Lecture 08

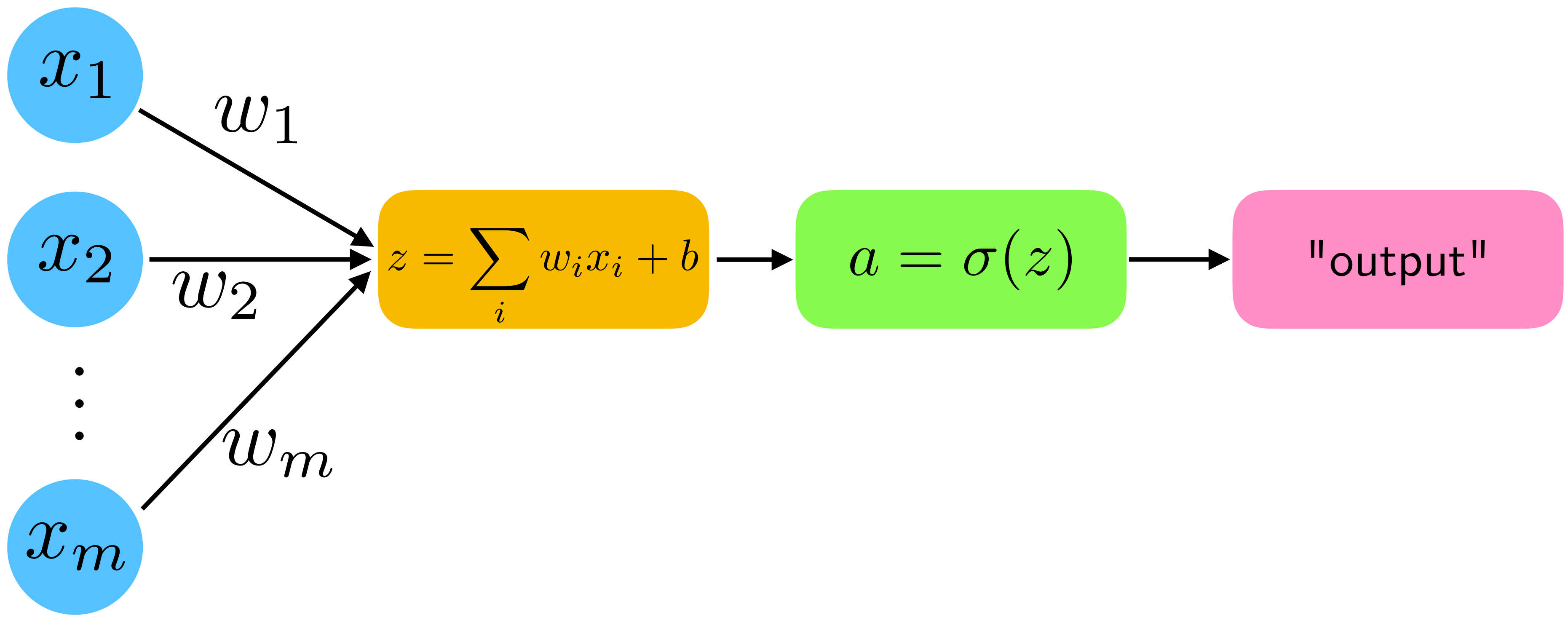
Logistic Regression and Multi-class Classification

STAT 479: Deep Learning, Spring 2019

Sebastian Raschka

http://stat.wisc.edu/~sraschka/teaching/stat479-ss2019/

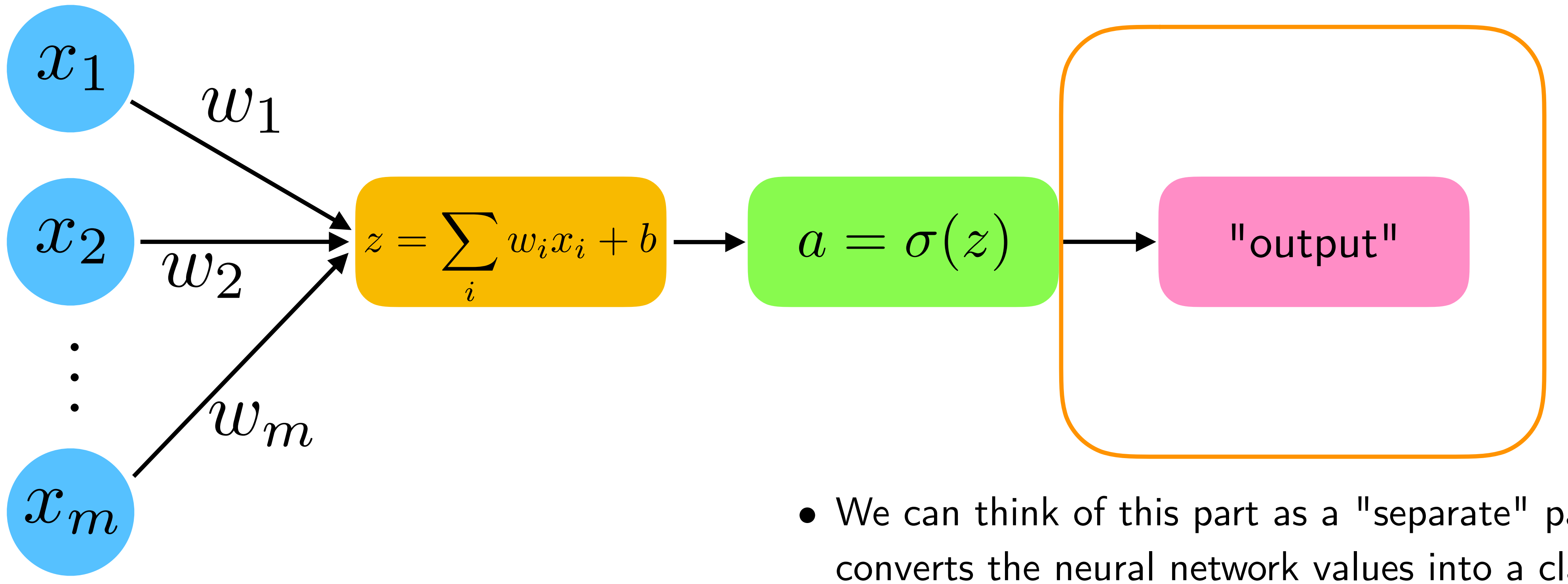
Homework 2 Recap



Generic Neuron representation

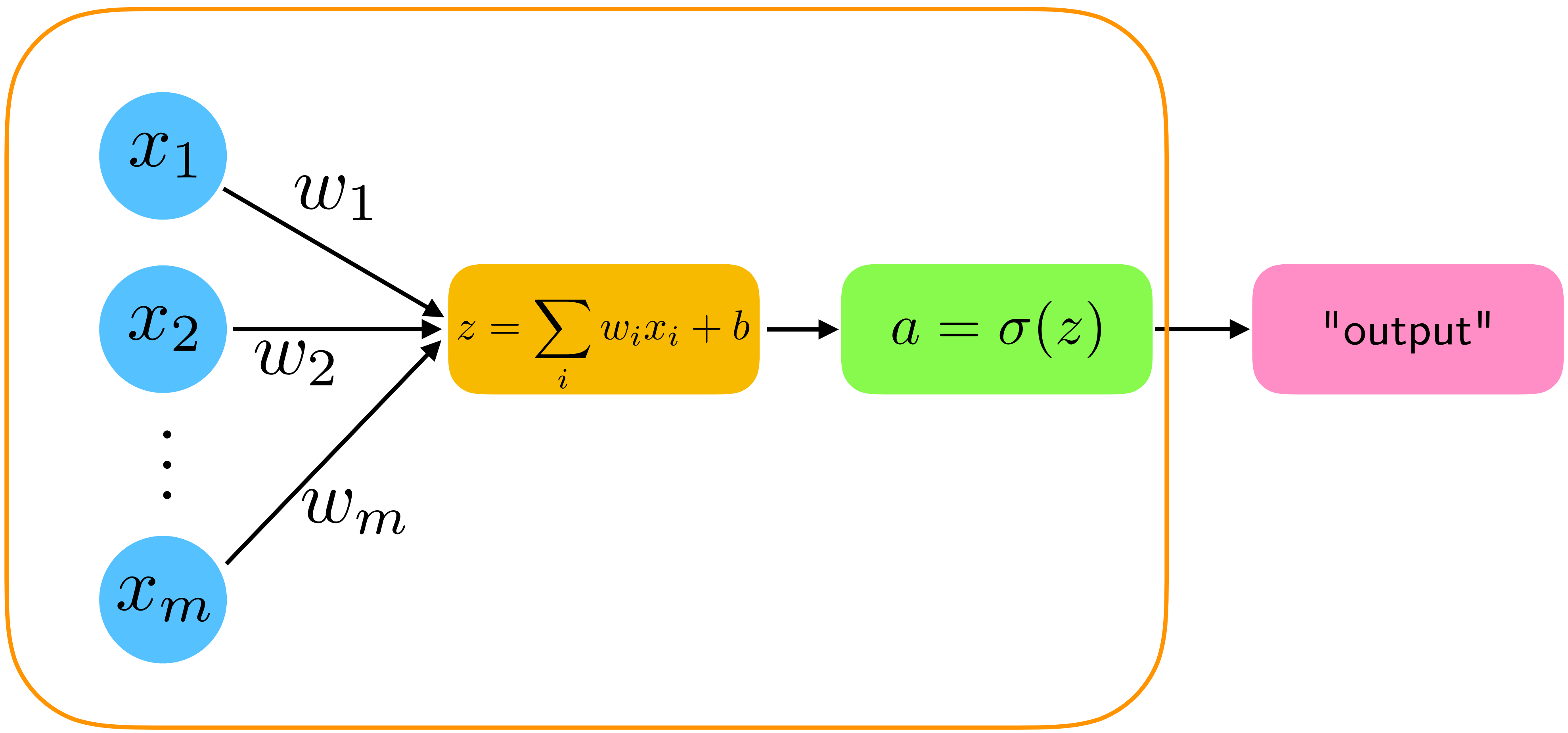
(Perceptron, ADALINE, Linear Regression, and later today: Logistic Regression)

Homework 2 Recap



- We can think of this part as a "separate" part that converts the neural network values into a class label, for example; e.g., via a threshold function
- Predicted class labels are not used during training (except by the Perceptron)
- ADALINE, Logistic Regression (later today), and all common types of multi-layer neural networks don't use predicted class labels for optimization as a threshold function is not smooth

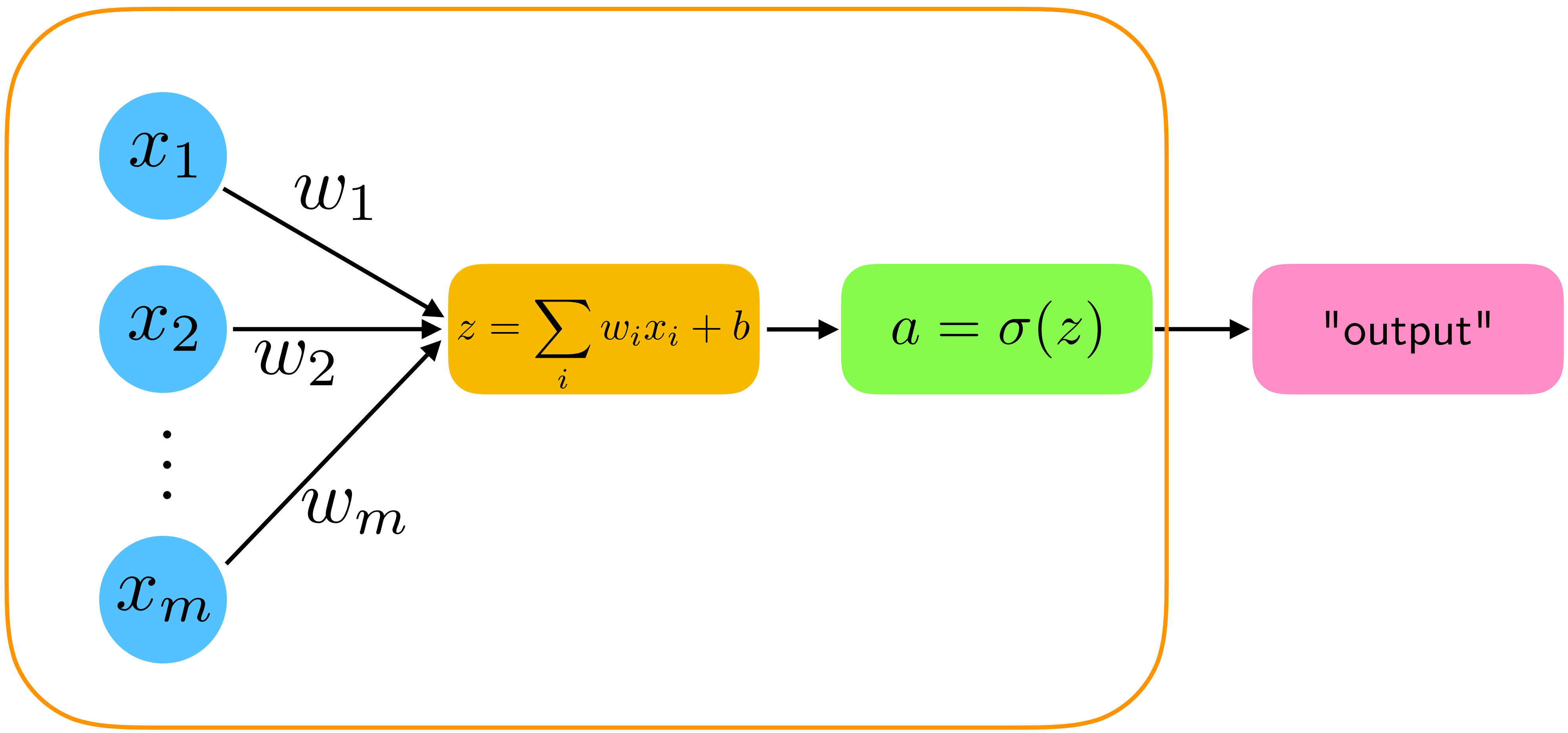
Homework 2 Recap



- For training, only this part matters!

