Deep Generative Models: Recurrent Neural Networks and Attention Mechanisms

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Taxonomy of Generative Models

What we've learned:
- Markov Models, HMMs, LDSs, RNNs

Deep Generative Models

What we've learned:
- PPCA
- VAE

Autoregressive models
(e.g., PixelCNN)

Flow-based models
(e.g., RealNVP)

Latent variable models

Energy-based models

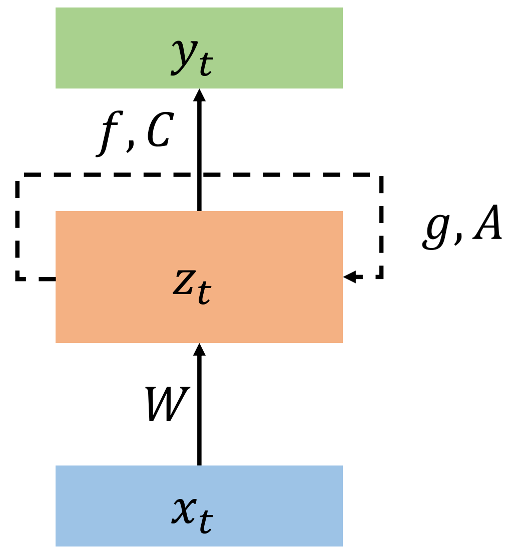
Implicit models
(e.g., GANs)

Prescribed models
(e.g., VAEs)

What we study now:
- Variants of RNN architectures
- Applications

Autoregressive Models

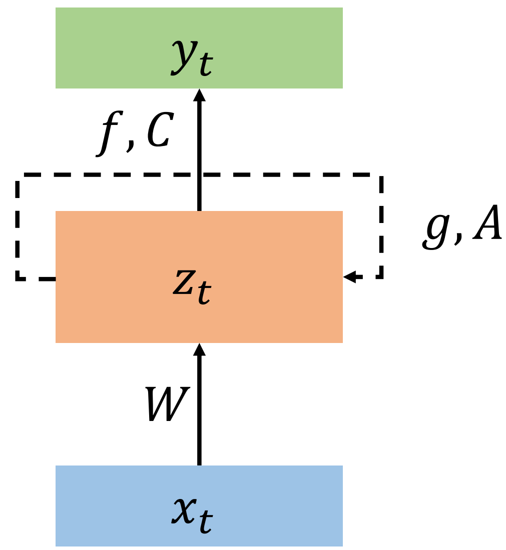
- Many kinds of models
  - Markov Chains
  - Hidden Markov Models
  - Markov Random Fields
  - Linear Dynamical Systems
  - **Recurrent Neural Networks**
  - Transformers



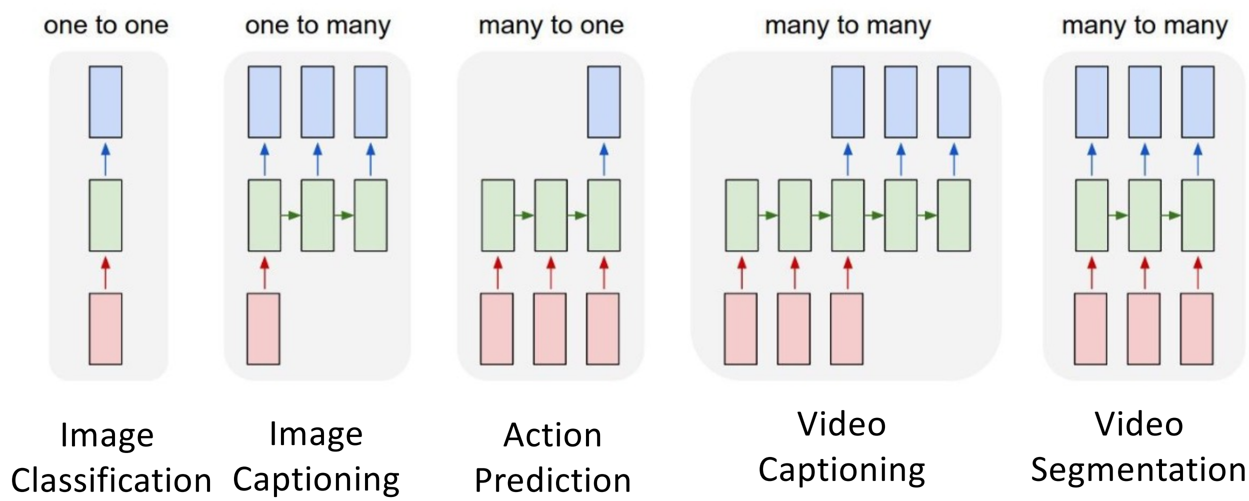
- Last lecture
  - **Model**: Introduced the vanilla RNN architecture
  - **Inference**: Unfolding
  - **Training**: Backpropagation Through Time
  - **Variants of RNNs**: LSTMs, GRUs

This Lecture

- We will continue on Recurrent Neural Networks
  - Sequence to Sequence Models
  - Align and Translate Model
  - Image Captioning



- Generalizations of Vanilla Neural Networks: RNNs can be very flexible, depending on the task!



Timeline in

- In today's and following lectures, we will see how the attention mechanism emerges into the well-know Transformer architecture today.

2014

Sequence to Sequence Learning with Neural Networks [Sutskever et al. (2014)]
- First application of RNNs to Machine Translation Tasks
- Introducing so-called "encoder-decoder" architectures

2015

Neural Machine Translation by Jointly Learning to Align and Translate [Bahdanau et al. (2015)]
- Using attention mechanism during the decoding process

2016

Show, Attend and Tell: Neural Image Caption Generation with Visual Attention [Xu et al. (2016)]
- First application of attention for image captioning
- Our first multi-modal application in this class!

2017

Attention Is All You Need [Vaswani et al. (2017)]
- Introduced the popular architecture known as Transformer
- Stacking attention layers together

Consider the task of Machine Translation

- Say we are given pairs of sentences, one with English and the other with Spanish
  - Original sentence: "I have a big cat but a small house."
  - Translated sentence: "Tengo un gato grande pero una casa pequeña."

