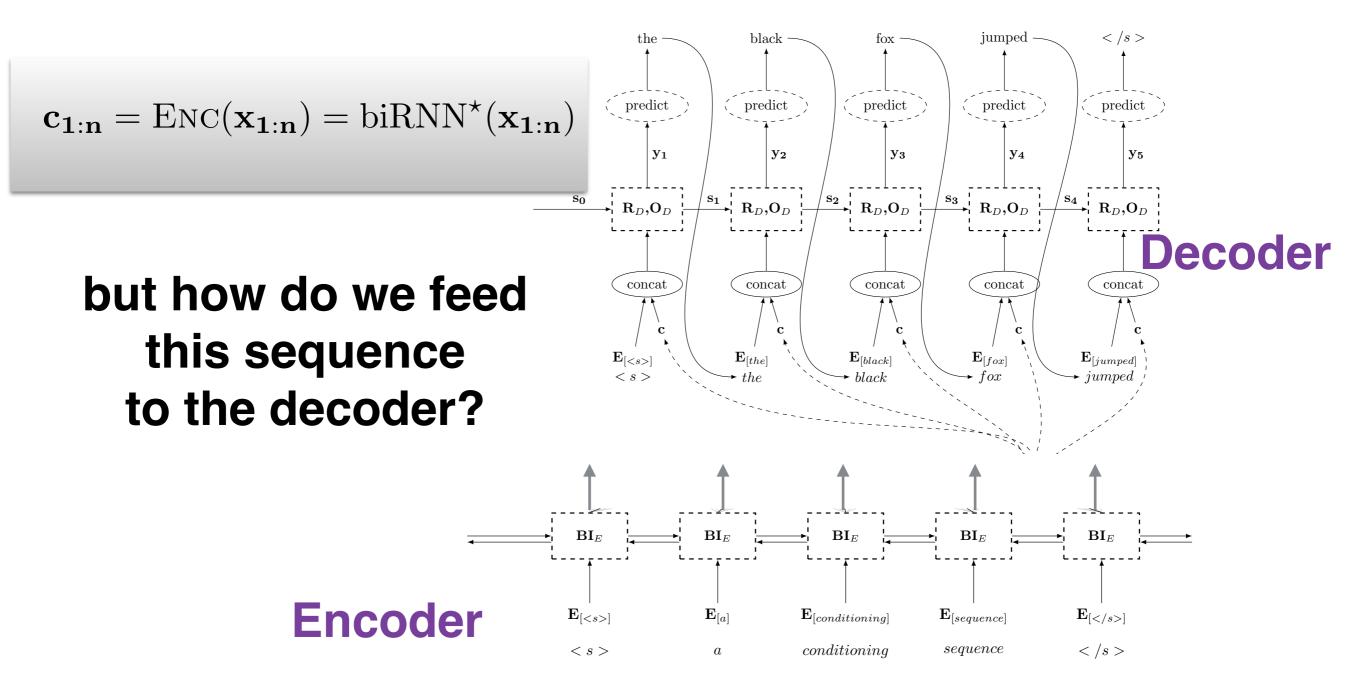
### Attention

 Instead of the encoder producing a single vector for the sentence, it will produce a one vector for each word.

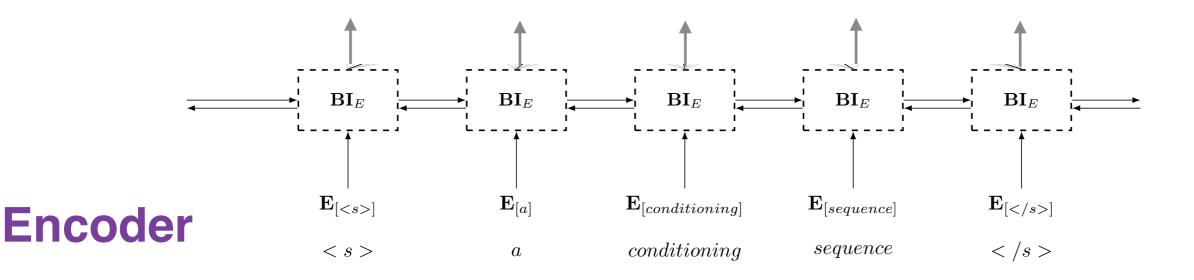






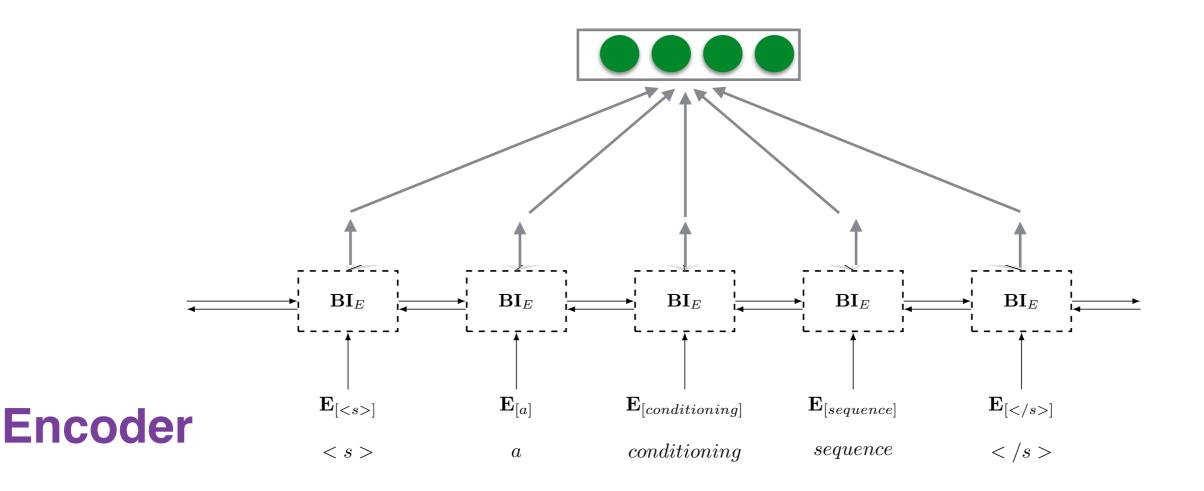


we can combine the different outputs into a single vector



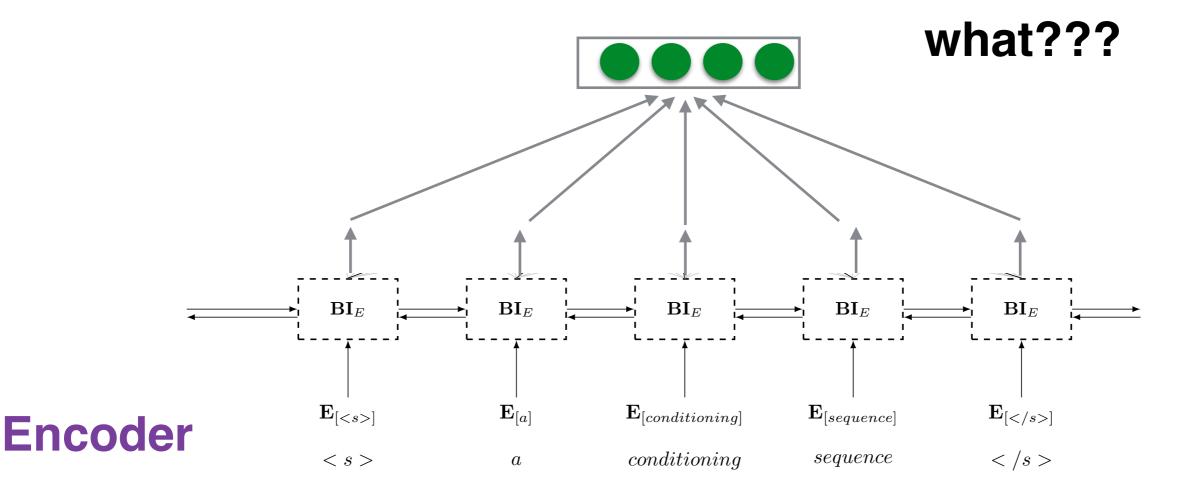
# Sequence to Sequence conditioned generation

we can combine the different outputs into a single vector



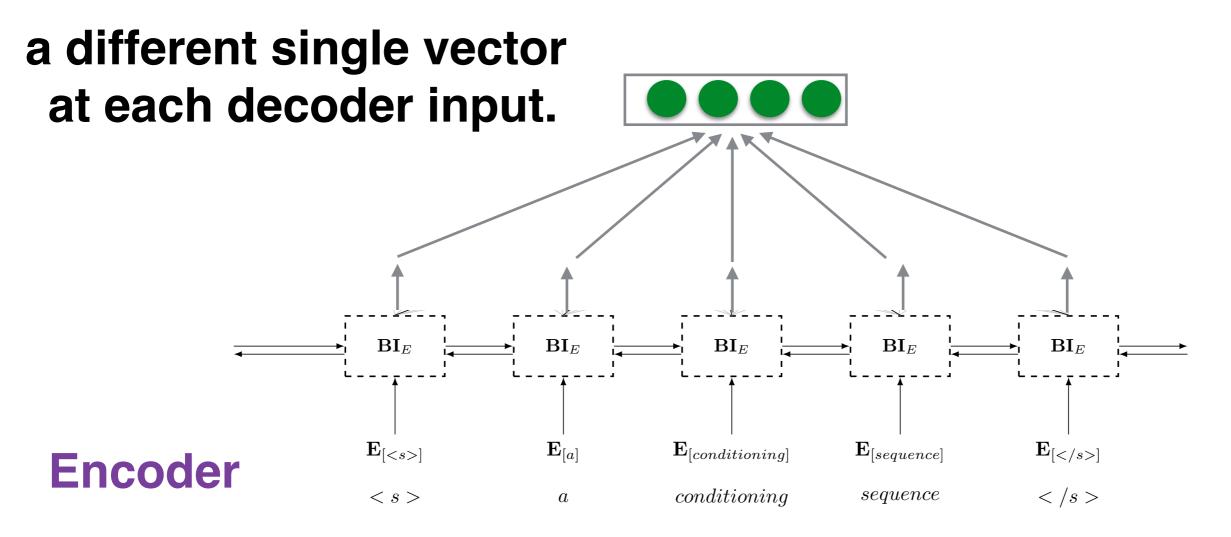
# Sequence to Sequence conditioned generation

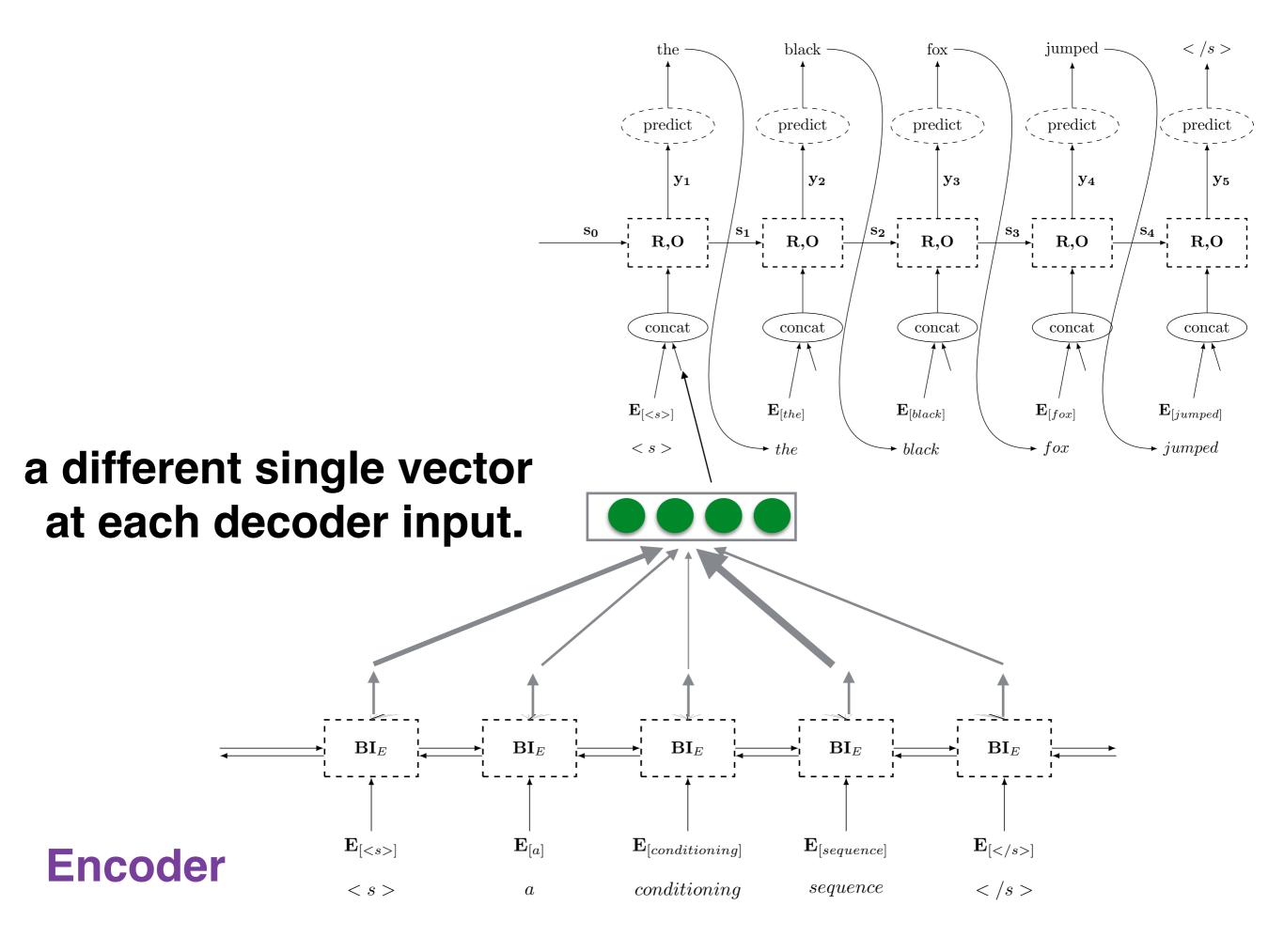
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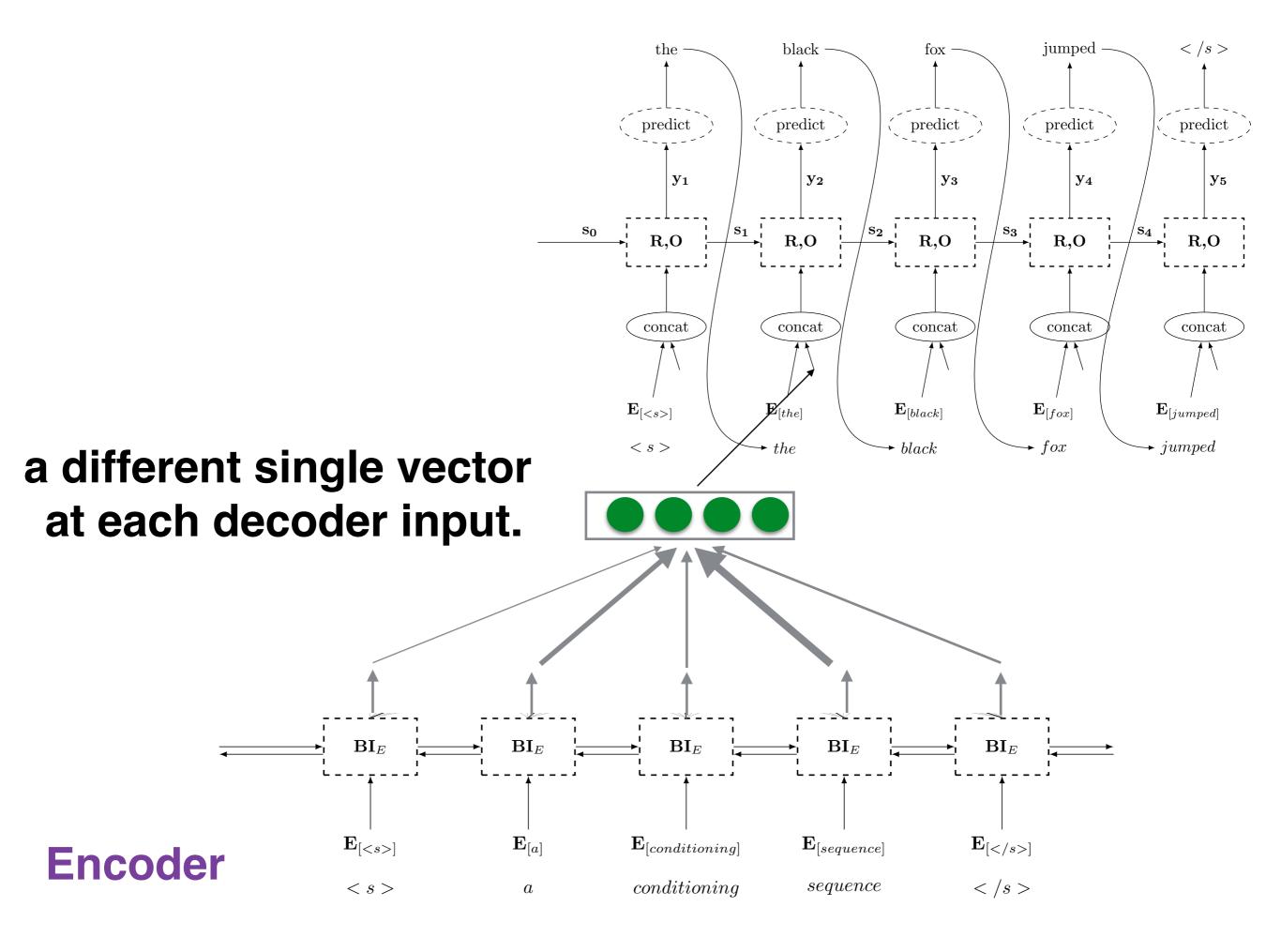


