Recurrent Neural Networks and Transformers

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Machine Learning

Outline

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Sequential Data

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  - T is call the ***horizon*** and may be different between $\boldsymbol{x}^{(n)}$ and $\boldsymbol{y}^{(n)}$ and across data points n's

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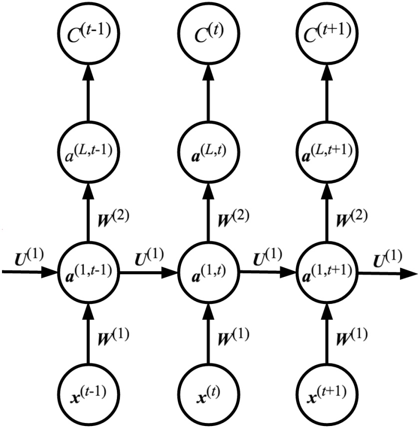

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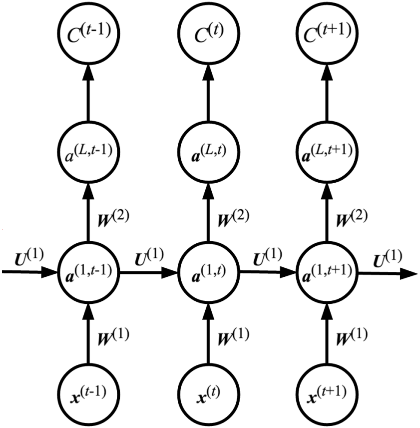

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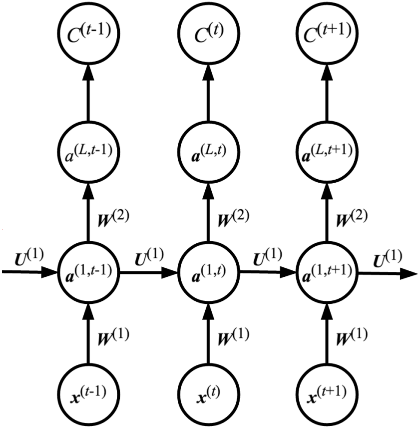

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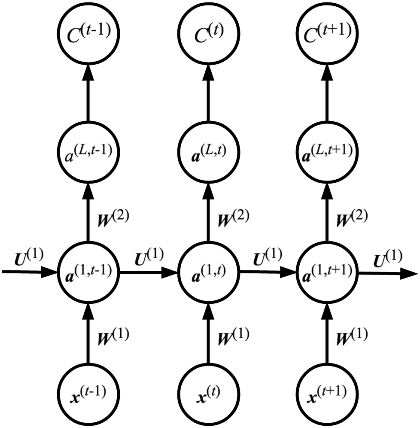

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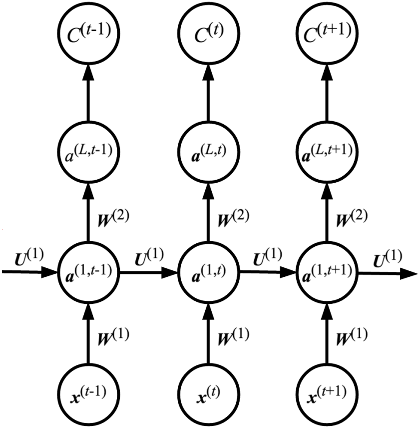
- $\mathbf{a}^{(\cdot,t)}$'s at deeper layers give more abstract summarizations



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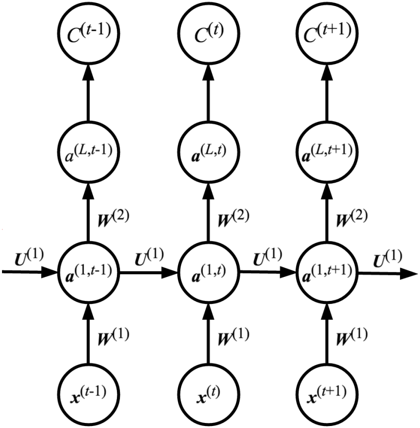

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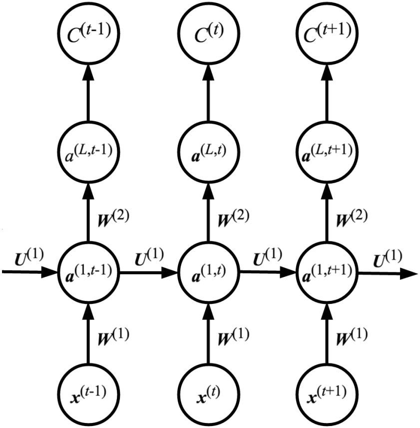

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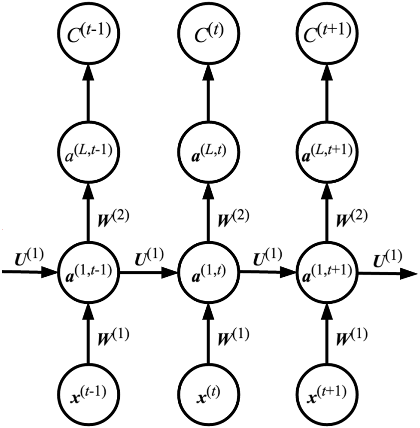
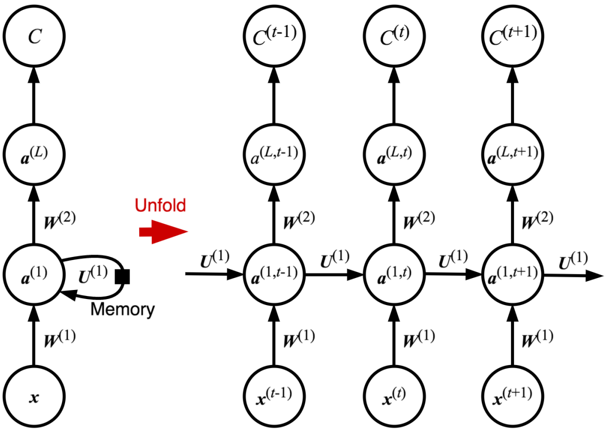
- Weights are ***shared*** across time instances
- Assumes that the "transition functions" are time invariant
- Our goal is to learn $\boldsymbol{U}^{(k)}$'s and $\boldsymbol{W}^{(k)}$'s for $k = 1, \cdots, L$



RNNs have Memory

- The computational graph of an RNN can be ***folded*** in time



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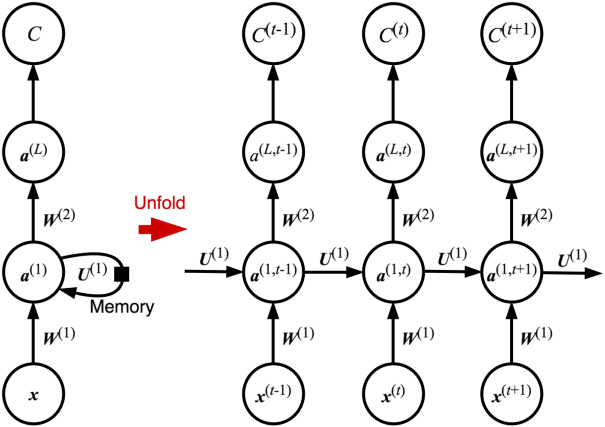
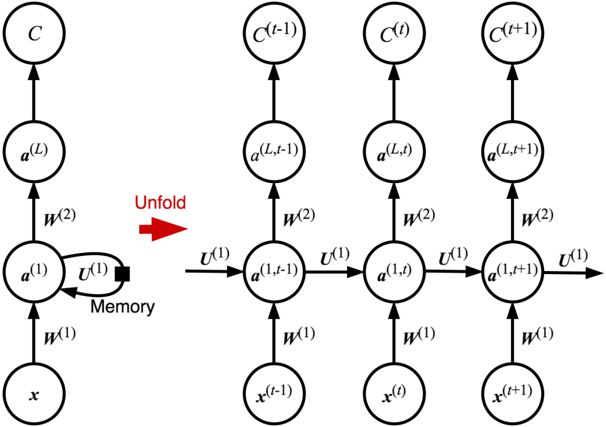
- Black squares denotes ***memory*** access



Output Layer (1/2)

- With multi-class $\mathbf{y}^{(t)}$,
  - $\mathbf{a}^{(L,t)}$ represents the probability of each class
  - $C^{(t)}$ is cross entropy
- How to obtain $\hat{\mathbf{y}}^{(t)}$ rom $\mathbf{a}^{(L,t)}$ at inference time?



Output Layer (2/2)

- ***Output sampling*** for multi-class tasks:
  - Greedy: sample $\hat{\mathbf{y}}^{(t)}$ from $\mathbf{a}^{(L,t)}$
  - Bean search: sample $\hat{\mathbf{y}}^{(t)}$ from the most probable paths of the join distribution $(\mathbf{a}^{(L,t)}, \mathbf{a}^{(L,t-1)}, \cdots \mathbf{a}^{(L,t-b)})$, where b is bean size
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- Problem: out of vocabulary or high dimensional $\mathbf{a}^{(L,t)}$

- Solution?

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- Problem: out of vocabulary or high dimensional $\mathbf{a}^{(L,t)}$

- Solution? ***Subword tokenization*** (to be discussed later)

RNNs vs CNNs for Sequential Data

- On processing a sequence of length T at each layer with
  - D-dimensional point input and output
  - F = the CNN filter/kernel size
  - #CNN filters $= D$

	#Weights	Computation	Autoregressive	Point Distance
CNN	$O(FD^2)$	$O(TFD^2)$	No	$O(\frac{T}{F})$
RNN	$O(D^2)$	$O(TD^2)$	Yes	$O(T)$

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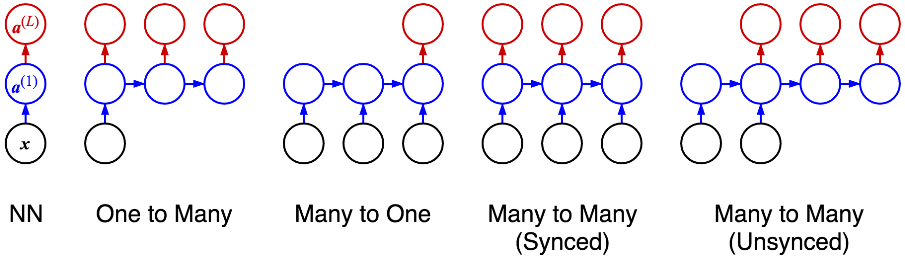
Input and Output

- $\boldsymbol{x}^{(t)}$'s and $\boldsymbol{y}^{(t)}$'s do ***not*** need to have one-to-one correspondence:



One2Many: Image Captioning

"A little girl sitting on a bed with a teddy bear."

