CSEP 517
Natural Language Processing

Neural Networks

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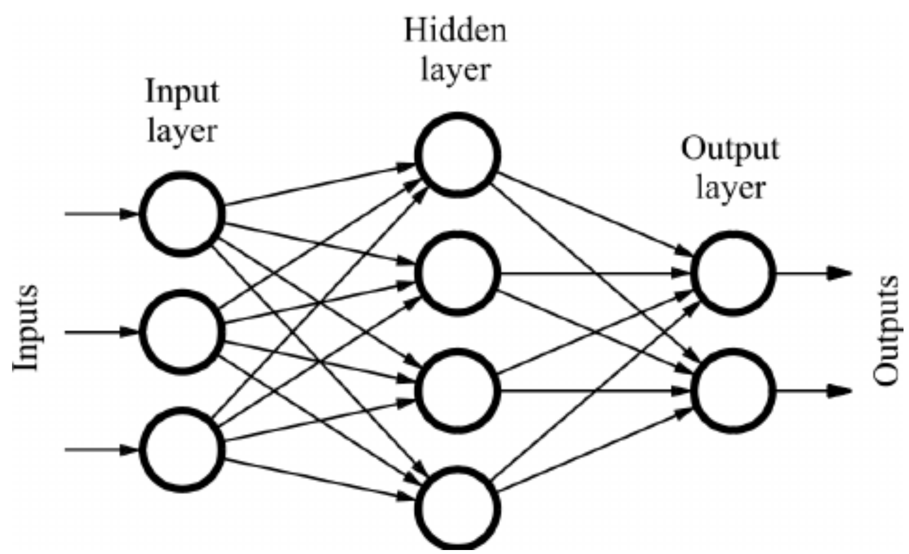
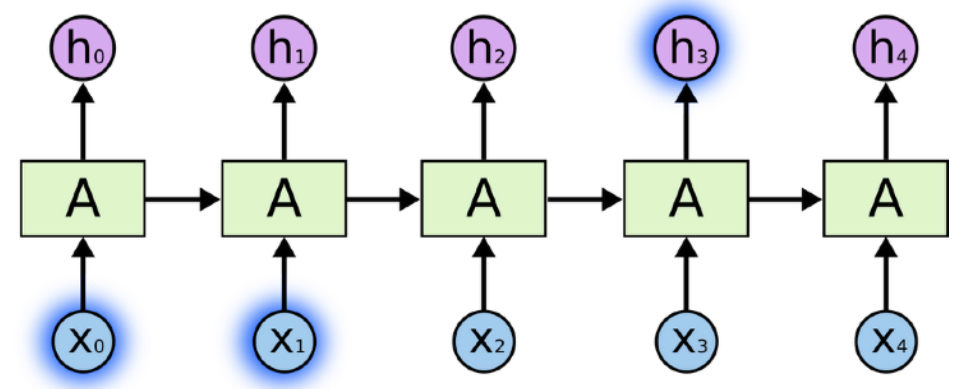
(Slides adapted from Danqi Chen, Chris Manning, Dan Jurafsky)

Neural networks for NLP

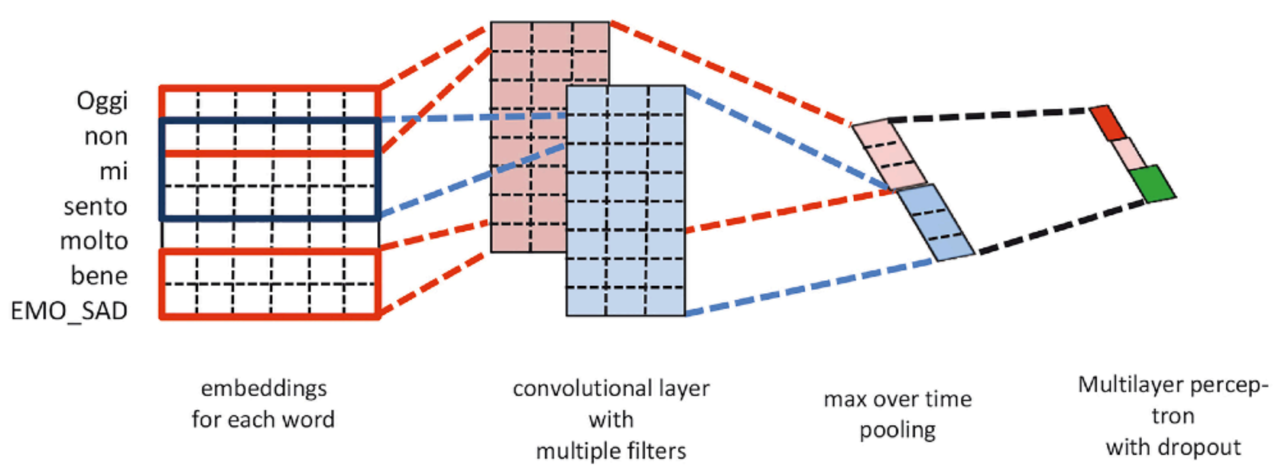
Feed-forward NNs



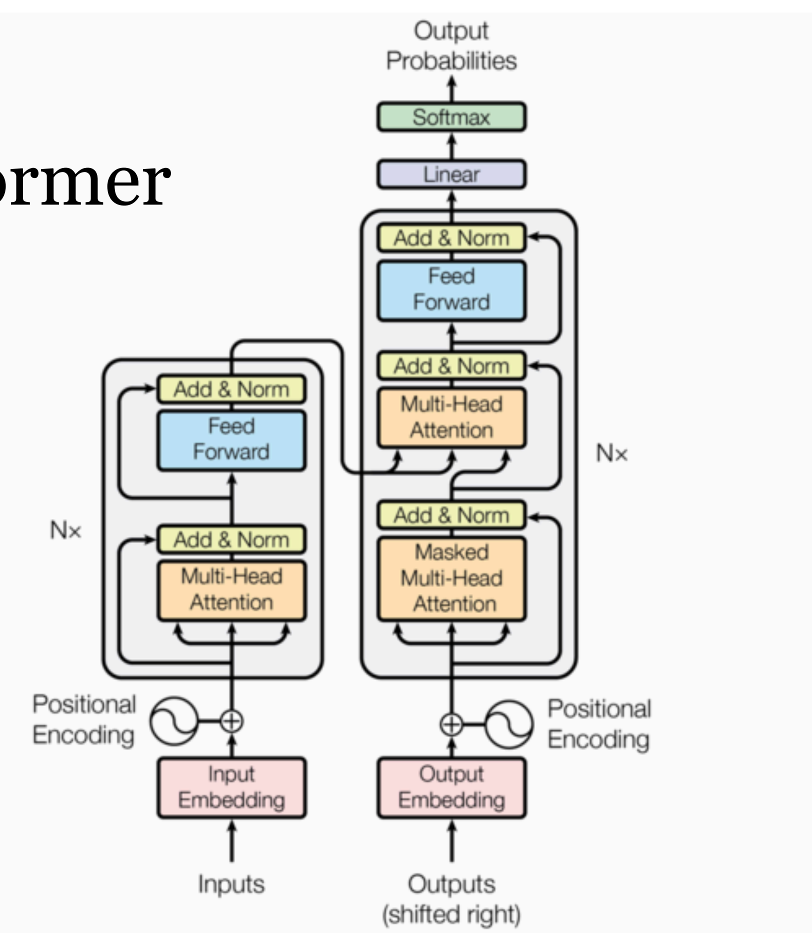
Recurrent NNs



Convolutional NNs



Transformer



Always coupled with word embeddings...

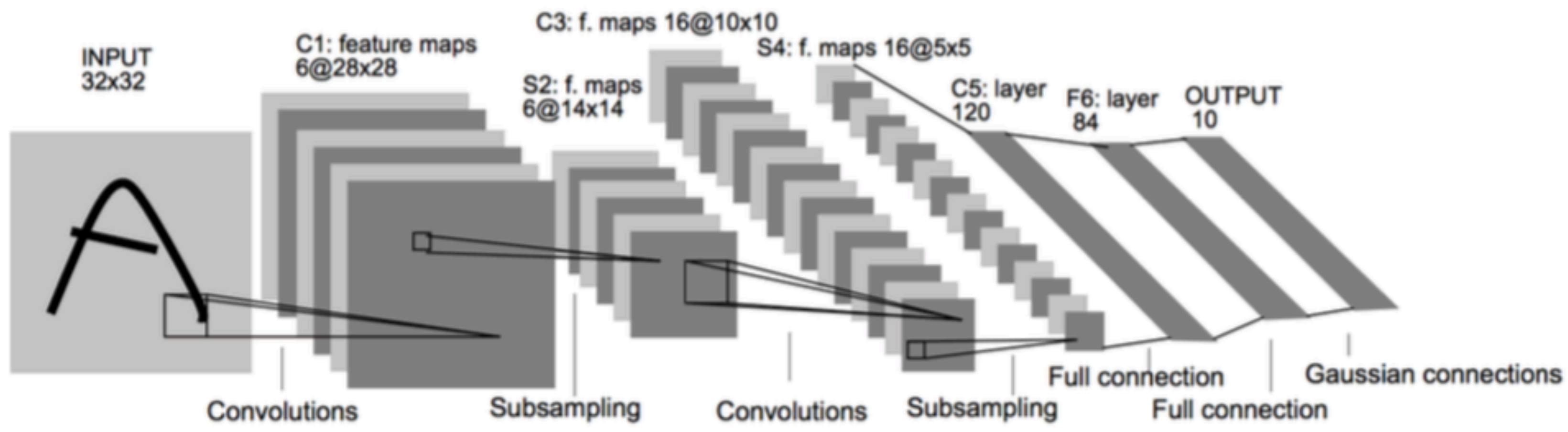
This Lecture

- Feedforward Neural Networks
- Applications
  - Neural Bag-of-Words Models
  - Feedforward Neural Language Models
- The training algorithm: Back-propagation

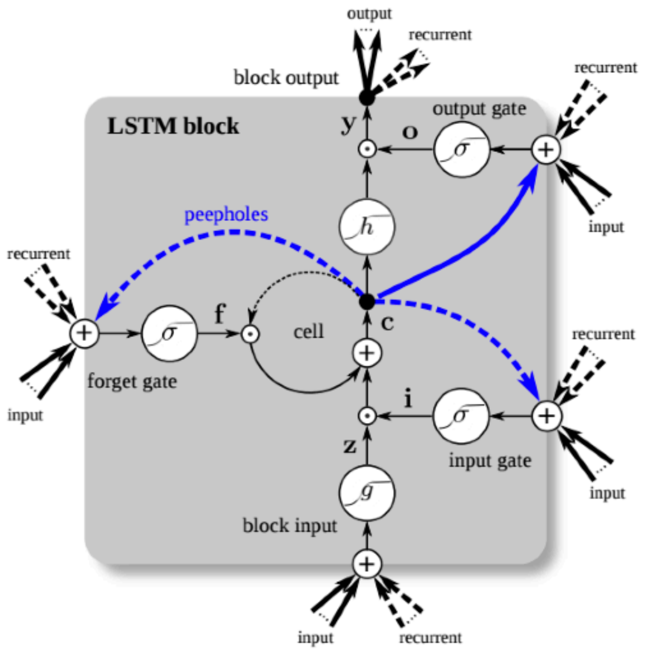
Neural Networks: History

NN "dark ages"

- Neural network algorithms date from the 80s
- ConvNets: applied to MNIST by LeCun in 1998



- Long Short-term Memory Networks (LSTMs): Hochreiter and Schmidhuber 1997



- Henderson 2003: neural shift-reduce parser, not SOTA

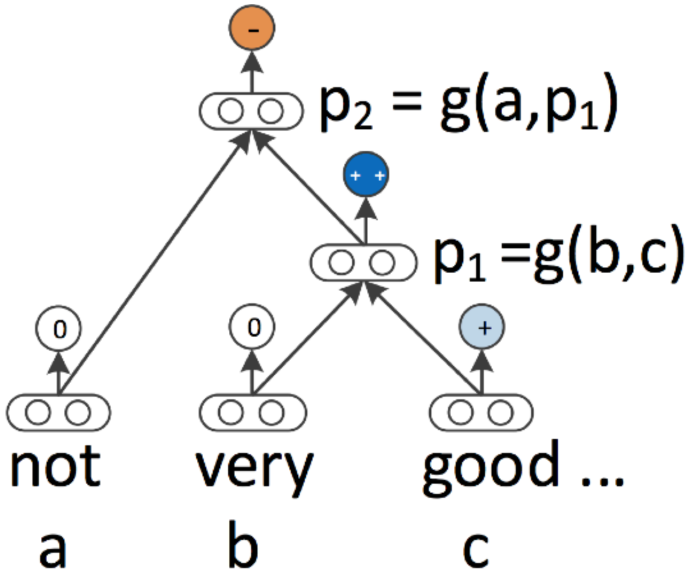
Credits: Greg Durrett

2008-2013: A glimmer of light

- Collobert and Weston 2011: "**NLP (almost) from Scratch**"
  - Feedforward NNs can replace "feature engineering"
  - 2008 version was marred by bad experiments, claimed SOTA but wasn't, 2011 version tied SOTA

- Krizhevskey et al, 2012: AlexNet for ImageNet Classification

- Socher 2011-2014: tree-structured RNNs working okay



Credits: Greg Durrett

2014: Stuff starts working

- Kim (2014) + Kalchbrenner et al, 2014: sentence classification
  - ConvNets work for NLP!
- Sutskever et al, 2014: sequence-to-sequence for neural MT
  - LSTMs work for NLP!
- Chen and Manning 2014: dependency parsing
  - Even feedforward networks work well for NLP!
- 2015: explosion of neural networks for everything under the sun

Credits: Greg Durrett

Why didn’t they work before?

