ENGINEERING
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McMaster University

Computational Natural Language Processing

Language Models and Recurrent Neural Nets

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Lecture Plan

1. A bit more about neural networks

Language modeling + RNNs

- 2. A new NLP task: **Language Modeling**

This is the most important concept in the class! It leads to GPT-3 and ChatGPT!

motivates

- 3. A new family of neural networks: **Recurrent Neural Networks (RNNs)**

Important and used in Ass1, but not the only way to build LMs

- 4. Problems with RNNs
- 5. Recap on RNNs/LMs

Reminders:

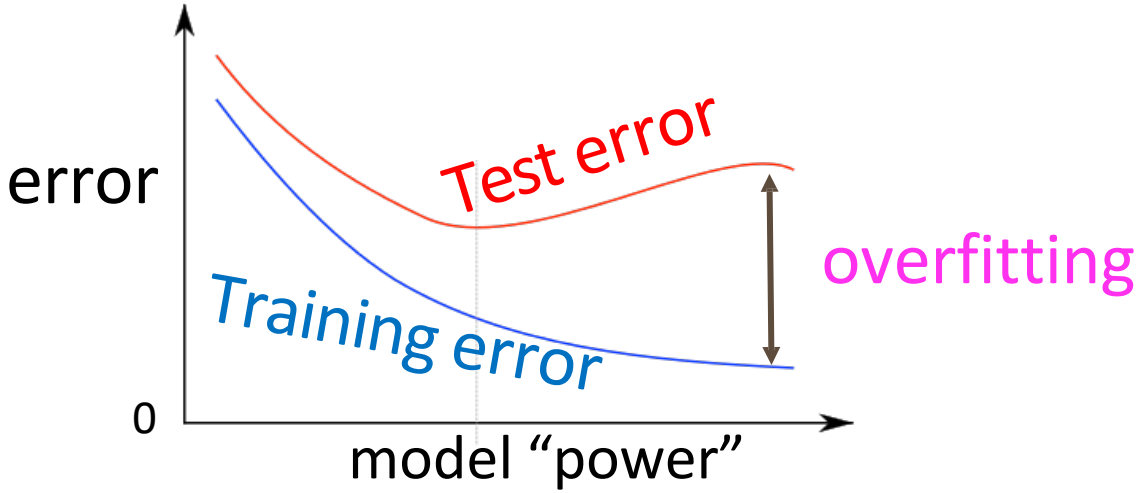
You should have started working on Assignment 1

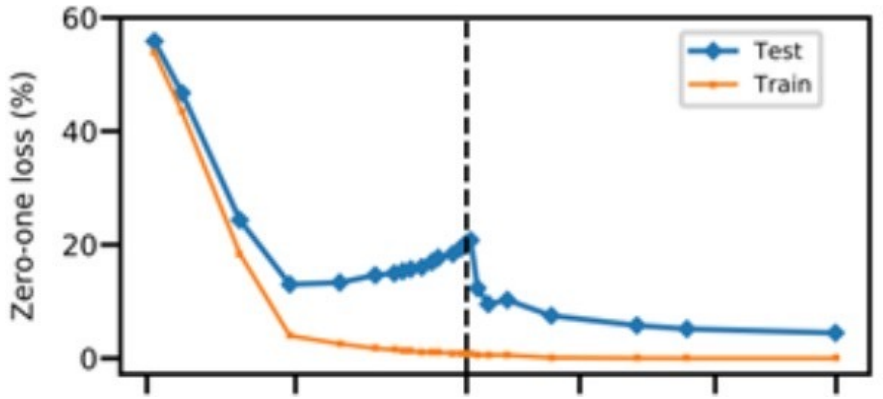
We have models with many parameters! Regularization!

- A full loss function includes **regularization** over all parameters θ, e.g., L2 regularization:

$$J(\theta) = \frac{1}{N}\sum_{i=1}^{N} -\log\left(\frac{e^{f_{y_i}}}{\sum_{c=1}^{C} e^{f_c}}\right) + \lambda \sum_k \theta_k^2$$

- Classic view: Regularization works to prevent overfitting when we have a lot of features (or later a very powerful/deep model, etc.)
- Now: Regularization produces models that generalize well when we have a "big" model
  - We do not care that our models overfit on the training data, even though they are **hugely** overfit



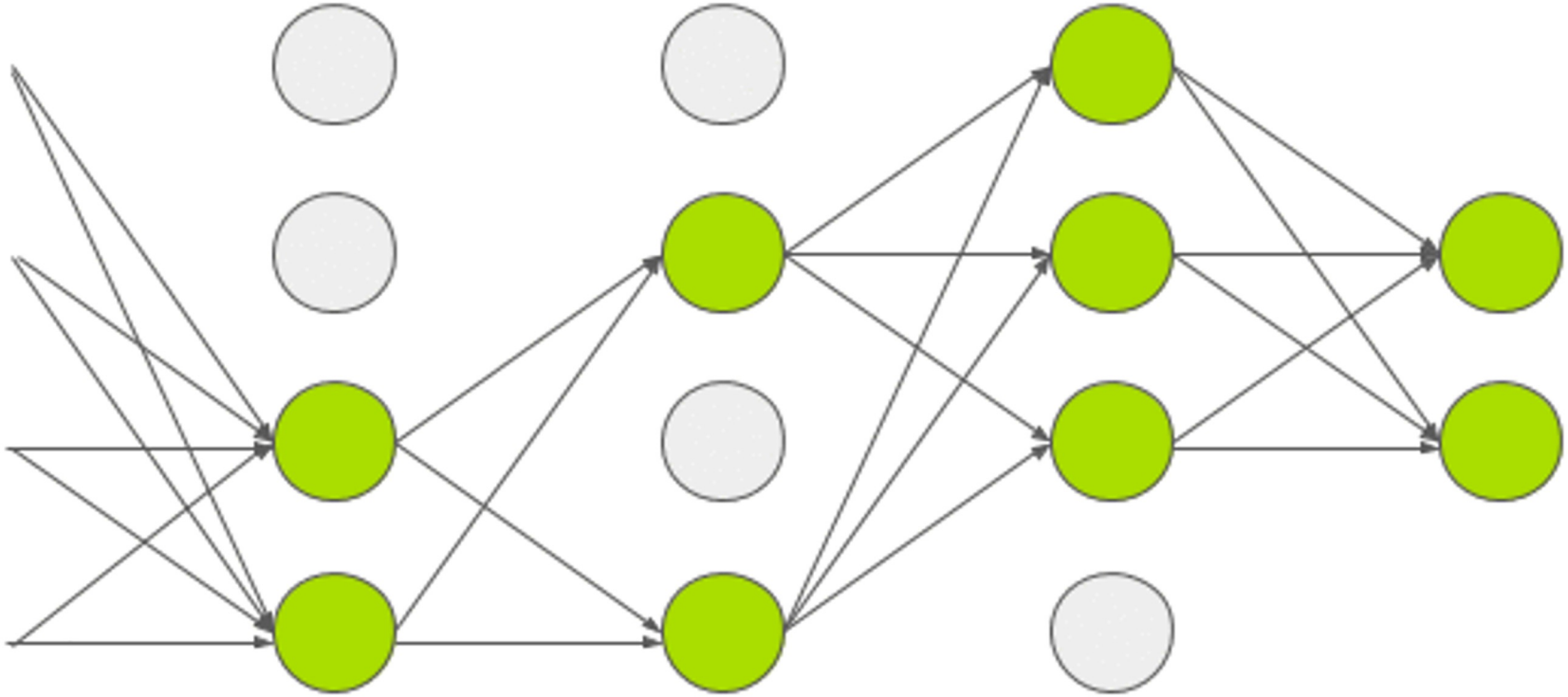


Dropout (Srivastava, Hinton, Krizhevsky, Sutskever, & Salakhutdinov 2012/JMLR 2014)

Preventing Feature Co-adaptation = Good Regularization Method! **Use it everywhere!**

- Training time: at each instance of evaluation (in online SGD-training), randomly set ~50% (*p*%) of the inputs to each neuron to 0
- Test time: halve the model weights (now twice as many)
- Except usually only drop first layer inputs a little (~15%) or not at all
- This prevents feature co-adaptation: A feature cannot only be useful in the presence of particular other features
- In a single layer: A kind of middle-ground between Naïve Bayes (where all feature weights are set independently) and logistic regression models (where weights are set in the context of all others)
- Can be thought of as a form of model bagging (i.e., like an ensemble model)
- Nowadays usually thought of as strong, feature-dependent regularizer [Wager, Wang, & Liang 2013]

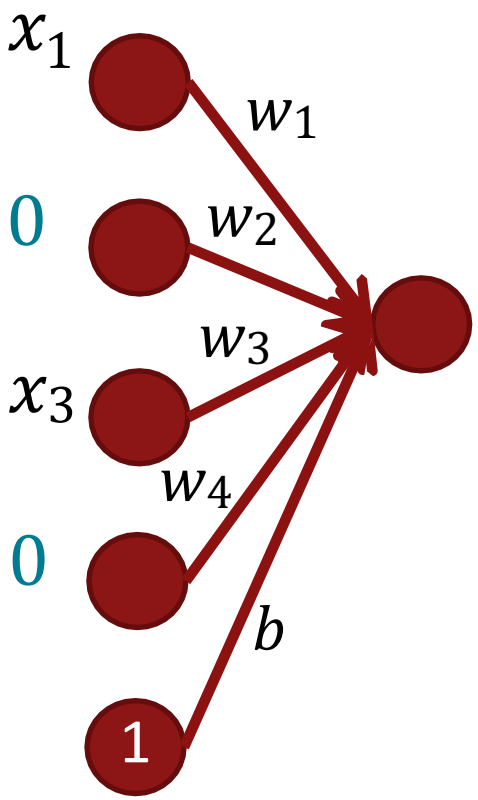
Dropout



Dropout (Srivastava, Hinton, Krizhevsky, Sutskever, & Salakhutdinov 2012/JMLR 2014)

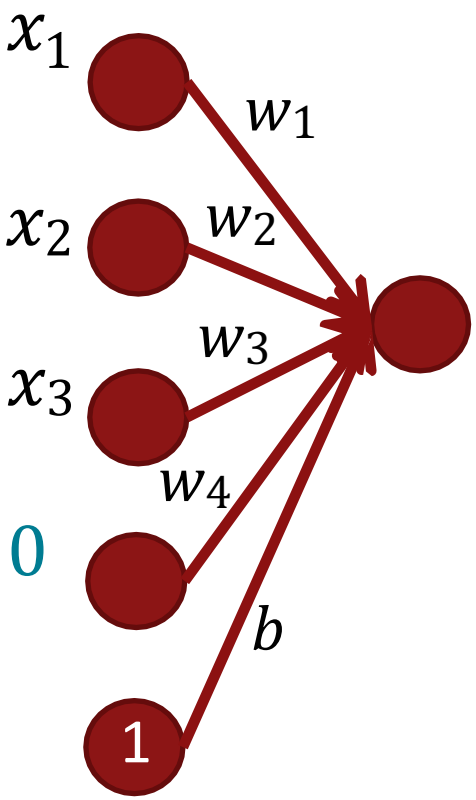
- During training
  - For each data point each time:
    - Randomly set input to 0 with probability p "dropout ratio" (often $p = 0.5$ except $p - 0.15$ for input layer) via dropout mask
- During testing
  - Multiply all weights by $1 - p$
  - No other dropout

Train 1



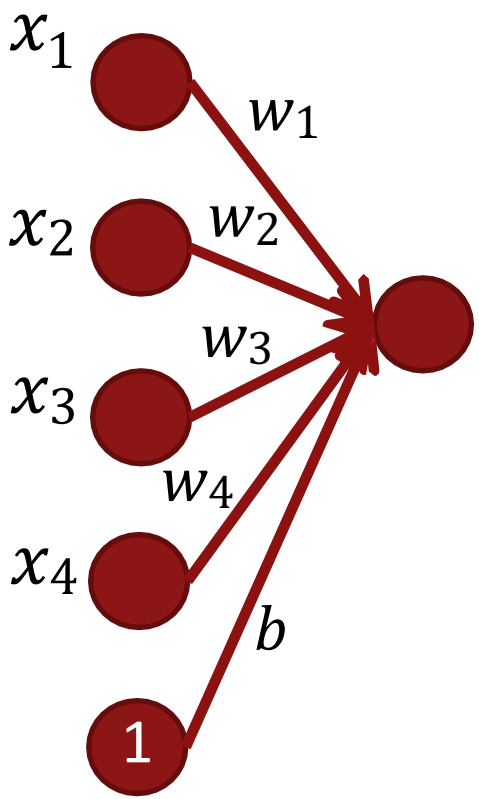
$y = w_1x_1 + w_3x_3 + b$

Train 2



$y = w_1x_1 + w_2x_2 + w_3x_3$

Test



$y = (1 - p)(w_1x_1 + w_2x_2 + w_3x_3 + w_4x_4)$

“Vectorization”

- E.g., looping over word vectors versus concatenating them all into one large matrix and then multiplying the softmax weights with that matrix:

```
from numpy import random
N = 500 # number of windows to classify
d = 300 # dimensionality of each window
C = 5 # number of classes
W = random.rand(C,d)
wordvectors_list = [random.rand(d,1) for i in range(N)]
wordvectors_one_matrix = random.rand(d,N)

%timeit [W.dot(wordvectors_list[i]) for i in range(N)]
%timeit W.dot(wordvectors_one_matrix)
```

- for loop: 1000 loops, best of 3: **639 µs** per loop
  Using single a C x N matrix: 10000 loops, best of 3: **53.8 µs** per loop
- Matrices are awesome!!! Always try to use vectors and matrices rather than for loops!
- The speed gain goes from 1 to 2 orders of magnitude with GPUs!

Parameter Initialization

- You normally must initialize weights to small random values (i.e., not zero matrices!)
  - To avoid symmetries that prevent learning/specialization
- Initialize hidden layer biases to 0 and output (or reconstruction) biases to optimal value if weights were 0 (e.g., mean target or inverse sigmoid of mean target)
- Initialize **all other weights** ~ Uniform(–*r*, *r*), with *r* chosen so numbers get neither too big or too small [later, the need for this is removed with use of layer normalization]
- Xavier initialization has variance inversely proportional to fan-in n_{in} (previous layer size) and fan-out n_{out} (next layer size):

$$\mathrm{Var}(W_i) = \frac{2}{n_{\mathrm{in}} + n_{\mathrm{out}}}$$

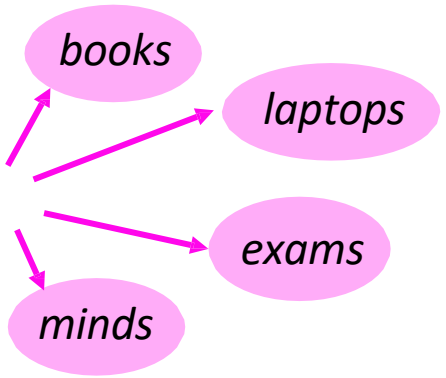
Optimizers

- Usually, plain SGD will work just fine!
  - However, getting good results will often require hand-tuning the learning rate
    - E.g., start it higher and halve it every *k* epochs (passes through full data, **shuffled** or sampled)
- For more complex nets, or to avoid worry, try more sophisticated "adaptive" optimizers that scale the adjustment to individual parameters by an accumulated gradient
  - These models give differential per-parameter learning rates
    - Adagrad ← Simplest member of family, but tends to "stall early"
    - RMSprop
    - Adam ← **A fairly good, safe place to begin in many cases**
    - AdamW
    - NAdamW ← Can be better with word vectors (W) and for speed (Nesterov acceleration)
    - …
  - Start them with an initial learning rate, around 0.001 ← Many have other hyperparameters

2. Language Modeling

- **Language Modeling** is the task of predicting what word comes next

the students opened their _____



- More formally: given a sequence of words $\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}, \ldots, \boldsymbol{x}^{(t)}$, compute the probability distribution of the next word $\boldsymbol{x}^{(t+1)}$:

$$P(\boldsymbol{x}^{(t+1)} | \ \boldsymbol{x}^{(t)}, \ldots, \boldsymbol{x}^{(1)})$$

where $\boldsymbol{x}^{(t+1)}$ can be any word in the vocabulary $V = \{\boldsymbol{w}_1, \ldots, \boldsymbol{w}_{|V|}\}$

- A system that does this is called a **Language Model**

Language Modeling

- You can also think of a Language Model as a system that assigns a probability to a piece of text

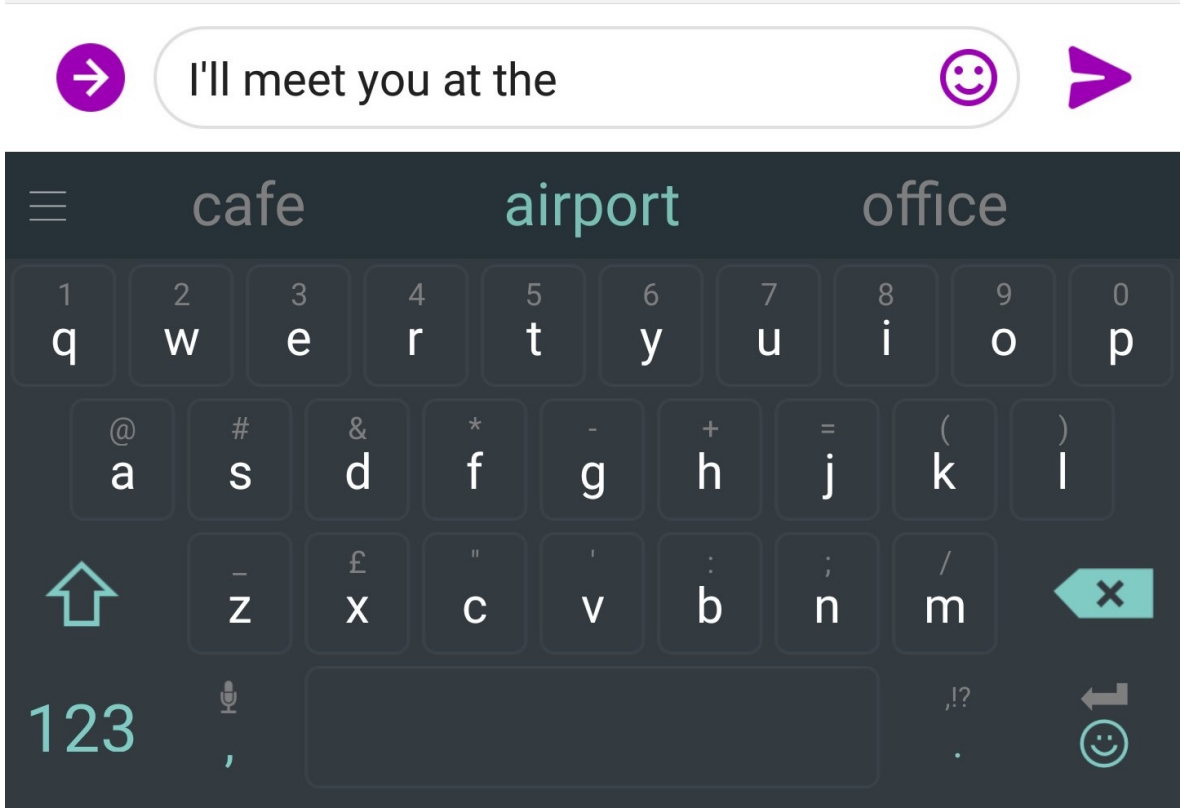
- For example, if we have some text $\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(T)}$, then the probability of this text (according to the Language Model) is:

$$P(\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(T)}) = P(\boldsymbol{x}^{(1)}) \times P(\boldsymbol{x}^{(2)} | \boldsymbol{x}^{(1)}) \times \cdots \times P(\boldsymbol{x}^{(T)} | \boldsymbol{x}^{(T-1)}, \ldots, \boldsymbol{x}^{(1)})$$

$$= \prod_{t=1}^{T} P(\boldsymbol{x}^{(t)} | \boldsymbol{x}^{(t-1)}, \ldots, \boldsymbol{x}^{(1)})$$

This is what our LM provides

You use Language Models every day!



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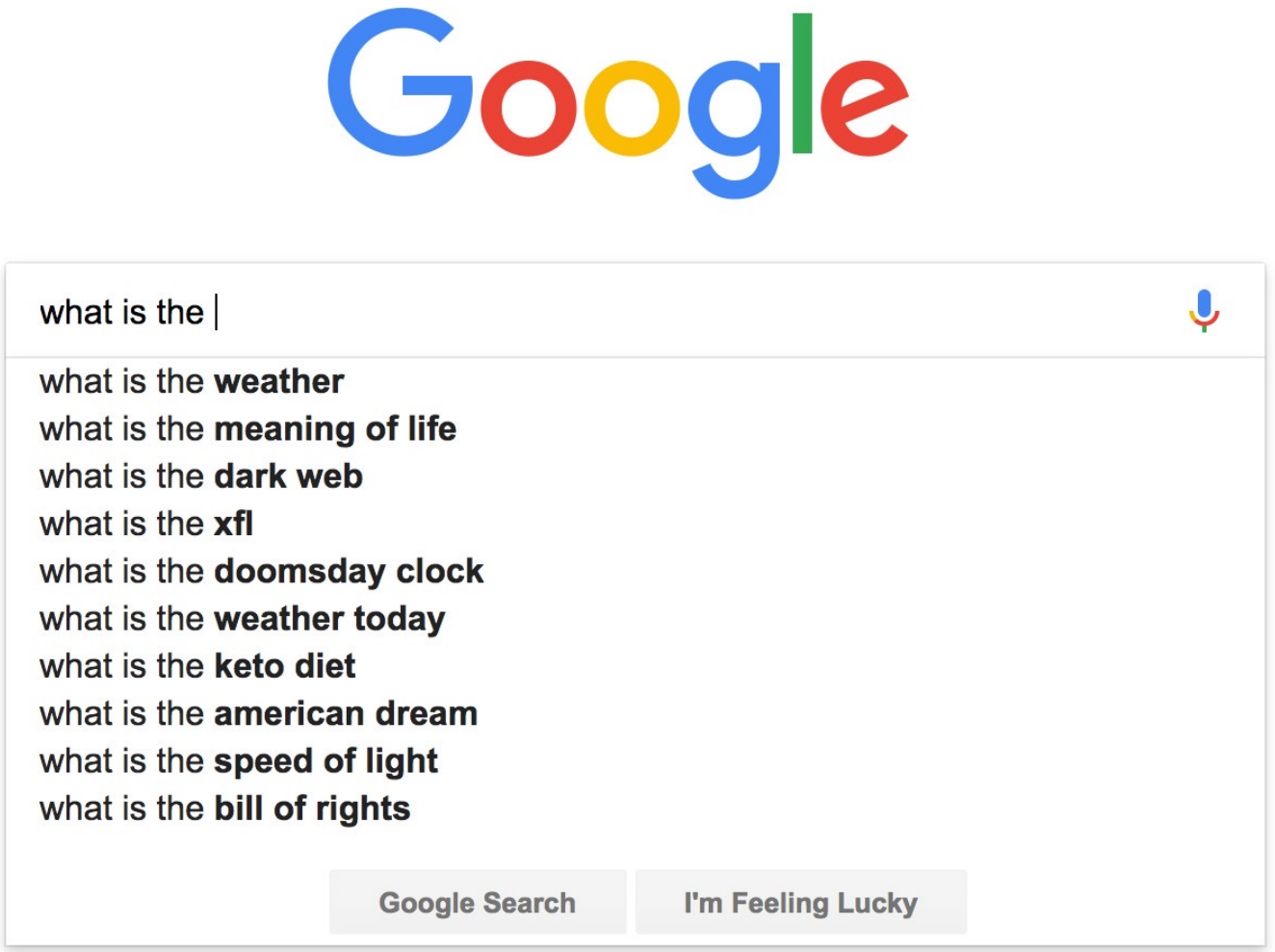


n-gram Language Models

the students opened their _____

- **Question**: How to learn a Language Model?
- **Answer** (pre- Deep Learning): learn an *n*-gram Language Model!

