CS 760: Machine Learning
Neural Networks

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Logistics

- **Announcements**:
  - Nothing new! HW 3 in progress. Ask proposal Q's!
- **Class roadmap:**

Thursday, Oct. 7	Neural Networks I
Tuesday, Oct. 12	Neural Networks II
Thursday, Oct. 14	Neural Networks III
Tuesday, Oct. 19	Neural Networks IV
Thursday, Oct. 21	Neural Networks V

All Neural Networks

Outline

- **Review & Perceptron Algorithm**
  - Definition, Training, Loss Equivalent, Mistake Bound
- **Neural Networks**
  - Introduction, Setup, Components, Activations
- **Training Neural Networks**
  - SGD, Computing Gradients, Backpropagation

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Review: Function Representations

- How much does it cost to "store" a function?
  - Last time in the context of PMFs
- Two representations for f

Lookup Table

x	f(x)
0	0
1	1
2	4
3	9
4	16
5	25

⋮

Expression

$$f(x) = x^2$$

Cost: if x is an integer between 0 and 99:

- Lookup table: **100** entries
- Expression: if quadratic, **3** coefficients ax^2+bx+c: store (1,0,0)

Review: Probability Functions

- Say our domain is $\{-1,+1\}^d$
- Function is $P(x_1, x_2, \ldots, x_d)$…
  - Suppose they're **independent** $P(x_1)P(x_2)\ldots P(x_n)$

Lookup Table

x	f(x)
-1,-1,-1,…,-1,-1	0.002
-1,-1,-1,…,-1,1	0.0032
-1,-1,-1,…,1,-1	0.12
-1,-1,-1….1,-1	0.00003
…	
1,1,1,…,1	0.328

Cost:
Lookup table: 2^d entries

Factorized Lookup Table

x_1	f(x)
-1	0.42
1	0.58

x_2	f(x)
-1	0.12
1	0.88

…

x_d	f(x)
-1	0.2
1	0.8

Cost: Lookup tables: **2d** entries

$0.002 = P(-1, -1, \ldots, -1) = 0.42 \times 0.12 \times \ldots \times 0.2$

Review: Probability Functions

- Say our domain is $\{-1,+1\}^d$
- Function is $P(x_1, x_2, \ldots, x_d)$…
  - If **independent** $P(x_1)P(x_2)\ldots P(x_n)$ and **identically distributed**

Lookup Table

x	f(x)
-1,-1,-1,…,-1,-1	0.002
-1,-1,-1,…,-1,1	0.0032
-1,-1,-1,…,1,-1	0.12
-1,-1,-1….1,-1	0.00003
…	
1,1,1,…,1	0.328

Cost:
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x_d	f(x)
-1	0.2
1	0.8

Cost: Lookup tables: **2d** entries

x_i	f(x)
-1	0.42
1	0.58

Cost: Lookup table: **2** entries

Review: Naïve Bayes Core Assumption

- Conditional **independence** of features:

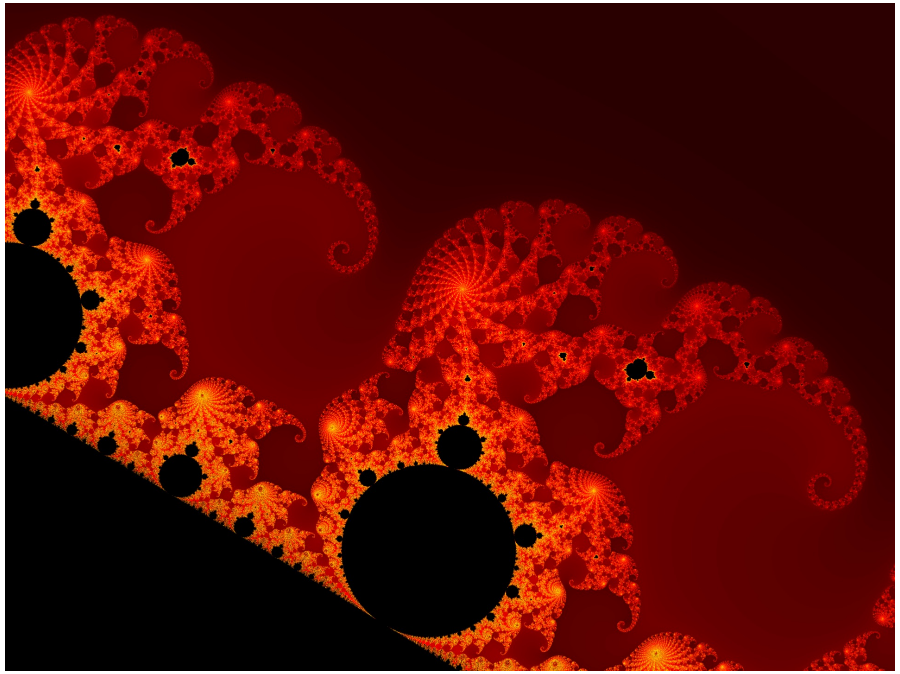
$$P(X_1, \ldots, X_K, Y) = P(X_1, \ldots, X_K | Y) P(Y)$$
$$= \left(\prod_{k=1}^{K} P(X_k | Y) \right) P(Y)$$

- What do we gain? With binary features, get 2 entries per feature
- So, number of probabilities

$$2^k \rightarrow 2k$$

Review: Function Representations

- More general: consider some object O
  - We did pairs (x,y) for function f
  - **Kolmogorov complexity** of O: shortest program that outputs O

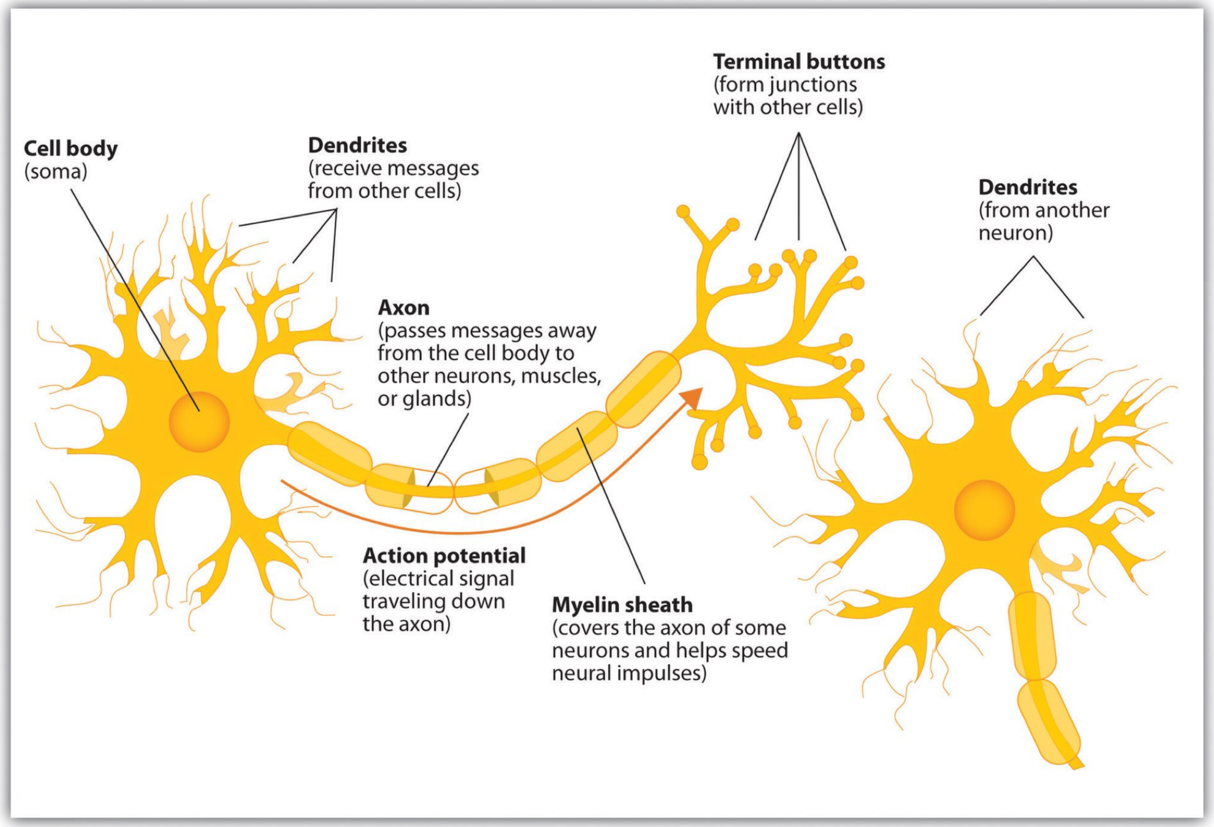


23 MB to store image (ie, bitmap)
A few bytes for program

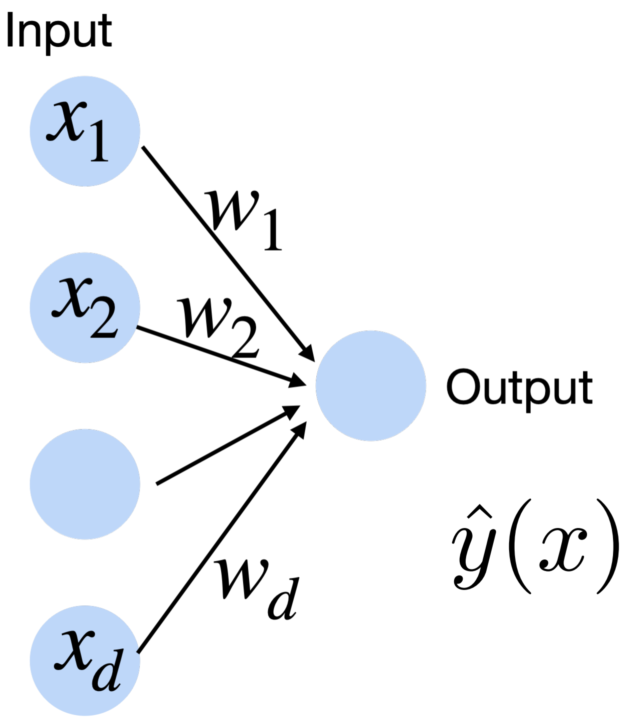
A. N. Kolmogorov

Neural networks: Origins

- *Artificial neural networks, connectionist models*
- Inspired by interconnected neurons in biological systems
  - Simple, homogenous processing units



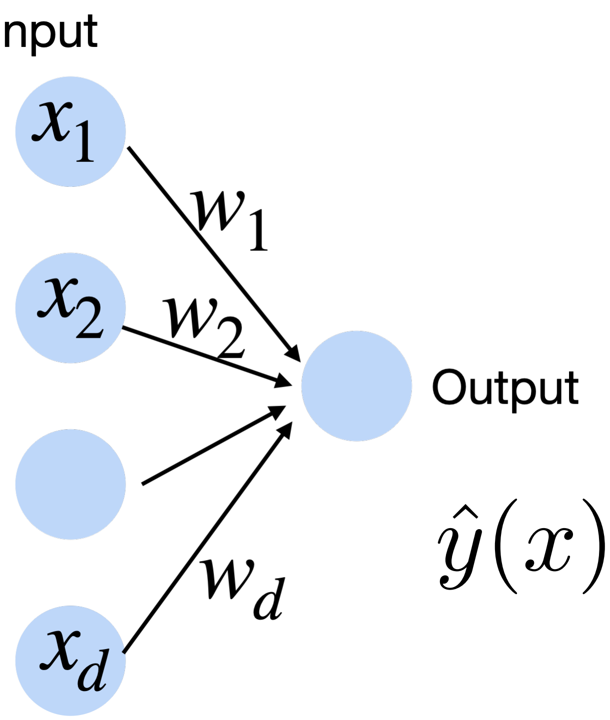
Perceptron: Simple Network



$$\hat{y}(x) = \begin{cases} 1 & w^T x \geq 0 \\ 0 & \text{otherwise} \end{cases}$$

[McCulloch & Pitts, **1943**; Rosenblatt, **1959**; Widrow & Hoff, **1960**]

Perceptron: Components



$$\hat{y}(x) = \begin{cases} 1 & w^T x \geq 0 \\ 0 & \text{otherwise} \end{cases}$$

$$f = w^T x \qquad \sigma(a) = \begin{cases} 1 & a \geq 0 \\ 0 & \text{otherwise} \end{cases} \qquad \hat{y}(x) = \sigma(w^T x)$$

Activation Function

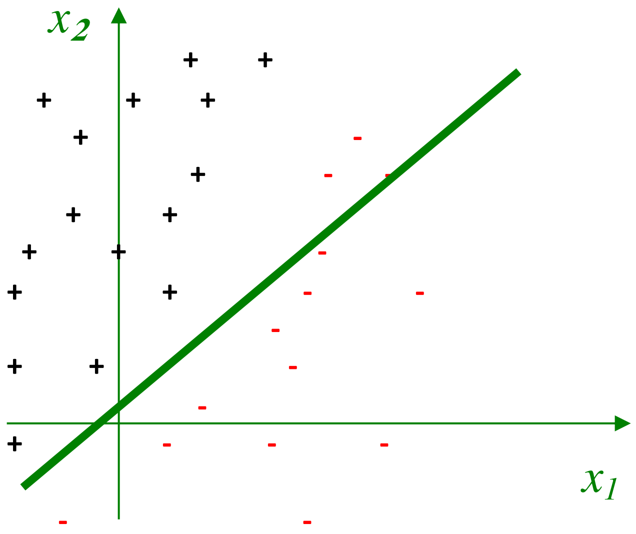
[McCulloch & Pitts, **1943**; Rosenblatt, **1959**; Widrow & Hoff, **1960**]

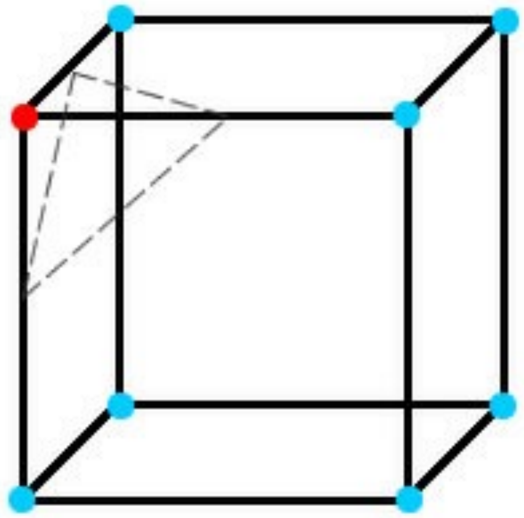
Perceptron: Representational Power

- Perceptrons can represent only *linearly separable* concepts

$$\hat{y}(x) = \begin{cases} 1 & w^T x \geq 0 \\ 0 & \text{otherwise} \end{cases}$$

