Introduction to Seq2Seq Modeling

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What are Sequence to Sequence Models?

- Generally used to convert one set of tokens into another
  - Many - to - Many RNN
- Bleak view: map a sequence of indexes to another independent set of indexes

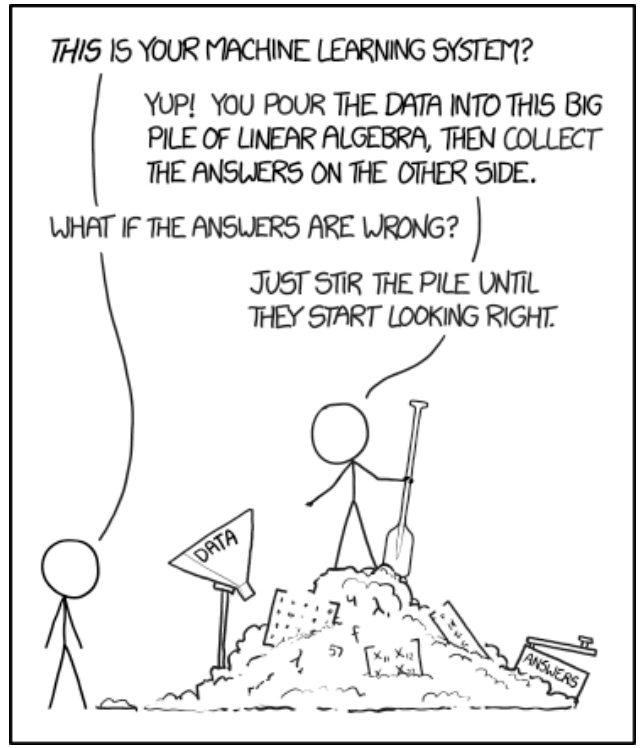


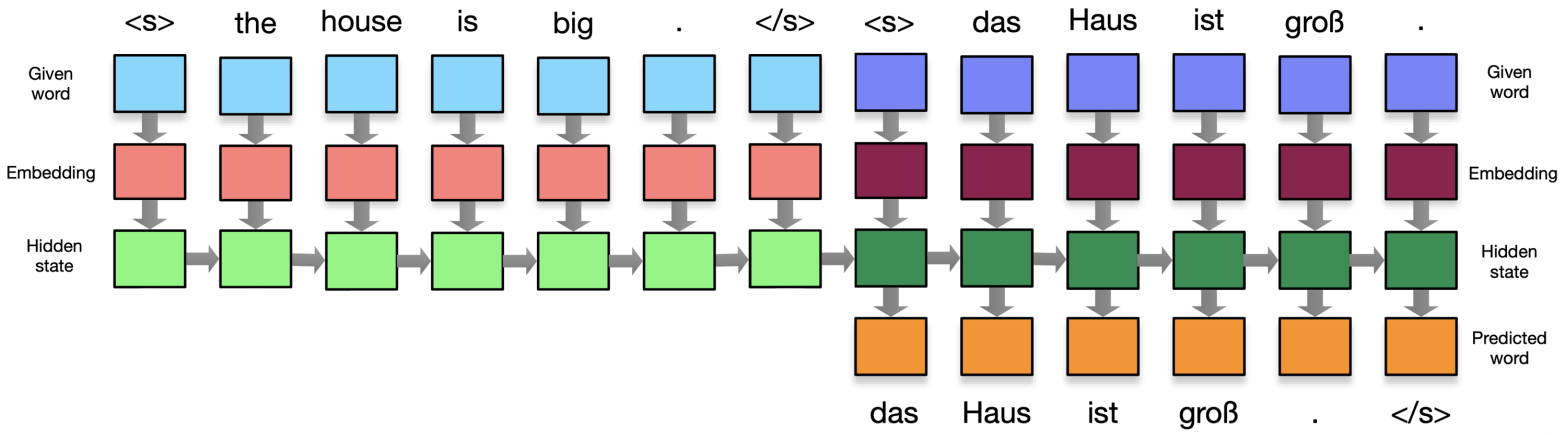
Figure: The pile gets soaked with data and starts to get mushy over time, so it's technically recurrent.

Encoder-Decoder Architecture

Overview: Encoders and Decoders

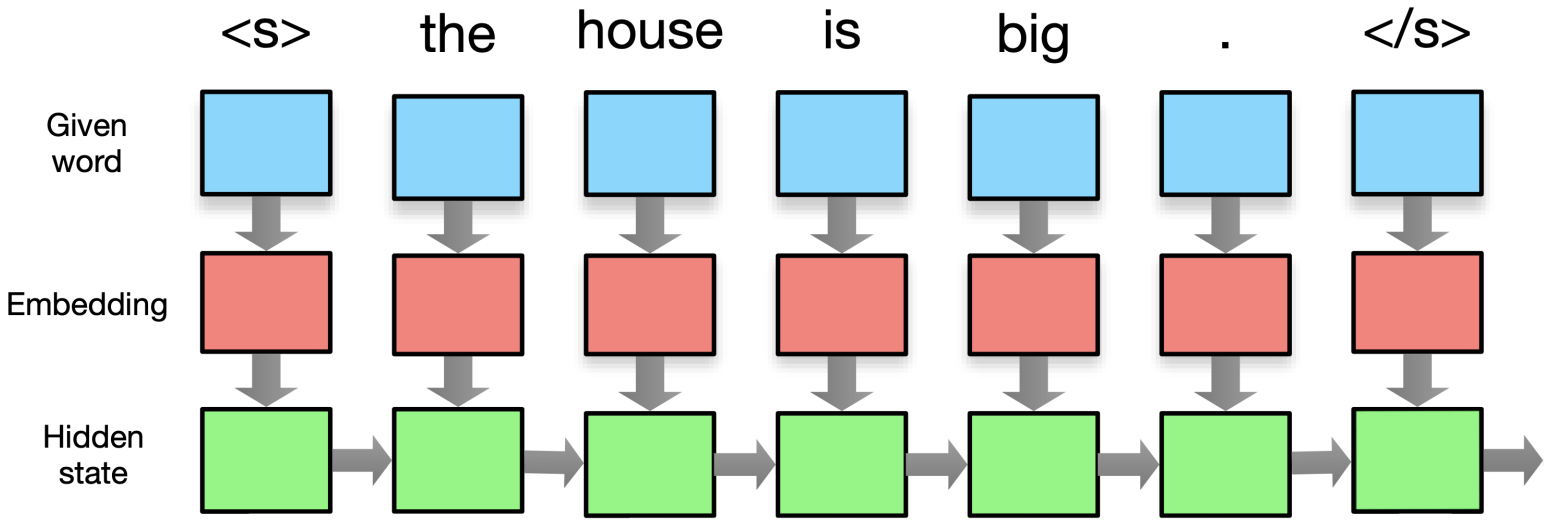
- We have 2 sub-networks: an **Encoder** and a **Decoder**
- Encoders
  - Give the source sentence meaning
- Decoders
  - Emit a variable-length sequence
- We will discuss how to connect the two for joint training

Overview: Encoders and Decoders



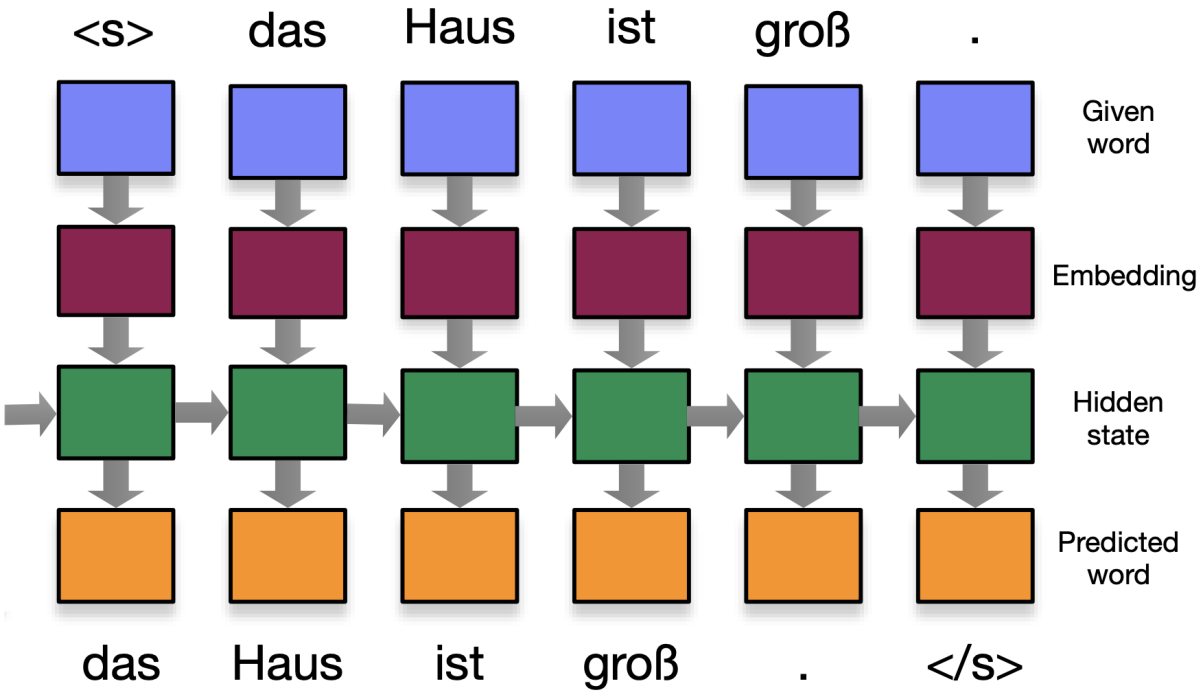
- Encapsulation allows for flexible design choices
- **Embeddings**
  - Pre-trained
  - DIY
- **Recurrent Layer**
  - Type
  - Depth
  - Directionality

What makes an Encoder?



- Recall: **Encoders** give the source sentence meaning
- Effectively a language model, without a layer to predict the next word
- Idea is to pass on the hidden state, and possibly use the encodings directly

What makes a Decoder?



