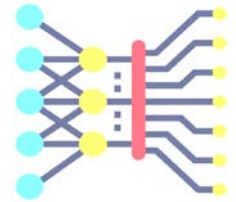


CS60010: Deep Learning

Spring 2023

Sudeshna Sarkar

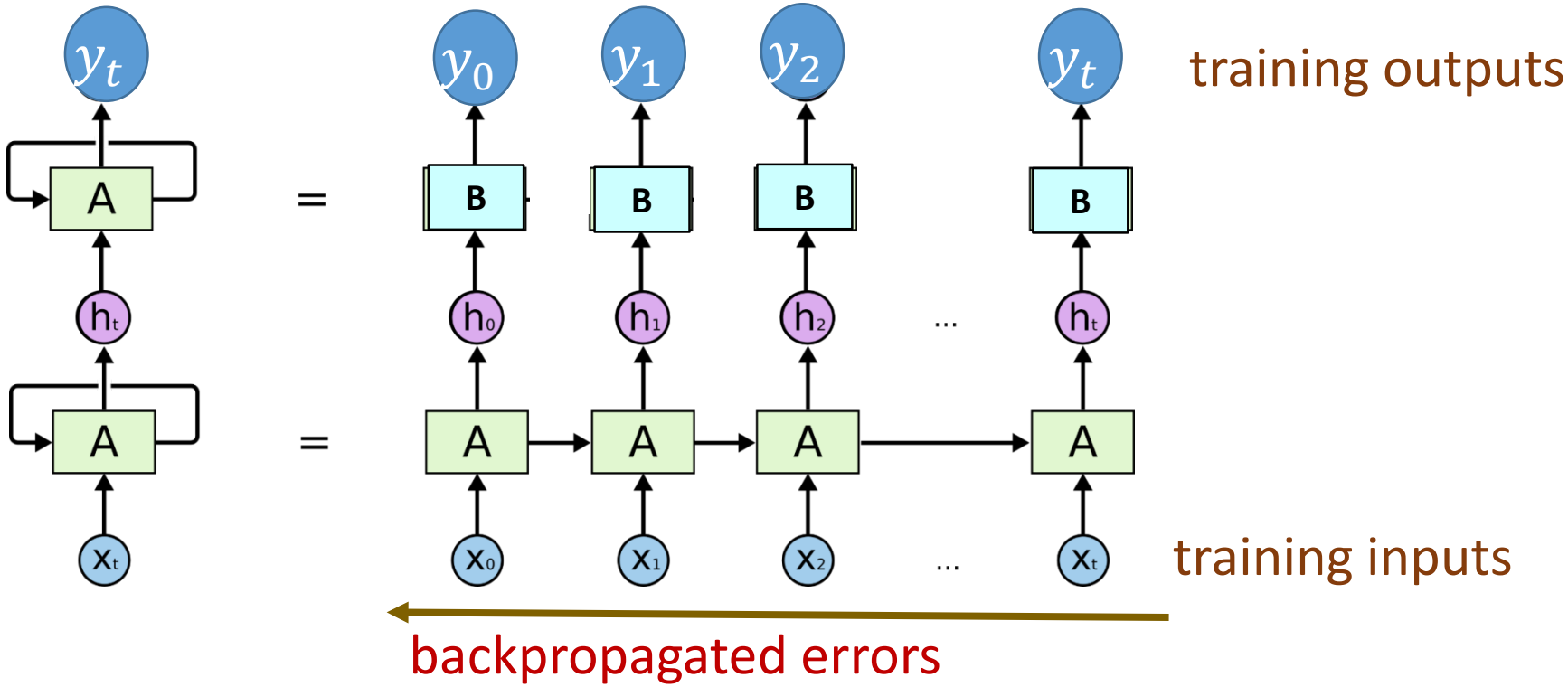
RNN Part 2

Sudeshna Sarkar

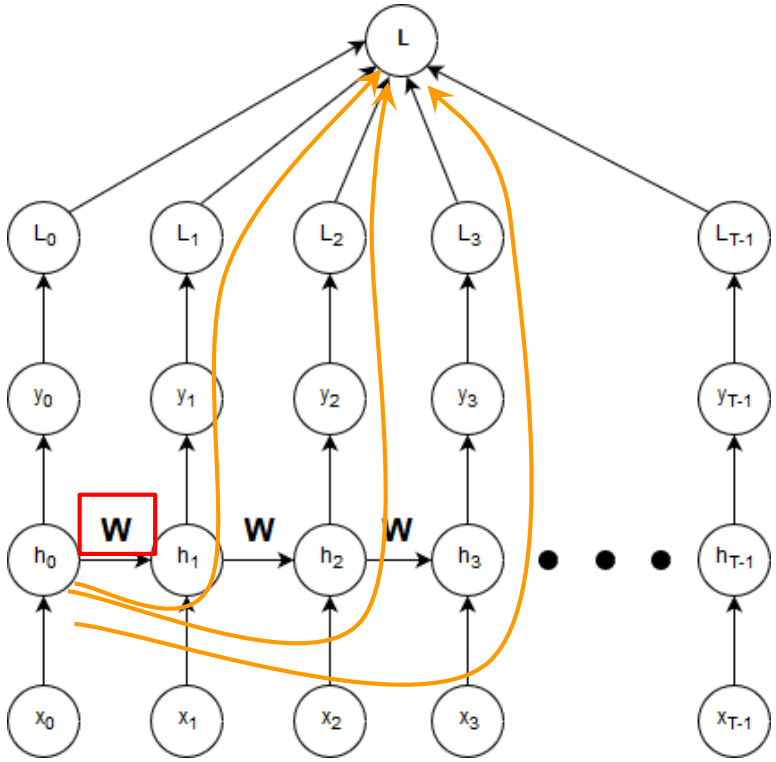
2 Mar 2023

Training RNN's

- RNNs can be trained using "backpropagation through time."
  - applying normal backprop to the unrolled network.



Backpropagation Through Time (BPTT)

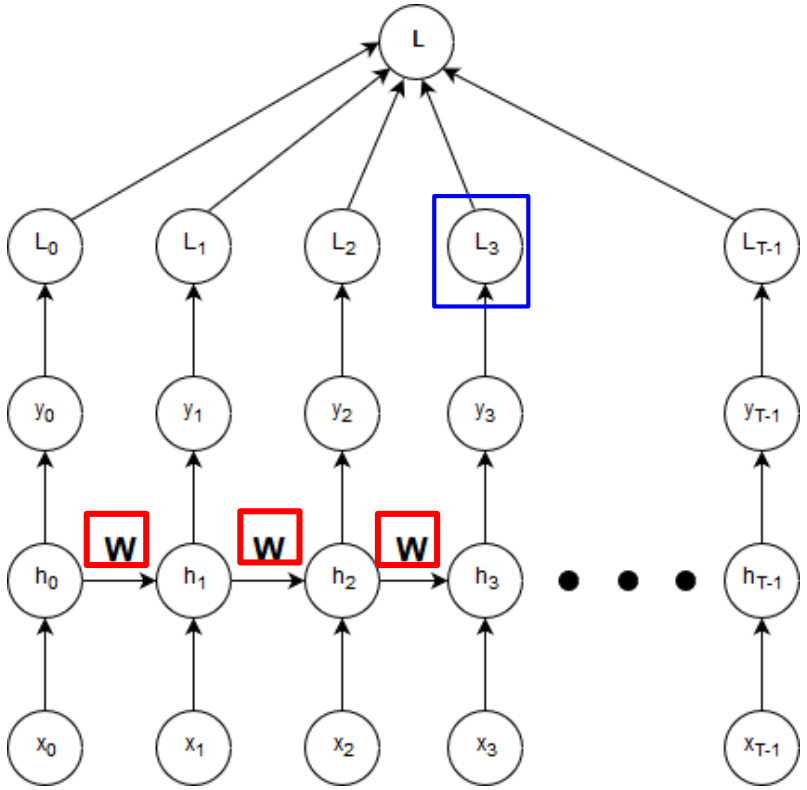


Update the weight matrix:

$$\mathbf{W} \rightarrow \mathbf{W} - \alpha \frac{\partial L}{\partial \mathbf{W}}$$

- Issue: **W** occurs each timestep
- **Every** path from **W** to L is one dependency
- Find all paths from **W** to L!

Backpropagation as two summations



1. First summation over L

$$\frac{\partial L}{\partial \mathbf{W}} = \sum_{j=0}^{T-1} \frac{\partial L_j}{\partial \mathbf{W}}$$

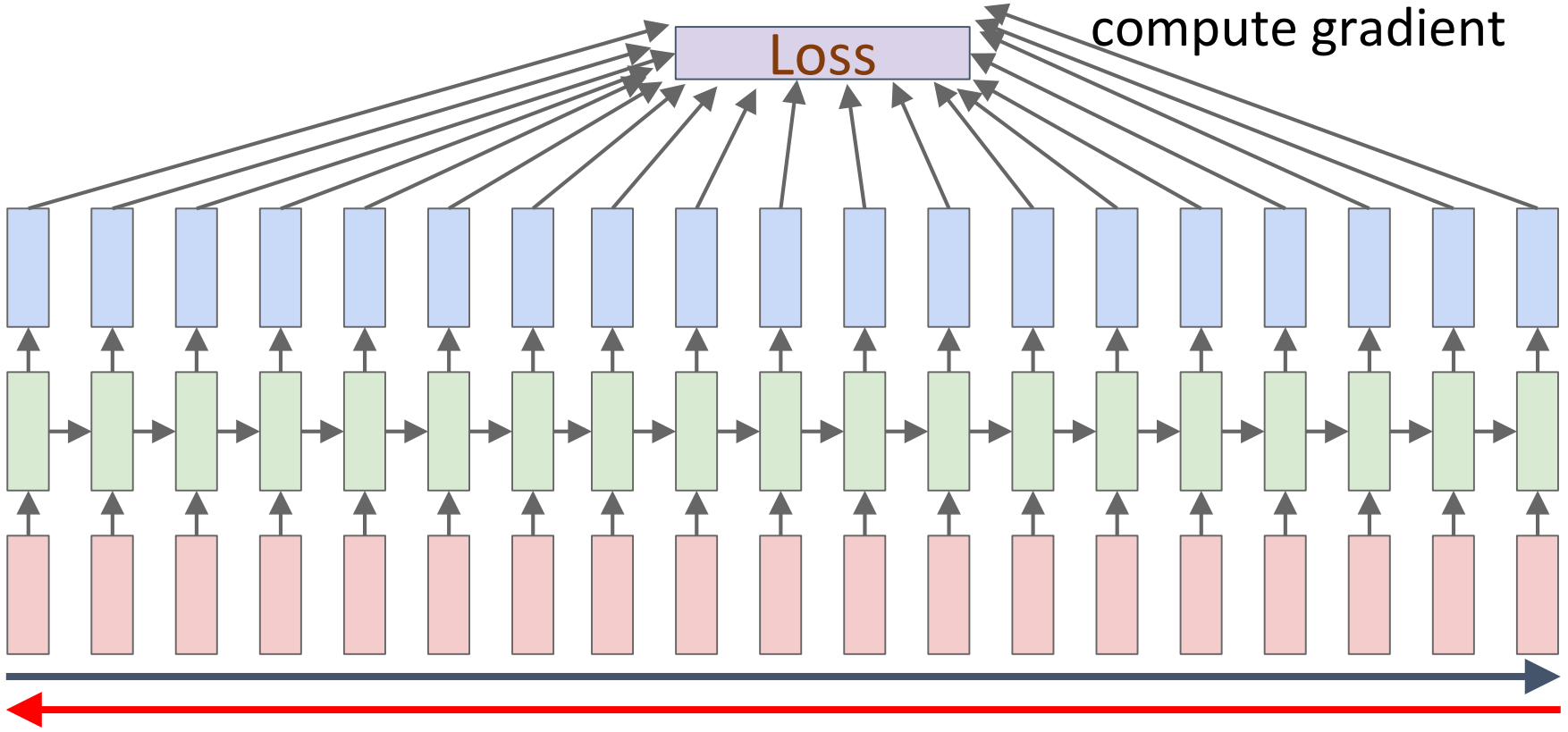
2. Second summation over h: Each L_j depends on the weight matrices *before it*

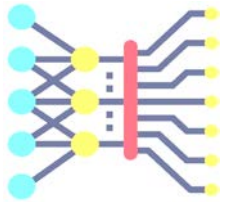
$$\frac{\partial L_j}{\partial \mathbf{W}} = \sum_{k=1}^{j} \frac{\partial L_j}{\partial h_k} \frac{\partial h_k}{\partial \mathbf{W}}$$

L_j depends on all h_k before it.

