Sequence to Sequence Models

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EPFL

HACKATHON

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Announcements

- **Class Online:** March 12th.
  - Event in the STCC, so we don’t have this room.
  - Lecture will be given remotely (and recorded)

Section Outline

- **Mitigating Vanishing Gradients:** LSTMs, GRUs
- **Sequence-to-sequence models:** Overview, Examples, Training
- **Sequence-to-sequence shortcomings:** Long-range dependencies, Temporal bottleneck
- **Improvements:** Attention mechanisms

Last Week Recap

- Recurrent neural networks can **theoretically** learn to model an **unbounded context length**
  - no increase in model size because weights are shared across time steps
- Practically, however, **vanishing gradients** stop vanilla RNNs from learning useful **long-range dependencies**

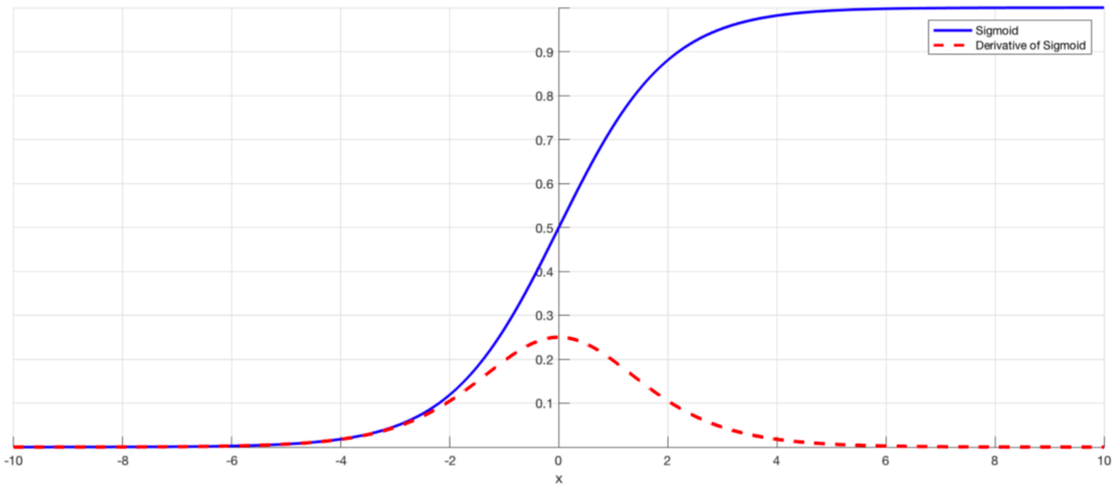
Vanishing Gradients

- **Learning Problem:** Long unrolled networks will crush gradients that backpropagate to earlier time steps

$$h_t = \sigma\left(W_{hx}x_t + W_{hh}h_{t-1} + b_h\right)$$

$$u = W_{hx}x_t + W_{hh}h_{t-1} + b_h$$

$$\frac{\partial h_t}{\partial h_{t-1}} = \frac{\partial \sigma(u)}{\partial u}\frac{\partial u}{\partial h_{t-1}} = W_{hh}\frac{\partial \sigma(u)}{\partial u}$$

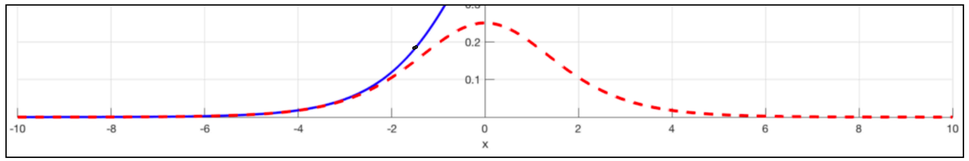


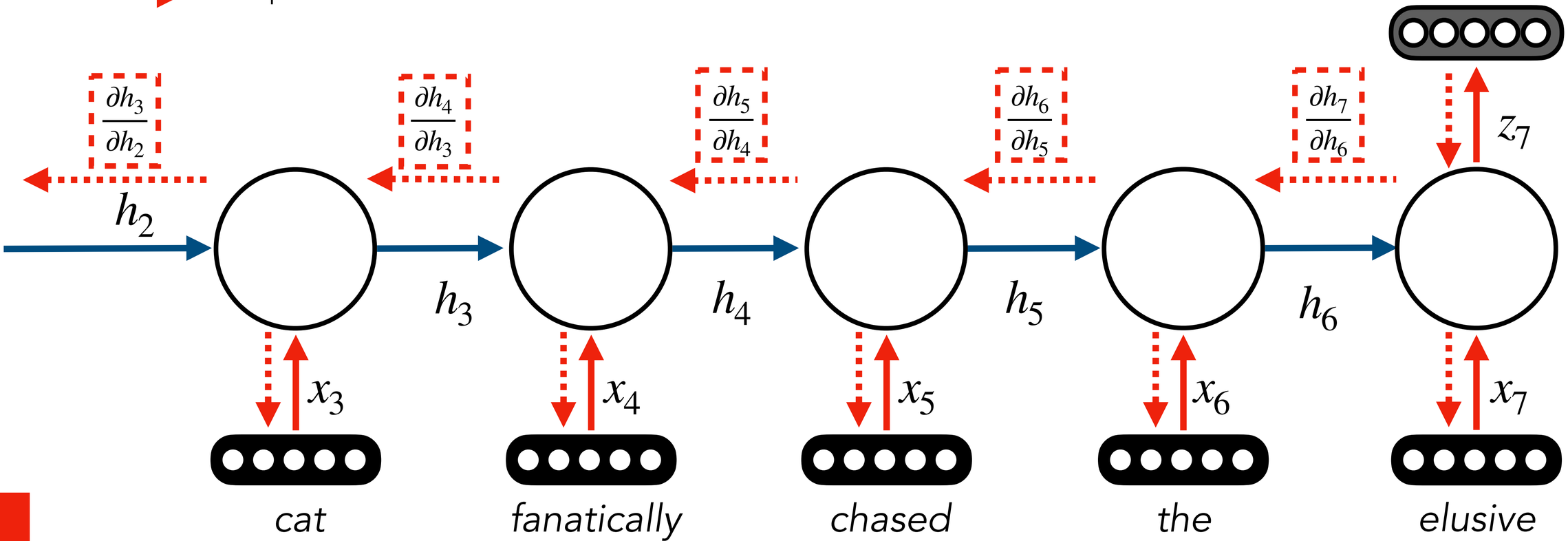
Vanishing Gradients

Gradient flow

Output flow

$$\frac{\partial h_t}{\partial h_{t-1}} = \frac{\partial \sigma(u)}{\partial u}\frac{\partial u}{\partial h_{t-1}} = W_{hh}\frac{\partial \sigma(u)}{\partial u}$$





Vanishing Gradients

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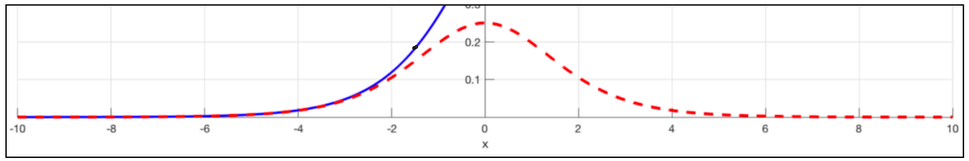


Gradient flow

Output flow

Problem in many recurrent neural networks,

Especially pronounced in Elman networks (Vanilla RNNs) due to the sigmoid activation

$\frac{\partial h_3}{\partial h_2}$

h_2

z_7

x_3 x_4 x_5 x_6 x_7

cat *fanatically* *chased* *the* *elusive*

Gated Recurrent Neural Networks

- Use gates to avoid dampening gradient signal every time step

$$h_t = \sigma\left(W_{hx}x_t + W_{hh}h_{t-1} + b_h\right)$$

Elman Network

$$h_t = h_{t-1} \odot \mathbf{f} + \mathbf{func}(x_t)$$

Gated Network Abstraction

f: forget gate

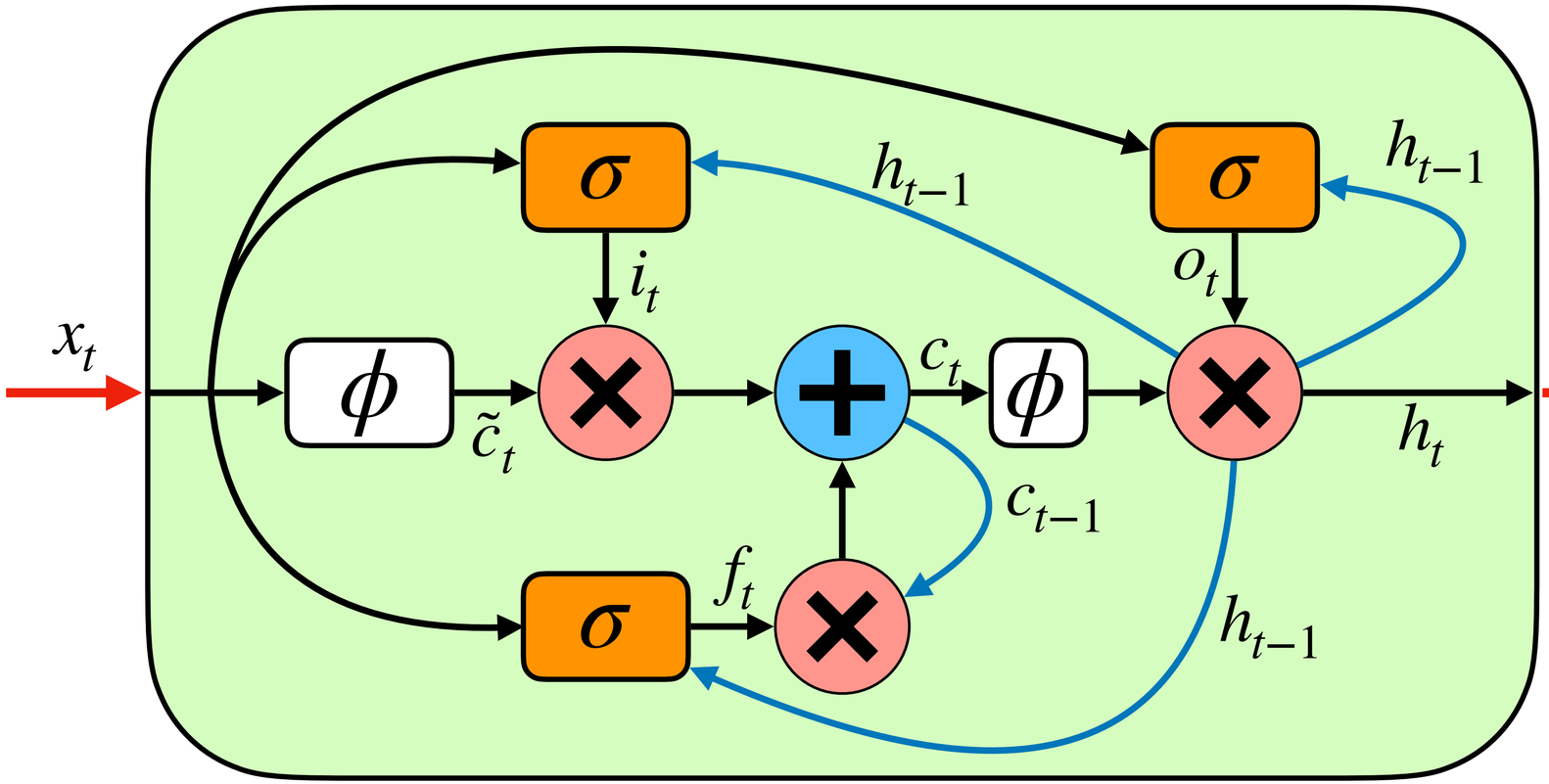
= control how much new info is added

= retains relevant past info

- Gate value **f** computes how much information from previous hidden state moves to the next time step —> 0 < **f** < 1

- Because h_{t-1} is no longer inside the activation function, it is not automatically constrained, reducing vanishing gradients!

Long Short Term Memory (LSTM)



Gates:

$$f_t = \sigma\left(W_{fx}x_t + W_{fh}h_{t-1} + b_f\right)$$
$$i_t = \sigma\left(W_{ix}x_t + W_{ih}h_{t-1} + b_i\right)$$
$$o_t = \sigma\left(W_{ox}x_t + W_{oh}h_{t-1} + b_o\right)$$

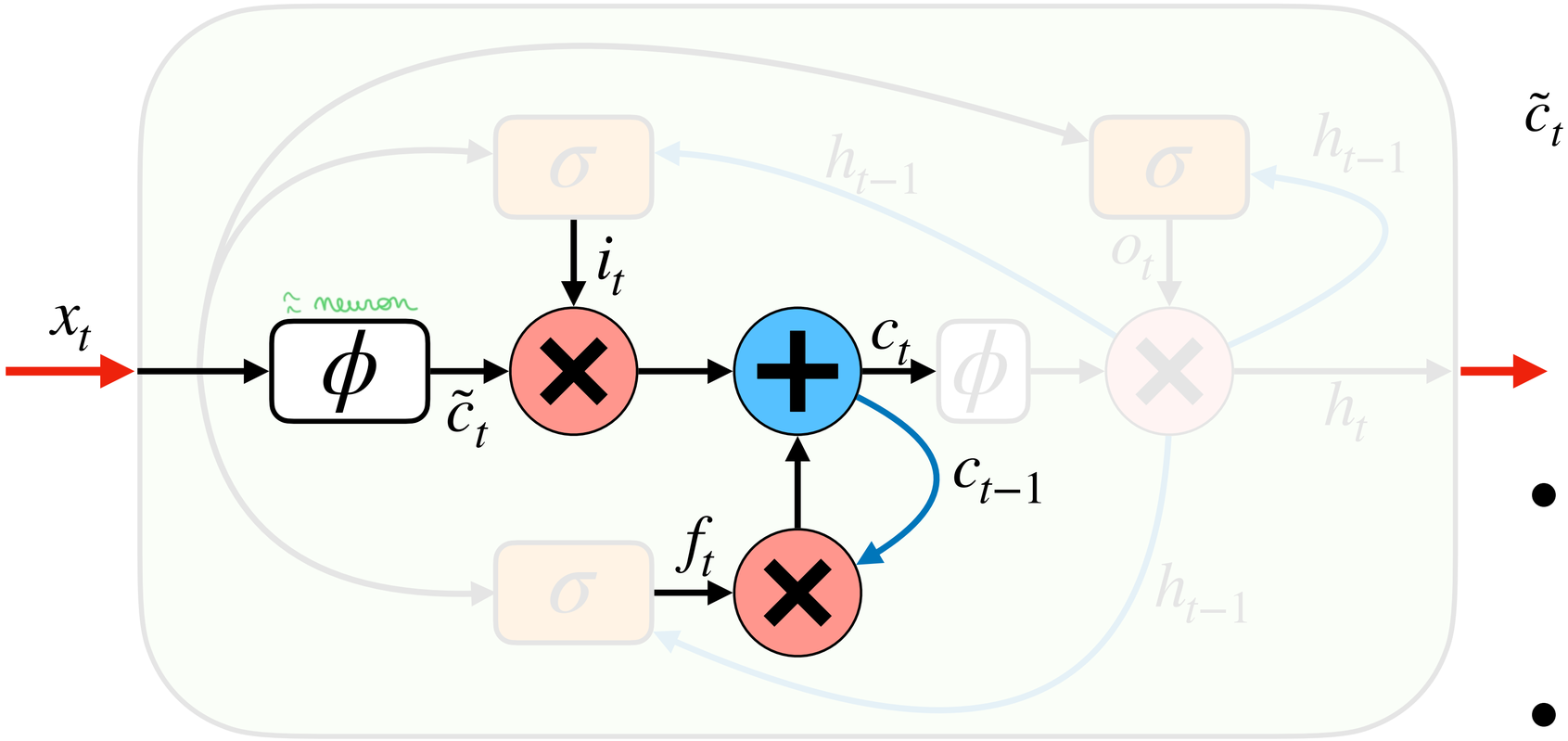
$$\tilde{c}_t = \phi\left(W_{cx}x_t + W_{ch}h_{t-1} + b_c\right)$$

$$c_t = i_t \times \tilde{c}_t + f_t \times c_{t-1}$$

$$h_t = o_t \times \phi(c_t)$$

(Hochreiter and Schmidhuber, 1997)

Cell State



$$\tilde{c}_t = \phi\left(W_{cx}x_t + W_{ch}h_{t-1} + b_c\right)$$

$$c_t = i_t \times \tilde{c}_t + f_t \times c_{t-1}$$

- Hidden state h_{t-1} is now short-term memory
- Cell state c_t tracks longer-term dependencies

What does the cell state track?