- **Datasets too small**: for MT, not really better until you have 1M+ parallel sentences (and really need a lot more)
- **Optimization not well understood**: good initialization, per-feature scaling + momentum (Adagrad/Adam) work best out-of-the-box
  - Regularization: dropout is pretty helpful
  - Computers not big enough: can’t run for enough iterations
- Inputs: need **word embeddings** to represent continuous semantics

Credits: Greg Durrett

The "Promise"

- Most NLP works in the past focused on human-designed representations and input features

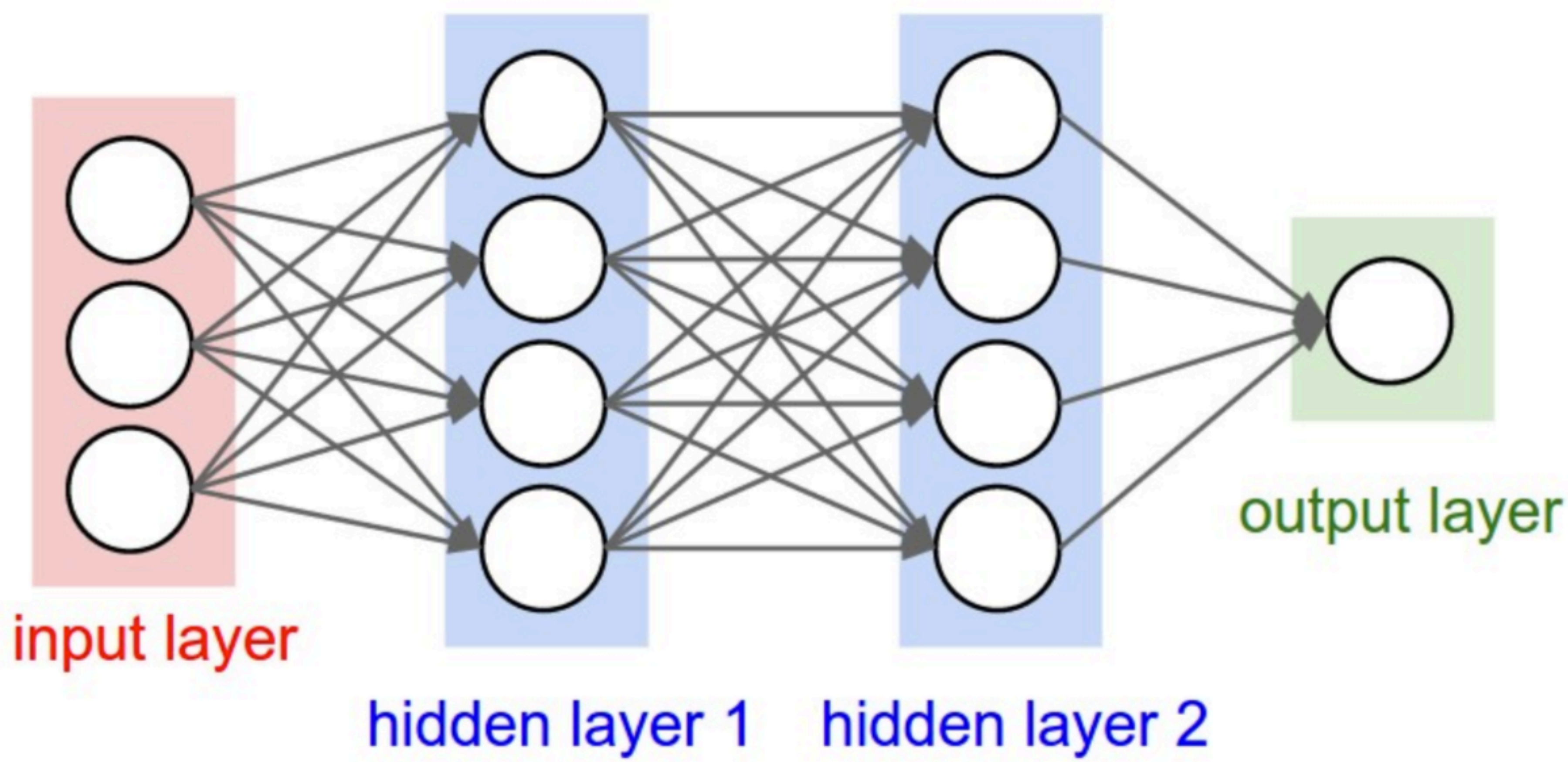
Var	Definition	Value in Fig. 5.2
x_1	count(positive lexicon) $\in$ doc)	3
x_2	count(negative lexicon) $\in$ doc)	2
x_3	$\begin{cases} 1 & \text{if "no"} \in \text{doc} \\ 0 & \text{otherwise} \end{cases}$	1
x_4	count(1st and 2nd pronouns $\in$ doc)	3
x_5	$\begin{cases} 1 & \text{if "!"} \in \text{doc} \\ 0 & \text{otherwise} \end{cases}$	0
x_6	log(word count of doc)	$\ln(64) = 4.15$

- **Representation learning** attempts to automatically learn good features and representations
- **Deep learning** attempts to learn multiple levels of representation on increasing complexity/abstraction

