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Designing, Visualizing and Understanding Deep Neural Networks (2021)

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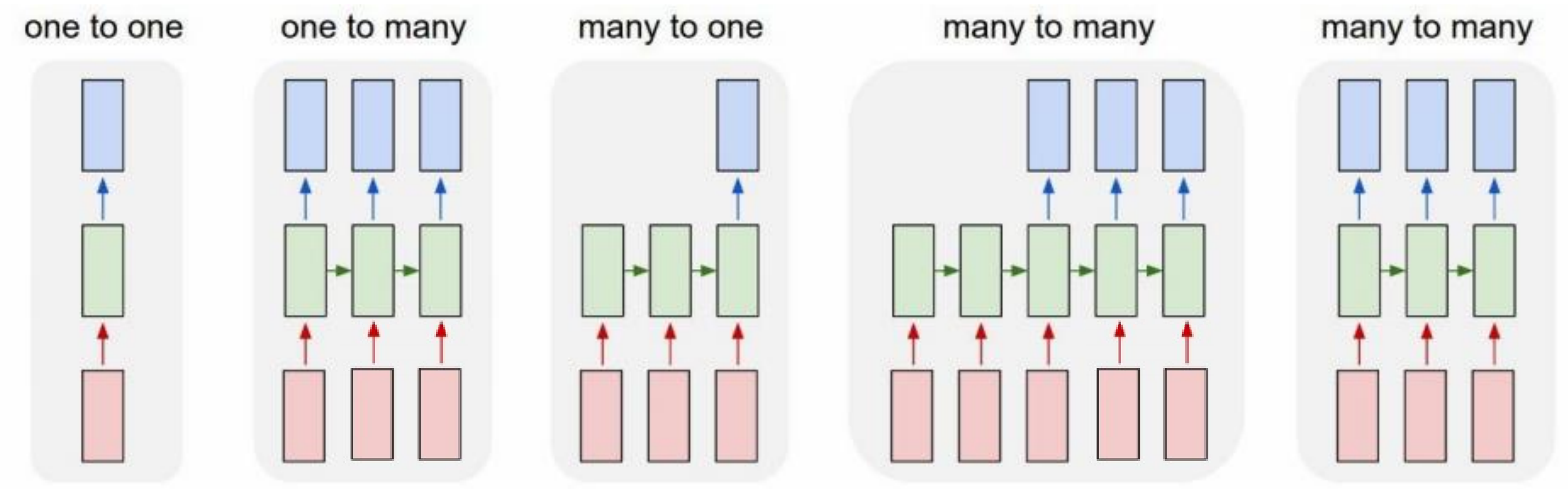
Sequence to Sequence Models

Designing, Visualizing and Understanding Deep Neural Networks

CS W182/282A

Instructor: Sergey Levine
UC Berkeley

Last time: RNNs and LSTMs



e.g., activity recognition

e.g., frame-level video annotation

e.g., image captioning

e.g., machine translation

Image: Andrej Karpathy

A basic neural language model

training data: natural sentences

I think therefore I am

I like machine learning

I am not just a neural network

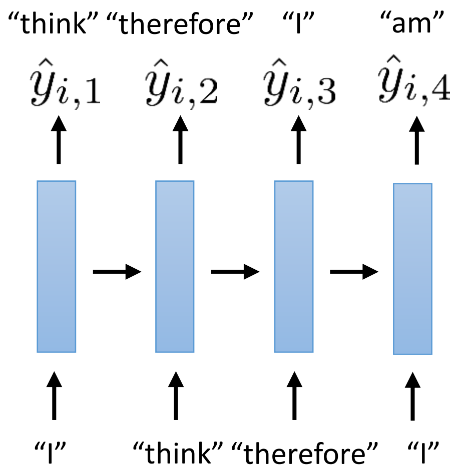
in reality there could be several million of these

how are these represented?

tokenize the sentence (each word is a token)

simplest: one-hot vector

more complex: word embeddings (we'll cover this later)



We'll talk about **real** language models much more later

$$x_{1,1} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

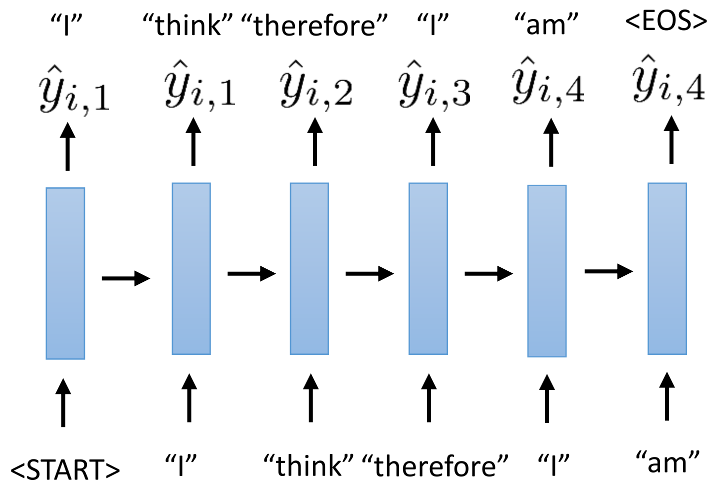
dimensionality = number of possible words

index of this word

A few details

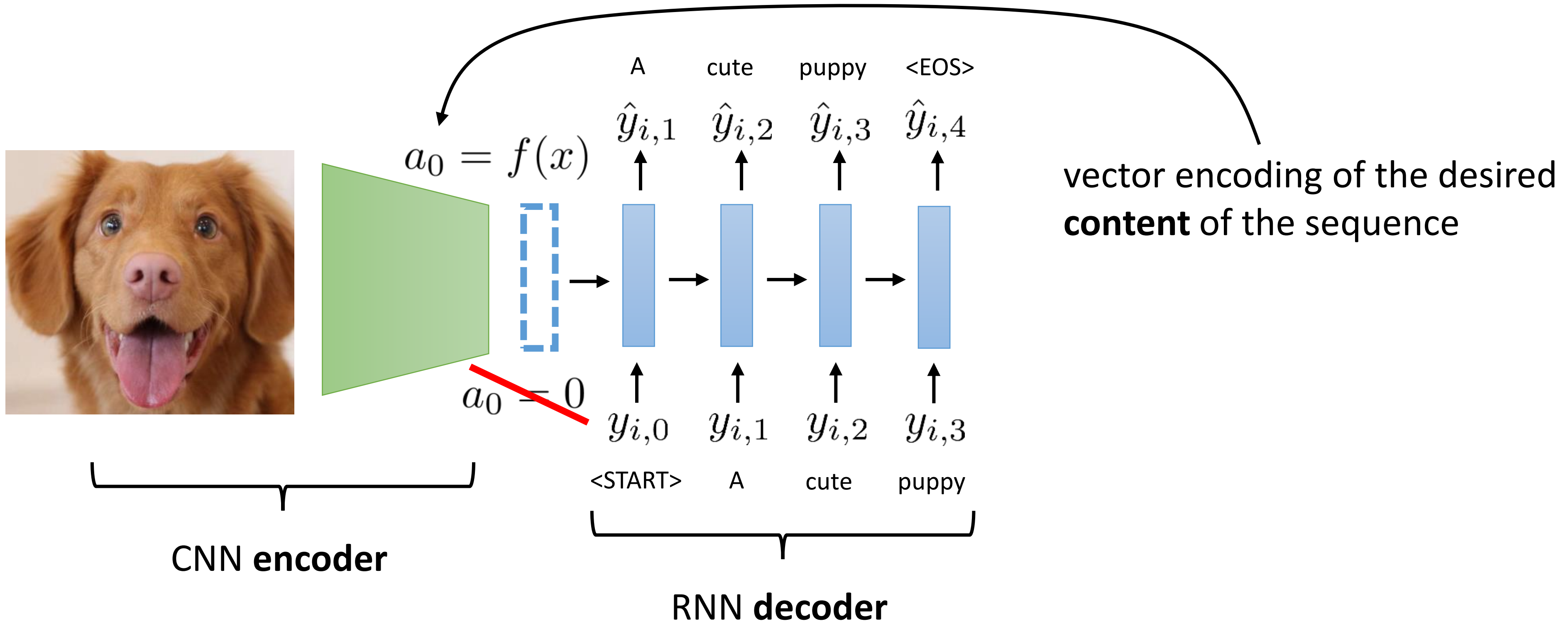
Question: how do we use such a model to **complete** a sequence (e.g., give it “I think…” and have it finish it?)