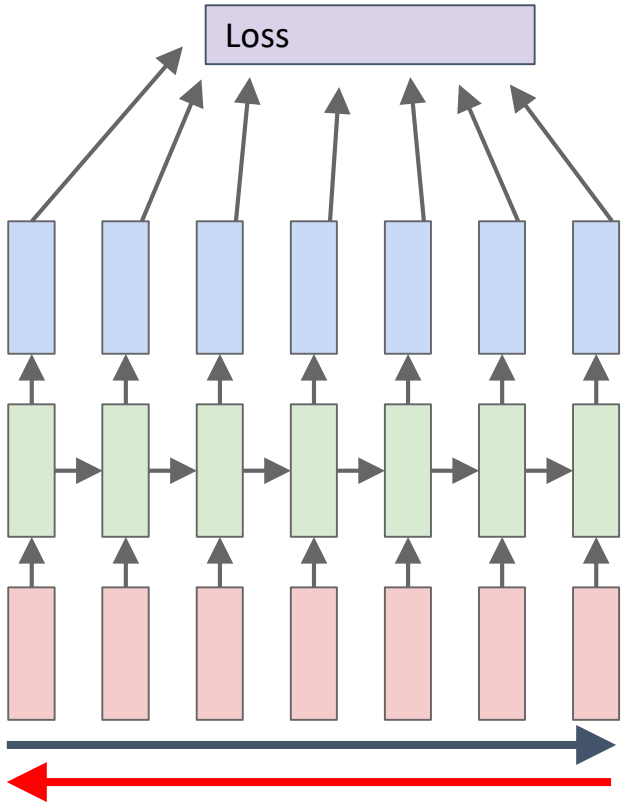
Backpropagation through time

Forward through entire sequence to compute loss, then backward through entire sequence to compute gradient

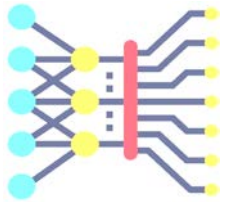




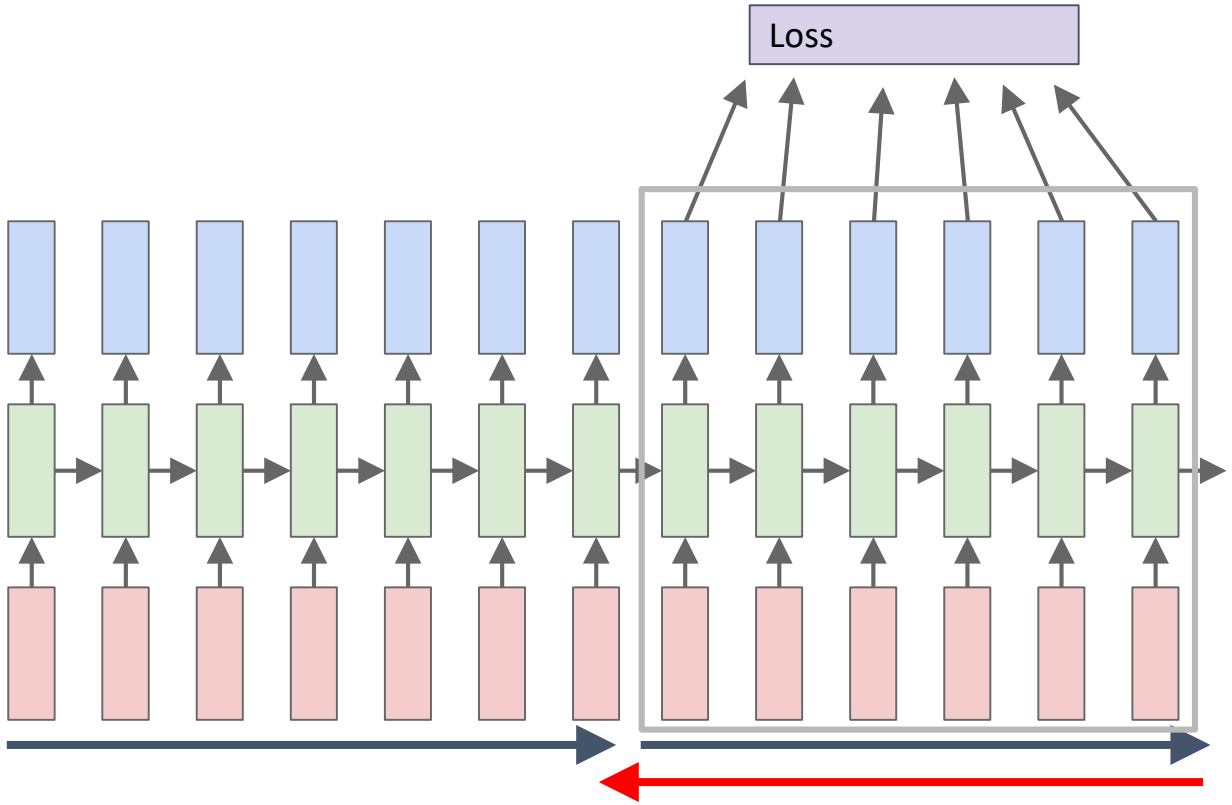
Truncated Backpropagation through time



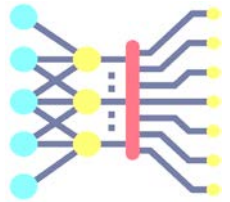
Run forward and backward through chunks of the sequence instead of whole sequence



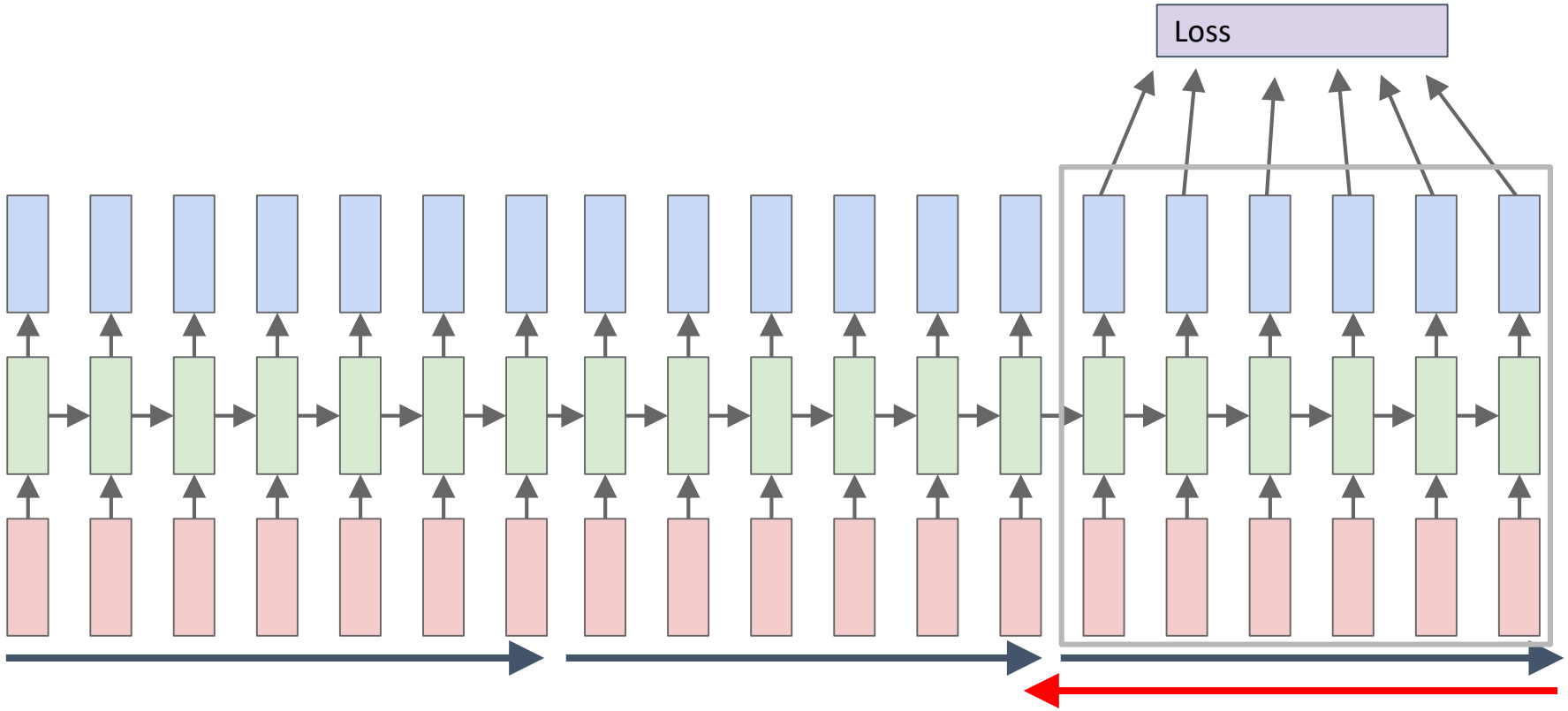
Truncated Backpropagation through time



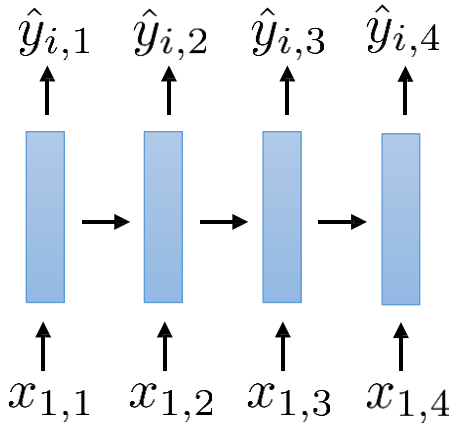
Carry hidden states forward in time forever, but only backpropagate for some smaller number of steps



Truncated Backpropagation through time



RNNs are extremely deep networks



If sequence length is 100, backpropagate through 100 steps.

vanishing gradients = gradient signal from later steps never reaches the earlier steps

this prevents the RNN from "remembering" things from the beginning!

"vanishing gradients"

$$\frac{d\mathcal{L}}{dW^{(1)}} = \frac{dz^{(1)}}{dW^{(1)}} \frac{da^{(1)}}{dz^{(1)}} \frac{dz^{(2)}}{da^{(1)}} \frac{d\mathcal{L}}{dz^{(2)}}$$

$$\frac{d\mathcal{L}}{dW^{(1)}} = J_1 J_2 J_3 \dots J_n \frac{d\mathcal{L}}{dz^{(n)}}$$

If we multiply many many numbers together, what will we get?

If most of the numbers are < 1, we get 0

If most of the numbers are > 1, we get infinity

We only get a reasonable answer if the numbers are all close to 1!

"exploding gradients"

could fix with gradient clipping

Promoting better gradient flow

$$C^{(t)} = Q\left(C^{(t-1)}, x^{(t)}\right)$$

Basic idea: we would really like the gradients to be close to 1

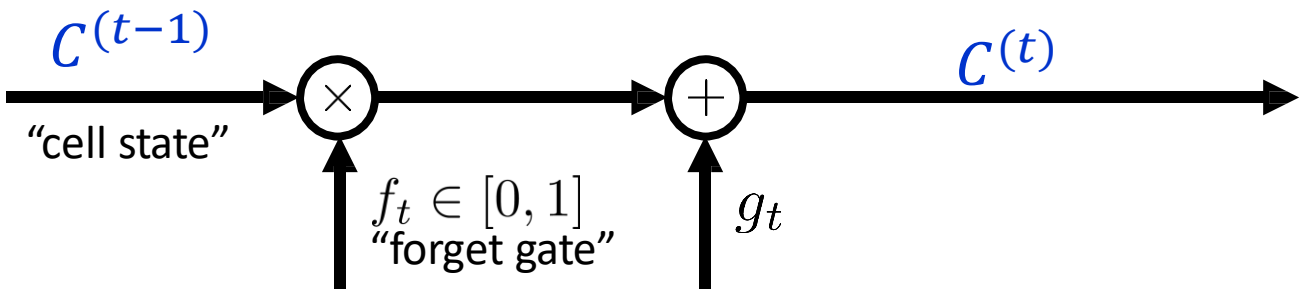
for each unit, we have a little "neural circuit" that decides whether to remember or overwrite

if "remembering," just copy the previous activation as it is

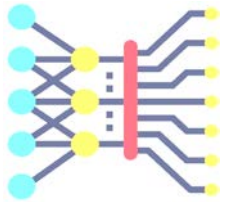
if "forgetting," just overwrite it with something based on the current input

$$C^{(t)} = C^{(t-1)} f_t + g_t$$

$$\frac{dQ}{dC^{(t-1)}} = f_t \in [0,1]$$



Gated RNNs

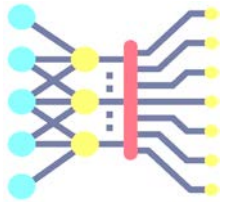


- **Gated RNNs** contain **gates** to control what information is passed through.