- Decision boundary given by:

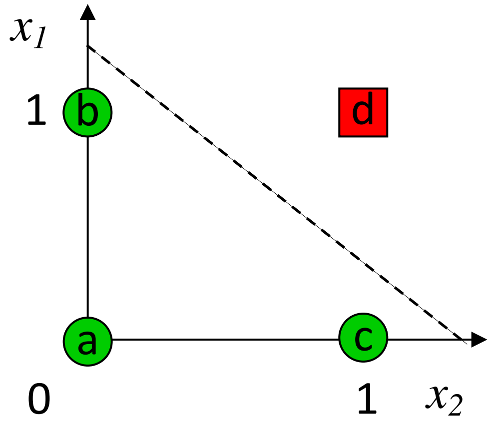




Which Functions are **Linearly Separable?**

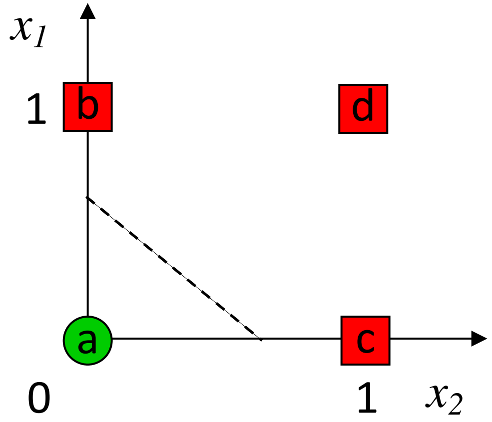
AND

	x_1	x_2	y
a	0	0	0
b	0	1	0
c	1	0	0
d	1	1	1



OR

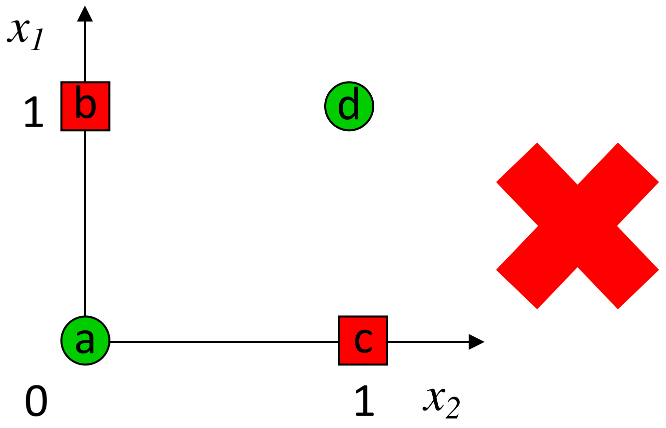
	x_1	x_2	y
a	0	0	0
b	0	1	1
c	1	0	1
d	1	1	1



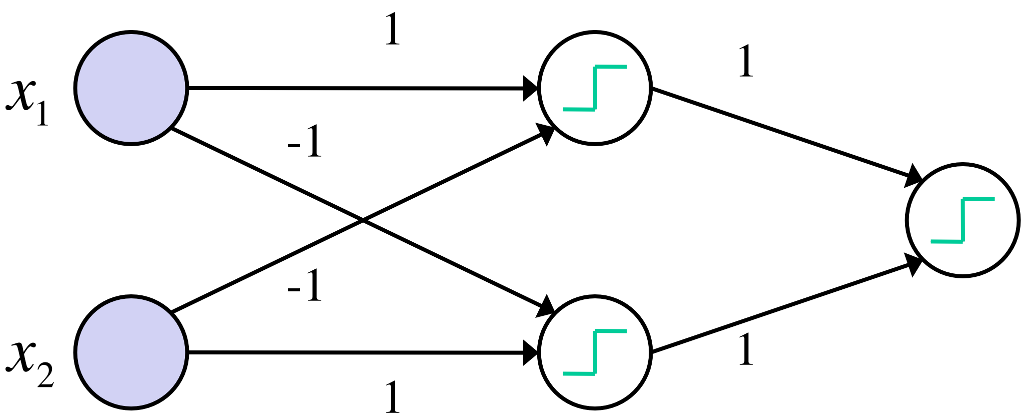
Which Functions are **Linearly Separable?**

<u>XOR</u>

	x_1	x_2	y
a	0	0	0
b	0	1	1
c	1	0	1
d	1	1	0



A multilayer perceptron can represent XOR!



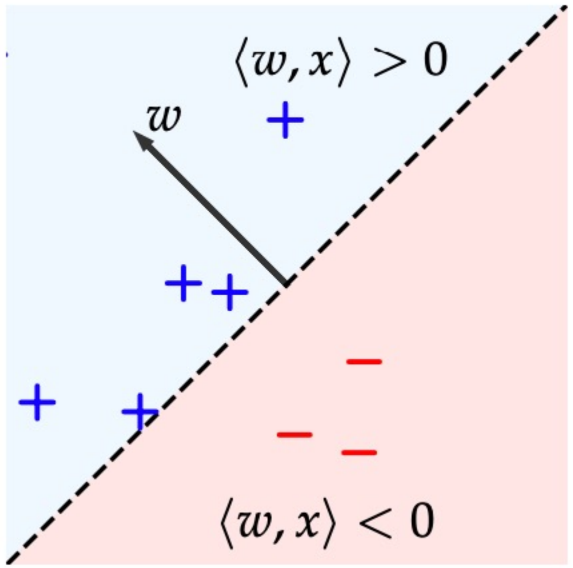
assume $w_0 = 0$ for all nodes

Perceptron: Training

- When are we correct?

$$y^{(i)} w^T x^{(i)} > 0$$

  - I.e., **signs** of prediction and label match



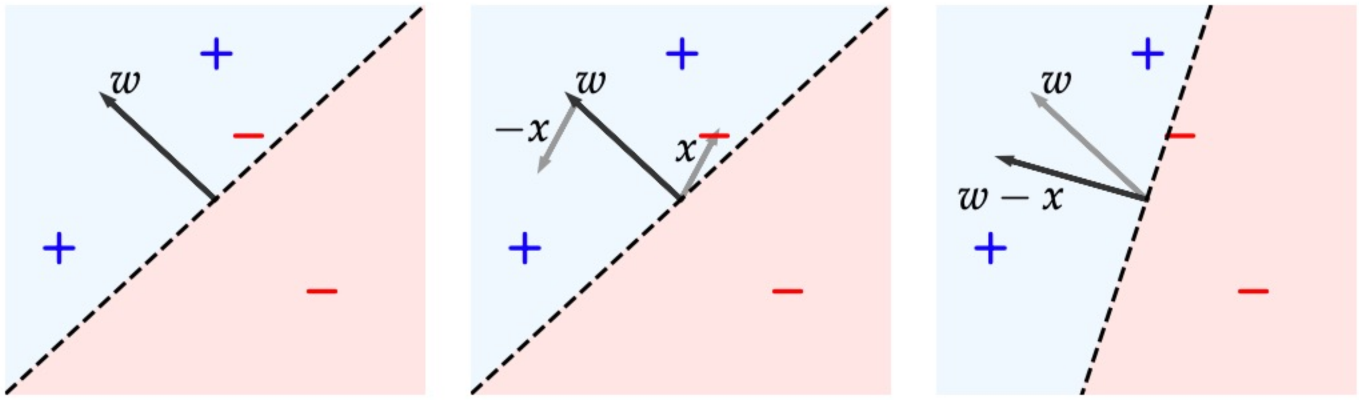
- In training, could ask for "margin": insist

$$y^{(i)} w^T x^{(i)} \geq c$$

  - More than we needed

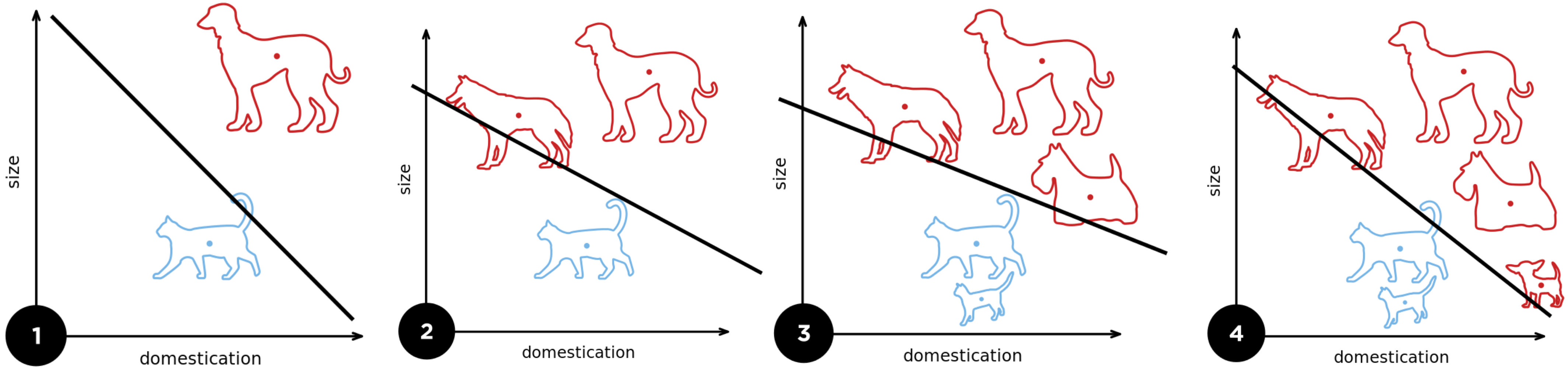
Perceptron: Training

- **Algorithm**:
  - Initialize at $w_0 = [0, \ldots, 0]^T$
  - At step t = 0,…
  - Select random index i,
  - If $y^{(i)} w^T x^{(i)} < 1$ then do $w_{t+1} = w_t + y^{(i)} x^{(i)}$
  - Else, $w_{t+1} = w_t$



Perceptron: Training

- **Algorithm training** example:



Perceptron: Training Comparison

- We're used to minimizing some loss function…
- Taking one example at a time…
    - Stochastic Optimization (like SGD!)

- **Step**: $w_{t+1} = w_t + y^{(i)} x^{(i)}$
    - What update to our prediction?

$$w_{t+1}^T x^{(i)} = w_t^T x^{(i)} + y^{(i)} \|x^{(i)}\|^2$$

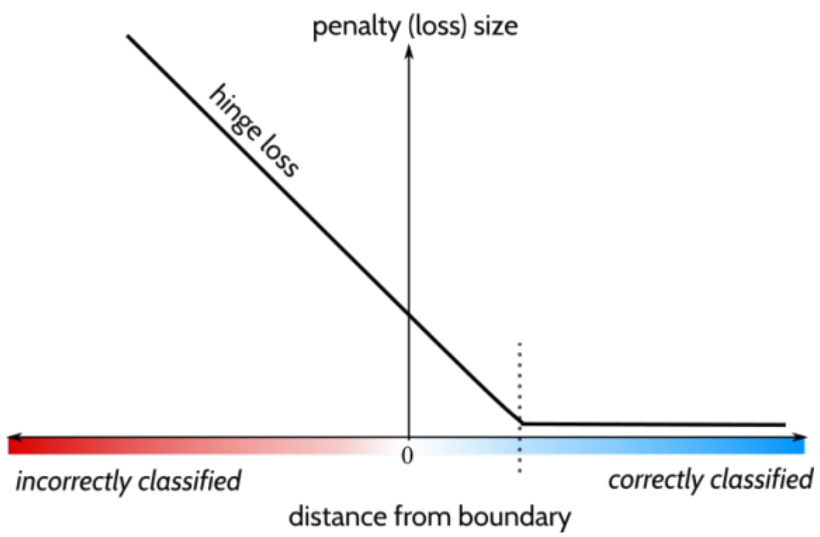
Perceptron: Training Comparison

- So: looks like **SGD** with a loss function L

SGD $$w_{t+1} = w_t - \alpha \nabla L(f(x^{(i)}, y^{(i)})$$

Perceptron $$w_{t+1} = w_t + y^{(i)} x^{(i)}$$

  - Need: gradient is 0 when we're right, $y^{(i)}x^{(i)}$ on mistakes



Hinge loss!