train model to output <EOS> token when sequence ends



If we want to come up with an entirely new sequence, start with a special <START> token

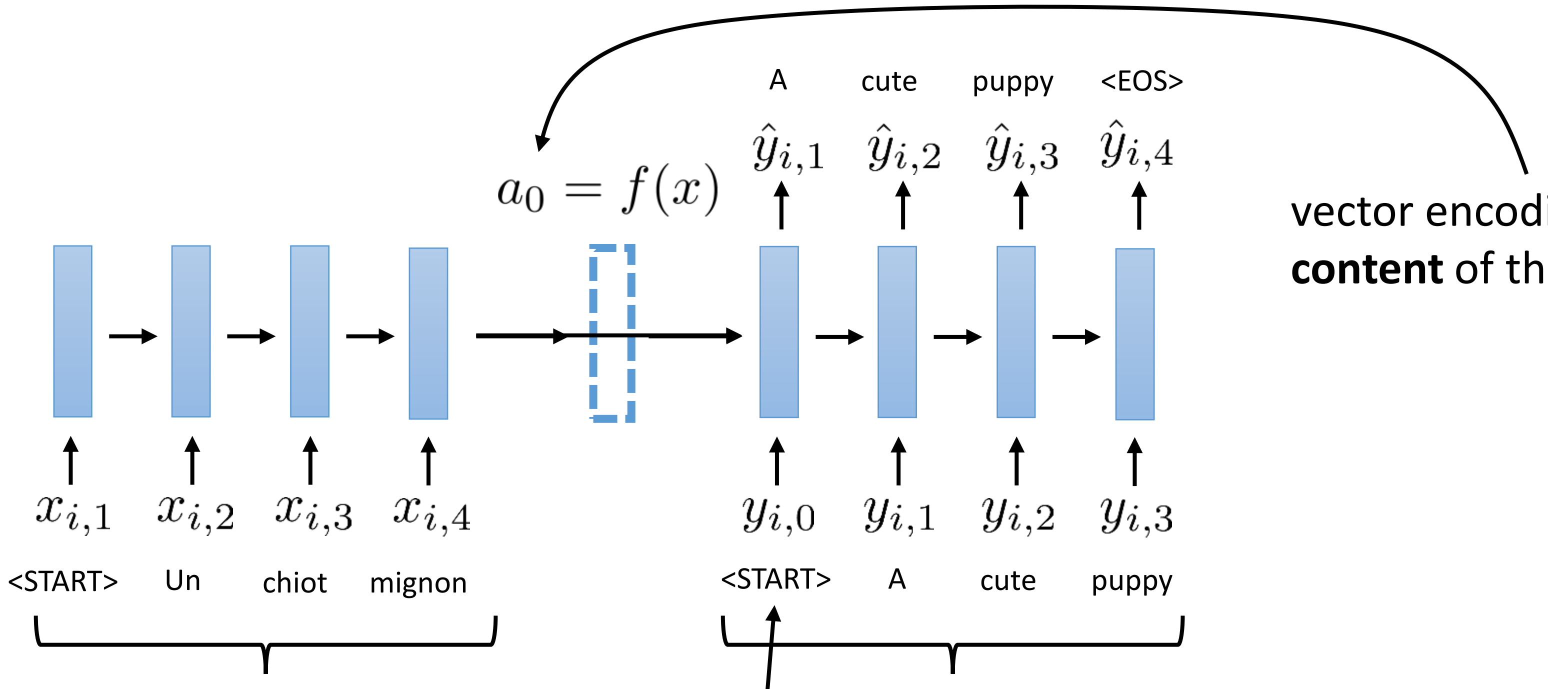
A conditional language model



What do we expect the training data to look like?

How do we tell the RNN **what** to generate?

What if we condition on *another* sequence?



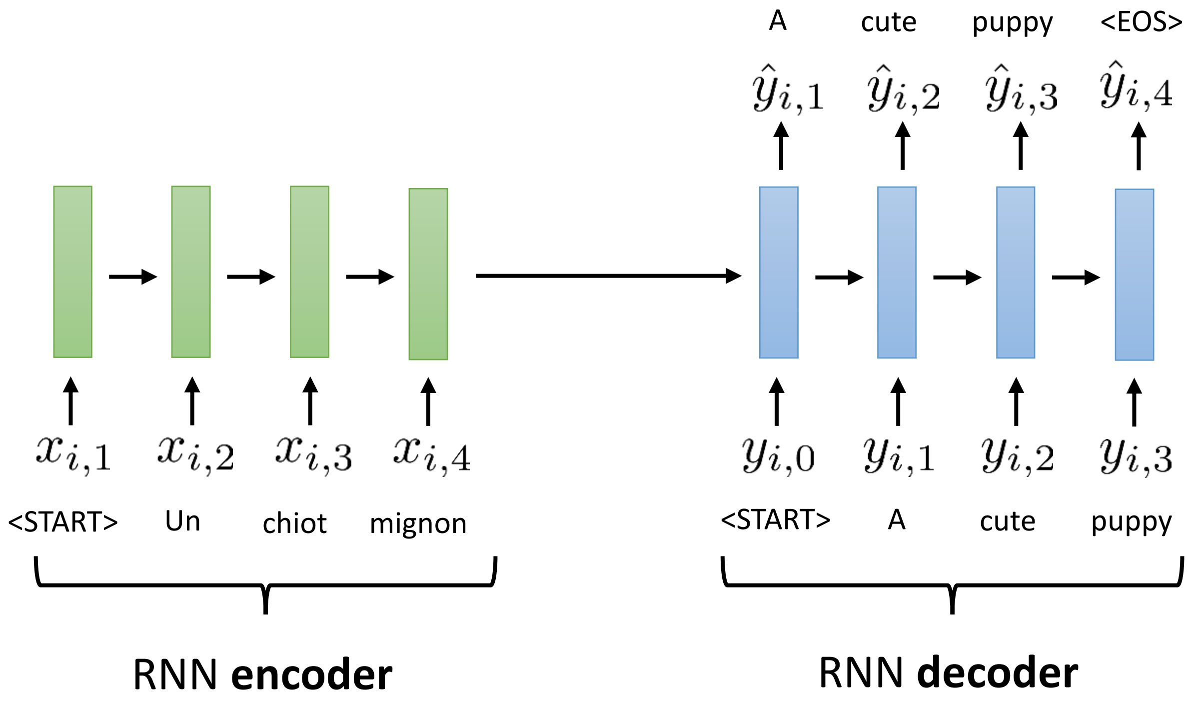
vector encoding of the desired **content** of the sequence

doubles as <EOS> token for input sequence

in reality the input sequence is often read **in reverse**

why?