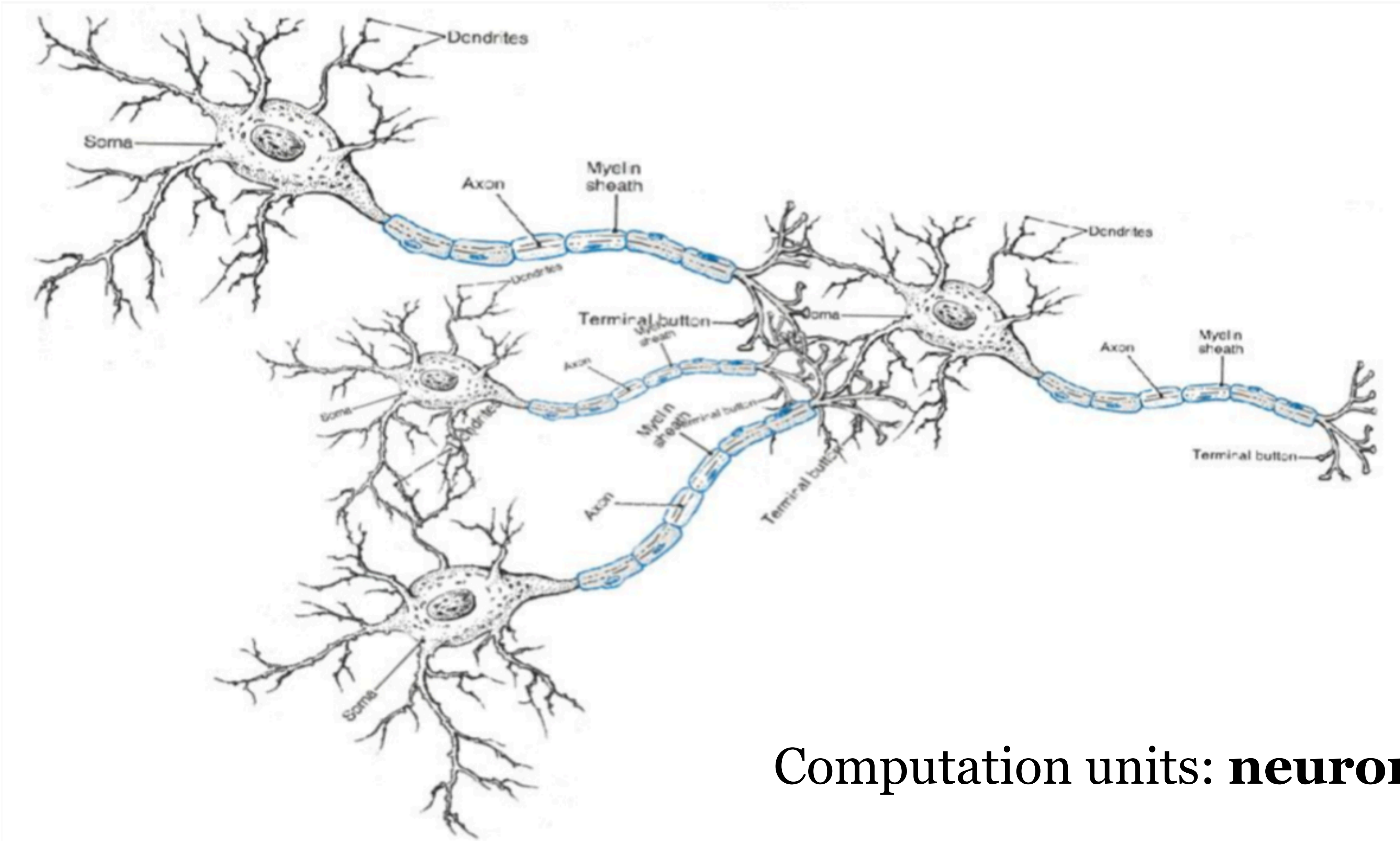
Feed-forward Neural Networks

Feed-forward NNs

- Input: $x_1, \ldots, x_d$
- Output: $y \in \{0,1\}$



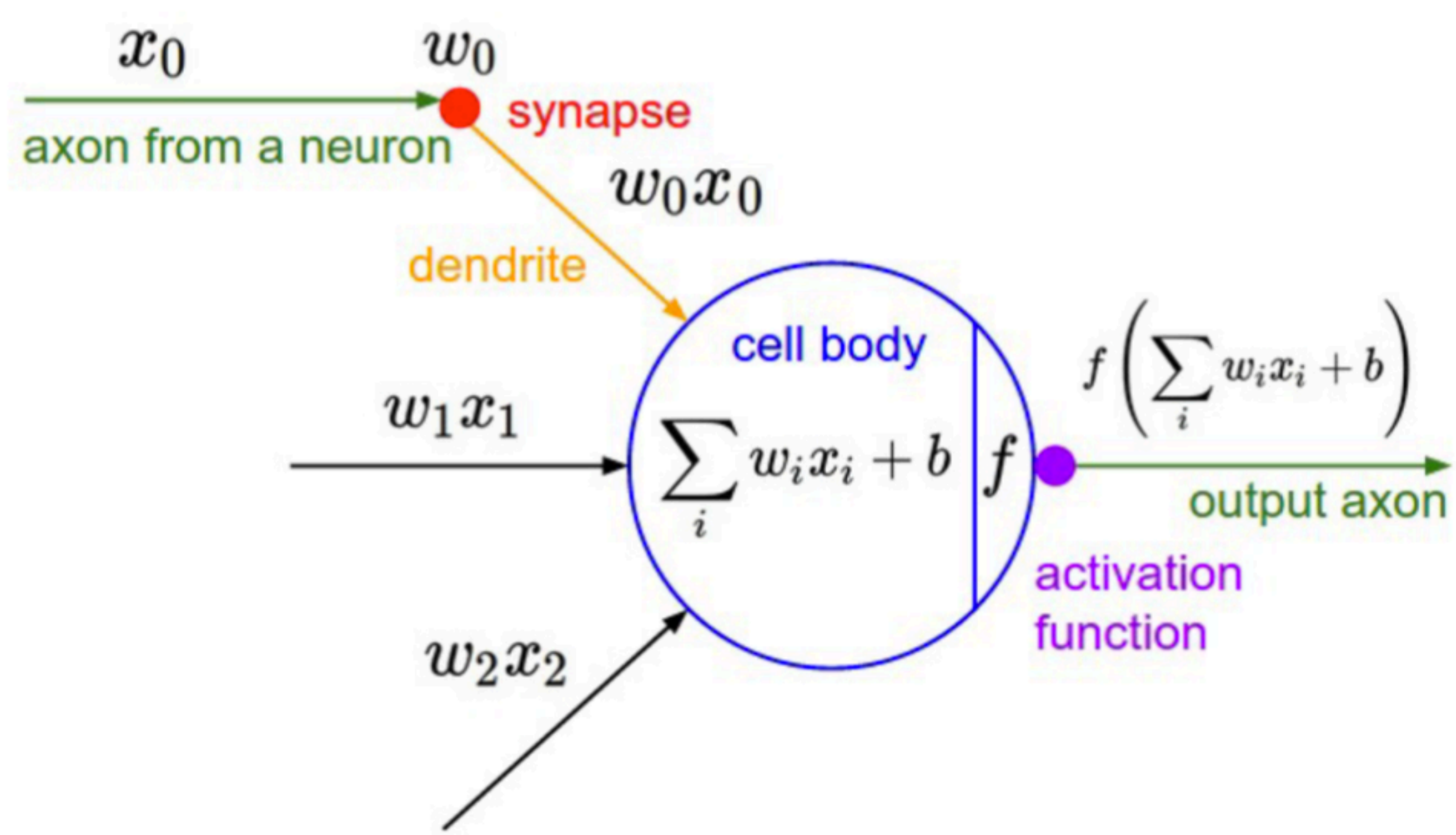
Neural computation



Computation units: **neurons**

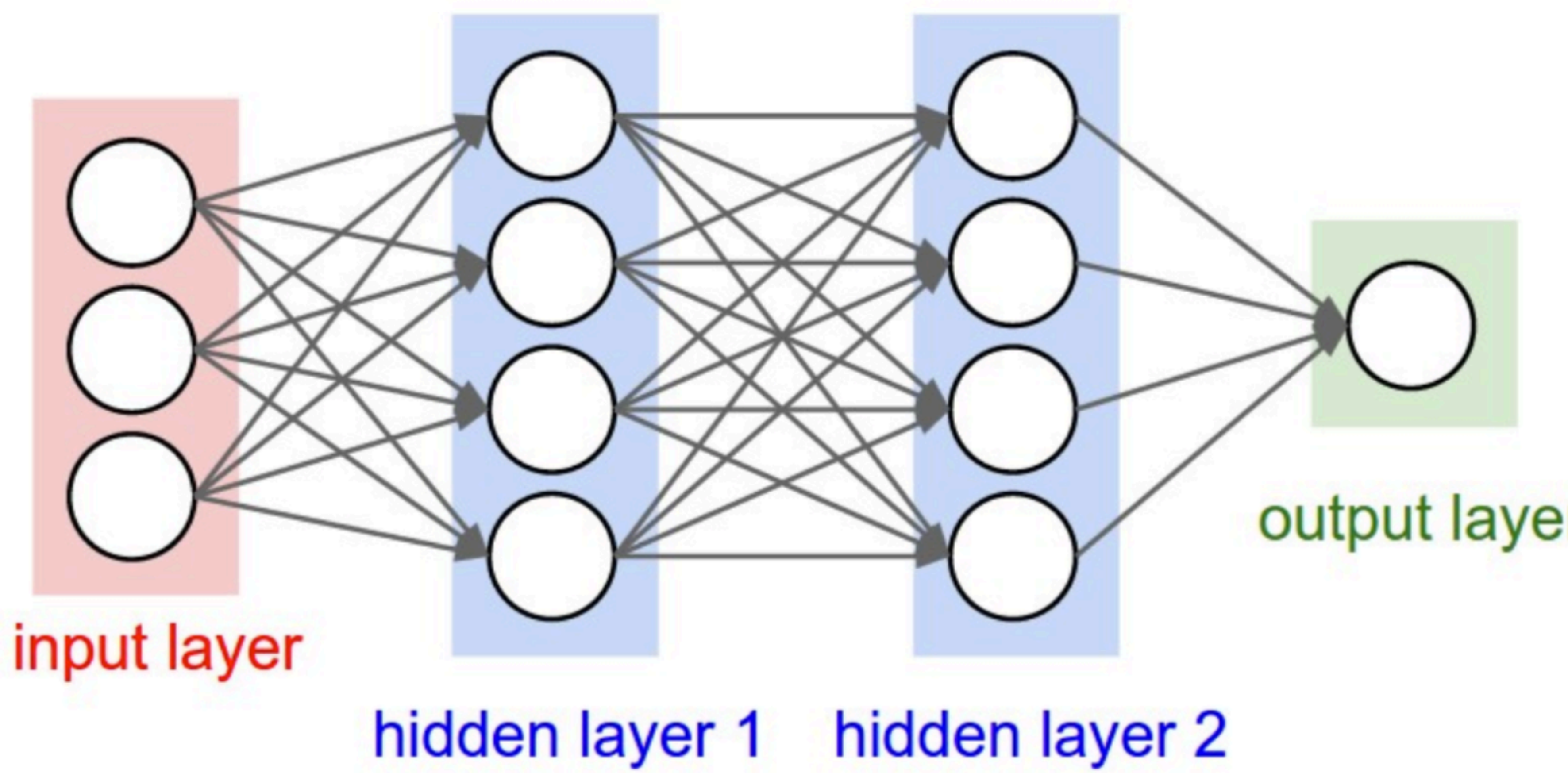
An artificial neuron

- A neuron is a computational unit that has scalar inputs and an output
- Each input has an associated weight.
- The neuron multiples each input by its weight, sums them, applied a **nonlinear function** to the result, and passes it to its output.

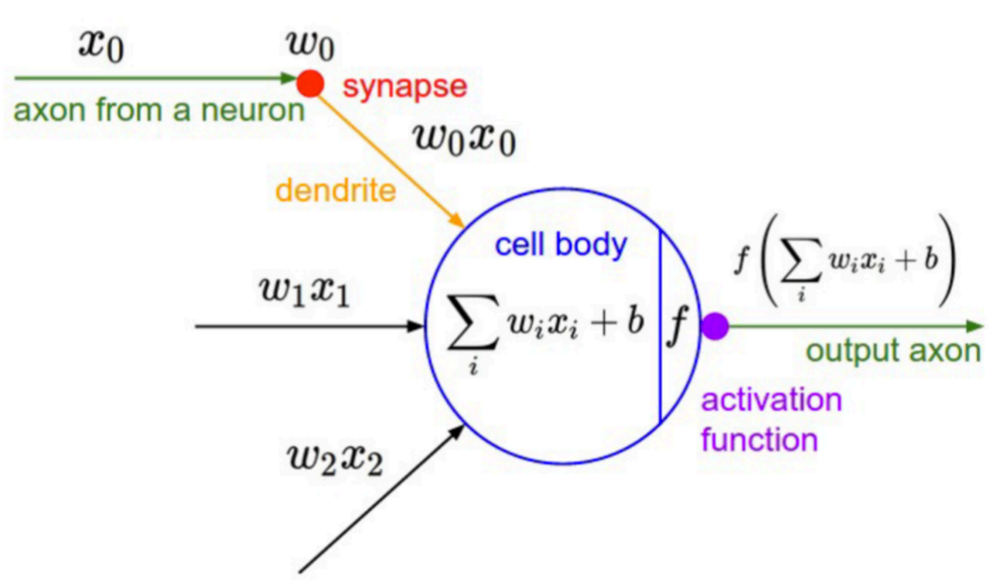


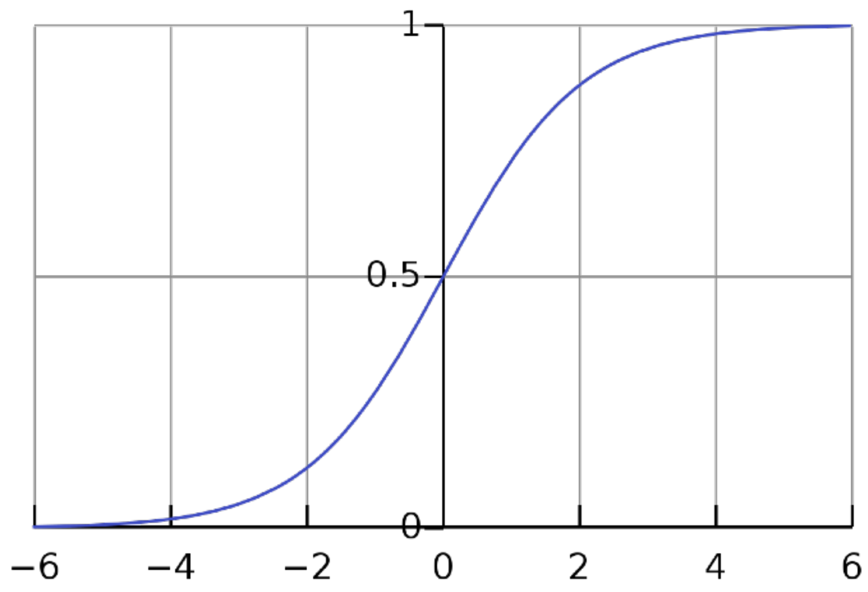
Neural networks

- The neurons are connected to each other, forming a **network**
- The output of a neuron may feed into the inputs of other neurons



