CS 760: Machine Learning
Neural Networks Continued

Fred Sala

University of Wisconsin-Madison

Oct. 12, 2021

Logistics

- **Announcements**:
  - HW 3 due today!
  - Proposal due **Thursday**!
- **Class roadmap:**

Tuesday, Oct. 12	Neural Networks II
Thursday, Oct. 14	Neural Networks III
Tuesday, Oct. 19	Neural Networks IV
Thursday, Oct. 21	Neural Networks V
Tuesday, Oct. 26	Practical Aspects of Training + Review

All Neural Networks

Outline

- **Neural Networks**
  - Introduction, Setup, Components, Activations
- **Training Neural Networks**
  - SGD, Computing Gradients, Backpropagation
- **Regularization**
  - Views, Data Augmentation, Other approaches

Outline

- **Neural Networks**
  - Introduction, Setup, Components, Activations
- **Training Neural Networks**
  - SGD, Computing Gradients, Backpropagation
- **Regularization**
  - Views, Data Augmentation, Other approaches

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

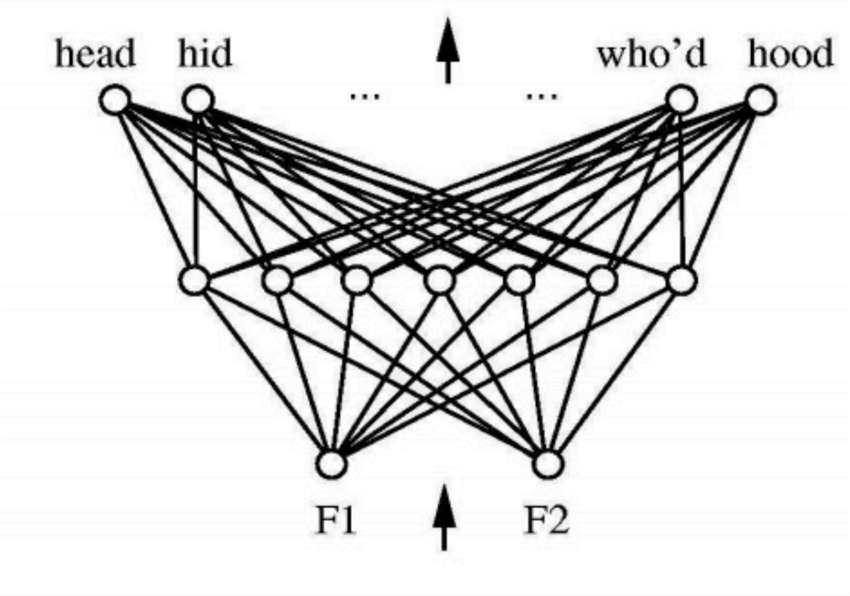


figure from Huang & Lippmann, *NIPS* 1988

Neural Network **Decision Regions**

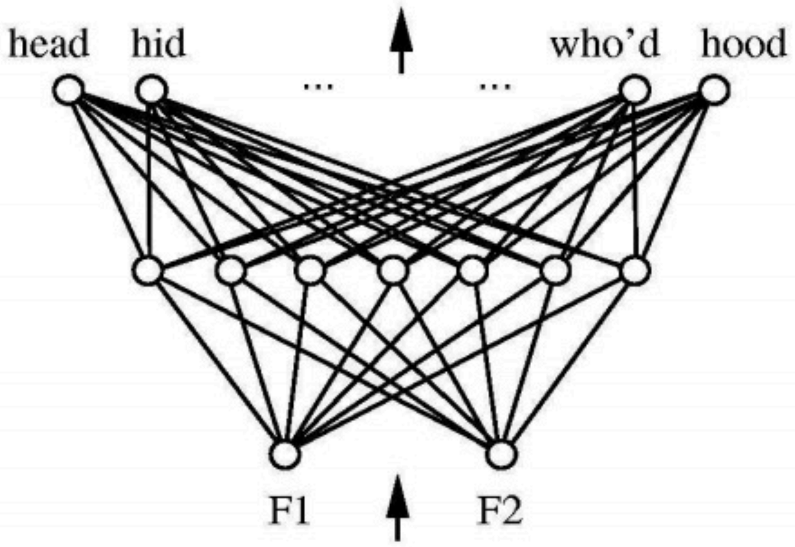
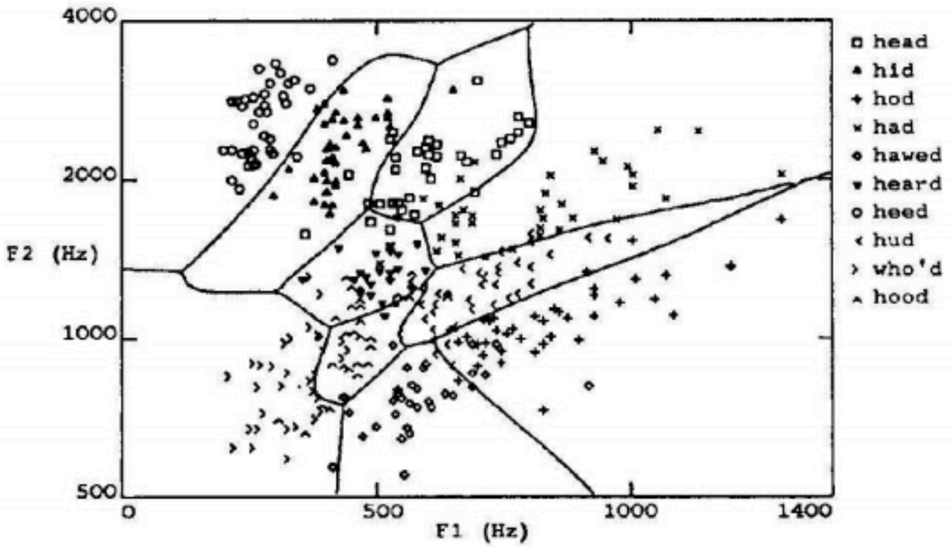
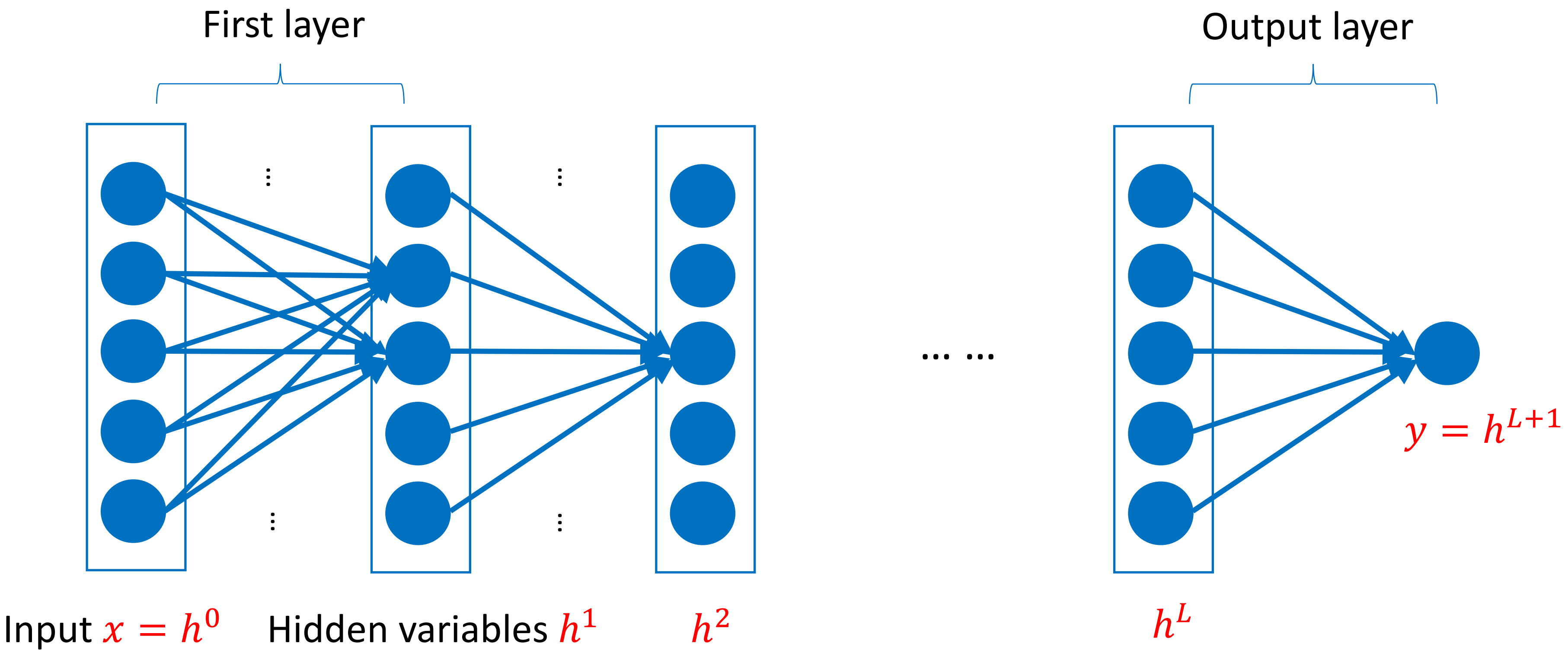


Figure from Huang & Lippmann, *NIPS* 1988



Neural Network Components

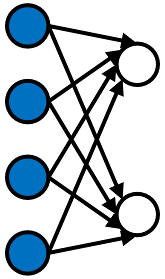
An $(L+1)$-layer network



Feature Encoding for NNs

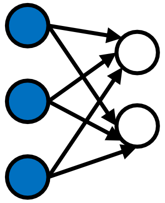
- Nominal features usually a one hot encoding

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



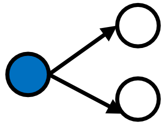
- Ordinal features: use a *thermometer* encoding

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



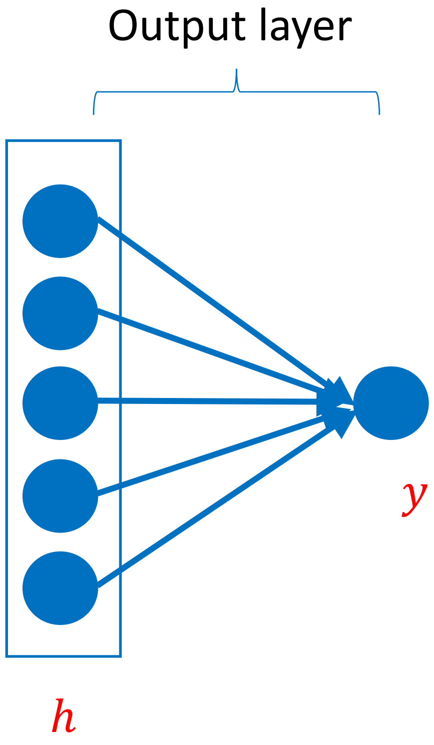
- Real-valued features use individual input units (may want to scale/normalize them first though)

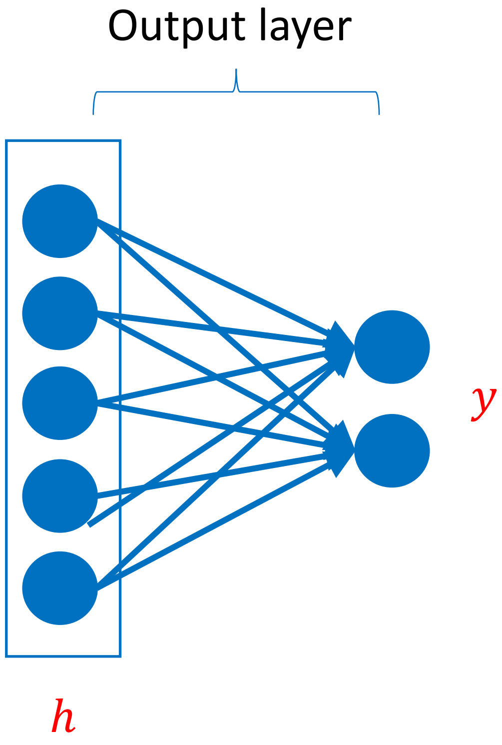
$$\text{precipitation} = \begin{bmatrix}0.68\end{bmatrix}$$



Output Layer: Examples

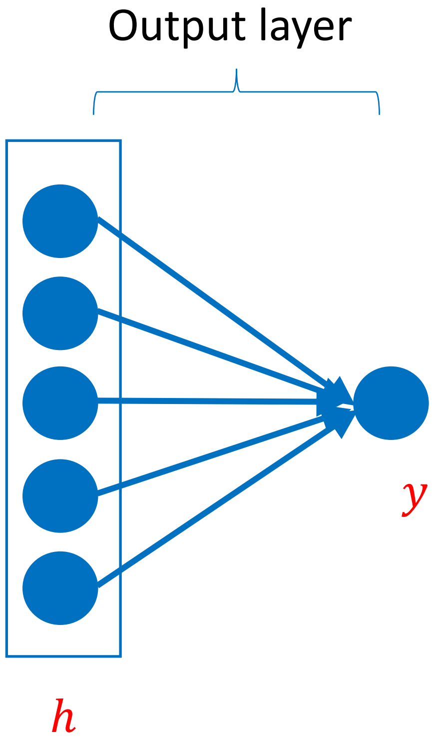
- Regression: $y = w^T h + b$
  - Linear units: no nonlinearity
- Multi-dimensional regression: $y = W^T h + b$
  - Linear units: no nonlinearity