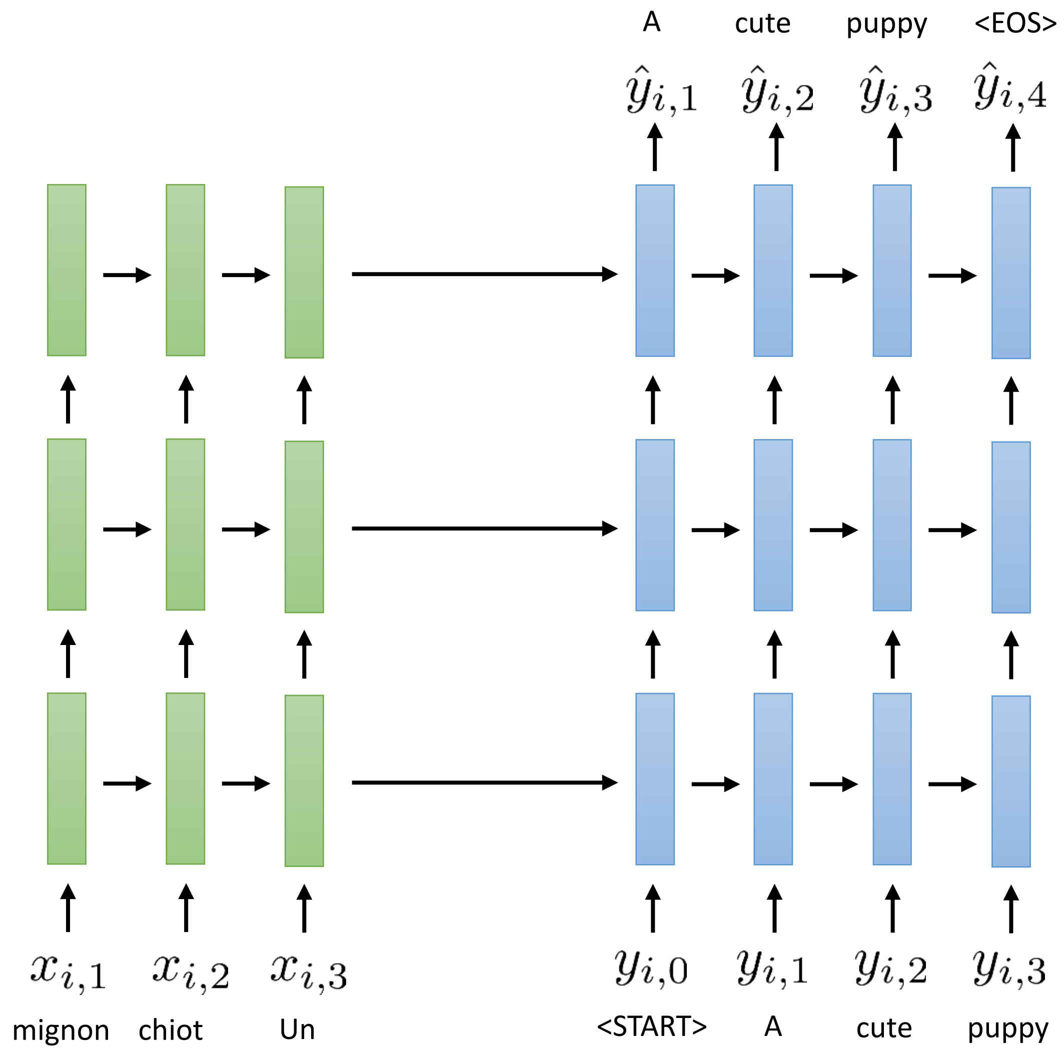
Sequence to sequence models



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

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

A more realistic example



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

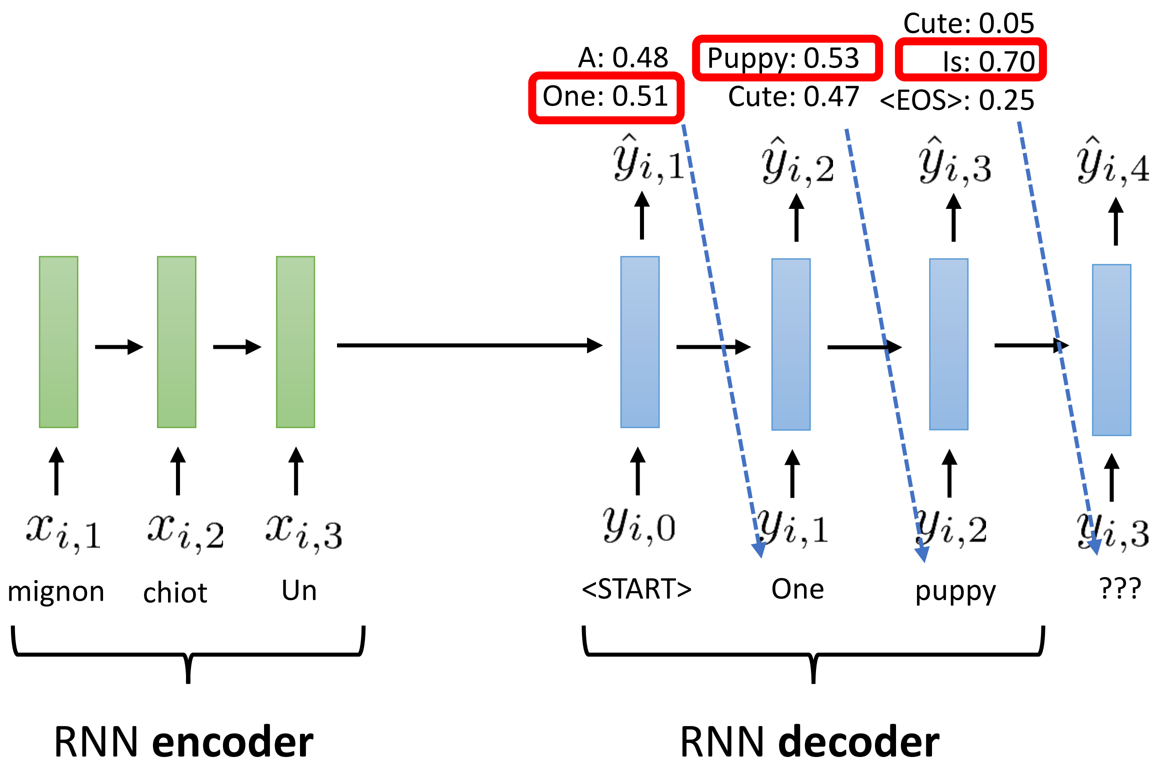
Not just for cute puppies!

- 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.

Decoding with beam search

Decoding the most likely sequence



notice we feed this in reverse, and don't need a "<START>" token on the encoder

What we *should* have done

what does each output represent?

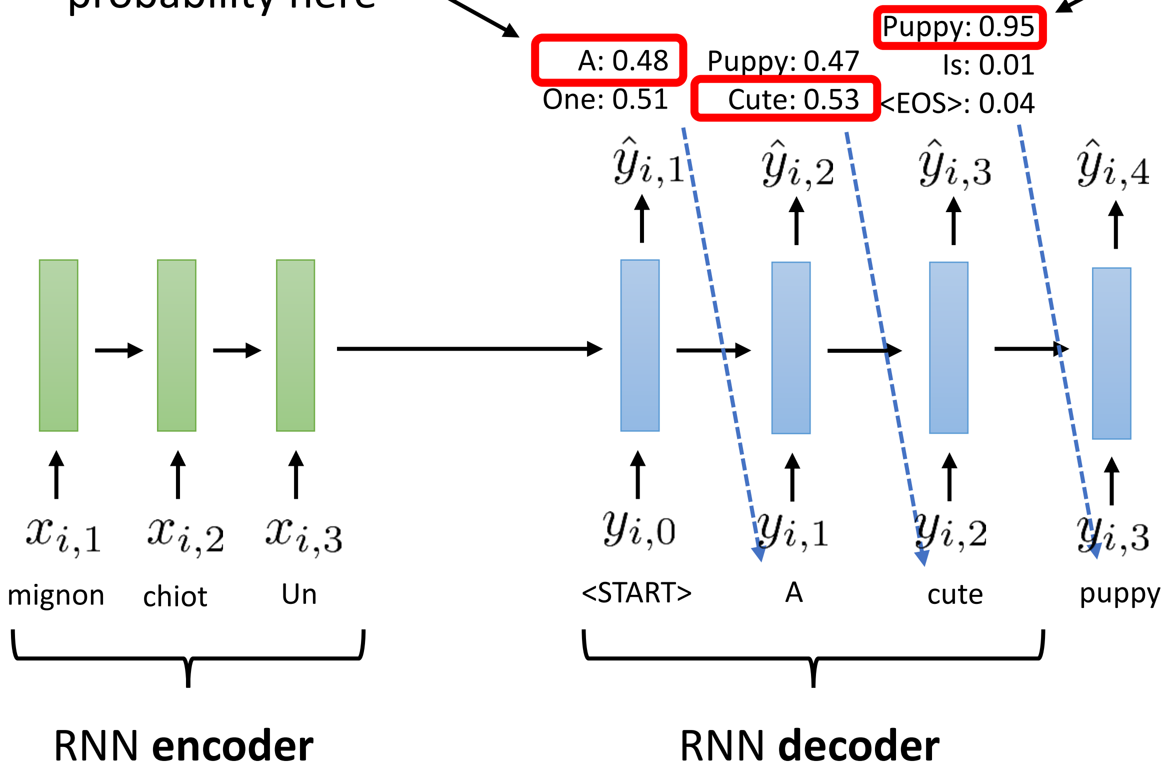
$$p(y_{i,t} | x_{i,1:T}, y_{i,0:t-1})$$

depends on whole input sequence

and output sequence so far!