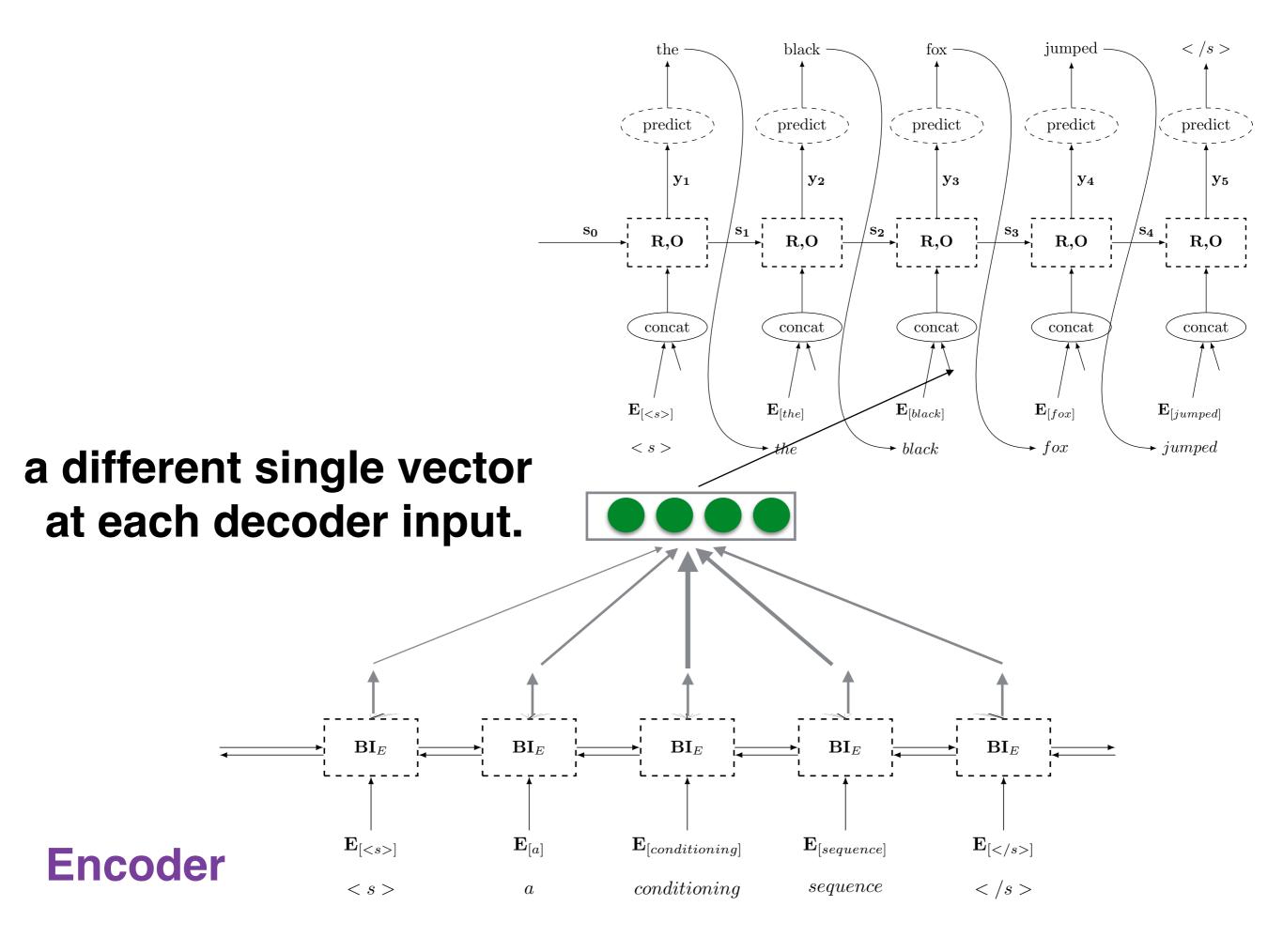
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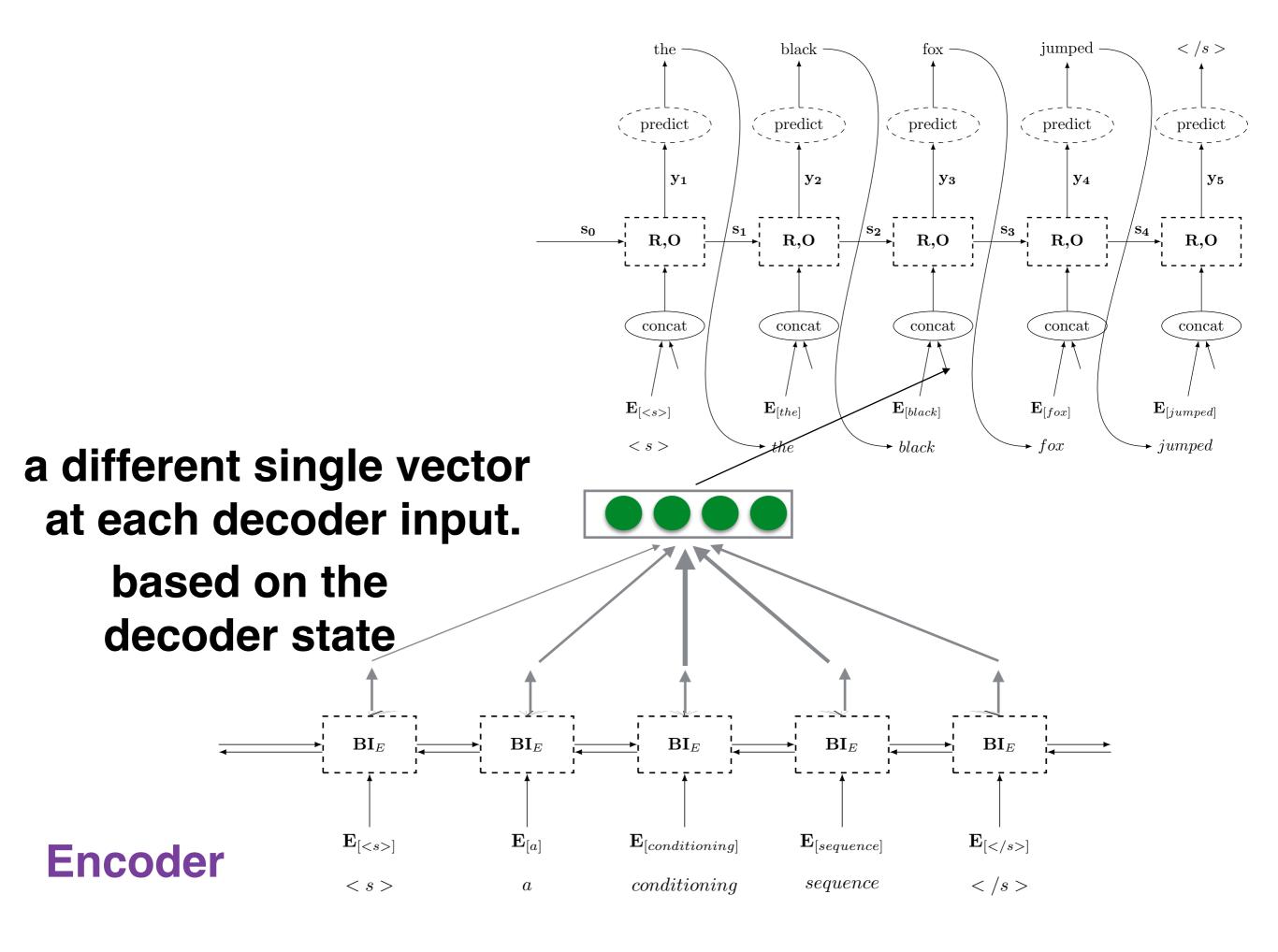
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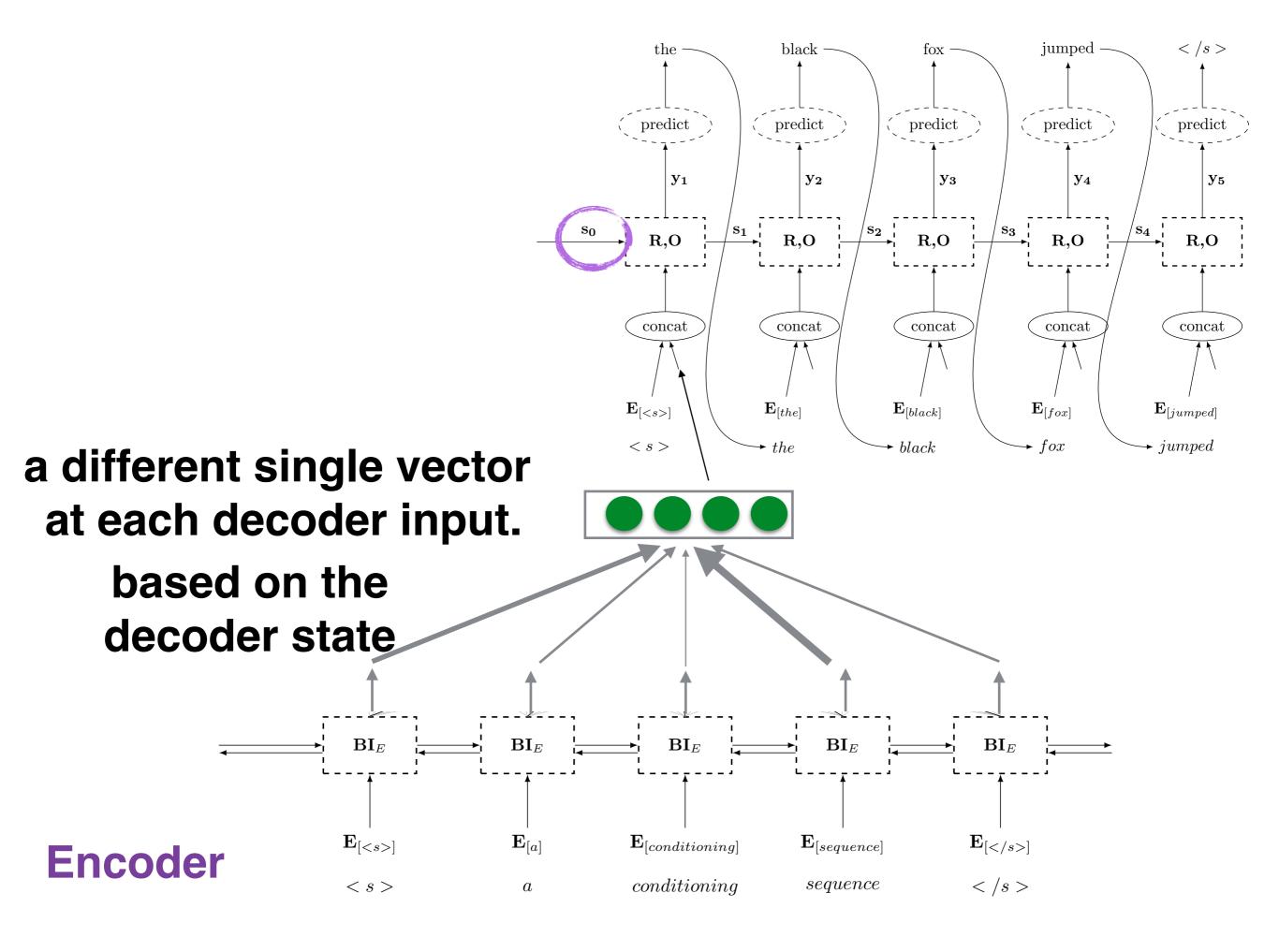


