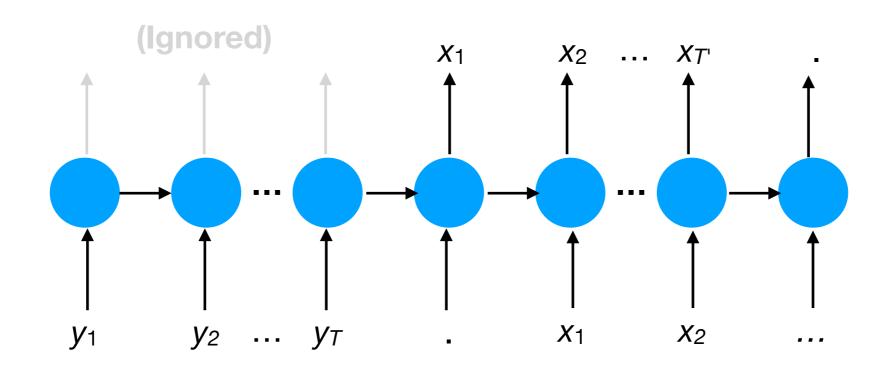
#### CS/DS 552: Class 14

Jacob Whitehill

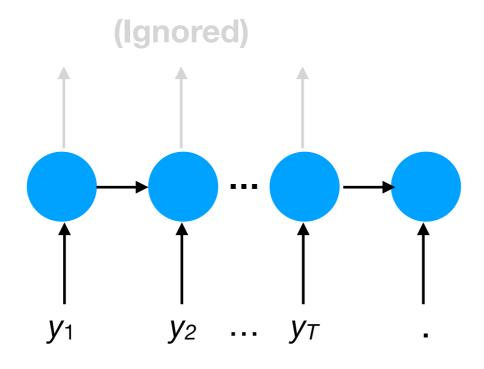
#### Machine translation

- Suppose we want to translate from one language to another.
- Language 1 vocabulary: { a, b, . }.
- Language 2 vocabulary: { u, v, w, . }.
- We add to both vocabularies a "." symbol that means end-of-sentence (EOS).

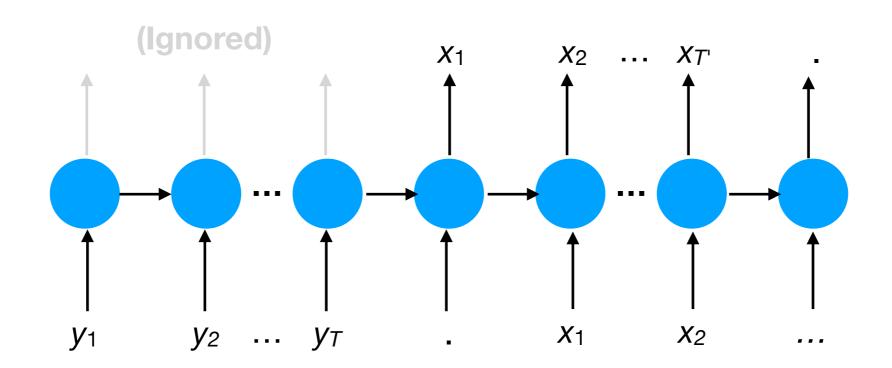
- We can construct an RNN to translate from the source language to the target language.
- Note that the length T of the input sentence is generally not equal to the length T' of the output sentence; hence, we cannot simply output one x<sub>t</sub> for each y<sub>t</sub>.



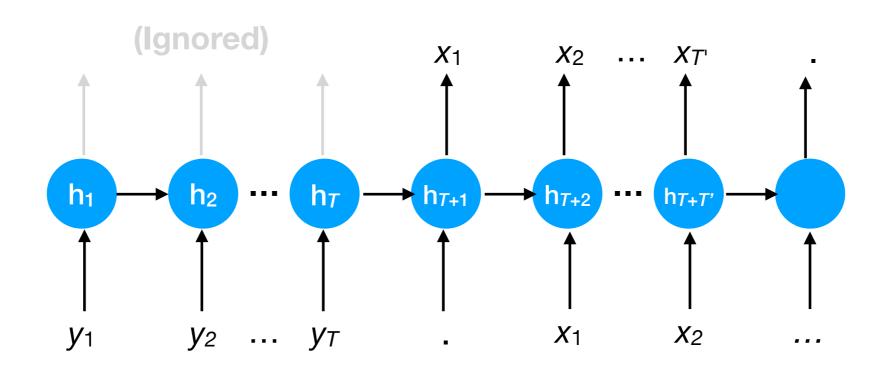
- We can construct an RNN to translate from the source language to the target language:
  - 1. We first input the T words of the input sentence as  $y_1$ , ...,  $y_T$ , followed by .



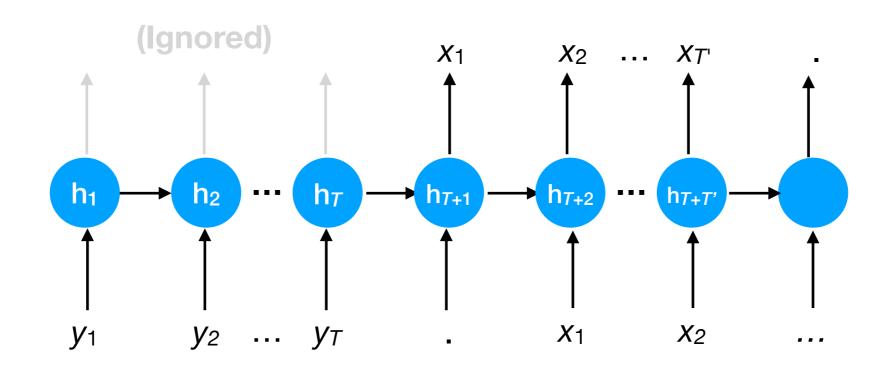
- We can construct an RNN to translate from the source language to the target language:
  - 1. We first input the T words of the input sentence as  $y_1$ , ...,  $y_T$ , followed by .
  - 2. We then obtain the T' words of the output sentence autoregressively as  $x_1, ..., x_{T'}$ , until the model outputs.



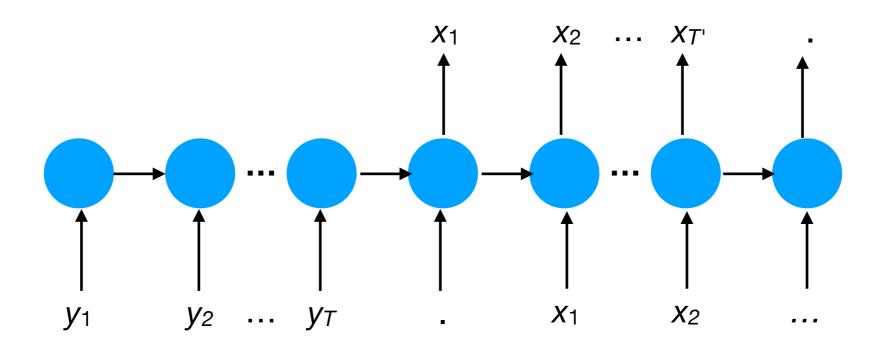
- The RNN's hidden state h<sub>t</sub> captures both the meaning of the input y and the summary of the output up to time t.
- $\mathbf{h}_t$  effectively "compresses" the variable-length history into a fixed-length representation (i.e., O(1) space).



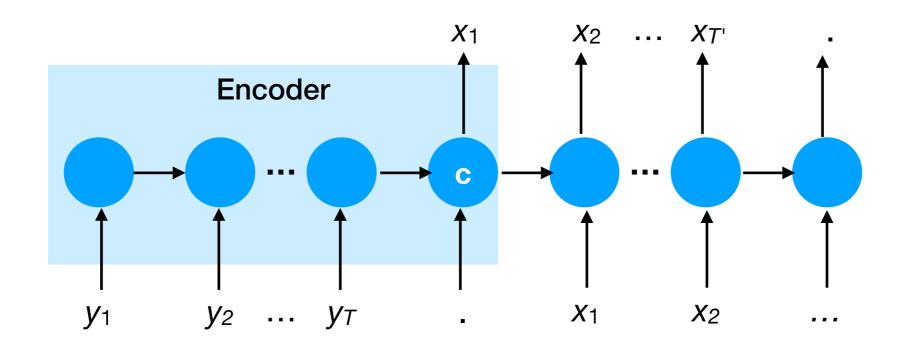
- This approach can work (and is the idea behind LLMs) but typically requires a very large model to be successful.
- Instead, it can be beneficial to break the machine translation problem into subtasks: "encoding" and "decoding".



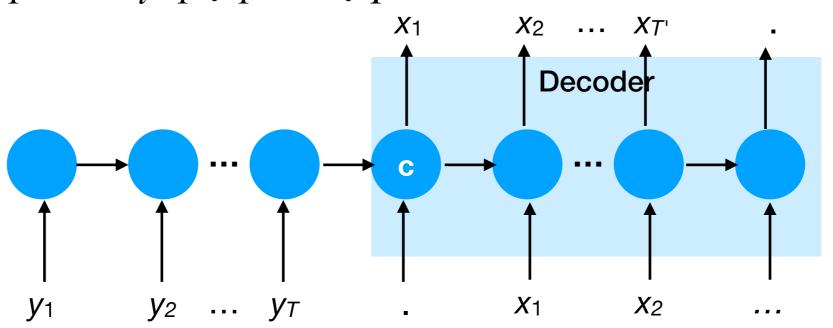
 We construct a sequence-to-sequence model consisting of an encoder RNN and a decoder RNN:



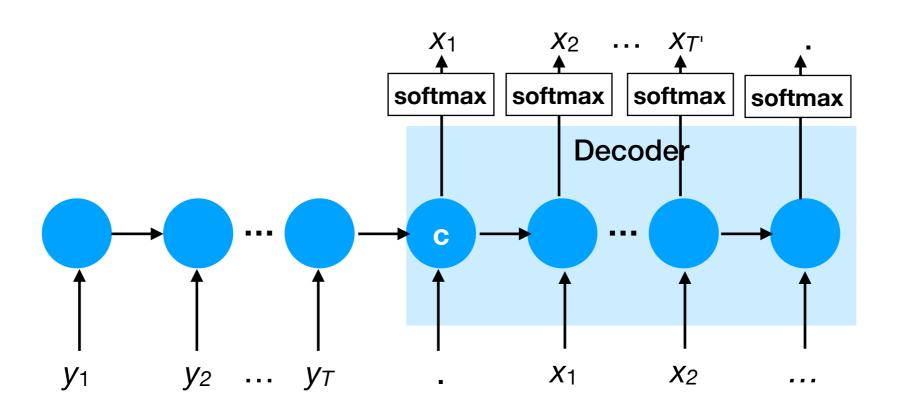
The encoder ingests the input sequence y<sub>1</sub>, ..., y<sub>T</sub> and produces a context vector c that captures y's meaning.



