

Logistics

- Homework 1 grades will be returned today
- **NEW:** starting Homework 2, we will take off one point if questions are not matched to pages on Gradescope
- Midterm: October 22nd
 - covers material through October 15th
 - mix of short answer and derivations
 - one double-sided 8.5x11 cheat sheet
 - review in-class on October 20th
- **NEW:** my office hours are now
 - Mondays 10:45 - 11:45
 - Tuesdays 1:20 - 2:20

Outline

- **Review: Neural Networks**

- Introduction, Setup, Components, Activations

- **Review: Training Neural Networks**

- SGD, Computing Gradients, Backpropagation

- **Regularization**

- Review, Penalties, Augmentation, Deep Net Approaches

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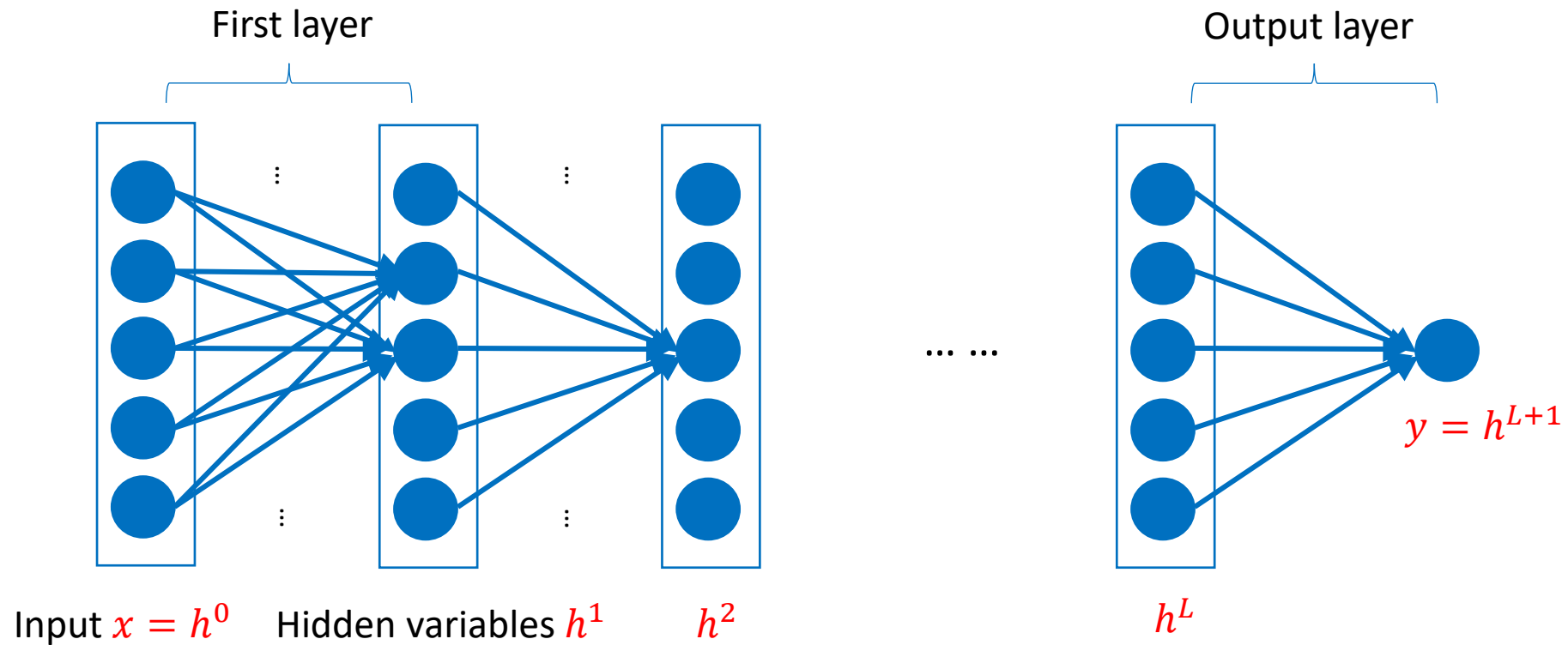
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Neural Network Components

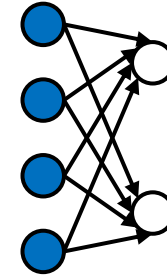
An $(L + 1)$ -layer network



Feature Encoding for NNs

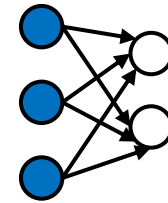
- Nominal features usually a one hot encoding

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



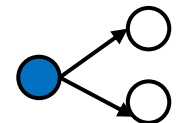
- Ordinal features: use a *thermometer* encoding

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



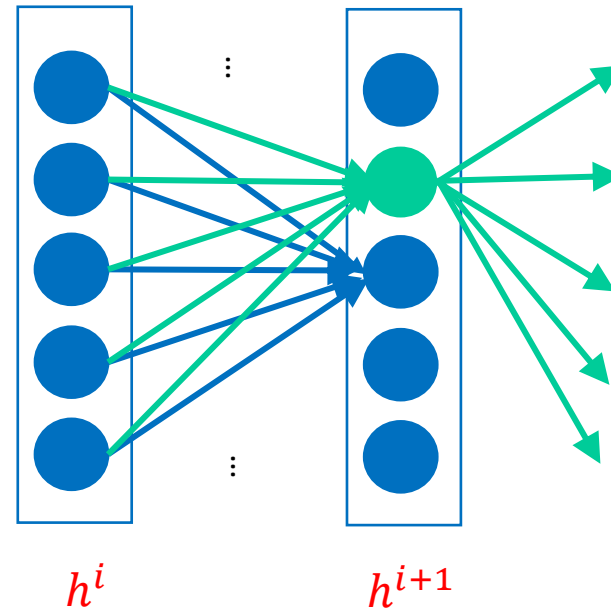
- Real-valued features use individual input units
(may want to scale/normalize them first though)

$$\text{precipitation} = [0.68]$$



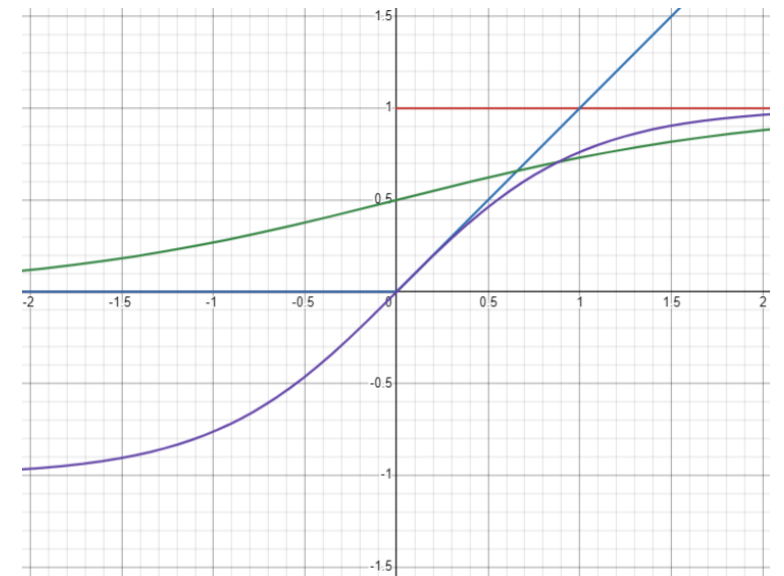
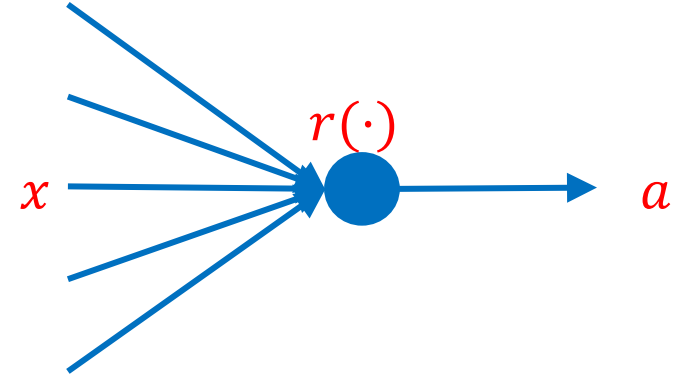
Hidden Layers

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



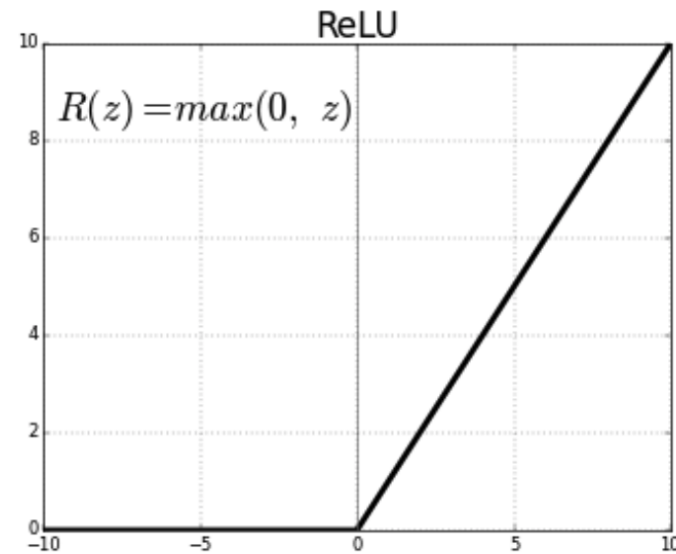
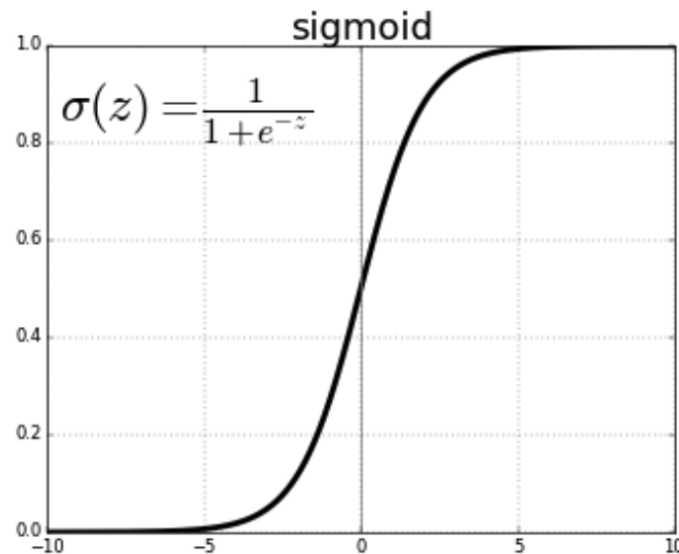
Hidden Layers

- Outputs $a = r(w^T x + b)$
- Typical activation function r
 - threshold $h(z) = 1_{\{z \geq 0\}}$
 - ReLU $\text{ReLU}(z) = z \cdot t(z) = \max\{0, z\}$
 - sigmoid $\sigma(z) = 1/(1 + \exp(-z))$
 - hyperbolic tangent $\tanh(z) = 2\sigma(2z) - 1$
- Why not **linear activation** functions?
 - Model would be linear.