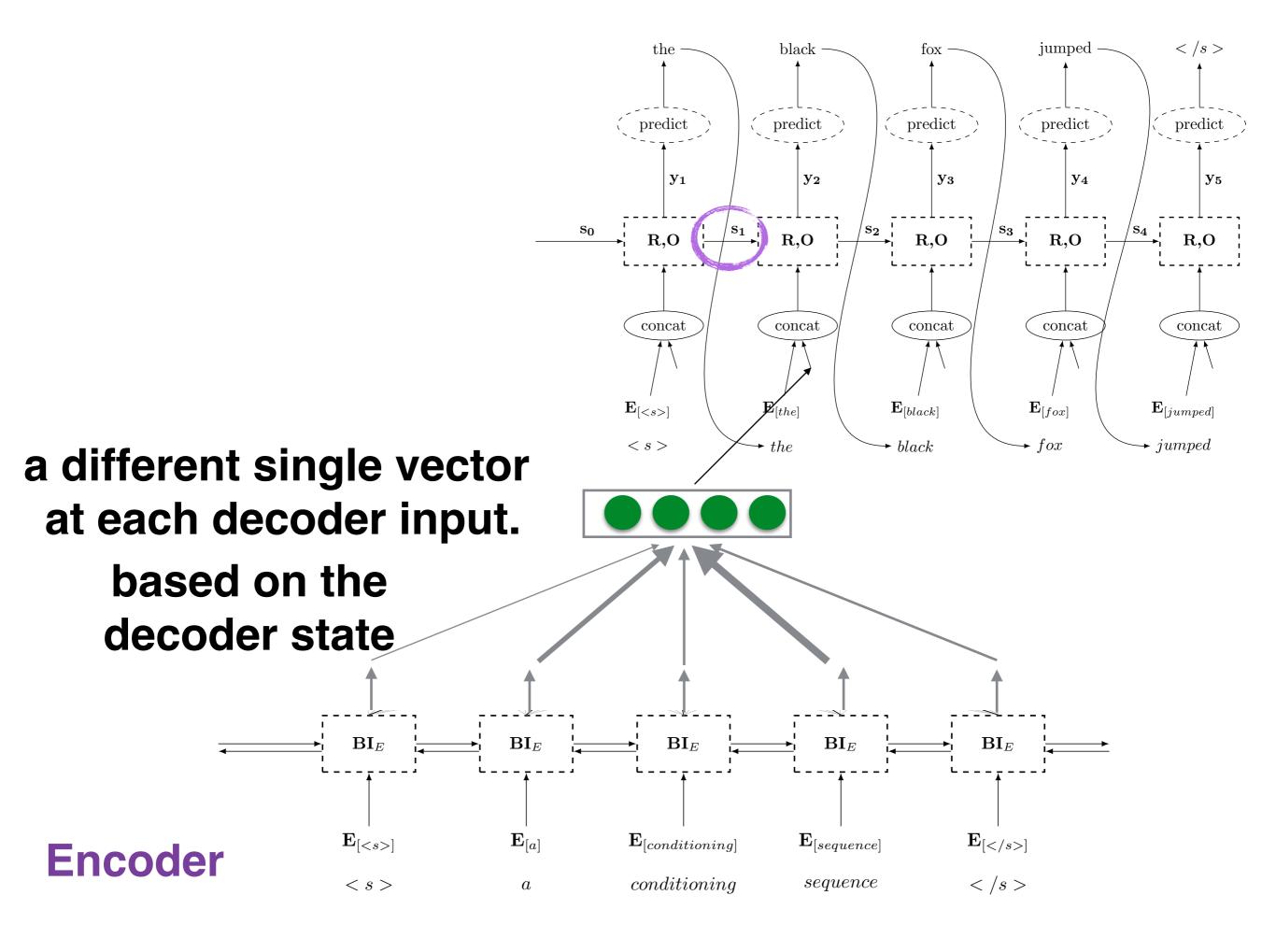


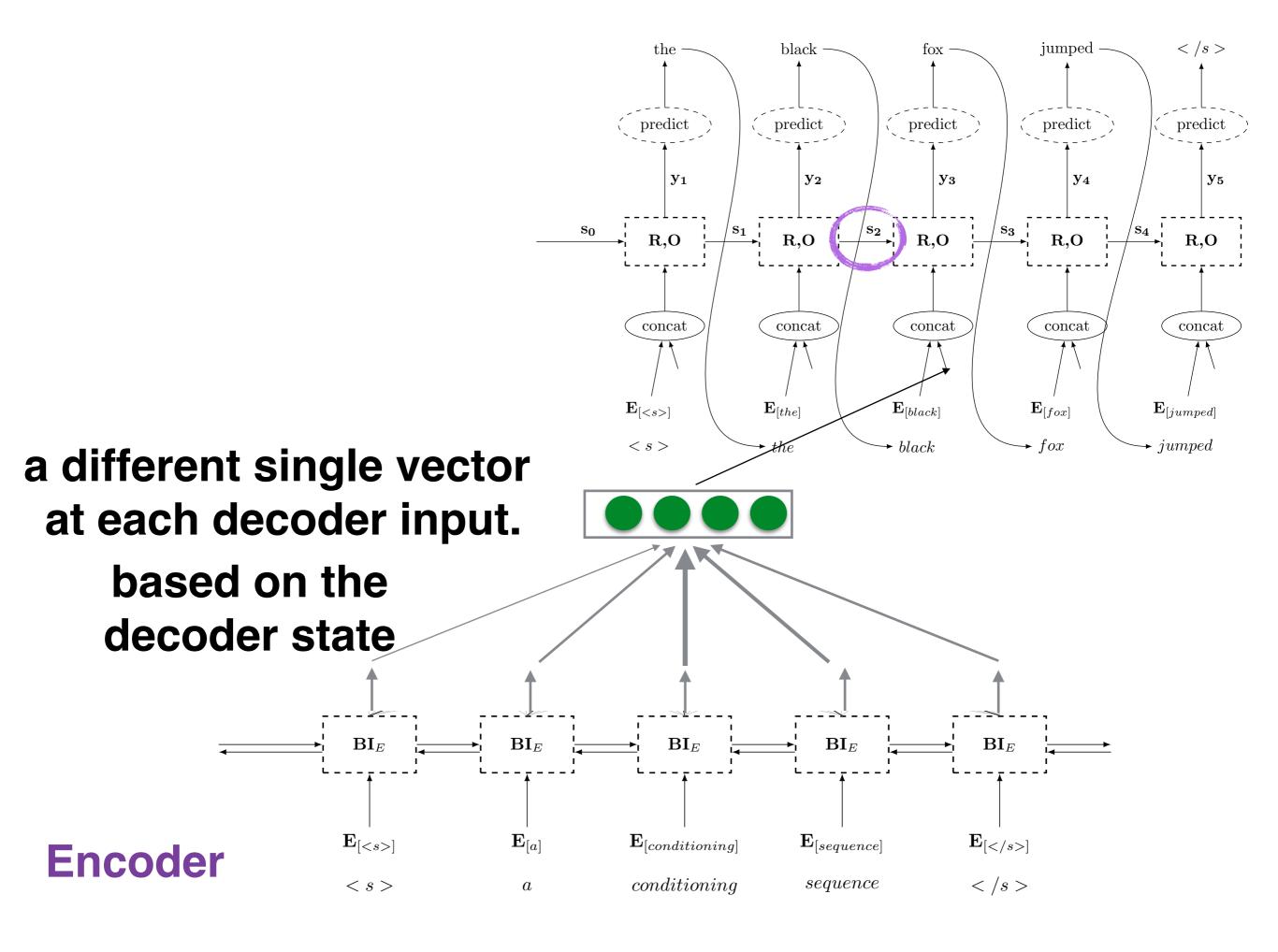












$$p(t_{j+1} = k \mid \hat{t}_{1:j}, \mathbf{x_{1:n}}) = f(O(\mathbf{s_{j+1}}))$$
  

$$\mathbf{s_{j+1}} = R(\mathbf{s_j}, [\mathbf{\hat{t}_j}; \mathbf{c^j}])$$
  

$$\mathbf{c^j} = \operatorname{attend}(\mathbf{c_{1:n}}, \hat{t}_{1:j})$$
  

$$\hat{t}_j \sim p(t_j \mid \hat{t}_{1:j-1}, \mathbf{x_{1:n}})$$

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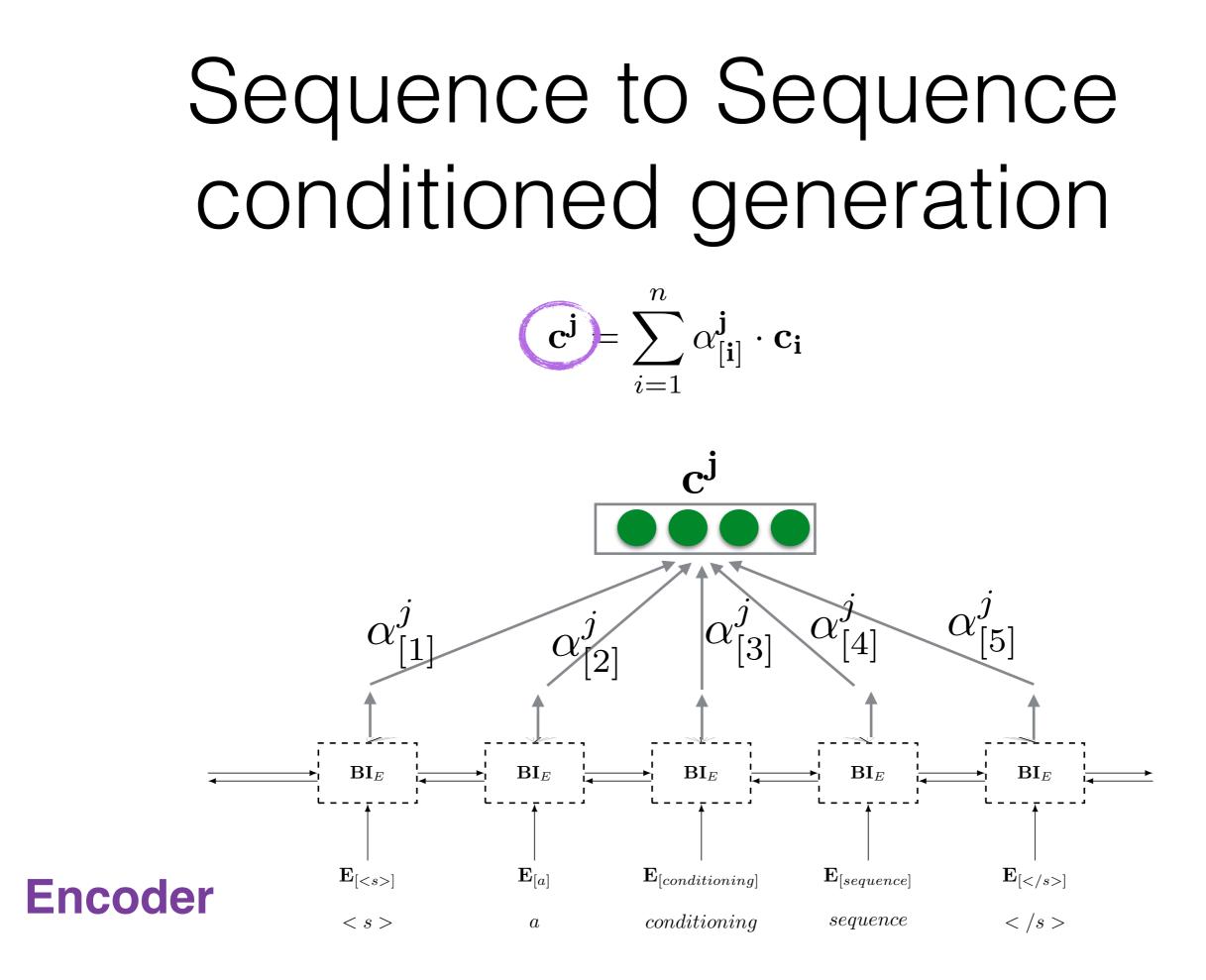
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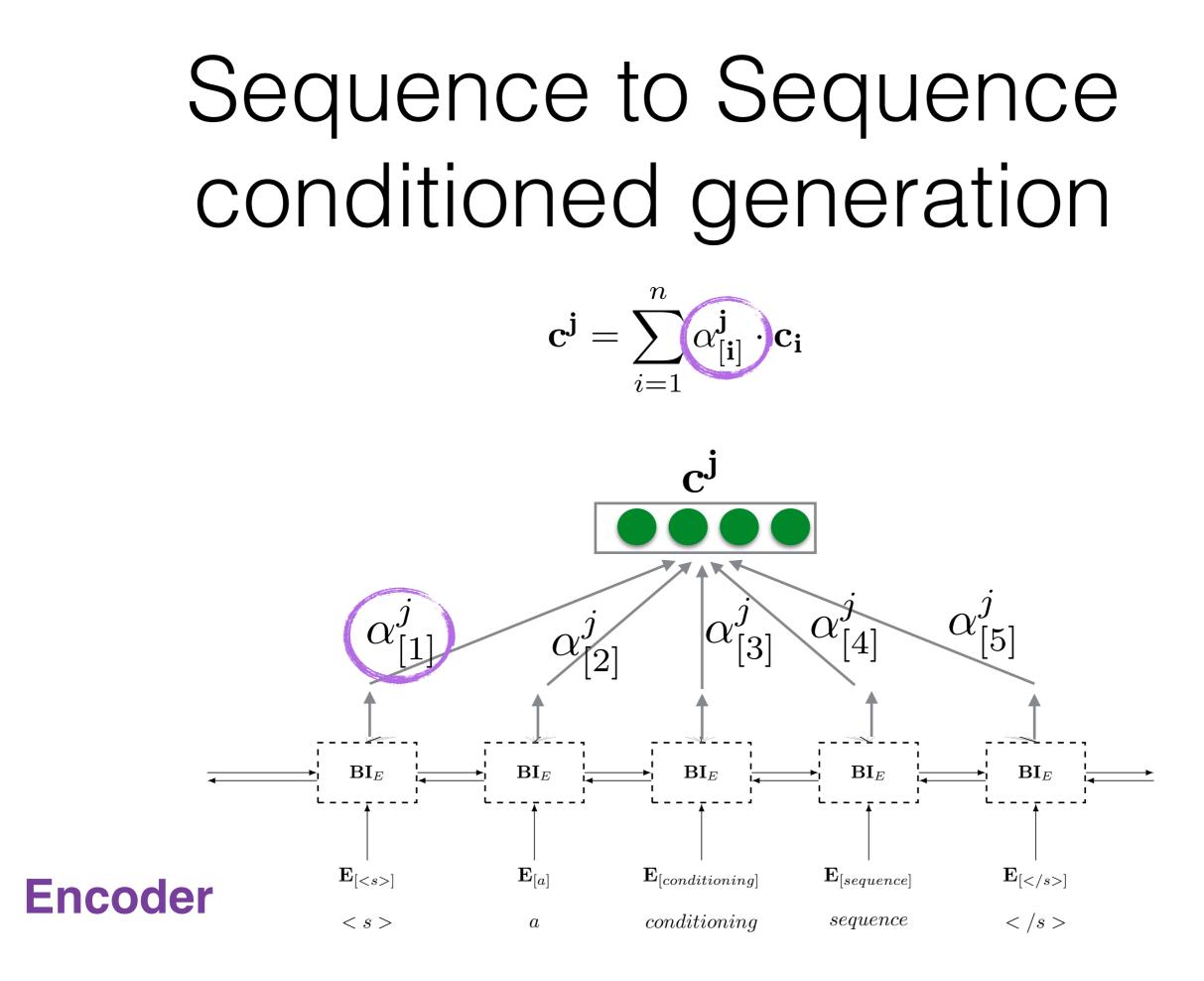
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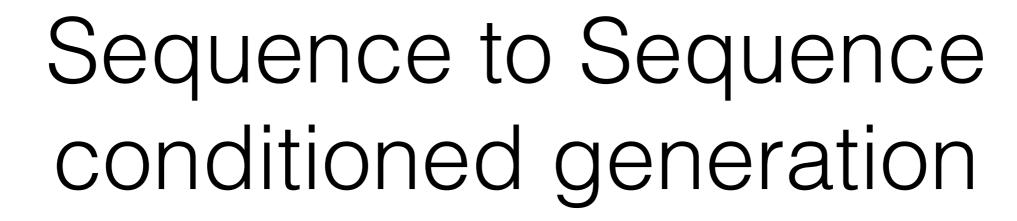
$$\mathbf{c}^j = \operatorname{attend}(\mathbf{c}_{1:n}, \hat{t}_{1:j})$$
  

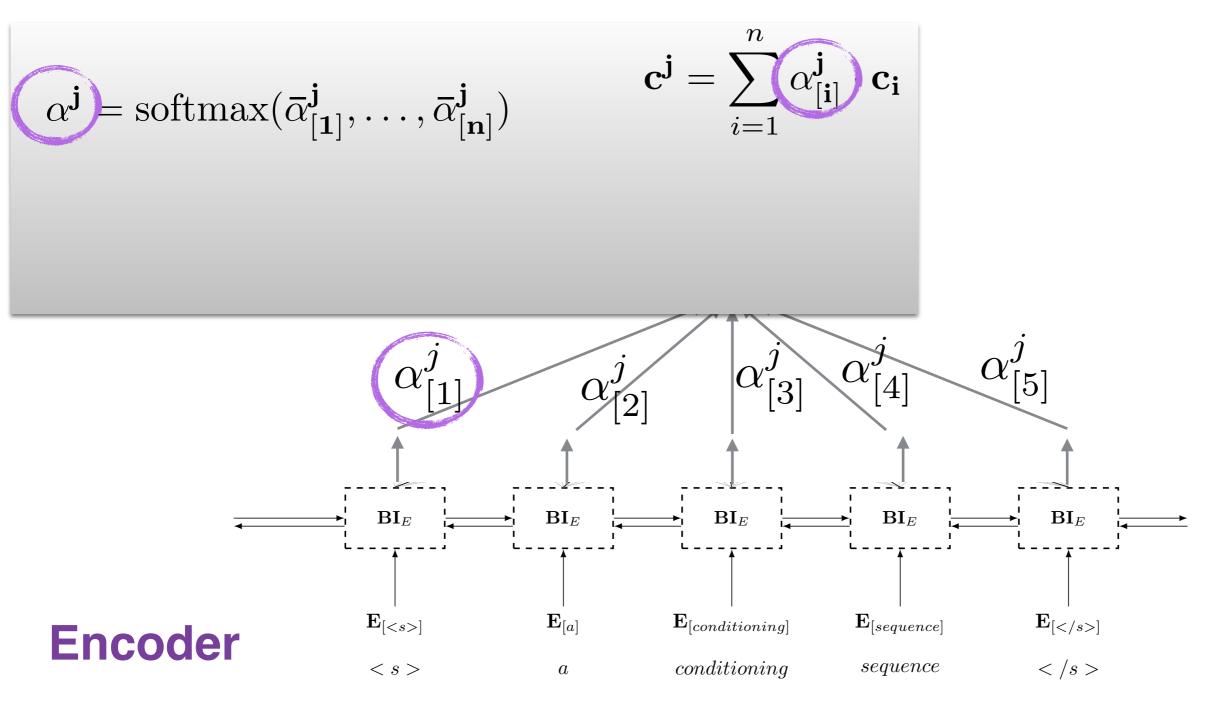
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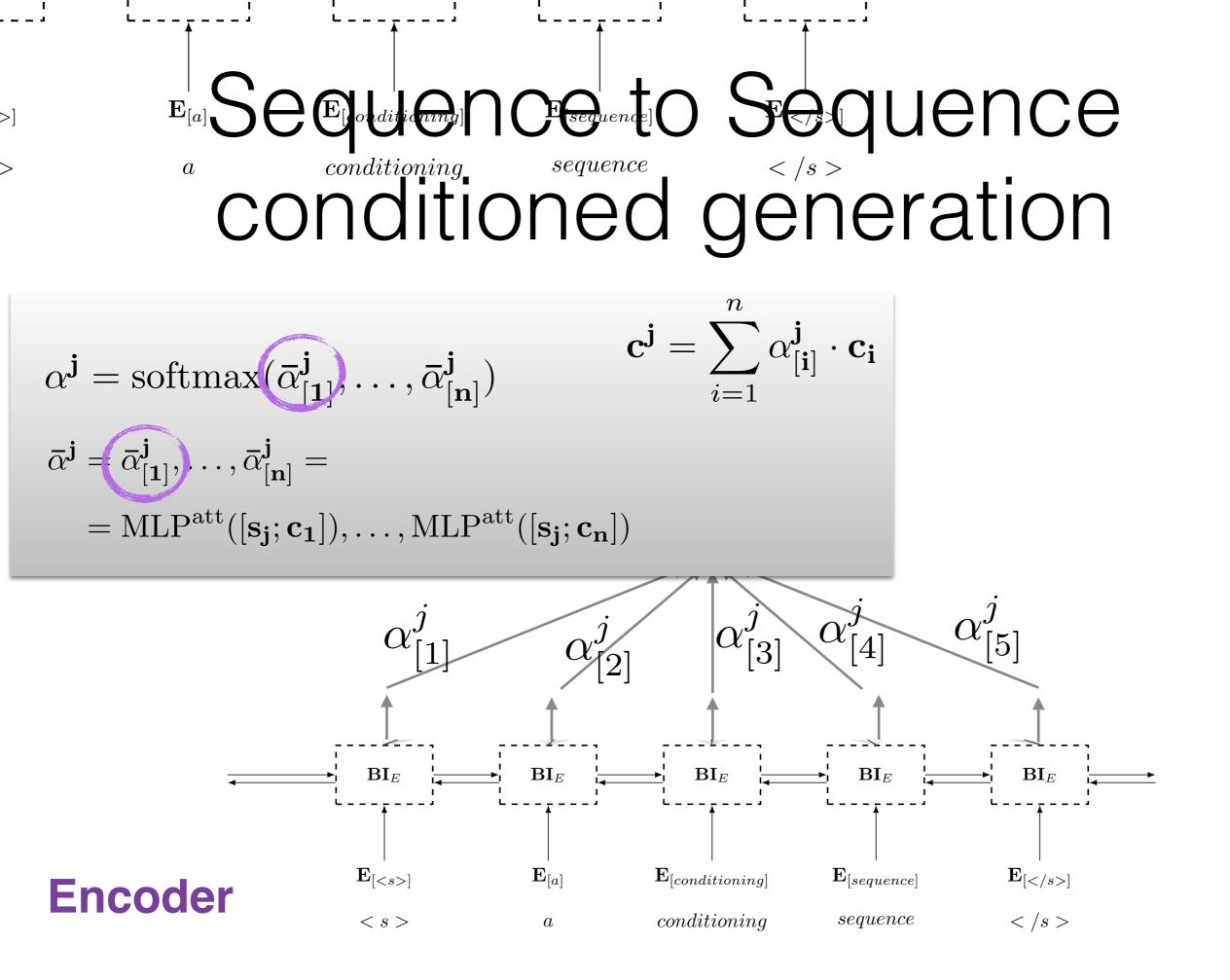
$$\mathbf{c}^j = \sum_{i=1}^n \alpha_{[i]}^j \cdot \mathbf{c}_i$$