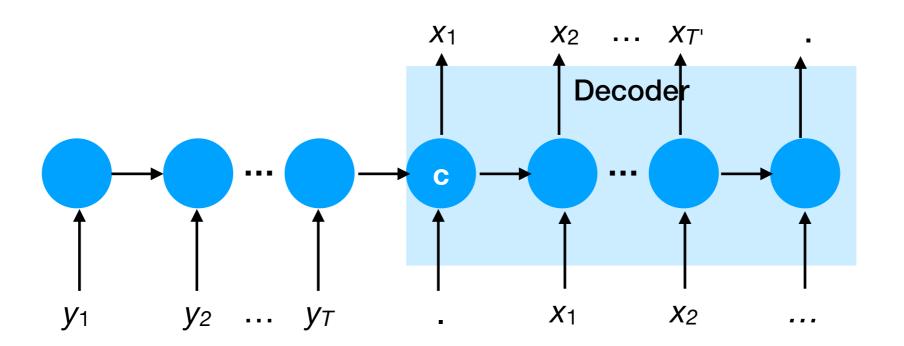
- The encoder ingests the input sequence  $y_1, ..., y_T$  and produces a context vector  $\mathbf{c}$  that captures  $\mathbf{y}$ 's meaning.
- The decoder uses the context vector to estimate  $P(x_t | x_1, ..., x_{t-1}, y_1, ..., y_T)$  at each timestep t.



• Since each  $x_t$  belongs to a finite set, we can compute  $P(x_t | x_1, ..., x_{t-1}, y_1, ..., y_T)$  using softmax.



• We can then autoregressively sample each  $x_t \sim P(x_t | x_1, ..., x_{t-1}, y_1, ..., y_T)$  to generate the sentence.



## Encoder-decoder model: training

 We train an encoder-decoder model to maximize the logprobability of producing the correct translation:

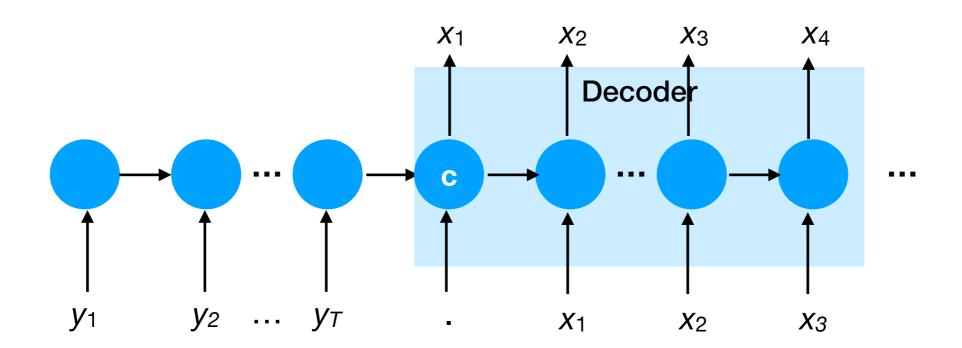
## Encoder-decoder model: training

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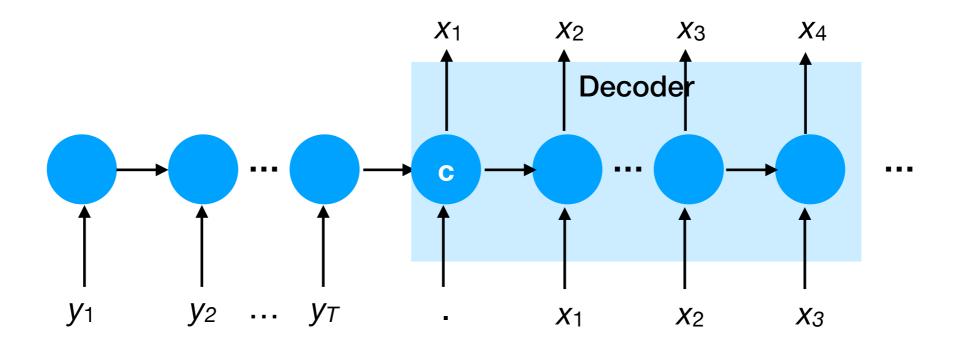
$$\log P(x_1,\ldots,x_{T'}\mid y_1,\ldots,y_T) = \log \prod_{t=1}^{T'} P(x_t\mid x_1,\ldots,x_{t-1},y_1,\ldots,y_T)$$

$$\begin{array}{c} \text{Minimize CE loss to} \\ \text{maximize log-} \\ \text{likelihood} \end{array} = \sum_{t=1}^{T'} \log P(x_t\mid x_1,\ldots,x_{t-1},y_1,\ldots,y_T)$$

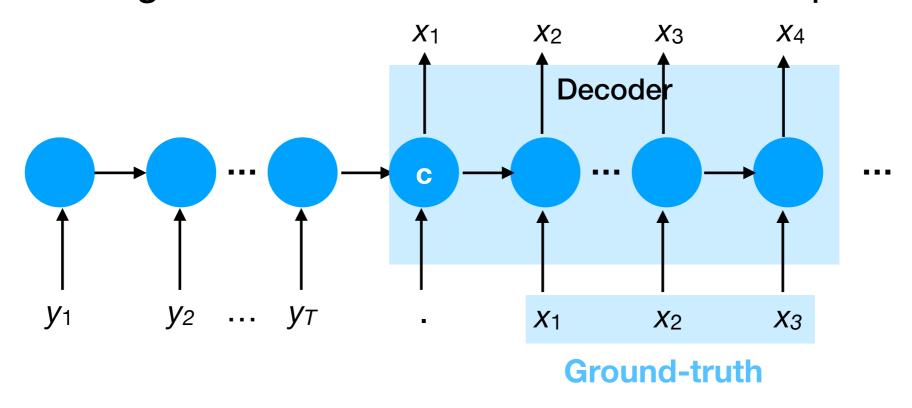
 Recall that the RNN auto-regressively feeds the predicted word x<sub>t</sub> back to the decoder at timestep t+1.



- However, at training time, we can use an alternative strategy since the correct output words are known.
- Instead of feeding the decoder the NN's predictions,

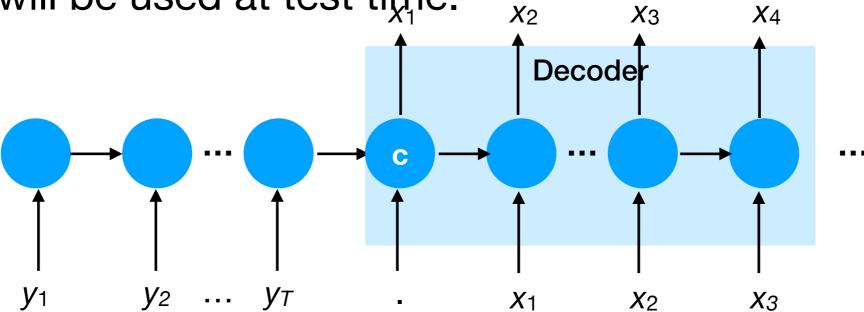


- However, at training time, we can use an alternative strategy since the correct output words are known.
- Instead of feeding the decoder the NN's predictions, we can feed the ground-truth values at each timestep.

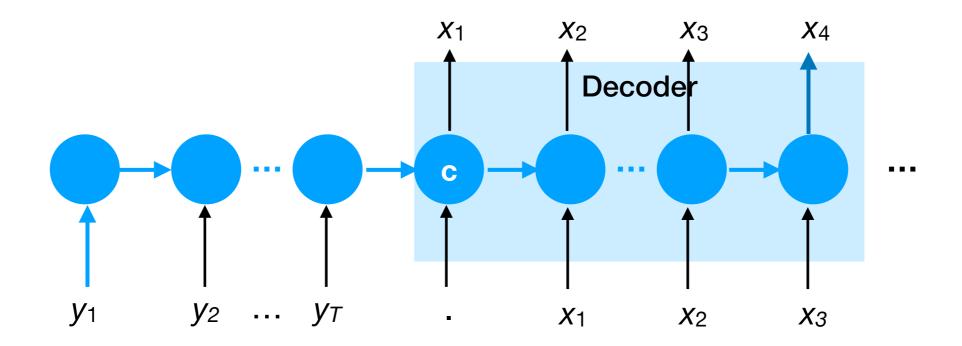


- This is called teacher forcing.
- Why helpful: we are feeding the NN the correct inputs rather than noisy ones.

 Why harmful: we are not training the NN consistently with how it will be used at test time.



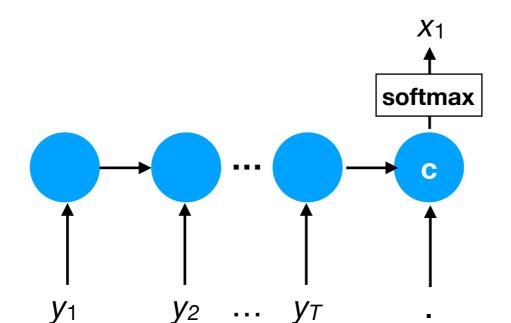
 Unfortunately, teacher forcing does not increase parallelism since the span is still O(T+T') due to the hidden state dependency.



# Encoder-decoder model: testing/inference

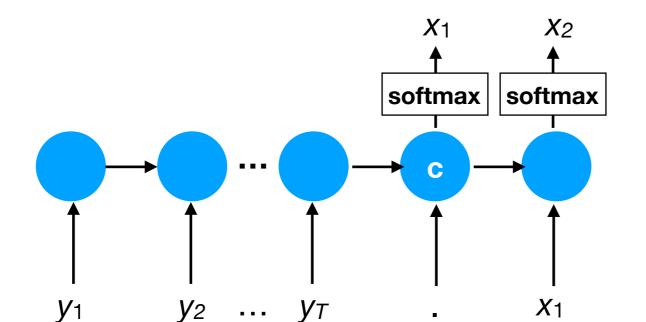
### Sampling each xt

- Given each  $P(x_t | x_1, ..., x_{t-1}, y_1, ..., y_T)$  estimated by the RNN, we can autoregressively sample a sentence **x**.
- Each such distribution is computed via softmax.



