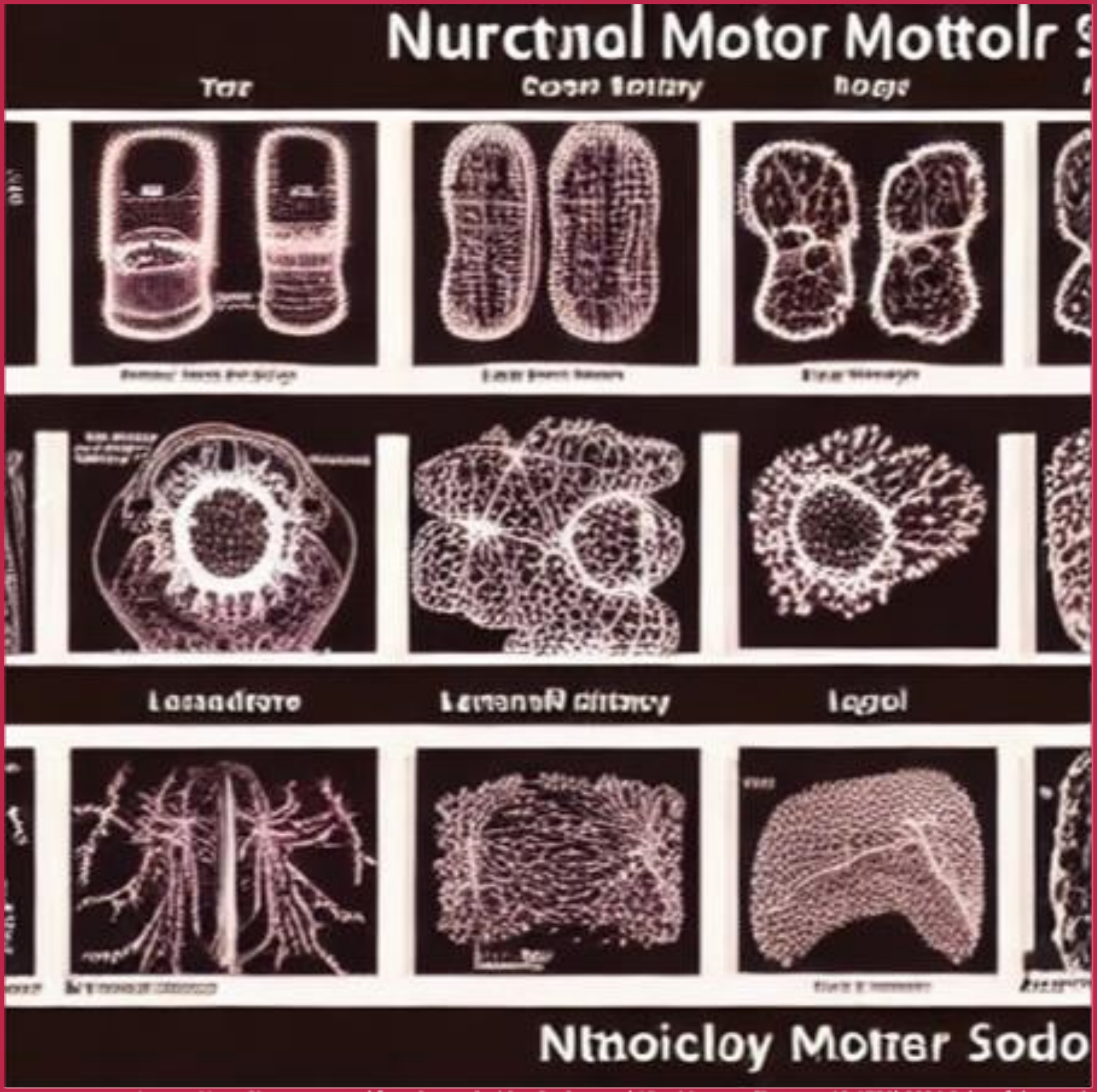


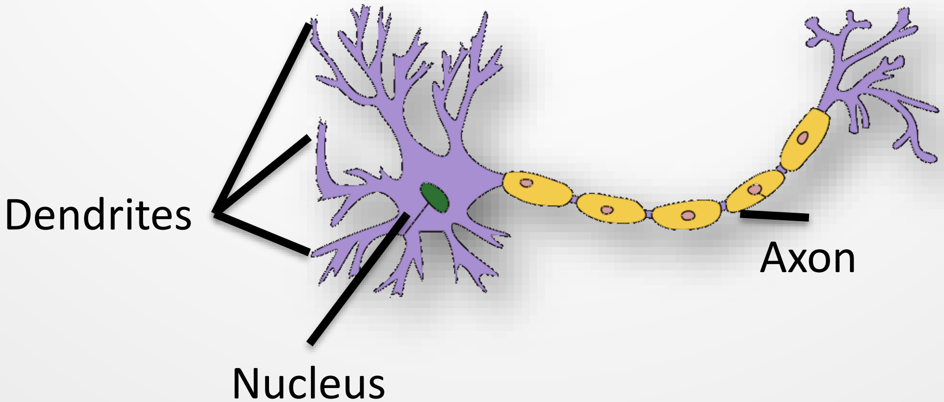
Image: AI text2img generated from lecture's title. *Background*: Viva Magenta (Pantone 18-1750) 2024 Color of the year!

Neural models of language

CSC401/2511 – Natural Language Computing – Fall 2024
Lecture 5
University of Toronto

Artificial neural networks

- **Artificial neural networks (ANNs)** were loosely inspired by networks of cytoplasmic protrusions in the brain.
  - Each unit has many inputs (~**dendrites**), one output (~**axon**).
  - The **nucleus** fires (sending an electric signal along the axon) given input from other neurons.
  - 'Learning' was formerly thought to occur at the **synapses** that connect neurons, either by amplifying or attenuating signals.

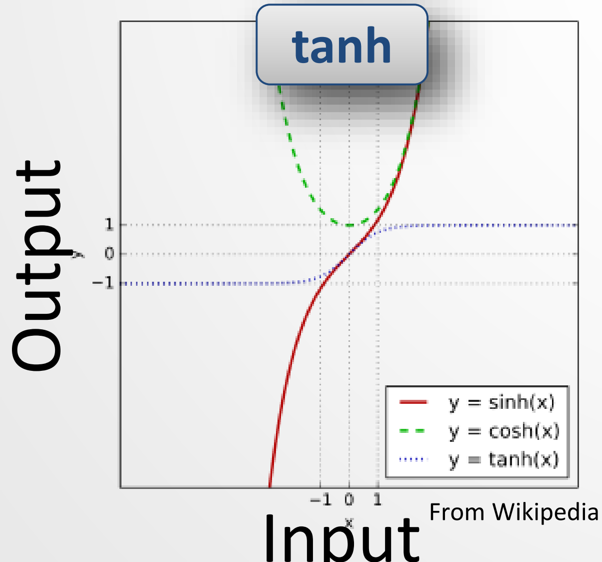


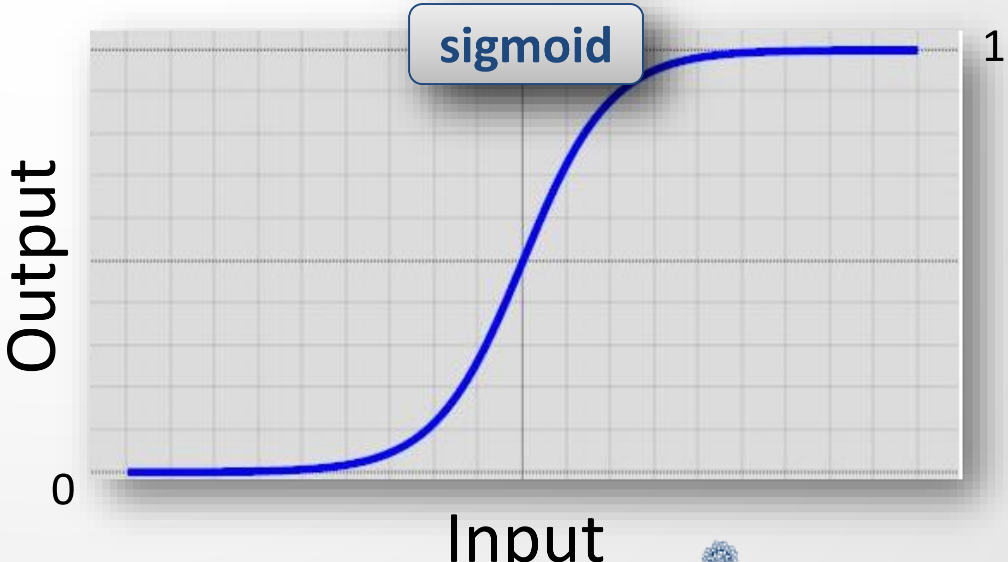
Feed-forward output

- Output is determined by an **activation function**, $g()$, which **can be non-linear (**of weighted input). Activation is empirically determined, but not learned as a parameter.
- Popular activation functions include **tanh** and the **sigmoid**:

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

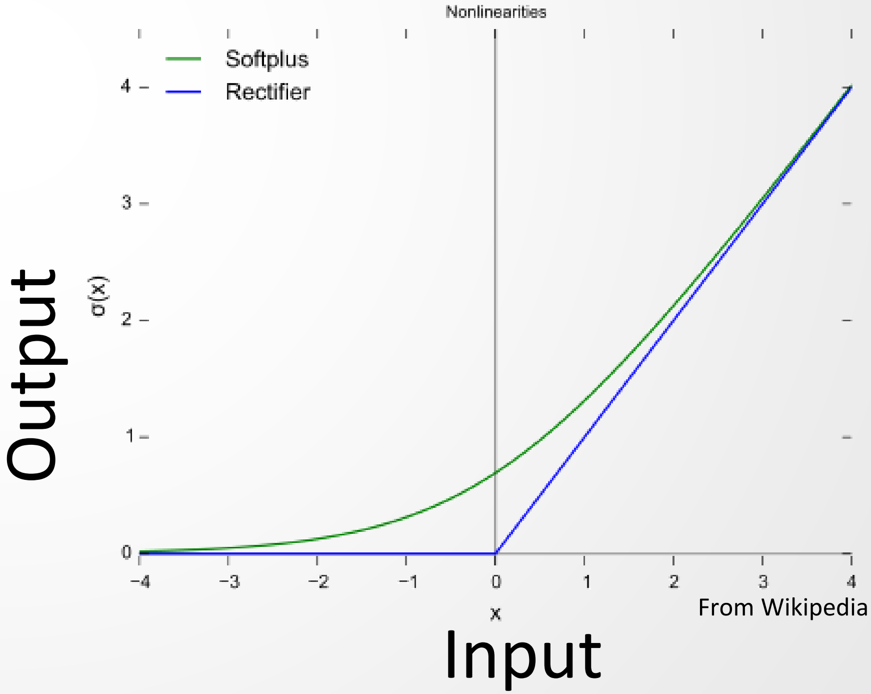
  - The sigmoid's derivative is the easily computable $\sigma' = \sigma \cdot (1 - \sigma)$





Rectified Linear Units (ReLUs)

- Since 2011, the **ReLU** $S = g(x) = \max(0, x)$ has become popular.
  - More appeals to biological plausibility, but sparse activation, and reduced likelihood of vanishing gradients are very practical reasons.
- A smooth approximation is the **softplus** $\log(1 + e^x)$, which has a simple derivative $1/(1 + e^{-x})$