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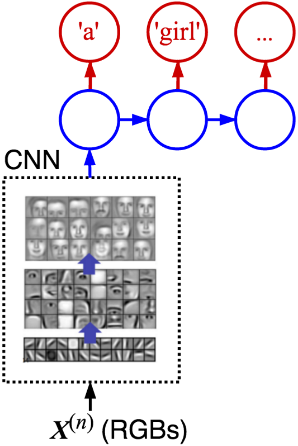
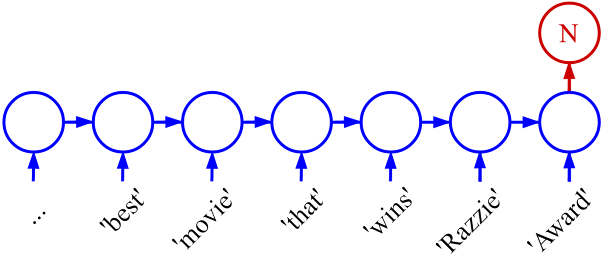


Many2One: Sentiment Analysis



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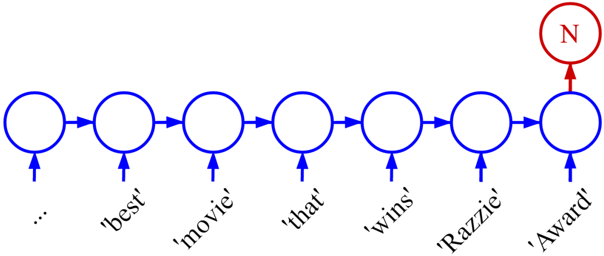
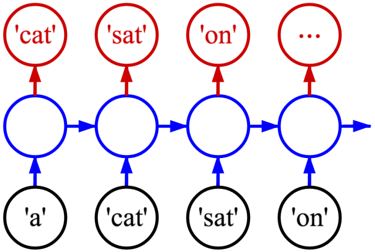


- A single word (e.g., "Razzie") can negate the entire input sentence

Many2Many (Synced): Language Modeling

- ***Language modeling***: predicting the next/nearby word based on the context



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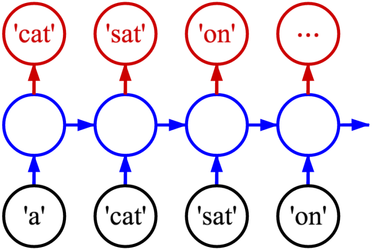
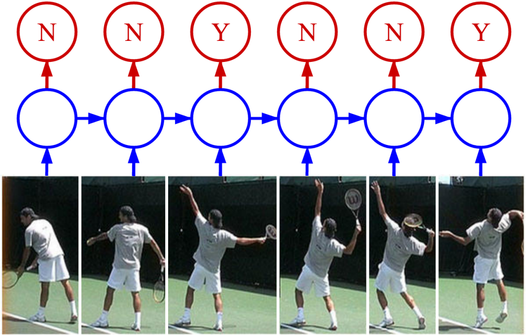


- Latent representations of RNN provide the context

Many2Many (Synced): Video Keyframe Tagging

- Video frame annotation:



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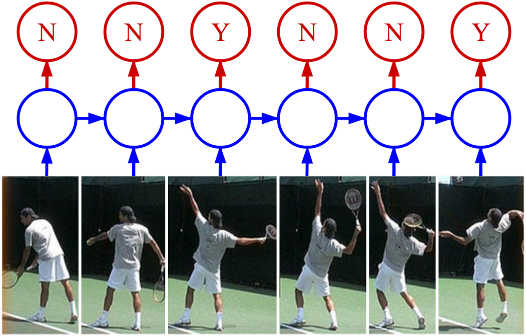
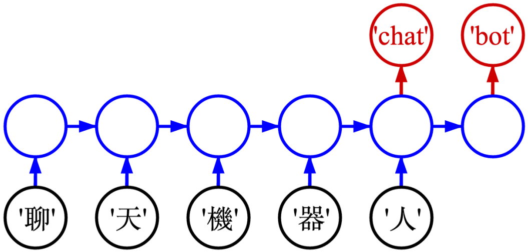


- Latent representations summarize "what's going on"

Many2Many (Unsynced): Machine Translation



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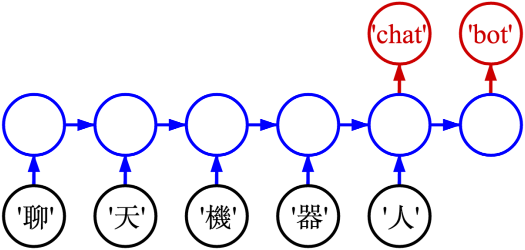

- Latent representations support ***encoding*** first, and then ***decoding***
- RNN learns the structure difference
- Also called ***sequence to sequence*** learning
  - Also used in other applications, e.g., chat bots

Bidirectional RNNs

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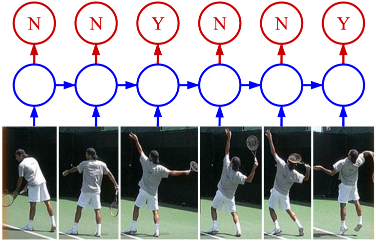

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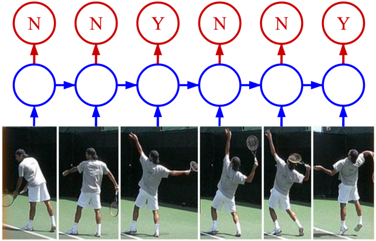

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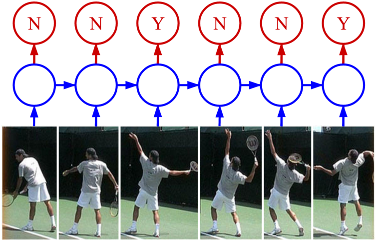
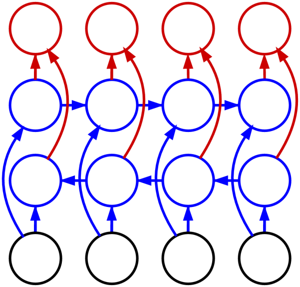
- ***Bidirectional RNNs***: output $\mathbf{a}^{(L,t)}$ depends on both $\mathbf{a}^{(k,t)}$'s and $\tilde{\mathbf{a}}^{(k,t)}$'s

$$\tilde{\mathbf{a}}^{(k,t)} = \mathrm{act}(\tilde{\boldsymbol{U}}^{(k)}\tilde{\mathbf{a}}^{(k,t+1)} + \tilde{\boldsymbol{W}}^{(k)}\tilde{\mathbf{a}}^{(k-1,t)})$$





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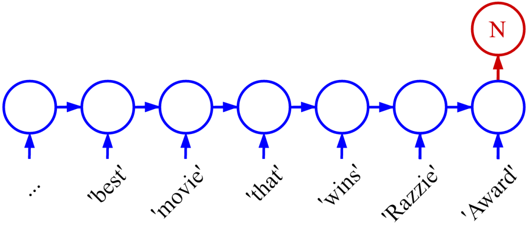

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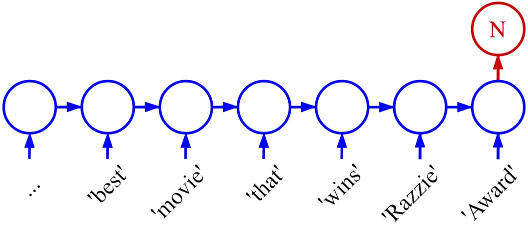
- In some applications, transitions are invariant in terms of other concepts



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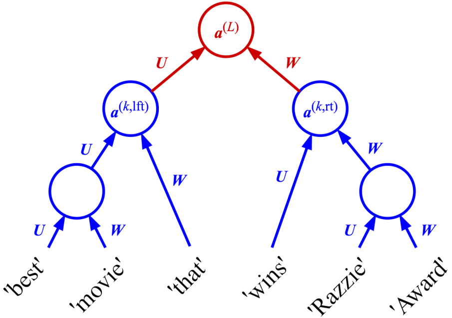

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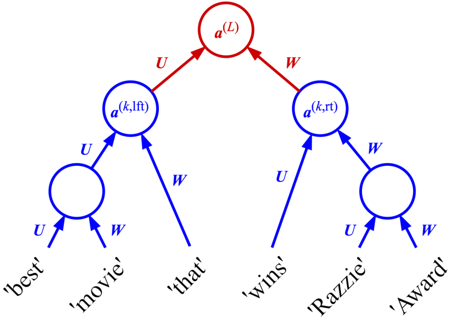

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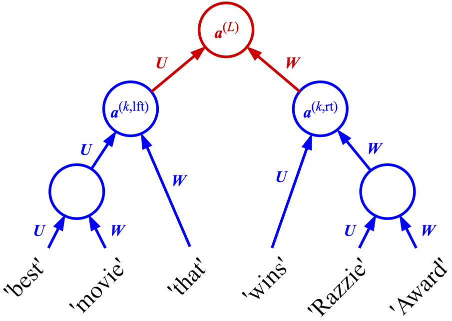
- Given sentence length T, $\mathbf{a}^{(L)}$ and $\mathbf{a}^{(1,\cdot)}$ can be $O(\log T)$ away in the best case



Outline

Cost Function of Vanilla RNNs

- Parameters to learn: $\Theta = \{\boldsymbol{W}^{(k)}, \boldsymbol{U}^{(k)}\}_k$ (bias terms omitted)
- Maximum likelihood:

$$
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&\arg\min_{\Theta} C(\Theta) \\
&\quad = \arg\min_{\Theta} -\log \mathrm{P}(\mathbf{X} \,|\, \Theta) \\
&\quad = \arg\min_{\Theta} -\textstyle\sum_{n,t} \log \mathrm{P}(\boldsymbol{y}^{(n,t)} \,|\, \boldsymbol{x}^{(n,t)}, \cdots, \boldsymbol{x}^{(n,1)}, \Theta) \\
&\quad = \arg\min_{\Theta} -\textstyle\sum_{n,t} C^{(n,t)}(\Theta)
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  - $\mathbf{y}^{(t)}$ depends only on $\mathbf{x}^{(1)}, \cdots, \mathbf{x}^{(t)}$
- For example, in binary classification:
- Assuming $\mathrm{P}(\mathbf{y}^{(n,t)} = 1 \,|\, \boldsymbol{x}^{(n,t)}, \cdots, \boldsymbol{x}^{(n,1)}) \sim \mathrm{Bernoulli}(\rho^{(t)})$, we have

$$
C^{(n,t)}(\Theta) = (\boldsymbol{a}^{(L,t)})^{y^{(n,t)}} (1 - \boldsymbol{a}^{(L,t)})^{(1-y^{(n,t)})}
$$

  - $\boldsymbol{a}^{(L,t)} = \rho^{(t)}$ are based on $\boldsymbol{a}^{(\cdot,t)}$'s, which summarize $\boldsymbol{x}^{(n,t)}, \cdots, \boldsymbol{x}^{(n,1)}$

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SGD-based Training

- RNN optimization problem can be solved using SGD:

$$\Theta^{(s+1)} \leftarrow \Theta^{(s)} - \eta \nabla_{\Theta} \sum_{n,t} C^{(n,t)}(\Theta^{(s)})$$

- Let $c^{(n,t)} = C^{(n,t)}(\Theta^{(s)})$, our goal is to evaluate $\frac{\partial c^{(n,t)}}{\partial U_{i,j}^{(k)}}$ and $\frac{\partial c^{(n,t)}}{\partial W_{i,j}^{(k)}}$
- Evaluation of $\frac{\partial c^{(n,t)}}{\partial W_{i,j}^{(k)}}$ is similar to that in DNNs and omitted
- We focus on:

$$\frac{\partial c^{(n,t)}}{\partial U_{i,j}^{(k)}} = \frac{\partial c^{(n,t)}}{\partial z_j^{(k,t)}} \cdot \frac{\partial z_j^{(k,t)}}{\partial U_{i,j}^{(k)}} = \delta_j^{(k,t)} \frac{\partial z_j^{(k,t)}}{\partial U_{i,j}^{(k)}}$$

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- We can get all second terms starting from the most shallow layer and ***earliest time***

Backward Pass through Time I

- The first term (error signal): $\delta_j^{(k,t)} = \frac{\partial c^{(n,t)}}{\partial z_j^{(k,t)}}$
- We have