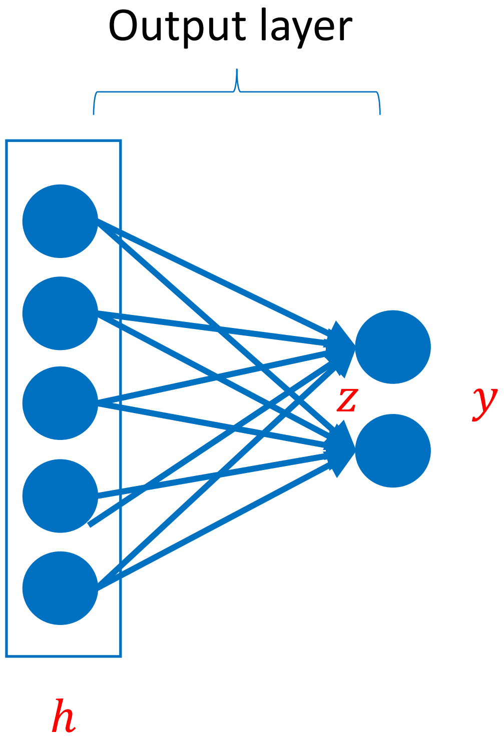




Output Layer: Examples

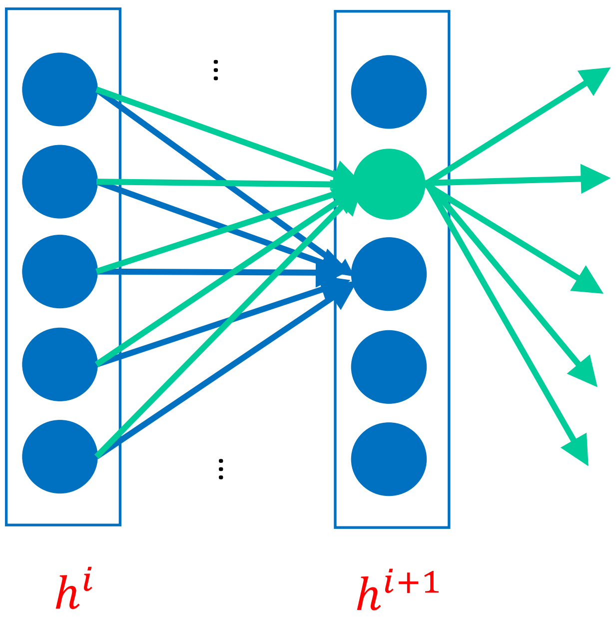
- Binary classification: $y = \sigma(w^T h + b)$
  - Corresponds to using logistic regression on h
- Multiclass classification:
  - $y = \mathrm{softmax}(z)$ where $z = W^T h + b$





Hidden Layers

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



Hidden Layers

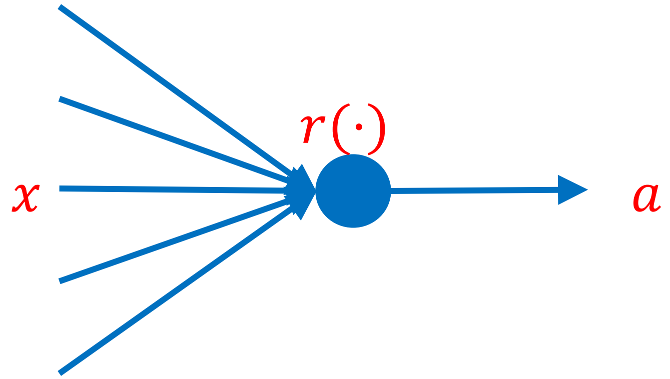
- Outputs $a = r(w^T x + b)$

Bias

Activation

Weight

- Typical activation function r
  - Sigmoid $\sigma(z) = 1/(1 + \exp(-z))$
  - Tanh $\tanh(z) = 2\sigma(2z) - 1$
  - ReLU $\mathrm{r}(z) = max[0, z]$
- Why not **linear activation** functions?
  - Model would be linear.