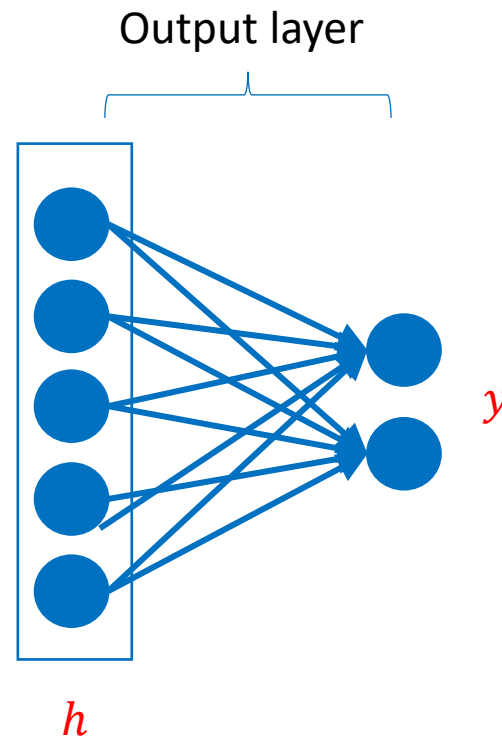
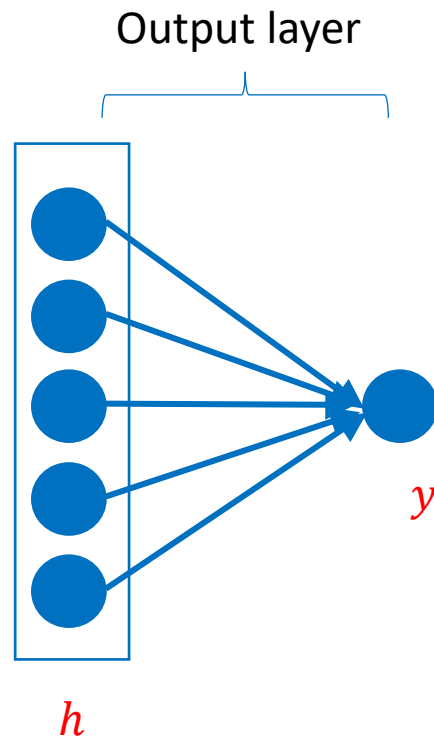
More on Activations

- Outputs $a = r(w^T x + b)$
 - Activation
 - Weight
 - Bias
- Consider **gradients**... saturating vs. nonsaturating



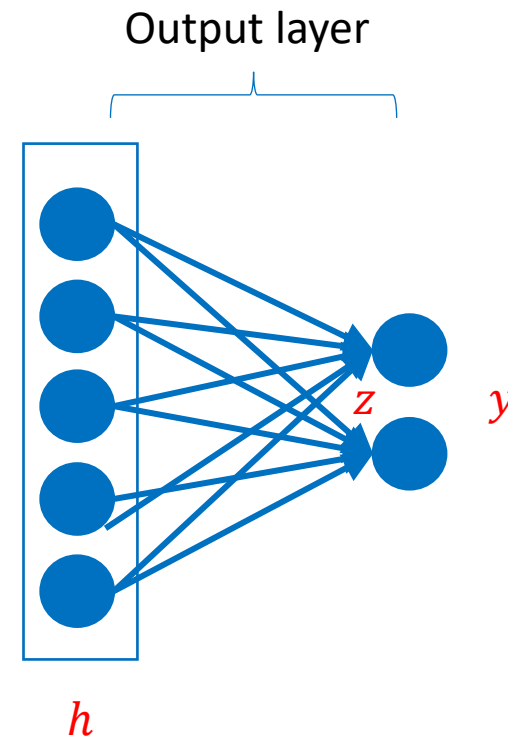
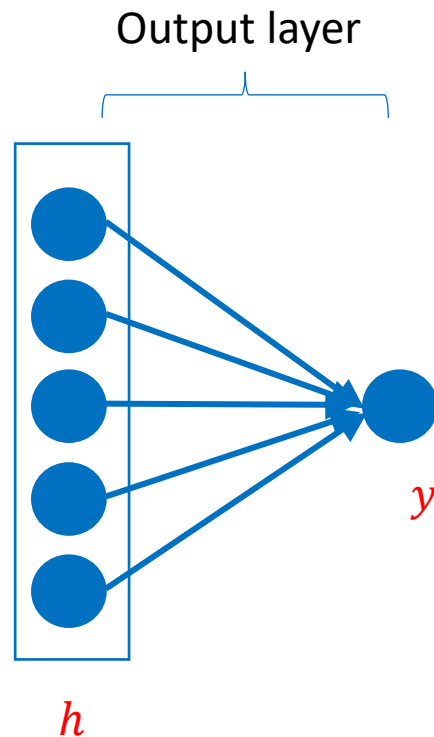
Output Layer: Examples