- Can visualise the activations of cell state (i.e., dimensions of **c**) and find semantic behaviour!
- Stack Overflow example:

```
#ifdef CONFIG_AUDITSYSCALL
static inline int audit_match_class_bits(int class, u32 *mask)
{
  int i;
  if (classes[class]) {
    for (i = 0; i < AUDIT_BITMASK_SIZE; i++)
      if (mask[i] & classes[class][i])
        return 0;
  }
  return 1;
}
```


Karpathy et al. (2015)

What does the cell state track?

- Can visualise the activations of cell state (i.e., dimensions of **c**) and find semantic behaviour!
- Stack Overflow example: **track indentation**

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}
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- War and Peace:

```
"You mean to imply that I have nothing to eat out of.... On the
contrary, I can supply you with everything even if you want to give
dinner parties," warmly replied Chichagov, who tried by every word he
spoke to prove his own rectitude and therefore imagined Kutuzov to be
animated by the same desire.

Kutuzov, shrugging his shoulders, replied with his subtle penetrating
smile: "I meant merely to say what I said."
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```

- War and Peace: **are we in a quote or not?**

```
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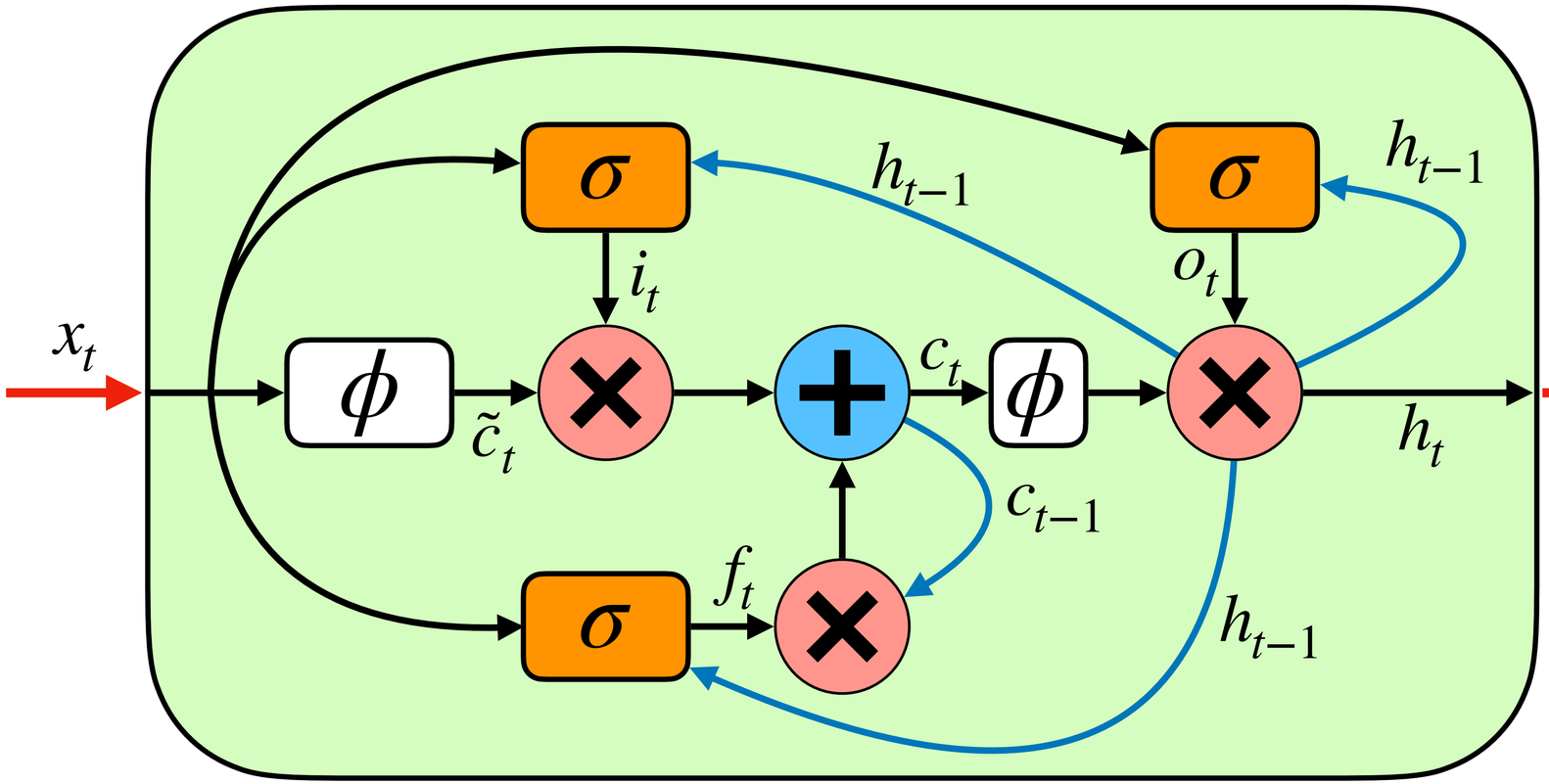
Long Short Term Memory (LSTM)



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$$o_t = \sigma\left(W_{ox}x_t + W_{oh}h_{t-1} + b_o\right)$$

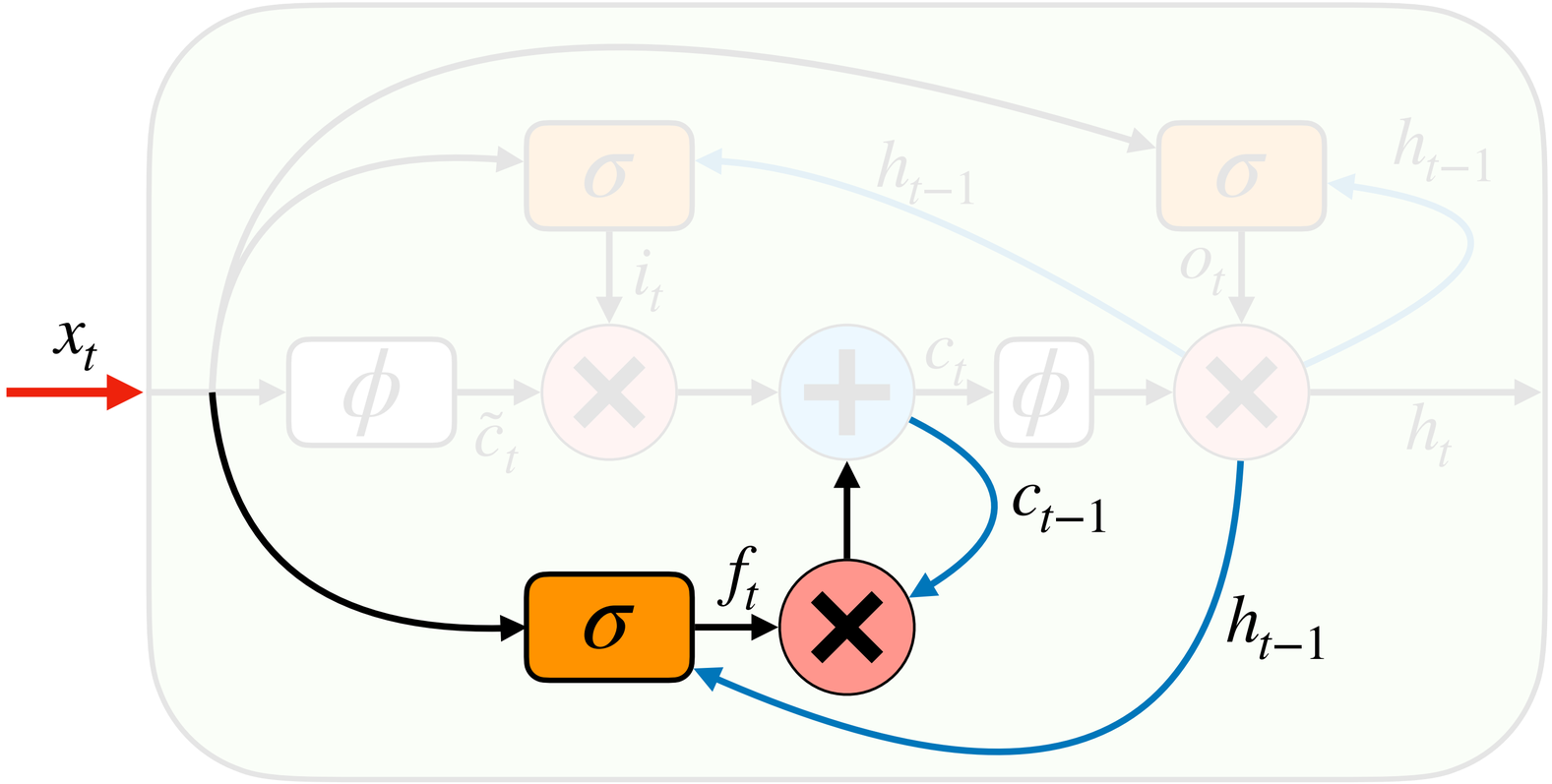
$$\tilde{c}_t = \phi\left(W_{cx}x_t + W_{ch}h_{t-1} + b_c\right)$$

$$c_t = i_t \times \tilde{c}_t + f_t \times c_{t-1}$$

$$h_t = o_t \times \phi(c_t)$$

Forget Gate

I went to **the** **lecture**



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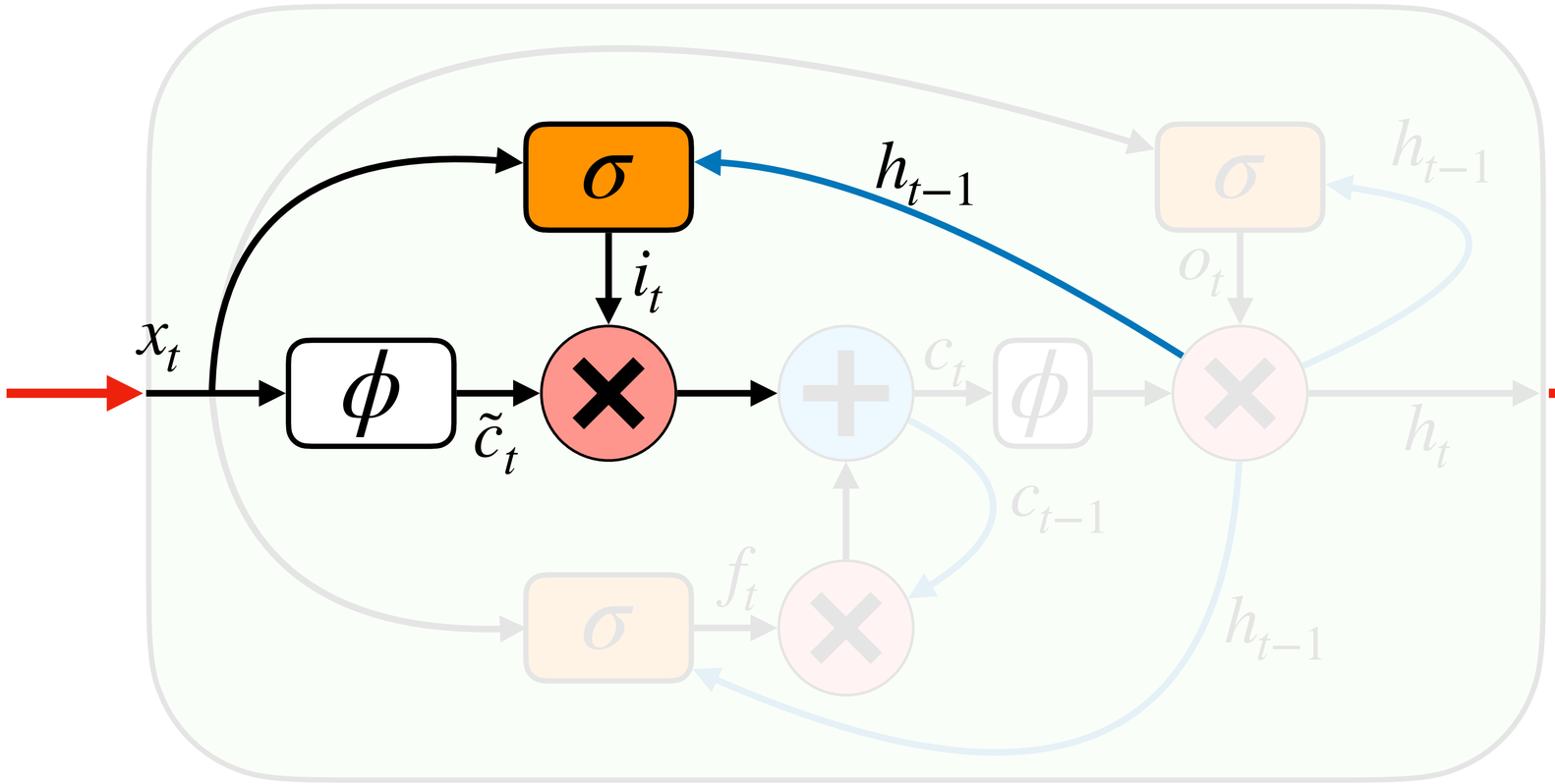
$$c_t = i_t \times \tilde{c}_t + f_t \times c_{t-1}$$

- Forget gate controls how much memory is forgotten
  - 1 -> remember the past
  - 0 -> forget everything up to now

Input Gate

I went to **the** **lecture**



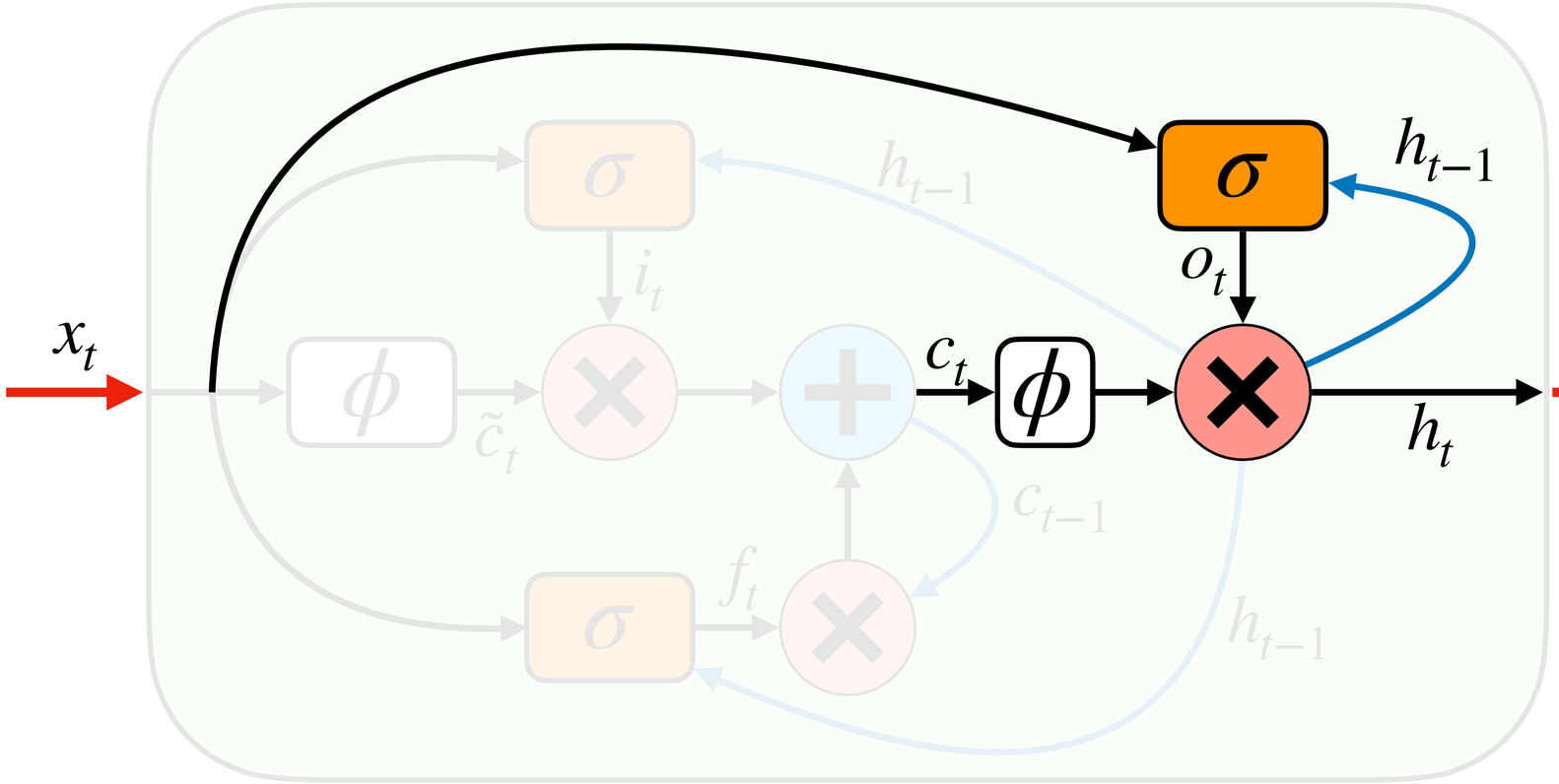
$$i_t = \sigma\left(W_{ix}x_t + W_{ih}h_{t-1} + b_i\right)$$

$$\tilde{c}_t = \phi\left(W_{cx}x_t + W_{ch}h_{t-1} + b_c\right)$$

$$c_t = i_t \times \tilde{c}_t + f_t \times c_{t-1}$$

- Input gate controls how new info is added to state memory
  - 0 -> ignore current time step
  - What might be ignored?