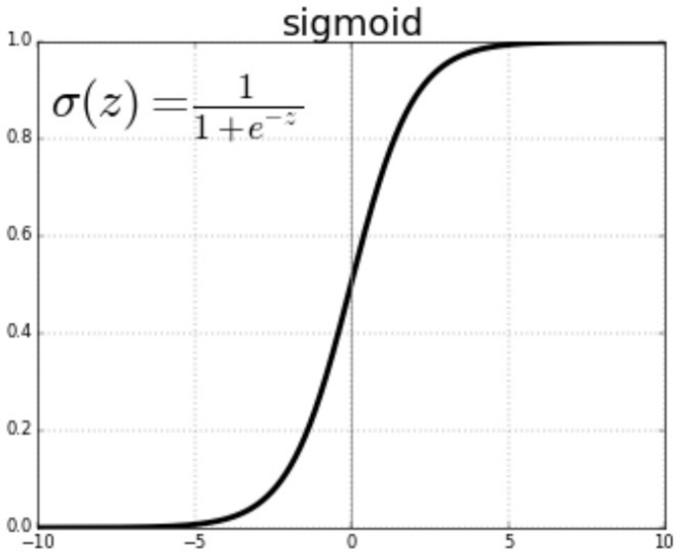
More on Activations

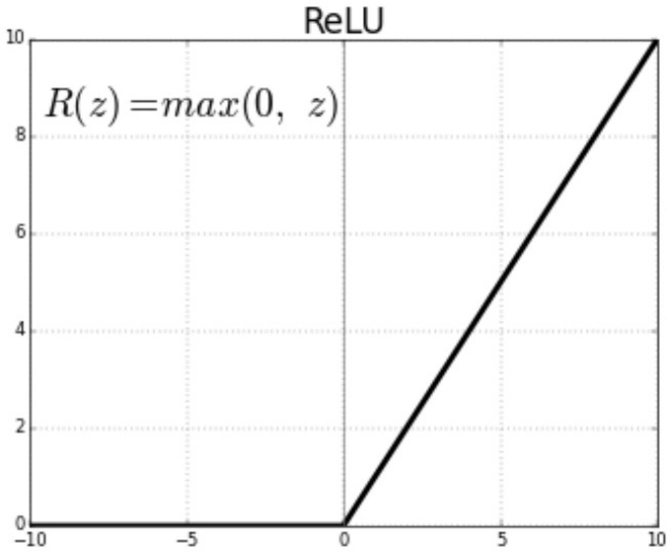
- Outputs $a = r(w^T x + b)$

Bias

Activation **Weight**

- Consider **gradients**… saturating vs. nonsaturating



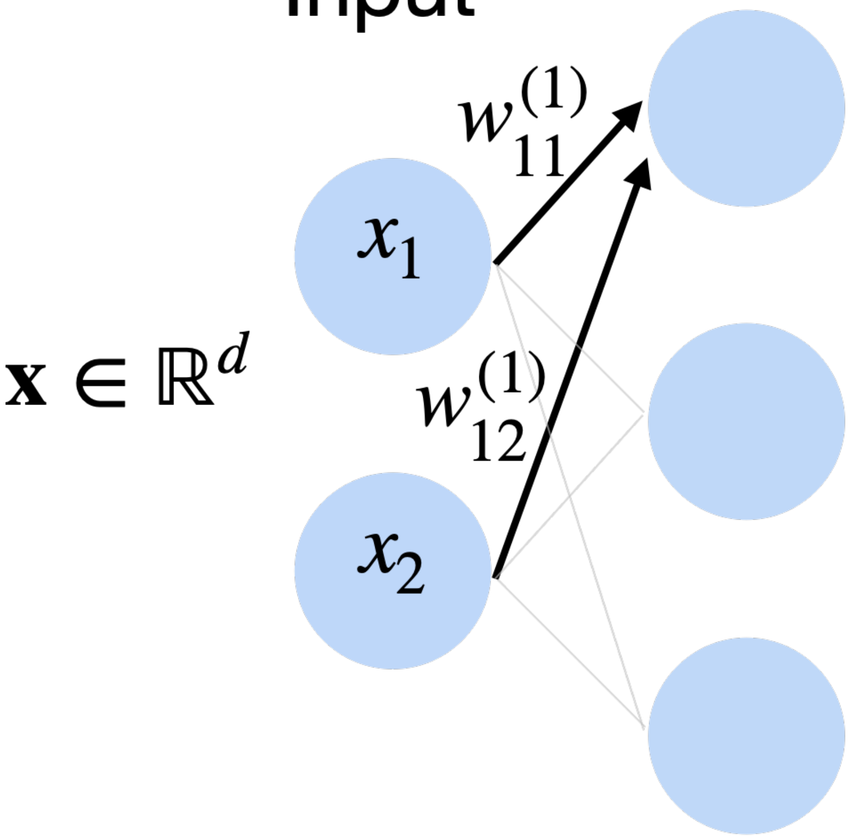


MLPs: Multilayer Perceptron

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

Hidden layer
3 neurons

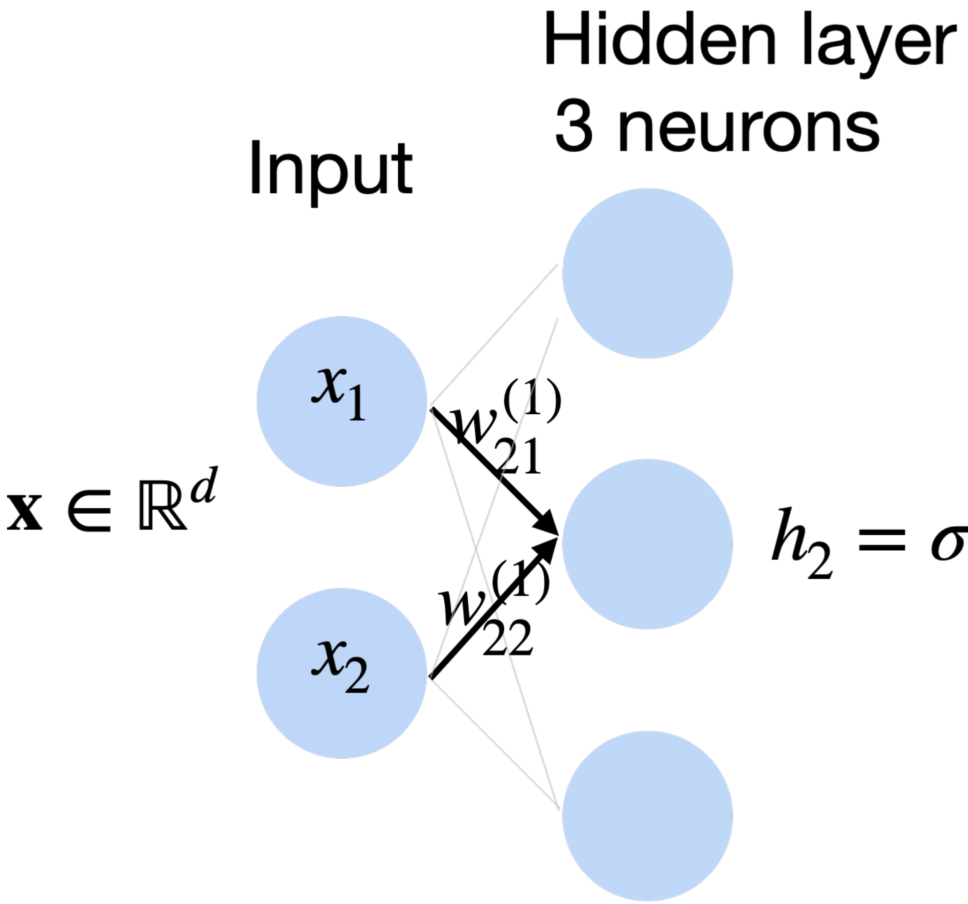
Input



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

MLPs: Multilayer Perceptron

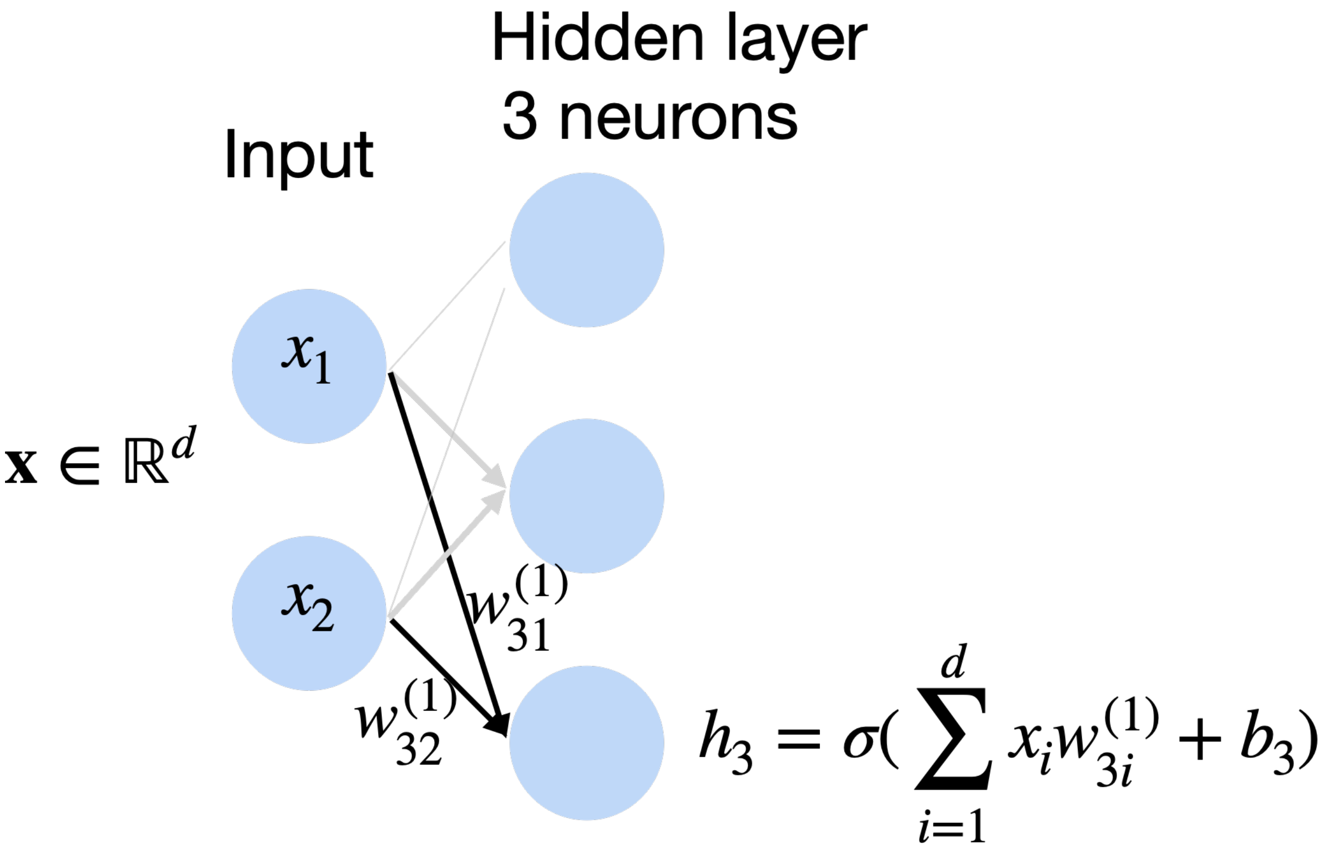
- **Ex**: 1 hidden layer, 1 output layer: depth 2



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

MLPs: Multilayer Perceptron

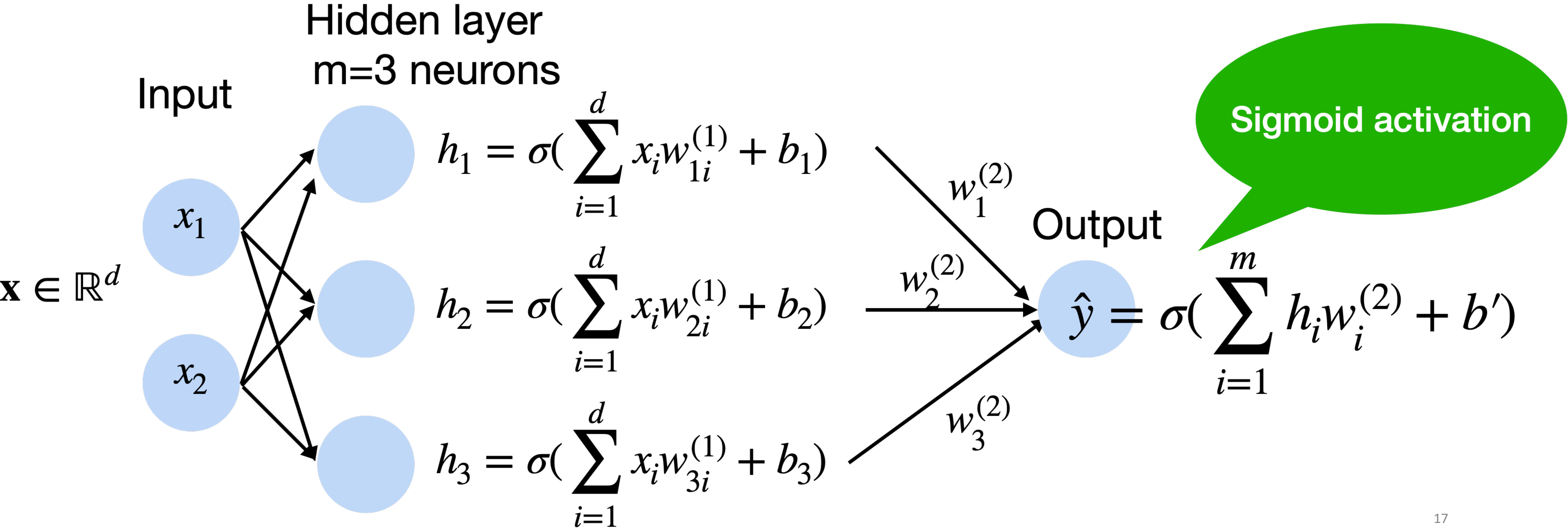
- **Ex**: 1 hidden layer, 1 output layer: depth 2



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

MLPs: Multilayer Perceptron

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



Input

Hidden layer
m=3 neurons

Output

Sigmoid activation

$\mathbf{x} \in \mathbb{R}^d$

x_1

x_2

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

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

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

$w_1^{(2)}$

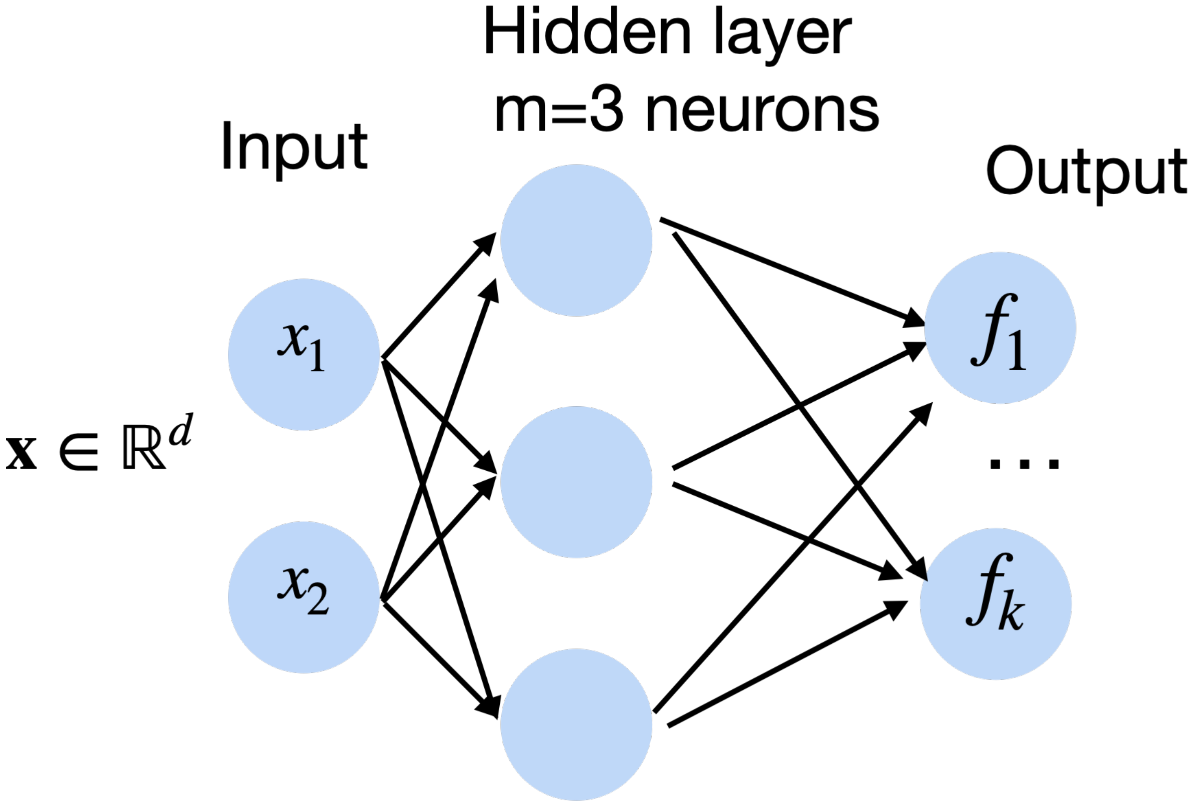
$w_2^{(2)}$

$w_3^{(2)}$

$$\hat{y} = \sigma(\sum_{i=1}^{m} h_i w_i^{(2)} + b')$$

Multiclass Classification Output

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

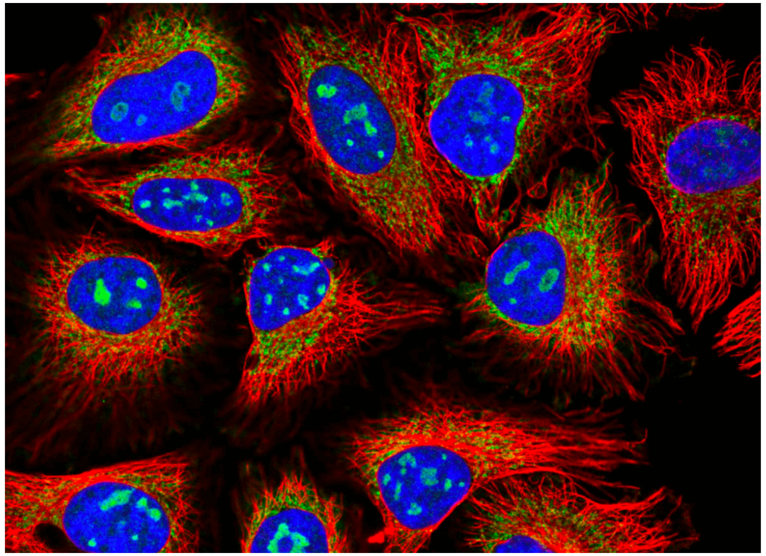


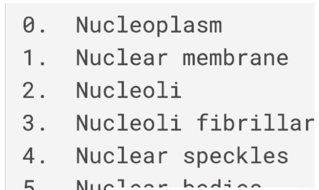
$$p(y \mid \mathbf{x}) = \text{softmax}(f)$$

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

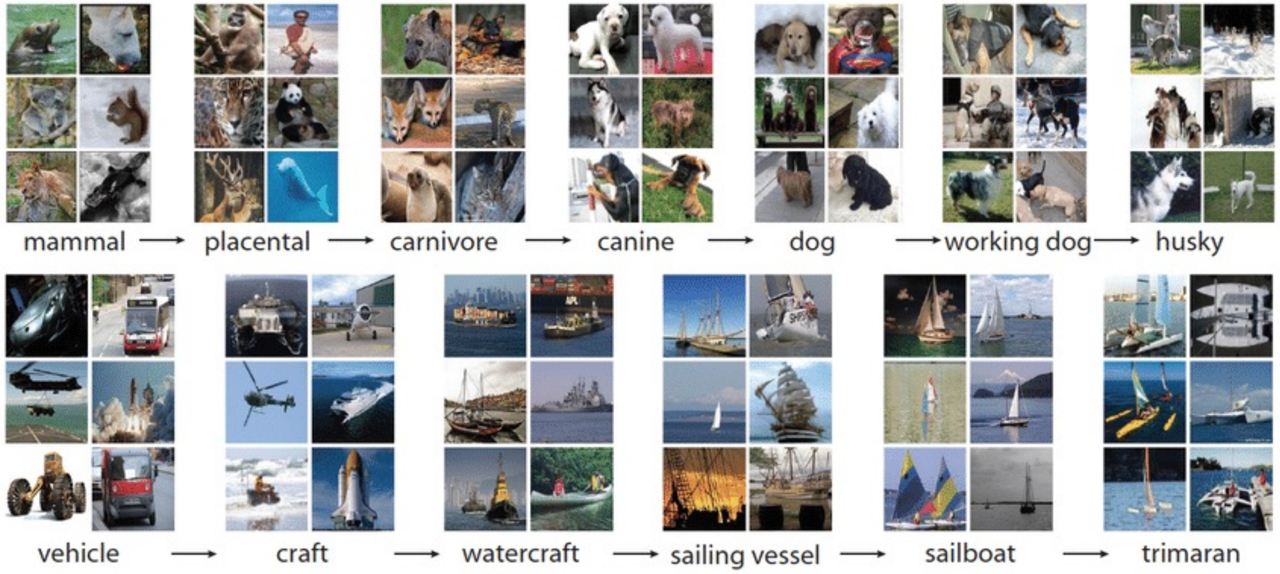
Multiclass Classification Examples

- Protein classification (Kaggle challenge)
- ImageNet





```
0.  Nucleoplasm
1.  Nuclear membrane
2.  Nucleoli
3.  Nucleoli fibrillar
4.  Nuclear speckles
5.  Nuclear bodies
6.  En
7.  Go
8.  Pe
9.  En
10.  L
11.  I
12.  A
13.  F
14.  M
15.  M
16.  C
```