$$\mathcal{L} = \frac{1}{n} \sum_i (y^{[i]} - a^{[i]})^2$$

Homework 2 Recap



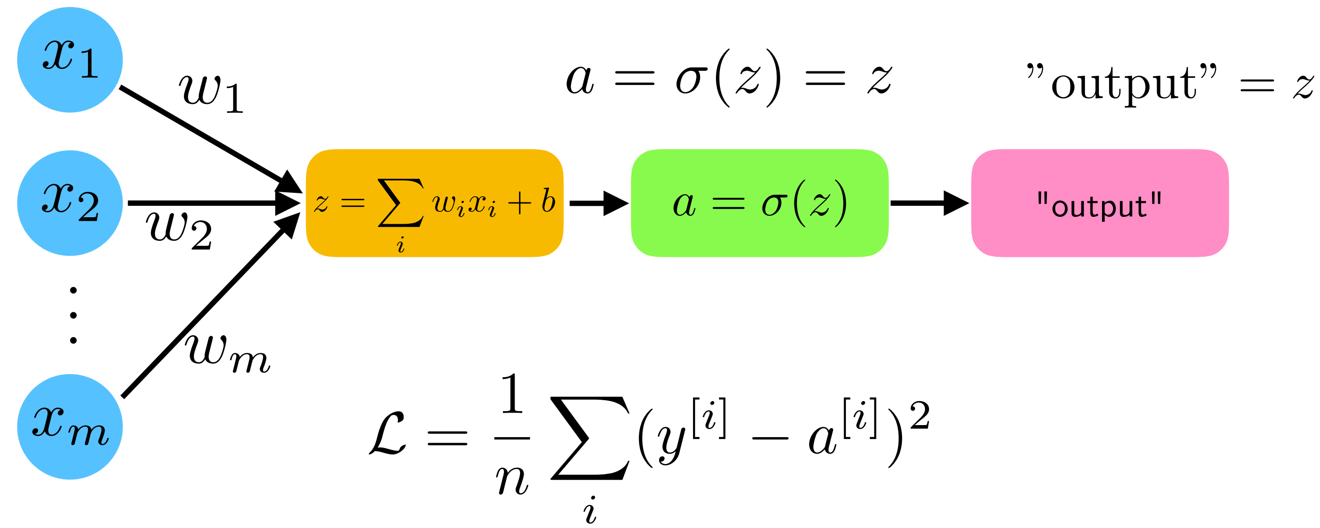
- For training, only this part matters!

$$\mathcal{L} = \frac{1}{n} \sum_i (y^{[i]} - a^{[i]})^2$$

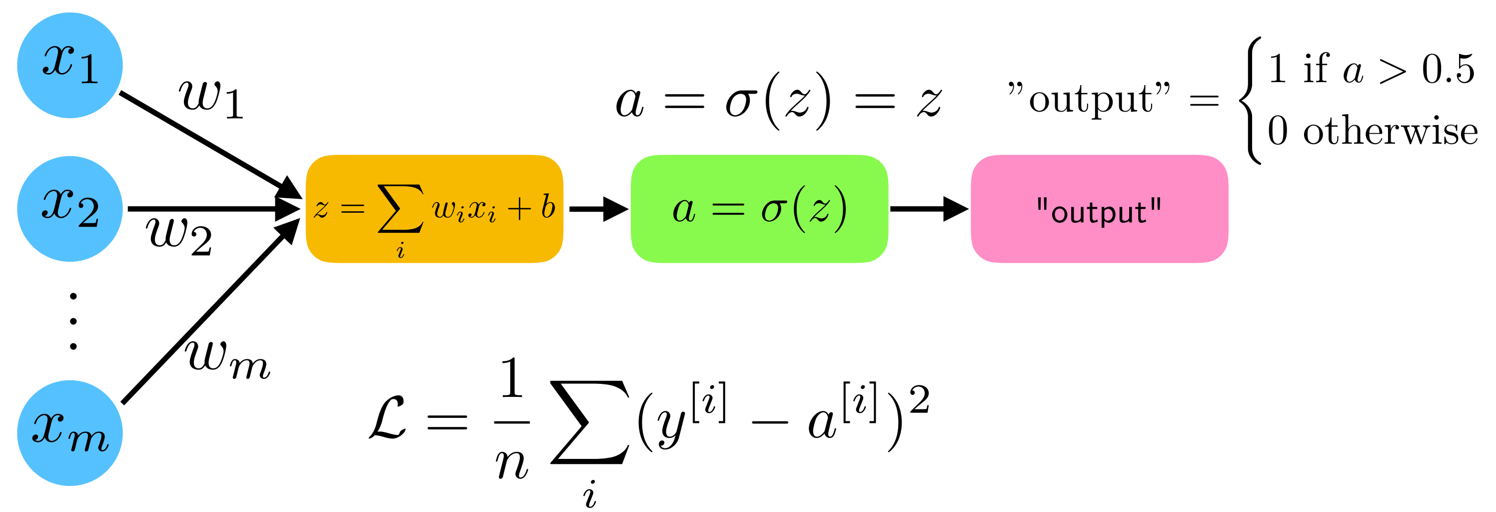
Want: $\frac{\partial \mathcal{L}}{\partial w_i}$ and $\frac{\partial \mathcal{L}}{\partial b}$

Homework 2 Recap

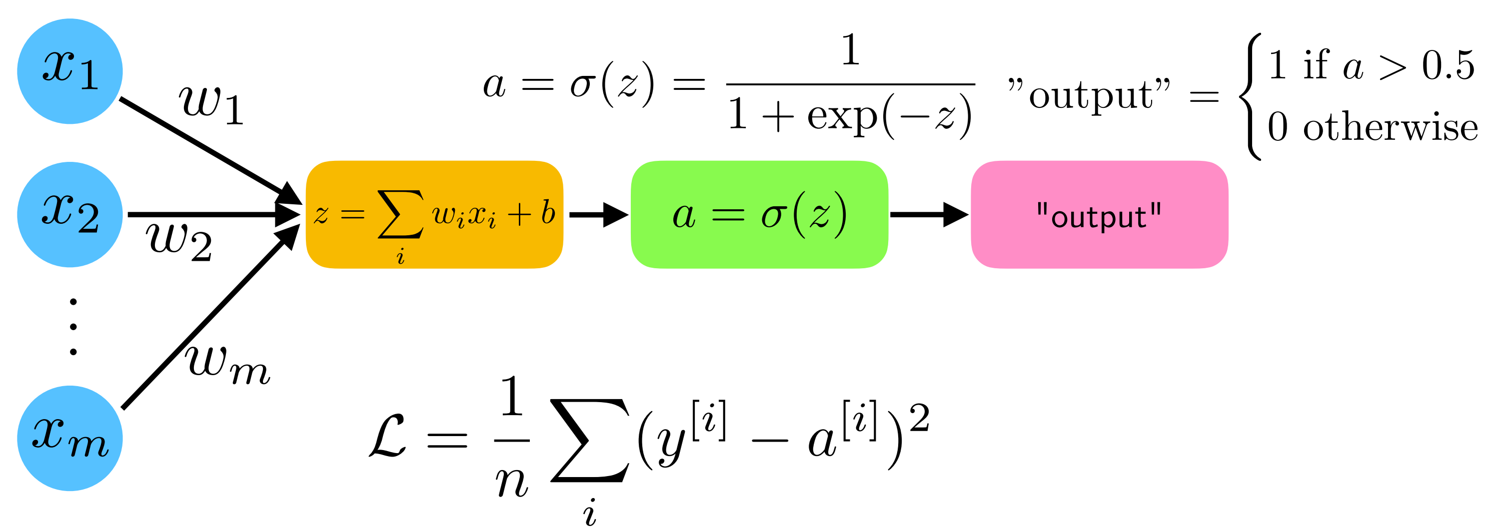
a) Linear regression



b) ADALINE

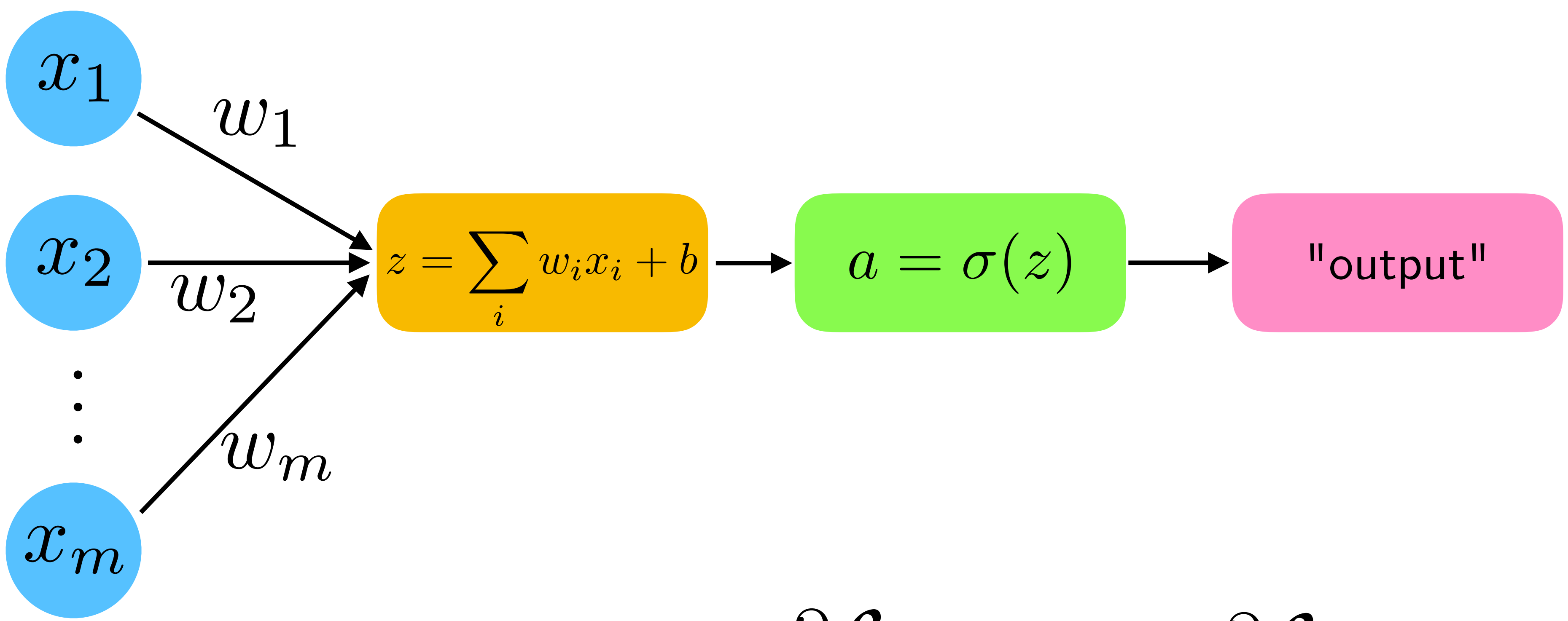


c) HW2 Neuron



Homework 2 Recap

$$\mathcal{L} = (y^{[i]} - a^{[i]})^2$$



Want: $\frac{\partial \mathcal{L}}{\partial w_i}$ and $\frac{\partial \mathcal{L}}{\partial b}$

Why could

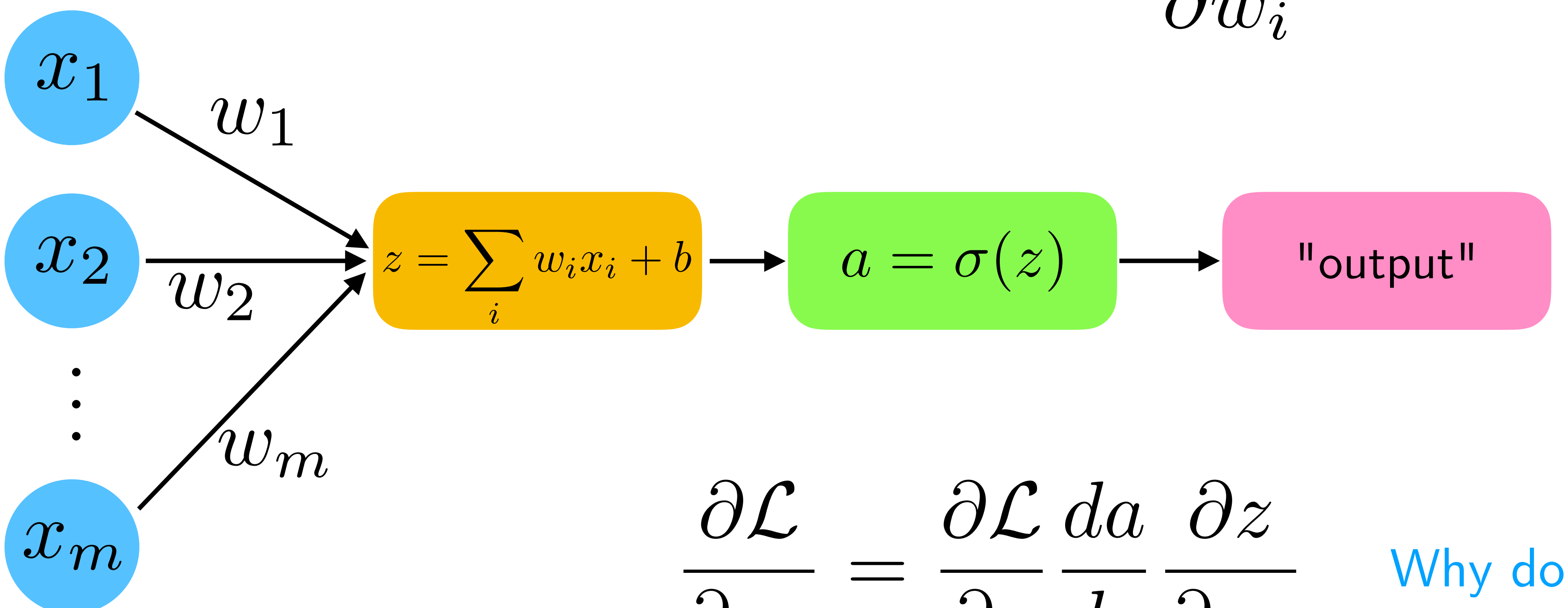
$$a = \sigma(z) = \frac{1}{1 + \exp(-z)}$$

be better than ADALINE's linear activation?

