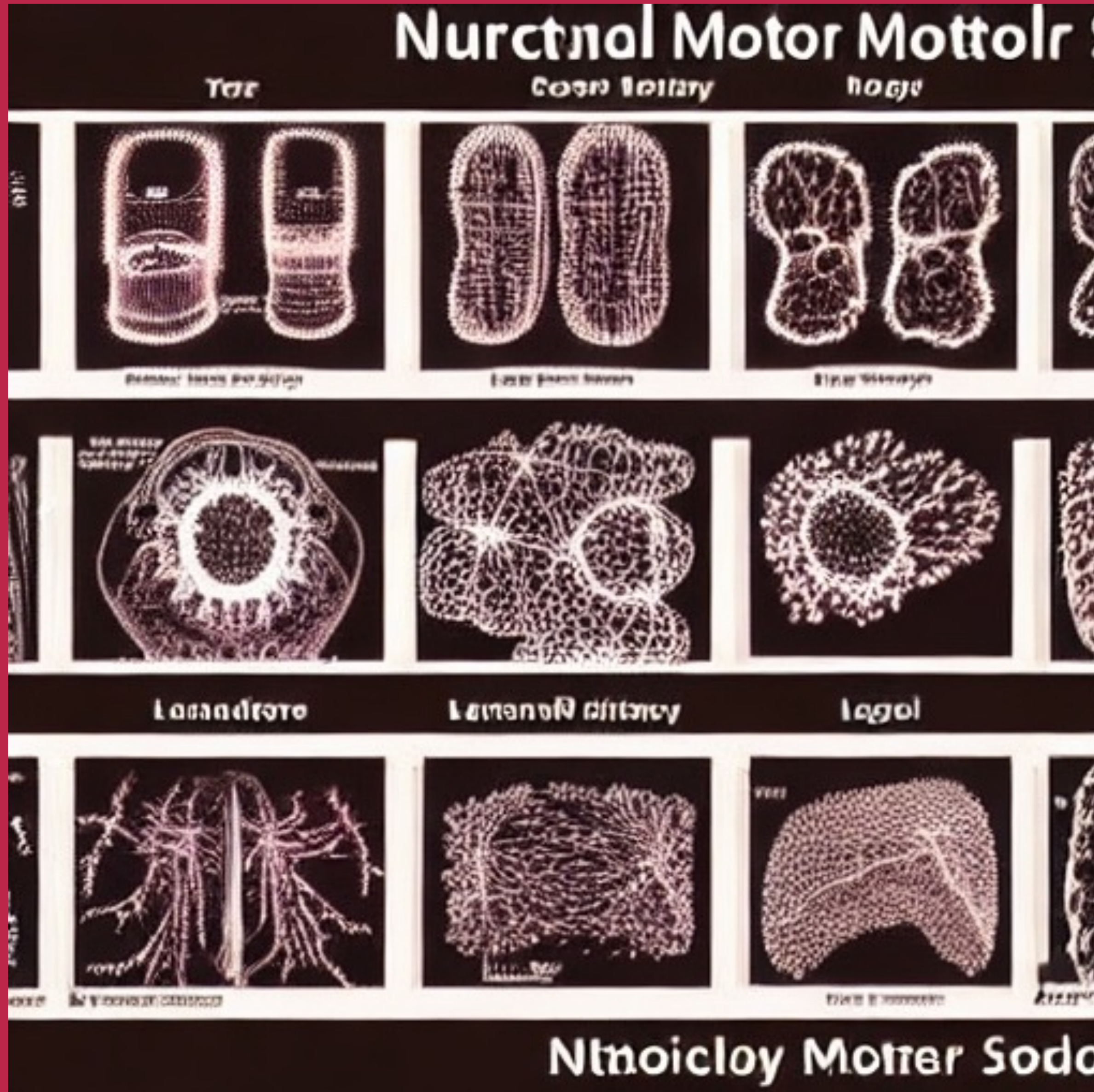


Image: AI text2img generated from lecture's title. *Background*: Viva Magenta (Pantone 18-1750) 2024 Color of the year!

Neural models of language

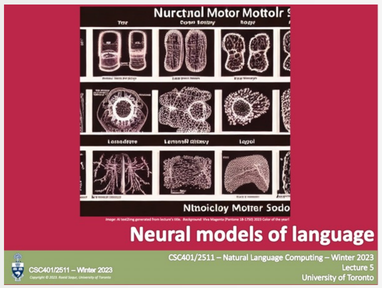
CSC401/2511 – Natural Language Computing – Winter 2024
Lecture 4
University of Toronto

Logistics

- Assignment 1: due Feb 9, 2024
- Assignment 2: release Feb 10, 2024
- Lectures:
  - Reading week break: Feb 19-23 (*no lectures, OHs*)
- Final exam: planned in-person
- Lecture feedback:
  - Anonymous
  - Please share any thoughts/suggestions

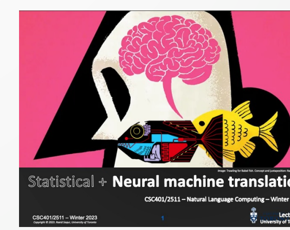
- **Questions?**

Lecture plan: Neural networks



Lecture 4 (**L4**): Neural Language Models (~2 sessions)
- Introduction
- Word-level representations (word2vec, CBOW)
- Neural language models
- Recurrent neural networks (RNN, LSTM)
- Contextual word embeddings

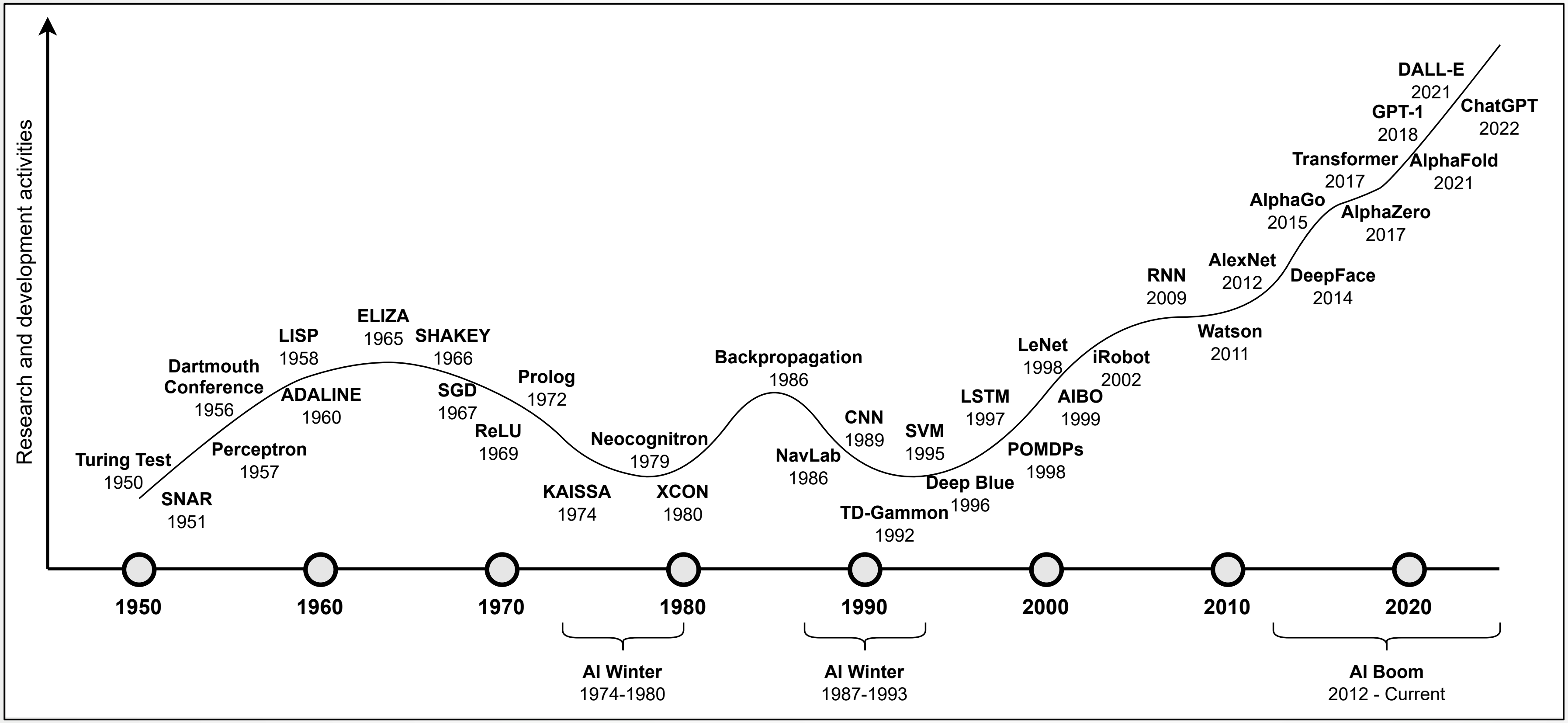
- Lecture 5 (**L5**): Machine Translation (MT) (~3 sessions)
  - Sequence-to-sequence (seq2seq) and attention models
  - Transformers



- Lecture 6 (**L6**): Transformer & Variants (~1 session)
  - Transformers deep-dive.

With material from Phil Blunsom, Piotr Mirowski, Adam Kalai, and James Zou

Historical Background



- **Artificial neural networks (ANNs)**
  - Not new. Few iterations, peaks and troughs with different monikers

1. Saqur, Raeid, et al. "Hype, Media Frenzy, and Mass Societal Hysteria: Perspectives on Human-imitative Intelligence.". ICVSS 2023

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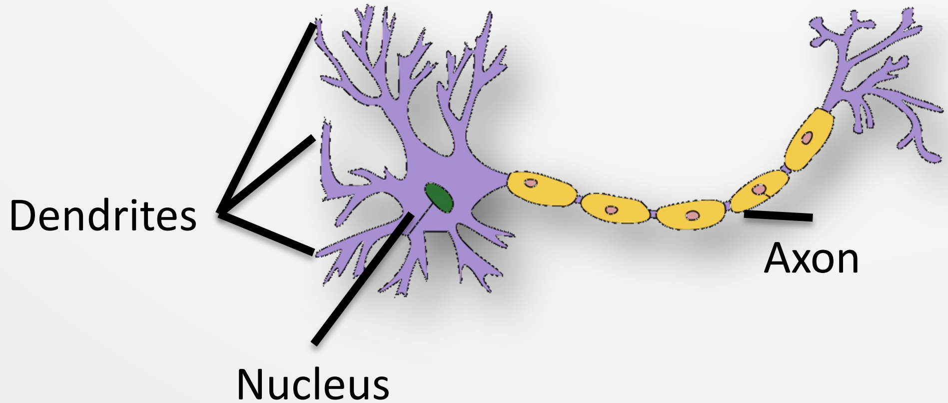
Artificial neural networks

- **Artificial neural networks (ANNs)** were (kind of) inspired from neurobiology (Widrow and Hoff, 1960).
  - Each unit has many inputs (**dendrites**), one output (**axon**).
  - The **nucleus** fires (sends an electric signal along the axon) given input from other neurons.
  - 'Learning' occurs at the **synapses** that connect neurons, either by amplifying or attenuating signals.



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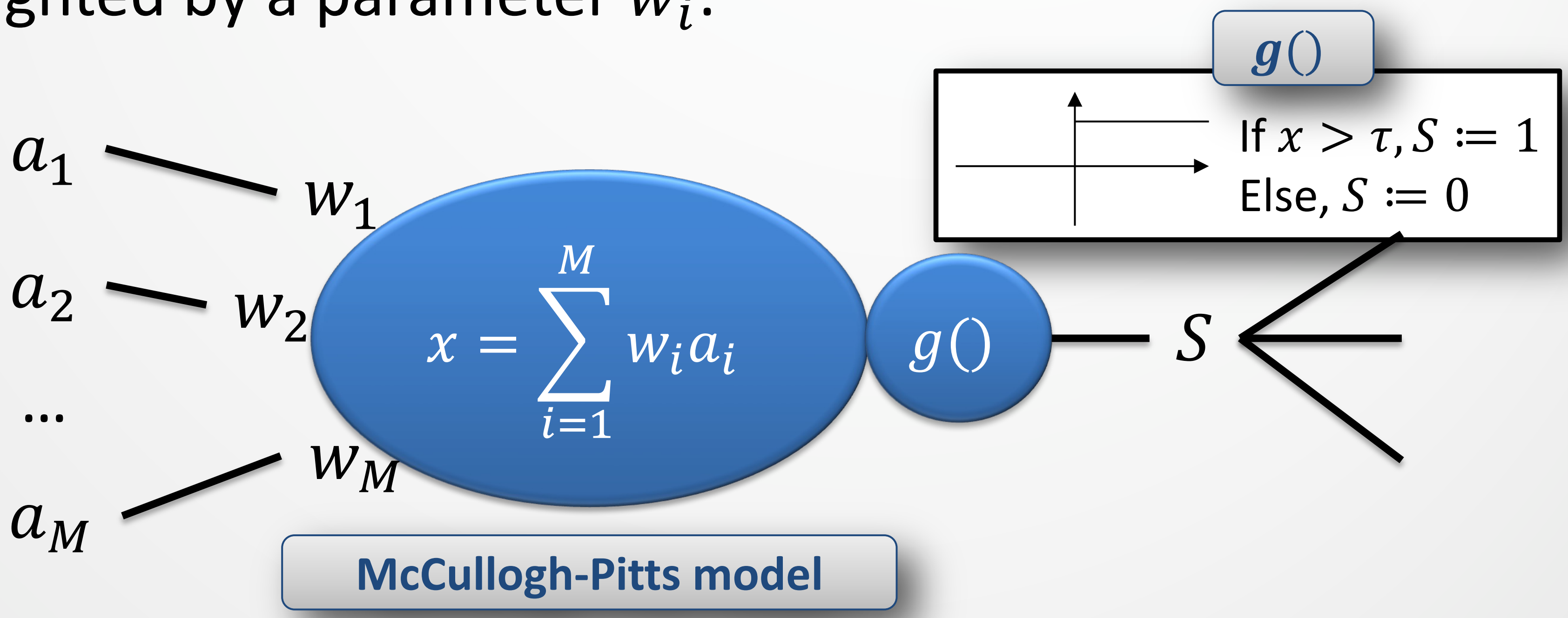
Perceptron: an artificial neuron

- Each neuron calculates a **weighted sum** of its inputs and compares this to a threshold, τ. If the sum exceeds the threshold, the neuron fires.
  - Inputs a_i are activations from adjacent neurons, each weighted by a parameter w_i.

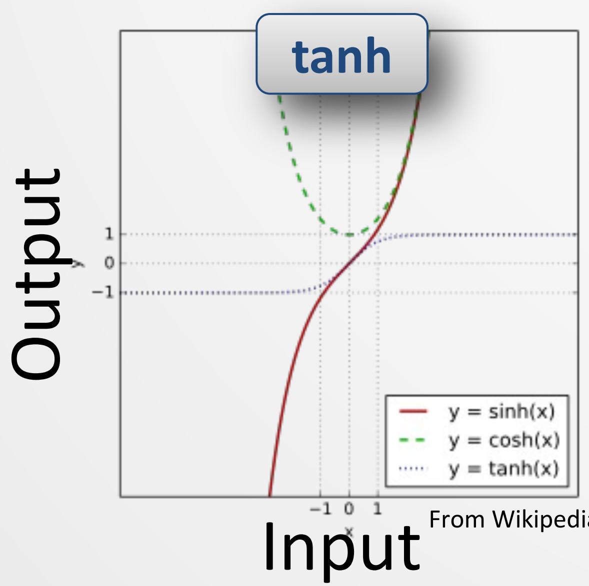


Perceptron output

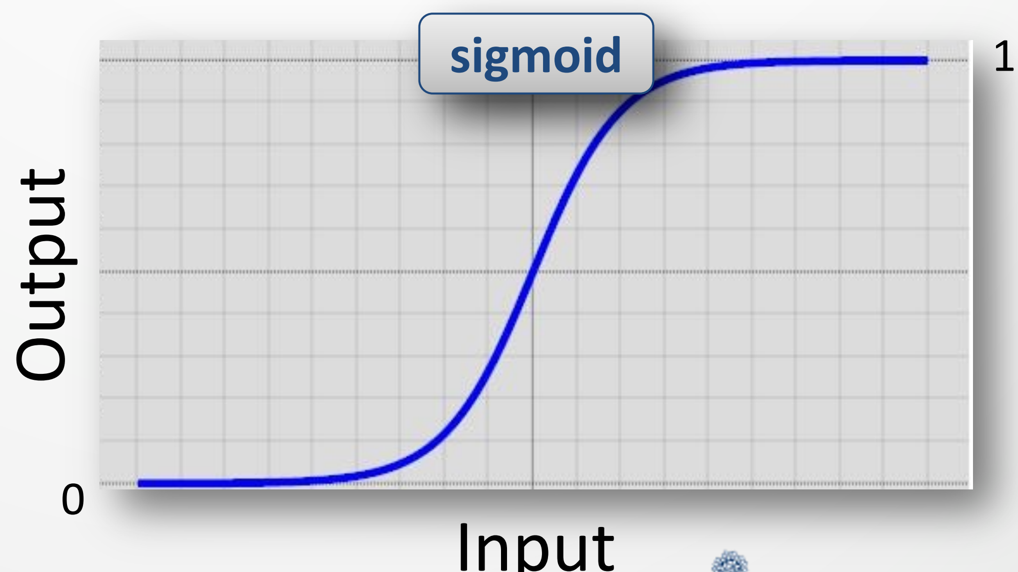
- Perceptron output is determined by **activation functions**, $g()$, which **can be non-linear functions** of weighted input.
- Popular activation functions include **tanh** and the **sigmoid**:

$$g(x) = \sigma(x) = \frac{1}{1 + e^{\rho x}}$$

  - The sigmoid's derivative is the easily computable $\sigma' = \sigma \cdot (1 - \sigma)$



From Wikipedia



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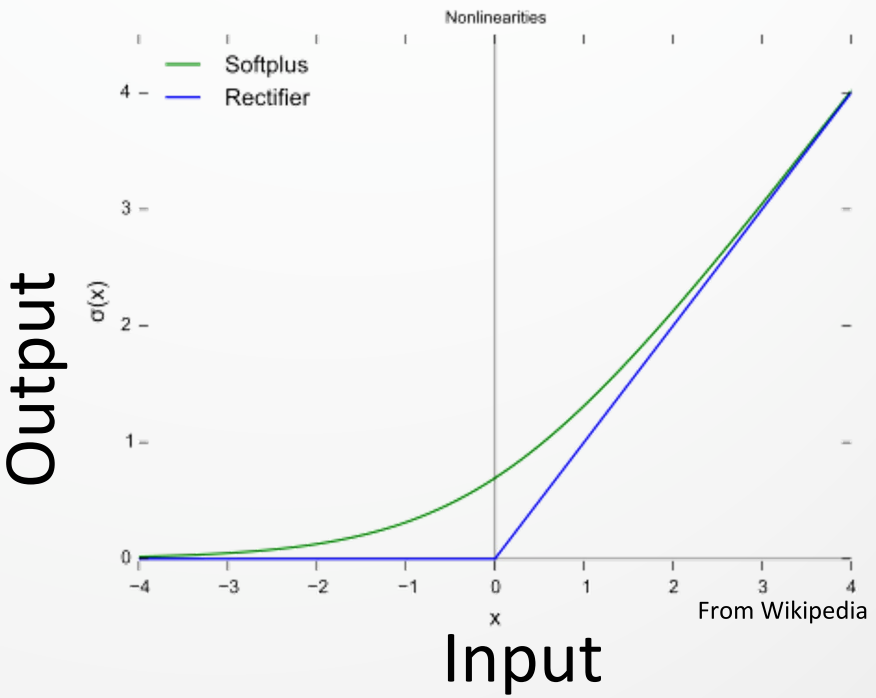
Rectified Linear Units (ReLUs)

- Since 2011, the **ReLU** $S = g(x) = \max(0, x)$ has become more popular.
  - More biologically plausible, sparse activation, limited (vanishing) gradient problems, efficient computation.
- A smooth approximation is the **softplus** $\log(1 + e^x)$, which has a simple derivative $1/(1 + e^{-x})$
- *Why do we care about the derivatives?*



X Glorot, A Bordes, Y Bengio (2011). Deep sparse rectifier neural networks. AISTATS.