Perceptron: Analysis

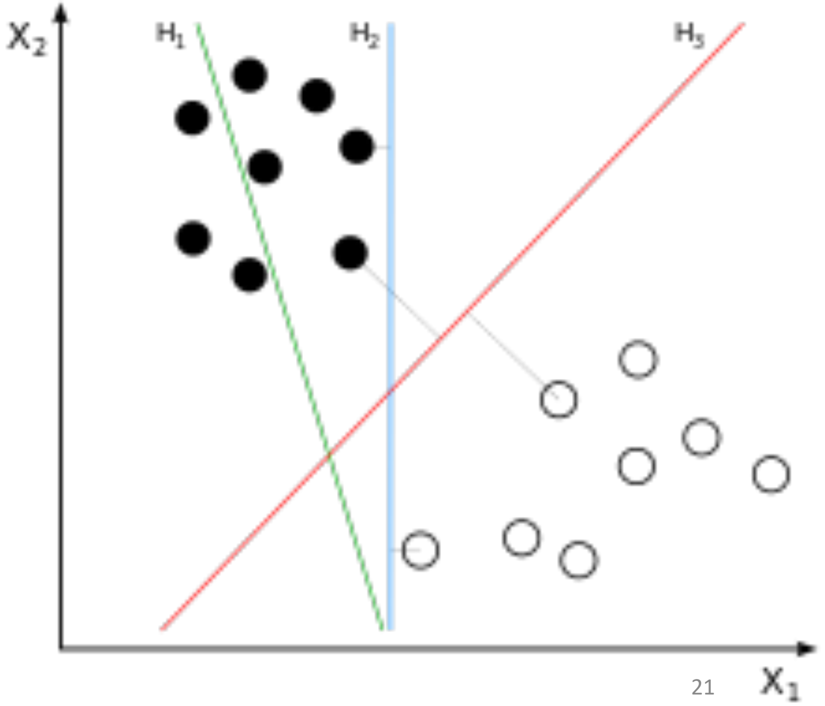
- Two aspects to analysis: **fitting training data** + **generalization**
- **Mistake bound**:
  - Hyperplane $$H_w = x : w^T x = 0$$
  - Margin

$$\gamma(S, w) = \min_{1 \leq i \leq n} \text{dist}(x_i, H_w)$$

$$\downarrow$$

$$|x^T w| / \|w\|$$

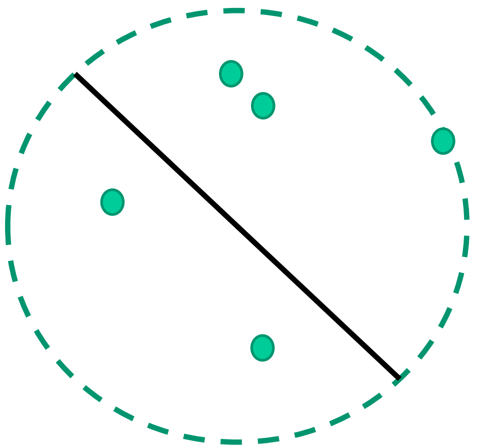
$$\gamma(S) = \max_{\|w\|=1} \gamma(S, w)$$



Perceptron: Mistake Bound

- Need some information about our data:

- **"Diameter"**: $D(S) = \max_{(x,y)\in S} \|x\|$



- **Mistake Bound Result**:
    - The total # of mistakes on a linearly separable set S is at most

$$(2 + D(S)^2)\gamma(S)^{-2}$$

Perceptron: Mistake Bound Interpretation

- **Mistake Bound Result**:
  - The total # of mistakes on a linearly separable set S is at most

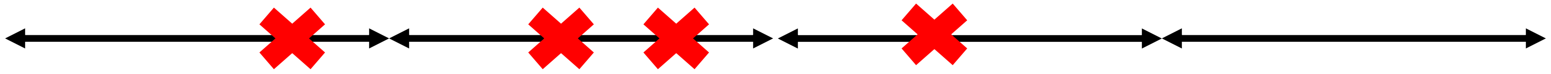
$$(2 + D(S)^2)\gamma(S)^{-2}$$

Diameter: Controls our biggest step.

Margin: Smaller means harder to find separator

- Scaling?

- **Implications**?
  - Run over dataset D repeatedly. # mistakes doesn't change
    - Eventually get perfect separation on a copy of D



Mistake Bound: Proof 1

- Let's prove the result.
  - Intuitive idea we exploit: **norm of weight vector** <-> # mistakes
- Start with changes in weight norm

$$\|w_{t+1}\|^2 = \|w_t + y^{(i_t)}x^{(i_t)}\|^2$$

If mistake

$$\|w_{t+1}\|^2 = \|w_t\|^2 + 2(y^{(i_t)})^T x^{(i_t)} + \|x^{(i_t)}\|^2$$

Margin

Diameter

$$\|w_{t+1}\|^2 \leq \|w_t\|^2 + 2 + D(S)^2$$

Mistake Bound: Proof 2

- This is true for each mistake

$$\|w_{t+1}\|^2 \leq \|w_t\|^2 + 2 + D(S)^2$$

- Let m_t be # mistakes by t step. Start at w_0 (norm 0). By w_t

$$\|w_t\| \leq \sqrt{m_t(2 + D(S)^2}$$

  - This was also a telescoping argument; recall proof of GD convergence

Mistake Bound: Proof 3

- Now we'll also lower bound norm
- Let w be a hyperplane that **separates, unit norm.** $\|w\| = 1$

$$w^T(w_{t+1} - w_t) = w^T(\underbrace{y^{(i_t)}x^{(i_t)}}_{\text{mistake}}) = \frac{|w^T x^{(i_t)}|}{\|w\|}$$

w classifies correctly ← $|w^T x^{(i_t)}|$

Norm 1 ← $\|w\|$

- But this is the margin for $x^{(it)}$, so:

$$\frac{|w^T x^{(i_t)}|}{\|w\|} \geq \gamma(S, w)$$

Mistake Bound: Proof 4

- So:

$$w^T(w_{t+1} - w_t) \geq \gamma(S, w)$$

- Let's look at our best solution: w_*, the maximum margin w
- From Cauchy-Schwartz $\|w_t\|\|w_*\| \geq w_*^T w_t$

- Let's set up a telescoping sum:

$$\|w_t\| \geq w_*^T w_t = \sum_{k=1}^{t} w_*^T (w_k - w_{k-1})$$

Mistake Bound: Proof 5

- Have: $w^T(w_{t+1} - w_t) \geq \gamma(S, w)$

$$||w_t|| \geq w_*^T w_t = \sum_{k=1}^{t} w_*^T (w_k - w_{k-1})$$

- Combine:

$$||w_t|| \geq w_*^T w_t = \sum_{k=1}^{t} w_*^T (w_k - w_{k-1}) \geq m_t \gamma(S)$$

0 for no mistake, Purple for mistake

- Note: $\gamma(S, w_*) = \gamma(S)$

Mistake Bound: Proof 6

- So, $m_t \gamma(S) \leq \|w_t\|$ $\|w_t\| \leq \sqrt{m_t(2 + D(S)^2}$

- I.e.,

$$m_t \gamma(S) \leq \sqrt{m_t(2 + D(S)^2)}$$

- Easy algebra gets us to $$m_t \leq \frac{2 + D(S)^2}{\gamma(S)^2}$$ ✔

Break & Quiz

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Multilayer Neural Network

- Input: two features from spectral analysis of a spoken sound
- Output: vowel sound occurring in the context “h__d”

output units

hidden units

input units

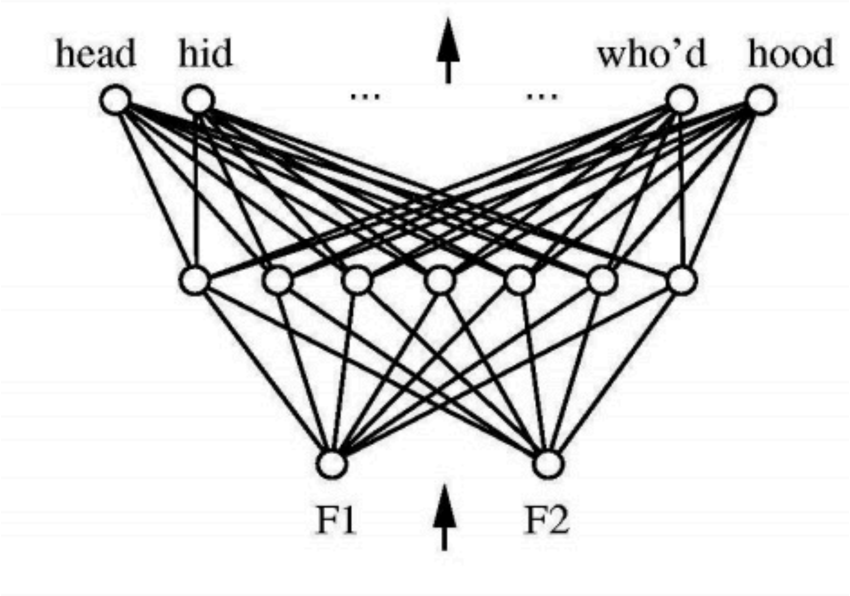


figure from Huang & Lippmann, *NIPS* 1988

Neural Network **Decision Regions**

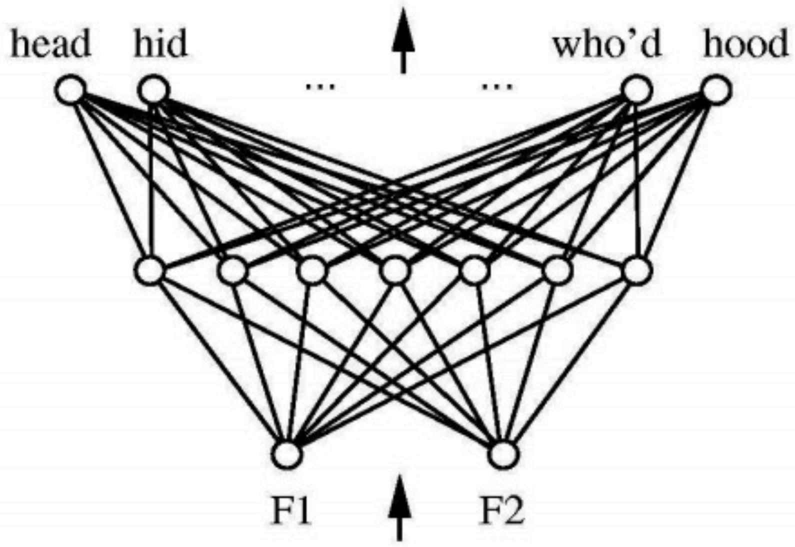
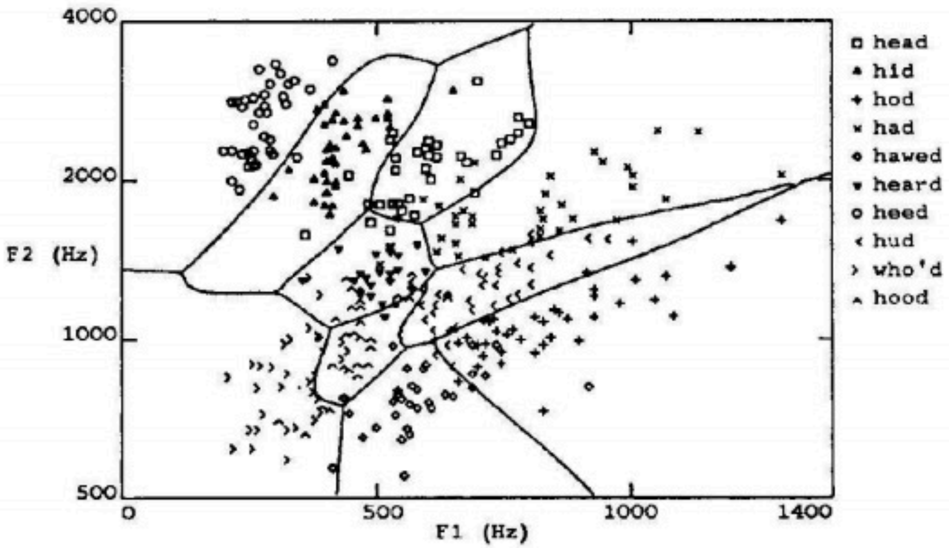
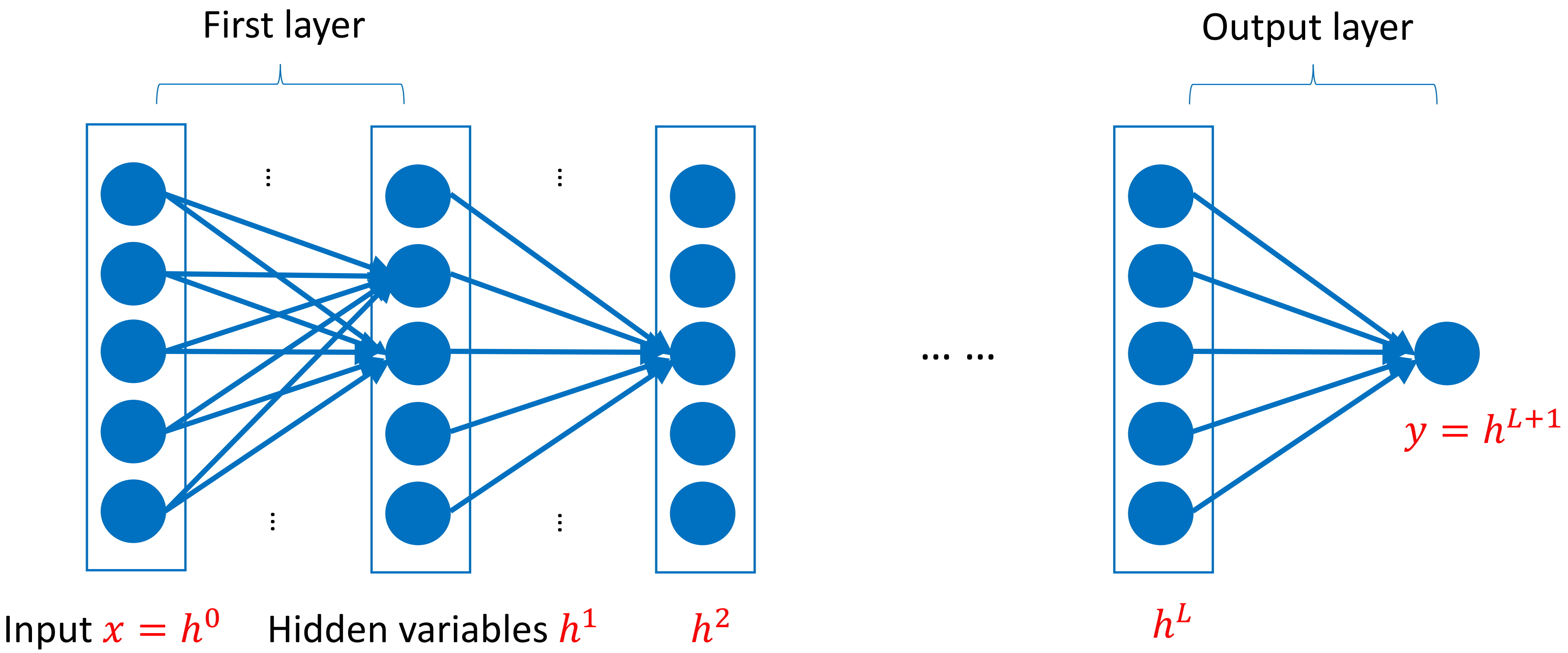


Figure from Huang & Lippmann, *NIPS* 1988



Neural Network Components

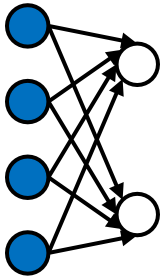
An $(L+1)$-layer network



Feature Encoding for NNs

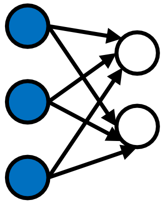
- Nominal features usually a one hot encoding

$$A = \begin{bmatrix}1\\0\\0\\0\end{bmatrix} \quad C = \begin{bmatrix}0\\1\\0\\0\end{bmatrix} \quad G = \begin{bmatrix}0\\0\\1\\0\end{bmatrix} \quad T = \begin{bmatrix}0\\0\\0\\1\end{bmatrix}$$