Break & Quiz

Outline

- **Neural Networks**
  - Introduction, Setup, Components, Activations
- **Training Neural Networks**
  - SGD, Computing Gradients, Backpropagation
- **Regularization**
  - Views, Data Augmentation, Other approaches

Training Neural Networks

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

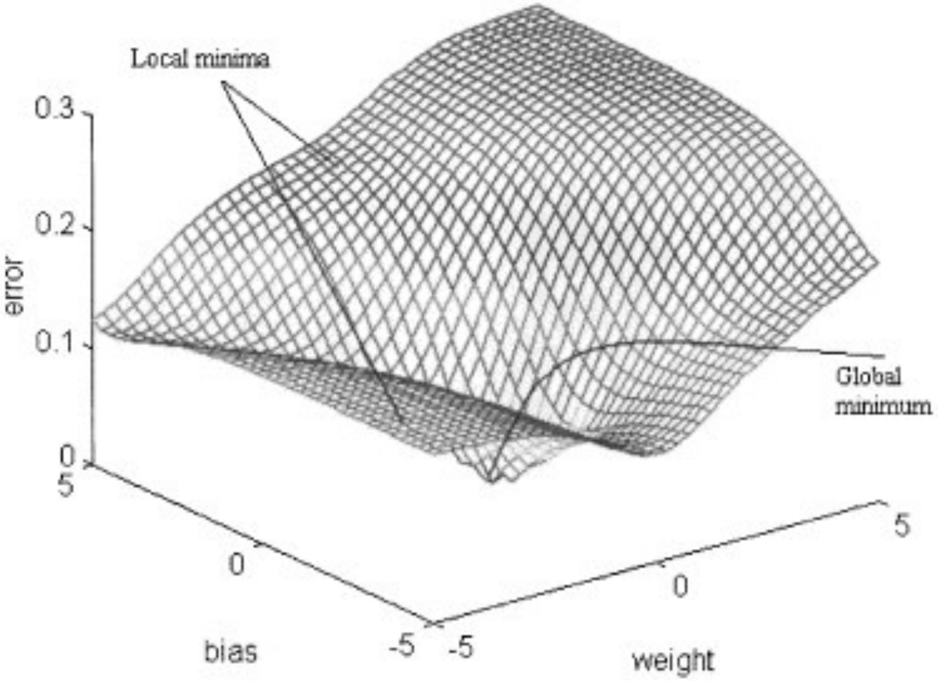


figure from Cho & Chow, *Neurocomputing* 1999

Training Neural Networks: SGD

- Algorithm:
  - Get $$D = \{(x^{(1)}, y^{(1)}), \ldots, (x^{(n)}, y^{(n)})\}$$
  - Initialize weights
  - Until stopping criteria met,
    - Sample training point. $(x^{(i)}, y^{(i)})$ without replacemet
    - Compute: $$f_{\text{network}}(x^{(i)})$$ ⟵ **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: $$w \leftarrow w - \alpha \nabla L^{(i)}(w)$$

Training Neural Networks: Minibatch SGD

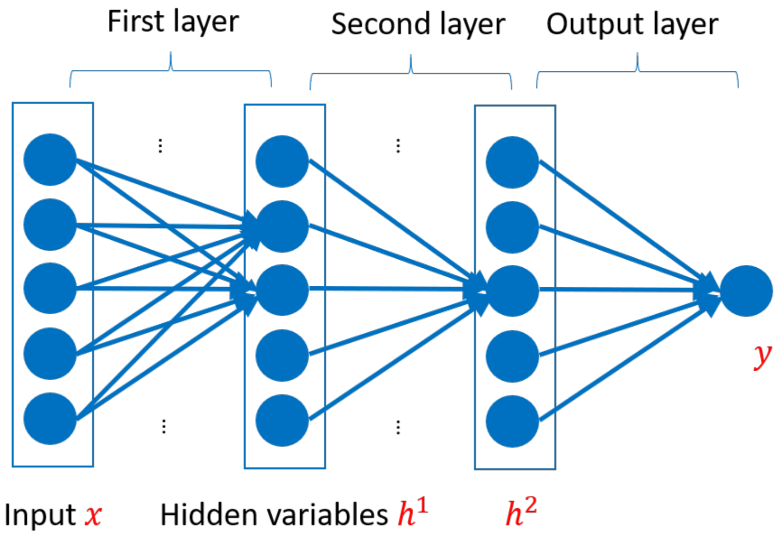
- Algorithm:
  - Get $D = \{(x^{(1)}, y^{(1)}), \ldots, (x^{(n)}, y^{(n)})\}$
  - Initialize weights
  - Until stopping criteria met,
    - Sample b points $j_1, j_2, \ldots, j_b$
    - Compute: $f_{\text{network}}(x^{(j_1)}), \ldots, f_{\text{network}}(x^{(j_b)})$ ← **Forward Pass**
    - Compute gradients: $\nabla L^{(j_1)}(w), \ldots, \nabla L^{(j_b)}(w)$ ← **Backward Pass**
    - Update weights:

$$w \leftarrow w - \frac{\alpha}{b} \sum_{k=1}^{b} \nabla L^{(j_k)}(w)$$

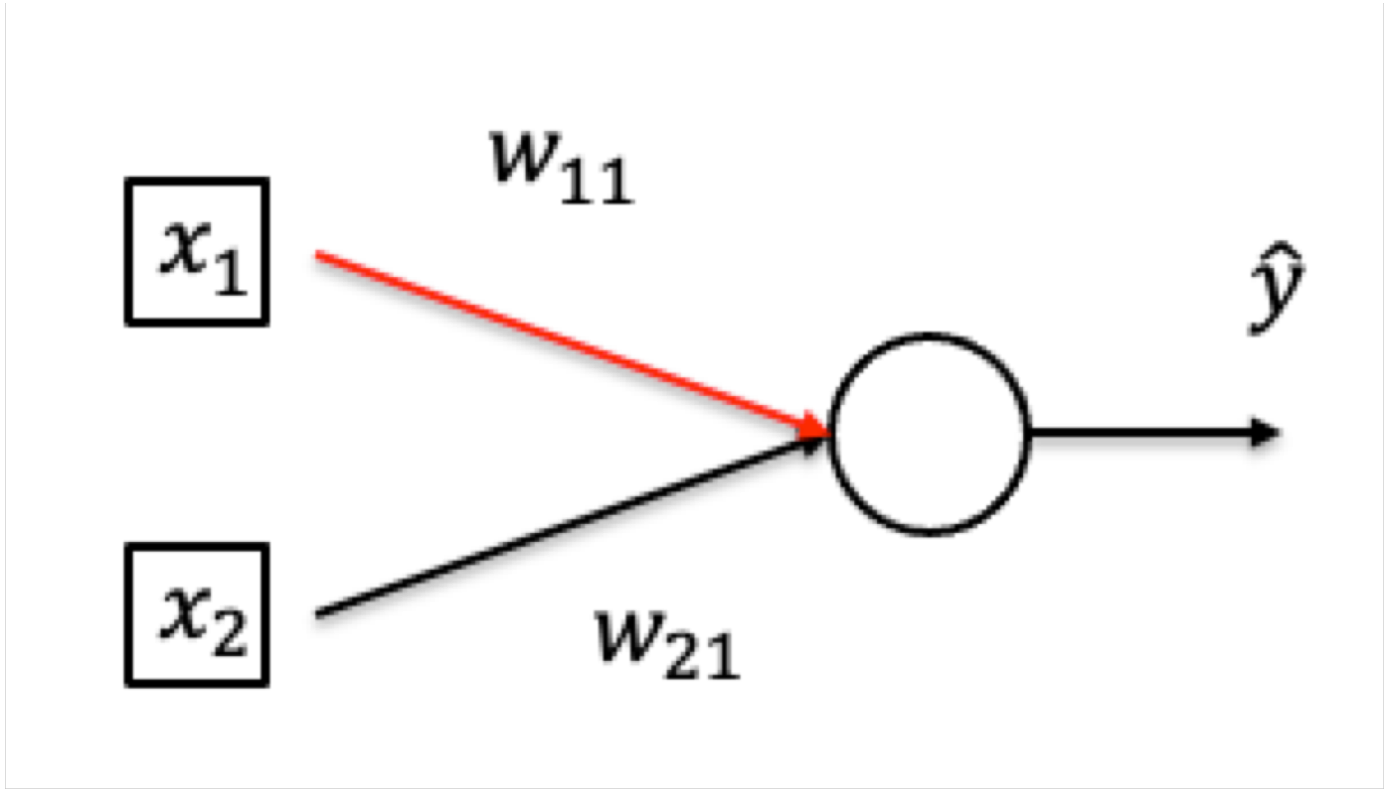
Training Neural Networks: Chain Rule

- Will need to compute terms like: $\frac{\partial L}{\partial w_1}$
  - But, L is a composition of:
    - Loss with output y
    - Output itself a composition of softmax with outer layer
    - Outer layer a combination of outputs from previous layer
    - Outputs from prev. layer a composition of activations and linear functions…
- Need the **chain rule**!
  - Suppose $L = L(g_1, \ldots, g_k)$ $g_j = g_j(w_1, \ldots, w_p)$
  - Then,

$$\frac{\partial L}{\partial w_i} = \sum_{j=1}^{k} \frac{\partial L}{\partial g_j} \frac{\partial g_j}{\partial w_i}$$