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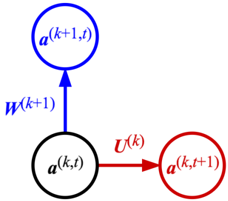
$$\begin{aligned}\delta_j^{(k,t)} &= \frac{\partial c^{(n,t)}}{\partial z_j^{(k,t)}} = \frac{\partial c^{(n,t)}}{\partial a_j^{(k,t)}} \cdot \frac{\partial a_j^{(k,t)}}{\partial z_j^{(k,t)}} = \frac{\partial c^{(n,t)}}{\partial a_j^{(k,t)}} \cdot \mathrm{act}'(z_j^{(k,t)}) \\ &= \left(\sum_s \frac{\partial c^{(n,t)}}{\partial z_s^{(k+1,t)}} \cdot \frac{\partial z_s^{(k+1,t)}}{\partial a_j^{(k,t)}} + \sum_s \frac{\partial c^{(n,t)}}{\partial z_s^{(k,t+1)}} \cdot \frac{\partial z_s^{(k,t+1)}}{\partial a_j^{(k,t)}} \right) \mathrm{act}'(z_j^{(k,t)})\end{aligned}$$



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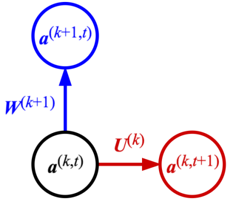

Backward Pass through Time II

$$\delta_j^{(k,t)} = \left(\sum_s \delta_s^{(k+1,t)} W_{j,s}^{(k+1)} + \sum_s \delta_s^{(k,t+1)} U_{j,s}^{(k)} \right) \mathrm{act}'(z_j^{(k,t)})$$

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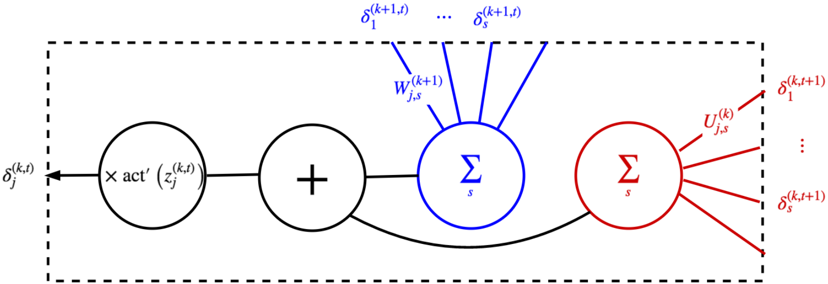
- We can evaluate all $\delta_j^{(k,t)}$'s starting from the deepest layer and ***latest time***



Backprop through Time (BPTT)

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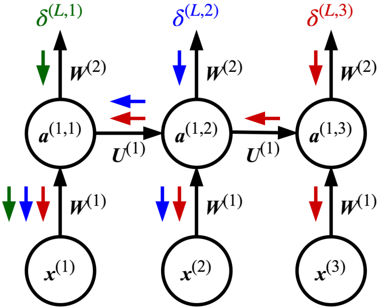
- ***BPTT***: single forward pass, ***multiple*** backward passes



Outline

Long-Term Dependencies

- Forward pass:

$$\boldsymbol{z}^{(k,t)} \leftarrow \boldsymbol{U}^{(k)\top}\boldsymbol{a}^{(k,t-1)} + \boldsymbol{W}^{(k)\top}\boldsymbol{a}^{(k-1,t)}$$

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- Backward pass:

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- If $a^{(k,i)}$ and $a^{(k,j)}$ are far away in time, their long-term dependency causes optimization problems

Exploding/Vanishing Gradient Problem

- Ignoring activation function and depth:

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- Exploding or vanishing gradients!

Cost Surface

- The cost surface of C is either very flat or steep
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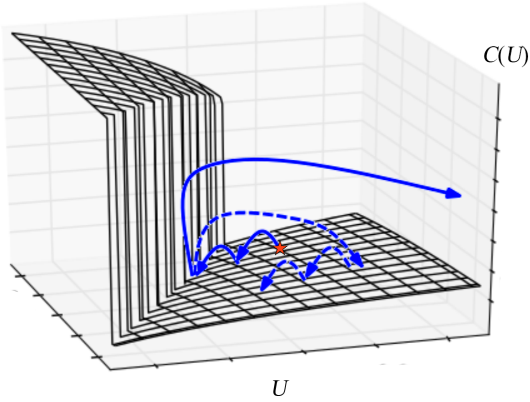

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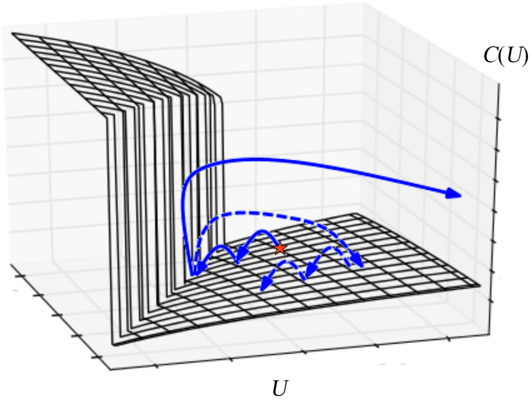
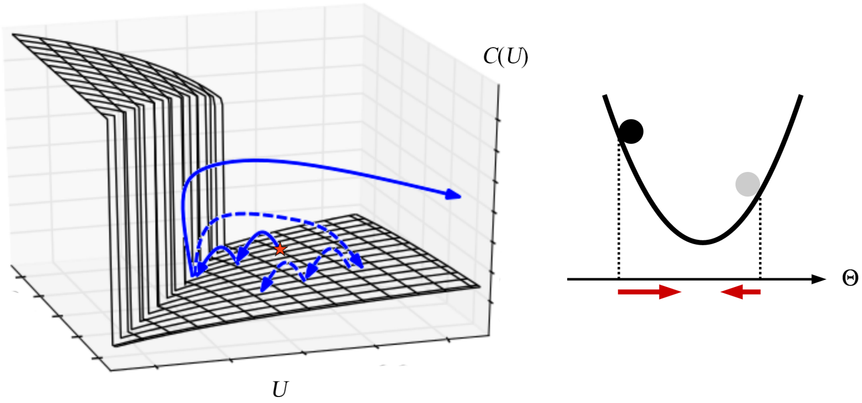


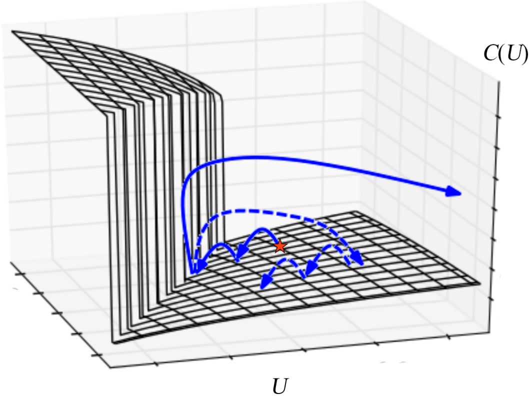
Nesterov Momentum

- Use Nesterov momentum to "brake" before hitting the wall



Gradient Clipping

- A simple way is to avoid the exploding gradient problem is to ***clip*** a gradient if it exceeds a predefined threshold
- Very effective in practice



RMS Prop

- Adaptive learning rate based on statistics of recent gradients:

$$\boldsymbol{r}^{(t+1)} \leftarrow \lambda \boldsymbol{r}^{(t)} + (1-\lambda)\boldsymbol{g}^{(t)} \odot \boldsymbol{g}^{(t)}$$

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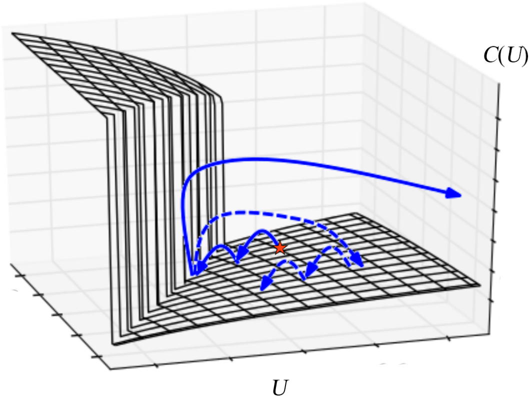

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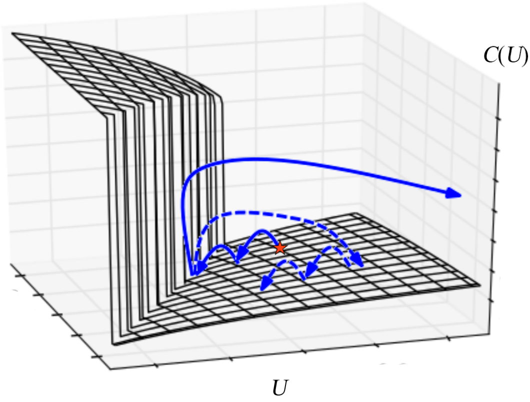

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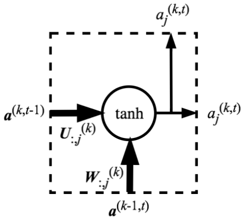

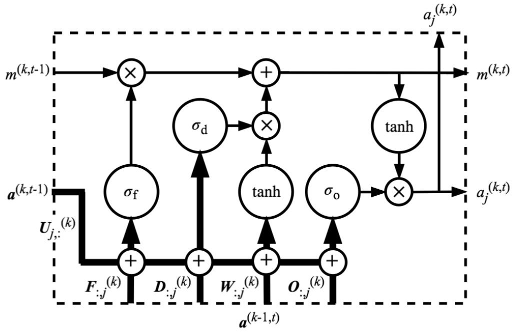

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- The j-th LSTM unit at depth k and time t:
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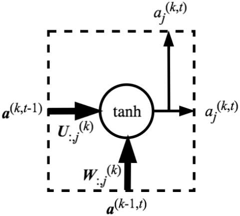

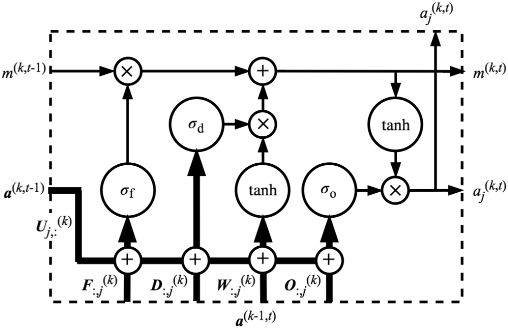

Long Short-Term Memory (LSTM)

- Idea: to create ***shortcut*** in each neuron for the error signals to flow backward more smoothly
- The j-th LSTM unit at depth k and time t:
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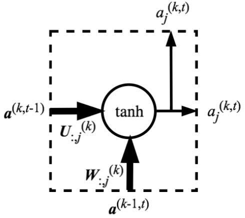

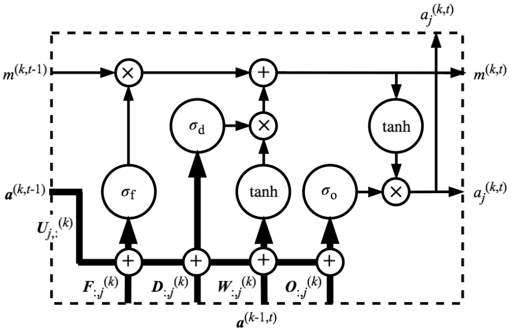

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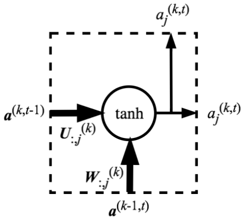