Output Gate



$$o_t = \sigma\left(W_{ox}x_t + W_{oh}h_{t-1} + b_o\right)$$

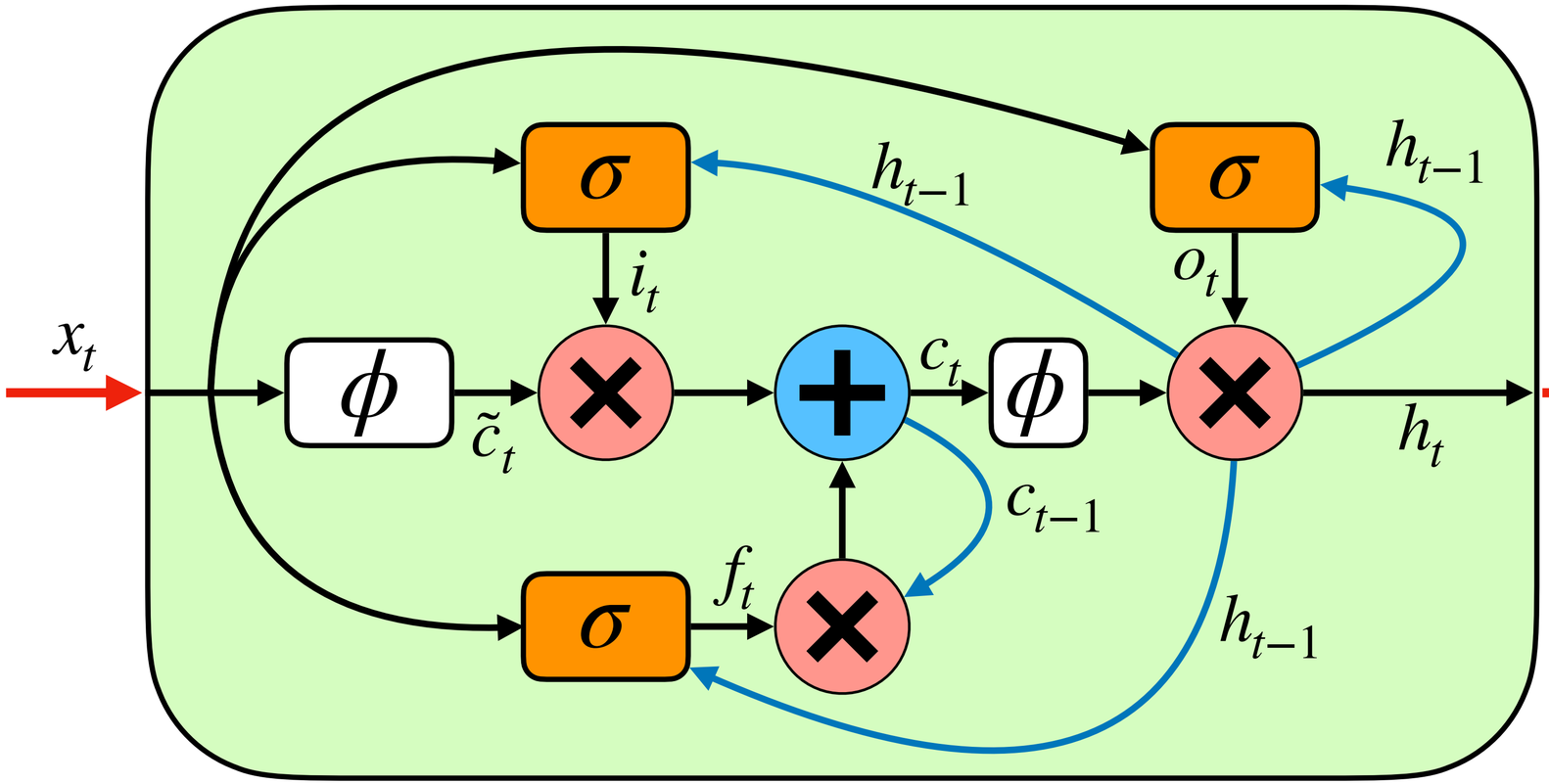
$$\tilde{c}_t = \phi\left(W_{cx}x_t + W_{ch}h_{t-1} + b_c\right)$$

$$c_t = i_t \times \tilde{c}_t + f_t \times c_{t-1}$$

$$h_t = o_t \times \phi(c_t)$$

- Output gate decides how the hidden state will influence gate values at next time step

Long Short Term Memory (LSTM)



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$$c_t = i_t \times \tilde{c}_t + f_t \times c_{t-1}$$

$$h_t = o_t \times \phi(c_t)$$

Questions!

- For what type of input might the model learn to make the input gate be 0 ?
- What happens if the forget gate is 0?
- What happens if both the forget gate and input gate are 0 ?
- What happens if both the forget gate and input gate are 1 ?

Gates:

$$f_t = \sigma\left(W_{fx}x_t + W_{fh}h_{t-1} + b_f\right)$$
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$$\tilde{c}_t = \phi\left(W_{cx}x_t + W_{ch}h_{t-1} + b_c\right)$$

$$c_t = i_t \times \tilde{c}_t + f_t \times c_{t-1}$$

$$h_t = o_t \times \phi(c_t)$$

Gated Recurrent Unit (GRU)

- Also uses gates to avoid dampening gradient signal every time step

$$h_t = (1 - \mathbf{z}) \odot h_{t-1} + \mathbf{z} \odot \textbf{func}(x_t, h_{t-1})$$

GRU

$$h_t = h_{t-1} \odot \mathbf{f} + \textbf{func}(x_t)$$

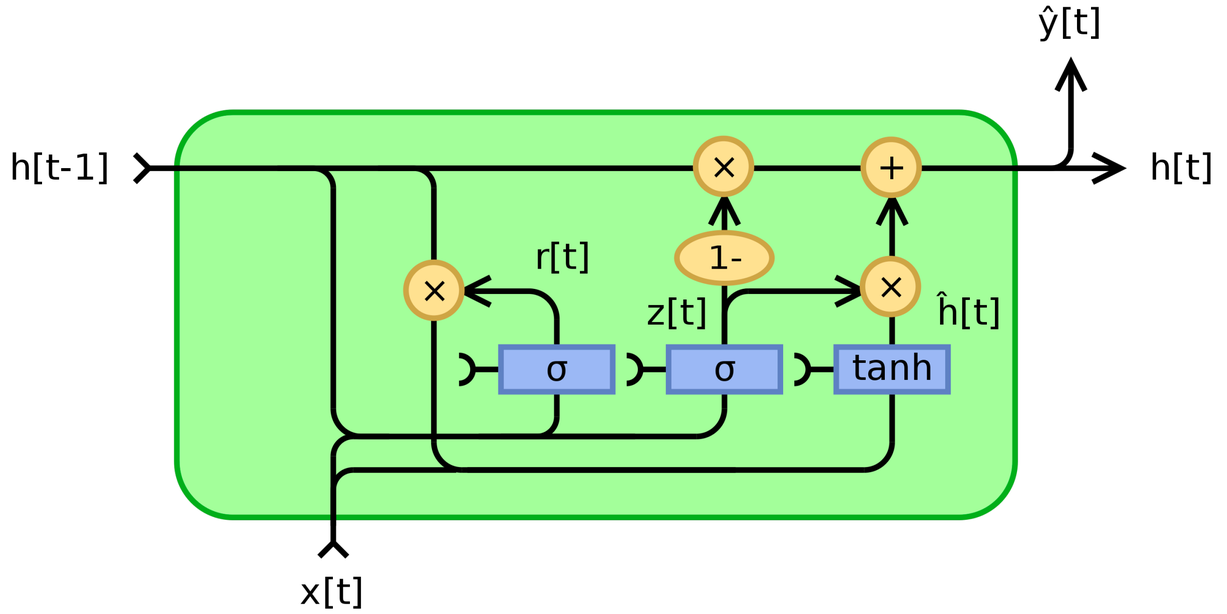
LSTM

- Works similarly to LSTM
  - Typically faster to train and sometimes works better than LSTMs
  - Theoretically less powerful (for example, it can't count)

Gated Recurrent Unit (GRU)

- **z** is update gate (used to update hidden state), **r** is reset gate (used to reset hidden state)

- The single hidden state and simpler update gate gives simpler mixing algorithm than in LSTMs

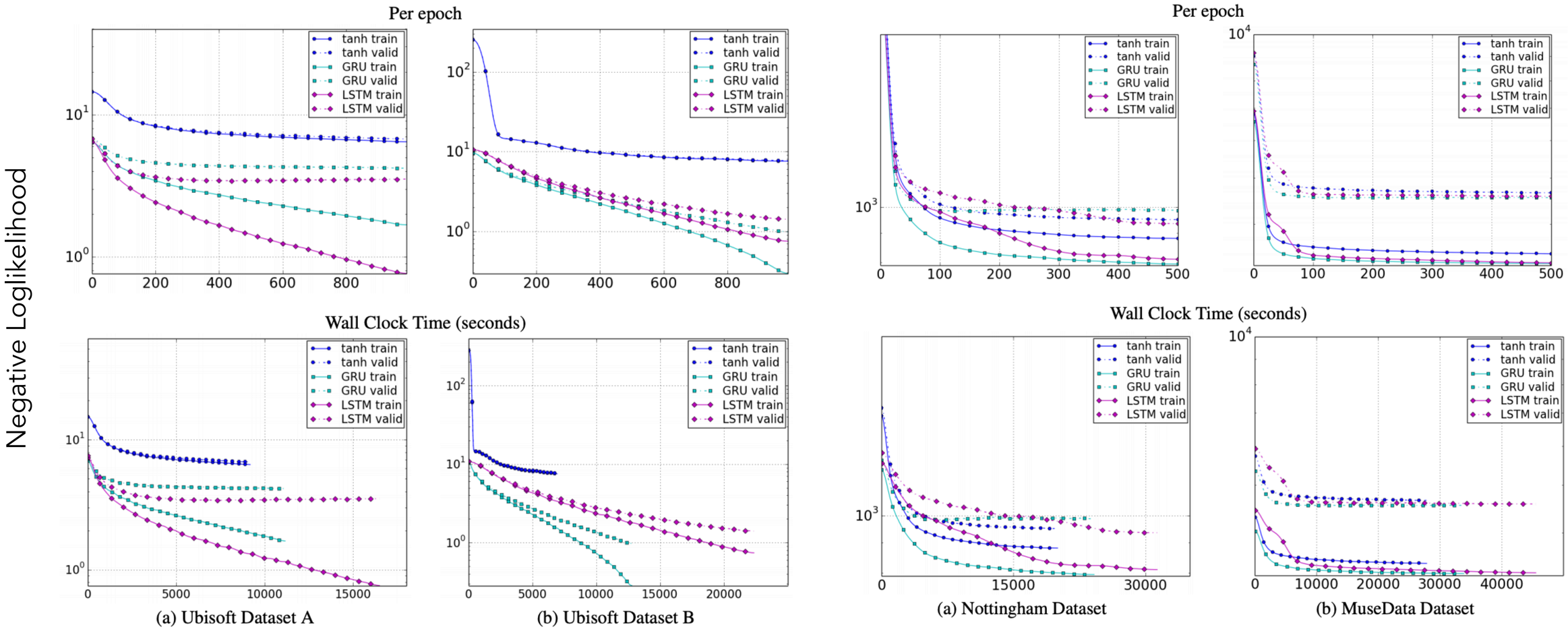


$$z_t = \sigma_g(W_z x_t + U_z h_{t-1} + b_z)$$
$$r_t = \sigma_g(W_r x_t + U_r h_{t-1} + b_r)$$
$$h_t = (1 - z_t) \circ h_{t-1} + z_t \circ \sigma_h(W_h x_t + U_h(r_t \circ h_{t-1}) + b_h)$$

Which is better?

Speech Signal Modeling

Music Modeling



(Chung et al, 2014)

Question

What are the advantages of using LSTMs and GRUs?

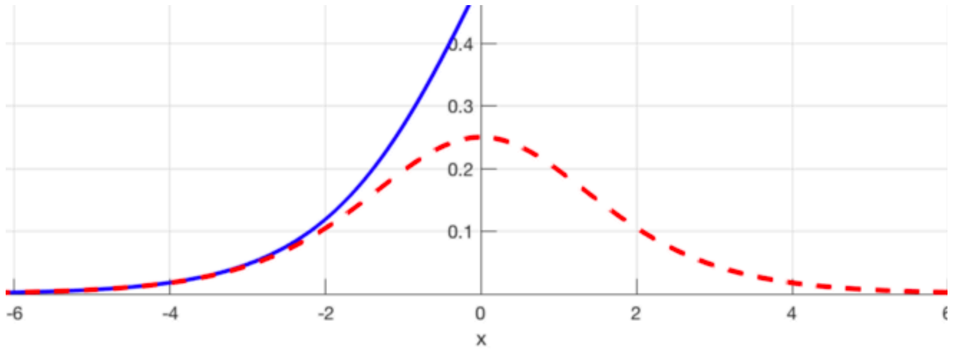
Vanishing Gradients?

Recurrent Neural Networks

State maintained by hidden state feedback

$$h_t = \sigma\left(W_{hx}x_t + W_{hh}h_{t-1} + b_h\right)$$

Gradient systemically squashed by sigmoid



Long Short Term Memory

State maintained by cell value

$$c_t = i_t \times \tilde{c}_t + f_t \times c_{t-1}$$

Gradient set by value of forget gate

$$\frac{\partial c_t}{\partial c_{t-1}} = f_t$$

Can still vanish, but only if forget gate closes!

Question

What's a disadvantage of using a LSTM or GRU?

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What's a disadvantage of using a LSTM or GRU?

$$f_t = \sigma\left(W_{fx}x_t + W_{fh}h_{t-1} + b_f\right)$$
$$i_t = \sigma\left(W_{ix}x_t + W_{ih}h_{t-1} + b_i\right)$$
$$o_t = \sigma\left(W_{ox}x_t + W_{oh}h_{t-1} + b_o\right)$$
$$\tilde{c}_t = \phi\left(W_{cx}x_t + W_{ch}h_{t-1} + b_c\right)$$
$$c_t = i_t \times \tilde{c}_t + f_t \times c_{t-1}$$
$$h_t = o_t \times \phi(c_t)$$

More parameters!

$$z_t = \sigma\left(W_{zh}h_t + b_z\right)$$
$$h_t = \sigma\left(W_{hx}x_t + W_{hh}h_{t-1} + b_h\right)$$

Question

Could there be better architectures than GRUs and LSTMs?

Optimal Architectures?