Gated Cells

LSTM, GRU, etc

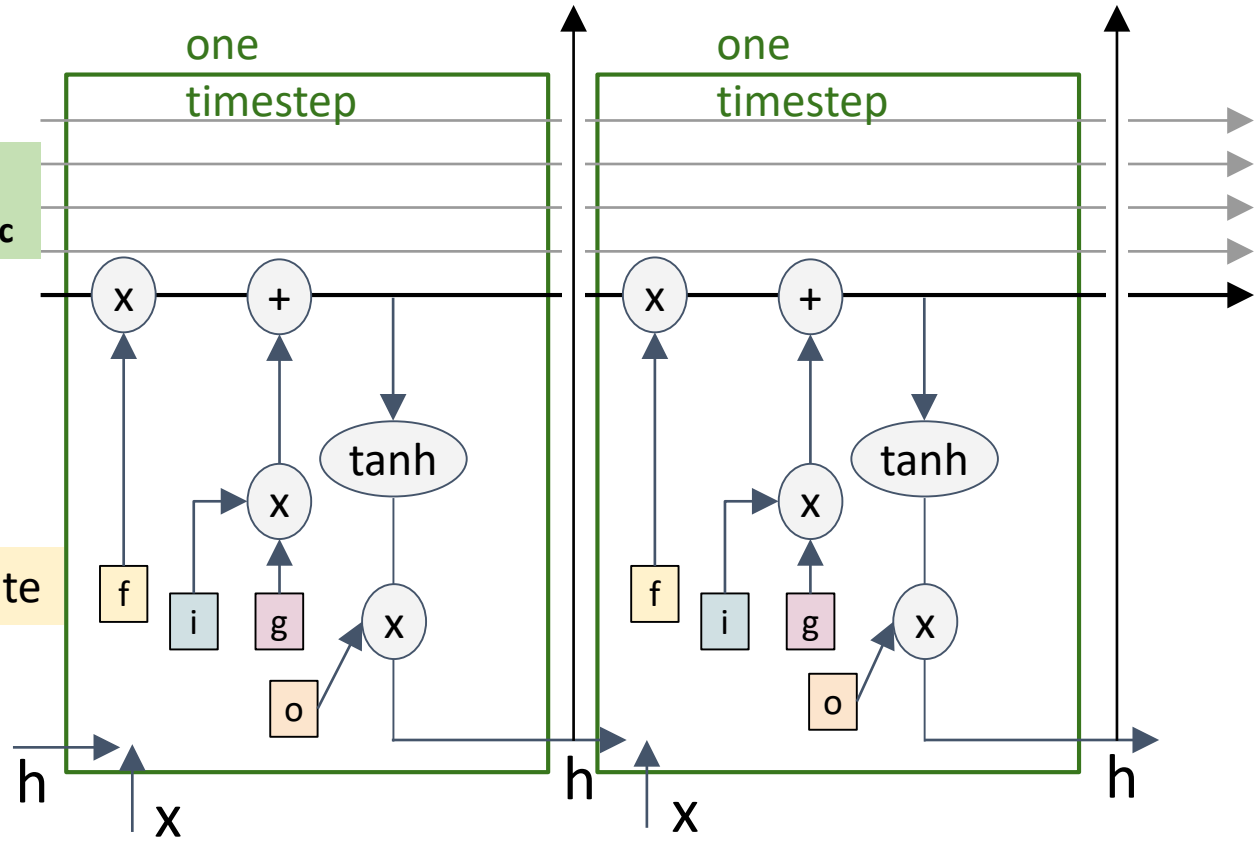
Long short-term memory (LSTM)



1. A special kind of RNN, capable of learning long-term dependencies.
2. Introduced by Hochreiter & Schmidhuber (1997)

LSTMs: learnable gates

$$
\begin{aligned}
g_t &= tanh(U_g h_{t-1} + W_g x_t) \\
i_t &= \sigma(U_i h_{t-1} + W_i x_t) \\
f_t &= \sigma(U_f h_{t-1} + W_f x_t) \\
o_t &= \sigma(U_o h_{t-1} + W_o x_t) \\
c_t &= f_t \odot c_{t-1} + i_t \odot g_t \\
h_t &= o_t \odot tanh(c_t)
\end{aligned}
$$



forget gate

RNN output at previous time step

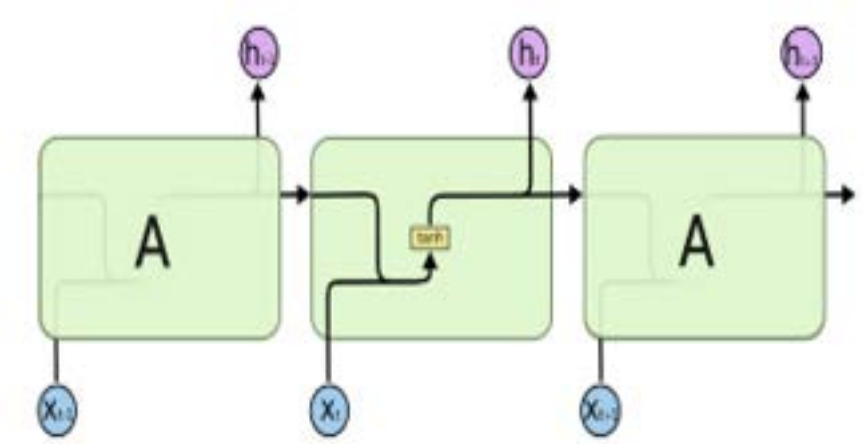
changes very little step to step!

"long term" memory

changes all the time (multiplicative)

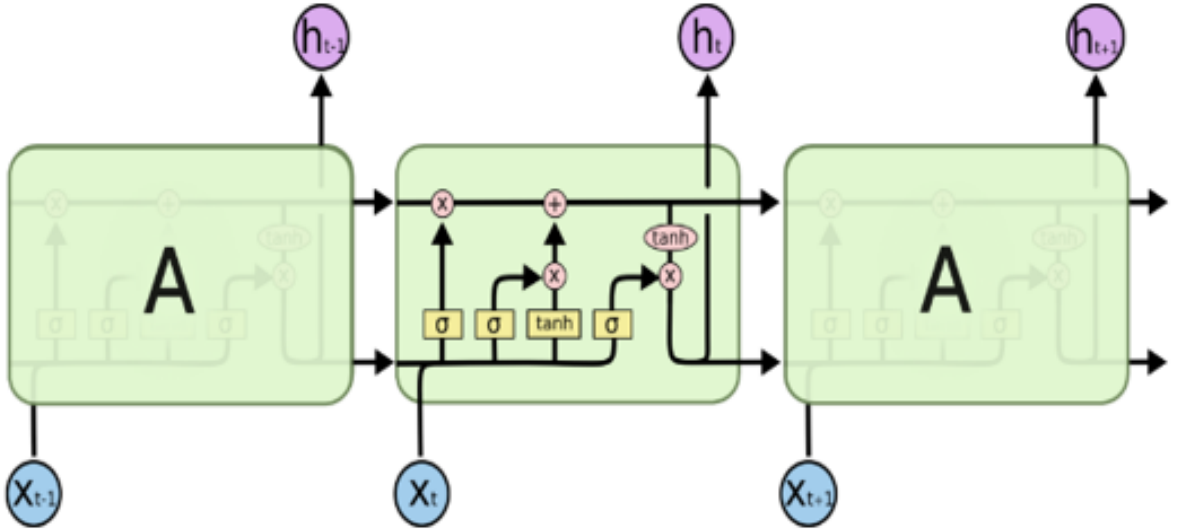
"short term" memory

Basic RNN unit



$$h_t = \tanh\left(W \begin{pmatrix} h_{t-1} \\ x_t \end{pmatrix}\right)$$

LSTM unit

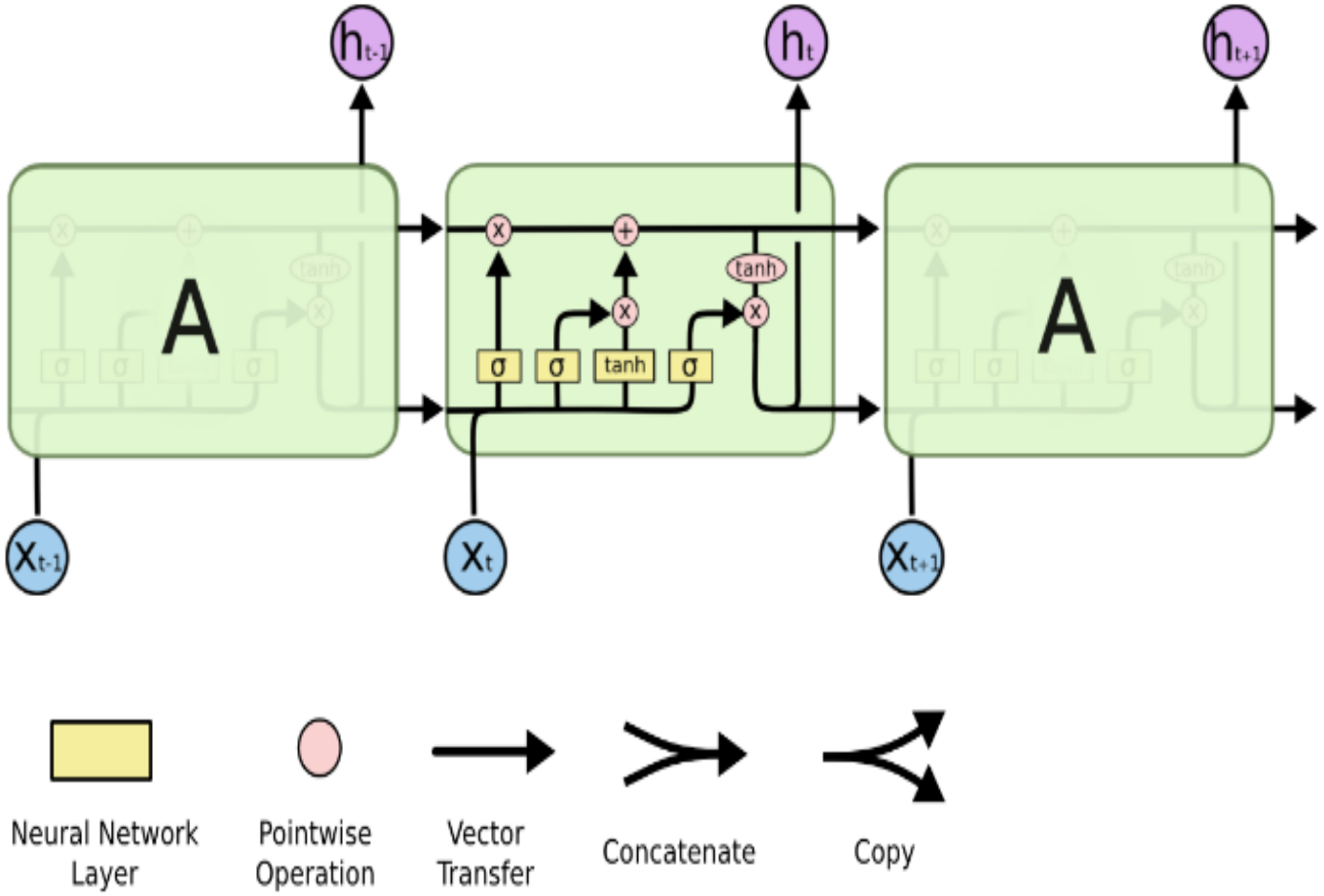


$$\begin{pmatrix} i \\ f \\ o \\ g \end{pmatrix} = \begin{pmatrix} \sigma \\ \sigma \\ \sigma \\ \tanh \end{pmatrix} W \begin{pmatrix} h_{t-1} \\ x_t \end{pmatrix}$$

$$c_t = f \odot c_{t-1} + i \odot g$$

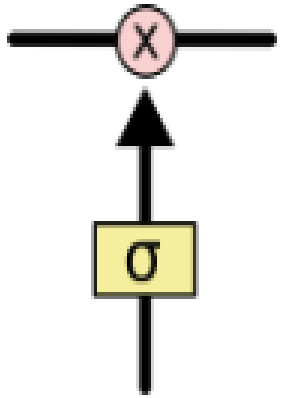
$$h_t = o \odot \tanh(c_t)$$

Long short-term memory

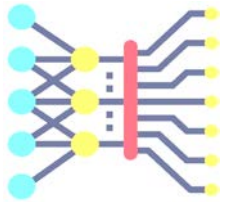


Information added or removed through gates.

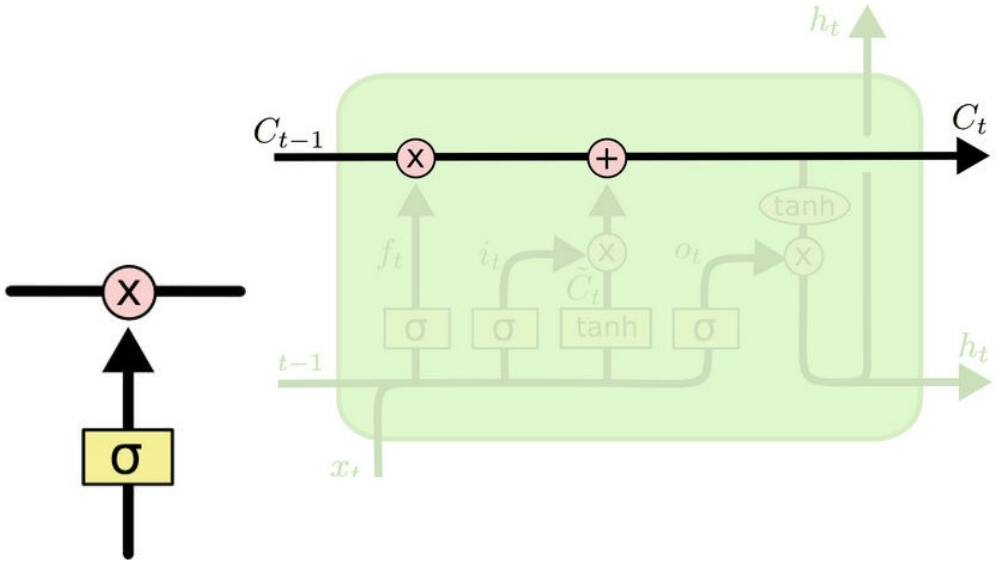
Ex: sigmoid net and pointwise multiplication