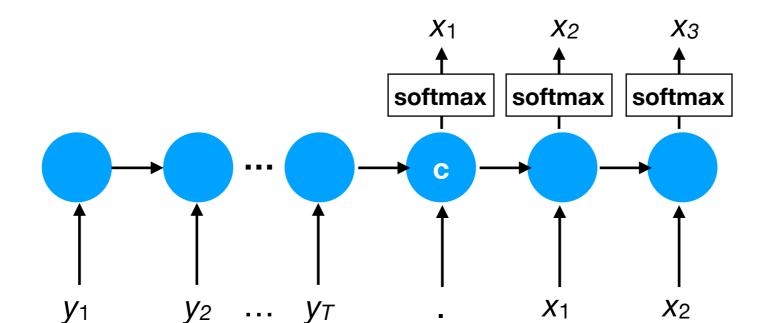
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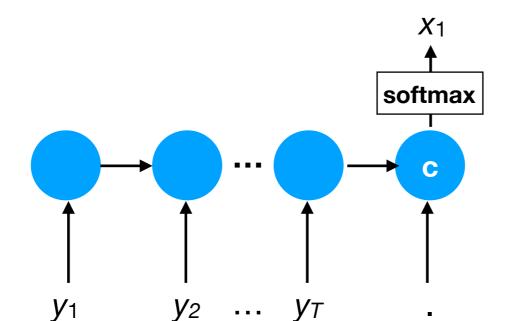
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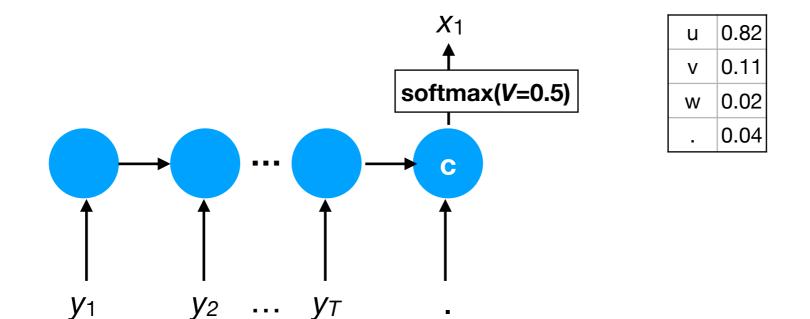
### Temperature

• Sometimes we may want to increase/decrease the amount of noise in each  $x_t$  to yield *more likely* or *more diverse* outputs.



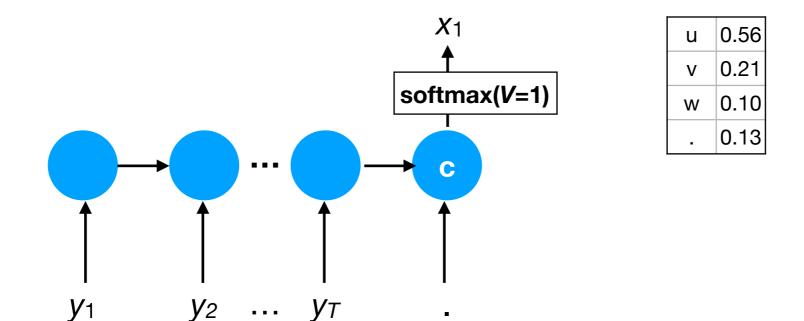
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- Sometimes we may want to increase/decrease the amount of noise in each  $x_t$  to yield *more likely* or *more diverse* outputs.
- We can achieve this by computing the softmax with a temperature V: softmax( $\mathbf{z}, V$ ) $_k = \frac{\exp(z_k/V)}{\sum_{k'=1}^K \exp(z_{k'}/V)}$
- Higher temperature V leads to more uniform probabilities.

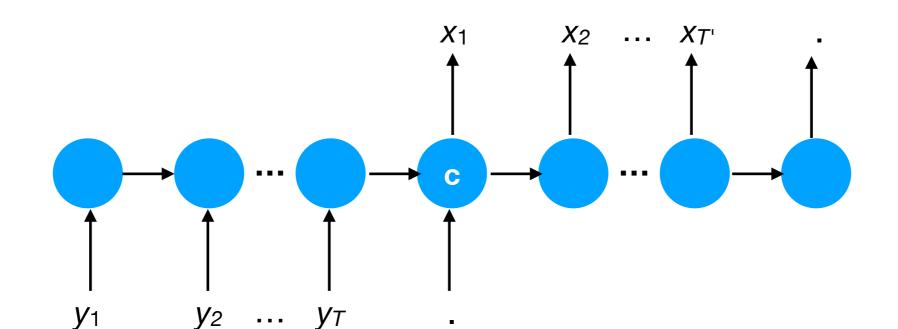


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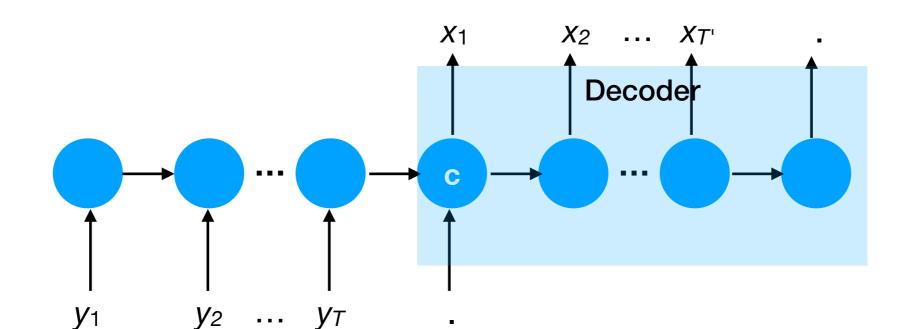


- We may wish to find the **most likely sentence**  $x_1, ..., x_{T'}$  that corresponds to the input sentence  $y_1, ..., y_T$ .
- How can we compute the likelihood  $P(x_1, ..., x_{T'} | y_1, ..., y_T)$ ?

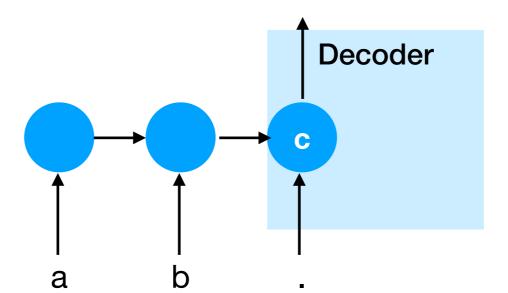


- Since  $P(x_1, ..., x_{T'} | y_1, ..., y_T)$  factorizes over t, we can:
  - 1. Pass a sentence  $y_1, ..., y_T$  into the RNN.
  - 2. Obtain the probability of each symbol  $x_t$ .
  - 3. Multiply the probabilities together:

$$P(x_1, x_2, x_3 | y_1, y_2) = P(x_1 | y_1, y_2) P(x_2 | y_1, y_2, x_1) P(x_3 | y_1, y_2, x_1, x_2)$$

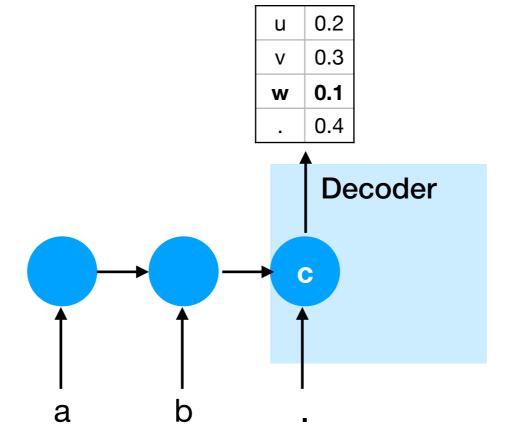


• Suppose  $y_1=a$ ,  $y_2=b$ ,  $y_3=$ . Then for  $x_1=w$ ,  $x_2=v$ , we have:



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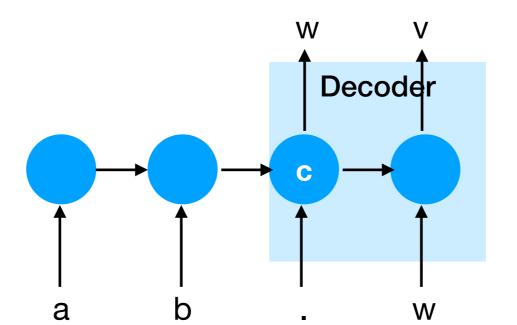
P("w v" | "a b.") = 0.1



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• Suppose  $y_1=a$ ,  $y_2=b$ ,  $y_3=$ . Then for  $x_1=w$ ,  $x_2=v$ , we have:

$$P(\text{"w v"} \mid \text{"a b."}) = 0.1 * 0.7 = 0.07$$



- Unfortunately, to search over all translations, there are exponentially (in T') many different probabilities  $P(x_1, ..., x_{T'} | y_1, ..., y_T)$  we would need to compute.
- Heuristic: perform a greedy **beam search** to keep track of the top-B most likely translations  $x_1, ..., x_T$ .

#### Beam search

#### Beam search

• Beam search is an efficient greedy heuristic that approximately optimizes:

$$\arg \max_{x_1,...,x_{T'}} p(x_1,...,x_{T'}|y_1,...,y_T)$$

#### Beam search

1. At each output timestep *t*, keep track of top-*B* most likely translations, where *B* is the **beam width**:

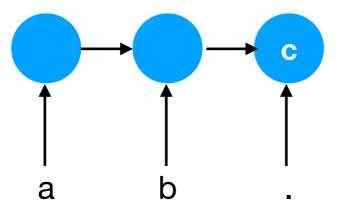
$$\{(x_1,\ldots,x_t)^{(1)},\ldots,(x_1,\ldots,x_t)^{(B)}\}$$

2. For each of our *B* candidates, we can compute:

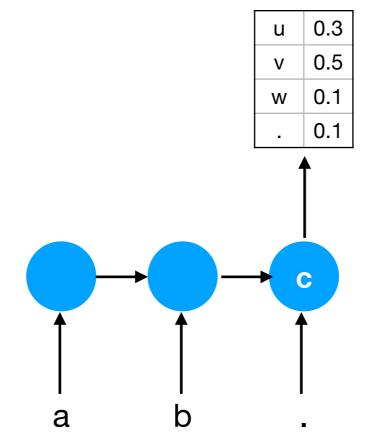
$$P(x_{t+1} \mid x_1, ..., x_t, y_1, ..., y_T)$$

- 3. If the output vocabulary has K words, then this results in  $B^*K$  possible sequences of length t+1.
- 4. From these *B\*K* choices, we select the top-*B* most likely translations of length *t*+1.

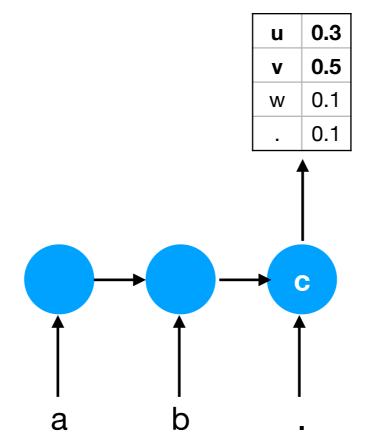
- Let input vocabulary={a, b, .} and output vocabulary={u, v, w, .}.
- Let beam width *B*=2.