A neuron can be a binary logistic regression unit

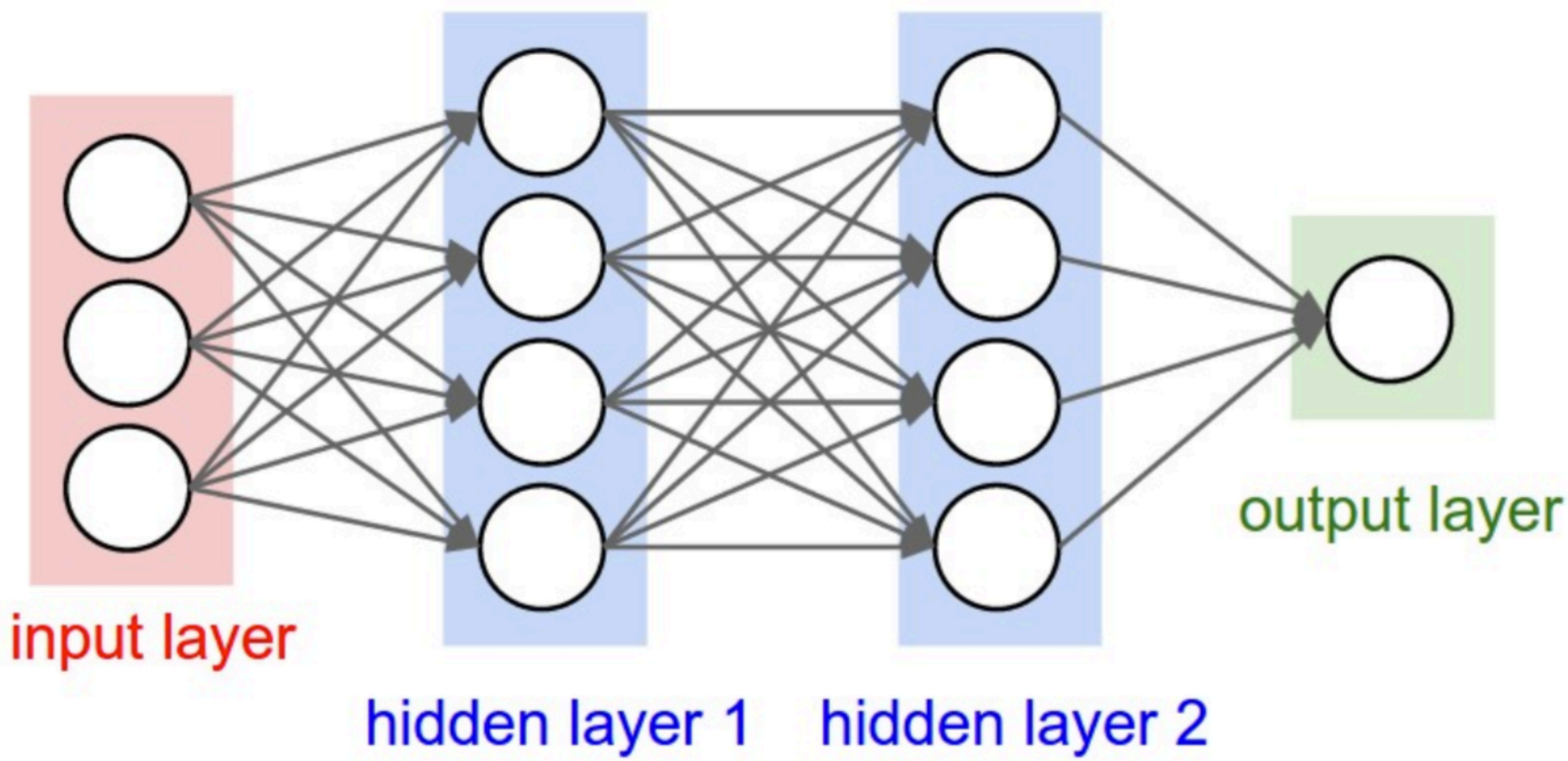




$$f(z) = \frac{1}{1 + e^{-z}}$$

$$h_{\mathbf{w},b}(\mathbf{x}) = f(\mathbf{w}^\intercal \mathbf{x} + b)$$

A neural network
= many layers of classifiers all learned at once, some providing features for others



- If we feed a vector of inputs through a bunch of logistic regression functions, then we get a vector of outputs…
- which we can feed into another logistic regression function

Mathematical Notation

- Input layer: $x_1, \ldots, x_d$
- Hidden layer 1: $h_1^{(1)}, h_2^{(1)}, \ldots, h_{d_1}^{(1)}$

$$h_1^{(1)} = f(W_{1,1}^{(1)} + W_{1,2}^{(1)} x_2 + \ldots + W_{1,d}^{(1)} x_d + b_1^{(1)})$$

$$h_2^{(1)} = f(W_{2,1}^{(1)} + W_{2,2}^{(1)} x_2 + \ldots + W_{2,d}^{(1)} x_d + b_2^{(1)})$$

$$\ldots$$

- Hidden layer 2: $h_1^{(2)}, h_2^{(2)}, \ldots, h_{d_2}^{(2)}$

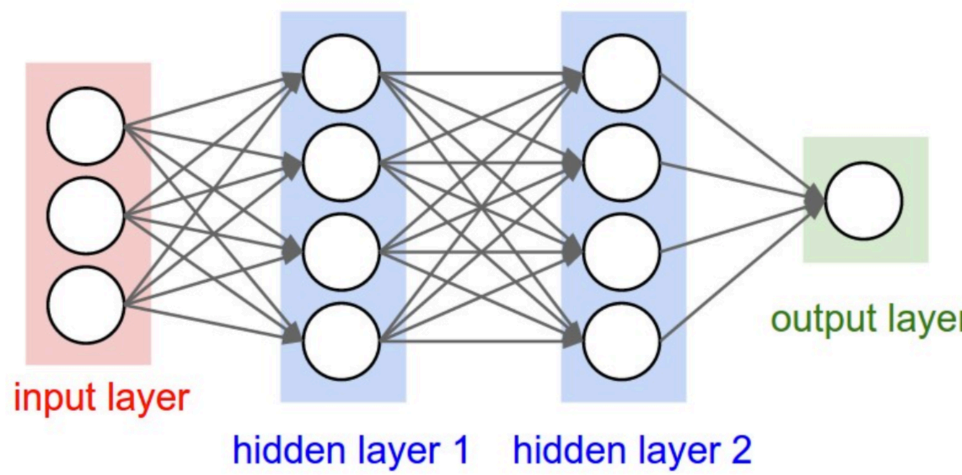
$$h_1^{(2)} = f(W_{1,1}^{(2)} h_1^{(1)} + W_{1,2}^{(2)} h_2^{(1)} + \ldots + W_{1,d_1}^{(2)} h_{d_1}^{(1)} + b_1^{(2)})$$

$$h_2^{(2)} = f(W_{2,1}^{(2)} h_1^{(1)} + W_{2,2}^{(2)} h_2^{(1)} + \ldots + W_{2,d_1}^{(2)} h_{d_1}^{(1)} + b_2^{(2)})$$

$$\ldots$$

- Output layer:

$$y = \sigma(w_1^{(o)} h_1^{(2)} + w_2^{(o)} h_2^{(2)} + \ldots + w_{d_2}^{(o)} h_{d_2}^{(2)} + b^{(o)})$$



Matrix Notation

- Input layer: $\mathbf{x} \in \mathbb{R}^d$
- Hidden layer 1:

$$\mathbf{h}_1 = f(\mathbf{W}^{(1)}\mathbf{x} + \mathbf{b}^{(1)}) \in \mathbb{R}^{d_1}$$

$$\mathbf{W}^{(1)} \in \mathbb{R}^{d_1 \times d}, \mathbf{b}^{(1)} \in \mathbb{R}^{d_1}$$

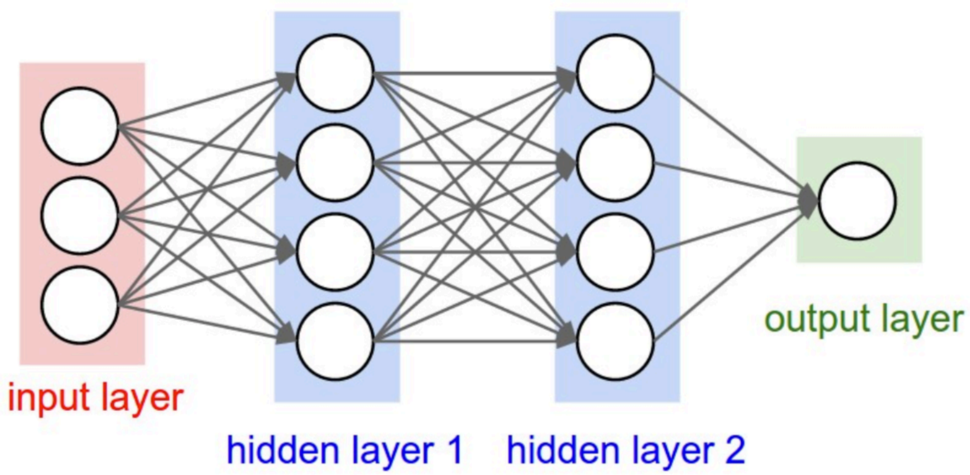
- Hidden layer 2:

$$\mathbf{h}_2 = f(\mathbf{W}^{(2)}\mathbf{h}_1 + \mathbf{b}^{(2)}) \in \mathbb{R}^{d_2}$$

$$\mathbf{W}^{(2)} \in \mathbb{R}^{d_2 \times d_1}, \mathbf{b}^{(2)} \in \mathbb{R}^{d_2}$$

- Output layer:

$$y = \sigma(\mathbf{w}^{(o)} \cdot \mathbf{h}_2 + b^{(o)})$$



*: f is applied element-wise

$$f([z_1, z_2, z_3]) = [f(z_1), f(z_2), f(z_3)]$$

Mathematical Notation, side by side

- Input layer: $x_1, \ldots, x_d$
- Hidden layer 1: $h_1^{(1)}, h_2^{(1)}, \ldots, h_{d_1}^{(1)}$

$$h_1^{(1)} = f(W_{1,1}^{(1)} + W_{1,2}^{(1)} x_2 + \ldots + W_{1,d}^{(1)} x_d + b_1^{(1)})$$

$$h_2^{(1)} = f(W_{2,1}^{(1)} + W_{2,2}^{(1)} x_2 + \ldots + W_{2,d}^{(1)} x_d + b_2^{(1)})$$

$$\ldots$$

- Hidden layer 2: $h_1^{(2)}, h_2^{(2)}, \ldots, h_{d_2}^{(2)}$

$$h_1^{(2)} = f(W_{1,1}^{(2)} h_1^{(1)} + W_{1,2}^{(2)} h_2^{(1)} + \ldots + W_{1,d_1}^{(2)} h_{d_1}^{(1)} + b_1^{(2)})$$

$$h_2^{(2)} = f(W_{2,1}^{(2)} h_1^{(1)} + W_{2,2}^{(2)} h_2^{(1)} + \ldots + W_{2,d_1}^{(2)} h_{d_1}^{(1)} + b_2^{(2)})$$

$$\ldots$$

- Output layer:

$$y = \sigma(w_1^{(o)} h_1^{(2)} + w_2^{(o)} h_2^{(2)} + \ldots + w_{d_2}^{(o)} h_{d_2}^{(2)} + b^{(o)})$$

- Input layer: $\mathbf{x} \in \mathbb{R}^d$
- Hidden layer 1:

$$\mathbf{h}_1 = f(\mathbf{W}^{(1)}\mathbf{x} + \mathbf{b}^{(1)}) \in \mathbb{R}^{d_1}$$

$$\mathbf{W}^{(1)} \in \mathbb{R}^{d_1 \times d}, \mathbf{b}^{(1)} \in \mathbb{R}^{d_1}$$

- Hidden layer 2:

$$\mathbf{h}_2 = f(\mathbf{W}^{(2)}\mathbf{h}_1 + \mathbf{b}^{(2)}) \in \mathbb{R}^{d_2}$$

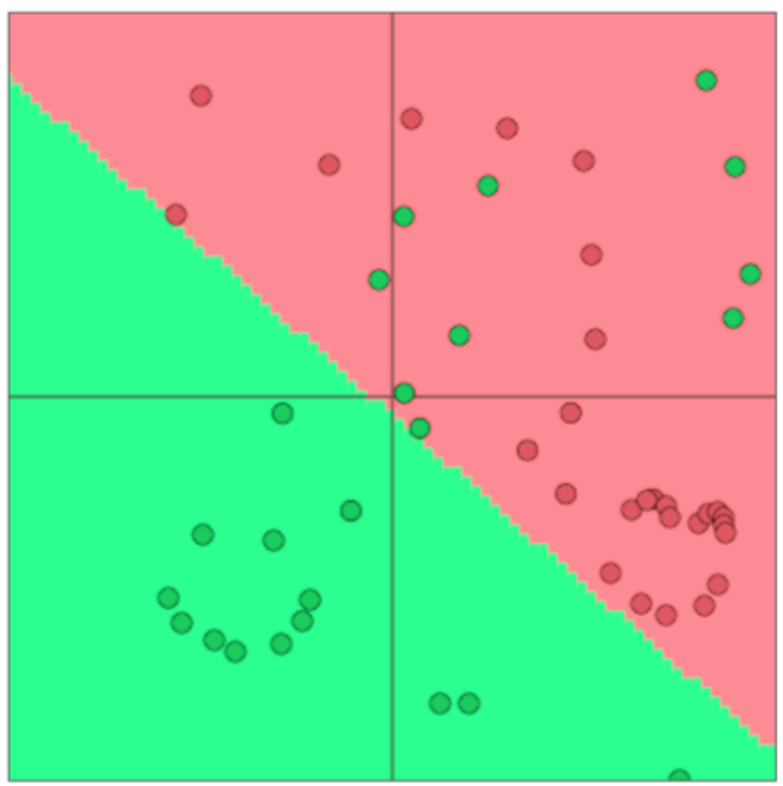
$$\mathbf{W}^{(2)} \in \mathbb{R}^{d_2 \times d_1}, \mathbf{b}^{(2)} \in \mathbb{R}^{d_2}$$