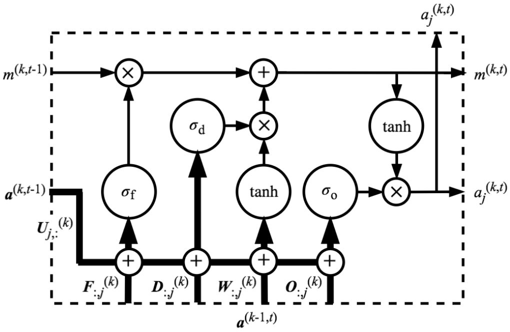

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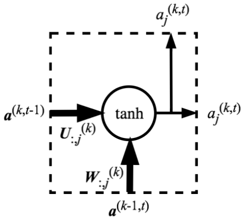
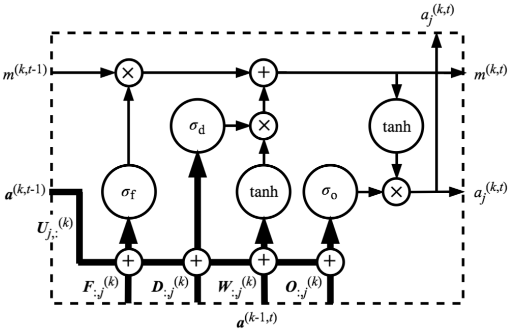
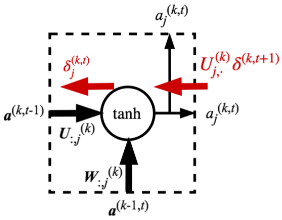
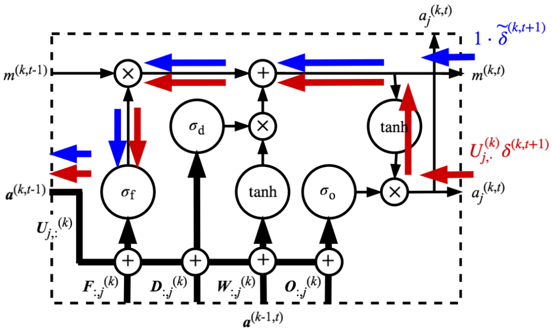




Error Signals

- Error signals now have a second path
  - If the forget gate is open, error signals won't decay (***blue arrows***)





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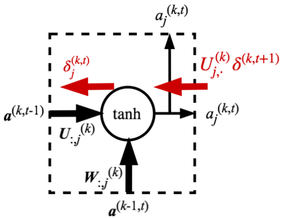

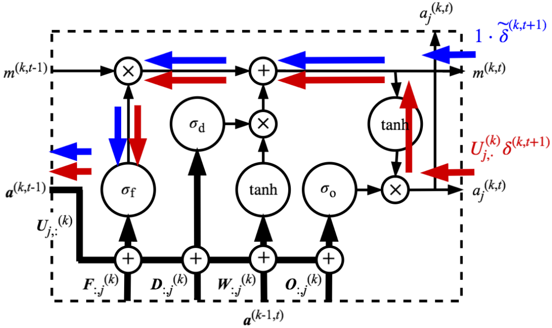

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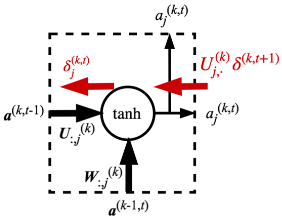
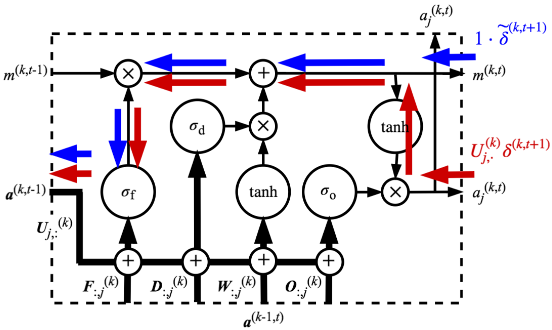
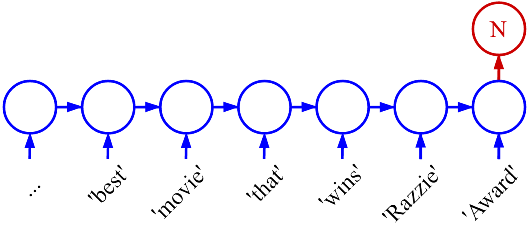
  - Avoids the vanishing gradients (but not exploding ones)
- When NN decides to close the forget gate, the vanishing gradient problem is irrelevant
- In practice, LSTM + gradient clipping works well together





Dynamic Representations for Sentiment Analysis



- LSTM units learn dynamic representations

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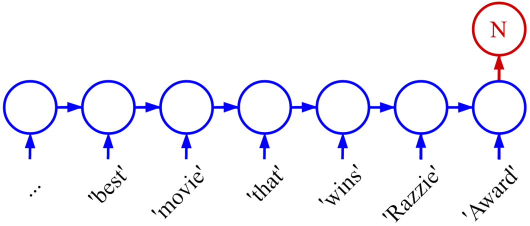

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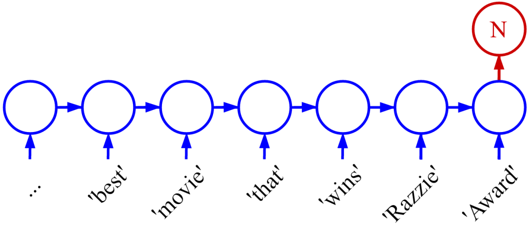

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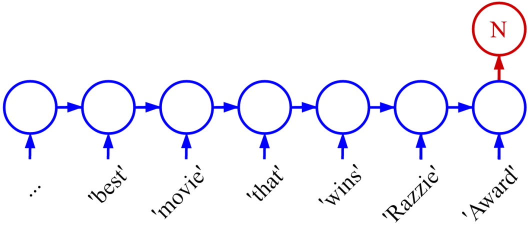

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- Closing forget gate for “Razzie”
  - To correct previous summarization and/or shift focus
- Closing input gate for “movie”
  - Not to learn, to keep the same summarization
- Closing output gate for “that”
  - To let the next neuron decide the activation/gate values by its own

Dynamic Representations for Language Models

Dynamic Representations for Language Models

- Neuron activations for language modeling [4] ▸ Interactive Tool

Learning Process of LSTMs

- Output at epoch 100:

  "*... tyntd-iafhatawiaoihrdemot lytdws e ,tfti, astai f ogoh...*"

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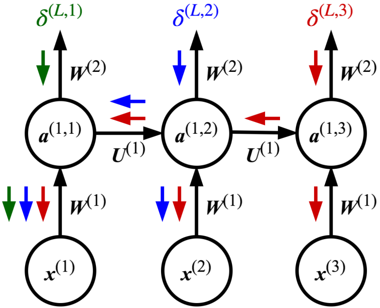
- At 2000 (topics and longer-term dependencies):

  “*... “Why do what that day,” replied Natasha, ...*”

Outline

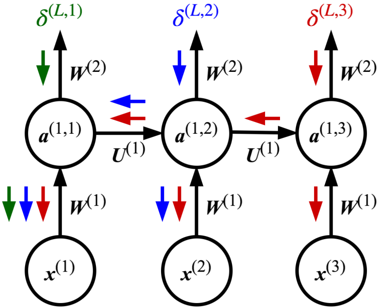
Parallelism

- A forward/backward pass through time in BPTT cannot be parallelized



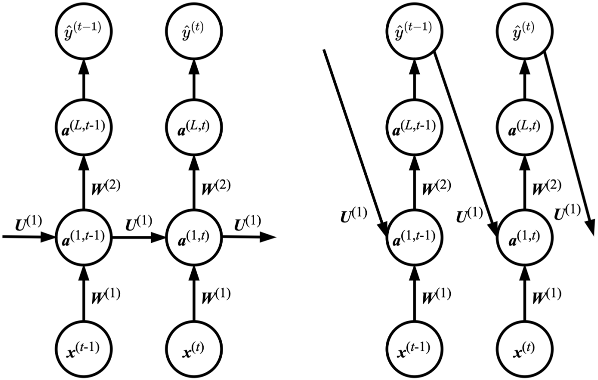
Parallelism

- A forward/backward pass through time in BPTT cannot be parallelized
- The ***hidden-to-hidden*** recurrent connections in a vanilla RNN create dependency between
  - $\boldsymbol{a}^{(k,t)}$'s in forward pass
  - $\delta^{(k,t)}$'s in backward pass



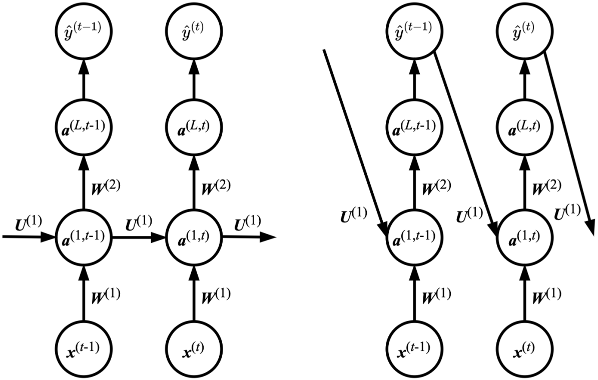
Output Recurrence and Teacher Forcing

- ***Teacher forcing***: replace hidden-to-hidden recurrence with output-to-hidden or output-to-input recurrence



Output Recurrence and Teacher Forcing

- *Teacher forcing*: replace hidden-to-hidden recurrence with output-to-hidden or output-to-input recurrence
- At training time, use ***correct labels*** $\boldsymbol{y}^{(\cdot)}$**'s** to train the model
  - So, the forward/backward pass through time can be parallelized
- At test time, switch back to using model output $\hat{\boldsymbol{y}}^{(\cdot)}$'s



Cost: Exposure Bias

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- Solution? Scheduled sampling
- At training time,
  1. Use $\boldsymbol{y}^{(\cdot)}$'s initially
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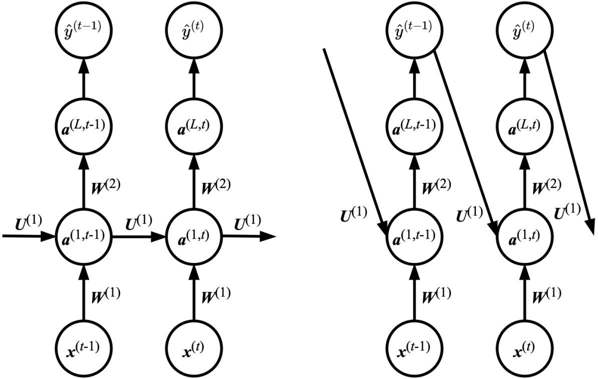
Cost: Reduced Expressiveness

- The vanilla RNNs are universal in the sense that they can simulate Turing machines [11]



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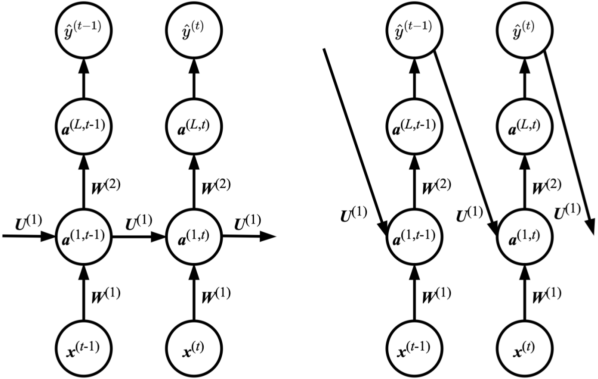

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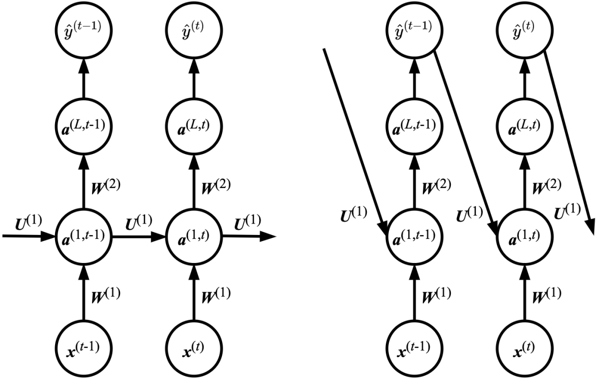
- The output $\boldsymbol{a}^{(L,\cdot)}$'s are explicitly trained to match training targets
  - Cannot capture all required information in the past to predict the future



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- In some RNNs, a hidden representation $\mathbf{a}^{(\cdot,t)}$ needs to support:
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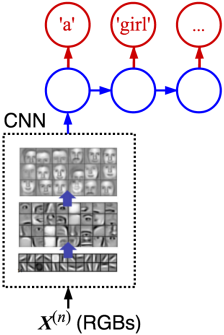
"A little girl sitting on a bed with a teddy bear."