Homework 2 Recap

$\mathcal{L} = (y^{[i]} - a^{[i]})^2$ For simplicity, suppose we have only 1 training example

Want: $\frac{\partial \mathcal{L}}{\partial w_i}$ and $\frac{\partial \mathcal{L}}{\partial b}$



$$\frac{\partial \mathcal{L}}{\partial w_i} = \frac{\partial \mathcal{L}}{\partial a} \frac{da}{dz} \frac{\partial z}{\partial w_i}$$

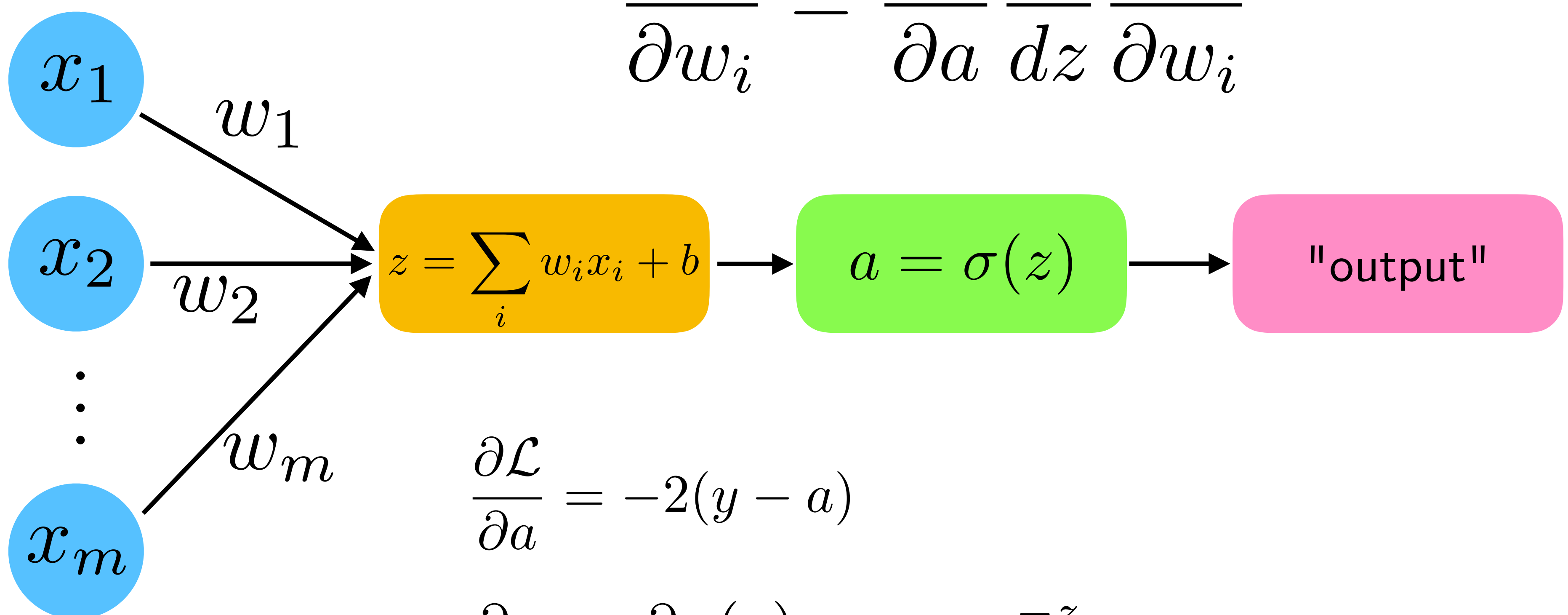
Why do I use a "d" here?

$$\frac{\partial \mathcal{L}}{\partial b} = \frac{\partial \mathcal{L}}{\partial a} \frac{da}{dz} \frac{\partial z}{\partial b}$$

Homework 2 Recap

$$\mathcal{L} = (y^{[i]} - a^{[i]})^2$$ For simplicity, suppose we have only 1 training example

$$\frac{\partial \mathcal{L}}{\partial w_i} = \frac{\partial \mathcal{L}}{\partial a} \frac{da}{dz} \frac{\partial z}{\partial w_i}$$



$$\frac{\partial \mathcal{L}}{\partial a} = -2(y - a)$$

$$\frac{\partial a}{\partial z} = \frac{\partial \sigma(z)}{\partial z} = \frac{e^{-z}}{(1 + e^{-z})^2} = \sigma(z) \cdot (1 - \sigma(z))$$

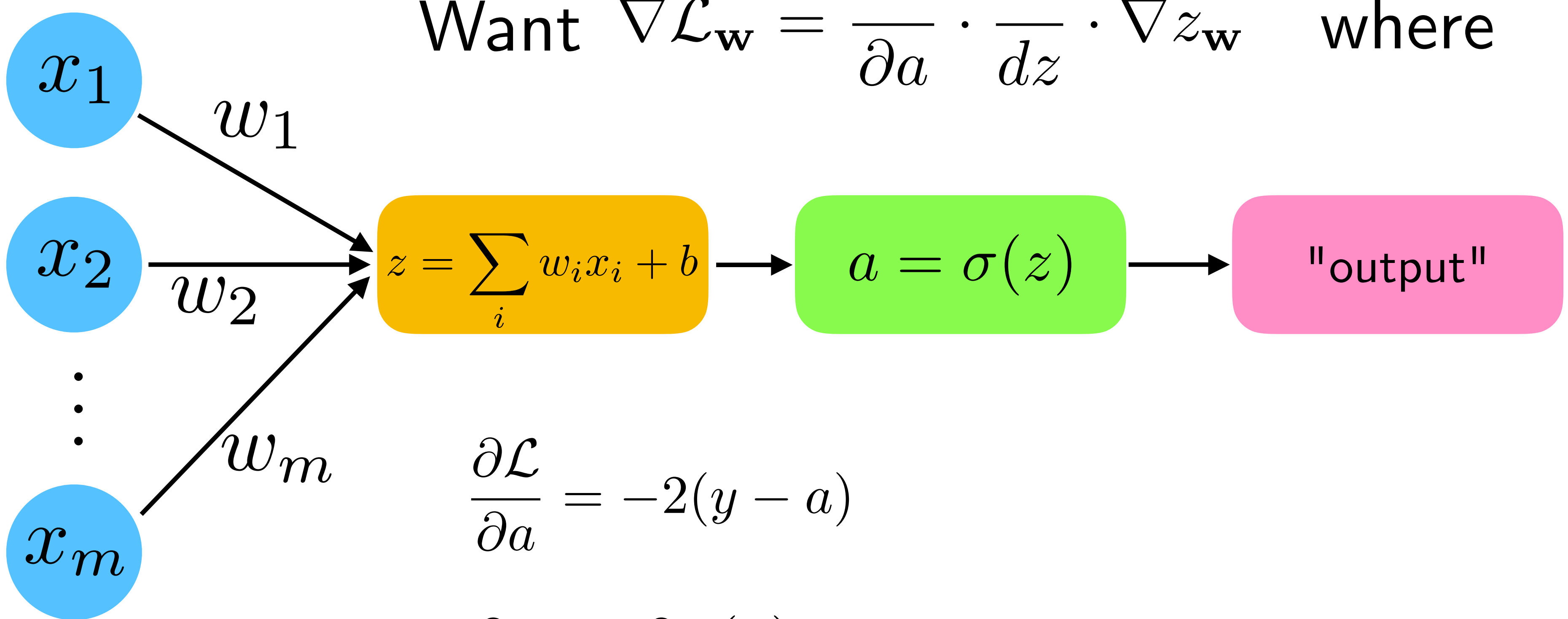
$$\frac{\partial z}{\partial w_i} = x_i$$

Homework 2 Recap

$\mathcal{L} = (y^{[i]} - a^{[i]})^2$ For simplicity, suppose we have only 1 training example

but multiple weights

Want $\nabla \mathcal{L}_{\mathbf{w}} = \frac{\partial \mathcal{L}}{\partial a} \cdot \frac{da}{dz} \cdot \nabla z_{\mathbf{w}}$ where $\nabla \mathcal{L}_{\mathbf{w}} = \begin{bmatrix} \frac{\partial \mathcal{L}}{w_1} \\ \frac{\partial \mathcal{L}}{w_2} \\ \vdots \\ \frac{\partial \mathcal{L}}{w_i} \end{bmatrix}$



$$\frac{\partial \mathcal{L}}{\partial a} = -2(y - a)$$

$$\frac{\partial a}{\partial z} = \frac{\partial \sigma(z)}{\partial z} = \frac{e^{-z}}{(1 + e^{-z})^2} = \sigma(z) \cdot (1 - \sigma(z))$$

$$\nabla_{\mathbf{w}} z = [x_1 \quad x_2 \quad \dots \quad x_m]^\top$$

Homework 2 Recap

Multiple training examples:

$$\mathcal{L} = (y^{[i]} - a^{[i]})^2 \longrightarrow \mathcal{L} = \frac{1}{n}\sum_i (y^{[i]} - a^{[i]})^2$$

$$\frac{\partial \mathcal{L}}{\partial w_i} = \frac{\partial \mathcal{L}}{\partial a}\frac{da}{dz}\frac{\partial z}{\partial w_i}$$

$$\frac{\partial \mathcal{L}}{\partial w_j} = \boxed{\frac{1}{n}\sum_{i=1}^{n}} -2(y^{[i]} - a^{[i]}) \cdot \sigma(z^{[i]}) \cdot (1 - \sigma(z^{[i]})) \cdot x_j^{[i]})$$

Only this part is new (compared to 1 training example)!

Homework 2 Recap

Multiple training examples:

$$\frac{\partial \mathcal{L}}{\partial w_i} = \frac{\partial \mathcal{L}}{\partial a} \frac{da}{dz} \frac{\partial z}{\partial w_i}$$

$$\frac{\partial \mathcal{L}}{\partial w_j} = \frac{1}{n} \sum_{i=1}^{n} -2(y^{[i]} - a^{[i]}) \cdot \sigma(z^{[i]}) \cdot (1 - \sigma(z^{[i]})) \cdot x_j^{[i]})$$

Vectorized:

$$\frac{\partial \mathcal{L}}{\partial w_j} = -\frac{2}{n} (\mathbf{y} - \mathbf{a}) \odot \sigma(\mathbf{z}) \odot (1 - \sigma(\mathbf{z}))\mathbf{x}_j^\top$$

Homework 2 Recap

Multiple training examples:

$$\frac{\partial \mathcal{L}}{\partial w_i} = \frac{\partial \mathcal{L}}{\partial a} \frac{da}{dz} \frac{\partial z}{\partial w_i}$$

$$\frac{\partial \mathcal{L}}{\partial w_j} = \frac{1}{n} \sum_{i=1}^{n} -2(y^{[i]} - a^{[i]}) \cdot \sigma(z^{[i]}) \cdot (1 - \sigma(z^{[i]})) \cdot x_j^{[i]})$$

Vectorized:

$$\frac{\partial \mathcal{L}}{\partial w_j} = -\frac{2}{n}(\mathbf{y} - \mathbf{a}) \odot \sigma(\mathbf{z}) \odot (1 - \sigma(\mathbf{z}))\mathbf{x}_j^\top$$

Can you spot the problem?