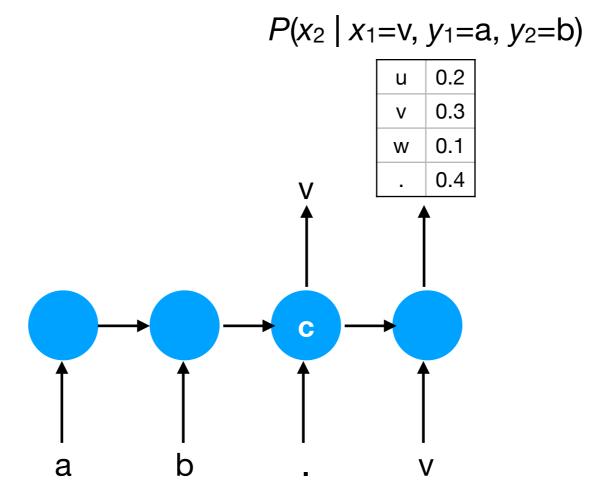
- Beam at *t*=0: {}
- At *t*=1, pick top-*B* most likely possible symbols:



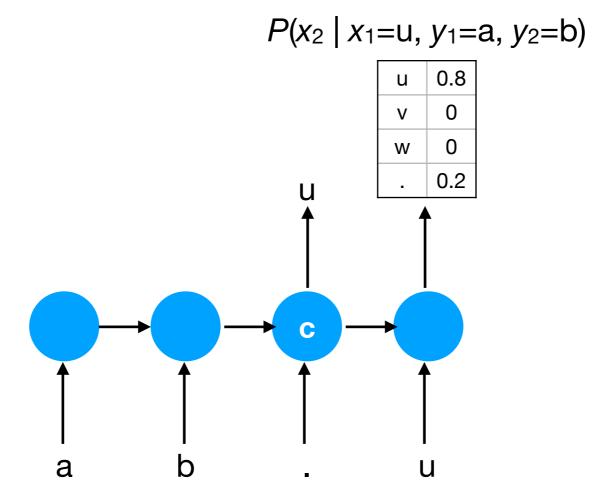
• Beam at t=1: {  $(x_1=v)$ ,  $(x_1=u)$  }



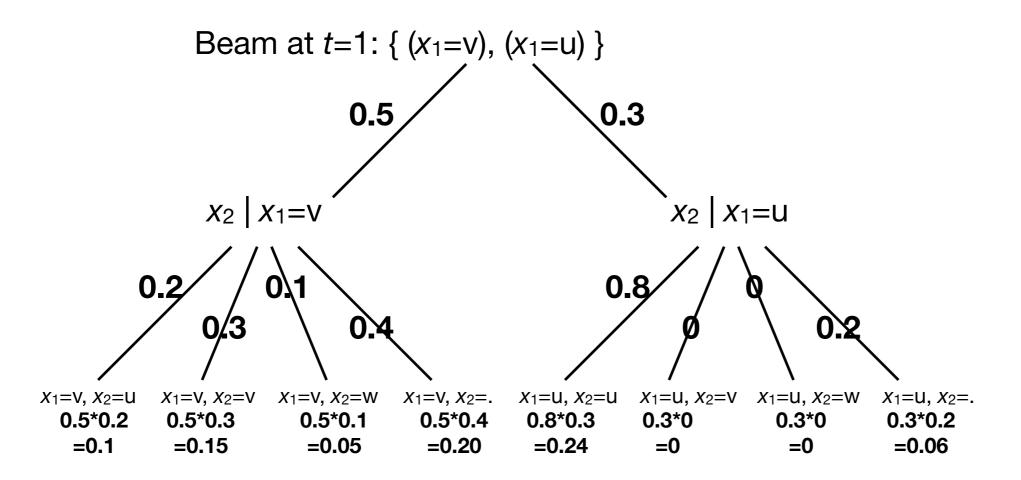
- 0.5 0.3 • Beam at *t*=1: { (**x**<sub>1</sub>=**v**), (x<sub>1</sub>=**u**) }
- At t=2, compute  $P(x_2 \mid x_1, y_1=a, y_2=b)$  for each  $(x_1)$  in the beam:



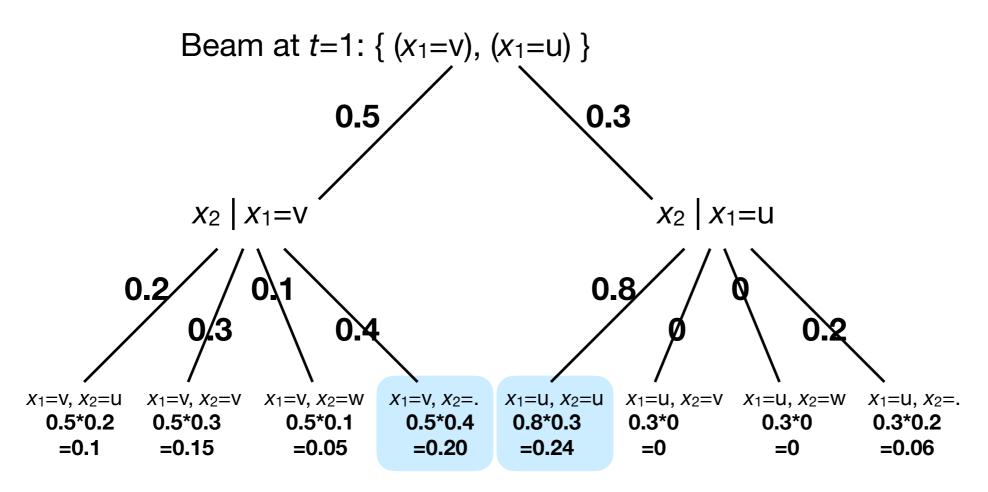
- Beam at t=1: {  $(x_1=v)$ ,  $(x_1=u)$  }
- At t=2, compute  $P(x_2 \mid x_1, y_1=a, y_2=b)$  for each  $(x_1)$  in the beam:



 This results in a total of B\*K=2\*4=8 possible sequences of length 2:



• We then pick the top-B most likely sequences as our next beam.

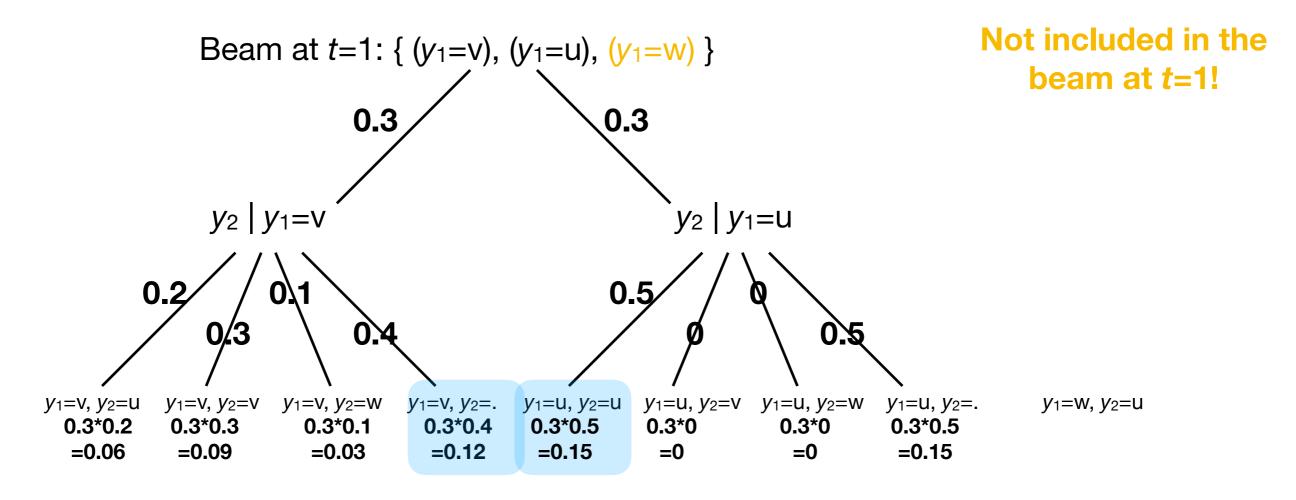


Beam at t=2: {  $(x_1=v, x_2=.), (x_1=u, x_2=u)$  }

 We repeat this procedure until all beam hypotheses end with "." (end-of-sentence), or for a fixed maximum number of timesteps.

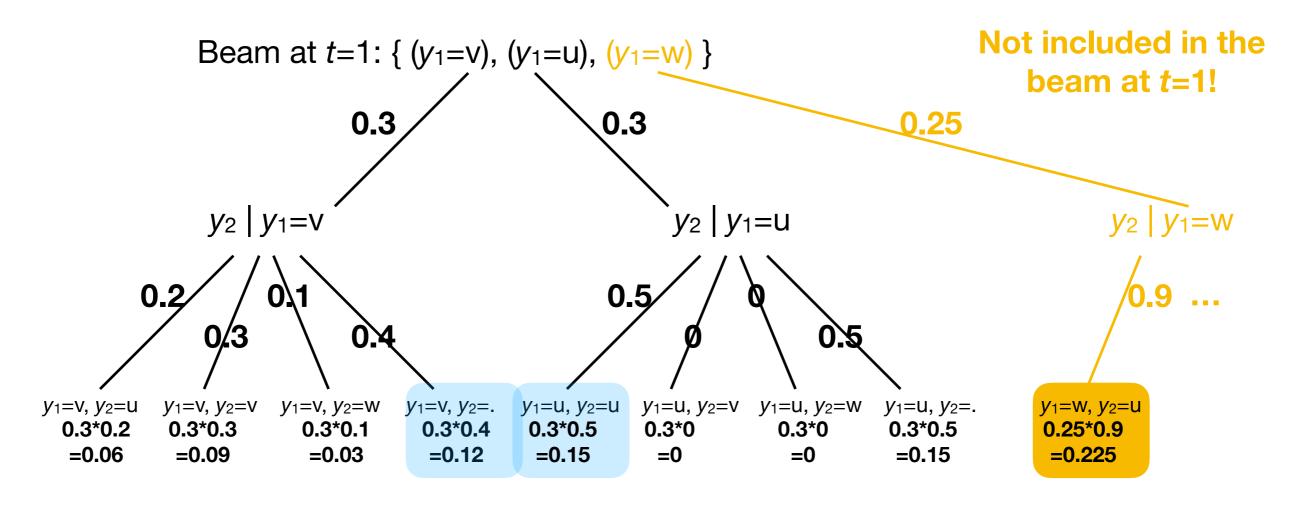
### Exercise

 For the vocabulary { u, v, w, . }, can you devise a scenario over 2 timesteps where beamsearch does not give the optimal answer?

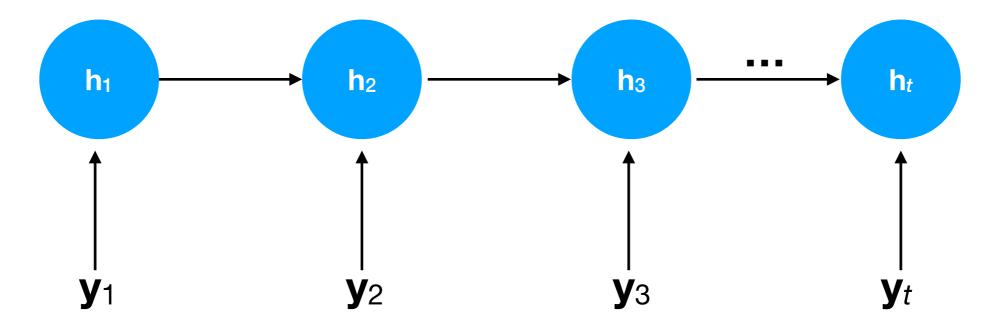


### **Exercise: Solution**

 For the vocabulary { u, v, w, . }, can you devise a scenario over 2 timesteps where beamsearch does not give the optimal answer?