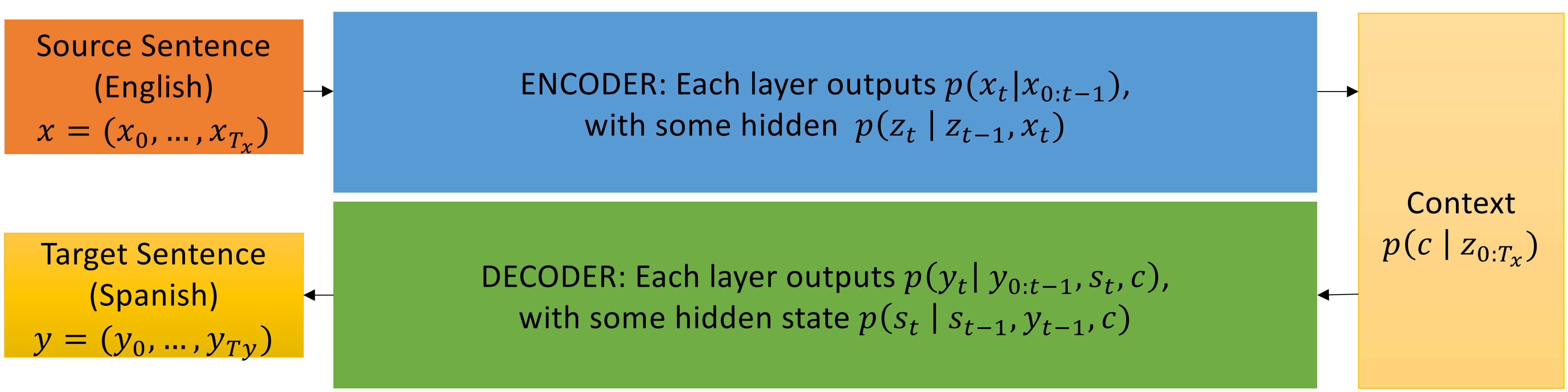
- In **Conditional Language Modeling (CLM)**, we want to compute

$$\hat{y}_{0:T_y} = \underset{y_{0:T_y}}{\operatorname{argmax}} P_\theta \left(y_{0:T_y} \,\middle|\, x_{0:T_x} \right)$$

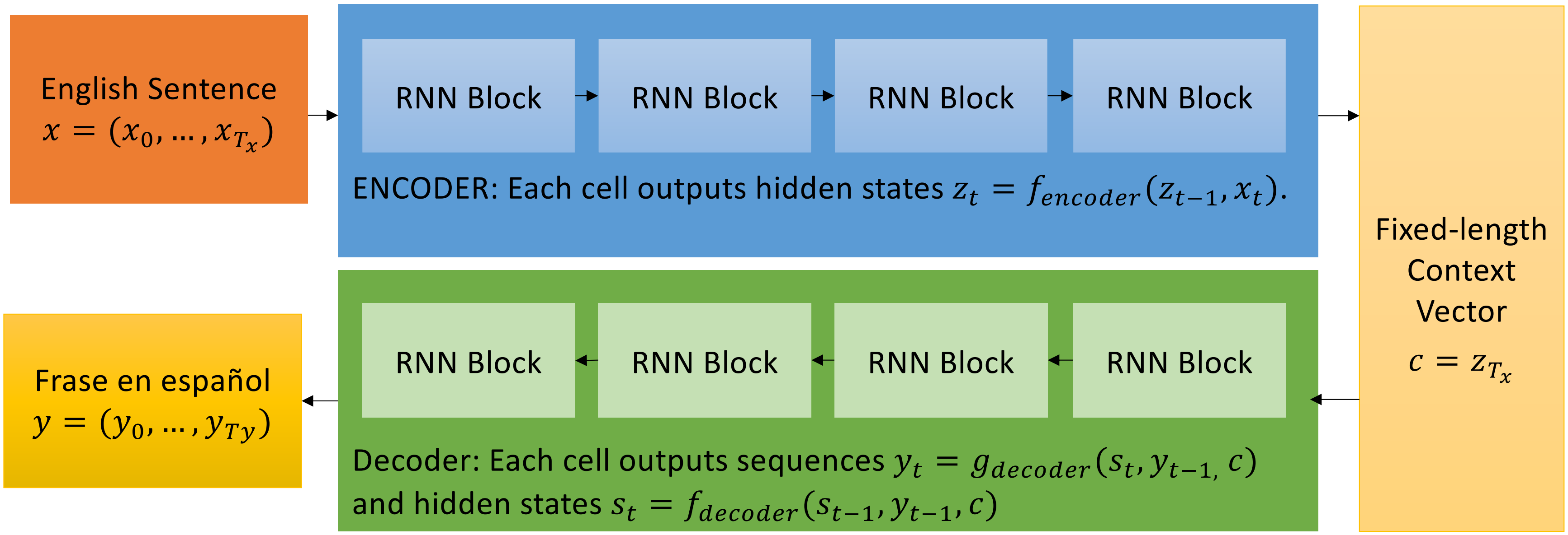
- Here:
  - $\hat{y}_{0:T_y}$ is the target sentence
  - $x_{0:T_x}$ is our original sentence
  - θ is the parameters of our language model
- So, what is our model? And how do we learn θ?

Overview

- The high-level idea is as follows:
  - A RNN allows us to encode our source sentence (English) $x_{0:T}$ to some latent (hidden) space $z_{0:T}$. This latent space encodes then semantics of the source sentence.
  - Once the semantics are captured, we want to decode it into the language we desire, i.e target sentence (Spanish) $y_{0:T}$.
- A similar structure can be found in VAEs, where we also have an encoder-decoder structure



RNN Encoder-Decoder Architecture



- Remarks on Architecture from Sutskever et al. (2014):
  - $f_{encoder}, f_{decoder}, g_{decoder}$ are parameterized by LSTM layers.
  - In theory, the context vector can be the output of a more complex function h that takes in the entire sequence of hidden states, i.e. $c = h(z_{0:T})$. But they found virtually no difference in performance when compared to only using the very last state.
  - $g_{encoder}$ is not needed since we are not “decoding” from the ENCODER block.