MUT1:

$$
\begin{aligned}
z &= \mathrm{sigm}(W_{\mathrm{xz}} x_t + b_{\mathrm{z}}) \\
r &= \mathrm{sigm}(W_{\mathrm{xr}} x_t + W_{\mathrm{hr}} h_t + b_{\mathrm{r}}) \\
h_{t+1} &= \tanh(W_{\mathrm{hh}}(r \odot h_t) + \tanh(x_t) + b_{\mathrm{h}}) \odot z \\
&+ h_t \odot (1 - z)
\end{aligned}
$$

MUT2:

$$
\begin{aligned}
z &= \mathrm{sigm}(W_{\mathrm{xz}} x_t + W_{\mathrm{hz}} h_t + b_{\mathrm{z}}) \\
r &= \mathrm{sigm}(x_t + W_{\mathrm{hr}} h_t + b_{\mathrm{r}}) \\
h_{t+1} &= \tanh(W_{\mathrm{hh}}(r \odot h_t) + W_{xh} x_t + b_{\mathrm{h}}) \odot z \\
&+ h_t \odot (1 - z)
\end{aligned}
$$

MUT3:

$$
\begin{aligned}
z &= \mathrm{sigm}(W_{\mathrm{xz}} x_t + W_{\mathrm{hz}} \tanh(h_t) + b_{\mathrm{z}}) \\
r &= \mathrm{sigm}(W_{\mathrm{xr}} x_t + W_{\mathrm{hr}} h_t + b_{\mathrm{r}}) \\
h_{t+1} &= \tanh(W_{\mathrm{hh}}(r \odot h_t) + W_{xh} x_t + b_{\mathrm{h}}) \odot z \\
&+ h_t \odot (1 - z)
\end{aligned}
$$

Arch.	Arith.	XML	PTB
Tanh	0.29493	0.32050	0.08782
LSTM	0.89228	0.42470	0.08912
LSTM-f	0.29292	0.23356	0.08808
LSTM-i	0.75109	0.41371	0.08662
LSTM-o	0.86747	0.42117	0.08933
LSTM-b	0.90163	0.44434	0.08952
GRU	0.89565	0.45963	0.09069
MUT1	**0.92135**	**0.47483**	0.08968
MUT2	0.89735	**0.47324**	0.09036
MUT3	0.90728	0.46478	**0.09161**

Arch.	5M-tst	10M-v	20M-v	20M-tst
Tanh	4.811	4.729	4.635	4.582 (97.7)
LSTM	4.699	4.511	4.437	4.399 (81.4)
LSTM-f	4.785	4.752	4.658	4.606 (100.8)
LSTM-i	4.755	4.558	4.480	4.444 (85.1)
LSTM-o	4.708	4.496	4.447	4.411 (82.3)
LSTM-b	4.698	4.437	4.423	**4.380 (79.83)**
GRU	4.684	4.554	4.559	4.519 (91.7)
MUT1	4.699	4.605	4.594	4.550 (94.6)
MUT2	4.707	4.539	4.538	4.503 (90.2)
MUT3	4.692	4.523	4.530	4.494 (89.47)

(Jozefowicz et al, 2015)

Recap

- Recurrent neural networks can **theoretically** learn to model an **unbounded context length**
  - no increase in model size because weights are shared across time steps
- Practically, however, **vanishing gradients** stop vanilla RNNs from learning useful **long-range dependencies**
- LSTMs and GRUs are variants of recurrent networks that mitigate the vanishing gradient problem
  - used for for **many sequence-to-sequence tasks (up next!)**

References

- Elman, J.L. (1990). Finding Structure in Time. *Cogn. Sci., 14*, 179-211.
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- Hochreiter, S., & Schmidhuber, J. (1997). Long Short-Term Memory. *Neural Computation, 9*, 1735-1780.
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- Greff, K., Srivastava, R.K., Koutník, J., Steunebrink, B.R., & Schmidhuber, J. (2015). LSTM: A Search Space Odyssey. *IEEE Transactions on Neural Networks and Learning Systems, 28*, 2222-2232.

Question

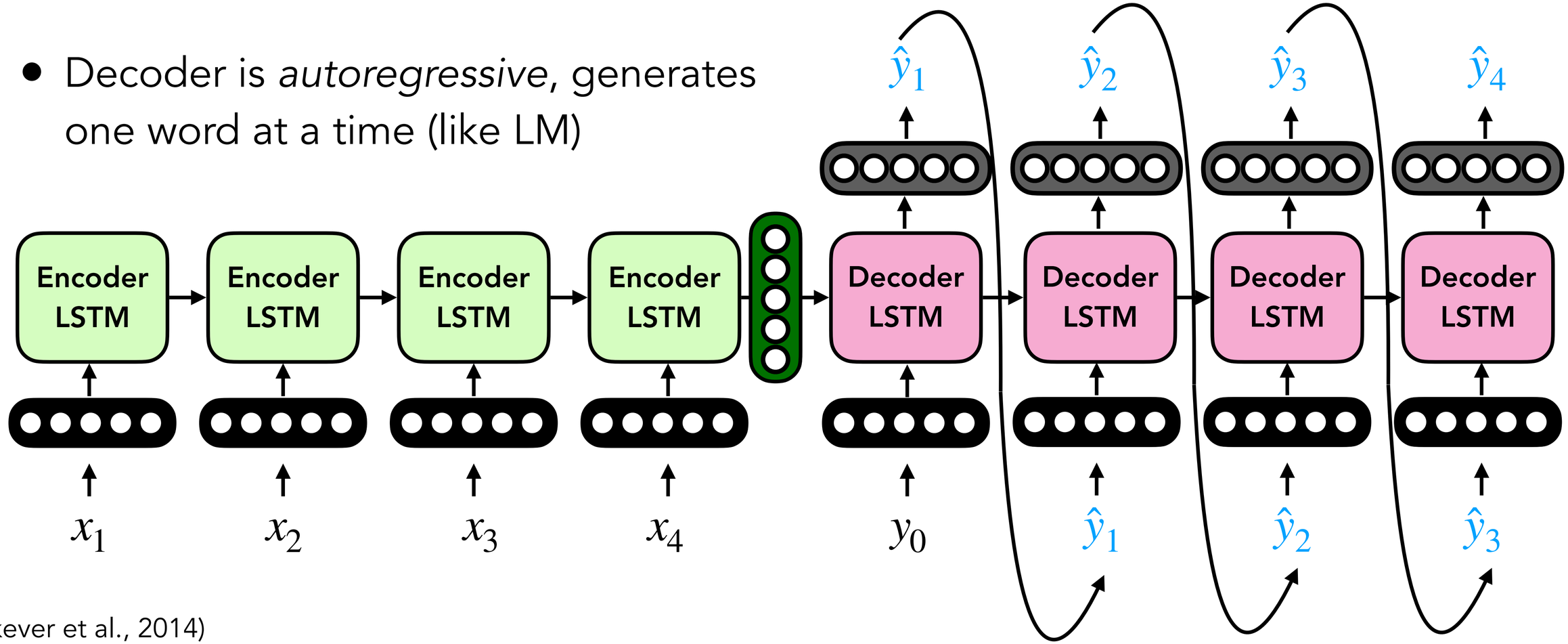
What could we do if the sequence we're encoding and the sequence we want to generate have different properties?

Example: Machine Translation

Encoder-Decoder Models

- Encode a sequence fully with one model (**encoder**) and use its representation to seed a second model that decodes another sequence (**decoder**)

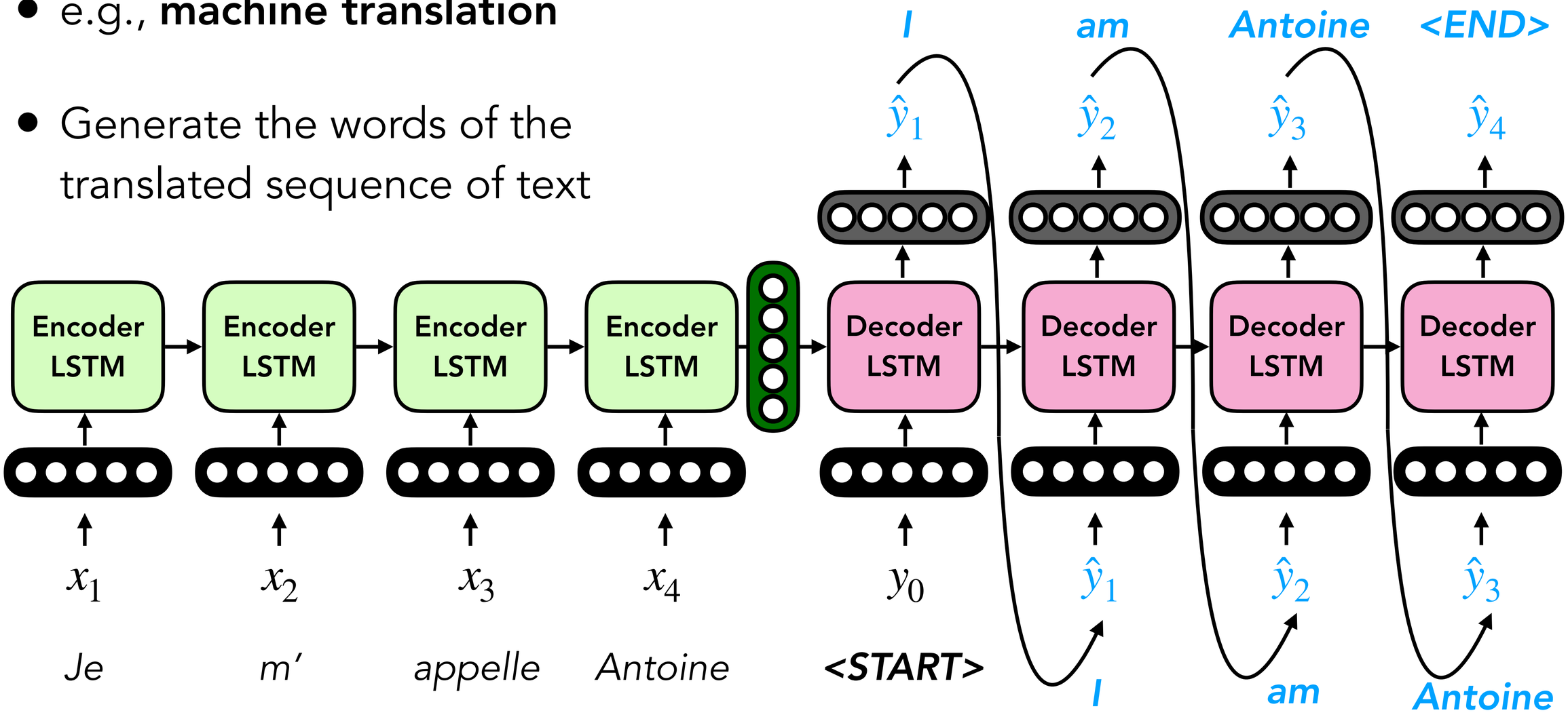
- Decoder is *autoregressive*, generates one word at a time (like LM)



(Sutskever et al., 2014)

Encoder-Decoder Models

- e.g., **machine translation**
- Generate the words of the translated sequence of text



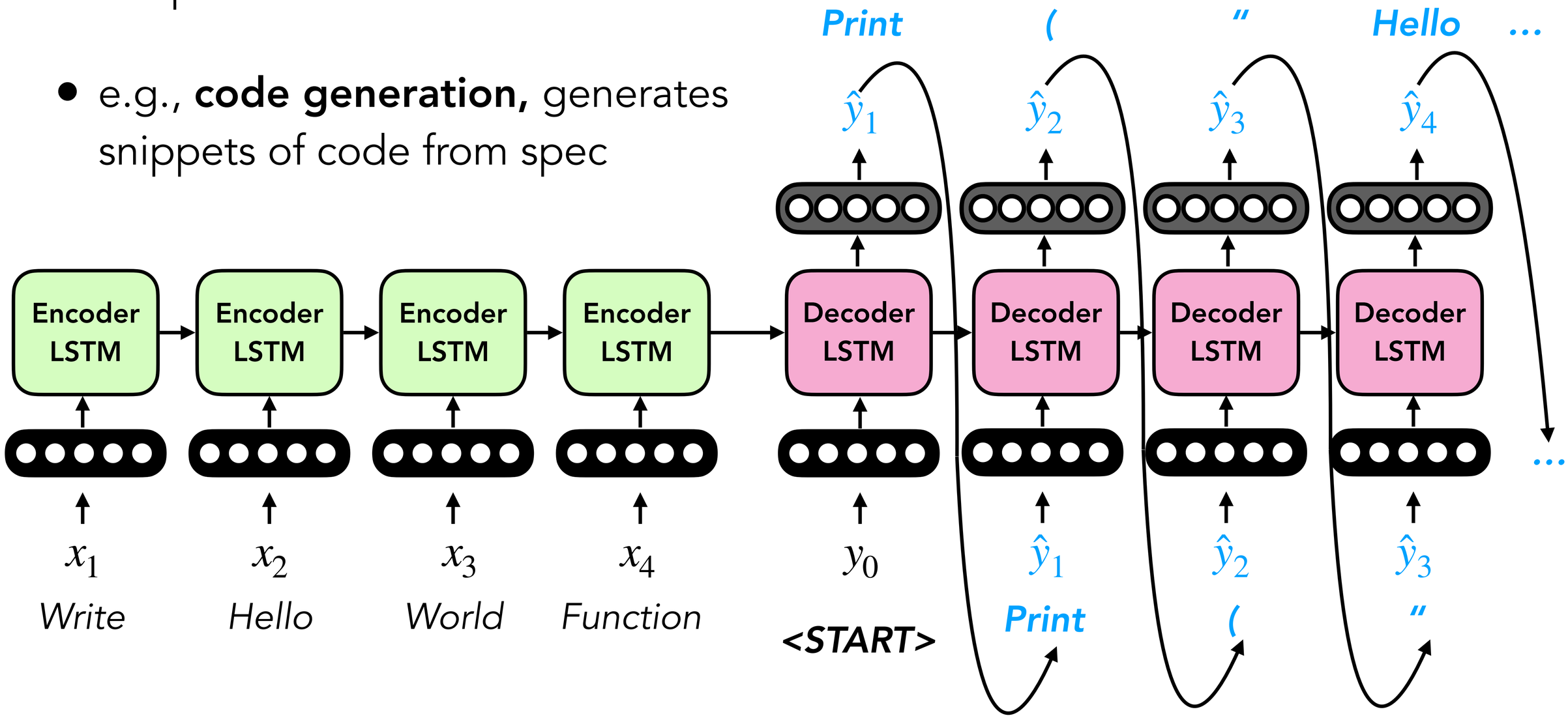
(Sutskever et al., 2014)

Question

What other tasks might have this property ?

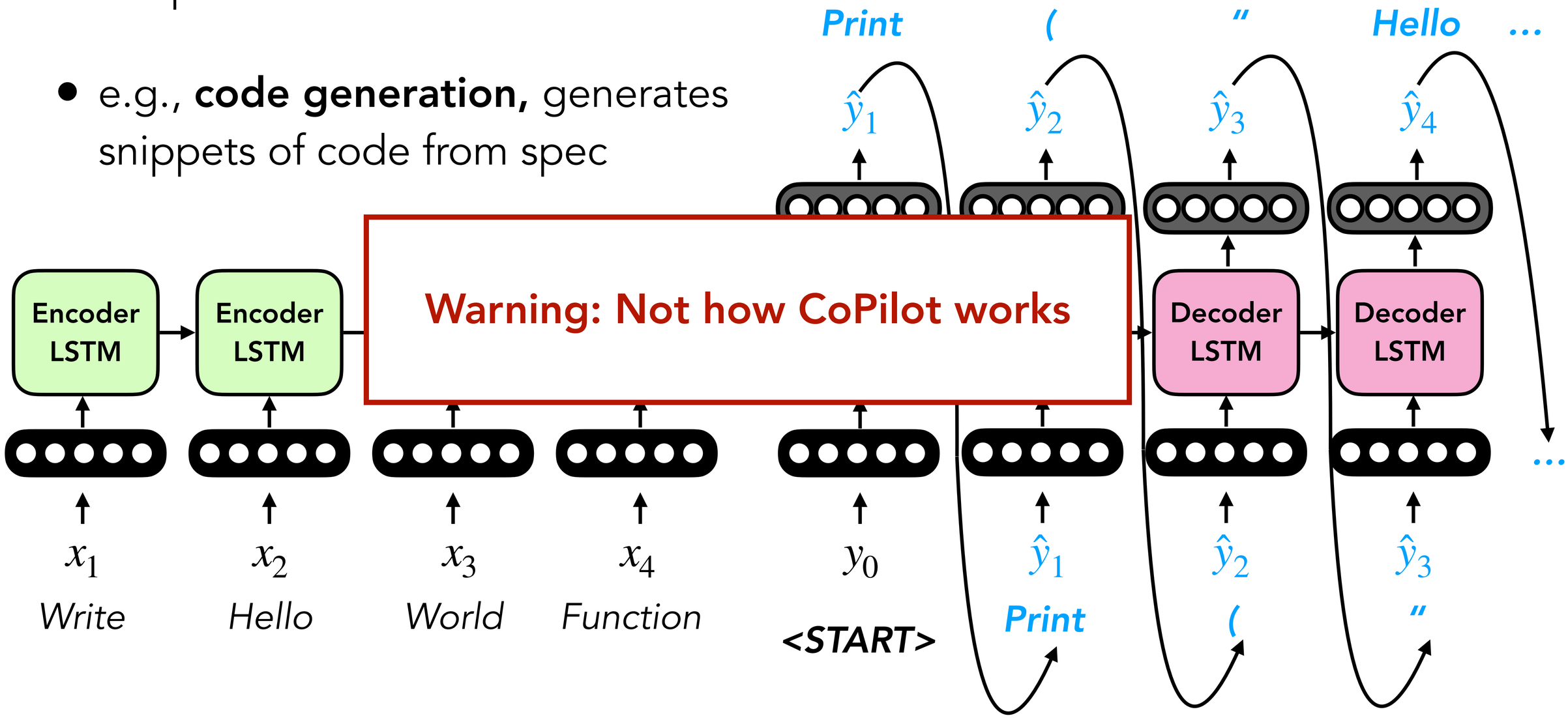
Encoder-Decoder Models

- Output can be other forms of text
- e.g., **code generation,** generates snippets of code from spec



