

CIS 7000 - Fall 2024

## The Pre-Transformer Era



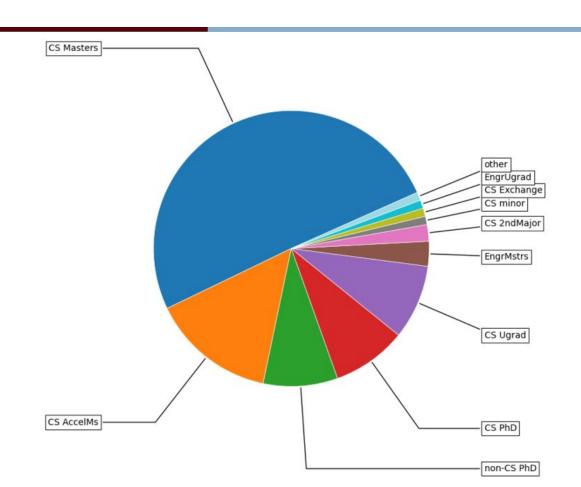
### Professor Mayur Naik

Slides adapted in part from UC Berkeley's CS182: Designing, Visualizing and Understanding Deep Neural Networks (Spring'21), Stanford's CS224N: Natural Language Processing with Deep Learning (Spring'24), and Chapters 7 and 8 of Jurafsky/Martin's book "Speech and Language Processing" (3rd ed).

### Recap of Last Lecture

- The Turing Test
- Overview of LLMs
  - How do LLMs work, What LLMs can do, Limitations of LLMs,
     What is the future
- Course Logistics

#### Who's In CIS 7000?



#### **Announcements**

 Homework 0 "Exploring LLMs" is due on Sunday Sept 8 at 11:59 pm ET. Available via Canvas and <a href="https://llm-class.github.io/homeworks.html">https://llm-class.github.io/homeworks.html</a>. Late submissions will not be accepted!

Homework 1 "Transformer from Scratch" will be released on Friday Sept 6; much more work than Homework 0! Due in 3 parts: Sun Sept 15 (Part 1), Sun Sept 22 (Part 2), and Sun Sept 29 at 11:59 pm ET (Final).

### Today's Agenda

- Background
  - Language Modeling, Perplexity Evaluation, Feedforward
     Neural Networks
- Recurrent Neural Networks (RNNs) and their Limitations
- Attention Mechanisms

### Background

- 1. Language Modeling
- 2. Perplexity Evaluation
- 3. Feedforward Neural Networks
  - a. Forward pass
  - b. Loss function
  - c. Back-propagation

### What is Language Modeling?

The task of computing  $P(w \mid h)$ , the probability distribution of possible words w from a vocabulary given some history (sequence of words) h.

... and thanks for all the \_\_\_\_ ~

fish	0.70
memories	0.10
support	0.05
help	0.05
love	0.04
time	0.02
work	0.02
fun	0.01
•••	

#### What is Language Modeling?

The task of computing  $P(w \mid h)$ , the probability distribution of possible words w from a vocabulary given some history (sequence of words) h.

Enables to compute probabilities of entire sentences by applying **chain rule of probability**:

$$P(w_1 \, w_2 \, \dots \, w_k) = P(w_1).P(w_2 \, | \, w_1).P(w_3 \, | \, w_{1:2})...P(w_k \, | \, w_{1:k-1}) = \prod_{i=1}^k P(w_i \, | \, w_{1:i-1})$$

Question: Why is this task important?

### Motivation for Language Modeling

- Generating more plausible sentences.
  - P("I saw a van") > P("eyes awe of an")
  - Many NLP applications: correcting grammar or spelling errors, machine translation, speech recognition, content summarization, conversational agents, etc.

 More importantly, Large Language Models are built by training them on this task!

### An Approximation

• A problem: computing  $P(w \mid h)$  exactly is infeasible for arbitrary history h since language is **creative** and h might have never occurred before!

Idea: the Markov assumption: approximate the history by just the last few words.

$$P(w_k|w_{1:k-1}) \approx P(w_k|w_{k-n+1:k-1})$$

 Example: n-gram models: look at n-1 words in the history. n=2 is bigrams, n=3 is trigrams, etc.

LLMs use \*much\* larger n, in the thousands or even millions!

### **Estimating Probabilities**

Goal: Train a language model  $P_{\theta}$  with parameters (weights)  $\theta$  such that  $P_{\theta}(h)$  computes a probability distribution over the vocabulary of all possible words.

Start with a dataset  $D_{train} = \{ (h_1, w_1), ..., (h_n, w_n) \}.$ 

Assumption: i.i.d. (independent and identically distributed)

Question: What is the objective of this model?