From Wikipedia

- *Why do we care about the derivatives?*

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

Parameter estimation

- 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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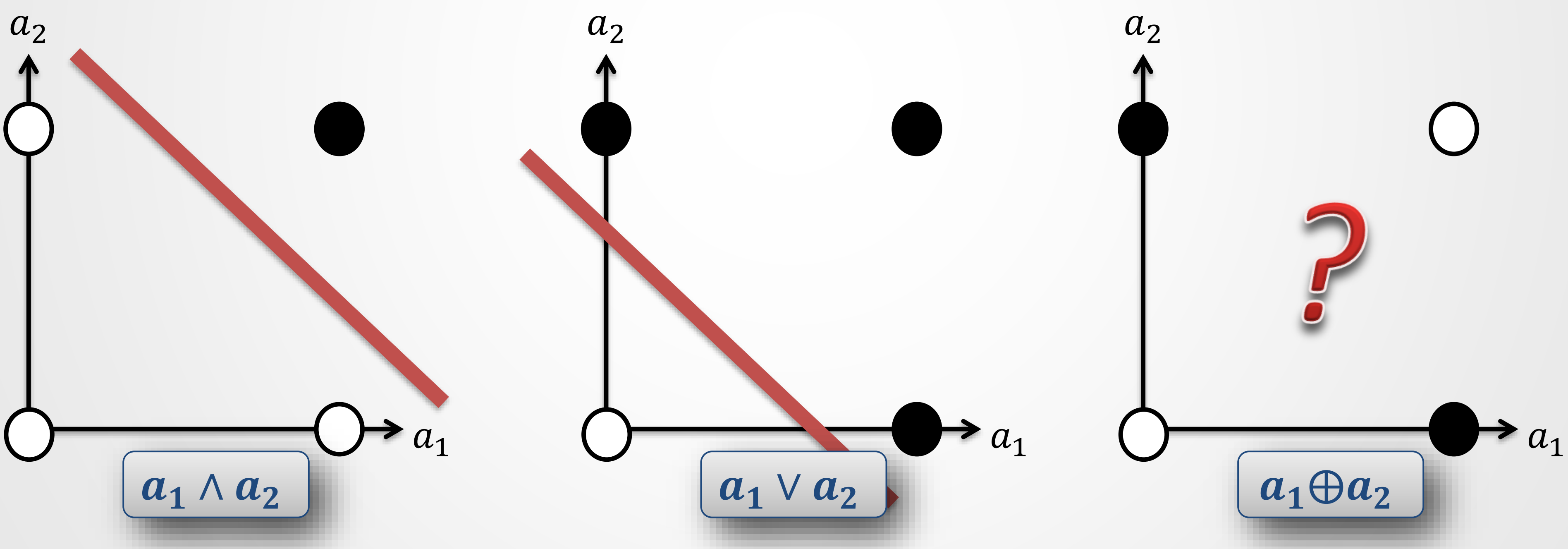
Threshold perceptra and XOR

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



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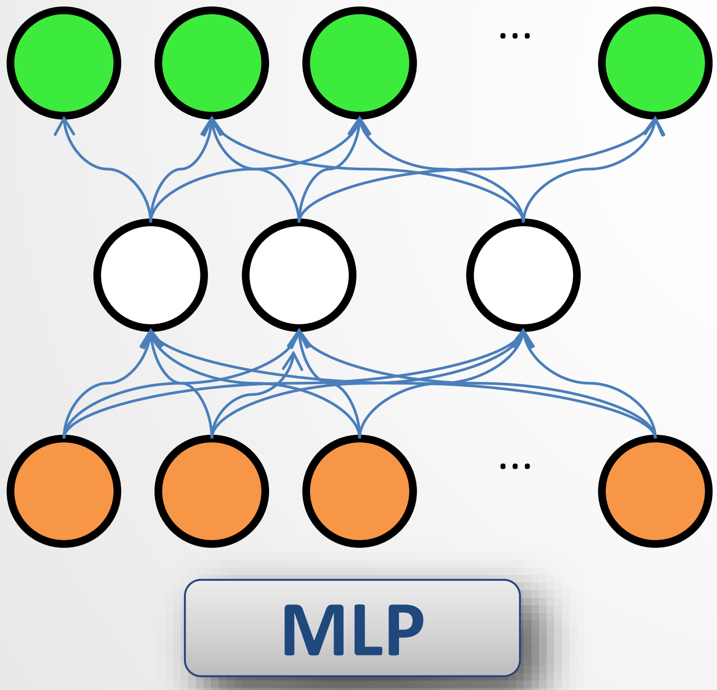
Multi-layer neural networks

- 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**. Sometimes, we even add noise.

Parameter estimation

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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Parameter estimation

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

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

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

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

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

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

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

Words

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

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

D

- In psychology, **word-feature representations** assign **features** to each index in a much denser vector.
  - E.g., concept-based features 'cheerful', 'emotional-tone'.

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

$d \ll D$

- Neither of these is learned.

Using word representations

Without a latent space,

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

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

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

EMBEDDING

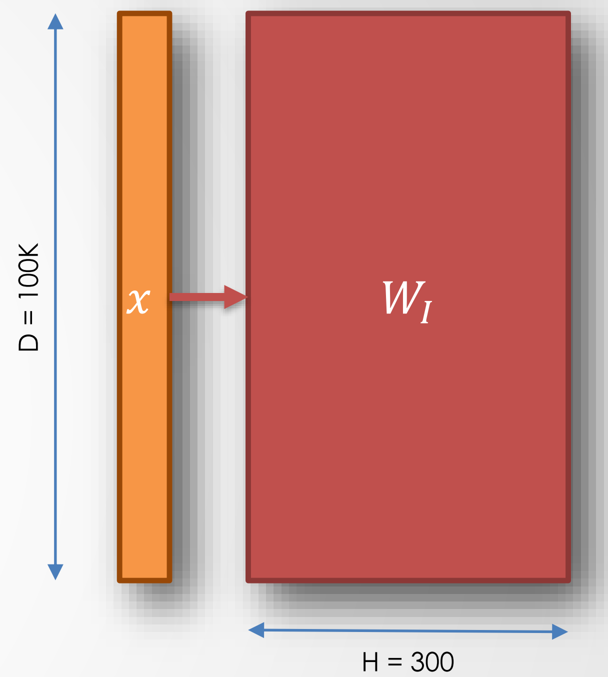
$$v_w = x^\intercal W_I$$

In latent space,

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

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

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



Reminder:

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

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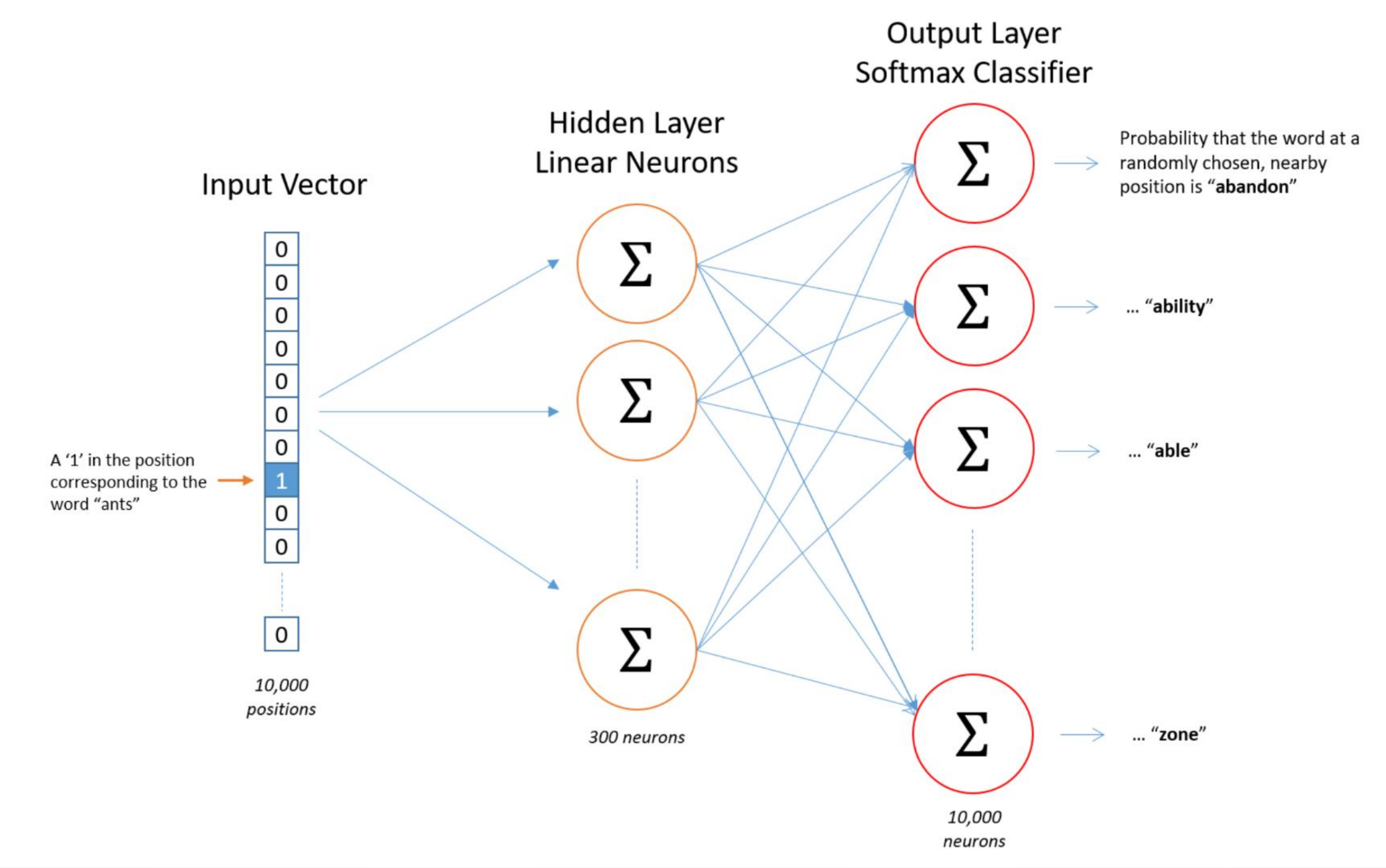
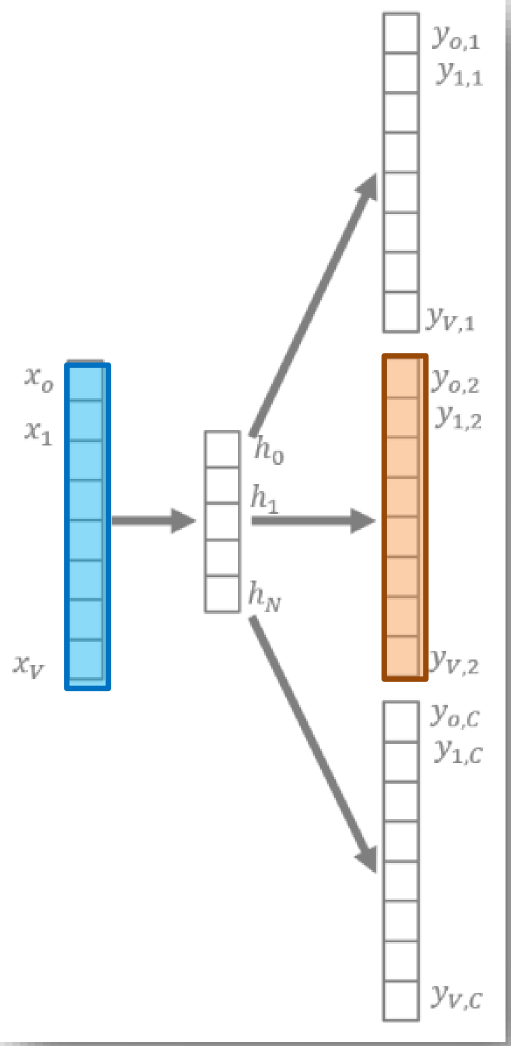
word2vec training regimen



Skip-grams with negative sampling

- Most word types do not appear together within a small window. The default process does not know this.
  - Also, not all that efficient – would be nice not to update $H \times D$ weights
  - **Contrastive learning:** push away from negative examples as well as towards positives.
- 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:
  - $$P(w_o|w_c) = \frac{\exp(v_o^T V_c)}{\sum_{w=1}^{D} \exp(v_w^T V_c)}$$