- **Definition:** An *n*-gram is a chunk of *n* consecutive words.
  - unigrams: “the”, “students”, “opened”, ”their”
  - bigrams: “the students”, “students opened”, “opened their”
  - trigrams: “the students opened”, “students opened their”
  - four-grams: “the students opened their”

- **Idea:** Collect statistics about how frequent different n-grams are and use these to predict next word.

n-gram Language Models

- First we make a Markov assumption: $x^{(t+1)}$ depends only on the preceding *n*-1 words

$$P(\boldsymbol{x}^{(t+1)}|\boldsymbol{x}^{(t)},\ldots,\boldsymbol{x}^{(1)}) = P(\boldsymbol{x}^{(t+1)}|\overbrace{\boldsymbol{x}^{(t)},\ldots,\boldsymbol{x}^{(t-n+2)}}^{n\text{-1 words}}) \quad \text{(assumption)}$$

prob of a n-gram

prob of a (n-1)-gram

$$= \frac{P(\boldsymbol{x}^{(t+1)},\boldsymbol{x}^{(t)},\ldots,\boldsymbol{x}^{(t-n+2)})}{P(\boldsymbol{x}^{(t)},\ldots,\boldsymbol{x}^{(t-n+2)})} \quad \text{(definition of conditional prob)}$$

- **Question:** How do we get these *n*-gram and (*n*-1)-gram probabilities?
- **Answer:** By counting them in some large corpus of text!

$$\approx \frac{\text{count}(\boldsymbol{x}^{(t+1)},\boldsymbol{x}^{(t)},\ldots,\boldsymbol{x}^{(t-n+2)})}{\text{count}(\boldsymbol{x}^{(t)},\ldots,\boldsymbol{x}^{(t-n+2)})} \quad \text{(statistical approximation)}$$

n-gram Language Models: Example

Suppose we are learning a 4-gram Language Model.

~~*as the proctor started the clock, the*~~ *students opened their* _____

discard

condition on this

$$P(\boldsymbol{w}|\text{students opened their}) = \frac{\text{count}(\text{students opened their } \boldsymbol{w})}{\text{count}(\text{students opened their})}$$

For example, suppose that in the corpus:

- "students opened their" occurred 1000 times
- "students opened their books" occurred 400 times
  - → P(books | students opened their) = 0.4
- "students opened their exams" occurred 100 times
  - → P(exams | students opened their) = 0.1

Should we have discarded the "proctor" context?

Sparsity Problems with n-gram Language Models

Sparsity Problem 1

Problem: What if *"students opened their w"* never occurred in data? Then *w* has probability 0!

(Partial) Solution: Add small δ to the count for every $w \in V$. This is called *smoothing*.

$$P(\boldsymbol{w}|\text{students opened their}) = \frac{\text{count}(\text{students opened their } \boldsymbol{w})}{\text{count}(\text{students opened their})}$$

Sparsity Problem 2

Problem: What if *"students opened their"* never occurred in data? Then we can't calculate probability for *any w*!

(Partial) Solution: Just condition on *"opened their"* instead. This is called *backoff*.

Note: Increasing *n* makes sparsity problems *worse.* Typically, we can't have *n* bigger than 5.

Storage Problems with n-gram Language Models

Storage: Need to store count for all *n*-grams you saw in the corpus.

$$P(\boldsymbol{w}|\text{students opened their}) = \frac{\text{count}(\text{students opened their } \boldsymbol{w})}{\text{count}(\text{students opened their})}$$

Increasing *n* or increasing corpus increases model size!

n-gram Language Models in practice

- You can build a simple trigram Language Model over a 1.7 million word corpus (Reuters) in a few seconds on your laptop

Business and financial news

today the _____

get probability distribution

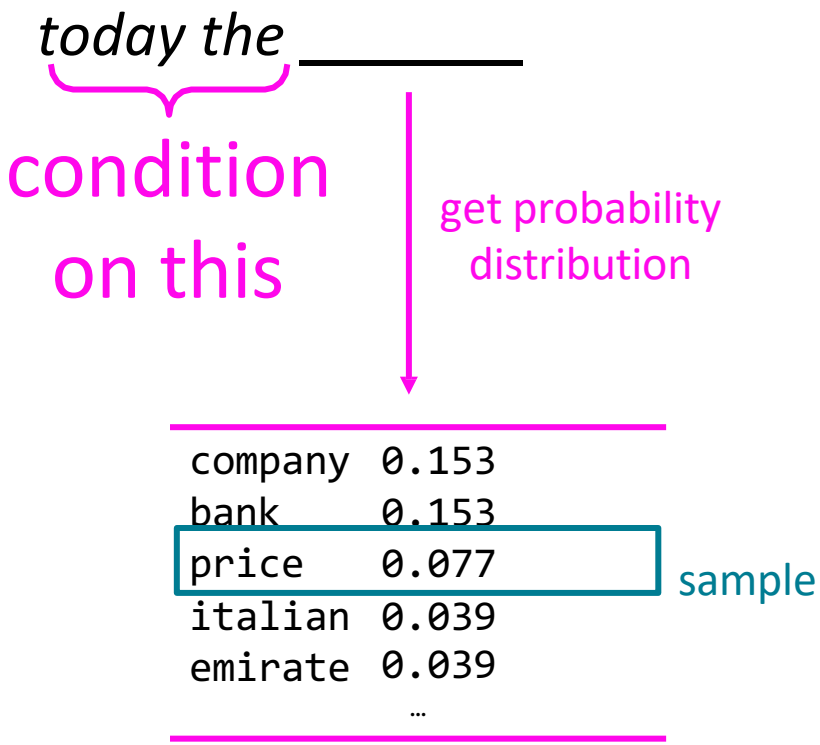
company	0.153
bank	0.153
price	0.077
italian	0.039
emirate	0.039
…	

Sparsity problem: not much granularity in the probability distribution

Otherwise, seems reasonable!

Generating text with a n-gram Language Model

You can also use a Language Model to generate text



Generating text with a n-gram Language Model

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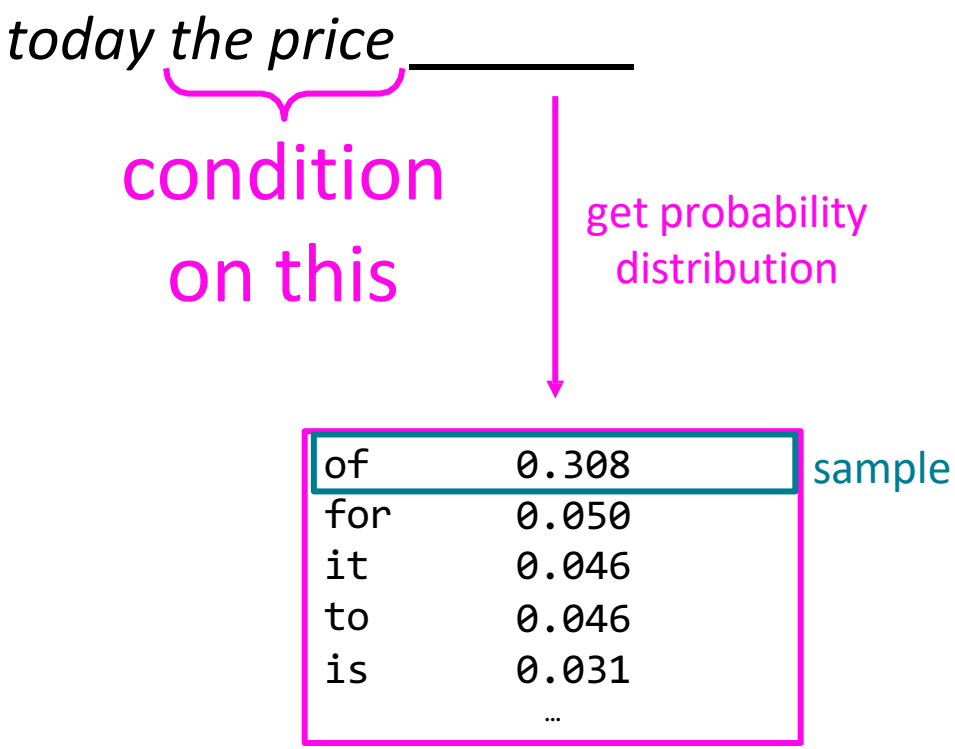
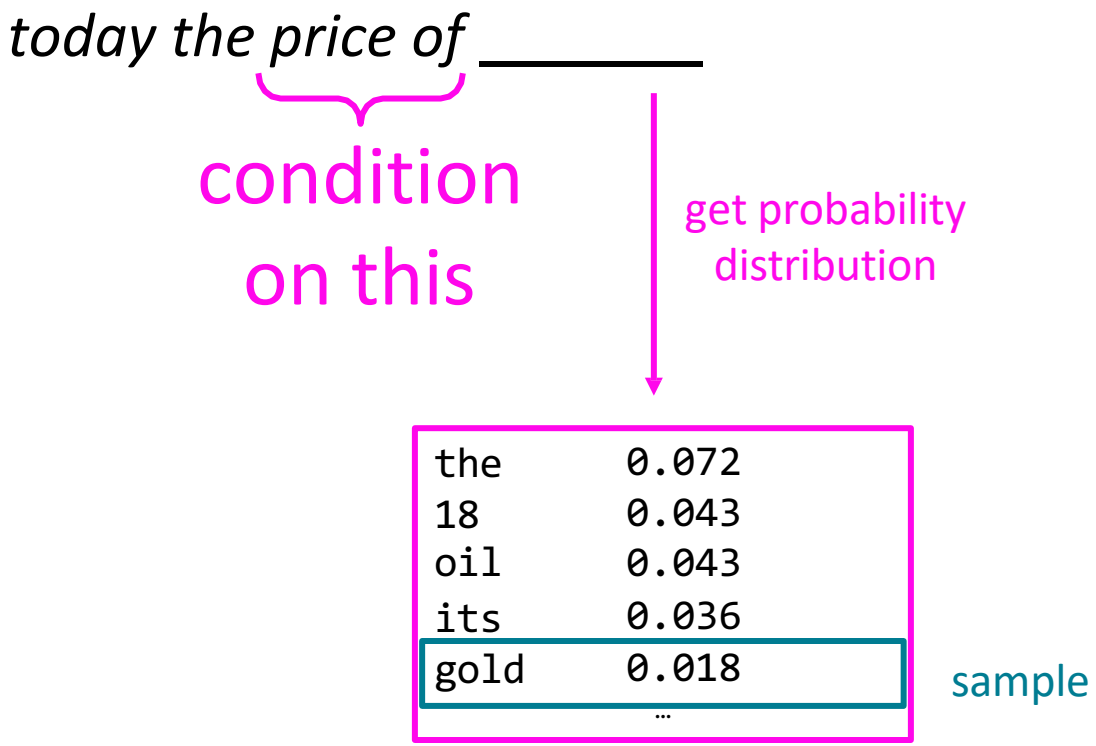


Generating text with a n-gram Language Model

You can also use a Language Model to generate text



Generating text with a n-gram Language Model

You can also use a Language Model to generate text

today the price of gold per ton , while production of shoe lasts and shoe industry , the bank intervened just after it considered and rejected an imf demand to rebuild depleted european stocks , sept 30 end primary 76 cts a share .

Surprisingly grammatical!

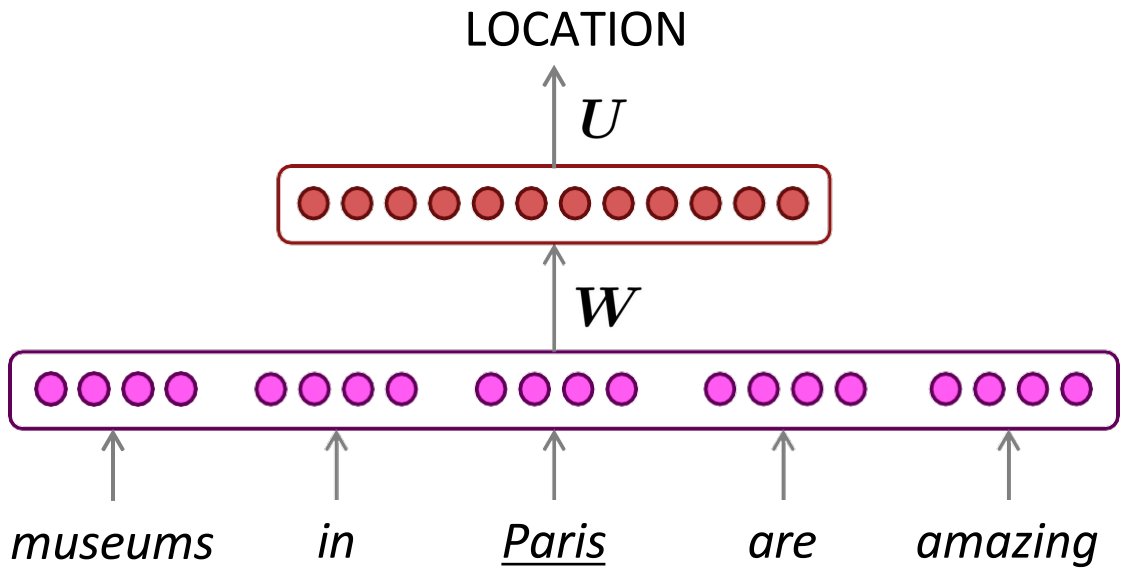
…but **incoherent.** We need to consider more than three words at a time if we want to model language well.

But increasing *n* worsens sparsity problem, and increases model size…

How to build a *neural* language model?

- Recall the Language Modeling task:
  - Input: sequence of words $\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}, \ldots, \boldsymbol{x}^{(t)}$
  - Output: prob. dist. of the next word $P(\boldsymbol{x}^{(t+1)} | \boldsymbol{x}^{(t)}, \ldots, \boldsymbol{x}^{(1)})$

- How about a window-based neural model?
  - We saw this applied to Named Entity Recognition in Lecture 2:



A fixed-window neural Language Model

~~as the proctor started the clock~~ *the students opened their* _____

discard

fixed window

A fixed-window neural Language Model

output distribution

$$\hat{\boldsymbol{y}} = \text{softmax}(\boldsymbol{U}\boldsymbol{h} + \boldsymbol{b}_2) \in \mathbb{R}^{|V|}$$

hidden layer

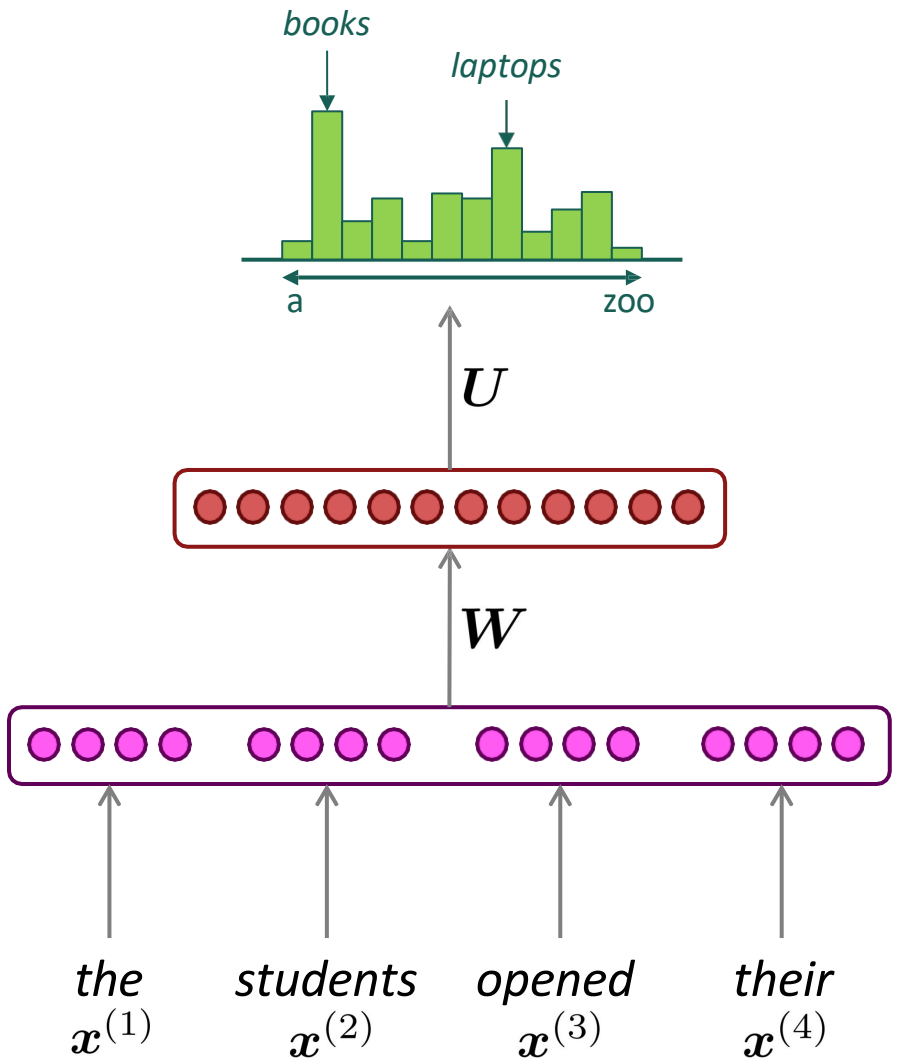
$$\boldsymbol{h} = f(\boldsymbol{W}\boldsymbol{e} + \boldsymbol{b}_1)$$

concatenated word embeddings

$$\boldsymbol{e} = [\boldsymbol{e}^{(1)}; \boldsymbol{e}^{(2)}; \boldsymbol{e}^{(3)}; \boldsymbol{e}^{(4)}]$$

words / one-hot vectors

$$\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}, \boldsymbol{x}^{(3)}, \boldsymbol{x}^{(4)}$$



A fixed-window neural Language Model

Approximately: Y. Bengio, et al. (2000/2003): A Neural Probabilistic Language Model

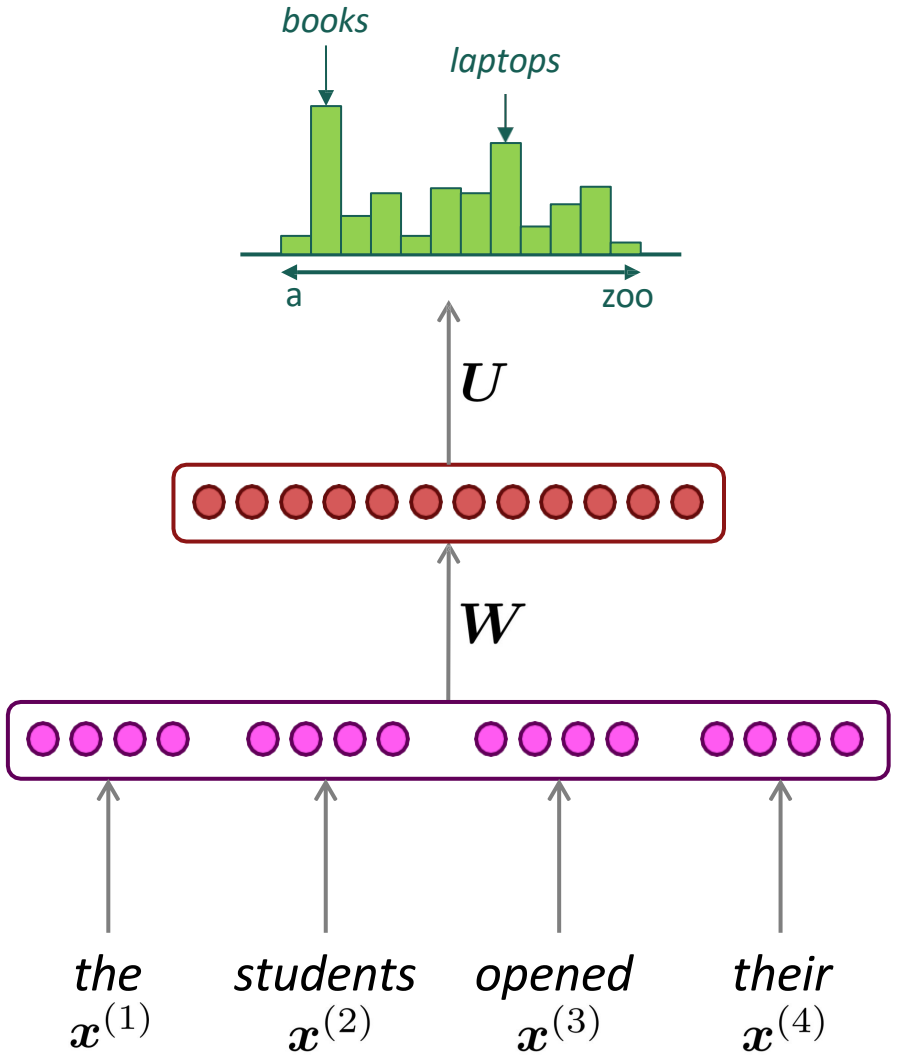
Improvements over *n*-gram LM:

- No sparsity problem
- Don't need to store all observed *n*-grams

Remaining **problems**:

- Fixed window is too small
- Enlarging window enlarges W
- Window can never be large enough!
- $x^{(1)}$ and $x^{(2)}$ are multiplied by completely different weights in W. No symmetry in how the inputs are processed.