Learning and Inference

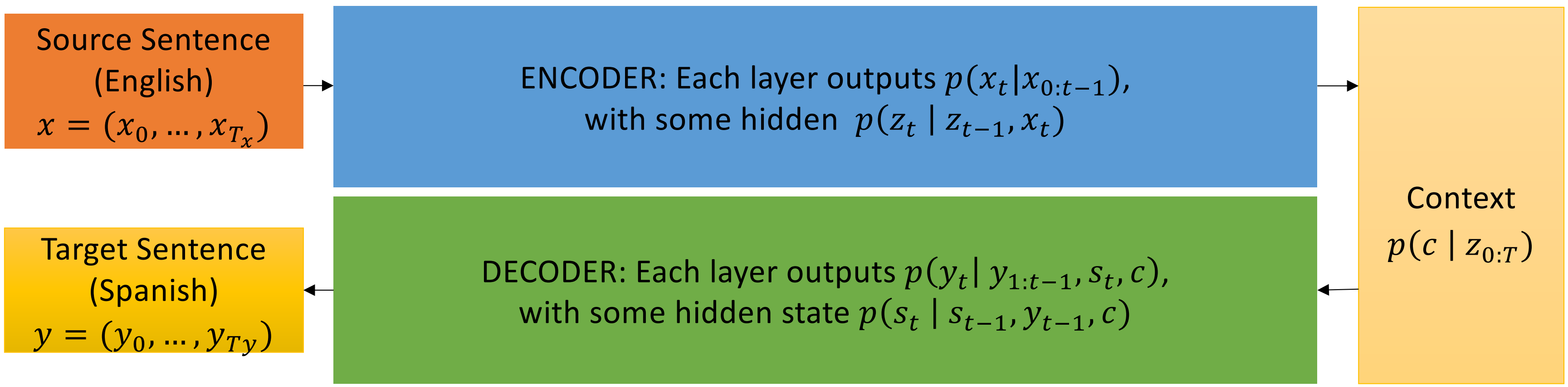
- **Learning:** Suppose we have the N samples $\left\{\left(x_{0:T_x}^{(n)}, y_{0:T_y}^{(n)}\right)\right\}_{n=1}^{N}$ of source-target sentence pairs. Similar to sentence classification, we can train the entire model end-to-end using cross entropy loss

$$\max_{\theta} \frac{1}{N} \sum_{n=1}^{N} \log P_{\theta}(y_{0:T_y}^{(n)} \mid x_{0:T_x}^{(n)})$$

- **Inference:** To decode, we simply select the target sentence with the highest probability. For a given $x_{0:T_x}$,

$$\begin{aligned}\hat{y}_{0:T_y} &= \operatorname{argmax}_{y_{0:T_y}} P_{\theta}\left(y_{0:T_y} \mid x_{0:T_x}\right) \\ &= \operatorname{argmax}_{y_{0:T_y}} \underbrace{P_{\theta}\left(y_{0:T_y} \mid c\right)}_{\text{Decoder} \rightarrow \text{Context}} \underbrace{P_{\theta}\left(c \mid x_{0:T_x}\right)}_{\text{Context} \leftarrow \text{Encoder}}\end{aligned}$$

Major Flaw in Fixed-context seq2seq Models

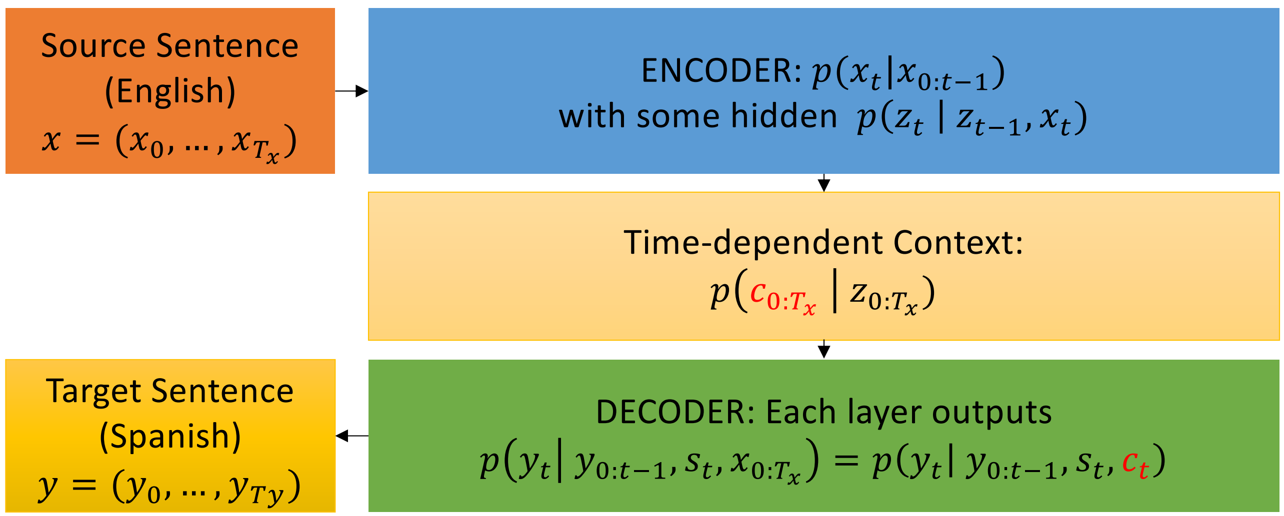


- However, there are obvious flaws to this design:
  - **Encoding**: the context c may not be able to capture earlier parts of the source sentence
  - **Fixed-length Context:** All the information from the source sentence is “jammed” into the single context vector c.

- As a result, this design often fails to capture long range dependences.

Improving seq2seq Models

- Q: How can we improve *fixed-context* seq2seq models?
  - A: one possibility is to make the context time-dependent!
  - If our new context can better capture the information from each word, then it should prove long-range dependencies.



- How should we model the probabilities $p\left(c_{0:T_x} \mid z_{0:T_x}\right)$ and $p(y_t | \, y_{0:t-1}, s_t, c_t)$?