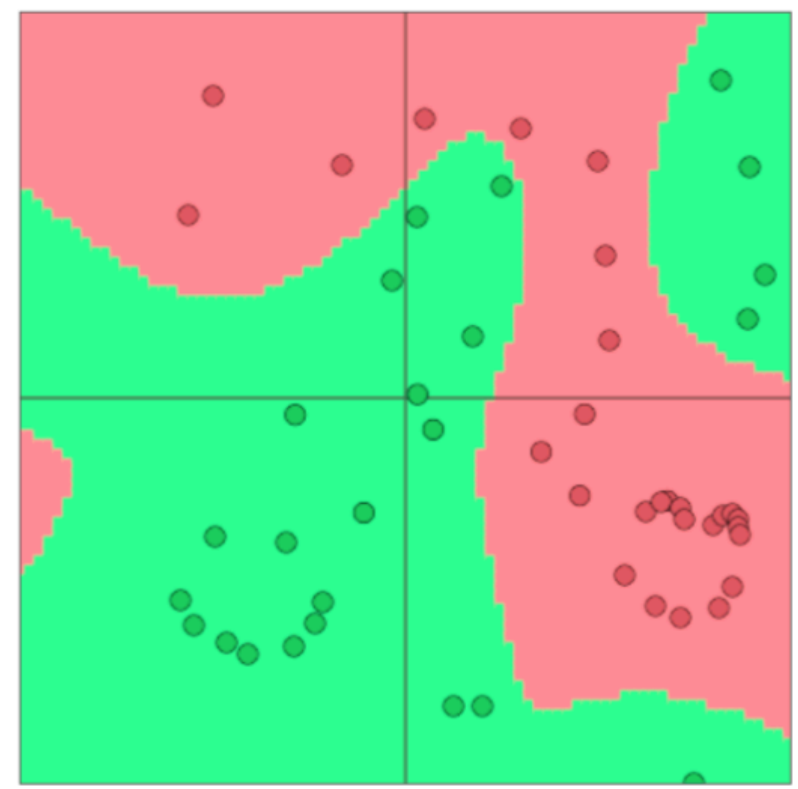
- Output layer:

$$y = \sigma(\mathbf{w}^{(o)} \cdot \mathbf{h}_2 + b^{(o)})$$

Why non-linearities?

- Neural networks can learn much more complex functions and nonlinear decision boundaries



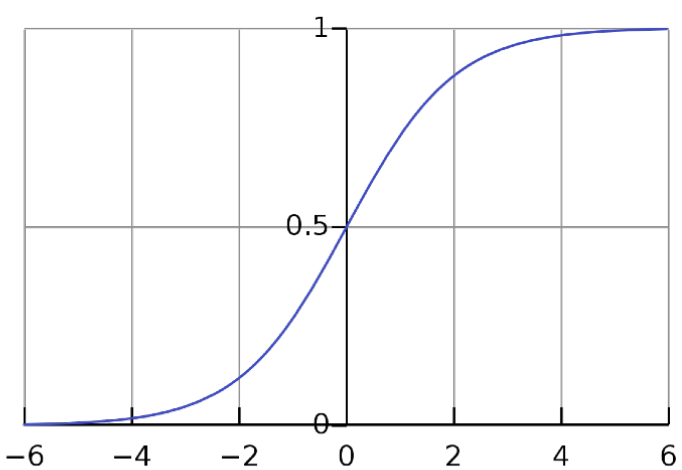


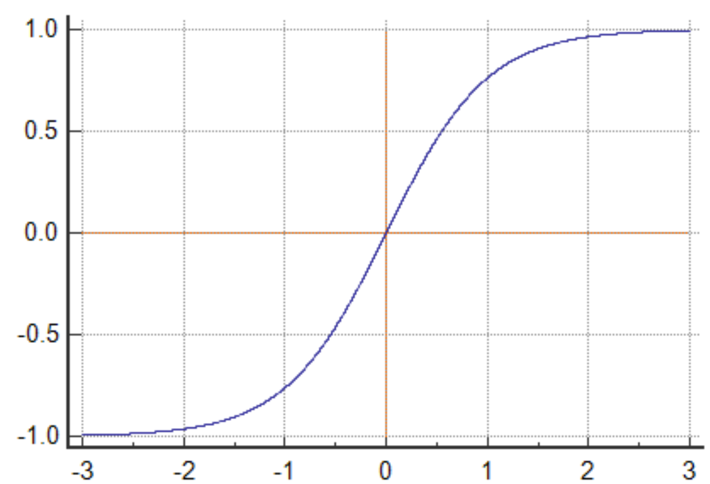
The capacity of the network increases with more hidden units and more hidden layers

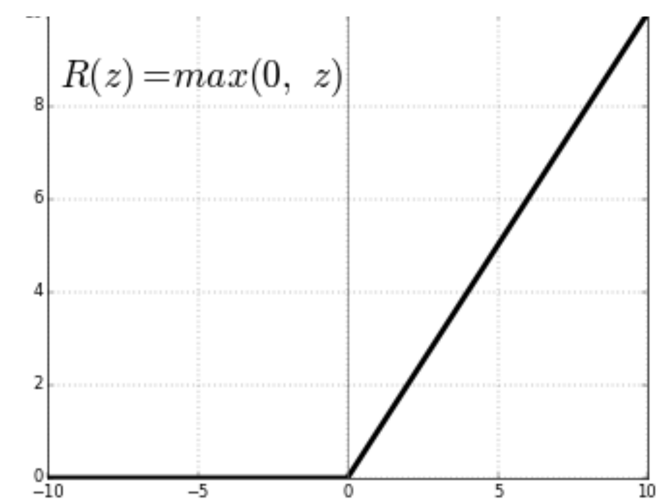
How if we remove activation function?

Activation functions

sigmoid	tanh	ReLU (rectified linear unit)
$f(z) = \dfrac{1}{1+e^{-z}}$	$f(z) = \dfrac{e^{2z}-1}{e^{2z}+1}$	$f(z) = \max(0, z)$







$$f'(z) = f(z) \times (1 - f(z))$$

$$f'(z) = 1 - f(z)^2$$

$$f'(z) = \begin{cases} 1 & z > 0 \\ 0 & z < 0 \end{cases}$$

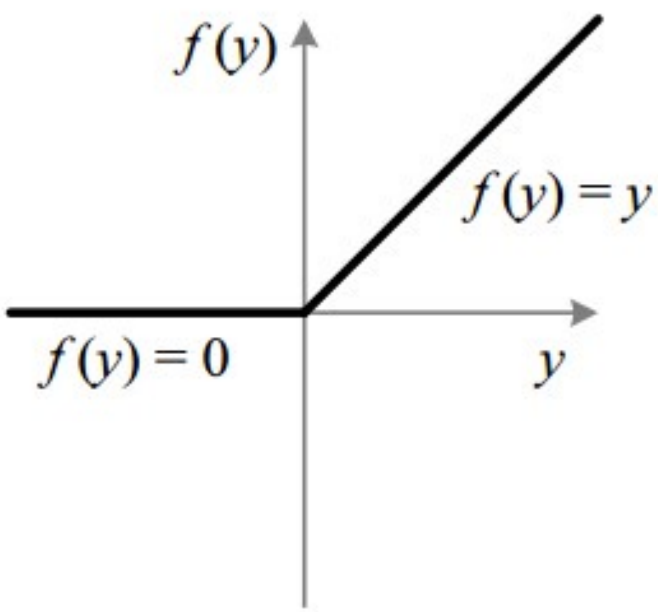
Advantages of ReLU?

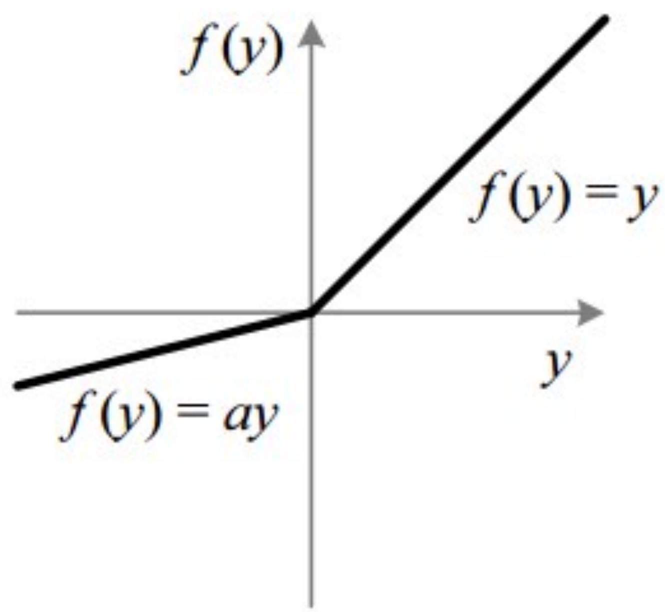
Activation functions

Problems of ReLU? "dead neurons"

Leaky ReLU

$$f(z) = \begin{cases} z & z \geq 0 \\ 0.01z & z < 0 \end{cases}$$





Loss functions

- Binary classification

$$y = \sigma(\mathbf{w}^{(o)} \cdot \mathbf{h}_2 + b^{(o)})$$

$$\mathcal{L}(y, y^*) = -y^* \log y - (1 - y^*) \log (1 - y)$$

- Regression

$$y = \mathbf{w}^{(o)} \cdot \mathbf{h}_2 + b^{(o)}$$

$$\mathcal{L}_{\mathrm{MSE}}(y, y^*) = (y - y^*)^2$$

- Multi-class classification (C classes)

$$y_i = \mathrm{softmax}_i(\mathbf{W}^{(o)}\mathbf{h}_2 + \mathbf{b}^{(o)}) \qquad \mathbf{W}^{(o)} \in \mathbb{R}^{C \times d_2}, \mathbf{b}^{(o)} \in \mathbb{R}^C$$

$$\mathcal{L}(y, y^*) = -\sum_{i=1}^{C} y_i^* \log y_i \qquad \mathrm{softmax}_i(x) = \frac{\exp(x_i)}{\sum_j \exp(x_j)}$$

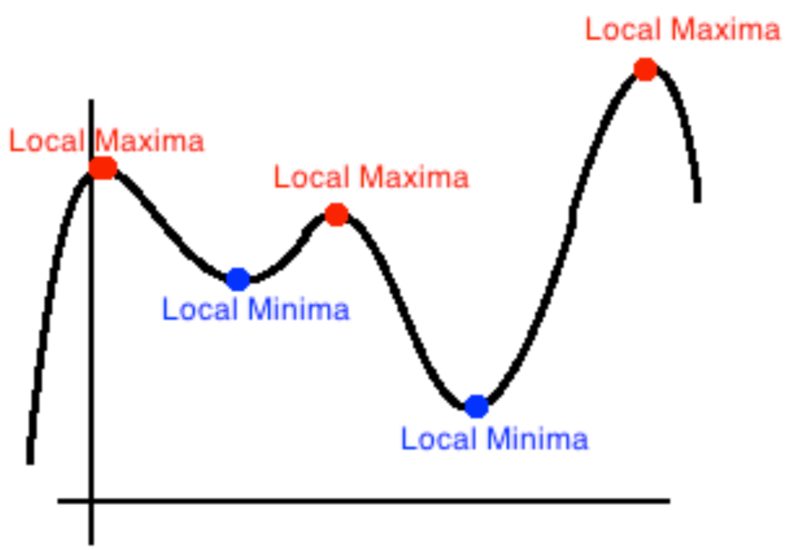
The question again becomes how to compute: $\nabla_\theta \mathcal{L}(\theta)$

$$\theta = \{\mathbf{W}^{(1)}, \mathbf{b}^{(1)}, \mathbf{W}^{(2)}, \mathbf{b}^{(2)}, \mathbf{w}^{(o)}, b^{(o)}\}$$

Optimization

$$\theta^{(t+1)} = \theta^{(t)} - \eta \nabla_\theta J(\theta)$$

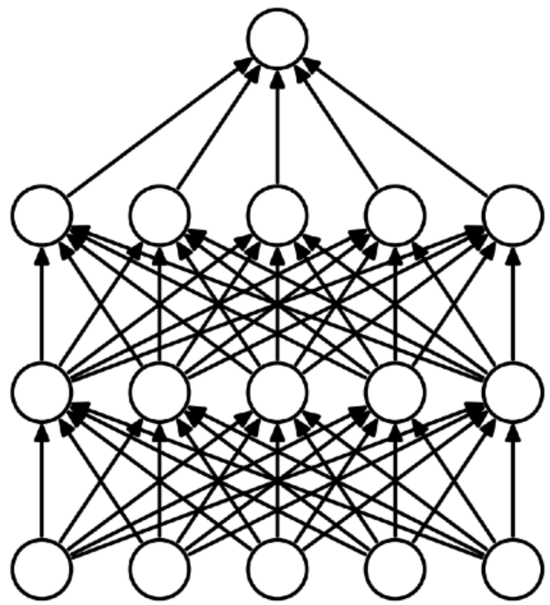
- Logistic regression is convex: one global minimum
- Neural networks are non-convex and not easy to optimize
- A class of more sophisticated "adaptive" optimizers that scale the parameter adjustment by an accumulated gradient.
    - **Adam**
    - Adagrad
    - RMSprop
    - ...