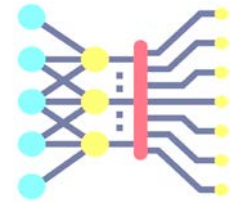
Core idea behind LSTM



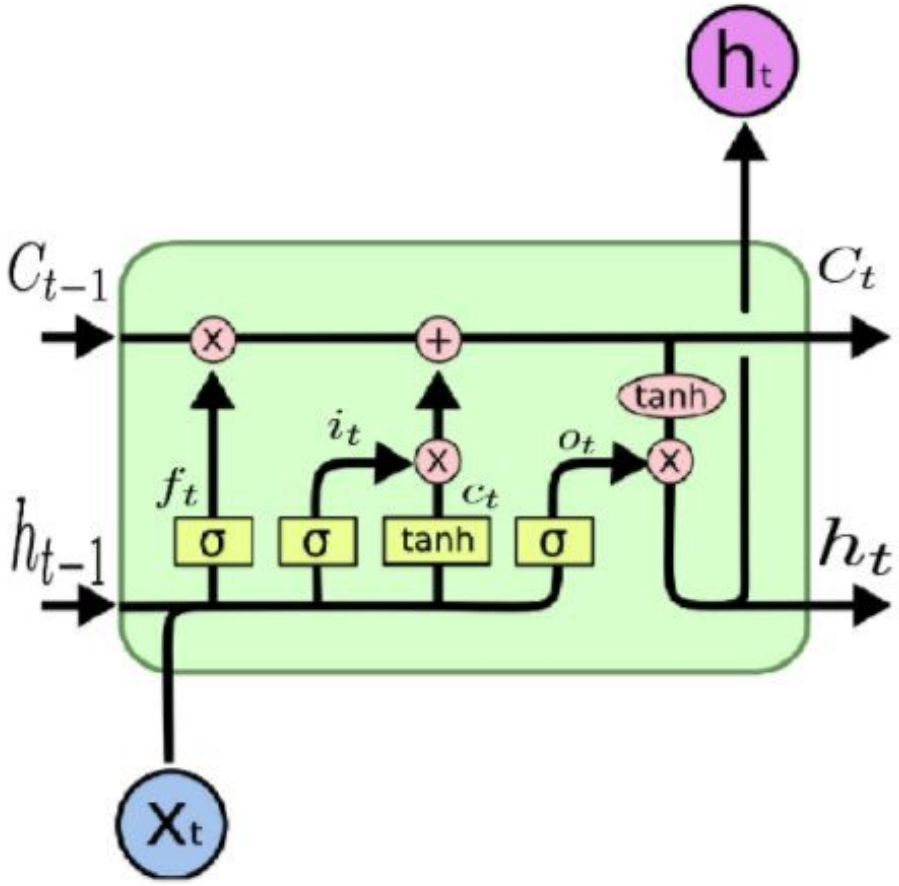
- Gates are an optional way to let information through.
- Three gates protect and control cell state



Long short-term memory



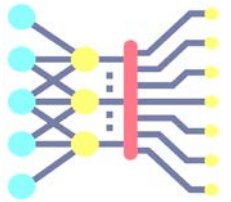
(1) Forget (2) Input (3) Update (4) Output



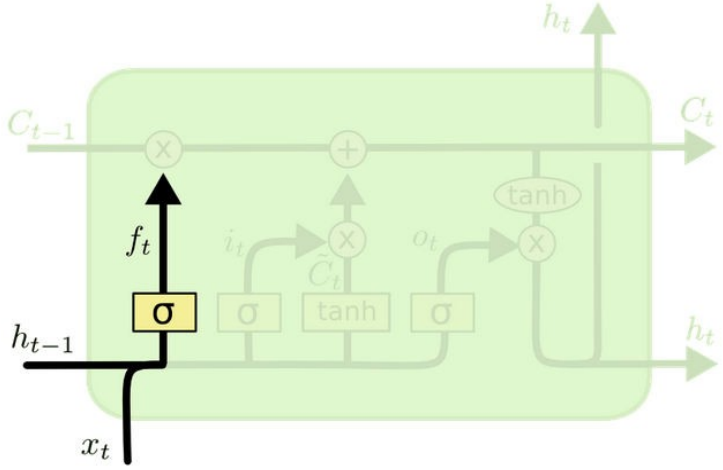
The key to LSTMs is the **cell state**,

It runs straight down the entire chain, with only some minor linear interactions.

LSM walk through: Step 1



- **Step 1:** decide what information we're going to throw away from the cell state : "forget gate layer."
- It looks at ht−1 and xt, and outputs a number between 0 and 1 for each number in the cell state Ct−1 for whether to forget.

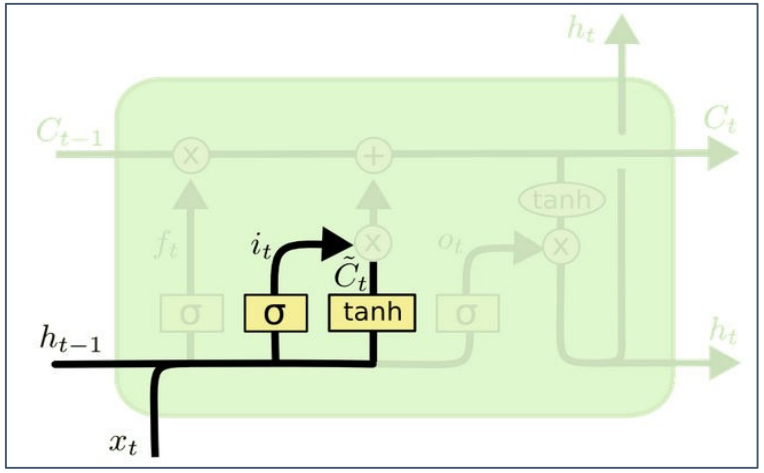


$$f_t = \sigma\left(W_f \cdot [h_{t-1}, x_t] \; + \; b_f\right)$$

- Language model: predict next word based on previous ones
  - Cell state may include the gender of the present subject so that the proper pronouns can be used
- When we see a new subject we want to forget old subject

LSTM walk through: Step 2

Decide what new information we're going to store in the cell state



$$i_t = \sigma\left(W_i \cdot [h_{t-1}, x_t] \; + \; b_i\right)$$

$$\tilde{C}_t = \tanh(W_C \cdot [h_{t-1}, x_t] \; + \; b_C)$$

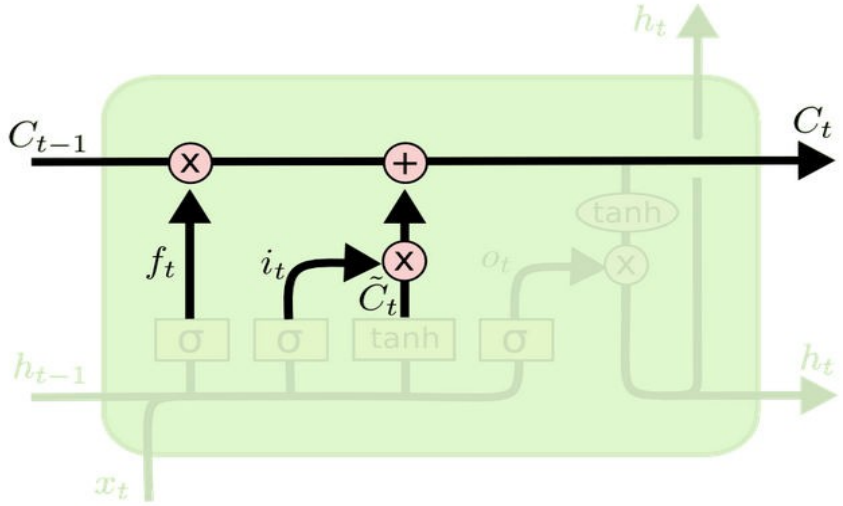
Two parts:
Input gate layer: decides which values we will update

Atanh layer creates a vector of new candidate values (C_t)˜ that could be added to the state.

In the Language model, we'd want to add the gender of the new subject to the cell state, to replace the old one we are forgetting

LSTM walk through: Step 3

- Update old cell state C_{t-1} into new cell state C_t.



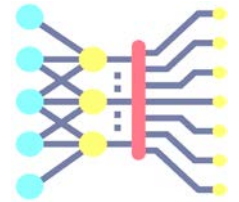
Multiply the old state by f_t, forgetting the things we decided to forget earlier.

- Then we add $i_t * \tilde{C}_t$.

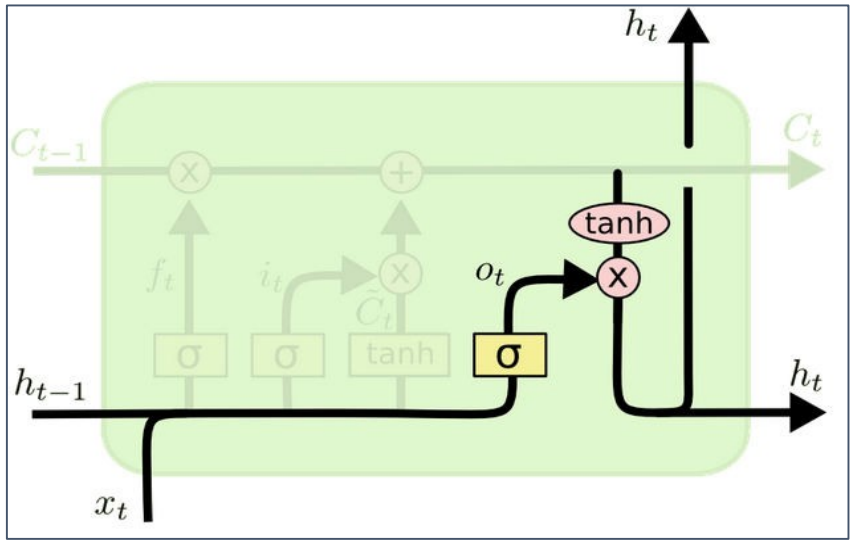
$$C_t = f_t * C_t + i_t * \tilde{C}_t$$

In the Language model, this is where we'd actually drop the information about the old subject's gender and add the new information, as we decided in previous steps

LSTM walk through: Step 4



Finally we decide what we are going to output



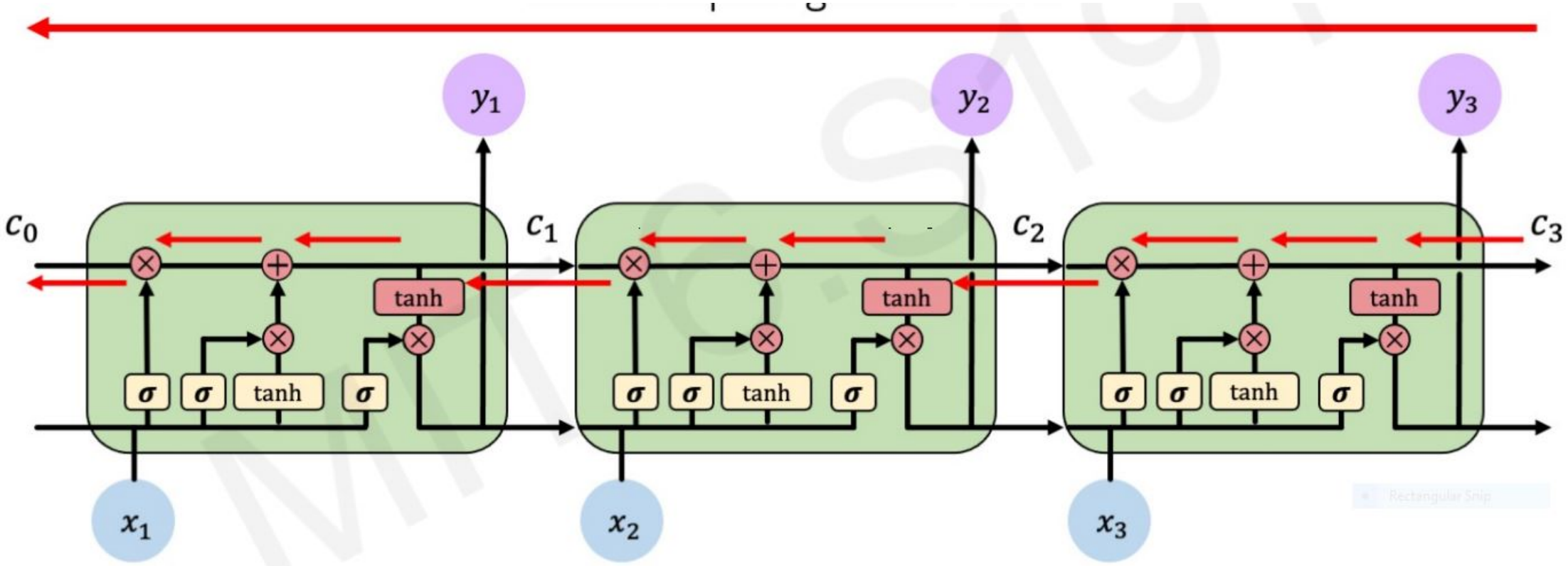
This output will be based on our cell state, but will be a filtered version.
First we run a sigmoid layer which decides what parts of cell state we're going to output. Then we put the cell state through tanh (to push values to be between -1 and 1) and multiply it by the output of the sigmoid gate, so that we output only the parts we decided to

For the Language model,
Since it just saw a subject it might want to output information relevant to a verb, in case that

$$o_t = \sigma\left(W_o\left[h_{t-1}, x_t\right] + b_o\right)$$

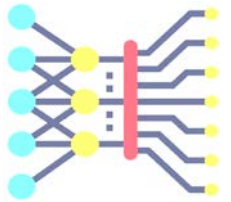
$$h_t = o_t * \tanh\left(C_t\right)$$

LSTM gradient flow is uninterrupted.