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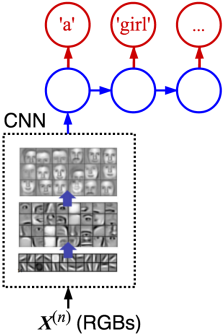

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- Can we ease the job of $\mathbf{a}^{(\cdot,t)}$?

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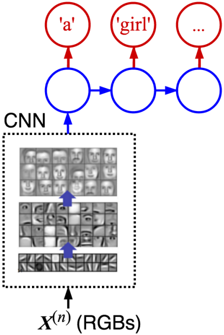

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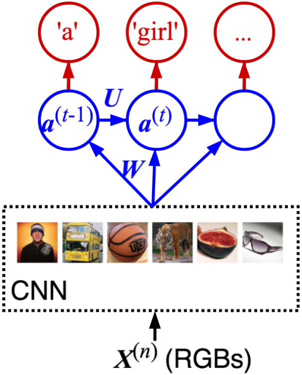

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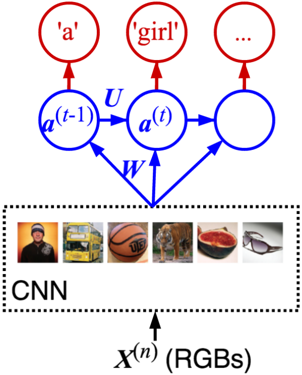

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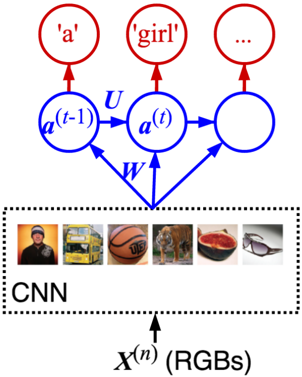

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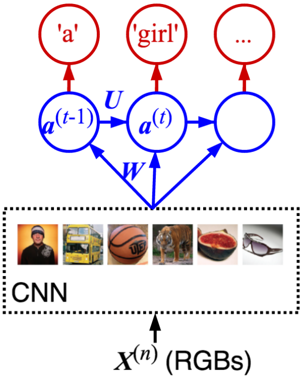
- Why not model the attention explicitly?
  - So we can see where $\mathbf{a}^{(\cdot,t)}$ is "looking at"



Attention Mechanism

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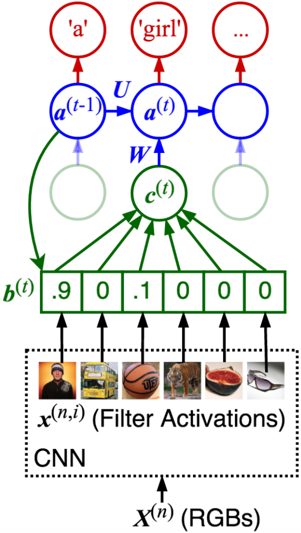

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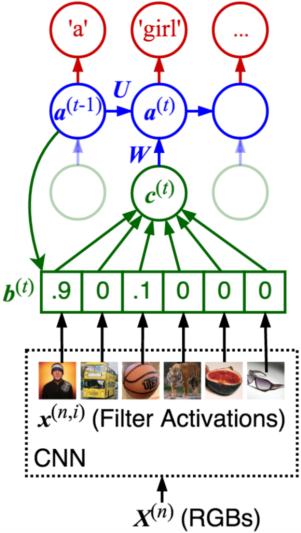

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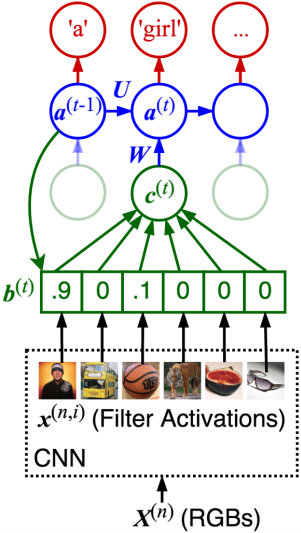

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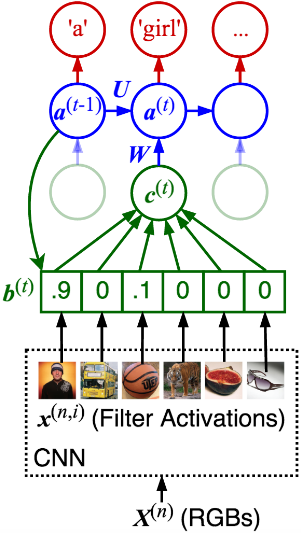

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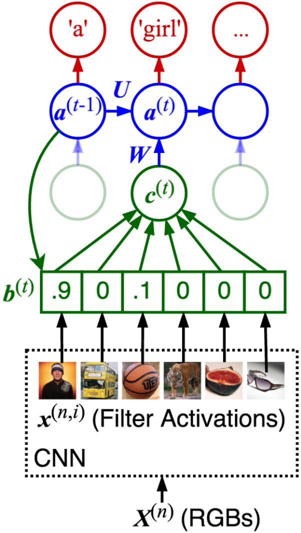
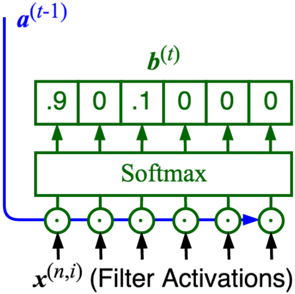
- Reduces size of $\boldsymbol{W}$ from $O(|\mathbf{X}| \cdot |\mathbf{a}^{(\cdot,t)}|)$ to $O(|\mathbf{x}^{(i)}| \cdot |\mathbf{a}^{(\cdot,t)}|)$
- How to obtain $\mathbf{b}^{(t)}$?



Computing Attention Vector

1. Use $\mathbf{a}^{(L-1,t-1)}$ as a "query" to get a match score for each input part by using, e.g., a simple NN [2, 13]:

$$z_i = \mathrm{act}(\boldsymbol{p}^\top \mathbf{a}^{(L-1,t-1)} + \boldsymbol{q}^\top \mathbf{x}^{(i)} + r)$$



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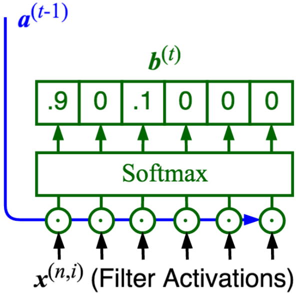
2. Normalize and concentrate on few larger scores by:

$$\mathrm{b}_i = \mathrm{softmax}(\mathrm{z})_i = \frac{\exp(\mathrm{z}_i)}{\sum_j \exp(\mathrm{z}_j)}$$



Computing Attention Vector

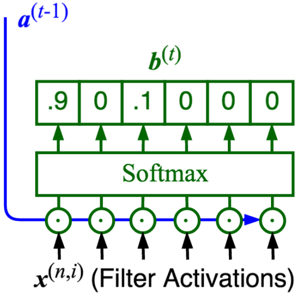
1. Use $\mathbf{a}^{(L-1,t-1)}$ as a "query" to get a match score for each input part by using, e.g., a simple NN [2, 13]:

$$\mathrm{z}_i = \mathrm{act}(\boldsymbol{p}^\top \mathbf{a}^{(L-1,t-1)} + \boldsymbol{q}^\top \mathbf{x}^{(i)} + r)$$

   - Jointly trained with the main RNN

2. Normalize and concentrate on few larger scores by:

$$\mathrm{b}_i = \mathrm{softmax}(\mathrm{z})_i = \frac{\exp(\mathrm{z}_i)}{\sum_j \exp(\mathrm{z}_j)}$$



Computing Attention Vector

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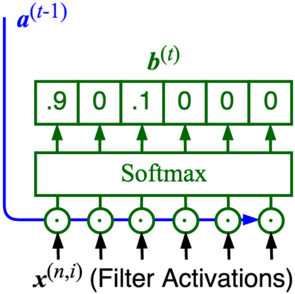
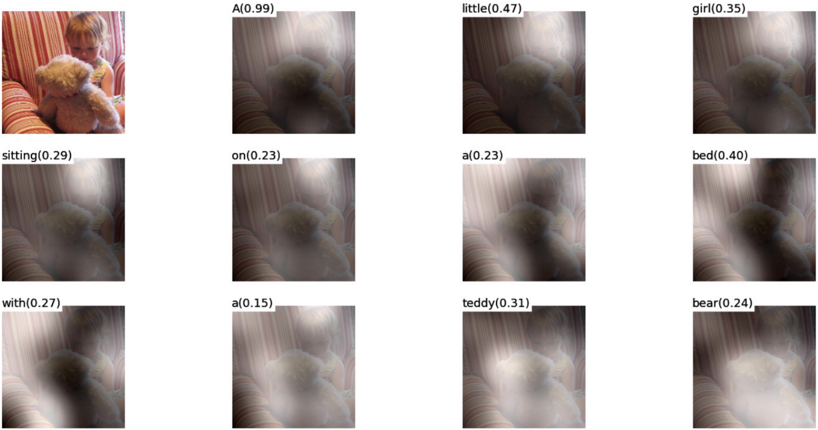
   - Jointly trained with the main RNN
   - $\boldsymbol{p}$, $\boldsymbol{q}$, and r are shared by different i's and t's (weight tying)

2. Normalize and concentrate on few larger scores by:

$$b_i = \mathrm{softmax}(z)_i = \frac{\exp(z_i)}{\sum_j \exp(z_j)}$$

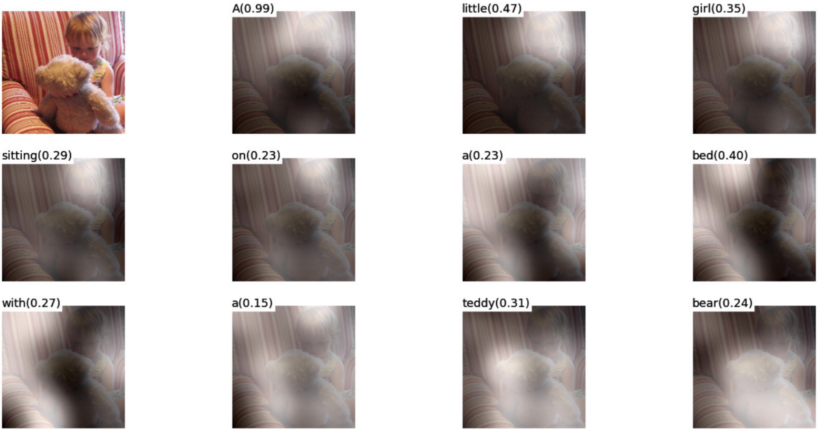


Visualizing Attention



- How to draw a mask?