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



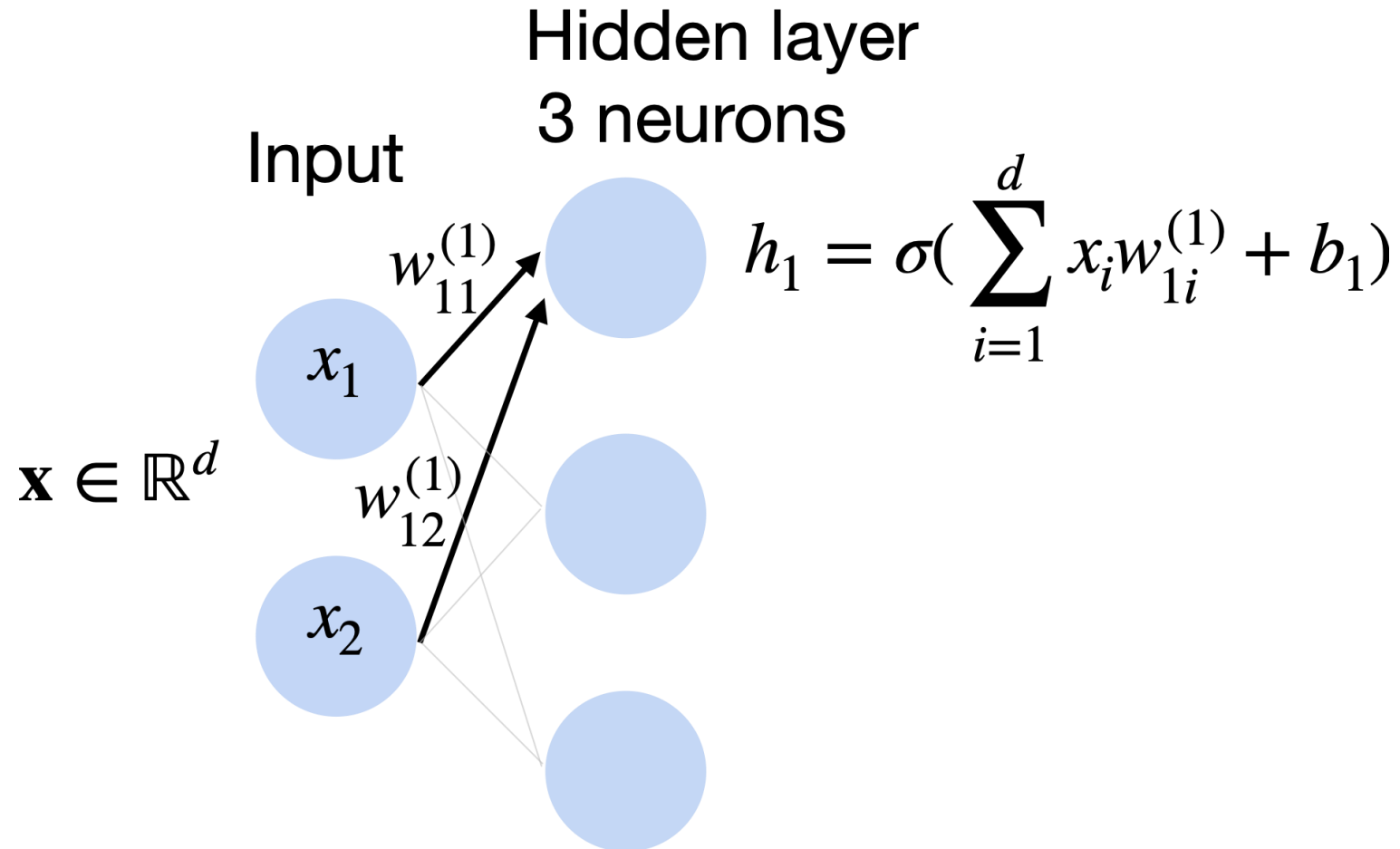
Output Layer: Examples

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



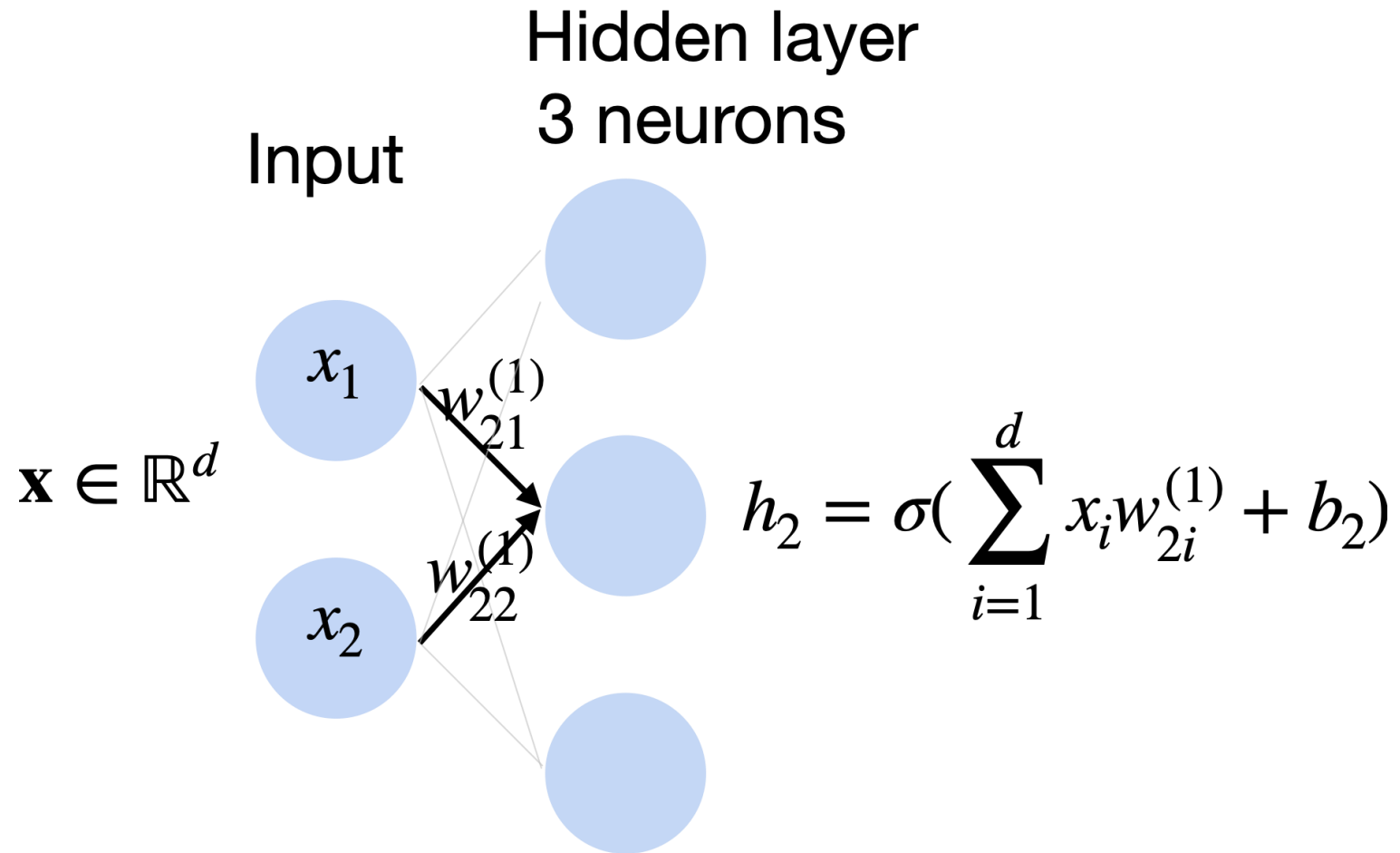
MLPs: Multilayer Perceptron

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



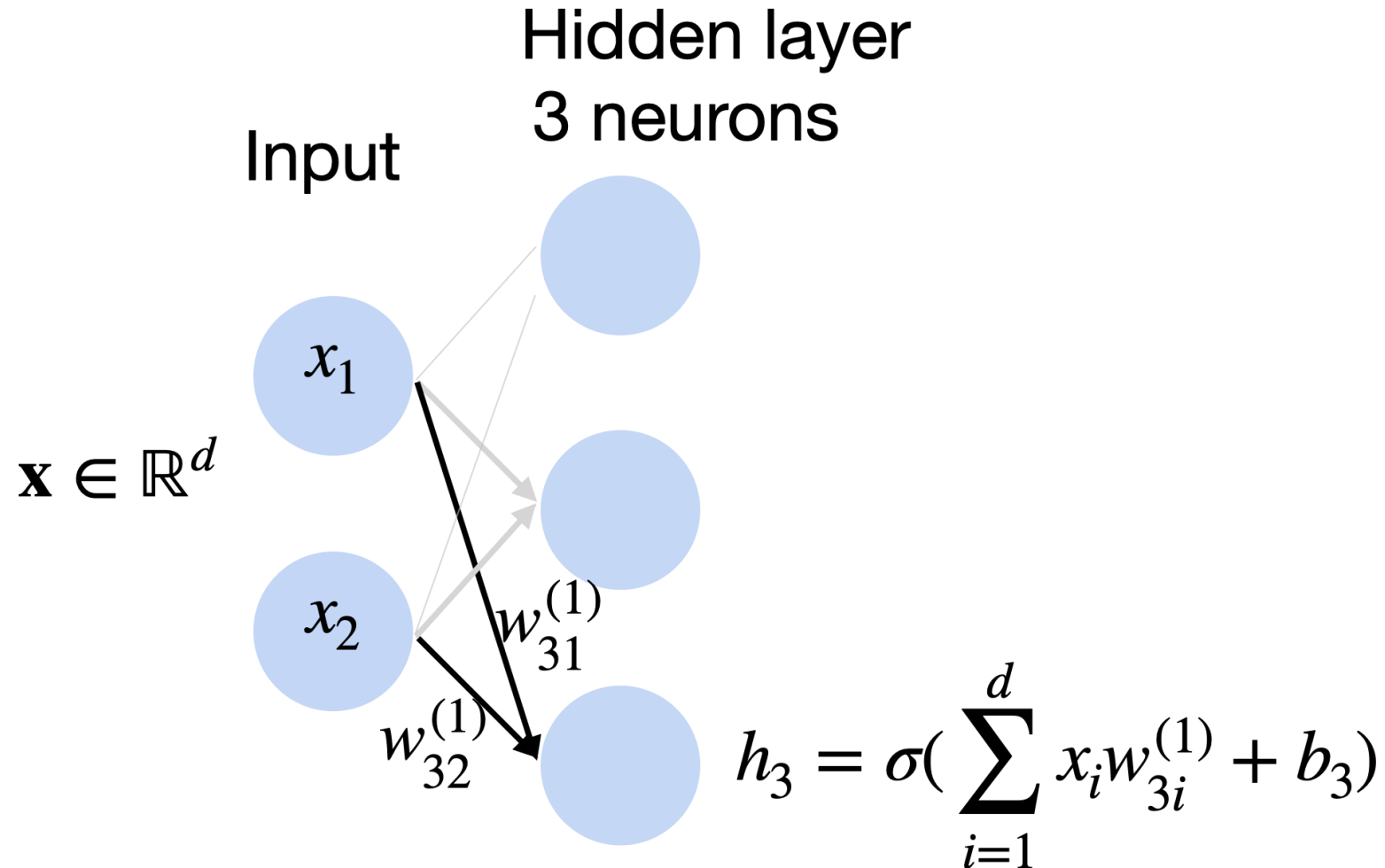
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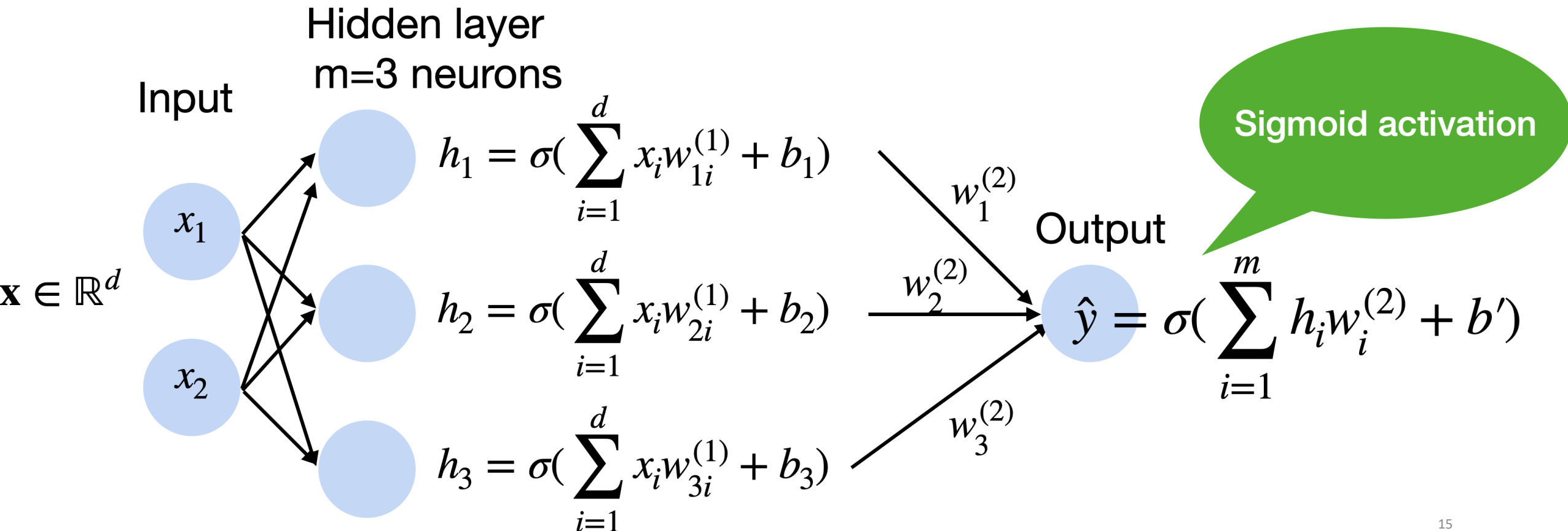
MLPs: Multilayer Perceptron

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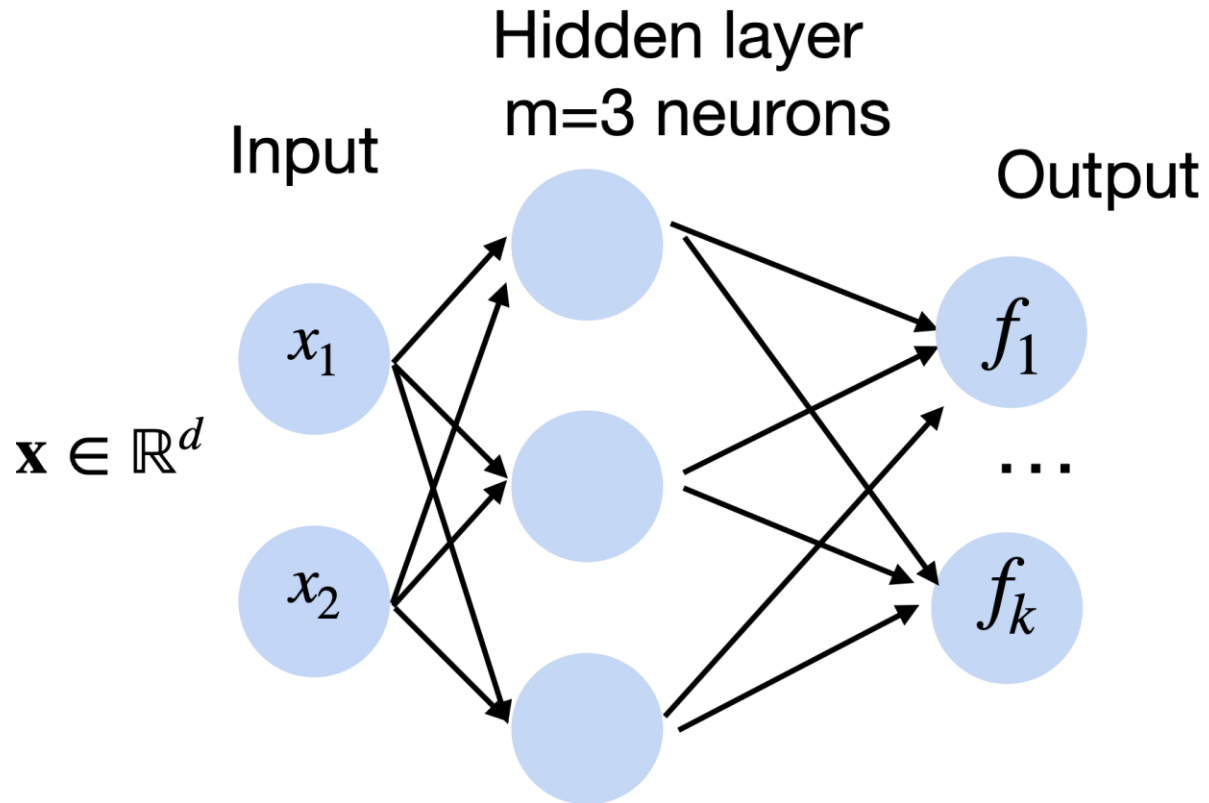
MLPs: Multilayer Perceptron

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



Multiclass Classification Output

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



$$p(y | \mathbf{x}) = \text{softmax}(f) \\ = \frac{\exp f_y(x)}{\sum_i^k \exp f_i(x)}$$





Break & Quiz

Q: Which of the following activation functions are typically **NOT** used in practice, and why not?

- a. sigmoid function $\sigma(z) = 1 / (1 + \exp(-z))$
- b. hyperbolic tangent $\tanh(z) = 2\sigma(z) - 1$
- c. threshold function $H(z) = 1_{z \geq 0}$
- d. linear (identity) function z
- e. Rectified linear unit $\text{ReLU}(z) = zH(z) = \max\{z, 0\}$

Q: Which of the following activation functions are **typically** NOT used in practice, and why not?

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- c. threshold function $H(z) = 1_{z \geq 0}$ 
- d. linear (identity) function z 
- e. Rectified linear unit $\text{ReLU}(z) = zH(z) = \max\{z, 0\}$

hard to optimize (derivative=0 everywhere except $z=0$, where it is undefined)

composition of linear functions is no more expressive than a single linear function

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Training Neural Networks

Training is done in the usual way: pick a loss and optimize it

- **Example:** 2 scalar weights

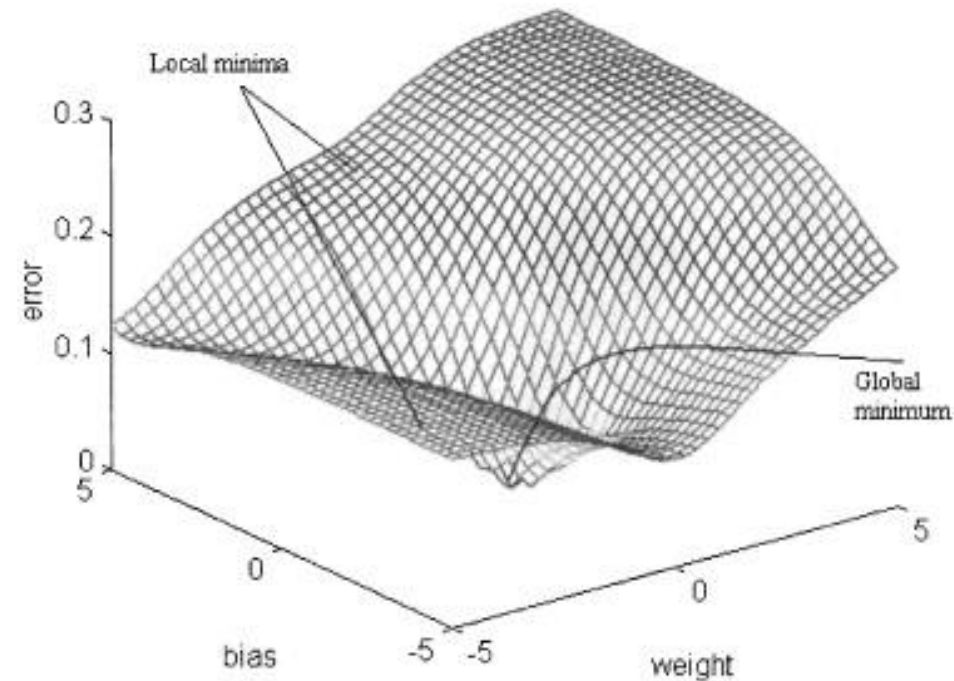


figure from Cho & Chow, *Neurocomputing* 1999

Training Neural Networks with SGD

Algorithm:

- Input dataset $D = \{(x^{(1)}, y^{(1)}), \dots, (x^{(n)}, y^{(n)})\}$
- Initialize weights
- Until stopping criterion is met:
 - For each training point $(x^{(i)}, y^{(i)})$ do
 - Compute prediction: $\hat{y}^{(i)} = f_w(x^{(i)})$ ← **Forward Pass**
 - Compute loss: $L^{(i)} = L(\hat{y}^{(i)}, y^{(i)})$ ← e.g. negative log-likelihood (NLL) loss
 $L(\hat{y}, y) = -y \log \hat{y} - (1 - y) \log(1 - \hat{y})$
 - Compute gradient: $\nabla_w L^{(i)} = (\partial_{w_1} L^{(i)}, \partial_{w_2} L^{(i)}, \dots, \partial_{w_m} L^{(i)})^T$ ← **Backward Pass**
 - Update weights: $w \leftarrow w - \alpha \nabla_w L^{(i)}$ ← **SGD step**