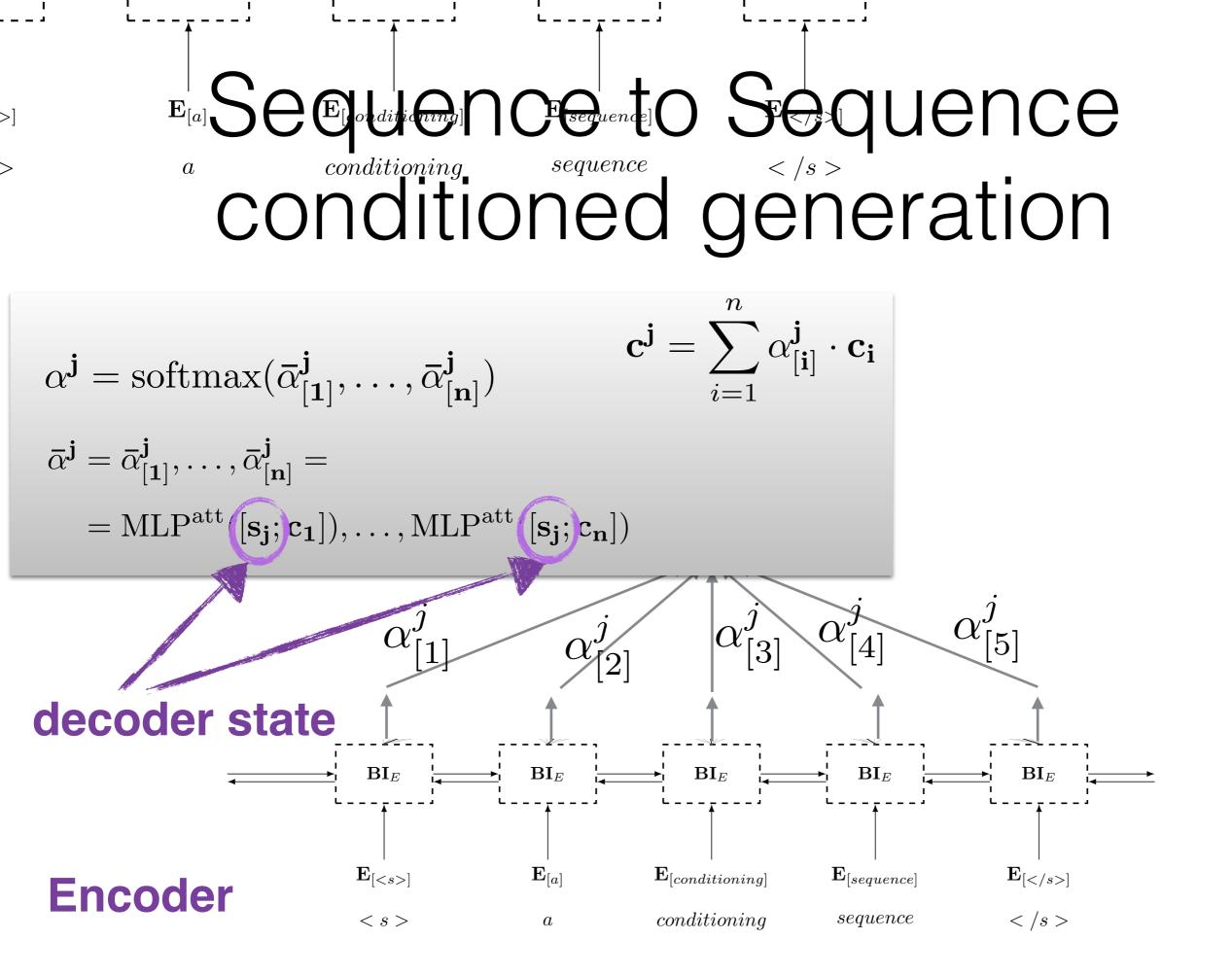












$$p(t_{j+1} = k \mid \hat{t}_{1:j}, \mathbf{x_{1:n}}) = f(O_{dec}(\mathbf{s_{j+1}}))$$
  

$$\mathbf{s_{j+1}} = R_{dec}(\mathbf{s_j}, [\hat{\mathbf{t}_j}; \mathbf{c^j}])$$
  

$$\mathbf{c^j} = \sum_{i=1}^n \alpha_{[i]}^j \cdot \mathbf{c_i}$$
  

$$\mathbf{c_{1:n}} = \operatorname{biRNN_{enc}^{\star}(\mathbf{x_{1:n}})}$$
  

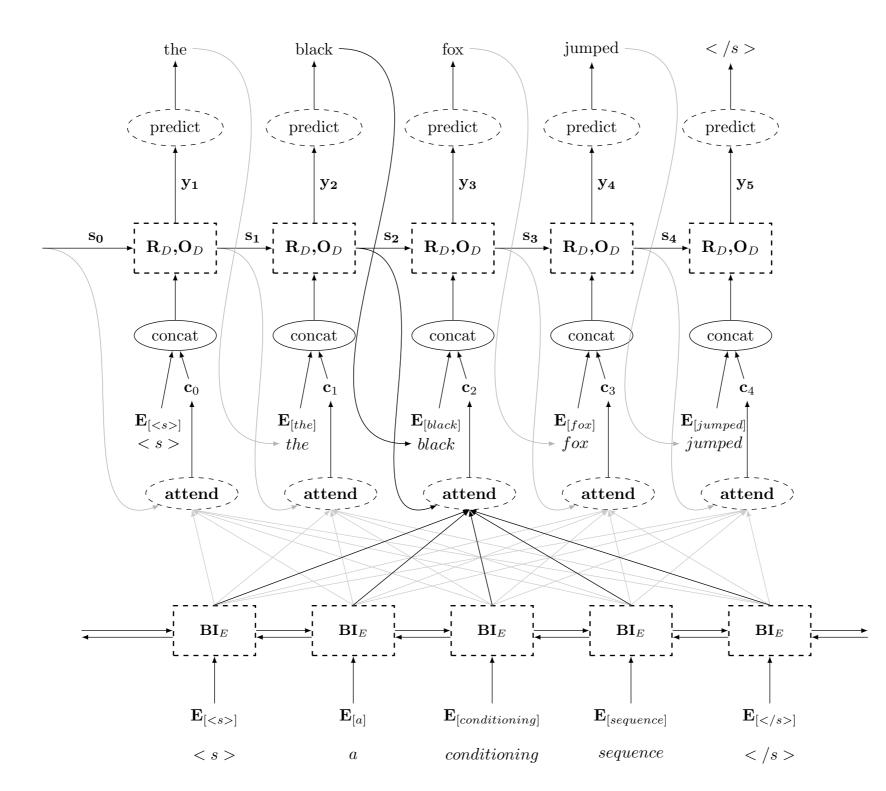
$$\alpha^j = \operatorname{softmax}(\overline{\alpha}_{[1]}^j, \dots, \overline{\alpha}_{[n]}^j)$$
  

$$\overline{\alpha}_{[i]}^j = \operatorname{MLP^{att}}([\mathbf{s_j}; \mathbf{c_i}])$$
  

$$\hat{t}_j \sim p(t_j \mid \hat{t}_{1:j-1}, \mathbf{x_{1:n}})$$
  

$$f(\mathbf{z}) = \operatorname{softmax}(\operatorname{MLP^{out}}(\mathbf{z}))$$

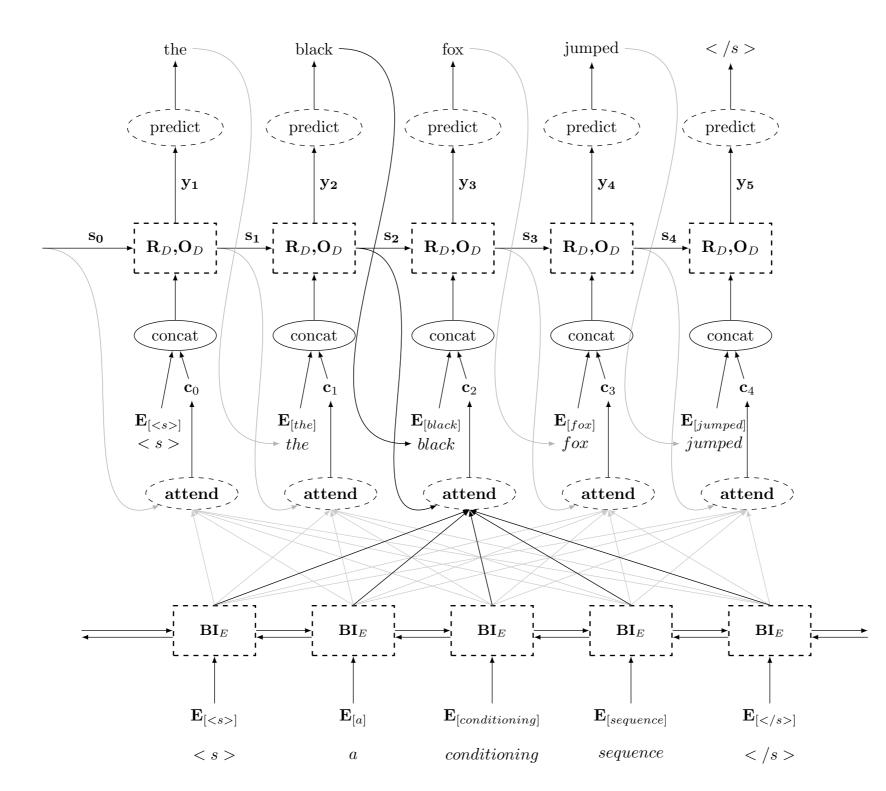
$$MLP^{att}([\mathbf{s_j}; \mathbf{c_i}]) = \mathbf{v} \tanh([\mathbf{s_j}; \mathbf{c_i}]\mathbf{U} + \mathbf{b})$$



- Encoder encodes a sequence of vectors, c1,...,Cn
- At each decoding stage, an MLP assigns a relevance score to each Encoder vector.
- The relevance score is based on  $c_i$  and the state  $s_j$
- Weighted-sum (based on relevance) is used to produce the conditioning context for decoder step j.

- Decoder "pays attention" to different parts of the encoded sequence at each stage.
- The attention mechanism is "soft" -- it is a mixture of encoder states.

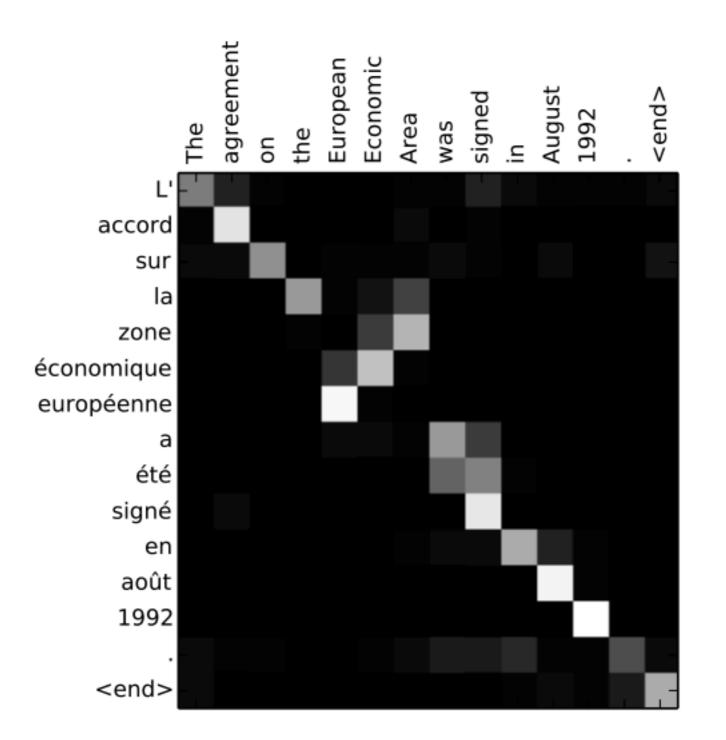
- The encoder acts as a read-only memory for the decoder.
- The decoder chooses what to read at each stage.



- Attention is very effective for sequence-tosequence tasks.
- Current state-of-the-art systems all use attention. (this is basically how Machine Translation works)

• Attention also makes models somewhat more interpretable.

(we can see where the model is "looking" at each stage of the prediction process)



ih the evening until 21 00, there was a further 5mm rain on the town, after 6, a 6 mm, which had already dropped to Sunday during the night

am Abend bis 21 Uhr fielen weitere 5mm Regen auf die Stadt, nach 6,@@ 6@@ mm, die bereits in der Nacht zum Sonntag nieder@@ gegangen waren

since then , the island authorities have tribed to put an end to the illegal behaviour of non-le@ alcoholic tourists in Mag@@ alu@@ t by minimizing the number of participants in the notorious alcohol@@ -free bar !

die Insel@@ behÄJrden haben seither versucht, das ordnungs@@ widrige Verhalten alkohol@@ isierter Urlauber in Mag@@ alu@@ f zu stoppen, indem die Anzahl der Teilnehmer an den berļchtigten alkohol@@ get@@ rĤnkten Knei@@ pent@@ ouren minimiert wurde

## Complexity

- Encoder decoder:
- Encoder-decoder with attention:

## Complexity

- Encoder decoder: O(n + m)
- Encoder-decoder with attention: O(n x m)

## Complexity

- Encoder decoder: O(n + m)
- Encoder-decoder with attention: O(n x m)

Where/how can you parallelize? in train time? in test time?