A good model is one that makes the data look probable. Therefore, choose  $\theta$  such that

$$P(D_{train}) = \prod_{i=1}^{n} P(h_i).P_{\theta}(w_i \mid h_i)$$
 is maximized.

## **Multiplying Probabilities**

$$P(D_{train}) = \prod_{i=1}^{n} P(h_i) \cdot P_{\theta}(w_i \mid h_i)$$
 Multiplying together many numbers <= 1

$$\log P(D_{train}) = \sum_{i=1}^{n} \log P(h_i) + \log P_{\theta}(w_i | h_i) = \sum_{i=1}^{n} \log P_{\theta}(w_i | h_i) + \text{const}$$

$$\theta^* \leftarrow \arg\max_{i=1} \sum_{i=1}^n \log P_{\theta}(w_i \mid h_i)$$
 maximum likelihood estimation (MLE)   
 This is our **loss function**

$$\theta^* \leftarrow \underset{\theta}{\operatorname{arg \, min}} - \frac{1}{n} \sum_{i=1}^n \log P_{\theta}(w_i \mid h_i)$$
 negative log likelihood (NLL)

Also called *cross-entropy*

#### **Evaluation: How Good is Our Model?**

Suppose we train  $P_{\theta}$  (more on how to do this later in today's lecture!)

How do we tell how good our LM is?

Does our LM prefer good sentences over bad ones?

 Assign higher probability to real or frequently observed sentences than ungrammatical or rarely observed ones?

Train the parameters of the LM on a **training set**  $(D_{train})$ .

Test the LM's performance on data we haven't seen.

- A **test set** is an unseen dataset different from D<sub>train</sub>, totally unused.
- An evaluation metric tells us how well our model does on test set.

#### **Extrinsic Evaluation of LMs**

Best evaluation for comparing LMs A and B.

Put each model in a task (e.g. spelling corrector, speech recognizer, machine translation system).

Run the task and get an accuracy for A and B.

- (e.g. how many misspelled words corrected properly, how many words translated properly).

Whichever model has higher accuracy is better.

Problem: Time-consuming.

#### Intrinsic Evaluation of LMs

Common intrinsic evaluation metric for LMs: perplexity.

Bad approximation unless the test data looks just like the training data.

Generally only useful in pilot experiments.

But it is helpful to think about (as long as extrinsic evaluation is also done).

Let's look at different intuitions of perplexity and define it!

### Intuition of Perplexity

**The Shannon Game**: how well can we predict the next word in a given sentence?

I always order pizza with cheese and \_\_\_\_\_

The 33rd President of the US was \_\_\_\_\_

I saw a \_\_\_\_\_

and 1e-100

mushrooms 0.1

A good LM is one that assigns a higher probability to the word that actually occurs.

### Perplexity

The best LM is one that best predicts an unseen test set  $D_{test}$ .

Perplexity is 2<sup>J</sup> where J is cross entropy loss on test set:  $J = -\frac{1}{n} \sum_{i=1}^{n} \log P_{\theta}(w_i \mid h_i)$ 

Perplexity >= 1. Lower is better.

Equivalently, perplexity of a sentence  $w_1 w_2 \dots w_n$  is  $P_{\theta}(w_1 w_2 \dots w_n)^{-\frac{1}{n}}$  which is

the same as 
$$\sqrt[n]{\dfrac{1}{\prod_{i=1}^n P_{ heta}(w_i|w_{1:i-1})}}$$

That is, it is the probability of the sentence normalized by the number of words.

### **Another Intuition of Perplexity**

Perplexity is the average branching factor at any point in a sentence.

Example 1: task is to recognize sentence of random digits. Average branching factor at each step is 10, so perplexity is 10.

Example 2: task is to recognize Operator (1 in 4), Sales (1 in 4), Tech Support (1 in 4), and 30,000 names (1 in 120,000 each). Perplexity is  $\sim$  53.

#### Lower Perplexity = Better Model

Training on 38 million words and testing on 1.5 million words from the WSJ.

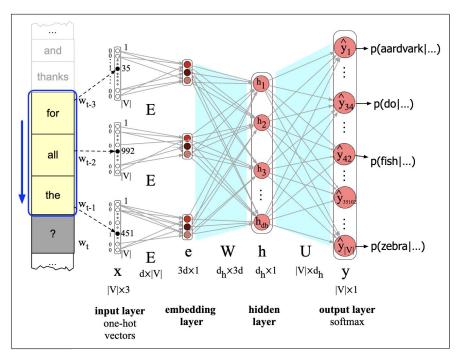
N-gram Order	Unigram	Bigram	Trigram
Perplexity	962	170	109

Further Reading: Hugging Face doc article on Perplexity of fixed-length models.