- Recall: **Decoders** provide a new sequence conditioned on the Encoder's hidden state
- Starts with the Encoder's hidden state, and predicts one token at a time
- Re-feed the predicted token back into the decoder

Word Embeddings: Practical Considerations

Recap: Word Embeddings

$$
\begin{array}{rcl}
\texttt{the} & \rightarrow & \begin{bmatrix} 1.23 & -0.58 & 0.22 & -0.80 & 0.61 \end{bmatrix} \\
\texttt{cat} & \rightarrow & \begin{bmatrix} -1.10 & 1.23 & 0.17 & -0.21 & 1.43 \end{bmatrix} \\
\texttt{is} & \rightarrow & \begin{bmatrix} -0.26 & 0.70 & 0.27 & 0.59 & -1.04 \end{bmatrix} \\
\texttt{black} & \rightarrow & \begin{bmatrix} -1.13 & -0.81 & -0.53 & -0.59 & 0.26 \end{bmatrix}
\end{array}
$$

- A trick to map tokens to vector representations

Recap: Pretrained Word Embeddings

- Co-occurence Matrix
- Pointwise Mutual Information
- SVD Co-occurence
- Ngram
- CBOW, Skip Gram
- GloVe
- Sentence Embeddings: ELMo

DIY Embeddings

- We can always train our own!

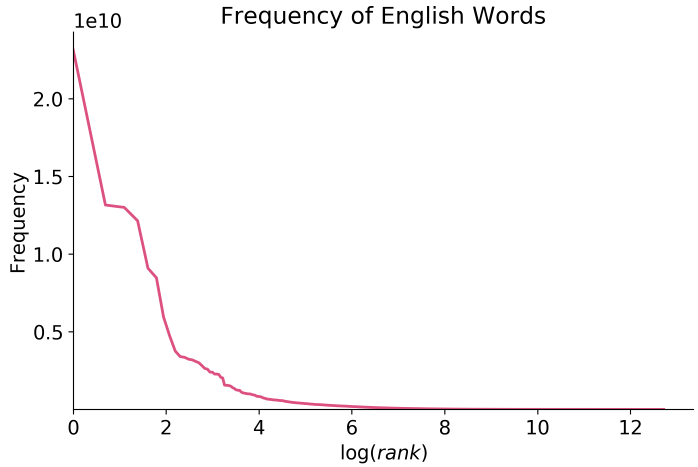
Special Tokens for Sequence Modeling

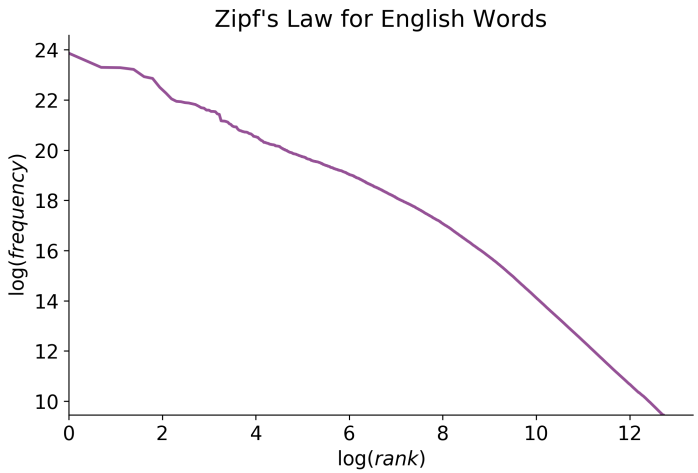
- ⟨PAD⟩ → Padding / Masking
- ⟨UNK⟩ → Unknown words
- ⟨SOS⟩ → Start of Sentence
- ⟨EOS⟩ → End of Sentence

⟨SOS⟩	Data	Science	is	the	⟨UNK⟩	!	⟨EOS⟩
⟨SOS⟩	I	⟨UNK⟩	for	S&P	.	⟨EOS⟩	⟨PAD⟩
⟨SOS⟩	Hello	World	!	⟨EOS⟩	⟨PAD⟩	⟨PAD⟩	⟨PAD⟩

Mangaging the Vocab Size

- Languages are unevenly distributed
- Many rare words, names $\rightarrow$ inflates the size of the vocabulary
- **Problem:**
  - Large embedding matrices for source, target language
  - Large output layers for prediction and softmax
- Naive Solution: Limit the vocab size to most frequent





Morphology, Compounding, and Transliteration

- Morphological Analysis

  tweet, *tweets*, *tweeted*, *tweeting*, *retweet*, ...

- Compound Splitting
  - homework $\rightarrow$ home·work
  - website $\rightarrow$ web·site
- Names, Places, Proper Nouns
  - Hoboken, Baltimore, Obama, Michelle
  - Can do Transliteration

Handling Numbers

- Do we really need to encode every number? **NO!**

`I pay 950.00 in May 2007` $>$ `I pay 2007 in May 950.00`

Handling Numbers

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  `I pay` 950.00 `in May` 2007 $>$ `I pay` 2007 `in May` 950.00

- **Solution 1:** Replace with a ⟨NUM⟩ token, but

  `I pay` ⟨NUM⟩ `in May` ⟨NUM⟩ $=$ `I pay` ⟨NUM⟩ `in May` ⟨NUM⟩

Handling Numbers

- Do we really need to encode every number? **NO!**

  I pay 950.00 in May 2007 > I pay 2007 in May 950.00

- **Solution 1:** Replace with a ⟨NUM⟩ token, but

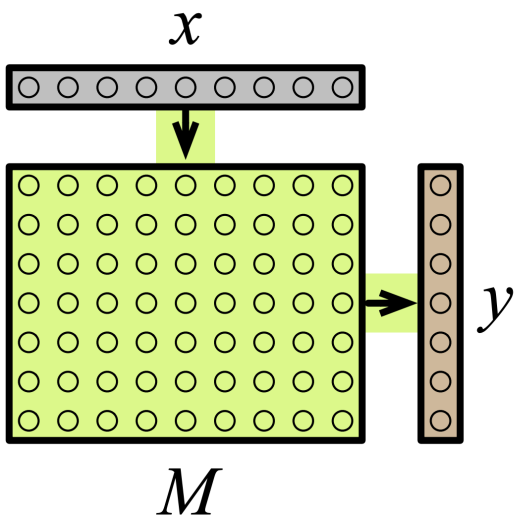
  I pay ⟨NUM⟩ in May ⟨NUM⟩ = I pay ⟨NUM⟩ in May ⟨NUM⟩

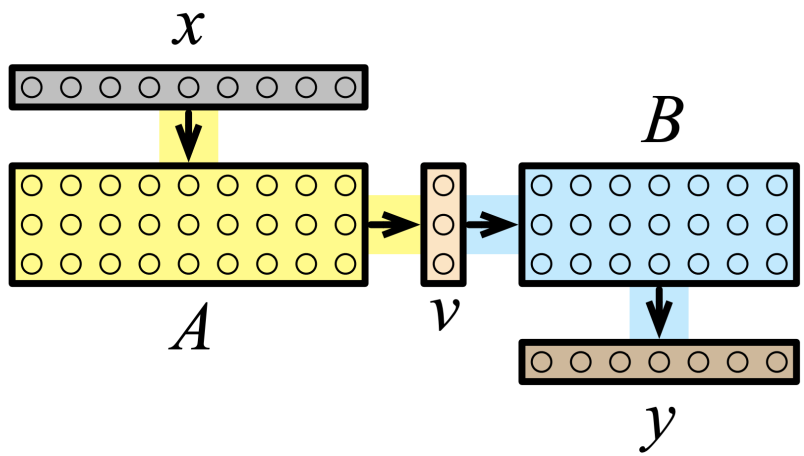
- **Solution 2:** Replace each digit with a unique symbol, e.g. 5

I pay 555.55 in May 5555 > I pay 5555 in May 555.55

- This reduces the need for embeddings, when we can simply do transliteration

Factored Decomposition





- **Problem:** Large input and output vectors
  - $|x| = 20,000$, $|y| = 50,000 \rightarrow |M| = 1,000,000,000$
- **Solution:** Use a bottleneck with smaller matrices A, B
  - $|v| = 100 \rightarrow |A| = 2,000,000$, $|B| = 5,000,000$
  - Total Parameters: $7,000,000$

Character-Based Models

- Instead use embeddings for character string
  `b e a u t i f u l`
- Idea is to induce embeddings for unseen morphological variants:
  `beautiful`
- Tokens are single characters, symbols, whitespace