    Computationally infeasible

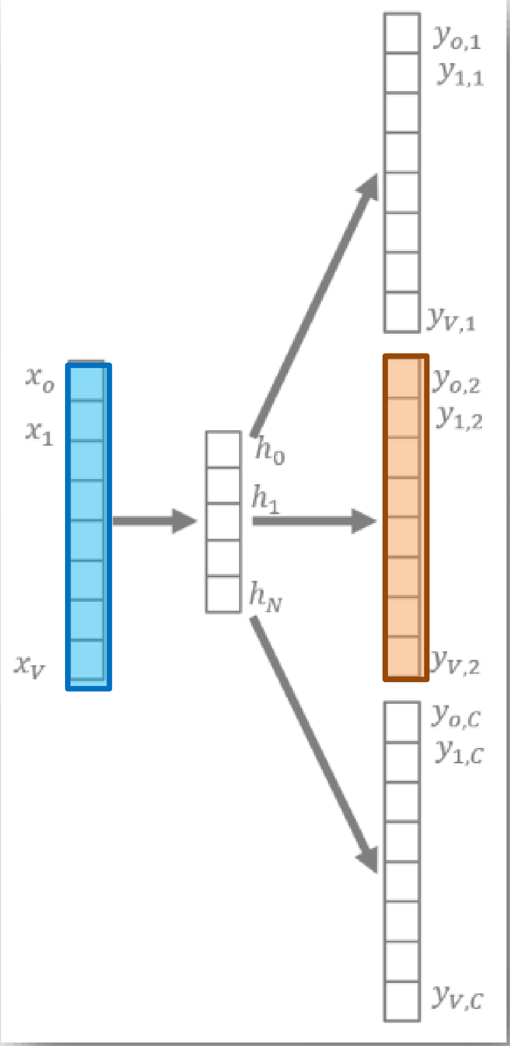
Skip-grams with negative sampling

- 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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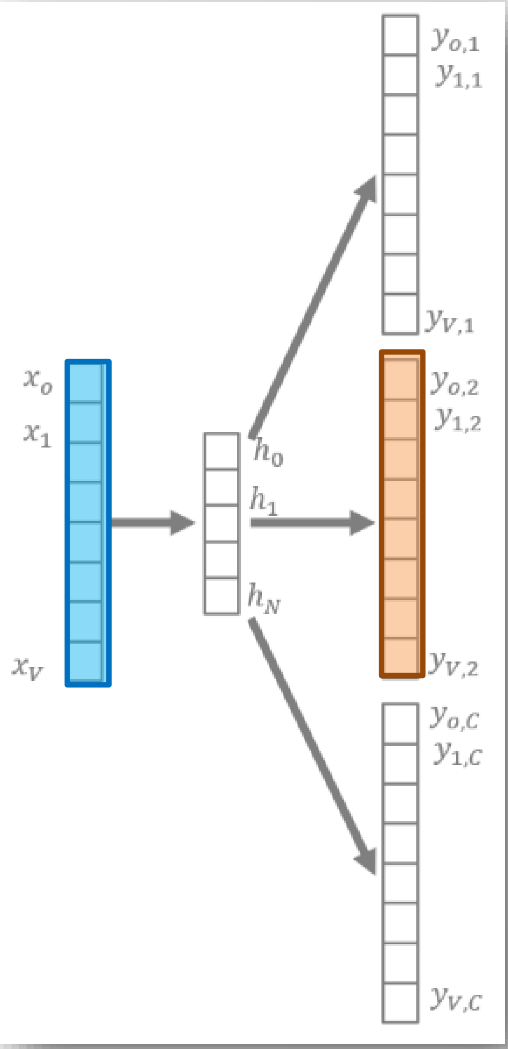
Skip-grams with negative sampling

- Choose a small number k of ‘negative’ words, then update the weights only for all the positive and 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.

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

- 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]

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RECURRENT NEURAL NETWORKS

Statistical language models

- Probability is conditioned on (window of) n previous words*
- A necessary (but incorrect) Markov assumption: each observation only factors through **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

Statistical language models

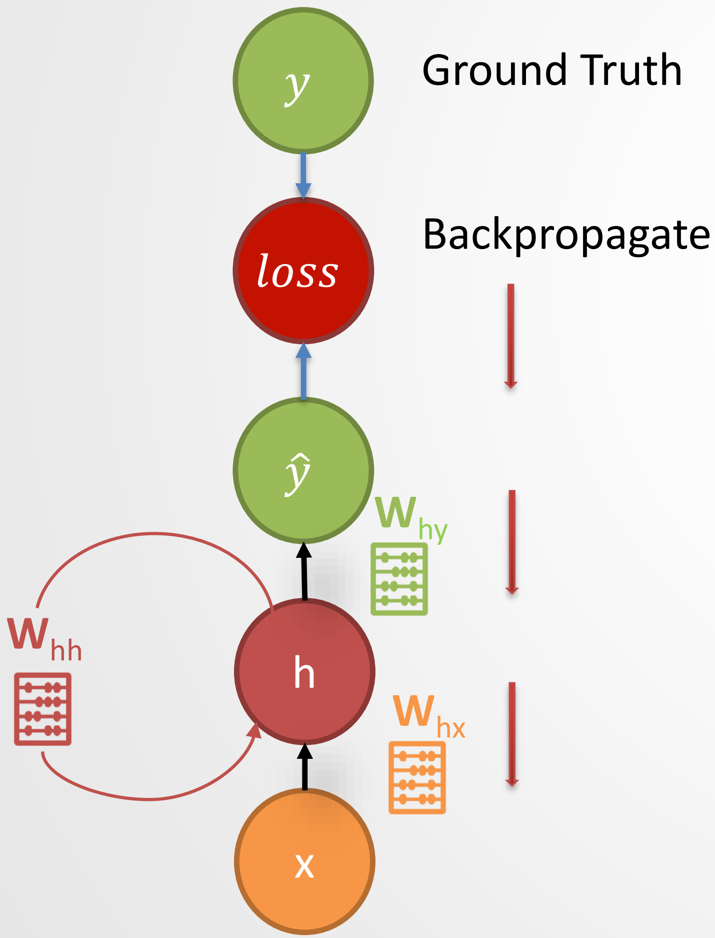
- Using higher n-gram counts (with smoothing) improves performance*

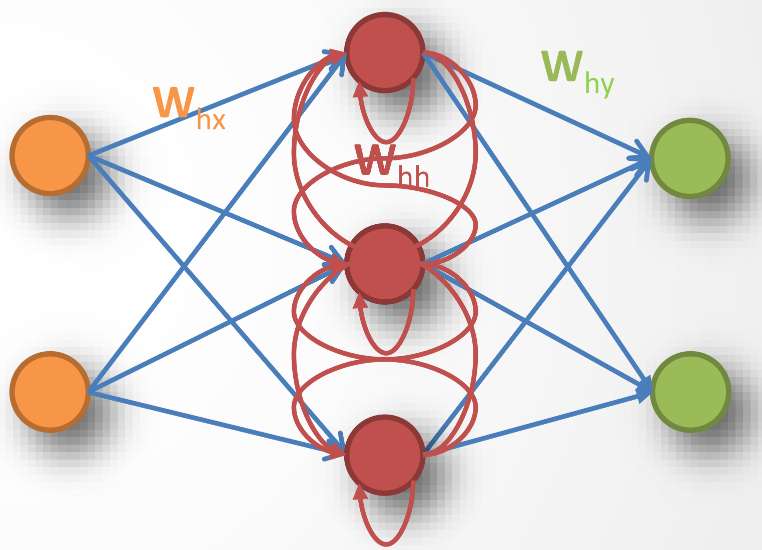
- *RNN intuition:*
  - Use as much history as we need to use
  - Use the **same set of weight** parameters for each word (or across all time steps) to keep the size of the network down
  - Memory requirement now scales with number of words

*From Lecture 2

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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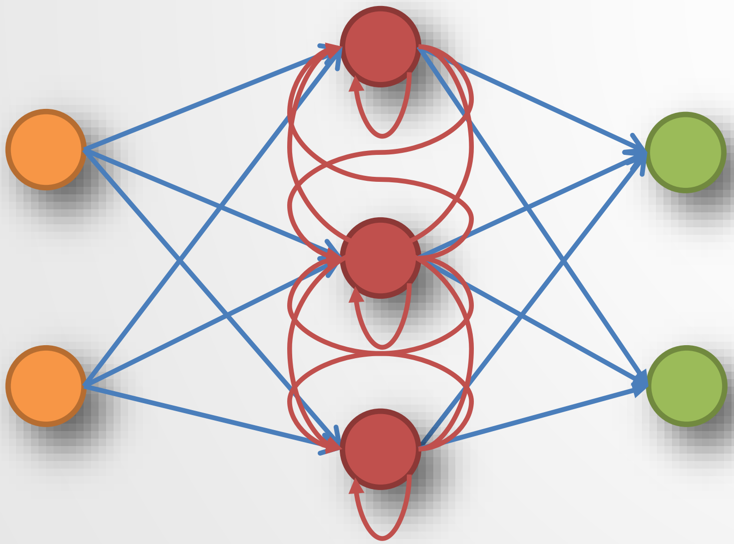
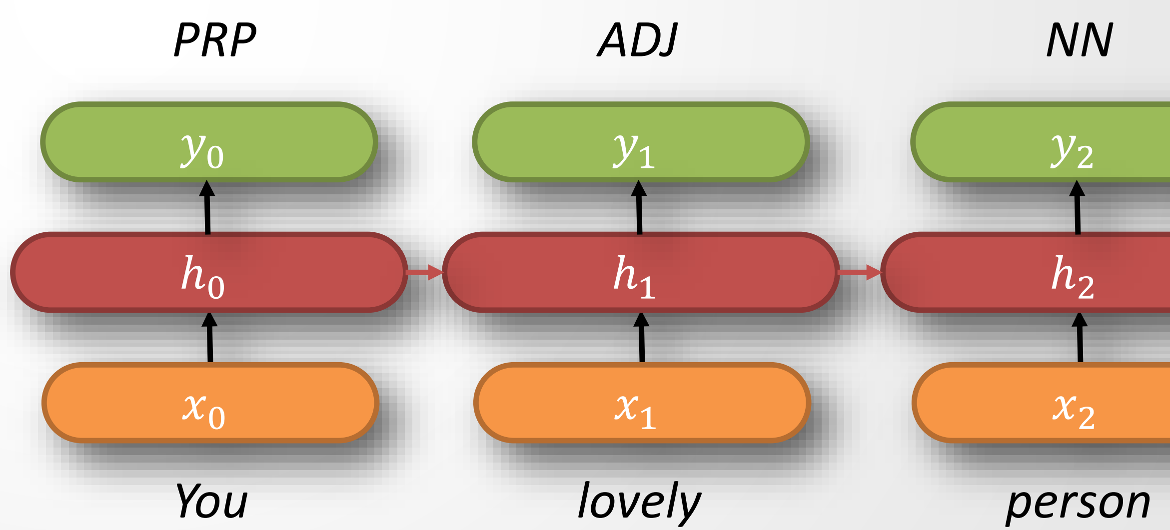
RNNs: Unrolling the h_i

- Copies of the same network can be applied (i.e., **unrolled**) at each point in a time series.
- Now we can use an approximation: backpropagation through time (BPTT).