Align and Translate [Bahdanau et al. (2015)]

- **Intuition:** Translation of the word x_t to y_t depends on the contexts of both the source sentence $x_{0:T}$ and target sentence $y_{0:T}$.
  - The latent space should be able to capture what is important

- Take our Spanish example:
  - Original sentence: "I have a big cat but a small house."
  - Translated sentence: "Tengo un gato grande pero una casa pequeña."
  - Notice that the translation doesn't exactly align
  - Hence we need a way to tell the model what part of the sentence to focus on

- **High-Level Idea**: During decoding, each context c_t to be a summary of the sources' hidden states $z_{0:T_x}$ and the target's current hidden states s_t

Align and Translate [Bahdanau et al. (2015)]

Source Sentence (English) $x = (x_0, \dots, x_{T_x})$

ENCODER: $p(x_t | x_{0:t-1}), p(z_t \mid z_{t-1}, x_t) = RNN(x_{0:T_x})$

Time-dependent Context: $p\left(c_{0:T_x} \mid z_{0:T_x}\right) = \text{Attention}$

Target Sentence (Spanish) $y = (y_0, \dots, y_{Ty})$

DECODER: sequence $y_t = g_{decoder}(y_{t-1}, s_t, c_t)$
with hidden states $s_t = f_{decoder}(s_{t-1}, y_{t-1}, c_t)$

- Define the probability of the target word y_t at time t as

$$p\left(y_t \middle| y_{0:t-1}, s_t, x_{0:T_x}\right) = g_{decoder}(y_{t-1}, s_t, c_t)$$

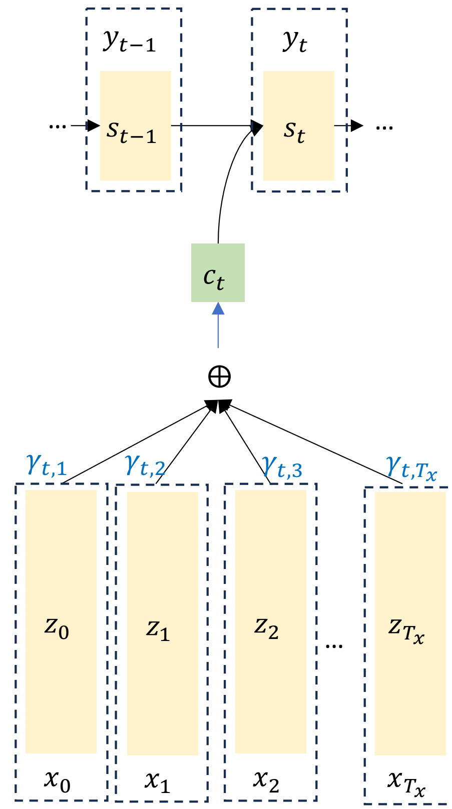
- Here $s_t = f_{decoder}(s_{t-1}, y_{t-1}, c_t)$ is hidden state of the RNN decoder that takes in the previous word y_t, the previous hidden state s_t, and a context vector c_t as input.
  - Similar to before, $f_{decoder}$ and $g_{decoder}$ are functions parameterized by neural networks.

Align and Translate

- Decoder: **context vector** c_t is computed as a weighted sum of the hidden states z_j:

$$c_t = \sum_{j=1}^{T_x} \gamma_{tj} z_j \qquad \gamma_{tj} = \frac{\exp(e_{tj})}{\sum_{k=1}^{T_x} \exp(e_{tk})} \qquad e_{tj} = a(s_{t-1}, z_j)$$

Context vector | Weights of hidden states | Alignment model



- Here:
  - c_t is the expected hidden state over all the hidden states with probability γ_{tj}.
  - γ_{tj} is the probability that the target word y_t is aligned to, or translated from, a source word x_j.
  - a is called the **Alignment model**
    - Computes how well the inputs around position j and the output at position t match
    - Typically chosen to be a feedforward neural network

Align and Translate

- In Bahdanau et al. (2015), they made the following design choices:
  - **Encoder**: Using a Bi-directional RNN, compute the *forward and backward* hidden states $\overrightarrow{h_t}$ and $\overleftarrow{h_t}$ using input $x = (x_0, \ldots, x_T)$. Concatenate them as one encoder hidden state $z_t = [\overrightarrow{h_t} \mid \overleftarrow{h_t}]$ (assume they are row vectors). Hidden states are also called *annotations.*
  - **Decoder:** Using a single direction RNN with Attention mechanism and alignment model

$$a(s_{i-1}, z_j) = v_a^\top \tanh(W_a s_{i-1} + U_a z_j)$$

- Ultimately, these design choices are flexible and application-dependent.

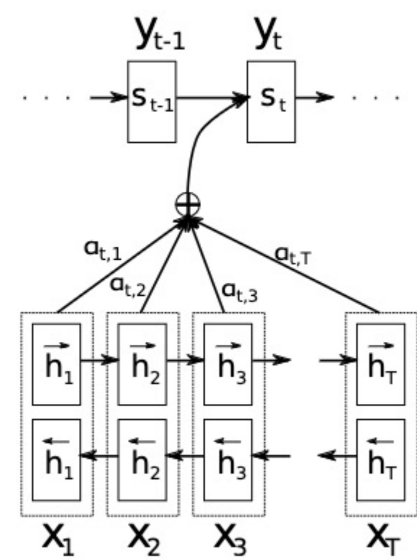


Figure 1: The graphical illustration of the proposed model trying to generate the t-th target word y_t given a source sentence $(x_1, x_2, \ldots, x_T)$.

Visualization of Annotations and Alignments

- Correlation between the source sentence (English) and target sentence (French)