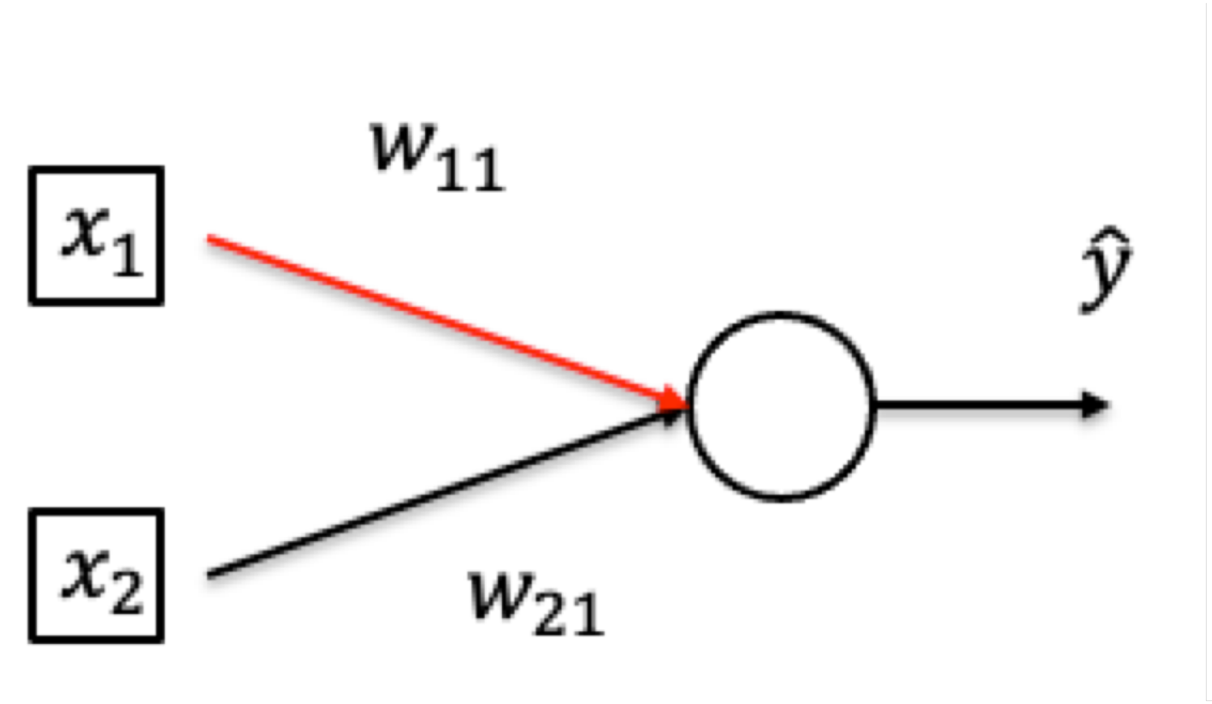


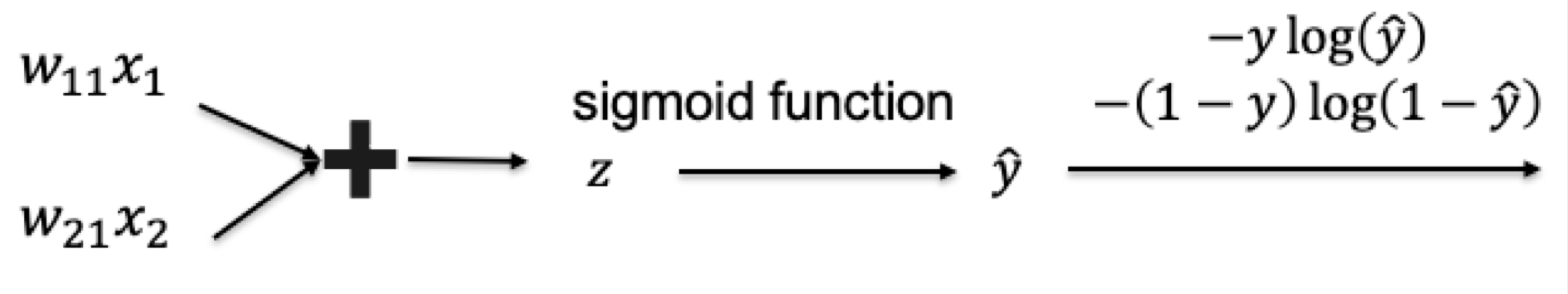
Computing Gradients



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

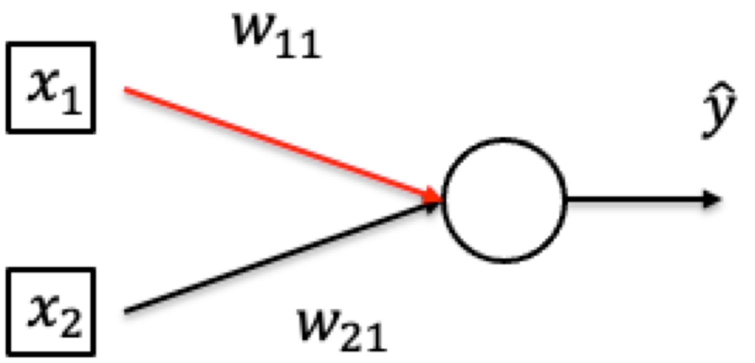
Computing Gradients

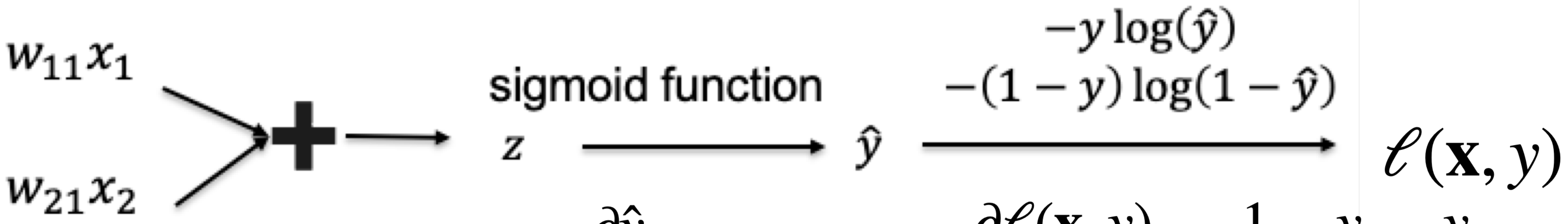




$\ell(\mathbf{x}, y)$

Computing Gradients





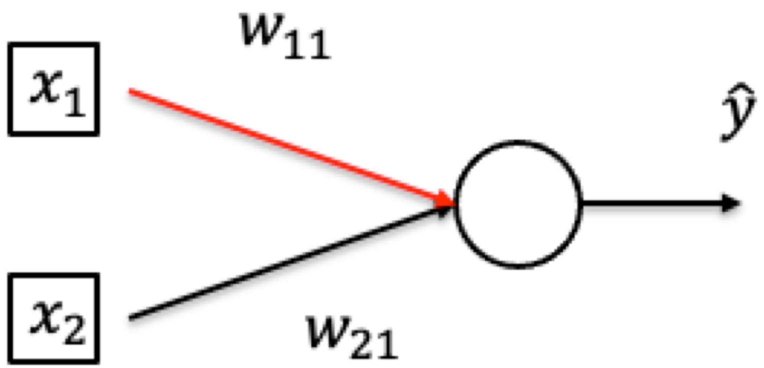
$$\frac{\partial \hat{y}}{\partial z} = \sigma'(z)$$

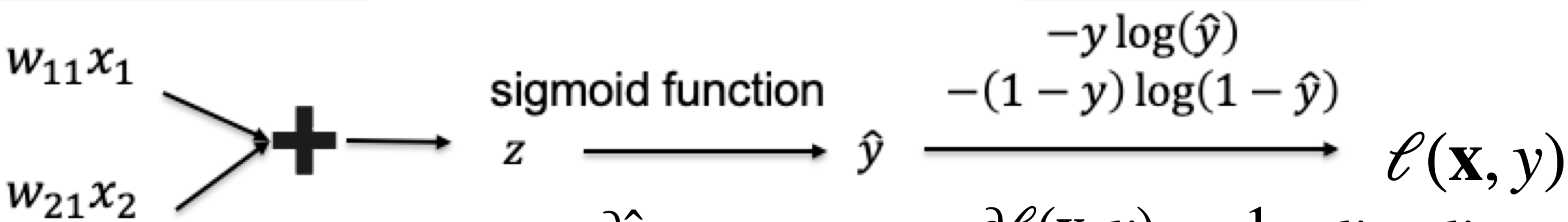
$$\frac{\partial \ell(\mathbf{x}, y)}{\partial \hat{y}} = \frac{1-y}{1-\hat{y}} - \frac{y}{\hat{y}}$$

- 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



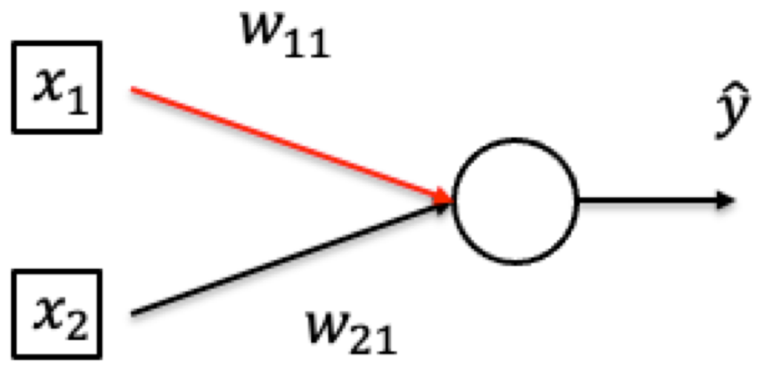


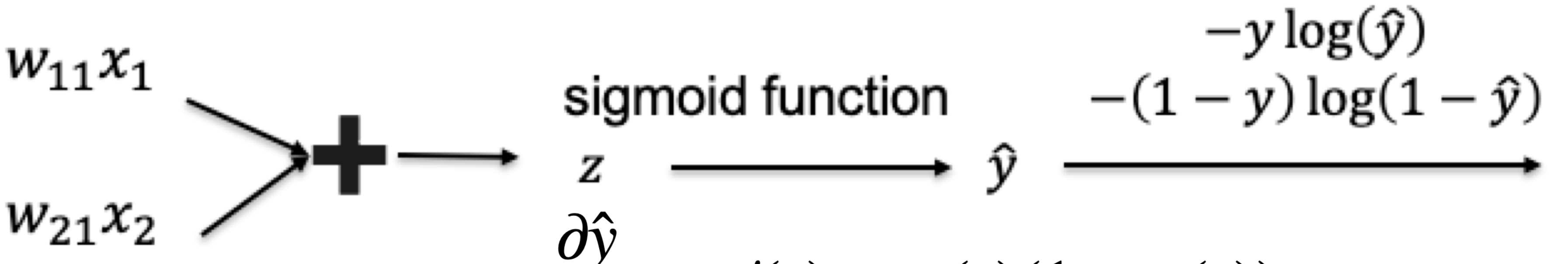
$$\frac{\partial \hat{y}}{\partial z} = \sigma'(z)$$

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

- 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





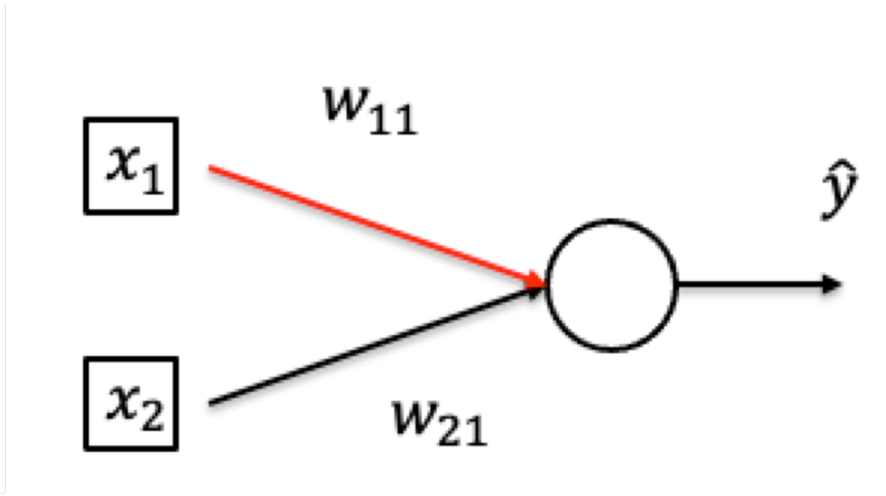
$\ell(\mathbf{x}, y)$

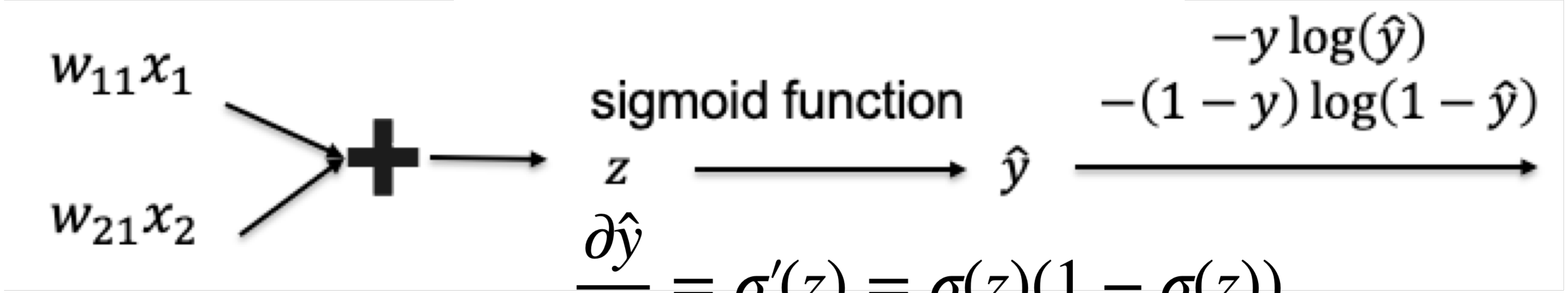
$$\frac{\partial \hat{y}}{\partial z} = \sigma'(z) = \sigma(z)(1-\sigma(z))$$

- By chain rule:

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

Computing Gradients





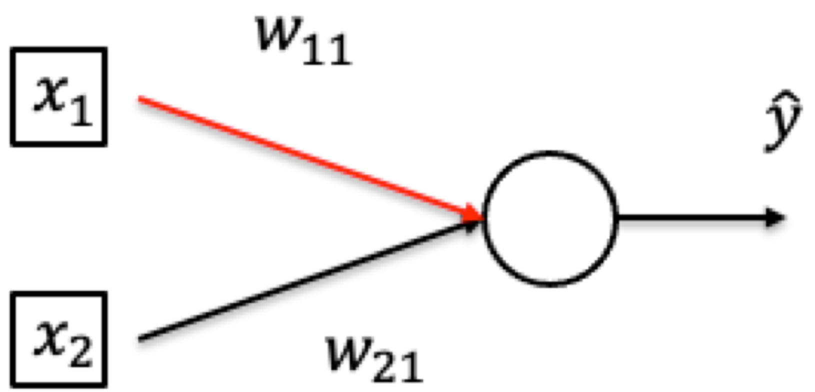
$\ell(\mathbf{x}, y)$

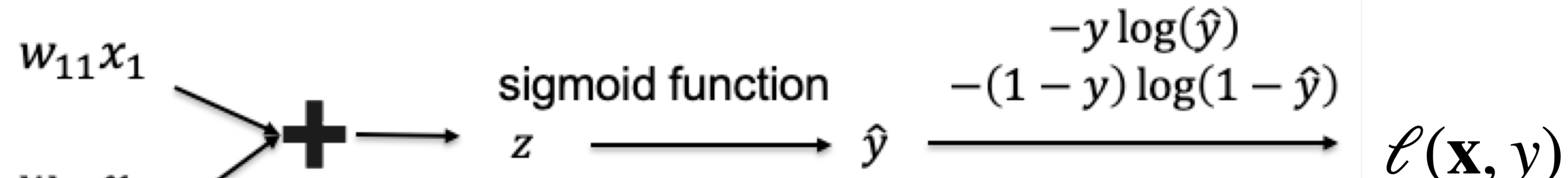
$$\frac{\partial \hat{y}}{\partial z} = \sigma'(z) = \sigma(z)(1-\sigma(z))$$