Encoder-Decoder Models

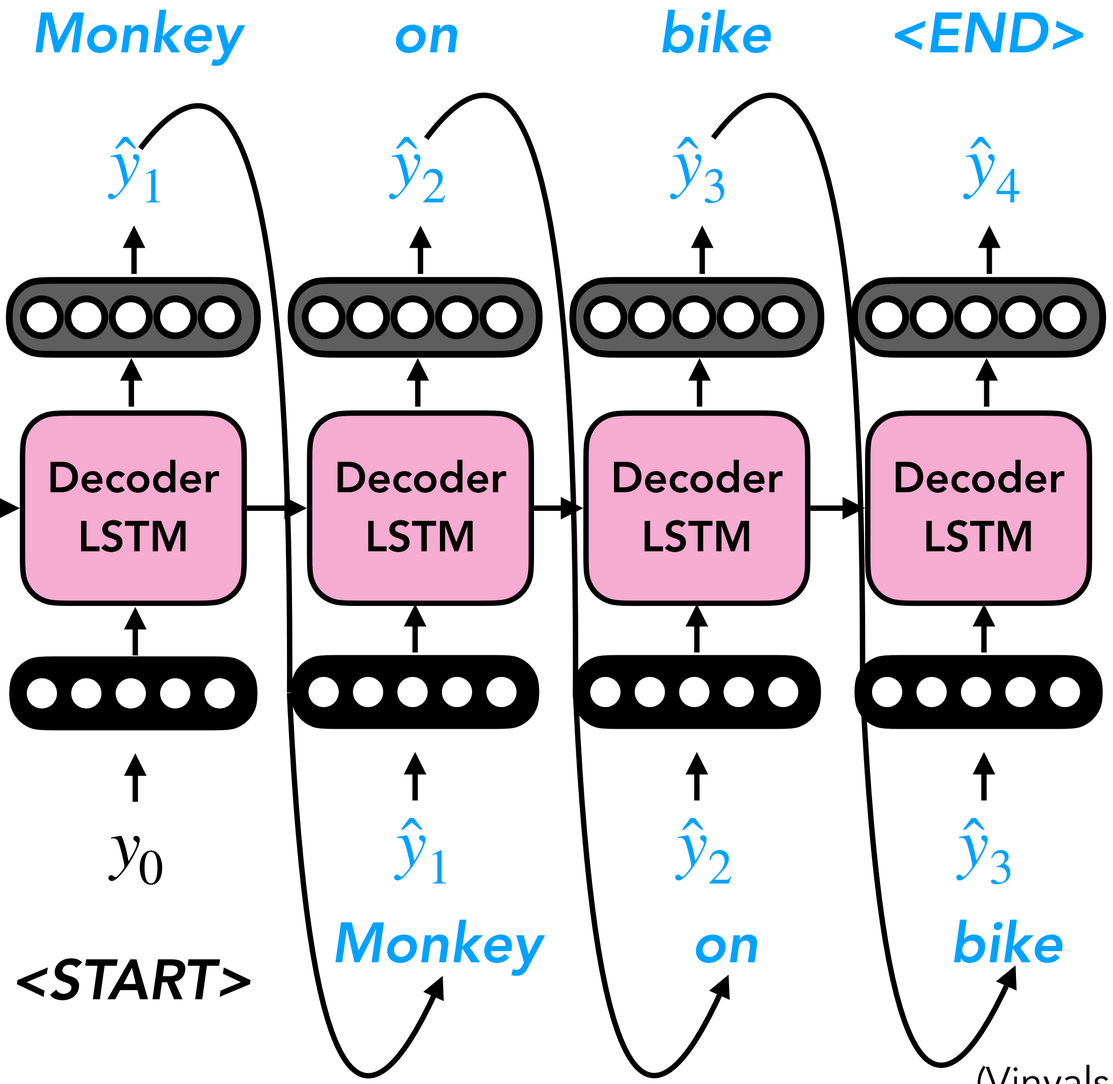
- Output can be other forms of text
- e.g., **code generation,** generates snippets of code from spec



Encoder-Decoder Models

- Input doesn't need to be text
- e.g., **image captioning**

Photo credit: J Hovenstine Studios

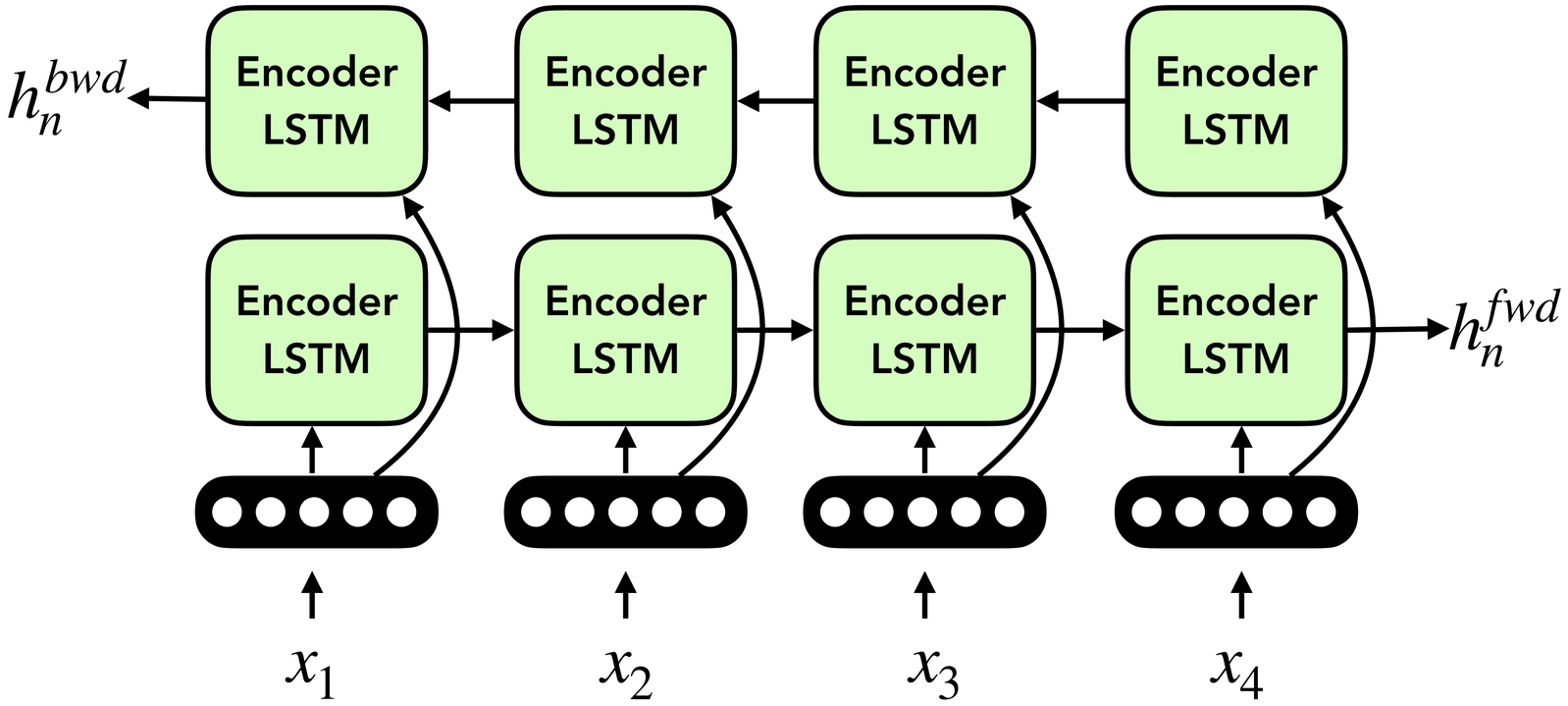


- Generate words of image description

(Vinyals et al., 2014)

Bidirectional Encoders

- Decoder needs to be unidirectional (autoregressive models can't know the future…)
- Encoder sequence representation augmented by encoding in both directions



(Schuster and Paliwal, 1997)

Bidirectional Encoders

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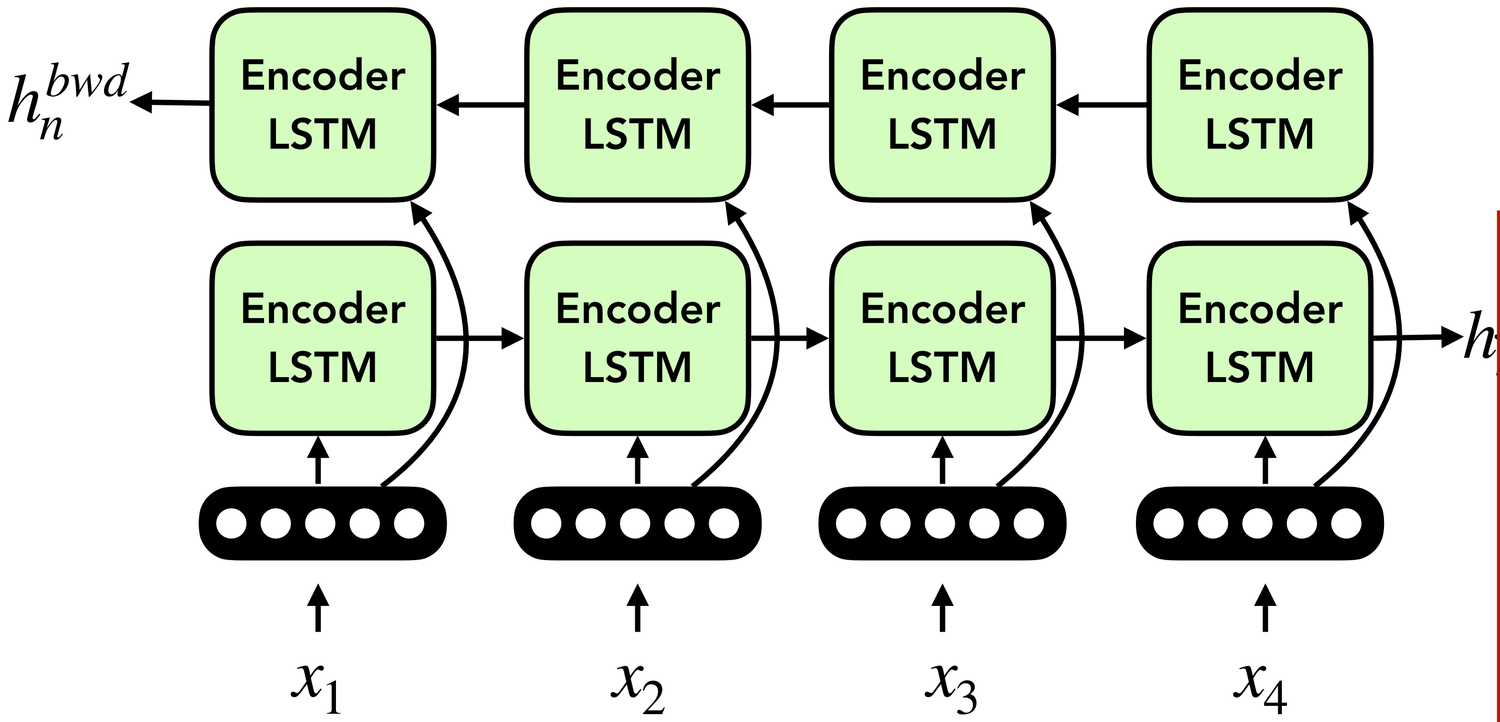

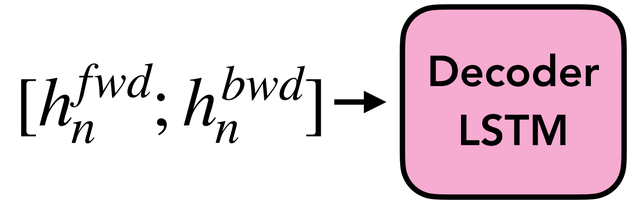

Does the decoder have to be twice the dimensionality of the encoder?

Bidirectional Encoders

- Decoder needs to be unidirectional (autoregressive models can't know the future…)
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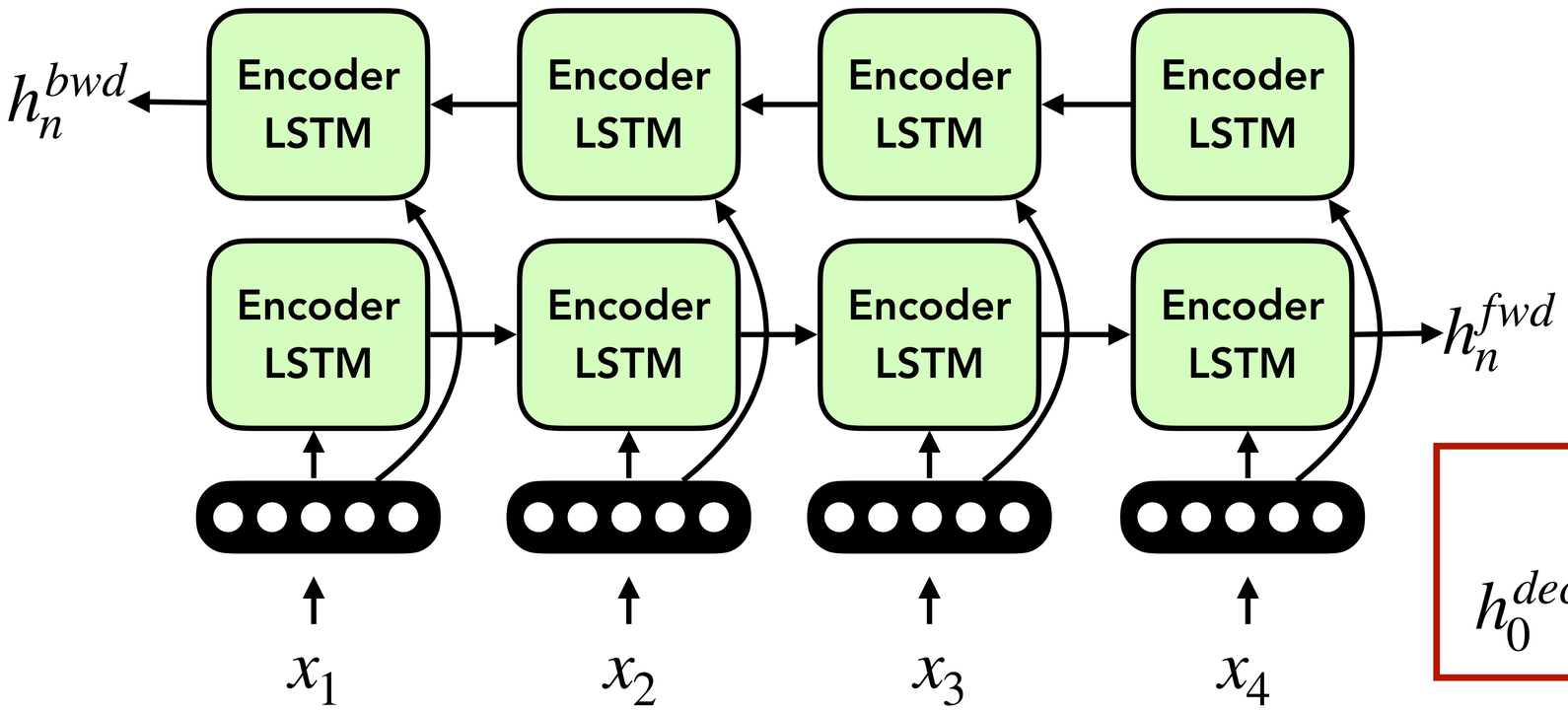
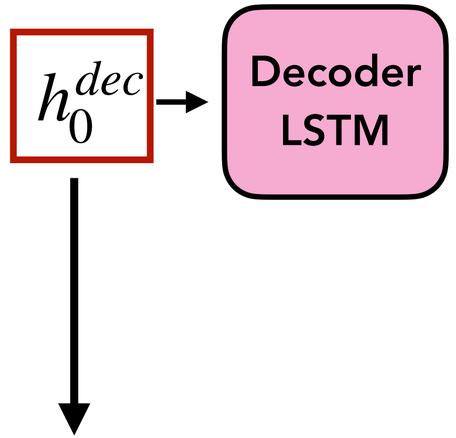