Training Neural Networks with minibatch SGD

Algorithm:

- Input dataset $D = \{(x^{(1)}, y^{(1)}), \dots, (x^{(n)}, y^{(n)})\}$
- Initialize weights
- Until stopping criterion is met:
 - Sample a **batch of b training points** i_1, \dots, i_b
 - Compute predictions: $\{\hat{y}^{(i_1)}, \dots, \hat{y}^{(i_b)}\} = \{f_w(x^{(i_1)}), \dots, f_w(x^{(i_b)})\}$
 - Compute avg. loss: $L^{(i_1, \dots, i_b)} = \frac{1}{b} \sum_{j=1}^b L(\hat{y}^{(i_j)}, y^{(i_j)})$
 - Compute gradient: $\nabla_w L^{(i_1, \dots, i_b)} = (\partial_{w_1} L^{(i_1, \dots, i_b)}, \dots, \partial_{w_m} L^{(i_1, \dots, i_b)})^\top$
 - Update weights: $w \leftarrow w - \alpha \nabla_w L^{(i_1, \dots, i_b)}$

Training Neural Networks: Chain Rule

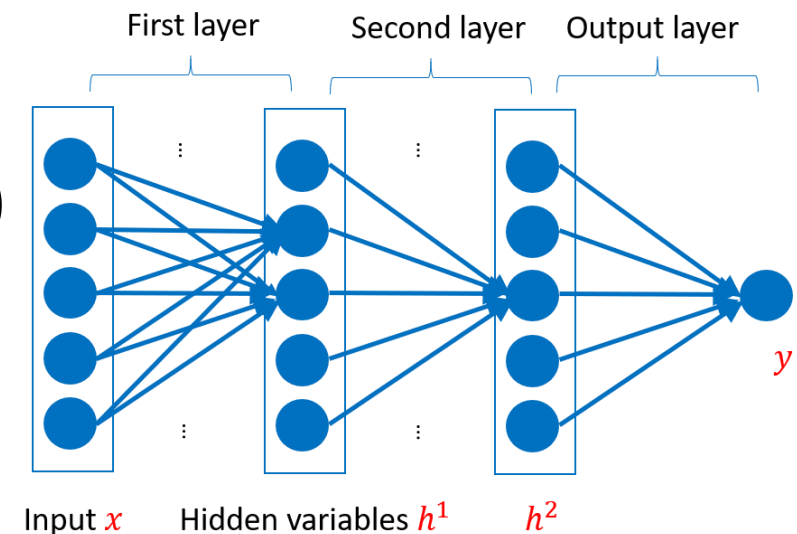
- Will need to compute terms like: $\frac{\partial L}{\partial w_1}$
- But, L is a composition of:
 - Loss with output y
 - Output itself a composition of softmax with outer layer
 - Outer layer a combination of outputs from previous layer
 - Outputs from prev. layer a composition of activations and linear functions...

- Need the **chain rule!**

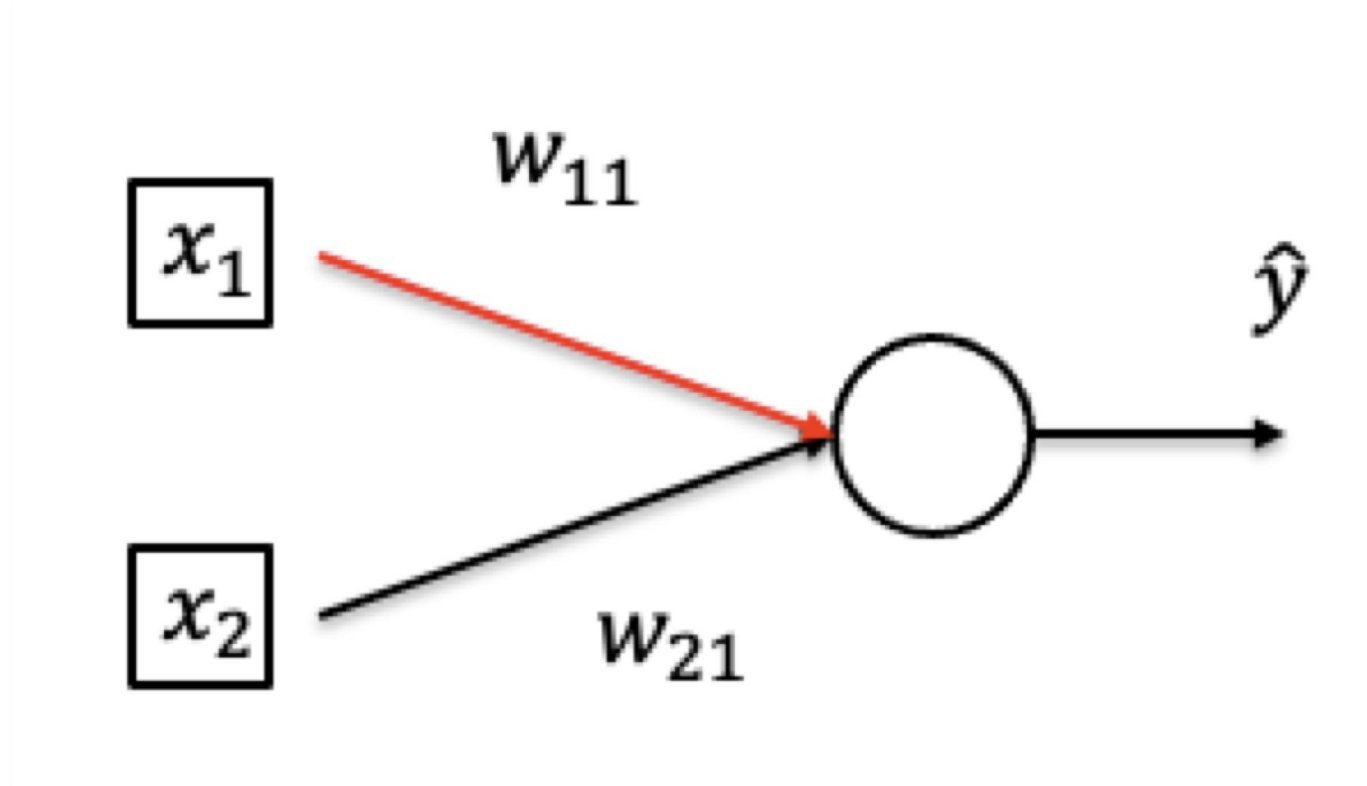
- Suppose $L = L(g_1, \dots, g_k)$ $g_j = g_j(w_1, \dots, w_p)$

- Then,

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

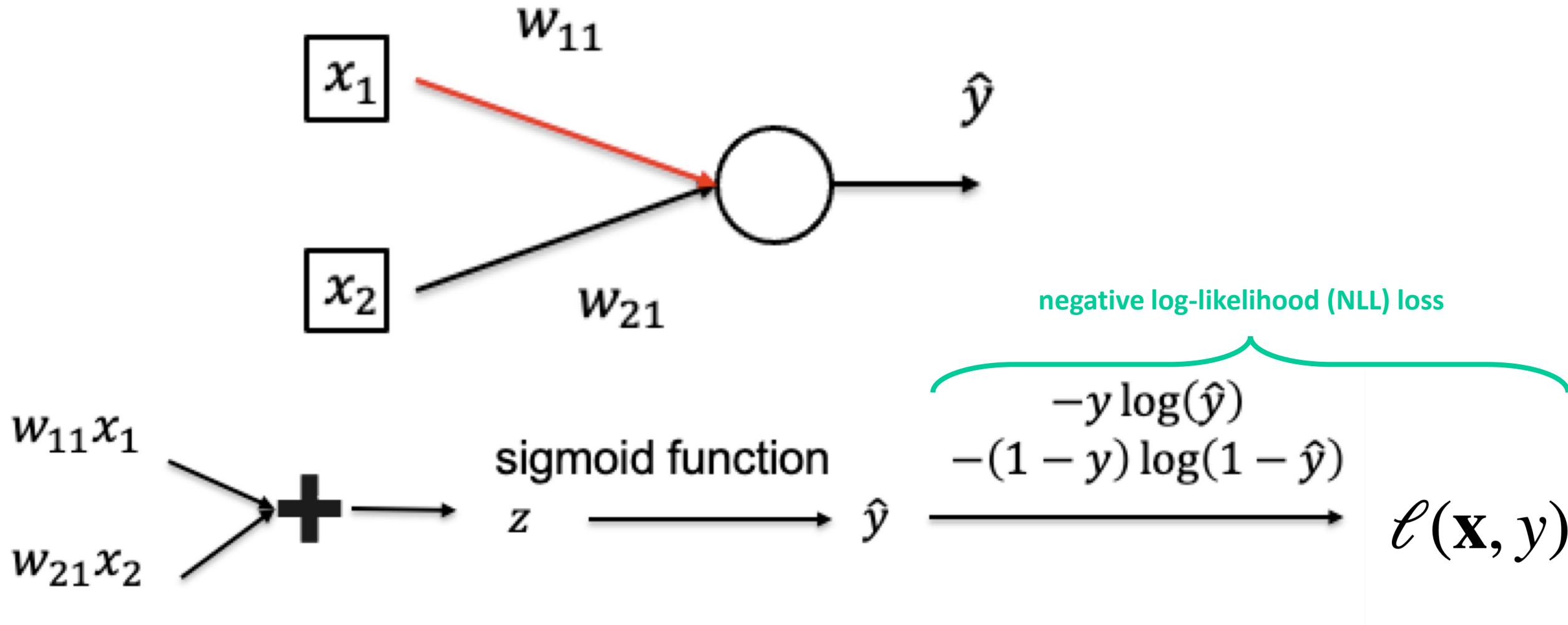


Computing Gradients

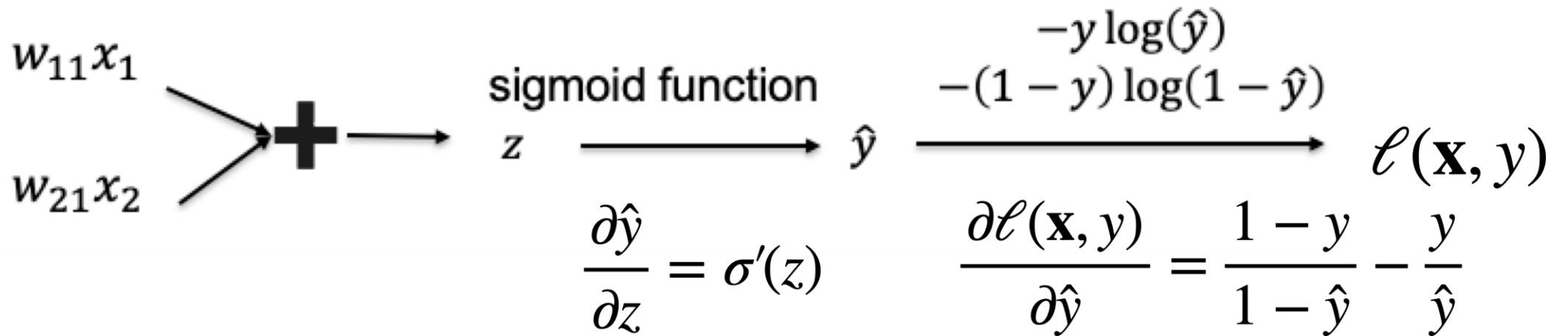
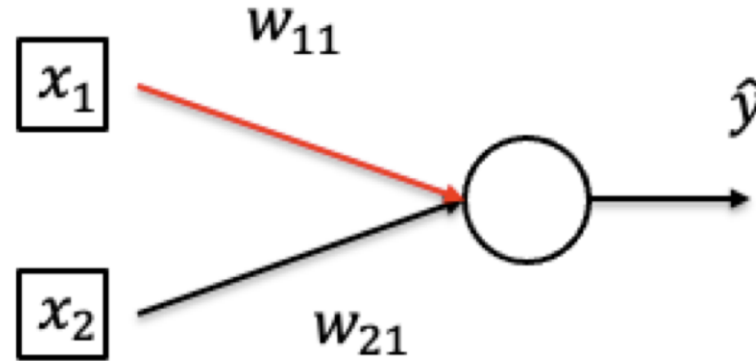