Perceptron learning

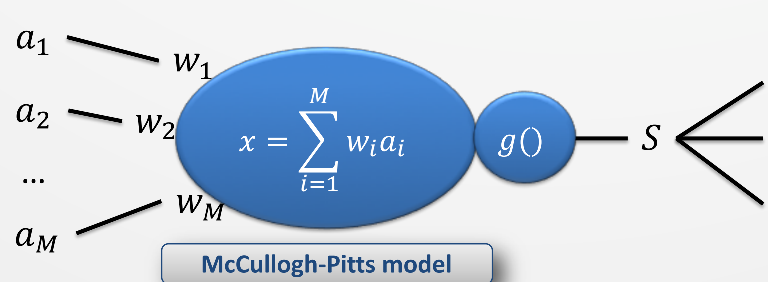
- Weights are adjusted in **proportion to the error** (i.e., the **difference** between the desired, y, and the actual output, S.
- The **derivative** g' allows us to assign blame proportionally.

- Given a small learning rate, α (e.g., 0.05), we can repeatedly adjust each of the weight parameters by

$$w_j := w_j + \alpha \cdot \sum_{i=1}^{R} Err_i \cdot g'(x_i) \cdot a_j[i]$$

} Assumes mean-square error objective

where $Err_i = (y_i - S_i)$, among R training examples.



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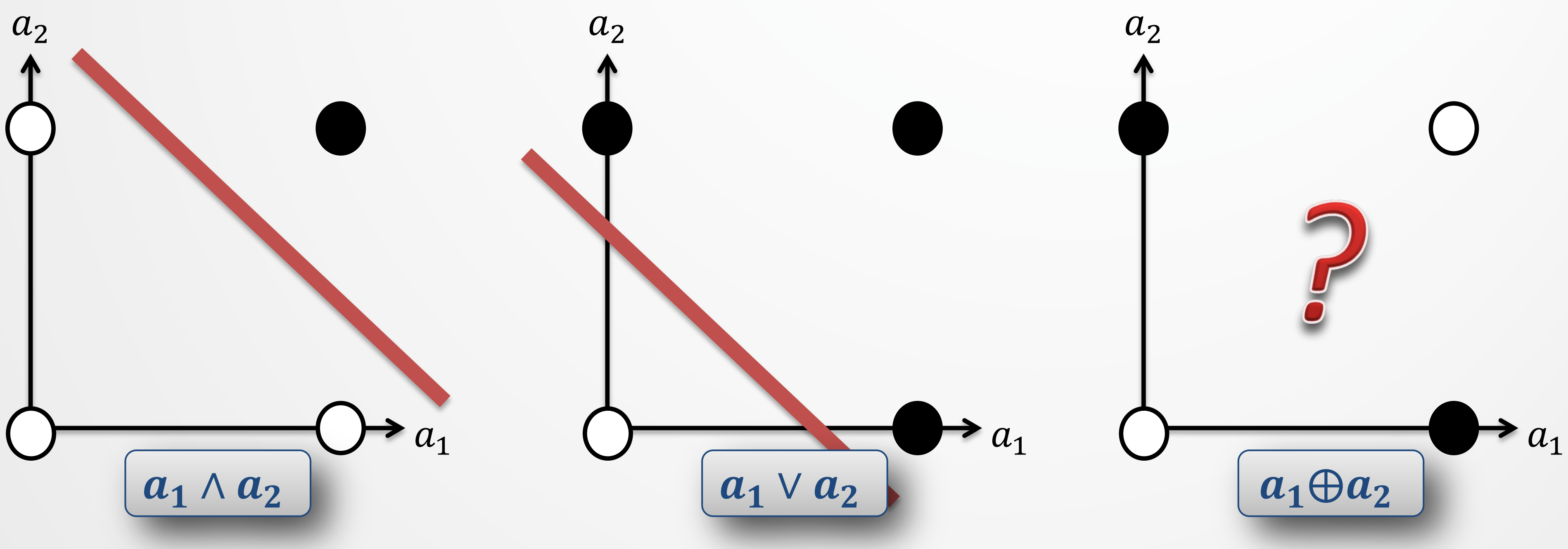
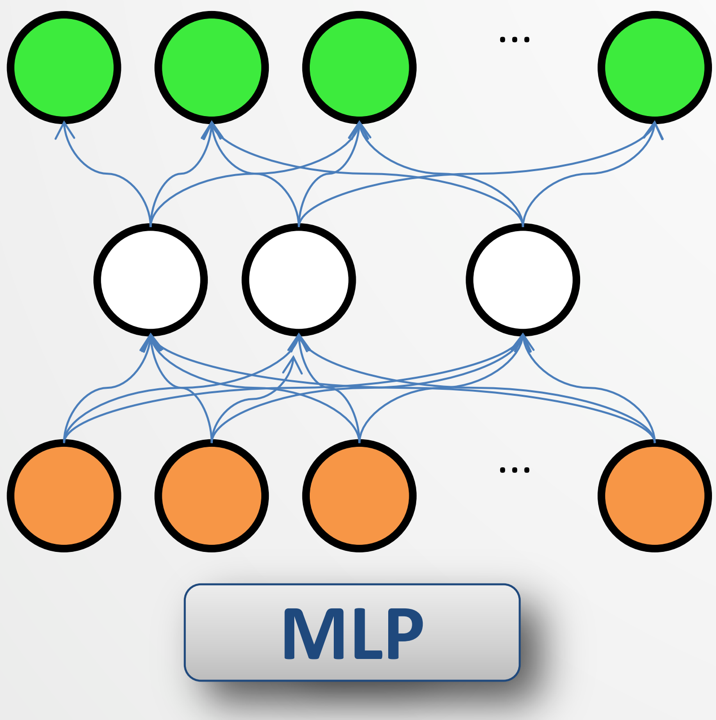
Threshold perceptra and XOR

- Some relatively simple logical functions cannot be learned by threshold perceptra (since they are not linearly separable).



Artificial neural networks

- Complex functions can be represented by layers of perceptron (**multi-layer perceptron, MLPs**).



- Inputs are passed to the **input layer.**
- **Activations** are propagated through **hidden layers** to the **output layer**.

- MLPs are quite **robust to noise**, and are trained specifically to reduce error.

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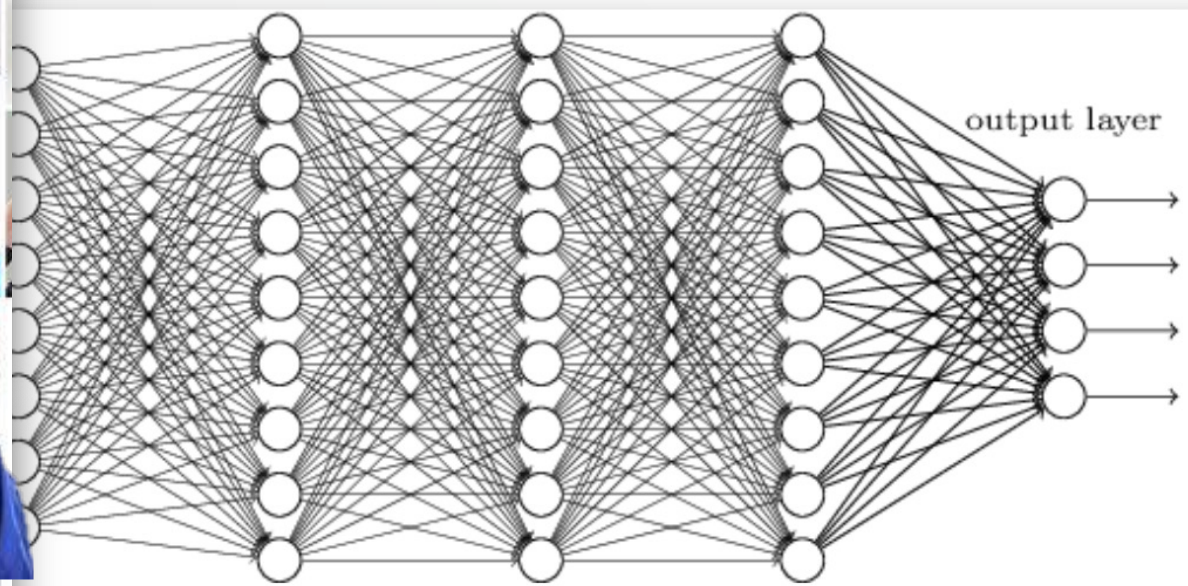
Deep



It's a cat.

Depression.

'hidden' representations are learned here

Can we find hidden patterns in words?

Words

- Given a corpus with D (e.g., $= 100K$) unique words, the **classical approach** is to uniquely assign **each word** with an index in D-dimensional vectors ('one-hot' representation).

lugubrious										
	0	**0**	**0**	**0**	**..**	**0**	**1**	**0**	**...**	**0**

D

- Classic **word-feature representation** assigns **features** to each index in a much denser vector.
  - E.g., psychology based features 'cheerful', 'emotional-tone'.

1	**0.8**	**2.5**	**0.81**	**...**	**99**

$d \ll D$

- Can we learn a dense representation? What will it give us?

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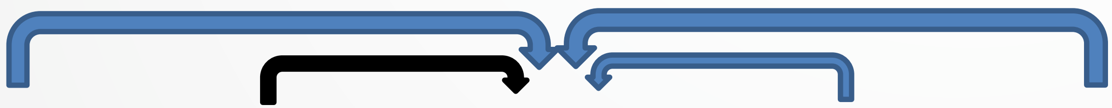
Learning word semantics

"*You shall know a word by the company it keeps.*"

— J.R. Firth (1957)

$$P(w_t = lugubrious | w_{t-1} = feeling, w_{t-2} = been, \ldots)$$



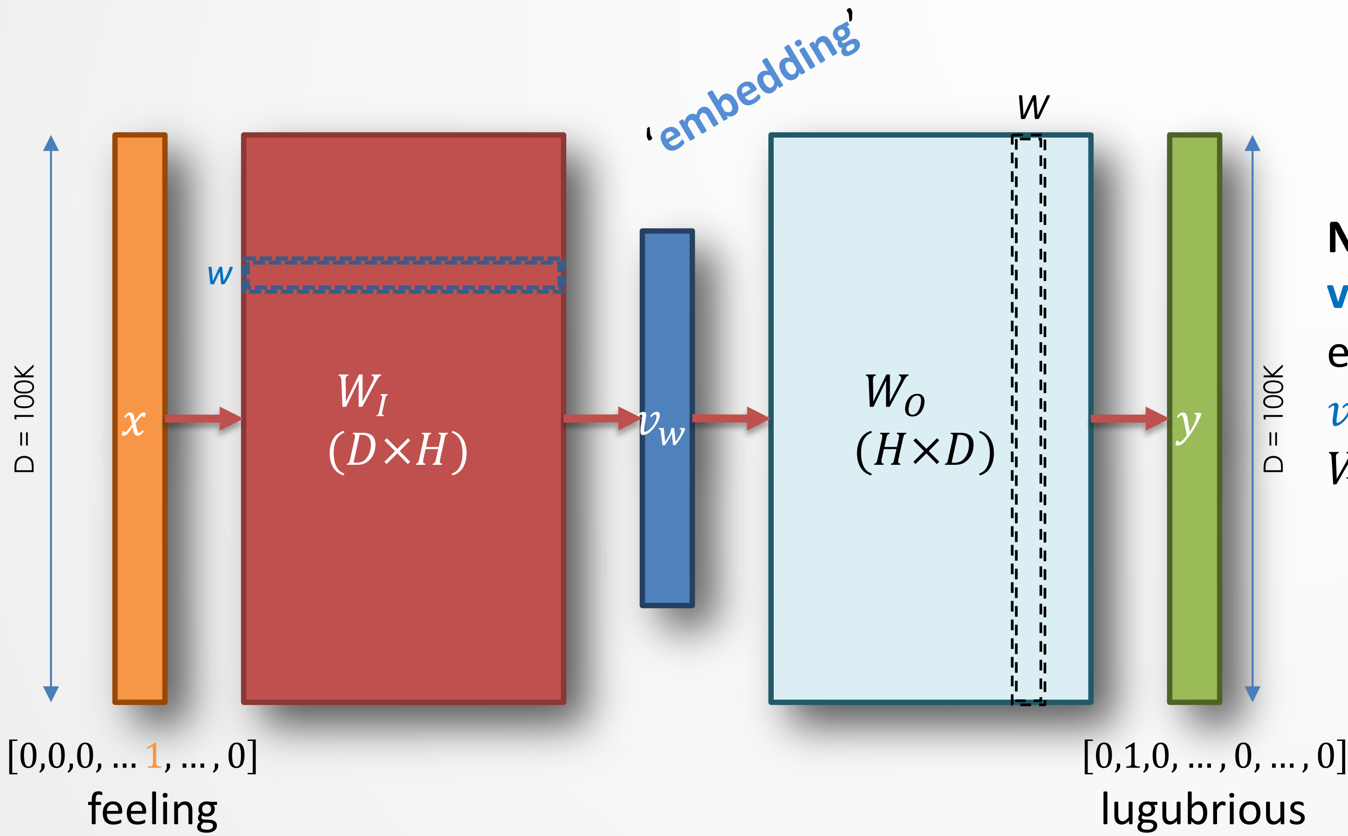
been	feeling	lugubrious	all	day
felt	a	lugubrious	sadness	in

…

Here, we're predicting the *center* word given the context.
This is called the '**continuous bag of words**' (**CBOW**) model[1].

[1] Mikolov T, Corrado G, Chen K, *et al.* Efficient Estimation of Word Representations in Vector Space. *Proc (ICLR 2013)* 2013;:1–12.
https://code.google.com/p/word2vec/

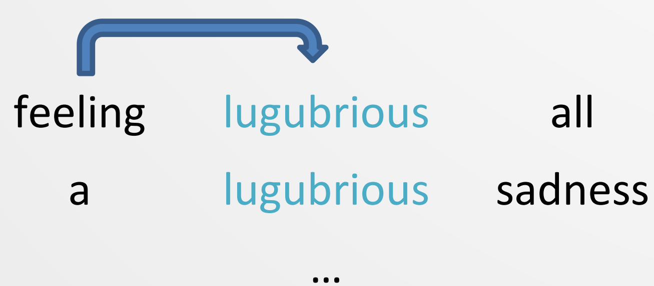
Continuous bag of words (1 word context)



Note: we have *two* **vector representations** of each word:

$v_w = x^{\intercal} W_I$ (w^{th} row of W_I)

$V_w = W_O^{\intercal} y$ (w^{th} col of W_O)



'**softmax**': $P(w_o|w_i) = \frac{\exp(V_{w_o}^{\intercal} v_{w_i})}{\sum_{w=1}^{W} \exp(V_w^{\intercal} v_{w_i})}$

Where

v_w is the 'input' vector for word w,

V_w is the 'output' vector for word w,

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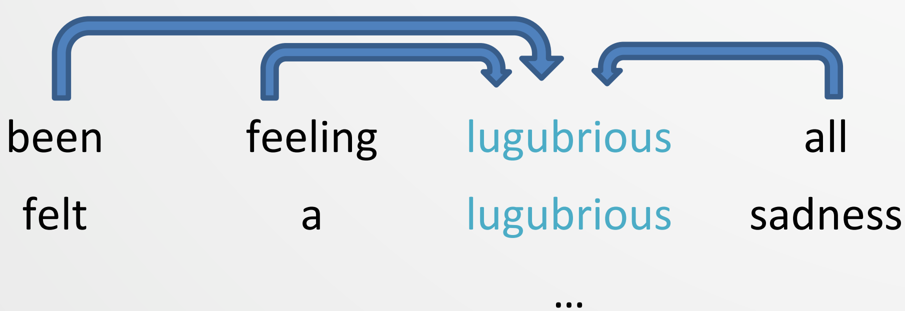
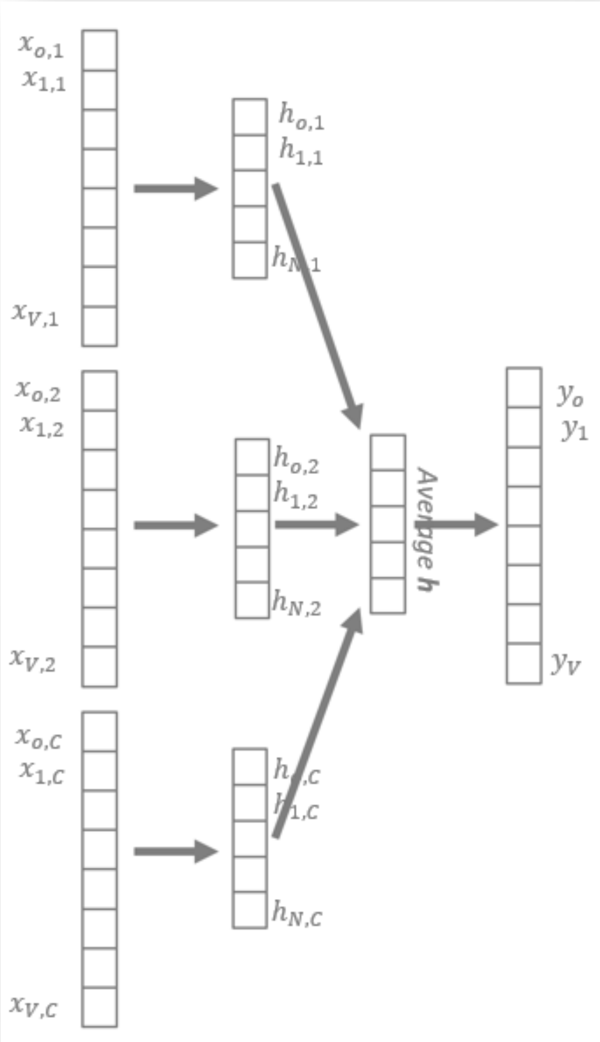
Continuous bag of words (C words context)

- If we want to use **more context**, C, we need to change the network architecture somewhat.
  - Each input word will produce one of C embeddings
  - We just need to add an **intermediate layer**, usually this just averages the embeddings.





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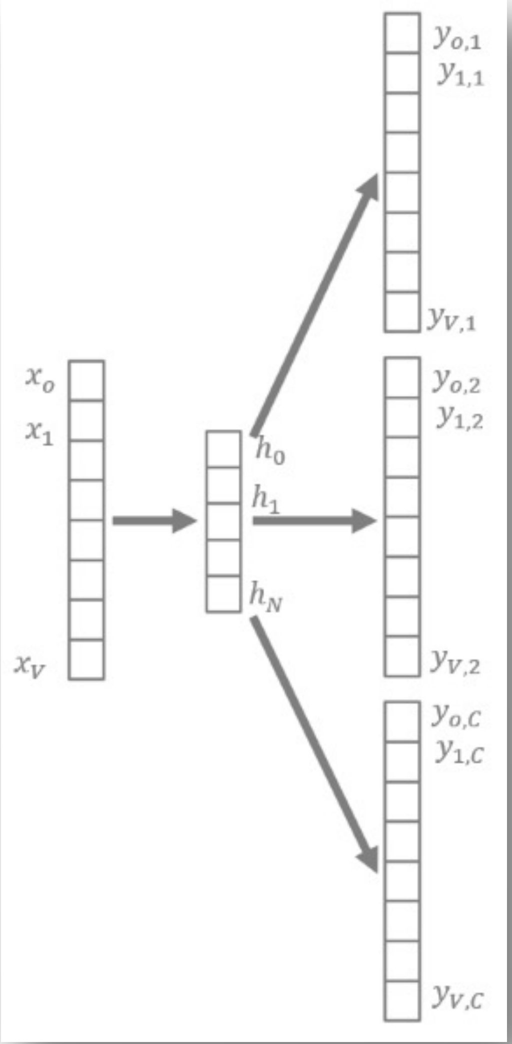
Skip-grams

- **Skip-grams** invert the task – we predict context words given the current word.

- According to Mikolov,
  Skip-gram: works well with small amounts of training data, represents rare words.