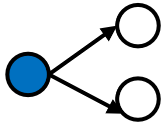
- Ordinal features: use a *thermometer* encoding

$$\text{small} = \begin{bmatrix}1\\0\\0\end{bmatrix} \quad \text{medium} = \begin{bmatrix}1\\1\\0\end{bmatrix} \quad \text{large} = \begin{bmatrix}1\\1\\1\end{bmatrix}$$



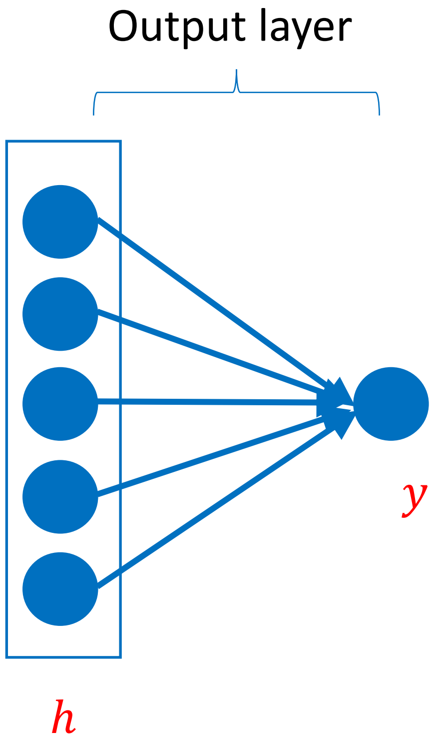
- Real-valued features use individual input units (may want to scale/normalize them first though)

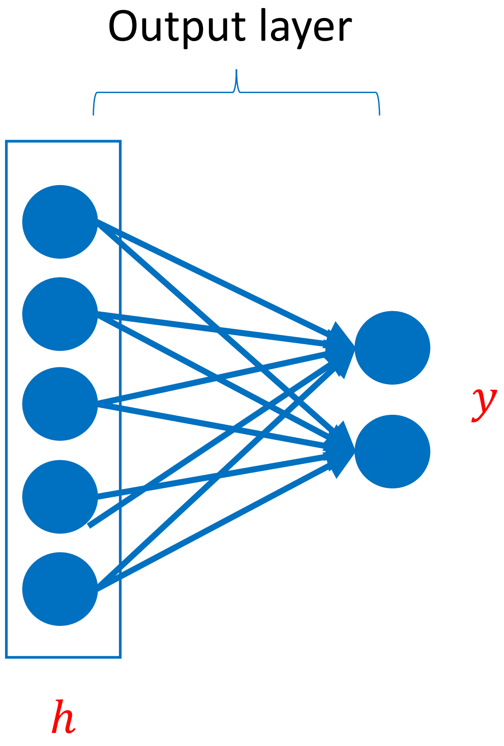
$$\text{precipitation} = \begin{bmatrix}0.68\end{bmatrix}$$



Output Layer: Examples

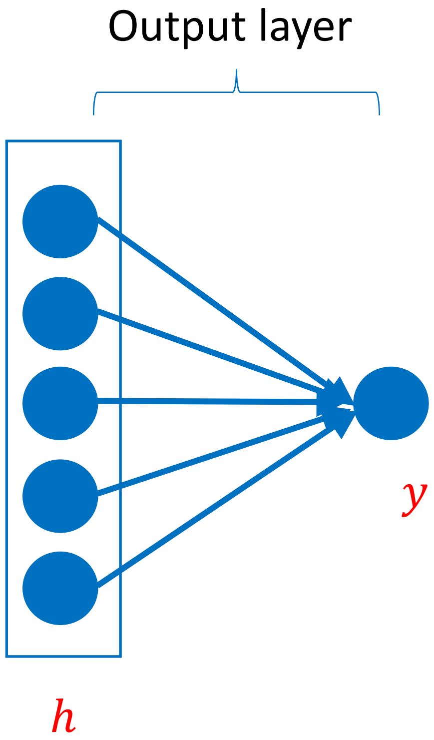
- Regression: $y = w^T h + b$
  - Linear units: no nonlinearity
- Multi-dimensional regression: $y = W^T h + b$
  - Linear units: no nonlinearity

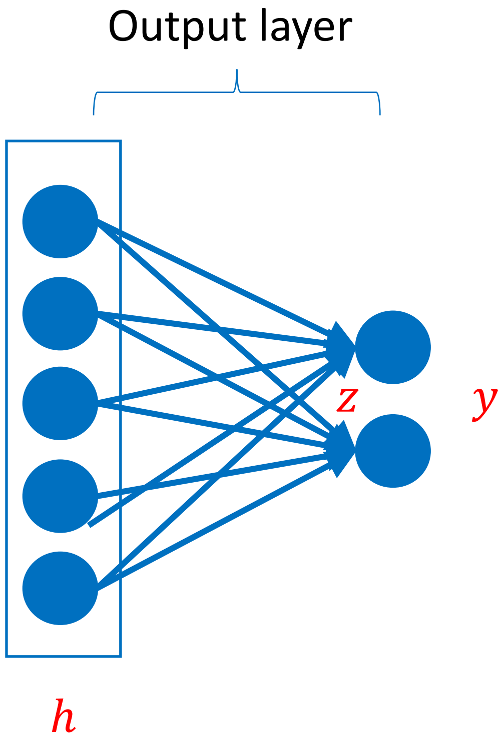




Output Layer: Examples

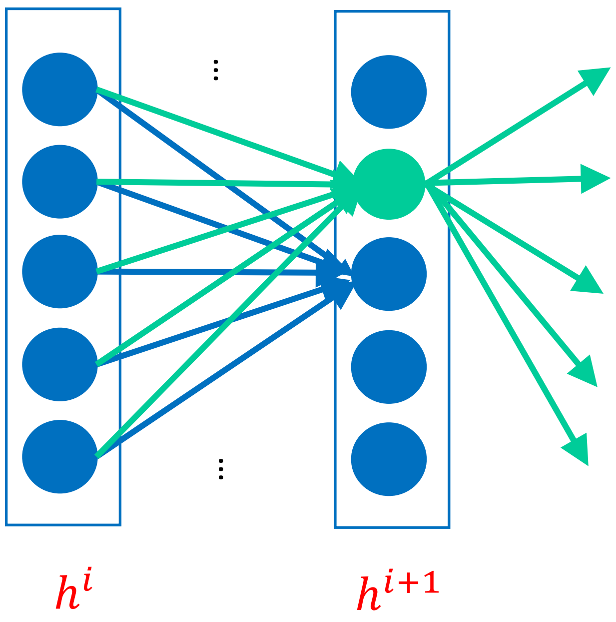
- Binary classification: $y = \sigma(w^T h + b)$
  - Corresponds to using logistic regression on h
- Multiclass classification:
  - $y = \text{softmax}(z)$ where $z = W^T h + b$





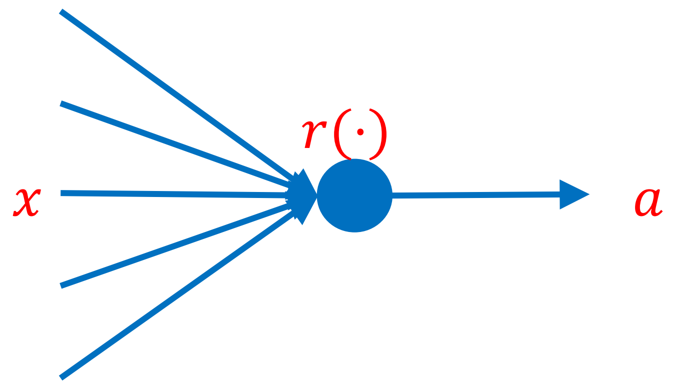
Hidden Layers

- Neuron takes weighted linear combination of the previous representation layer
  - Outputs one value for the next layer



Hidden Layers

- Outputs $a = r(w^T x + b)$

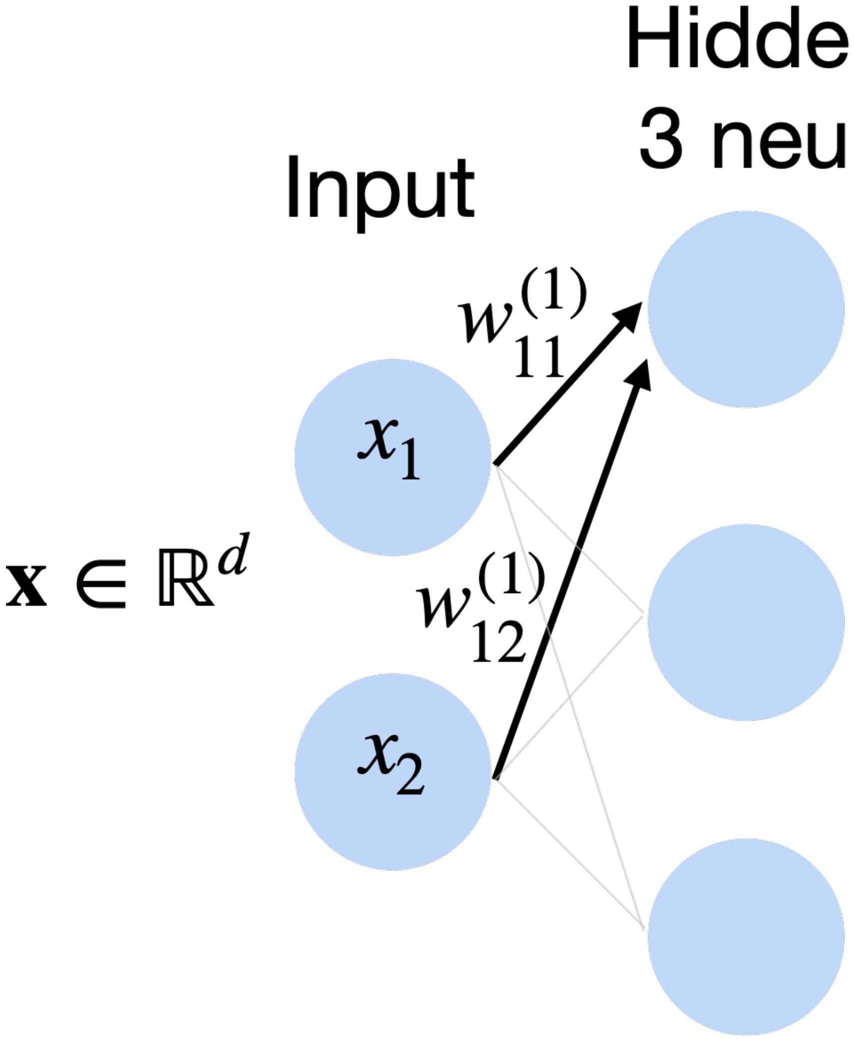


- Typical activation function r
  - Threshold $\mathrm{t}(z) = \mathbb{I}[z \geq 0]$
  - Sigmoid $\sigma(z) = 1/(1 + \exp(-z))$
  - Tanh $\tanh(z) = 2\sigma(2z) - 1$

- Why not **linear activation** functions?
  - Model would be linear.

MLPs: Multilayer Perceptron

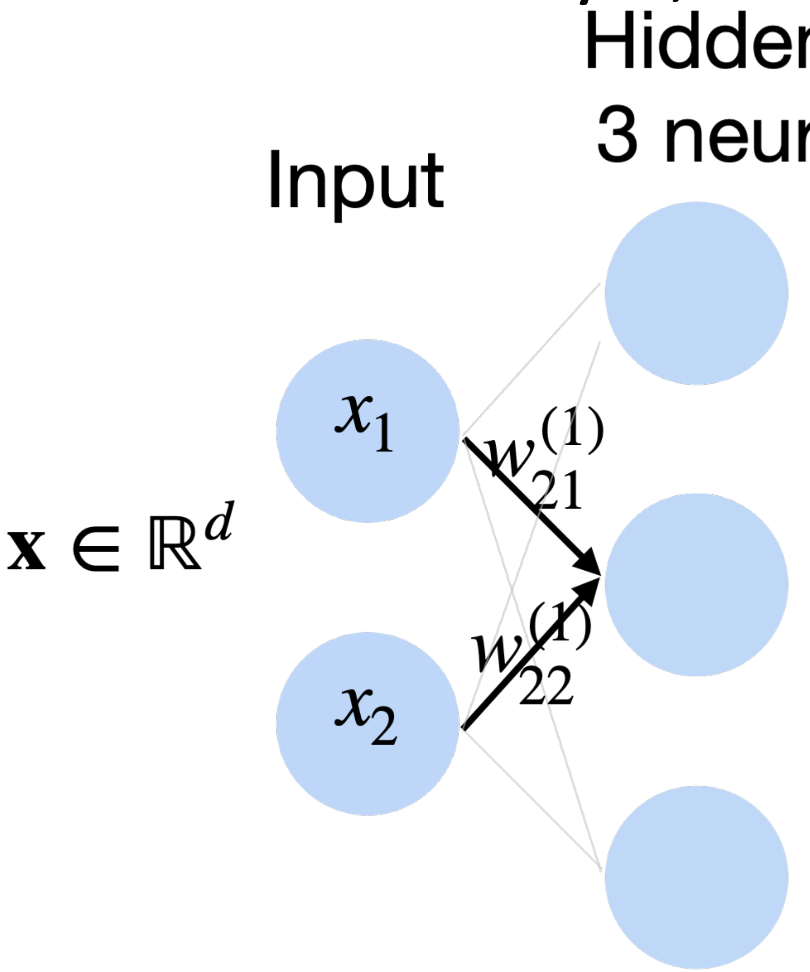
- **Ex**: 1 hidden layer, 1 output layer: depth 2