$\rightarrow$

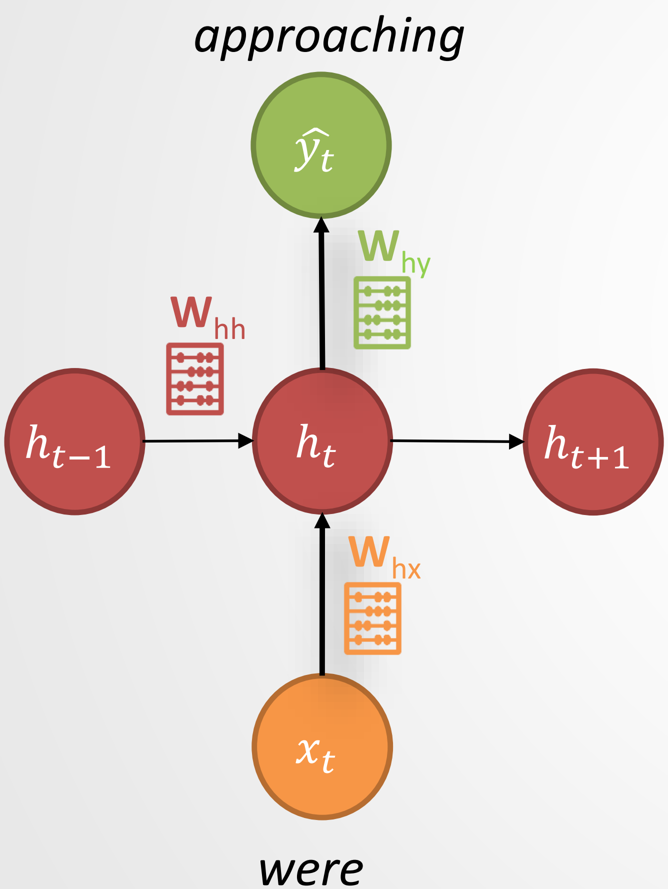


$$h_t = g(W_I[\boldsymbol{h_{t-1}}; \boldsymbol{x}] + c)$$
$$\boldsymbol{y_t} = W_O \boldsymbol{h_t} + b$$

RNNs: One time step snapshot

Two riders .. approaching .. horses.

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



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

- At a single time-step:

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

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

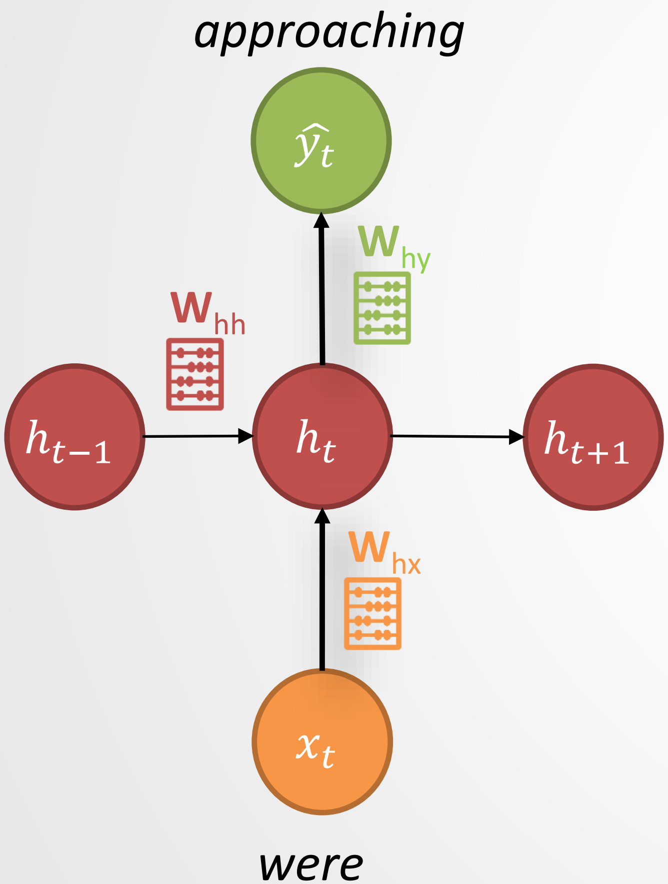
$$\hat{y_t} = softmax\,(W_{hy}\boldsymbol{h_t} + b)$$

```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 $\boldsymbol{X}$: $x_1, x_2, \dots, x_t, x_{t+1}, \dots, x_T$



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

$\hat{y} \in \mathbb{R}^{|V|}$ 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

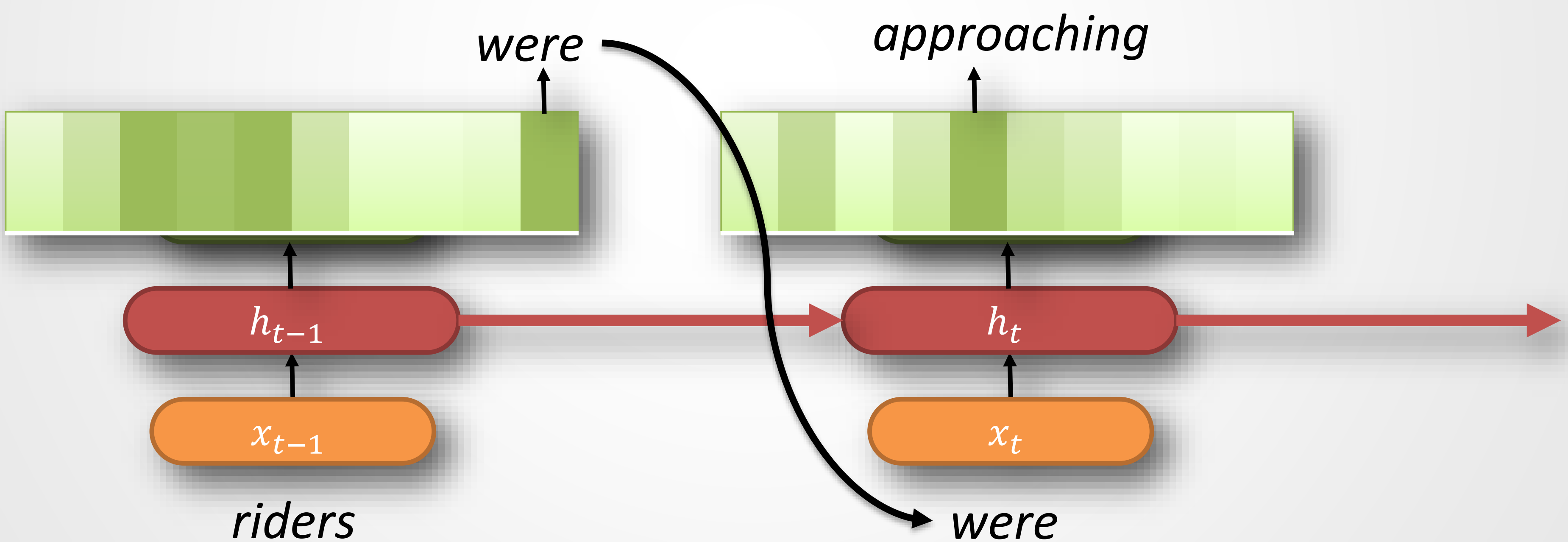
- Same **cross-entropy** loss function

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

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

Sampling from a RNN LM

- If $|h_i| < |V|$, we've already reduced the number of parameters relative to trigrams.
- Good news: NN encodings tend to be very compact.



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

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

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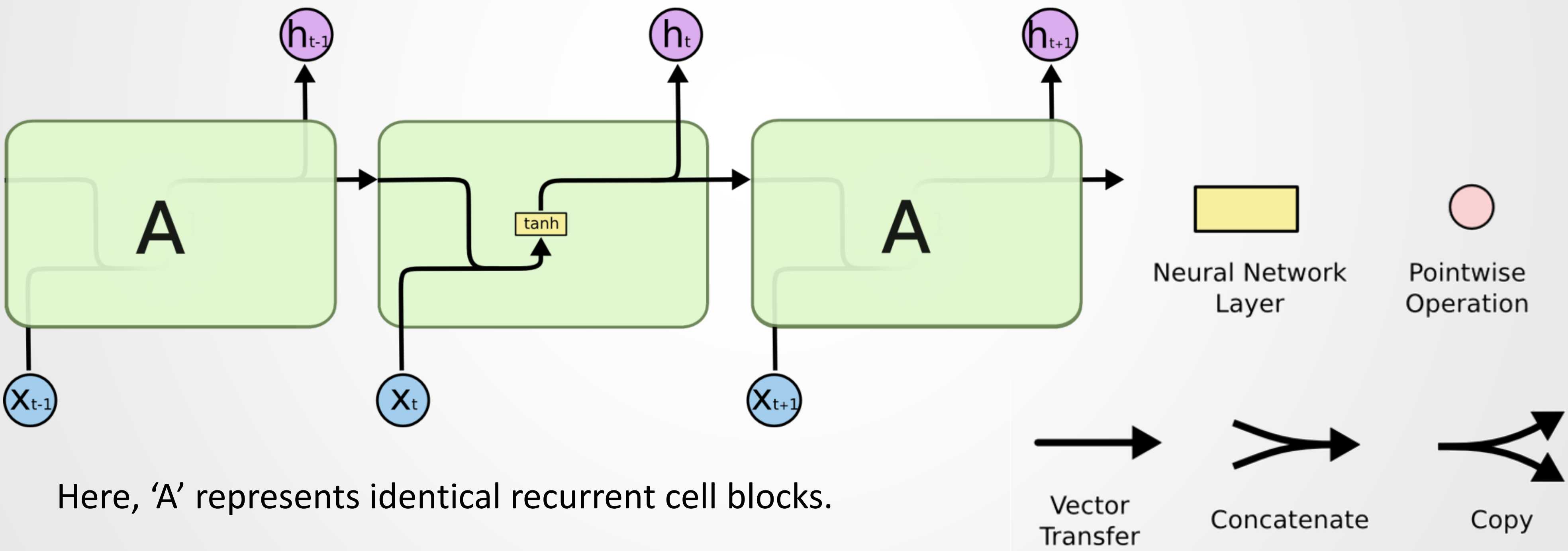
RNNs and retrograde amnesia

- Bad news: gradients don't multiply out well over long distances (**gradient decay).**
- Can we spend some parameters to store extra information?



Here, 'A' represents identical recurrent cell blocks.

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

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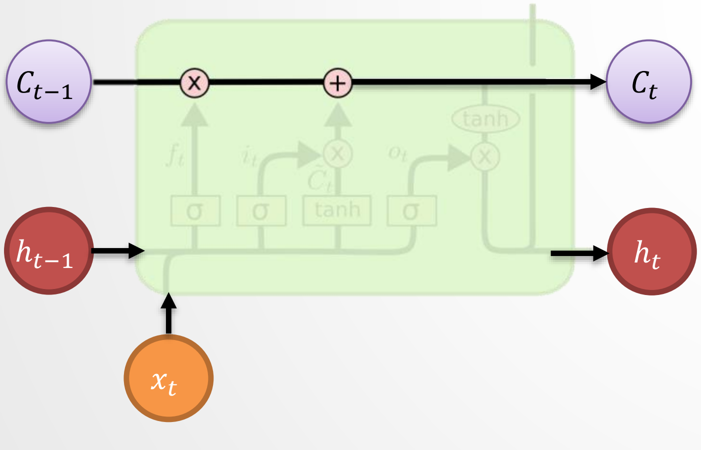
RNNs and retrograde amnesia

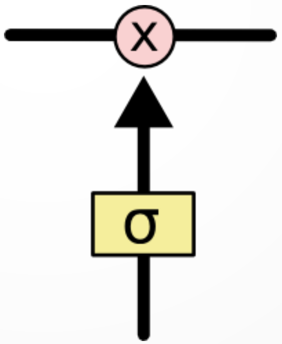
- **Catastrophic forgetting** is common.