  CBOW: several times faster to train, slightly better accuracy for frequent words



Mikolov T, Corrado G, Chen K, *et al.* Efficient Estimation of Word Representations in Vector Space. *Proc (ICLR 2013)* 2013;:1–12. https://arxiv.org/pdf/1301.3781.pdf

Actually doing the learning

- Given H-dimensional embeddings, and V word types, our parameters, θ, are:

$$\theta = \begin{bmatrix} v_a \\ v_{aardvark} \\ \vdots \\ v_{zymurgy} \\ V_a \\ V_{aardvark} \\ \vdots \\ V_{zymurgy} \end{bmatrix} \in \mathbb{R}^{2V \times H}$$

Actually doing the learning

We have many options. Gradient descent is popular.
Given T tokens of training data, optimize objective:

$$J(\theta) = \frac{1}{T}\sum_{t=1}^{T}\sum_{-c<j<c,j\neq 0} \log P(w_{t+j}|w_t)$$

And we want to update vectors $V_{w_{t+j}}$ then v_{w_t} within θ

$$\theta^{(new)} = \theta^{(old)} - \alpha \nabla_\theta J(\theta)$$

So, we'll need to take the derivative of the (log of the) softmax function:

$$P(w_o|w_i) = \frac{\exp(V_{w_o}^\intercal v_{w_i})}{\sum_{w=1}^{W}\exp(V_w^\intercal v_{w_i})}$$

Where v_w is the 'input' vector for word w,
and V_w is the 'output' vector for word w,

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Actually doing the learning

We need the derivative of the (log of the) softmax function:

$$\frac{\delta}{\delta v_{w_t}} \log P(w_{t+j}|w_t) = \frac{\delta}{\delta v_{w_t}} \log \frac{\exp(V_{w_{t+j}}^{\intercal} v_{w_t})}{\sum_{w=1}^{W} \exp(V_w^{\intercal} v_{w_t})}$$

$$= \frac{\delta}{\delta v_{w_t}} \left[\log \exp\left(V_{w_{t+j}}^{\intercal} v_{w_t}\right) - \log \sum_{w=1}^{W} \exp(V_w^{\intercal} v_{w_t}) \right]$$

$$= V_{w_{t+j}} \qquad - \frac{\delta}{\delta v_{w_t}} \log \sum_{w=1}^{W} \exp(V_w^{\intercal} v_{w_t})$$

[apply the chain rule $\frac{\delta f}{\delta v_{w_t}} = \frac{\delta f}{\delta z} \frac{\delta z}{\delta v_{w_t}}$]

$$= V_{w_{t+j}} - \sum_{w=1}^{W} p(w|w_t) V_w$$

More details: http://arxiv.org/pdf/1411.2738.pdf

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Using word representations

Without a latent space,

lugubrious = $[0,0,0,\ldots,0,1,0,\ldots,0]$, &

sad = $[0,0,0,\ldots,0,0,1,\ldots,0]$ so

Similarity = $\cos(x,y) = 0.0$

EMBEDDING

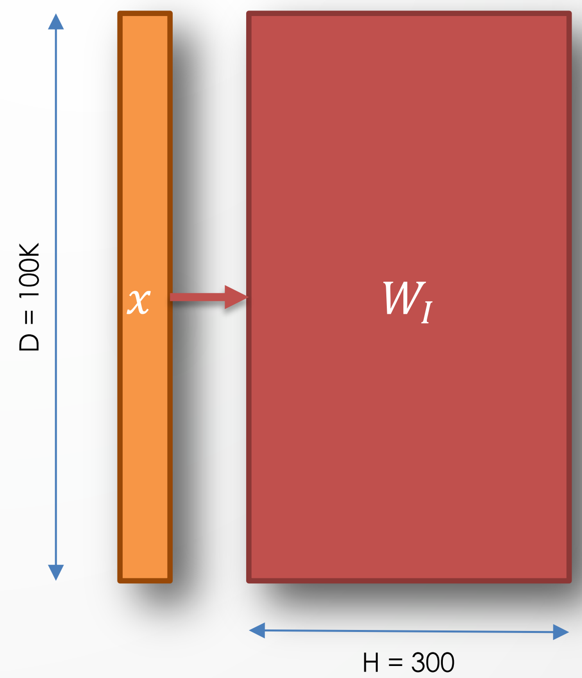
$$v_w = x^\intercal W_I$$

In latent space,

lugubrious = $[0.8,0.69,0.4,\ldots,0.05]_H$, &

sad = $[0.9,0.7,0.43,\ldots,0.05]_H$ so

Similarity = $\cos(x,y) = 0.9$



Reminder:

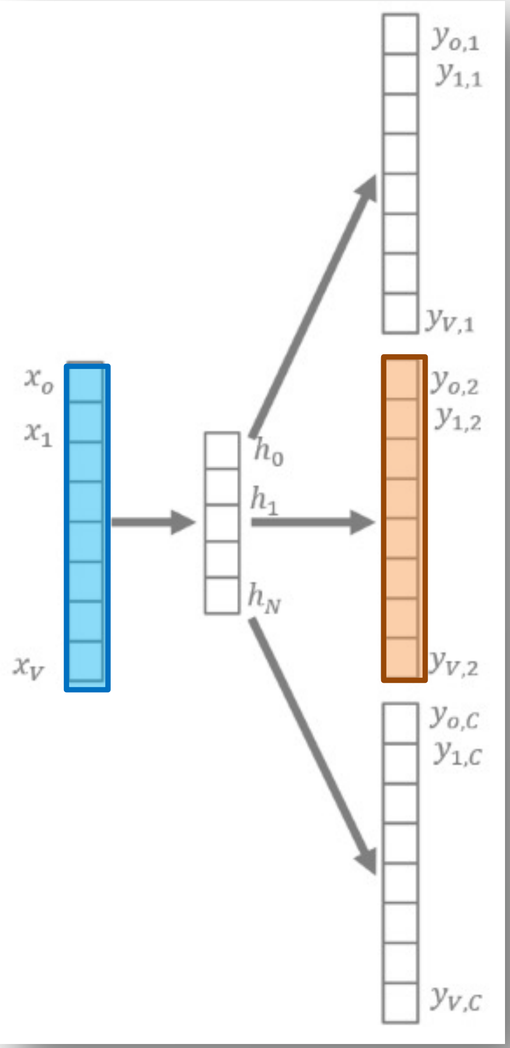
$$\cos(u,v) = \frac{u \cdot v}{||u|| \times ||v||}$$

Skip-grams with negative sampling

- The default process is inefficient.
  - For one – **what a waste of time**!
    We don't want to update $H \times D$ weights!
  - For two – **we want to avoid confusion**!
    'Hallucinated' (negative) contexts should be minimized.

- For the observed (true) pair (*lugubrious*, *sadness*), only the output neuron for *sadness* should be 1, and all $D - 1$ others should be 0.

- Mathematical Intuition:
  - $P(w_o|w_c) = \dfrac{\exp(v_o^T V_c)}{\sum_{w=1}^{D} \exp(v_w^T V_c)}$ } Computationally infeasible



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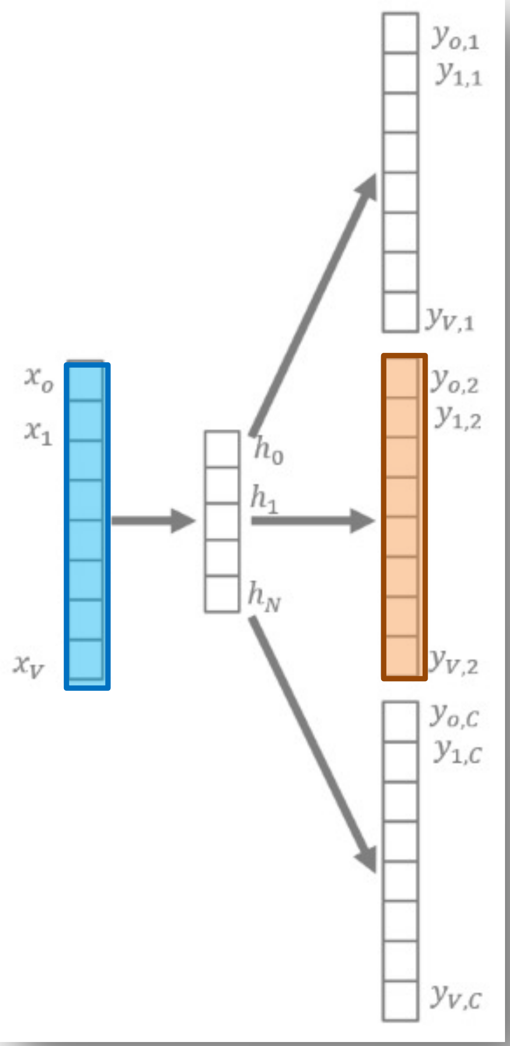
Skip-grams with negative sampling

- We want to **maximize** the association of ***observed*** (positive) contexts:

  lugubrious *sad*
  lugubrious *feeling*
  lugubrious *tired*

- We want to **minimize** the association of '***hallucinated***' contexts:

  lugubrious *happy*
  lugubrious *roof*
  lugubrious *truth*



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Skip-grams with negative sampling

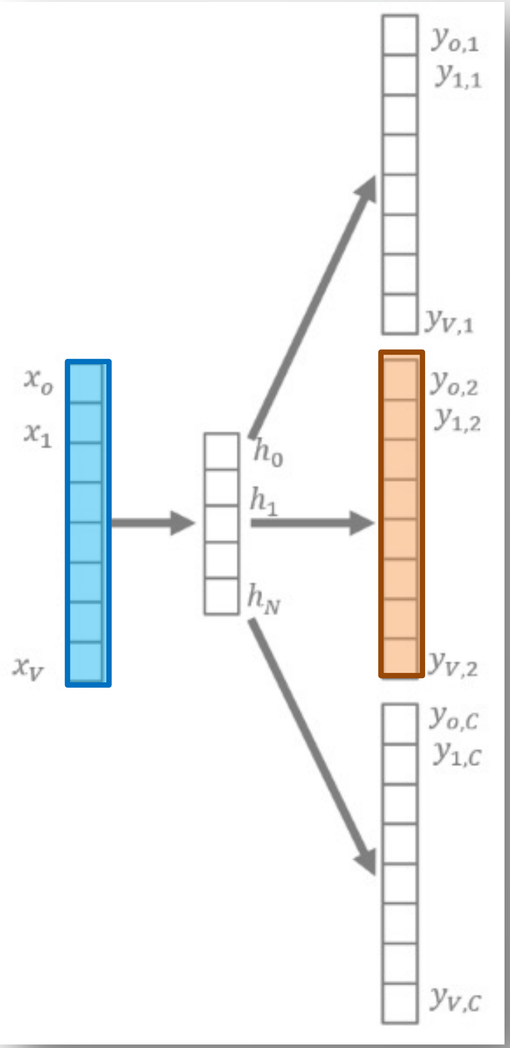
- Choose a small number k of 'negative' words, and just update the weights for the 'positive' word plus the k 'negative' words.
  - $5 \leq k \leq 20$ can work in practice for fewer data.
  - For $D = 100K$, we only update 0.006% of the weights in the output layer.

$$J(\theta) = \log \sigma(v_o^T v_c) + \sum_{i=1}^{k} \mathbb{E}_{j \sim P(w)} [\log \sigma(-v_i^T v_c)]$$

Unigram dist.

- Mimno and Thompson (2017) choose the top k words by modified unigram probability:

$$P^*(w_{t+1}) = \frac{C(w_{t+1})^{\frac{3}{4}}}{\sum_w C(w)^{\frac{3}{4}}}$$



Mimno, D., & Thompson, L. (2017). The strange geometry of skip-gram with negative sampling. *EMNLP 2017*. [link]

Smell the GloVe

- **GloVe** ('**Glo**bal **Ve**ctors') is an alternative method of obtaining word embeddings.
  - Instead of predicting words at particular positions, look at the **co-occurrence matrix** within the corpus

$$X = \begin{array}{c|cccccccc} & I & like & enjoy & deep & learning & NLP & flying & . \\ \hline I & 0 & 2 & 1 & 0 & 0 & 0 & 0 & 0 \\ like & 2 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ enjoy & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ deep & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\ learning & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ NLP & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \\ flying & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 \\ . & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 \end{array}$$

Word w_i occurs $X_{i,j} (= X_{j,i})$ times with word w_j, within some context window (e.g., 10 words, a sentence, …).

Pennington J, Socher R, Manning CD. (2014) GloVe: Global Vectors for Word Representation. *Proc EMNLP 2014*:1532–43. https://nlp.stanford.edu/projects/glove/

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Smell the GloVe

- Populating the co-occurrence matrix requires a complete pass through the corpus, but needs only be done once.
- Let $P_{i,j} = P(w_j | w_i) = X_{i,j} / X_i$,

Table 1: Co-occurrence probabilities for target words *ice* and *steam* with selected context words from a 6 billion token corpus. Only in the ratio does noise from non-discriminative words like *water* and *fashion* cancel out, so that large values (much greater than 1) correlate well with properties specific to ice, and small values (much less than 1) correlate well with properties specific of steam.

Probability and Ratio	$k = solid$	$k = gas$	$k = water$	$k = fashion$
$P(k\|ice)$	1.9×10^{-4}	6.6×10^{-5}	3.0×10^{-3}	1.7×10^{-5}
$P(k\|steam)$	2.2×10^{-5}	7.8×10^{-4}	2.2×10^{-3}	1.8×10^{-5}
$P(k\|ice)/P(k\|steam)$	8.9	8.5×10^{-2}	1.36	0.96

Pennington J, Socher R, Manning CD. (2014) GloVe: Global Vectors for Word Representation. *Proc EMNLP 2014.* https://nlp.stanford.edu/projects/glove/

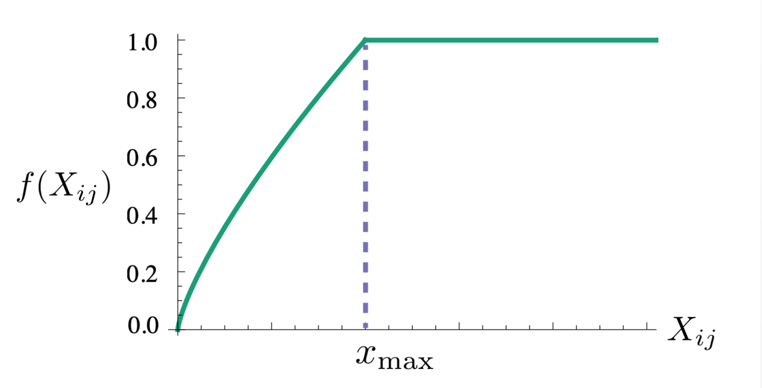
Aside – smell the GloVe

- Minimize $J = \sum_{i,j=1}^{V} f(X_{i,j}) \left(v_{w_i}^T v_{w_j} + b_i + \widetilde{b_j} - \log X_{i,j} \right)^2$

  where, b_i and $\widetilde{b_j}$ are input and output bias terms associated with w_i and w_j, respectively, V is vocab. size

- Weighting function $f(X_{i,j})$:

$$f(x) = \begin{cases} (x/x_{\max})^{\alpha} & \text{if } x < x_{\max} \\ 1 & \text{otherwise} \end{cases}.$$



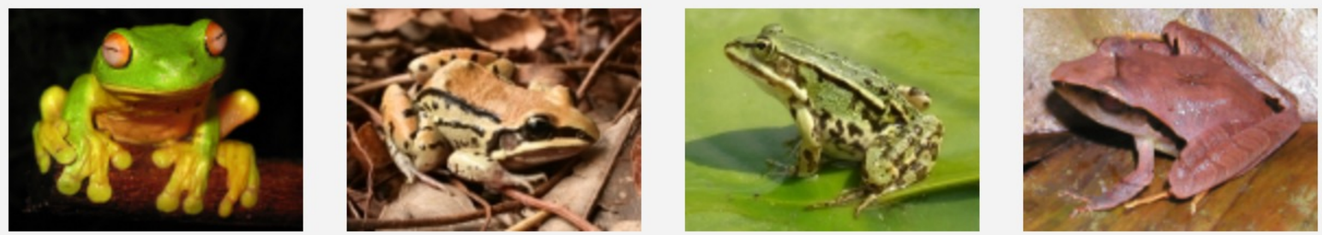
Weighting function *f* with alpha = ¾, x_{max} = 100

1. $f(0) = 0$. If f is viewed as a continuous function, it should vanish as $x \to 0$ fast enough that the $\lim_{x\to 0} f(x) \log^2 x$ is finite.
2. $f(x)$ should be non-decreasing so that rare co-occurrences are not overweighted.
3. $f(x)$ should be relatively small for large values of x, so that frequent co-occurrences are not overweighted.

Aside – evaluation

- **Intrinsic evaluation**: popular [redacted] method was to cherry-pick a few *k*-nearest neighbours examples that match expectations.

0. *frog*
1. frogs
2. toad
3. litoria
4. leptodactylidae
5. rana
6. lizard
7. eleutherodactylus



3. litoria 4. leptodactylidae 5. rana 7. eleutherodactylus

- **Extrinsic evaluation**: embed resulting vectors into a variety of tasks[1,2].

SuperGLUE GLUE

Leaderboard Version: **2.0**

Rank	Name	Model	URL	Score	BoolQ	CB	COPA	MultiRC	ReCoRD	RTE	WiC	WSC	AX-b	AX-g
1	Liam Fedus	SS-MoE		91.0	92.3	96.9/98.0	99.2	89.2/65.2	95.0/94.2	93.5	77.4	96.6	72.3	96.1/94.1
2	Microsoft Alexander v-team	Turing NLR v5		90.9	92.0	95.9/97.6	98.2	88.4/63.0	96.4/95.9	94.1	77.1	97.3	67.8	93.3/95.5
3	ERNIE Team - Baidu	ERNIE 3.0		90.6	91.0	98.6/99.2	97.4	88.6/63.2	94.7/94.2	92.6	77.4	97.3	68.6	92.7/94.7