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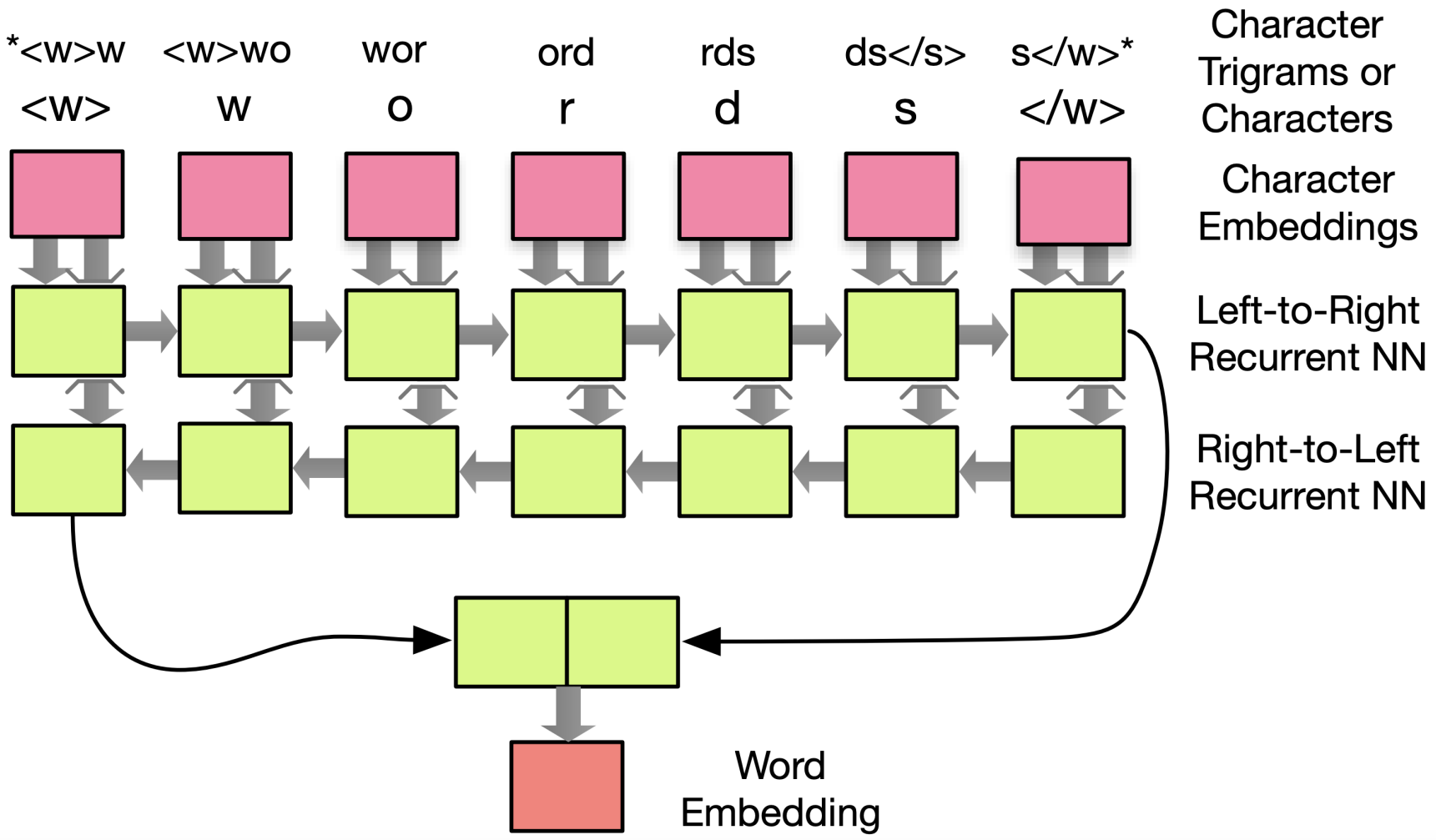
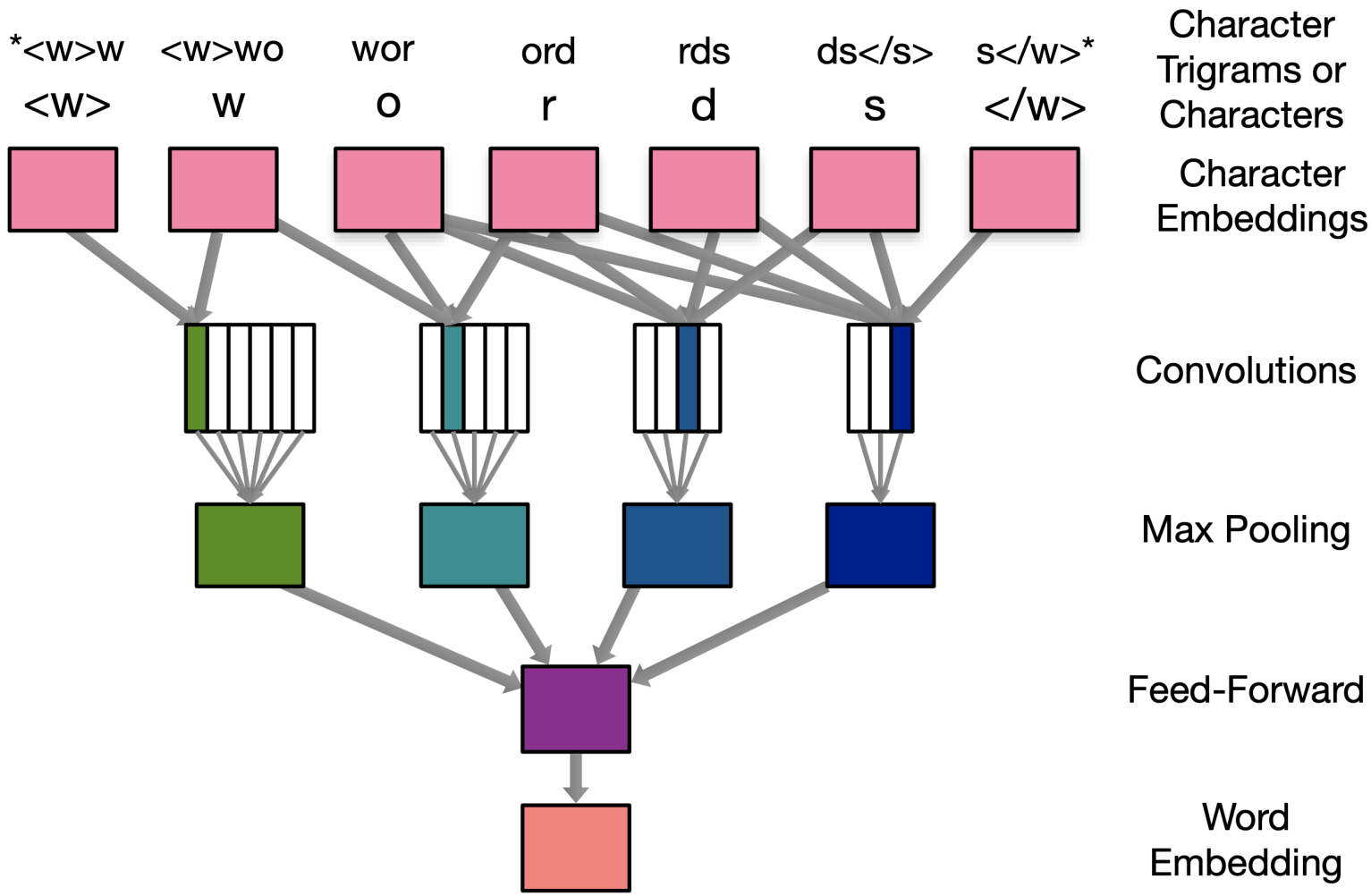
- Instead use embeddings for character string
  `b e a u t i f u l`
- Idea is to induce embeddings for unseen morphological variants:
  `beautiful`
- Tokens are single characters, symbols, whitespace
- Generally poor performance

Character-Based Models



Character-Based Models



BPE Subwords

t h e · f a t · c a t · i s · i n · t h e · t h i n · b a g

t h → th	th e · f a t · c a t · i s · i n · th e · th i n · b a g
a t → at	th e · f at · c at · i s · i n · th e · th i n · b a g
i n → in	th e · f at · c at · i s · in · th e · th in · b a g
th e → the	the · f at · c at · i s · in · the · th in · b a g

- Breaks words into subwords
  - Starts with the character set
  - Merges the most frequent pairs, one per iteration
- Unsupervised (accidental) morphology (frequency suffixes)

BPE Tokenization on HHGTTG

- Unique Characters: 101
- Unique BPE Tokens (1K iterations): 1,093
- Unique BPE Tokens (5K iterations): 4,817
- Unique Tokens: 9,541

```
there is a the@@ ory which st@@ at@@ es that if ever any@@ one
di@@ sc@@ o@@ ver@@ s ex@@ ac@@ tly what the universe is for
and why it is here , it will in@@ stan@@ tly di@@ s@@ ap@@ pe@@ ar
and be re@@ pl@@ ac@@ ed by something even more bi@@ zar@@ re
and in@@ ex@@ p@@ li@@ c@@ able .
there is another the@@ ory which st@@ at@@ es that
this has al@@ re@@ ad@@ y happ@@ ened .
in the beg@@ in@@ ning the universe was cre@@ ated .
this has made a lot of people very an@@ gr@@ y and
been wi@@ de@@ ly re@@ gar@@ ded as a b@@ ad mo@@ ve .
```

Modeling Recurrent Relations

Vanilla RNNs

$$h_t = \tanh\left(\overbrace{W_{ih}x_t + b_{ih}}^{input} + \underbrace{W_{hh}h_{t-1} + b_{hh}}_{hidden}\right)$$

- h_t is the hidden state at time t
- x_t is the input at time t
- h_{t-1} is the previous hidden state
- h_0 is initialized to $\mathbf{0}$

Long Short Term Memory (LSTM)

$$
\begin{aligned}
\text{Gates} \rightarrow & \begin{cases}
i_t = \sigma(W_{ii} x_t + b_{ii} + W_{hi} h_{t-1} + b_{hi}) \\
f_t = \sigma(W_{if} x_t + b_{if} + W_{hf} h_{t-1} + b_{hf}) \\
o_t = \sigma(W_{io} x_t + b_{io} + W_{ho} h_{t-1} + b_{ho}) \\
g_t = \tanh(W_{ig} x_t + b_{ig} + W_{hg} h_{t-1} + b_{hg})
\end{cases} \\
\text{Outputs} \rightarrow & \begin{cases}
c_t = f_t \odot c_{t-1} + i_t \odot g_t \\
h_t = o_t \odot \tanh(c_t)
\end{cases}
\end{aligned}
$$

- h_t is the hidden state at time t
- c_t is the cell state at time t
- x_t is the input at time t

Gated Recurrent Units (GRU)

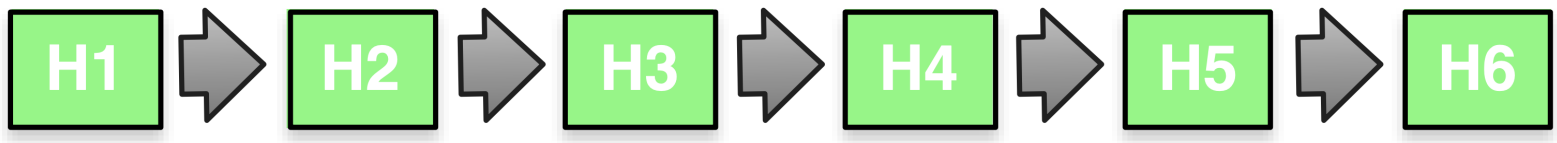
$$\text{Gates} \rightarrow \begin{cases} r_t = \sigma(W_{ir} x_t + b_{ir} + W_{hr} h_{(t-1)} + b_{hr}) \\ z_t = \sigma(W_{iz} x_t + b_{iz} + W_{hz} h_{(t-1)} + b_{hz}) \\ n_t = \tanh(W_{in} x_t + b_{in} + r_t \odot (W_{hn} h_{(t-1)} + b_{hn})) \end{cases}$$

$$\text{Outputs} \rightarrow \begin{cases} h_t = (1 - z_t) \odot n_t + z_t \odot h_{(t-1)} \end{cases}$$