Feedforward Neural Network for

Language Modeling

#### Architecture and Illustration of Forward Pass



Sketch of feedforward neural language model with N=3.

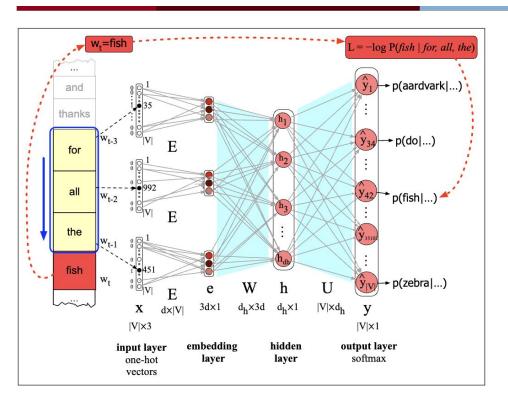
At each timestep *t* the network computes a *d*-dimensional embedding for each context word (by multiplying a one-hot vector by embedding matrix **E**), and concatenates the 3 resulting embeddings to get the embedding layer **e**.

The embedding vector **e** is multiplied by a weight matrix **W** and then an activation function is applied element-wise to produce the hidden layer **h**, which is then multiplied by another weight matrix **U**.

Finally, a softmax output layer predicts at each node i the probability that the next word  $w_t$  will be vocabulary word  $V_i$ .

Y. Benjio et al. A Neural Probabilistic Language Model. JMLR 2003.

### Loss Function: Negative Log Likelihood (NLL)

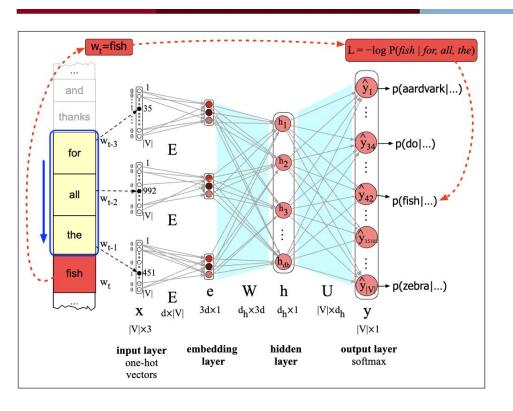


The parameter update for stochastic gradient descent for cross-entropy loss L from step s to s+1 is:

$$oldsymbol{ heta}^{s+1} = oldsymbol{ heta}^s - \eta rac{\partial \left[ -\log p(w_t|w_{t-1},...,w_{t-n+1}) 
ight]}{\partial oldsymbol{ heta}}$$

This gradient can be computed in any standard neural network framework (e.g. Pytorch) which will then backpropagate through  $\theta = \mathbf{E}, \mathbf{W}, \mathbf{U}$ .

#### Forward Pass and Loss Function in Equations



$$e = [E x_{t-3}; E x_{t-2}; E x_{t-1}]$$

$$h = \sigma (W e)$$

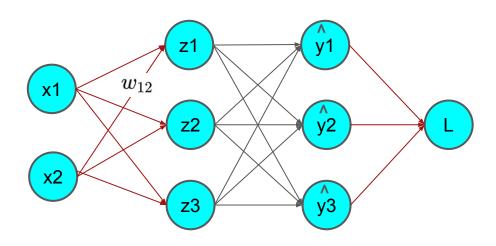
$$z = U h$$

$$\hat{\mathbf{y}} = \operatorname{softmax}(\mathbf{z})$$

$$\mathbf{L} = -\mathbf{y} (\log \hat{\mathbf{y}})^{\mathsf{T}}$$

where **y** is one-hot vector representing ground truth.

Let's consider a simple feedforward network:

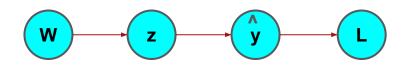


$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \ \mathbf{W} = \begin{bmatrix} w_{11} & w_{12} \\ w_{21} & w_{22} \\ w_{31} & w_{32} \end{bmatrix} \ \mathbf{z} = \begin{bmatrix} w_{11}x_1 + w_{12}x_2 \\ w_{21}x_1 + w_{22}x_2 \\ w_{31}x_1 + w_{32}x_2 \end{bmatrix} \ \hat{\mathbf{y}} = \begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \hat{y}_3 \end{bmatrix} \ L = -\sum_{i=1}^3 y_i \log(\hat{y}_i)$$

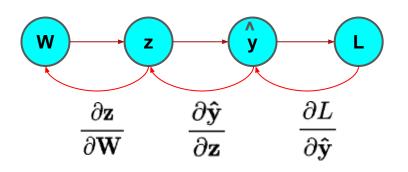
where y is one-hot vector representing ground truth.