Visualizing Attention

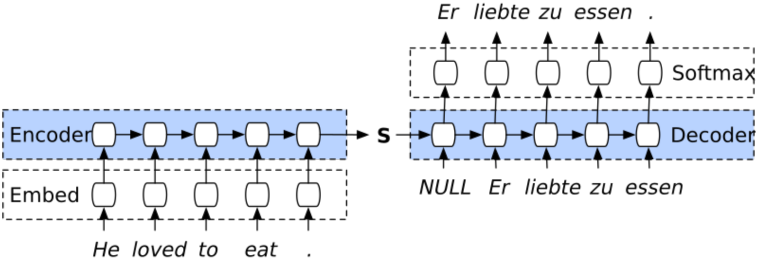


- How to draw a mask? Threat $\mathbf{c}^{(t)} = \sum_i b_i^{(t)} \mathbf{x}^{(i)}$ as image and enlarge it

Outline

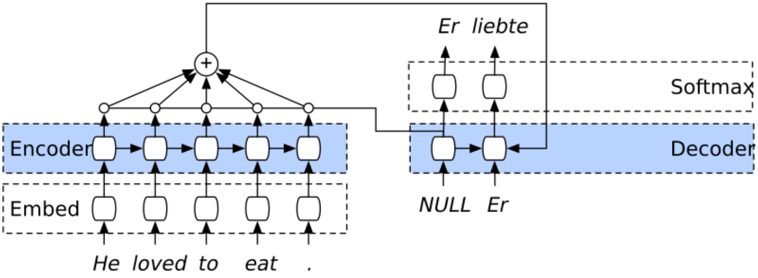
GoogleNMTv1: Encoder-Decoder

- LSTM-based RNN
- Hidden state S encodes an entire input sequence
- Then supplied to the decoder



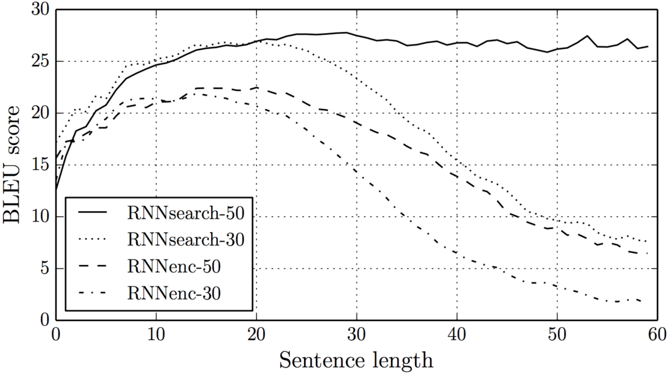
GoogleNMTv2: Attention-based Encoder-Decoder

- No feed-forward connection between the encoder and decoder
- Instead, uses previous output as query to get attention and next output
  - Allows for retrieving different parts of input sentence depending on decoding context



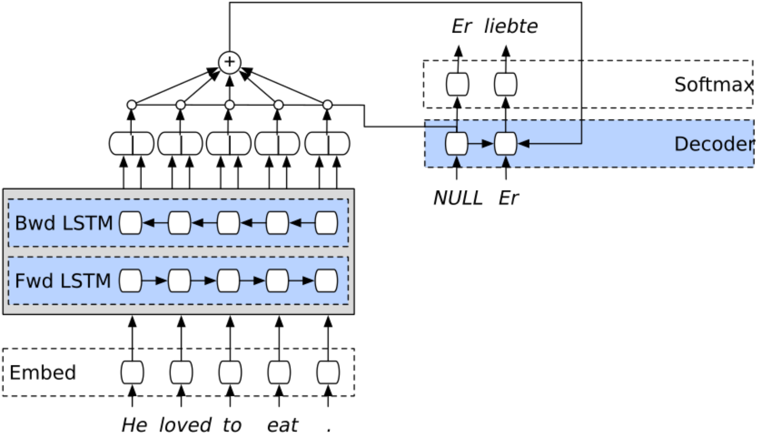
Long Sequences

- Attention-based model generates long sequences better



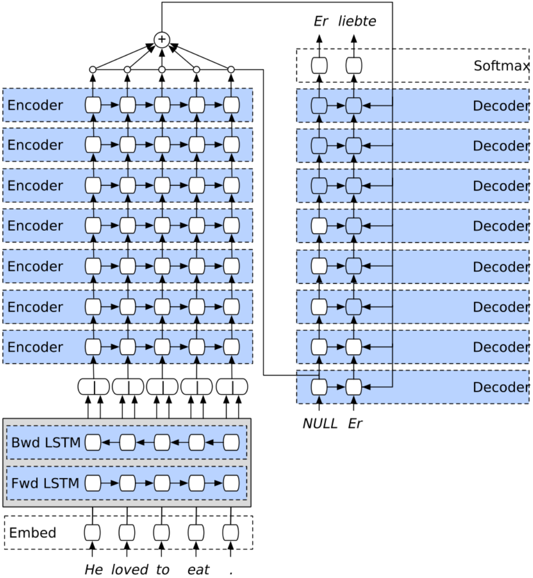
GoogleNMTv3: Bidirectional Encoder Layer

- Takes into account future words when summarizing input sequence
- Better determines the meaning/context



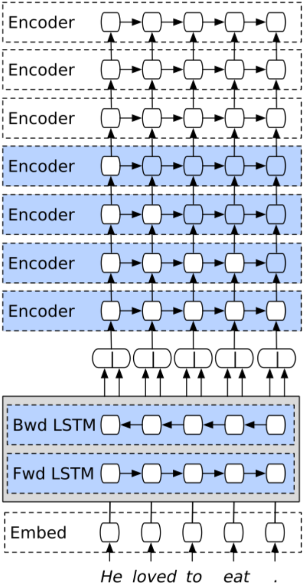
GoogleNMTv4: Going Deep

- Encoder:
  - ***1*** bi-directional layer
  - 7 uni-directional layers
- Decoder:
  - 8 uni-directional layers
  - ***Lowest*** decoder layer for querying attention

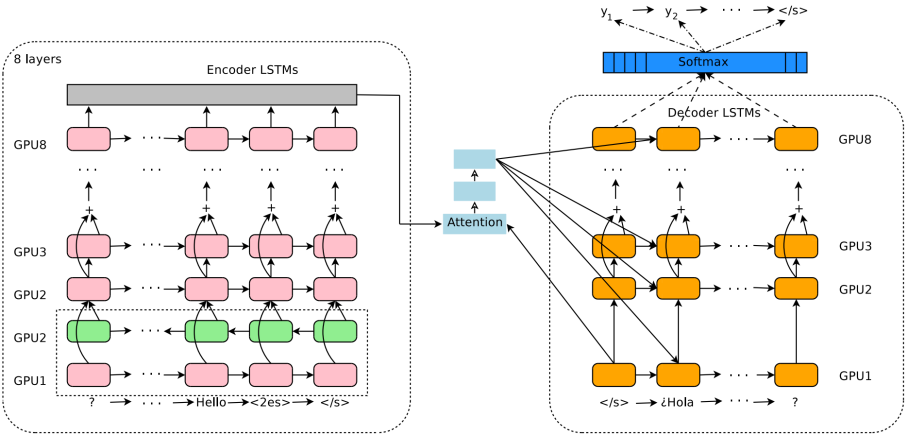


GoogleNMTv5: Parallelization

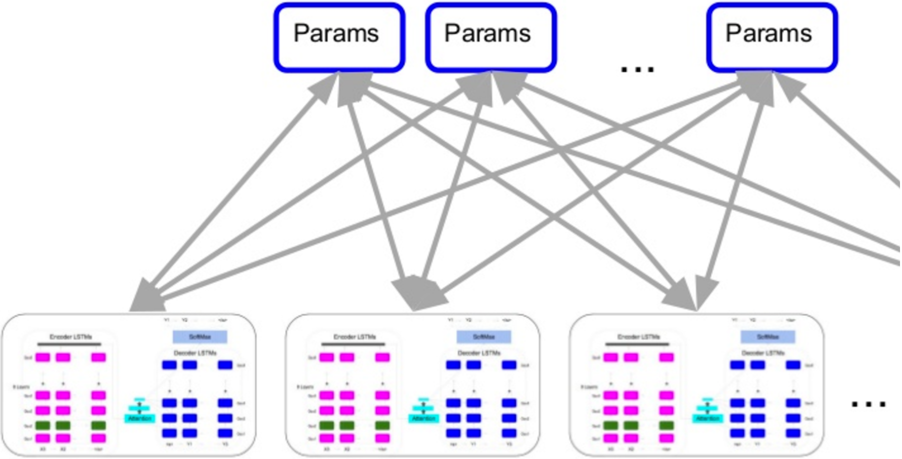
- Each layer trained by a GPU
- Forward pass:
  - Encoder: 7 uni-directional encoder layers trained in a pipeline
  - Decoder: pipeline starts as soon as encoder layers are ready
- Backward pass:
  - Teacher forcing



Model Parallelism (1 Machine, 8 GPUs)

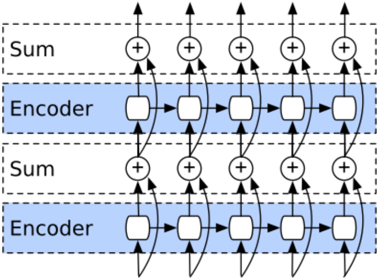


Data Parallelism (Multiple Param Servers)



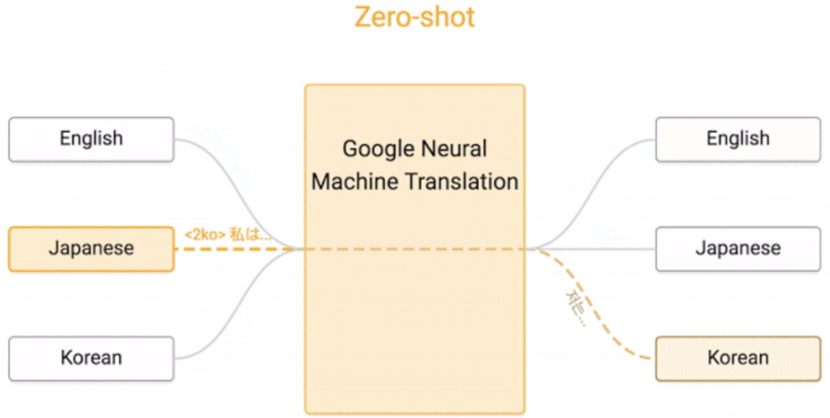
GoogleNMTv6: Residuals

- Upper layer learns the ***delta*** function to the lower one
- Easier to train a deep NN



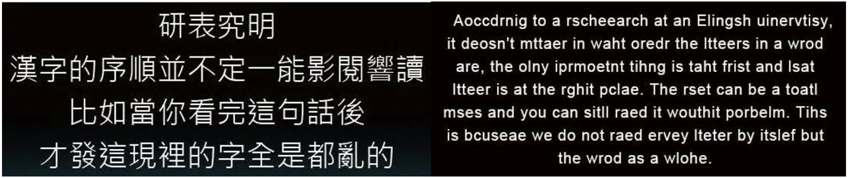
GoogleNMTv7: Multilingual & Zero-Shot Translation

- Training: input $\boldsymbol{x}$ augmented with task identifier (language pair)
  - E.g., (eng, jp), (kr, en), (jp, en)
- Inference: ***unknown*** language-pair identifier
  - E.g., (kr, jp)

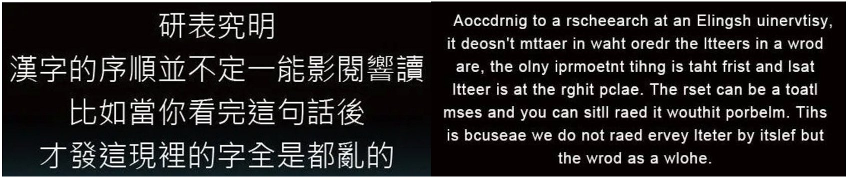


Outline

How Humans Process Text?