slightly lower probability here

much higher probability here



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

notice we feed this in reverse, and don't need a "<START>" token on the encoder

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

probabilities at each time step

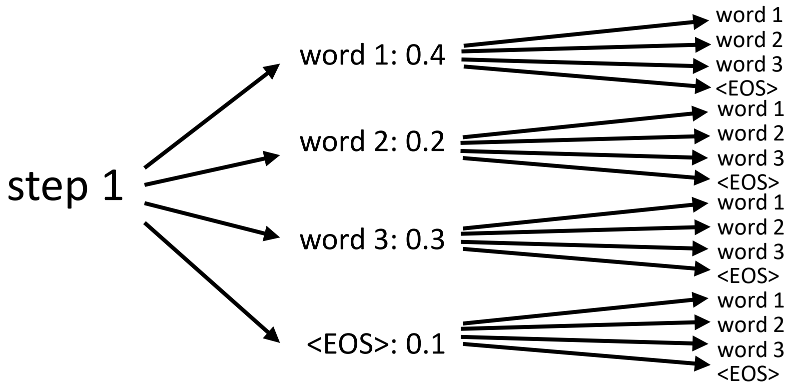
How many possible decodings are there?

Word 1: 0.4	Word 1: 0.1	Word 1: 0.7	Word 1: 0.1	Word 1: 0.0	
Word 2: 0.2	Word 2: 0.5	Word 2: 0.1	Word 2: 0.8	Word 2: 0.1	....
Word 3: 0.3	Word 3: 0.2	Word 3: 0.1	Word 3: 0.0	Word 3: 0.0	
<EOS>: 0.1	<EOS>: 0.2	<EOS>: 0.1	<EOS>: 0.1	<EOS>: 0.9	

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

Fortunately, the **structure** of this problem makes some simple **approximate search** methods work **very well**

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

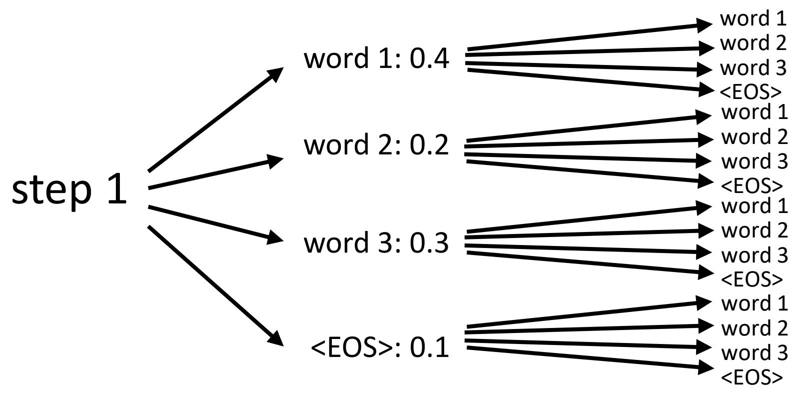
This is not true in general! This is a guess based on what we know about sequence decoding.

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



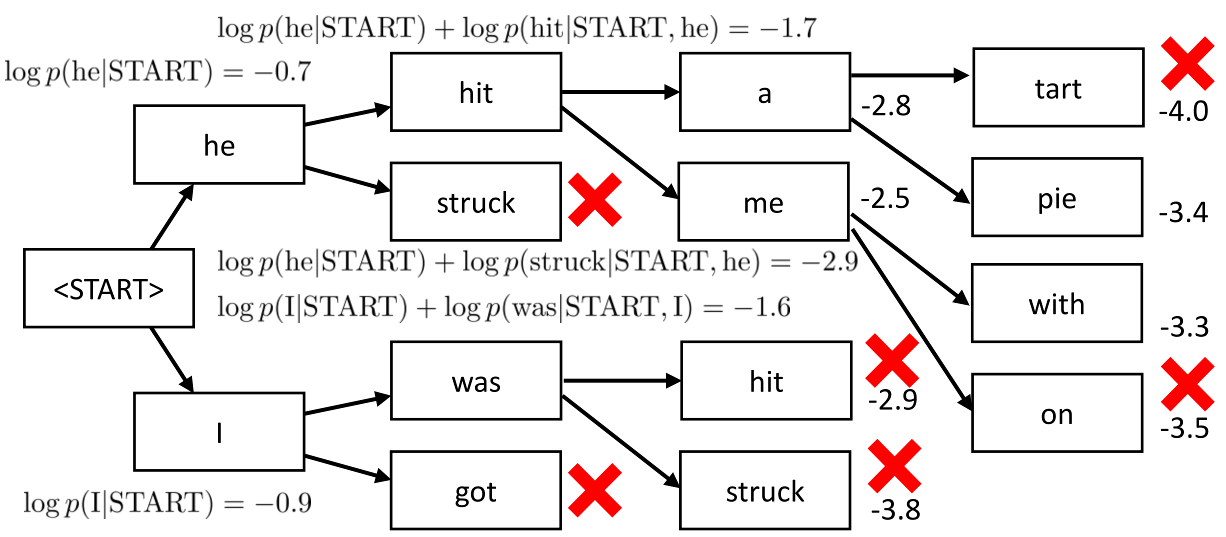
Beam search example

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

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

Example (CS224n, Christopher Manning): **translate (Fr->En):** <u>il a m'entarté</u> (he hit me with a pie)

k = 2 (track the 2 most likely hypotheses) 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

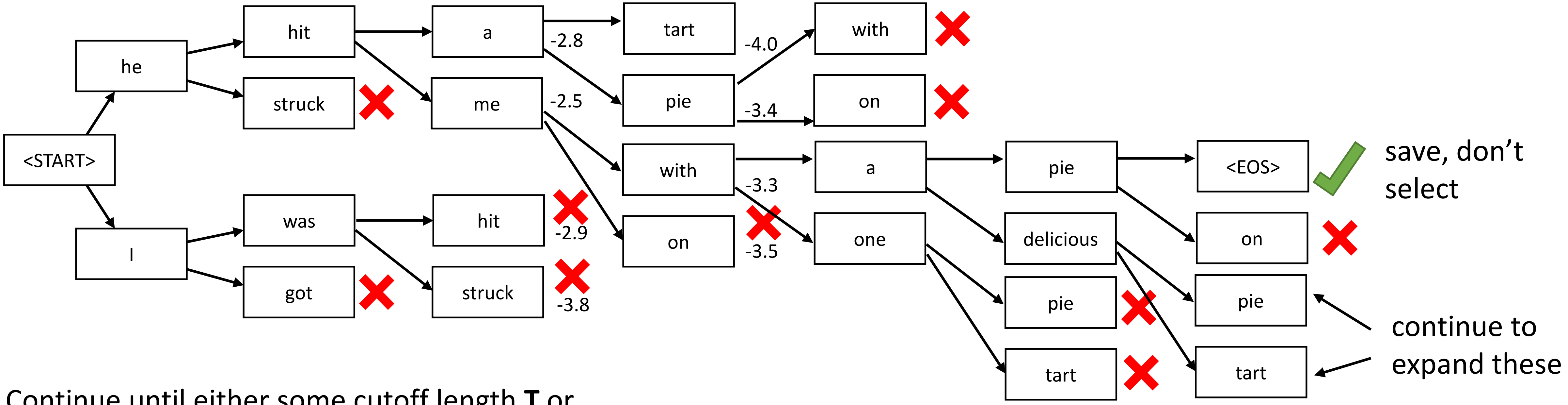
2. sort the resulting k^2 length t sequences by their *total* log-probability
3. keep the top k
4. advance each hypothesis to time $t+1$

When do we stop decoding?