- h_t is the hidden state at time t
- x_t is the input at time t

Aside: Different Perspectives on Deep Recurrent Models

- So far we've only seen Left to Right Sequencing



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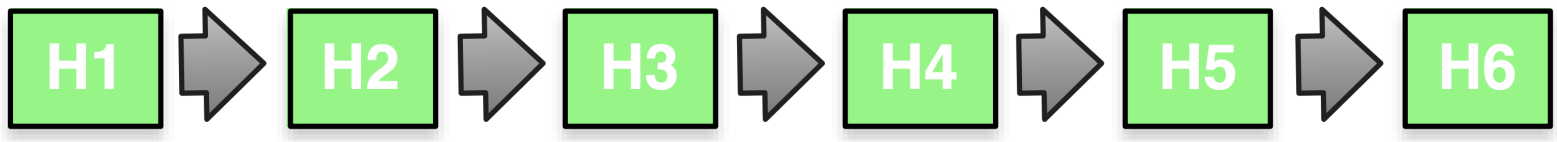
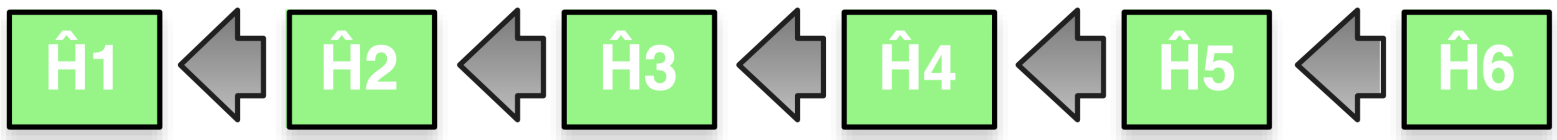


- Why not Right to Left?



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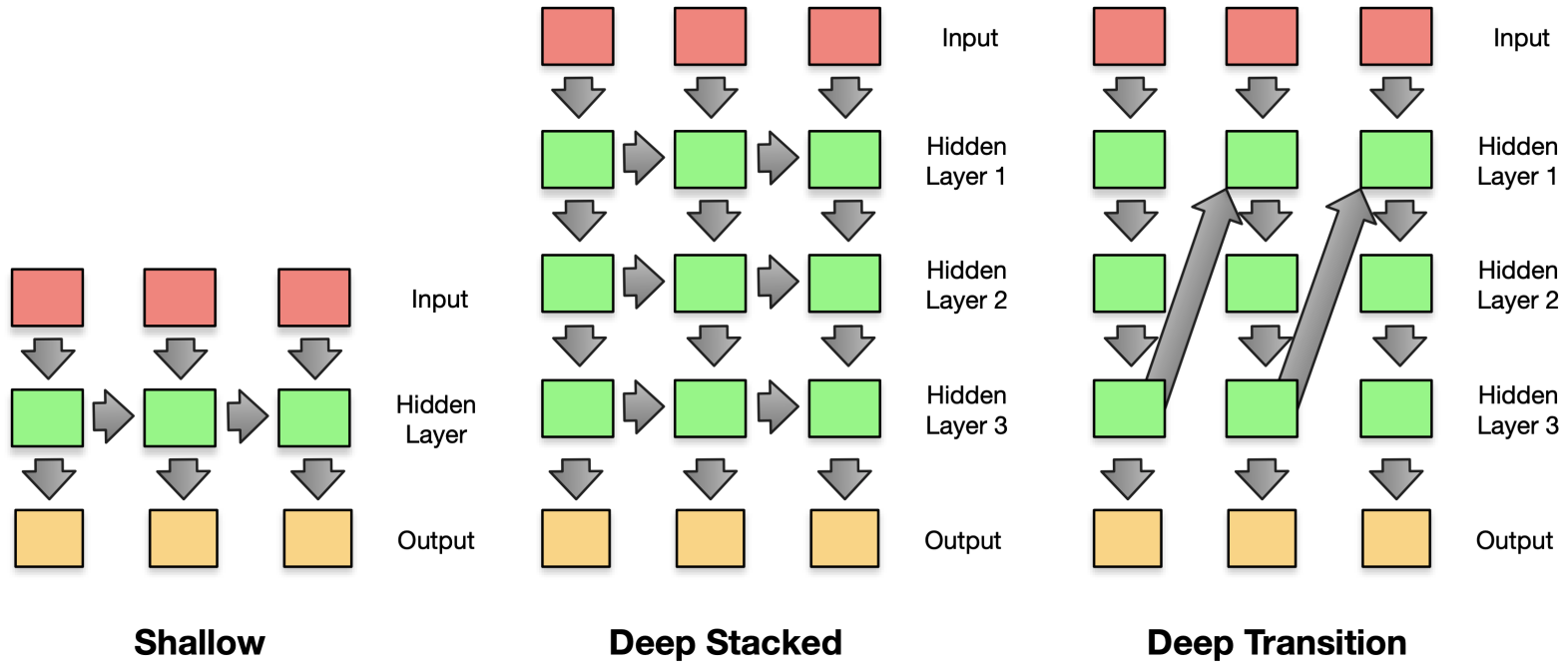
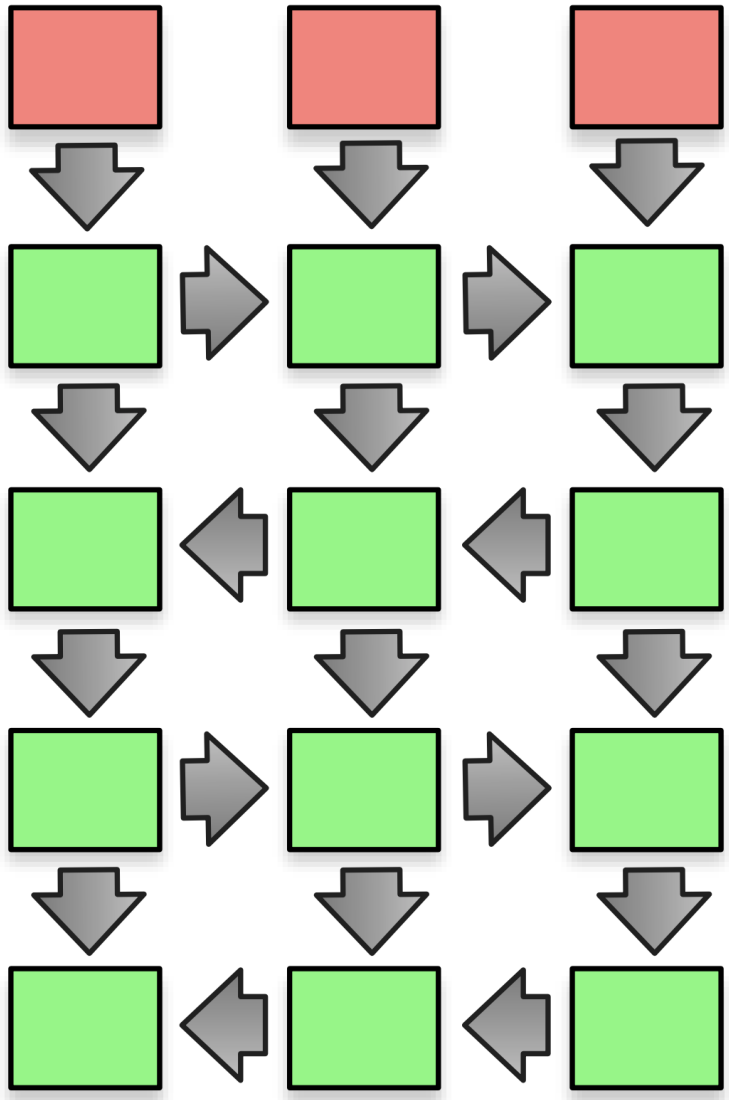
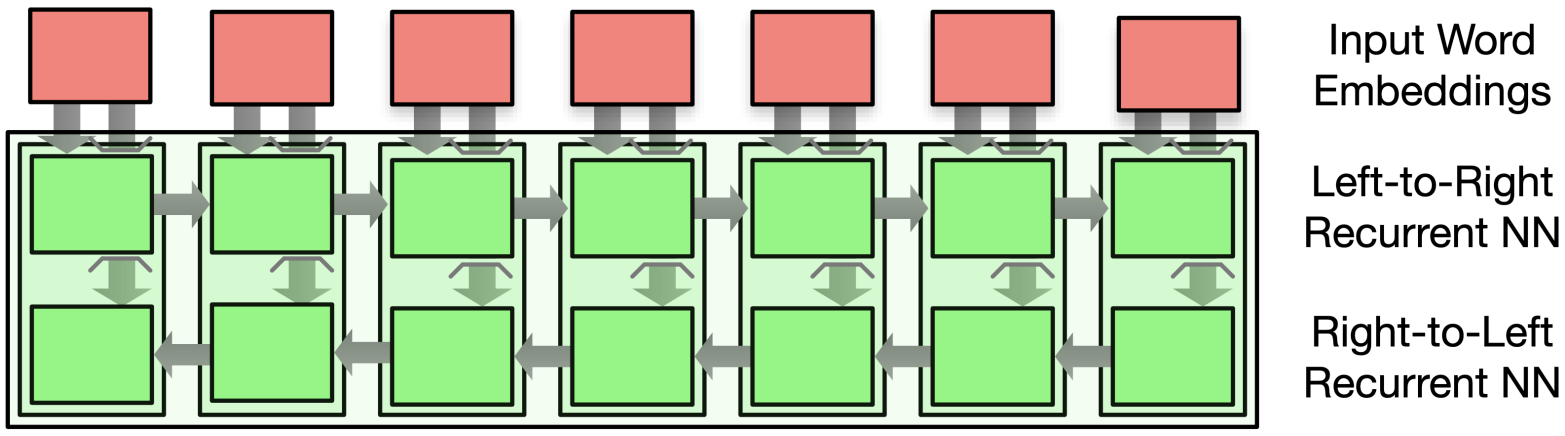


- Experiment with different stacking techniques

Alternating Recurrent Directions



Bidirectional Sequence Modeling



- Can capture both left and right context
- Implementation usually concatenates RNN states