  - E.g., the **relevant** context in "*The teacher taught transformers terribly telling tiring, tortuous theories …*" has likely been **overwritten** by the time h_{13} is produced.

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

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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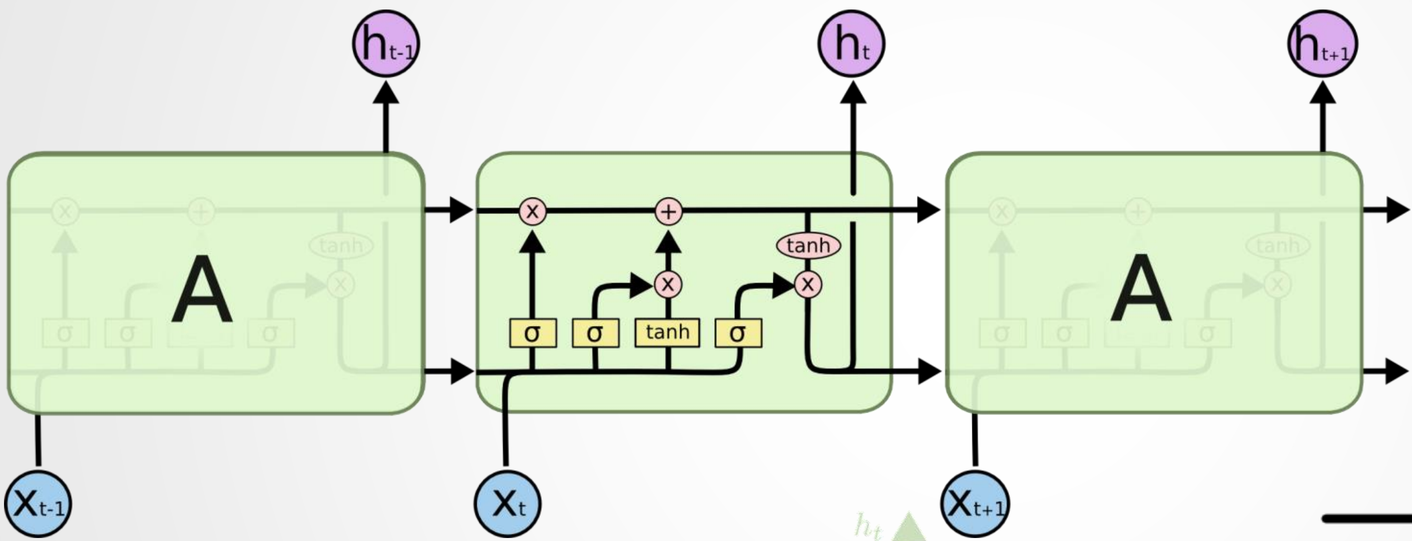
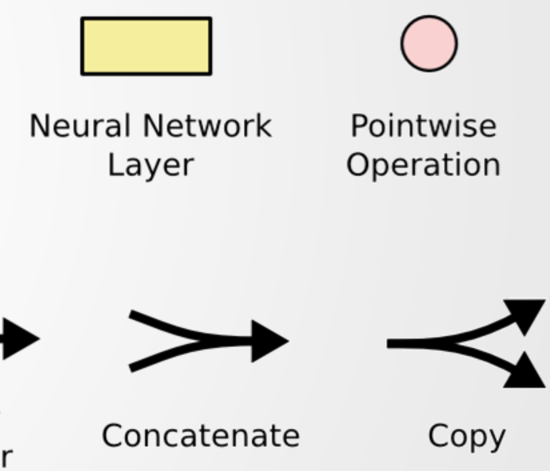
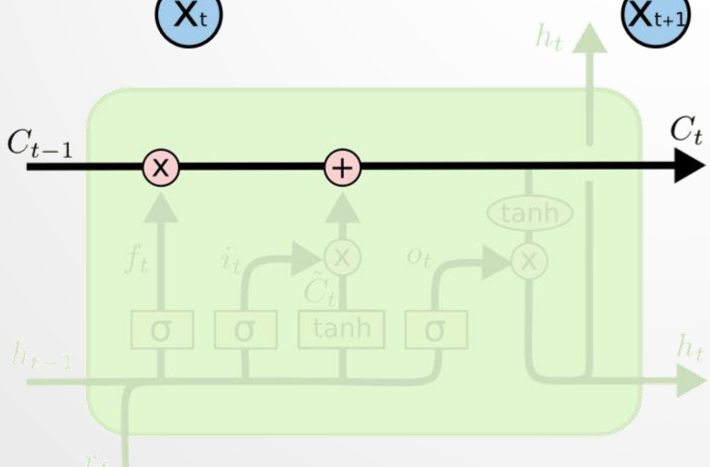
LSTM – core ideas

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



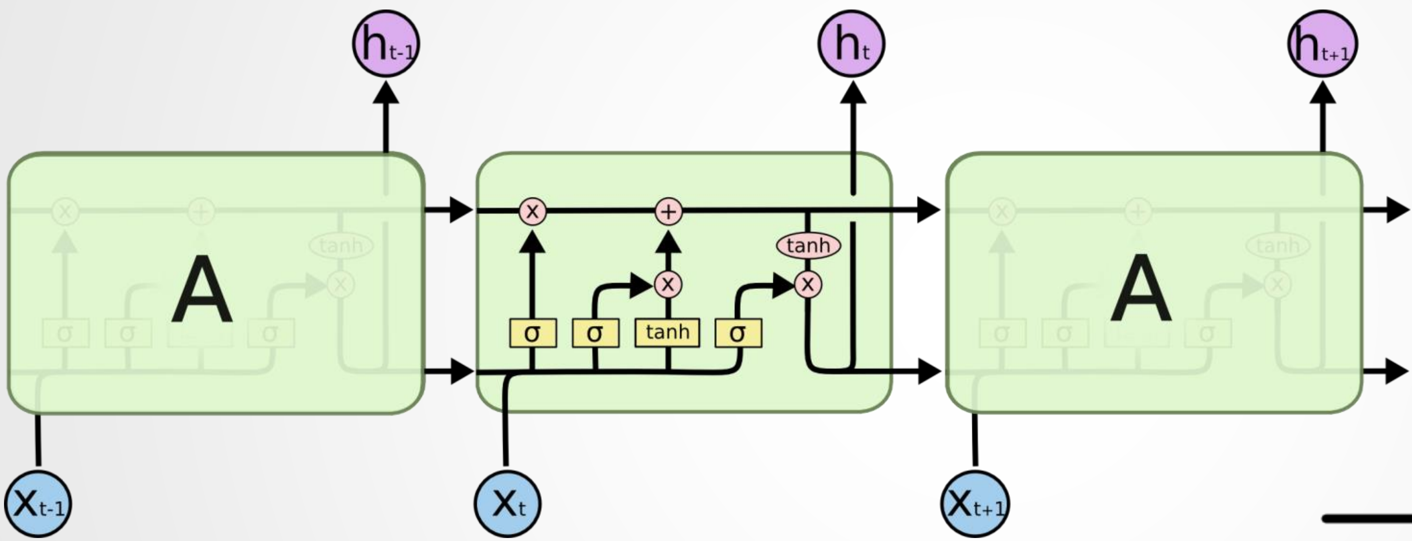


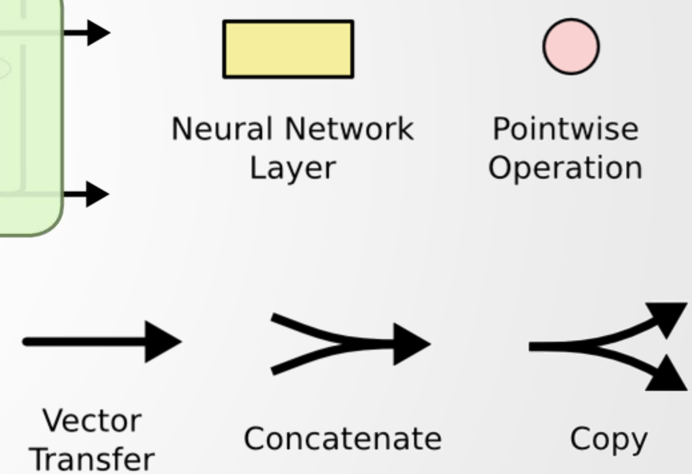


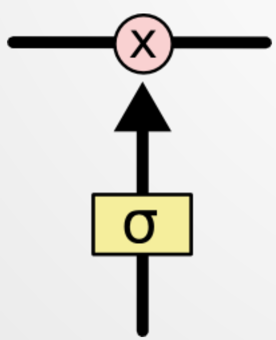
The **cell state** is a special vector stream that runs through the entire chain and **stores long-term information.**

LSTM – core ideas

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



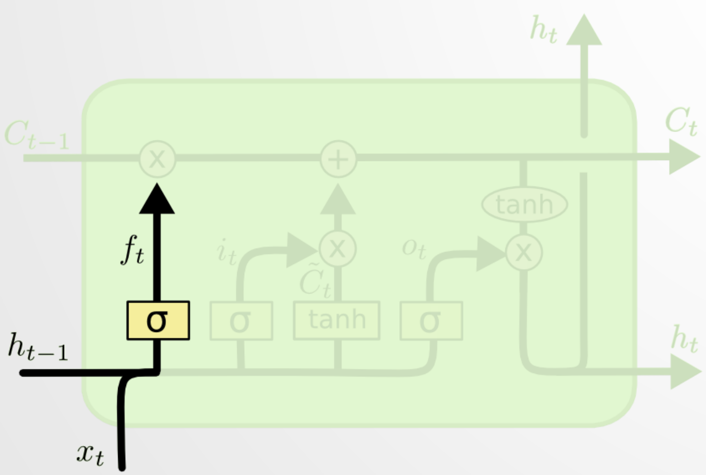




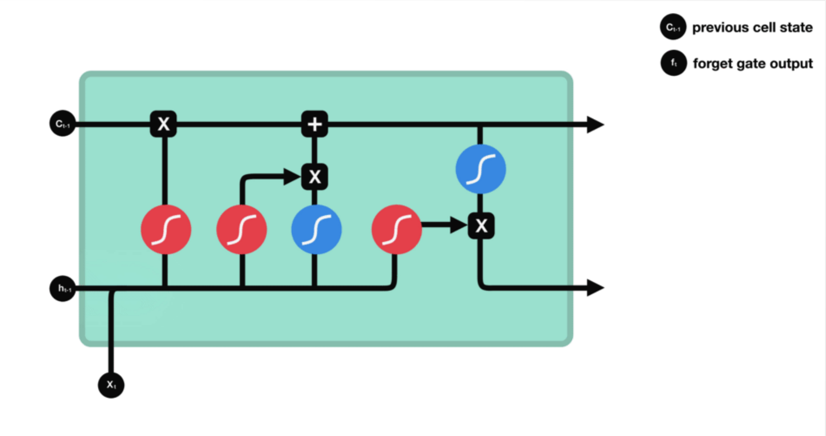
Gates decide what information should be withheld in the cell state.
They are a **sigmoid** followed by a pointwise ×.
Values near 0 block information; values near 1 pass information.

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 readily interpretable.)

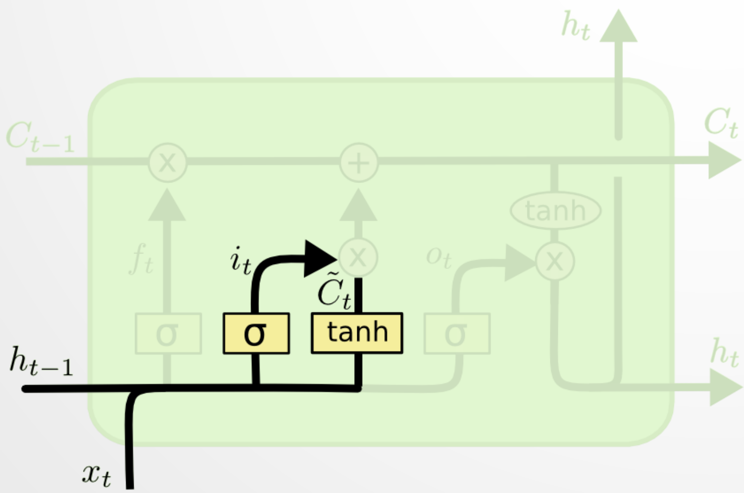


$$f_t = \sigma\left(W_f \cdot [h_{t-1}, x_t] + b_f\right)$$



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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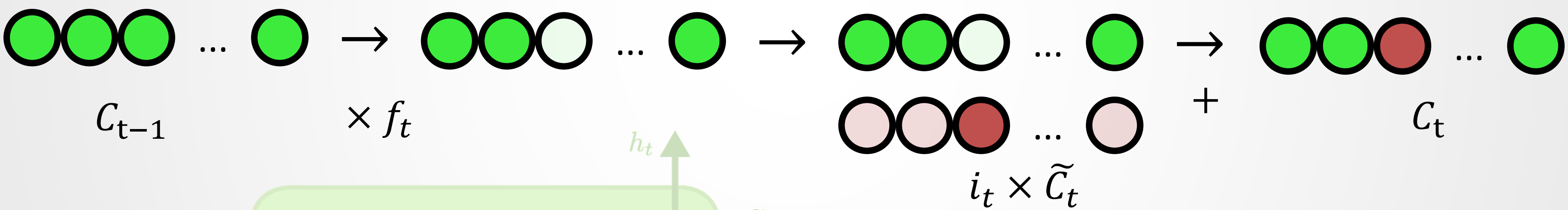
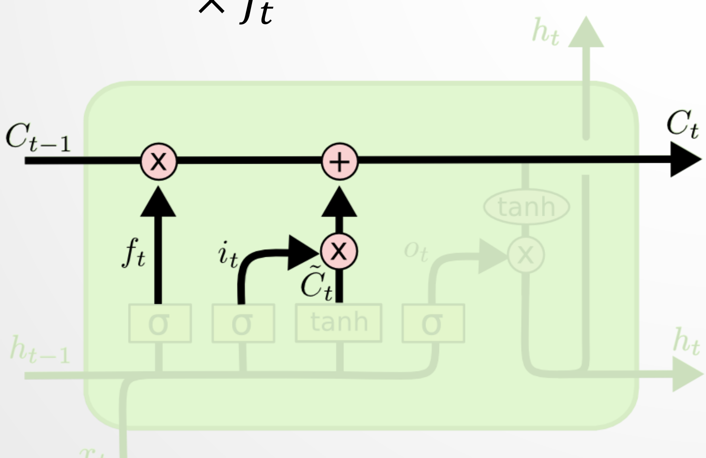
LSTM step 3: update the cell state