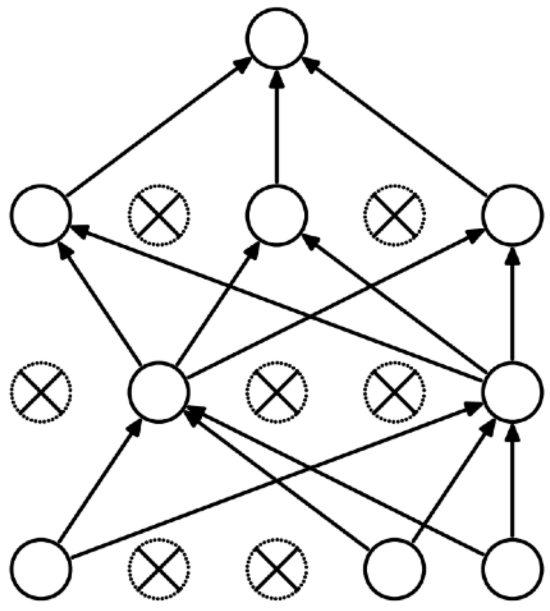
(Ruder 2016): An overview of gradient descent optimization algorithms

Dropout

- Form of regularization NNs
- Idea: “Handicap” NN by removing hidden units **stochastically**
  - set each hidden unit in a layer to 0 with probability p during training ($p = 0.5$ usually works well)
  - scale outputs by $1/(1-p)$
  - hidden units forced to learn more general patterns
- Test time: Simply compute identity



(a) Standard Neural Net

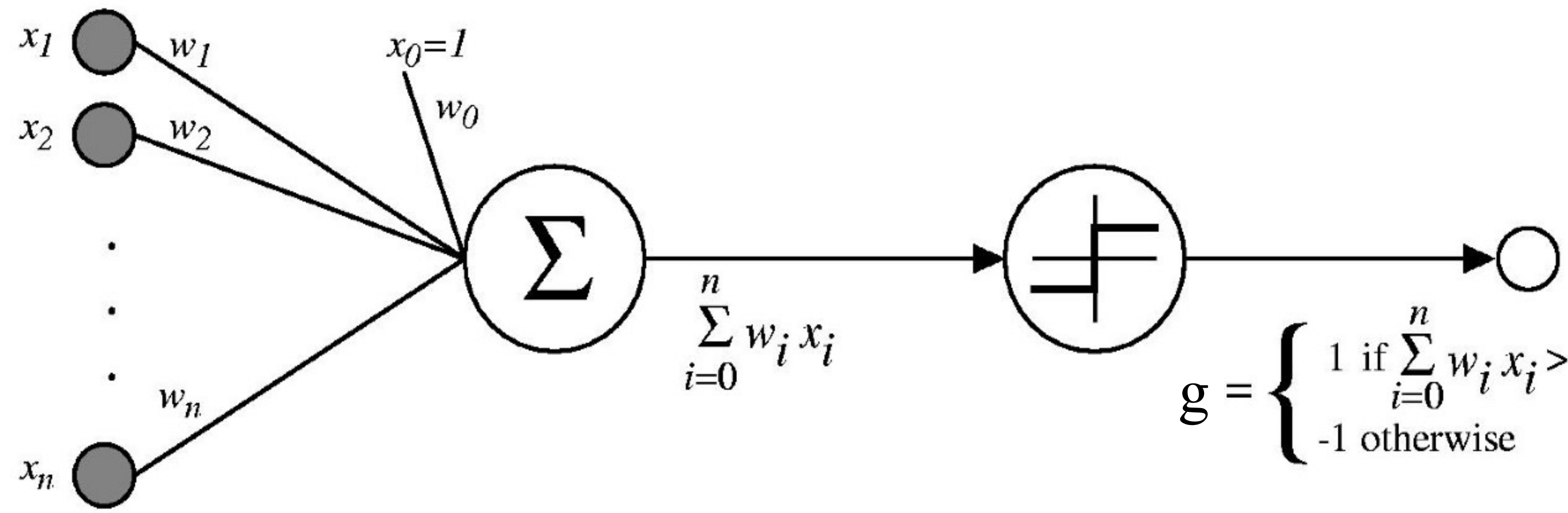


(b) After applying dropout.

What can we compute with NNs?

Perceptron, linear classification, Boolean functions: $x_i \in \{0,1\}$

- Can learn $x_1 \vee x_2$?
  - $-0.5 + x_1 + x_2$
- Can learn $x_1 \wedge x_2$?
  - $-1.5 + x_1 + x_2$



- Can learn any conjunction or disjunction?
  - $0.5 + x_1 + \ldots + x_n$
  - $(-n+0.5) + x_1 + \ldots + x_n$
- Can learn majority?
  - $(-0.5*n) + x_1 + \ldots + x_n$
- What are we missing? The dreaded XOR!, etc.

Going beyond linear classification

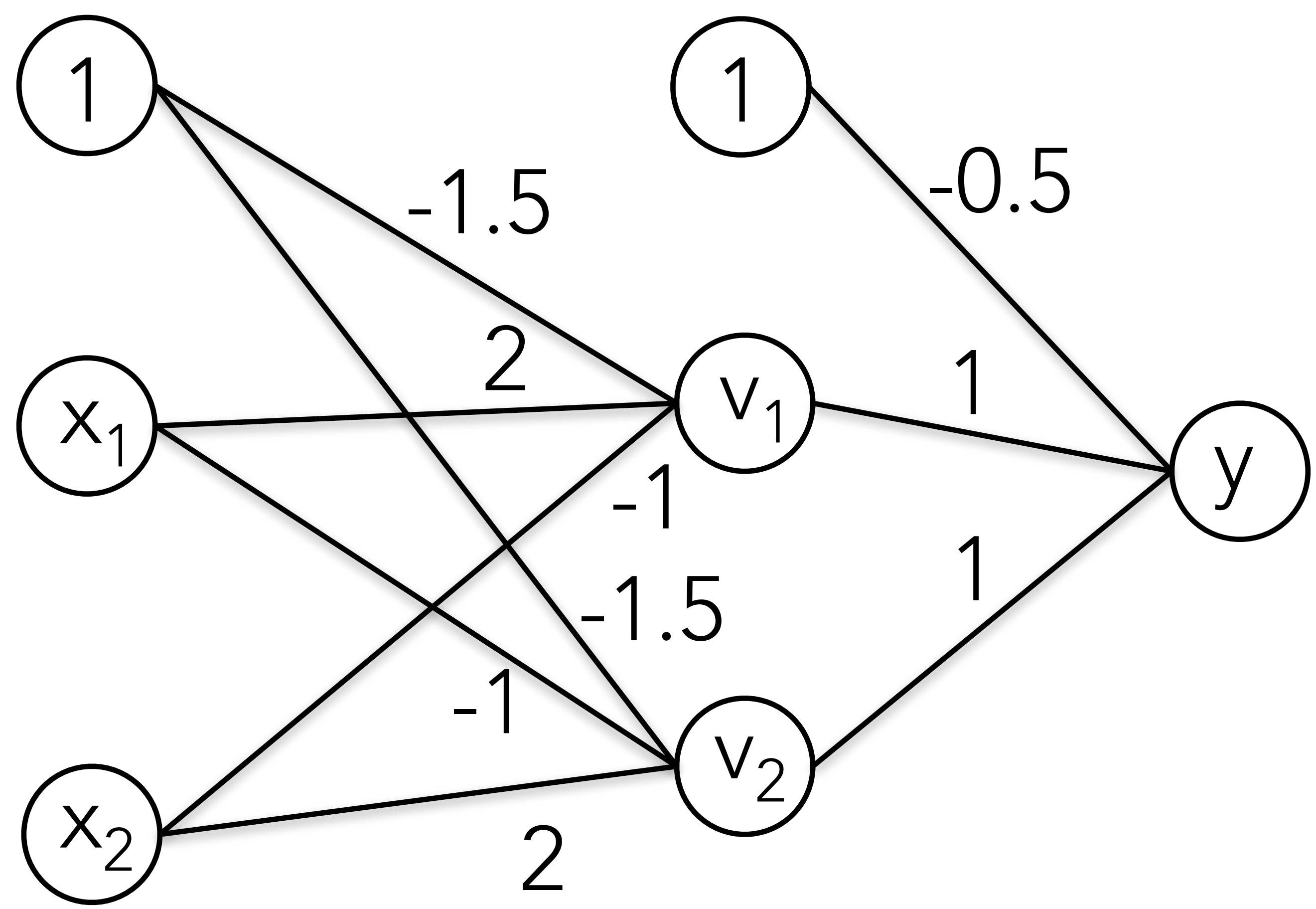
Solving the XOR problem

$$y = x_1 \text{ XOR } x_2 = (x_1 \wedge \neg x_2) \vee (x_2 \wedge \neg x_1)$$

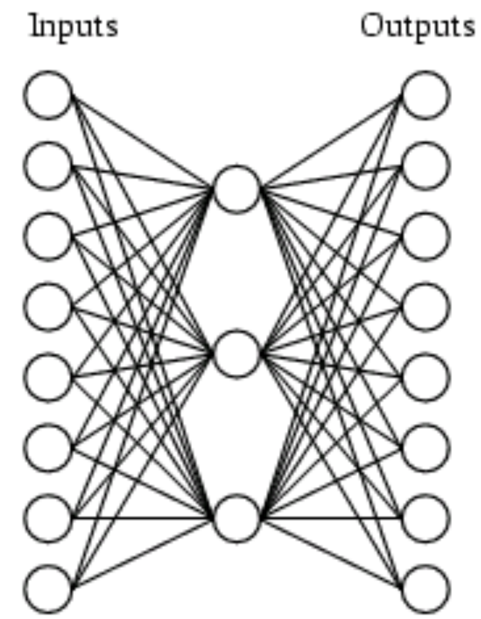
$$v_1 = (x_1 \wedge \neg x_2)$$
$$= -1.5 + 2x_1 - x_2$$

$$v_2 = (x_2 \wedge \neg x_1)$$
$$= -1.5 + 2x_2 - x_1$$

$$y = v_1 \vee v_2$$
$$= -0.5 + v_1 + v_2$$



Example data for NN with hidden layer



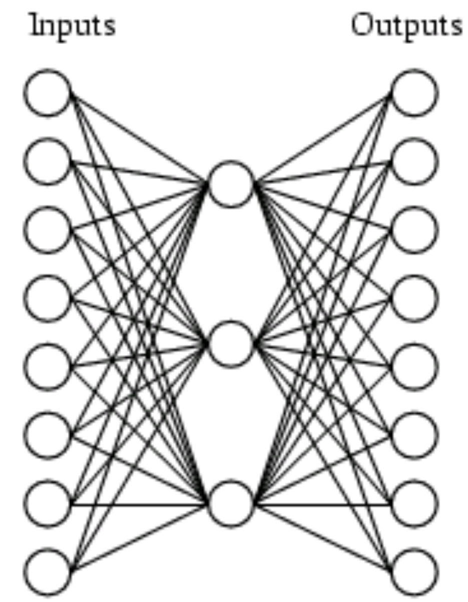
A target function:

Input		Output
10000000	$\rightarrow$	10000000
01000000	$\rightarrow$	01000000
00100000	$\rightarrow$	00100000
00010000	$\rightarrow$	00010000
00001000	$\rightarrow$	00001000
00000100	$\rightarrow$	00000100
00000010	$\rightarrow$	00000010
00000001	$\rightarrow$	00000001

Can this be learned??