Aside: Dimensionality of Inputs and Outputs

Type	RNN	LSTM	GRU
In	B, L, H_{in}	B, L, H_{in}	B, L, H_{in}
h_{t-1}	$B, N_L \cdot N_D, H_{out}$	$B, N_L \cdot N_D, H_{out}$	$B, N_L \cdot N_D, H_{out}$
c_{t-1}	-	$B, N_L \cdot N_D, H_{out}$	-
h_t	$B, N_L \cdot N_D, H_{out}$	$B, N_L \cdot N_D, H_{out}$	$B, N_L \cdot N_D, H_{out}$
c_t	-	$B, N_L \cdot N_D, H_{out}$	-
Out	$B, L, N_D \cdot H_{out}$	$B, L, N_D \cdot H_{out}$	$B, L, N_D \cdot H_{out}$

- B is the batch size
- L is the sequence length
- N_D is the number of directions
- N_L is the number of layers
- H_{in}, H_{out} are the input and hidden size

Aside: The Influence of Padding in RNNs

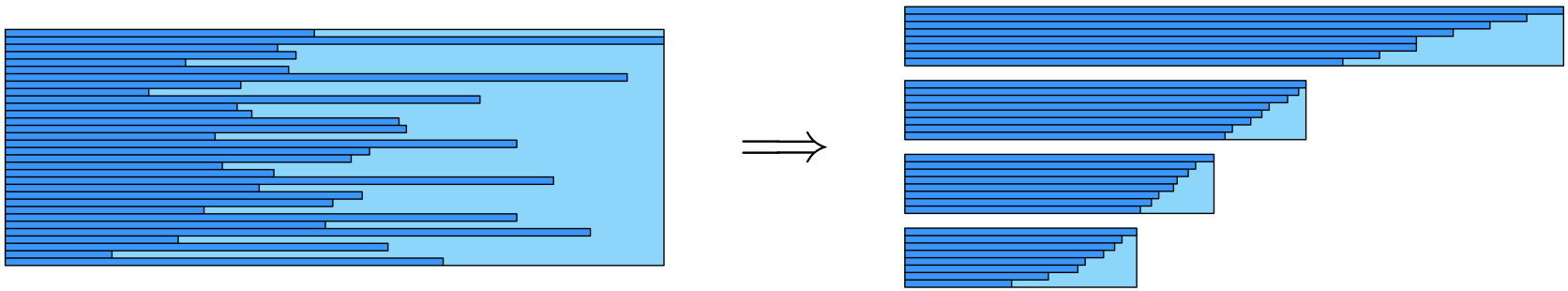
- Assume the embedding $E[\langle \text{PAD} \rangle] = \mathbf{0}$
- Are we safe?

Aside: The Influence of Padding in RNNs

- Assume the embedding $E[\langle \text{PAD} \rangle] = \mathbf{0}$
- Are we safe? **NO!**
- Because of the bias term, zero input does not result in a zero output
  - This alters the hidden state being passed onto the next iteration
- Don't even think about the mess bidirectionals become...
- **Question:** Does this mean we learn the amount of padding for a given sequence?

Training Considerations

Increasing Throughput through Batching



- We can pad sentences of different lengths to increase batch size
- While also minimizing the use of padding
- Matrix Operations are faster

Teacher Forcing

- Instead of refeeding the predicted token, replace it with the true token randomly
- This is only done during training, not inference

$$y_{i+1} = \begin{cases} \text{argmax}_j \, \theta_i & \mathcal{U}(0,1) < \text{TF} \\ t_{i+1} & \textit{else} \end{cases}$$

- t_{i+1} is the true token
- TF is the teacher forcing ratio

Cross Entropy and Label Smoothing

$$\ell(\mathbf{x}, y_i) = -\log\left(\frac{\exp x_{y_i}}{\sum_j \exp x_j}\right)$$
$$= -\underbrace{x_{y_i}}_{max} + \underbrace{\log \sum_j \exp x_j}_{min}$$

- Softmax and Cross-Entropy loss assign all the probability mass to a single word
  - LogSumExp is minimized on confident predictions
- Solution: smooth the distribution

Cross Entropy and Label Smoothing

- Softmax

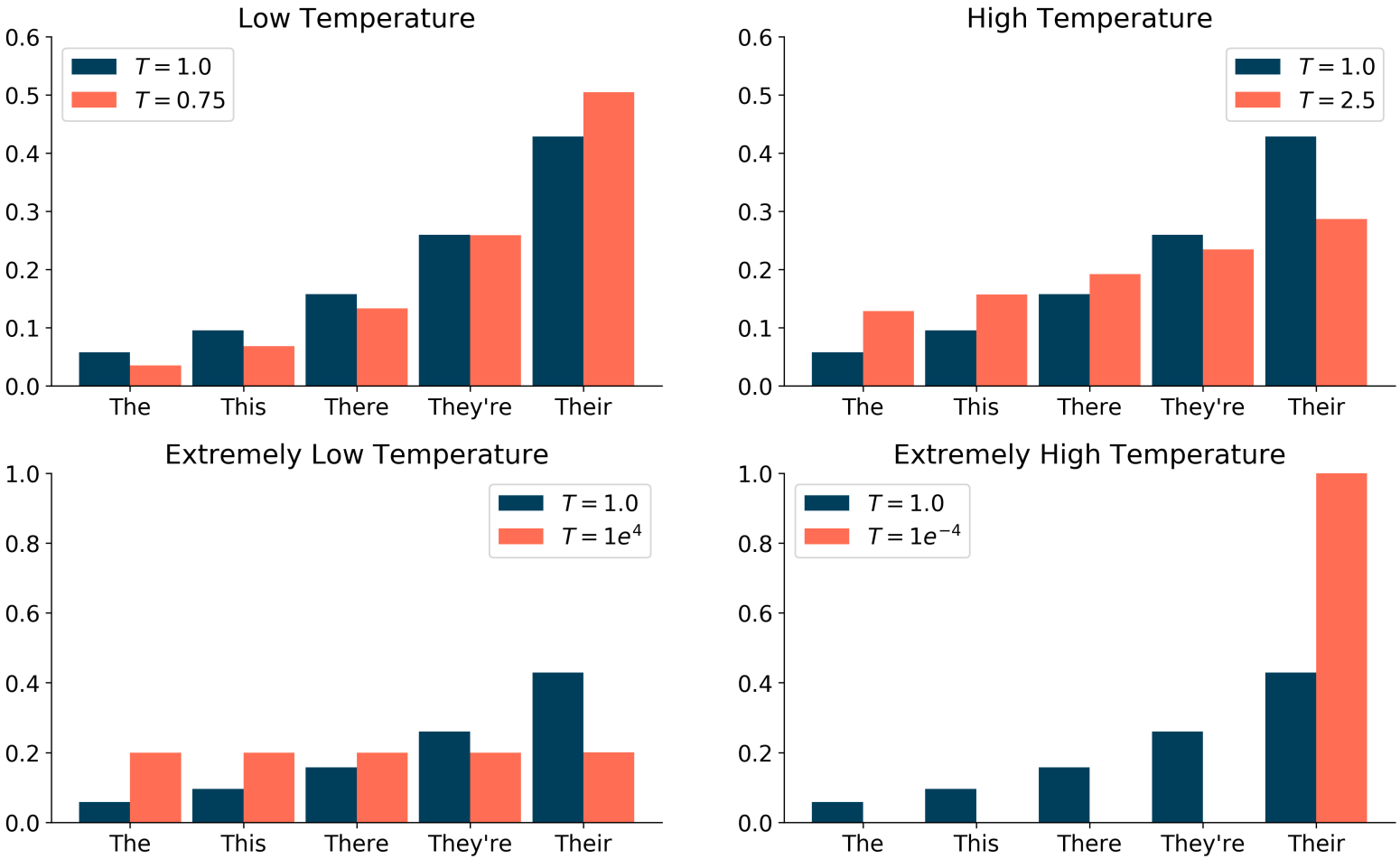
$$p(y_i) = \frac{\exp x_{y_i}}{\sum_j \exp x_j}$$

- Smoothed Softmax with Temperature T

$$p(y_i) = \frac{\exp\left(x_{y_i}/T\right)}{\sum_j \exp\left(x_j/T\right)}$$

- As $T \to \infty$, the distribution is smoother, uniform
- AS $T \to 0$, the distribution approaches a kronecker delta centered on the class with the most mass
- **Question:** Why do we divide instead of adding/subtracting?

Visualizing Temperature



Monte Carlo Decoding

- Recall how we select the next token:
  - **Greedy:** Top token weight
  - **Teacher Forcing:** Randomly select the true token
- Note that the outputs are a distribution over the target vocabulary
- **Use these weights in a multinomial to randomly select a continuation**

$$y_{i+1} \sim \text{Multinomial}\left(\theta_i\right)$$

Different Token Decoding Schemes

- **Greedy:**

$$y_{i+1} = \underset{j}{\text{argmax}}\, \theta_i$$

- **Teacher Forcing:**

$$y_{i+1} = \begin{cases} \text{argmax}_j\, \theta_i & \mathcal{U}(0,1) < \text{TF} \\ t_{i+1} & \textit{else} \end{cases}$$

- **Monte Carlo:**

$$y_{i+1} \sim \text{Multinomial}\,(\theta_i)$$

- θ_i are the output weights from the Decoder
- t_{i+1} is the true token at position $i+1$
- TF is the teacher forcing ratio

Masked Loss

- Remember, we don't care what gets predicted after seeing a ⟨EOS⟩
- Hence, we need to mask out the loss for predicted tokens associated with ⟨PAD⟩

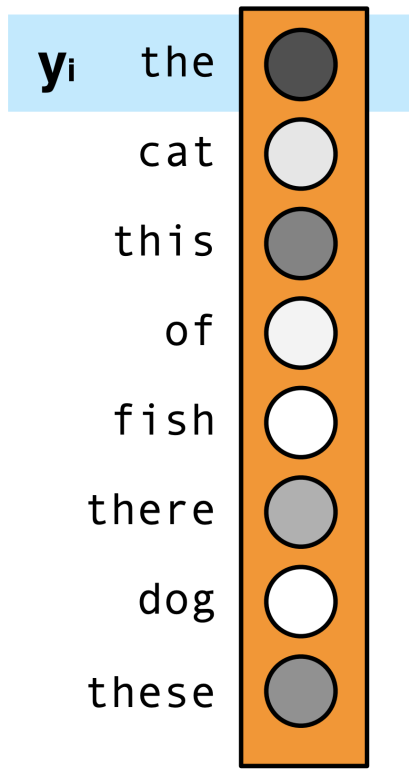
pred	→	*le*	*le*	*chat*	*chat*	*chat*	*chat*
		↓	↓	↓	↓	↓	↓
		ℓ	ℓ	ℓ	ℓ	ℓ	0
		↑	↑	↑	↑	↑	↑
true	→	*le*	*chat*	*est*	*noir*	⟨EOS⟩	⟨PAD⟩