- 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, $i_t \times \tilde{C}_t$.
  - Finally, write this information to the new cell state C_t.





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

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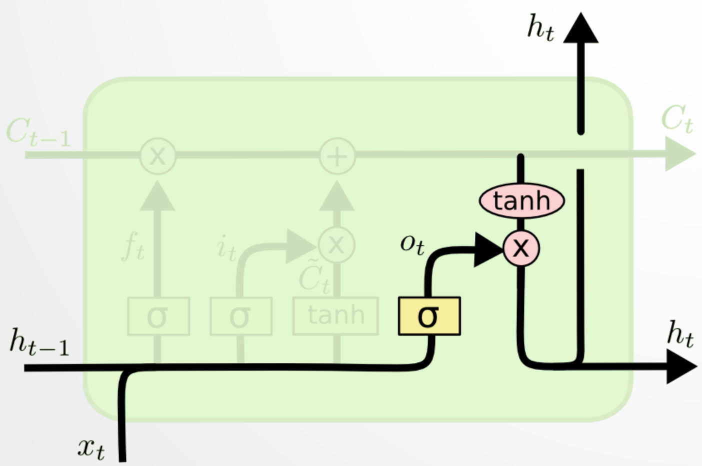
LSTM step 4: output and feedback

- 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).

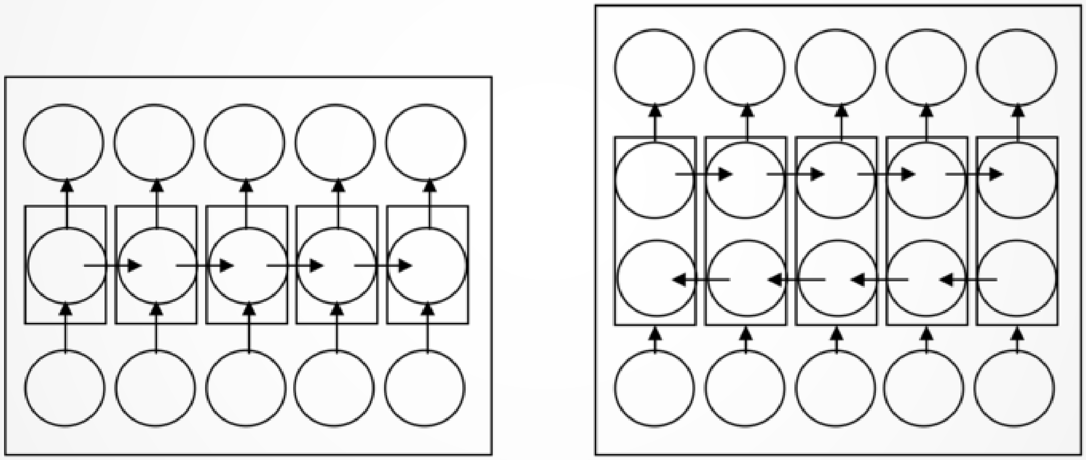


$$o_t = \sigma(W_o[h_{t-1}, x_t] + b_o)$$

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

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.

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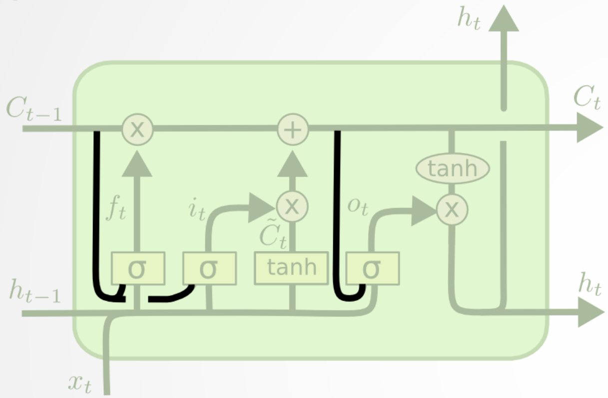
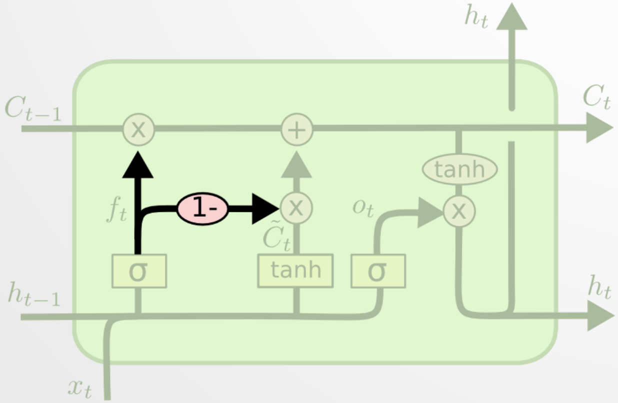
Variants of LSTMs

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



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

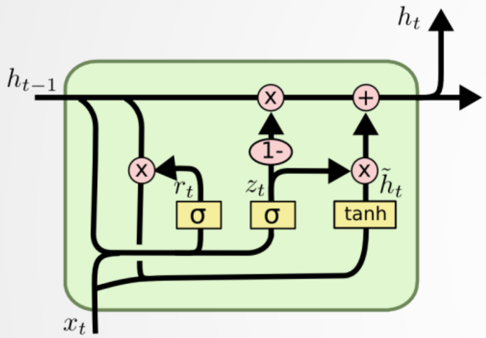
- We can **couple** the '*forget*' and '*input*' gates.
  - Joint decisioning is more efficient.



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

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)

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

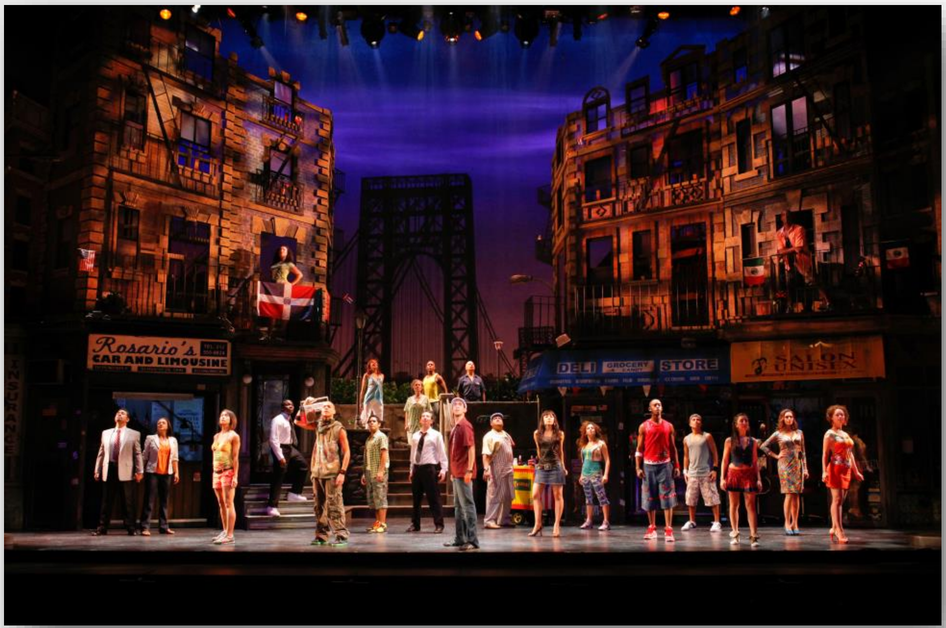
$h_t = (1 - z_t) * h_{t-1} + z_t * \tilde{h}_t$

- 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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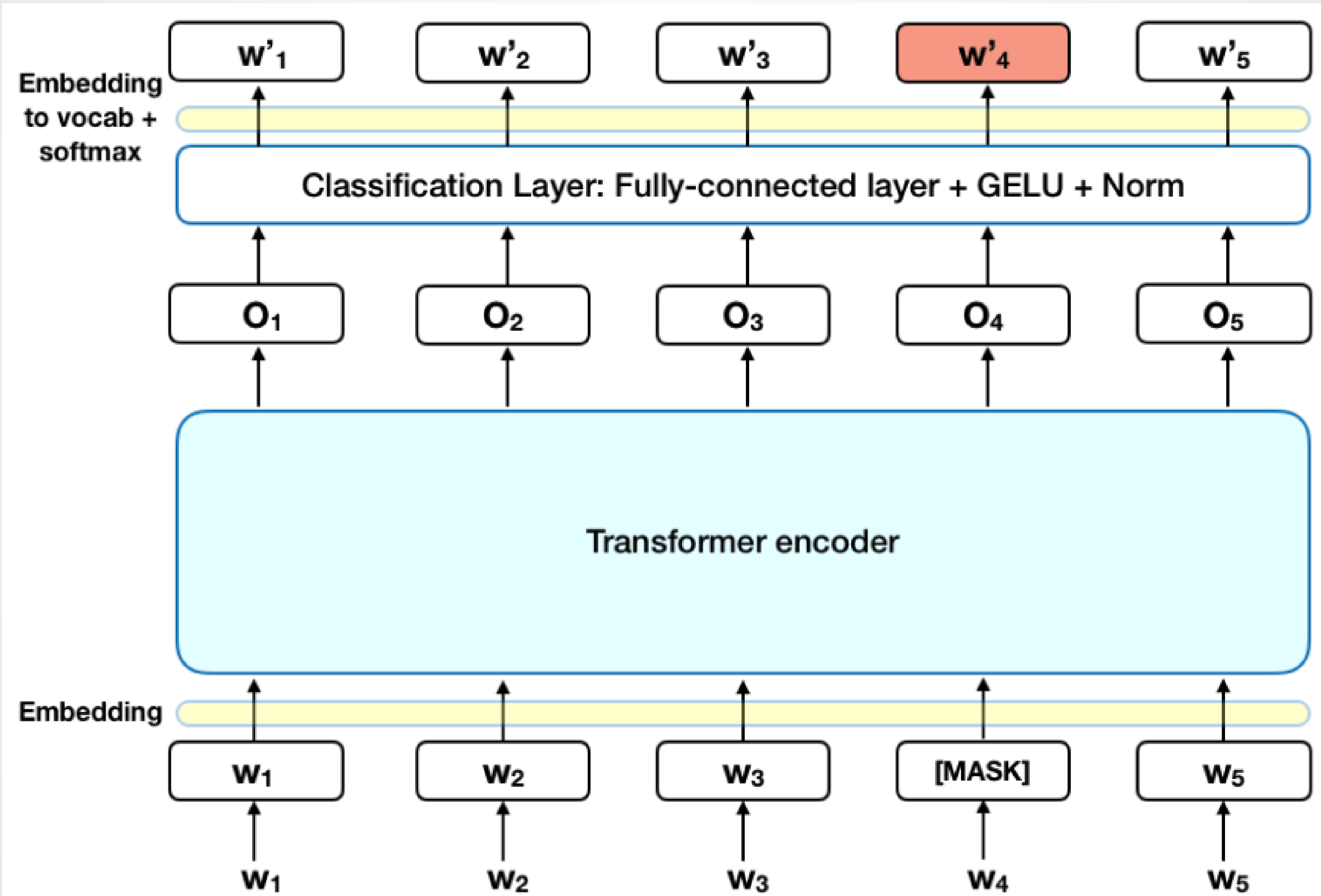
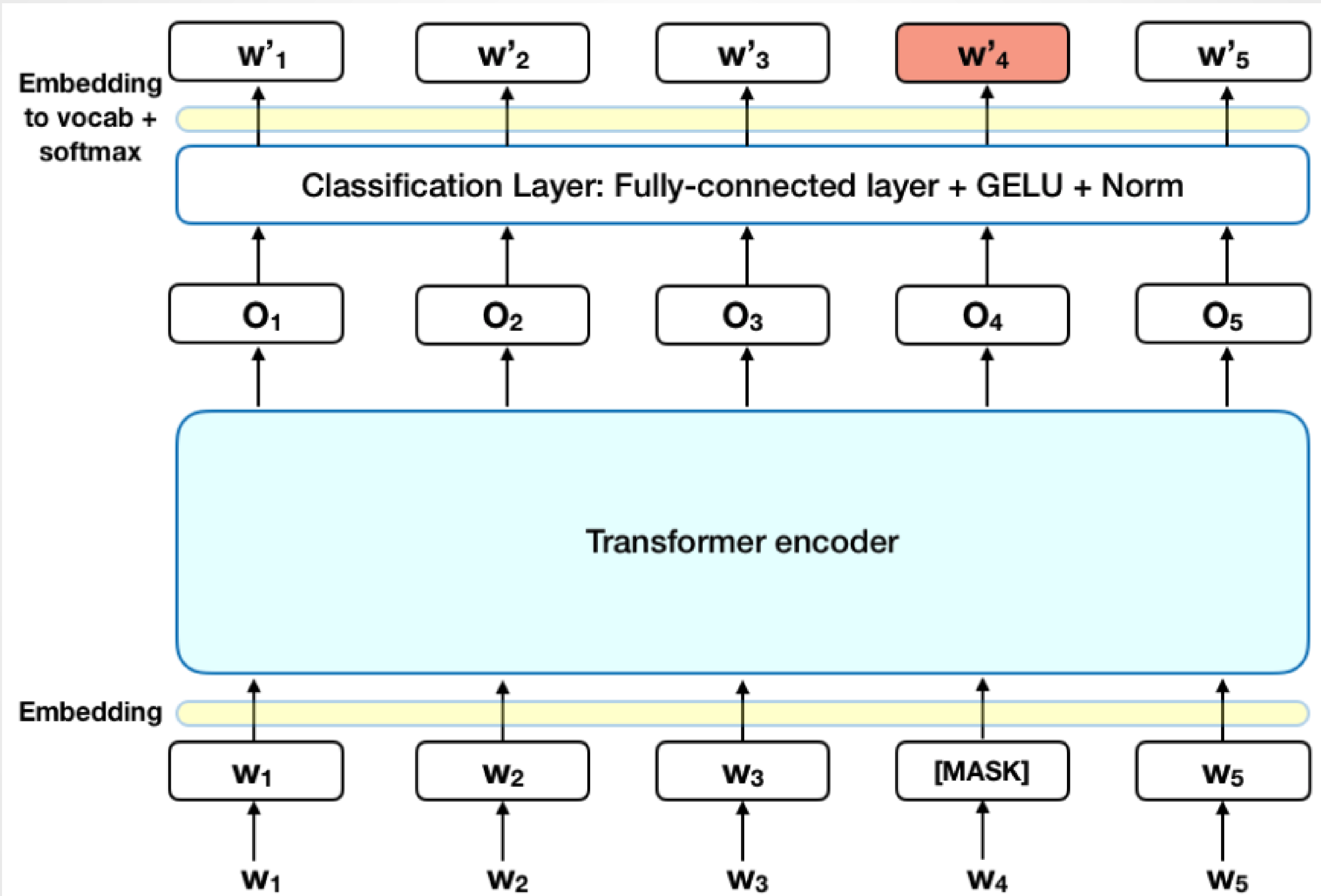
• BERT

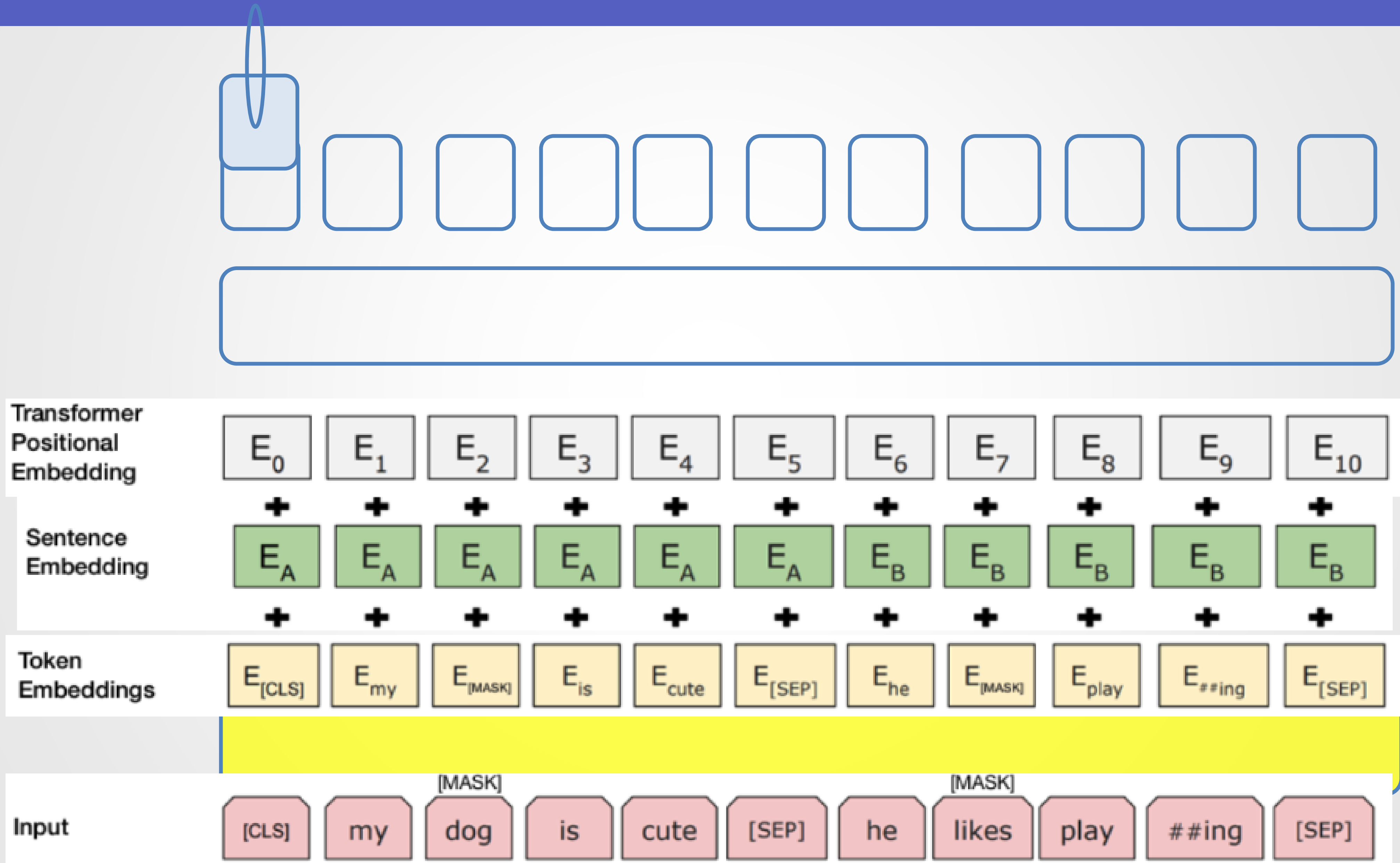


w'_1
w'_2
w'_3
w'_4
w'_5
Embedding to vocab + softmax