- Able to show that some target words “attend” to multiple target words

- Diagonal: x_t matches with y_t
- Cross-Diagonal: context dependent

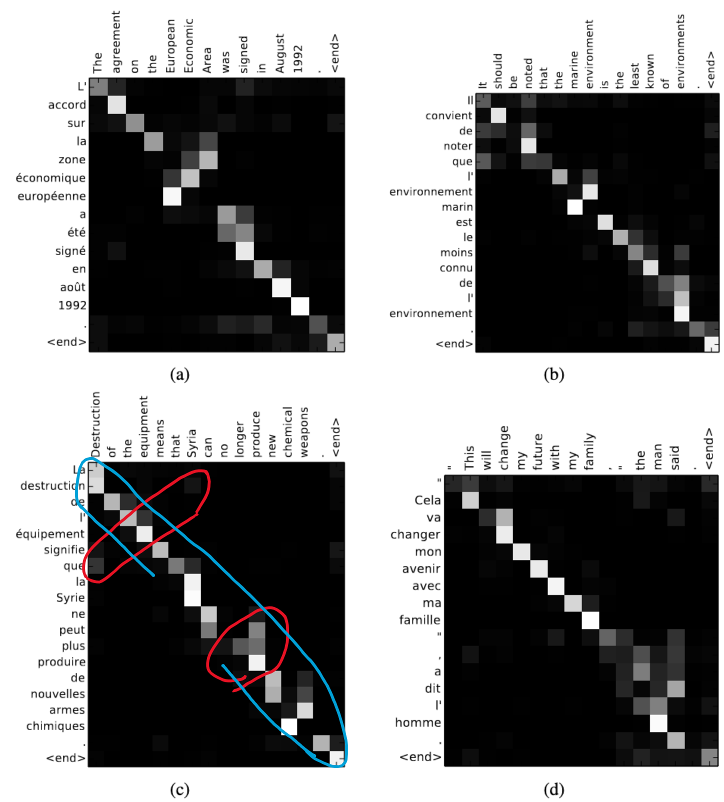


Figure 3: Four sample alignments found by RNNsearch-50. The x-axis and y-axis of each plot correspond to the words in the source sentence (English) and the generated translation (French), respectively. Each pixel shows the weight α_{ij} of the annotation of the j-th source word for the i-th target word (see Eq. (6)), in grayscale (0: black, 1: white). (a) an arbitrary sentence. (b–d) three randomly selected samples among the sentences without any unknown words and of length between 10 and 20 words from the test set.

Recap

- Today we covered two seq2seq models:
  - Encoder-Decoder with fixed context [Sutskever et al. (2014)]
  - Time-dependent context with Attention Mechanism [Bahdanau et al. (2015)]

- Comparing seq2seq models
  - Bi-directional RNNs instead of LSTMs
  - **Alignment model** instead of single fixed-vector hidden states
  - Have context vector c_t that depends on the timestep

- Next lecture:
  - Using attention mechanism for image captioning
  - Is attention all your need?

Deep Generative Models: VAE+RNN for Image Captioning

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Encoder-Decoder Architectures

- Encoder-Decoder Architectures allow us to
  - Learn a meaningful hidden representation for our input
  - Via a Decoder, make use of our hidden representation for downstream tasks
- So far, our main motivation has been driven by Language
  - Machine Translation, Text Summarization, etc
- What about Cross Modalities? Language-to-Vision?

Up Next

- Today we will talk about Image Caption Generation using a combination of Variational Auto Encoders (VAEs) and Recurrent Neural Networks (RNNs)

- Introduced in Xu et al (2016) “Show, Attend and Tell: Neural Image Caption Generation with Visual Attention”

- Task: Given an image, generate a sentence that describes the image
  - Can be seen as a combination of Object Detection and Machine Translation

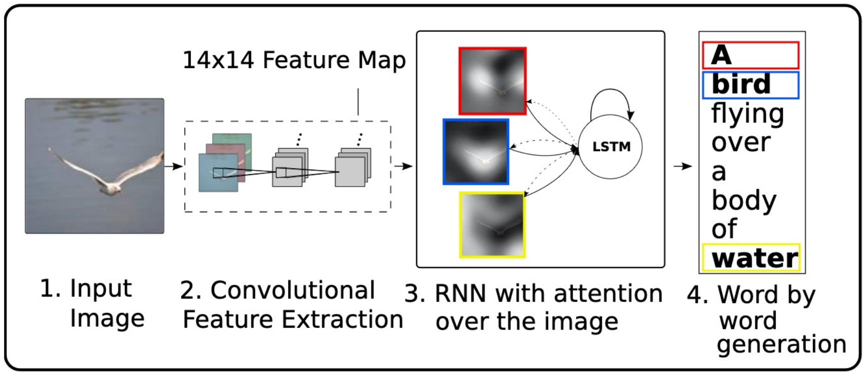
A bird flying over a body of water.

A woman throwing a frisbee in a park.

Task

- Today we will talk about Image Caption Generation using a combination of Variational Auto Encoders (VAEs) and Recurrent Neural Networks (RNNs)

- Our overall pipeline:

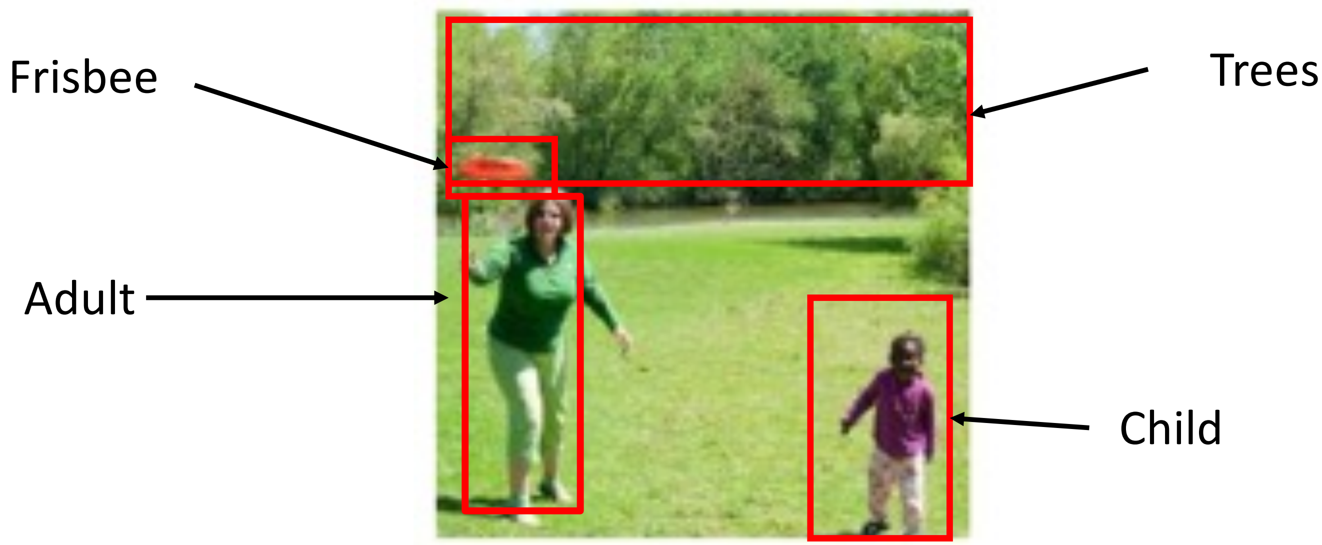


- Similar to any language task, suppose we are given a vocabulary of size K, a sentence of length T can be presented by each word being a one-hot embedding

$$y = \{y_0, \dots, y_T\}, y_t \in \mathbb{R}^K$$

Image Encoder

- An image can have many sources of information



- Ideally our hidden representation should be meaningful, in the sense that it should capture all the semantic parts of the image