[1] https://gluebenchmark.com/tasks
[2] https://super.gluebenchmark.com/tasks

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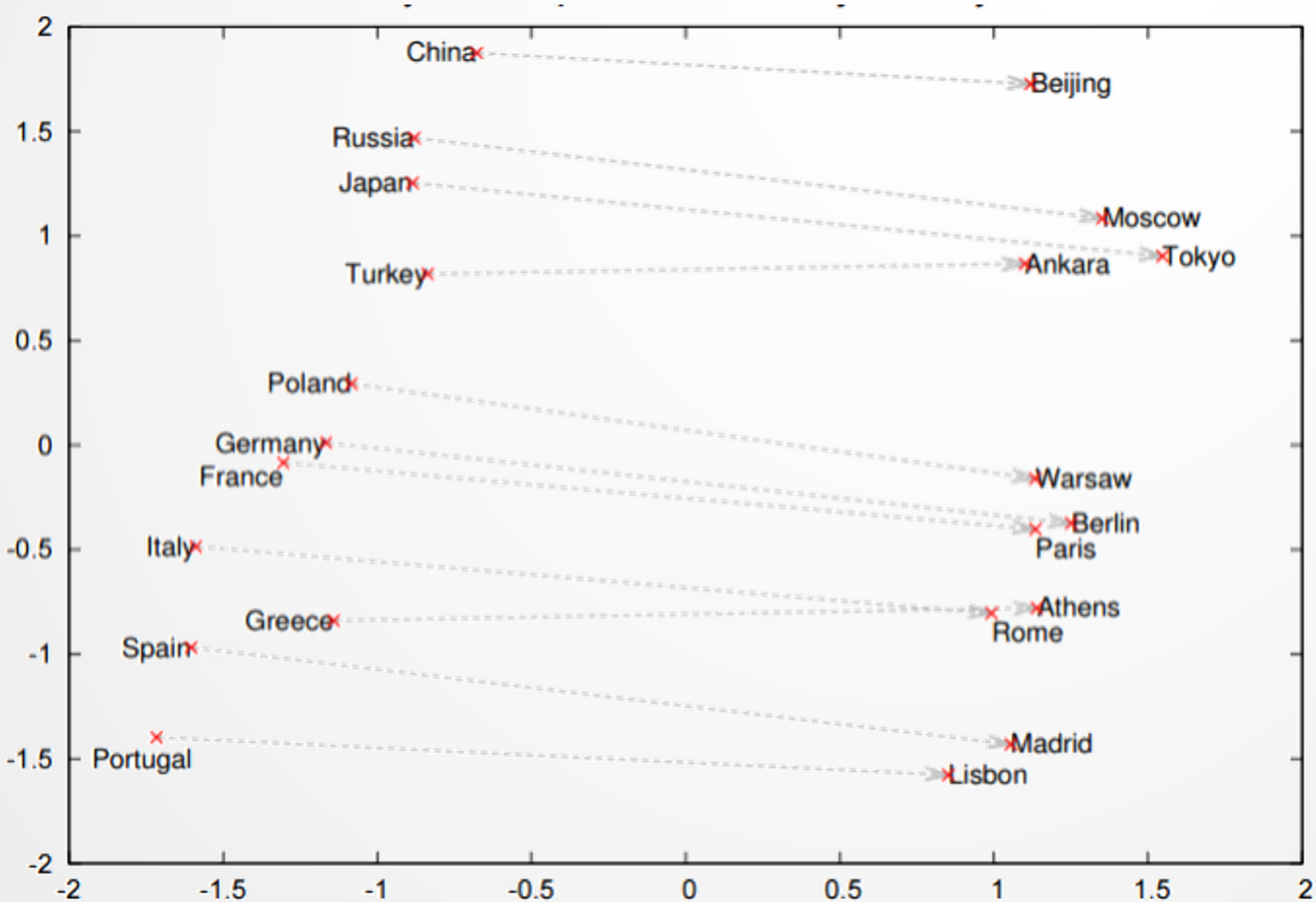
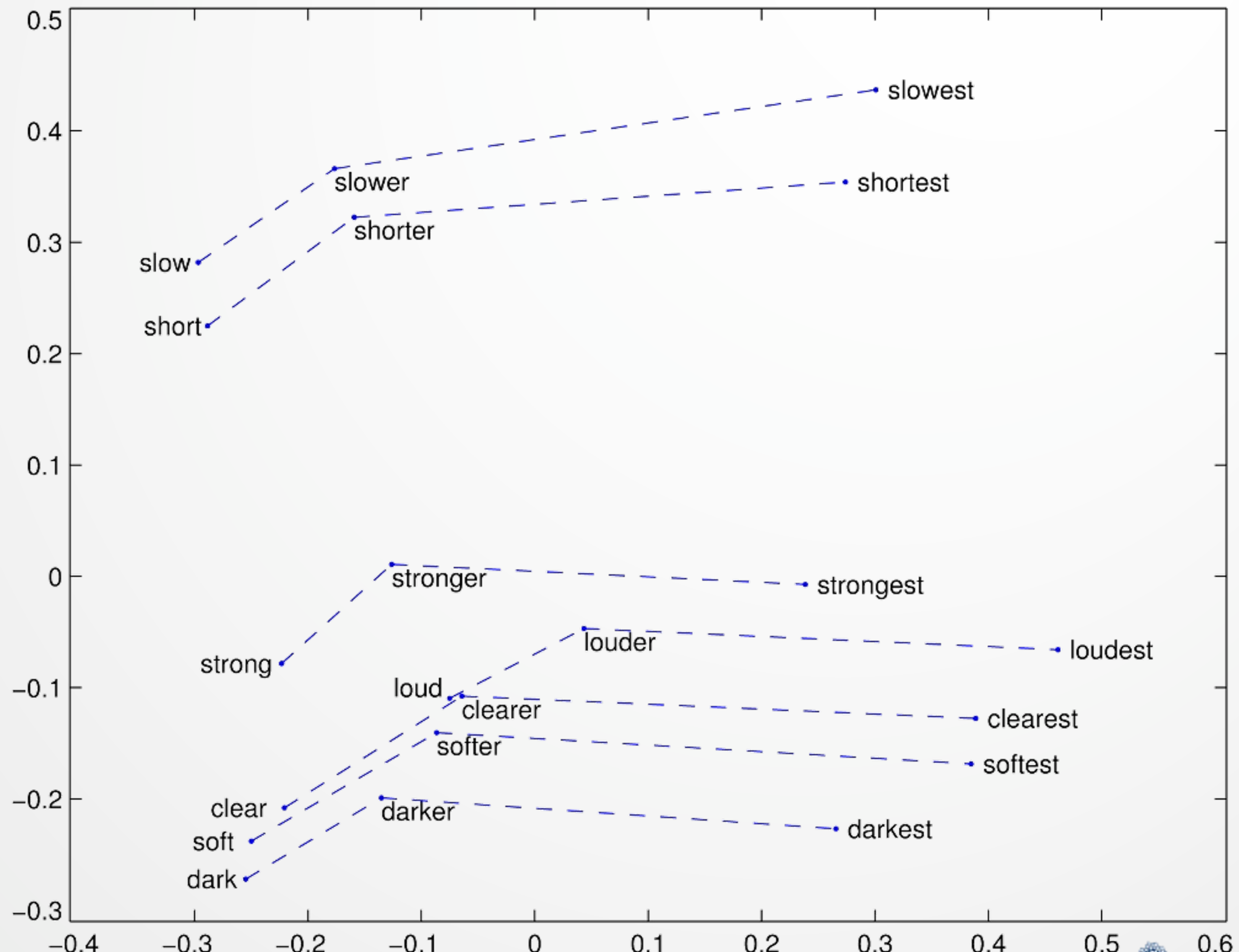
Linguistic regularities in vector space



Trained on the Google news corpus with over 300 billion words.

Linguistic regularities in vector space



(from GloVe)

Linguistic regularities in vector space

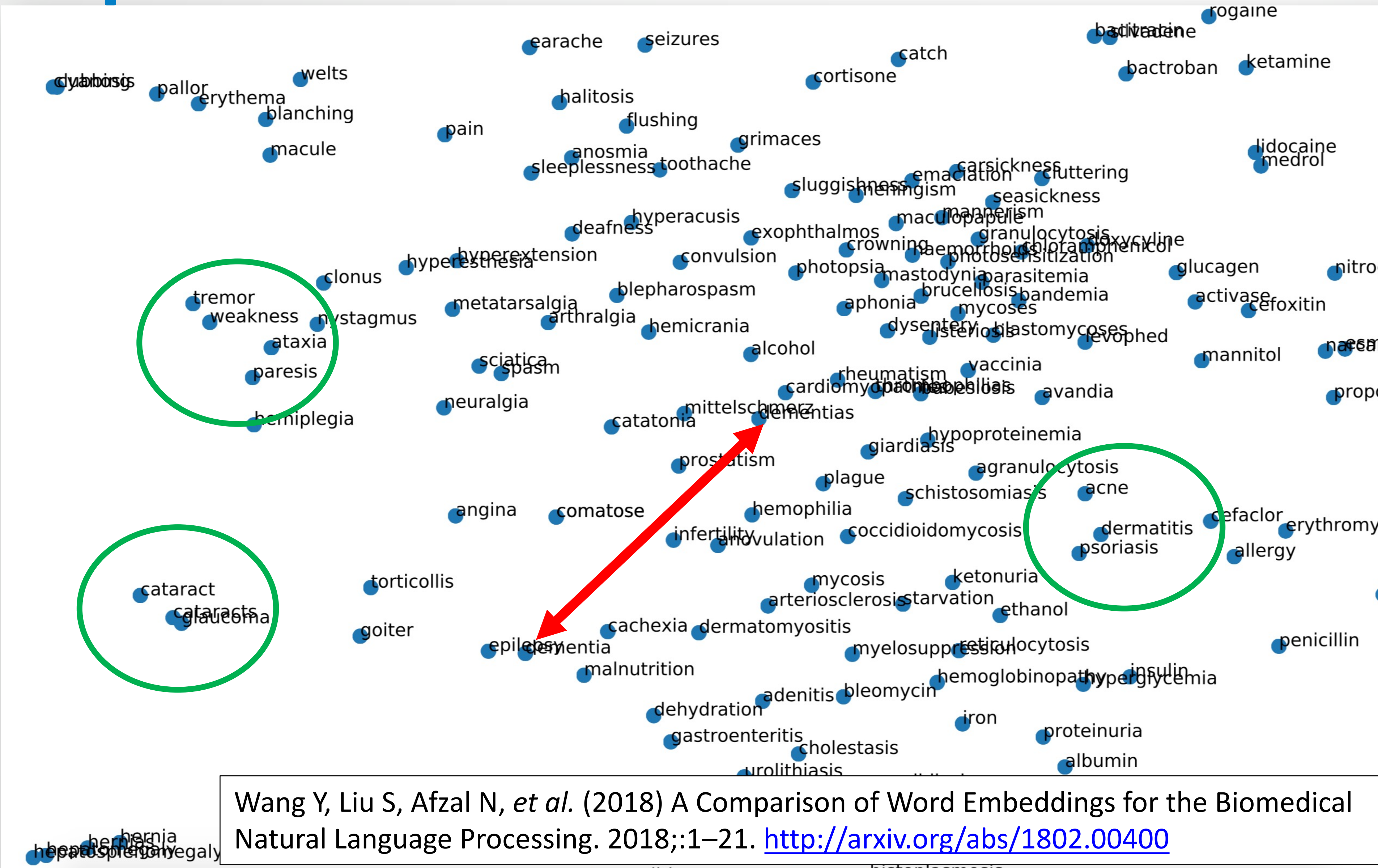
Expression	Nearest token
Paris – France + Italy	Rome
Bigger – big + cold	Colder
Sushi – Japan + Germany	bratwurst
Cu – copper + gold	Au
Windows – Microsoft + Google	Android

Analogies: apple:apples :: octopus:octopodes

Hypernymy: shirt:clothing :: chair:furniture

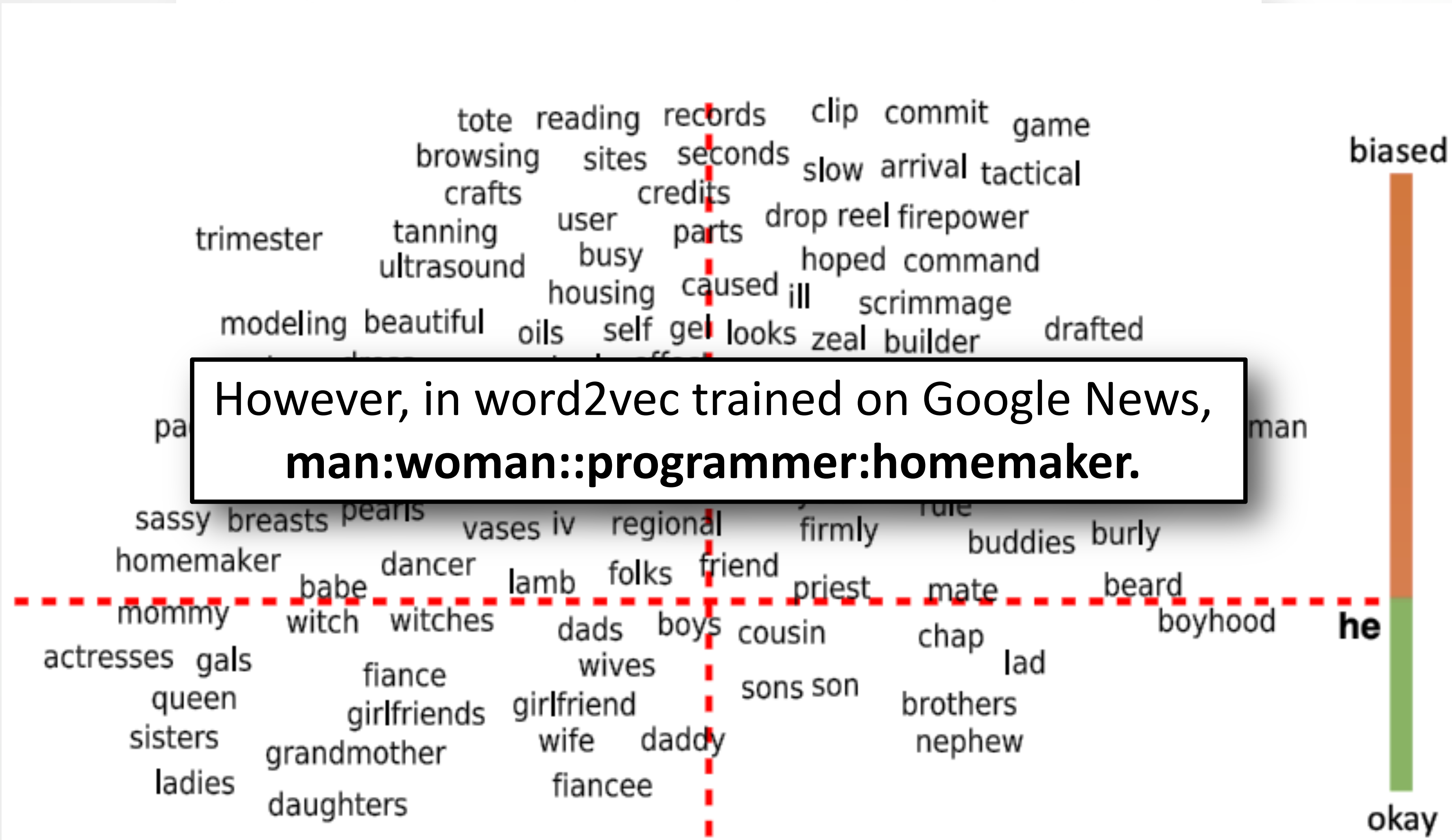
Semantic: queen – king ≈ woman – man

Importance of in-domain data



Wang Y, Liu S, Afzal N, *et al.* (2018) A Comparison of Word Embeddings for the Biomedical Natural Language Processing. 2018;:1–21. http://arxiv.org/abs/1802.00400

Biases: let's talk about gender



However, in word2vec trained on Google News,
man:woman::programmer:homemaker.

Bolukbasi T, Chang K, Zou J, *et al.* Man is to Computer Programmer as Woman is to Homemaker? Debiasing Word Embeddings. In: *NIPS*. 2016. 1–9.

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Biases: let’s talk about gender

Man is to Computer Programmer as Woman is to Homemaker? Debiasing Word Embeddings

Tolga Bolukbasi[1], **Kai-Wei Chang**[2], **James Zou**[2], **Venkatesh Saligrama**[1,2], **Adam Kalai**[2]
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Abstract

The blind application of machine learning runs the risk of amplifying biases present in data. Such a danger is facing us with *word embedding*, a popular framework to represent text data as vectors which has been used in many machine learning and

Extreme *she*	Extreme *he*
1. homemaker	1. maestro
2. nurse	2. skipper
3. receptionist	3. protege
4. librarian	4. philosopher
5. socialite	5. captain
6. hairdresser	6. architect
7. nanny	7. financier
8. bookkeeper	8. warrior
9. stylist	9. broadcaster
10. housekeeper	10. magician

Gender stereotype *she*-*he* analogies

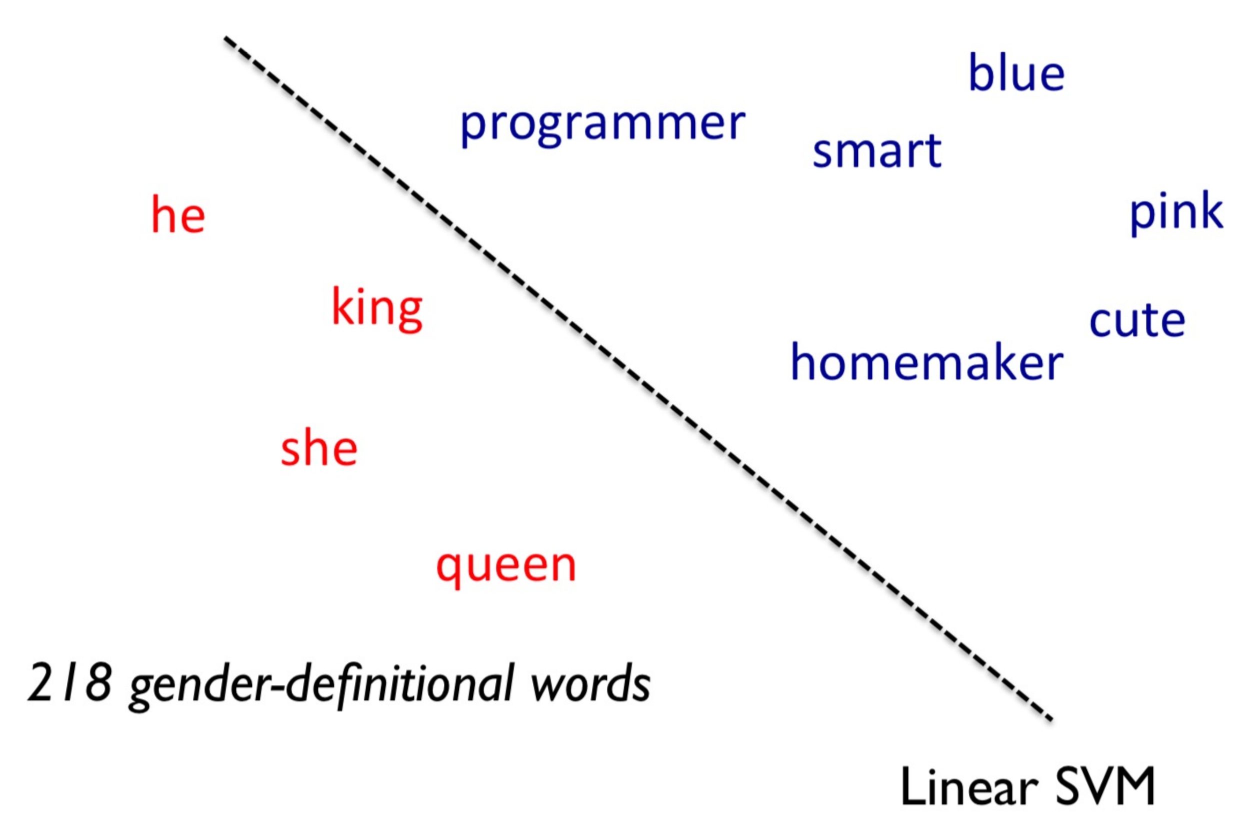
sewing-carpentry	registered nurse-physician	housewife-shopkeeper
nurse-surgeon	interior designer-architect	softball-baseball
blond-burly	feminism-conservatism	cosmetics-pharmaceuticals
giggle-chuckle	vocalist-guitarist	petite-lanky
sassy-snappy	diva-superstar	charming-affable
volleyball-football	cupcakes-pizzas	lovely-brilliant

Gender appropriate *she*-*he* analogies

queen-king	sister-brother	mother-father
waitress-waiter	ovarian cancer-prostate cancer	convent-monastery

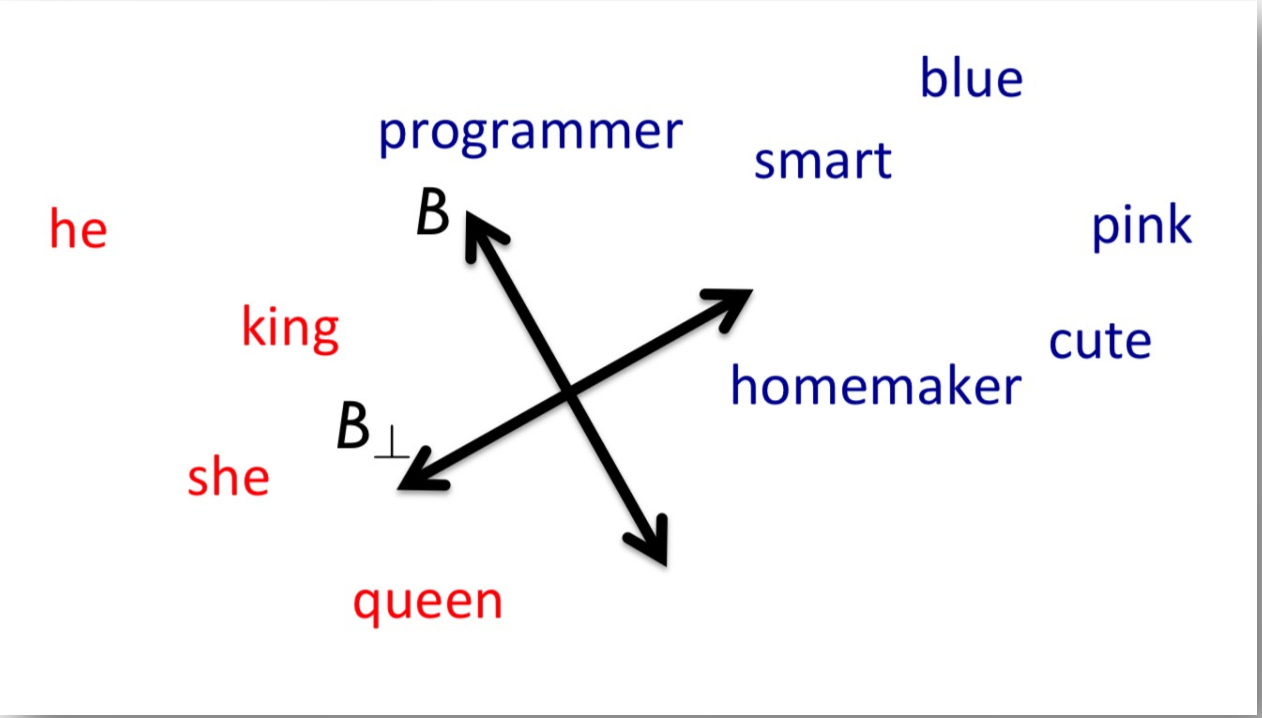
Solution?