Project beforehand:

$$h_0^{dec} = W_{dec}[h_n^{fwd}; h_n^{bwd}] + b_{dec}$$

Training Encoder-Decoder Models

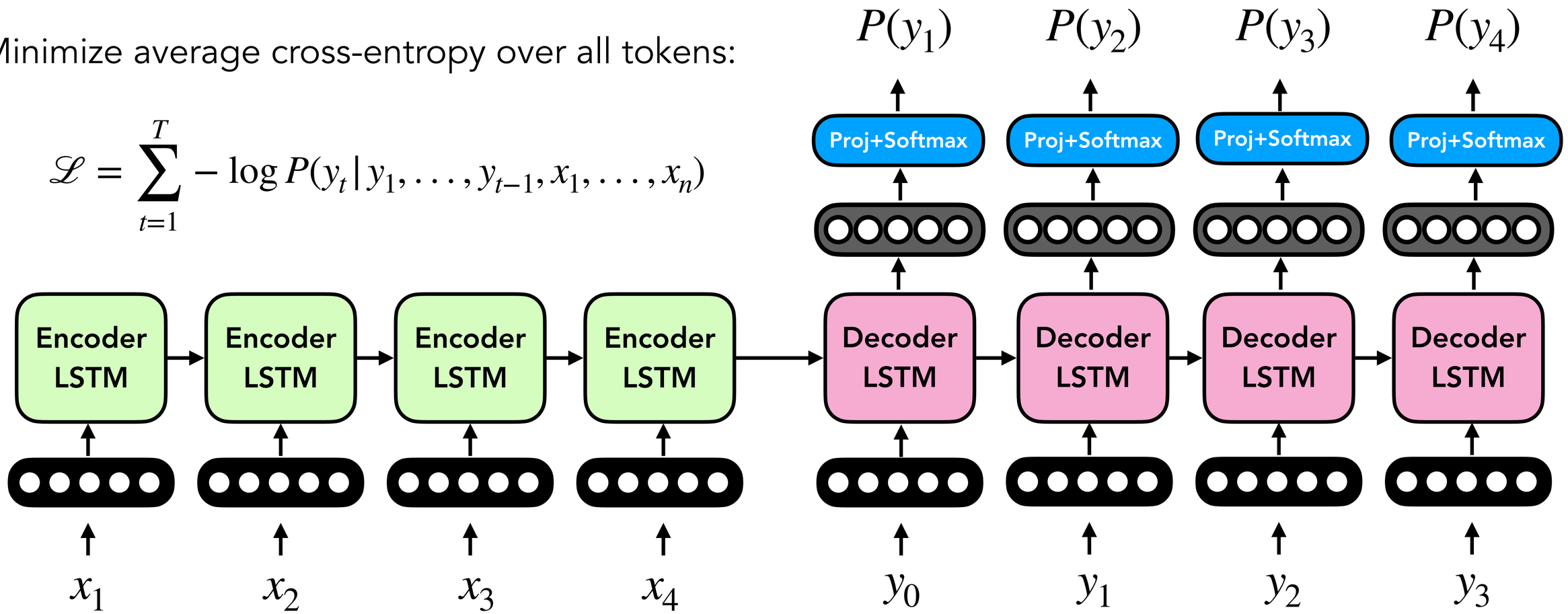
- With a language model, we had practically unlimited data!
  - We were only learning which words followed others, so any text would do!
- With encoder-decoder models, we are learning which sequences align with others
  - **Machine Translation**: Need paired data across languages (sentences that have the same meaning)
  - **Image Captioning**: Need paired image-text data (images and their description)
  - **Code Generation**: Need paired code-text data (e.g., code and their comments)
  - And so on… for other tasks!

Training Encoder-Decoder Models

Similar to training a language model!

Minimize average cross-entropy over all tokens:

$$\mathscr{L} = \sum_{t=1}^{T} -\log P(y_t \,|\, y_1, \ldots, y_{t-1}, x_1, \ldots, x_n)$$



Note: Change in notation — Encoder inputs are now subscripted by *n* and decoder outputs subscripted by *t*

Training Encoder-Decoder Models

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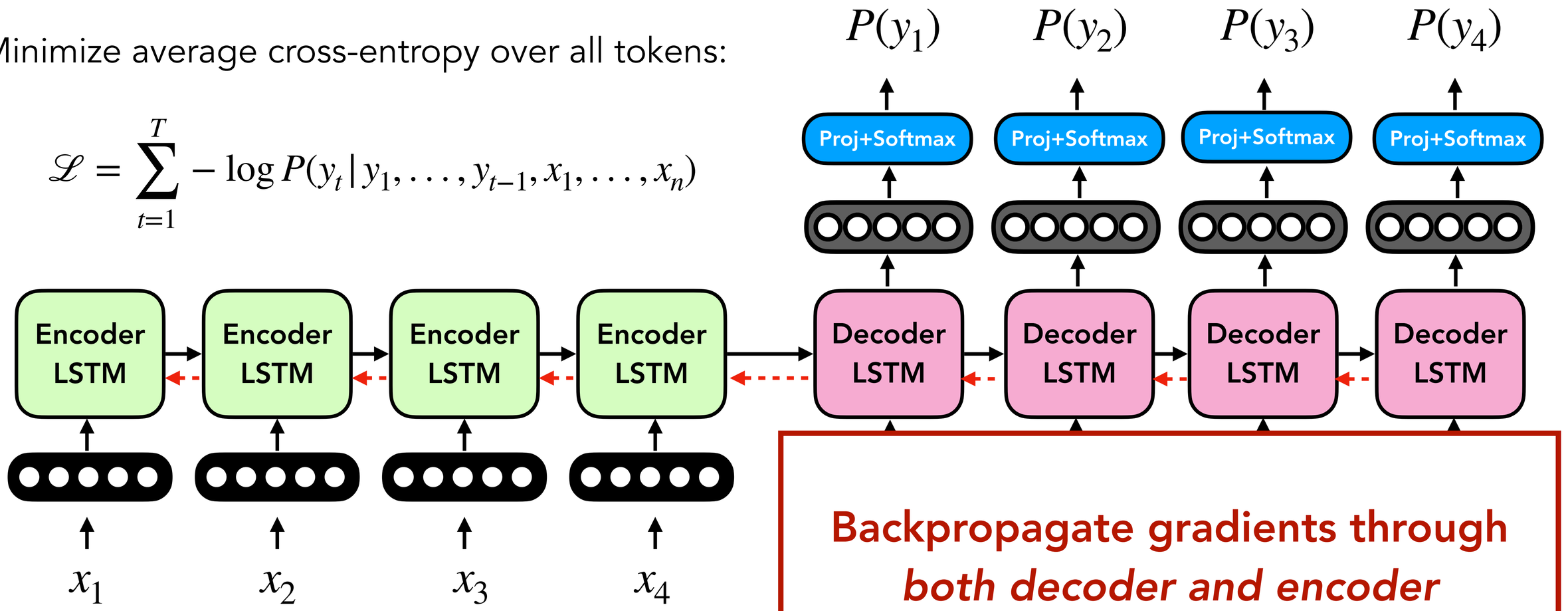

Backpropagate gradients through *both decoder and encoder*

Training Encoder-Decoder Models

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  - We were only learning which words followed others, so any text would do!
- With encoder-d quences align with others
  - **Machine Translat** t have the same meaning)
  - **Image Captioning**: Need paired image-text data (images and their description)
  - **Code Generation**: Need paired code-text data (e.g., code and their comments)
  - And so on… for other tasks!

Warning: Paired data can be much more challenging to find in the wild

“you can’t cram the meaning of a whole %&@#&ing sentence into a single $*(&@ing vector!”

— Ray Mooney (NLP professor at UT Austin)

Issue with Recurrent Models

- State represented as a single vector —> massive compression of information
- At every step, it must be re-computed, making it challenging to learn long-range dependencies without ignoring immediate ones

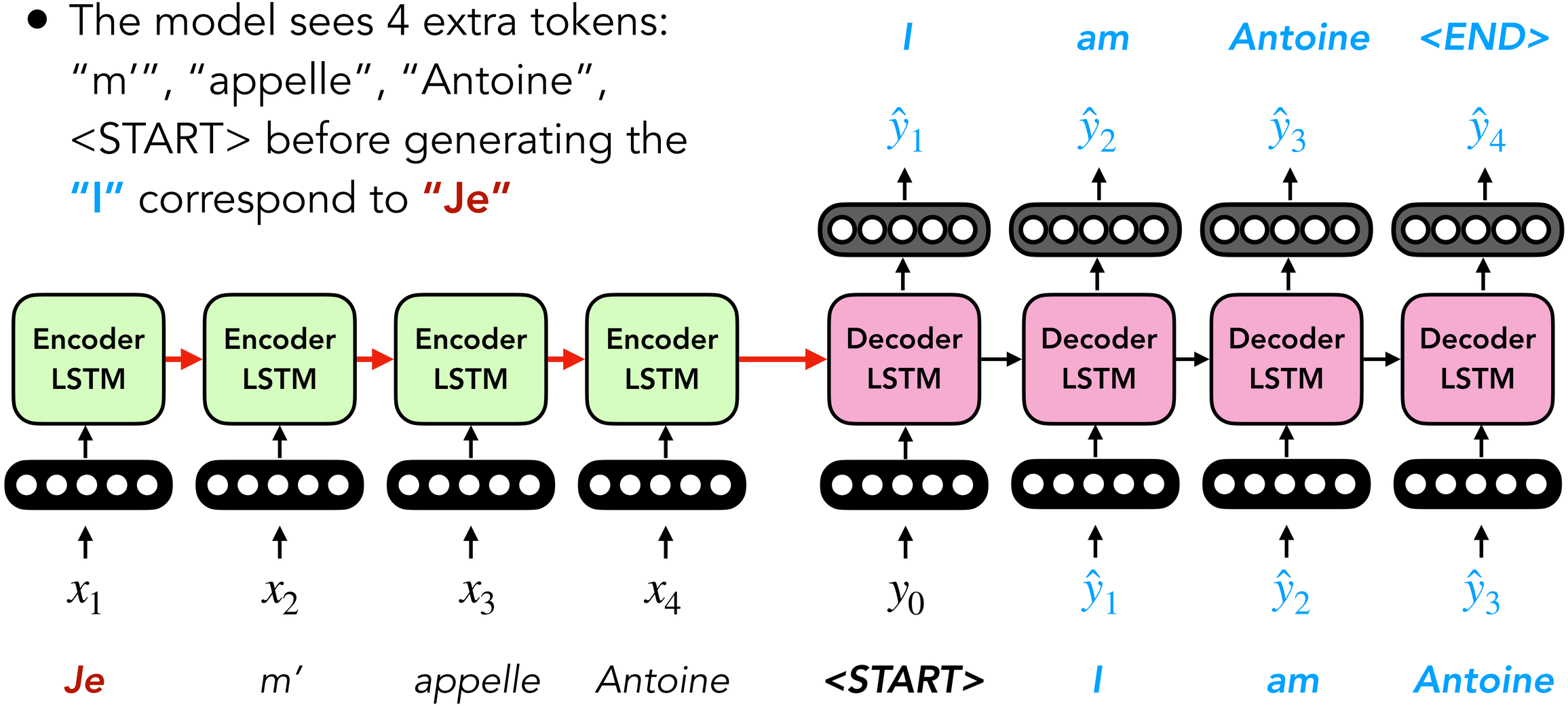
> *They tuned, discussed for a moment, then struck up a lively* ***jig****. Everyone joined in, turning the courtyard into an even more chaotic scene, people now* ***dancing*** *in circles,* ***swinging*** *and* ***spinning*** *in circles, everyone making up their own* ***dance steps****. I felt my feet tapping, my body wanting to move. Aside from writing, I 've always loved* **dancing** .

- Nearby words should affect each other more than farther ones, but RNNs make it challenging to learn **any** long-range interactions

LAMBADA dataset, 2016

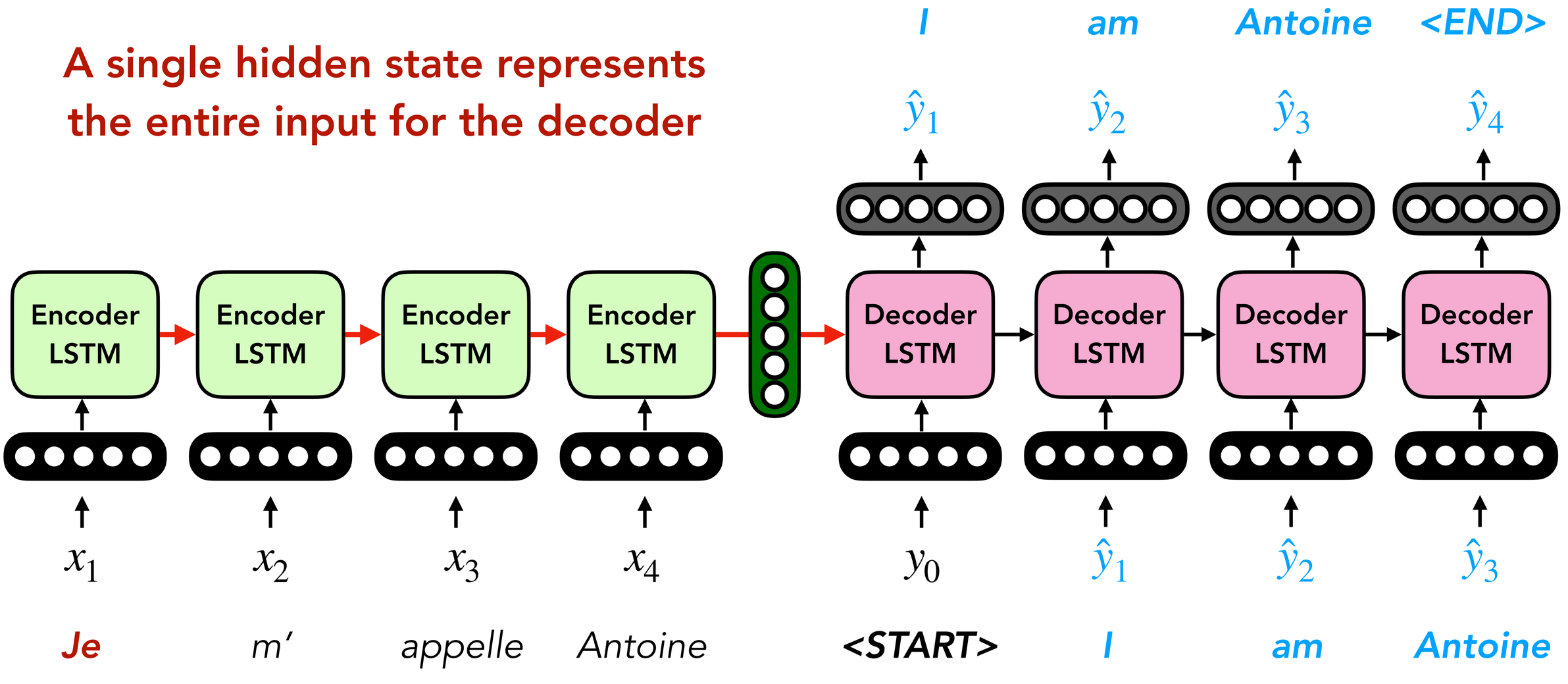
Toy Example

- The model sees 4 extra tokens: "m'", "appelle", "Antoine", <START> before generating the **"I"** correspond to **"Je"**



(Sutskever et al., 2014)