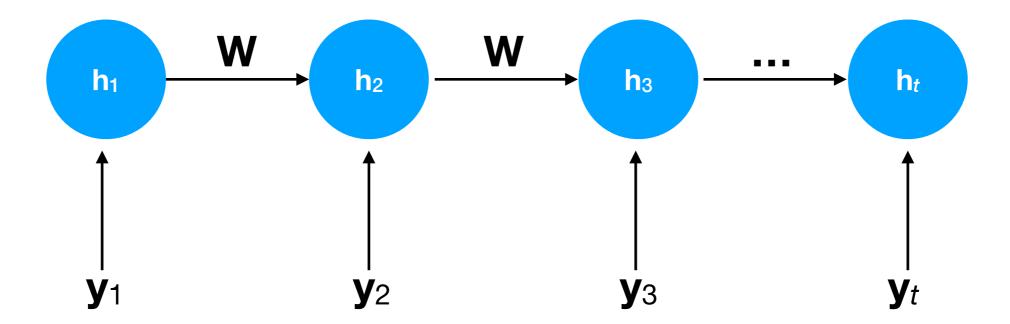


- In practice, the hidden states { h<sub>t</sub> } of basic RNNs have difficulty storing information long-term.
- Basic RNNs are also highly unstable to train.



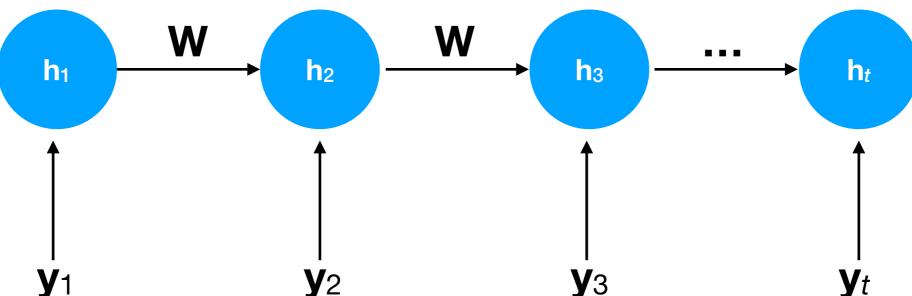
• To see why, suppose we remove non-linearity and consider what happens when we repeatedly multiply  $\mathbf{h}_t$  by  $\mathbf{W}$ .

$$\mathbf{h}_t = \mathbf{W}^t \mathbf{h}_1 + \dots$$



• To see why, suppose we remove non-linearity and consider what happens when we repeatedly multiply  $\mathbf{h}_t$  by  $\mathbf{W}$ .

$$\mathbf{h}_t = \mathbf{W}^t \mathbf{h}_1 + \dots$$
  $= \mathbf{U} \mathbf{\Lambda}^t \mathbf{U}^ op \mathbf{h}_1 + \dots$  if  $\mathbf{W}$  is diagonalizable



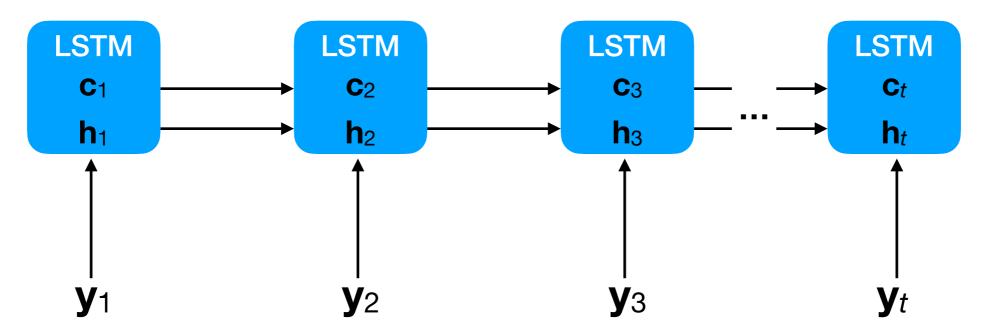
Unless all W's eigenvalues have magnitude ≈1, h<sub>1</sub>'s contribution to h<sub>t</sub> will tend to explode to infinity or vanish to 0.

$$\mathbf{h}_t = \mathbf{W}^t \mathbf{h}_1 + \dots$$

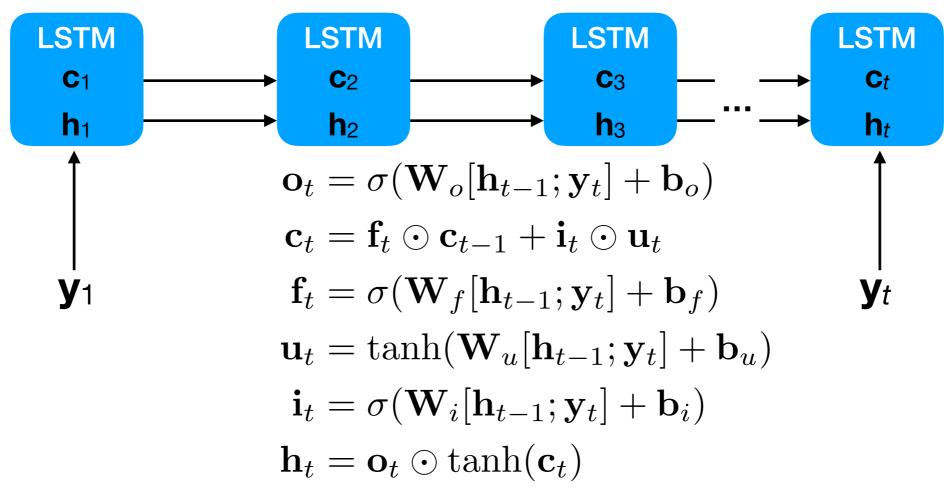
$$= \mathbf{U} \mathbf{\Lambda}^t \mathbf{U}^{ op} \mathbf{h}_1 + \dots$$

$$\downarrow \mathbf{h}_1 \qquad \qquad \downarrow \mathbf{h}_2 \qquad \qquad \downarrow \mathbf{h}_3 \qquad \qquad \downarrow \mathbf{h}_t$$

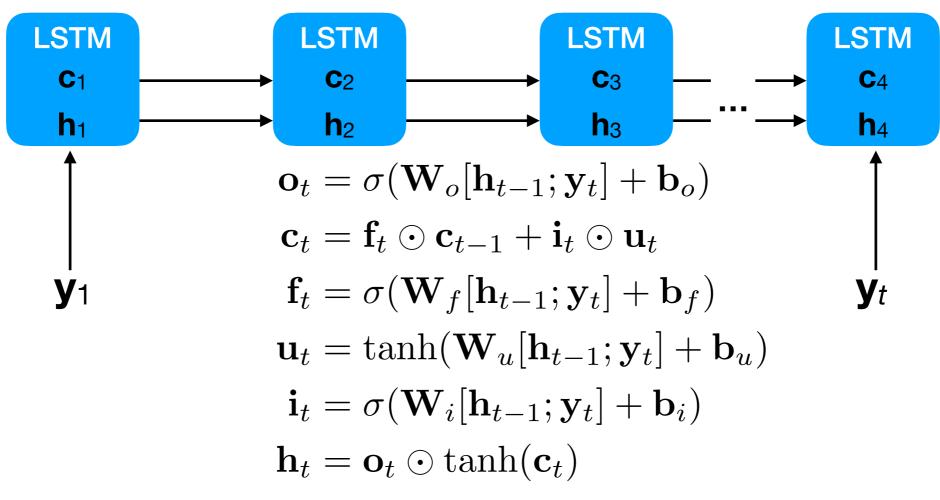
- A long short-term memory (LSTM) RNN improves on this by making it easy to store information over long timespans.
- It contains both a hidden state  $\mathbf{h}_t$  and a **cell state**  $\mathbf{c}_t$ , using the input  $\mathbf{y}_t$ .



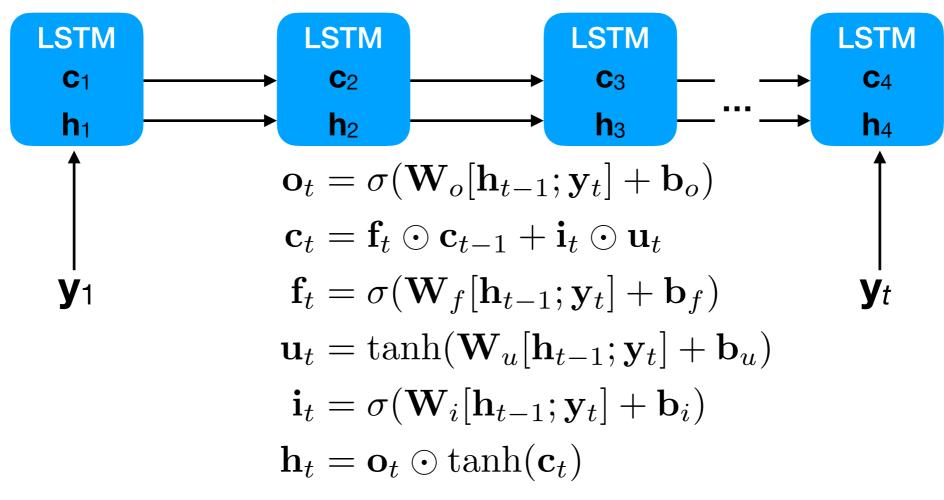
- Input gates  $i_t$  control what parts of input  $y_t$  are allowed into  $c_t$ .
- Forgetting gates  $f_t$  control what parts of  $c_{t-1}$  are allowed into  $c_t$ .
- Output gates  $o_t$  control what parts of  $c_t$  are allowed into  $h_t$ .



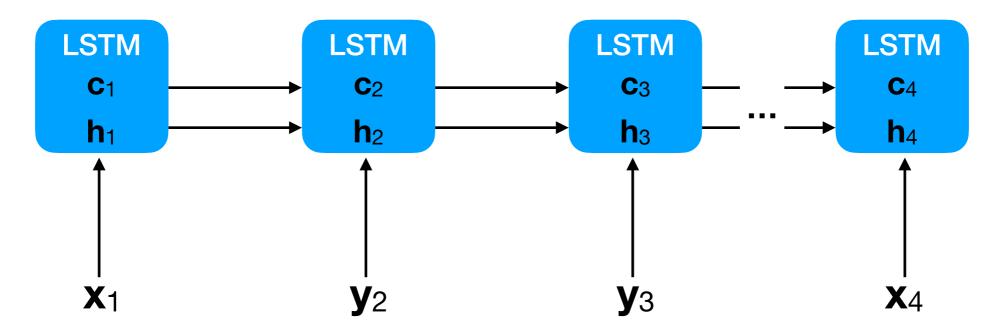
• If the  $\mathbf{f}_t = \mathbf{1}$ , then  $\mathbf{c}_t$  will maintain its value over time without exploding/vanishing.