# Beyond Seq2Seq

- Can think of a general design pattern in neural nets:
  - Input: sequence, query
    - Encode the input into a sequence of vectors
    - Attend to the encoded vectors, based on query (weighted sum, determined by query)
    - Predict based on the attended vector

## Attention More Abstractly

- Input sequence X<sub>1</sub>,...,X<sub>n</sub>
- Query vector q
- Attention weights a [1,...,n] = softmax(score(q,x1), ..., score(q,xn))
- Result vector v = sum a<sub>i\*</sub>x<sub>i</sub>
  - = sum softmax(score( $\mathbf{q}, \mathbf{x}_1$ ), ..., score( $\mathbf{q}, \mathbf{x}_n$ ))<sub>[i]\*</sub> $\mathbf{x}_i$

### How to Attend?

v: attended vec, q: query vec

• MLP:

 $\mathbf{u}g(\mathbf{W^1v}+\mathbf{W^2q})$ 

• dot product:

• biaffine transform:

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• biaffine transform:

#### $\mathbf{v}^{ op}\mathbf{W}\mathbf{q}$

## How to Attend?

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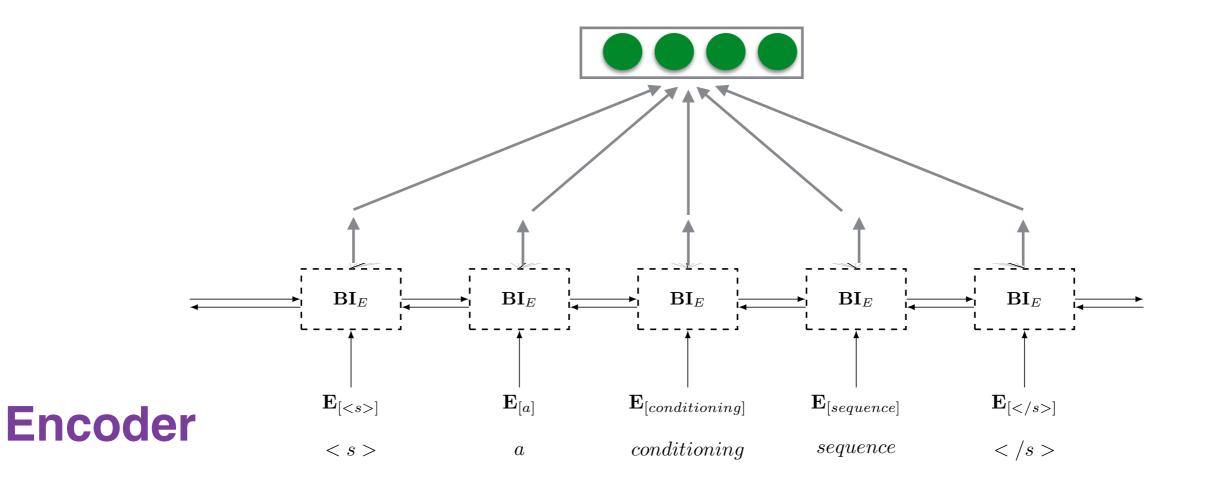
• biaffine transform:

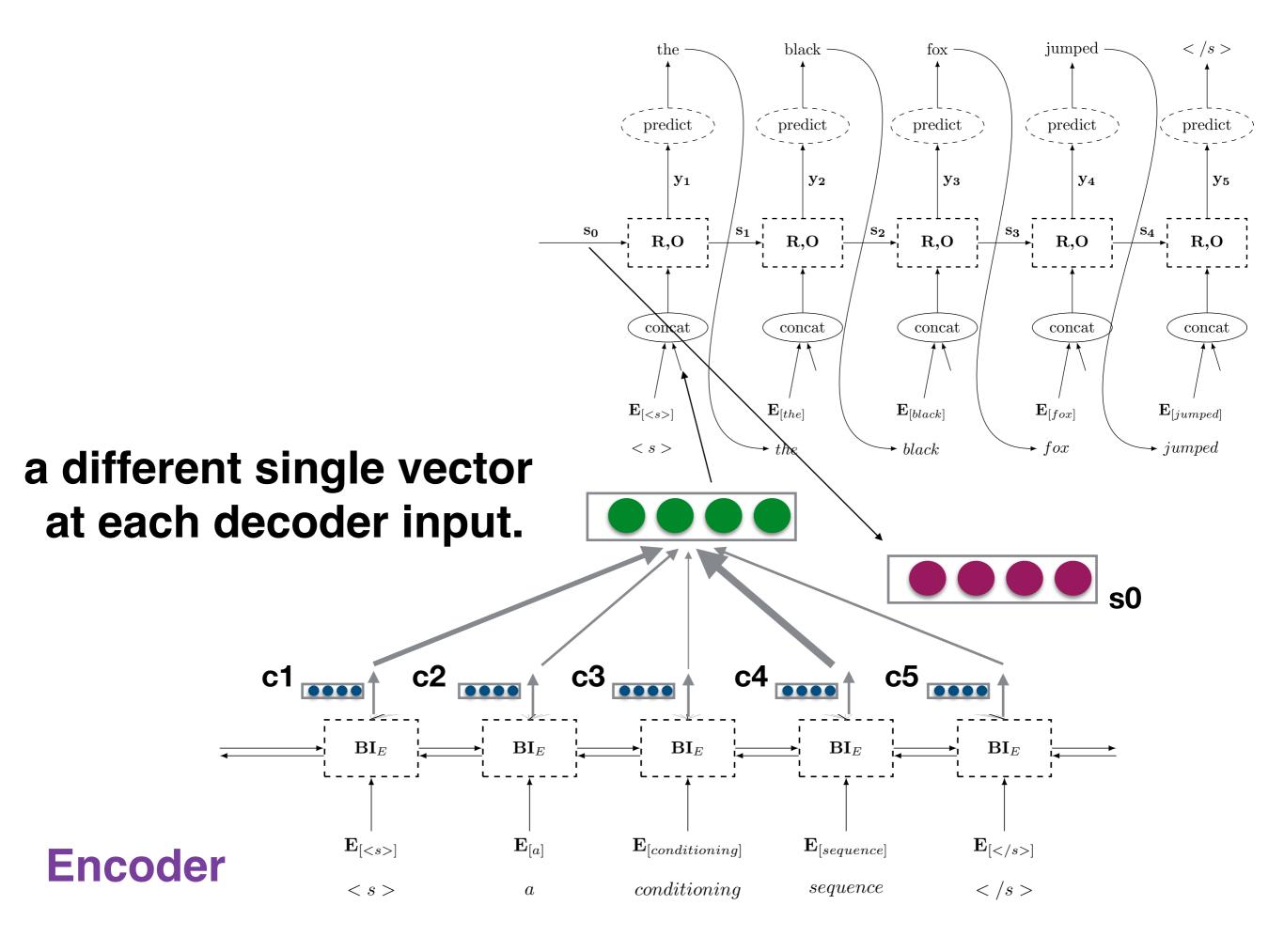
**Pros? Cons?** 

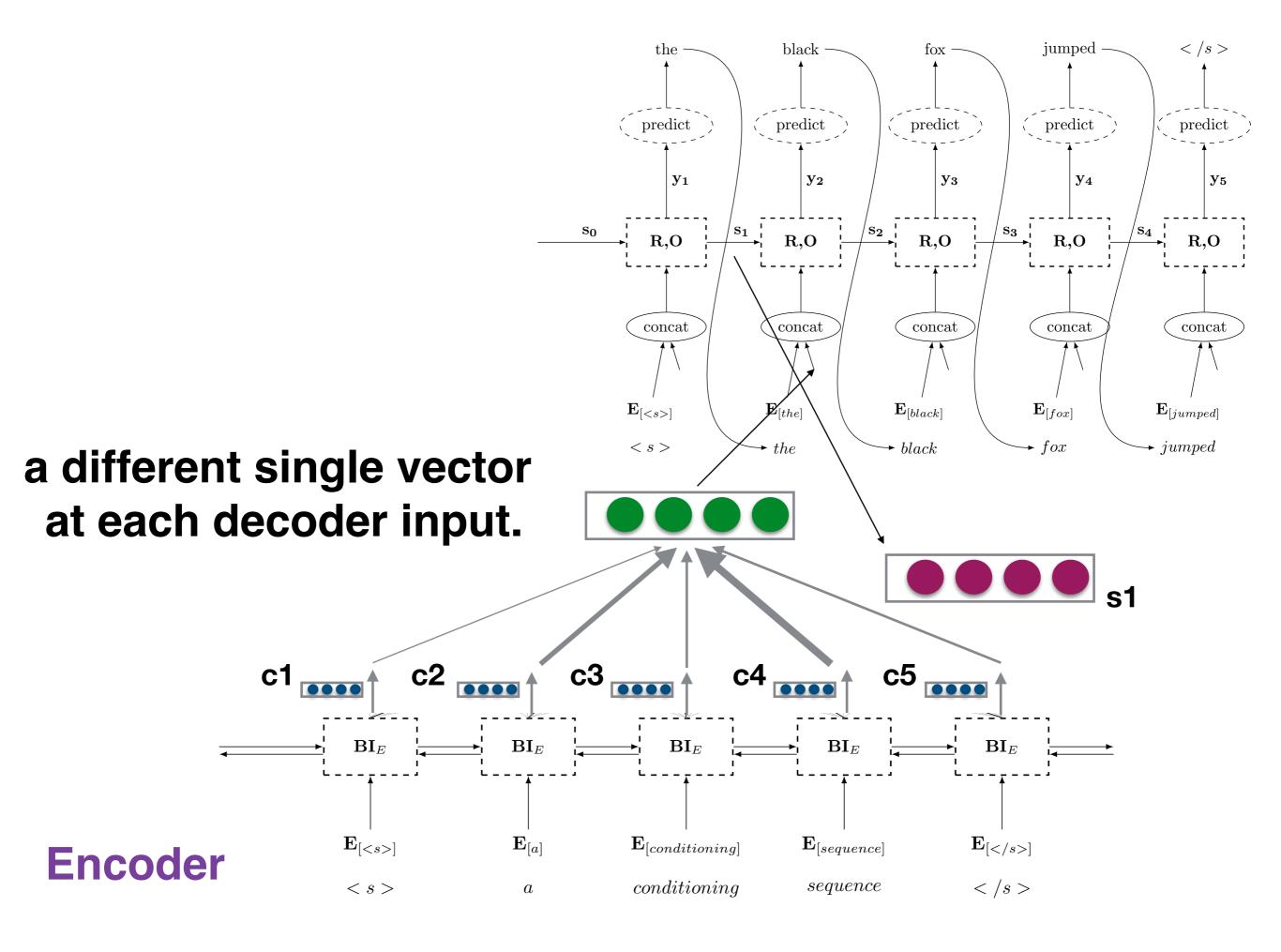
$$\mathbf{v}^ op \mathbf{W} \mathbf{q}$$

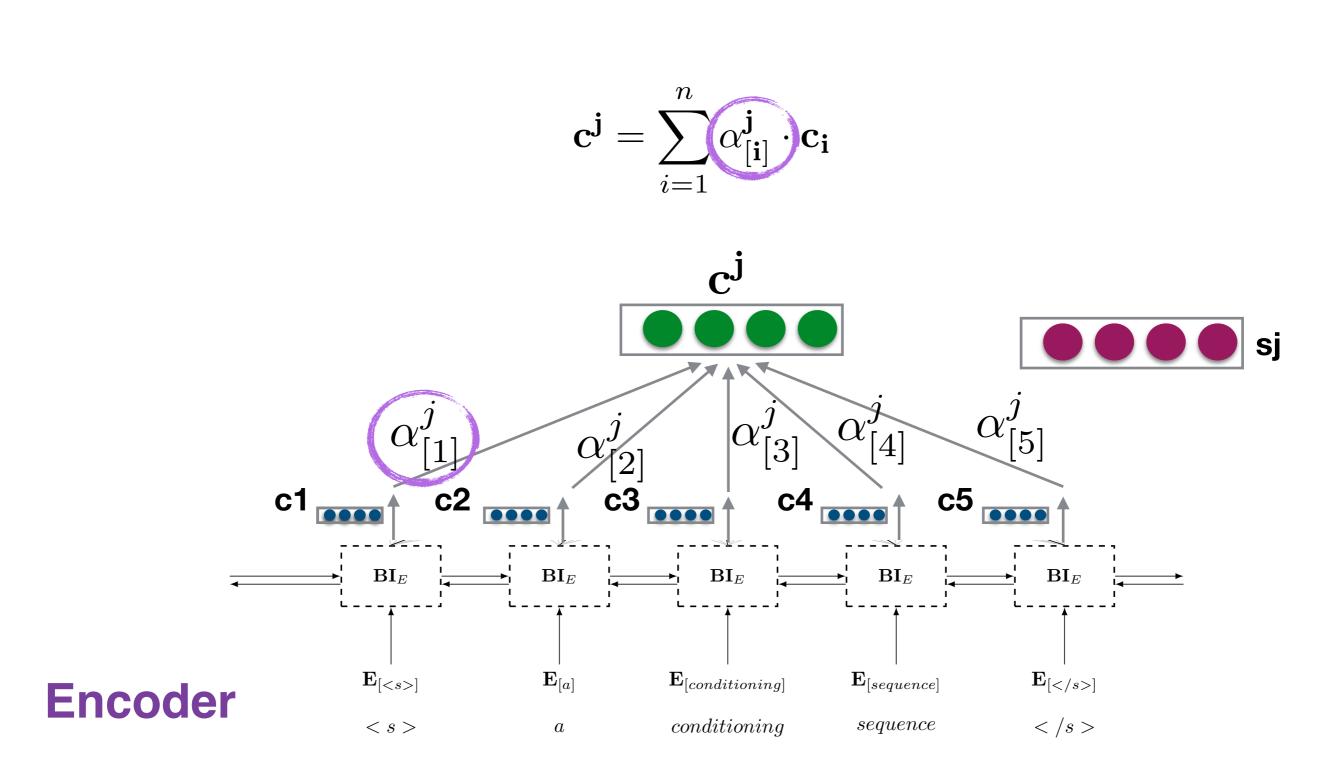
### attention: more graphically

### we can combine the different outputs into a single vector









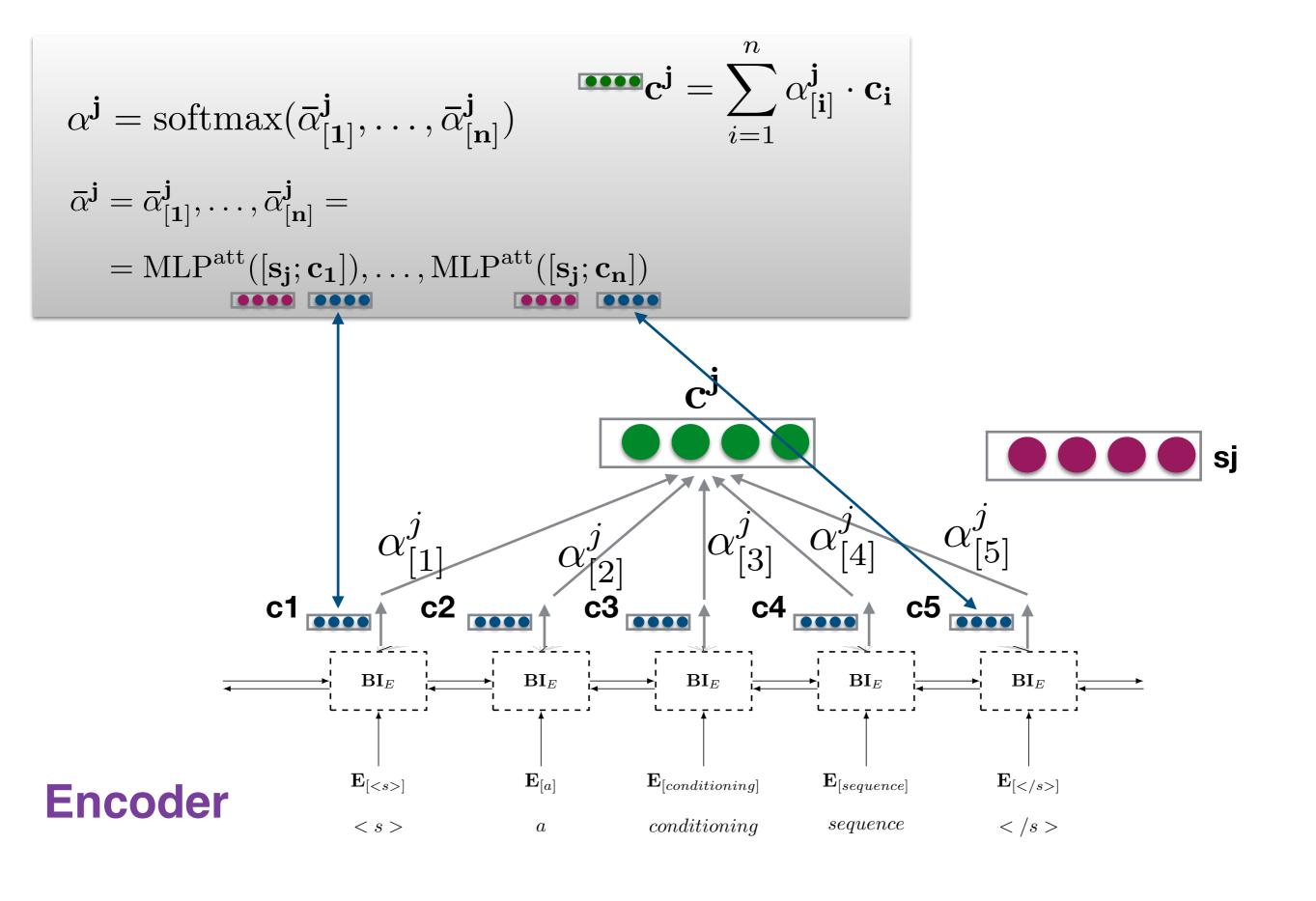


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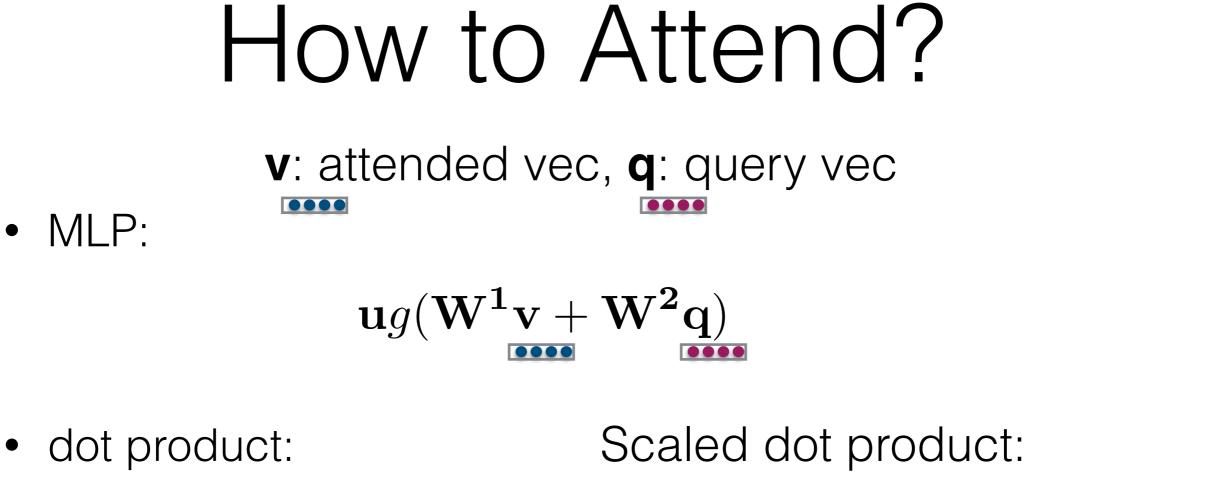
ocquence

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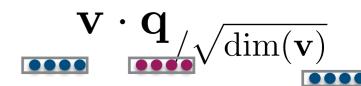
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- Input sequence X<sub>1</sub>,...,X<sub>n</sub>
- Query vector **q**
- Attention weights a [1,...,n]
   = softmax(score(q,x1), ..., score(q,xn))
- Result vector v = sum a<sub>i\*</sub>x<sub>i</sub>
  - = sum softmax(score( $\mathbf{q}, \mathbf{x}_1$ ), ..., score( $\mathbf{q}, \mathbf{x}_n$ ))<sub>[i]\*</sub> $\mathbf{x}_i$



• dot product:

 $\mathbf{v} \cdot \mathbf{q}$ 



• biaffine transform:

$$\mathbf{v}^{ op}\mathbf{W}\mathbf{q}$$

### Alternatives

- Soft vs. **Hard** attention
- Why use a biRNN encoder and not just the use word-vectors (embeddings) directly?
- What if the sequences are **mostly monotonic**?