$$h_1 = \sigma(\sum_{i=1}^{d} x_i w_{1i}^{(1)} + b_1)$$

MLPs: Multilayer Perceptron

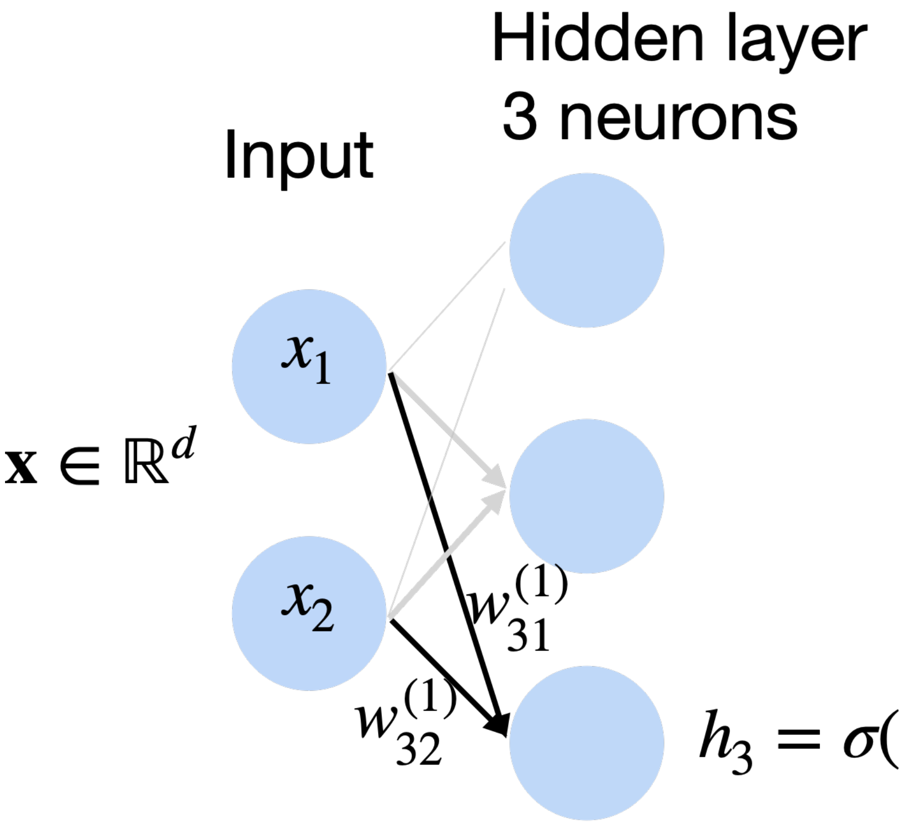
- **Ex**: 1 hidden layer, 1 output layer: depth 2



$$h_2 = \sigma\left(\sum_{i=1}^{d} x_i w_{2i}^{(1)} + b_2\right)$$

MLPs: Multilayer Perceptron

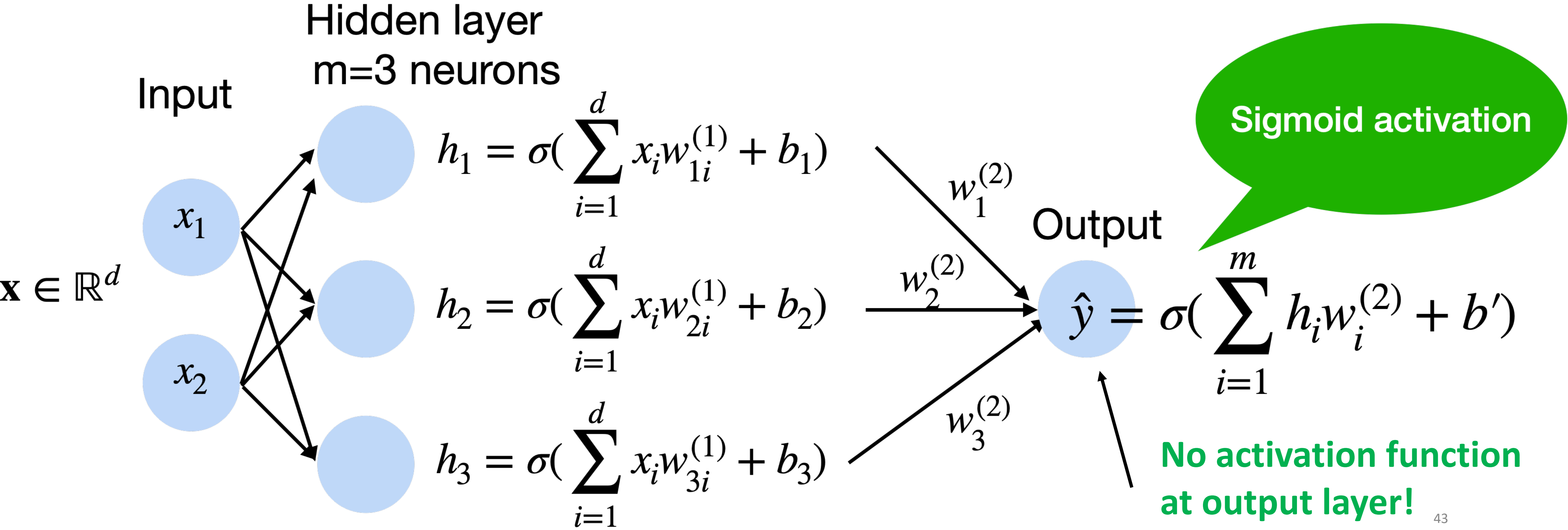
- **Ex**: 1 hidden layer, 1 output layer: depth 2



$$h_3 = \sigma(\sum_{i=1}^{d} x_i w_{3i}^{(1)} + b_3)$$

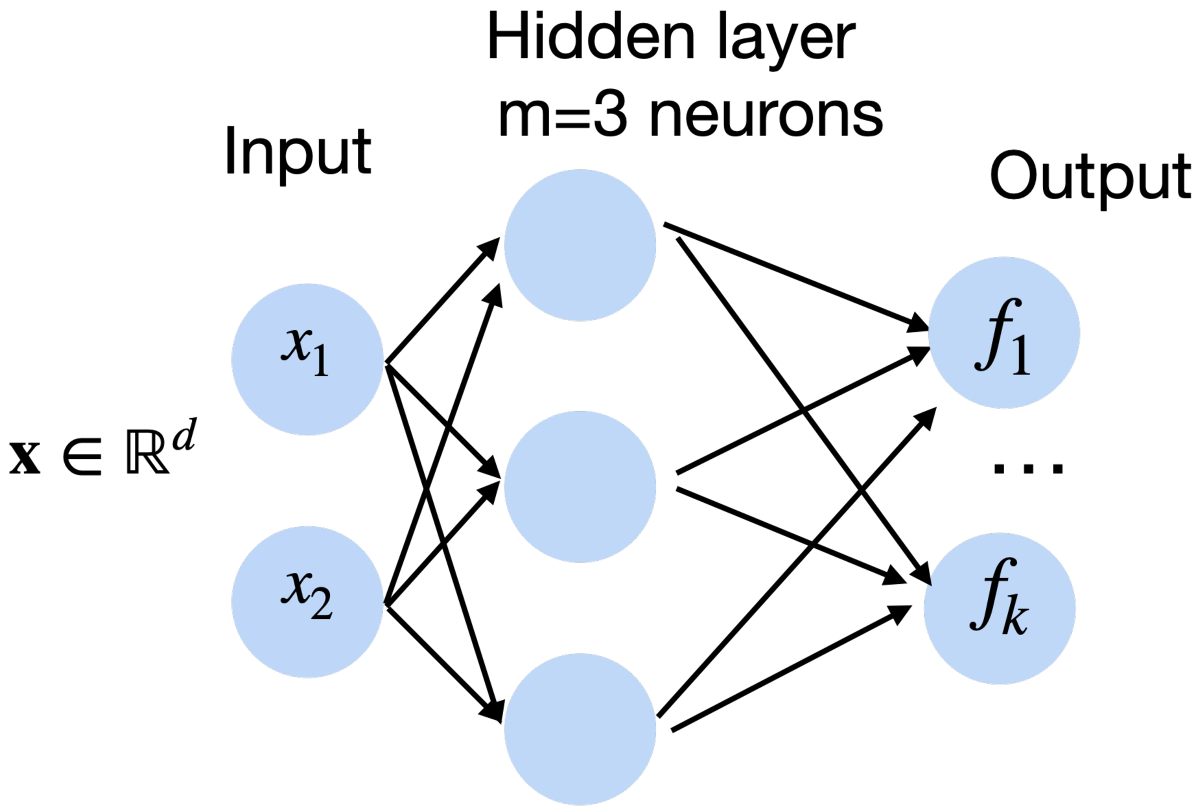
MLPs: Multilayer Perceptron

- **Ex**: 1 hidden layer, 1 output layer: depth 2



Multiclass Classification Output

- Create k output units
- Use softmax (just like logistic regression)

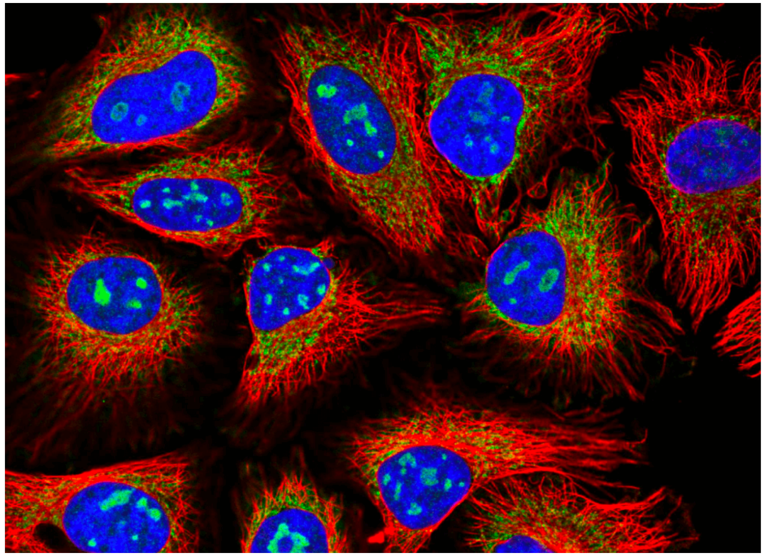


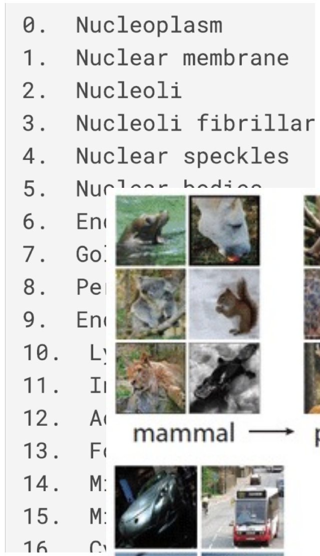
$$p(y \mid \mathbf{x}) = \text{softmax}(f)$$

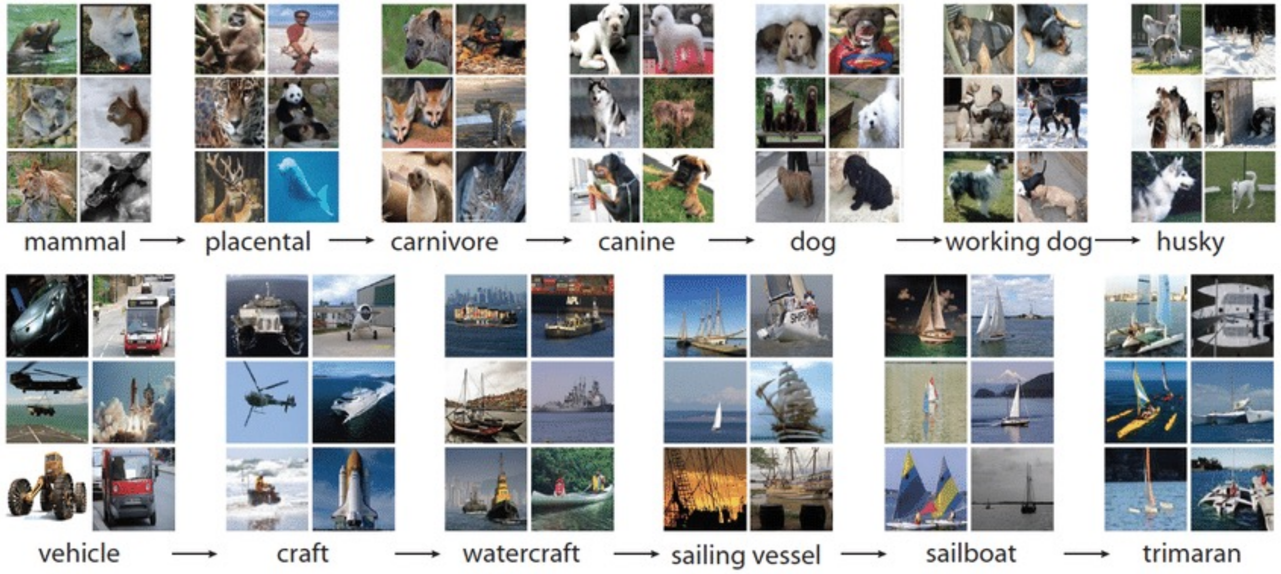
$$= \frac{\exp f_y(x)}{\sum_i^k \exp f_i(x)}$$

Multiclass Classification Examples

- Protein classification (Kaggle challenge)
- ImageNet







Break & Quiz

Outline

- **Review & Perceptron Algorithm**
  - Definition, Training, Loss Equivalent, Mistake Bound
- **Neural Networks**
  - Introduction, Setup, Components, Activations
- **Training Neural Networks**
  - SGD, Computing Gradients, Backpropagation

Training Neural Networks

- Training the usual way. Pick a loss and optimize
- **Example**: 2 scalar weights