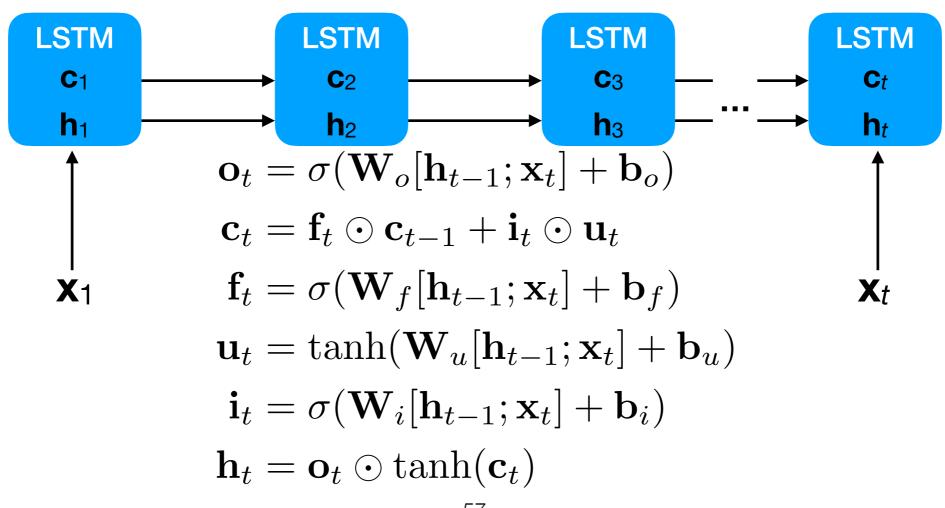
- If the  $f_t=1$ , then  $c_t$  will maintain its value over time without exploding/vanishing.
- Which components of  $\mathbf{c}_t$  are "retrieved" from long-term storage depends on  $\mathbf{y}_t$  and  $\mathbf{h}_{t-1}$ .



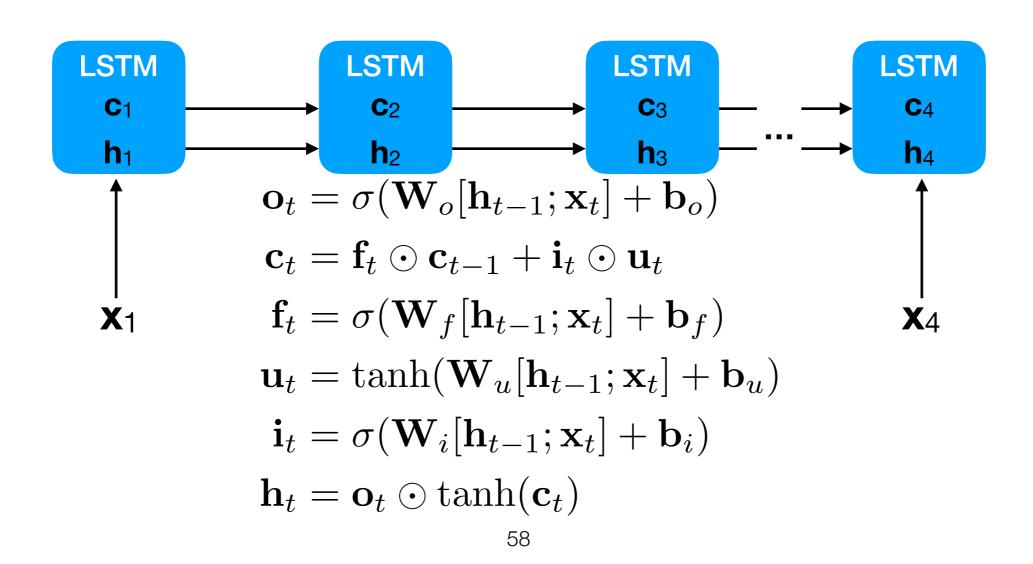
- In practice, LSTMs are much easier to train than basic RNNs.
- The memory cell  $\mathbf{c}_t$  selectively stores & forgets information from the input.
- It is still limited since it tries to summarize an entire history in one vector.



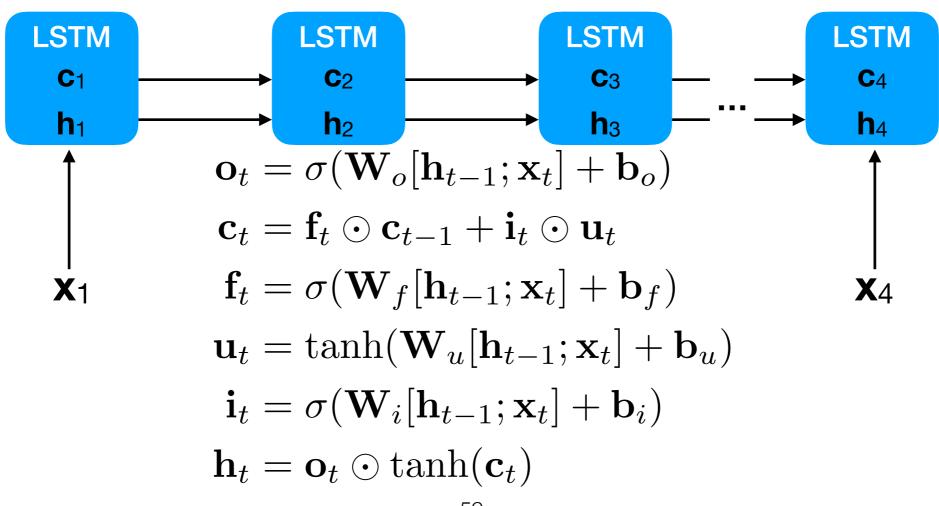
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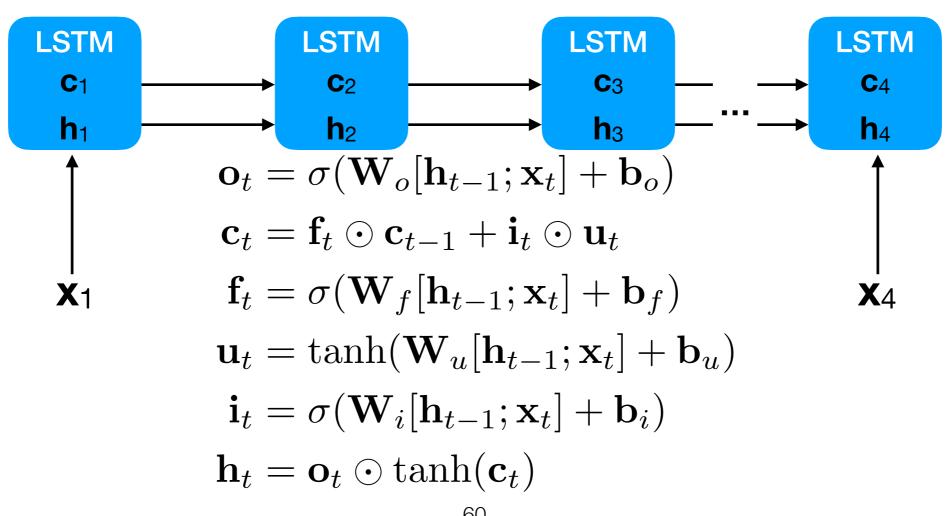
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- In practice, LSTMs are much easier to train than basic RNNs.
- However, the memory cell  $\mathbf{c}_t$  provides only limited storage since it summarizes an entire memory history into a single vector.



 The simplest way to sum up n numbers is sequential (with O(n) time):

```
total = 0
for i in range(n):
    total += nums[i]
```

$$total = 13$$

3	1	0	2	4	1	0	2	
---	---	---	---	---	---	---	---	--

 However, we can also parallelize this by computing sums in a tree:

Rule: parent = child1 + child2

3	1	0	2	4	1	0	2

 However, we can also parallelize this by computing sums in a tree:

Rule: parent = child1 + child2

 4
 2
 5
 2

 3
 1
 0
 2
 4
 1
 0
 2

 However, we can also parallelize this by computing sums in a tree:

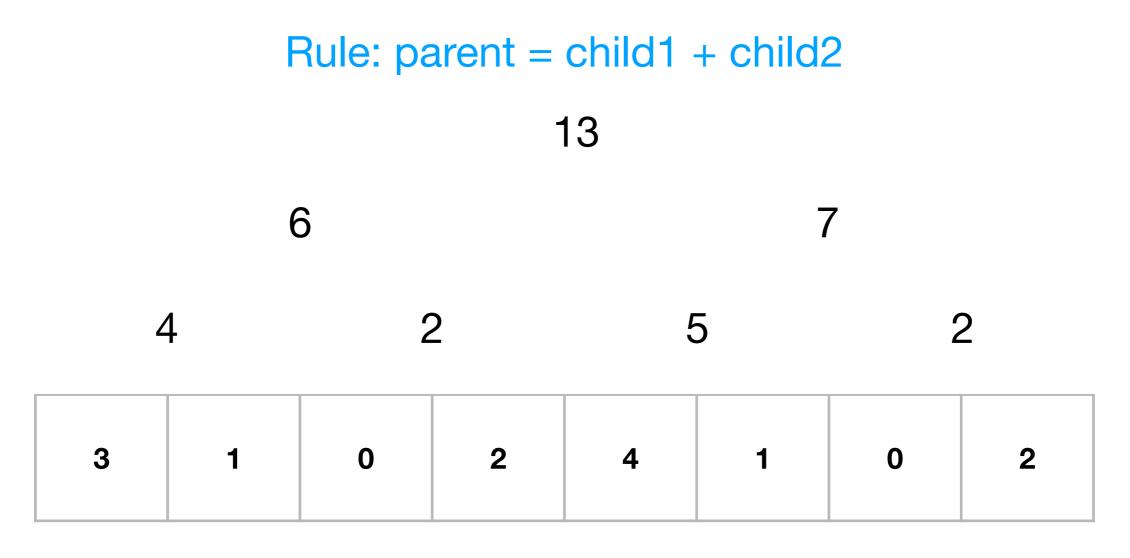
Rule: parent = child1 + child2

 6
 7

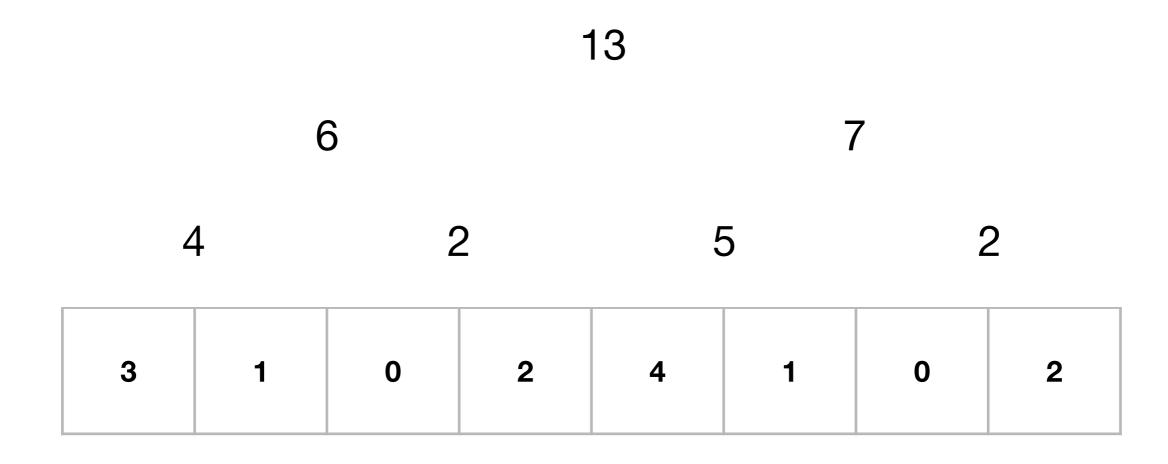
 4
 2
 5
 2

 3
 1
 0
 2
 4
 1
 0
 2

 However, we can also parallelize this by computing sums in a tree:



Now the computational cost is only O(log n).