- **Solution:** Zero out elements by either:
  - Multiply pad outputs by 0
  - Specify the label to ignore in Cross Entropy call

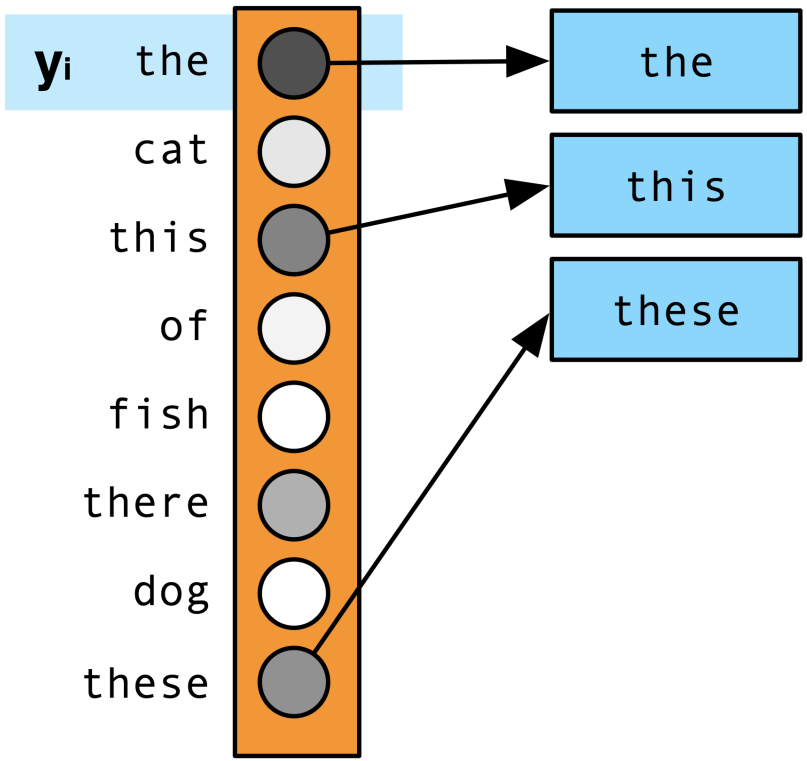
$$\ell(\mathbf{x}, y_i) = \mathbb{1}_{\{y_i \neq \langle \text{PAD} \rangle\}} \cdot \left(-x_{y_i} + \log \sum_j \exp x_j \right)$$

Decoding: Making better Translations

Beam Search



Beam Search



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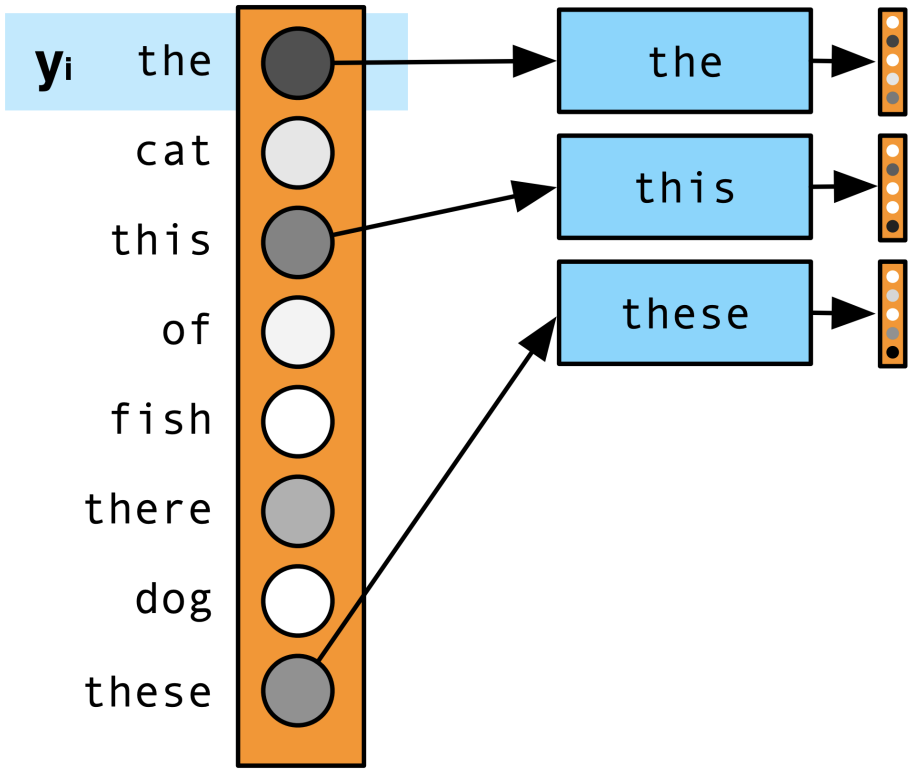

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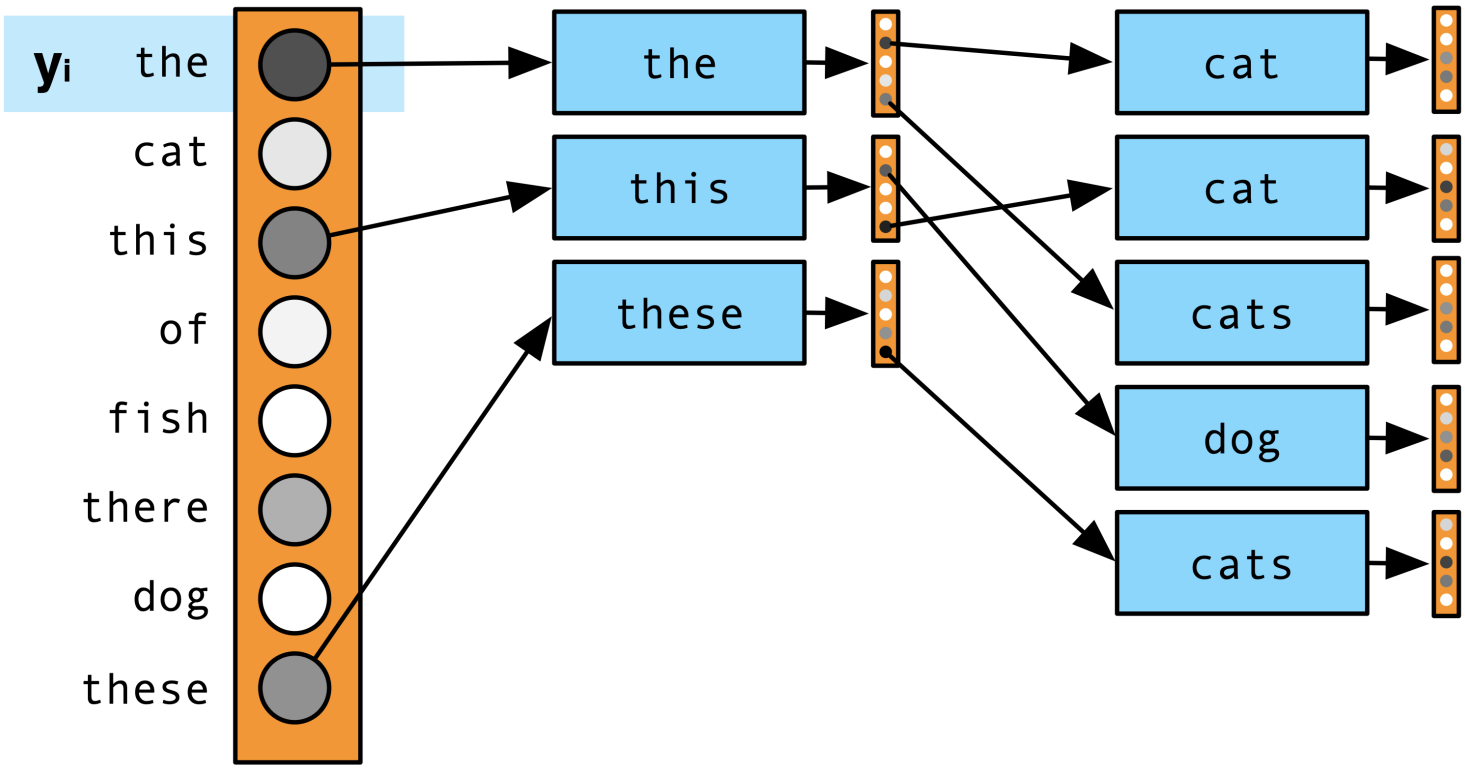
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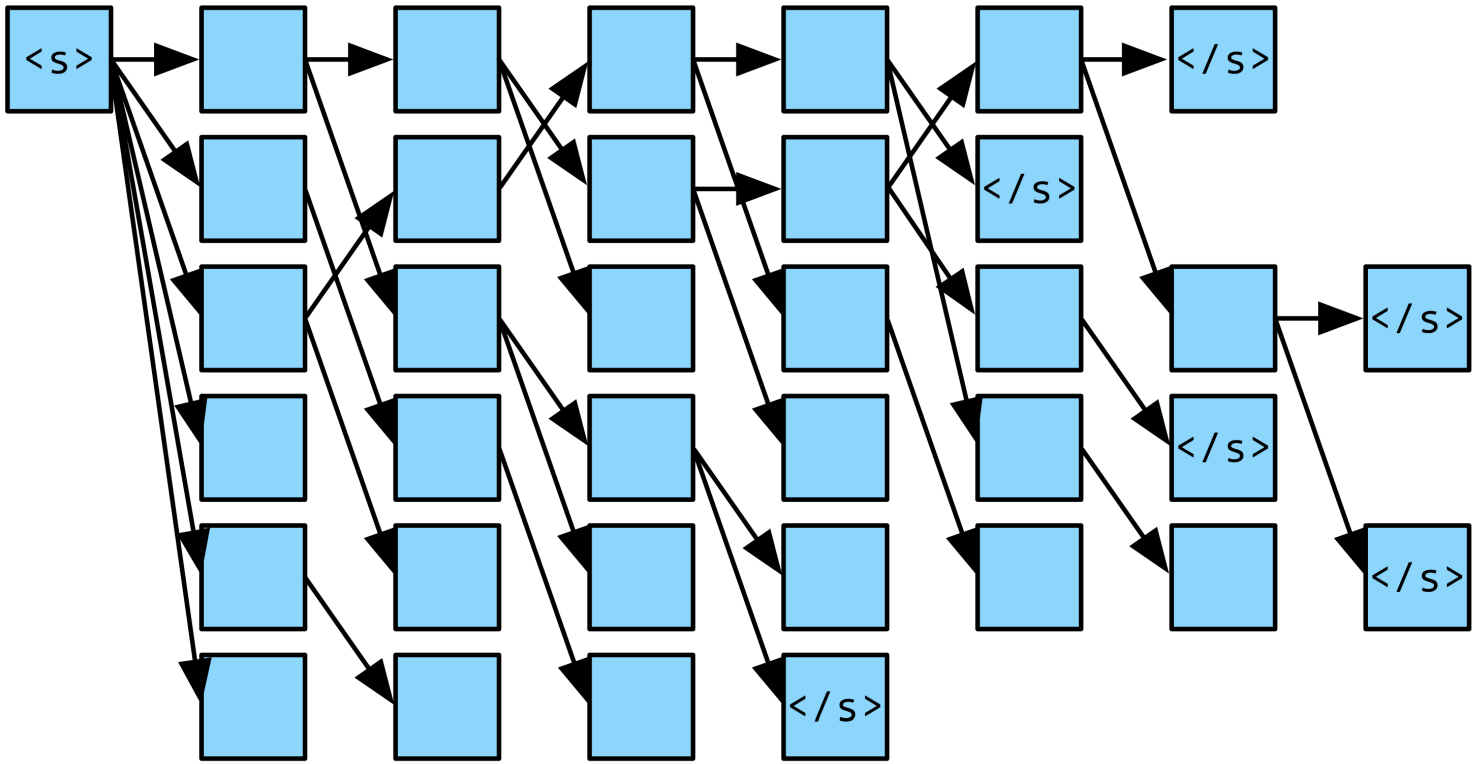
Beam Search