Let’s say 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 log p = -4.5

he threw a pie log p = -3.2 this is best, right?

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

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

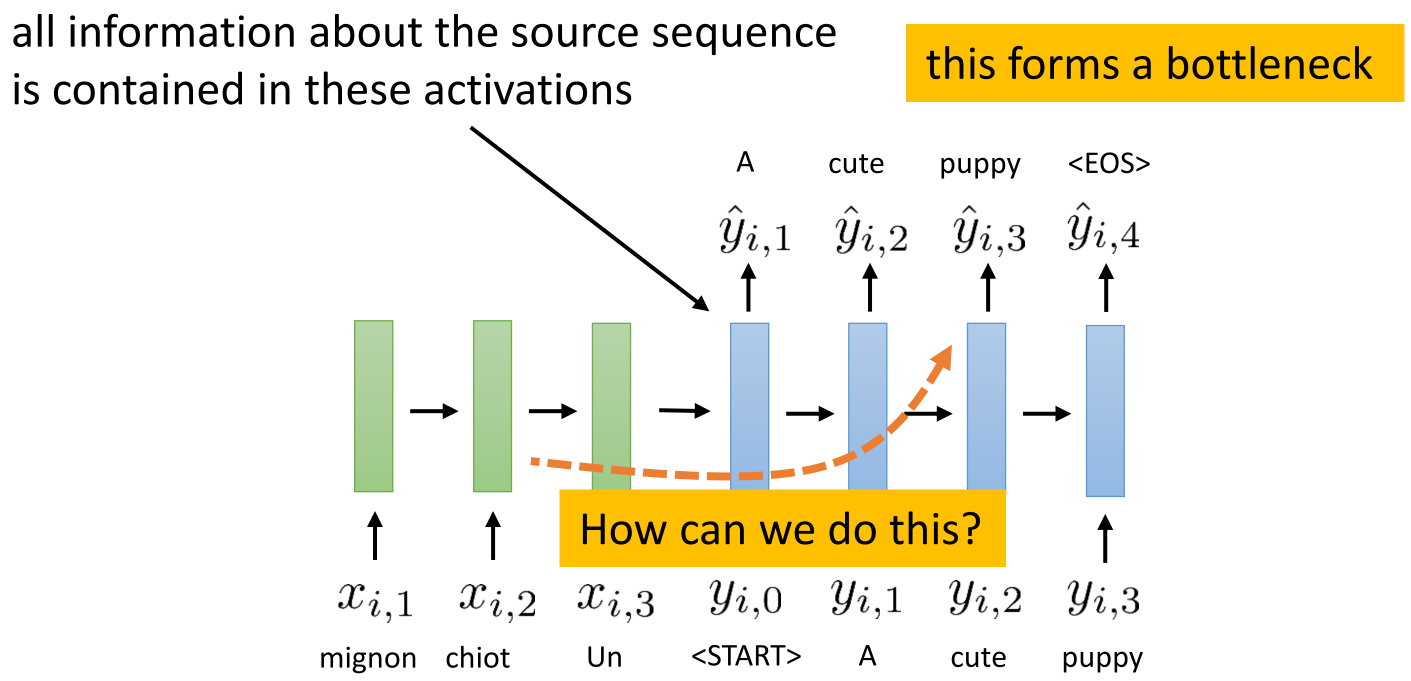
at each time step t:

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

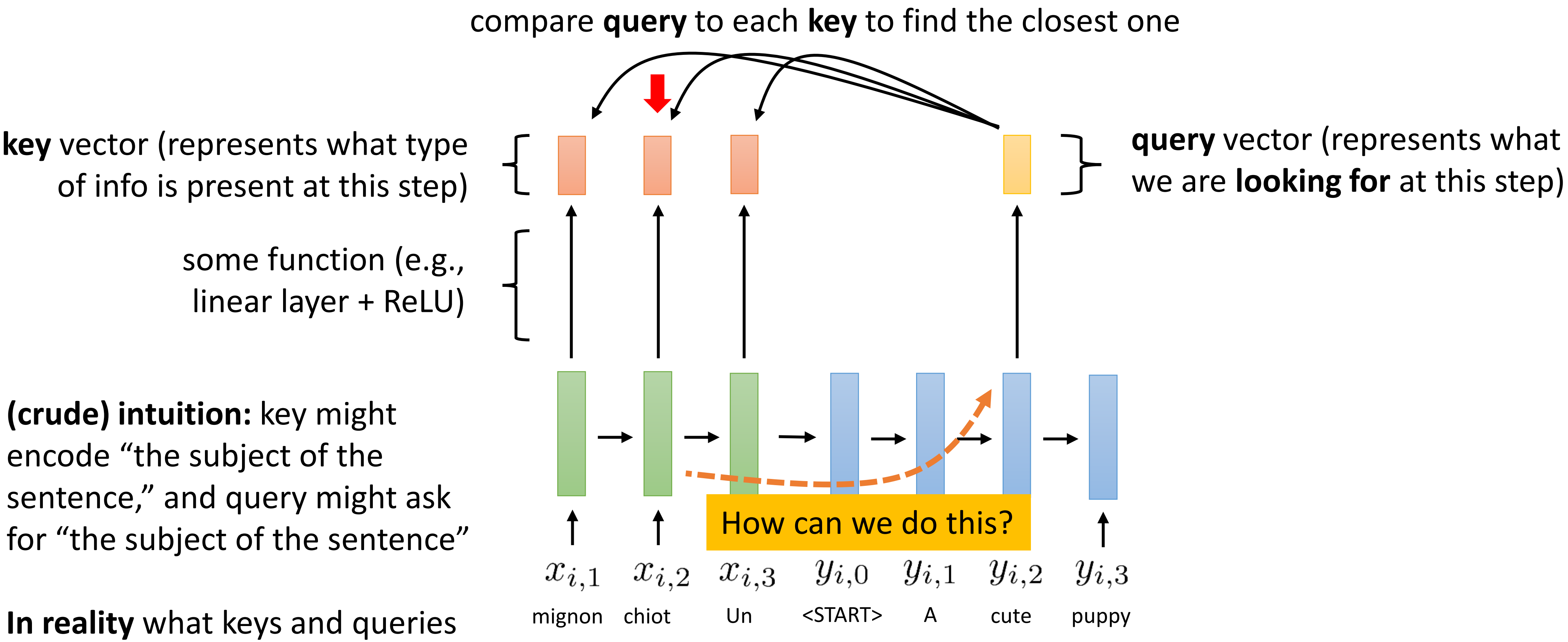
Attention

The bottleneck problem



Idea: what if we could somehow "peek" at the source sentence while decoding?

Can we "peek" at the input?



(crude) intuition: key might encode "the subject of the sentence," and query might ask for "the subject of the sentence"

In reality what keys and queries mean is **learned** – we do not have to select it manually!

Attention

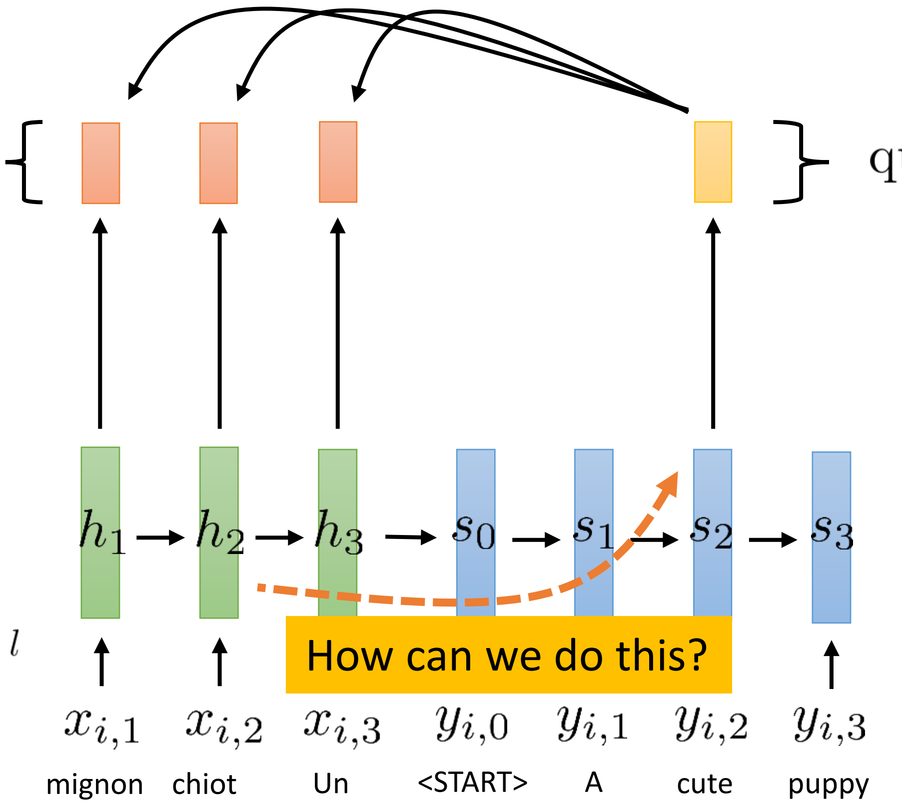
attention score for (encoder) step t to (decoder) step l