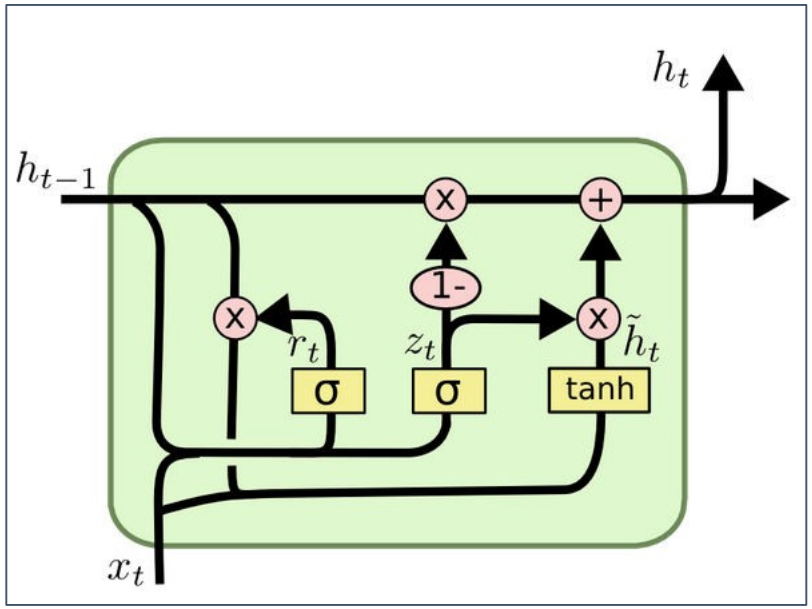


Backpropagation from c_t to c_{t-1} only elementwise multiplication by f, no matrix multiply by W

Gated Recurrent Unit (GRU)



- A dramatic variant of LSTM
  - It combines the forget and input gates into a single update gate
  - It also merges the cell state and hidden state, and makes some other changes
  - The resulting model is simpler than LSTM models



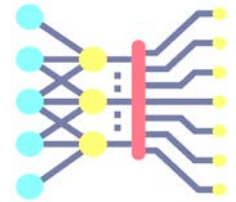
$$z_t = \sigma\left(W_z \cdot [h_{t-1}, x_t]\right)$$

$$r_t = \sigma\left(W_r \cdot [h_{t-1}, x_t]\right)$$

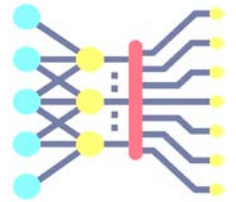
$$\tilde{h}_t = \tanh\left(W \cdot [r_t * h_{t-1}, x_t]\right)$$

$$h_t = (1 - z_t) * h_{t-1} + z_t * \tilde{h}_t$$

Notes

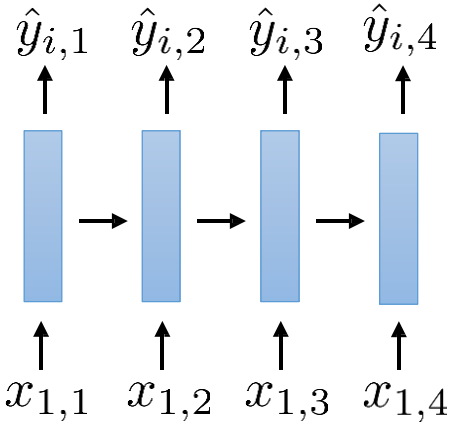


- Vanilla RNNs are simple but don’t work very well
- Common to use LSTM or GRU: their additive interactions improve gradient flow
- Backward flow of gradients in RNN can explode or vanish. Exploding is controlled with gradient clipping. Vanishing is controlled with additive interactions (LSTM)
- LSTM units are OK – they work fine in many cases, and dramatically improve over naïve RNNs
  - Still require lot of hyperparameter tuning
- LSTM cells are complicated, but once implemented, they can be used the same as any other type of layer.



Using RNNs

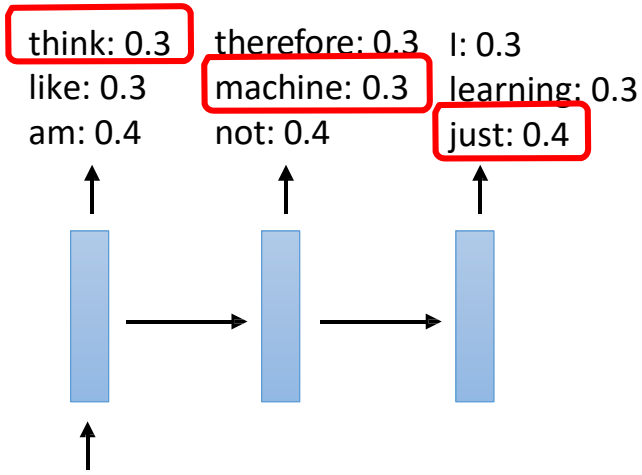
Autoregressive models and structured prediction



most problems that require multiple outputs have strong **dependencies** between these outputs

this is sometimes referred to as **structured** prediction

Example: text generation



I think therefore I am

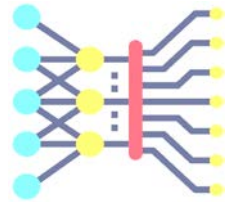
I like machine learning

I am not just a neural network

we get a nonsense output even though the network had exactly the right probabilities!

Key idea: past outputs should influence future outputs!

Autoregressive models and structured prediction



How do we train it?

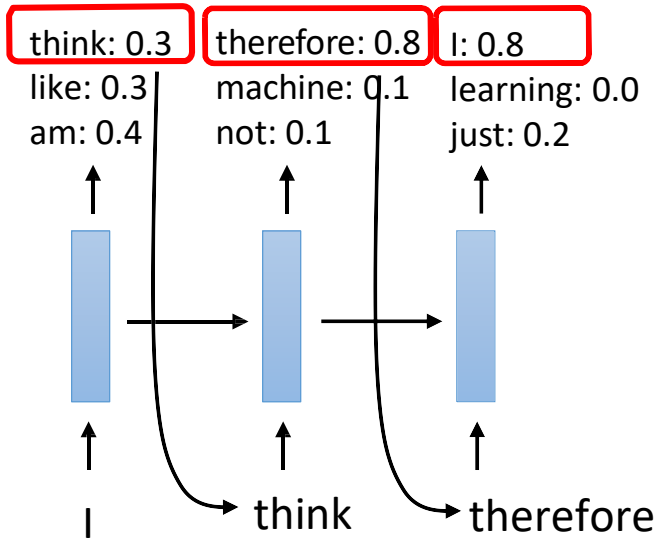
Basic version: just set inputs to be entire training sequences, and ground truth outputs to be those same sequences (offset by one step)

$$x_{1:5} = (\text{“I”}, \text{“think”}, \text{“therefore”}, \text{“I”}, \text{“am”})$$

$$y_{1:5} = (\text{“think”}, \text{“therefore”}, \text{“I”}, \text{“am”}, \text{stop\_token})$$

This teaches the network to output “am” if it sees “I think therefore I”

Example: text generation



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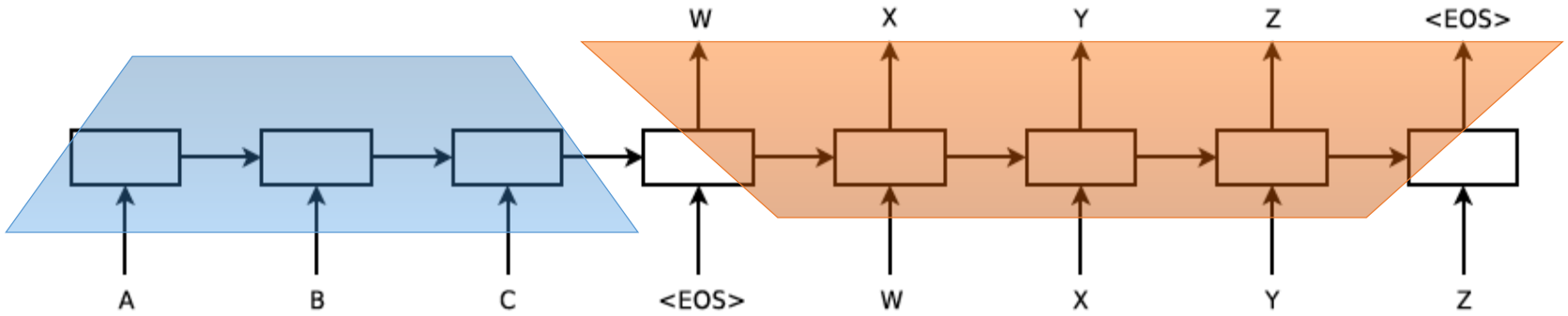
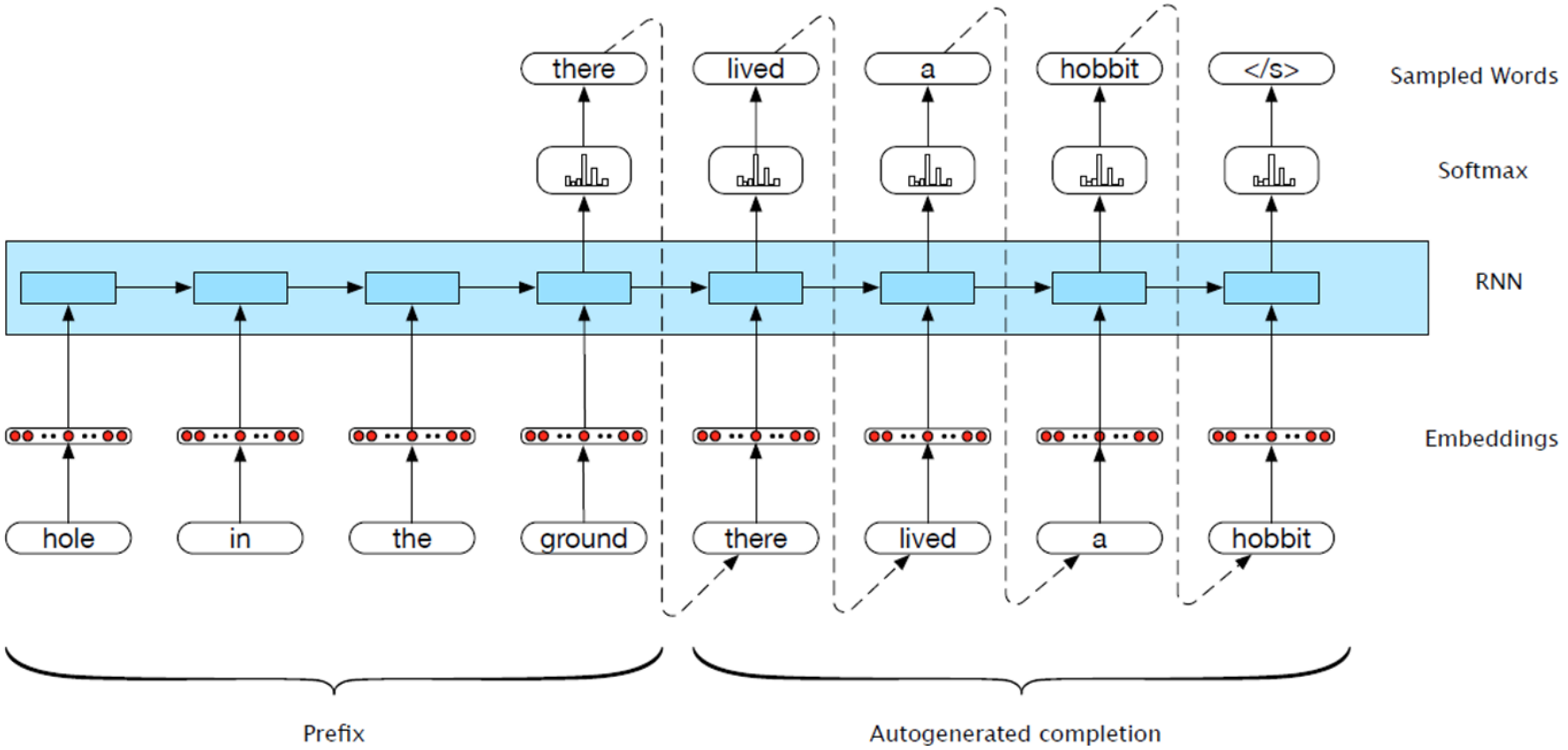
Neural Machine Translation