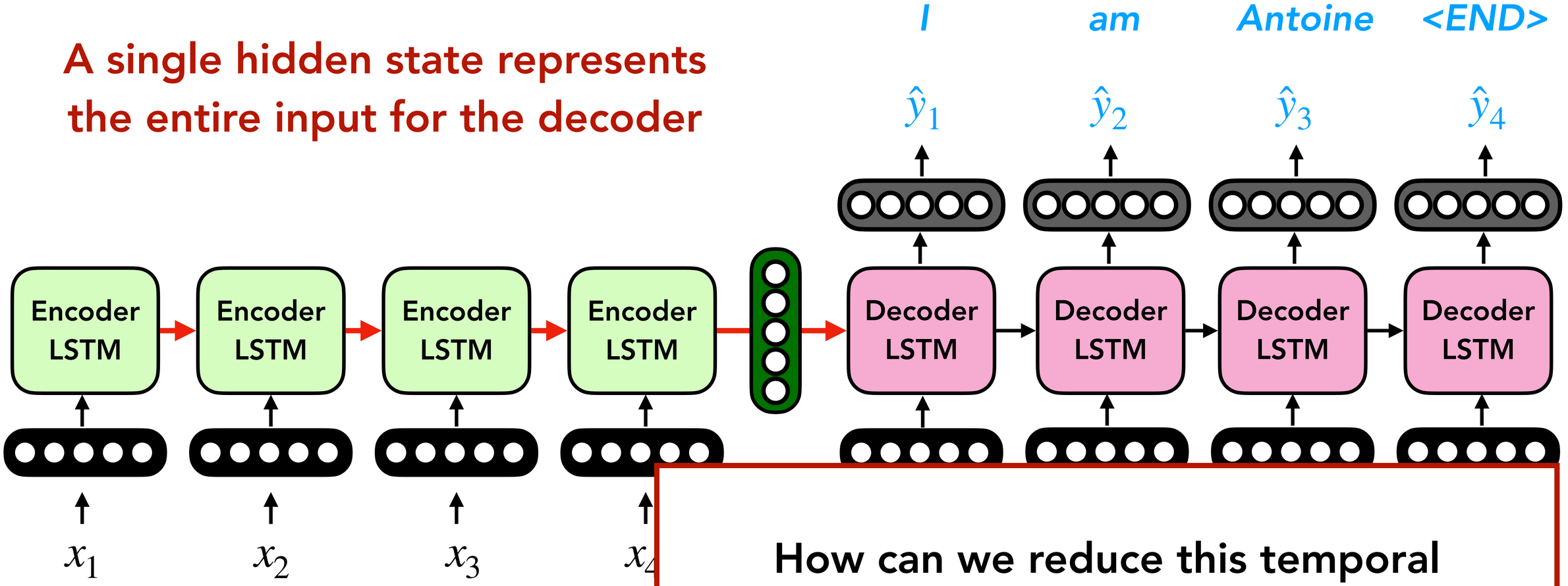
Toy Example



(Sutskever et al., 2014)

Toy Example

A single hidden state represents the entire input for the decoder



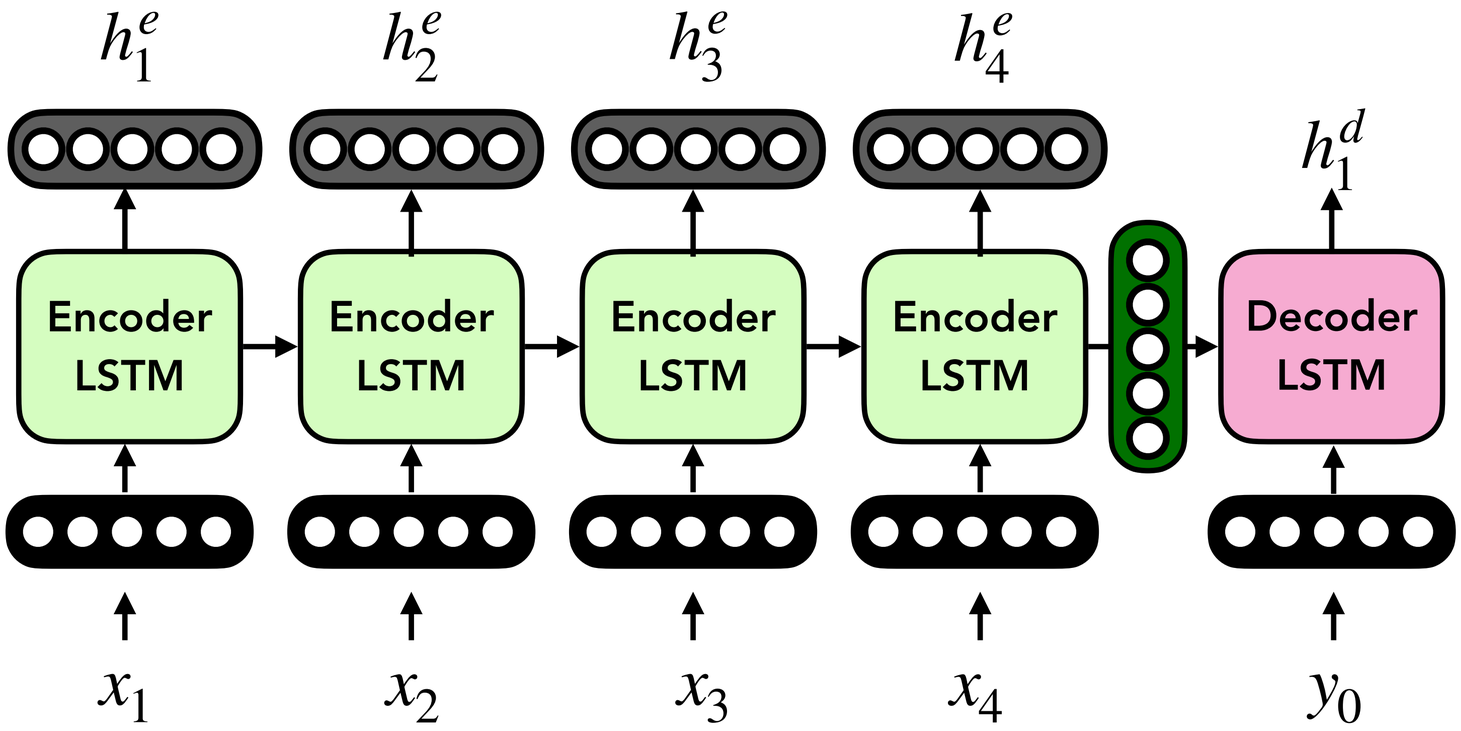
How can we reduce this temporal bottleneck ?

(Sutskever et al., 2014)

Solution

Attention!

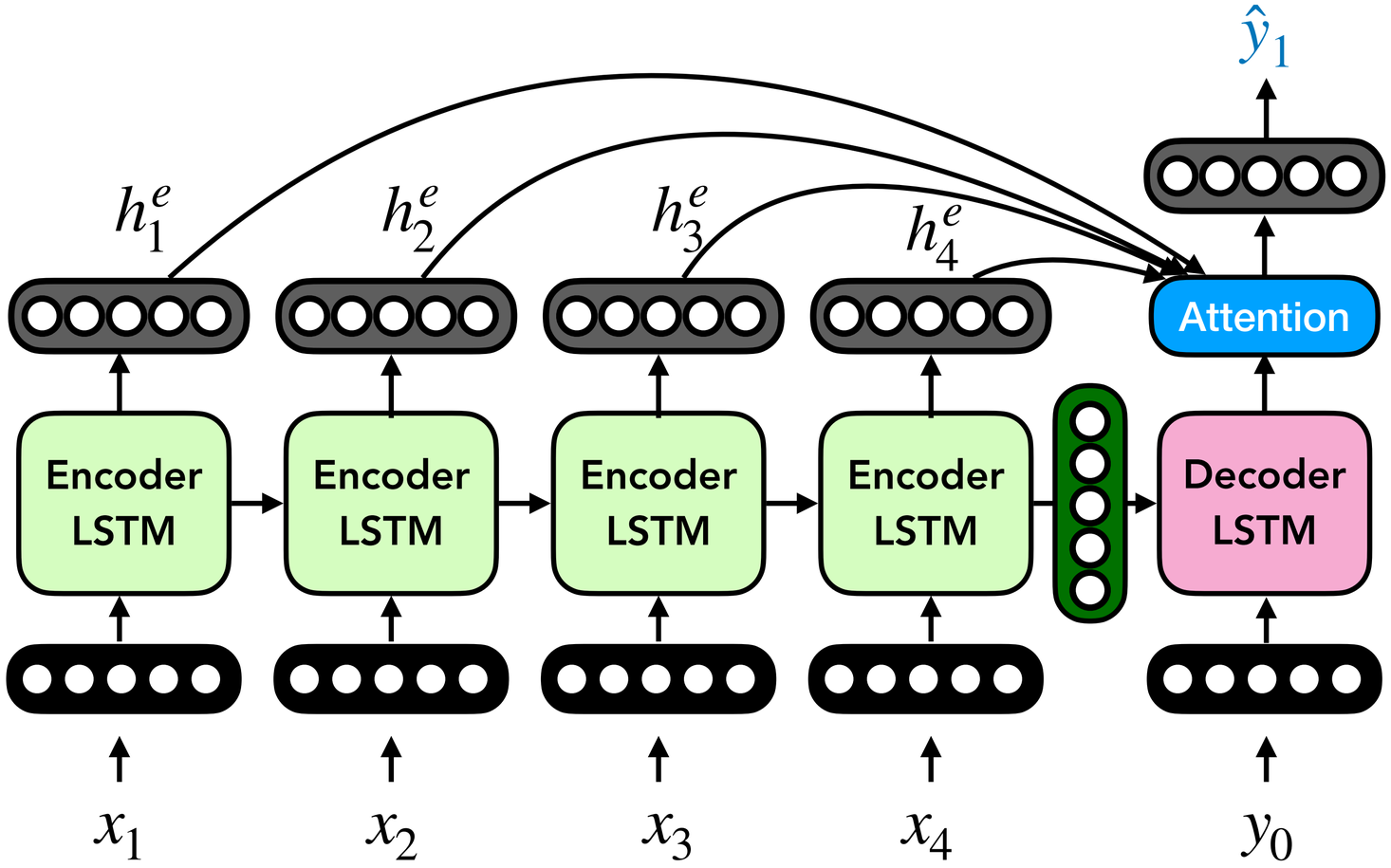
Attentive Encoder-Decoder Models



- **Recall:** At each encoder time step, there is an output of the RNN!

(Bahdanau et al., 2015)

Attentive Encoder-Decoder Models



- **Recall:** At each encoder time step, there is an output h_n^e of the RNN!
- **Idea:** Use the output of the Decoder LSTM to compute an **attention** (i.e., a mixture) over all the h_n^e outputs of the encoder LSTM
- **Intuition:** focus on different parts of the input at each time step

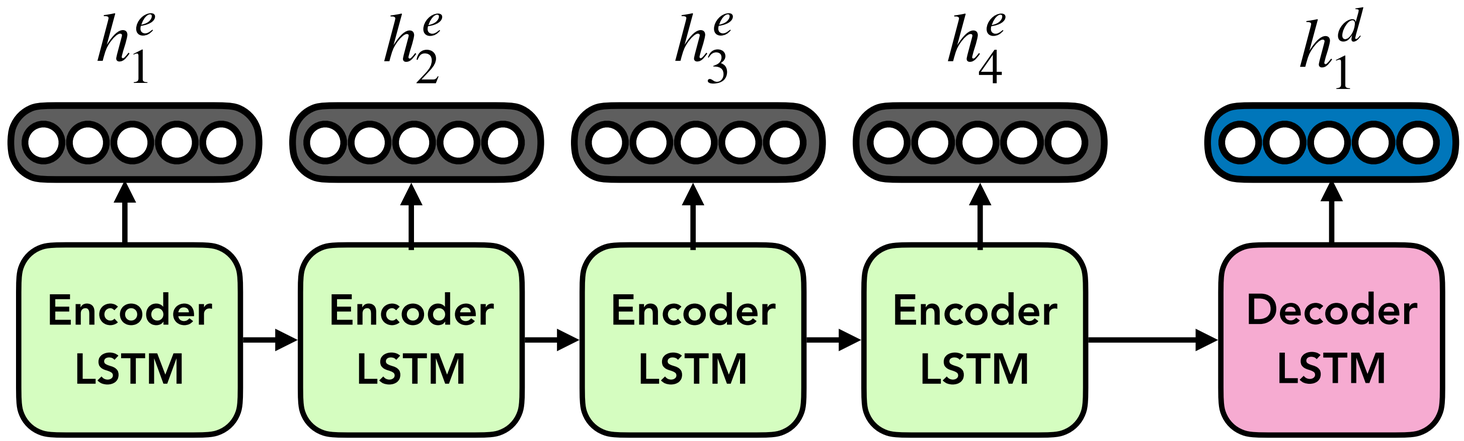
(Bahdanau et al., 2015)

What is attention?

- Attention is a **weighted average over a set of inputs**

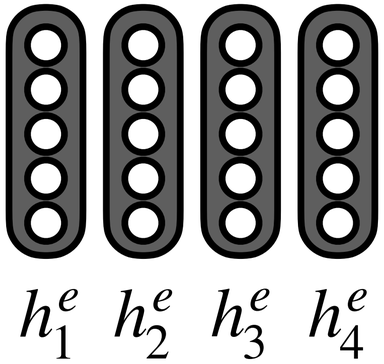
h_n^e = encoder output hidden states

- How should we compute this weighted average?



Attention Function

- **Compute** pairwise similarity between each encoder hidden state and decoder hidden state (“idea of what to decode”)



h_n^e = encoder output hidden states

Also known as a “keys”

h_t^d = decoder output hidden state

Also known as a “query”

Attention Function

- **Compute** pairwise similarity between each encoder hidden state and decoder hidden state ("idea of what to decode")

h_n^e = encoder output hidden states

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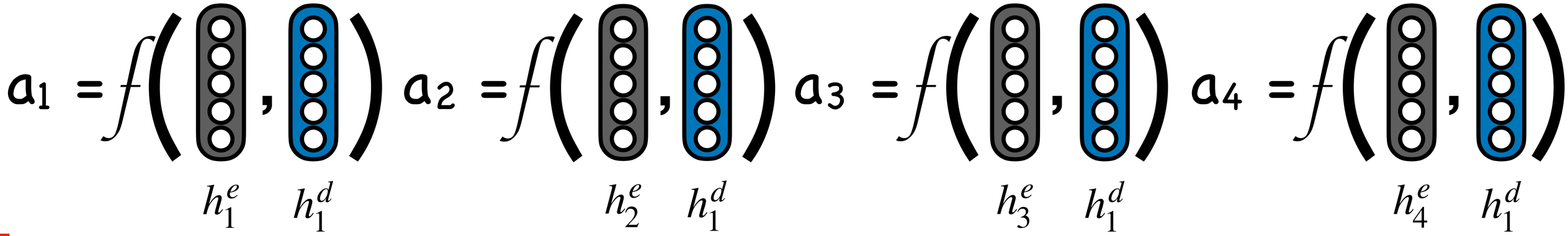


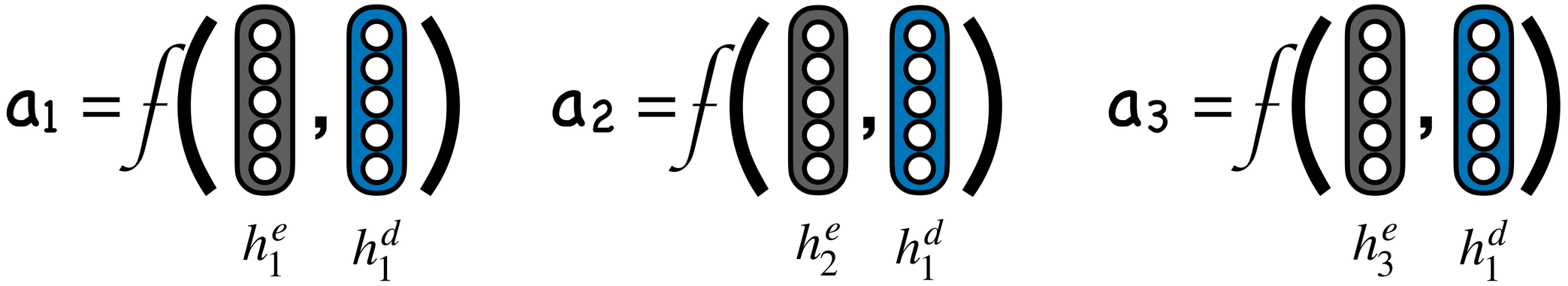
- **We have a single query vector for multiple key vectors**

Attention Function

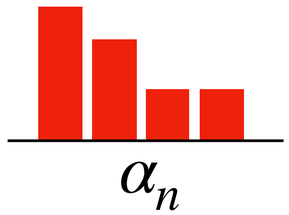
Attention Function	Formula
Multiplicative	$a = h^e \mathbf{W} h^d$
Linear	$a = v^T \phi(\mathbf{W}[h^e; h^d])$
Scaled Dot Product	$a = \frac{(\mathbf{W}h^e)^T(\mathbf{U}h^d)}{\sqrt{d}}$

Attention Function

- **Compute** pairwise similarity between each encoder hidden state and decoder hidden state ("idea of what to decode")