Homework 2 Recap

Multiple training examples:

$$\frac{\partial \mathcal{L}}{\partial w_i} = \frac{\partial \mathcal{L}}{\partial a} \frac{da}{dz} \frac{\partial z}{\partial w_i}$$

$$\frac{\partial \mathcal{L}}{\partial w_j} = \frac{1}{n} \sum_{i=1}^{n} -2(y^{[i]} - a^{[i]}) \cdot \sigma(z^{[i]}) \cdot (1 - \sigma(z^{[i]})) \cdot x_j^{[i]})$$

Vectorized:

$$\frac{\partial \mathcal{L}}{\partial w_j} = -\frac{2}{n}(\mathbf{y} - \mathbf{a}) \odot \sigma(\mathbf{z}) \odot (1 - \sigma(\mathbf{z}))\mathbf{x}_j^\top$$

In code, this is ok, in proper math, this is a vector of 1's now

Homework 2 Recap

Multiple training examples:

$$\frac{\partial \mathcal{L}}{\partial w_i} = \frac{\partial \mathcal{L}}{\partial a} \frac{da}{dz} \frac{\partial z}{\partial w_i}$$

$$\frac{\partial \mathcal{L}}{\partial w_j} = \frac{1}{n} \sum_{i=1}^{n} -2(y^{[i]} - a^{[i]}) \cdot \sigma(z^{[i]}) \cdot (1 - \sigma(z^{[i]})) \cdot x_j^{[i]})$$

$$\frac{\partial \mathcal{L}}{\partial w_j} = -\frac{2}{n}(\mathbf{y} - \mathbf{a}) \odot \sigma(\mathbf{z}) \odot (1 - \sigma(\mathbf{z}))\mathbf{x}_j^\top \quad \text{where} \quad \mathbf{x} \in \mathbb{R}^{m \times 1}$$

Multiple training examples and features:

$$\nabla_{\mathbf{w}} \mathcal{L} = \Big(-\frac{2}{n}(\mathbf{y} - \mathbf{a}) \odot \sigma(\mathbf{z}) \odot (1 - \sigma(\mathbf{z}))^\top \mathbf{X}\Big)^\top \quad \text{where} \quad \mathbf{X} \in \mathbb{R}^{n \times m}$$

$$\nabla_{\mathbf{w}} \mathcal{L} = \mathbf{X}^\top \Big(-\frac{2}{n}(\mathbf{y} - \mathbf{a}) \odot \sigma(\mathbf{z}) \odot (1 - \sigma(\mathbf{z}))\Big)$$

Homework 2 Recap

$\mathcal{L} := 0, \quad w_1 := 0, \quad w_2 := 0, \quad b := 0$

for i =1 to i=n:

$$z^{[i]} = w^T x^{[i]} + b$$

$$a^{[i]} = \sigma\left(z^{[i]}\right)$$

$$\mathcal{L} \pm (y^{[i]} - a^{[i]})^2$$

$$\frac{\partial \mathcal{L}}{\partial z^{[i]}} = -2(y^{[i]} - a^{[i]}) \cdot \sigma(z^{[i]})(1 - \sigma(z^{[i]})$$

$$\frac{\partial \mathcal{L}}{\partial w_1} \pm x_1^{[i]} \frac{\partial \mathcal{L}}{\partial z^{[i]}}$$

$$\frac{\partial \mathcal{L}}{\partial w_2} \pm x_2^{[i]} \frac{\partial \mathcal{L}}{\partial z^{[i]}}$$

$$\frac{\partial \mathcal{L}}{\partial b} \pm \frac{\partial \mathcal{L}}{\partial z^{[i]}}$$

If still confused, think of the previous slide as a for-loop;
we simply "vectorized" it :)

$\mathcal{L} := \mathcal{L}/n$

$$\frac{\partial \mathcal{L}}{\partial w_1} := \frac{\partial \mathcal{L}}{\partial w_1}/n, \quad \frac{\partial \mathcal{L}}{\partial w_2} := \frac{\partial \mathcal{L}}{\partial w_2}/n, \quad \frac{\partial \mathcal{L}}{\partial b} := \frac{\partial \mathcal{L}}{\partial b}/n$$

Homework 2 Recap

Lastly, about the sigmoid derivative ...

$$
\begin{aligned}
\frac{d}{dz}\sigma(z) &= \frac{d}{dz}\frac{1}{1+e^{-z}} \\
&= \frac{d}{dz}\left(1+e^{-z}\right)^{-1} \quad \text{[apply chain rule]} \\
&= -(1+e^{-z})^{-2} \cdot \frac{d}{dz}(1+e^{-z}) \quad \text{[apply sum rule]} \\
&= -(1+e^{-z})^{-2} \cdot \left(\frac{d}{dz}1 + \frac{d}{dz}e^{-z}\right) \\
&= -(1+e^{-z})^{-2} \cdot \frac{d}{dz}e^{-z} \quad \text{[apply chain rule]} \\
&= -(1+e^{-z})^{-2} \cdot e^{-z}\frac{d}{dz}(-z) \\
&= -(1+e^{-z})^{-2} \cdot \left(-e^{-z}\right) \\
&= \frac{1}{(1+e^{-z})^2} \cdot e^{-z} \\
&= \frac{e^{-z}}{(1+e^{-z})^2}
\end{aligned}
$$

Homework 2 Recap

Simplifying the sigmoid derivative ...

$$
\begin{aligned}
\frac{e^{-z}}{(1+e^{-z})^2} &= \frac{e^{-z}}{1+e^{-z}} \cdot \frac{1}{1+e^{-z}} \\
&= \frac{-1+1+e^{-z}}{1+e^{-z}} \cdot \frac{1}{1+e^{-z}} \\
&= \left(\frac{-1}{1+e^{-z}} + \frac{1+e^{-z}}{1+e^{-z}}\right) \cdot \frac{1}{1+e^{-z}} \\
&= \left(\frac{-1}{1+e^{-z}} + 1\right) \cdot \frac{1}{1+e^{-z}} \\
&= \left(1 - \frac{1}{1+e^{-z}}\right) \cdot \frac{1}{1+e^{-z}} \\
&= \big(1 - \sigma(z)\big) \cdot \sigma(z)
\end{aligned}
$$

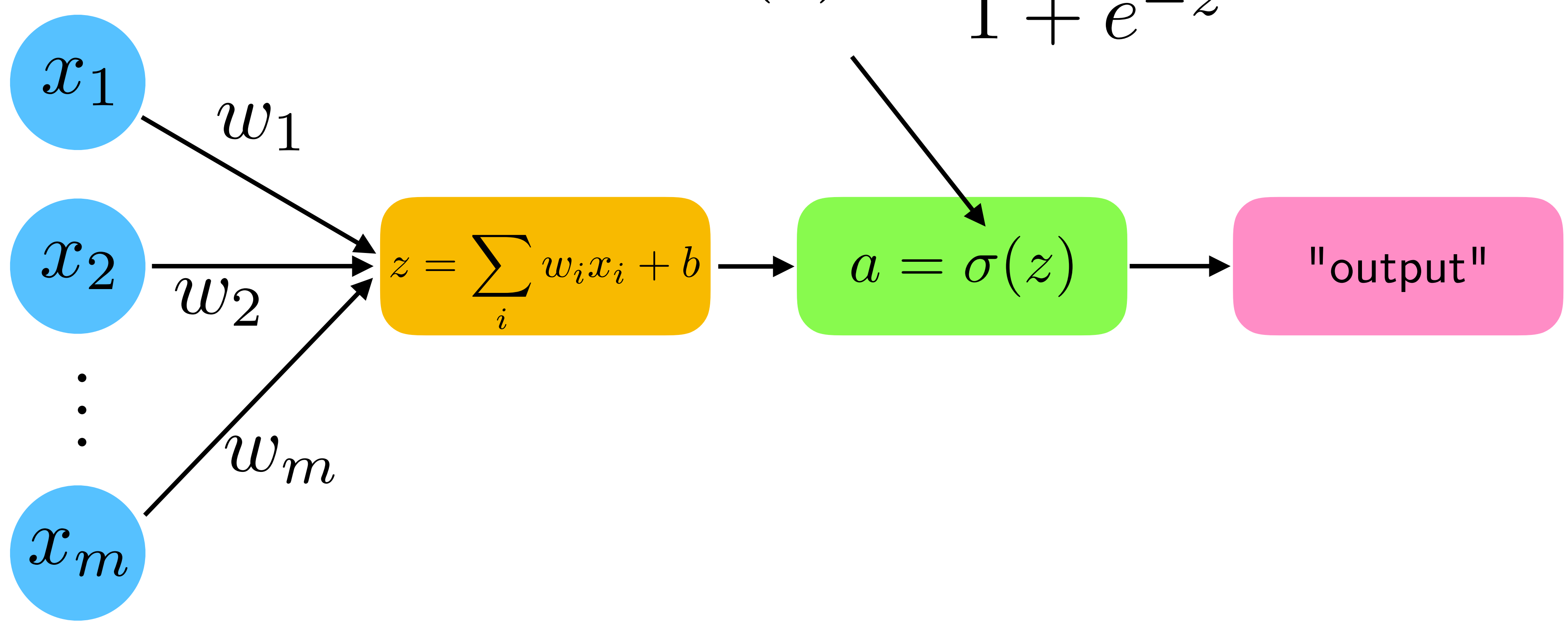
$$\frac{d\sigma(z)}{dz} = \frac{e^{-z}}{(1+e^{-z})^2} = \sigma(z) \cdot (1 - \sigma(z))$$

Logistic Regression for Binary Classification

Logistic Regression Neuron

For binary classes $y \in \{0, 1\}$

"logistic sigmoid" $\sigma(z) = \frac{1}{1 + e^{-z}}$

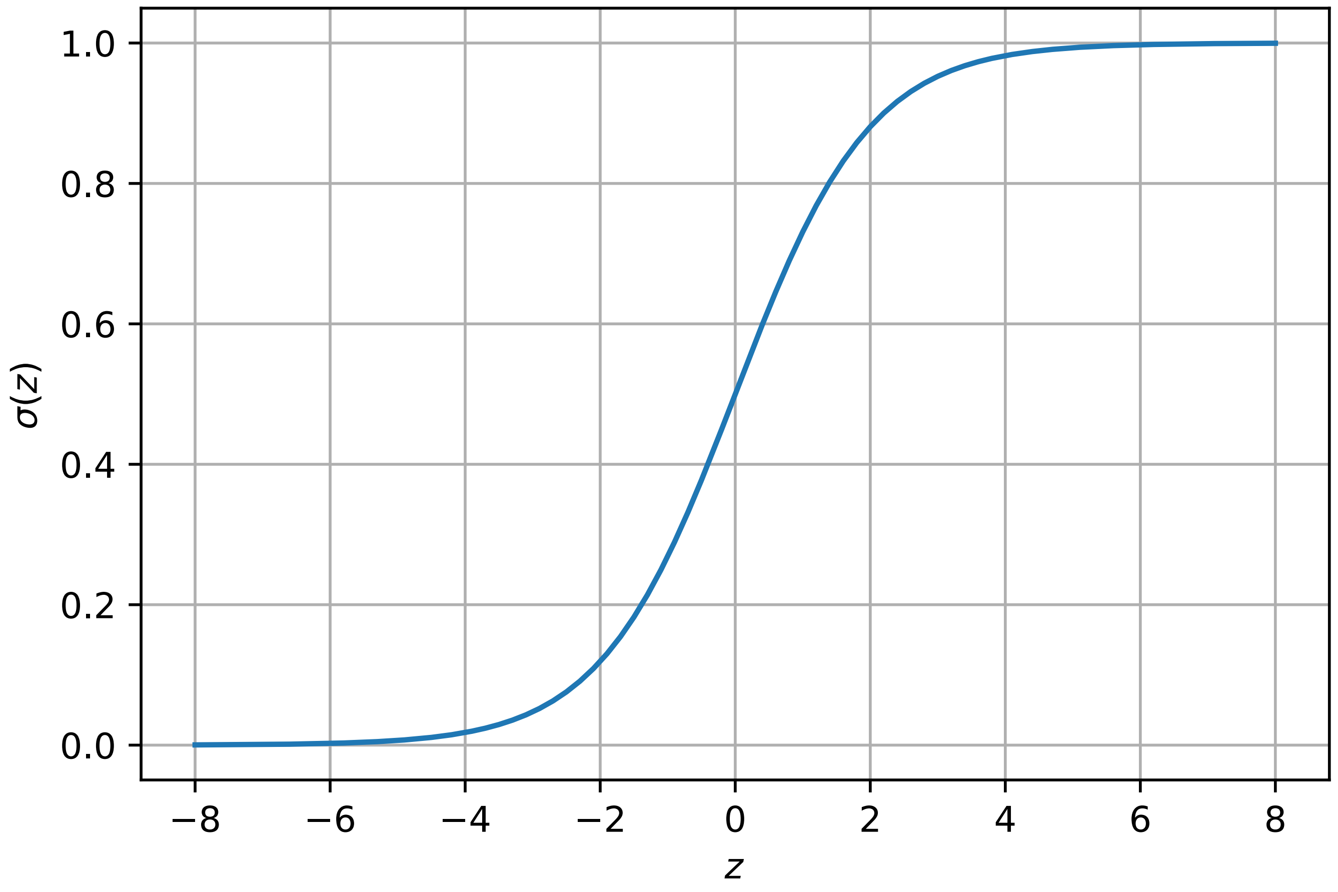


- Same as before, except different loss function
- in ADALINE and HW, we minimized the MSE loss:

$$\text{MSE} = \frac{1}{n} \sum_i (a^{[i]} - y^{[i]})^2$$

Logistic Sigmoid Function

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



Logistic Regression

$$h(\mathbf{x}) = \sigma(\mathbf{w}^\top \mathbf{x})$$

$$P(y|\mathbf{x}) = \begin{cases} h(\mathbf{x}) & \text{if } y = 1 \\ 1 - h(\mathbf{x}) & \text{if } y = 0 \end{cases}$$

want $\quad P(y=0|\mathbf{x}) \approx 1 \quad \text{if } y = 0$

$$P(y=1|\mathbf{x}) \approx 1 \quad \text{if } y = 1$$

Logistic Regression

$$h(\mathbf{x}) = \sigma(\mathbf{w}^\top \mathbf{x})$$

$$P(y|\mathbf{x}) = \begin{cases} h(\mathbf{x}) & \text{if } y = 1 \\ 1 - h(\mathbf{x}) & \text{if } y = 0 \end{cases}$$

here, hypothesis is just our activation function output

$$h(\mathbf{x}) = a$$

want $\quad P(y = 0|\mathbf{x}) \approx 1 \quad \text{if } y = 0$

$$P(y = 1|\mathbf{x}) \approx 1 \quad \text{if } y = 1$$

Logistic Regression

$$h(\mathbf{x}) = \sigma(\mathbf{w}^\top \mathbf{x})$$

$$P(y|\mathbf{x}) = \begin{cases} h(\mathbf{x}) & \text{if } y = 1 \\ 1 - h(\mathbf{x}) & \text{if } y = 0 \end{cases}$$

rewrite more compactly

want $$P(y = 0|\mathbf{x}) \approx 1 \quad \text{if } y = 0$$
$$P(y = 1|\mathbf{x}) \approx 1 \quad \text{if } y = 1$$

$$P(y|\mathbf{x}) = a^y (1 - a)^{(1-y)}$$

Logistic Regression

And for multiple training examples, we want to maximize:

$$P\big(y^{[i]}, ..., y^{[n]} | \mathbf{x}^{[1]}, ..., \mathbf{x}^{[n]}\big) = \prod_{i=1}^{n} P\big(y^{[i]} | \mathbf{x}^{[i]}\big)$$

You may remember this as *Maximum Likelihood Estimation* from your other stats classes.