where 
$$\mathbf{y}_i = rac{\sum_{j=1}^3 e^{z_j}}{\sum_{j=1}^3 e^{z_j}}$$
  $\begin{bmatrix} \hat{y}_1 \ \hat{y}_2 \ \hat{y}_2 \end{bmatrix}$   $L = -\sum_{i=1}^3 y_i \log(\hat{y}_i)$ 

Computation Graph: (linear in this example but a DAG in general)



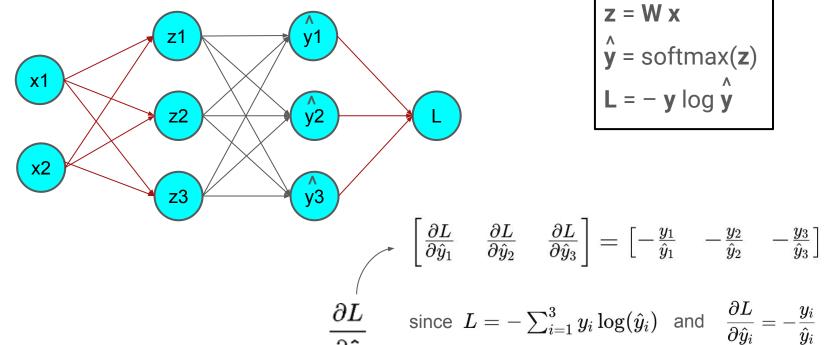
**Backward Differentiation:** 



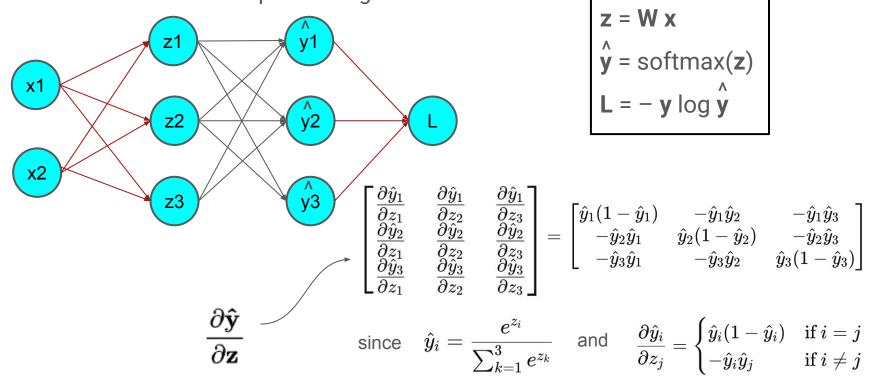
$$\frac{\partial L}{\partial \mathbf{W}} = \frac{\partial L}{\partial \hat{\mathbf{y}}} \cdot \frac{\partial \hat{\mathbf{y}}}{\partial \mathbf{z}} \cdot \frac{\partial \mathbf{z}}{\partial \mathbf{W}}$$

(by chain rule of probability)

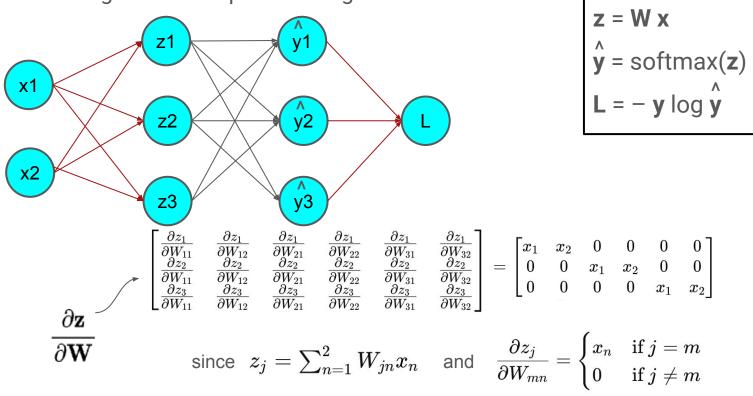
Gradient of Loss with Respect to Predicted Probabilities:



Jacobian of Softmax with Respect to Logits:



Jacobian of Logits with Respect to Weights:



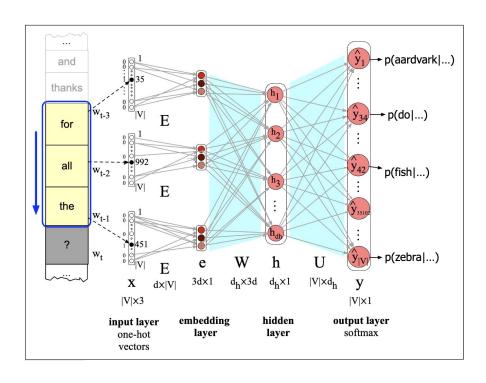
Putting it all together:

$$z = W x$$
  
 $\hat{y} = softmax(z)$   
 $L = -y log \hat{y}$ 

$$= \begin{bmatrix} -\frac{y_1}{\hat{y}_1} & -\frac{y_2}{\hat{y}_2} & -\frac{y_3}{\hat{y}_3} \end{bmatrix} \cdot \begin{bmatrix} \hat{y}_1(1-\hat{y}_1) & -\hat{y}_1\hat{y}_2 & -\hat{y}_1\hat{y}_3 \\ -\hat{y}_2\hat{y}_1 & \hat{y}_2(1-\hat{y}_2) & -\hat{y}_2\hat{y}_3 \\ -\hat{y}_3\hat{y}_1 & -\hat{y}_3\hat{y}_2 & \hat{y}_3(1-\hat{y}_3) \end{bmatrix} \cdot \begin{bmatrix} x_1 & x_2 & 0 & 0 & 0 & 0 \\ 0 & 0 & x_1 & x_2 & 0 & 0 \\ 0 & 0 & 0 & 0 & x_1 & x_2 \end{bmatrix}$$

$$= \begin{bmatrix} (\hat{y}_1 - y_1)x_1 & (\hat{y}_1 - y_1)x_2 & (\hat{y}_2 - y_2)x_1 & (\hat{y}_2 - y_2)x_2 & (\hat{y}_3 - y_3)x_1 & (\hat{y}_3 - y_3)x_2 \end{bmatrix}$$

#### Pros/Cons of Feedforward Neural Network as Language Model



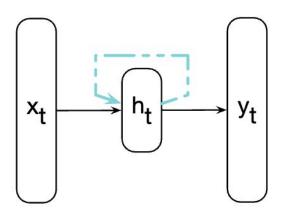
#### Improvements over n-gram LM:

- No sparsity problem.
- No need to store all observed n-grams.

#### Remaining problems:

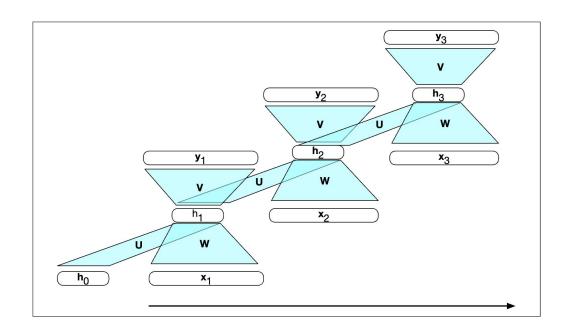
- Fixed window is too small.
- Model size (W) increases for longer input context.
- Window can never be large enough!
- Each x<sub>i</sub> is multiplied by completely different weights in W, so no symmetry in how the inputs are processed.

#### **Recurrent Neural Networks**



$$\mathbf{h}_{t} = \sigma (\mathbf{U} \mathbf{h}_{t-1} + \mathbf{W} \mathbf{x}_{t})$$
  
 $\mathbf{y}_{t} = \operatorname{softmax}(\mathbf{V} \mathbf{h}_{t})$ 

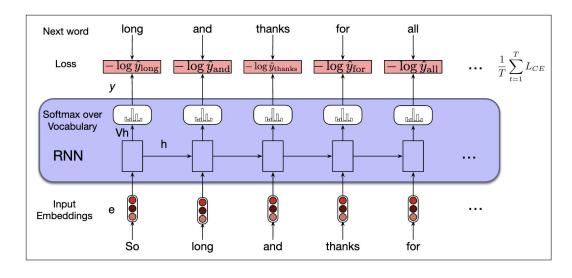
#### Recurrent Neural Networks: Forward Pass



$$\mathbf{h_0} = 0$$
  
for  $\mathbf{t} = 1$  to length( $\mathbf{x}$ ) do  
 $\mathbf{h_t} = \sigma (\mathbf{U} \mathbf{h_{t-1}} + \mathbf{W} \mathbf{x_t})$   
 $\mathbf{y_t} = \operatorname{softmax}(\mathbf{V} \mathbf{h_t})$   
return  $\mathbf{y}$ 

The matrices **U**, **V** and **W** are shared across time, while new values for **h** and **y** are calculated with each time step.