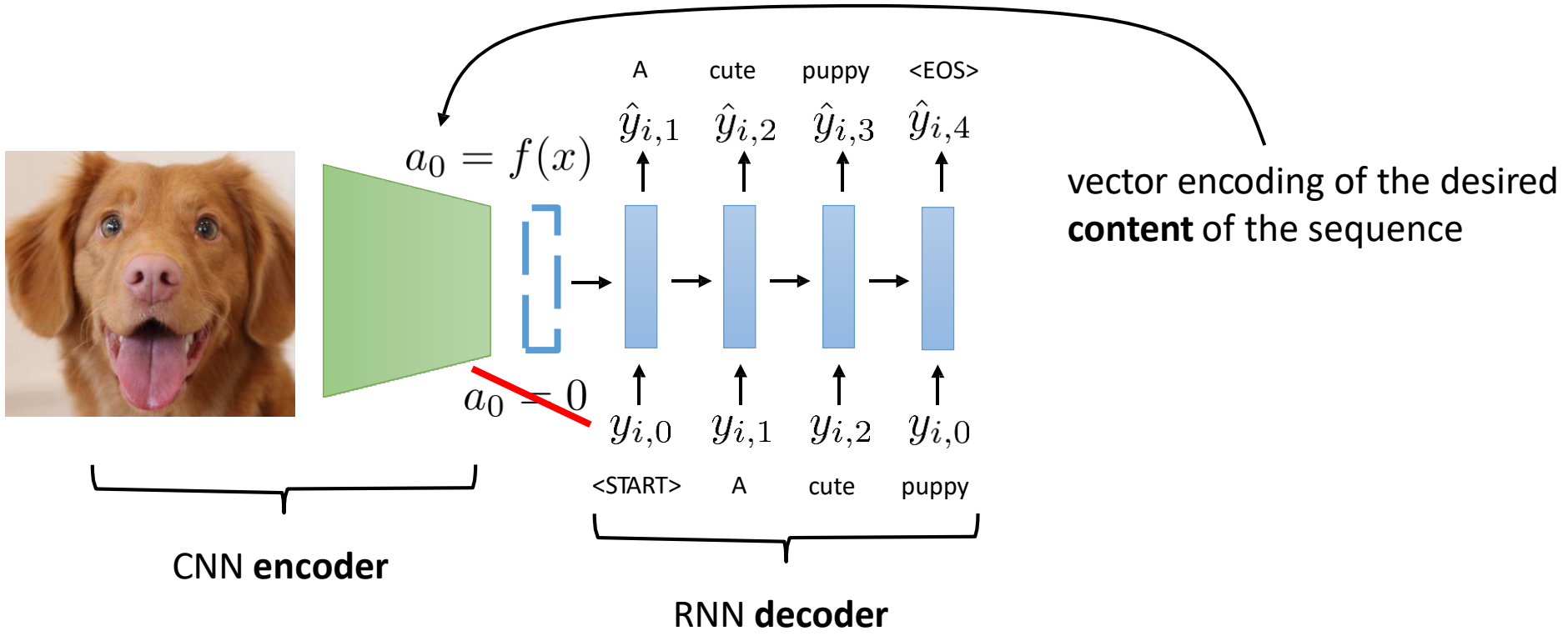
Sutskever et al. 2014

Generation with prefix: Conditional Language Model

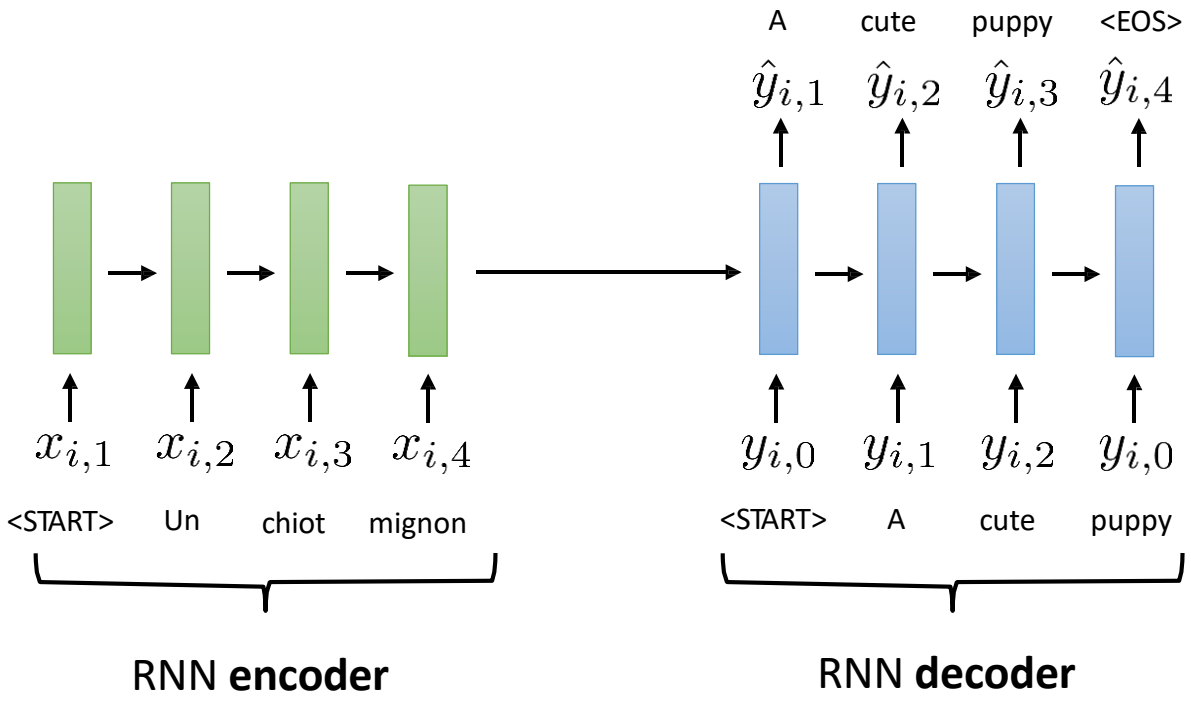


$$h_t = g(h_{t-1}, x_t)$$
$$y_t = f(h_t)$$

A conditional language model



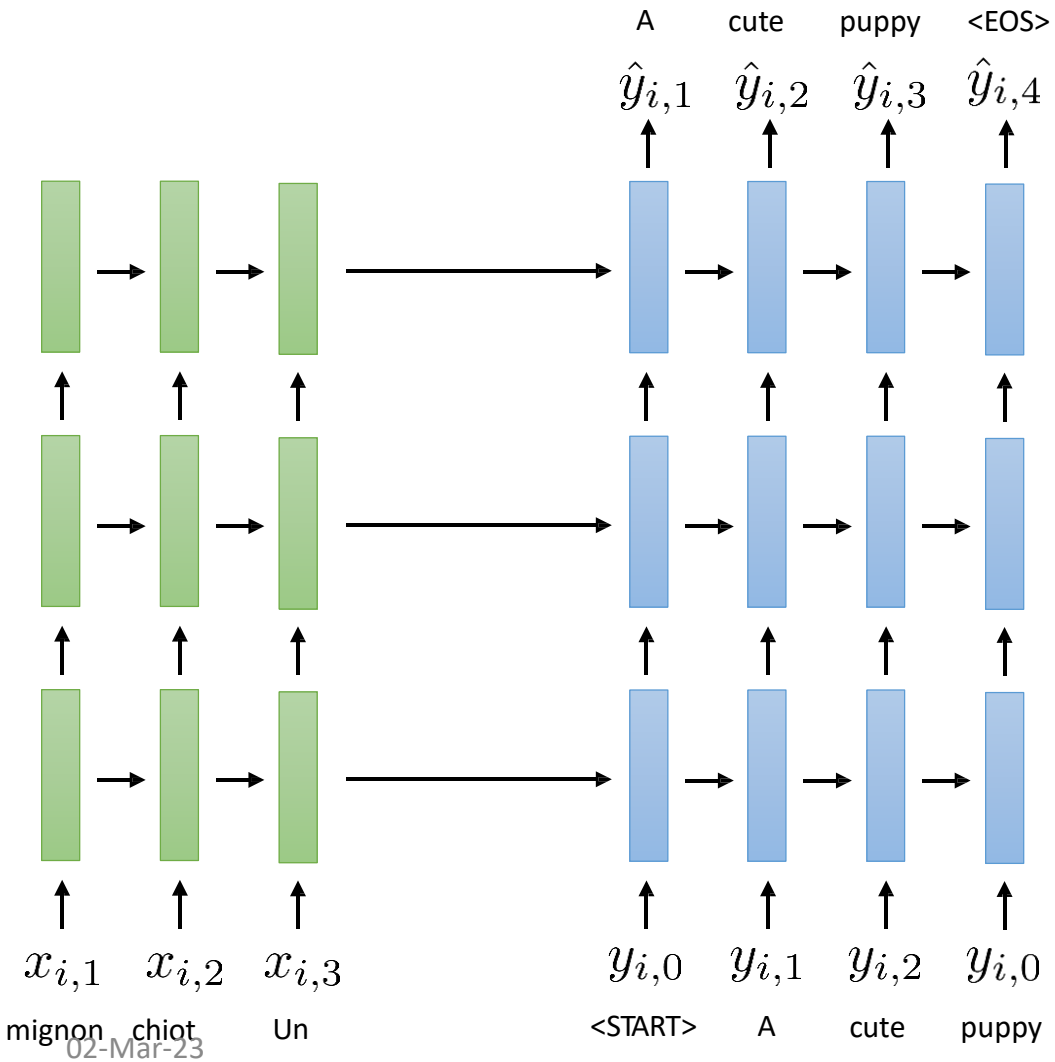
Sequence to sequence models



typically two **separate** RNNs (with different weights)

trained **end-to-end** on paired data (e.g., pairs of French & English sentences)

Deeper models

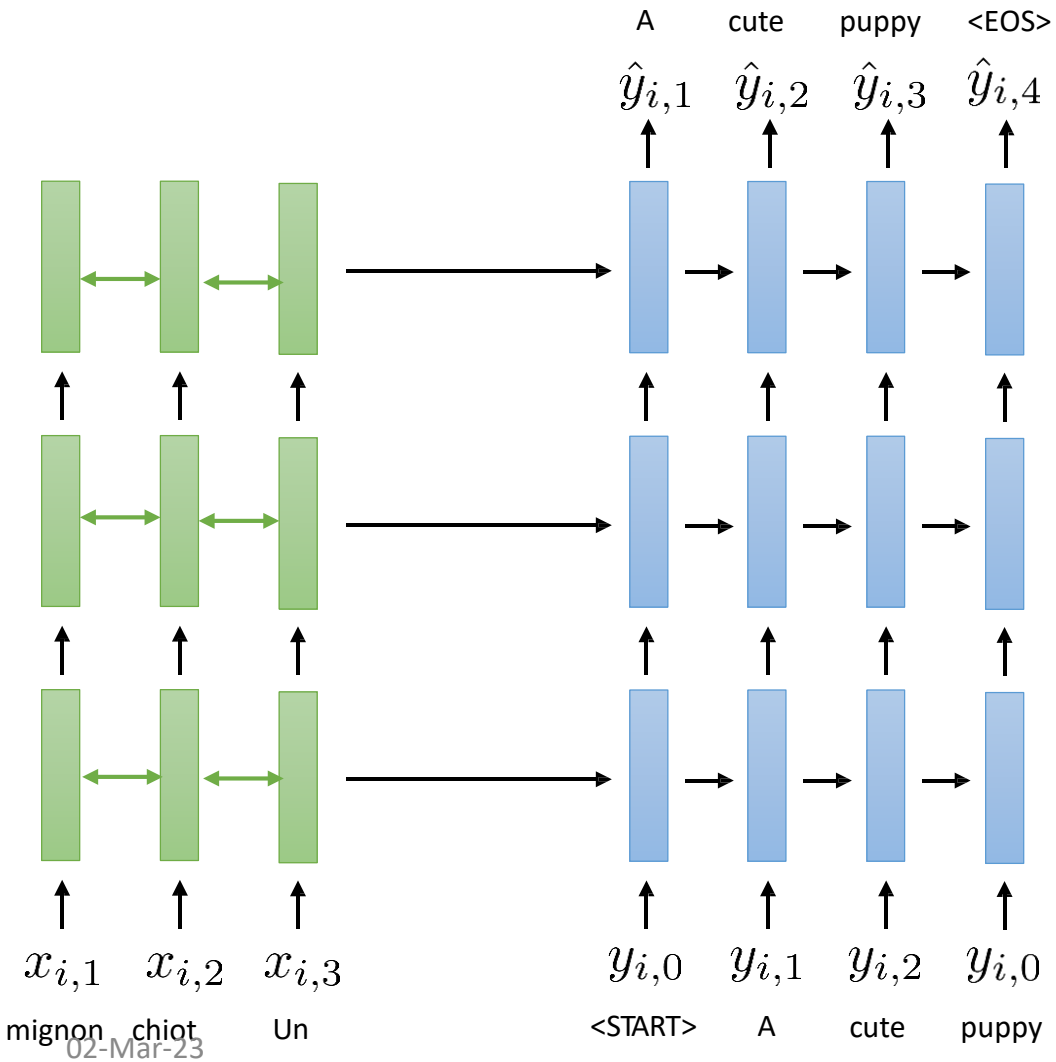


- Multiple RNN layers
- Each RNN layer uses LSTM cells (or GRU)
- Trained end-to-end on pairs of sequences
- Sequences can be different lengths

- Translate **one language** into **another language**
- Summarize a **long sentence** into a **short sentence**
- Respond to a **question** with an **answer**
- Code generation? **text** to **Python code**

For more, see: Ilya Sutskever, Oriol Vinyals, Quoc V. Le. **Sequence to Sequence Learning with Neural Networks**. 2014.