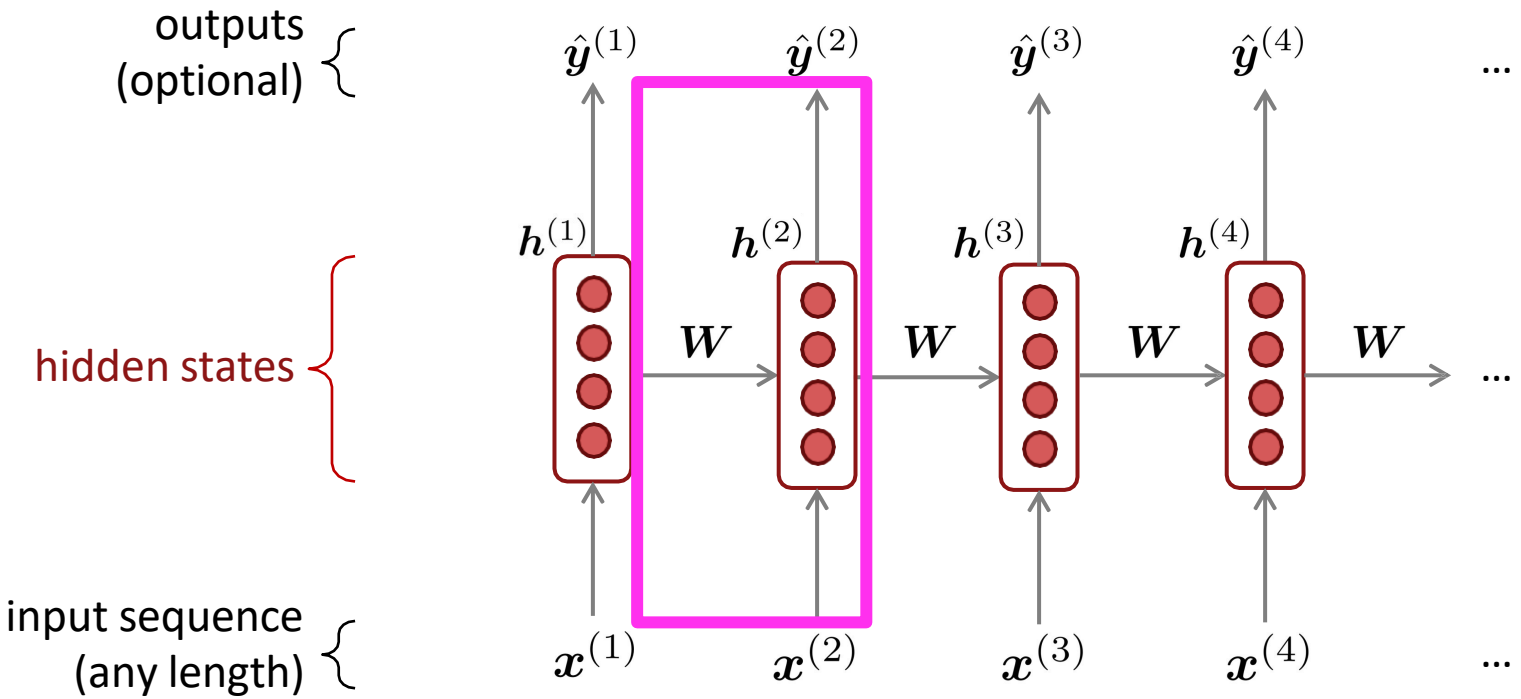
We need a neural architecture that can process *any length input*



3. Recurrent Neural Networks (RNN)

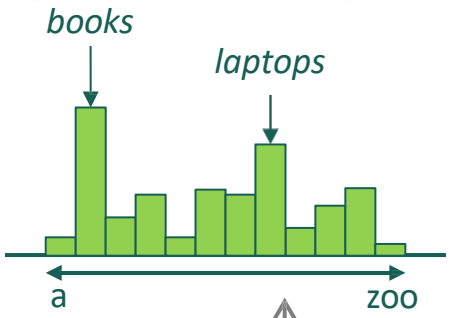
A family of neural architectures

Core idea: Apply the same weights *W repeatedly*



A Simple RNN Language Model

$\hat{\boldsymbol{y}}^{(4)} = P(\boldsymbol{x}^{(5)}|\text{the students opened their})$



output distribution

$$\hat{\boldsymbol{y}}^{(t)} = \text{softmax}\left(\boldsymbol{U}\boldsymbol{h}^{(t)} + \boldsymbol{b}_2\right) \in \mathbb{R}^{|V|}$$

hidden states

$$\boldsymbol{h}^{(t)} = \sigma\left(\boldsymbol{W}_h\boldsymbol{h}^{(t-1)} + \boldsymbol{W}_e\boldsymbol{e}^{(t)} + \boldsymbol{b}_1\right)$$

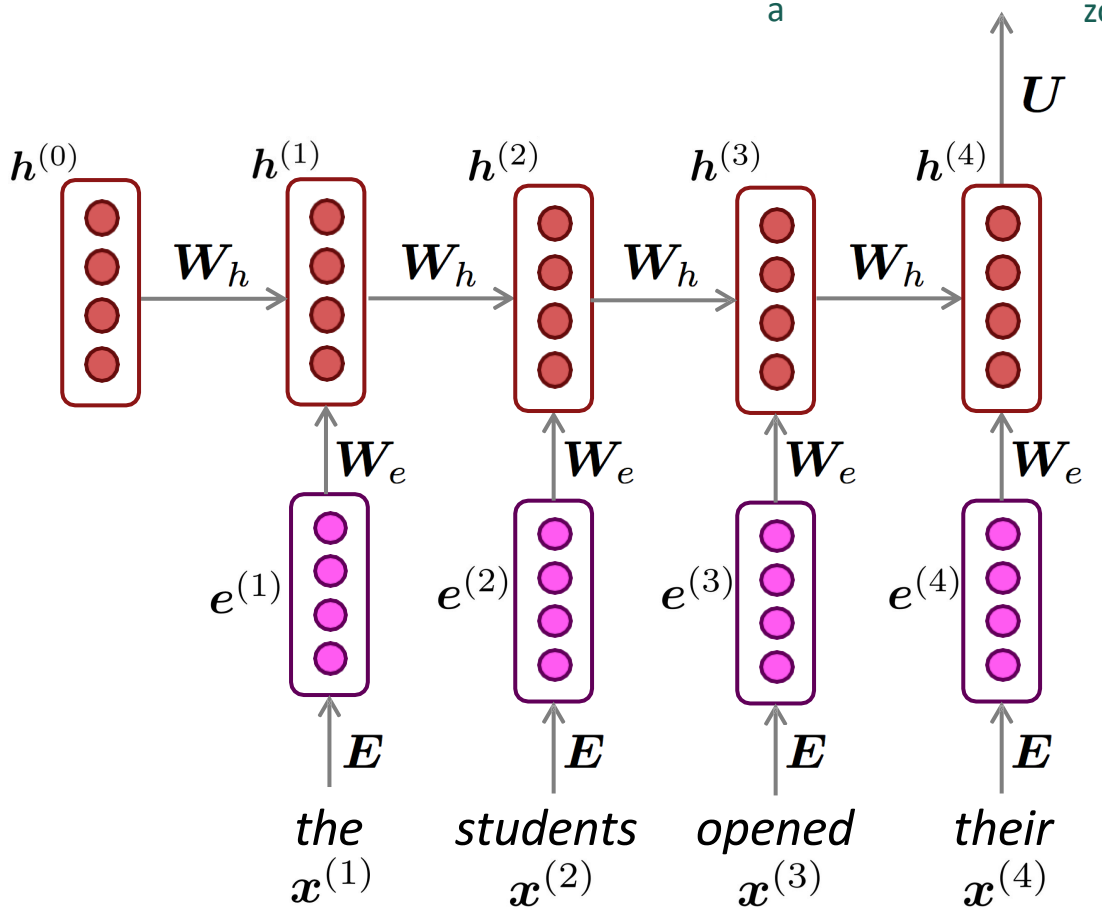
$\boldsymbol{h}^{(0)}$ is the initial hidden state

word embeddings

$$\boldsymbol{e}^{(t)} = \boldsymbol{E}\boldsymbol{x}^{(t)}$$

words / one-hot vectors

$$\boldsymbol{x}^{(t)} \in \mathbb{R}^{|V|}$$



***Note**: this input sequence could be much longer now!*

RNN Language Models

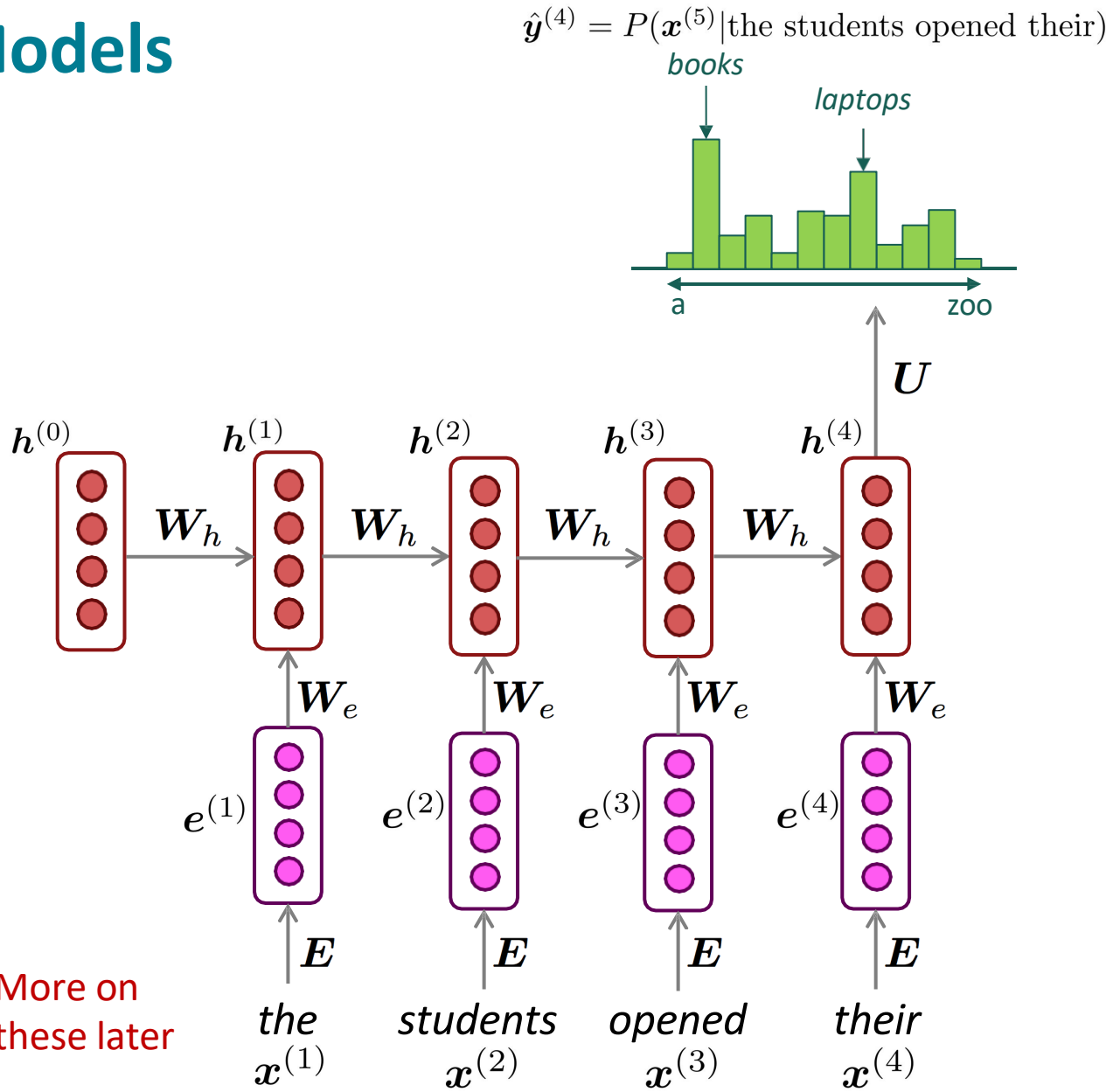
RNN **Advantages**:

- Can process any length input
- Computation for step *t* can (in theory) use information from many steps back
- Model size doesn't increase for longer input context
- Same weights applied on every timestep, so there is symmetry in how inputs are processed.

RNN **Disadvantages**:

- Recurrent computation is slow
- In practice, difficult to access information from many steps back

More on these later



Training an RNN Language Model

- Get a big corpus of text which is a sequence of words $\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(T)}$
- Feed into RNN-LM; compute output distribution $\hat{\boldsymbol{y}}^{(t)}$ for *every step t*.
  - i.e., predict probability dist of *every word*, given words so far

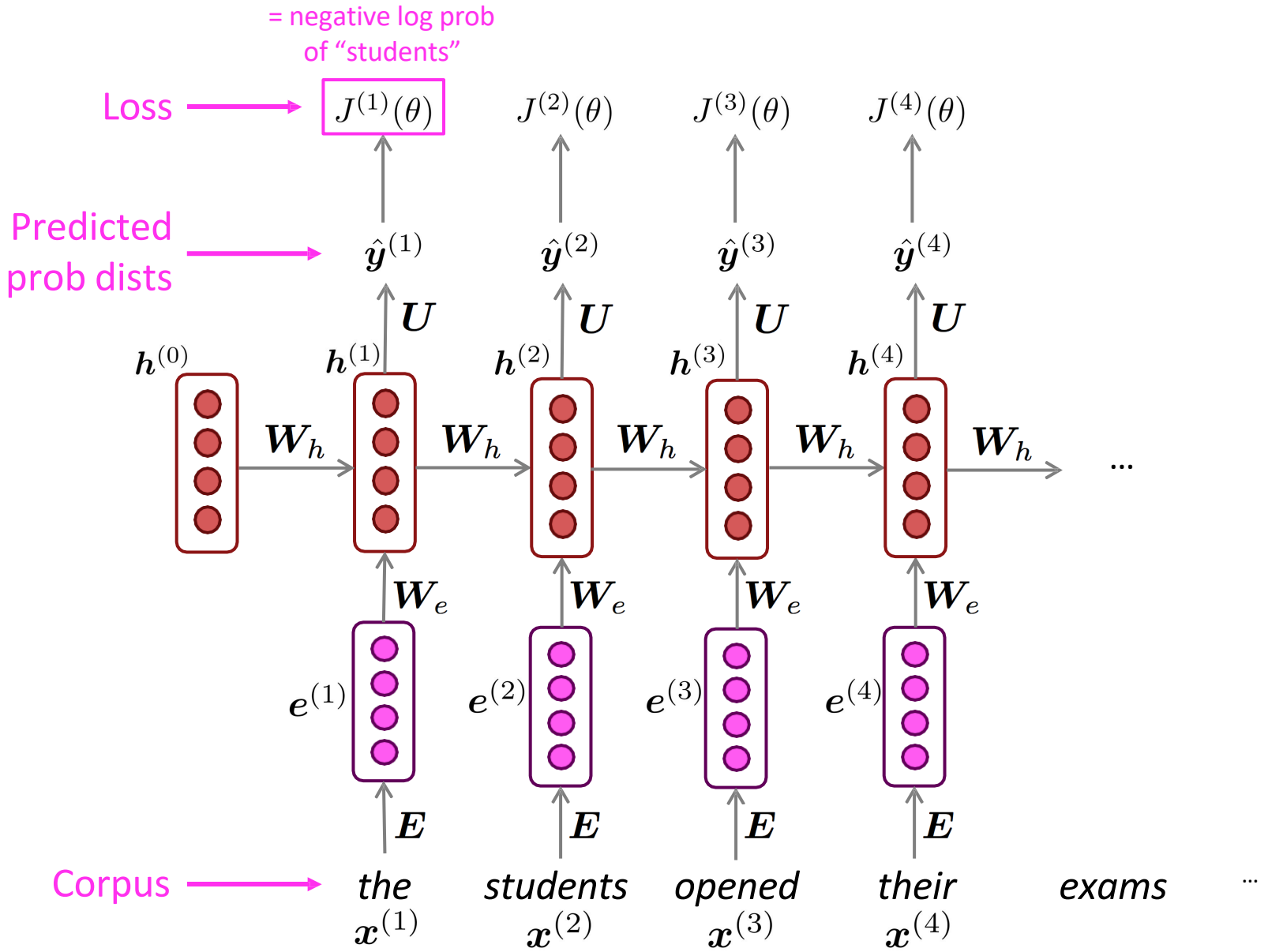
- Loss function on step *t* is cross-entropy between predicted probability distribution $\hat{\boldsymbol{y}}^{(t)}$, and the true next word $\boldsymbol{y}^{(t)}$ (one-hot for $\boldsymbol{x}^{(t+1)}$):

$$J^{(t)}(\theta) = CE(\boldsymbol{y}^{(t)}, \hat{\boldsymbol{y}}^{(t)}) = -\sum_{w \in V} \boldsymbol{y}_w^{(t)} \log \hat{\boldsymbol{y}}_w^{(t)} = -\log \hat{\boldsymbol{y}}_{\boldsymbol{x}_{t+1}}^{(t)}$$

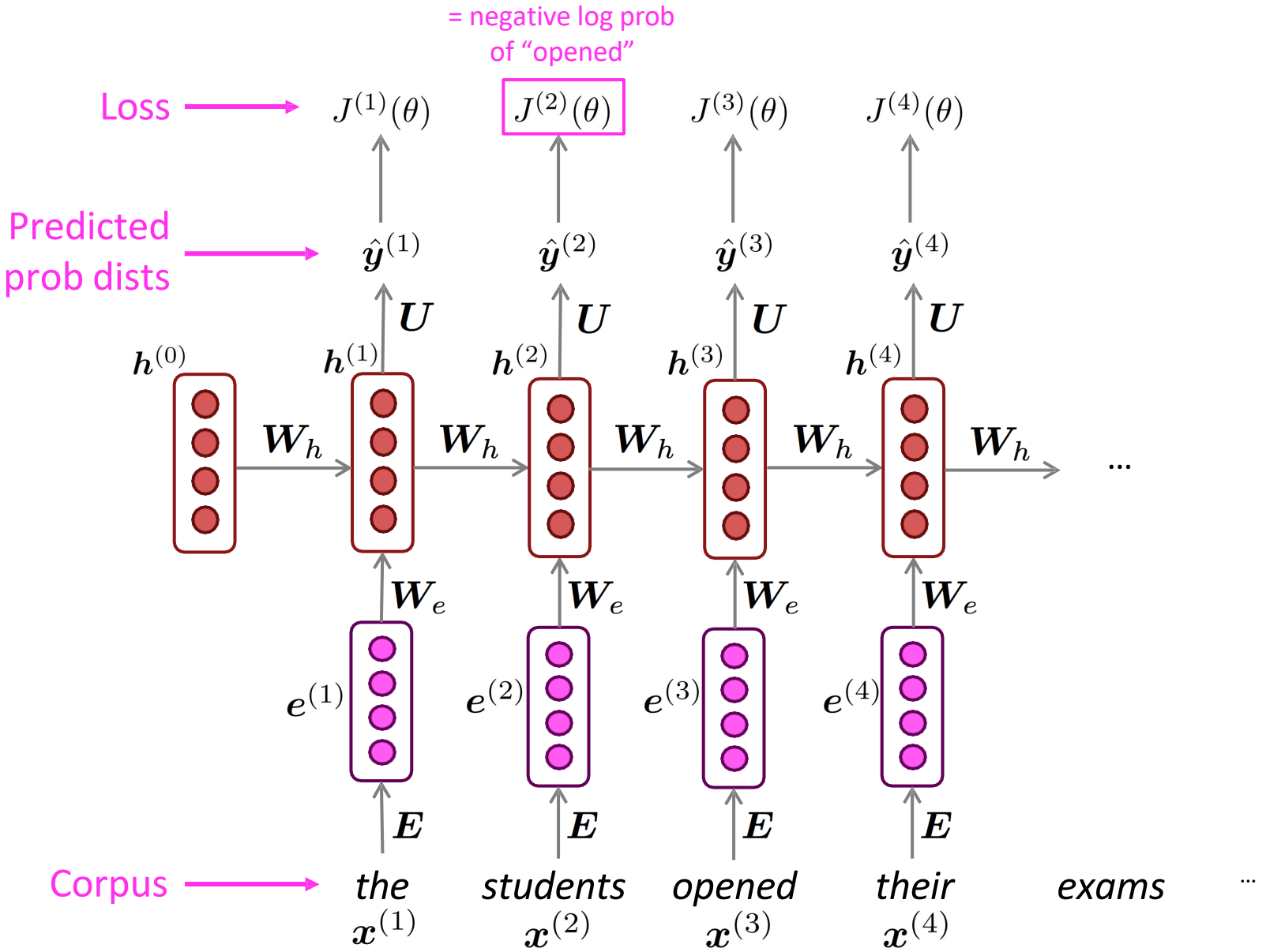
- Average this to get overall loss for entire training set:

$$J(\theta) = \frac{1}{T} \sum_{t=1}^{T} J^{(t)}(\theta) = \frac{1}{T} \sum_{t=1}^{T} -\log \hat{\boldsymbol{y}}_{\boldsymbol{x}_{t+1}}^{(t)}$$