1. Hand-pick words S_0 that are ’gender definitional’.
   ‘Neutral’ words are the complement, $N = V \setminus S_0$.



Solution?

2. Project away gender subspace from gender-neutral words, $w \coloneqq w - w \cdot B$ for $w \in N$, where B is the gender subspace.



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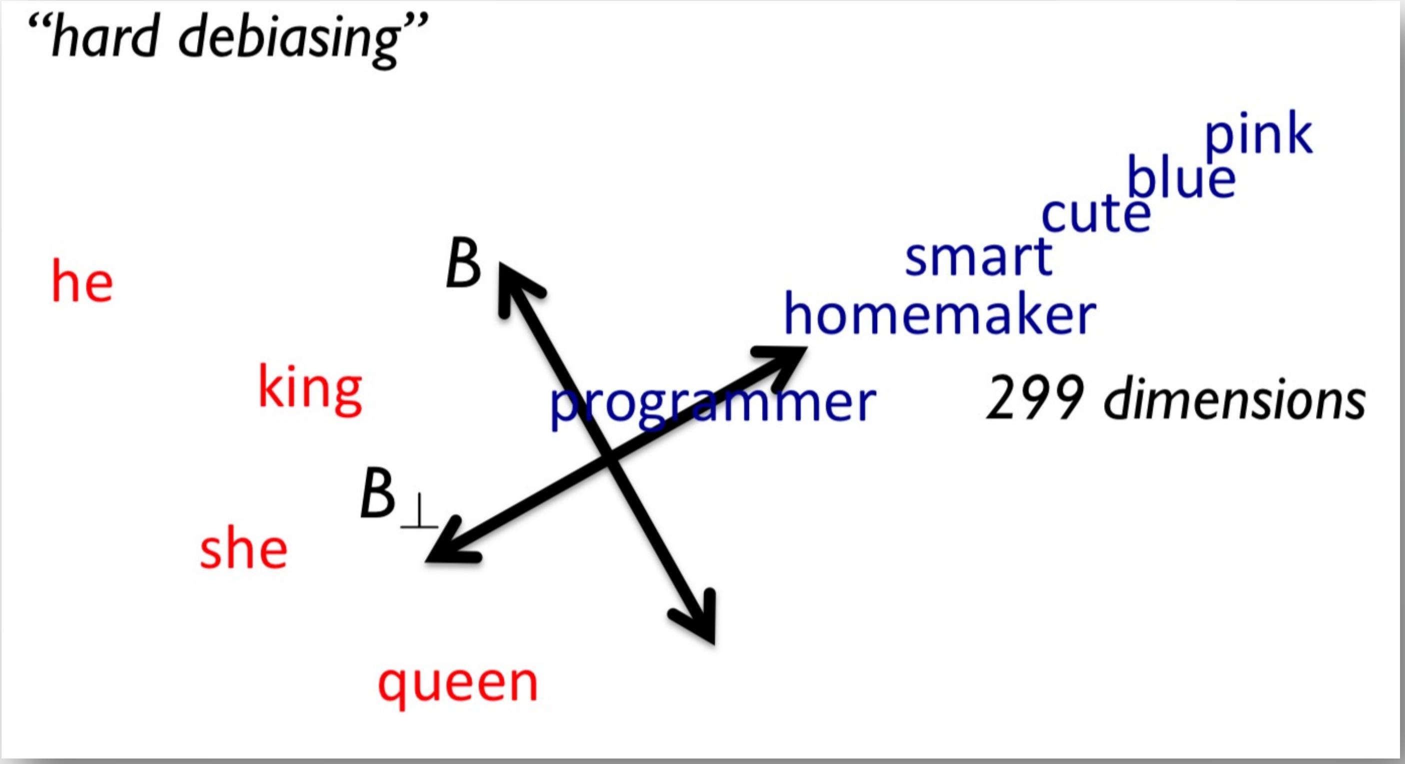
Solution?

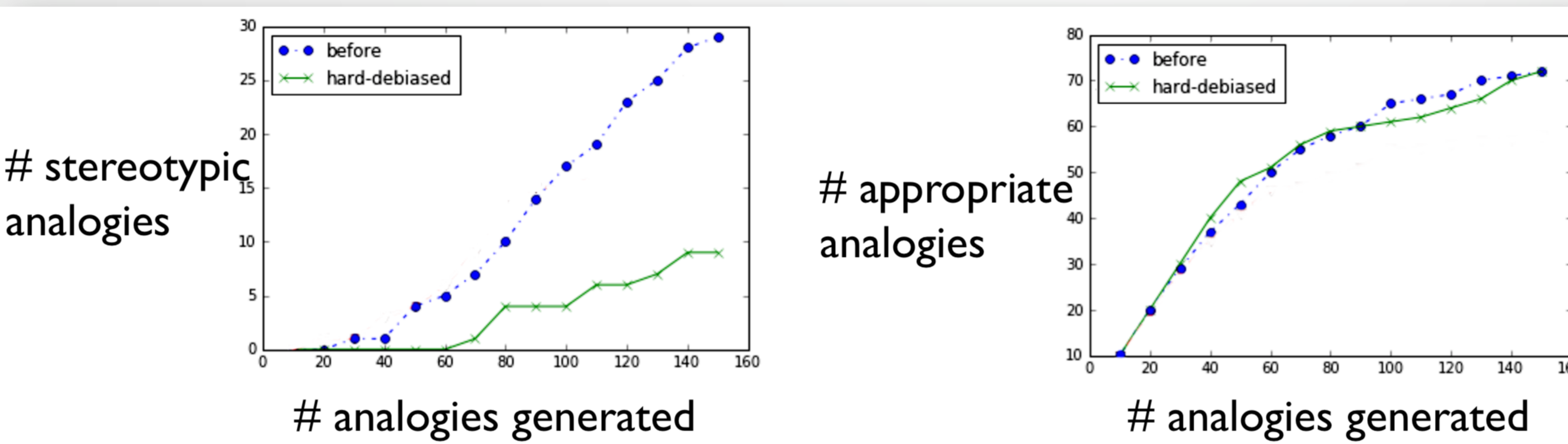
2. Project away gender subspace from gender-neutral words, $w := w - w \cdot B$ for $w \in N$, where B is the gender subspace.



Results

- Generate many analogies, see which ones preserve gender stereotypes.

He:*Blue* :: She: *?*		Irrelevant.
He:*Doctor* :: She: *?*		Stereotypic. He:Doctor-> She: __
He:Brother :: She: *?*		Appropriate. he:brother -> she:sister



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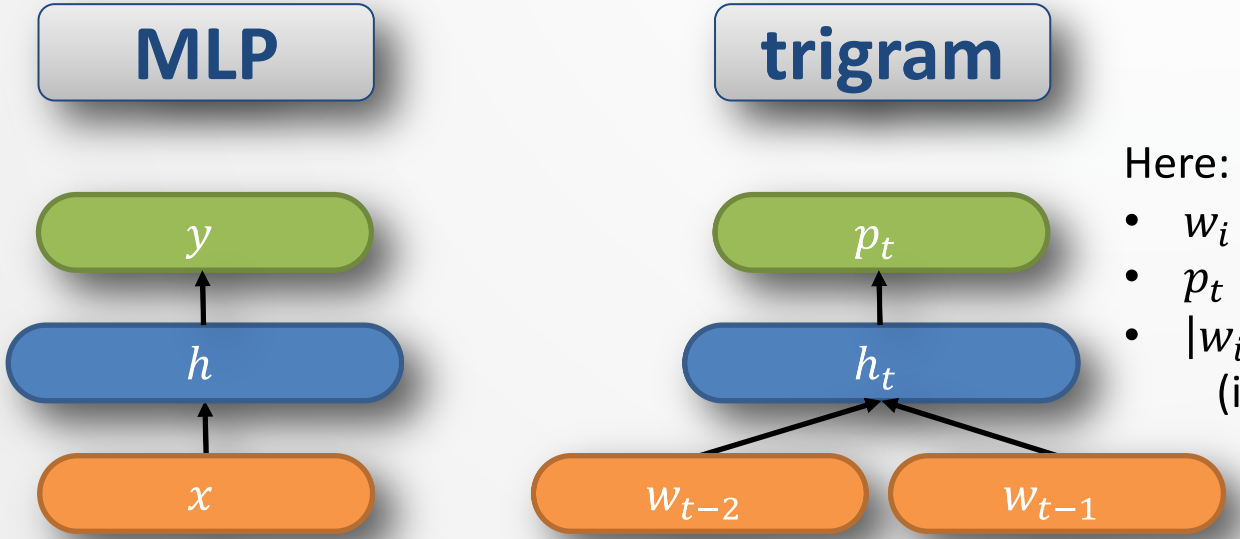
NEURAL LANGUAGE MODELS

Trigram models

- CBOW: prediction of current word w_t given w_{t-1}.
- Let's reconsider predicting w_t given multiple w_{t-j}?
  - I.e., let's think about **language modelling.**



$h = g(W_I \boldsymbol{x} + c)$
$\boldsymbol{y} = W_O \boldsymbol{h} + b$

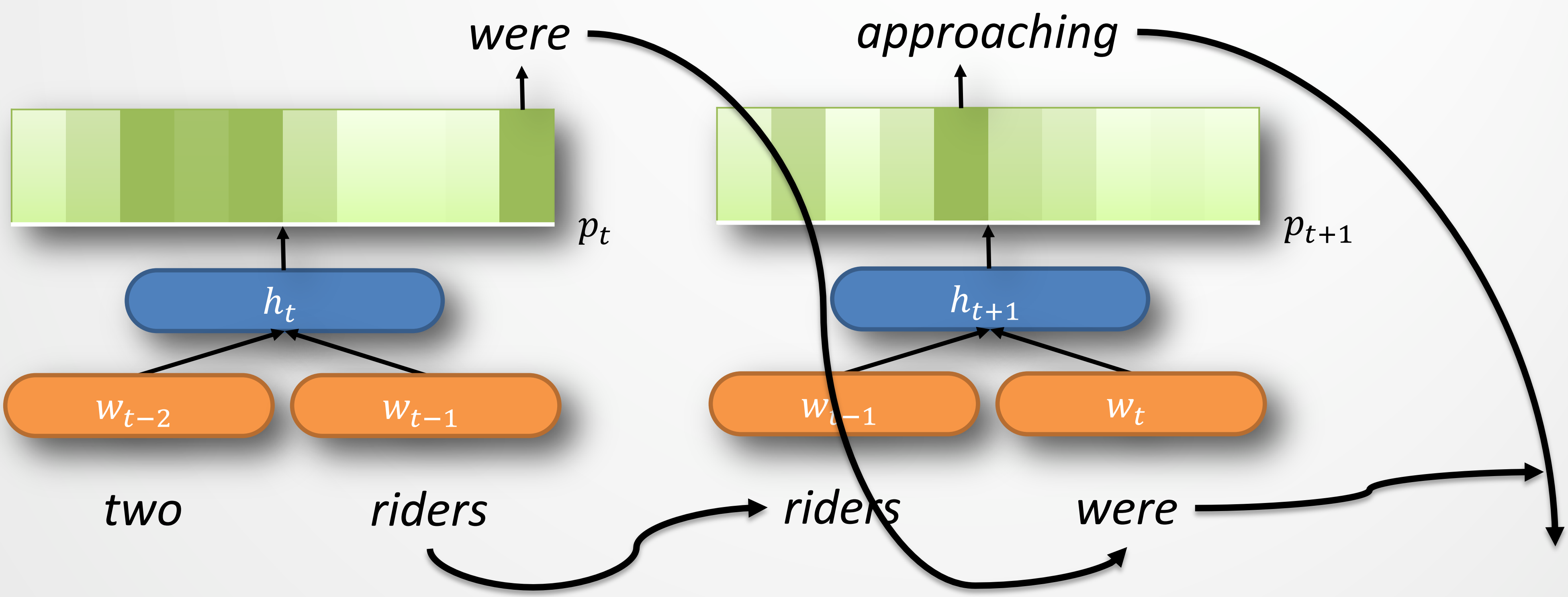
$h_t = g(W_I[\boldsymbol{w_{t-2}}; \boldsymbol{w_{t-1}}] + c)$
$\boldsymbol{p_t} = softmax(W_O \boldsymbol{h_t} + b)$

Here:

- w_i is a one-hot vector,
- p_t is a distribution, and
- $|w_i| = |p_t| = |V|$ (i.e., the size of the vocabulary)

Sampling from trigram models

- Since $p_t \sim P(w_t | w_{t-2}\ w_{t-1})$, we just feed forward and sample from the output vector.



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Training trigram models

- Here's one approach:

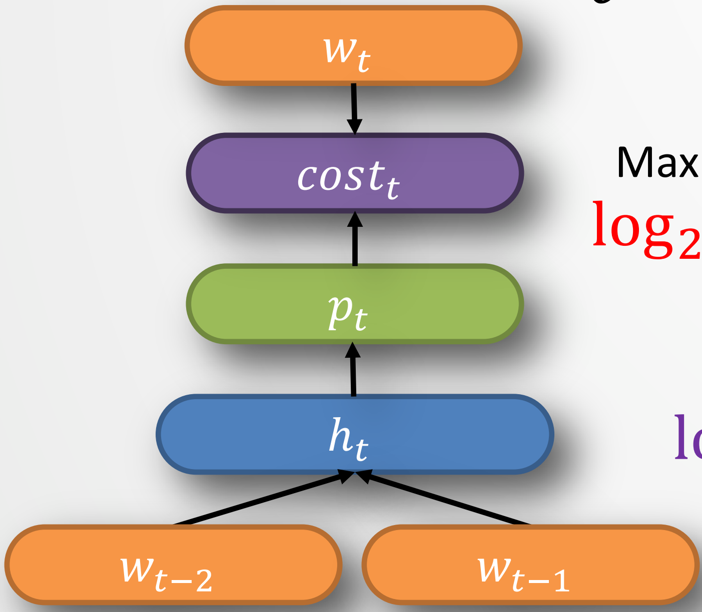
1. Randomly choose a batch (e.g., 10K consecutive words)
2. Propagate words through the current model
3. Obtain word likelihoods (loss)
4. Back-propagate loss
5. Gradient step to update model
6. Go to (1)

Training trigram models

- The typical training objective is the cross entropy (see Lecture 3) of the corpus C given the model M:

$$\mathcal{F} = H(C; M) = -\frac{\log_2 P_M(C)}{\|C\|}$$

Minimize



Maximize

$$\log_2 P_M(C) = \log_2 \prod_{t=0}^{T} P(w_t) = \sum_{t=0}^{T} \log_2 P(w_t)$$

$$\log_2 P(w_t) = w_t^{\mathsf{T}} \log p_t$$

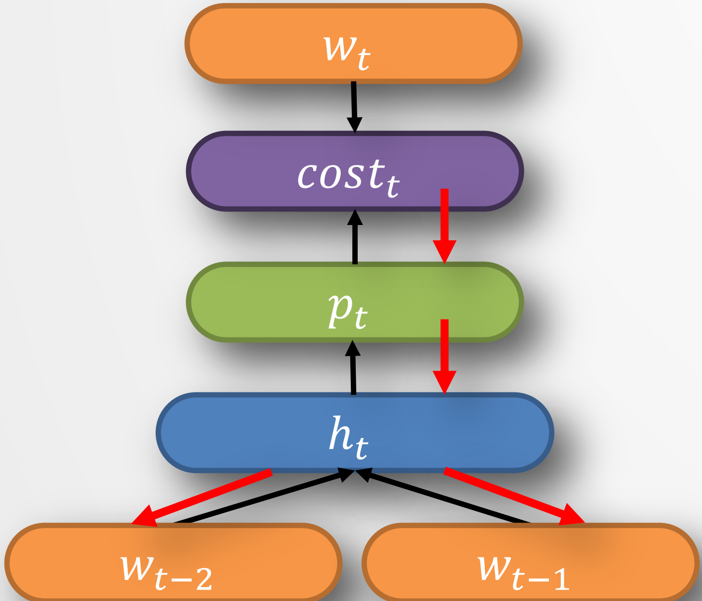
$h_t = g(W_I[\mathbf{w_{t-2}}; \mathbf{w_{t-1}}] + c)$
$\mathbf{p_t} = softmax(W_O \mathbf{h_t} + b)$

Here:

- w_i is a one-hot vector, and
- p_t is a distribution.

Training trigram models

- Compute our gradients, using $\mathcal{F} = -\frac{\log_2 P_M(C)}{\|C\|}$ and $\log_2 P(w_t) = w_t^\intercal \log p_t$ and back-propagate.



$$\frac{\delta \mathcal{F}}{\delta \mathrm{W}_O} = -\frac{1}{\|C\|}\sum_t \frac{\delta cost_t}{\delta p_t}\frac{\delta p_t}{\delta W_O}$$

$$\frac{\delta \mathcal{F}}{\delta \mathrm{W}_I} = -\frac{1}{\|C\|}\sum_t \frac{\delta cost_t}{\delta p_t}\frac{\delta p_t}{\delta h_t}\frac{\delta h_t}{\delta W_I}$$

$h_t = g(W_I[\boldsymbol{w_{t-2}}; \boldsymbol{w_{t-1}}] + c)$
$\boldsymbol{p_t} = softmax(W_O \boldsymbol{h_t} + b)$

Here:

- w_i is a one-hot vector, and
- p_t is a distribution.

Evaluating trigram (language) models

- Popular, intrinsic measure is *perplexity* (over unseen sentences)
- Information theoretic measure of how well a probability model predicts a sample – lower is better

- Given a text corpus C of n words $(w_1, \ldots, w_n)$, and a language model, $LM = \mathrm{P}(w_i | w_{1:i-1})$

$$\mathrm{Perplexity}_C(\mathrm{LM}) = 2^{-\frac{1}{n}\sum_{i=1}^{n} \log_2 LM(w_i | w_{1:i-1})}$$
$$= 2^{-\frac{\log_2 P_{LM}(C)}{||C||}}$$
$$= 2^{H(C;\, LM)}$$

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So what?

- ☺ Neural language models of this type:
  - Can generalize better than MLE LMs to unseen *n*-grams,
  - Can use *semantic* information as in word2vec.

$$P(the\ cat\ sat\ on\ the\ \boldsymbol{mat}) \approx P(the\ cat\ sat\ on\ the\ \boldsymbol{rug})$$

- ☹ Neural language models of this type:
  - Can take *relatively* long to train. "GPUs kill the Earth."
  - Number of parameters scale poorly with increasing context. Large vocab and training corpus is prohibitive.

Let's improve both of these issues…

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Dealing with that bottleneck

- Traditional datasets for neural language modeling include:
  - AP News (14M tokens, 17K types)
  - HUB-4 (1M tokens, 25K types)
  - Google News (6B tokens, 1M types)
  - Wikipedia (3.2B tokens, 2M types)

- Datasets for **medical/clinical** LM include:
  - EMRALD/ICES (3.5B tokens, 13M types)

- Much of the computational effort is in the initial embedding, and in the softmax.
  - Can we simplify and speed up the process?