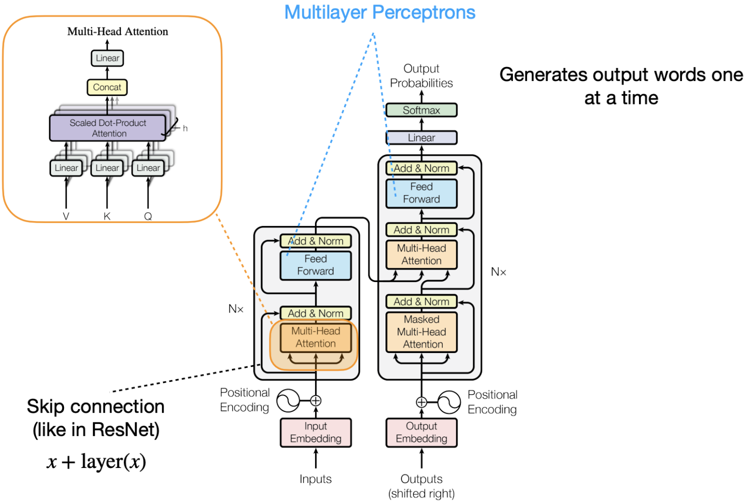


How Humans Process Text?



- ***Not entirely sequential*** as in RNNs
- ***Not recursively based on local patterns*** as in CNNs
- Any other "better" architectures?

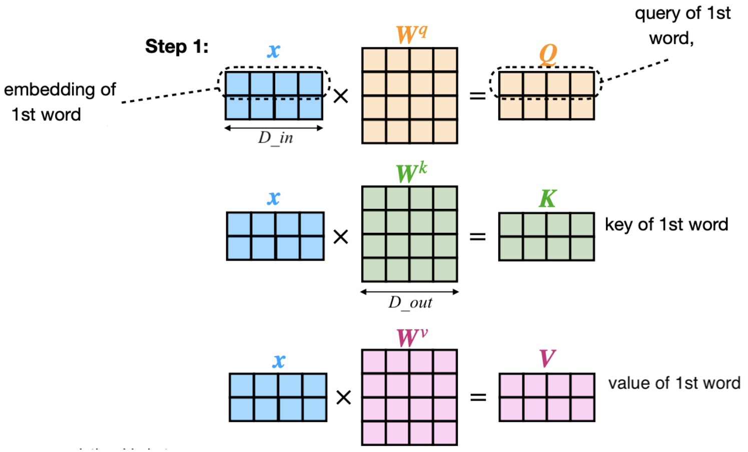
Attention is All You Need [12]



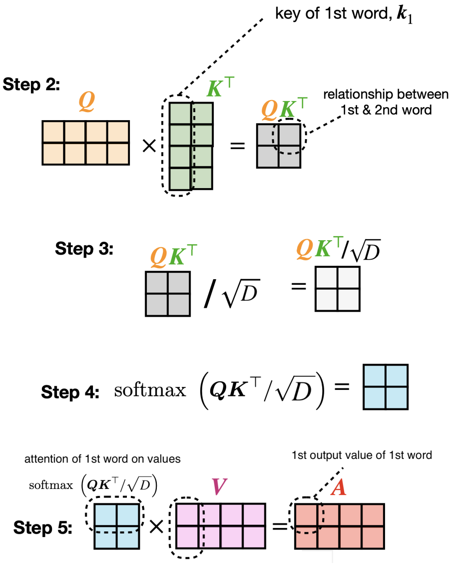
- RNN layers are replaced with *self-* and *cross-attention* blocks

Self-Attention

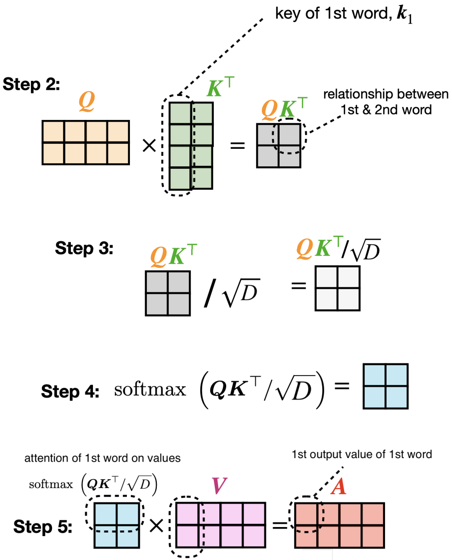
- Weights to learn at each layer: $\boldsymbol{W}_{\text{query}}, \boldsymbol{W}_{\text{key}}, \boldsymbol{W}_{\text{value}} \in \mathbb{R}^{D \times D}$
- Batch, non-autoregressive processing of sequences



Self-Attention

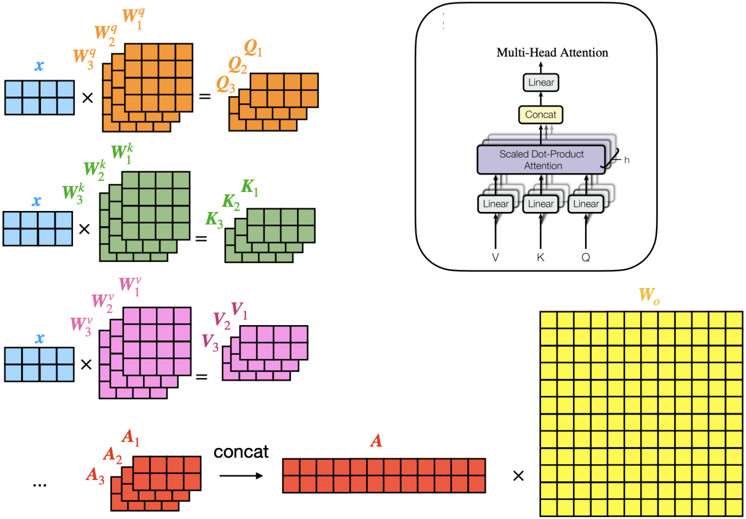


Self-Attention



- Input: $\boldsymbol{A}^{(l-1)} \in \mathbb{R}^{T \times D}$ (T tokens, each with dimension D)
- Output: $\boldsymbol{A}^{(l)} \in \mathbb{R}^{T \times D}$ (T tokens, each with dimension D)
  - ***Context*** augmented
  - E.g, "**train** a model" vs. "get on a **train**"

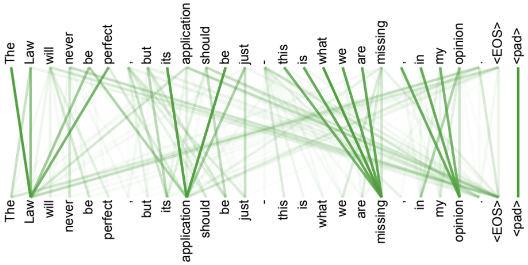
Multi-head Self-Attention

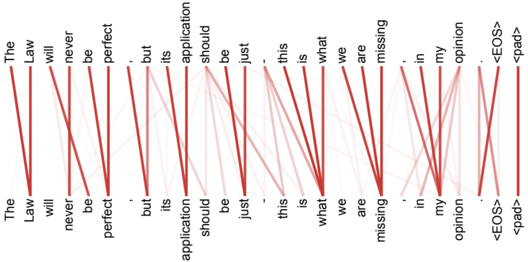


- Given H heads, we have $\boldsymbol{W}_{\text{query}}^{(h)}, \boldsymbol{W}_{\text{key}}^{(h)}, \boldsymbol{W}_{\text{value}}^{(h)} \in \mathbb{R}^{D \times \frac{D}{H}}$ and $\boldsymbol{A} \in \mathbb{R}^{T \times D}$

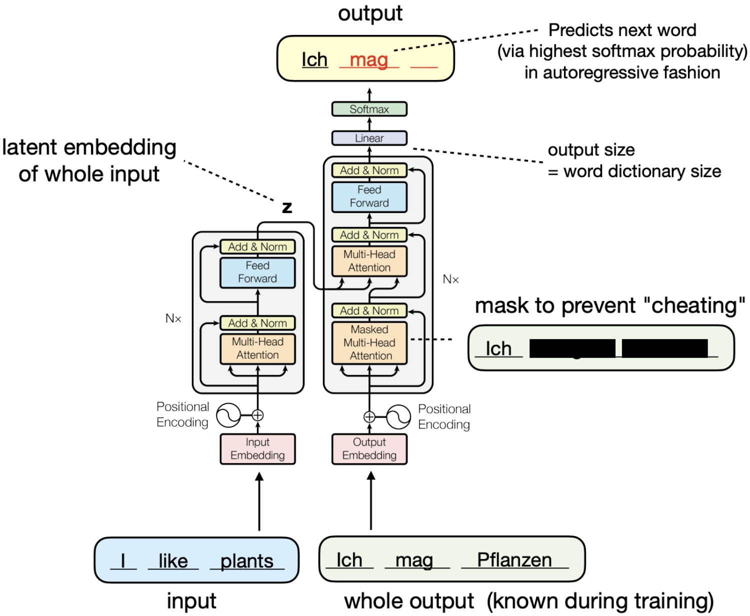
Same Sequence, Different Context Augmentations

Step 4: $\text{softmax}\left(\boldsymbol{Q}\boldsymbol{K}^\top/\sqrt{D}\right) =$



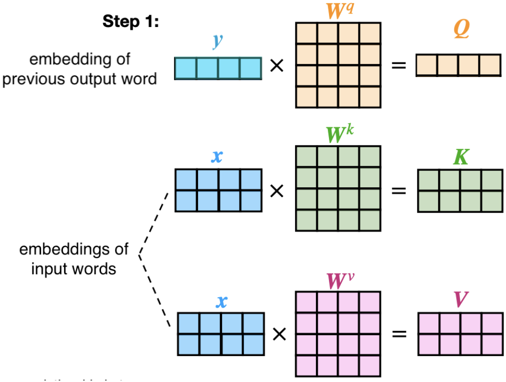


Masked Self-Attention for Autoregressive Output

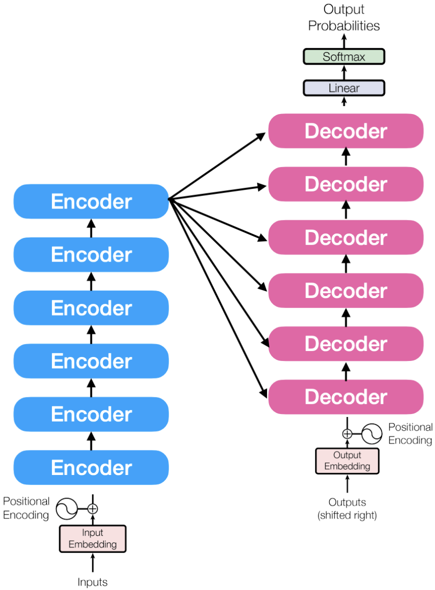


Cross-Attention for Autoregressive Output

- When generating each output token, attend each output token on entire context
  - The last output token as query (autoregressive)
  - Input + previous output tokens (context) as keys and values
  - Dimension of attention matrix: $1 \times$ context length