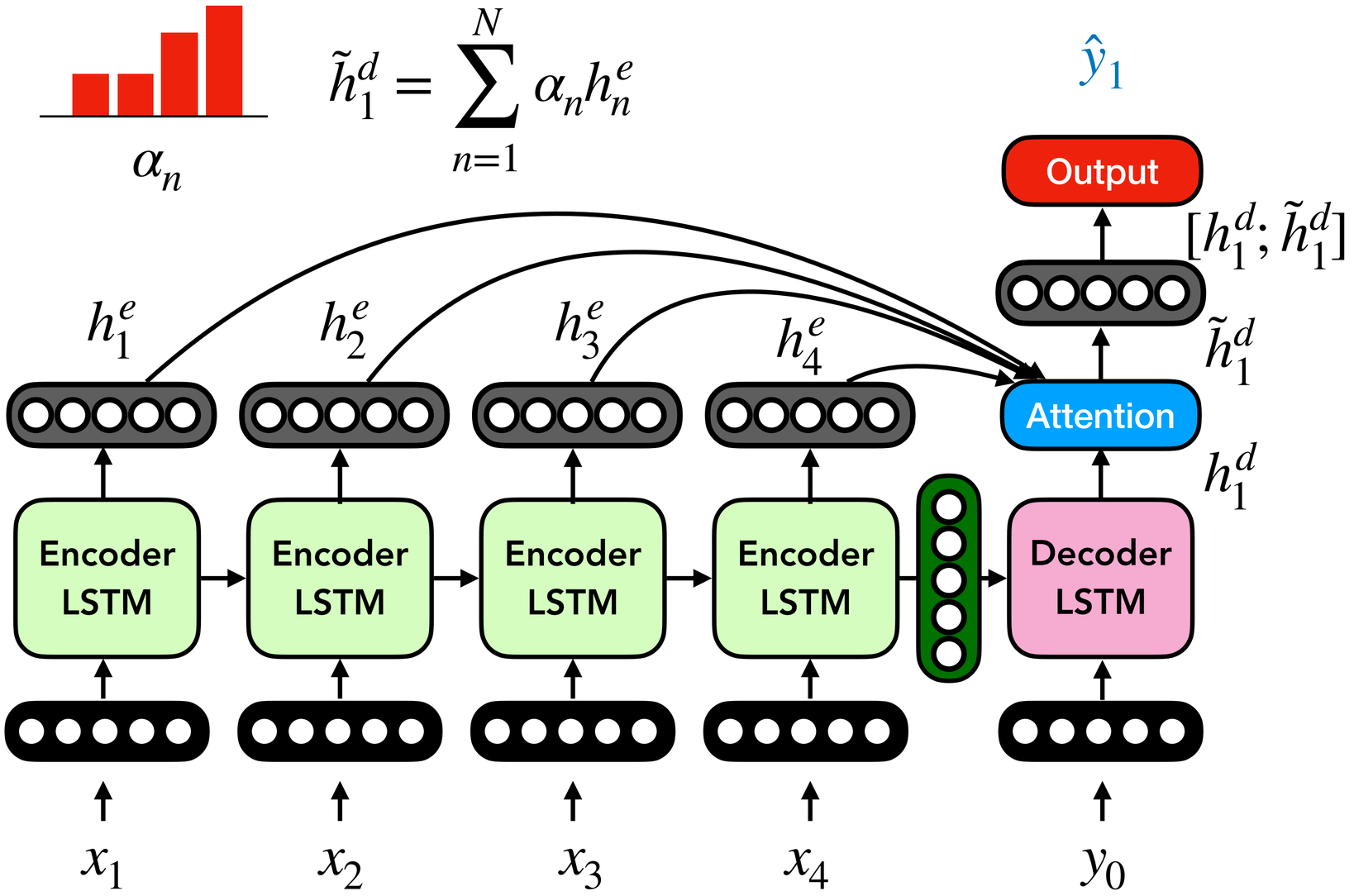


- **Convert** pairwise similarity scores to probability **distribution** (using softmax!) over encoder hidden states and compute weighted average:

Softmax! $\alpha_n = \frac{e^{a_n}}{\sum_j e^{a_j}}$ →  → $\tilde{h}_1^d = \sum_{n=1}^{N} \alpha_n h_n^e$

Here h_n^e is known as the "value"

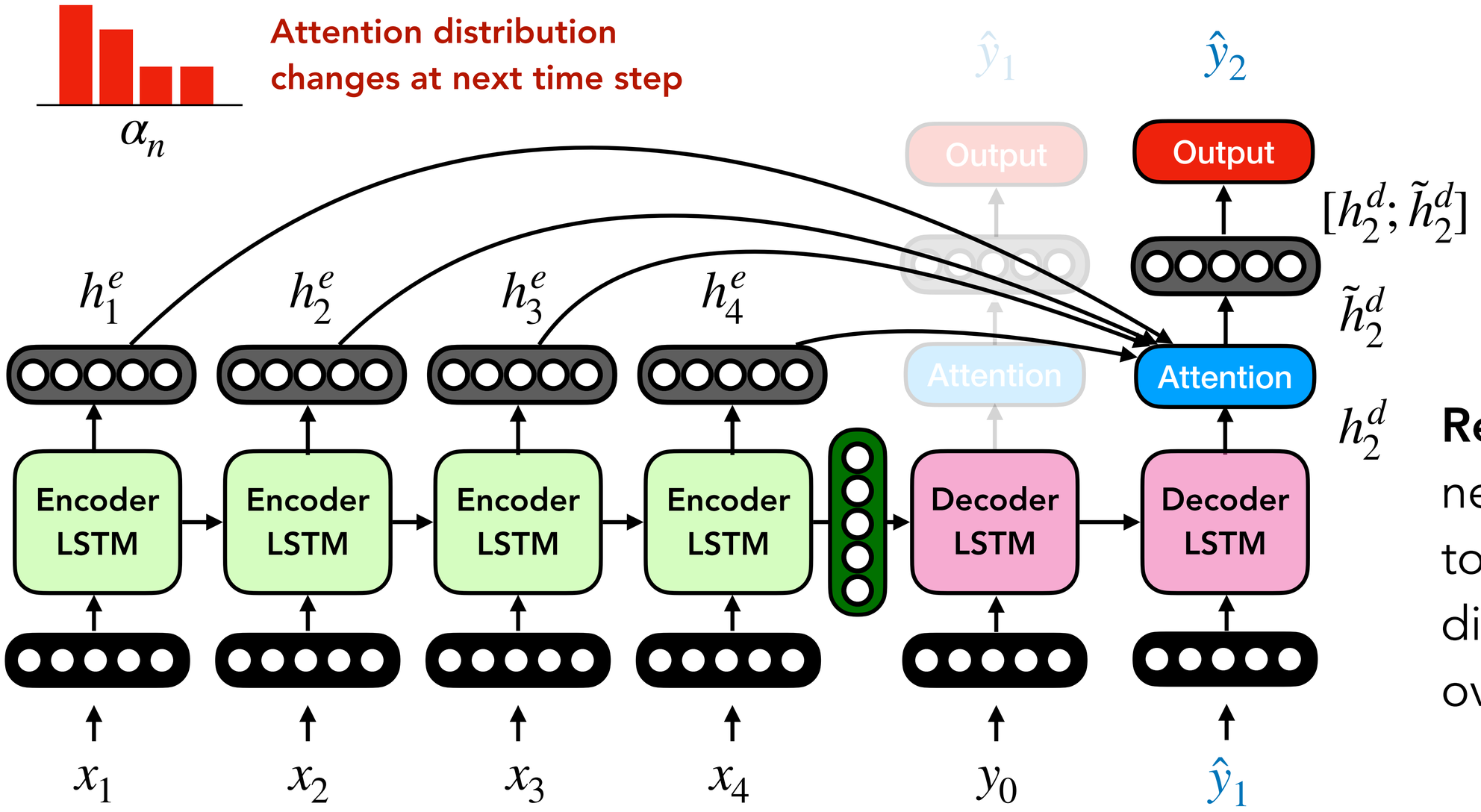
Attentive Encoder-Decoder Models



- **Intuition:** $\tilde{h}_1^d$ contains information about encoder hidden states that got **high** attention
- Typically, $\tilde{h}_1^d$ is concatenated (or composed in some other manner) with h_1^d (the original decoder state) before being passed to the **output** layer
- **Output** layer predicts the most likely output token $\hat{y}_1$

(Bahdanau et al., 2015)

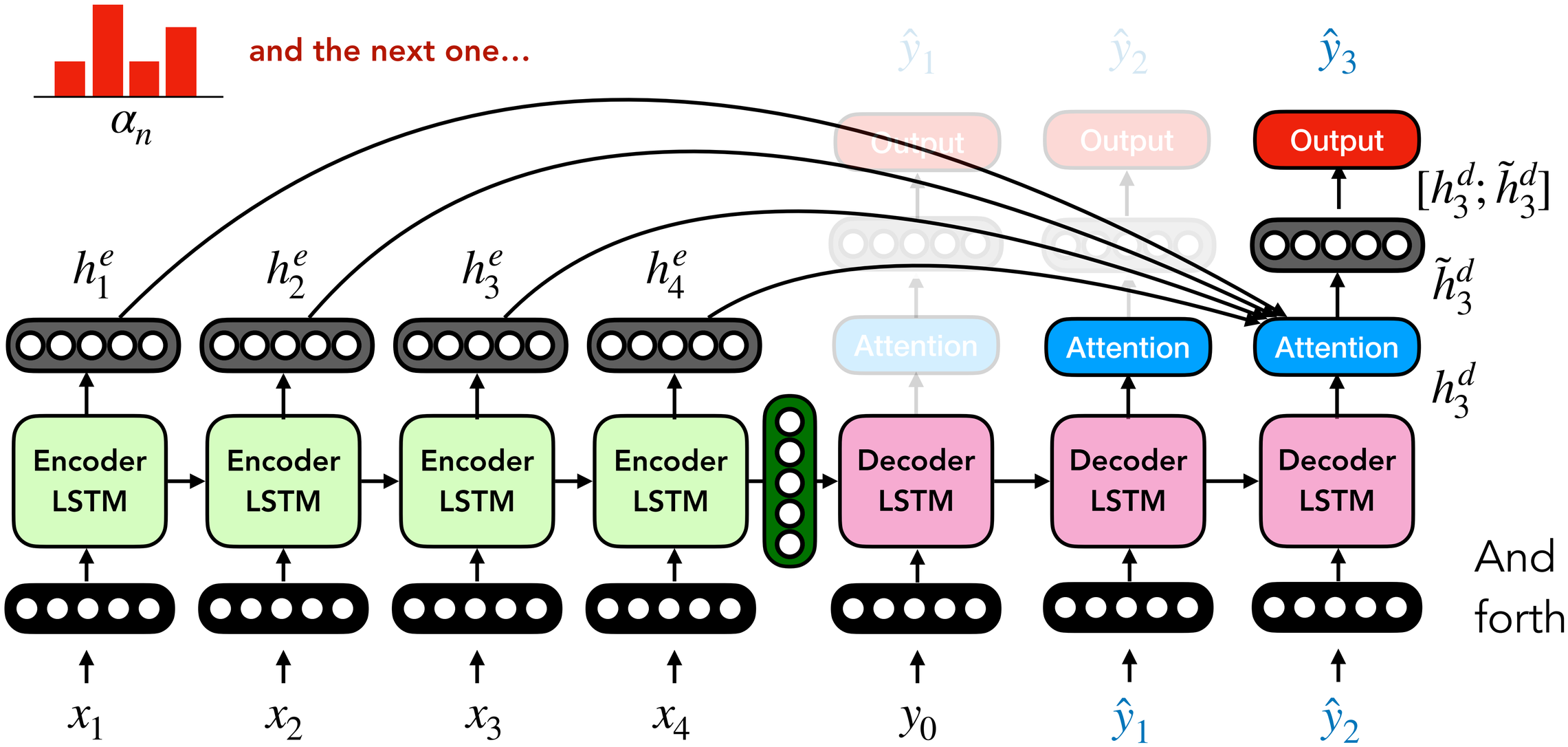
Attentive Encoder-Decoder Models



Repeat in next time step to get new distribution over states

(Bahdanau et al., 2015)

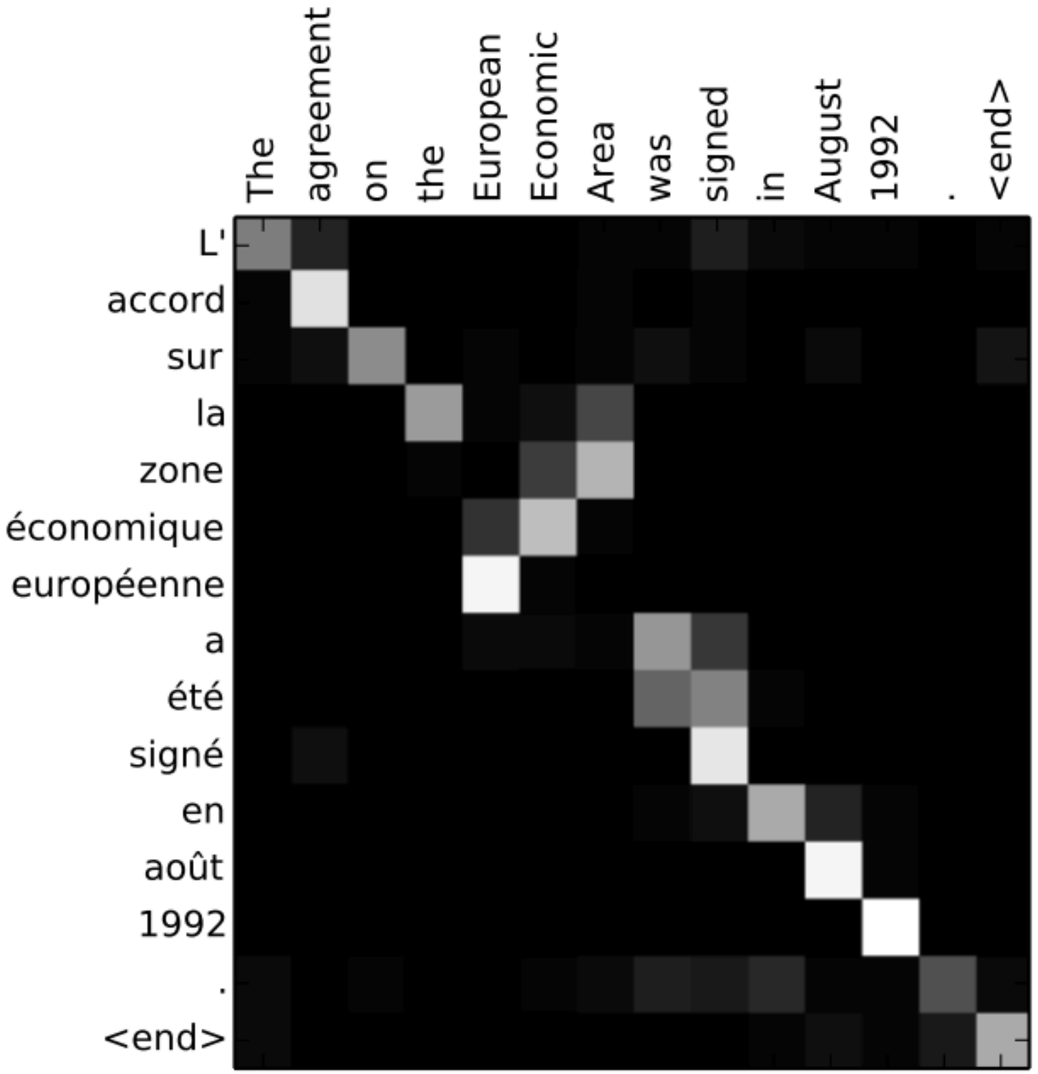
Attentive Encoder-Decoder Models



(Bahdanau et al., 2015)

Interpretability?

- **Main Idea:** Attention can be visualised based on the score given to each encoder hidden state
- What is focused on when each word is generated?
- Training with attention gives us implicit alignment for free!



Question

How does attention address the temporal bottleneck in sequence to sequence models?

Direct connections between decoder states and encoder hidden states

Attention Recap

- **Main Idea:** Decoder computes a weighted sum of encoder outputs
  - Compute pairwise score between each encoder hidden state and initial decoder hidden state ("idea of what to decode")
- Many possible functions for computing scores (dot product, bilinear, etc.)
- **Temporal Bottleneck Fixed! Direct link** between decoder and encoder states
  - Helps with vanishing gradients!
- **Interpretability** allows us to investigate model behavior!
- Attention is **agnostic** to the type of RNN used in the encoder and decoder!

Question

In what range can an attention weight fall ?

[0, 1]

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