Training an RNN Language Model



Training an RNN Language Model



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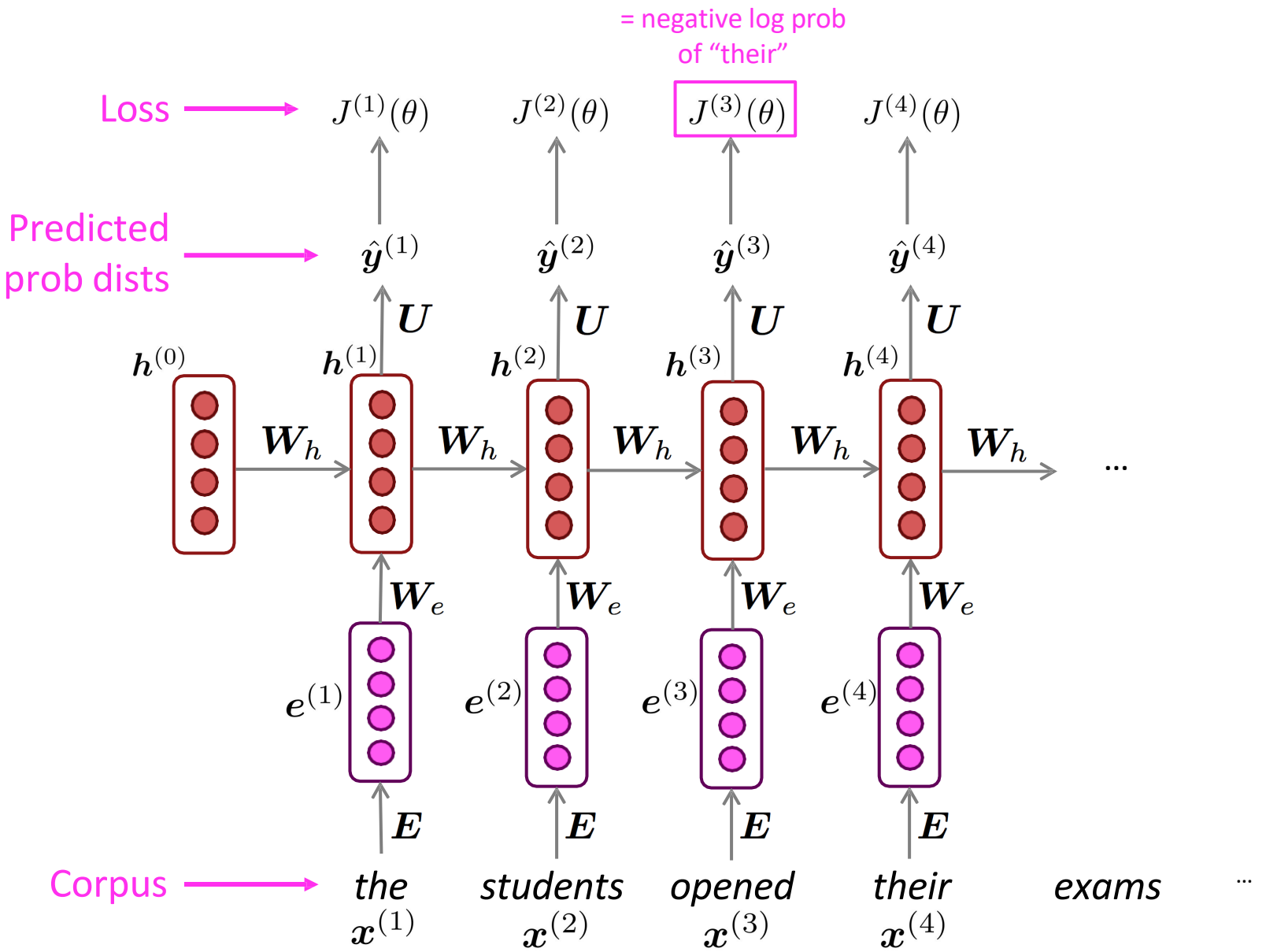
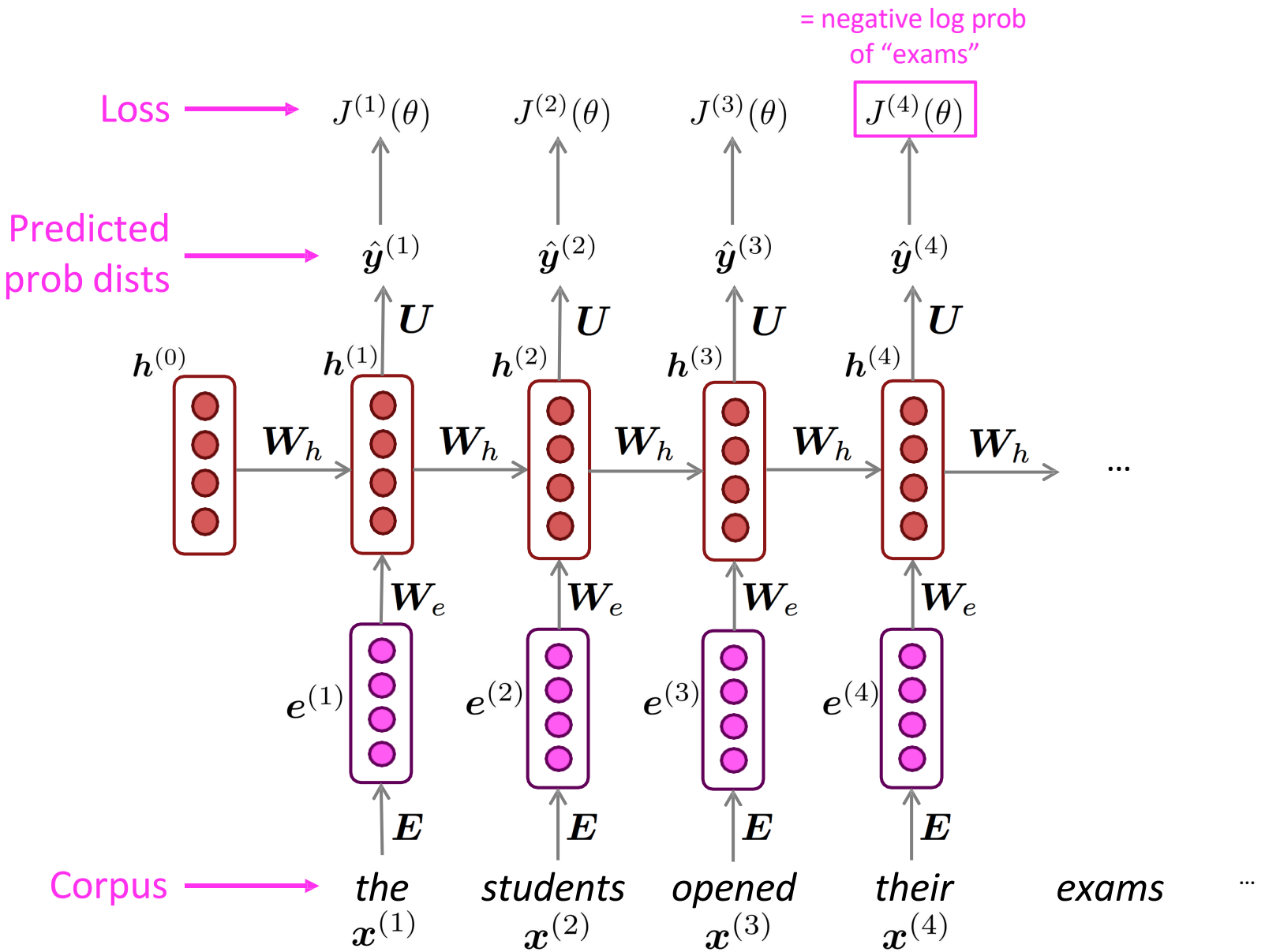
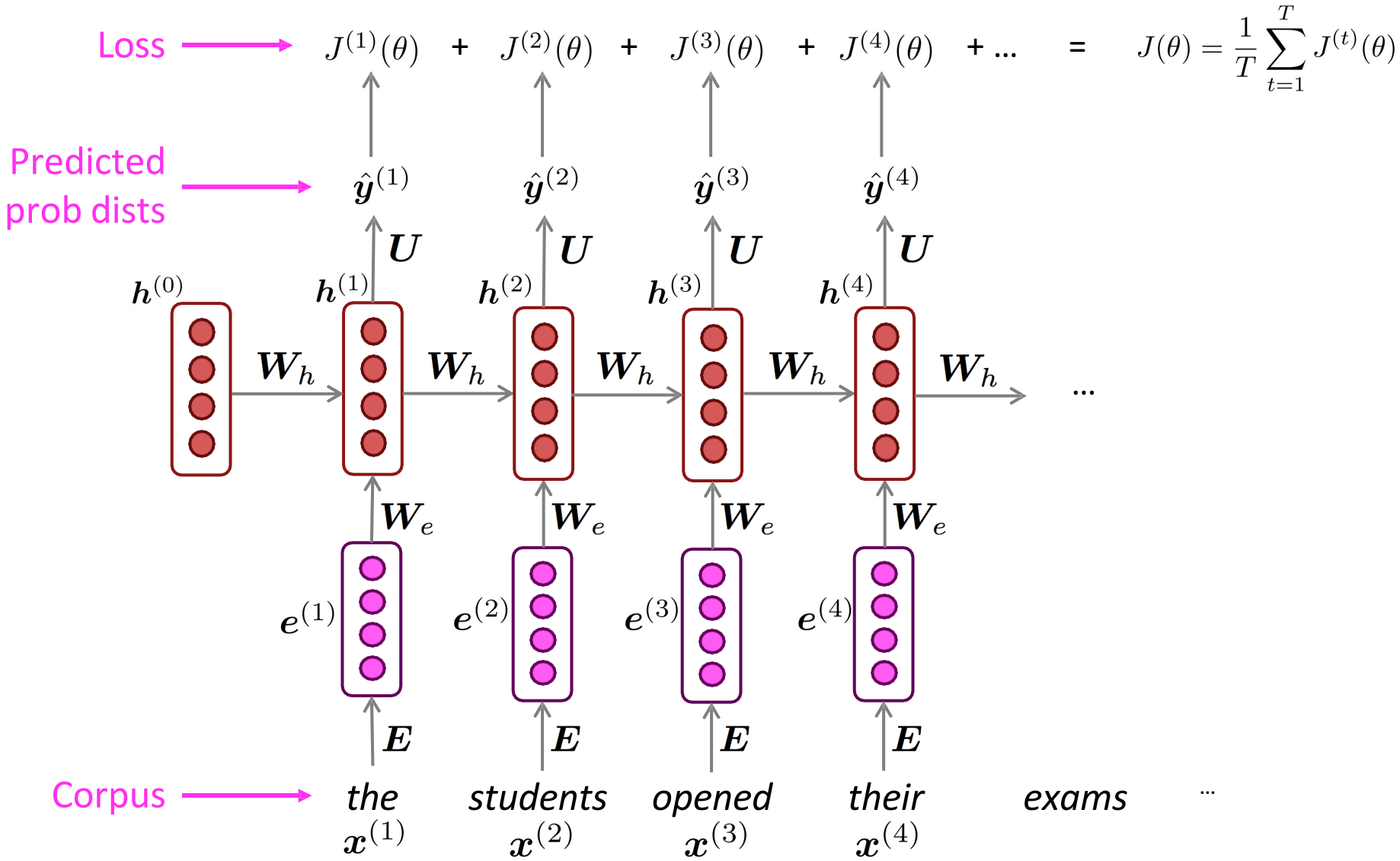


Training an RNN Language Model



Training an RNN Language Model

"Teacher forcing"



Training a RNN Language Model

- However: Computing loss and gradients across entire corpus $\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(T)}$ at once is too expensive (memory-wise)!

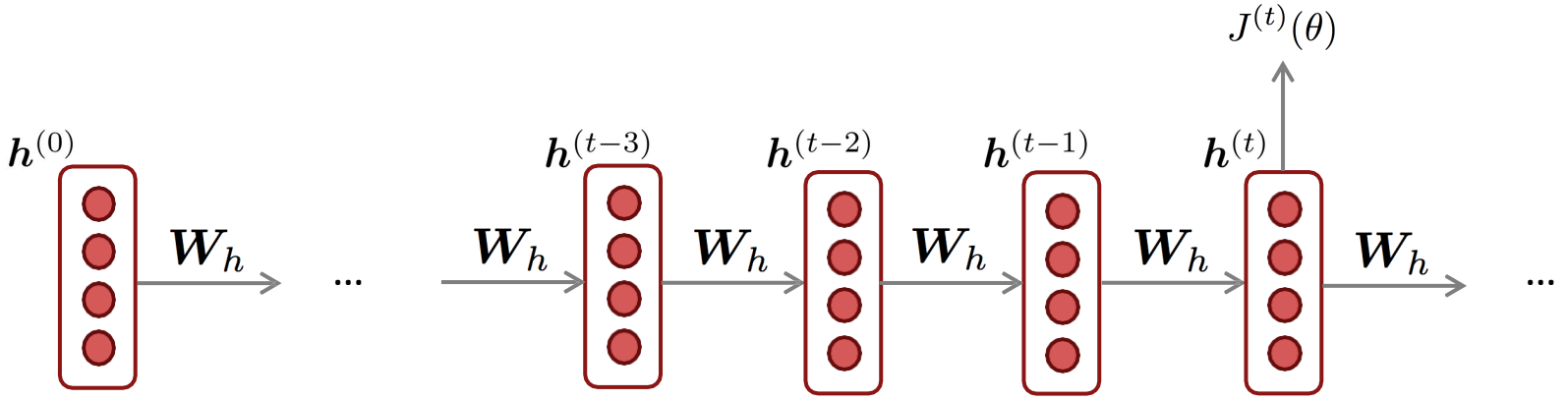
$$J(\theta) = \frac{1}{T} \sum_{t=1}^{T} J^{(t)}(\theta)$$

- In practice, consider $\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(T)}$ as a sentence (or a document)

- Recall: Stochastic Gradient Descent allows us to compute loss and gradients for small chunk of data, and update.

- Compute loss $J(\theta)$ for a sentence (actually, a batch of sentences), compute gradients and update weights. Repeat on a new batch of sentences.

Backpropagation for RNNs



Question: What's the derivative of $J^{(t)}(\theta)$ w.r.t. the repeated weight matrix $\boldsymbol{W}_h$?

Answer: $$\frac{\partial J^{(t)}}{\partial \boldsymbol{W_h}} = \sum_{i=1}^{t} \left. \frac{\partial J^{(t)}}{\partial \boldsymbol{W_h}} \right|_{(i)}$$

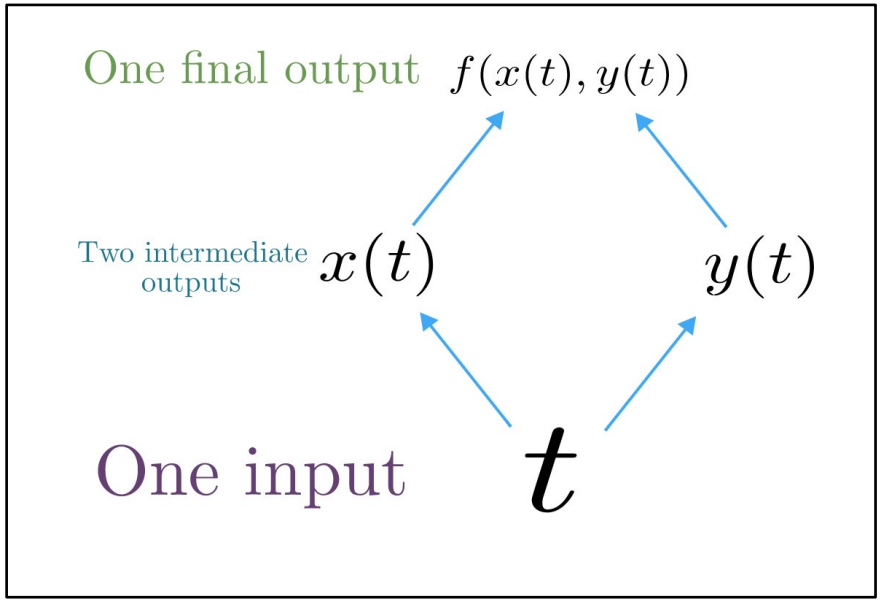
"The gradient w.r.t. a repeated weight is the sum of the gradient w.r.t. each time it appears"

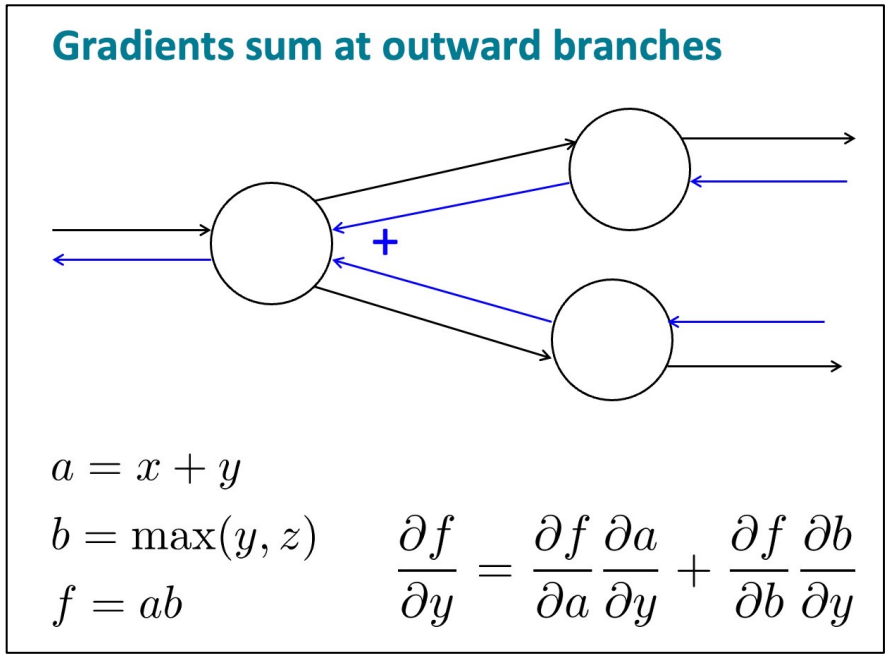
Why?

Multivariable Chain Rule

- Given a multivariable function $f(x, y)$, and two single variable functions $x(t)$ and $y(t)$, here's what the multivariable chain rule says:

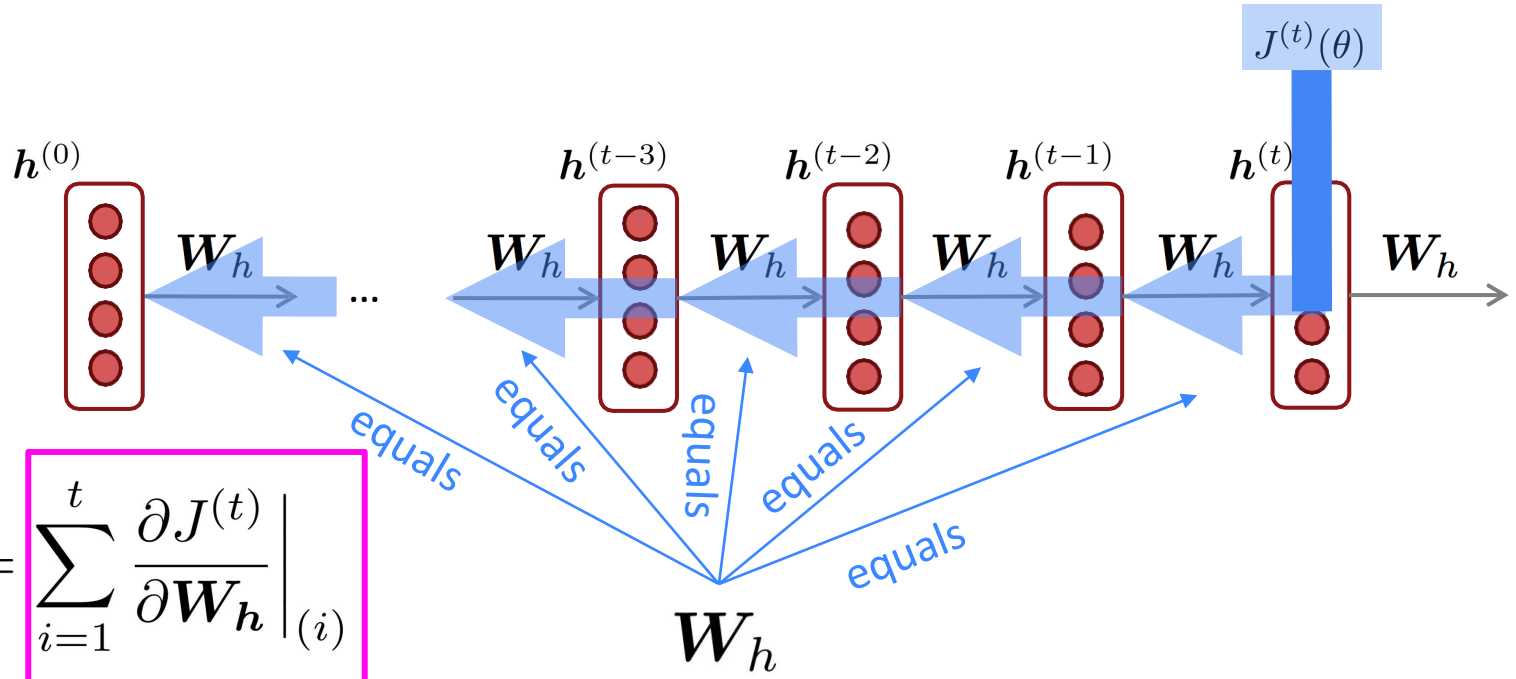
$$\underbrace{\frac{d}{dt} f(x(t), y(t))}_{\text{Derivative of composition function}} = \frac{\partial f}{\partial x}\frac{dx}{dt} + \frac{\partial f}{\partial y}\frac{dy}{dt}$$





Source:
https://www.khanacademy.org/math/multivariable-calculus/multivariable-derivatives/differentiating-vector-valued-functions/a/multivariable-chain-rule-simple-version

Training the parameters of RNNs: Backpropagation for RNNs



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

$$\frac{\partial J^{(t)}}{\partial \boldsymbol{W_h}} = \sum_{i=1}^{t} \frac{\partial J^{(t)}}{\partial \boldsymbol{W_h}}\bigg|_{(i)}$$

Question: How do we calculate this?