### Attention vs. No Attention

• When would you use an Encoder-Decoder without attention?

### RNNs --> Transformers

#### **Attention Is All You Need**

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Łukasz Kaiser\* Google Brain lukaszkaiser@google.com

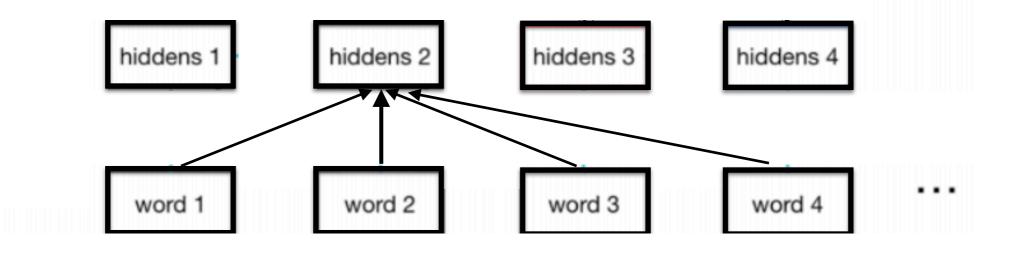
Illia Polosukhin\*<sup>‡</sup> illia.polosukhin@gmail.com

#### replace RNN with attention-based mechanism

- Main concepts to know:
  - Self-attention
  - Multi-head attention
- Also think about: why do this? what is the motivation?

#### Self attention

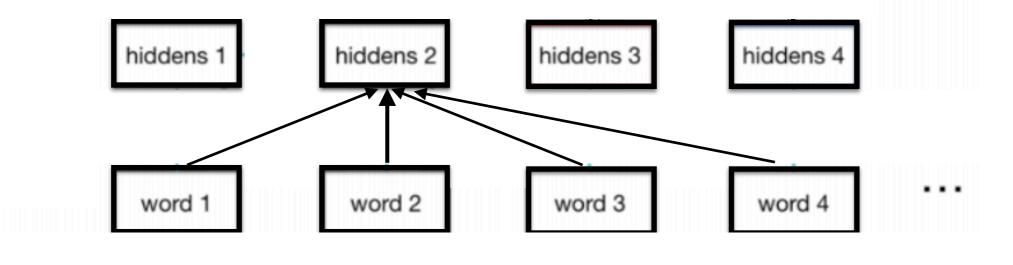
each token attends to all tokens in previous layer



#### Self attention

each token attends to all tokens in previous layer

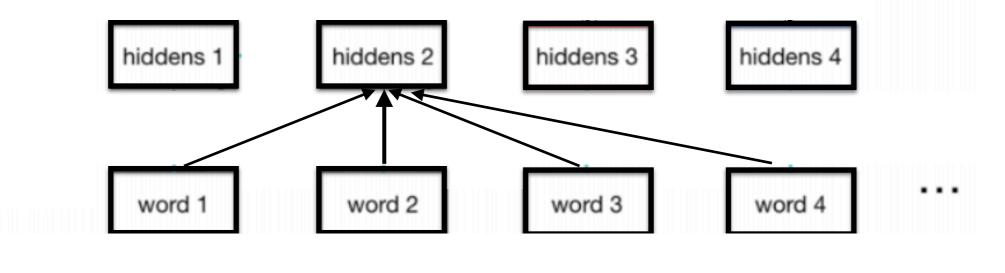
 $att_{x_i} = softmax(dot(x_i, x_1), dot(x_i, x_2), ..., dot(x_i, x_n))_{[i]}x_i$ 



#### Self attention

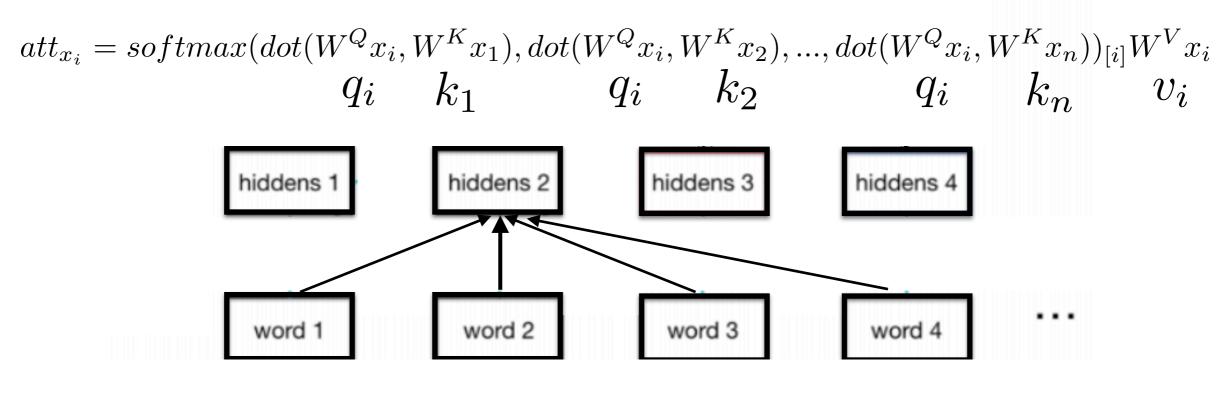
#### each token attends to all tokens in previous layer transform x into Q, K, V

 $att_{x_{i}} = softmax(dot(W^{Q}x_{i}, W^{K}x_{1}), dot(W^{Q}x_{i}, W^{K}x_{2}), ..., dot(W^{Q}x_{i}, W^{K}x_{n}))_{[i]}W^{V}x_{i}$ 

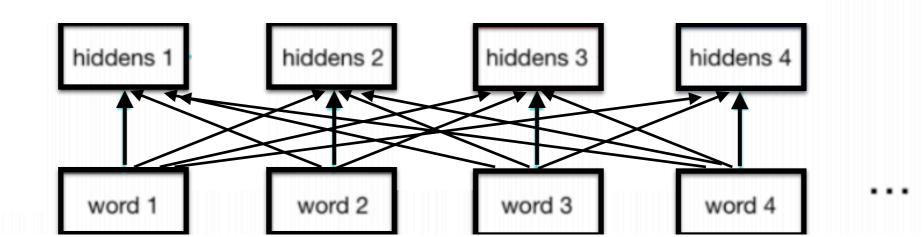


#### Self attention

each token attends to all tokens in previous layer transform x into Q, K, V



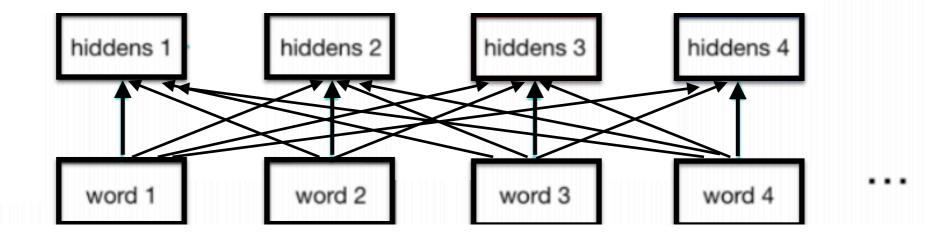
#### Self attention



#### Self attention

matrix form:

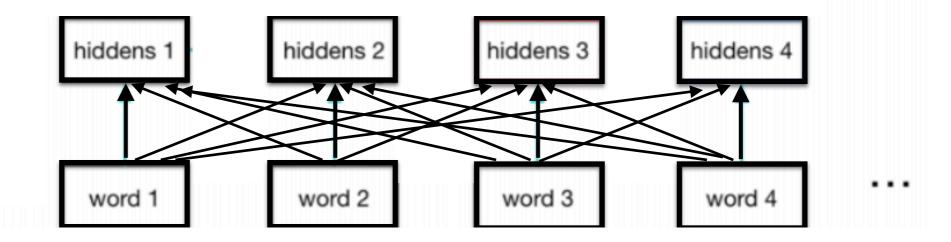
Attention $(Q, K, V) = \operatorname{softmax}(QK^T)V$ 



#### Self attention

matrix form + scaled attention:

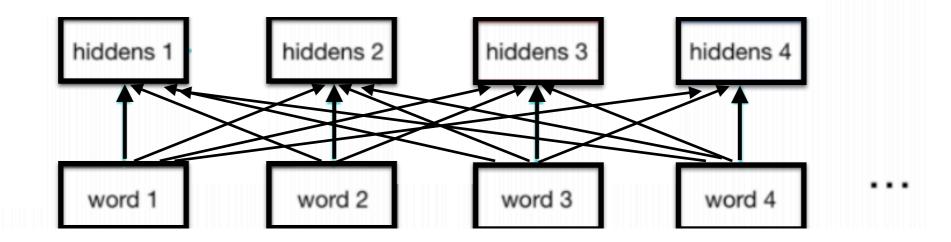
$$\operatorname{Attention}(Q, K, V) = \operatorname{softmax}(\frac{QK^T}{\sqrt{d_k}})V$$



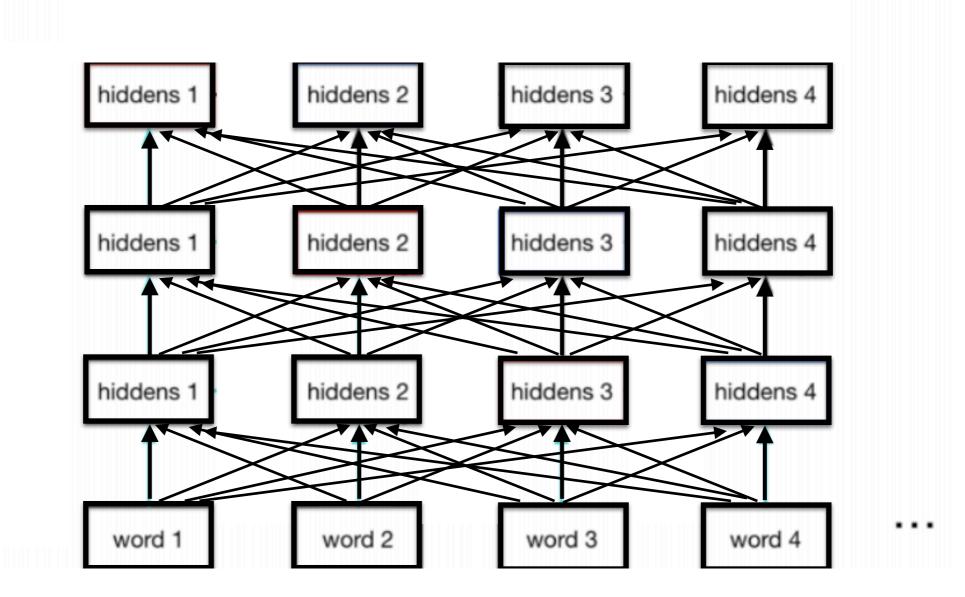
We suspect that for large values of  $d_k$ , the dot products grow large in magnitude, pushing the softmax function into regions where it has extremely small gradients <sup>4</sup>. To counteract this effect, we scale the dot products by  $\frac{1}{\sqrt{d_k}}$ .

matrix form + scaled attention:

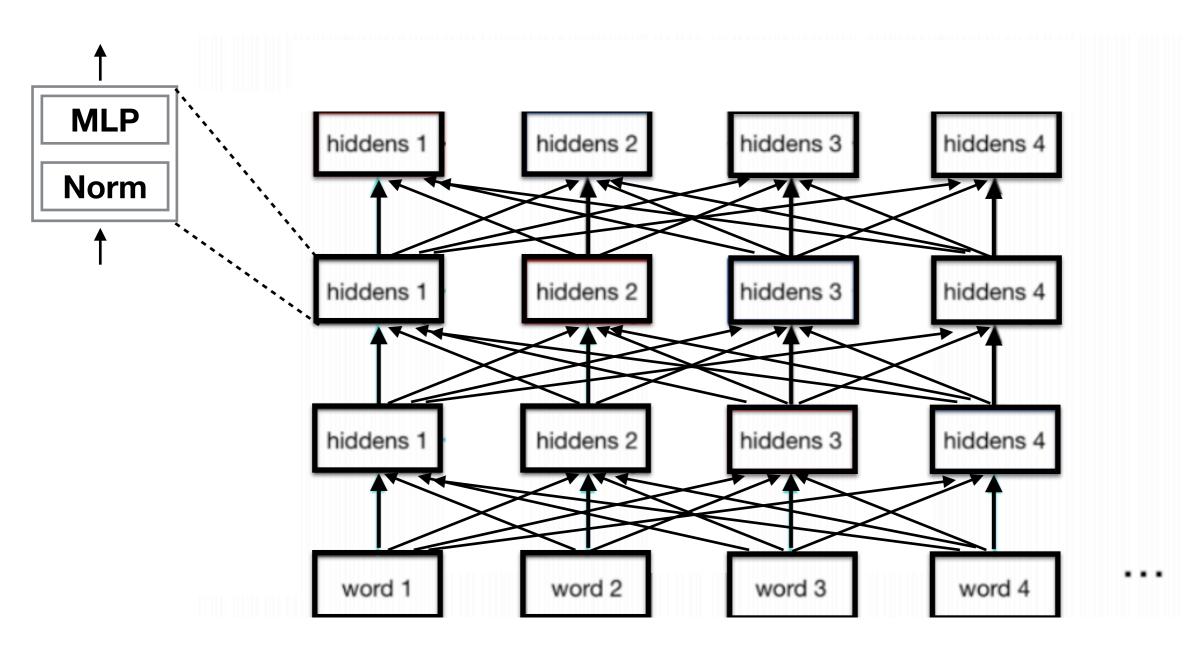
$$\operatorname{Attention}(Q, K, V) = \operatorname{softmax}(\frac{QK^T}{\sqrt{d_k}})V$$