Dealing with that bottleneck

- **Replace** rare words with <out-of-vocabulary> token.
- **Subsample** frequent words.

e.g., <unk>

- Hierarchical softmax.
- Noise-contrastive estimation.
- Negative sampling.

[Morin & Bengio, 2005, Mikolov et al, 2011, 2013b;
Mnih & Teh 2012, Mnih & Kavukcuoglu, 2013]

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Hierarchical softmax with grouping

- Group words into distinct classes, c, e.g., by frequency.
  - E.g., c_1 is top 5% of words by frequency, c_2 is the next 5%, …
- Factorize $p(w_o|w_i) = p(w_o|w_i, C) = \sum p(c|w_i)p(w_o|w_i, c)$

'**softmax**': $P(w_o|w_i) = \frac{\exp(V_{w_o}^{\intercal} v_{w_i})}{\sum_{w=1}^{|V|} \exp(V_w^{\intercal} v_{w_i})}$ ⇒ $\frac{\exp(c_j v_{w_i})}{\sum_c \exp(c v_{w_i})} \times \frac{\exp(V_{w_o}^{\intercal} v_{w_i})}{\sum_{w \in c} \exp(V_w^{\intercal} v_{w_i})}$

Where

v_w is the 'input' vector for word w,
V_w is the 'output' vector for word w,

[Mikolov et al, 2011, Auli et al, 2013]

RECURRENT NEURAL NETWORKS

Statistical language models

- Probability is conditioned on (window of) n previous words*
- A necessary (but incorrect) Markov assumption: each observation only depends on **a short linear history** of length *L*.

$$P(w_n|w_{1:(n-1)}) \approx P(w_n|w_{(n-L+1):(n-1)})$$

- Probabilities are estimated by computing unigrams and bigrams

$$P(s) = \prod_{i=1}^{t} P(w_i|w_{i-1})$$

bigram

$$P(s) = \prod_{i=2}^{t} P(w_i|w_{i-2}w_{i-1})$$

trigram

*From Lecture 2

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Statistical language models

- Using higher n-gram counts (with smoothing) improves performance*
- *Computational burden:* too many n-grams (combinations)
  - Infeasible RAM requirements
- *RNN intuition:*
  - Use the **same set of weight** parameters for each word (or across all time steps)
  - Condition the neural network on all previous words (or time steps)
  - Memory requirement now scales with number of words

*From Lecture 2

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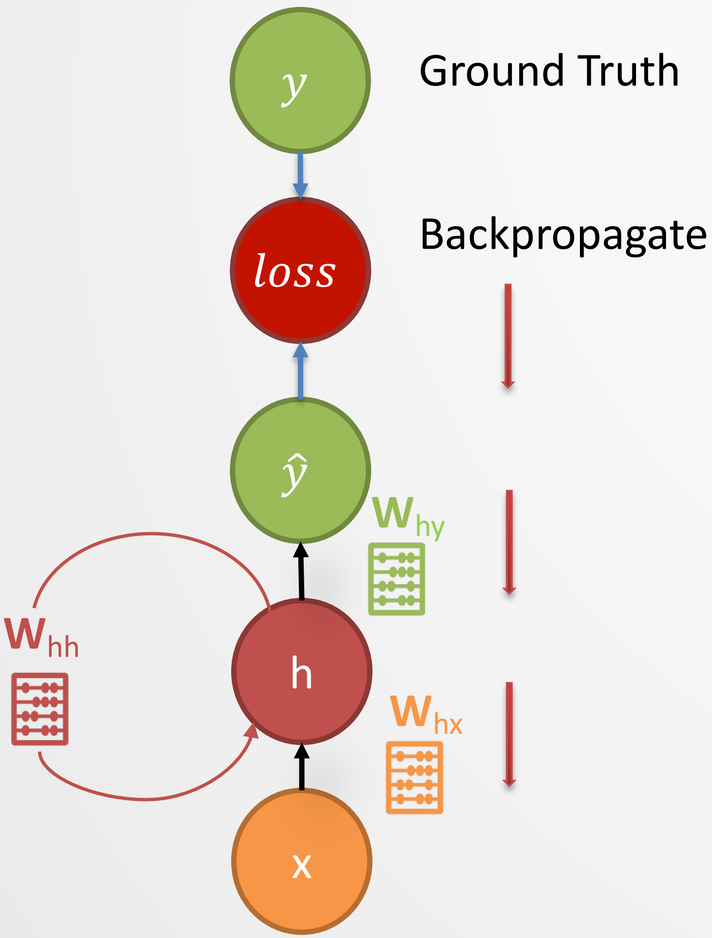
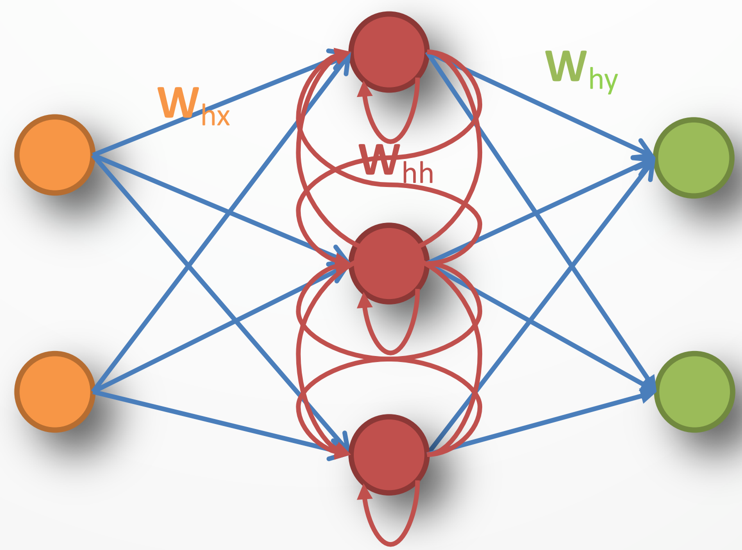
Recurrent neural networks (RNNs)

- An RNN has **feedback** connections in its structure so that it '*remembers*' previous states, when reading a sequence.





Elman network feed hidden units back

Jordan network (not shown) feed output units back

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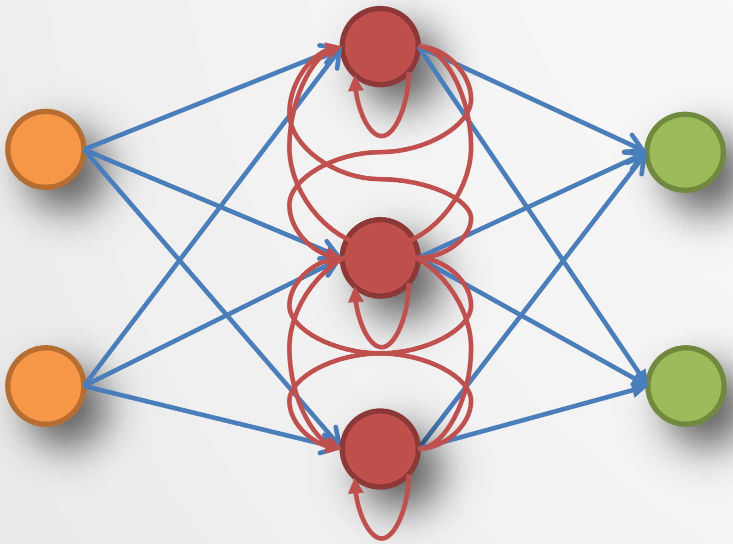
RNNs: Unrolling the $\boldsymbol{h_i}$

- Copies of the same network can be applied (i.e., **unrolled**) at each point in a time series.
  - These can be applied to various tasks.



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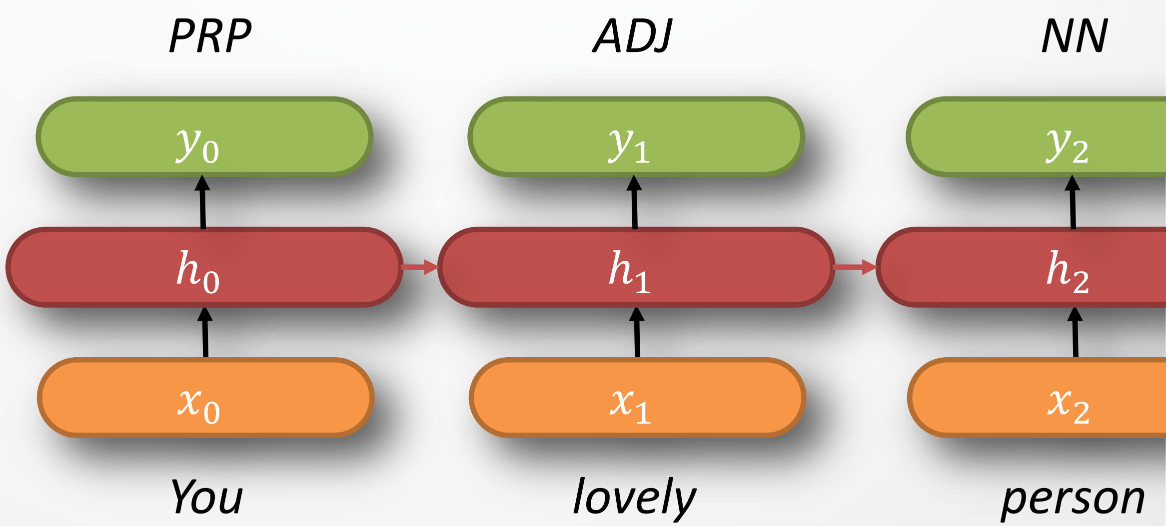

$$h_t = g(W_I[\boldsymbol{h_{t-1}}; \boldsymbol{x}] + c)$$
$$\boldsymbol{y_t} = W_O \boldsymbol{h_t} + b$$

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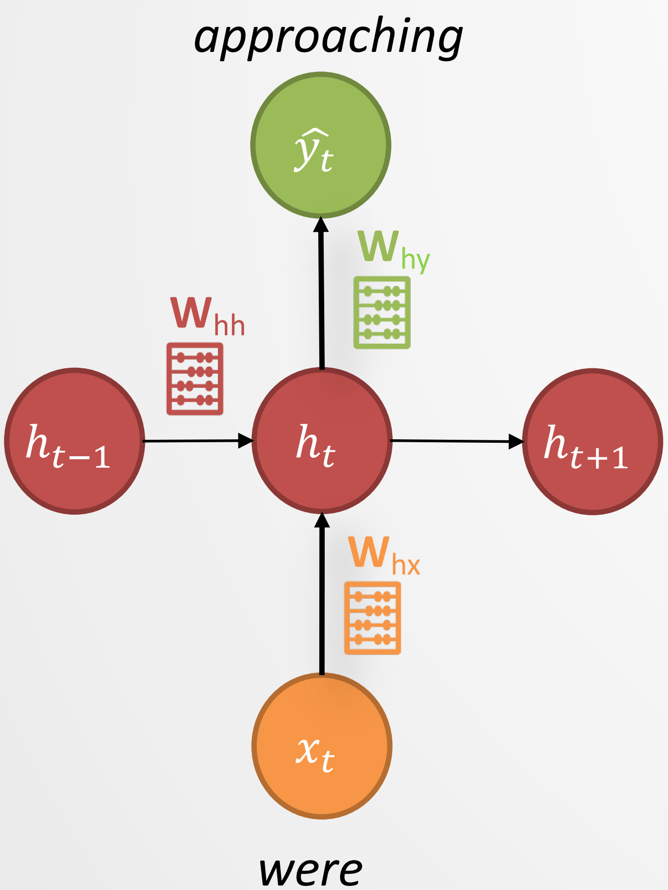
RNNs: One time step snapshot

Two riders .. approaching .. horses.

- Given a list of word vectors $\boldsymbol{X}$: $x_1, x_2, \ldots, x_t, x_{t+1}, \ldots, x_T$



$$P(x_{t+1} = v_j | x_t, \ldots, x_1) = \widehat{y_{t,j}}$$

- At a single time-step:

$$h_t = g([W_{hh}\boldsymbol{h_{t-1}} + W_{hx}\boldsymbol{x_t}] + c)$$

$$h_t = g(W_I[\boldsymbol{h_{t-1}}; \boldsymbol{x_t}] + c) \quad \text{(equivalent notation)}$$

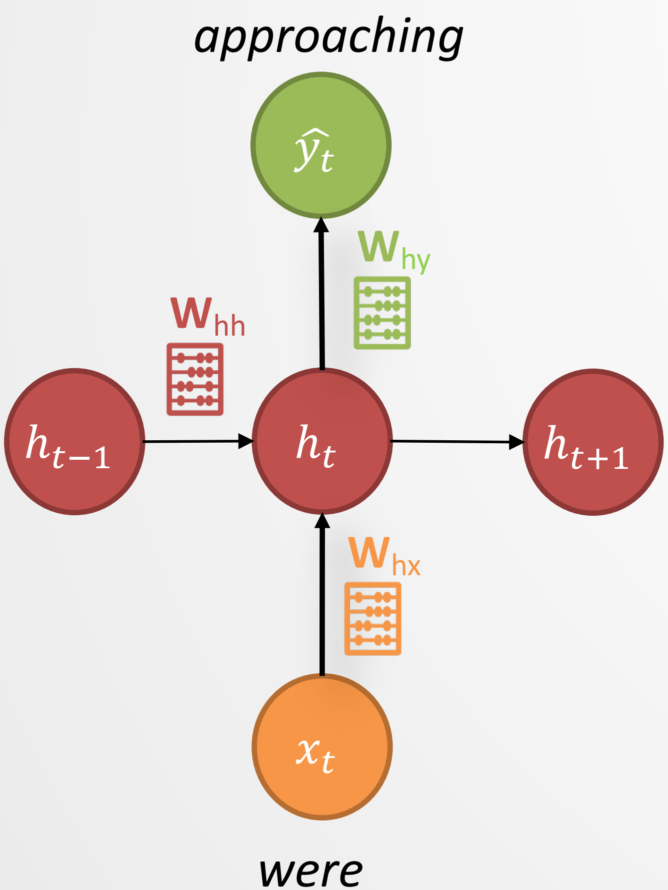
$$\widehat{y_t} = softmax\,(W_{hy}\boldsymbol{h_t} + b)$$

```python
import numpy as np

def softmax(x):
    f_x = np.exp(x) / np.sum(np.exp(x))
    return f_x

class RNN:
    # ...
    def step(self, x, is_normalized=False):
        # update the hidden state
        self.h = np.tanh(np.dot(self.W_hh, self.h) + np.dot(self.W_xh, x))

        # compute the output vector
        y = np.dot(self.W_hy, self.h)

        return softmax(y) if is_normalized else y
```

RNNs: Training

Two riders .. approaching .. horses.

- Given a list of word vectors $\boldsymbol{X}$: $x_1, x_2, \ldots, x_t, x_{t+1}, \ldots, x_T$



$$P(x_{t+1} = v_j | x_t, \ldots, x_1) = \widehat{y_{t,j}}$$

$\hat{y} \in \mathbb{R}^{|V|}$ is a probability distribution over the vocabulary

The output $\widehat{y_{t,j}}$ is the word (index) prediction of the next word (**$\mathbf{x}_{t+1}$**)

Evaluation

- Same **cross-entropy** loss function

$$J^{(t)}(\theta) = -\sum_{j=1}^{|V|} \underbrace{y_{t,j}}_{\text{Ground truth}} \log \underbrace{\hat{y}_{t,j}}_{\text{prediction}}$$

- **Perplexity**: 2^J (lower is better)

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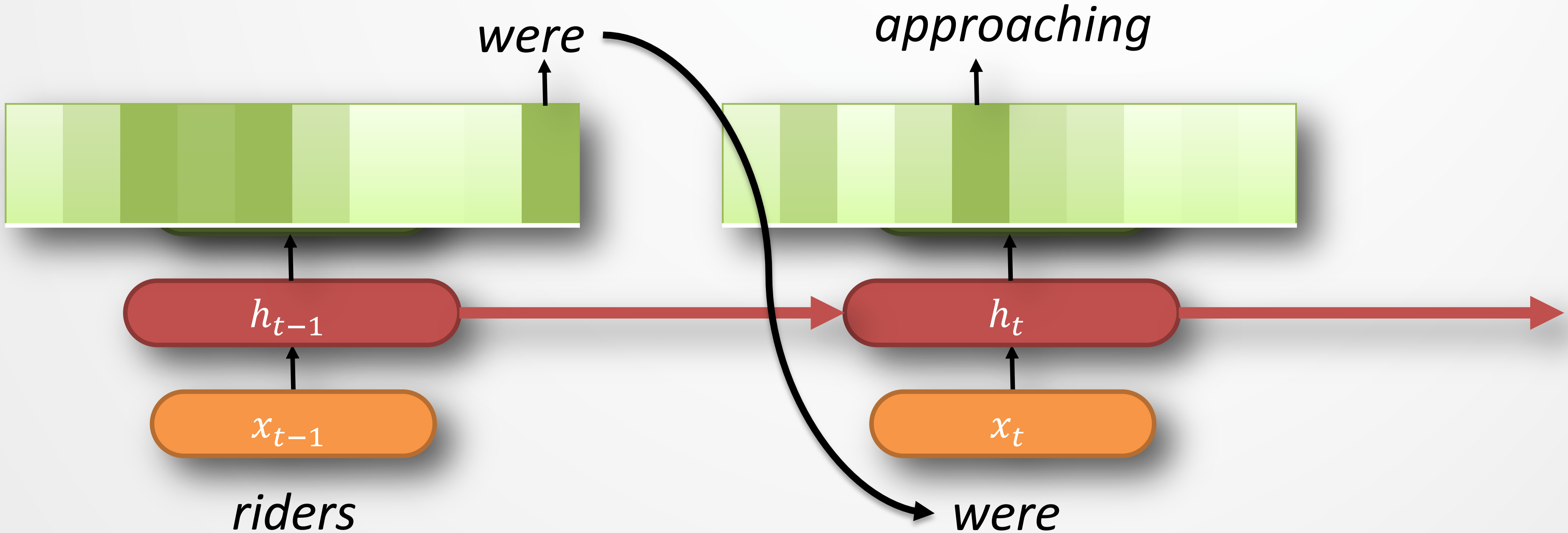
Sampling from a RNN LM

- If $|h_i| < |V|$, we've already reduced the number of parameters from the trigram NN.
  - In 'theory', information is maintained in h_i across arbitrary lengths of time…

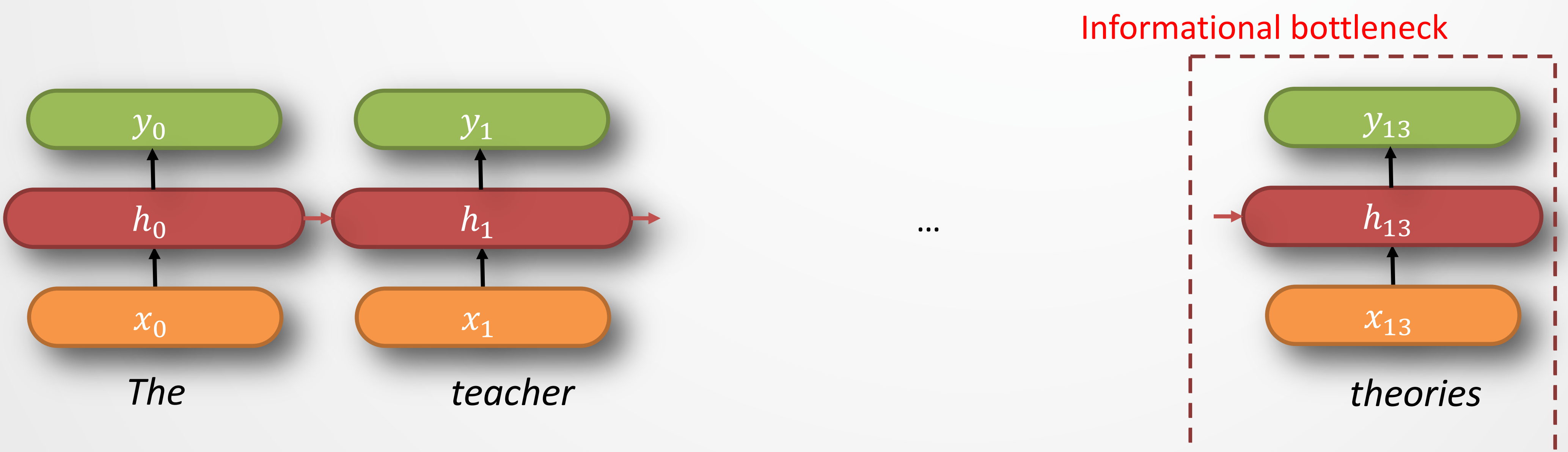


$h_t = g([W_{hh}\boldsymbol{h_{t-1}}; W_{hx}\boldsymbol{x_t}] + c)$
$\hat{y}_t = softmax\,(W_{hy}\boldsymbol{h_t} + b)$