Want to compute $\frac{\partial \ell(\mathbf{x}, y)}{\partial w_{11}}$

Computing Gradients



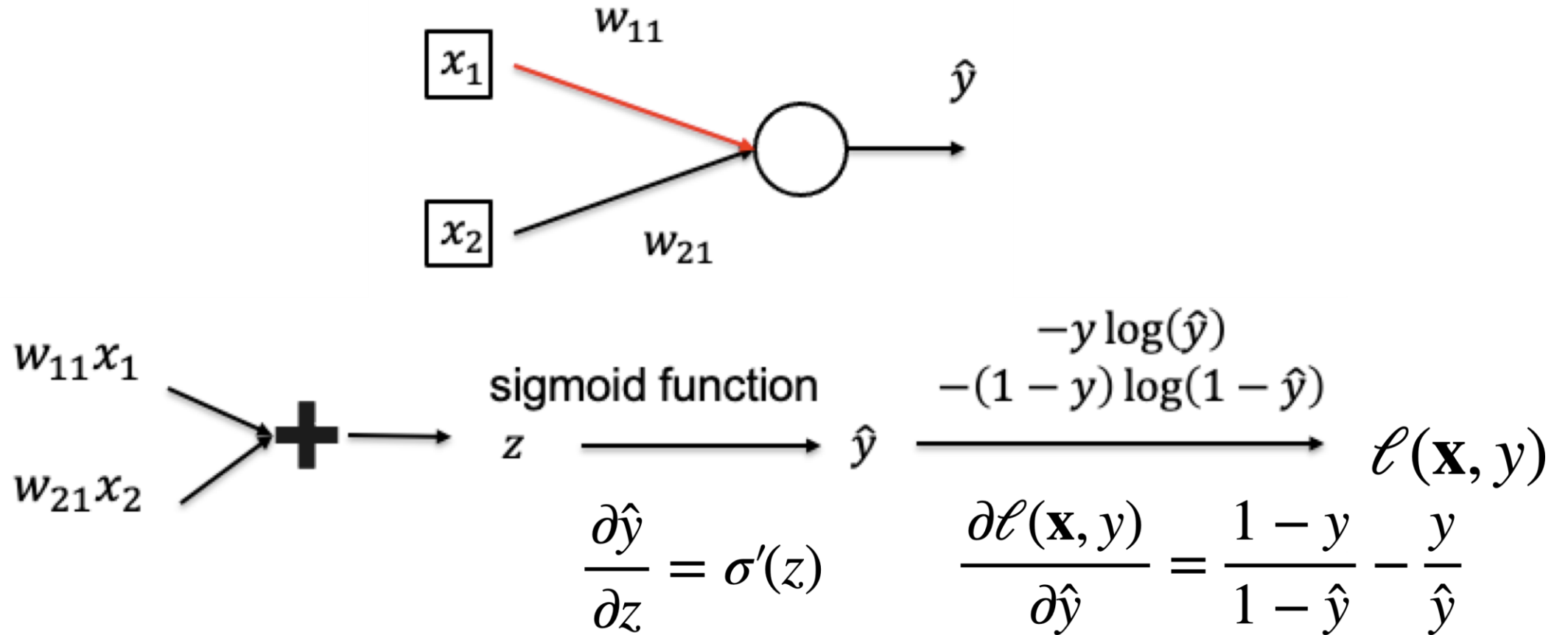
Computing Gradients



By chain rule:

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

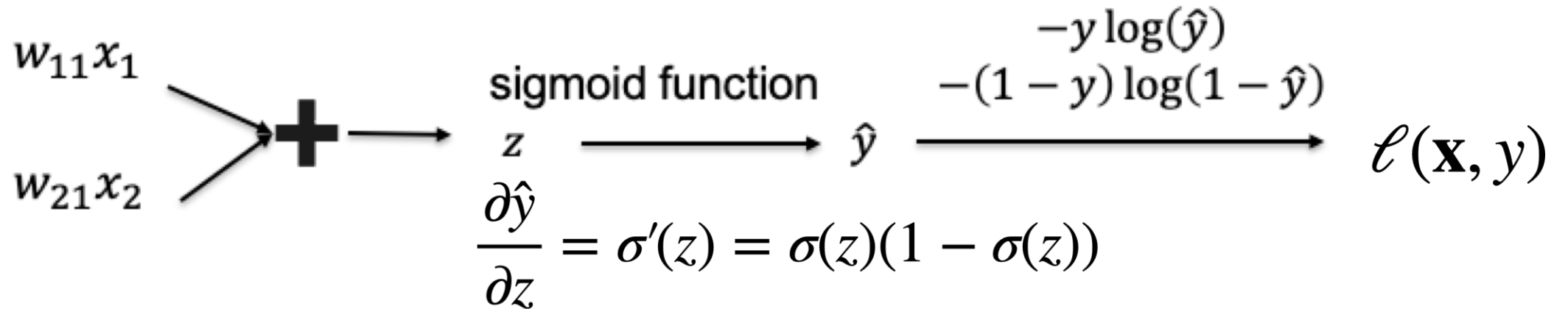
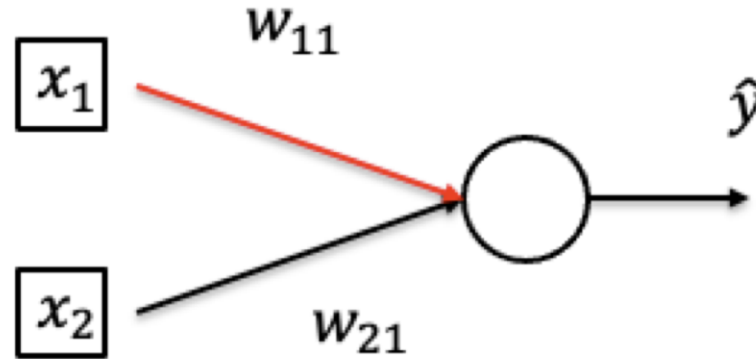
Computing Gradients



By chain rule:

$$\frac{\partial \ell}{\partial w_{11}} = \frac{\partial \ell}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial z} x_1$$

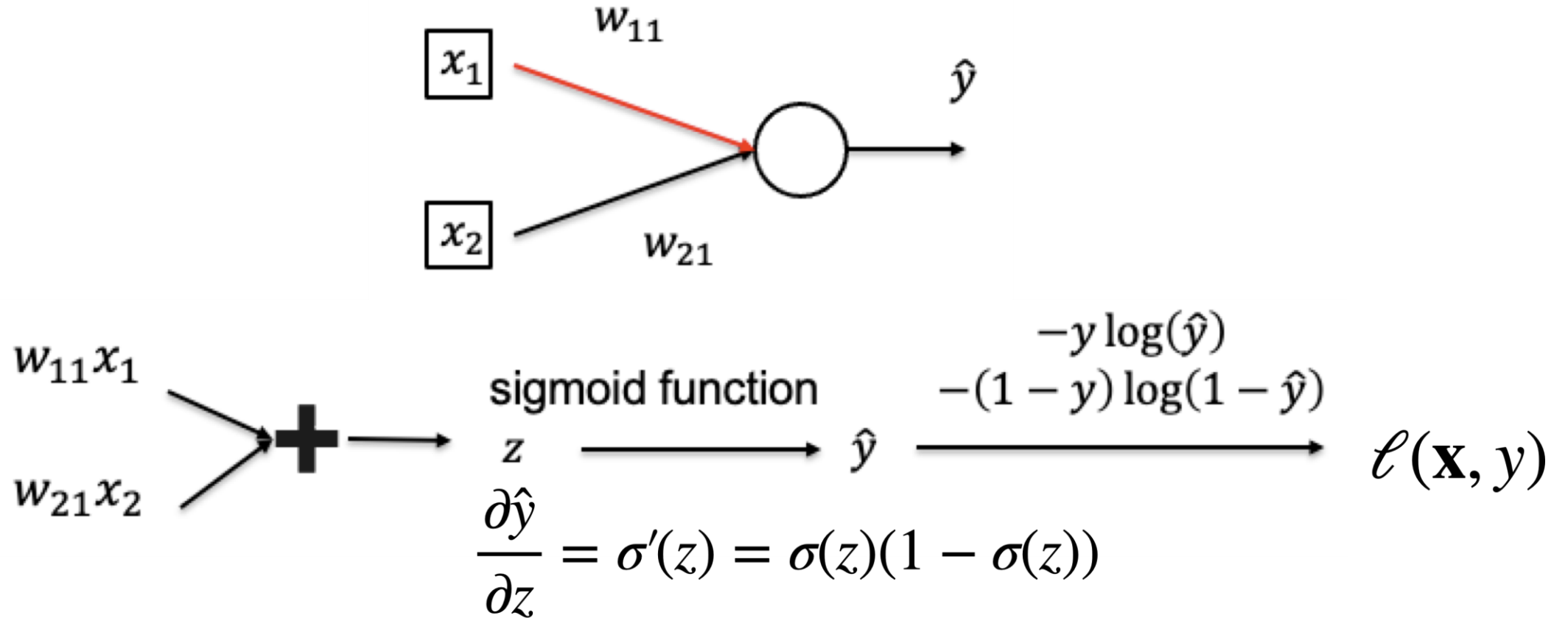
Computing Gradients



By chain rule:

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

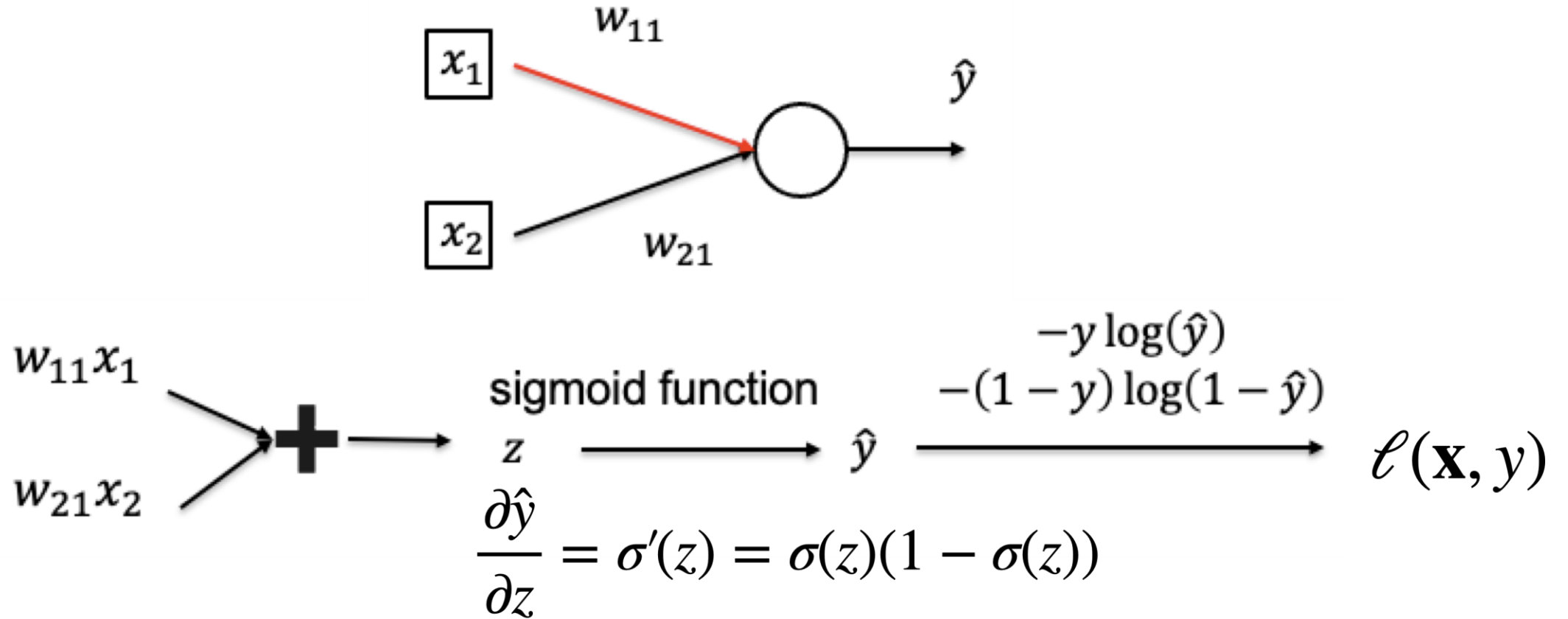
Computing Gradients



By chain rule:

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

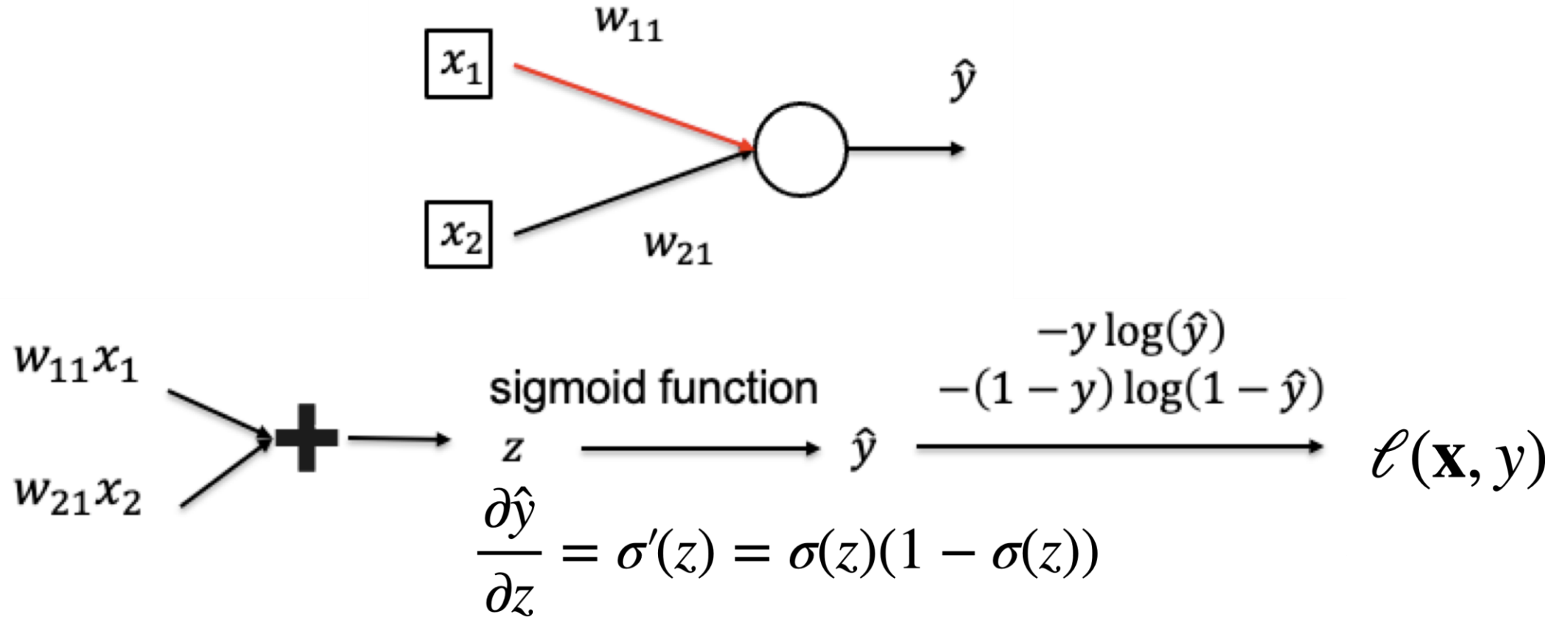
Computing Gradients



By chain rule:

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

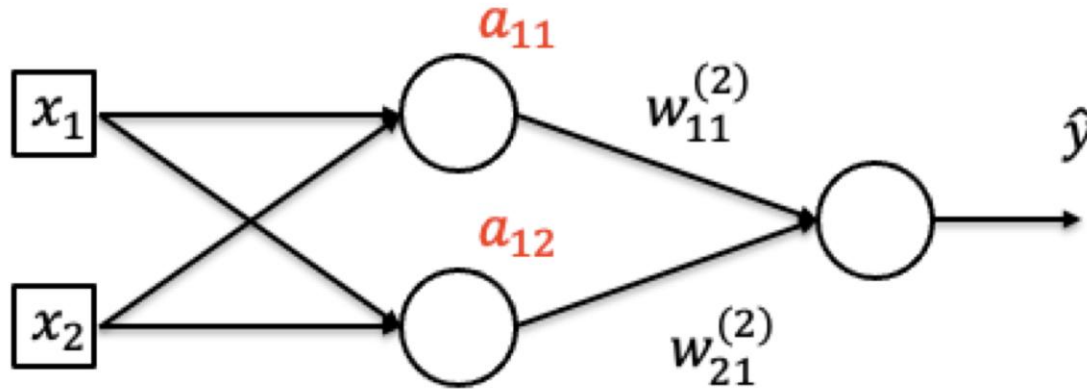
Computing Gradients



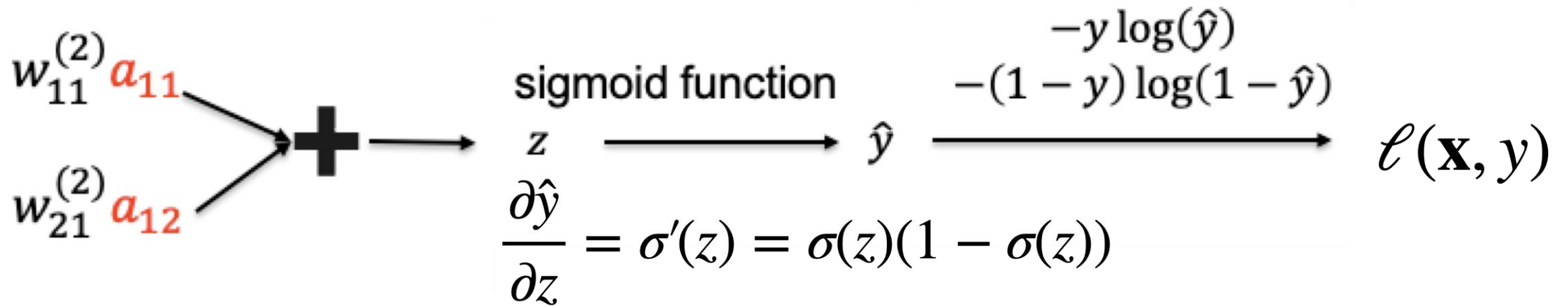
By chain rule:

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

Computing Gradients: More Layers

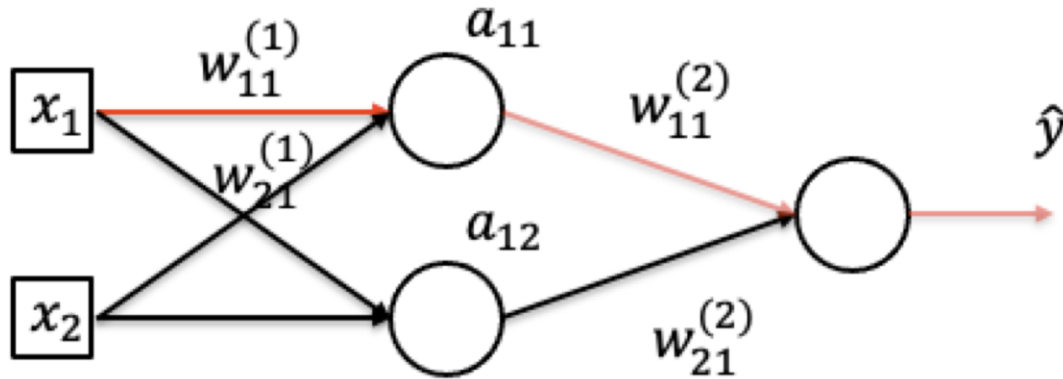


Make it deeper



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



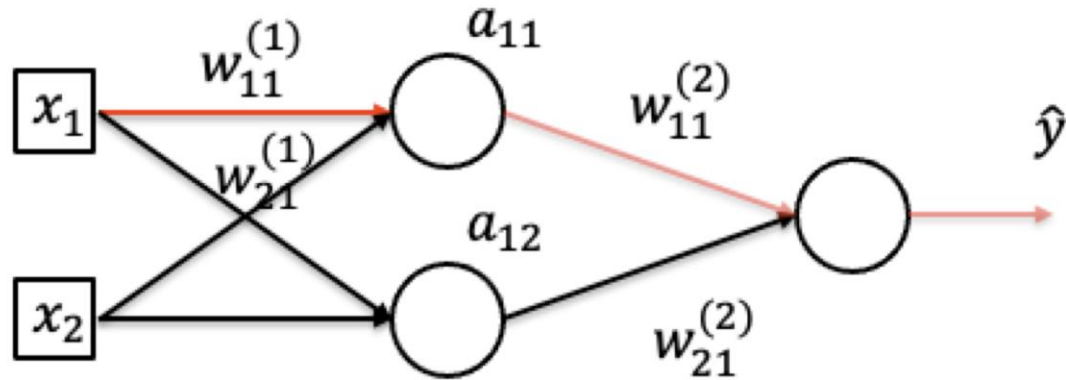
$$\begin{array}{c}
 w_{11}^{(1)} x_1 \\
 w_{21}^{(1)} x_2
 \end{array}
 \rightarrow \text{+} \rightarrow z_{11} \xrightarrow{\sigma(z_{11})} a_{11} \xrightarrow{\frac{\partial l}{\partial a_{11}} = (\hat{y} - y) w_{11}^{(2)}} l(x, y)$$

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

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



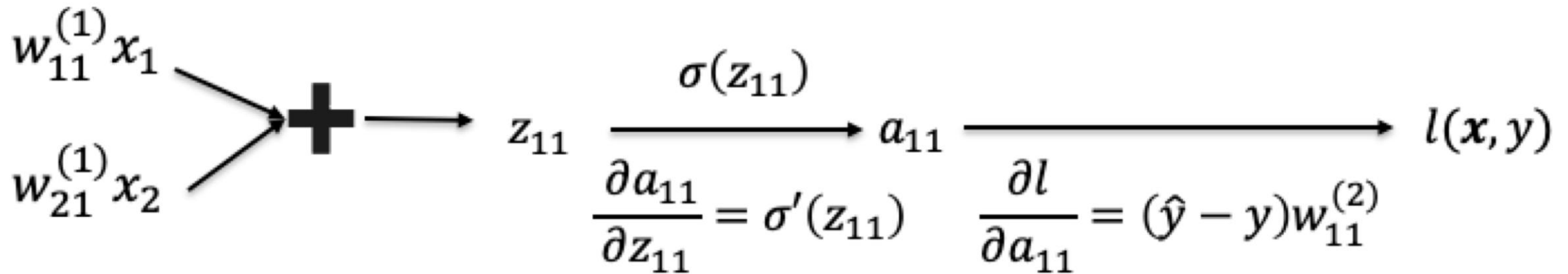
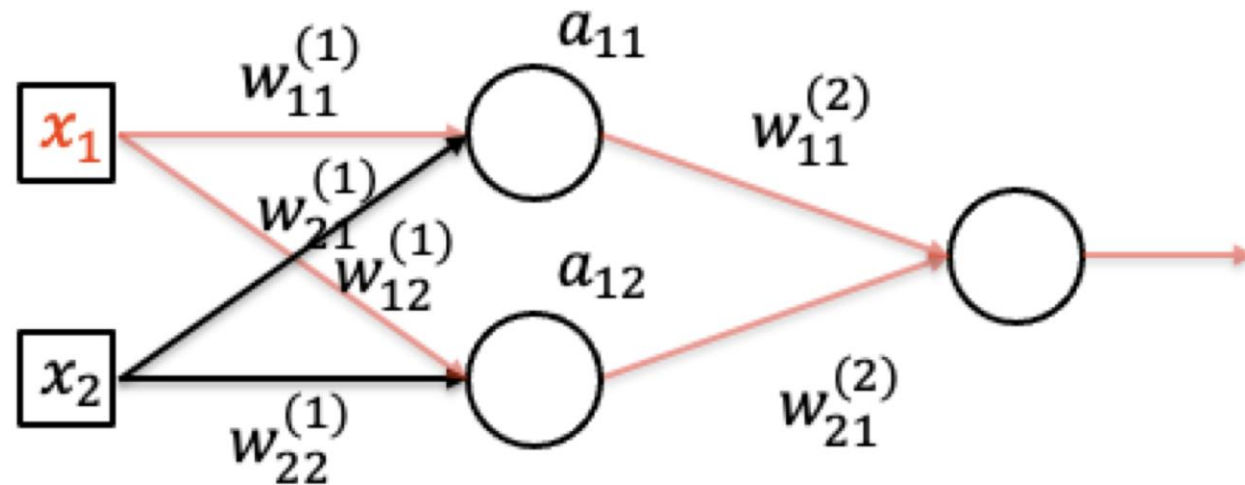
Computational graph for the forward pass of the first hidden node. Inputs $w_{11}^{(1)}x_1$ and $w_{21}^{(1)}x_2$ are summed to produce z_{11} . z_{11} is passed through the activation function σ to produce a_{11} . a_{11} is then multiplied by $w_{11}^{(2)}$ to produce the loss $l(x, y)$.