Classification Layer: Fully-connected layer + GELU + Norm
O_1
O_2
O_3
O_4
O_5
Transformer encoder
Embedding
w_1
w_2
w_3
[MASK]
w_5
w_1
w_2
w_3
w_4
w_5

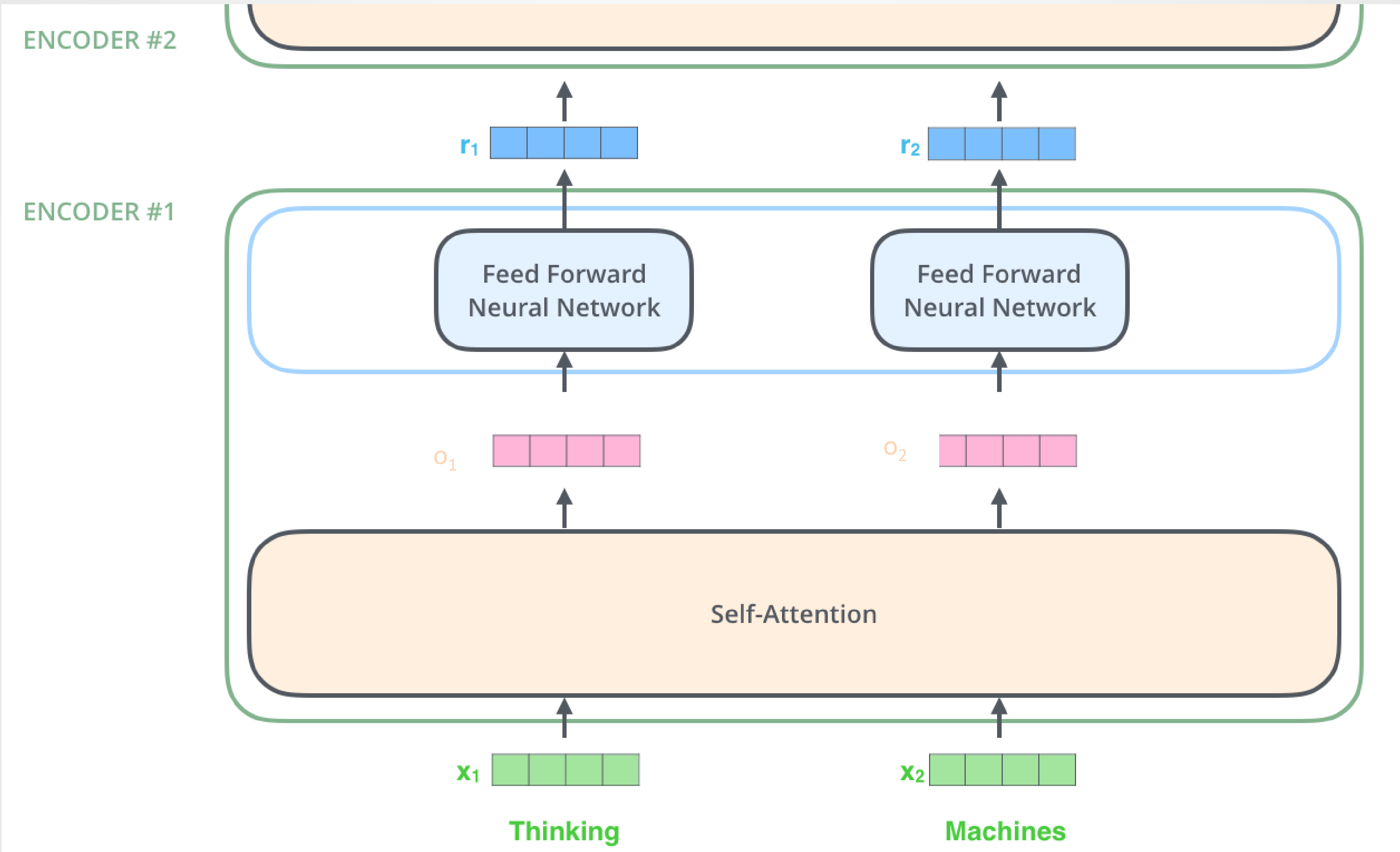
.Training task 1: Masking



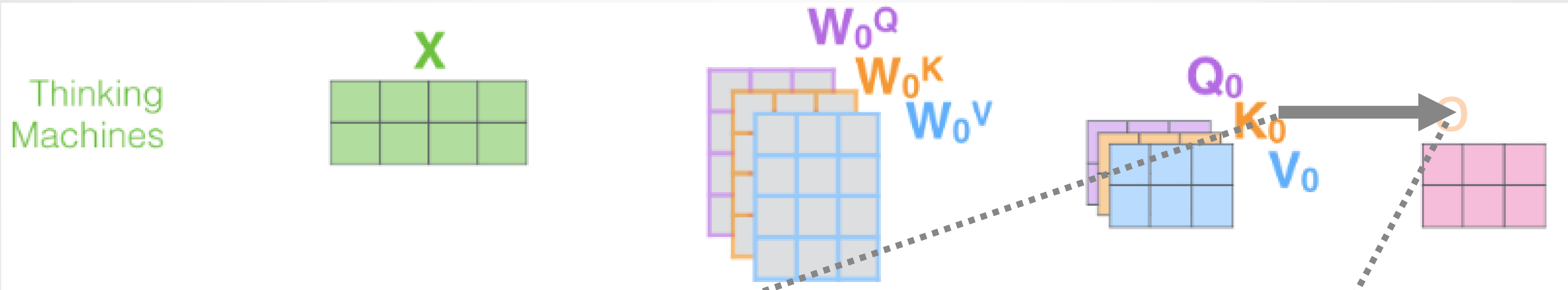
.Training task 2: Next Sent.



.Transformers

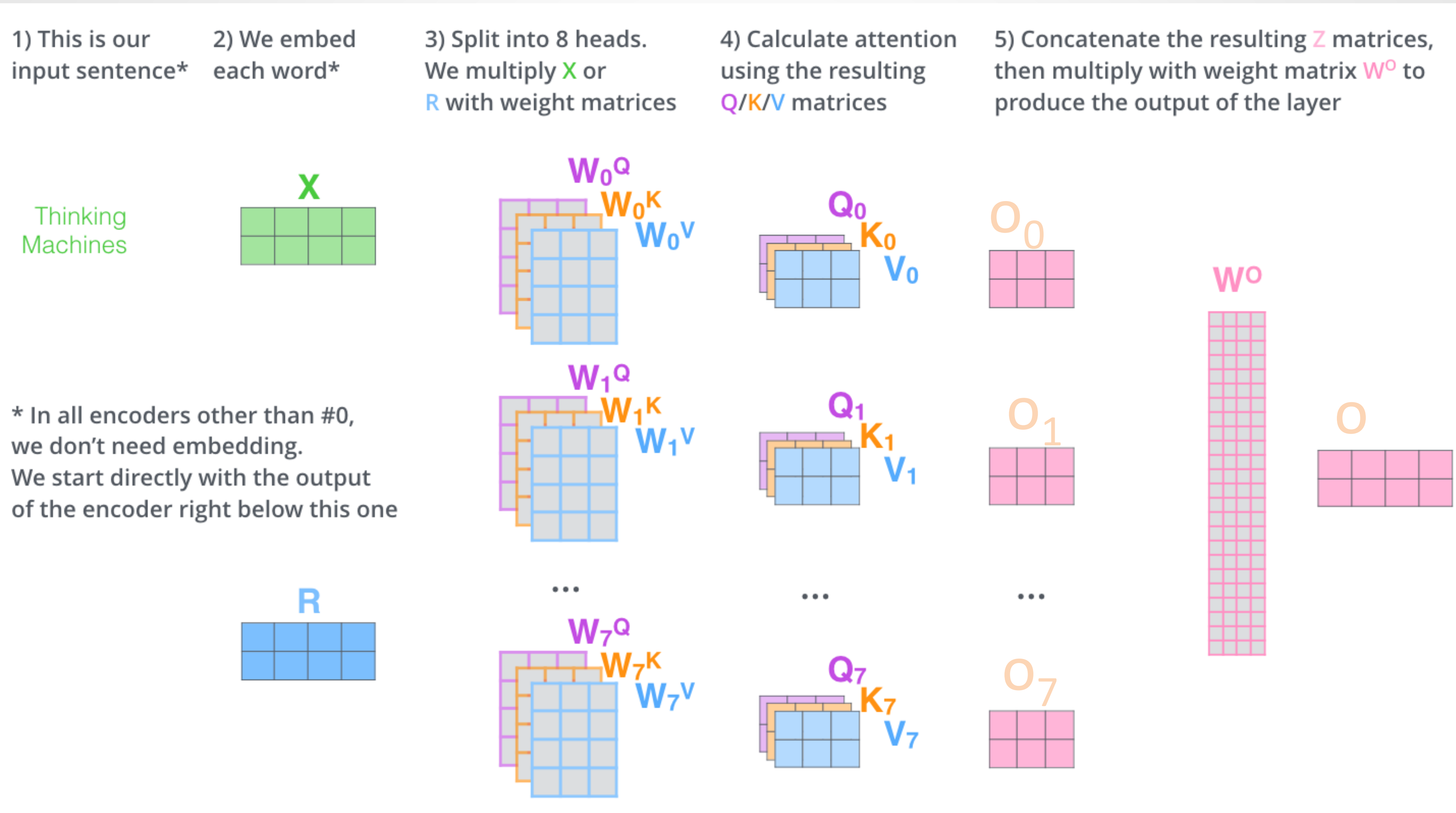


.Self-attention



$$\alpha_{ij} = \frac{\exp\left(q_i^T k_j\right)}{\sum_{l=1}^{n} \exp\left(q_i^T k_l\right)} \qquad o_i = \sum_{j=1}^{n} \alpha_{ij} v_j$$

.Multiheaded Self attention



.Positional encodings

$$\vec{p_t} = \begin{bmatrix} \sin(\omega_1 . t) \\ \cos(\omega_1 . t) \\ \\ \sin(\omega_2 . t) \\ \cos(\omega_2 . t) \\ \\ \vdots \\ \\ \sin(\omega_{d/2} . t) \\ \cos(\omega_{d/2} . t) \end{bmatrix}_{d \times 1}$$

$$\vec{p_t}^{(i)} = f(t)^{(i)} := \begin{cases} \sin(\omega_k . t), & \text{if } i = 2k \\ \cos(\omega_k . t), & \text{if } i = 2k+1 \end{cases}$$

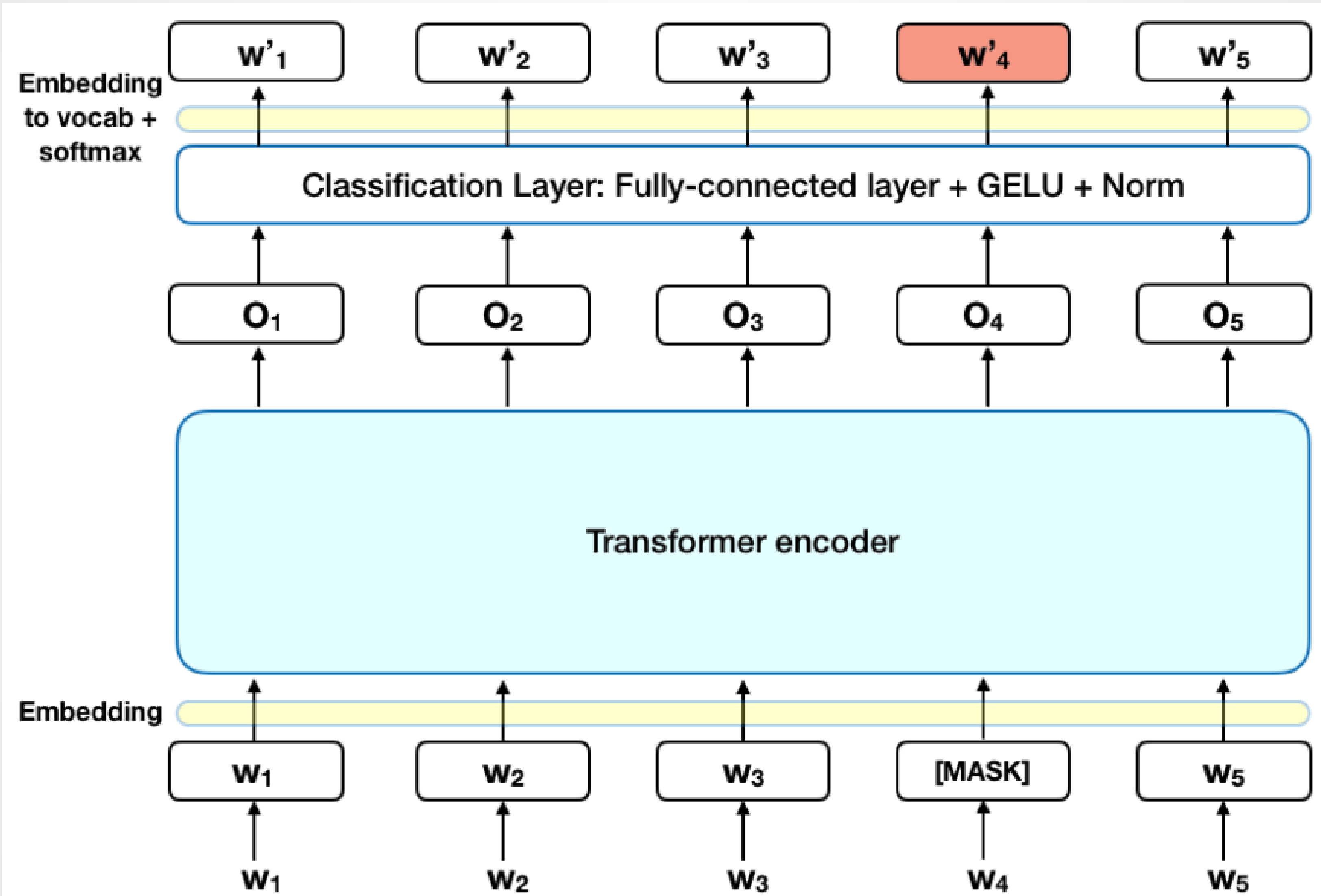
where

$$\omega_k = \frac{1}{10000^{2k/d}}$$

.Huh?

- Encodings of any two distinct positions are distinct
- Each position maps to only one encoding
- Test sentences may be longer than training
- Distance between two positions should be constant across sentences (of varying lengths).

.Training task 1: Masking



The truth about masking

- Real easy to do well on MASKed position and nothing else
- Real easy to learn to copy the context-independent embedding
- So…
  - 80% of the time: MASK
  - 10% of the time: correct word
  - 10% of the time: another random word