Karpathy (2015), [The Unreasonable Effectiveness of Recurrent Neural Networks]

RNNs and retrograde amnesia

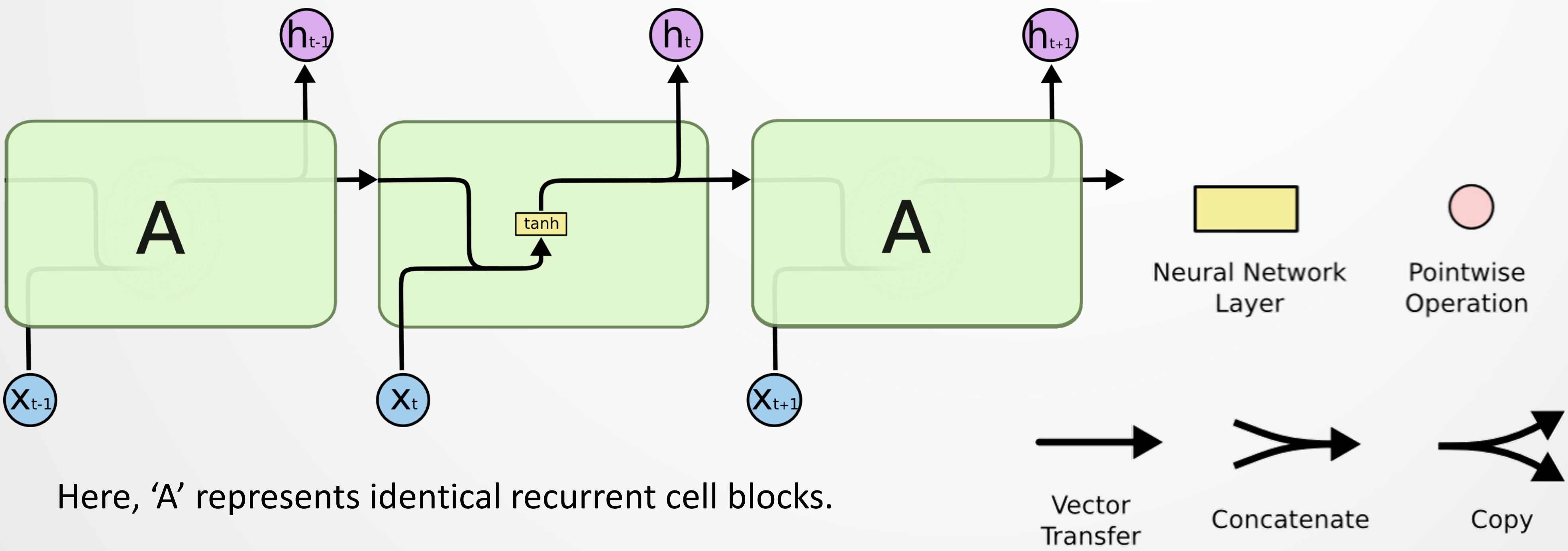
- Unfortunately, **catastrophic forgetting** is common.
  - E.g., the **relevant** context in "*The teacher taught transformers terribly telling tiring, tortuous theories* ..." has likely been **overwritten** by the time h_{13} is produced.



Bengio Y, Simard P, Frasconi P. (1994) Learning Long-Term Dependencies with Gradient Descent is Difficult. IEEE Trans. Neural Networks.;**5**:157–66. doi:10.1109/72.279181

RNNs and retrograde amnesia

- One challenge with RNNs is that the **gradient** decays quickly as one pushes it back in time. Can we store relevant information?

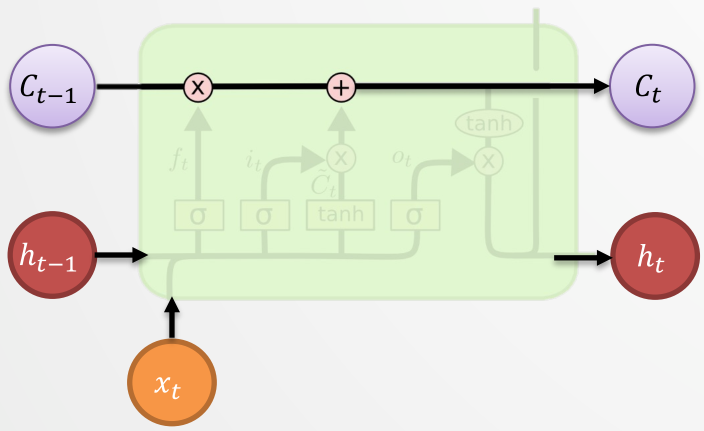


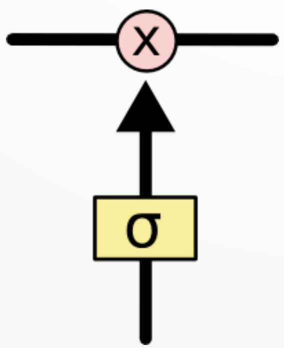
Here, 'A' represents identical recurrent cell blocks.

Imagery and sequence from http://colah.github.io/posts/2015-08-Understanding-LSTMs/

Long short-term memory (LSTM)

- Within each *recurrent unit or cell*:
  - Self-looping recurrence for ***cell state*** *using vector C*
  - Information flow regulating structures called ***gates***





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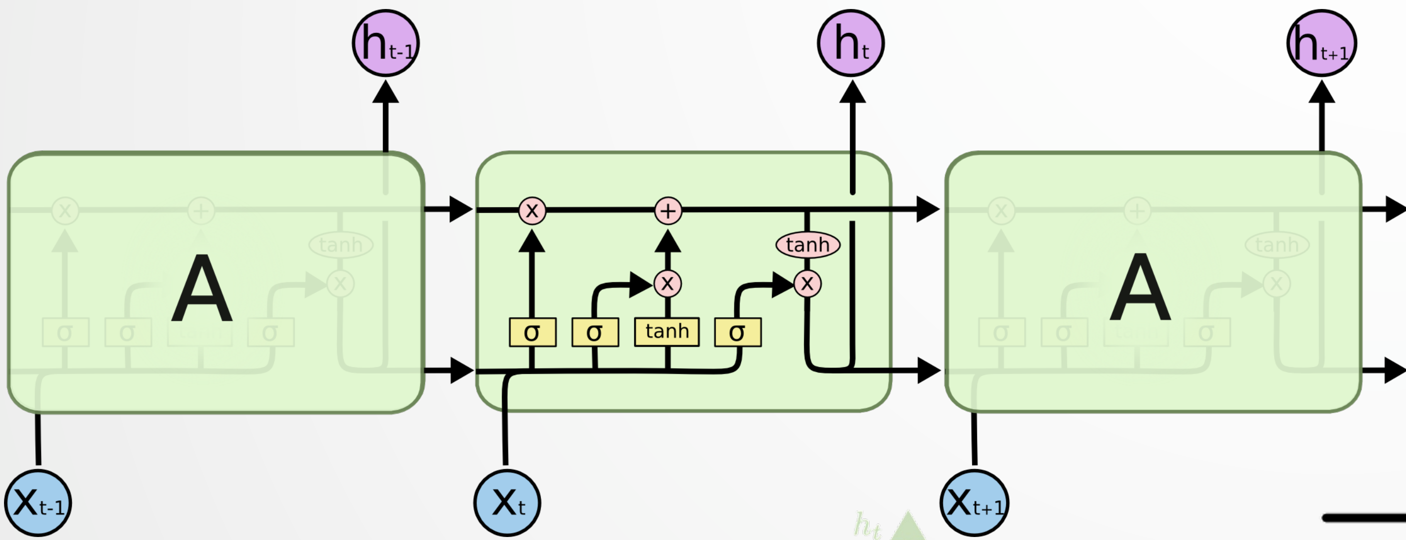
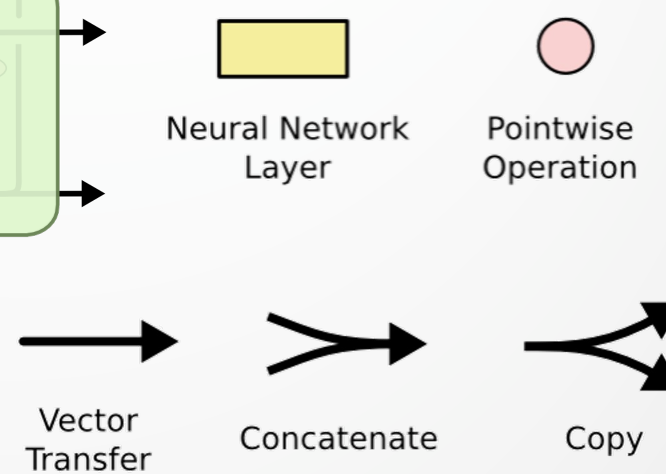
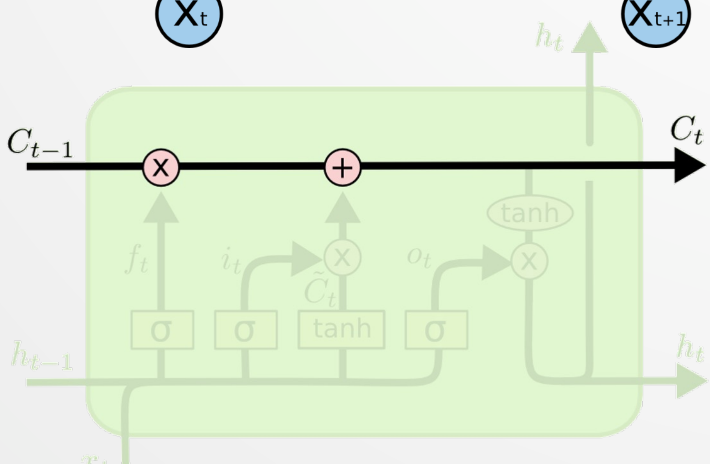
LSTM – core ideas

- In each **cell** (i.e. recurrent unit) in an LSTM, there are four interacting neural network layers.







The **cell state** is a special vector stream that runs through the entire chain and **stores the long-term information.**

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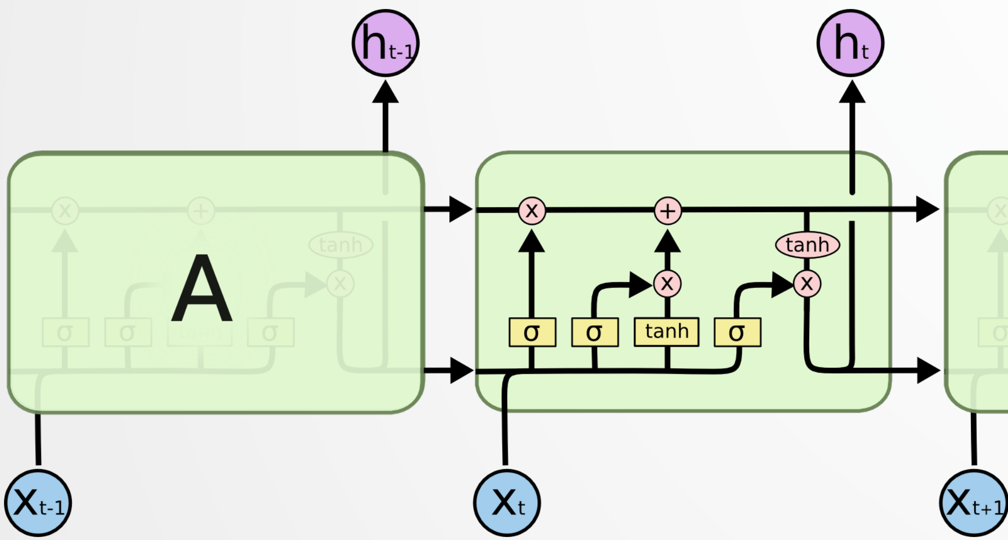
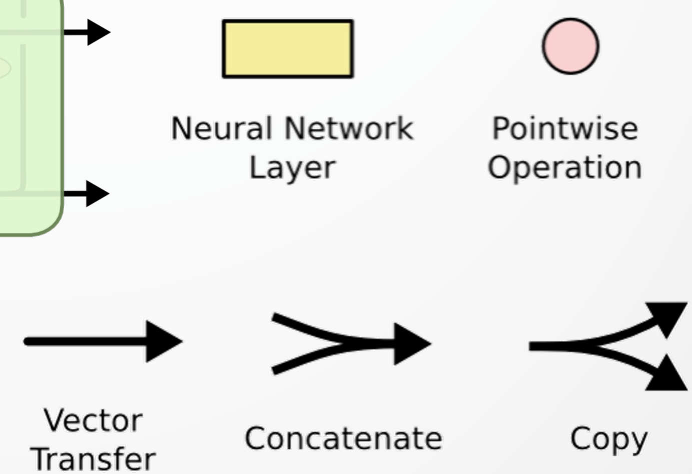
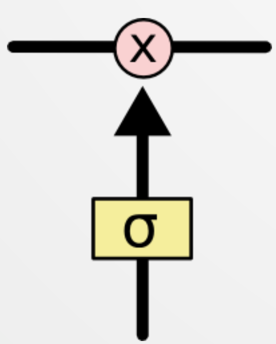
LSTM – core ideas

- In each **cell** (i.e. recurrent unit), there are four interacting neural network layers.



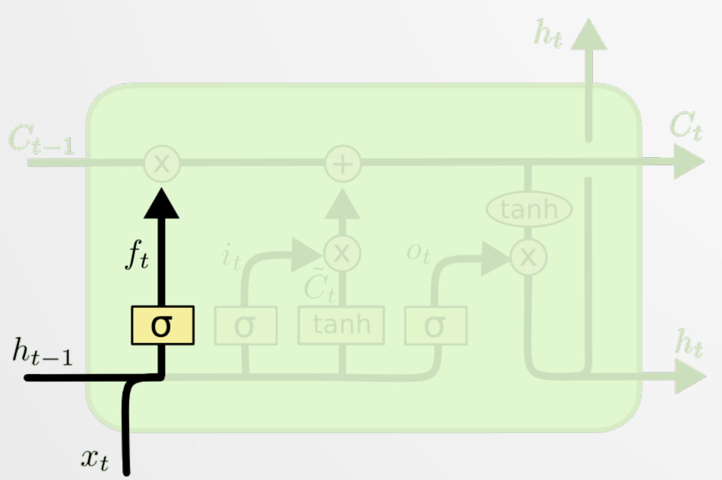




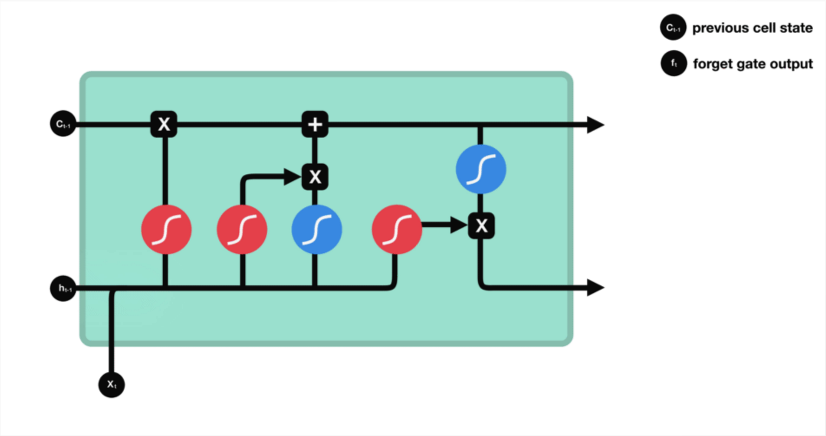
Gates decide what information should be withheld in the cell state.
They are a **sigmoid** followed by a pointwise ×.
Values near 0 block information; values near 1 pass information.

LSTM step 1: decide what to forget

- The **forget gate layer** compares h_{t-1} and the current input x_t to decide which elements in cell state C_{t-1} to keep and which to turn off.
  - E.g., the cell state might 'remember' the number (sing./plural) of the current subject, in order to predict appropriately conjugated verbs, but decide to forget it when a new subject is mentioned at x_t.
    - (There's scant evidence that such information is so explicit.)

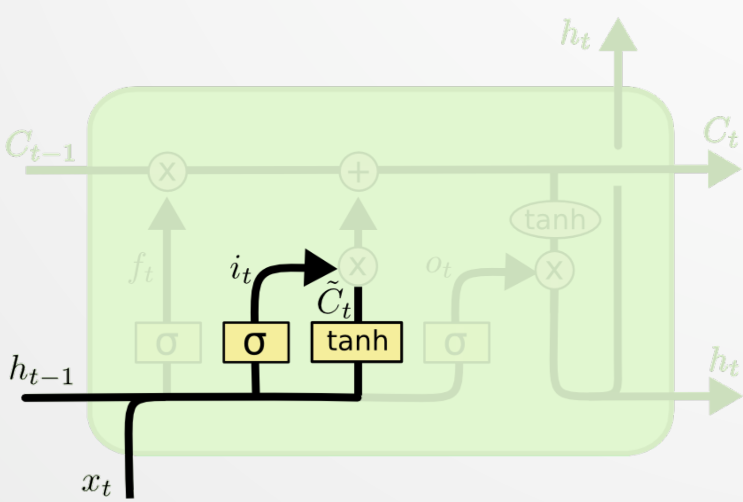


$$f_t = \sigma\left(W_f \cdot [h_{t-1}, x_t] \; + \; b_f\right)$$



LSTM step 2: decide what to store

- The **input gate layer** has two steps.
  - First, a sigmoid layer **σ** decides which cell units to update.
  - Next, a **tanh** layer creates new candidate values $\widetilde{C}_t$.
  - E.g., the σ can turn on the 'number' units, and the tanh can push information on the current subject.
  - The σ layer is important – we don't want to push information on units (i.e., latent dimensions) for which we have no information.



$$i_t = \sigma\left(W_i \cdot [h_{t-1}, x_t] \ + \ b_i\right)$$

$$\tilde{C}_t = \tanh(W_C \cdot [h_{t-1}, x_t] \ + \ b_C)$$

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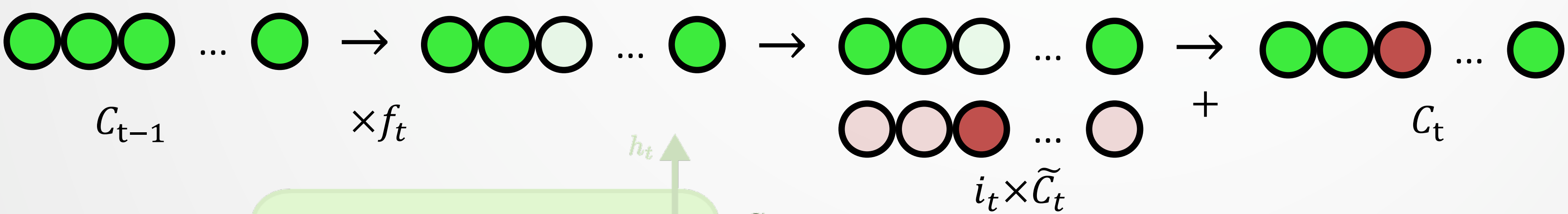
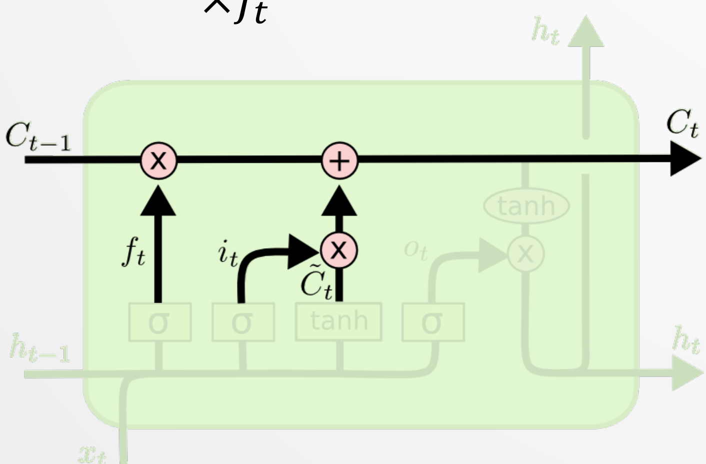
LSTM step 3: update the cell state

- Update C_{t-1} to C_t.
  - First, forget what we want to forget: multiply C_{t-1} by f_t.
  - Then, create a 'mask vector' of information we want to store, $i_t \times \widetilde{C}_t$.
  - Finally, write this information to the new cell state C_t.





$$C_t = f_t \times C_{t-1} + i_t \times \widetilde{C}_t$$

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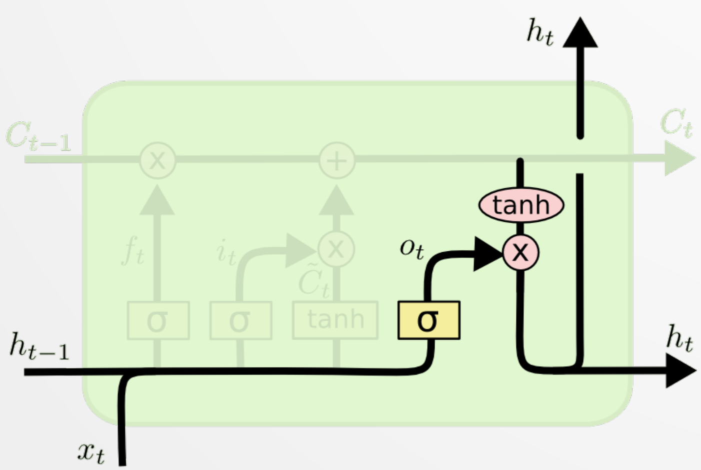
LSTM step 4: output and feedback

- Output something, o_t, based on the current x_t and h_{t-1}.
- Combine the output with the cell to give your h_t.
  - Normalize cell C_t on [-1,1] using tanh and combine with o_t

- In some sense, C_t is **long-term** memory and h_t is the **short-term memory** (hence the name).