#### Self attention

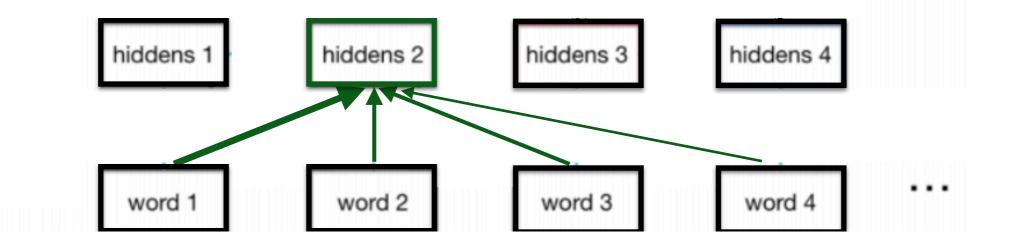


### Each attention layer is followed by Layer-norm and MLP



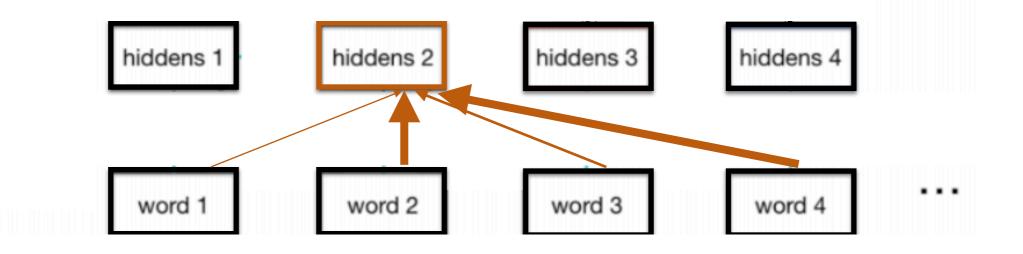
#### multi-head attention

one attention pattern



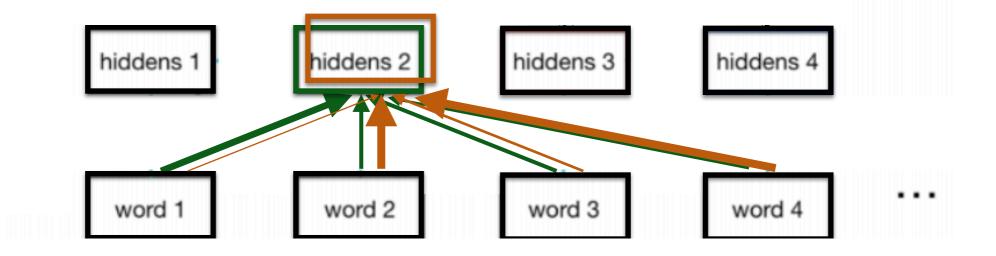
#### multi-head attention

another attention pattern



#### multi-head attention

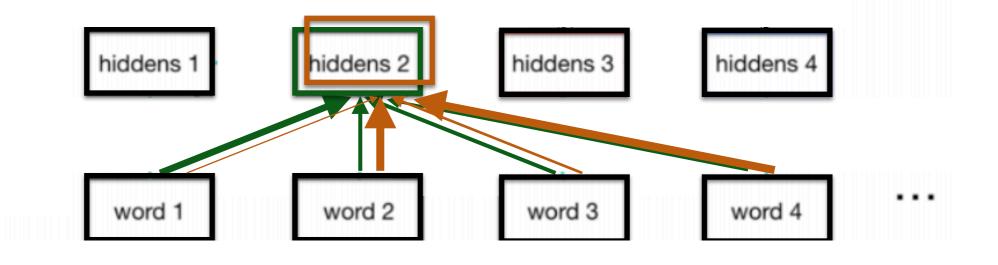
why chose if we can just have several?



#### multi-head attention

why chose if we can just have several?

 $MultiHead(Q, K, V) = Concat(head_1, ..., head_h)W^O$ 



#### multi-head attention

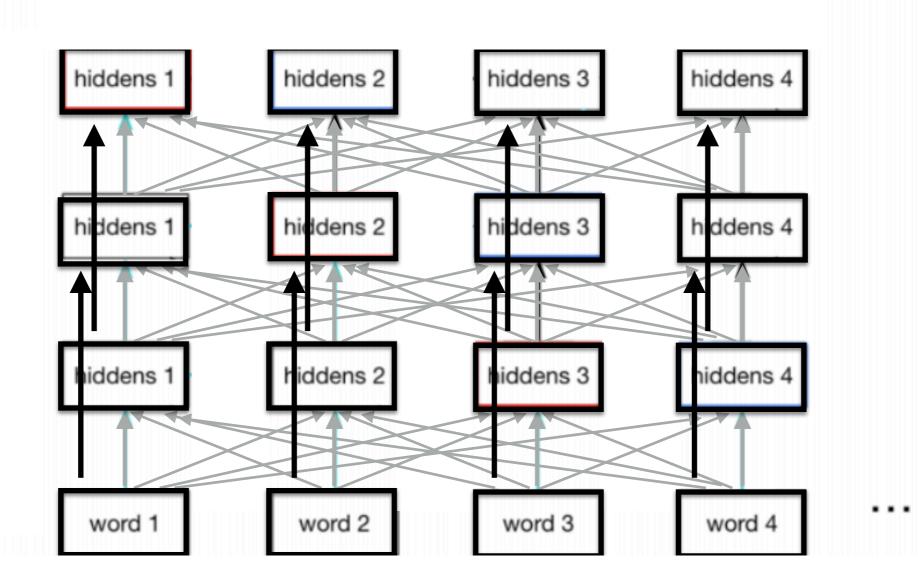
why chose if we can just have several?

 $\begin{aligned} \text{MultiHead}(Q, K, V) &= \text{Concat}(\text{head}_1, ..., \text{head}_h)W^O \\ \end{aligned}$ where  $\text{head}_i = \text{Attention}(QW_i^Q, KW_i^K, VW_i^V) \end{aligned}$ 

Where the projections are parameter matrices  $W_i^Q \in \mathbb{R}^{d_{\text{model}} \times d_k}$ ,  $W_i^K \in \mathbb{R}^{d_{\text{model}} \times d_k}$ ,  $W_i^V \in \mathbb{R}^{d_{\text{model}} \times d_v}$ and  $W^O \in \mathbb{R}^{hd_v \times d_{\text{model}}}$ .

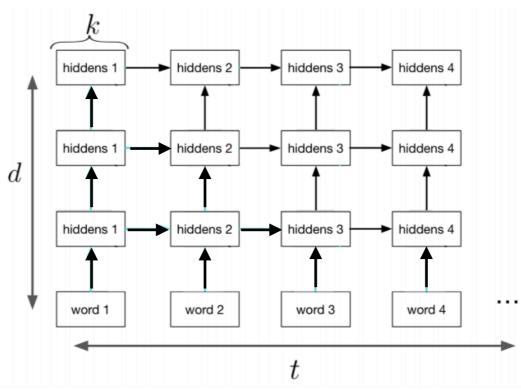
In this work we employ h = 8 parallel attention layers, or heads. For each of these we use  $d_k = d_v = d_{\text{model}}/h = 64$ . Due to the reduced dimension of each head, the total computational cost is similar to that of single-head attention with full dimensionality.

#### **Skip connections**



# Cost vs Opportunity

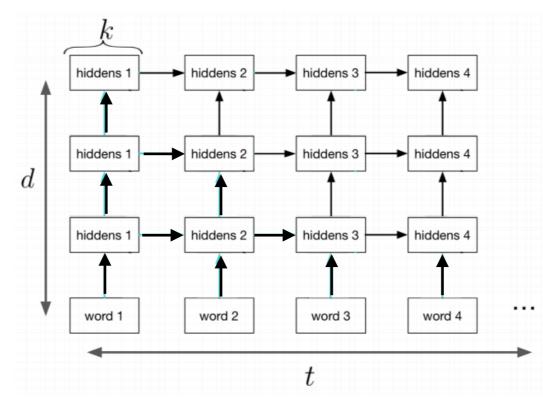
 Consider a standard d layer RNN from Lecture 13 with k hidden units, training on a sequence of length t.



- There are k<sup>2</sup> connections for each hidden-to-hidden connection. A total of t × k<sup>2</sup> × d connections.
- We need to store all  $t \times k \times d$  hidden units during training.
- Only  $k \times d$  hidden units need to be stored at test time.

## Cost vs Opportunitv

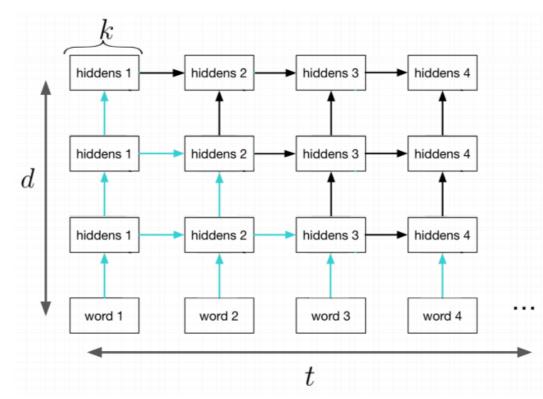
 Consider a standard d layer RNN from Lecture 13 with k hidden units, training on a sequence of length t.



• Which hidden layers can be computed in parallel in this RNN?

## Cost vs Opportunitv

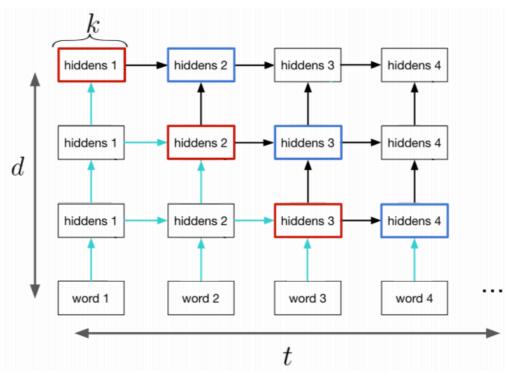
 Consider a standard d layer RNN from Lecture 13 with k hidden units, training on a sequence of length t.



• Which hidden layers can be computed in parallel in this RNN?

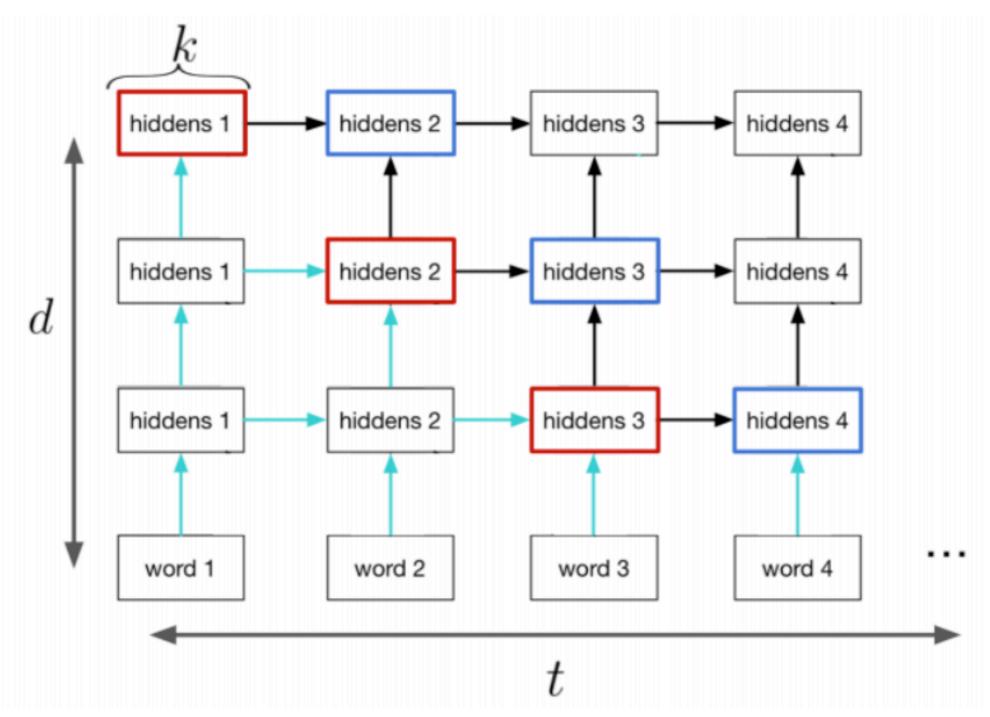
# Cost vs Opportunity

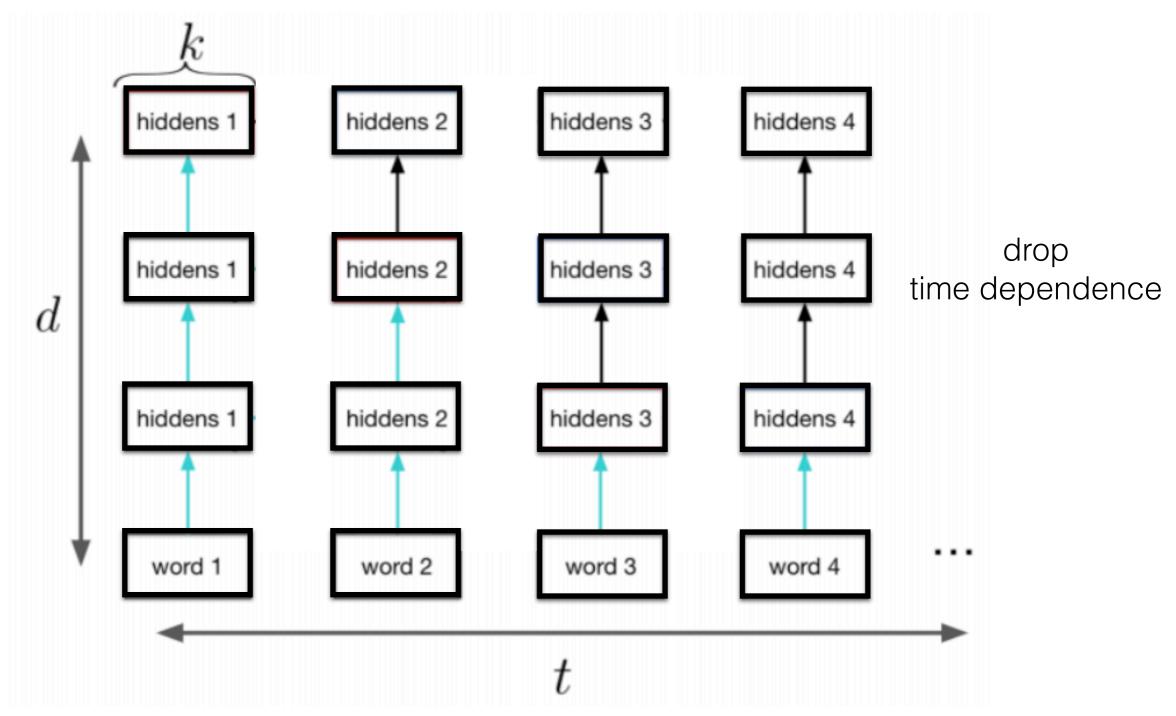
 Consider a standard d layer RNN from Lecture 13 with k hidden units, training on a sequence of length t.

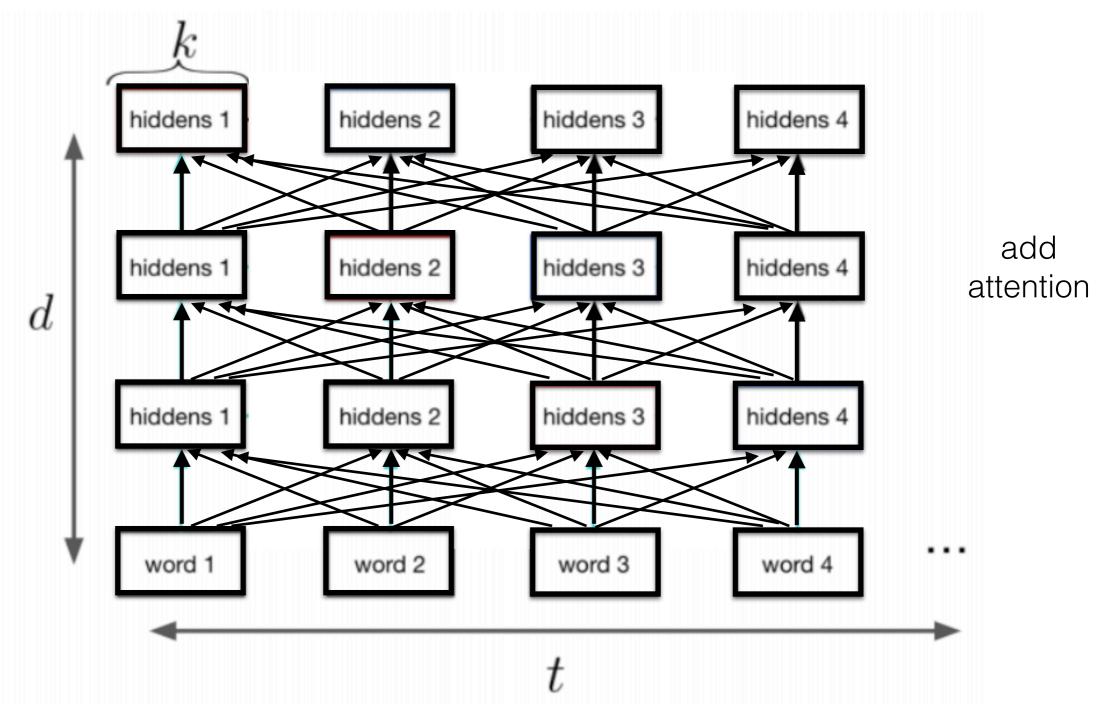


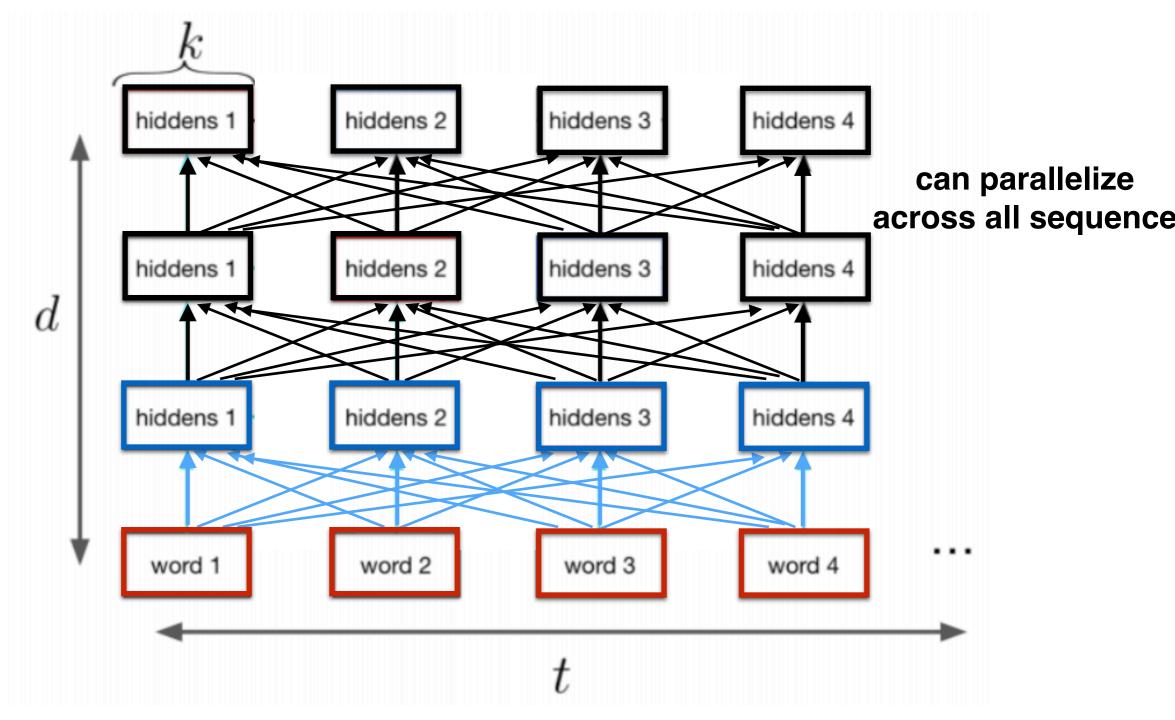
- Both the input embeddings and the outputs of an RNN can be computed in parallel.
- The blue hidden units are independent given the red.
- The numer of sequential operation is still propotional to t.