#### Recurrent Neural Networks: Training

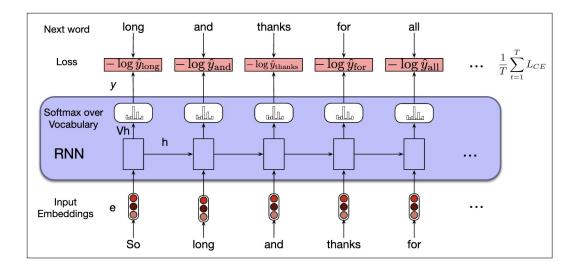


At each word position  $\mathbf{t}$  of the input, the model takes word  $\mathbf{w}_{\mathbf{t}}$  together with  $\mathbf{h}_{\mathbf{t-1}}$ , encoding information from the preceding  $\mathbf{w}_{1:\mathbf{t-1}}$ , and uses them to compute a probability distribution over possible next words so as to compute the model's loss for the next word  $\mathbf{w}_{\mathbf{t+1}}$ .

Then we move to the next word, ignore what the model predicted for the next word and instead use the correct word  $\mathbf{w}_{t+1}$  along with the prior history encoded to estimate the probability of word  $\mathbf{w}_{t+2}$ .

This idea that we always provide the model the correct history sequence to predict the next word (rather than feeding the model its best case from the previous time step) is called **teacher forcing**.

#### Recurrent Neural Networks: Backpropagation

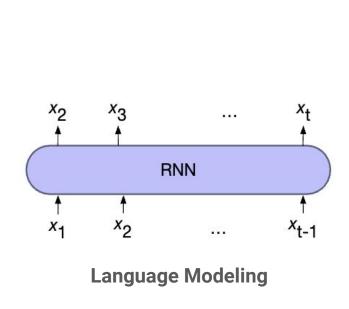


Backpropagate over timesteps **t** = **T**, ... ,**1**, summing gradients as you go. This algorithm is called "backpropagation through time".

Computing loss and gradients over entire corpus at once is too expensive (memory-wise). In practice, consider (a batch of) sentences at a time.

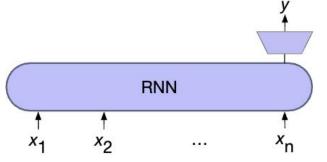
In practice, often "truncated" after ~20 timesteps for training efficiency reasons.

#### RNN Architectures for Different NLP Tasks



# Sequence Labeling

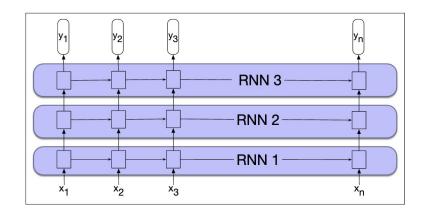
Applications:
Part-of-speech
tagging,
Named entity
recognition



# **Sequence Classification**

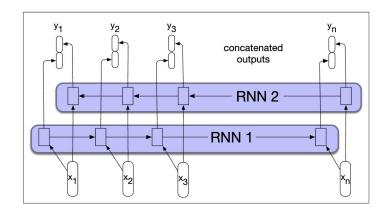
Applications: sentiment analysis, spam detection

#### Variations of RNNs



**Stacking** 

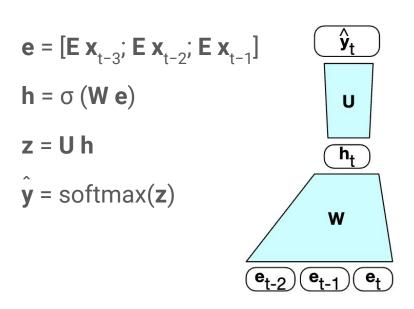
The output of a lower level serves as the input to higher levels with the output of the last network serving as the final output. The resulting network induces representations at differing levels of abstraction across layers.



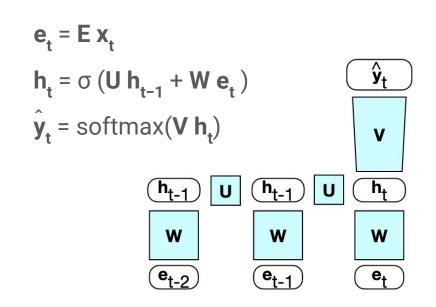
**Bidirectional** 

Separate models are trained in the forward and backward directions, with the output of each model at each time point concatenated to represent the bidirectional state at that time point.

#### Feedforward vs. Recurrent Neural Network as Language Model



**Feedforward Neural Network** 



**Recurrent Neural Network** 

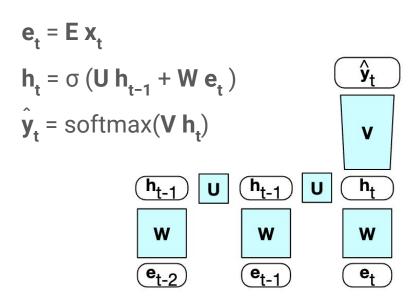
#### Pros/Cons of Recurrent Neural Network as Language Model

#### Pros:

- Can process any length input!
- Computation for step t can (in theory)
  use information from many steps back.
- Model size (W) doesn't increase for longer input context.
- Each x<sub>i</sub> is multiplied by same weights in W, so there is symmetry in how inputs are processed.