$$\begin{aligned} & w_{11}^{(1)}x_1 + w_{21}^{(1)}x_2 \rightarrow z_{11} \xrightarrow{\sigma(z_{11})} a_{11} \xrightarrow{\frac{\partial l}{\partial a_{11}} = (\hat{y} - y)w_{11}^{(2)}} l(x, y) \\ & \frac{\partial a_{11}}{\partial z_{11}} = \sigma'(z_{11}) \end{aligned}$$

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

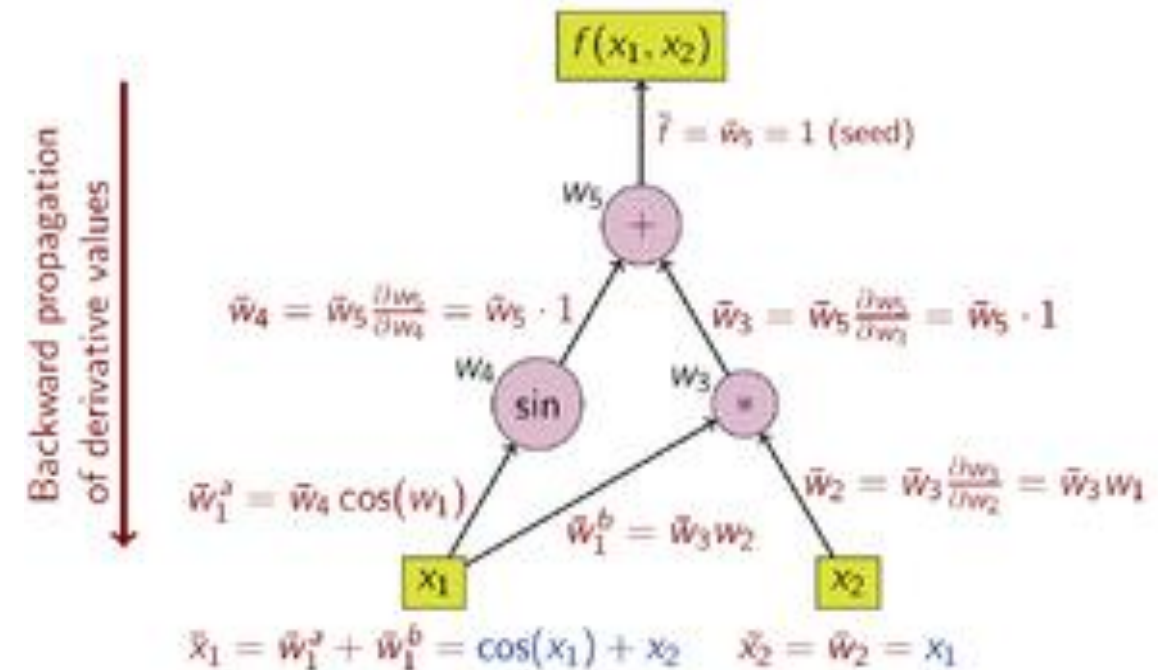


By chain rule:

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

Backpropagation

- So to compute derivative w.r.t specific weights we **propagate** loss information **back** through the network
- Today we do this by automatic differentiation (**autodiff**) for arbitrarily complex computation graphs
- Go backwards from top to bottom, recursively computing gradients



Wiki



Break & Quiz

True or False: Backprop is an optimization algorithm.

a. False; some optimization algorithms use the output of backprop.

True or False: Backprop is a weight-updating algorithm

a. False; gradient-based optimization algorithms like SGD use the output of backprop to update the weights.

True or False: Backprop is a gradient-computation algorithm

a. True

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Review: Regularization

Any method to **prevent overfitting** or **help optimization**

So far, we've seen one approach: penalty-based regularization

$$\operatorname{argmin}_{\theta} \frac{1}{n} \sum_{i=1}^n \text{loss}_i(\theta) + \lambda R(\theta)$$

- $R(\theta) = \frac{1}{2} \|\theta\|_2^2$ (Ridge)
- $R(\theta) = \|\theta\|_1$ (LASSO)

Penalty-based regularization of convex losses

Helps **prevent overfitting** by reducing the hypothesis space

- equivalent to constraint formulation for convex penalties R :

$$\operatorname{argmin}_{\theta} \frac{1}{n} \sum_{i=1}^n \text{loss}_i(\theta) + \lambda R(\theta) = \operatorname{argmin}_{R(\theta) \leq \tau} \frac{1}{n} \sum_{i=1}^n \text{loss}_i(\theta)$$

- LASSO known to yield **sparse** parameters θ

Ridge **helps optimization** by making the objective **strongly convex**

- gives objective positive curvature at every point
- gradient descent on strongly convex + smooth losses has suboptimality $O((1 - \kappa)^T)$ after T iterations, vs. $O(1/T)$ with regular convexity

Ridge (ℓ_2) regularization of general losses

- 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**

ℓ_1 regularization of general losses

- 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

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

- Effects like sparsity less well-understood than convex case

Data Augmentation

Augmentation: transform + add new samples to dataset

- Transformations: based on domain
- Idea: build **invariances** into the model
 - Ex: if all images have same alignment, model learns to use it
- Keep the label the same!



Data Augmentation: Examples

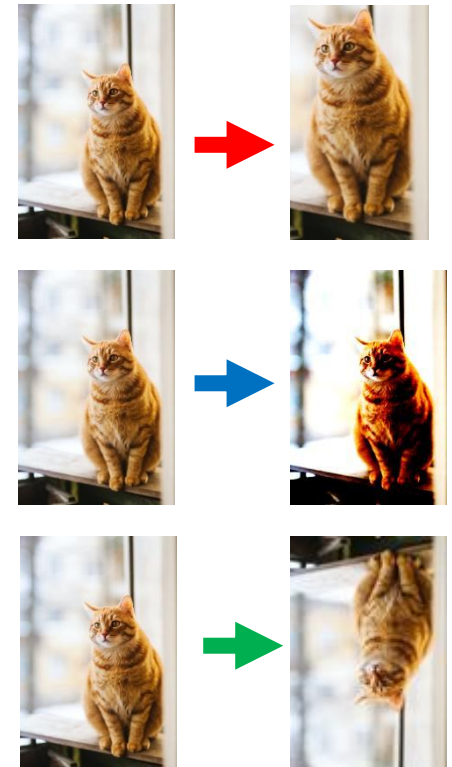
Examples of transformations for images

- **Crop** (and zoom)
- **Color** (change contrast/brightness)
- **Rotations+** (translate, stretch, shear, etc.)

Many more possibilities. Combine as well!

Q: how to know what performs best?

A: cross-validation



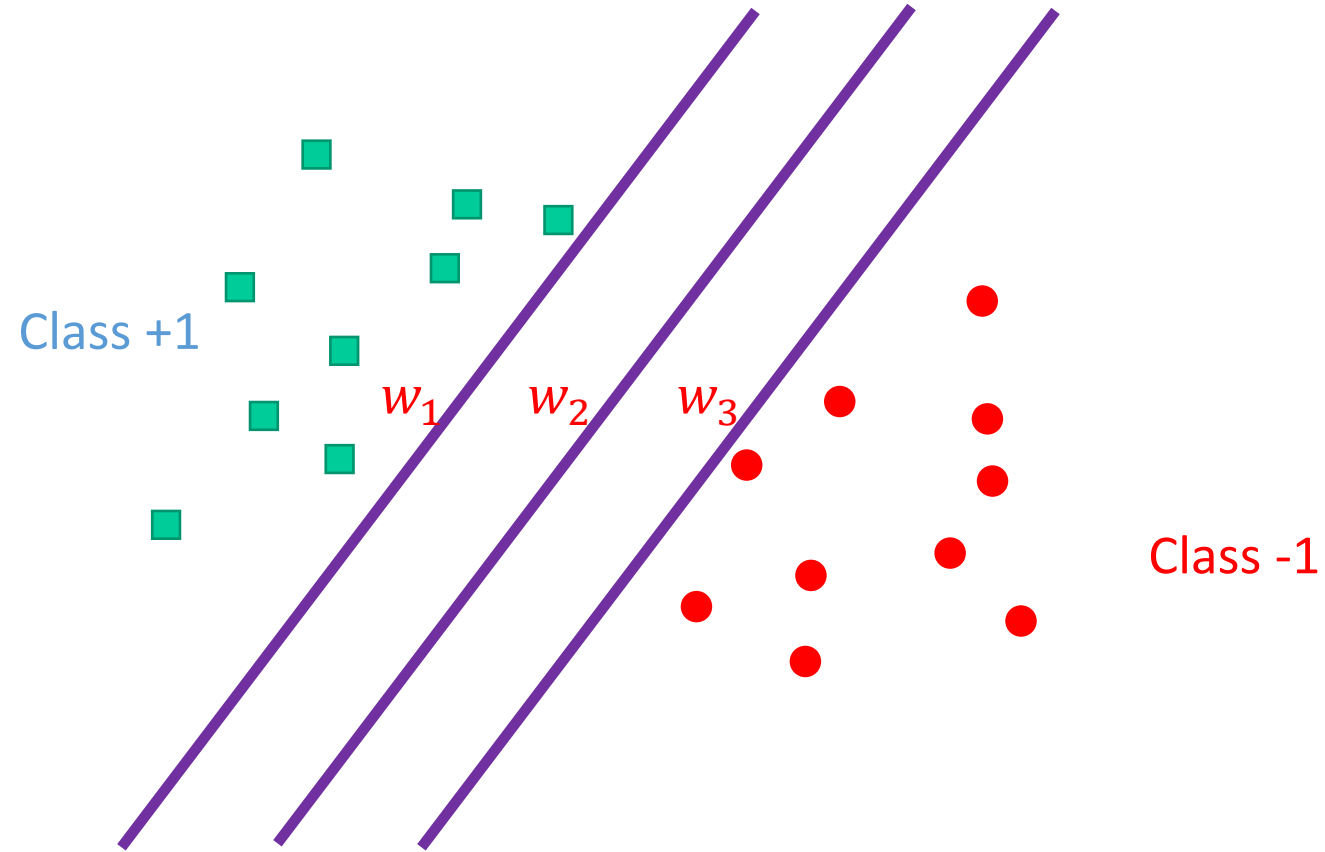
Data Augmentation: Other Domains

Not just for image data. For example, on text:

- Substitution
 - E.g. “It is a **great** day” → “It is a **wonderful** day”
 - Use a thesaurus for particular words
 - Or use a model. Pre-trained word embeddings, language models
- Back-translation
 - “Given the low budget and production limitations, this movie is very good.”
→ “There are few budget items and production limitations to make this film a really good one”