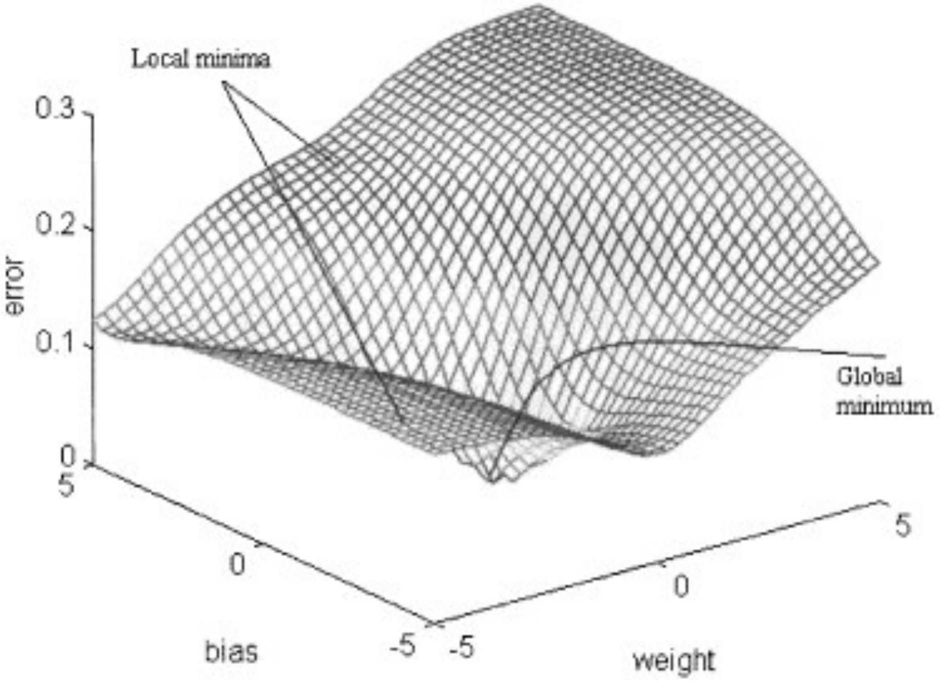
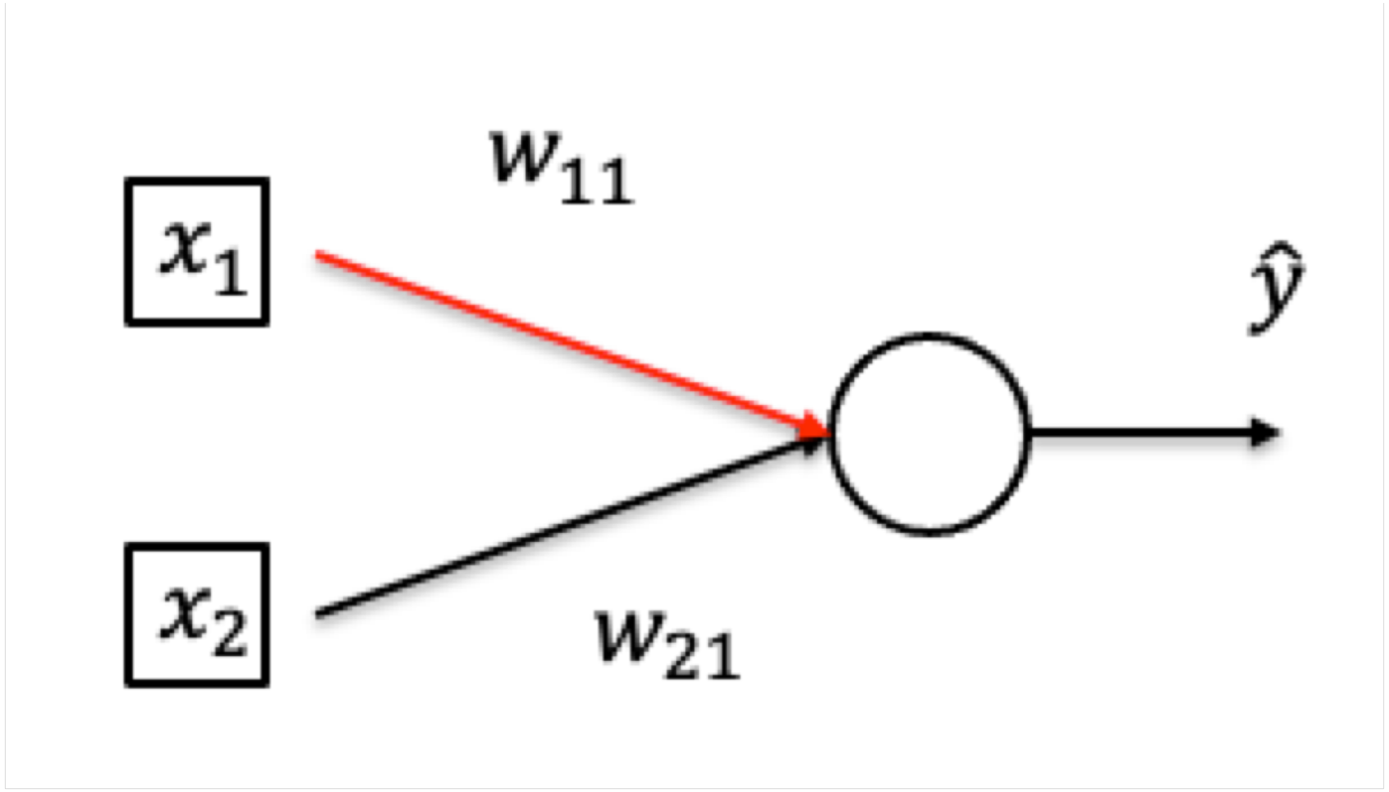


figure from Cho & Chow, *Neurocomputing* 1999

Training Neural Networks

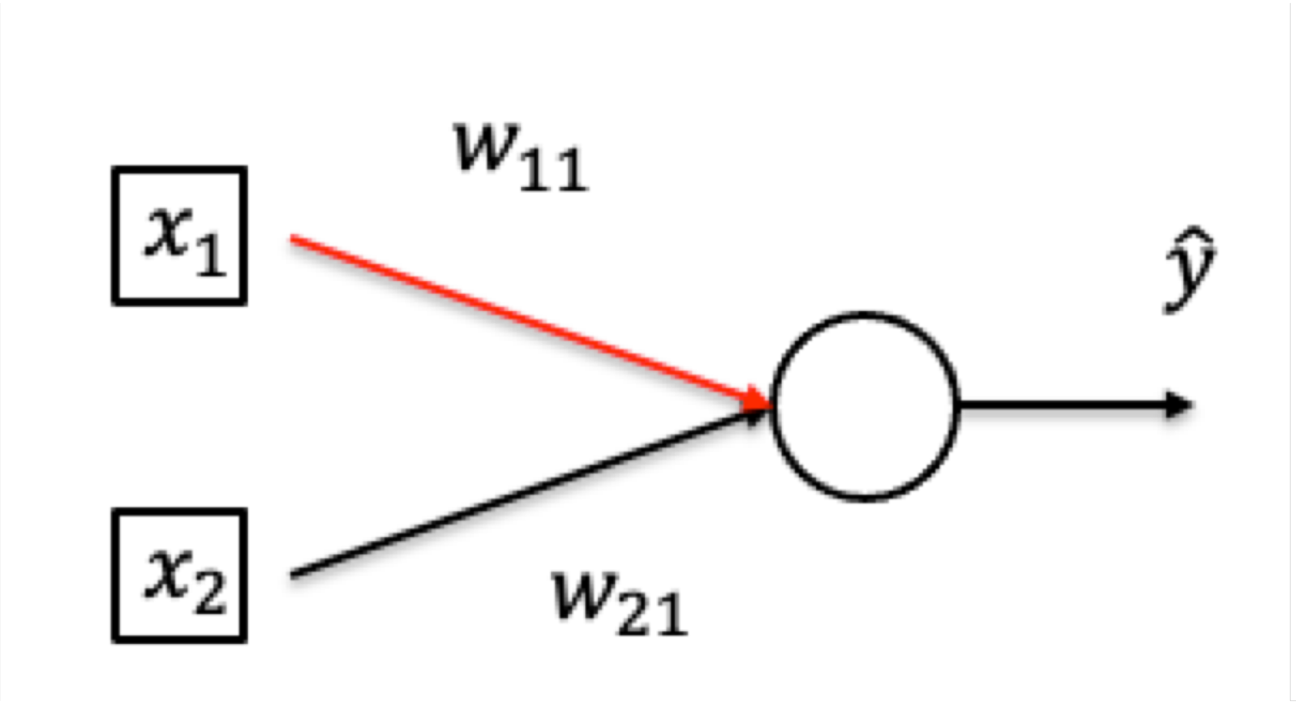
- Algorithm:
  - Get $$D = \{(x^{(1)}, y^{(1)}), \ldots, (x^{(n)}, y^{(n)})\}$$
  - Initialize weights
  - Until stopping criteria met,
    - For each training point $(x^{(i)}, y^{(i)})$
    - Compute: $f_{\text{network}}(x^{(d)})$ ⟵ **Forward Pass**
    - Compute gradient: $\nabla L^{(i)}(w) = \left[\frac{\partial L^{(d)}}{\partial w_0}, \frac{\partial L^{(d)}}{\partial w_1}, \ldots, \frac{\partial L^{(d)}}{\partial w_m}\right]^T$ ⟵ **Backward Pass**
    - Update weights: $$w \leftarrow w - \alpha \nabla L^{(i)}(w)$$

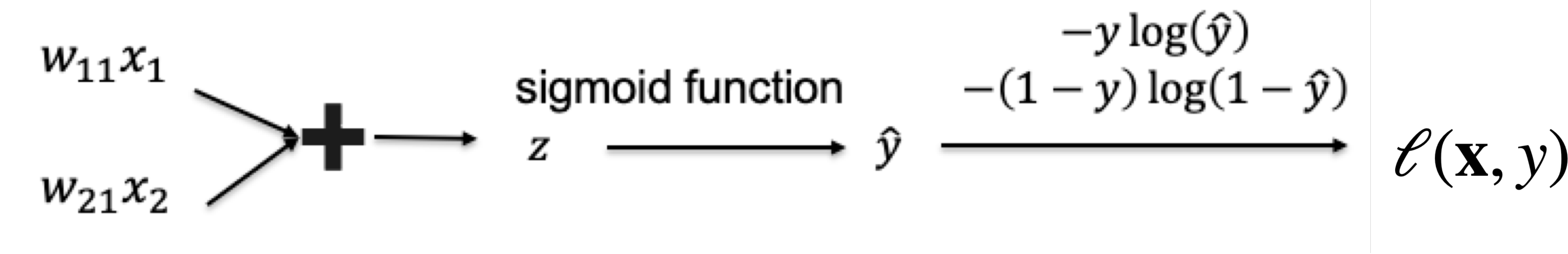
Computing Gradients



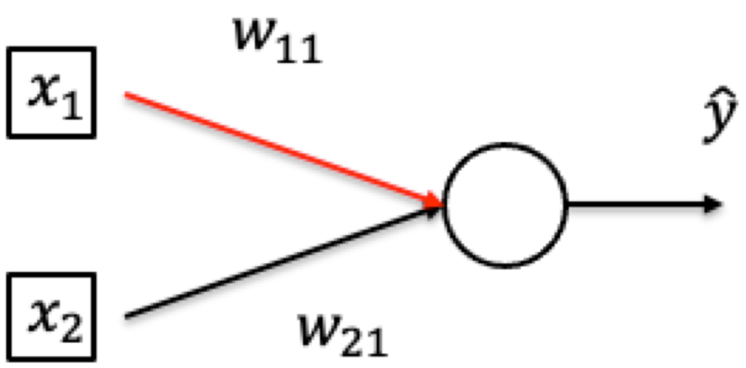
- Want to compute $\dfrac{\partial \ell(\mathbf{x}, y)}{\partial w_{11}}$

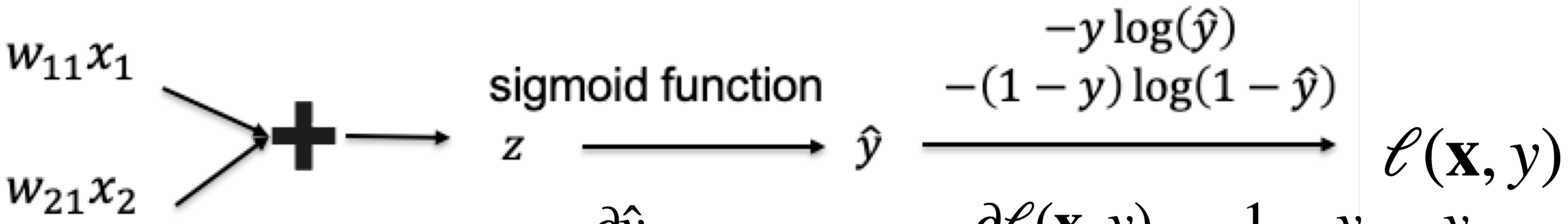
Computing Gradients





Computing Gradients





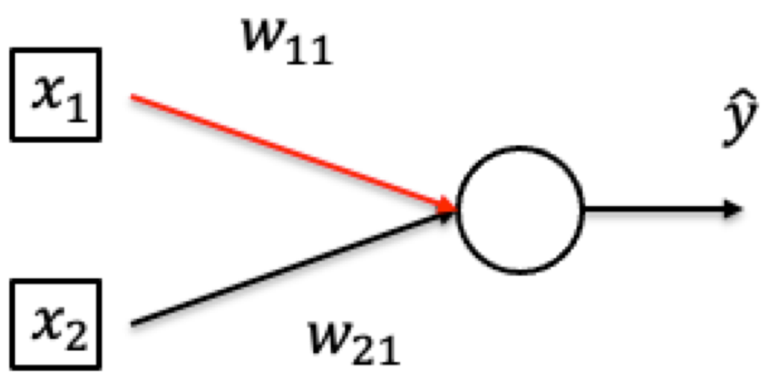
$$\frac{\partial \hat{y}}{\partial z} = \sigma'(z)$$

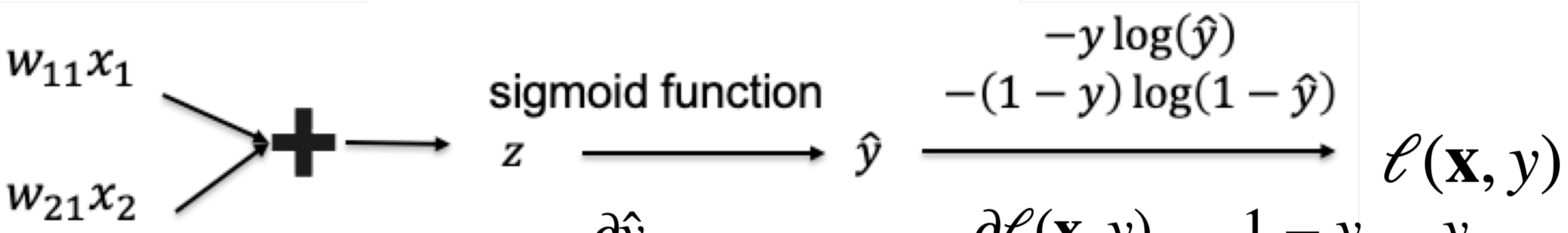
$$\frac{\partial \ell(\mathbf{x}, y)}{\partial \hat{y}} = \frac{1-y}{1-\hat{y}} - \frac{y}{\hat{y}}$$

- By chain rule:

$$\frac{\partial l}{\partial w_{11}} = \frac{\partial l}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial z} \frac{\partial z}{\partial w_{11}}$$