Likelihood "Loss"

$$
\begin{aligned}
L(\mathbf{w}) &= P(\mathbf{y} \mid \mathbf{x}; \mathbf{w}) \\
&= \prod_{i=1}^{n} P\big(y^{(i)} \mid x^{(i)}; \mathbf{w}\big) \\
&= \prod_{i=1}^{n} \Big(\sigma\big(z^{(i)}\big)\Big)^{y^{(i)}} \Big(1 - \sigma\big(z^{(i)}\big)\Big)^{1-y^{(i)}}
\end{aligned}
$$

Log-Likelihood "Loss"

$$
\begin{aligned}
L(\mathbf{w}) &= P(\mathbf{y} \mid \mathbf{x}; \mathbf{w}) \\
&= \prod_{i=1}^{n} P\big(y^{(i)} \mid x^{(i)}; \mathbf{w}\big) \\
&= \prod_{i=1}^{n} \Big(\sigma\big(z^{(i)}\big)\Big)^{y^{(i)}} \Big(1 - \sigma\big(z^{(i)}\big)\Big)^{1-y^{(i)}}
\end{aligned}
$$

In practice, it is easier to maximize the (natural) log of this equation, which is called the log-likelihood function:

$$
\begin{aligned}
l(\mathbf{w}) &= \log L(\mathbf{w}) \\
&= \sum_{i=1}^{n} \Big[y^{(i)} \log\Big(\sigma\big(z^{(i)}\big)\Big) + \big(1 - y^{(i)}\big) \log\Big(1 - \sigma\big(z^{(i)}\big)\Big)\Big]
\end{aligned}
$$

Negative Log-Likelihood Loss

In practice, it is even more convenient to minimize negative log-likelihood instead of maximizing log-likelihood:

$$
\begin{aligned}
\mathcal{L}(\mathbf{w}) &= -l(\mathbf{w}) \\
&= -\sum_{i=1}^{n} \left[y^{(i)} \log\left(\sigma\big(z^{(i)}\big)\right) + \left(1 - y^{(i)}\right) \log\left(1 - \sigma\big(z^{(i)}\big)\right) \right]
\end{aligned}
$$

(in code, we also usually add a $1/n$ scaling factor for further convenience, where n is the number of training examples or number of examples in a minibatch)

Logistic Regression Loss

- So, "doing logistic regression" is similar to what we have done before
- in ADALINE and HW2, we minimized the MSE loss:

$$\text{MSE} = \frac{1}{n} \sum_{i} (a^{[i]} - y^{[i]})^2$$

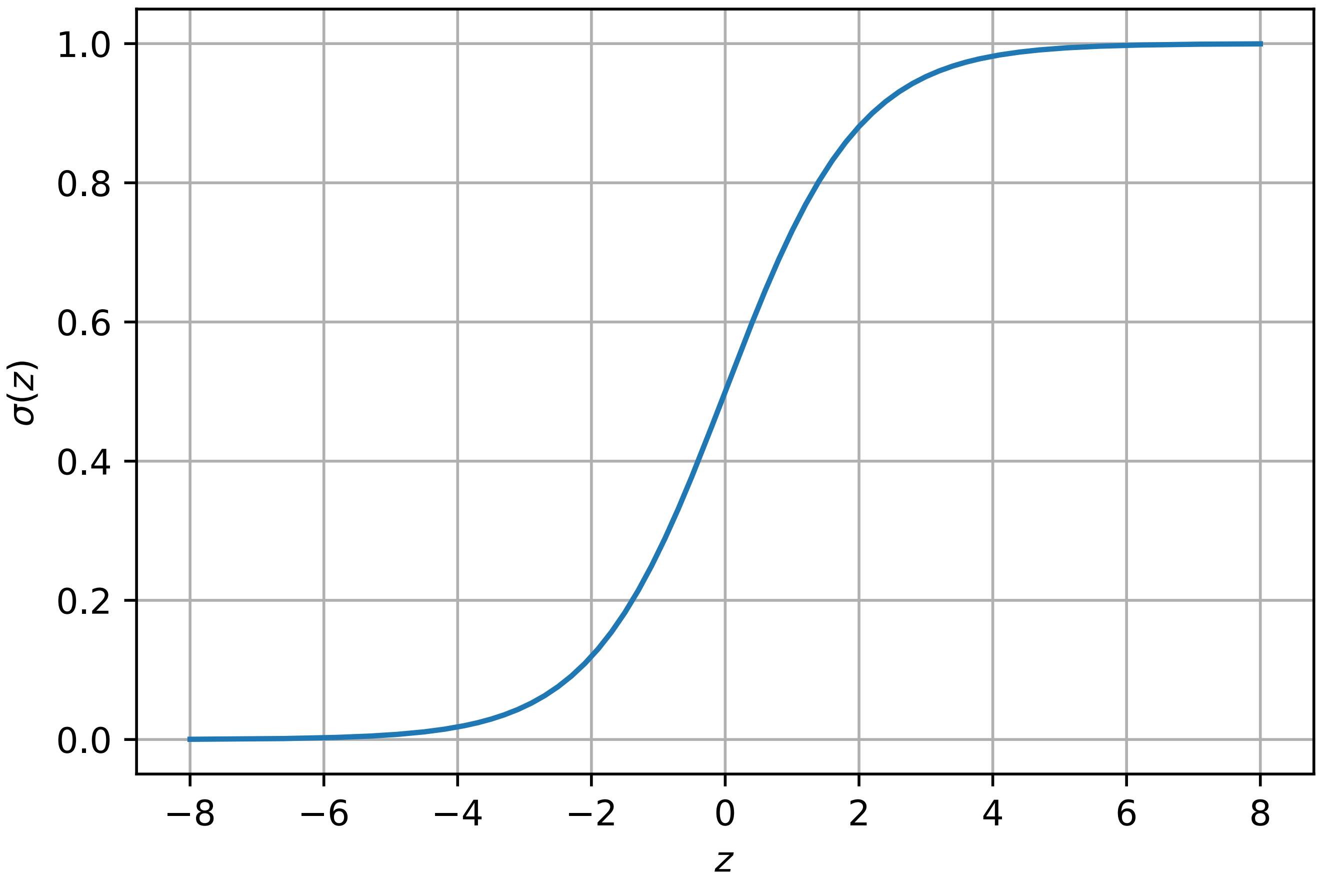
- However, the difference is that in Logistic Regression, we maximize the likelihood
- Maximizing likelihood is the same as maximizing the log-likelihood, but the latter is numerically more stable
- Maximizing the log-likelihood is the same as minimizing the negative log-likelihood, which is convenient, so we don't have to change our code and can still use gradient descent (instead of gradient ascent)

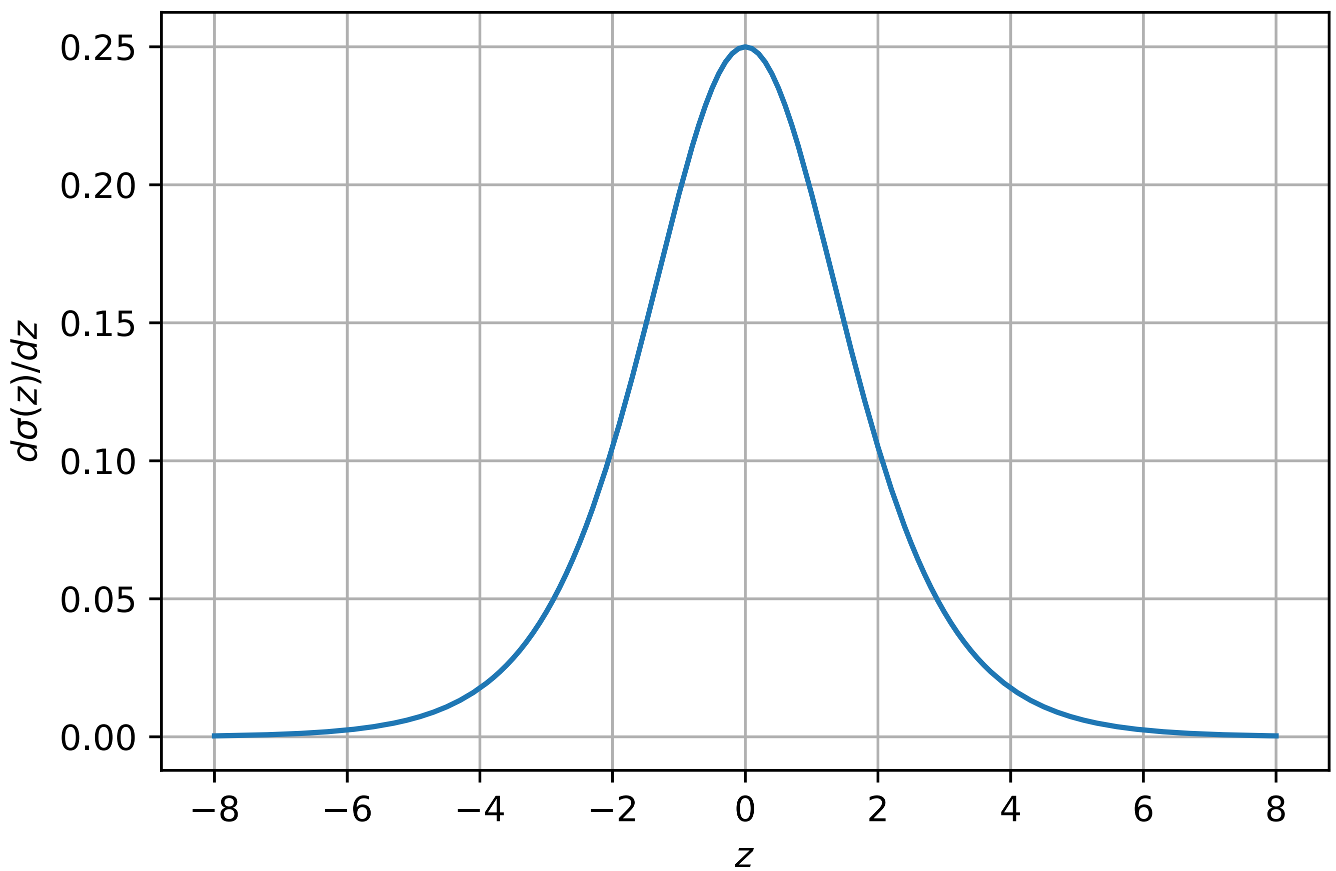
Logistic Sigmoid Derivative

Generally, another nice property of the logistic sigmoid (in multi-layer nets) is that it has nice derivatives!

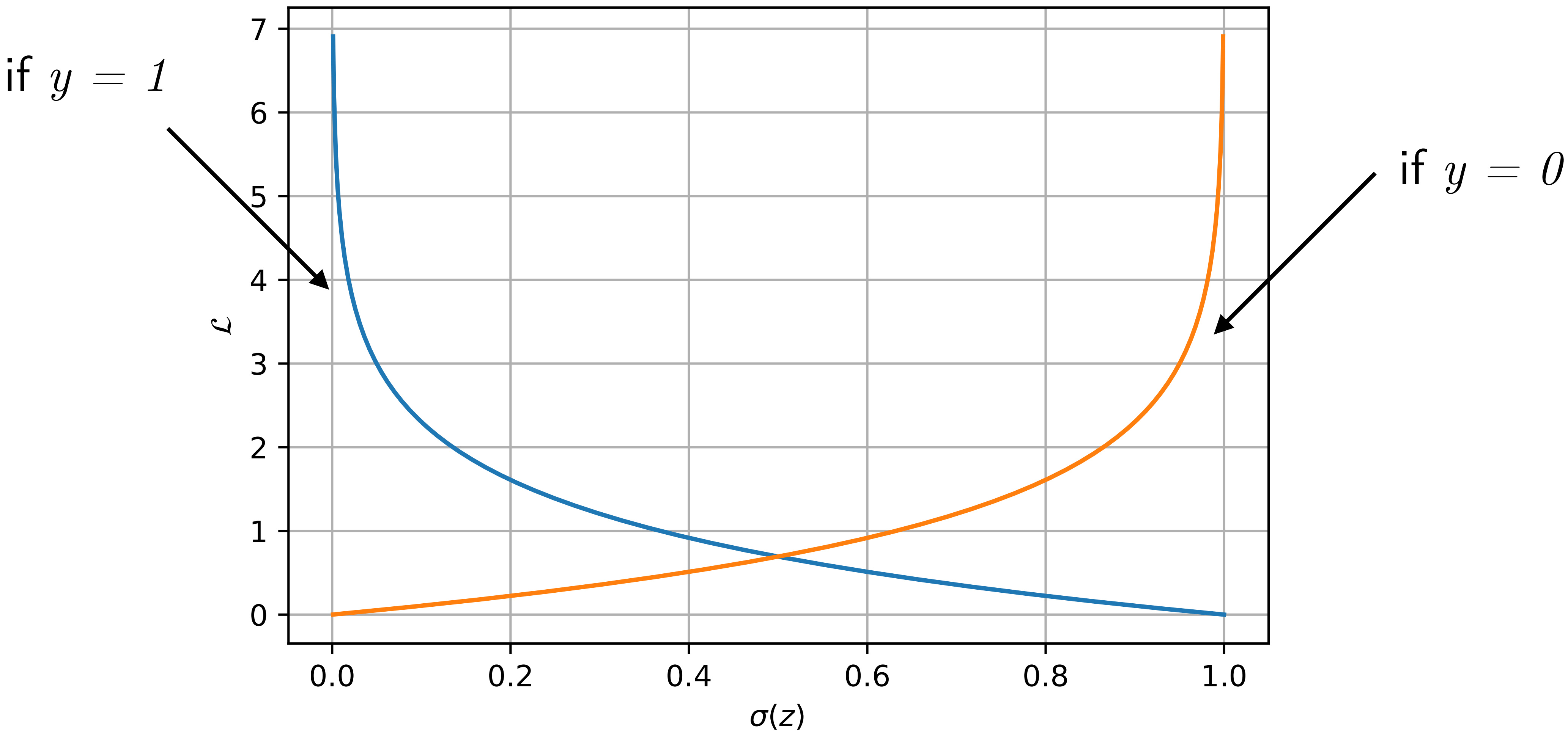
$$\sigma(z) = \frac{1}{1 + e^{-z}}$$

$$\frac{d}{dz}\sigma(z) = \frac{e^{-z}}{(1 + e^{-z})^2} = \sigma(z)(1 - \sigma(z))$$