Learned weights for hidden layer

A network:



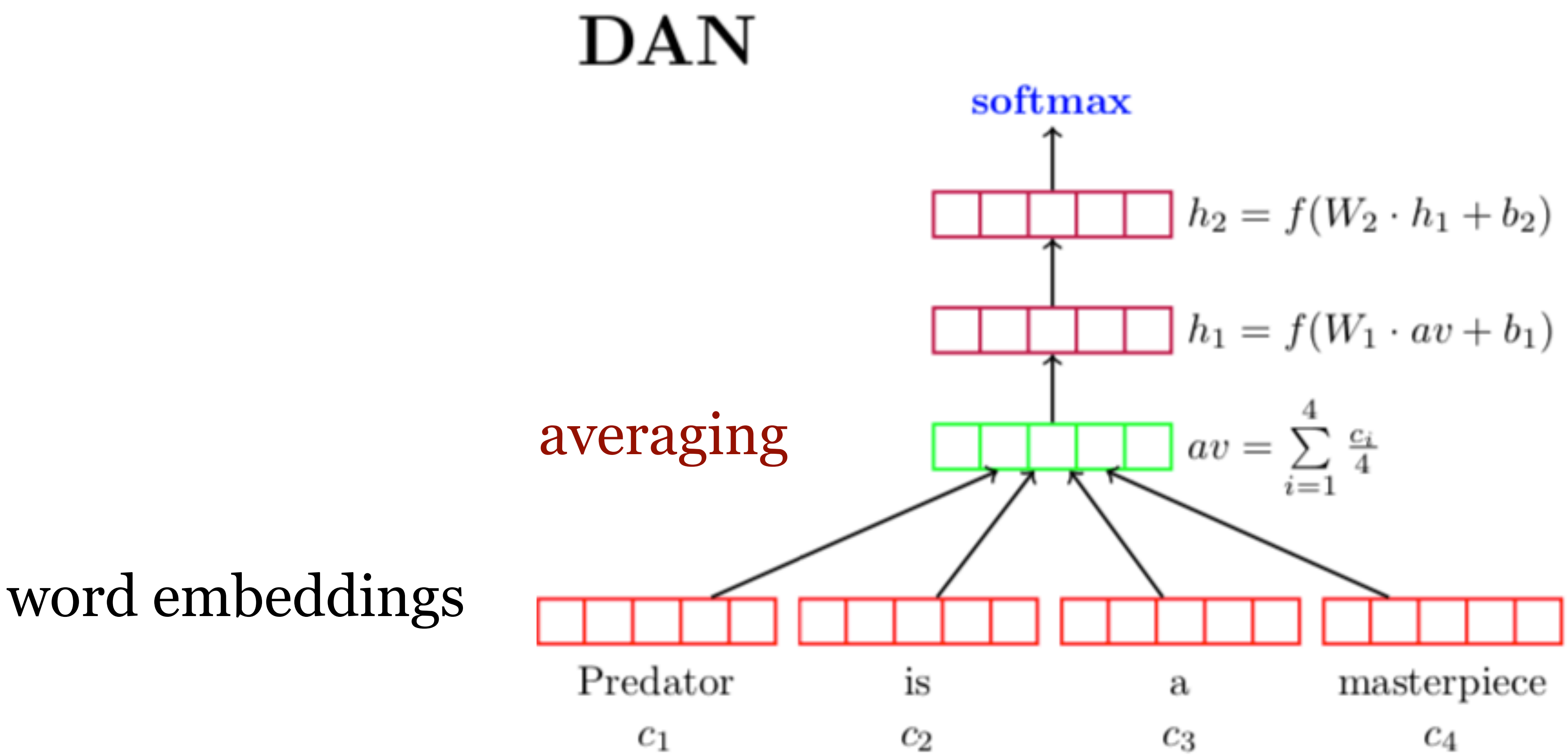
Learned hidden layer representation:

Input		Hidden Values				Output
10000000	→	.89	.04	.08	→	10000000
01000000	→	.01	.11	.88	→	01000000
00100000	→	.01	.97	.27	→	00100000
00010000	→	.99	.97	.71	→	00010000
00001000	→	.03	.05	.02	→	00001000
00000100	→	.22	.99	.99	→	00000100
00000010	→	.80	.01	.98	→	00000010
00000001	→	.60	.94	.01	→	00000001

Applications

Neural Bag-of-Words (NBOW)

- Deep Averaging Networks (DAN) for Text Classification



(Iyyer et 2015): Deep Unordered Composition Rivals Syntactic Methods for Text Classification

Word embeddings: re-train or not?

- Word embeddings can be treated as parameters too!

$$\theta = \{\mathbf{W}^{(1)}, \mathbf{b}^{(1)}, \mathbf{W}^{(2)}, \mathbf{b}^{(2)}, \mathbf{w}^{(o)}, b^{(o)}, \mathbf{E}_{emb}\}$$

- When the training set is small, don't re-train word embeddings (think of them as features!).

Why?

- Most cases: initialize word embeddings using pre-trained ones (word2vec, Glove) and re-train them for the task

"good" vs "bad"

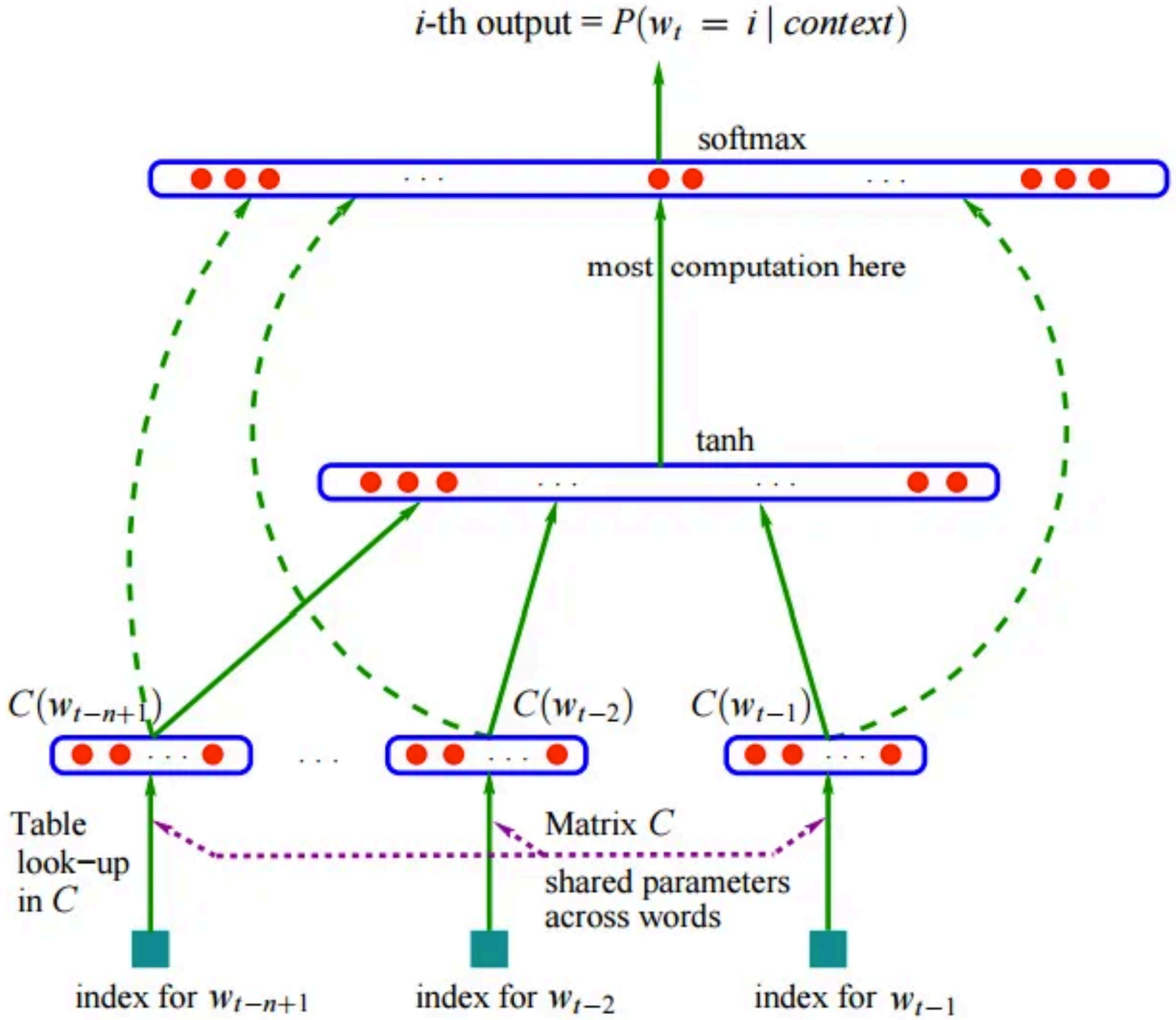
- When you have enough data, you can just randomly initialize them and train from scratch (e.g. machine translation)

Neural Bag-of-Words (NBOW)

Model	RT	SST fine	SST bin	IMDB	Time (s)
DAN-ROOT	—	46.9	85.7	—	**31**
DAN-RAND	77.3	45.4	83.2	88.8	136
DAN	80.3	47.7	86.3	89.4	136
NBOW-RAND	76.2	42.3	81.4	88.9	91
NBOW	79.0	43.6	83.6	89.0	91
BiNB	—	41.9	83.1	—	—
NBSVM-bi	79.4	—	—	91.2	—

Feedforward Neural LMs

- N-gram models: $P(\text{mat}|\text{the cat sat on the})$



- Input layer (context size n = 5):

$$\mathbf{x} = [\mathbf{e}_{\text{the}}; \mathbf{e}_{\text{cat}}; \mathbf{e}_{\text{sat}}; \mathbf{e}_{\text{on}}; \mathbf{e}_{\text{the}}] \in \mathbb{R}^{dn}$$

concatenation

- Hidden layer

$$\mathbf{h} = \tanh(\mathbf{W}\mathbf{x} + \mathbf{b}) \in \mathbb{R}^{h}$$

- Output layer (softmax)

$$\mathbf{z} = \mathbf{U}\mathbf{h} \in \mathbb{R}^{|V|}$$

$$P(w = i \mid \text{context}) = softmax_i(\mathbf{z})$$

(Bengio et 2003): A Neural Probabilistic Language Model

Backpropagation

How to compute gradients?

Backpropagation

- It's taking derivatives and applying chain rule!
- We'll **re-use** derivatives computed for higher layers in computing derivatives for lower layers so as to minimize computation
- Good news is that modern automatic differentiation tools did all for you!
    - Implementing backprop by hand is like programming in assembly language.