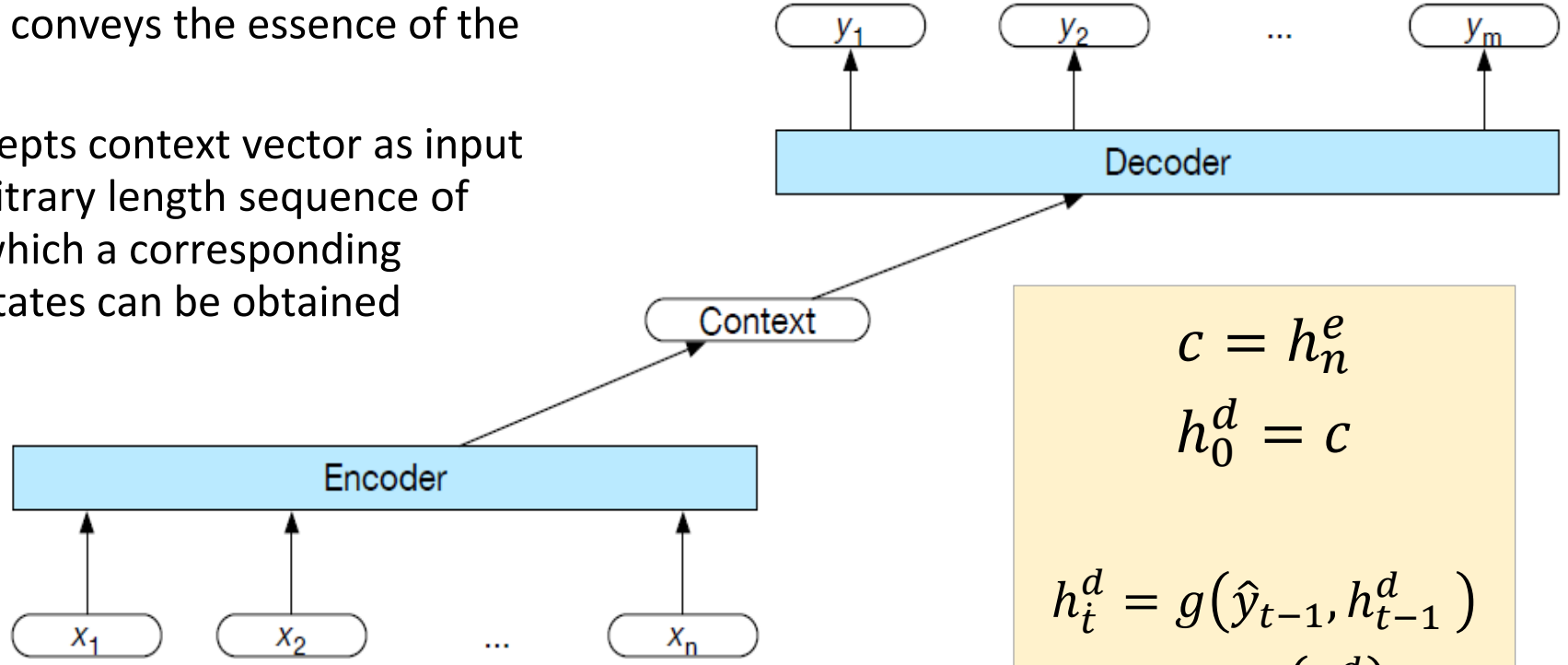
Bidirectional models



Encoder-decoder networks

- An **encoder** that accepts an input sequence and generates a corresponding sequence of contextualized representations
- A **context vector** that conveys the essence of the input to the decoder
- A **decoder**, which accepts context vector as input and generates an arbitrary length sequence of hidden states, from which a corresponding sequence of output states can be obtained

simple RNNs, LSTMs, GRUs, stacked Bi-LSTMs widely used CNN



$$c = h_n^e$$

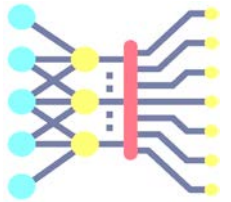
$$h_0^d = c$$

$$h_t^d = g\left(\hat{y}_{t-1}, h_{t-1}^d\right)$$

$$Z_t = f\left(h_t^d\right)$$

$$y_t = \text{soft}\max\ (z_t)$$

Decoder Weaknesses



The context vector *c only* available at the beginning of the generation process.

- Its influence became less-and-less important as the output sequence was generated.

- Solution: Make *c* available at each step in the decoding process,
  1. when generating the hidden states in the deocoder
  2. while producing the generated output.

$$c = h_n^e$$

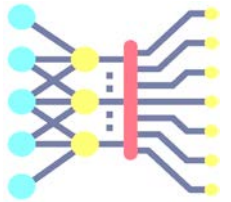
$$h_0^d = c$$

$$h_t^d = g\left(\hat{y}_{t-1}, h_{t-1}^d, c\right)$$

$$Z_t = f\left(h_t^d\right)$$

$$y_t = \text{soft}\max\left(\hat{y}_{t-1}, z_t, c\right)$$

Choosing the best output

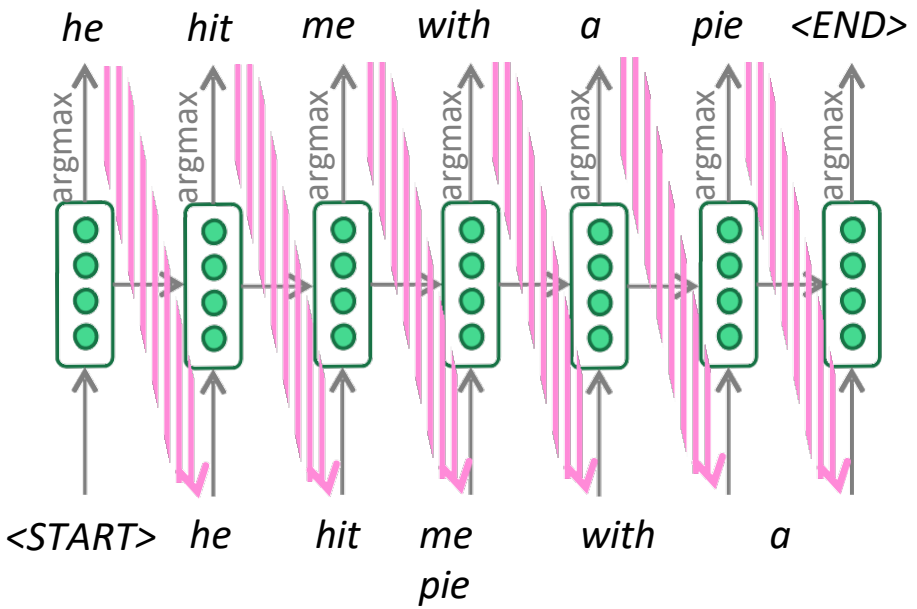


- For neural generation, we can sample from the softmax distribution.

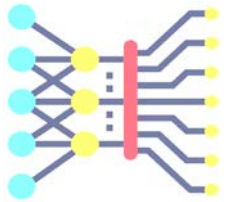
- In MT where we're looking for a specific output sequence, sampling isn't useful.
- Greedy Dcoding: we choose the most likely output at each time step by taking the argmax over the softmax output

$$\hat{y} = \text{argmax} P(y_i | y_{<i})$$

Greedy decoding

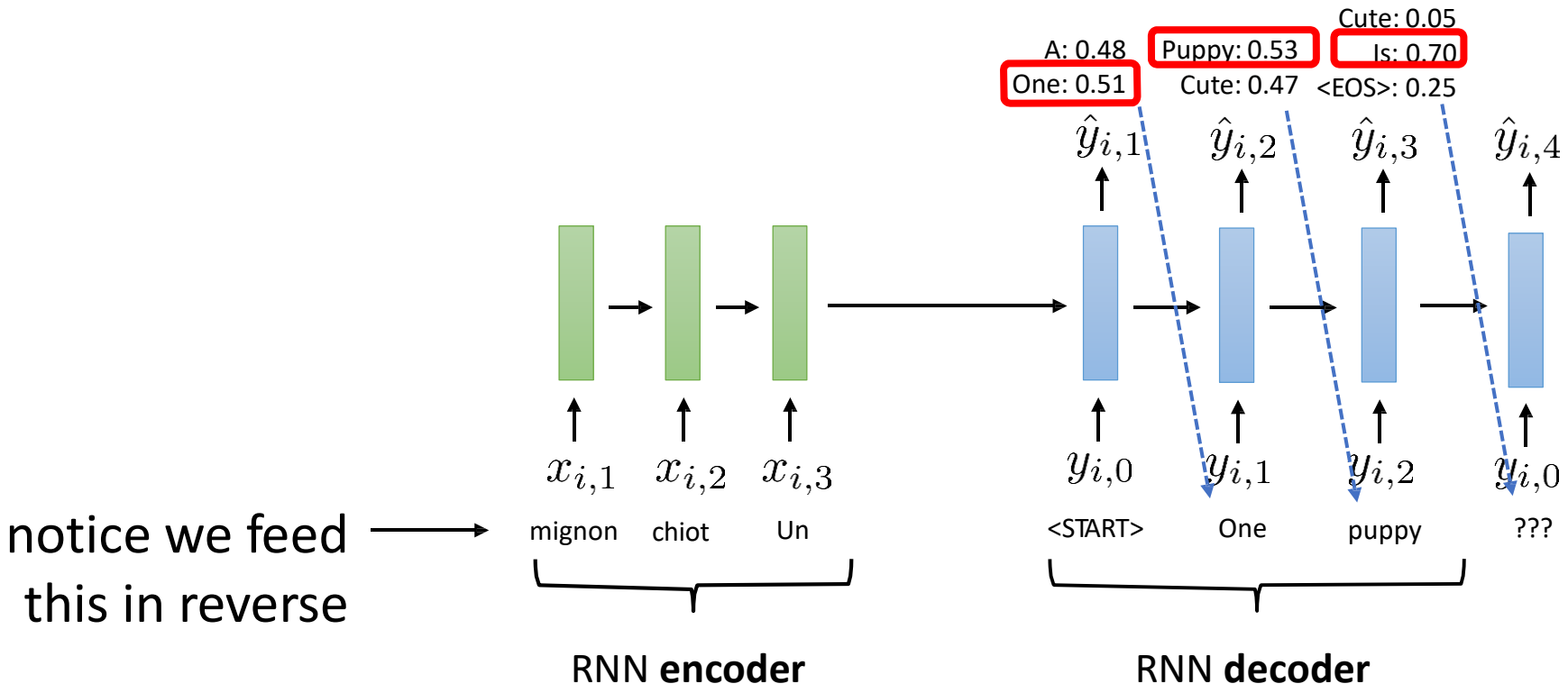


greedy decoding : take most probable word on each step



Decoding with beam search

Decoding the most likely sequence



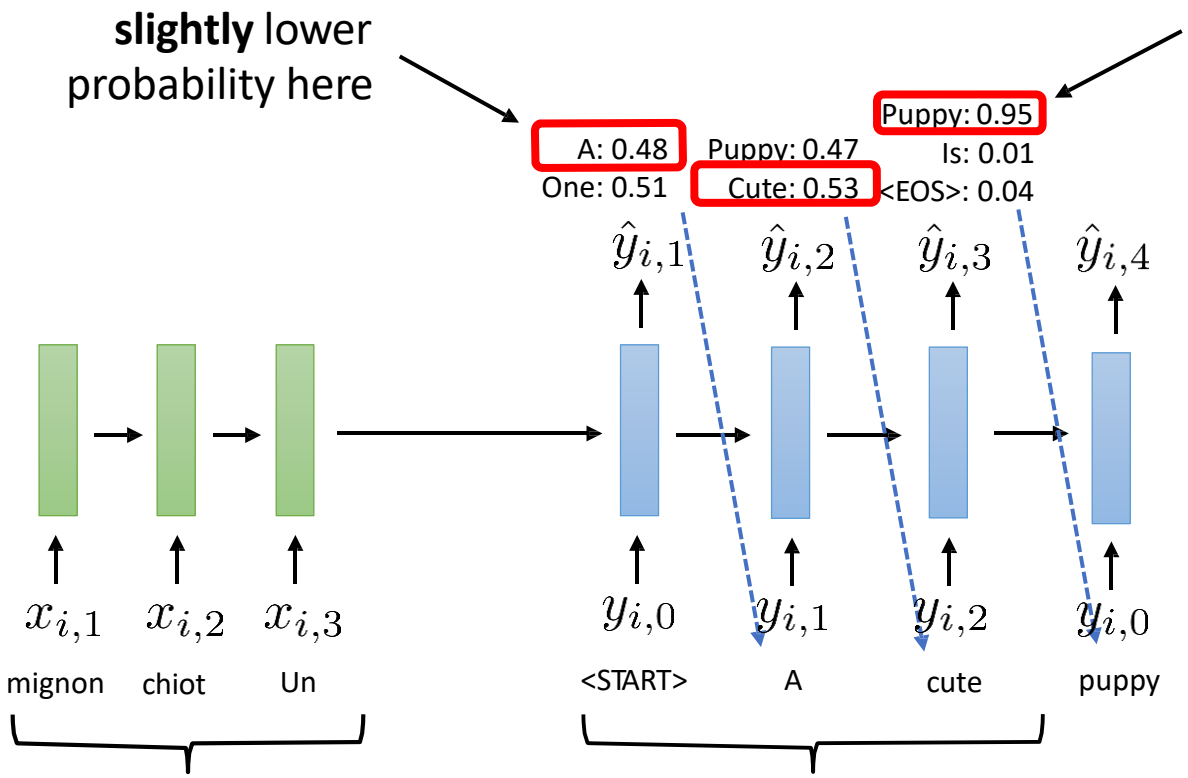
What we *should* have done

what does each output represent?

$$p(y_{i,t}|x_{i,1:T}, y_{i,0:t-1})$$

depends on whole input sequence

and output sequence so far!