Image Encoder: Convolutional Neural Networks

- To capture these meaningful features, we will feed the image through a (pre-trained) Convolutional Neural Network

- Then use the feature vectors x_i of earlier convolutional layers to represent low-level features

- Denote each part by

$$x = [x_1 | \dots | x_L] \in \mathbb{R}^{T_x \times D}$$

where T_x is the number of low-level features of dimension D

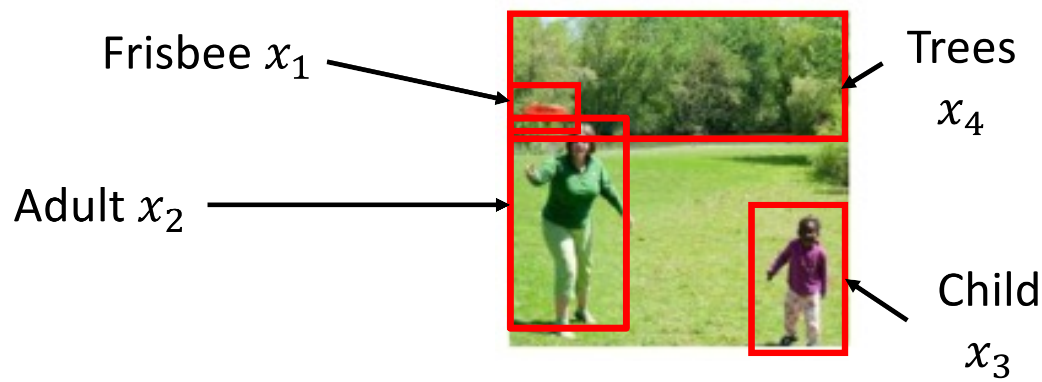
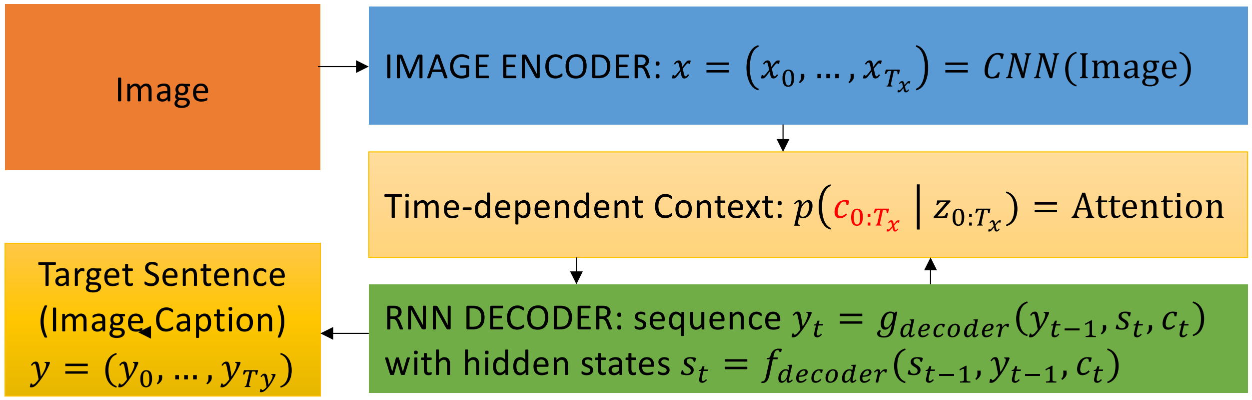


Figure above: In an ideal situation, each semantic part is presented by a low-level feature vector x_i.

Decoder: LSTM with Context



- Similar to Align and Translate, now we have to design the context vectors
  - For image captioning, we will use attention mechanisms to attend to different locations of the image

- So How is the context vector $\widehat{c_t}$ computed using our image features $x_1 \dots x_{T_x}$?

Decoder: Context Vector and Attention

- c_t is a context vector that presents the relevant part of the image input at time t
- There are two ways to compute c_t :
  - Option 1: ϕ = **Hard Attention**: only one of the T_x image locations is chosen
  - Option 2: ϕ = **Soft Attention:** all of them is weighted in some way
- Similar to Align and Translate model, we can define:

A person is standing on a beach with a surfboard.

$$c_t = \phi(x_1, \dots, x_L, \gamma_{t,1}, \dots, \gamma_{t,L})$$

Some function ϕ of using the attention weights and features to combine a context vector.

$$\gamma_{tj} = \frac{\exp(e_{tj})}{\sum_{k=1}^{T_x} \exp(e_{tk})}$$

Weights, for which of the L positions to attend to

$$e_{ti} = a(x_i, s_{t-1})$$

"Attention Model"
a multi-layer perceptron

Image Features $x_1, \dots, x_{T_x}$
Decoder's Hidden Features $s_1, \dots, s_T$

First option for ϕ: Stochastic Hard Attention

- Stochastic Hard Attention implies we use a “on-off” way to choose which location of the image to focus
  - Meaning we can only choose one location each time
- Let $\hat{\gamma}_t \in \{0,1\}^L$ be a *one-hot* location variable that represents where the model decides to focus attention when generating the t^{th} word.
- We can treat the attention locations as intermediate latent random variables

$$p(\hat{\gamma}_{t,i} = 1 \,|\hat{\gamma}_{1:t-1}, x_1, \dots, x_L) = \gamma_{t,i} \qquad\qquad \hat{c}_t = \sum_{k=1}^{T_x} \hat{\gamma}_{t,k} x_k$$

- This means we can treat γ_t as a categorical distribution:

$$\hat{\gamma}_t \sim \text{Categorical}(\gamma_{t,1}, \dots, \gamma_{t,T_x})$$

- And we can just sample this distribution during inference to obtain samples for the context $\hat{c}_t$.