- By chain rule:

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

Computing Gradients

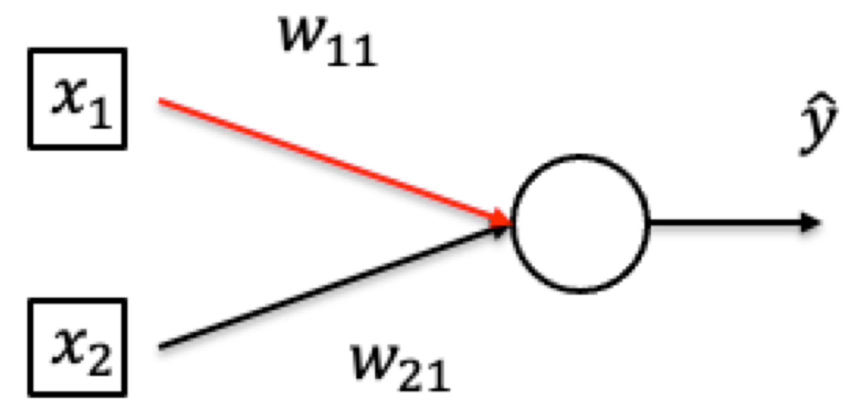


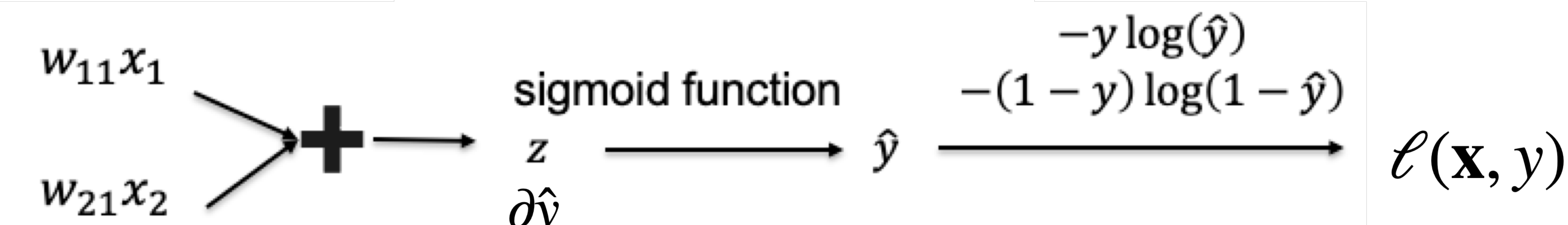


$$\frac{\partial \hat{y}}{\partial z} = \sigma'(z) = \sigma(z)(1-\sigma(z))$$

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

Computing Gradients

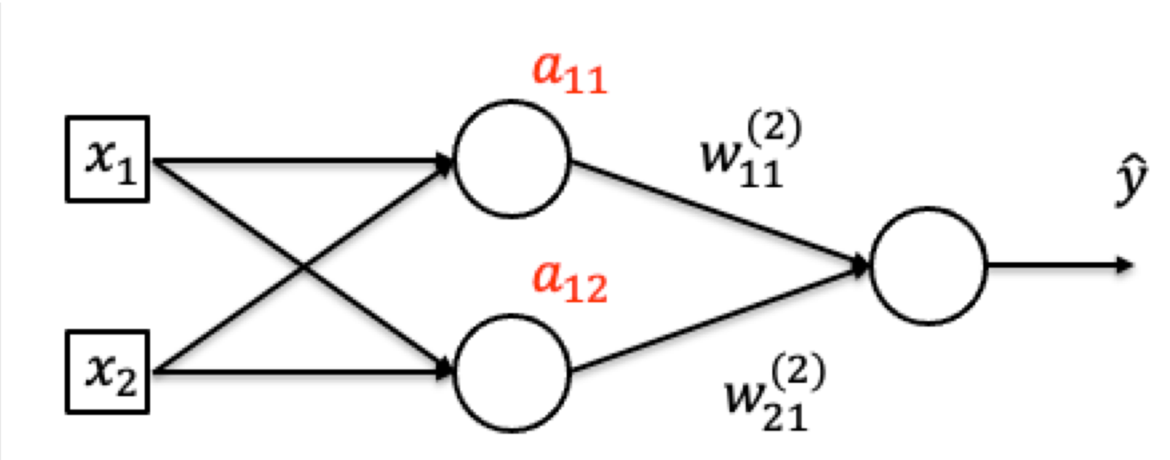




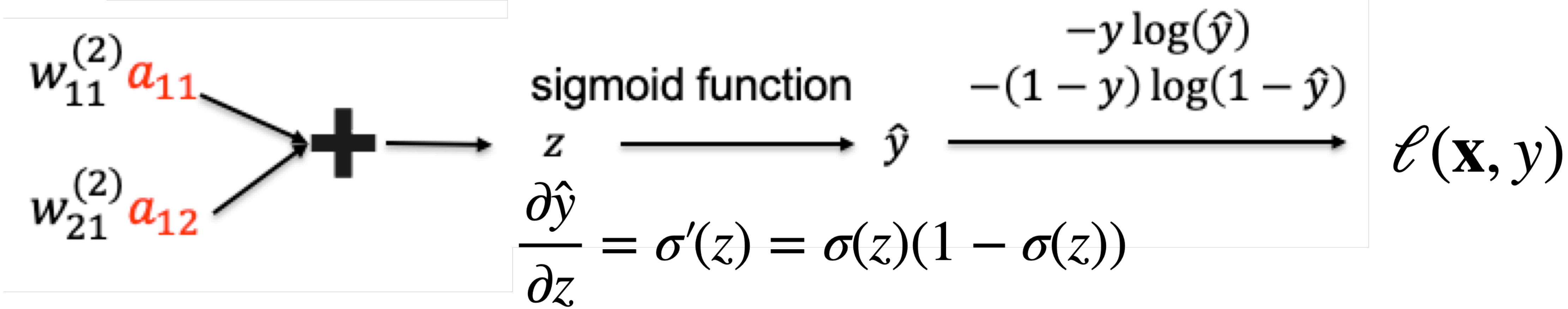
$$\frac{\partial \hat{y}}{\partial z} = \sigma'(z) = \sigma(z)(1-\sigma(z))$$

- 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



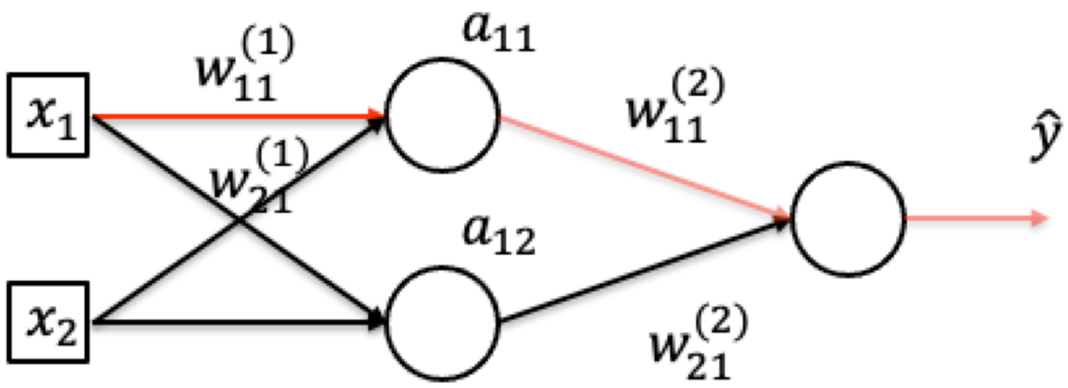
Make it deeper

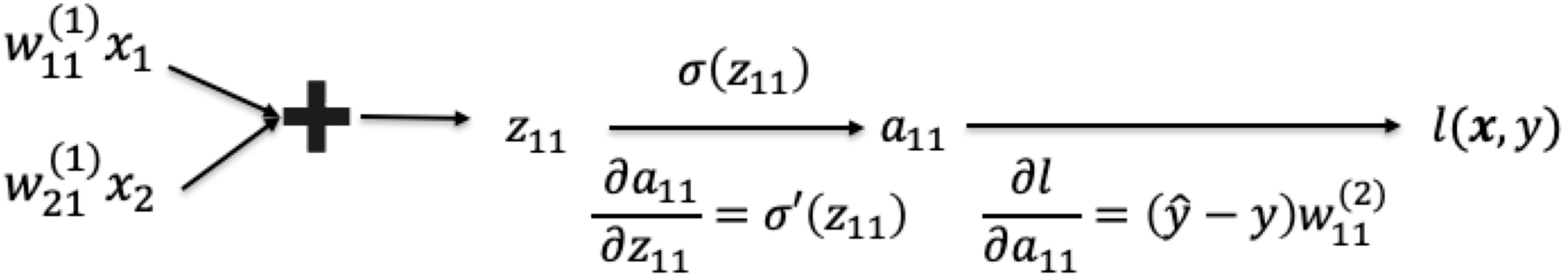


$$\frac{\partial \hat{y}}{\partial z} = \sigma'(z) = \sigma(z)(1-\sigma(z))$$

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

Computing Gradients: More Layers



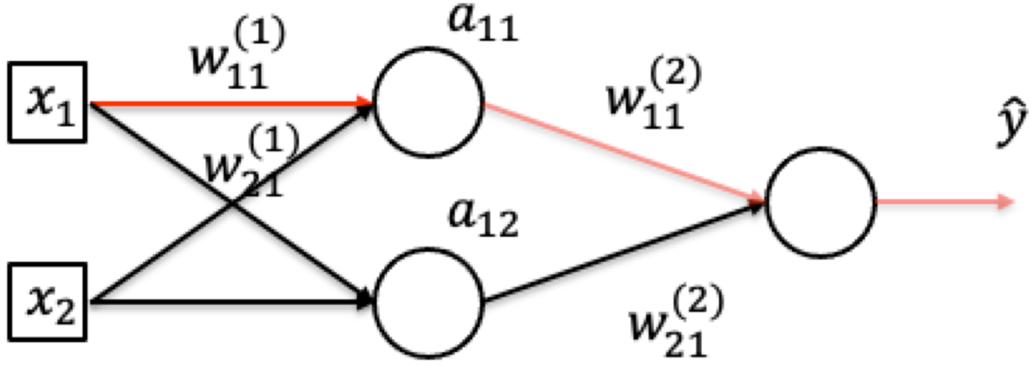


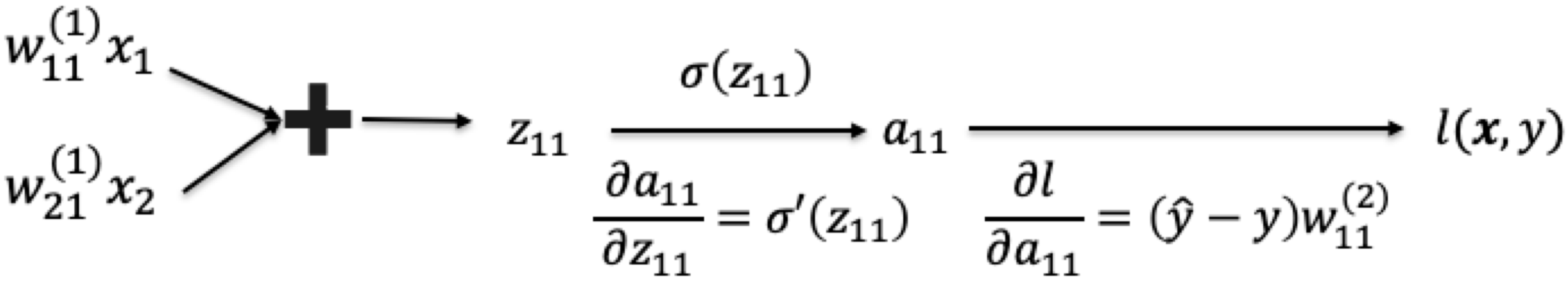
$$\frac{\partial a_{11}}{\partial z_{11}} = \sigma'(z_{11})$$