Loss for a Single Training Example



$$\mathcal{L}(\mathbf{w}) = -y^{(i)} \log\left(\sigma\left(z^{(i)}\right)\right) + \left(1 - y^{(i)}\right) \log\left(1 - \sigma\left(z^{(i)}\right)\right)$$

Learning Rule

Same gradient descent rule as before, for which we need

$$\frac{\partial \mathcal{L}}{\partial w_j} = \frac{\partial \mathcal{L}}{\partial a} \frac{da}{dz} \frac{\partial z}{\partial w_j}$$

$$\frac{\partial \mathcal{L}}{\partial a} = \left(y \frac{1}{a} - (1-y) \frac{1}{1-a} \right)$$

$$\frac{da}{dz} = \frac{e^{-z}}{(1+e^{-z})^2} = a \cdot (1-a)$$

$$\frac{\partial z}{w_j} = x_j$$

Learning Rule

Same gradient descent rule as before, for which we need

$$\frac{\partial \mathcal{L}}{\partial w_j} = \frac{\partial \mathcal{L}}{\partial a} \frac{da}{dz} \frac{\partial z}{\partial w_j}$$

$$\frac{\partial \mathcal{L}}{\partial a} = \left(y \frac{1}{a} - (1-y) \frac{1}{1-a} \right)$$

$$\frac{da}{dz} = \frac{e^{-z}}{(1+e^{-z})^2} = a \cdot (1-a)$$

$$\frac{\partial z}{w_j} = x_j$$

$$\longrightarrow \quad \frac{\partial \mathcal{L}}{\partial z} = y - a$$

Learning Rule for Logistic Regression

Same gradient descent rule as for ADALINE & Linear Regression, for which we need

$$\frac{\partial \mathcal{L}}{\partial w_j} = \frac{\partial \mathcal{L}}{\partial a} \frac{da}{dz} \frac{\partial z}{\partial w_j}$$

$$\frac{\partial \mathcal{L}}{\partial a} = -\left(y\frac{1}{a} - (1-y)\frac{1}{1-a}\right)$$

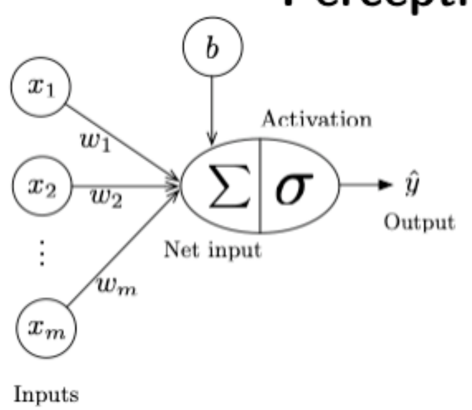
$$\frac{da}{dz} = \frac{e^{-z}}{(1+e^{-z})^2} = a \cdot (1-a) \longrightarrow \frac{\partial \mathcal{L}}{\partial z} = y - a \longrightarrow \frac{\partial \mathcal{L}}{\partial w_j} = (y-a)x_j$$

$$\frac{\partial z}{w_j} = x_j$$

Learning Rule for Logistic Regression

Remember the Perceptron & ADALINE Lectures?

Perceptron Recap



$$\sigma\left(\sum_{i=1}^{m} x_i w_i + b\right) = \sigma\left(\mathbf{x}^T\mathbf{w} + b\right) = \hat{y}$$

$$\sigma(z) = \begin{cases} 0, & z \leq 0 \\ 1, & z > 0 \end{cases}$$

$$b = -\theta$$

Let $\mathcal{D} = (\langle \mathbf{x}^{[1]}, y^{[1]} \rangle, \langle \mathbf{x}^{[2]}, y^{[2]} \rangle, ..., \langle \mathbf{x}^{[n]}, y^{[n]} \rangle) \in (\mathbb{R}^m \times \{0,1\})^n$

1. Initialize $\mathbf{w} := 0^{m-1}$, $\mathbf{b} := 0$
2. For every training epoch:
   - A. For every $\langle \mathbf{x}^{[i]}, y^{[i]} \rangle \in \mathcal{D}$:
     - (a) $\hat{y}^{[i]} := \sigma(\mathbf{x}^{[i]T}\mathbf{w} + b)$ ← Compute output (prediction)
     - (b) $\text{err} := (y^{[i]} - \hat{y}^{[i]})$ ← Calculate error
     - (c) $\mathbf{w} := \mathbf{w} + err \times \mathbf{x}^{[i]}$, $b := b + err$ ← Update parameters

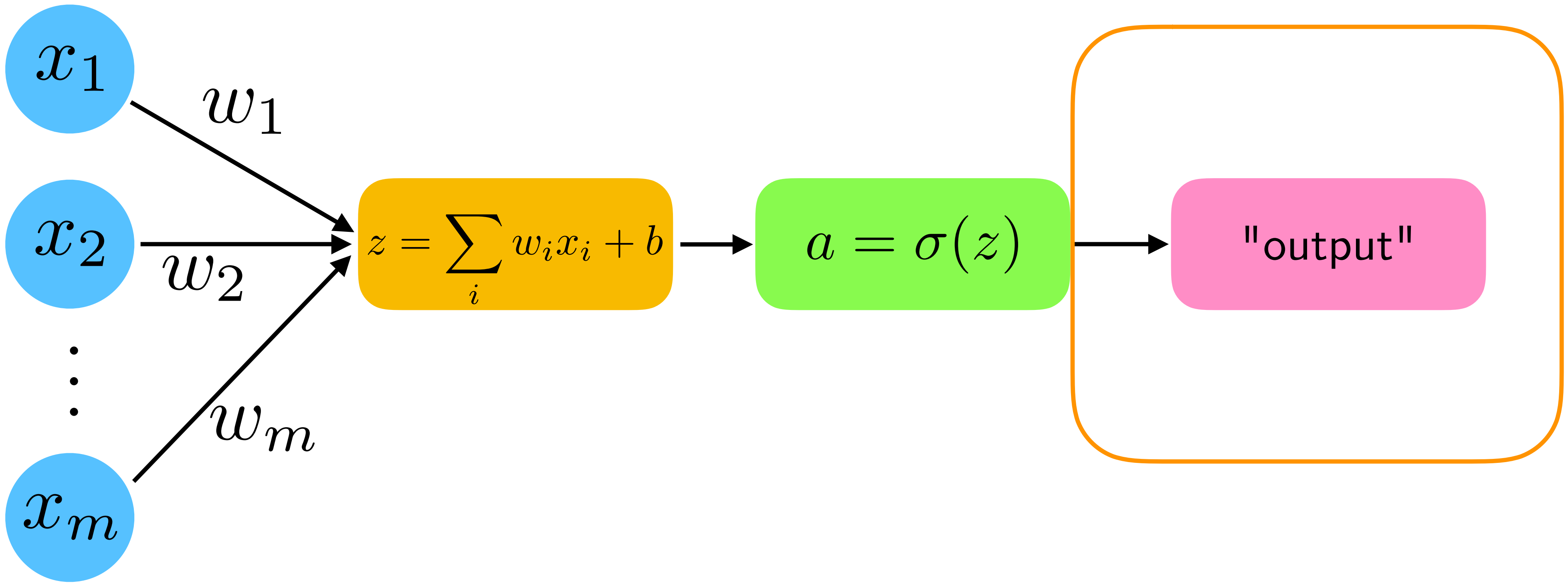
$$\frac{\partial \mathcal{L}}{\partial w_j} = (y - a)x_j$$

$$\Delta w := \text{"negative gradient"}$$
$$= -\frac{\partial \mathcal{L}}{\partial w_j}$$

$$w := w + \eta \cdot \Delta w$$

Update for each batch/minibatch with learning rate

Class Label Predictions with Logistic Regression



In logistic regression, we can use

$$\hat{y} := \begin{cases} 1 & \text{if } \sigma(z) > 0.5 \\ 0 & \text{otherwise} \end{cases}$$

which is the same as

$$\hat{y} := \begin{cases} 1 & \text{if } z > 0.0 \\ 0 & \text{otherwise} \end{cases}$$

- We can think of this part as a "separate" part that converts the neural network values into a class label, for example; e.g., via a threshold function
- Predicted class labels are not used during training (except by the Perceptron)
- ADALINE, Logistic Regression, and all common types of multi-layer neural networks don't use predicted class labels for optimization as a threshold function is not smooth

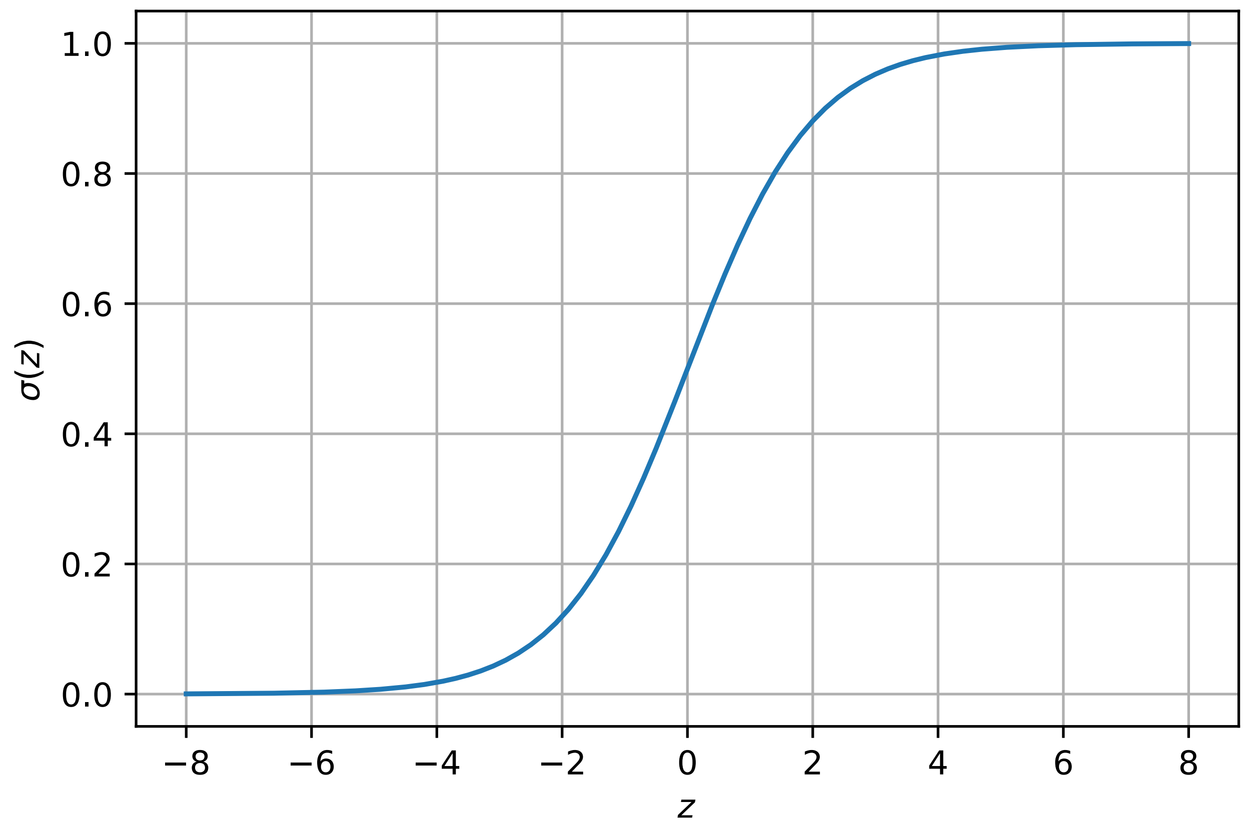
About the Term "Logits"