Computing Gradients

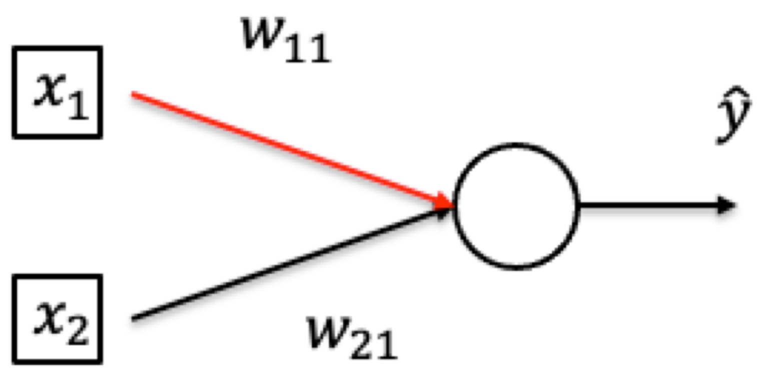


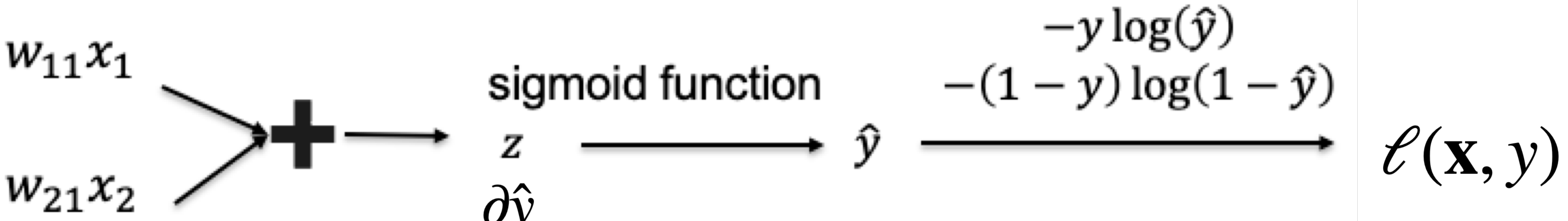


$$\frac{\partial \hat{y}}{\partial z} = \sigma'(z) \qquad \frac{\partial \ell(\mathbf{x}, y)}{\partial \hat{y}} = \frac{1-y}{1-\hat{y}} - \frac{y}{\hat{y}}$$

- By chain rule: $$\frac{\partial l}{\partial w_{11}} = \frac{\partial l}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial z} x_1$$

Computing Gradients



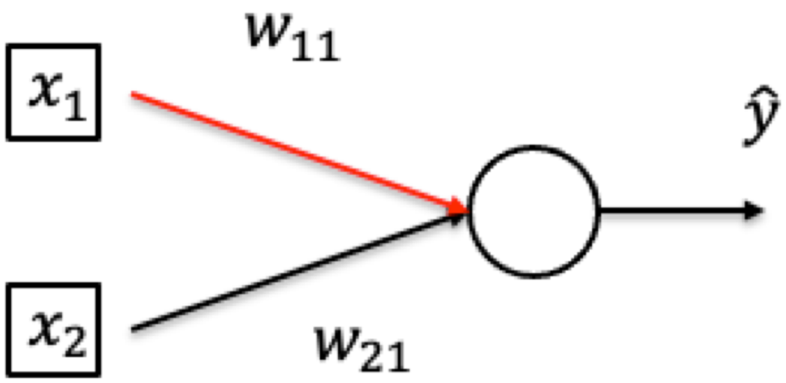


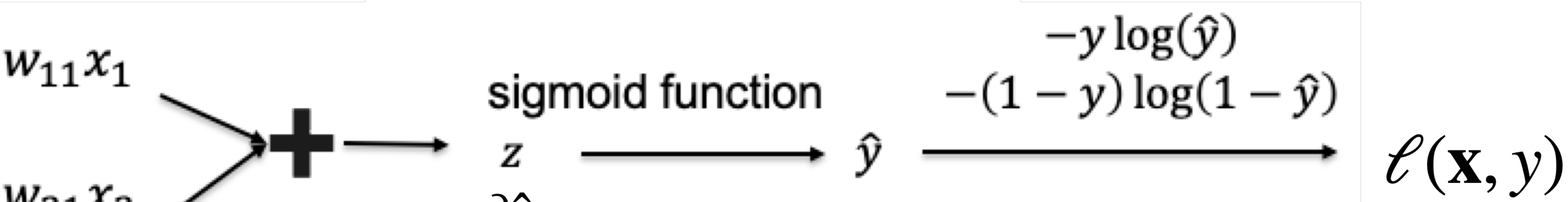
$$\frac{\partial \hat{y}}{\partial z} = \sigma'(z) = \sigma(z)(1-\sigma(z))$$

- By chain rule:

$$\frac{\partial l}{\partial w_{11}} = \frac{\partial l}{\partial \hat{y}} \hat{y}(1-\hat{y})x_1$$

Computing Gradients

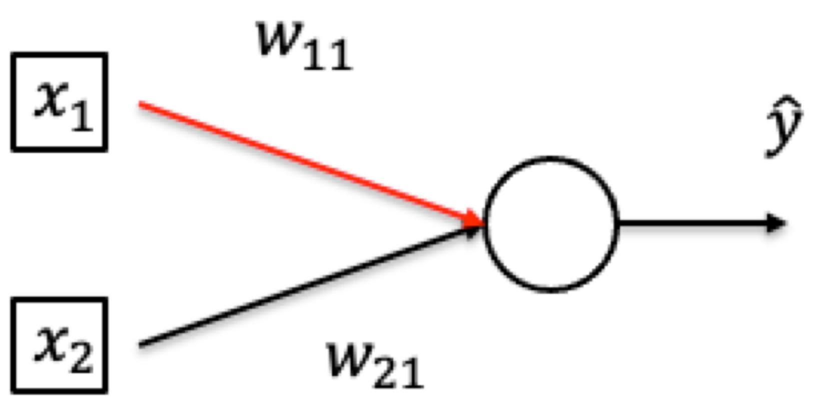


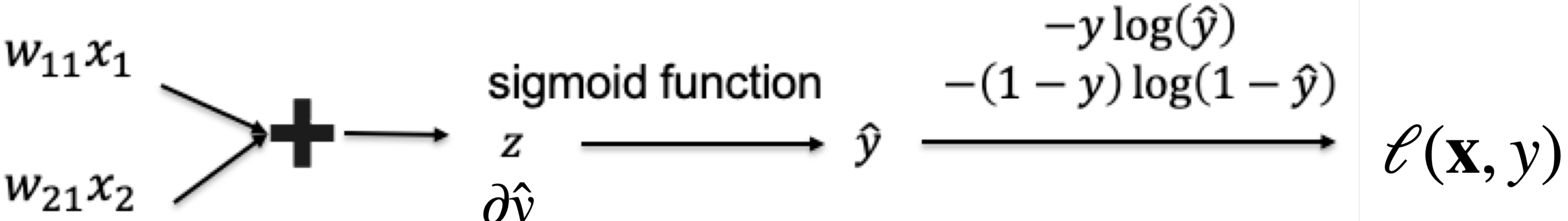


$$\frac{\partial \hat{y}}{\partial z} = \sigma'(z) = \sigma(z)(1 - \sigma(z))$$

- By chain rule: $$\frac{\partial l}{\partial w_{11}} = \left(\frac{1-y}{1-\hat{y}} - \frac{y}{\hat{y}}\right)\hat{y}(1-\hat{y})x_1$$

Computing Gradients

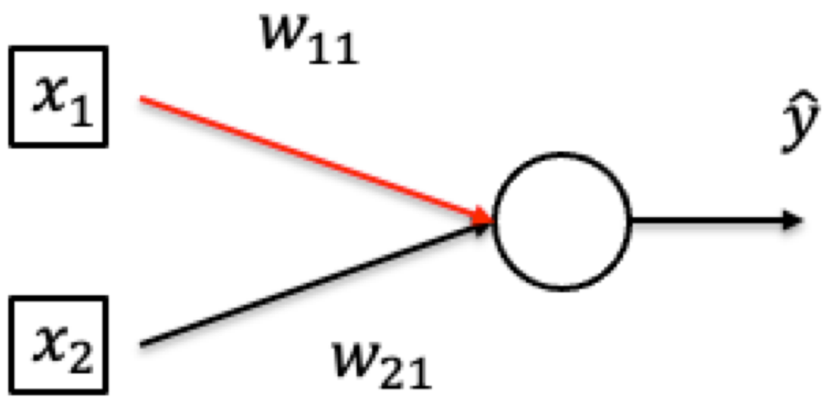


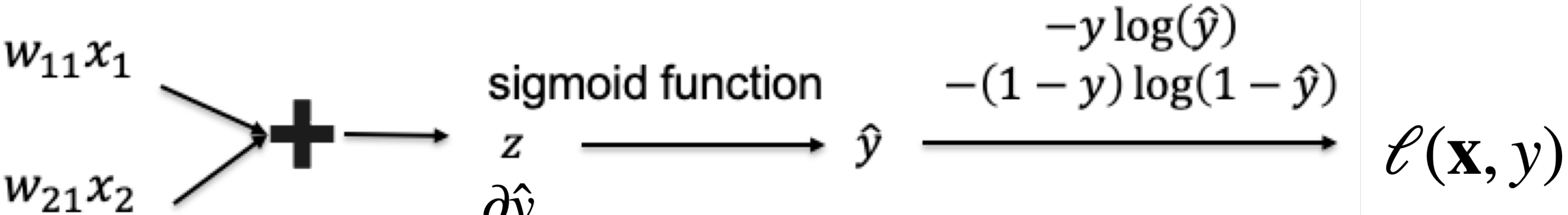


$$\frac{\partial \hat{y}}{\partial z} = \sigma'(z) = \sigma(z)(1 - \sigma(z))$$

- By chain rule: $\frac{\partial l}{\partial w_{11}} = (\hat{y} - y)x_1$

Computing Gradients



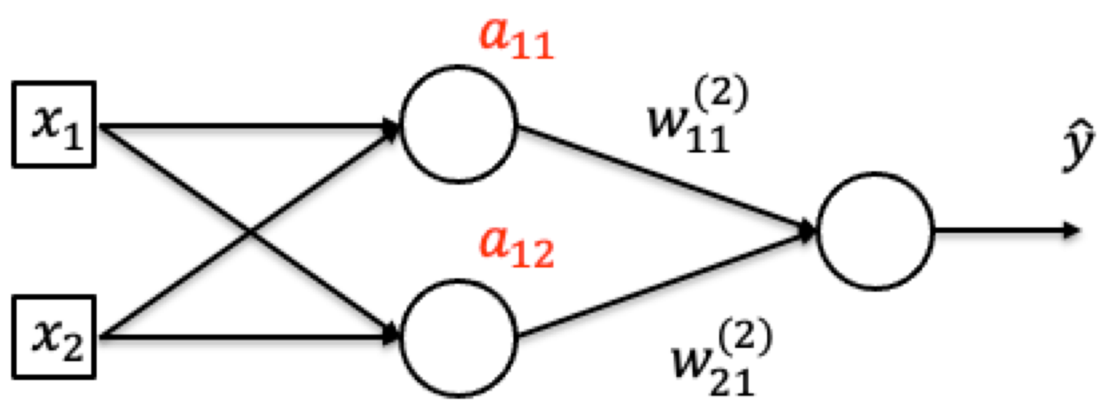


$$\frac{\partial \hat{y}}{\partial z} = \sigma'(z) = \sigma(z)(1-\sigma(z))$$

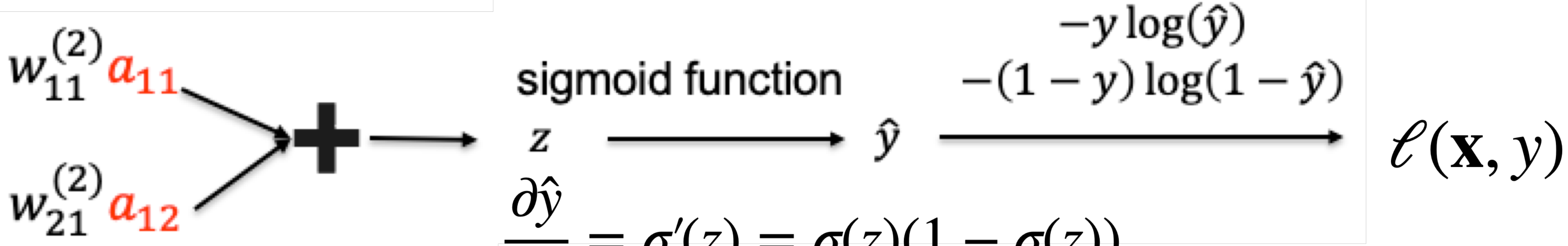
- By chain rule:

$$\frac{\partial l}{\partial x_1} = \frac{\partial l}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial z} w_{11} = (\hat{y} - y) w_{11}$$