What if we also want to compute all the prefix-sums?

p	3	4	4	6	10	11	11	13
X	3	1	0	2	4	1	0	2

- What if we also want to compute all the prefix-sums?
- A simple sequential algorithm is:

$$p[0] = x[0]$$
  
for i in range(1, n):  
 $p[i] = p[i-1] + x[i]$ 

• Total work is O(n) and span is O(n).

p	3	4	4	6	10	11	11	13
X	3	1	0	2	4	1	0	2

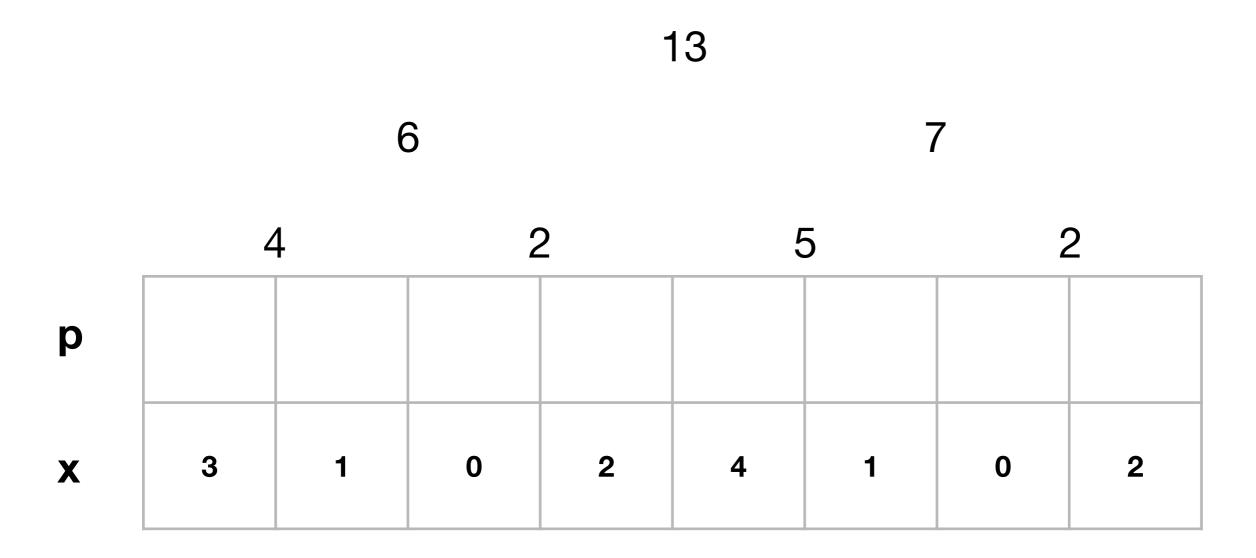
Can we parallelize this?

р	3	4	4	6	10	11	11	13	
X	3	1	0	2	4	1	0	2	

• Can we parallelize this? Yes, using a two-pass recursion.

p	3	4	4	6	10	11	11	13
X	3	1	0	2	4	1	0	2

• We first recursively compute sums pairwise.



- We first recursively compute sums pairwise.
- At this point, we can set p [7]=13.
  13

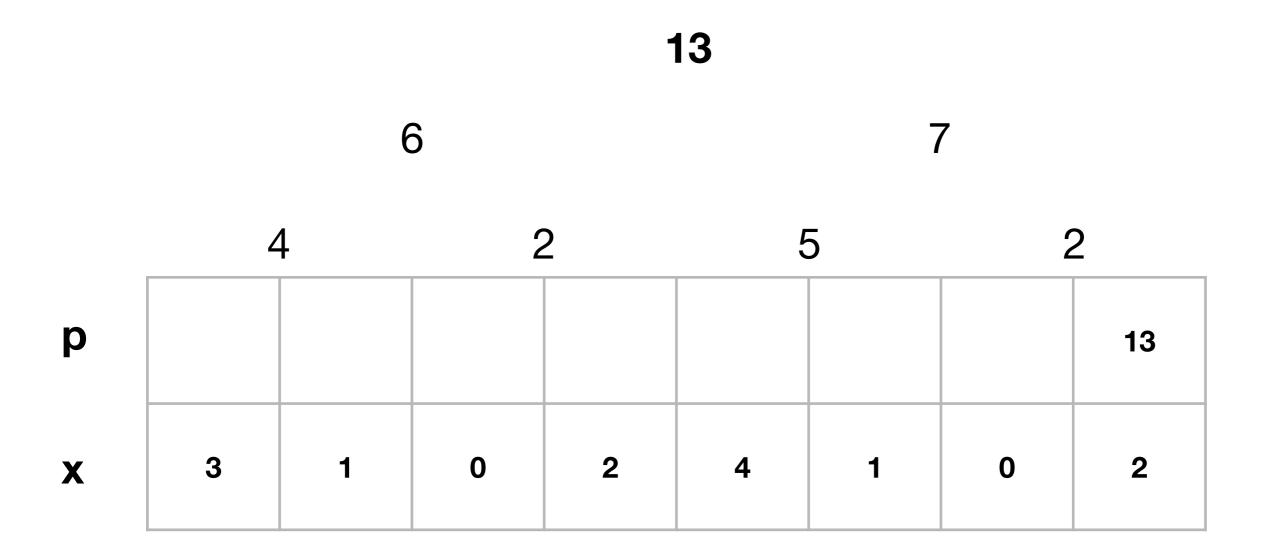
6 7

4 2 5 2

p 13

x 3 1 0 2 4 1 0 2

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13
6 7
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13

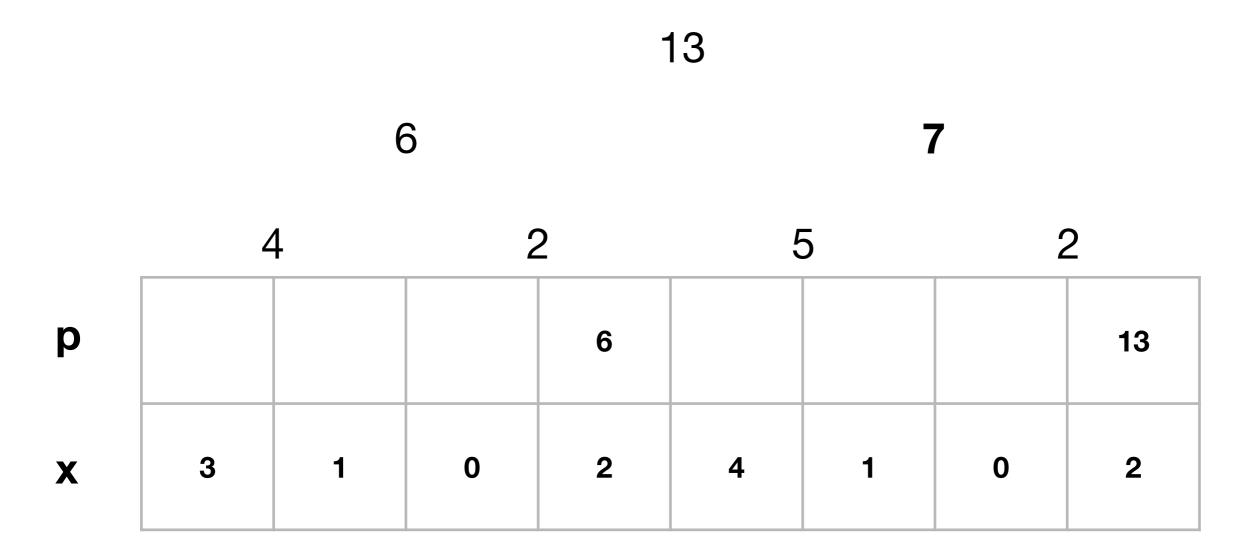
• Thus, p[3]=6.

6

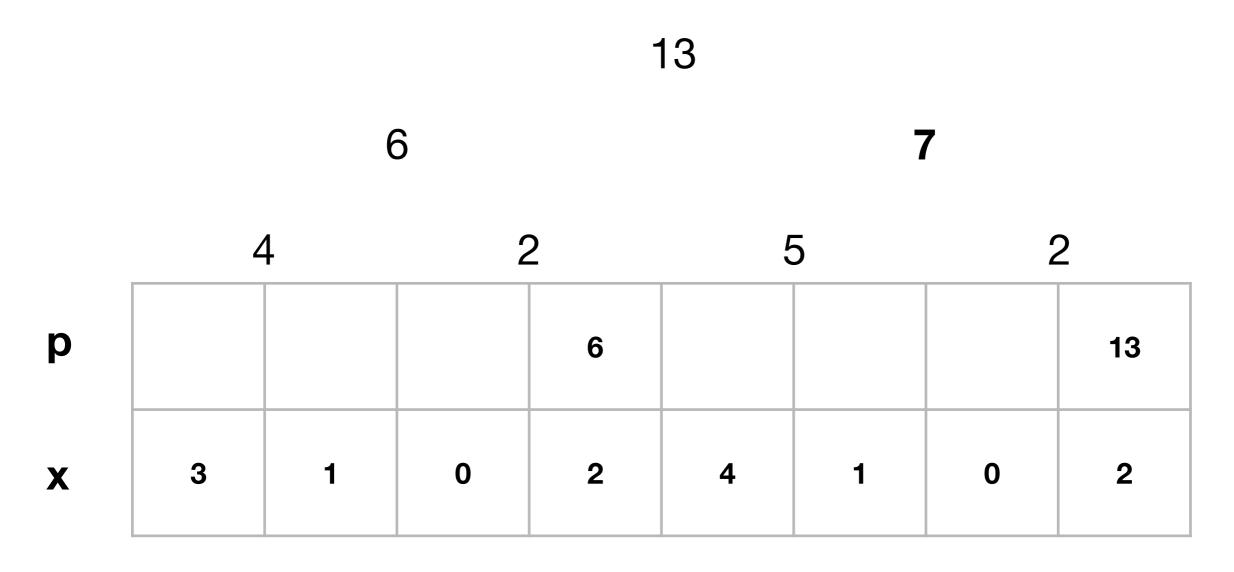
7

	4	1	2	2	5	5		2
p				6				13
X	3	1	0	2	4	1	0	2

• Recursing into 13's right sub-tree (7)



• Recursing into 13's right sub-tree (7), we know that the sum of x [4:6] was 5.