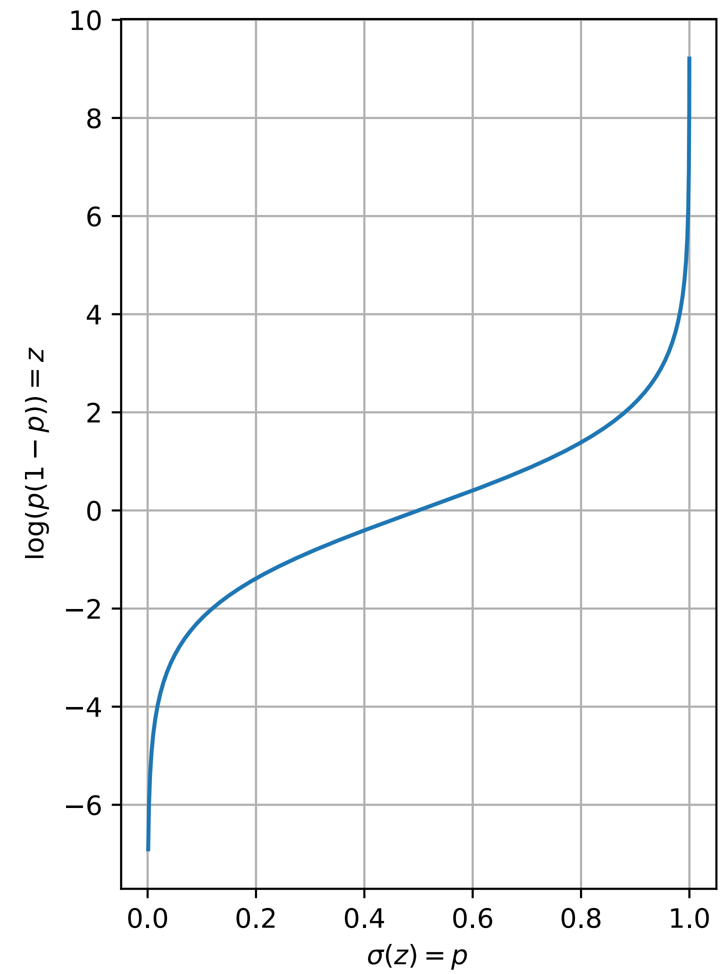
"Logits" is a very commonly used Deep Learning jargon;
probably inspired by the logits for logistic regression

- In deep learning, the ***logits*** are the ***net inputs*** of the the last neuron layer
- In statistics, we call the ***log-odds*** the ***logits***
- In logistic regression, the ***logits*** are naturally $\mathbf{w}^\top \mathbf{x}$ ...
- ... because ***log-odds*** is just short for "logarithm of the odds": log($\mathrm{p}/(1$ - $\mathrm{p})$)
- In other words, the ***logits*** are the inverse of the logistic sigmoid function

About the Term "Logits"

"Logits" is a very commonly used Deep Learning jargon;
probably inspired by the logits for logistic regression





$$\sigma(z) = \frac{1}{1 + \exp(-z)}$$

$$logit(\sigma(z)) = \log(\sigma(z)/(1 - \sigma(z)) = z$$

About the Term "Binary Cross Entropy"

- Negative log-likelihood and binary cross entropy are equivalent
- They are just formulated in different contexts
- Cross entropy comes from the "information theory" (computer science) perspective
- For those who took my previous STAT479: Machine Learning class, we have seen regular entropy in the context of decision trees (but with $\log_2$ instead of the natural log)

  https://github.com/rasbt/stat479-machine-learning-fs18/blob/master/06_trees/06_trees_notes.pdf

- Then, we kind of covered cross entropy in the t-SNE lecture. I.e.,
  KL-divergence = CrossEntropy - Entropy
  https://github.com/rasbt/stat479-machine-learning-fs18/blob/master/14_feat-extract/14_feat-extract_slides.pdf

$$H_{\mathbf{a}}(\mathbf{y}) = -\sum_{i} \Big(y^{[i]} \log(a^{[i]}) + (1 - y^{[i]}) \log(1 - a^{[i]}) \Big)$$

Binary Cross Entropy

$$H_{\mathbf{a}}(\mathbf{y}) = \sum_{i=1}^{n} \sum_{k=1}^{K} -y_k^{[i]} \log \left(a_k^{[i]} \right)$$

(Multi-category) Cross Entropy for K different class labels

PyTorch Loss-Input Confusion (Cheatsheet)

https://github.com/rasbt/stat479-deep-learning-ss19/blob/master/other/pytorch-lossfunc-cheatsheet.md

Logistic Regression Coding Example

https://github.com/rasbt/stat479-deep-learning-ss19/blob/master/L08_logistic/code/logistic-regression.ipynb

Logistic Regression for Multi-class Classification:

Multinomial Logistic Regression/ Softmax Regression

MNIST - 60k Handwritten Digits

http://yann.lecun.com/exdb/mnist/

Balanced dataset:

- 10 classes (digits 0-9)
- 10k digits per class

Image dimensions: 28x28x1

In NCHW, an image batch of 128 examples would be a tensor with dimensions (128, 1, 28, 28)

- Training set images: train-images-idx3-ubyte.gz (9.9 MB, 47 MB unzipped, and 60,000 examples)
- Training set labels: train-labels-idx1-ubyte.gz (29 KB, 60 KB unzipped, and 60,000 labels)
- Test set images: t10k-images-idx3-ubyte.gz (1.6 MB, 7.8 MB, unzipped and 10,000 examples)
- Test set labels: t10k-labels-idx1-ubyte.gz (5 KB, 10 KB unzipped, and 10,000 labels)

MNIST - 60k Handwritten Digits

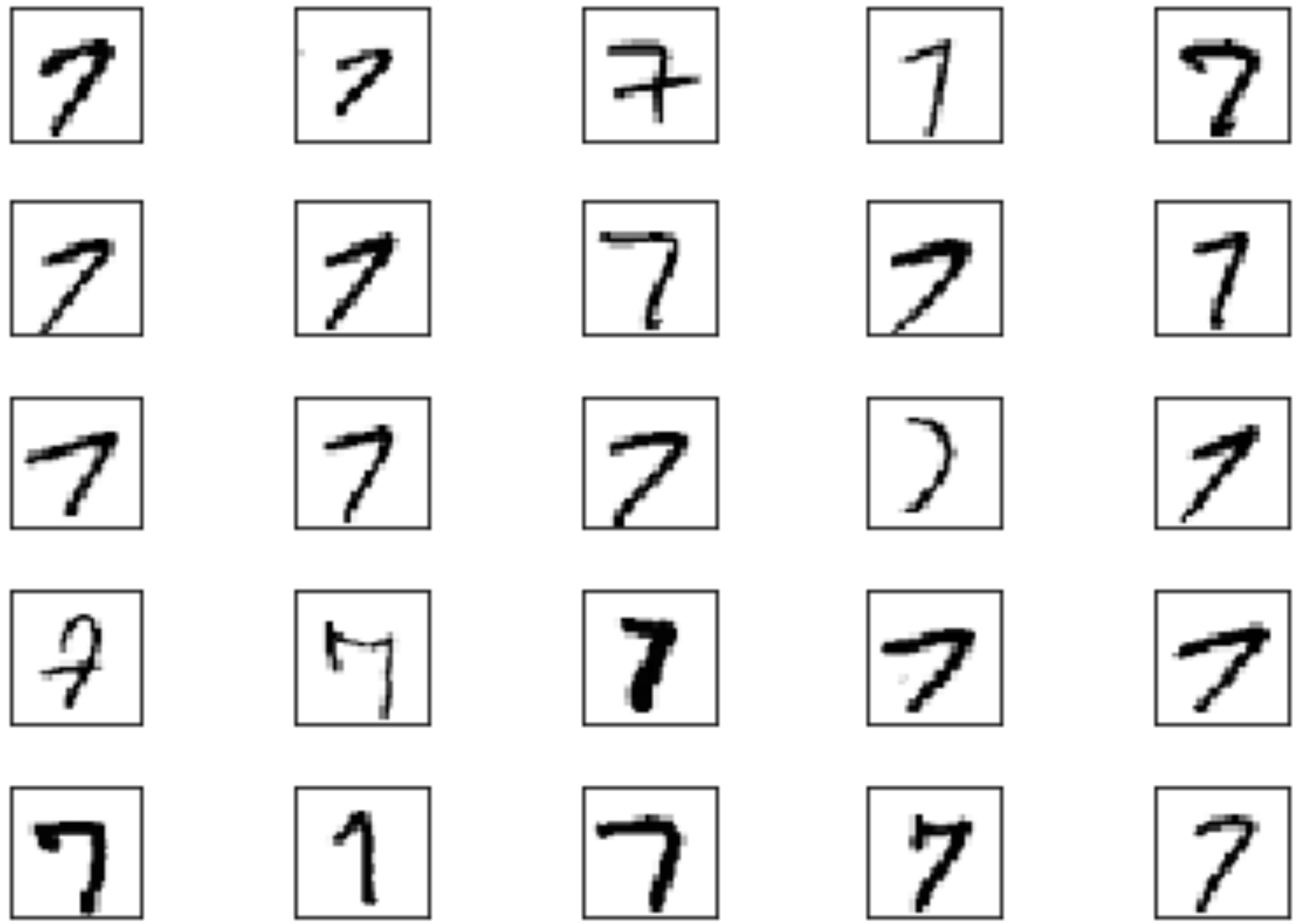


Illustration of different "7"s

Data Representation (unstructured data; images)

Convolutional Neural Networks (later)

```
Image batch dimensions: torch.Size([128, 1, 28, 28])
Image label dimensions: torch.Size([128])
```

← "NCHW" representation

```
print(images[0].size())
```

```
torch.Size([1, 28, 28])
```

```
images[0]
```

```
tensor([[[0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000,
          0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000,
          0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000,
          0.0000, 0.0000, 0.0000, 0.0000],
         [0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000,
          0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000,
          0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000,
          0.0000, 0.0000, 0.0000, 0.0000],
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          0.0000, 0.0000, 0.0000, 0.0000],

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          0.0000, 0.0000, 0.0000, 0.0000],
         [0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000,
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          0.0000, 0.0000, 0.0000, 0.0000],
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          0.0000, 0.0000, 0.0000, 0.0667, 0.0745, 0.5412, 0.9725, 0.9922,
          0.9922, 0.9922, 0.6275, 0.0549, 0.0000, 0.0000, 0.0000, 0.0000,
```

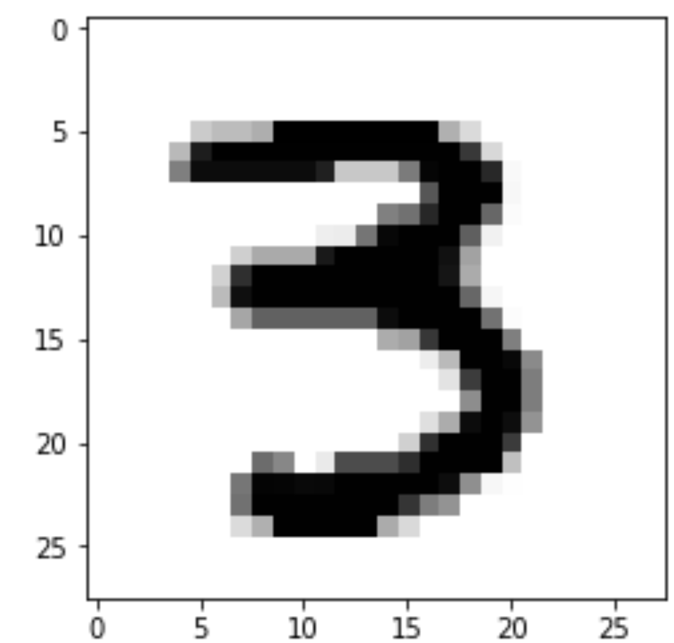

Note that I normalized pixels by factor 1/255 here

Data Representation (unstructured data; images)

Softmax regression: "traditional method"