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

- 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

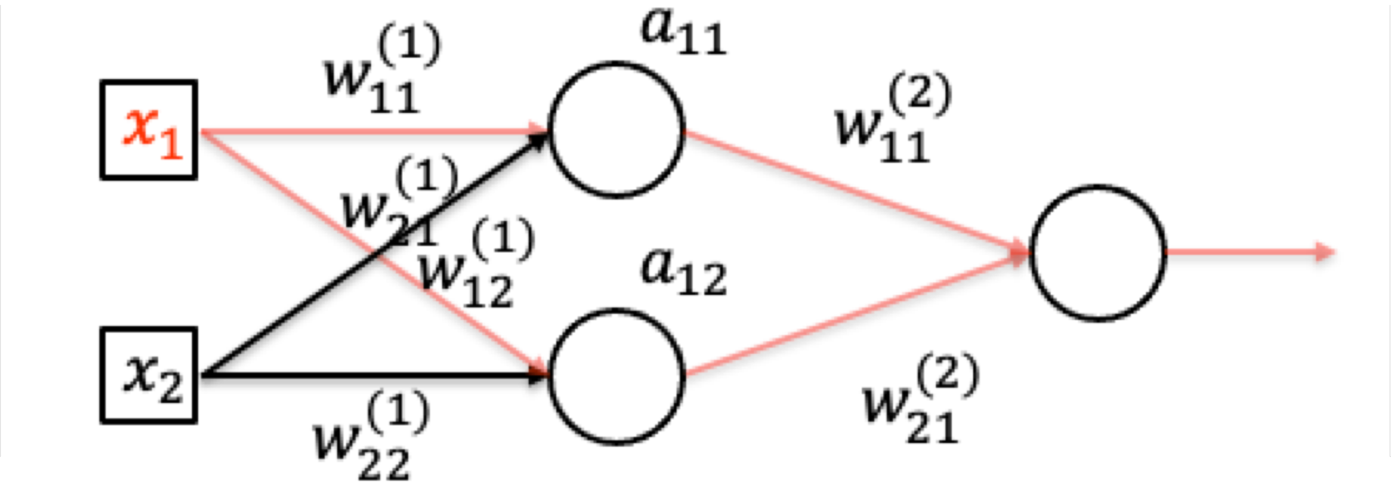


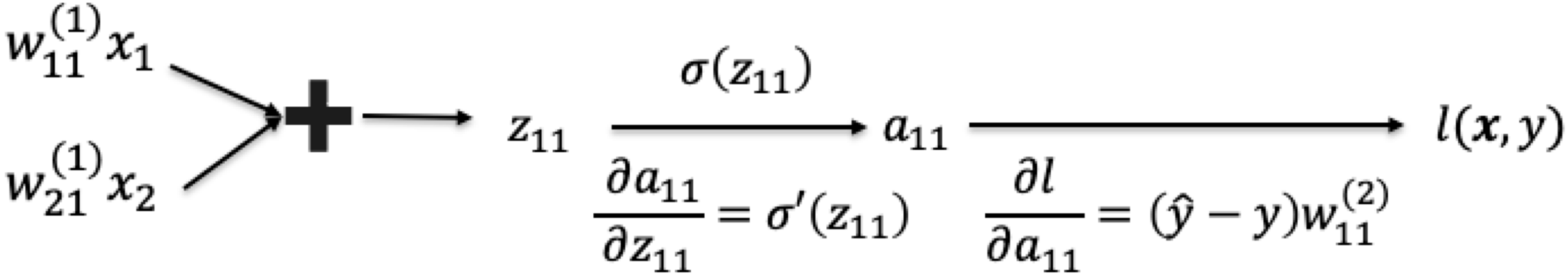


$$\frac{\partial a_{11}}{\partial z_{11}} = \sigma'(z_{11}) \qquad \frac{\partial l}{\partial a_{11}} = (\hat{y} - y)w_{11}^{(2)}$$

- 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





$$w_{11}^{(1)}x_1 \quad w_{21}^{(1)}x_2 \quad + \longrightarrow z_{11} \xrightarrow{\sigma(z_{11})} a_{11} \longrightarrow l(x, y)$$

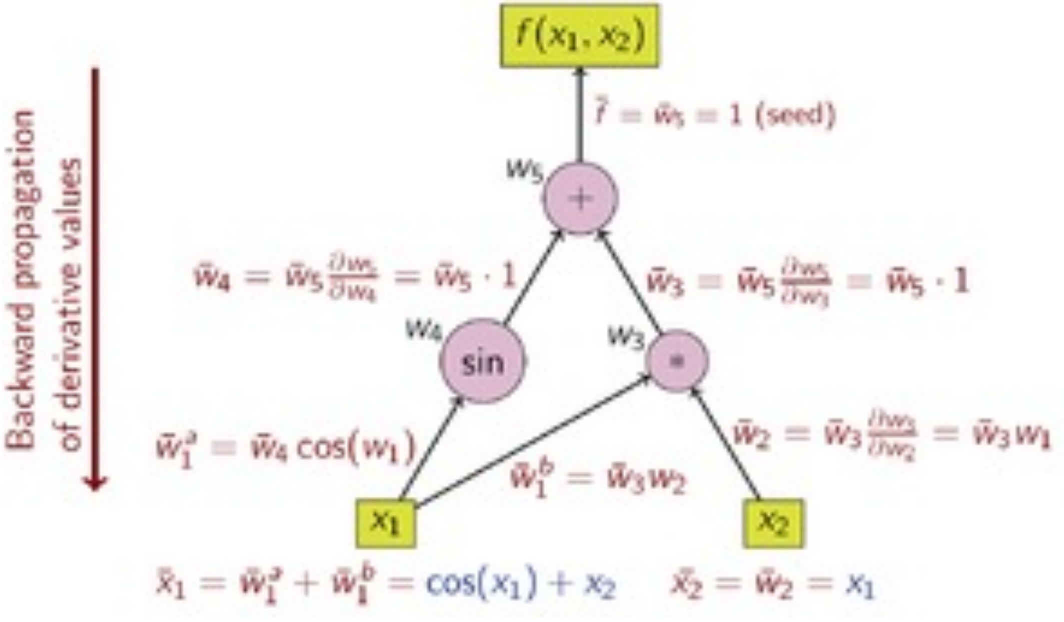
$$\frac{\partial a_{11}}{\partial z_{11}} = \sigma'(z_{11}) \qquad \frac{\partial l}{\partial a_{11}} = (\hat{y} - y)w_{11}^{(2)}$$

- By chain rule:

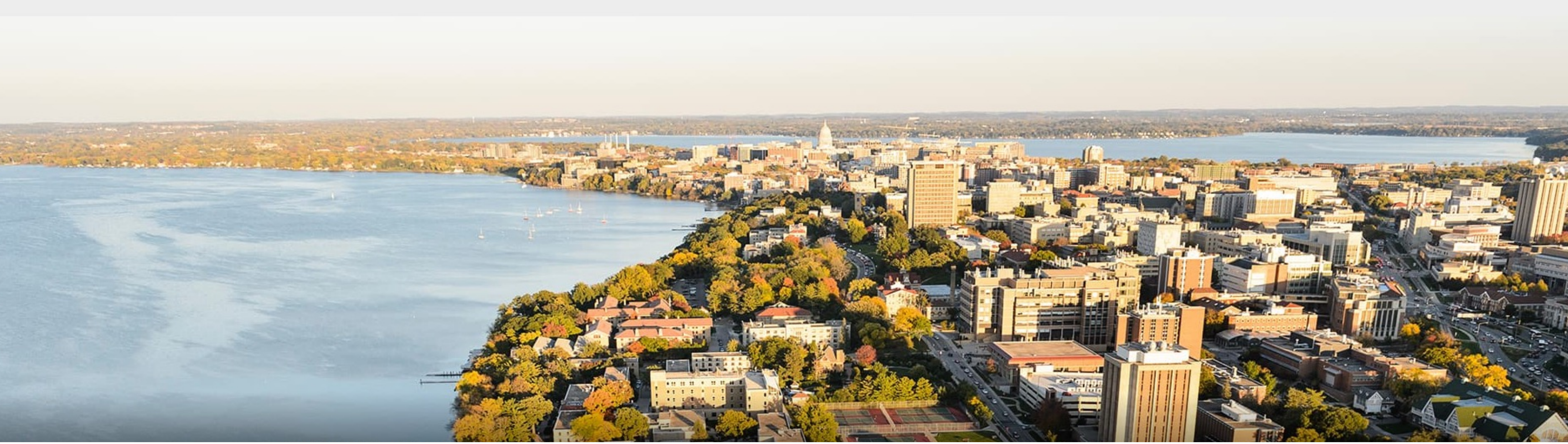
$$\frac{\partial l}{\partial x_1} = \frac{\partial l}{\partial a_{11}}\frac{\partial a_{11}}{\partial x_1} + \frac{\partial l}{\partial a_{12}}\frac{\partial a_{12}}{\partial x_1}$$

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
- Go backwards from top to bottom, recursively computing gradients



Wiki



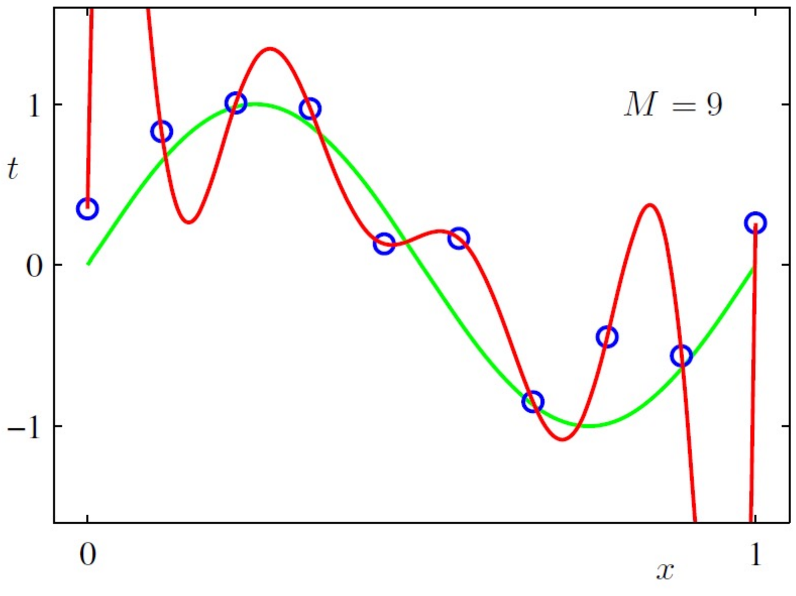
Break & Quiz

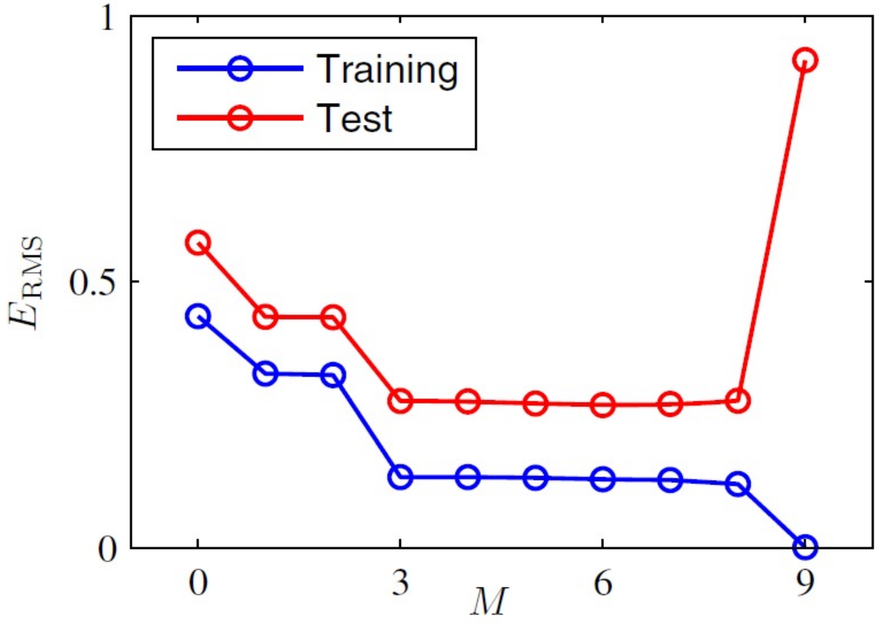
Outline

- **Neural Networks**
  - Introduction, Setup, Components, Activations
- **Training Neural Networks**
  - SGD, Computing Gradients, Backpropagation
- **Regularization**
  - Views, Data Augmentation, Other approaches

Review: Overfitting

- What is it? When empirical loss and expected loss are different
- Possible solutions:
  - Larger data set
  - Throwing away useless hypotheses also helps (**regularization**)





Review: Regularization

- In general: any method to **prevent overfitting** or **help optimization**

- One approach: additional terms in the optimization objective

- Different “views”
  - Hard constraint,
  - Soft constraint,
  - Bayesian view

Regularization: Hard Constraint View

- Training objective / parametrized version

$$\min_{f} \hat{L}(f) = \frac{1}{n}\sum_{i=1}^{n} l(f, x_i, y_i)$$

subject to: $f \in \boldsymbol{\mathcal{H}}$

$$\min_{\theta} \hat{L}(\theta) = \frac{1}{n}\sum_{i=1}^{n} l(\theta, x_i, y_i)$$

subject to: $\theta \in \Omega$

- When Ω measured by some quantity R

$$\min_{\theta} \hat{L}(\theta) = \frac{1}{n}\sum_{i=1}^{n} l(\theta, x_i, y_i)$$

subject to: $R(\theta) \leq r$

$$\min_{\theta} \hat{L}(\theta) = \frac{1}{n}\sum_{i=1}^{n} l(\theta, x_i, y_i)$$

subject to: $||\theta||_2^2 \leq r^2$

L2 Regularization

Regularization: Soft Constraint View

- Equivalent to, for some parameter $\lambda^* > 0$

$$\min_{\theta} \hat{L}_R(\theta) = \frac{1}{n}\sum_{i=1}^{n} l(\theta, x_i, y_i) + \lambda^* R(\theta)$$

- For L2,

$$\min_{\theta} \hat{L}_R(\theta) = \frac{1}{n}\sum_{i=1}^{n} l(\theta, x_i, y_i) + \lambda^* ||\theta||_2^2$$

- Comes from **Lagrangian duality**

Regularization: Bayesian Prior View

- Recall our MAP version of training. Bayes law:

$$p(\theta \mid \{x_i, y_i\}) = \frac{p(\theta)p(\{x_i, y_i\}|\theta)}{p(\{x_i, y_i\})}$$

- MAP:

$$\max_{\theta} \log p(\theta \mid \{x_i, y_i\}) = \min_{\theta} - \underbrace{\log p(\theta)}_{\text{Regularization}} - \underbrace{\log p(\{x_i, y_i\} \mid \theta)}_{\text{MLE loss}}$$

- L2: Corresponds to normal $p(x \mid y, \theta)$, **normal prior** $p(\theta)$

Choice of View?