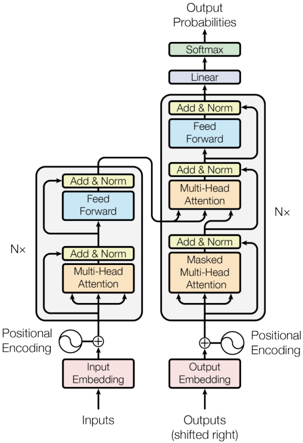


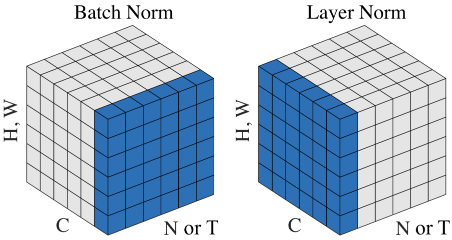
Going Deep



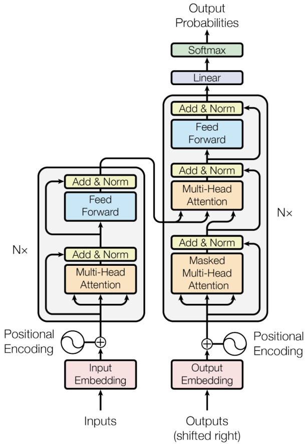
Output
Probabilities
Softmax
Linear
Decoder
Decoder
Decoder
Decoder
Decoder
Decoder
Encoder
Encoder
Encoder
Encoder
Encoder
Encoder
Positional
Encoding
Output
Embedding
Outputs
(shifted right)
Positional
Encoding
Input
Embedding
Inputs

Layer Normalization



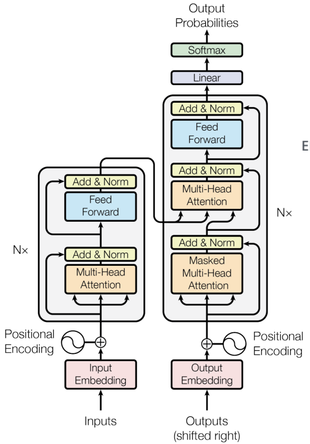


Positional Encoding



- "John loves Mary" $\neq$ "Mary loves John"
- So far, augmented context does ***not*** change when the input words change order

Positional Encoding



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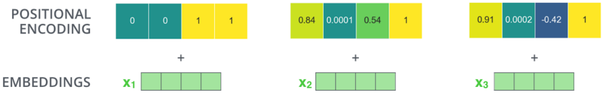
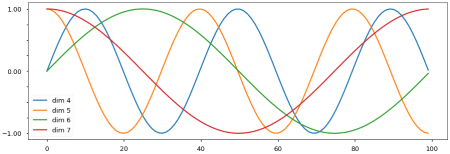


- Each word position corresponds to multiple $\sin(\cdot)$ / $\cos(\cdot)$ values of different periods



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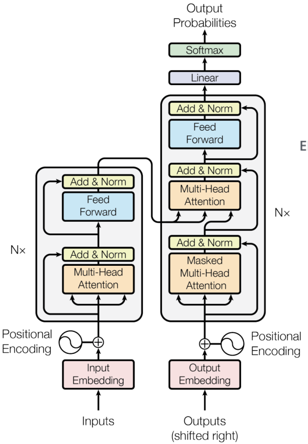

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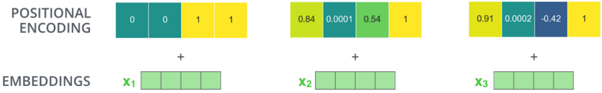
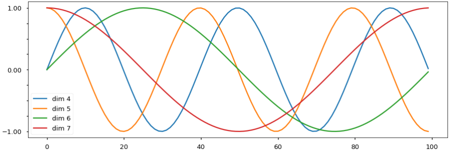


- Each word position corresponds to multiple $\sin(\cdot)$ / $\cos(\cdot)$ values of different periods
  - Why not linear values (e.g, 1, 2, 3, ...)?



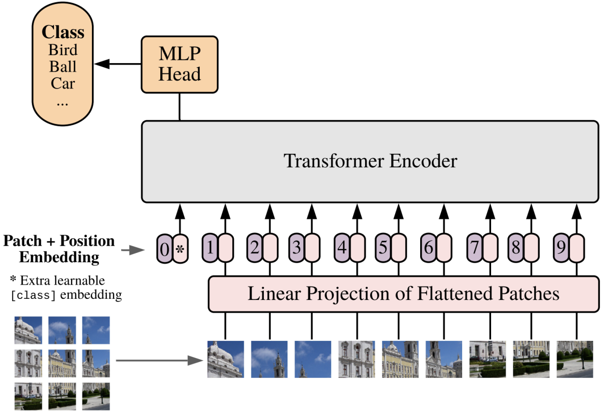
Remarks I: RNNs vs. CNNs vs. Transformers

- On processing a sequence of length T at each layer with
  - D-dimensional point input and output
  - F = the CNN filter/kernel size
  - #CNN filters = D
  - #attention heads = H
  - Query, key, and value size = $\frac{D}{H}$

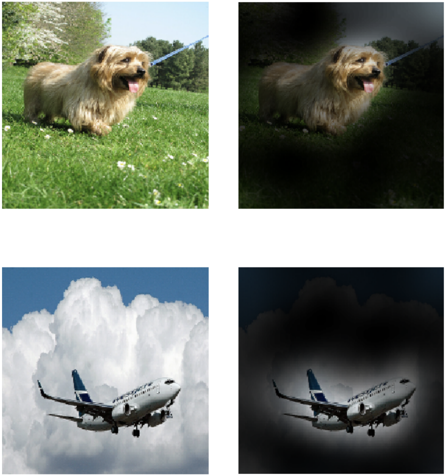
	#Weights	Computation	Auto-reg.	Point Dist.
CNN	$O(FD^2)$	$O(TFD^2)$	No	$O(\frac{T}{F})$
RNN	$O(D^2)$	$O(TD^2)$	Yes	$O(T)$
Self-attention	$O(D^2)$	$O(TD^2 + T^2D)$	No	$O(1)$

Remarks II: Vision Transformers (ViT) [3]

- Splits an image into 16×16 patches (words)
- Like BERT, uses [CLS] input word to get class predictions



Attention



Outline

Sequence Tokenization

- Word-level
  - High input/output dimension (D)
  - Out-of-vocabulary (OOV) problem
  - "old" $\neq$ "older" $\neq$ "oldest"
- Char-level
  - Long sequence (T)

Sequence Tokenization

- Word-level
  - High input/output dimension (D)
  - Out-of-vocabulary (OOV) problem
  - "old" $\neq$ "older" $\neq$ "oldest"
- Char-level
  - Long sequence (T)
- Subword-level?
  - How to deal with OOV problem?
  - How to support different languages?

Byte Pair Encoding (BPE) [10]

- Given a training set of words
  1. Uses Unicode bytes as base symbols $\{\boldsymbol{s}^{(1)}, \boldsymbol{s}^{(2)}, \cdots\}$
  2. Merge two symbol $\boldsymbol{s}^{(i)}$ and $\boldsymbol{s}^{(j)}$ having highest $\Pr(\boldsymbol{s}^{(i)})$ and $\Pr(\boldsymbol{s}^{(j)})$
  3. Repeat step 2 until target #symbols is met

	Vocabulary	Encoded Sentence
Initialization	['a', 'c', 'b', 'e', 'i', '</w>', 'k', 'm', 'o', 'n', 'p', 's', 'r', 'u', 't', 'v', 'x']	v i e t n a m </w> t a k e s </w> m e a s u r e s </w> t o </w> b o o s t </w> r i c e </w> e x p o r t s </w>
After 1 merge operation	['a', 'c', 'b', 'e', 'p', '</w>', 'k', 'm', 'o', 'n', 'i', 's', 'r', 'u', 't', 'v', 'x', 's</w>']	v i e t n a m </w> t a k e s</w> m e a s u r e s</w> t o </w> b o o s t </w>r i c e </w> e x p o r t s</w>
After 10 merge operations	['</w>', 'vi', 'as', 'es</w>', 's</w>', 'nam', 'to', 'ri', 't</w>', 'ort', 'a', 'c', 'b', 'e', 'k', 'm', 'o', 'p', 's', 'r', 'u', 't', 'x']	vi e t nam </w> t a k es</w> m e as u r es</w> to </w> b o o s t</w> ri c e </w> e x p ort s</w>
After 34 merge operations	['takes</w>', 'measures</w>', 'exports</w>', 'boost</w>', 'rice</w>', 'vietnam</w>', 'to</w>']	vietnam</w> takes</w> measures</w> to</w> boost</w> rice</w> exports</w>

Other Variants

- BPE is used by GPT
- WordPiece [9]:
  - Merge $\boldsymbol{s}^{(i)}$ and $\boldsymbol{s}^{(j)}$ having highest $\frac{\Pr(\boldsymbol{s}^{(i)},\boldsymbol{s}^{(j)})}{\Pr(\boldsymbol{s}^{(i)})\Pr(\boldsymbol{s}^{(j)})}$
  - Used by BERT
- Unigram Language Model [6]
  - Top-down, probabilistic
- SentencePiece [7]
  - Treat space "_" as symbols to support difference languages
  - Merge algorithm: BPE or Unigram Language Model
  - Used by ALBERT, XLNet, Marian, T5

Reference I

[1] Martin Arjovsky, Amar Shah, and Yoshua Bengio.
Unitary evolution recurrent neural networks.
arXiv preprint arXiv:1511.06464, 2015.

[2] Dzmitry Bahdanau, Kyunghyun Cho, and Yoshua Bengio.
Neural machine translation by jointly learning to align and translate.
arXiv preprint arXiv:1409.0473, 2014.

[3] Alexey Dosovitskiy, Lucas Beyer, Alexander Kolesnikov, Dirk Weissenborn, Xiaohua Zhai, Thomas Unterthiner, Mostafa Dehghani, Matthias Minderer, Georg Heigold, Sylvain Gelly, et al.
An image is worth 16x16 words: Transformers for image recognition at scale.
arXiv preprint arXiv:2010.11929, 2020.

Reference II

[4] Andrej Karpathy, Justin Johnson, and Li Fei-Fei.
Visualizing and understanding recurrent networks.
arXiv preprint arXiv:1506.02078, 2015.

[5] David Krueger and Roland Memisevic.
Regularizing rnns by stabilizing activations.
arXiv preprint arXiv:1511.08400, 2015.

[6] Taku Kudo.
Subword regularization: Improving neural network translation models with multiple subword candidates.
arXiv preprint arXiv:1804.10959, 2018.

[7] Taku Kudo and John Richardson.
Sentencepiece: A simple and language independent subword tokenizer and detokenizer for neural text processing.
arXiv preprint arXiv:1808.06226, 2018.

Reference III

[8] Quoc V Le, Navdeep Jaitly, and Geoffrey E Hinton.
A simple way to initialize recurrent networks of rectified linear units.
arXiv preprint arXiv:1504.00941, 2015.

[9] Mike Schuster and Kaisuke Nakajima.
Japanese and korean voice search.
In *2012 IEEE international conference on acoustics, speech and signal processing (ICASSP)*, pages 5149–5152. IEEE, 2012.

[10] Rico Sennrich, Barry Haddow, and Alexandra Birch.
Neural machine translation of rare words with subword units.
arXiv preprint arXiv:1508.07909, 2015.

[11] Eduardo D Sontag.
On the computational power of neural nets'.
JOURNAL OF COMPUTER AND SYSTEM SCIENCES, 50:132–150, 1995.

Reference IV

[12] Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N Gomez, Łukasz Kaiser, and Illia Polosukhin.
Attention is all you need.
Advances in neural information processing systems, 30, 2017.

[13] Kelvin Xu, Jimmy Ba, Ryan Kiros, Kyunghyun Cho, Aaron Courville, Ruslan Salakhutdinov, Richard S Zemel, and Yoshua Bengio.
Show, attend and tell: Neural image caption generation with visual attention.
arXiv preprint arXiv:1502.03044, 2(3):5, 2015.