Stochastic Hard Attention (Learning)

- While it is intuitive to parameterize $\hat{\gamma}_t \sim \text{Categorical}(\gamma_{t,1}, \ldots, \gamma_{t,T_x})$, it raises the question of how to train the entire model end-to-end?
  - This is the same issue we face in VAEs!
  - Hence we can use the **Variational Lower Bound** approach
- To backpropagate through the entire model, we need to define **a variational lower bound** on the marginal log-likelihood $\log p(y_{0:T} \mid x_{1:T_x})$ of observing the sequence of words $y_{0:T}$ given image features x
- Quick Recall: Let X and Z be a random variable, jointly distributed with distribution p_θ. If $p_\theta(X)$ is the marginal distribution of X and $p_\theta(Z|X)$ is the conditional distribution of Z given X. Then for any sample $x \sim p_\theta$ and any distribution q_ψ, we have

$$\log p_\theta(x) \geq \mathbb{E}_{z \sim q_\psi}[\log \frac{p_\theta(x,z)}{q_\psi(z)}]$$

Stochastic Hard Attention (Learning)

- Just like our VAE model, we may now consider our context $p(c)$ as our latent variable. Then we can derive the ELBO.

- Define
  - ψ as the parameters of the encoder $q(c \mid x)$, the distribution of context vectors from CNNs.
  - θ as the parameters of the decoder $p(y \mid c, x)$, the image captioner.
- The Evidence Lower Bound L_s:

$$\begin{aligned} L_{\theta,\psi}(c, x, y) &= \sum_c q_\psi(c \mid x) \log p_\theta(y \mid c, x) \\ &\leq \log \sum_c q_\psi(c \mid x) p_\theta(y \mid c, x) \qquad \text{(Jensen's Inequality)} \\ &= \log p_\theta(y \mid x) \qquad \text{(Marginal Log-Likelihood)} \end{aligned}$$

Stochastic Hard Attention (Learning)

- Our Lower Bound: $L_{\theta,\psi}(c,x,y) = \sum_c q_\psi(c \mid x) \log p_\theta(y \mid c, x)$
- To learn we will need the gradient. For **both parameter** $W = \{\theta, \psi\}$ in our RNN, we can estimate the gradient using Monte Carlo sampling approximation.

- The exact derivative for the ELBO objective (derivation next slide):

$$\frac{\partial L}{\partial W} = \sum_c q_\psi(c \mid x) \left[\frac{\partial \log p_\theta(y \mid c, x)}{\partial W} + \log p_\theta(y \mid c, x) \frac{\partial \log q_\psi(c \mid x)}{\partial W}\right]$$

- The estimated derivative using Monte Carlo sampling approximation, with $\hat{\gamma}_t \sim \text{Categorical}(\gamma_{t,1}, \dots, \gamma_{t,L})$ and $\hat{c}_t = \sum_{k=1}^{T_x} \hat{\gamma}_{t,k} x_k$:

$$\frac{\partial L}{\partial W} = \frac{1}{M} \sum_{m=1}^{M} \left[\frac{\partial \log p_\theta(y \mid \hat{c}^{(m)}, x)}{\partial W} + \log p_\theta(y \mid \hat{c}^{(m)}, x) \frac{\partial \log q_\psi(\hat{c}^{(m)} \mid x)}{\partial W}\right]$$

Derivation of the Gradient for Exact ELBO

- $L_{\theta,\psi}(c,x,y) = \sum_c q_\psi(c \mid x) \log p_\theta(y \mid c,x)$

$$\frac{\partial L_{\theta,\psi}(c,x,y)}{\partial W}$$

$$= \sum_c q_\psi(\, c \mid x\,) \frac{\partial \log p_\theta(y|c,x)}{\partial W} + \frac{\partial q_\psi(c \mid x)}{\partial W} \log p_\theta(y \mid c,x) \qquad \text{(chain rule)}$$

$$= \sum_c q_\psi(\, c \mid x\,) \frac{\partial \log p_\theta(y|c,x)}{\partial W} + q_\psi(c \mid x) \frac{\partial \log q_\psi(c \mid x)}{\partial W} \log p_\theta(y \mid c,x)$$

$$= \sum_c q_\psi(\, c \mid x\,) [\frac{\partial \log p_\theta(\, y|c,x\,)}{\partial W} + \frac{\partial \log q_\psi\,(c \mid x)}{\partial W} \log p_\theta(y \mid c,x)]$$

- The third line uses the identity $\frac{\partial q_\psi(c \mid x)}{\partial W} = q_\psi(c \mid x) \frac{\partial \log q_\psi(c \mid x)}{\partial W}$

Second option for ϕ: Deterministic “Soft” Attention

- Recall our three equations:

$$c_t = \phi(x_1, \dots, x_L, \gamma_{t,1}, \dots, \gamma_{t,L}) \qquad \gamma_{tj} = \frac{\exp(e_{tj})}{\sum_{k=1}^{T_x} \exp(e_{tk})} \qquad e_{ti} = a(x_i, s_{t-1})$$

- Hard Attention method requires us to ample the attention location c_t each time
- Instead, we can take the expectation of the context vector c_t directly