Computing Gradients: More Layers



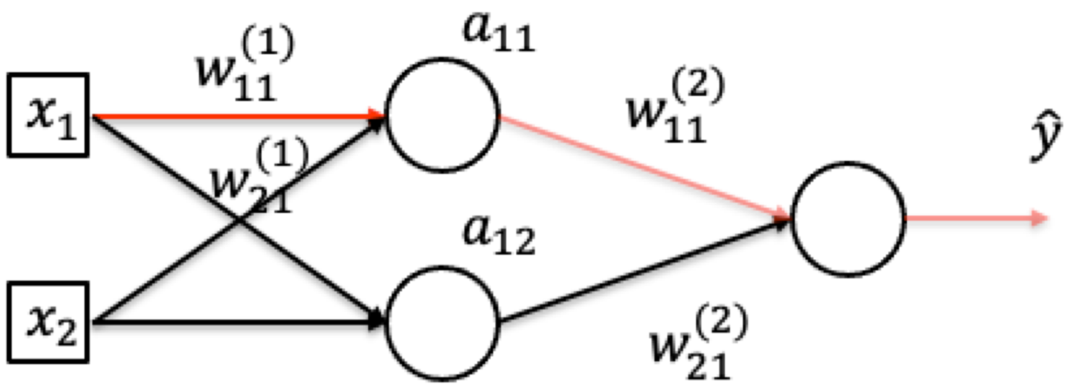
Make it deeper

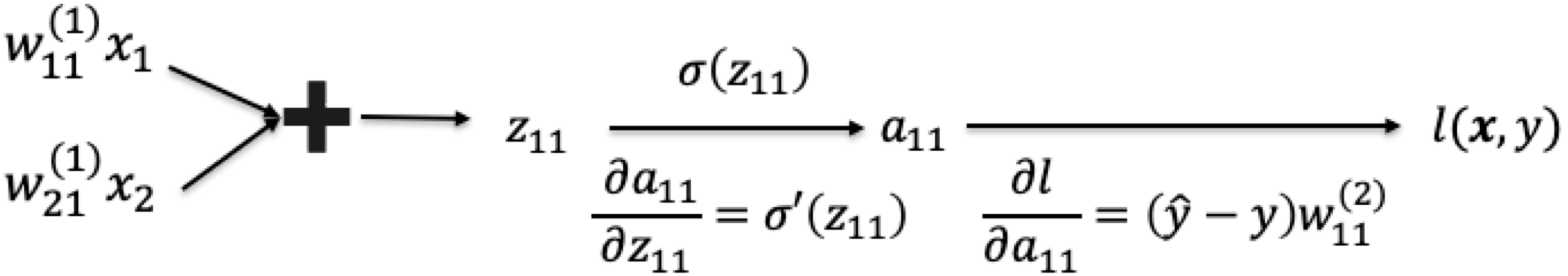


$$\frac{\partial \hat{y}}{\partial z} = \sigma'(z) = \sigma(z)(1 - \sigma(z))$$

- By chain rule: $\frac{\partial l}{\partial a_{11}} = (\hat{y} - y) w_{11}^{(2)}, \quad \frac{\partial l}{\partial a_{12}} = (\hat{y} - y) w_{21}^{(2)}$

Computing Gradients: More Layers

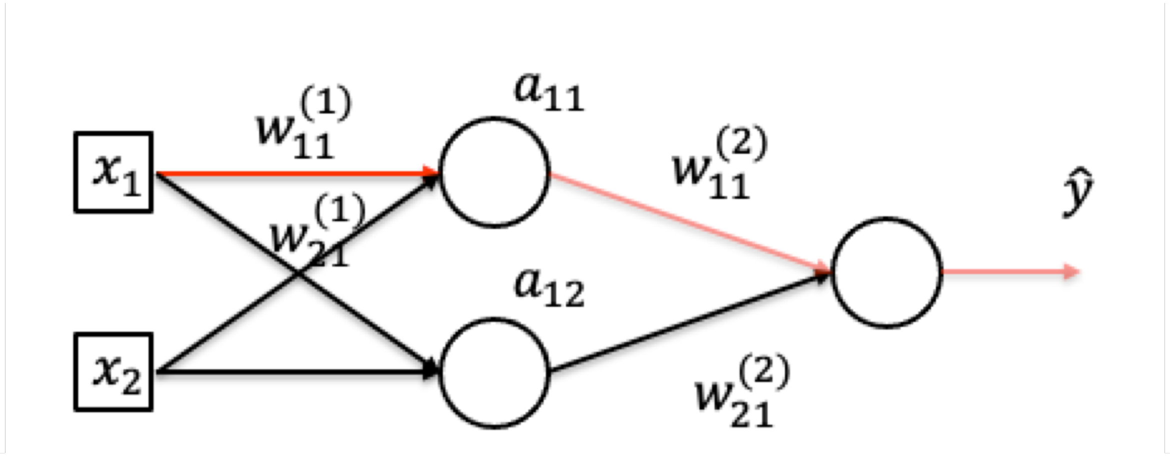


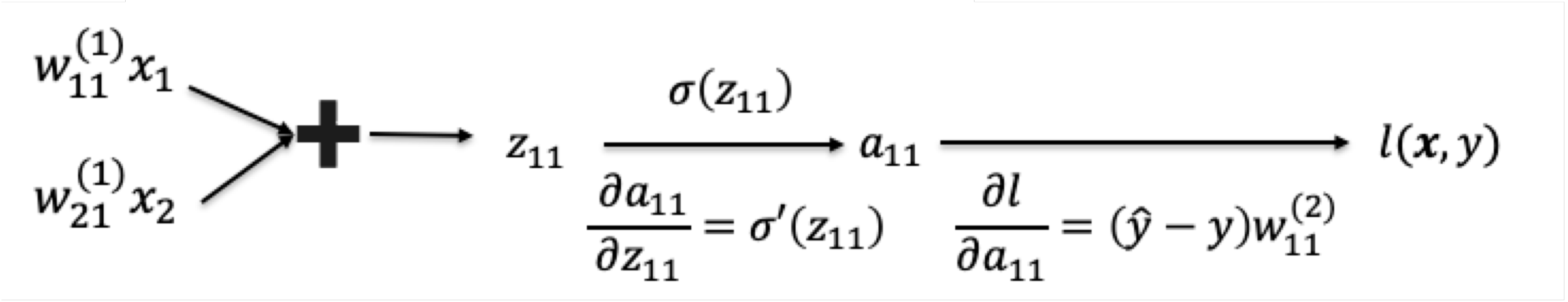


- By chain rule:

$$\frac{\partial l}{\partial w_{11}} = \frac{\partial l}{\partial a_{11}} \frac{\partial a_{11}}{\partial w_{11}^{(1)}} = (\hat{y} - y) w_{11}^{(2)} \frac{\partial a_{11}}{\partial w_{11}^{(1)}}$$

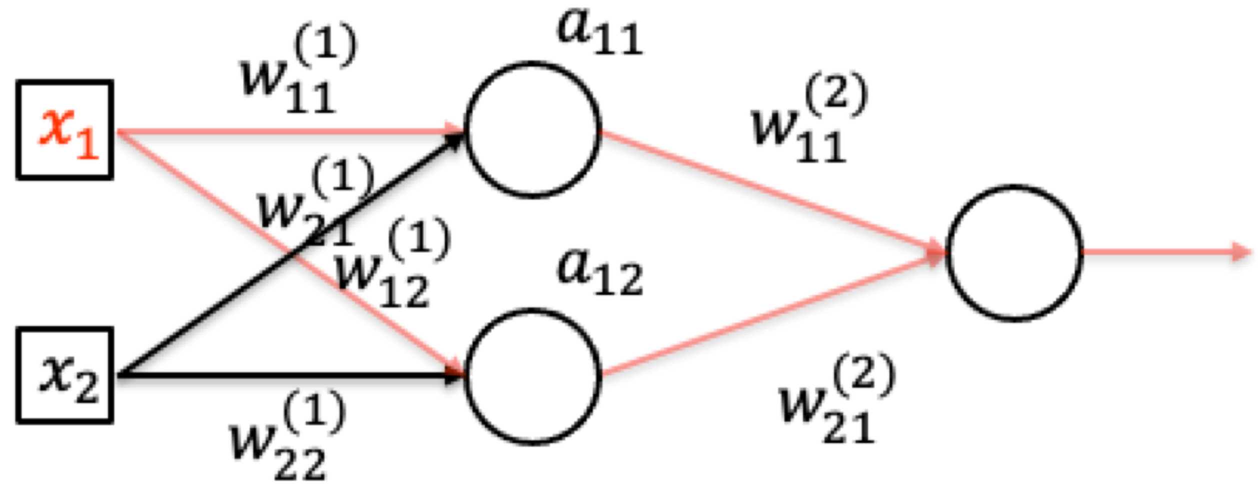
Computing Gradients: More Layers

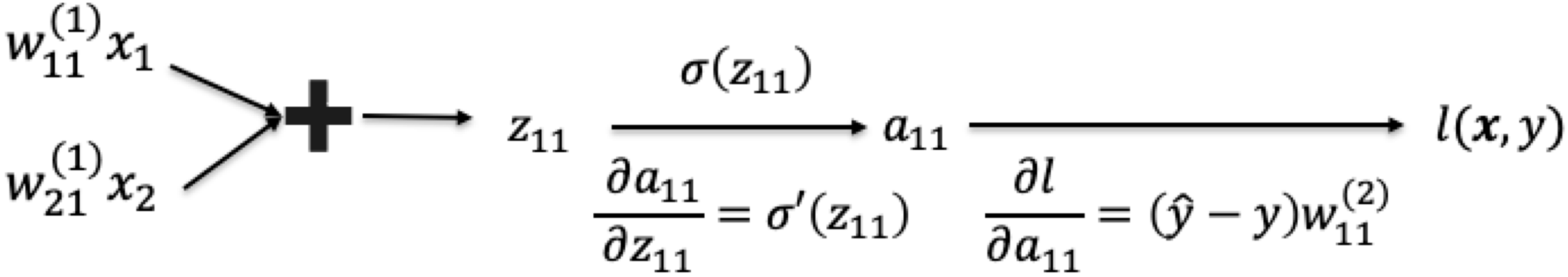




- By chain rule: $\frac{\partial l}{\partial w_{11}} = \frac{\partial l}{\partial a_{11}} \frac{\partial a_{11}}{\partial w_{11}^{(1)}} = (\hat{y} - y) w_{11}^{(2)} a_{11} (1 - a_{11}) x_1$

Computing Gradients: More Layers



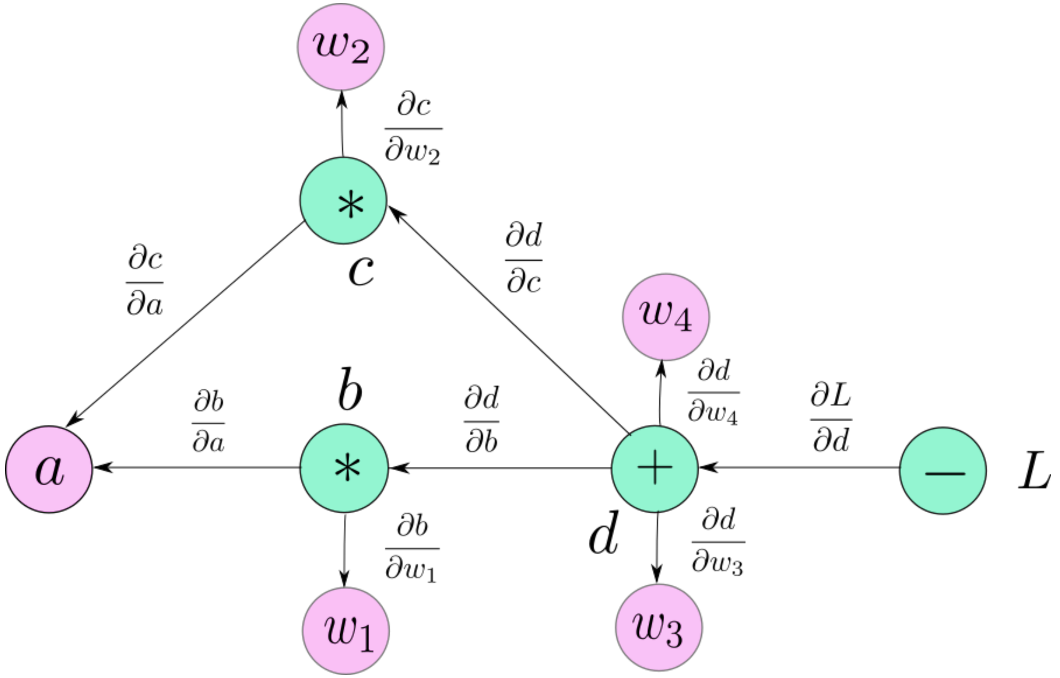


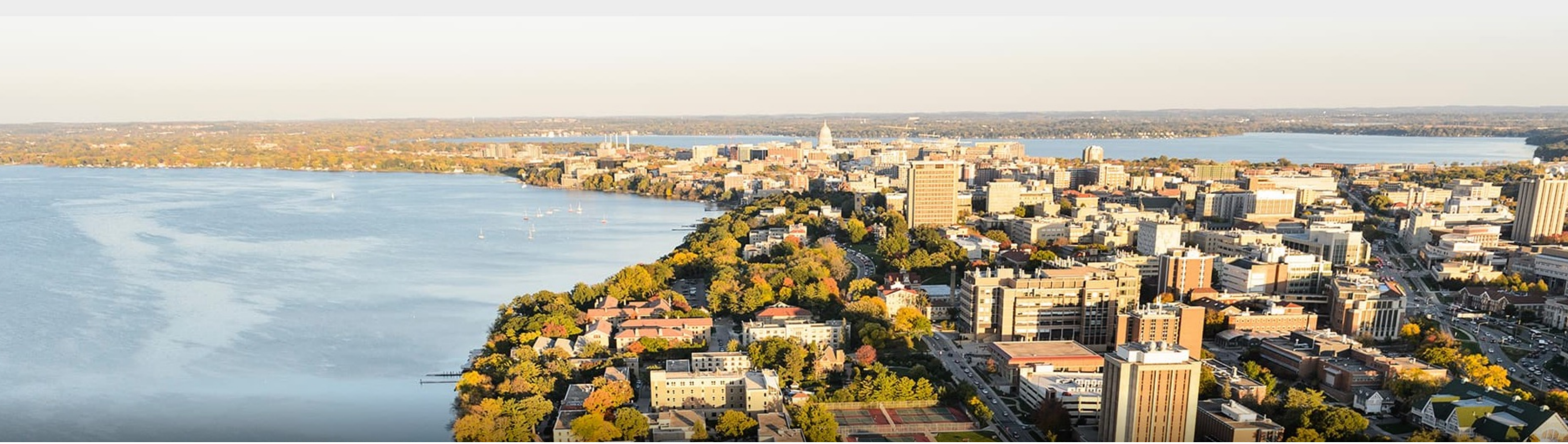
- By chain rule:

$$\frac{\partial l}{\partial x_1} = \frac{\partial l}{\partial a_{11}}\frac{\partial a_{11}}{\partial x_1} + \frac{\partial l}{\partial a_{12}}\frac{\partial a_{12}}{\partial x_1}$$

Backpropagation

- Now we can compute derivatives for particular neurons, but we want to automate this process
- Set up a computation graph and run on the graph





Thanks Everyone!

Some of the slides in these lectures have been adapted/borrowed from materials developed by Mark Craven, David Page, Jude Shavlik, Tom Mitchell, Nina Balcan, Elad Hazan, Tom Dietterich, Pedro Domingos, Jerry Zhu, Yingyu Liang, Volodymyr Kuleshov