Answer: Backpropagate over timesteps $i = t, \ldots, 0$, summing gradients as you go. This algorithm is called **"backpropagation through time"** [Werbos, P.G., 1988, *Neural Networks* **1**, and others]

Apply the multivariable chain rule:

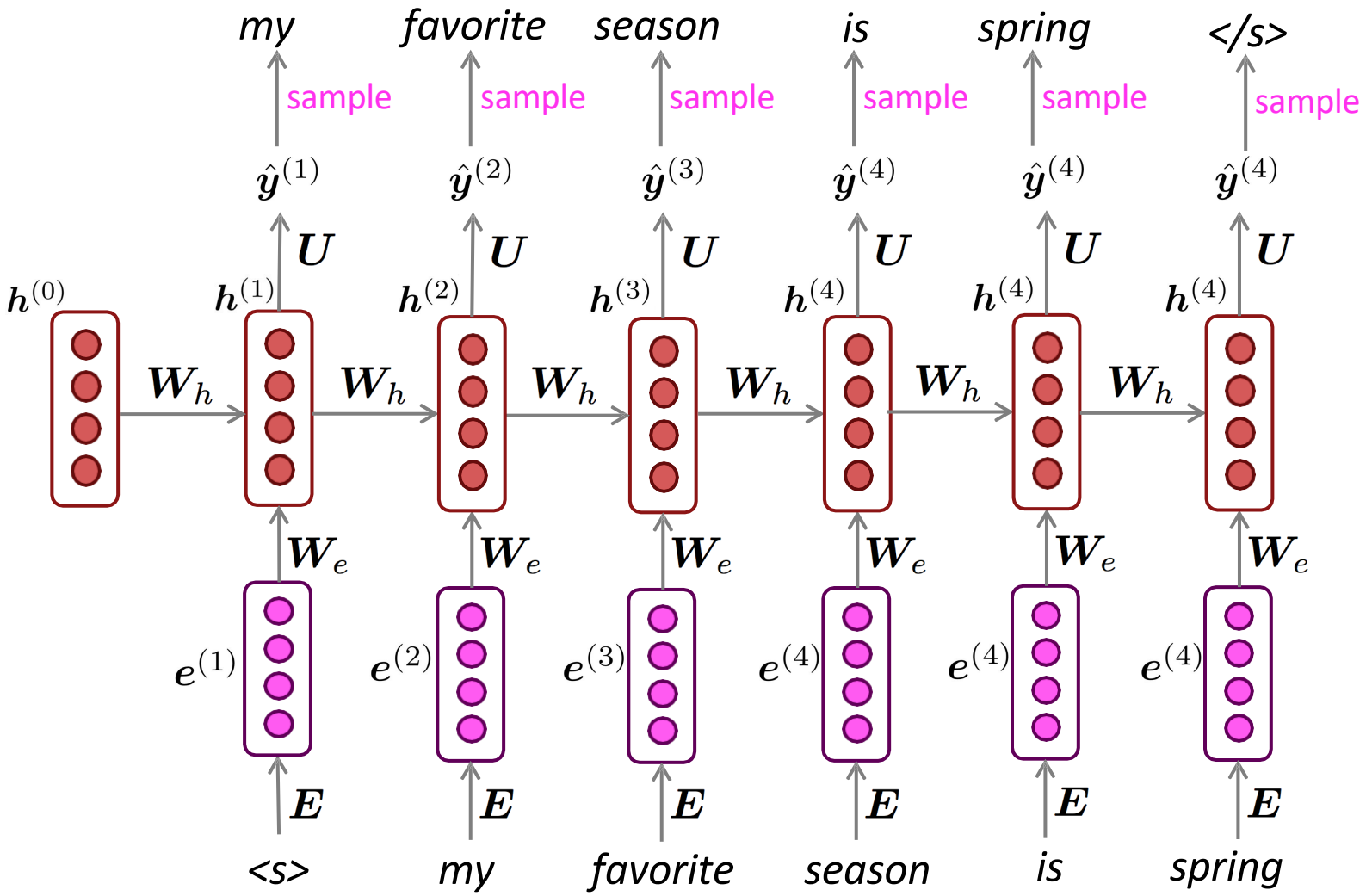
$$\frac{\partial J^{(t)}}{\partial \boldsymbol{W}_h} = \sum_{i=1}^{t} \frac{\partial J^{(t)}}{\partial \boldsymbol{W}_h}\bigg|_{(i)} \frac{\partial \boldsymbol{W}_h|_{(i)}}{\partial \boldsymbol{W}_h}$$

$= 1$

$$= \sum_{i=1}^{t} \frac{\partial J^{(t)}}{\partial \boldsymbol{W}_h}\bigg|_{(i)}$$

Generating with an RNN Language Model ("Generating roll outs")

Just like an n-gram Language Model, you can use a RNN Language Model to generate text by repeated sampling. Sampled output becomes next step's input.



Generating text with an RNN Language Model

Let's have some fun!

- You can train an RNN-LM on any kind of text, then generate text in that style.
- RNN-LM trained on Obama speeches:

The United States will step up to the cost of a new challenges of the American people that will share the fact that we created the problem. They were attacked and so that they have to say that all the task of the final days of war that I will not be able to get this done.

Source: https://medium.com/@samim/obama-rnn-machine-generated-political-speeches-c8abd18a2ea0

Generating text with an RNN Language Model

Let's have some fun!

- You can train an RNN-LM on any kind of text, then generate text in that style.
- RNN-LM trained on *Harry Potter*:

"Sorry," Harry shouted, panicking—"I'll leave those brooms in London, are they?"

"No idea," said Nearly Headless Nick, casting low close by Cedric, carrying the last bit of treacle Charms, from Harry's shoulder, and to answer him the common room perched upon it, four arms held a shining knob from when the spider hadn't felt it seemed. He reached the teams too.

Source: https://medium.com/deep-writing/harry-potter-written-by-artificial-intelligence-8a9431803da6

Generating text with an RNN Language Model

Let’s have some fun!

- You can train an RNN-LM on any kind of text, then generate text in that style.
- RNN-LM trained on recipes:

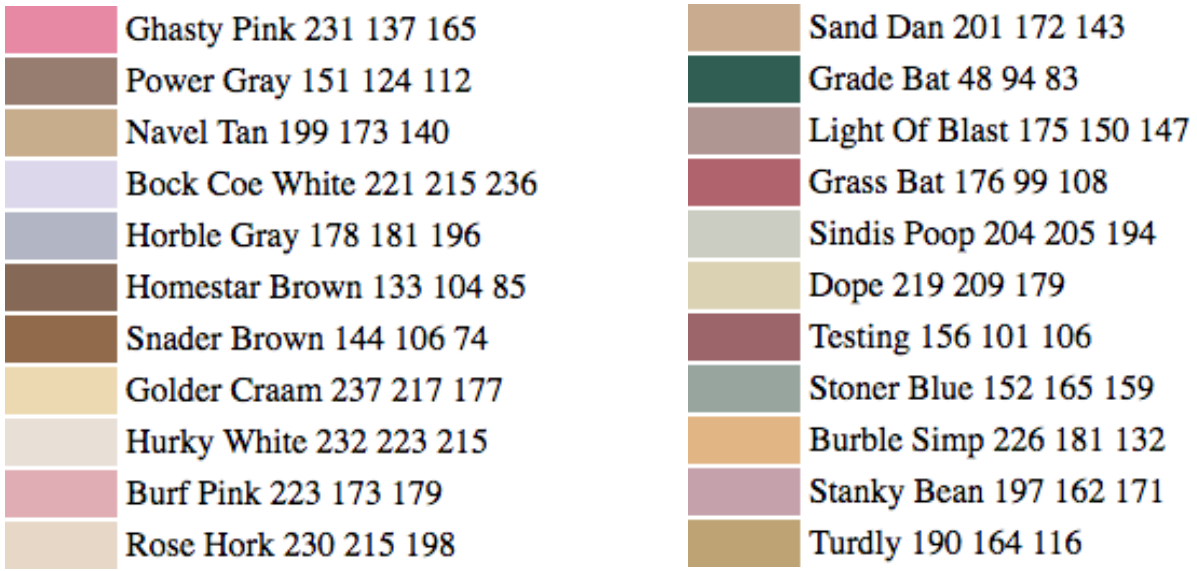
```
      Title: CHOCOLATE RANCH BARBECUE
Categories: Game, Casseroles, Cookies, Cookies
      Yield: 6 Servings

      2 tb Parmesan cheese -- chopped
      1 c  Coconut milk
      3    Eggs, beaten

  Place each pasta over layers of lumps. Shape mixture into the moderate oven and simmer
  until firm. Serve hot in bodied fresh, mustard, orange and cheese.

  Combine the cheese and salt together the dough in a large skillet; add the ingredients
  and stir in the chocolate and pepper.
```

Source: https://gist.github.com/nylki/1efbaa36635956d35bcc

Generating text with a RNN Language Model

Let's have some fun!

- You can train a RNN-LM on any kind of text, then generate text in that style.
- RNN-LM trained on paint color names:



This is an example of a character-level RNN-LM (predicts what character comes next)

Source: http://aiweirdness.com/post/160776374467/new-paint-colors-invented-by-neural-network

Evaluating Language Models

- The standard evaluation metric for Language Models is perplexity.

$$\text{perplexity} = \prod_{t=1}^{T} \left(\frac{1}{P_{\text{LM}}(\boldsymbol{x}^{(t+1)} | \ \boldsymbol{x}^{(t)}, \ldots, \boldsymbol{x}^{(1)})} \right)^{1/T}$$

Normalized by number of words

Inverse probability of corpus, according to Language Model

- This is equal to the exponential of the cross-entropy loss $J(\theta)$:

$$= \prod_{t=1}^{T} \left(\frac{1}{\hat{\boldsymbol{y}}^{(t)}_{\boldsymbol{x}_{t+1}}} \right)^{1/T} = \exp\left(\frac{1}{T} \sum_{t=1}^{T} -\log \hat{\boldsymbol{y}}^{(t)}_{\boldsymbol{x}_{t+1}} \right) = \exp(J(\theta))$$

Lower perplexity is better!

RNNs greatly improved perplexity over what came before

n-gram model →

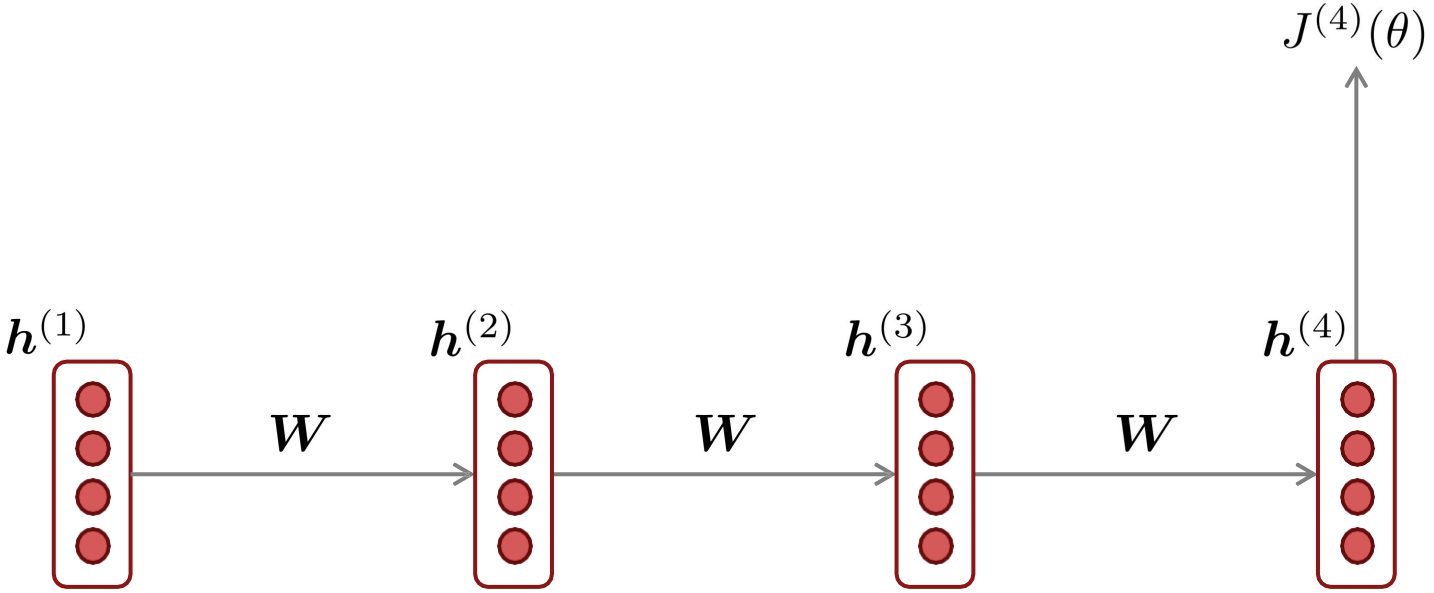
Increasingly complex RNNs ↓

Model	Perplexity
Interpolated Kneser-Ney 5-gram (Chelba et al., 2013)	67.6
RNN-1024 + MaxEnt 9-gram (Chelba et al., 2013)	51.3
RNN-2048 + BlackOut sampling (Ji et al., 2015)	68.3
Sparse Non-negative Matrix factorization (Shazeer et al., 2015)	52.9
LSTM-2048 (Jozefowicz et al., 2016)	43.7
2-layer LSTM-8192 (Jozefowicz et al., 2016)	30
Ours small (LSTM-2048)	43.9
Ours large (2-layer LSTM-2048)	39.8

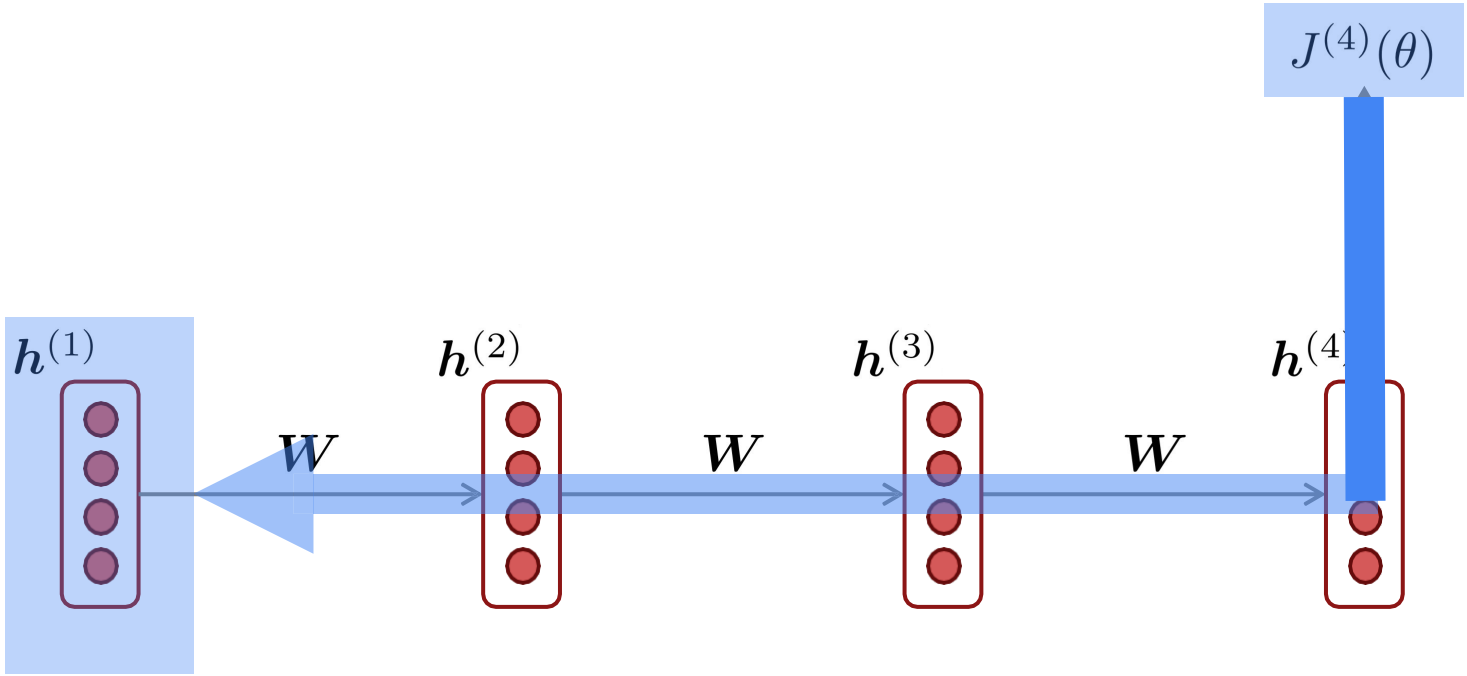
↓ Perplexity improves (lower is better)

Source: https://research.fb.com/building-an-efficient-neural-language-model-over-a-billion-words/

4. Problems with RNNs: Vanishing and Exploding Gradients

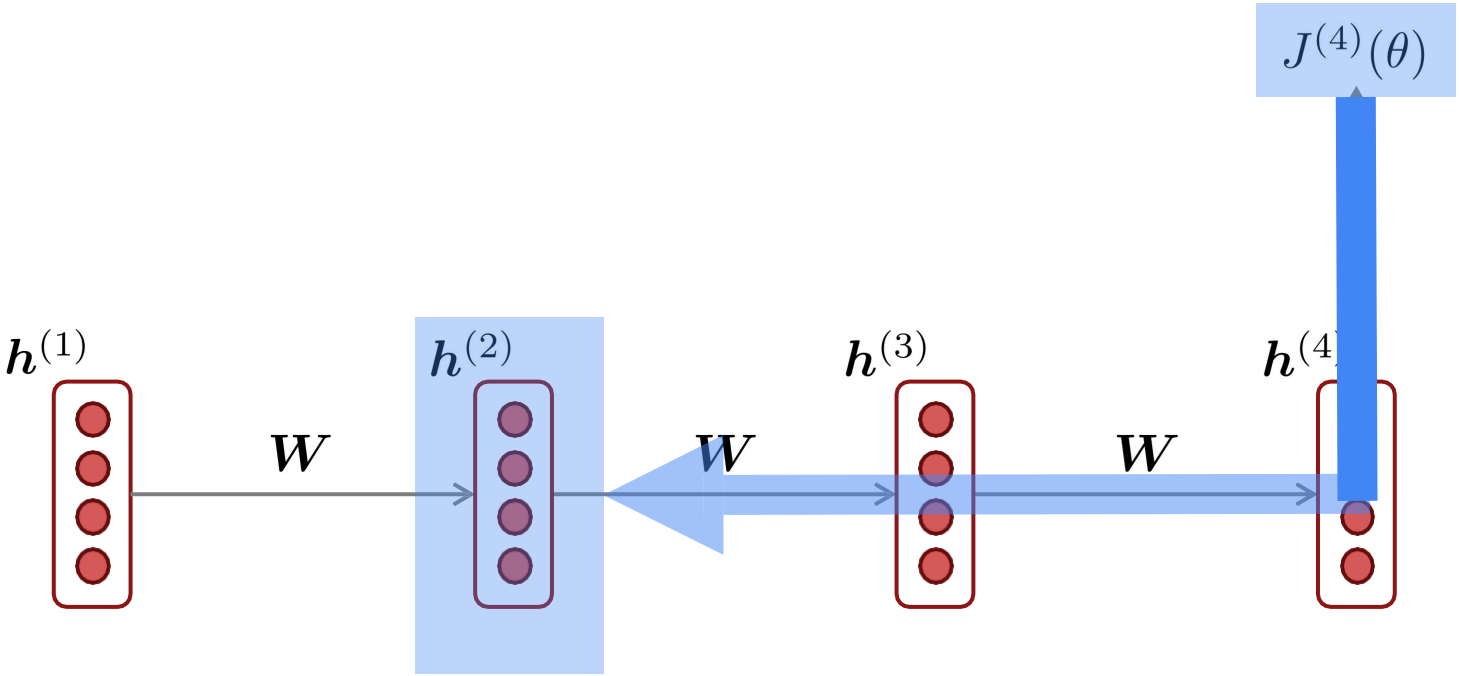


Vanishing gradient intuition



$$\frac{\partial J^{(4)}}{\partial \boldsymbol{h}^{(1)}} = \ ?$$

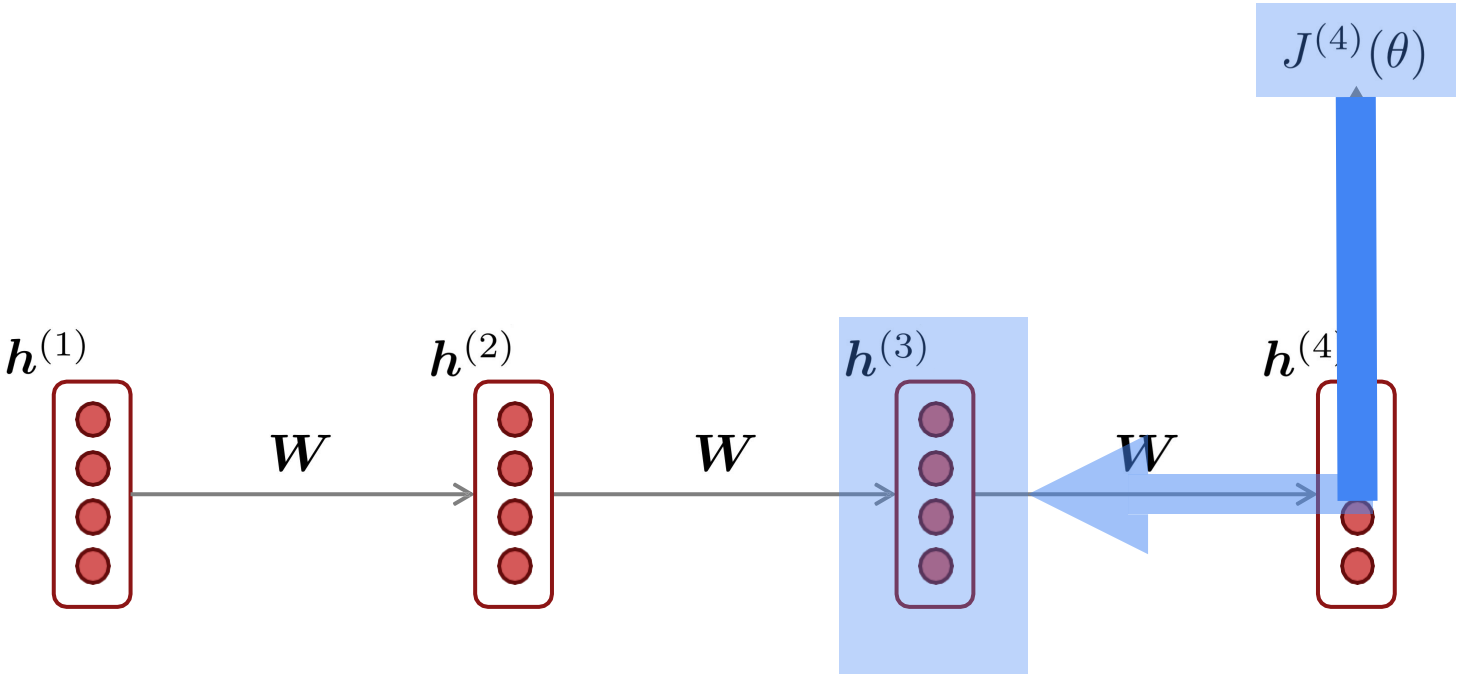
Vanishing gradient intuition



$$\frac{\partial J^{(4)}}{\partial \boldsymbol{h}^{(1)}} = \frac{\partial \boldsymbol{h}^{(2)}}{\partial \boldsymbol{h}^{(1)}} \times \frac{\partial J^{(4)}}{\partial \boldsymbol{h}^{(2)}}$$

chain rule!