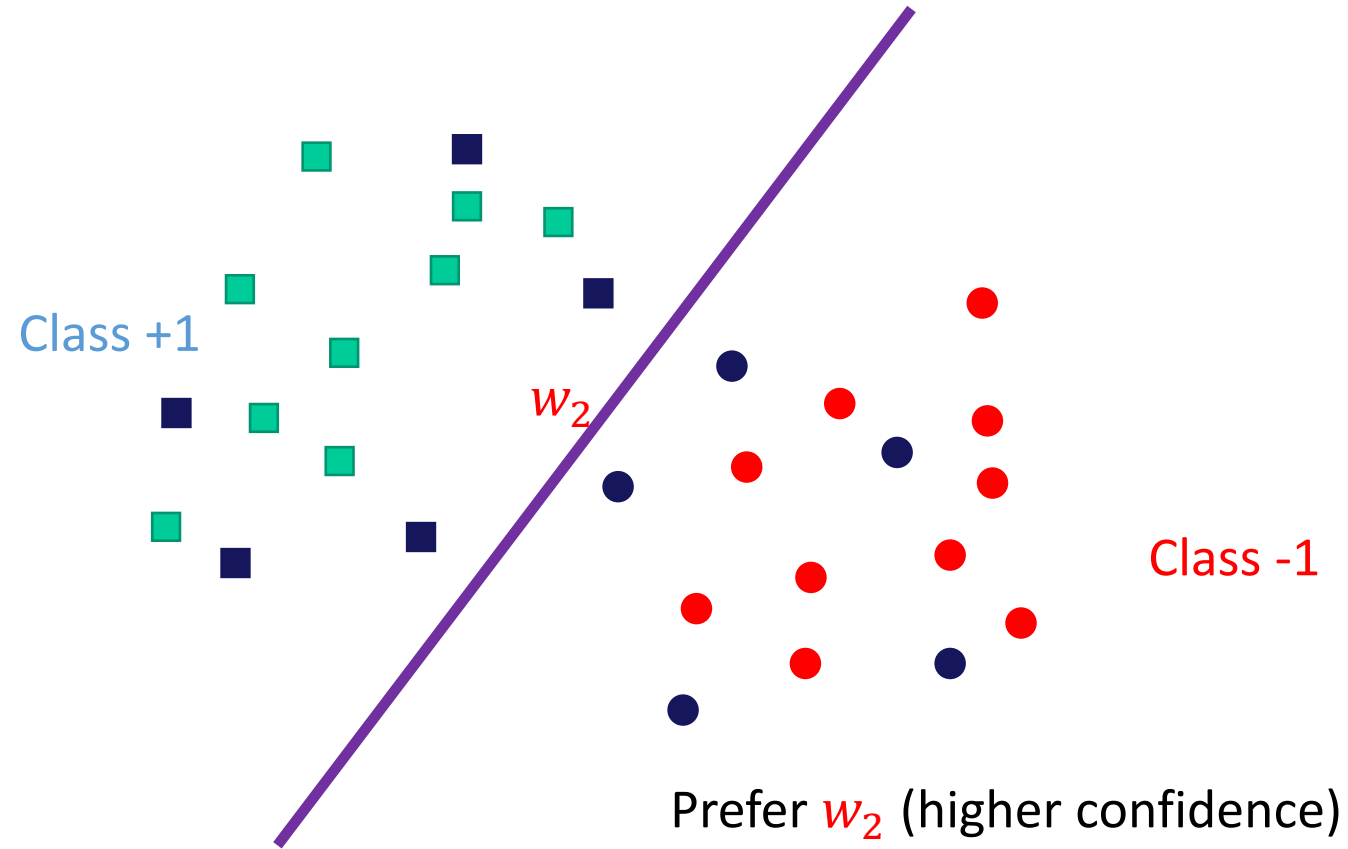
Adding Noise

- What if we have many solutions?



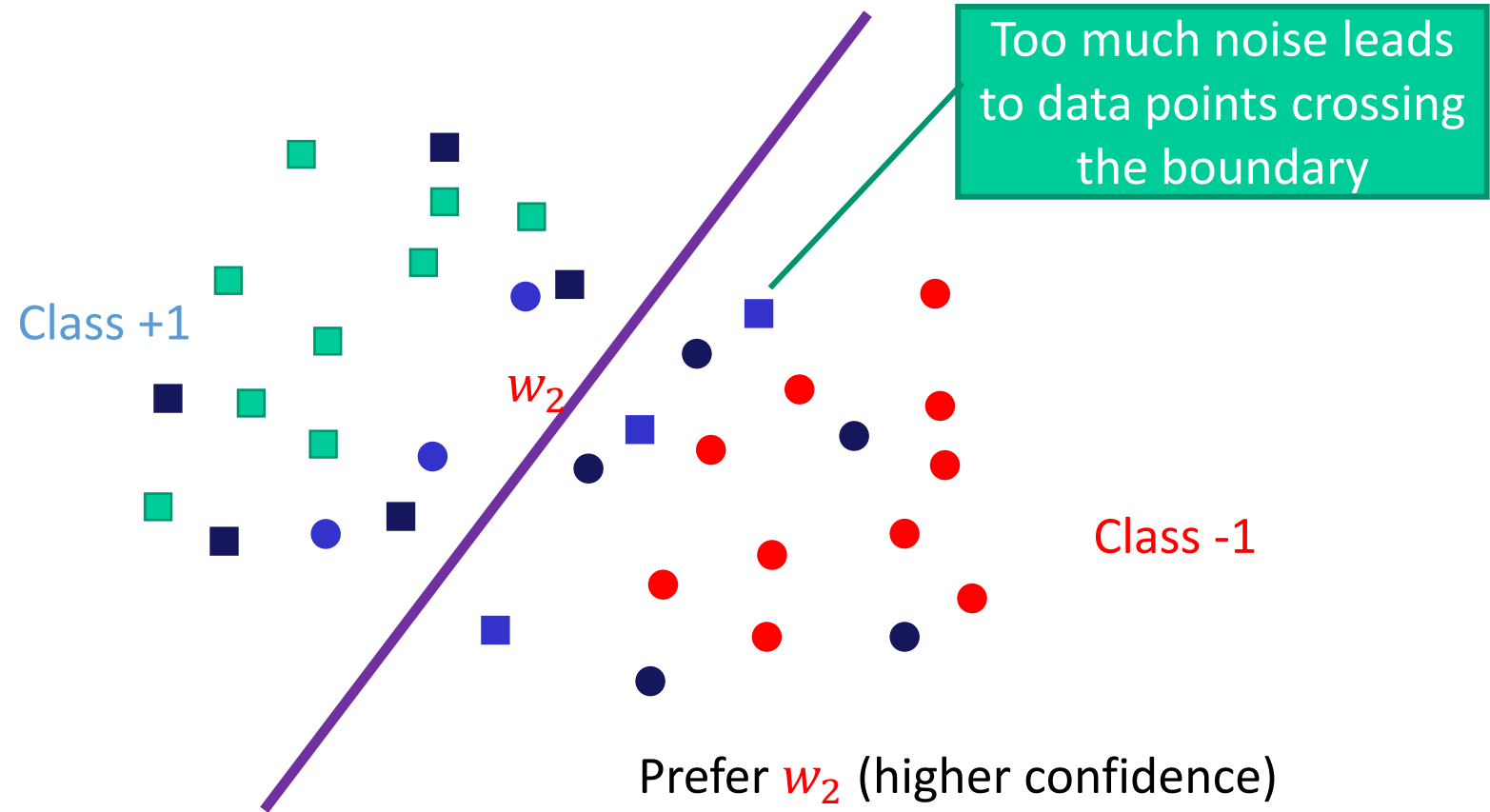
Adding Noise

- Adding some amount of noise helps us pick solution:



Adding Noise

- Too much: hurts instead



Adding Noise: Equivalence to Weight Decay

- Suppose the hypothesis is $f(x) = w^T x$, noise is $\epsilon \sim N(0, \lambda I)$
- After adding noise, the loss is

$$L(f) = \mathbb{E}_{x,y,\epsilon} [f(x + \epsilon) - y]^2 = \mathbb{E}_{x,y,\epsilon} [f(x) + w^T \epsilon - y]^2$$

$$L(f) = \mathbb{E}_{x,y,\epsilon} [f(x) - y]^2 + 2\mathbb{E}_{x,y,\epsilon} [w^T \epsilon (f(x) - y)] + \mathbb{E}_{x,y,\epsilon} [w^T \epsilon]^2$$

$$L(f) = \mathbb{E}_{x,y,\epsilon} [f(x) - y]^2 + \lambda \|w\|^2$$

Early Stopping

Idea: don't train to too small training error

- limits the volume of parameter space reachable from the initialization

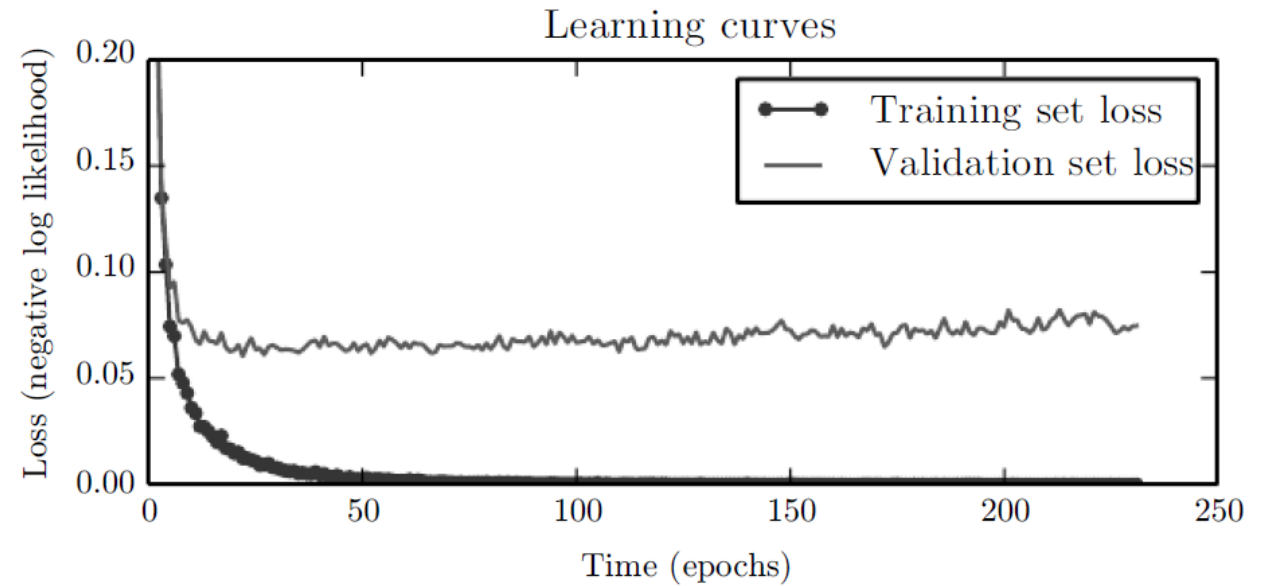


Figure from *Deep Learning*,
Goodfellow, Bengio and Courville

Practically: when training, also output validation error

- every time validation error improved, store a copy of the weights
- when validation error not improved for some time, stop
- return the copy of the weights stored

Dropout

Basic idea: randomly select a subset of weights to update

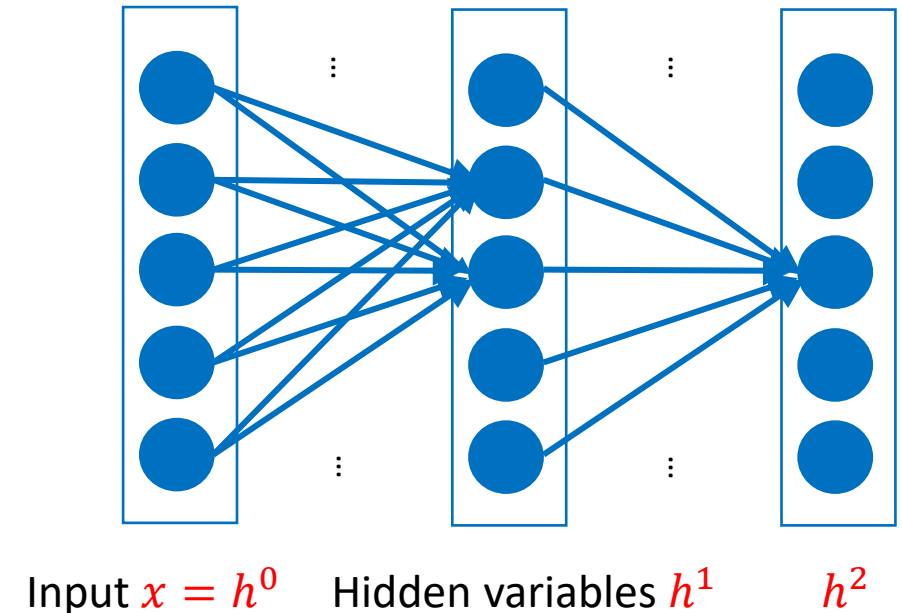
- In each update step
 - Randomly sample a different binary mask to all the input and hidden units
 - Multiply the mask bits with the units and do the update as usual
- At test time: use all of the weights
- Typical dropout probabilities:
 - 0.2 for inputs weights
 - 0.5 for hidden units

Batch Normalization

Basic idea: standardize inputs to each layer of a neural network

- recall: it is often beneficial to standardize the i th **input** feature x_i by passing $(x_i - \mu_i)/\sigma_i$ to the model; statistics μ_i and σ_i are computed on the training data
- **batch normalization** standardizes the outputs h^L of each layer L before passing them to layer L+1, with **statistics computed on each batch**

Supposed to help optimization, but its mechanism is poorly understood



Summary of regularization

Linear models dominated by **well-understood** penalty-based approaches such as Ridge and LASSO

Neural network regularization is less understood:

- some (weight decay, data augmentation) are applicable to or adapted from linear models
- some (dropout, batch-norm) specific to deep nets
- usually selected via a mix of **trial-and-error** + **formal validation**



Thanks Everyone!

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