$e_{t,l} = k_t \cdot q_l$

RNN encoder activations at step t

key: $k_t = k(h_t)$

query: $q_l = q(s_l)$



learned function

e.g., $k_t = \sigma(W_k h_t + b_k)$

not differentiable!

intuitively: send h_t for $\arg\max_t e_{t,l}$ to step l

let $\alpha_{\cdot,l} = \text{softmax}(e_{\cdot,l})$

$$\alpha_{t,l} = \frac{\exp(e_{t,l})}{\sum_{t'} \exp(e_{t',l})}$$

send $a_l = \sum_t \alpha_{t,l} h_t$ ⟵ approximates h_t for $\arg\max_t e_{t,l}$

what does "send" mean?

who receives it?

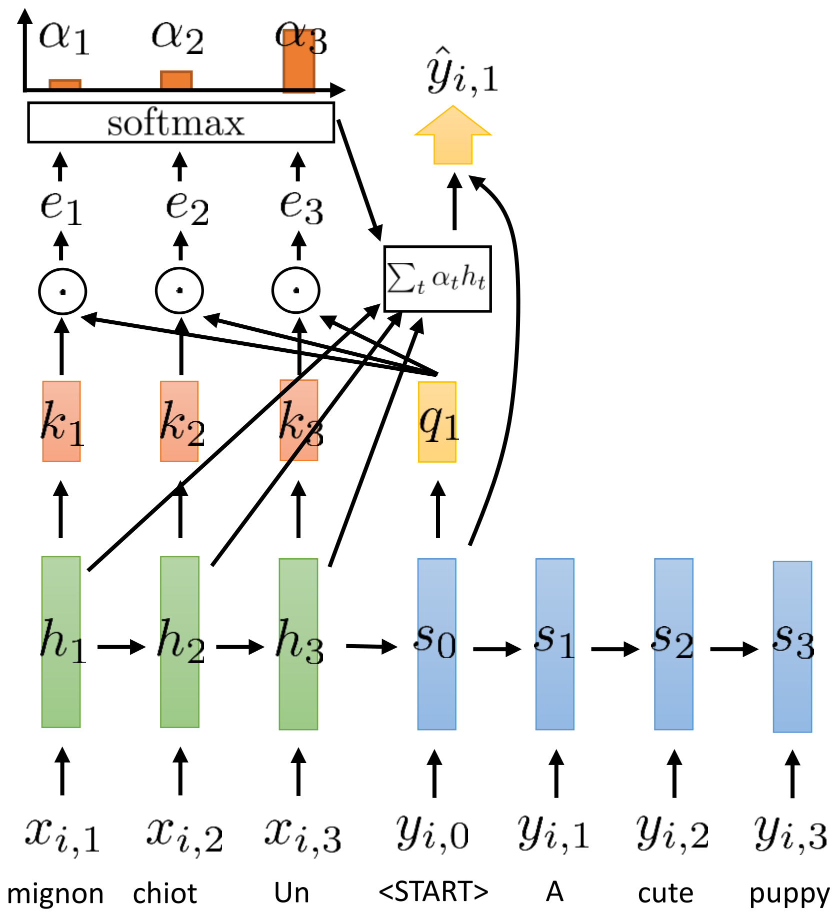
output: $\hat{y}_l = f(s_l, a_l)$

next RNN layer if using multi-layer (stacked) RNN

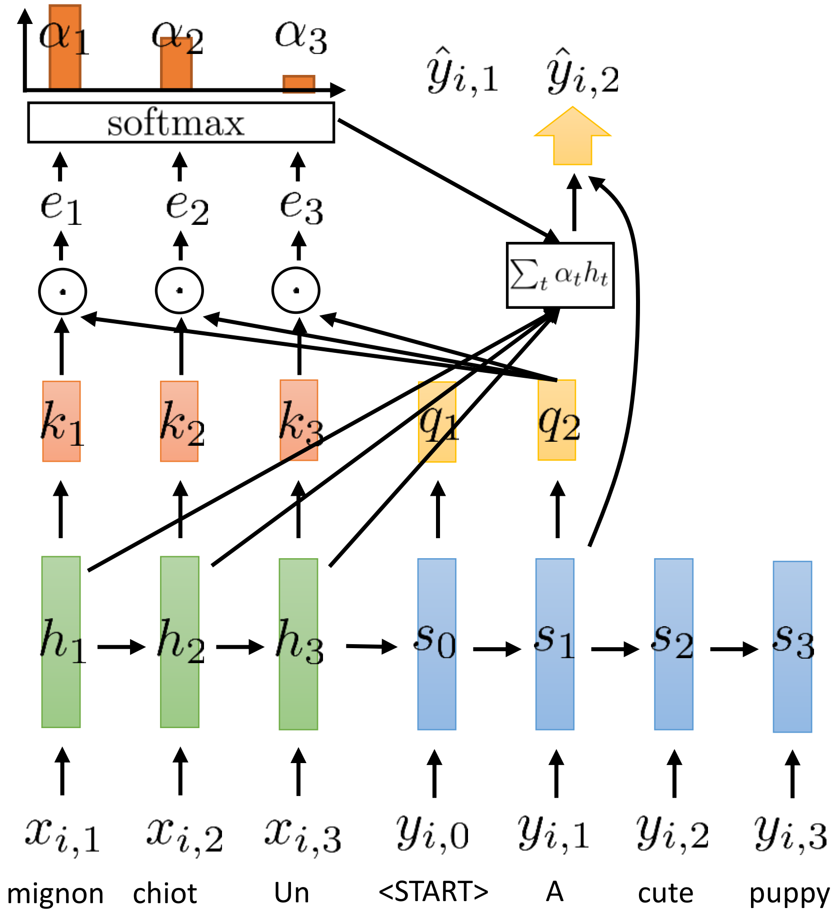
next decoder step $\bar{s}_l = \begin{bmatrix} s_{l-1} \\ a_{l-1} \\ x_l \end{bmatrix}$

(kind of like appending a to the input)