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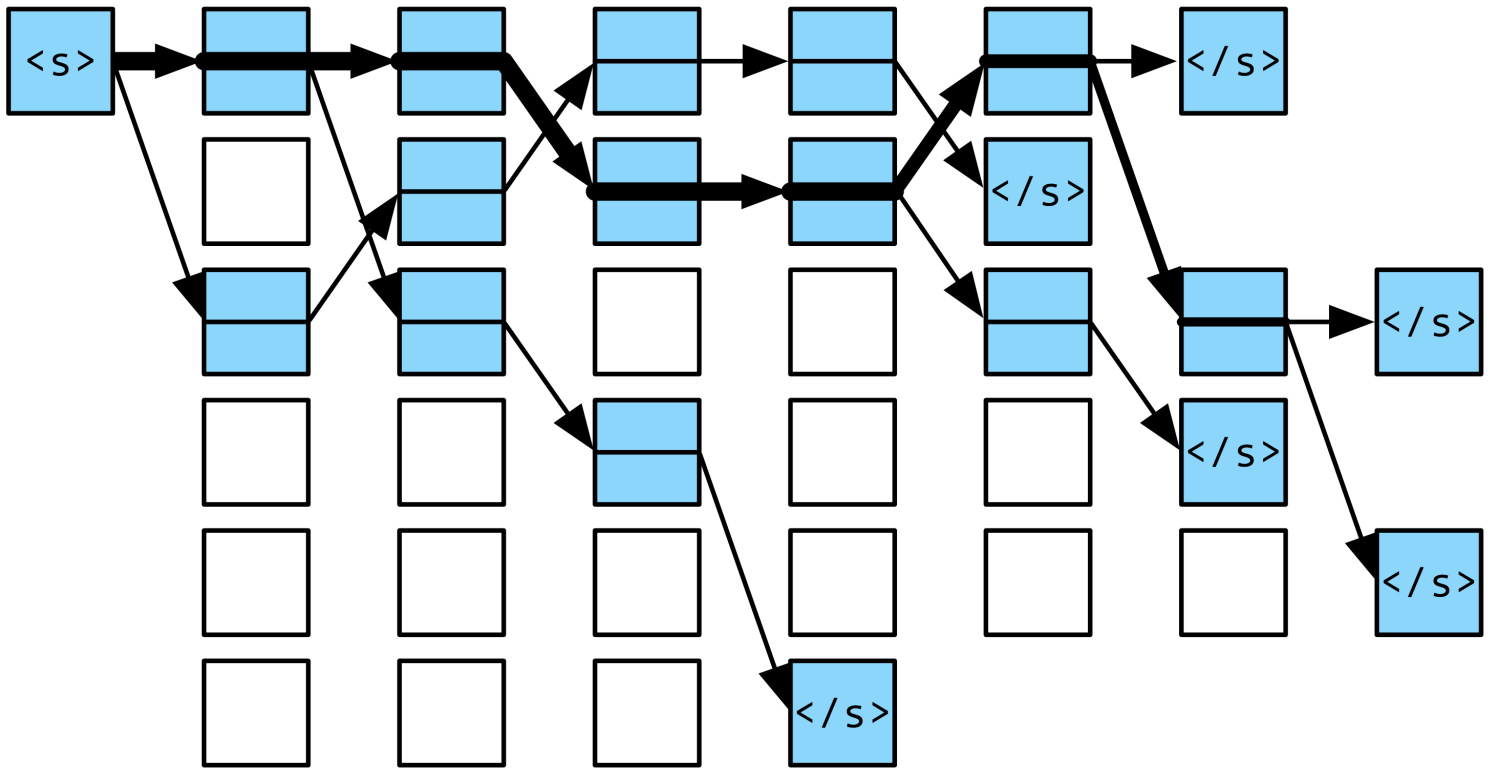
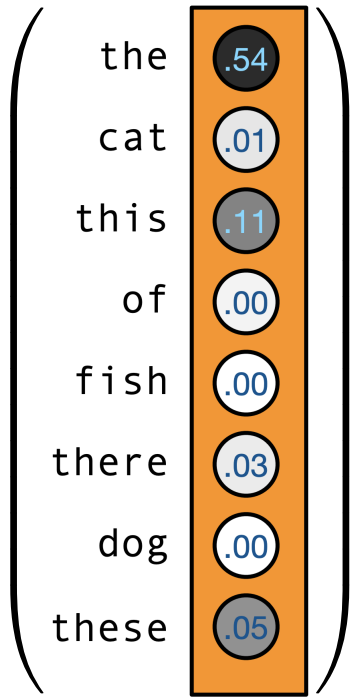


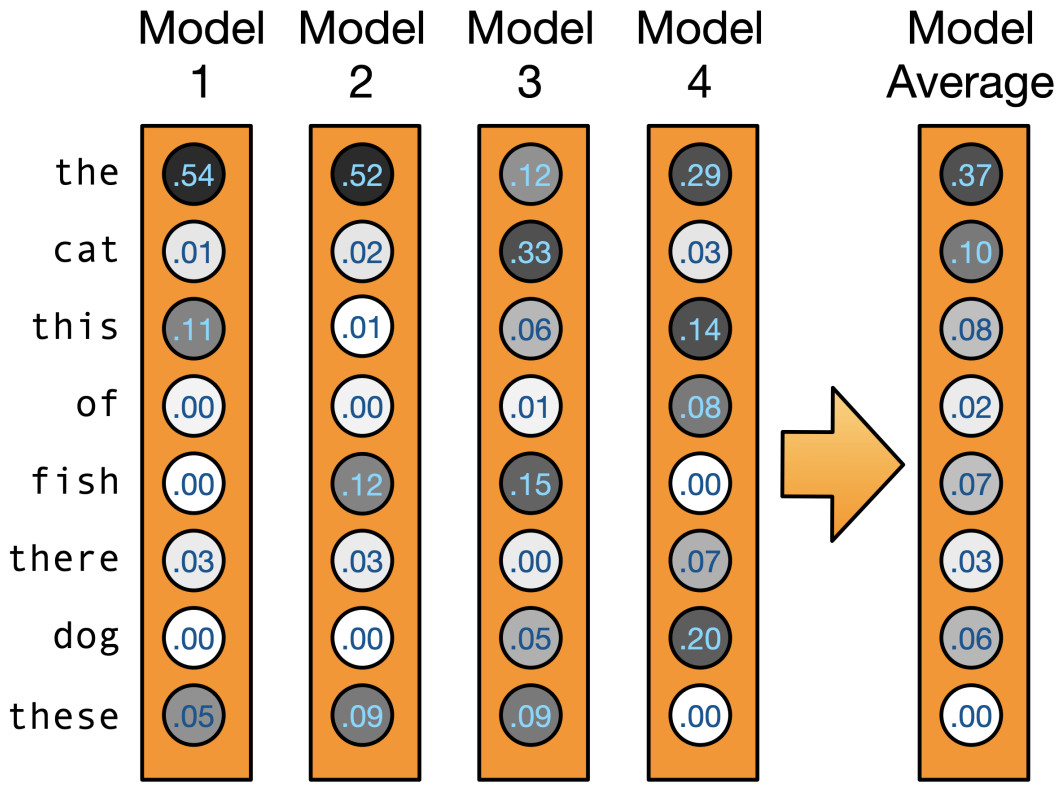
Monte Carlo Beam Search

$$y_{i+1} \sim \text{Multinomial}$$



- Why not sample n words based on their probabilities?
- Adds more diversity to beam search results

Ensembling



- Why not average different models?
- Random initialization leads to different local solutions
- Could also use model dumps from different iterations

Applications

Recall: Encoders, Decoders, and Seq2Seq Models

- **Encoders** given a sequence meaning
- **Decoders** generate a new sequence
- **Seq2Seq** generate sequences conditioned on another sequence

What to use for which application?