- Typical choice for optimization: soft-constraint

$$\min_{\theta} \hat{L}_R(\theta) = \hat{L}(\theta) + \lambda R(\theta)$$

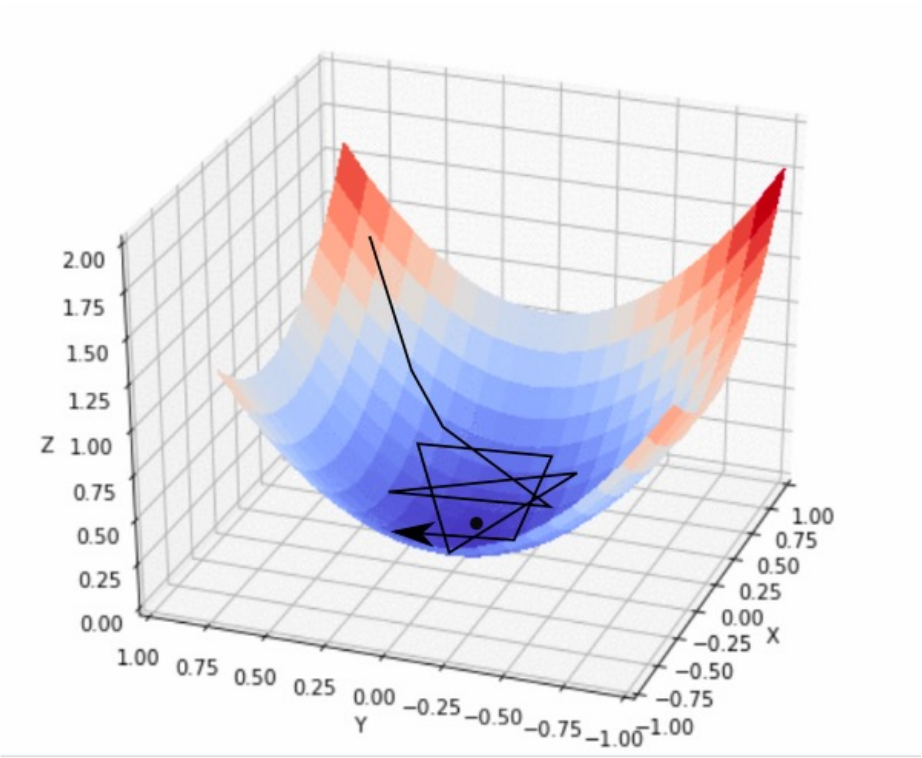
- Hard constraint / Bayesian view: conceptual / for derivation
- Hard-constraint preferred if
  - Know the explicit bound $R(\theta) \leq r$
- Bayesian view preferred if
  - Domain knowledge easy to represent as a prior

Examples: L2 Regularization

- Again,

$$\min_{\theta} \hat{L}_R(\theta) = \hat{L}(\theta) + \frac{\lambda}{2} ||\theta||_2^2$$

- Questions: what are the
  - Effects on (stochastic) gradient descent?
  - Effects on the optimal solution?



L2 Regularization: **Effect on GD**

- Gradient of regularized objective

$$\nabla\hat{L}_R(\theta) = \nabla\hat{L}(\theta) + \lambda\theta$$

- Gradient descent update

$$\theta \leftarrow \theta - \eta\nabla\hat{L}_R(\theta) = \theta - \eta\,\nabla\hat{L}(\theta) - \eta\lambda\theta$$

$$= (1-\eta\lambda)\theta - \eta\,\nabla\hat{L}(\theta)$$

- In words, **weight decay**

L2 Regularization: **Effect on Optimal Solution**

- Consider a quadratic approximation around θ^*

$$\hat{L}(\theta) \approx \hat{L}(\theta^*) + (\theta - \theta^*)^T \nabla \hat{L}(\theta^*) + \frac{1}{2}(\theta - \theta^*)^T H (\theta - \theta^*)$$

- Since θ^* is optimal, $\nabla \hat{L}(\theta^*) = 0$

$$\hat{L}(\theta) \approx \hat{L}(\theta^*) + \frac{1}{2}(\theta - \theta^*)^T H (\theta - \theta^*)$$

$$\nabla \hat{L}(\theta) \approx H(\theta - \theta^*)$$

L2 Regularization: **Effect on Optimal Solution**

- Gradient of regularized objective: $\nabla \hat{L}_R(\theta) \approx H(\theta - \theta^*) + \lambda\theta$

- On the optimal θ_R^*: $0 = \nabla \hat{L}_R(\theta_R^*) \approx H(\theta_R^* - \theta^*) + \lambda\theta_R^*$

$$\theta_R^* \approx (H + \lambda I)^{-1} H\theta^*$$

- H has eigendecomp. $H = Q\Lambda Q^T$, assume $(\Lambda + \lambda I)^{-1}$ exists:

$$\theta_R^* \approx (H + \lambda I)^{-1} H\theta^* = Q(\Lambda + \lambda I)^{-1}\Lambda Q^T\theta^*$$

- Effect: **rescale along eigenvectors of *H***

L2 Regularization: **Effect on Optimal Solution**

Effect: rescale along eigenvectors of H

Visual Example:

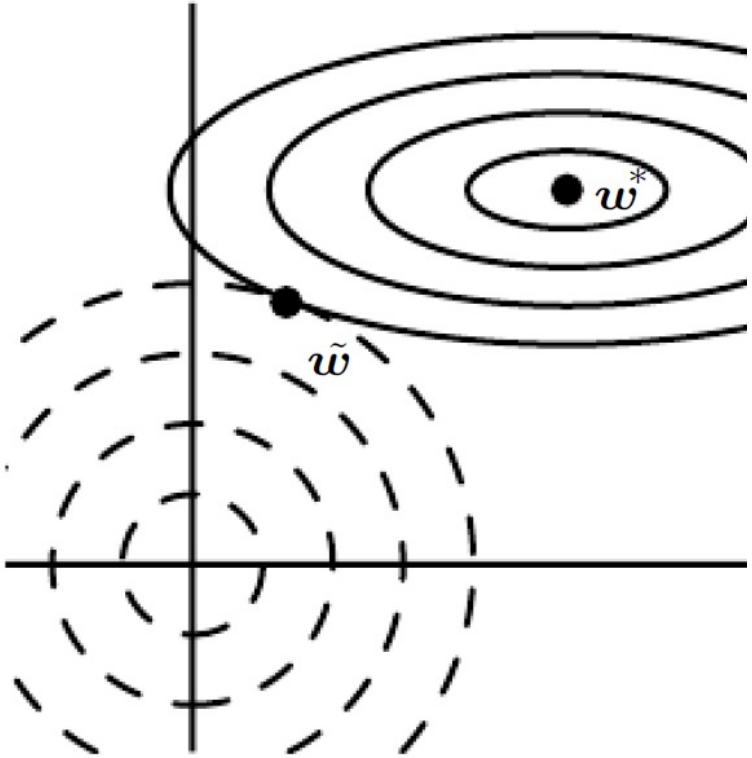


Figure from *Deep Learning*,
Goodfellow, Bengio and Courville

L1 Regularization: **Effect on GD**

$$\min_{\theta} \hat{L}_R(\theta) = \hat{L}(\theta) + \lambda||\theta||_1$$

- Effect on (stochastic) gradient descent:
- Gradient of regularized objective

$$\nabla\hat{L}_R(\theta) = \nabla\hat{L}(\theta) + \lambda\text{sign}(\theta)$$

where **sign** applies to each element in θ

- Gradient descent update

$$\theta \leftarrow \theta - \eta\nabla\hat{L}_R(\theta) = \theta - \eta\,\nabla\hat{L}(\theta) - \eta\lambda\text{sign}(\theta)$$

L1 Regularization: **Effect on Optimal Solution**

- Again,

$$\hat{L}(\theta) \approx \hat{L}(\theta^*) + \frac{1}{2}(\theta - \theta^*)^T H(\theta - \theta^*)$$

- Further assume that H is diagonal and positive $(H_{ii} > 0, \forall i)$
  - **not true in general** but assume for getting some intuition

- The regularized objective is (ignoring constants)

$$\hat{L}_R(\theta) \approx \sum_i \frac{1}{2} H_{ii}(\theta_i - \theta_i^*)^2 + \lambda|\theta_i|$$

L1 Regularization: **Effect on Optimal Solution**

- The regularized objective is (ignoring constants)

$$\hat{L}_R(\theta) \approx \sum_i \frac{1}{2} H_{ii}(\theta_i - \theta_i^*)^2 + \lambda|\theta_i|$$

- The optimal θ_R^*

$$(\theta_R^*)_i \approx \begin{cases} \max\left\{\theta_i^* - \dfrac{\lambda}{H_{ii}}, 0\right\} & \text{if } \theta_i^* \geq 0 \\ \min\left\{\theta_i^* + \dfrac{\lambda}{H_{ii}}, 0\right\} & \text{if } \theta_i^* < 0 \end{cases}$$

- Compact expression for the optimal θ_R^*

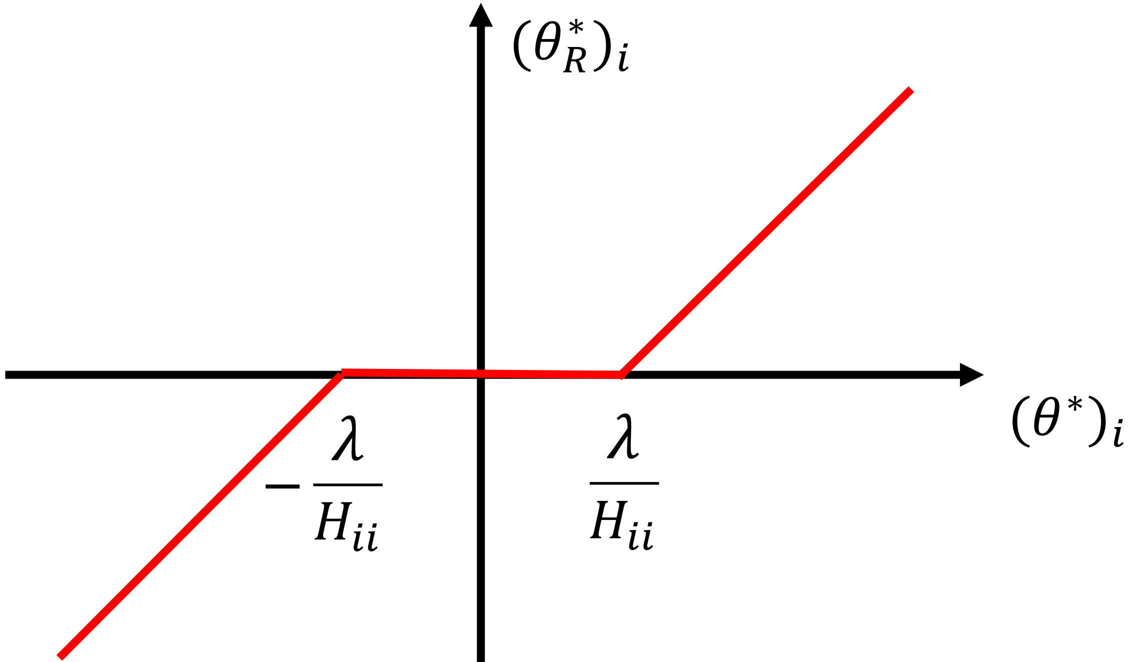
$$(\theta_R^*)_i \approx \operatorname{sign}(\theta_i^*) \max\{|\theta_i^*| - \frac{\lambda}{H_{ii}}, 0\}$$

L1 Regularization: **Effect on Optimal Solution**

- The optimal θ_R^*

$$(\theta_R^*)_i \approx \begin{cases} \max\left\{\theta_i^* - \frac{\lambda}{H_{ii}}, 0\right\} & \text{if } \theta_i^* \geq 0 \\ \min\left\{\theta_i^* + \frac{\lambda}{H_{ii}}, 0\right\} & \text{if } \theta_i^* < 0 \end{cases}$$

- Effect: **induces sparsity**



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, Sharon Li