• Recursing into 13's right sub-tree (7), we know that the sum of x [4:6] was 5.

• Thus, p[6]=p[4]+5.

13

6

7

		1	2	2	Ę	5	2	2
p				6		11		13
X	3	1	0	2	4	1	0	2

• By similar logic, we can compute:

13
6
7

4
2
5
2

p
6
10
11
13

x
3
1
0
2
4
1
0
2

• By similar logic, we can compute:

p X

• By similar logic, we can compute:

p X

• Using this **parallel scan**, we reduce the span to  $O(\log n)$ .

p X

 Clearly, we can generalize this approach to the prefix-sum of *vectors* by performing (and parallelizing) the scan channel-wise, e.g.:

P	3, -1	4, 3	4, 5	6, 3	10, 3	11, 6	11, 7	13, 8
X	3, -1	1, 4	0, 2	2, -2	4, 0	1, 3	0, 1	2, 1

• We can also generalize it to the prefix-sums of multiples of the **X**, i.e.,  $p_i = \sum_{i'=1}^i (a \times x_i) = p_{i-1} + a \times x_i$ .

• The example below is for a=2.

P	6, -2	8, 6	8, 10	12, 6	12, 6	22, 12	22, 14	26, 16
X	3, -1	1, 4	0, 2	2, -2	4, 0	1, 3	0, 1	2, 1

- We can further generalize this idea from addition (+) to any binary associative operator ⊕.
- $\oplus$  is associative iff  $x \oplus (y \oplus z) = (x \oplus y) \oplus z \quad \forall x, y, z$
- Examples include scalar addition, scalar multiplication, matrix addition, matrix multiplication.

P	0, -1	4, 3	4, 5	6, 3	6, 3	11, 6	11, 7	13, 8
X	3, -1	1, 4	0, 2	2, -2	4, 0	1, 3	0, 1	2, 1

• What if we want to compute  $p_i = b \times p_{i-1} + x_i$  for all i?

P								
X	3	1	0	2	4	1	0	2

# Exercise

- What if we want to compute  $p_i = b \times p_{i-1} + x_i$  for all *i*?
- Manually compute the answers for b=2:

P								
X	3	1	0	2	4	1	0	2

# Solution

- What if we want to compute  $p_i = b \times p_{i-1} + x_i$  for all i?
- Manually compute the answers for b=2:

P	3	7	14	30	64	129	258	518
X	3	1	0	2	4	1	0	2

- Can we parallelize  $p_i = b \times p_{i-1} + x_i$  for all i?
- We need an associative operator. Maybe  $x \oplus y = bx + y$ ?
- Let's try it out...

P	3	7	14	30	64	129	258	518
X	3	1	0	2	4	1	0	2

- Our operator:  $x \oplus y = bx + y$ 
  - $3 \oplus 1 = b * 3 + 1 = 2 * 3 + 1 = 7$

P

X

3 7

• Our operator:  $x \oplus y = bx + y$ 

• 
$$3 \oplus 1 = b * 3 + 1 = 2 * 3 + 1 = 7$$

• 
$$7 \oplus 0 = 2 * 7 + 0 = 14$$

_	
	Ì

3	7	14
3	1	0

• Our operator:  $x \oplus y = bx + y$ 

• 
$$3 \oplus 1 = b * 3 + 1 = 2 * 3 + 1 = 7$$

• 
$$7 \oplus 0 = 2 * 7 + 0 = 14$$

Looking good so far!

3	7	14	30	64	129	258	518
3	1	0	2	4	1	0	2

• Unfortunately,  $x \oplus y = bx + y$  is not associative:

• 
$$1 \oplus 0 = 2 * 1 + 0 = 2$$

• 
$$3 \oplus 2 = 2 * 3 + 2 = 8$$

• Hence,  $(3 \oplus 1) \oplus 0 \neq 3 \oplus (1 \oplus 0)$ .

3	7	14	30	64	129	258	518
3	1	0	2	4	1	0	2

• Unfortunately,  $x \oplus y = bx + y$  is not associative:

• 
$$1 \oplus 0 = 2 * 1 + 0 = 2$$

• 
$$3 \oplus 2 = 2 * 3 + 2 = 8$$
 Needed to multiply by  $b^2!$ 

• Hence,  $(3 \oplus 1) \oplus 0 \neq 3 \oplus (1 \oplus 0)$ .

P	3	7	14	30	64	129	258	518
X	3	1	0	2	4	1	0	2

- We need a way of storing the current power of b.
- Hence, we will use 2 numbers (u,v) to represent each step of the computation.
- Operator:  $(u, v) \oplus (u', v') = (b^{v'}u + u', v + v')$
- We initialize  $(u, v)=(x_i, 1)$  for each i.

P	3	7	14	30	64	129	258	518
X	3	1	0	2	4	1	0	2

• Operator:  $(u, v) \oplus (u', v') = (b^{v'}u + u', v + v')$ 

• 
$$(3,1) \oplus (1,1) = (2^1 * 3 + 1, 2) = (7,2)$$

•  $(7,2) \oplus (0,1) = (2^1 * 7 + 0,3) = (14,3)$ 

P	3	7	14	30	64	129	258	518
X	3	1	0	2	4	1	0	2

• Operator:  $(u, v) \oplus (u', v') = (b^{v'}u + u', v + v')$ 

• 
$$(1,1) \oplus (0,1) = (2^1,2) = (2,2)$$

• 
$$(3,1) \oplus (2,2) = (2^2 * 3 + 2,3) = (14,3)$$

This operator is associative.

P	3	7	14	30	64	129	258	518	
X	3	1	0	2	4	1	0	2	

• We can thus use a parallel scan to compute  $p_i = b \times p_{i-1} + x_i$  with span  $O(\log n)$ .

(518,8)

(30,4)

(38,4)

(7,2)

(2,2)

(9,2)

(2,2)

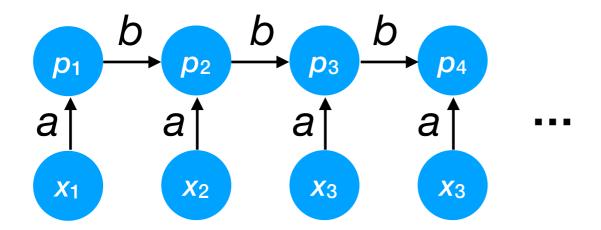
P

3	7	14	30	64	129	258	518
3	1	0	2	4	1	0	2

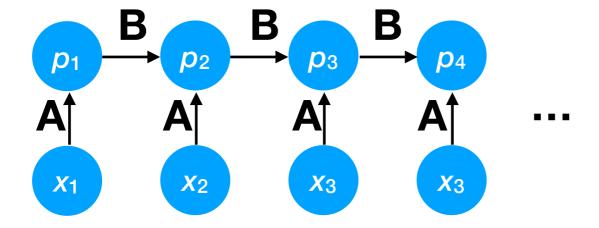
• Putting all the parts together, we can use a parallel scan to compute prefix-sums of the form  $p_i = b \times p_{i-1} + ax_i$ .

P	3	7	14	30	64	129	258	518
X	3	1	0	2	4	1	0	2

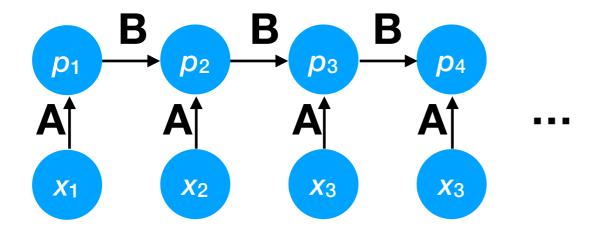
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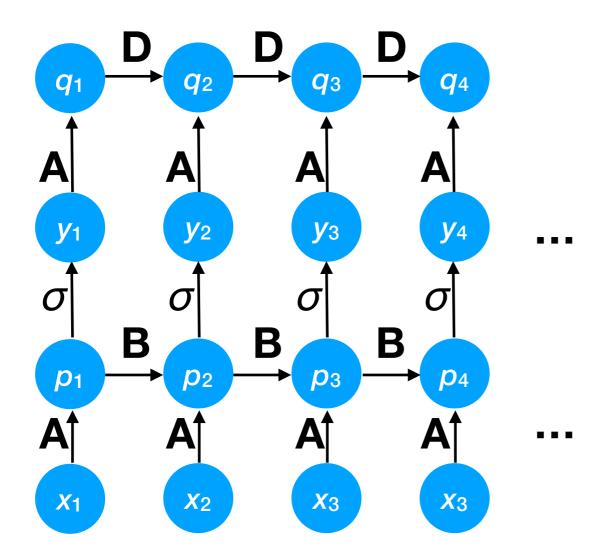
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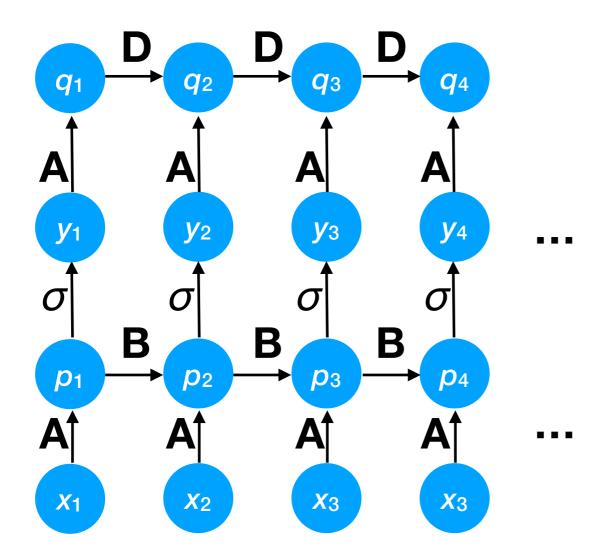
- Putting all the parts together, we can use a parallel scan to compute prefix-sums of the form  $\mathbf{p}_i = \mathbf{B}\mathbf{p}_{i-1} + \mathbf{A}x_i$ .
- This is equivalent to a linear RNN.



 While not sufficient by itself, it can be a powerful component in a larger NN with nonlinearities, e.g.:



• It is also one of the key ideas behind structured state space models (S3), e.g., Mamba.



# Exercises

# Exercise 1

- Suppose that, in a diffusion, we want to "merge" two faces  $\mathbf{x}^{(1)}$  and  $\mathbf{x}^{(2)}$  at some timestep t by computing  $\mathbf{z}_{t}^{(1)}$  and  $\mathbf{z}_{t}^{(2)}$ , averaging to get  $\mathbf{z}_{t} = (\mathbf{z}_{t}^{(1)} + \mathbf{z}_{t}^{(2)})/2$ , and then sampling  $\mathbf{x} \sim P(\mathbf{x} \mid \mathbf{z}_{t})$ ?
- What is (slightly) wrong with this?

# Exercise 2

- Consider the statement:
  - The fundamental goal of a VAE is to minimize reconstruction error while also keeping the KL divergence between Q(z | x) and P(z) low.
- In which sense is this statement true?
- In which sense is it false?