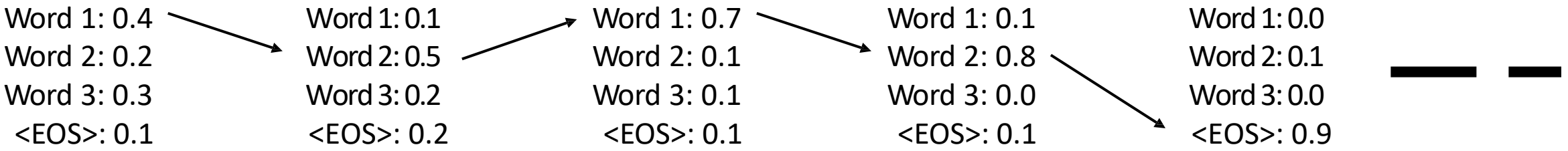


If we want to maximize the product of **all** probabilities, we should not just greedily select the highest probability on the first step!

$$p(y_{i,1:T_y}|x_{i,1:T}) = \prod_{t=1}^{T_y} p(y_{i,t}|x_{i,1:T}, y_{i,0:t-1})$$

probabilities at each time step

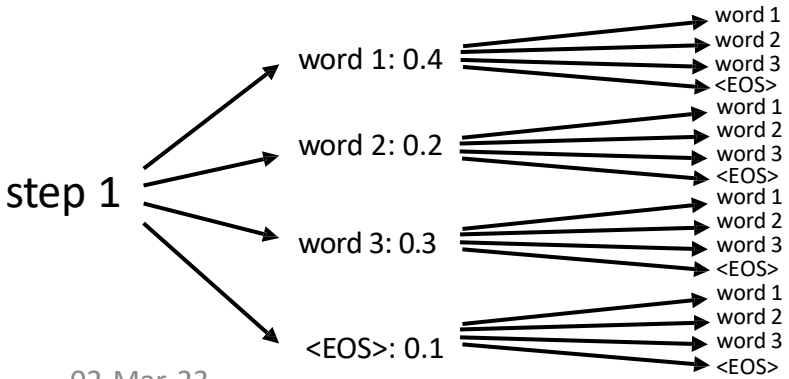
How many possible decodings are there?



for M words, in general there are M^T sequences of length T

any one of these might be the optimal one!

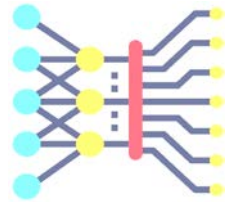
Decoding is a **search** problem



We could use *any* tree search algorithm But exact search in this case is **very** expensive

The **structure** of this problem makes some simple **approximate search** methods work **very well**

Beam search decoding



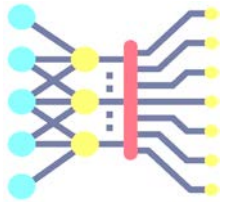
- Core idea: On each step of decoder, keep track of the *k* most probable partial translations (which we call *hypotheses*)
  - *k* is the beam size (in practice around 5 to 10)
- A hypothesis $y_1, \ldots, y_t$ has a score which is its log probability:

$$\text{score}(y_1, \ldots, y_t) = \log P_{\text{LM}}(y_1, \ldots, y_t | x) = \sum_{i=1}^{t} \log P_{\text{LM}}(y_i | y_1, \ldots, y_{i-1}, x)$$

  - Scores are negative, and higher score is better
  - We search for high-scoring hypotheses, tracking top *k* on each step

- Beam search is not guaranteed to find optimal solution
- But much more efficient than exhaustive search!

Decoding with approximate search



Basic intuition: while choosing the **highest-probability** word on the first step may not be optimal, choosing a **very low-probability** word is very unlikely to lead to a good result

Equivalently: we can't be greedy, but we can be *somewhat* greedy

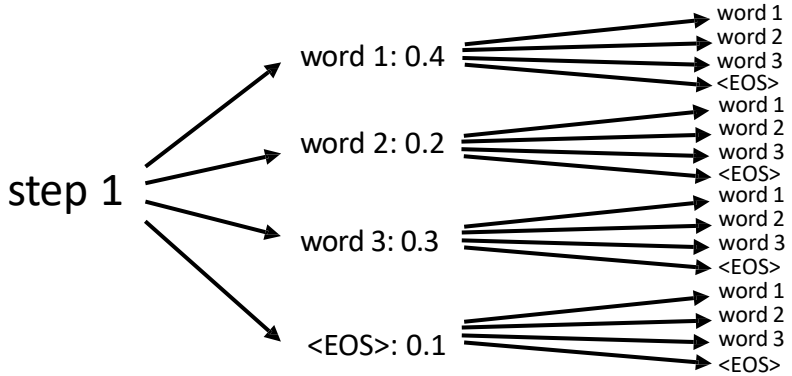
Beam search intuition**:** store the **k** best sequences **so far**, and update each of them.

special case of **k** = 1 is just

greedy decoding often use **k**

around 5-10

Decoding is a **search** problem



Beam search example

$$p(y_{i,1:T_y}|x_{i,1:T}) = \prod_{t=1}^{T_y} p(y_{i,t}|x_{i,1:T}, y_{i,0:t-1})$$

$$\log p(y_{i,1:T_y}|x_{i,1:T}) = \sum_{t=1}^{T_y} \log p(y_{i,t}|x_{i,1:T}, y_{i,0:t-1})$$

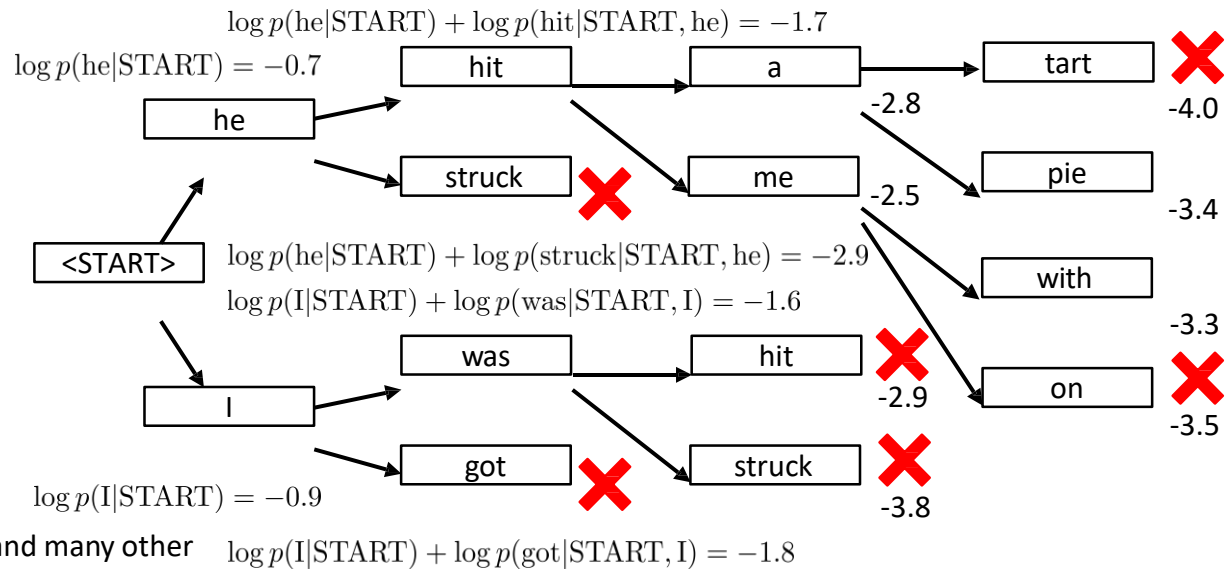
in practice, we **sum up** the log probabilities as we go (to avoid underflow)

Example

k = 2 (track the 2 most likely hypotheses)

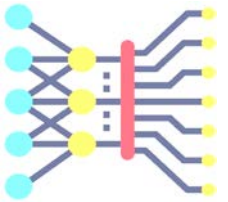
translate (Fr->En): il a m'entarté (he hit me with a pie)

no perfectly equivalent English word, makes this hard



…and many other choices with lower log-prob

Beam search summary



$$\log p(y_{i,1:T_y}|x_{i,1:T}) = \sum_{t=1}^{T_y} \log p(y_{i,t}|x_{i,1:T}, y_{i,0:t-1})$$

there are k of these

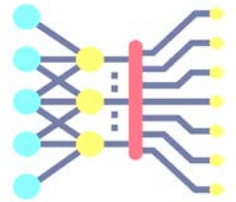
at each time step t:

1. for each hypothesis $y_{1:t-1,i}$ that we are tracking:
   find the top k tokens $y_{t,i,1}, \ldots, y_{t,i,k}$

very easy, we get this from the softmax log-probs

2. sort the resulting k^2 length t sequences by their *total* log-probability
3. keep the top k
4. advance each hypothesis to time $t+1$

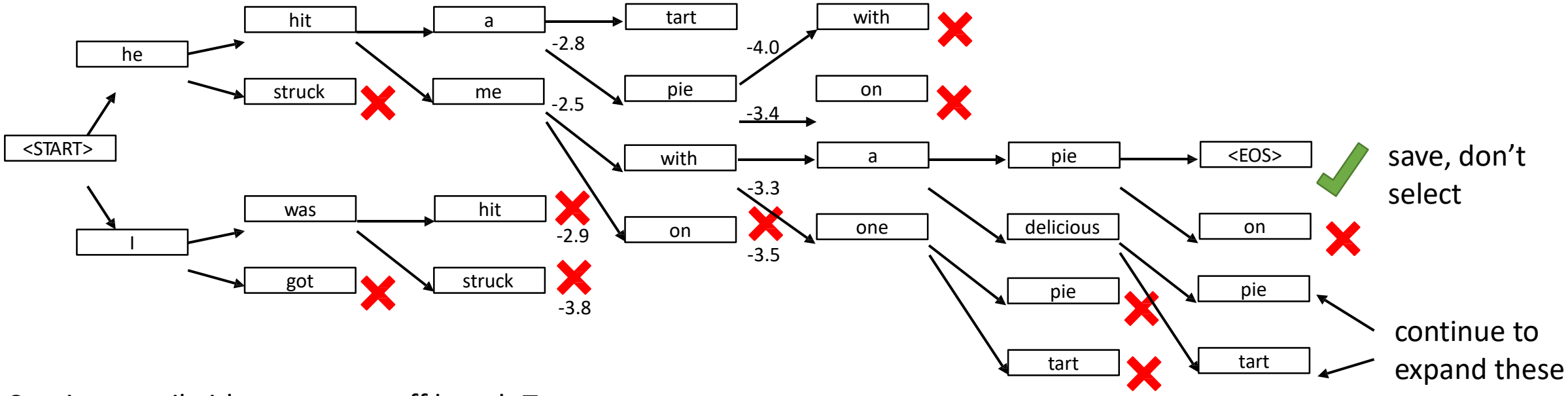
When do we stop decoding?



Suppose one of the highest-scoring hypotheses ends in <END>

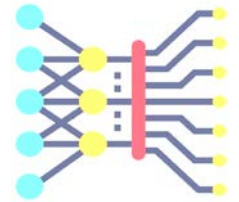
Save it, along with its score, but do **not** pick it to expand further (there is nothing to expand)

Keep expanding the **k** remaining best hypotheses



Continue until either some cutoff length **T** or until we have **N** hypotheses that end in <EOS>

Which sequence do we pick?



At the end we might have something like this:

he hit me with a pie he — log p = -4.5

threw a pie — log p = -3.2

I was hit with a pie that he threw — log p = -7.2

$$\log p(y_{i,1:T}|x_{i,1:T}) = \sum_{t=1}^{T} \log p(y_{i,t}|x_{i,1:T}, y_{i,0:t-1})$$

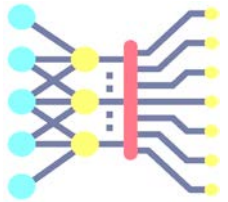
Problem: p < 1 **always**, hence log p < 0 **always**

The **longer** the sequence the **lower** its total score (more negative numbers added together)

Simple "fix": just divide by sequence length

$$\text{score}(y_{i,1:T}|x_{i,1:T}) = \frac{1}{T} \sum_{t=1}^{T} \log p(y_{i,t}|x_{i,1:T}, y_{i,0:t-1})$$

Beam search summary



$$\text{score}(y_{i,1:T}|x_{i,1:T}) = \frac{1}{T}\sum_{t=1}^{T}\log p(y_{i,t}|x_{i,1:T}, y_{i,0:t-1})$$

at each time step t:

1. for each hypothesis $y_{1:t-1,i}$ that we are tracking:
   find the top k tokens $y_{t,i,1}, \ldots, y_{t,i,k}$
2. sort the resulting k^2 length t sequences by their *total* log-probability
3. save any sequences that end in EOS
4. keep the top k
5. advance each hypothesis to time $t+1$ if $t < H$

return saved sequence with highest score