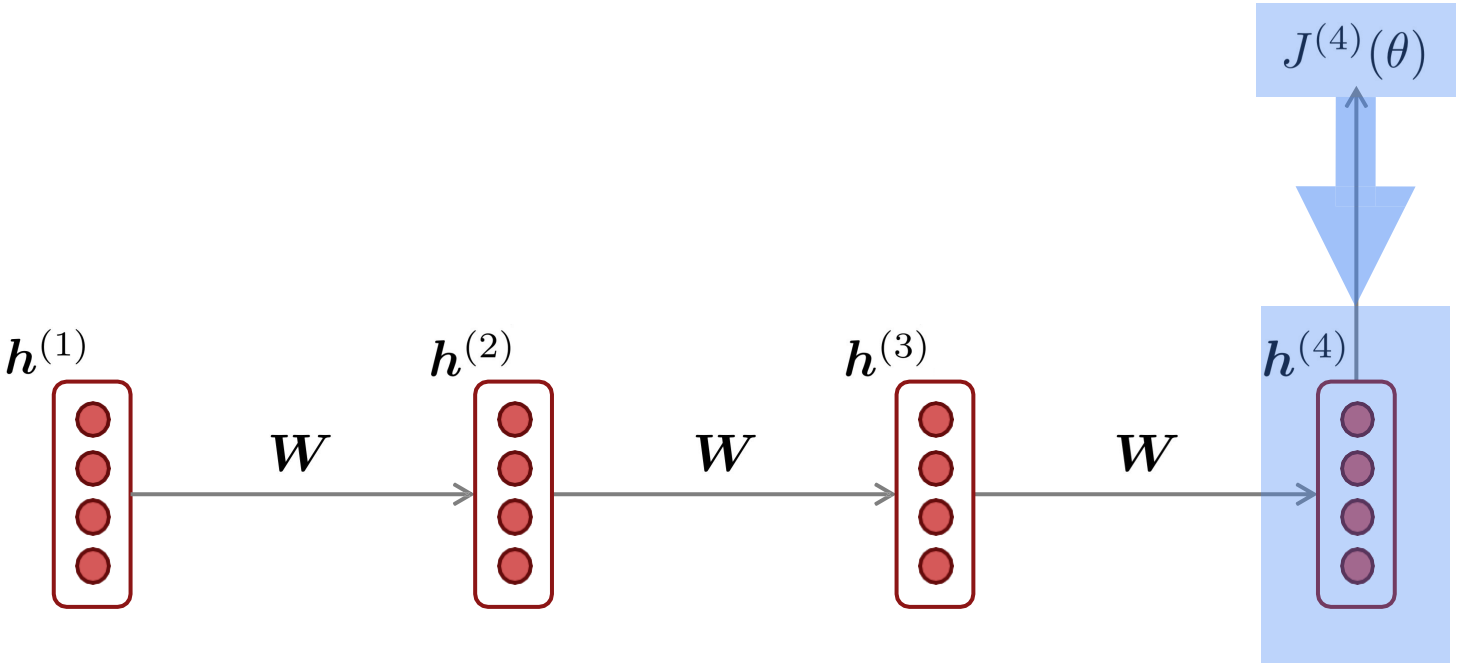
Vanishing gradient intuition



$$\frac{\partial J^{(4)}}{\partial \boldsymbol{h}^{(1)}} = \frac{\partial \boldsymbol{h}^{(2)}}{\partial \boldsymbol{h}^{(1)}} \times \frac{\partial \boldsymbol{h}^{(3)}}{\partial \boldsymbol{h}^{(2)}} \times \frac{\partial J^{(4)}}{\partial \boldsymbol{h}^{(3)}}$$

chain rule!

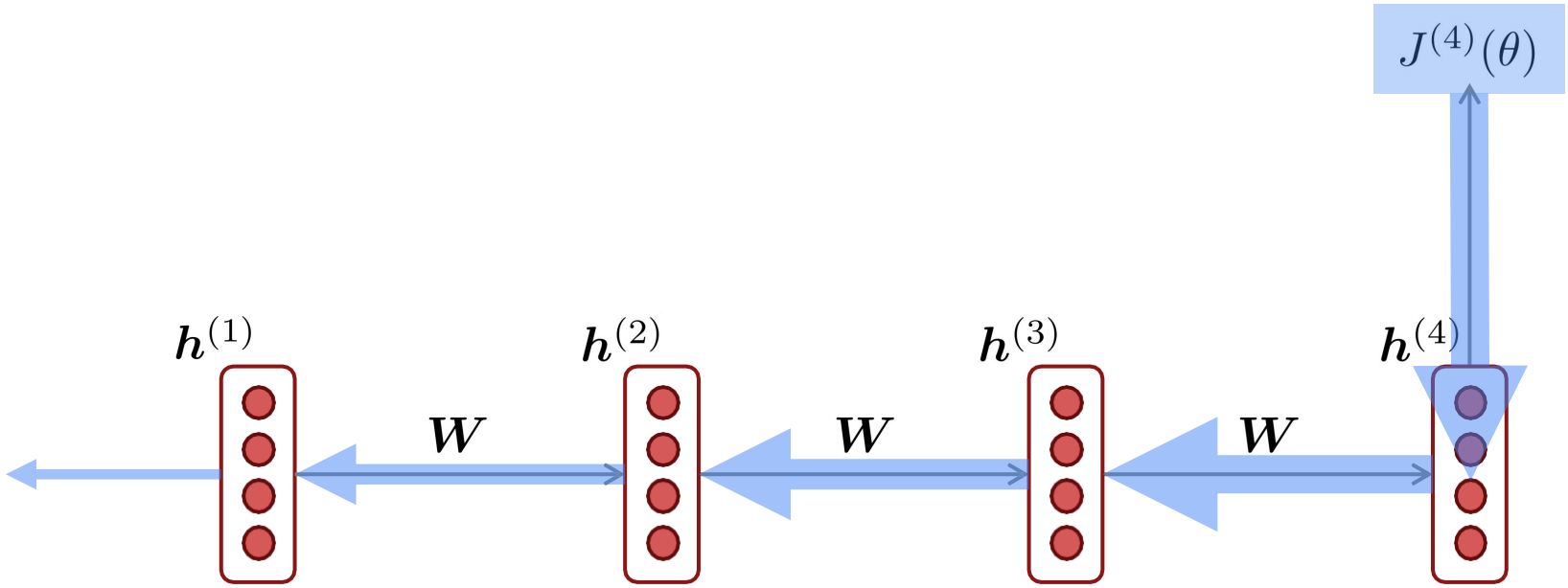
Vanishing gradient intuition



$$\frac{\partial J^{(4)}}{\partial \boldsymbol{h}^{(1)}} = \frac{\partial \boldsymbol{h}^{(2)}}{\partial \boldsymbol{h}^{(1)}} \times \frac{\partial \boldsymbol{h}^{(3)}}{\partial \boldsymbol{h}^{(2)}} \times \frac{\partial \boldsymbol{h}^{(4)}}{\partial \boldsymbol{h}^{(3)}} \times \frac{\partial J^{(4)}}{\partial \boldsymbol{h}^{(4)}}$$

chain rule!

Vanishing gradient intuition



$$\frac{\partial J^{(4)}}{\partial h^{(1)}} = \frac{\partial h^{(2)}}{\partial h^{(1)}} \times \frac{\partial h^{(3)}}{\partial h^{(2)}} \times \frac{\partial h^{(4)}}{\partial h^{(3)}} \times \frac{\partial J^{(4)}}{\partial h^{(4)}}$$

What happens if these are small?

Vanishing gradient problem:
When these are small, the gradient signal gets smaller and smaller as it backpropagates further

Vanishing gradient proof sketch (linear case)

ONLY READ IF INTERESTED

- Recall: $$\boldsymbol{h}^{(t)} = \sigma\left(\boldsymbol{W}_h \boldsymbol{h}^{(t-1)} + \boldsymbol{W}_x \boldsymbol{x}^{(t)} + \boldsymbol{b}_1\right)$$
- What if σ were the identity function, $\sigma(x) = x$?

$$\frac{\partial \boldsymbol{h}^{(t)}}{\partial \boldsymbol{h}^{(t-1)}} = \operatorname{diag}\left(\sigma'\left(\boldsymbol{W}_h \boldsymbol{h}^{(t-1)} + \boldsymbol{W}_x \boldsymbol{x}^{(t)} + \boldsymbol{b}_1\right)\right) \boldsymbol{W}_h \qquad \text{(chain rule)}$$

$$= \boldsymbol{I}\, \boldsymbol{W}_h = \boldsymbol{W}_h$$

- Consider the gradient of the loss $J^{(i)}(\theta)$ on step i, with respect to the hidden state $\boldsymbol{h}^{(j)}$ on some previous step j. *Let* $\ell = i - j$

$$\frac{\partial J^{(i)}(\theta)}{\partial \boldsymbol{h}^{(j)}} = \frac{\partial J^{(i)}(\theta)}{\partial \boldsymbol{h}^{(i)}} \prod_{j<t\leq i} \frac{\partial \boldsymbol{h}^{(t)}}{\partial \boldsymbol{h}^{(t-1)}} \qquad \text{(chain rule)}$$

$$= \frac{\partial J^{(i)}(\theta)}{\partial \boldsymbol{h}^{(i)}} \prod_{j<t\leq i} \boldsymbol{W}_h = \frac{\partial J^{(i)}(\theta)}{\partial \boldsymbol{h}^{(i)}} \boldsymbol{W}_h^{\ell} \qquad \text{(value of } \frac{\partial \boldsymbol{h}^{(t)}}{\partial \boldsymbol{h}^{(t-1)}}\text{)}$$

If W_h is "small", then this term gets exponentially problematic as ℓ becomes large

Source: "On the difficulty of training recurrent neural networks", Pascanu et al, 2013. http://proceedings.mlr.press/v28/pascanu13.pdf (and supplemental materials), at http://proceedings.mlr.press/v28/pascanu13-supp.pdf

Vanishing gradient proof sketch (linear case)

ONLY READ IF INTERESTED

- What's wrong with $\boldsymbol{W}_h^\ell$?
- Consider if the eigenvalues of $\boldsymbol{W}_h$ are all less than 1: (sufficient but not necessary)

$$\lambda_1, \lambda_2, \ldots, \lambda_n < 1$$
$$\boldsymbol{q}_1, \boldsymbol{q}_2, \ldots, \boldsymbol{q}_n \text{ (eigenvectors)}$$

- We can write $\frac{\partial J^{(i)}(\theta)}{\partial \boldsymbol{h}^{(i)}} \boldsymbol{W}_h^\ell$ using the eigenvectors of $\boldsymbol{W}_h$ as a basis:

$$\frac{\partial J^{(i)}(\theta)}{\partial \boldsymbol{h}^{(i)}} \boldsymbol{W}_h^\ell = \sum_{i=1}^{n} c_i \lambda_i^\ell \boldsymbol{q}_i \approx \mathbf{0} \text{ (for large } \ell)$$

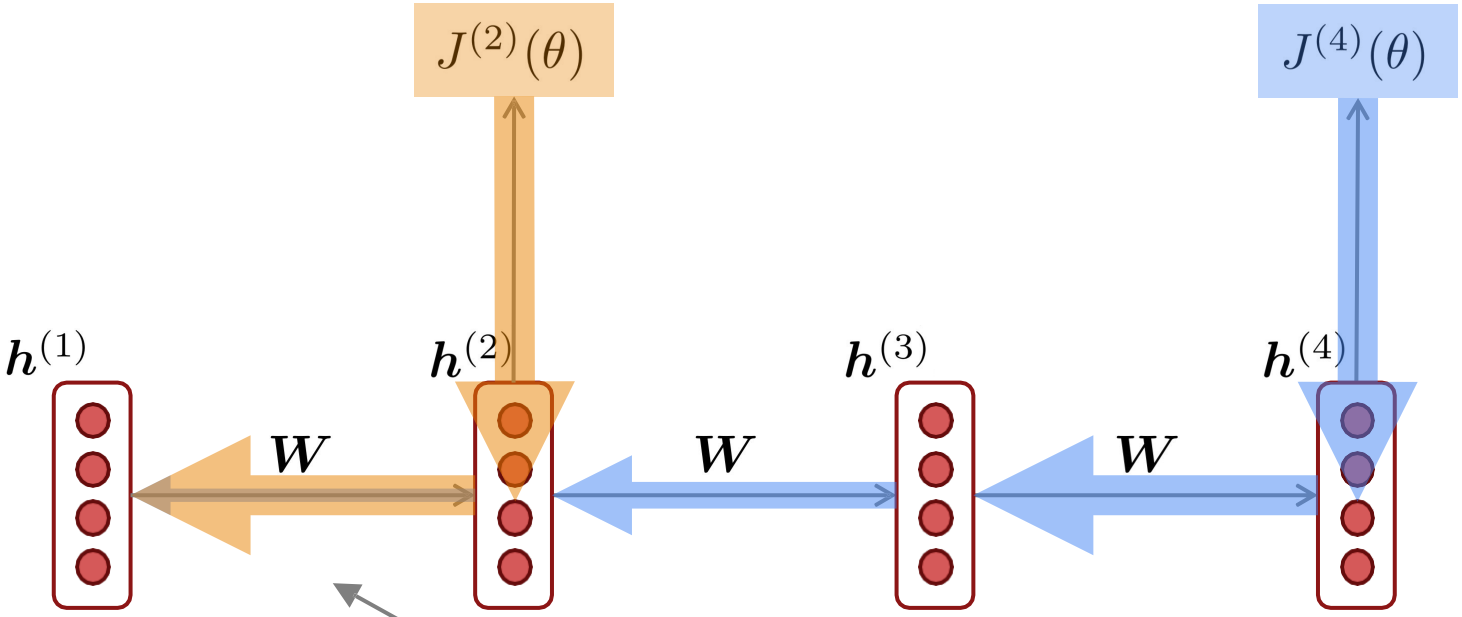
Approaches 0 as ℓ grows, so gradient vanishes

- What about nonlinear activations σ (i.e., what we use?)
  - Pretty much the same thing, except the proof requires $\lambda_i < \gamma$

for some γ dependent on dimensionality and σ

Source: "On the difficulty of training recurrent neural networks", Pascanu et al, 2013. http://proceedings.mlr.press/v28/pascanu13.pdf (and supplemental materials), at http://proceedings.mlr.press/v28/pascanu13-supp.pdf

Why is vanishing gradient a problem?



Gradient signal from far away is lost because it's much smaller than gradient signal from close-by.

So, model weights are updated only with respect to near effects, not long-term effects.

Effect of vanishing gradient on RNN-LM

- **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 7th 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

Why is exploding gradient a problem?

- If the gradient becomes too big, then the SGD update step becomes too big:

$$\theta^{new} = \theta^{old} - \overbrace{\alpha}^{\text{learning rate}} \underbrace{\nabla_\theta J(\theta)}_{\text{gradient}}$$

- This can cause bad updates: we take too large a step and reach a weird and bad parameter configuration (with large loss)
  - You think you've found a hill to climb, but suddenly you're in Iowa

- In the worst case, this will result in Inf or NaN in your network
(then you have to restart training from an earlier checkpoint)

Gradient clipping: solution for exploding gradient

- **Gradient clipping**: if the norm of the gradient is greater than some threshold, scale it down before applying SGD update

Algorithm 1 Pseudo-code for norm clipping

$\hat{\mathbf{g}} \leftarrow \frac{\partial \mathcal{E}}{\partial \theta}$
if $\|\hat{\mathbf{g}}\| \geq threshold$ **then**
  $\hat{\mathbf{g}} \leftarrow \frac{threshold}{\|\hat{\mathbf{g}}\|}\hat{\mathbf{g}}$
end if

- **Intuition**: take a step in the same direction, but a smaller step

- In practice, **remembering to clip gradients is important**, but exploding gradients are an easy problem to solve

Source: "On the difficulty of training recurrent neural networks", Pascanu et al, 2013. http://proceedings.mlr.press/v28/pascanu13.pdf

How to fix the vanishing gradient problem?

- The main problem is that *it's too difficult for the RNN to learn to preserve information over many timesteps*.

- In a vanilla RNN, the hidden state is constantly being rewritten

$$\boldsymbol{h}^{(t)} = \sigma\left(\boldsymbol{W}_h \boldsymbol{h}^{(t-1)} + \boldsymbol{W}_x \boldsymbol{x}^{(t)} + \boldsymbol{b}\right)$$

- First off next time: How about an RNN with separate memory which is added to?
  - LSTMs

- And then: Creating more direct and linear pass-through connections in model
  - Attention, residual connections, etc.

Long Short-Term Memory RNNs (LSTMs)

- A type of RNN proposed by Hochreiter and Schmidhuber in 1997 as a solution to the problem of vanishing gradients
  - Everyone cites that paper but really a crucial part of the modern LSTM is from Gers et al. (2000) 💜💜
- Only started to be recognized as promising through the work of S's student Alex Graves c. 2006
  - Work in which he also invented CTC (connectionist temporal classification) for speech recognition
- But only really became well-known after Hinton brought it to Google in 2013
  - Following Graves having been a postdoc with Hinton

Hochreiter and Schmidhuber, 1997. Long short-term memory. https://www.bioinf.jku.at/publications/older/2604.pdf
Gers, Schmidhuber, and Cummins, 2000. Learning to Forget: Continual Prediction with LSTM. https://dl.acm.org/doi/10.1162/089976600300015015
Graves, Fernandez, Gomez, and Schmidhuber, 2006. Connectionist temporal classification: Labelling unsegmented sequence data with recurrent neural nets. https://www.cs.toronto.edu/~graves/icml_2006.pdf

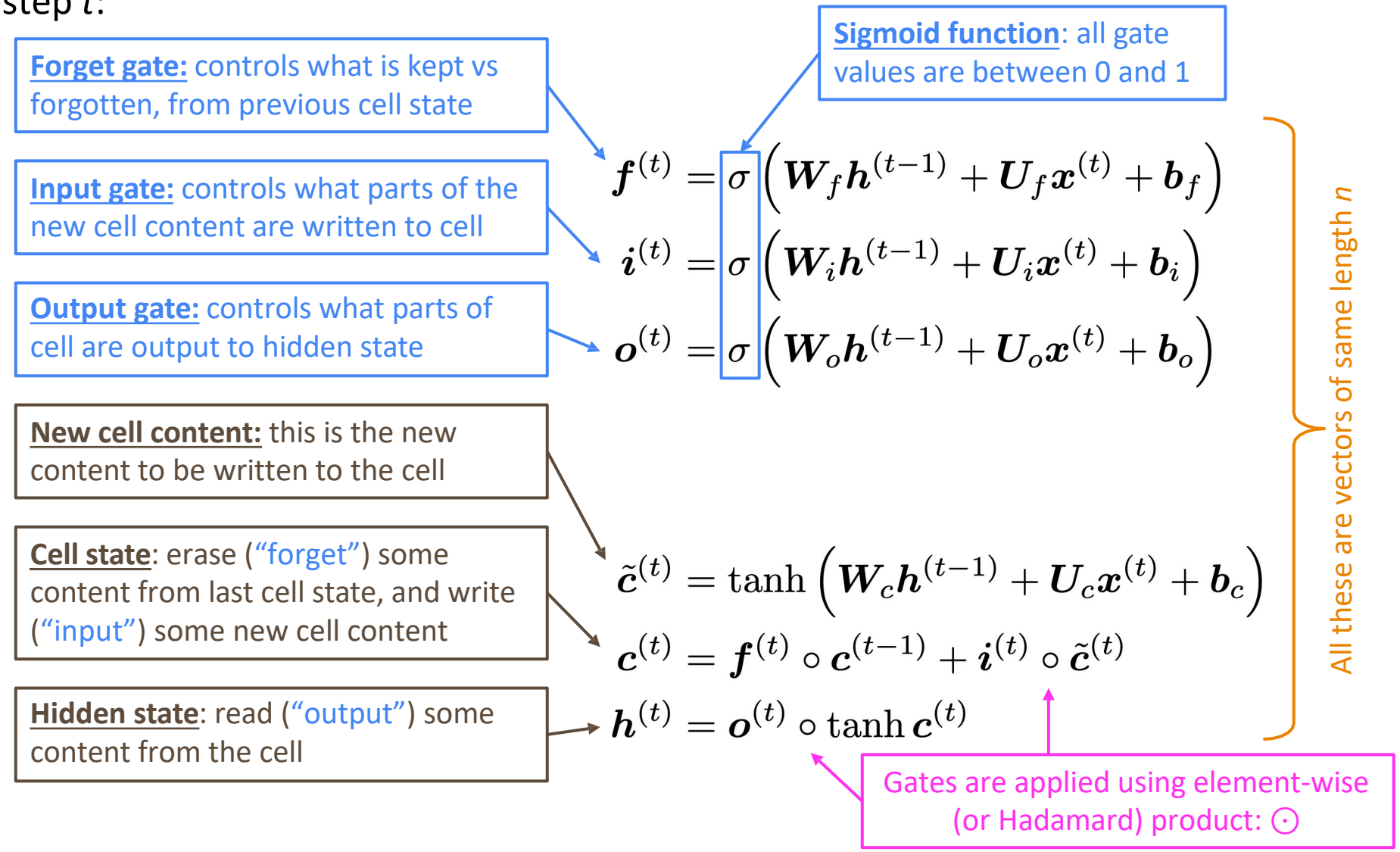
Long Short-Term Memory RNNs (LSTMs)