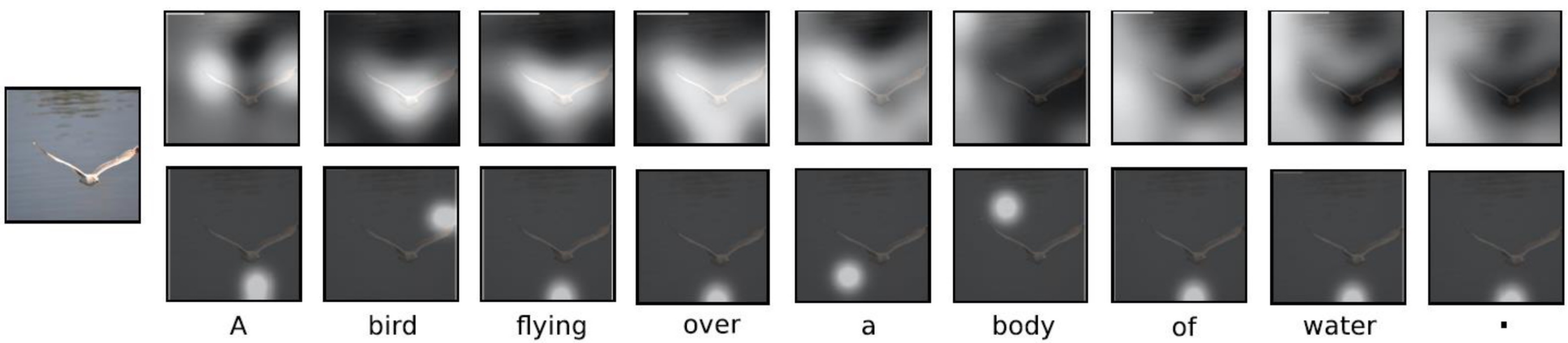
$$c_t = \phi(x_1, \dots, x_L, \gamma_{t,1}, \dots, \gamma_{t,L}) = \sum_{i=1}^{T_x} \gamma_{t,i} x_i$$

- Then this would no longer be a ”on-off” mechanism, but a weighted sum of low-level features instead.

- Lucky for us, this is differentiable end-to-end using cross entropy

Soft Attention vs Hard Attention

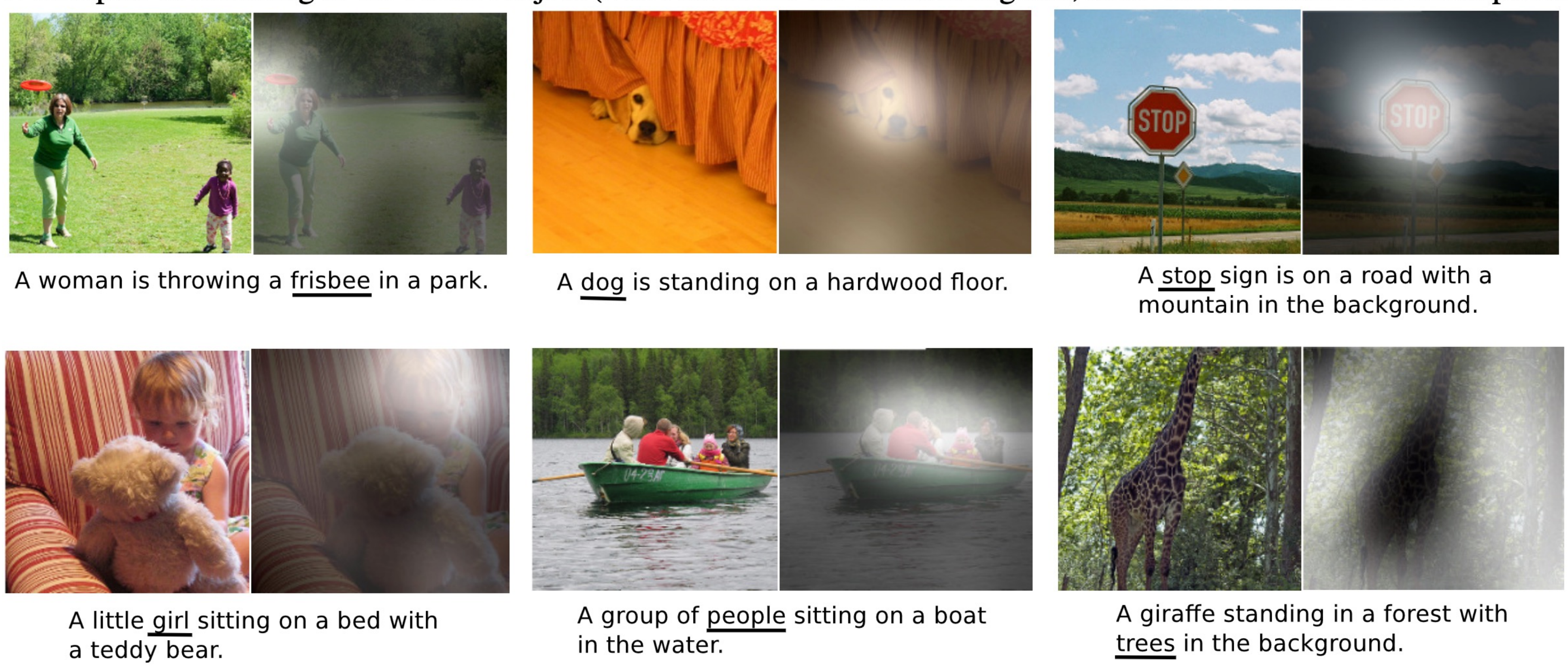
Soft attention



Hard attention

Examples of Image Caption Generation

Figure 3. Examples of attending to the correct object (*white* indicates the attended regions, *underlines* indicated the corresponding word)



Examples of Image Caption Generation

Figure 5. Examples of mistakes where we can use attention to gain intuition into what the model saw.

A large white bird standing in a forest.

A woman holding a clock in her hand.

A man wearing a hat and
a hat on a skateboard.

A person is standing on a beach
with a surfboard.

A woman is sitting at a table
with a large pizza.

A man is talking on his cell phone
while another man watches.

Wrap-up

- We introduced a Multi-modal Encoder-Decoder architecture method to do image caption
  - Generative: parameterize location variable with categorial variable (Hard Attention), use MCMC to sample and learn the RNN decoder.
  - Discriminative: use weighted sum (Soft Attention) and train everything end-to-end.

- We have shown the brief history of Attention mechanism
  - Sequence to Sequence with Neural Networks for Machine Translation
    - The use of fixed-length single context vector to decode c
  - Align and Translate for Machine Translation
    - The use of multiple time-dependent context vectors c_t
  - Image Captioning
    - Soft and Hard Attention

Why do RNNs fall short? And what can we do?

- Hard to capture long-term dependencies
  - Require modification to architectures
- Training Issues: Vanishing/Exploding Gradients
- Hard to handle varying length sequences
- Sequential nature make them hard to process in parallel

- **Solution to all of this:**
- Let’s not depend on recurrence anymore
- Let’s just rely “Attention” completely to capture global dependencies