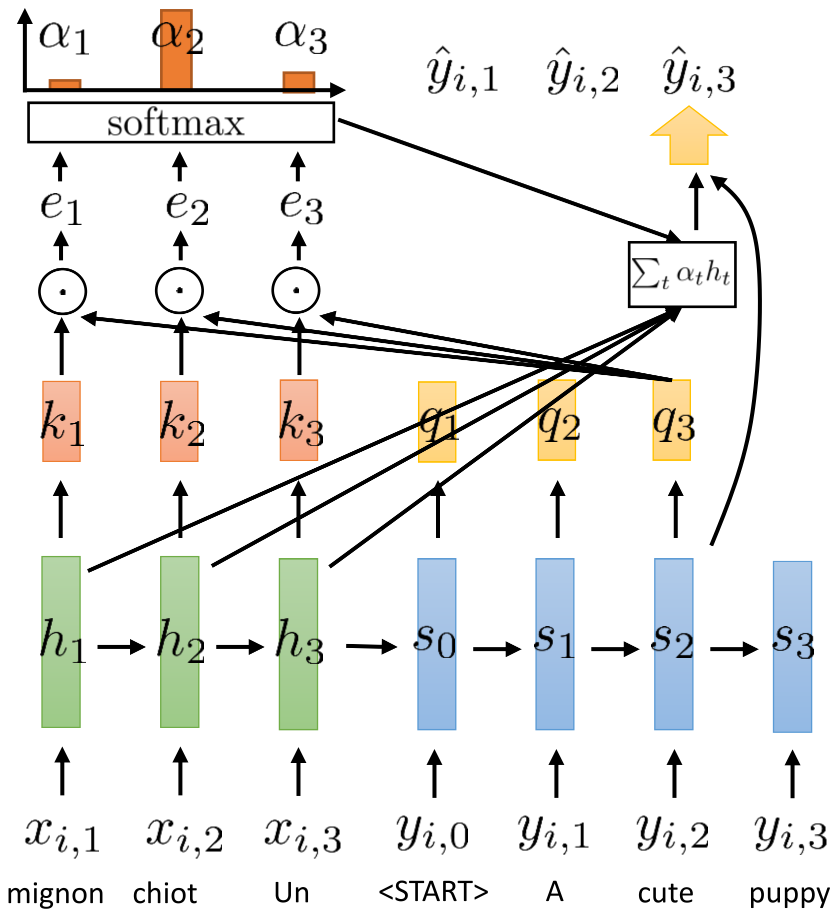
Attention Walkthrough (Example)



Attention Walkthrough (Example)



Attention Walkthrough (Example)



Attention Equations

Encoder-side:

$k_t = k(h_t)$

Decoder-side:

$q_l = q(s_l)$

$e_{t,l} = k_t \cdot q_l$

$$\alpha_{t,l} = \frac{\exp(e_{t,l})}{\sum_{t'} \exp(e_{t',l})}$$

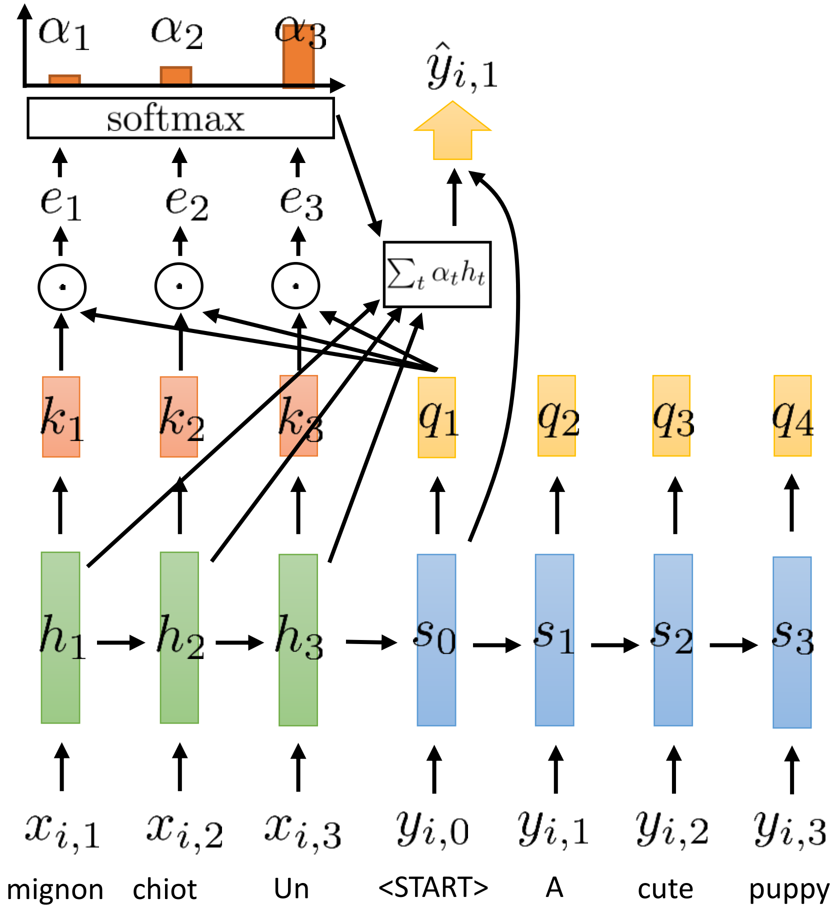
$$a_l = \sum_t \alpha_t h_t$$

Could use this in various ways:

concatenate to hidden state: $\begin{bmatrix} s_{l-1} \\ a_{l-1} \\ x_l \end{bmatrix}$

use for readout, e.g.: $\hat{y}_l = f(s_t, a_l)$

concatenate as input to next RNN layer



Attention Variants

Simple key-query choice: k and q are identity functions

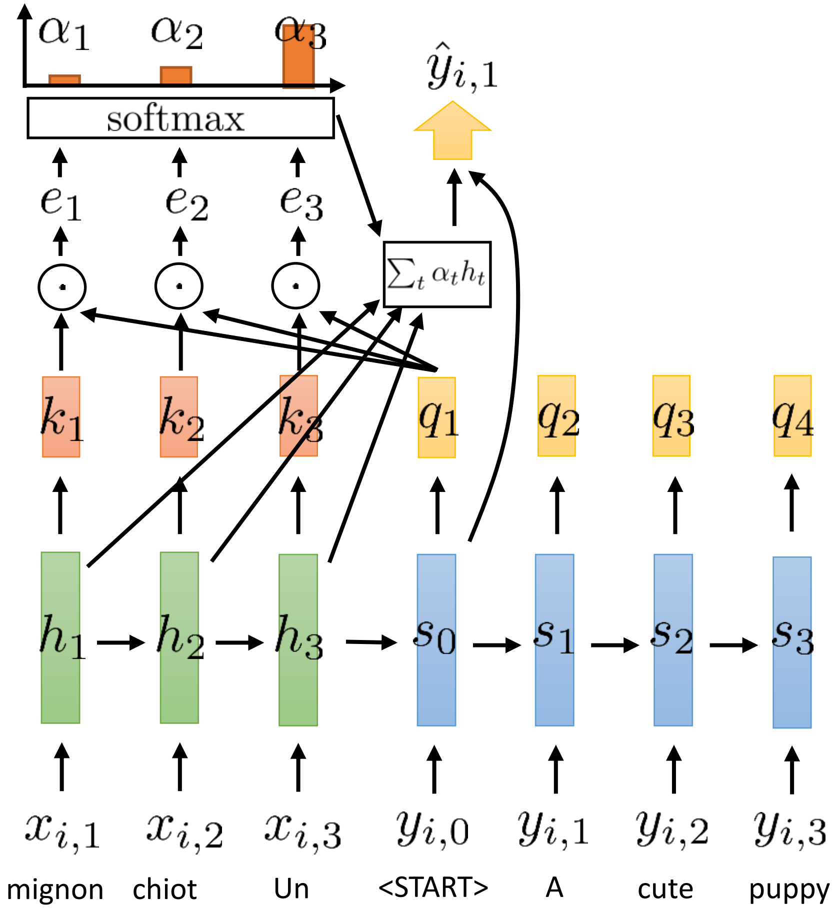
$$k_t = h_t \qquad q_l = s_l$$

Decoder-side:

$$e_{t,l} = h_t \cdot s_l$$

$$\alpha_{t,l} = \frac{\exp(e_{t,l})}{\sum_{t'} \exp(e_{t',l})}$$

$$a_l = \sum_t \alpha_t h_t$$



Attention Variants

Linear multiplicative attention:

$$k_t = W_k h_t \qquad q_l = W_q s_l$$

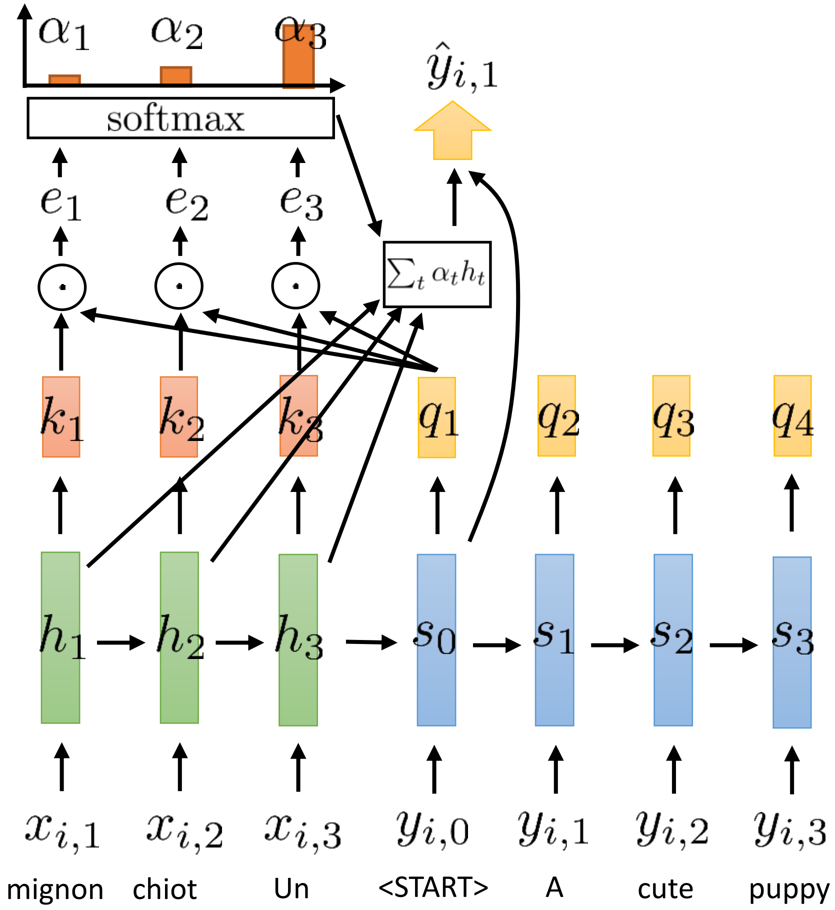
Decoder-side:

just learn this matrix

$$e_{t,l} = h_t^T W_k^T W_q s_l = h_t^T W_e s_l$$

$$\alpha_{t,l} = \frac{\exp(e_{t,l})}{\sum_{t'} \exp(e_{t',l})}$$

$$a_l = \sum_t \alpha_t h_t$$



Attention Variants

Learned value encoding:

Encoder-side:

$$k_t = k(h_t)$$

Decoder-side:

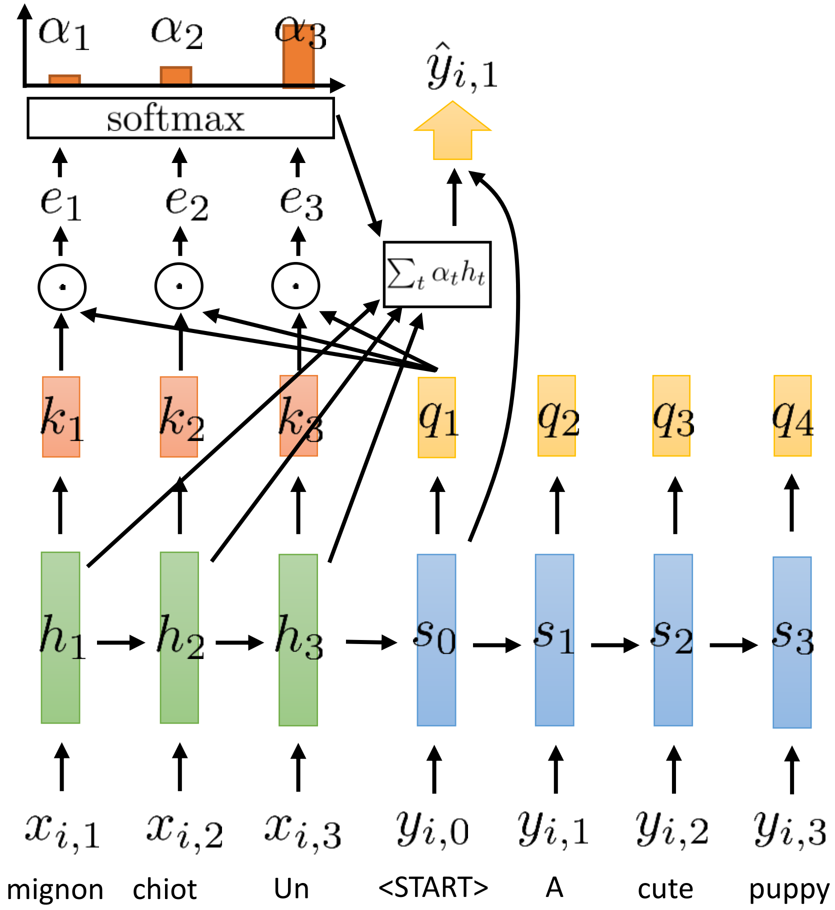
$$q_l = q(s_l)$$

$$e_{t,l} = k_t \cdot q_l$$

$$\alpha_{t,l} = \frac{\exp(e_{t,l})}{\sum_{t'} \exp(e_{t',l})}$$

$$a_l = \sum_t \alpha_t v(h_t)$$

some learned function



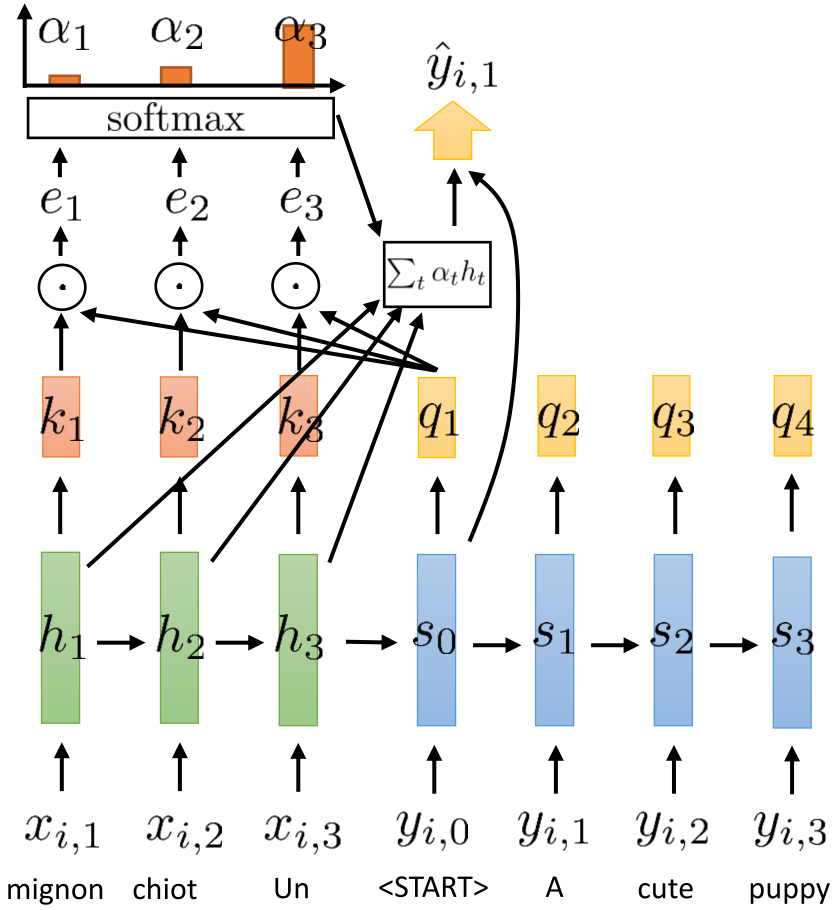
Attention Summary

Every encoder step t produces a key k_t

Every decoder step l produces a query q_l

Decoder gets "sent" encoder activation h_t corresponding to largest value of $k_t \cdot q_l$

actually gets $\sum_t \alpha_t h_t$



Why is this **good**?

- Attention is **very** powerful, because now all decoder steps are connected to **all** encoder steps!
- Connections go from O(T) to O(1)
- Gradients are much better behaved (O(1) propagation length)
- Becomes very important for very long sequences
- Bottleneck is much less important
- This works much better in practice

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