- On step *t*, there is a hidden state $\boldsymbol{h}^{(t)}$ and a cell state $\boldsymbol{c}^{(t)}$
  - Both are vectors length *n*
  - The cell stores long-term information
  - The LSTM can read, erase, and write information from the cell
    - The cell becomes conceptually rather like RAM in a computer

- The selection of which information is erased/written/read is controlled by three corresponding gates
  - The gates are also vectors of length *n*
  - On each timestep, each element of the gates can be open (1), closed (0), or somewhere in-between
  - The gates are dynamic: their value is computed based on the current context

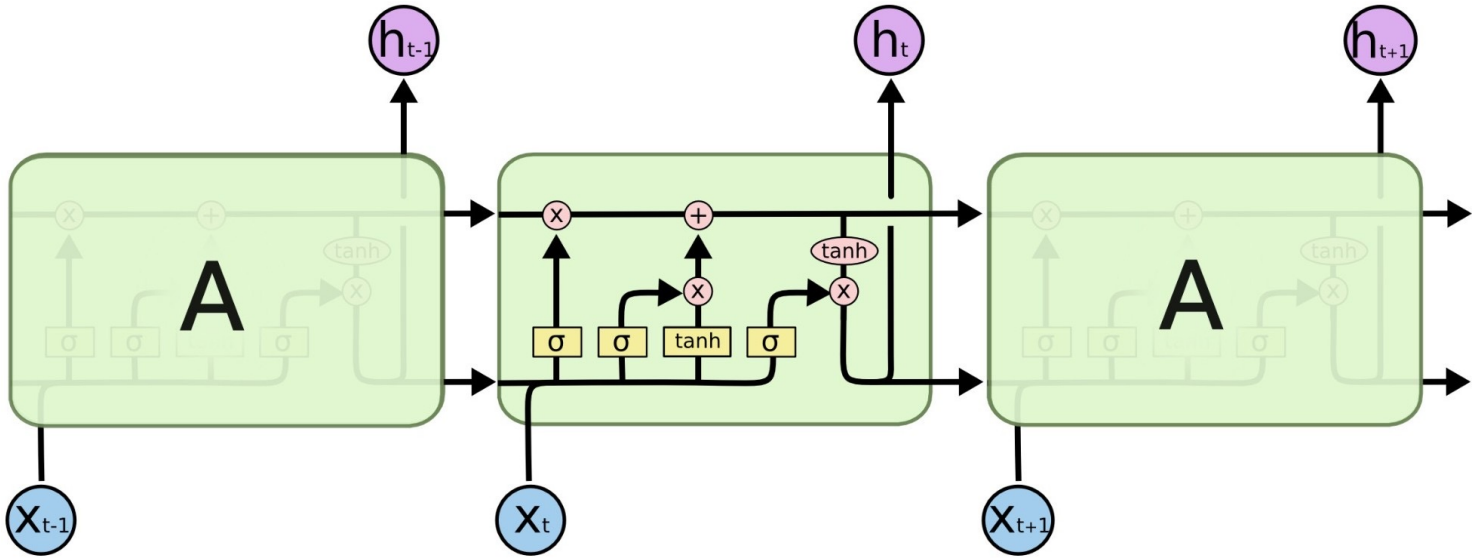
Long Short-Term Memory (LSTM)

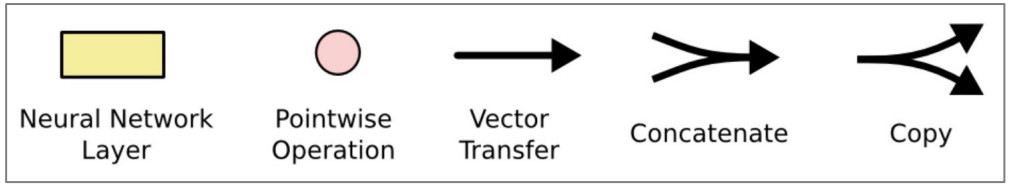
We have a sequence of inputs $x^{(t)}$, and we will compute a sequence of hidden states $h^{(t)}$ and cell states $c^{(t)}$. On timestep t:



Long Short-Term Memory (LSTM)

You can think of the LSTM equations visually like this:

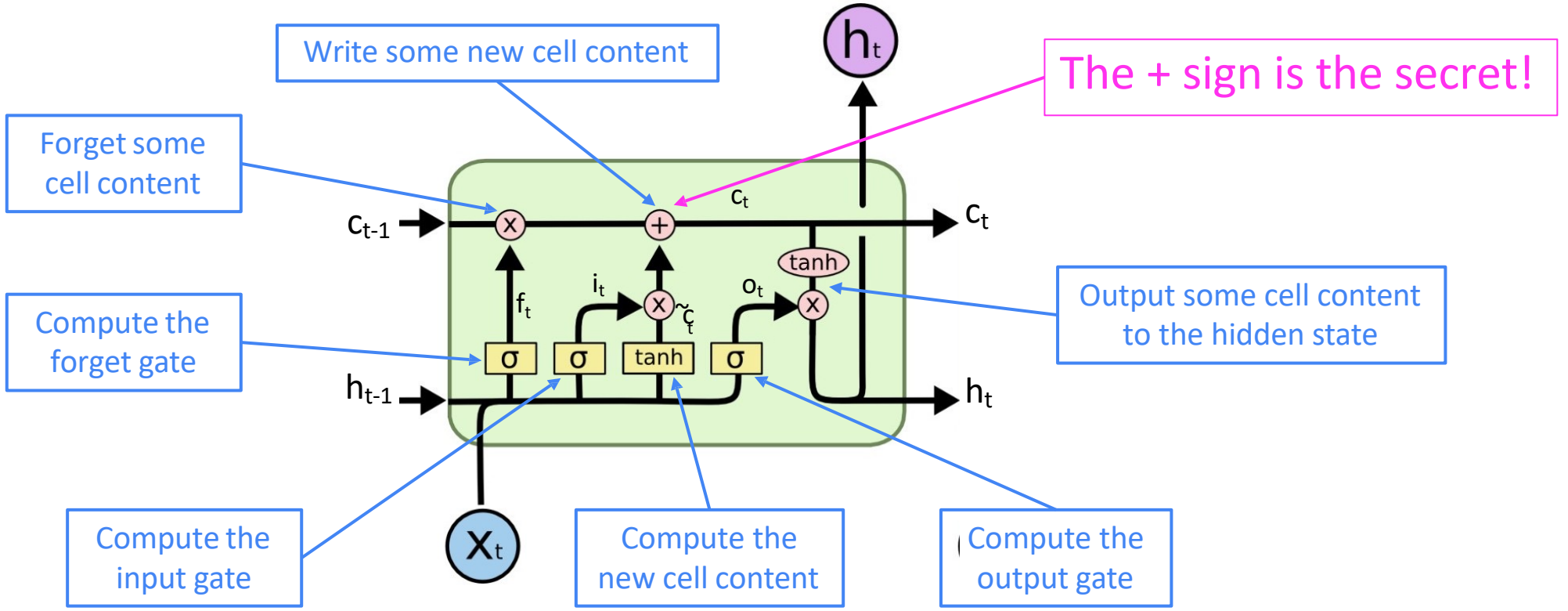




Source: http://colah.github.io/posts/2015-08-Understanding-LSTMs/

Long Short-Term Memory (LSTM)

You can think of the LSTM equations visually like this:



Source: http://colah.github.io/posts/2015-08-Understanding-LSTMs/

How does LSTM solve vanishing gradients?

- The LSTM architecture makes it much easier for an RNN to preserve information over many timesteps
  - e.g., if the forget gate is set to 1 for a cell dimension and the input gate set to 0, then the information of that cell is preserved indefinitely.
  - In contrast, it's harder for a vanilla RNN to learn a recurrent weight matrix W_h that preserves info in the hidden state
  - In practice, you get about 100 timesteps rather than about 7

- However, there are alternative ways of creating more direct and linear pass-through connections in models for long distance dependencies

Is vanishing/exploding gradient just an RNN problem?

- No! It can be a problem for all neural architectures (including feed-forward and convolutional), especially very deep ones.
  - Due to chain rule / choice of nonlinearity function, gradient can become vanishingly small as it backpropagates
  - Thus, lower layers are learned very slowly (i.e., are hard to train)
- Another solution: lots of new deep feedforward/convolutional architectures add more direct connections (thus allowing the gradient to flow)

For example:

- Residual connections aka "ResNet"
- Also known as skip-connections
- The identity connection preserves information by default
- This makes deep networks much easier to train

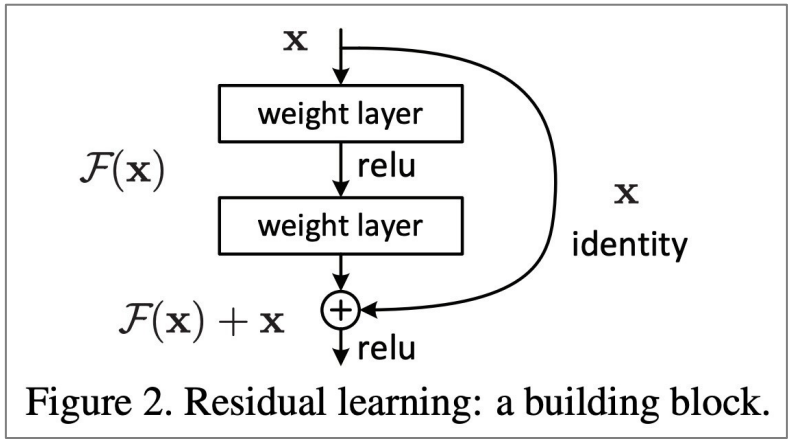


Figure 2. Residual learning: a building block.

"Deep Residual Learning for Image Recognition", He et al, 2015. https://arxiv.org/pdf/1512.03385.pdf

LSTMs: real-world success

- In 2013–2015, LSTMs started achieving state-of-the-art results
  - Successful tasks include handwriting recognition, speech recognition, machine translation, parsing, and image captioning, as well as language models
  - LSTMs became the dominant approach for most NLP tasks

- Now (2019–2023), Transformers have become dominant for all tasks
  - For example, in **WMT** (a Machine Translation conference + competition):
    - In WMT 2014, there were 0 neural machine translation systems (!)
    - In WMT 2016, the summary report contains "RNN" 44 times (and these systems won)
    - In WMT 2019: "RNN" 7 times, "Transformer" 105 times

Source: "Findings of the 2016 Conference on Machine Translation (WMT16)", Bojar et al. 2016, http://www.statmt.org/wmt16/pdf/W16-2301.pdf
Source: "Findings of the 2018 Conference on Machine Translation (WMT18)", Bojar et al. 2018, http://www.statmt.org/wmt18/pdf/WMT028.pdf
Source: "Findings of the 2019 Conference on Machine Translation (WMT19)", Barrault et al. 2019, http://www.statmt.org/wmt18/pdf/WMT028.pdf

5. Recap

- **Language Model**: A system that predicts the next word

- **Recurrent Neural Network**: A family of neural networks that:
  - Take sequential input of any length
  - Apply the same weights on each step
  - Can optionally produce output on each step

- Recurrent Neural Network ≠ Language Model

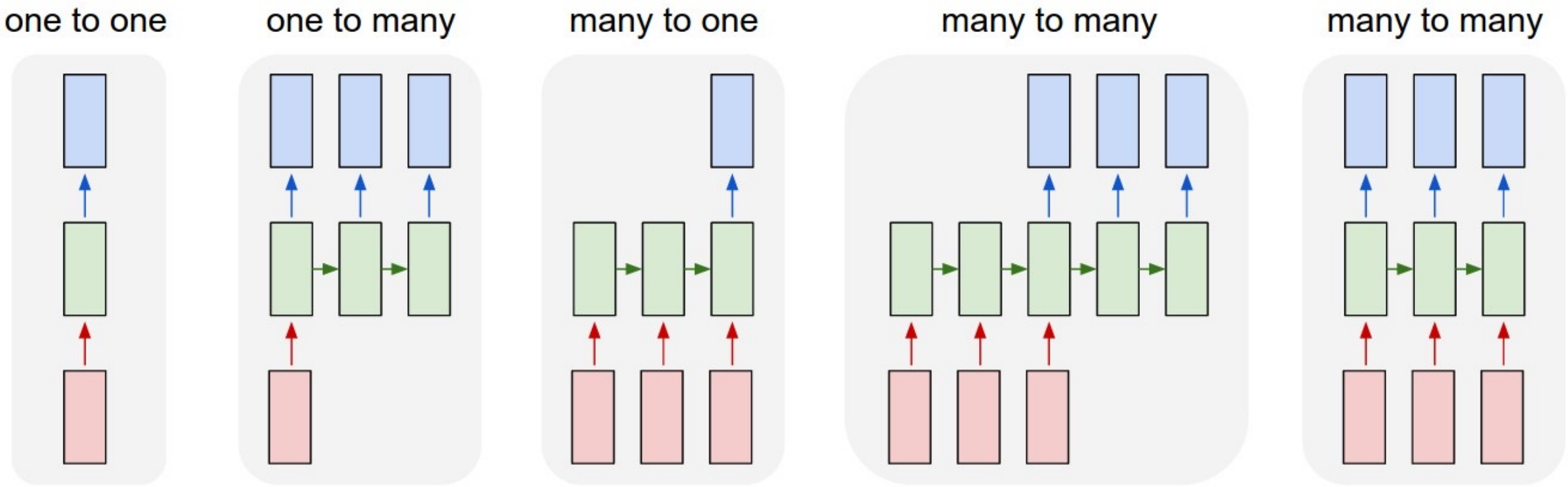
- We've shown that RNNs are a great way to build a LM (despite some problems)

- RNNs are also useful for much more!

Why should we care about Language Modeling?

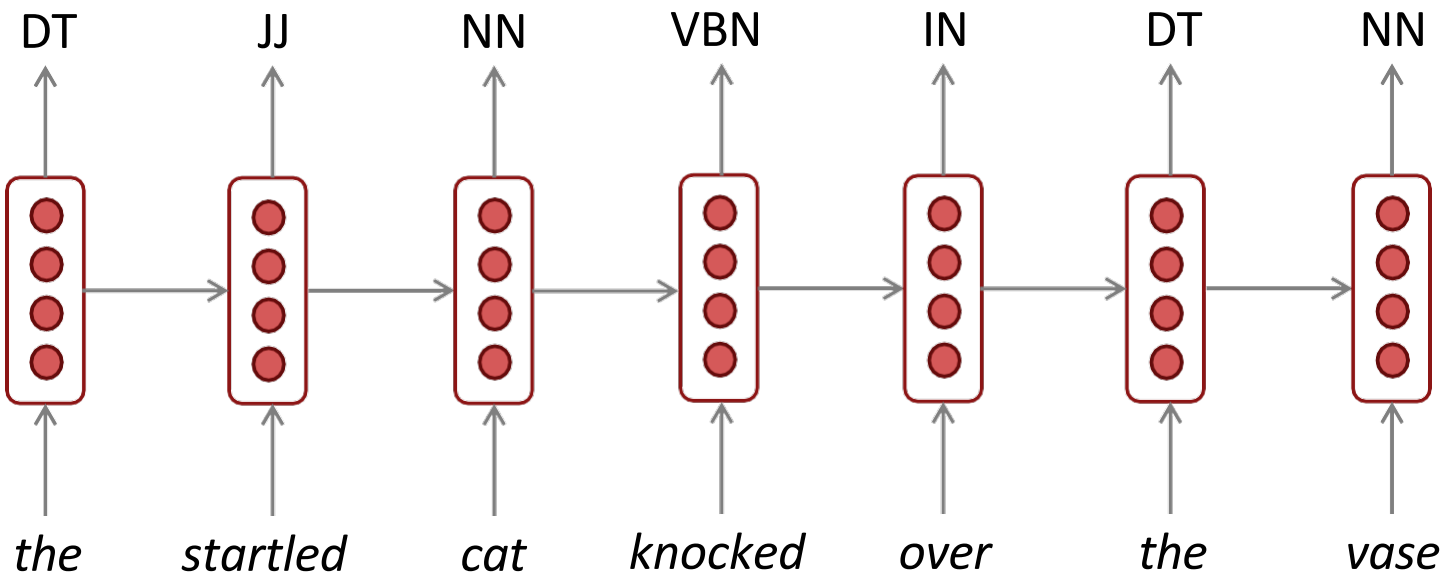
- Language Modeling is a benchmark task that helps us measure our progress on predicting language use
- Language Modeling is a subcomponent of many NLP tasks, especially those involving generating text or estimating the probability of text:
    - Predictive typing
    - Speech recognition
    - Handwriting recognition
    - Spelling/grammar correction
    - Authorship identification
    - Machine translation
    - Summarization
    - Dialogue
    - etc.
- Everything else in NLP has now been rebuilt upon Language Modeling: GPT-3 is an LM!

Other RNN Architectures



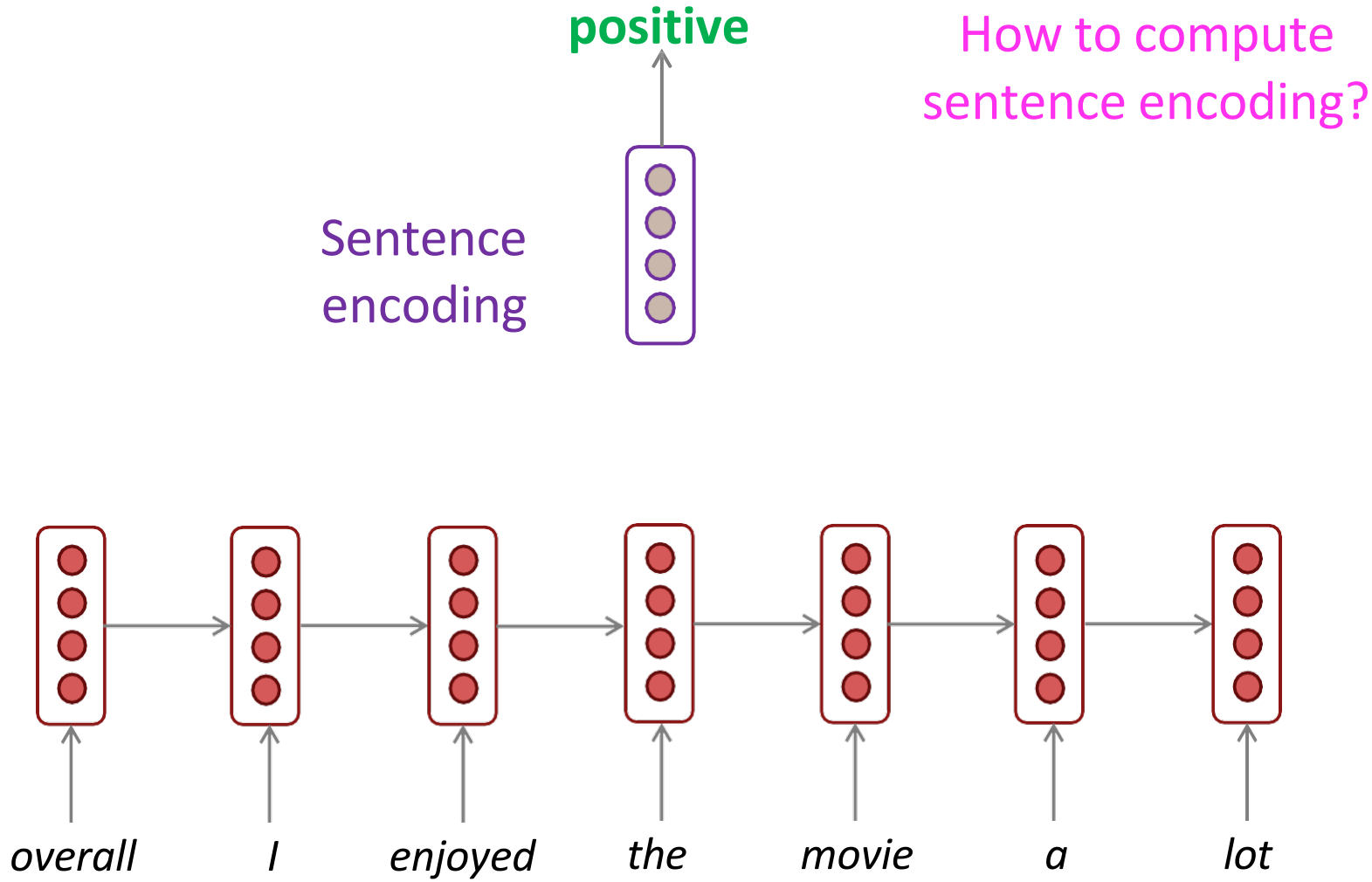
Other RNN uses: RNNs can be used for sequence tagging