Deriving gradients for Feedforward NNs

Input: $\mathbf{x}$ $\qquad \mathbf{x} \in \mathbb{R}^d$

$$\mathbf{h}_1 = \tanh(\mathbf{W}_1 \mathbf{x} + \mathbf{b}_1) \qquad \mathbf{W}_1 \in \mathbb{R}^{d_1 \times d} \quad \mathbf{b}_1 \in \mathbb{R}^{d_1}$$

$$\mathbf{h}_2 = \tanh(\mathbf{W}_2 \mathbf{h}_1 + \mathbf{b}_2) \qquad \mathbf{W}_2 \in \mathbb{R}^{d_2 \times d_1} \quad \mathbf{b}_2 \in \mathbb{R}^{d_2}$$

$$y = \sigma(\mathbf{w}^\intercal \mathbf{h_2} + b) \qquad \mathbf{w} \in \mathbb{R}^{d_2}$$

$$\mathcal{L}(y, y^*) = -y^* \log y - (1 - y^*) \log (1 - y)$$

$$\frac{\partial L}{\partial \mathbf{w}} = \ ? \qquad \frac{\partial L}{\partial b} = \ ?$$

$$\frac{\partial L}{\partial \mathbf{W}_2} = \ ? \qquad \frac{\partial L}{\partial \mathbf{b}_2} = \ ?$$

$$\frac{\partial L}{\partial \mathbf{W}_1} = \ ? \qquad \frac{\partial L}{\partial \mathbf{b}_1} = \ ?$$

Deriving gradients for Feedforward NNs

$$\mathbf{z}_1 = \mathbf{W}_1\mathbf{x} + \mathbf{b}_1 \quad \mathbf{h}_1 = \tanh(\mathbf{z}_1)$$

$$\mathbf{z}_2 = \mathbf{W}_2\mathbf{h}_1 + \mathbf{b}_2 \quad \mathbf{h}_2 = \tanh(\mathbf{z}_2)$$

$$y = \sigma(\mathbf{w}^\intercal \mathbf{h_2} + b)$$

Forward Propagation ↓

$$\frac{\partial \mathcal{L}}{\partial b} = y - y^* \qquad \frac{\partial \mathcal{L}}{\partial \mathbf{w}} = (y - y^*)\mathbf{h}_2 \qquad \frac{\partial \mathcal{L}}{\partial \mathbf{h}_2} = (y - y^*)\mathbf{w}$$

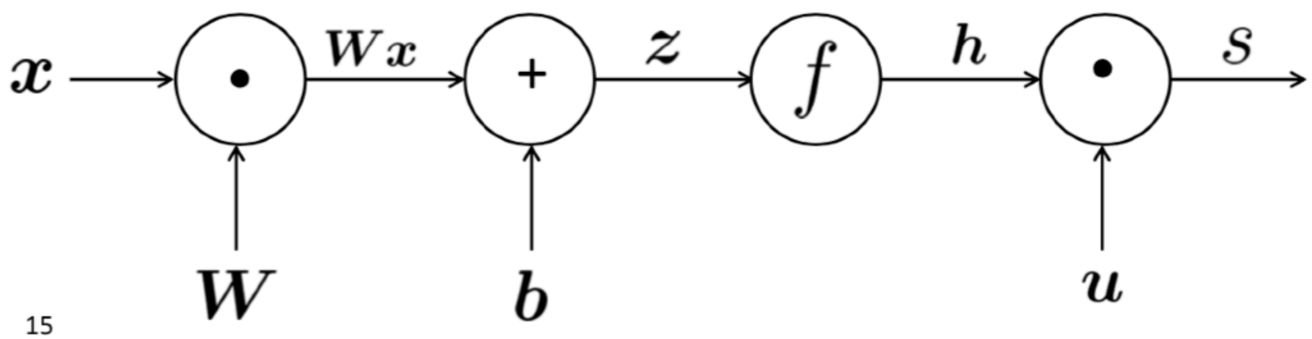
Backward Propagation ↓

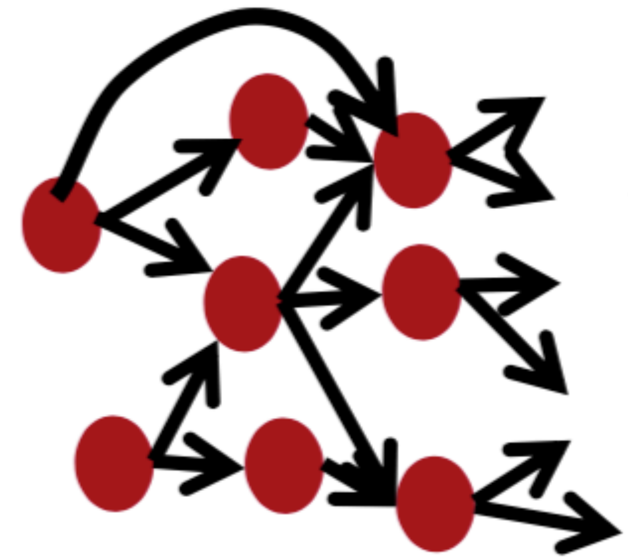
$$\frac{\partial L}{\partial \mathbf{z}_2} = (1 - \mathbf{h}_2^2) \circ \frac{\partial L}{\partial \mathbf{h}_2}$$

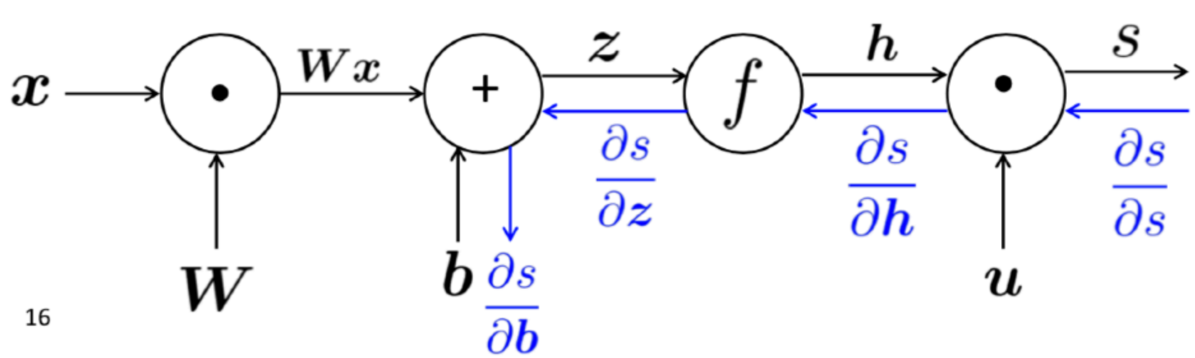
$$\frac{\partial L}{\partial \mathbf{W}_2} = \frac{\partial L}{\partial \mathbf{z}_2}\mathbf{h}_1^\intercal \qquad \frac{\partial L}{\partial \mathbf{b}_2} = \frac{\partial L}{\partial \mathbf{z}_2} \qquad \frac{\partial L}{\partial \mathbf{h}_1} = \mathbf{W}_2^\intercal \frac{\partial L}{\partial \mathbf{z}_2}$$

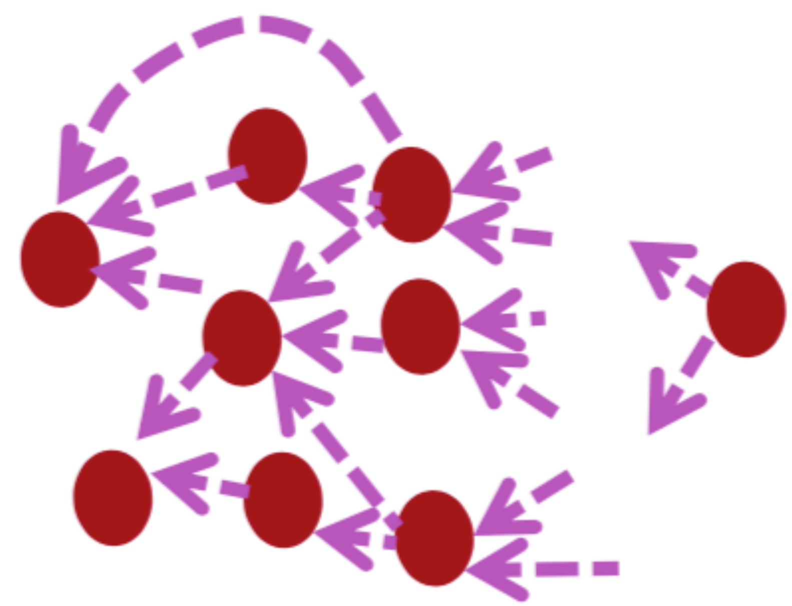
$$\frac{\partial L}{\partial \mathbf{z}_1} = (1 - \mathbf{h}_1^2) \circ \frac{\partial L}{\partial \mathbf{h}_1} \qquad \frac{\partial \mathcal{L}}{\partial \mathbf{W}_1} = \frac{\partial \mathcal{L}}{\partial \mathbf{z_1}}\mathbf{x}^\intercal \qquad \frac{\partial \mathcal{L}}{\partial \mathbf{b}_1} = \frac{\partial \mathcal{L}}{\partial \mathbf{z_1}}$$

Computational graphs







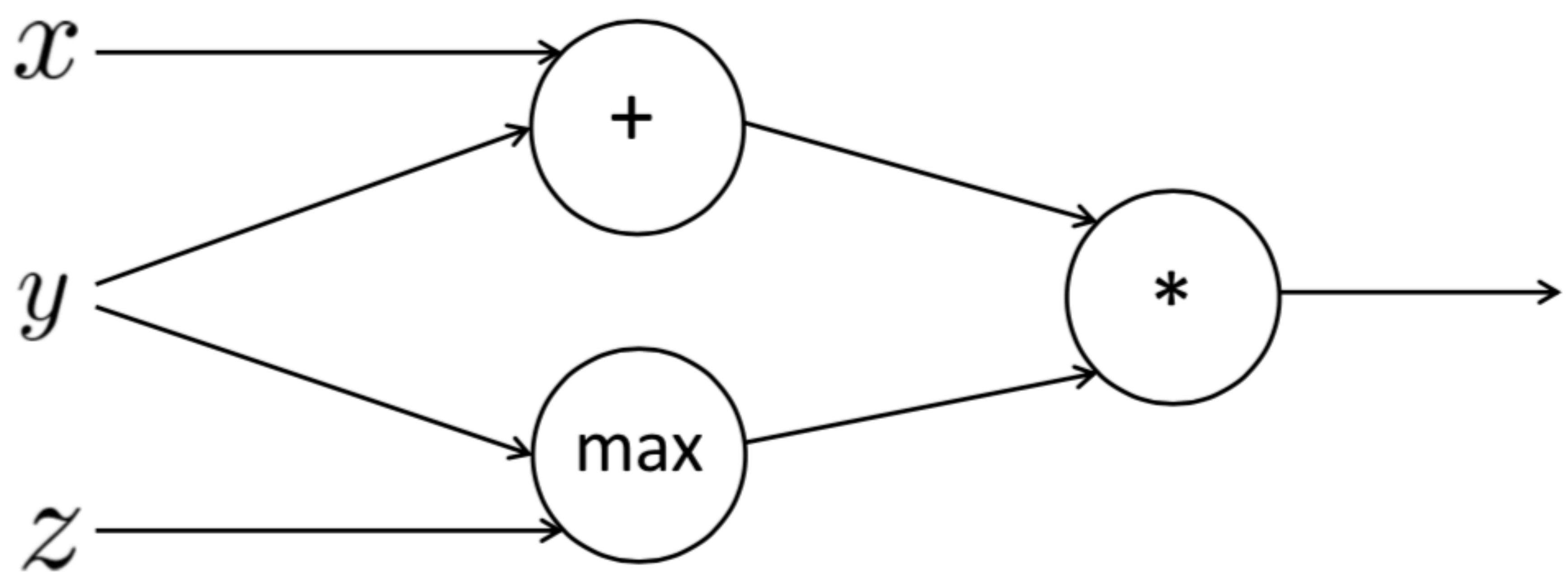


Credits: Chris Manning

An example

$$f(x, y, z) = (x + y)\max(y, z)$$
$$x = 1, y = 2, z = 0$$

$$a = x + y$$
$$b = \max(y, z)$$
$$f = ab$$



Compute the gradients yourself!

Backpropagation in general computational graph

- Forward propagation: visit nodes in topological sort order
  - Compute value of node given predecessors
- Backward propagagation:
  - Initialize output gradient as 1
  - Visit nodes in reverse order and compute gradient wrt each node using gradient wrt successors

$$\frac{\partial L}{\partial x} = \sum_{i=1}^{n} \frac{\partial \mathcal{L}}{\partial y_i} \frac{\partial y_i}{\partial x}$$

$$\{y_1, \ldots, y_n\} = \text{ successors of } x$$