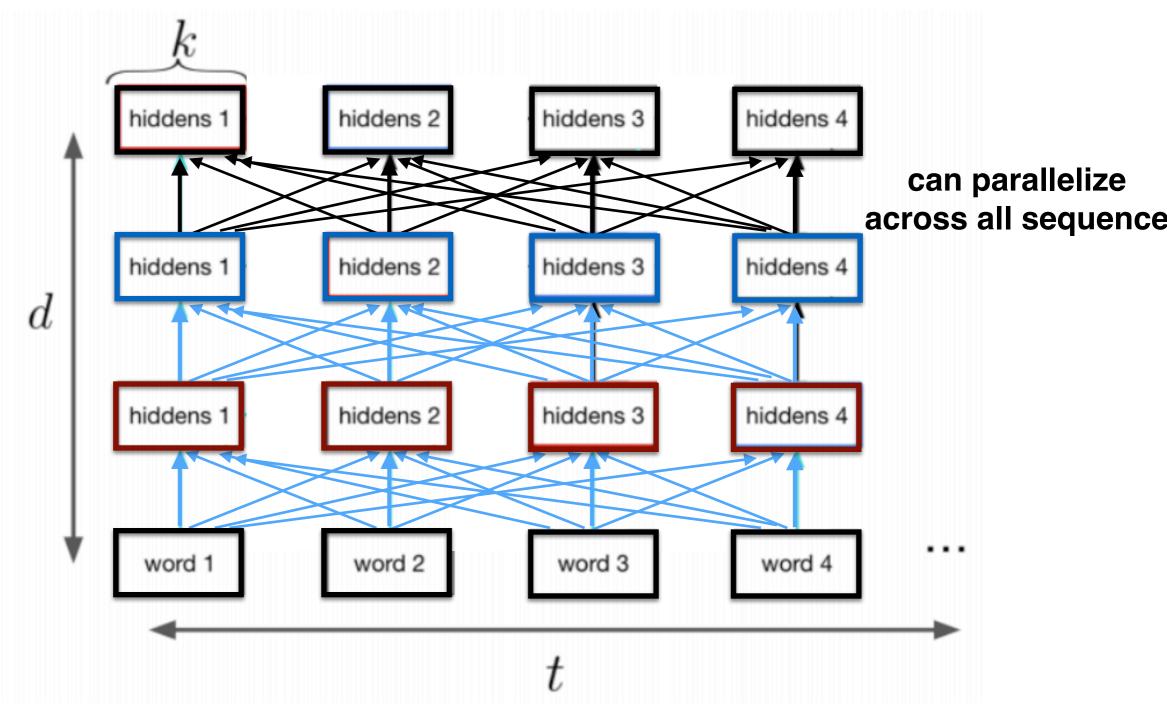
### Cost vs Opportunity RNN to Self-attention



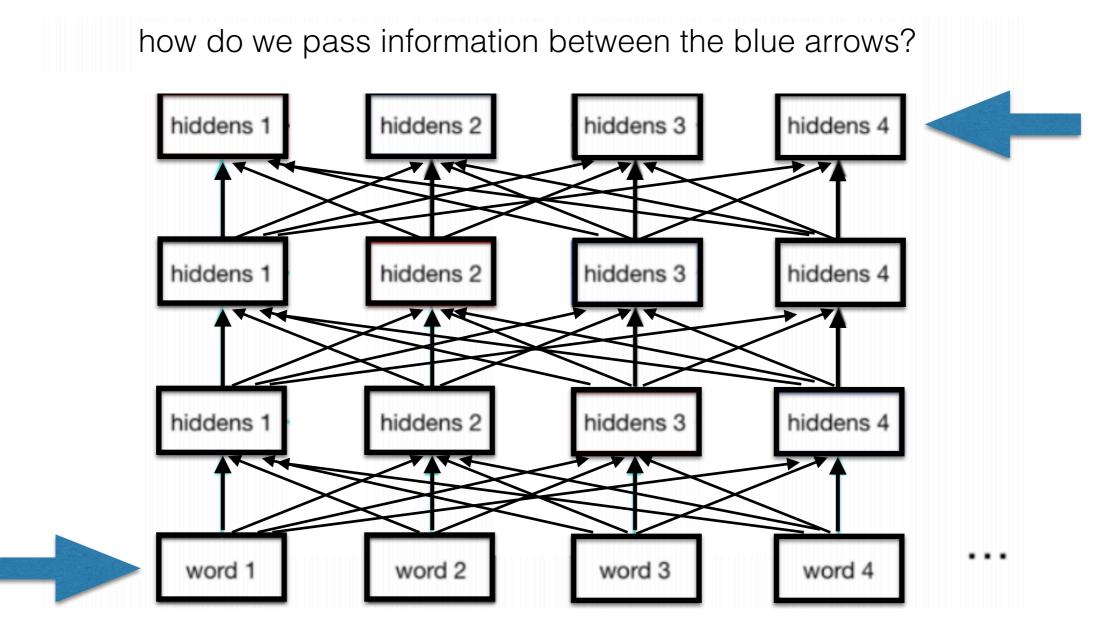








### Information flow

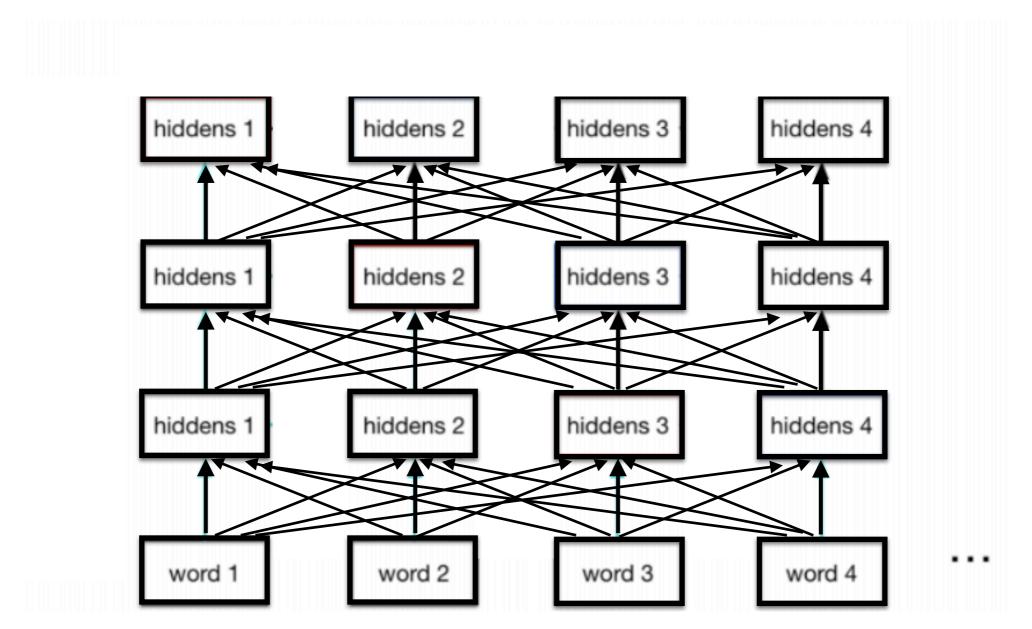


#### Transformer VS **RNN** case Information flow how do we pass information between the blue arrows? hiddens 1 hiddens 2 hiddens 3 hiddens 4 hiddens 2 hiddens 1 hiddens 3 hiddens 4 hiddens 1 hiddens 2 hiddens 3 hiddens 4 . . . word 1 word 2 word 3 word 4

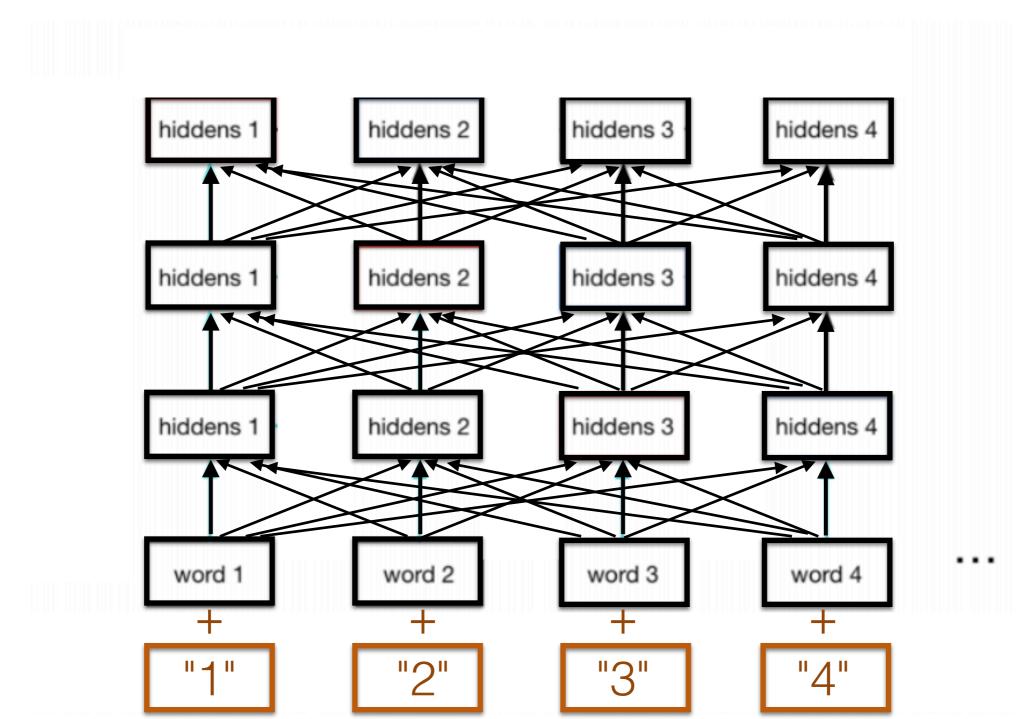
Table 1: Maximum path lengths, per-layer complexity and minimum number of sequential operations for different layer types. n is the sequence length, d is the representation dimension, k is the kernel size of convolutions and r the size of the neighborhood in restricted self-attention.

Layer Type	Complexity per Layer	Sequential Operations	Maximum Path Length
Self-Attention	$O(n^2 \cdot d)$	O(1)	O(1)
Recurrent	$O(n \cdot d^2)$	O(n)	O(n)
Convolutional	$O(k\cdot n\cdot d^2)$	O(1)	$O(log_k(n))$
Self-Attention (restricted)	$O(r \cdot n \cdot d)$	O(1)	O(n/r)

### **Positional information**



#### **Positional information**



# Transformer: more details

### http://nlp.seas.harvard.edu/2018/04/03/attention.html

harvardnlp 💔

Members PI Code Publications

The Annotated Transformer

Apr 3, 2018

### http://jalammar.github.io/illustrated-transformer/

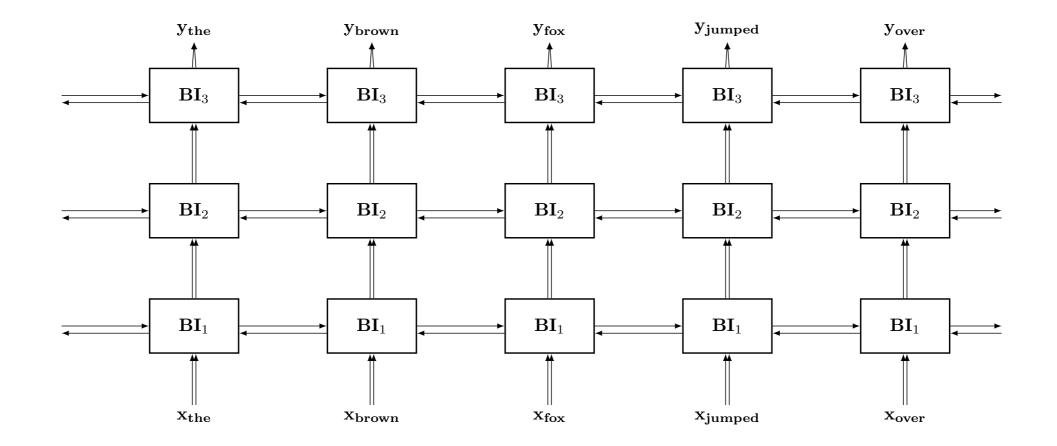


Jay Alammar Visualizing machine learning one concept at a time

**The Illustrated Transformer** 

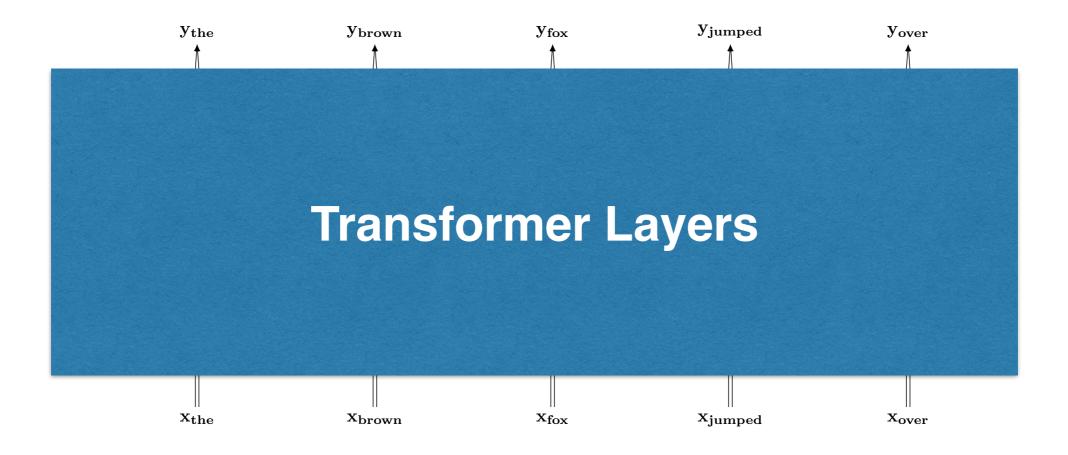
### good explanations, have a look.

# **BiRNN -> Transformer**



Deep biRNN

# **BiRNN -> Transformer**



- An alternative to RNN
- Replace recurrence with attention to all tokens.
- More computation. More parallelism. Shorter connections between data points.

# To summarize

- RNNs are very capable learners of sequential data.
- n -> 1: RNN acceptor
- n -> n : biRNN (transducer)
- 1 -> m : conditioned generation (conditioned LM)
- n -> m : conditioned generation (encoder-decoder)
- n -> m : encoder-decoder with attention