- **Encoders**
  - POS Tagging
  - Sentence Embeddings
  - Anything where you are given the sentence at test time
- **Decoders**
  - Text Generation
  - Language Modeling
  - Anything where you need to create a sequence at test time
- **Seq2Seq**
  - Translation
  - Speech Recognition
  - Summarization
  - Question/Answering
  - Anything where you convert a sequence into another sequence

Bill's Application: Column Segmention

Problem Statement: Column Segmentation

Year Ended December 31	Totals
2018	$ 155,458.46
2019	155,458.46
2020	155,458.46
2021	155,458.46
2022	155,458.46
2023-2026	505,870.61
	1,283,162.91
Less imputed interest	(174,862.64)
Net Present Value of Minimum Lease Payments	1,108,300.27
Less: Current Maturities	(118,236.87)
Long-Term Capital Lease Obligations	$ 990,063.40

→

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Lease Payments	1,108,300.27
Less: Current Maturities	-118,236.87
Long-Term Capital Lease Obligations	$990,063.40

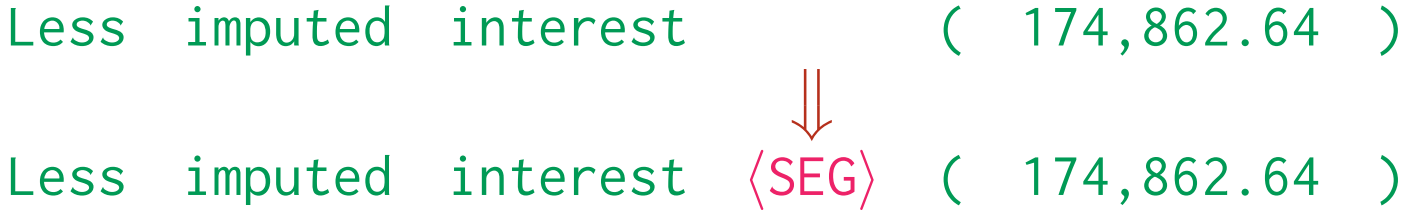
- Given a sequence of text, can we predict where to insert columns?

Issue: Vocabulary Size

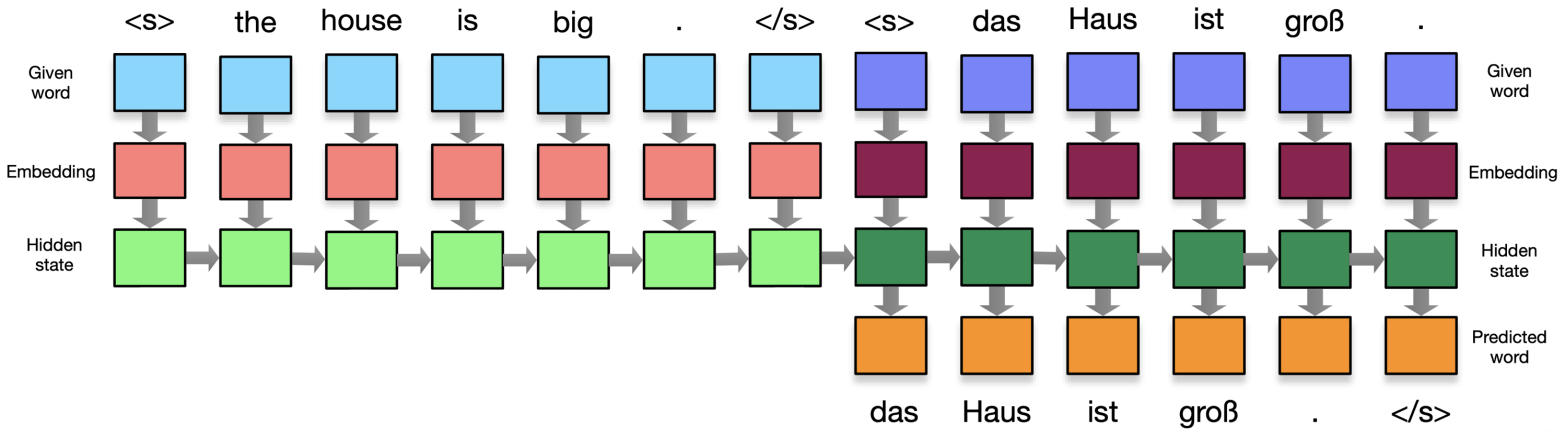
- Is the text actually important?
- Over 10K unique tokens, mostly numbers
- **Solutions:**
  - Token $\rightarrow$ Part-of-Speech
  - Numeric Value $\rightarrow \langle \text{NUM} \rangle$
- Reduces vocabulary size to 21 tokens

Regular Seq2Seq

- Translation Task
- Given a sequence of tokens
- Translate into the same set of tokens, but with a special ⟨SEG⟩ token



Seq2Seq Architecture




```
Seq2Seq(
  (encoder): Encoder(
    (embedding): Embedding(21, 256)
    (gru): GRU(256, 128, num_layers=2, batch_first=True)
  )
  (decoder): Decoder(
    (embedding): Embedding(22, 256)
    (gru): GRU(256, 128, num_layers=2, batch_first=True)
    (fc): Linear(in_features=128, out_features=22, bias=True)
  )
)
The model has 508,438 trainable parameters
```

Seq2Seq: Sample Results

```
>  num num num punct
=  num ⟨SEG⟩ num ⟨SEG⟩ num ⟨SEG⟩ punct
<  num ⟨SEG⟩ num ⟨SEG⟩ num ⟨SEG⟩ punct

>  adj num num num
=  adj ⟨SEG⟩ num ⟨SEG⟩ num ⟨SEG⟩ num
<  adj ⟨SEG⟩ num ⟨SEG⟩ num ⟨SEG⟩ num num num num num

>  verb noun noun noun noun noun verb
=  verb ⟨SEG⟩ noun noun ⟨SEG⟩ noun noun noun ⟨SEG⟩ verb
<  verb noun ⟨SEG⟩ ⟨SEG⟩ noun noun noun noun ⟨SEG⟩ noun ···
```

Secondary Approach: Throw away the decoder

- Just use an encoder, with an output layer
- For every token, predict if we should insert a ⟨SEG⟩
- No longer have to learn the actual sequence

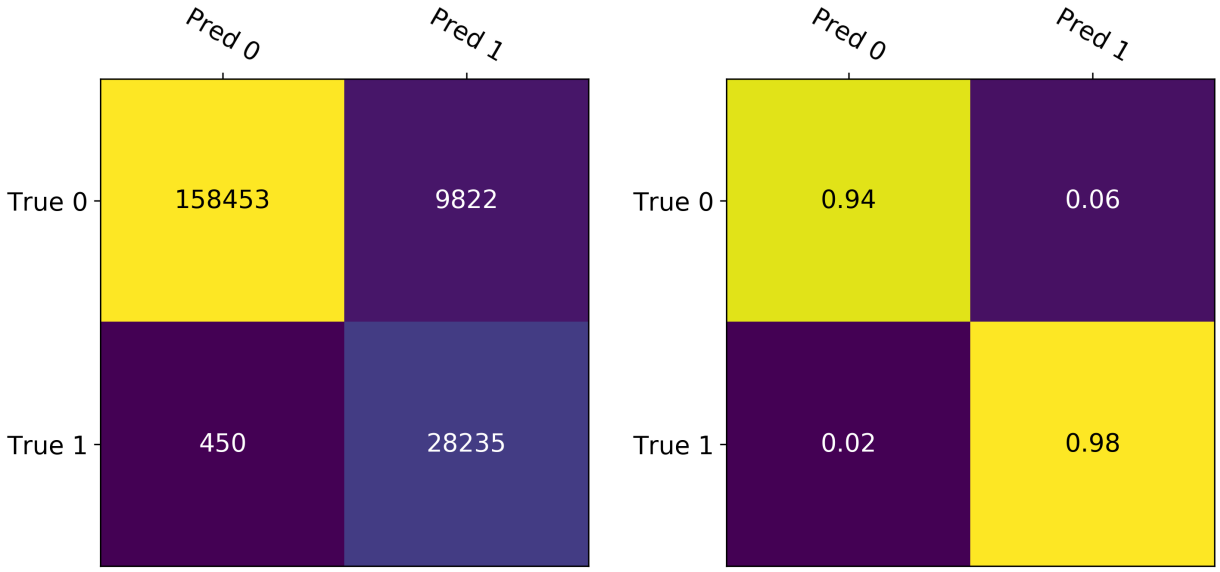
```
Classifier(
  (encoder): Encoder(
    (embedding): Embedding(21, 256)
    (gru): GRU(256, 128, num_layers=2, batch_first=True, bidirectional=True)
  )
  (linear): Linear(in_features=256, out_features=1, bias=True)
)
The model has 598,529 trainable parameters
```

Secondary Approach: Training Labels

- Labels are now binary vectors, where $x_i = 1$ implies that there is a ⟨SEG⟩ between x_i and x_{i+1}

```
Less  imputed  interest          (  174,862.64  )
 0       0         1             0       0       0
Less  imputed  interest  ⟨SEG⟩   (  174,862.64  )
```

Secondary Approach: Sample Results



	Precision	Recall	F1-Score	Support
Label: 0	1.00	0.94	0.97	168,275
Label: 1	0.74	0.98	0.85	28,685
accuracy			0.95	196,960
macro avg	0.87	0.96	0.91	196,960
weighted avg	0.96	0.95	0.95	196,960

Future Plans

- Features
  - Use segment location information
  - Tesseract gives bounding box information
- Encoder Structure
  - Convolution
  - Transformer
- Ensembling
  - Treat rows as independent, then aggregate predicted column segments
  - Jointly train on all sequences in a table, mixing the individual rows

Tools, References, and Further Reading

Papers

- Sutskever et al., Sequence to Sequence Learning with Neural Networks
- Cho et al., Learning Phrase Representations using RNN Encoder-Decoder for Statistical Machine Translation
- Sennrich et al., Neural Machine Translation of Rare Words with Subword Units
- Koehn, Neural Machine Translation
- Koehn, Six Challenges for Neural Machine Translation

Tutorials

- Pytorch
  - Official PyTorch Seq2Seq Tutorial
  - PyTorch Seq2Seq with Torchtext
  - Ben Trevett Seq2Seq Tutorial
- Tensorflow
  - NMT with Attention

Libraries

- Facebook: fairseq (PyTorch)
- Open NMT (PyTorch)
- Open NMT (Tensorflow)

Thank You!