#### Cons:

- Recurrent computation is slow (cannot be parallelized).
- In practice, it is difficult to access information from many steps back.



#### Vanishing Gradient Problem!

RNN extensions such as LSTMs (or other varieties like GRUs) are commonly used.

### Effect of Vanishing Gradient on RNN-Based Language Model

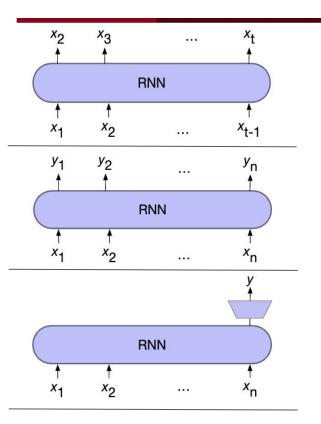
**LM task:** When she tried to print her tickets, she found that the printer was out of toner. She went to the stationery store to buy more toner. It was very overpriced. After installing the toner into the printer, she finally printed her \_\_\_\_\_\_

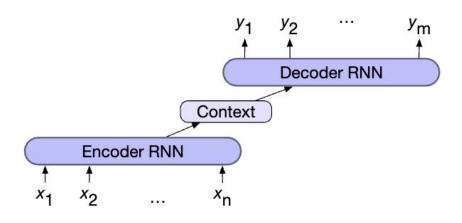
To learn from this training example, the RNN-LM needs to model the dependency between "tickets" on the 7 step and the target word "tickets" at the end.

But if the gradient is small, the model can't learn this dependency. So, the model is unable to predict similar long-distance dependencies at test time.

More on vanishing/exploding gradient problems in training RNNs: R. Pascanu et al. On the difficulty of training recurrent neural networks. ICML 2013.

#### Encoder-Decoder or Seq2Seq Architecture



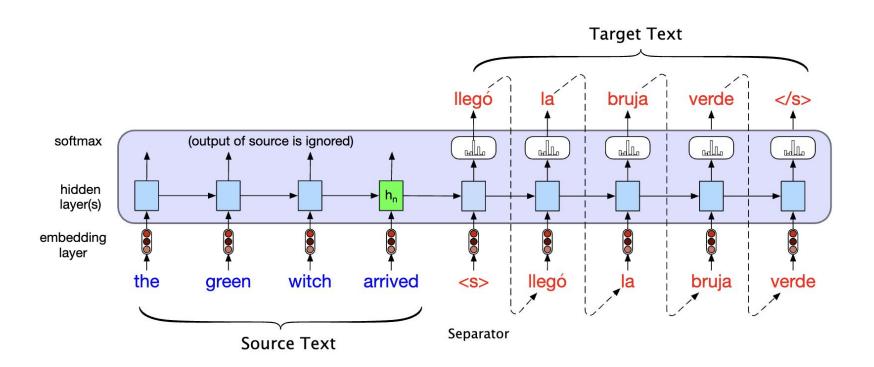


Taking an input sequence and translating it to an output sequence that is of a different length than the input, and doesn't align with it in a word-to-word way.

Many applications: machine translation, summarization, question-answering, dialogue, ...

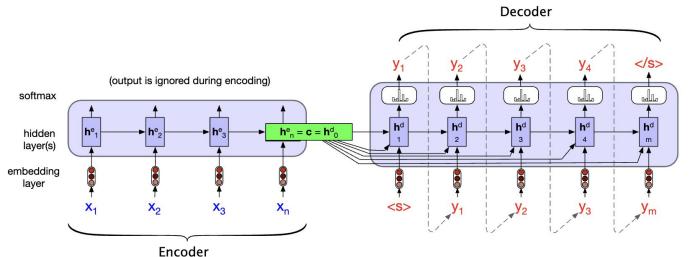
I. Sutskever et al. Sequence to Sequence Learning with Neural Networks. NeurIPS 2014.

### Illustrative Example: Machine Translation



#### Encoder-Decoder RNN, More Formally

The final hidden state of the encoder RNN,  $\mathbf{h_n}^e$ , serves as the context for the decoder in its role as  $\mathbf{h_0}^d$  in the decoder RNN, and is also made available to each decoder hidden state.



$$\mathbf{c} = \mathbf{h}_{n}^{e}$$

$$\mathbf{h}_{0}^{d} = \mathbf{c}$$

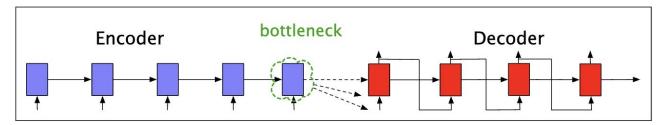
$$\mathbf{h}_{i}^{d} = g(\hat{\mathbf{y}}_{i-1}, \mathbf{h}_{i-1}^{d}, \mathbf{c})$$

$$\hat{\mathbf{y}}_{i} = \operatorname{softmax}(\mathbf{h}_{i}^{d})$$

where **g** is a stand-in for some flavor of RNN.