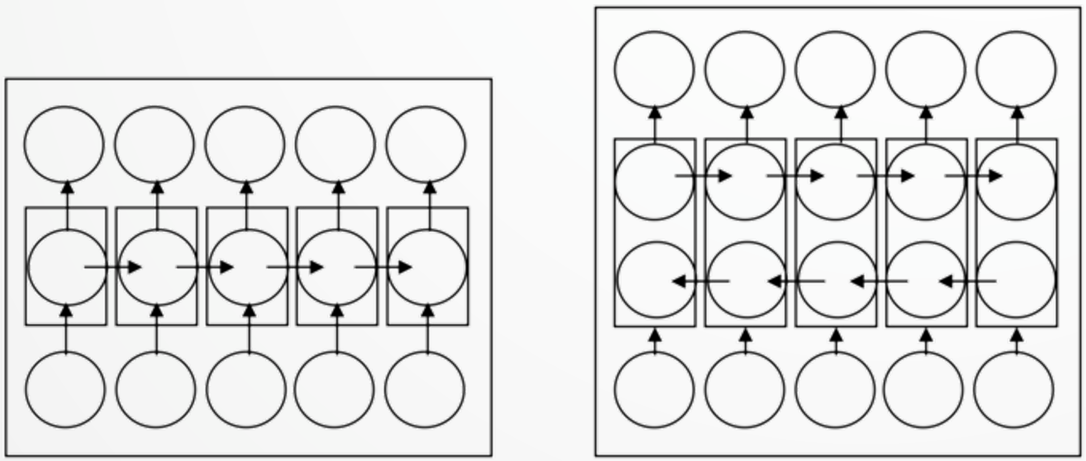


$$o_t = \sigma(W_o[h_{t-1}, x_t] + b_o)$$

$$h_t = o_t \times \tanh(C_t)$$

Variants of LSTMs

- There are many variations on LSTMs.
  - ‘*Bidirectional LSTMs*’ (and bidirectional RNNs generally), learn. (Similar: *Multi-stack RNNs)*



(a) (b)

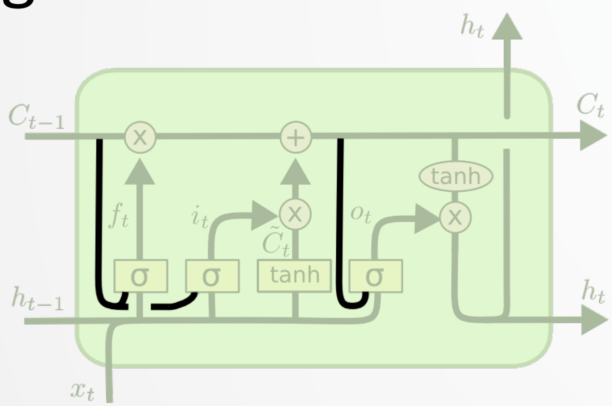
Structure overview

(a) unidirectional RNN
(b) bidirectional RNN

Schuster, Mike, and Kuldip K. Paliwal. (1997) Bidirectional recurrent neural networks. *Signal Processing, IEEE Transactions on* **45(**11) (1997): 2673-2681.2.

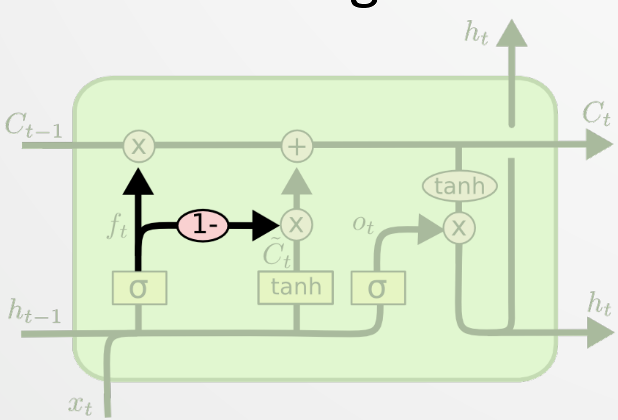
Variants of LSTMs

- Gers & Schmidhuber (2000) add '**peepholes**' that allow all sigmoids to read the cell state.



$$f_t = \sigma\left(W_f \cdot [\boldsymbol{C_{t-1}}, h_{t-1}, x_t] \; + \; b_f\right)$$
$$i_t = \sigma\left(W_i \cdot [\boldsymbol{C_{t-1}}, h_{t-1}, x_t] \; + \; b_i\right)$$
$$o_t = \sigma\left(W_o \cdot [\boldsymbol{C_t}, h_{t-1}, x_t] \; + \; b_o\right)$$

- We can **couple** the '*forget*' and '*input*' gates.
  - Joint decisioning is more efficient.



$$C_t = f_t * C_{t-1} + (\mathbf{1} - \boldsymbol{f_t}) * \tilde{C}_t$$

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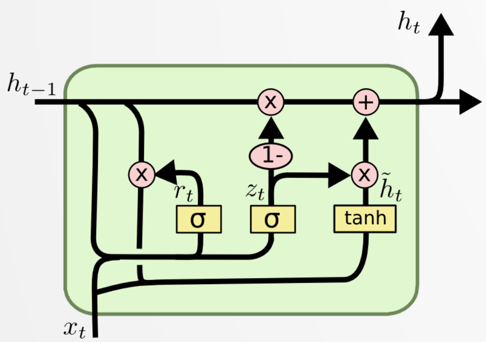
Aside - Variants of LSTMs

- **Gated Recurrent units** (GRUs; Cho *et al* (2014)) go a step further and also merge the cell and hidden states.



$z_t = \sigma\left(W_z \cdot [h_{t-1}, x_t]\right)$ **Update** gate

$r_t = \sigma\left(W_r \cdot [h_{t-1}, x_t]\right)$ **Reset** gate (0: replace units in h_{t-1} with those in x_t)

$\tilde{h}_t = \tanh\left(W \cdot [r_t * h_{t-1}, x_t]\right)$

$h_t = (1 - z_t) * h_{t-1} + z_t * \tilde{h}_t$

- Which of these variants is best? Do the differences matter?
  - Greff, et al. (2015) do a nice comparison of popular variants, finding that **they're all about the same**
  - Jozefowicz, et al. (2015) tested more than ten thousand RNN architectures, finding some that worked better than LSTMs on certain tasks.

CONTEXTUAL WORD EMBEDDINGS

Deep contextualized representations

- What does the word *play* mean?

AllenNLP

Peters ME, Neumann M, Iyyer M, *et al.* (2018) Deep contextualized word representations. Published Online First: 2018. doi:10.18653/v1/N18-1202; http://arxiv.org/abs/1802.05365

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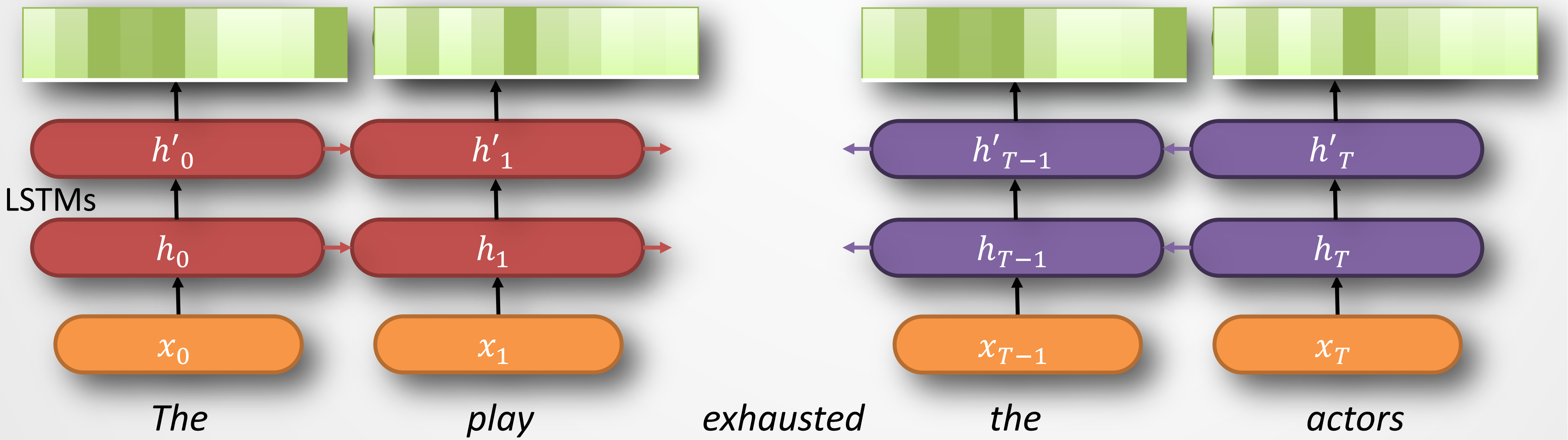
ELMo: Embeddings from Language Models

- Instead of a fixed embedding for each word **type**, ELMo considers the entire sentence before embedding each **token**.
  - It uses a **bi-directional** LSTM trained on a specific task.
  - Outputs are softmax probabilities on words, as before.



Peters, Mathew E., et al. "Deep contextualized word representations. (2018)." *arXiv preprint arXiv:1802.05365* (2018).

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ELMo: Embeddings from Language Models

For each token, a L-layer biLM computes (2L+1) representations:

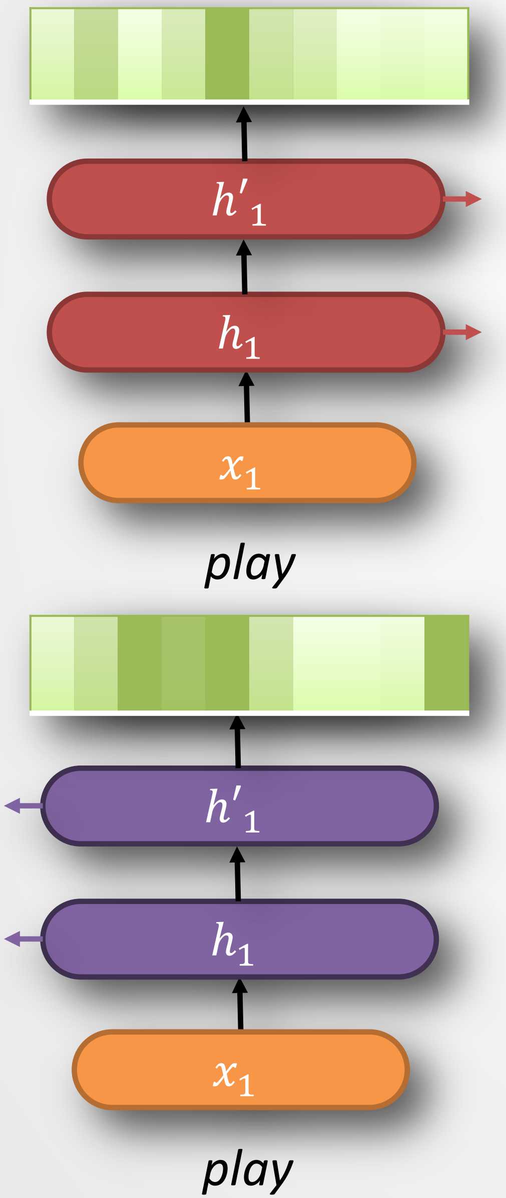
$$\begin{aligned} R_k &= \{\mathbf{x}_k^{LM}, \overrightarrow{\mathbf{h}}_{k,j}^{LM}, \overleftarrow{\mathbf{h}}_{k,j}^{LM} \mid j = 1, \ldots, L\} \\ &= \{\mathbf{h}_{k,j}^{LM} \mid j = 0, \ldots, L\}, \end{aligned}$$

- Task specific weighting produces the final embedding for word token k.

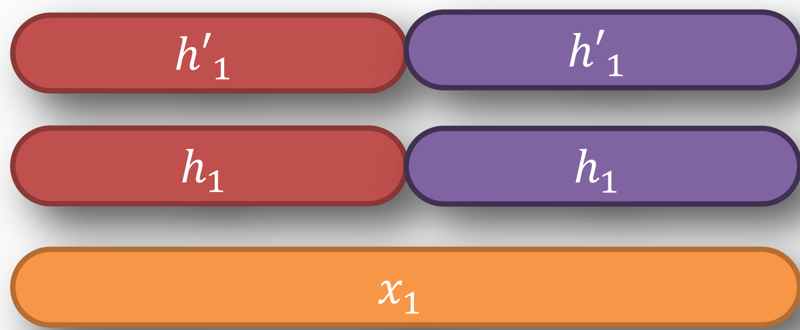
$$\mathbf{ELMo}_k^{task} = E(R_k; \Theta^{task}) = \gamma^{task} \sum_{j=0}^{L} s_j^{task} \mathbf{h}_{k,j}^{LM}$$

- where R_K is the set of all L hidden layers, $\mathbf{h}_{k,j}$
  s_j^{task} is the task's weight on the layer, and
  γ^{task} is a weight on the entire task

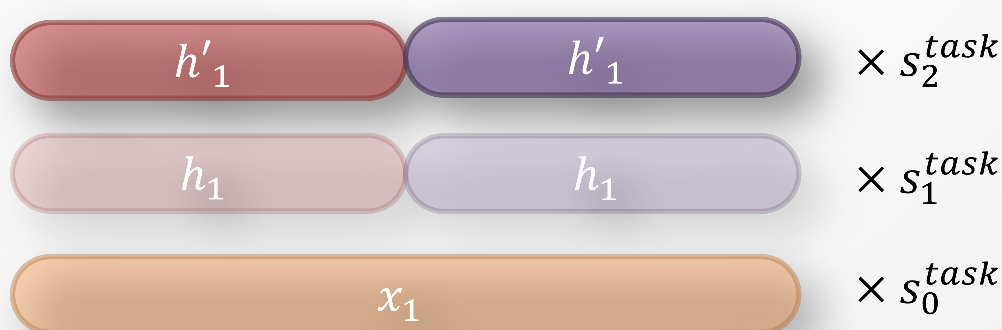
ELMo: Embeddings from Language Models



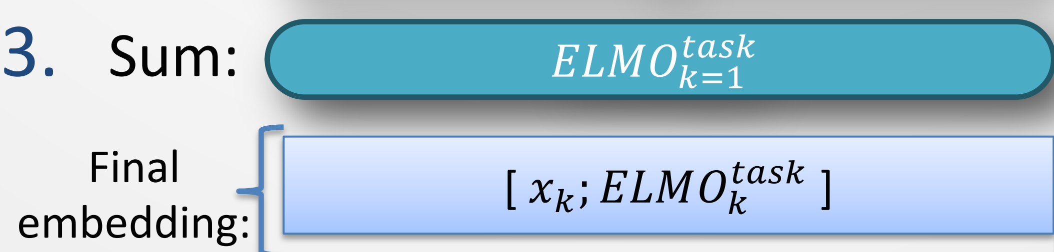
1. Concatenate



2. Multiply by weight vectors



3. Sum:



ELMo: Embeddings from Language Models

- What does the word *play* mean?

	Source	Nearest Neighbors
GloVe	play	playing, game, games, played, players, plays, player, Play, football, multiplayer
biLM	Chico Ruiz made a spectacular play on Alusik 's grounder {...}	Kieffer , the only junior in the group , was commended for his ability to hit in the clutch , as well as his all-round excellent play .
	Olivia De Havilland signed to do a Broadway play for Garson {...}	{...} they were actors who had been handed fat roles in a successful play , and had talent enough to fill the roles competently , with nice understatement .

Table 4: Nearest neighbors to "play" using GloVe and the context embeddings from a biLM.

Peters ME, Neumann M, Iyyer M, *et al.* (2018) Deep contextualized word representations. Published Online First: 2018. doi:10.18653/v1/N18-1202; http://arxiv.org/abs/1802.05365

ELMo: Embeddings from Language Models

	Task	Previous SOTA		Our Baseline	ELMo + Baseline	Increase (Absolute/ Relative)
Q&A	SQuAD	Liu et al. (2017)	84.4	81.1	85.8	4.7 / 24.9%
Textual entailment	SNLI	Chen et al. (2017)	88.6	88.0	88.7 ± 0.17	0.7 / 5.8%
Semantic role labelling	SRL	He et al. (2017)	81.7	81.4	84.6	3.2 / 17.2%
Coreference resolution	Coref	Lee et al. (2017)	67.2	67.2	70.4	3.2 / 9.8%
Name entity resolution	NER	Peters et al. (2017)	91.93 ± 0.19	90.15	92.22 ± 0.10	2.06 / 21%
Sentiment analysis	SST-5	McCann et al. (2017)	53.7	51.4	54.7 ± 0.5	3.3 / 6.8%

Table 1: Test set comparison of ELMo enhanced neural models with state-of-the-art single model baselines across six benchmark NLP tasks. The performance metric varies across tasks – accuracy for SNLI and SST-5; F_1 for SQuAD, SRL and NER; average F_1 for Coref. Due to the small test sizes for NER and SST-5, we report the mean and standard deviation across five runs with different random seeds. The "increase" column lists both the absolute and relative improvements over our baseline.

Neural networks research

- Research in neural networks is exciting, expansive, and explorative.
- We have many **hyper-parameters** we can tweak
  (e.g., activation functions, number and size of layers).
- We have many **architectures** we can use
  (e.g., deep networks, LSTMs, attention mechanisms).

- Given the fevered hype, it's important to retain our scientific skepticism.
  - What are our **biases** and expectations?
  - When are neural networks the **wrong choice**?
  - How are we actually **evaluating** these systems?