e.g., **part-of-speech tagging**, named entity recognition



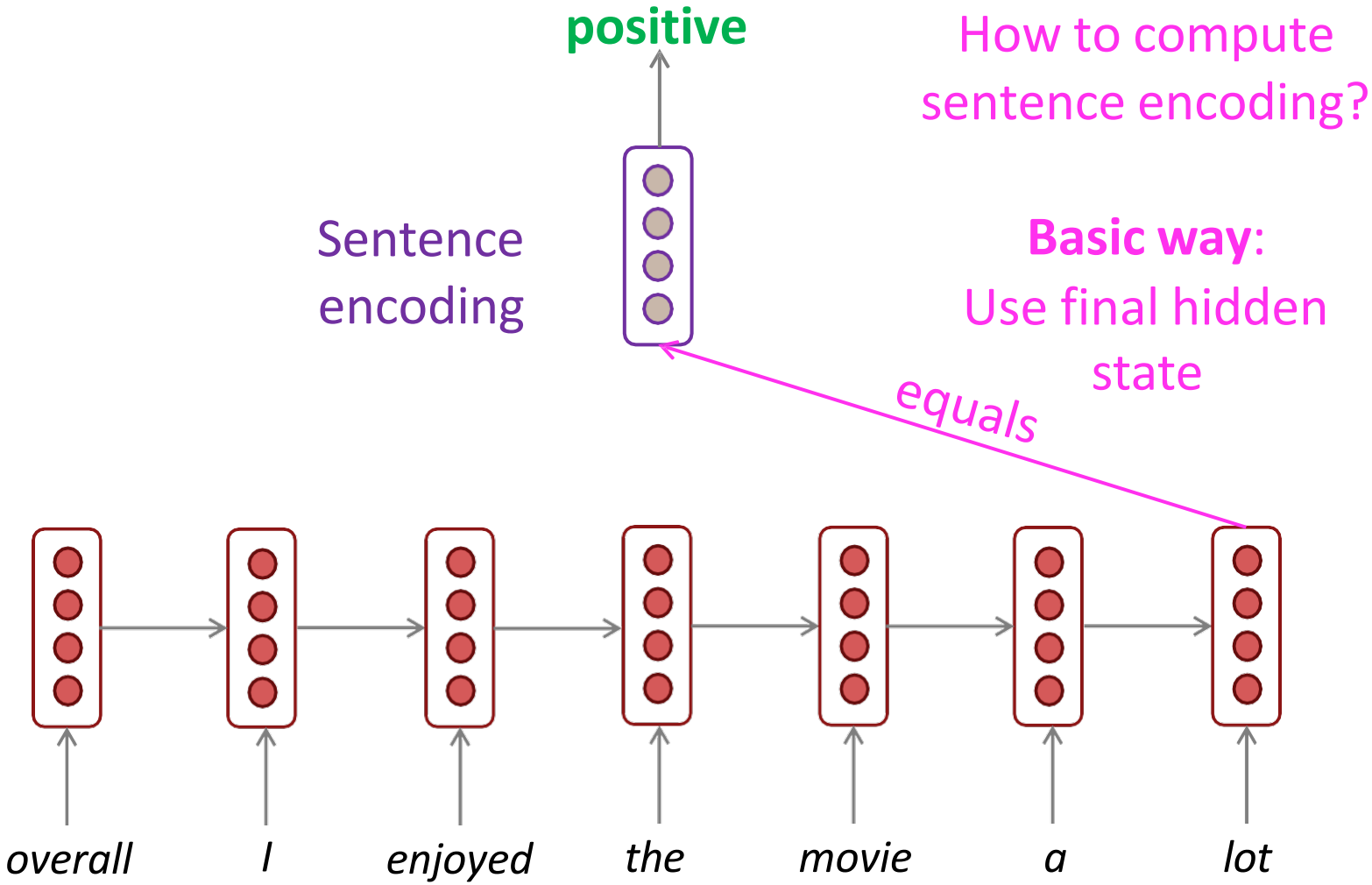
RNNs can be used for sentence classification

e.g., sentiment classification



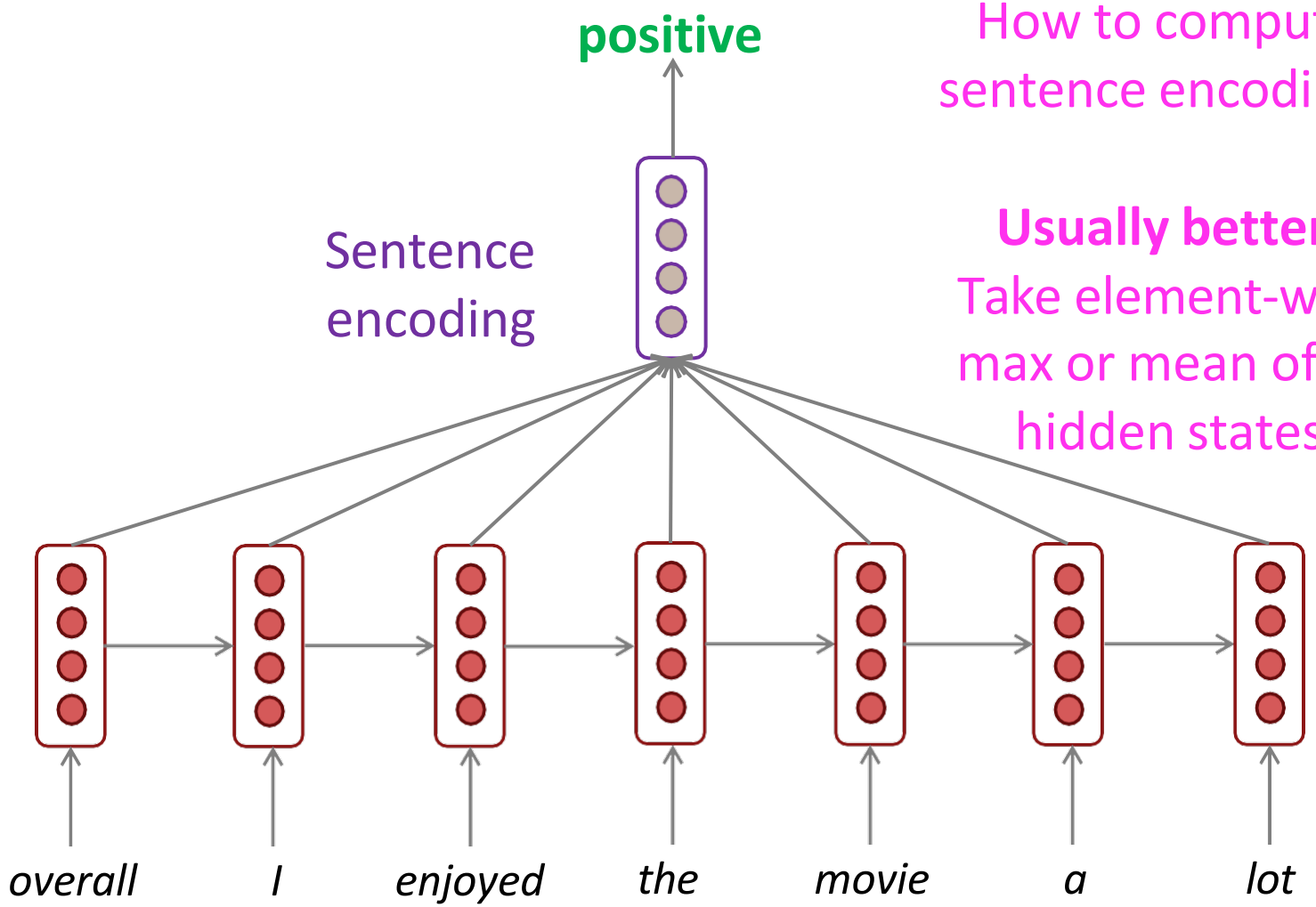
RNNs can be used for sentence classification

e.g., sentiment classification



RNNs can be used for sentence classification

e.g., sentiment classification



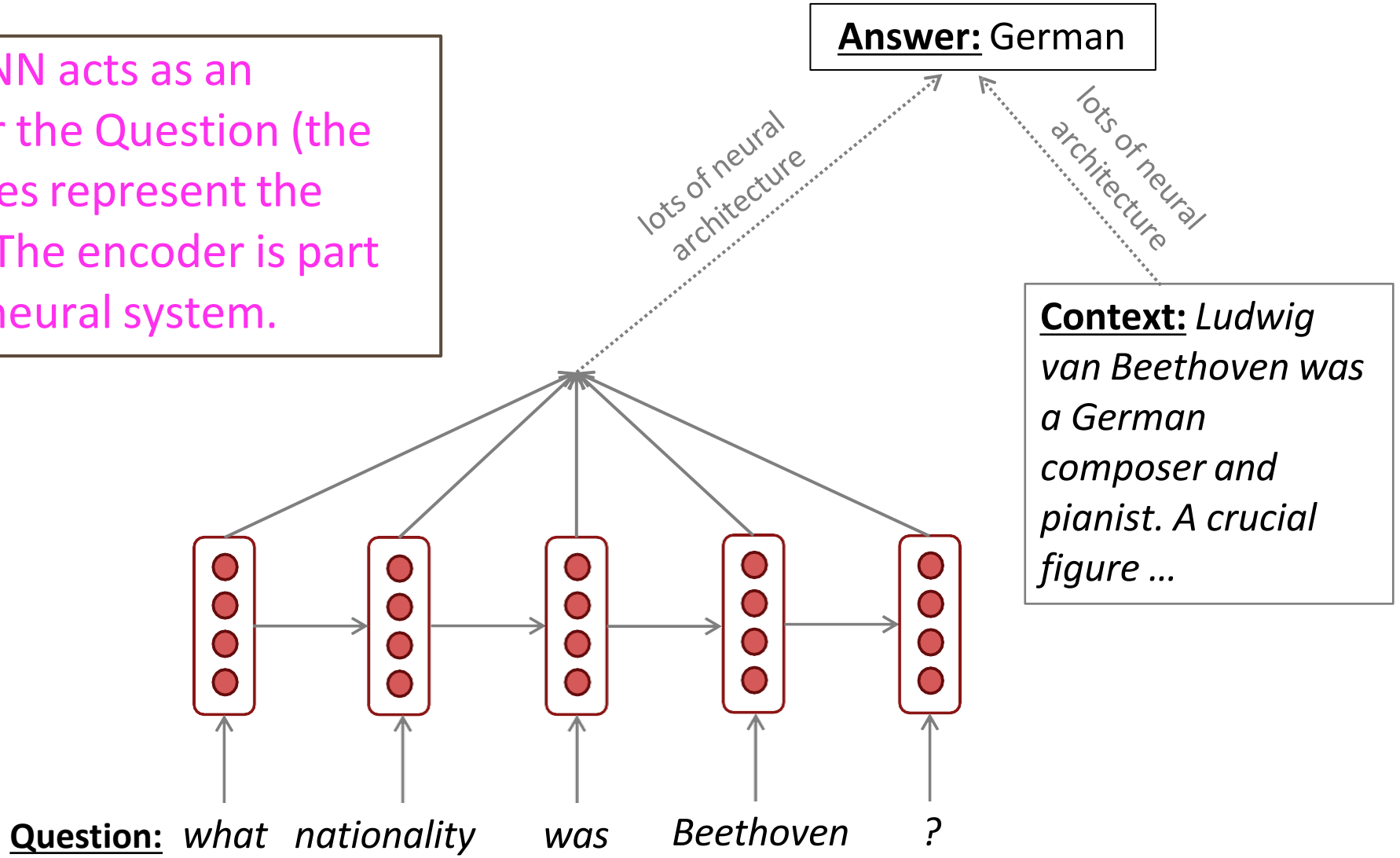
How to compute sentence encoding?

Usually better: Take element-wise max or mean of all hidden states

RNNs can be used as an encoder module

e.g., **question answering**, machine translation, *many other tasks!*

Here the RNN acts as an **encoder** for the Question (the hidden states represent the Question). The encoder is part of a larger neural system.

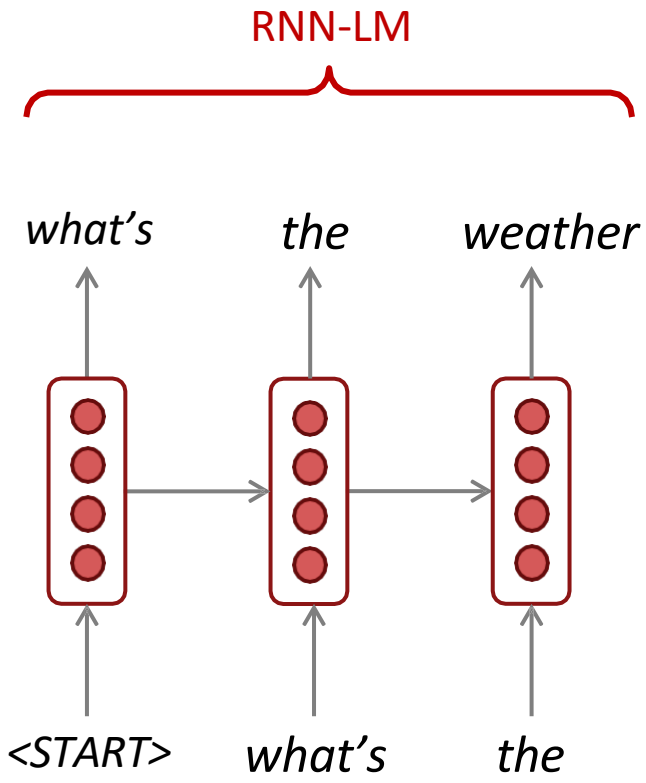


RNN-LMs can be used to generate text

e.g., **speech recognition**, machine translation, summarization

Input (audio)

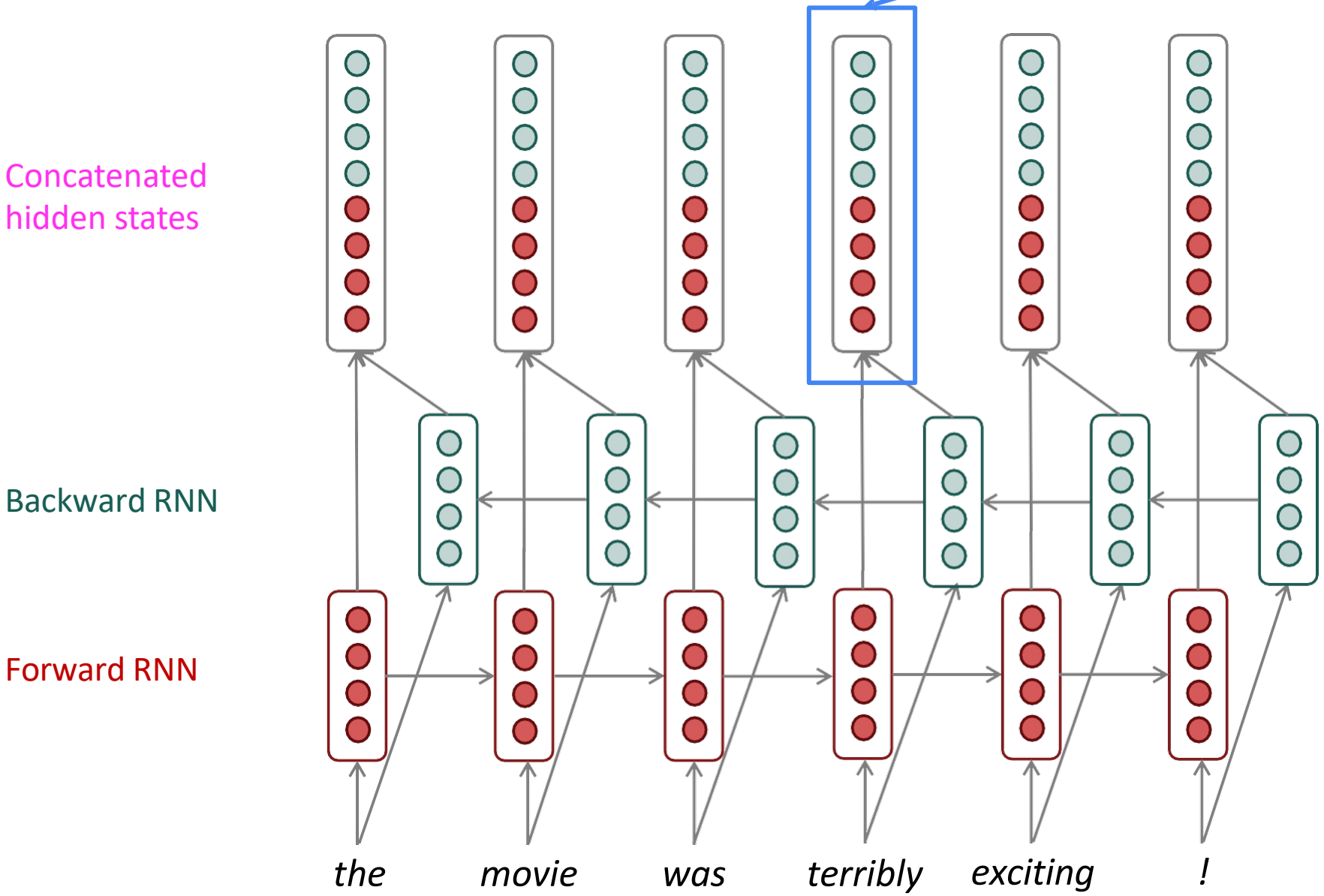
conditioning



This is an example of a *conditional language model*.
We'll see Machine Translation in much more detail next lectures.

Bidirectional RNNs

This contextual representation of “terribly” has both left and right context!



Bidirectional RNNs

- Note: bidirectional RNNs are only applicable if you have access to the entire input sequence
  - They are **not** applicable to Language Modeling, because in LM you *only* have left context available.

- If you do have entire input sequence (e.g., any kind of encoding), bidirectionality is powerful (you should use it by default).

- For example, BERT (**Bidirectional** Encoder Representations from Transformers) is a powerful pretrained contextual representation system built on bidirectionality.
  - You will learn more about transformers, including BERT, in a couple of weeks!

Multi-layer RNNs

- RNNs are already “deep” on one dimension (they unroll over many timesteps)

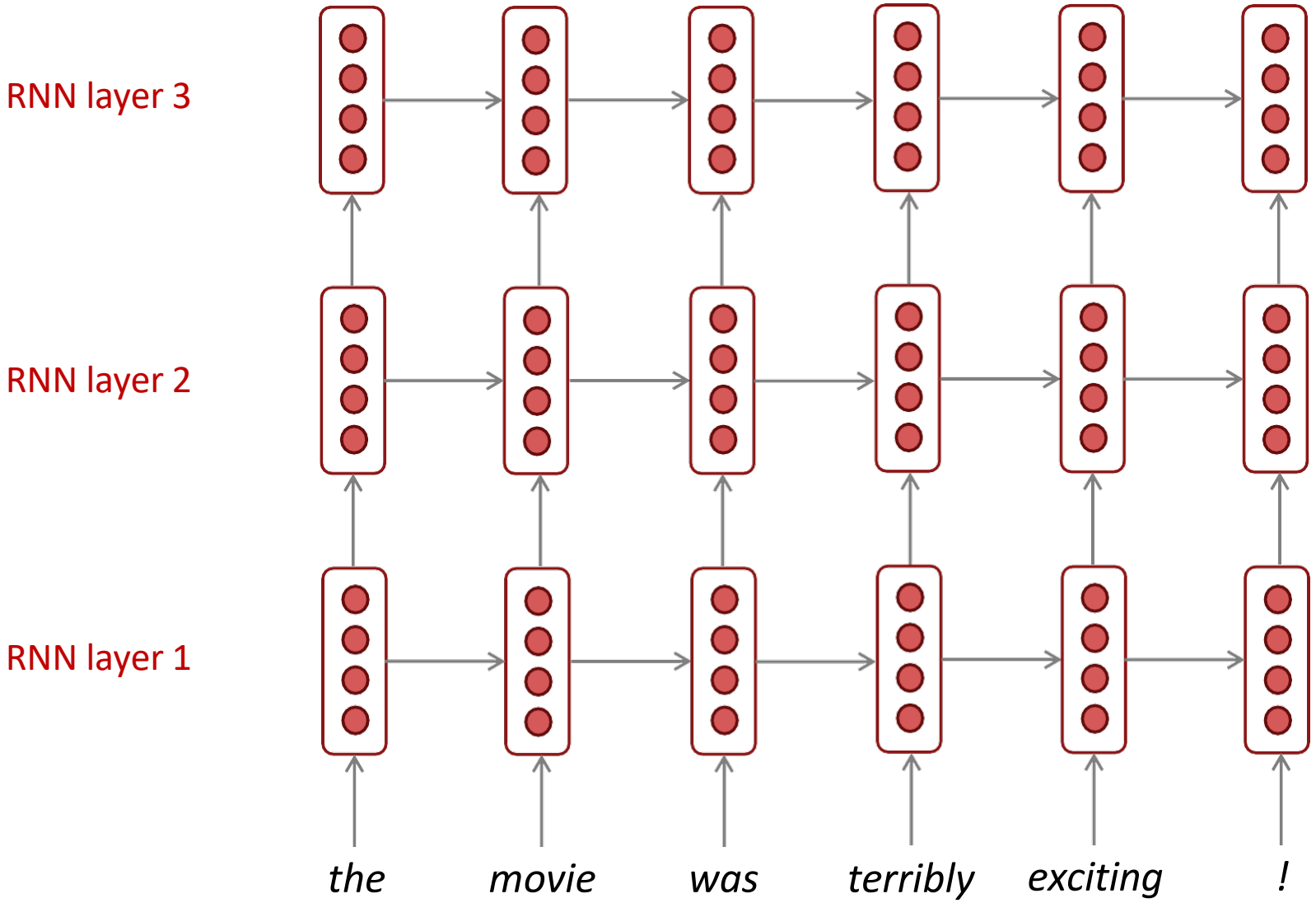
- We can also make them “deep” in another dimension by applying multiple RNNs – this is a multi-layer RNN.

- This allows the network to compute more complex representations
  - The lower RNNs should compute lower-level features and the higher RNNs should compute higher-level features.

- Multi-layer RNNs are also called *stacked RNNs*.

Multi-layer RNNs

The hidden states from RNN layer *i* are the inputs to RNN layer *i*+1



Multi-layer RNNs in practice

- Multi-layer or stacked RNNs allow a network to compute more complex representations – they work better than just have one layer of high-dimensional encodings!
  - The lower RNNs should compute lower-level features and the higher RNNs should compute higher-level features.
- High-performing RNNs are usually multi-layer (but aren't as deep as convolutional or feed-forward networks)
- For example: In a 2017 paper, Britz et al. find that for Neural Machine Translation, 2 to 4 layers is best for the encoder RNN, and 4 layers is best for the decoder RNN
  - Often 2 layers is a lot better than 1, and 3 might be a little better than 2
  - Usually, skip-connections/dense-connections are needed to train deeper RNNs (e.g., 8 layers)
- Transformer-based networks (e.g., BERT) are usually deeper, like 12 or 24 layers.
  - You will learn about Transformers later; they have a lot of skipping-like connections

"Massive Exploration of Neural Machine Translation Architecutres", Britz et al, 2017. https://arxiv.org/pdf/1703.03906.pdf

Terminology

The RNN described in this lecture = **simple**/vanilla/**Elman** RNN 

You learned about other RNN flavors

like LSTM  and GRU  and multi-layer RNNs 

By the end of the course: You will understand phrases like
"stacked bidirectional LSTMs with residual connections and self-attention"