#### The Bottleneck Problem

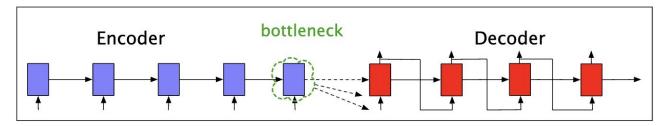
Requiring the context **c** to be only the encoder's final hidden state forces all the information from the entire source sentence to pass through this representational bottleneck!



D. Bahdanau et al. Neural Machine Translation by Jointly Learning to Align and Translate. ICLR 2015.

#### Attention Mechanism: A Solution to the Bottleneck Problem

Requiring the context **c** to be only the encoder's final hidden state forces all the information from the entire source sentence to pass through this representational bottleneck!



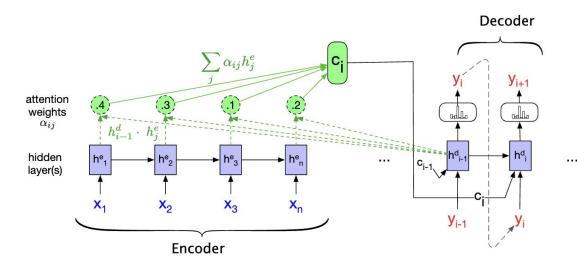
 $\mathbf{c} = \mathbf{h}_{n}^{e}$   $\mathbf{h}_{0}^{d} = \mathbf{c}$   $\mathbf{h}_{i}^{d} = g(\hat{\mathbf{y}}_{i-1}, \mathbf{h}_{i-1}^{d}, \mathbf{c}_{i})$   $\hat{\mathbf{y}}_{i} = softmax(\mathbf{h}_{i}^{d})$ 

Instead of a static context vector  $\mathbf{c}$ , dynamically generated a context vector  $\mathbf{c}_{\mathbf{i}}$  for each decoding step  $\mathbf{i}$  that takes all encoder hidden states into account in its derivation.

$$c_i = f(h_1^e, ..., h_n^e)$$

D. Bahdanau et al. Neural Machine Translation by Jointly Learning to Align and Translate. ICLR 2015.

#### **Dot-Product Attention**



Finally compute a fixed-length context vector for the current decoder state by taking a weighted average over all the encoder hidden states.

First step in computing  $\mathbf{c}_i$ : How much to focus on each encoder state  $\mathbf{h}_i^e$ , or how relevant it is to the decoder state captured in  $\mathbf{h}_{i-1}^d$ .

$$score(h_{i-1}^{d}, h_{j}^{e}) = h_{i-1}^{d} \cdot h_{j}^{e}$$

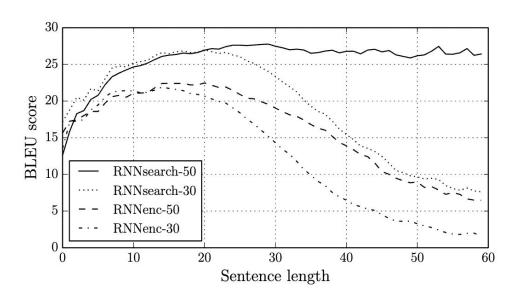
Then normalize the weights.

$$\mathbf{q}_{ij} = \text{softmax}(\text{score}(\mathbf{h}_{i-1}^{d}, \mathbf{h}_{j}^{e}))$$

$$c_i = \sum_j \alpha_{ij} h_j^e$$

More sophisticated scoring function:  $\mathbf{h_{i-1}}^d \mathbf{W} \mathbf{h_i}^e$  using learned weights  $\mathbf{W}$ .

### Experimental Results With vs. Without Attention Mechanism



Performance of RNN encoder-decoder models trained on sentences of length upto 30 or 50:

RNNsearch - with attention RNNenc - without attention

D. Bahdanau et al. Neural Machine Translation by Jointly Learning to Align and Translate. ICLR 2015.

#### Up Next ...

 Mon Sept 9: Tutorial on "From Pytorch to Hugging Face: How to run your own LLM".

Topics: Pytorch framework and Hugging Face Transformers library.

• Wed Sept 11: Lecture on The Transformer Architecture.

*Topics:* Self-Attention, Transformer Block, Input/Output Processing, Types of Transformers, Training and Inference, Case Studies (BERT, GPT-2, Mixtral).