[0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0,
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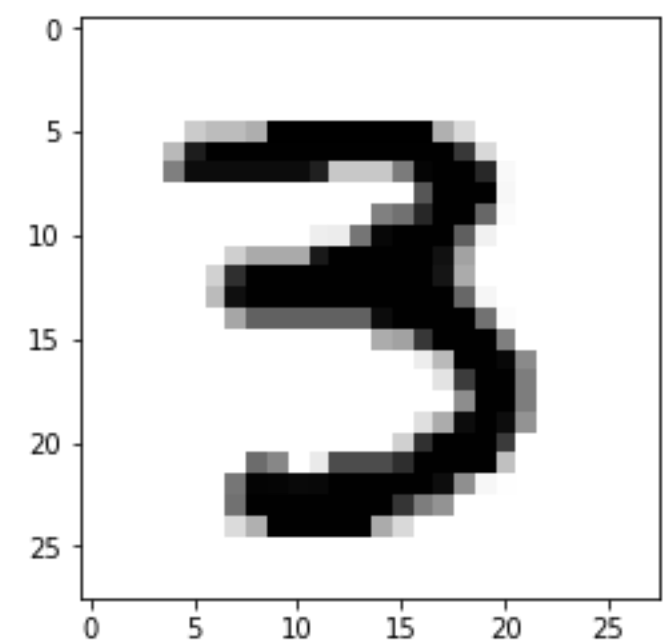
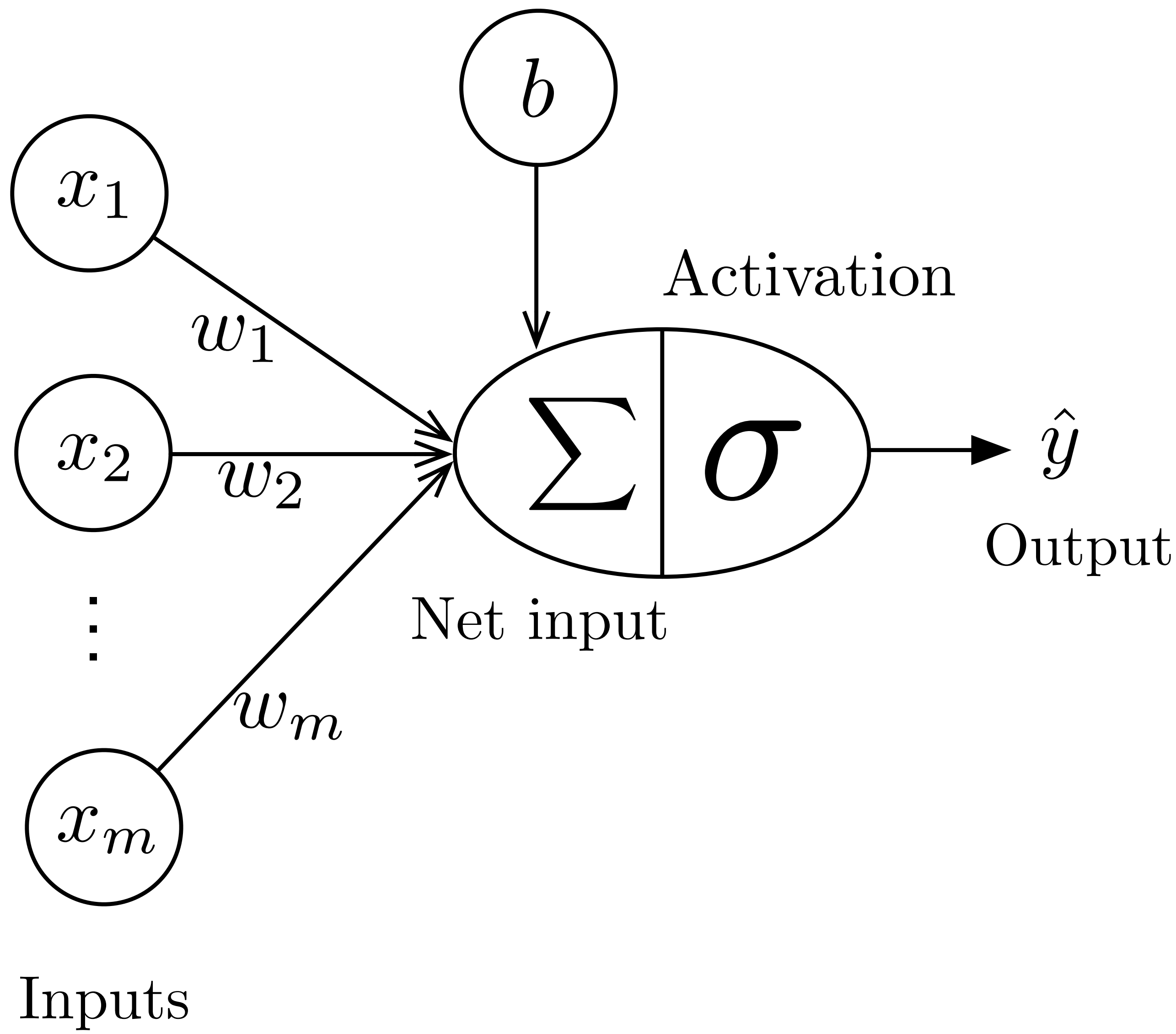
Represent digit as a long vector of pixels



Note that I normalized pixels by factor 1/255 here

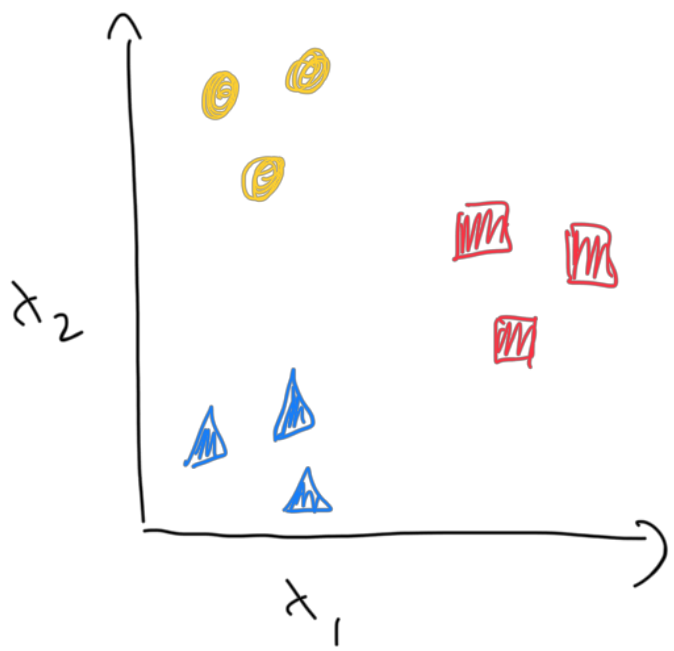
Previous Approach for Binary Classes

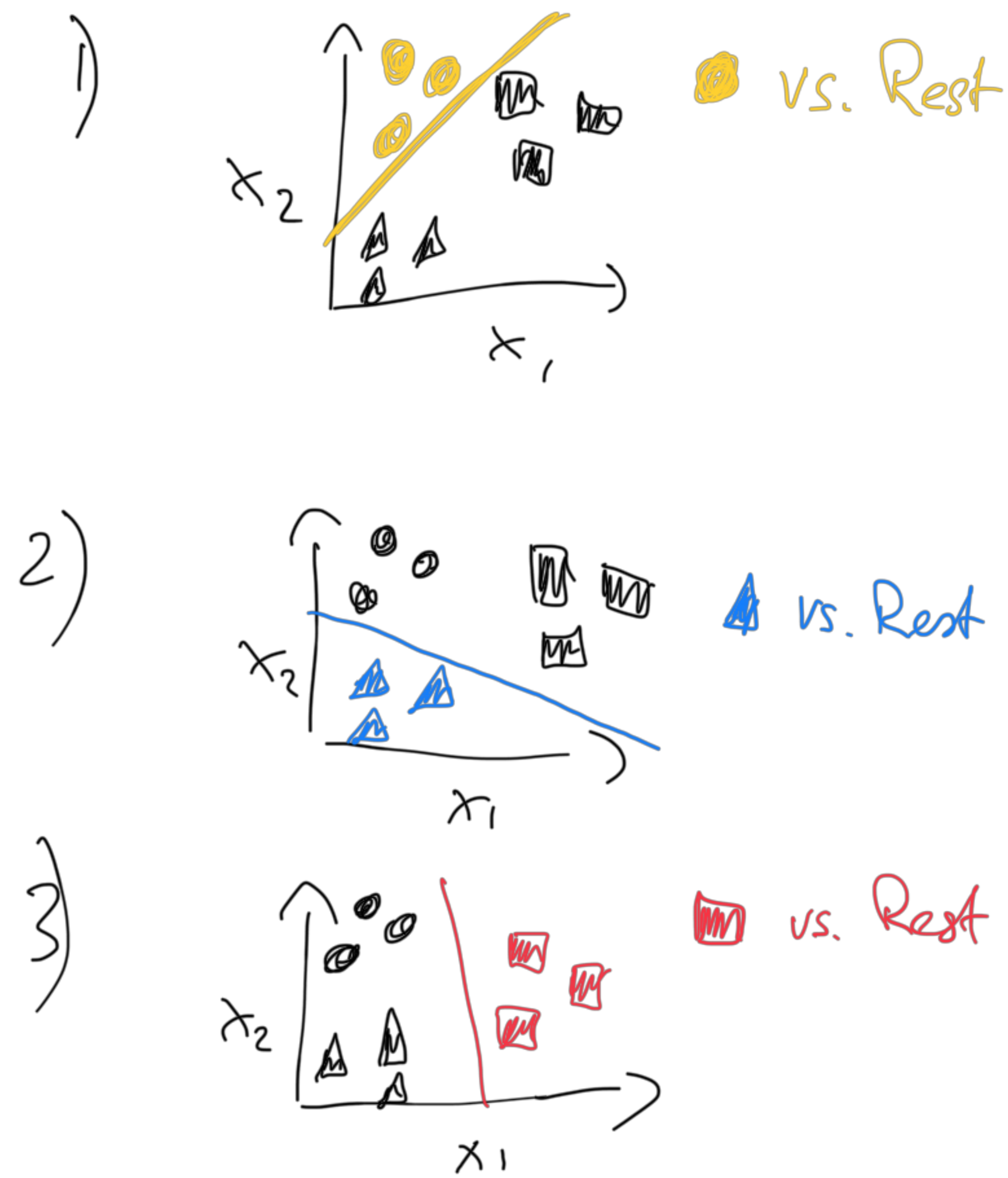


In logistic regression, the activation can be interpreted as $p(y=1|x)$

Multi-Class Classification with Multiple Binary Classifiers

One-vs-Rest (OvR) / One-vs-All (OvA)

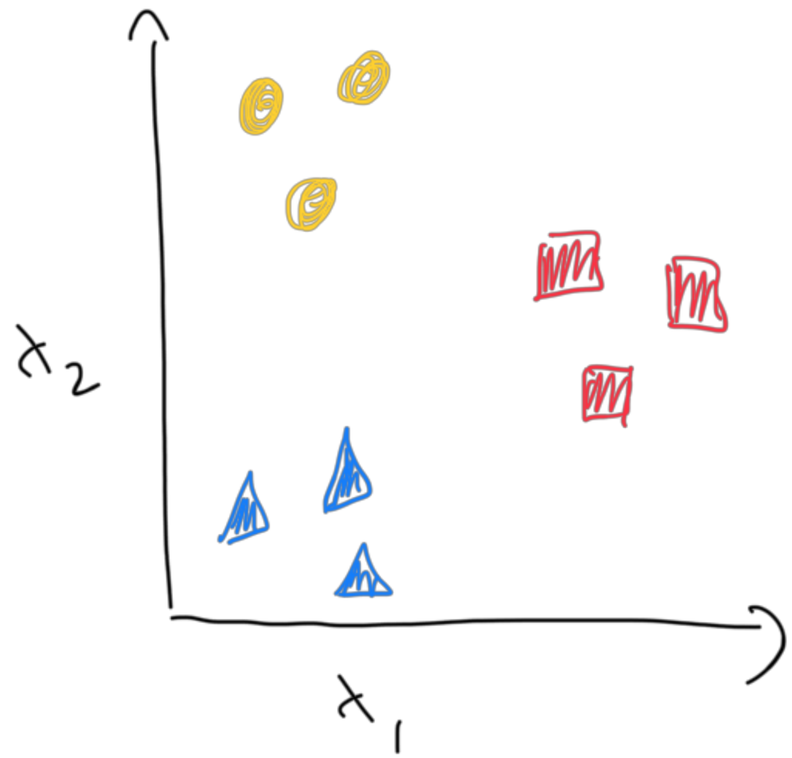


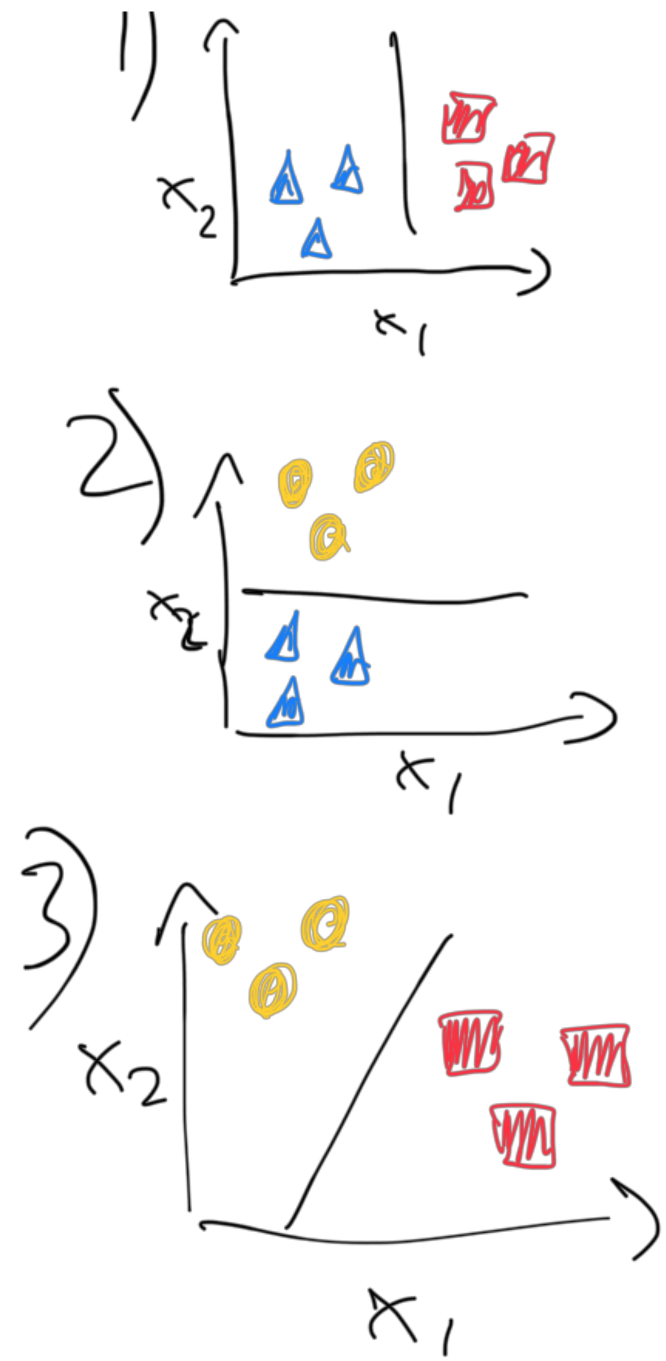


Then, choose the class with the highest confidence score

Multi-Class Classification with Multiple Binary Classifiers

One-vs-One (OvO) / All-vs-All (AvA)





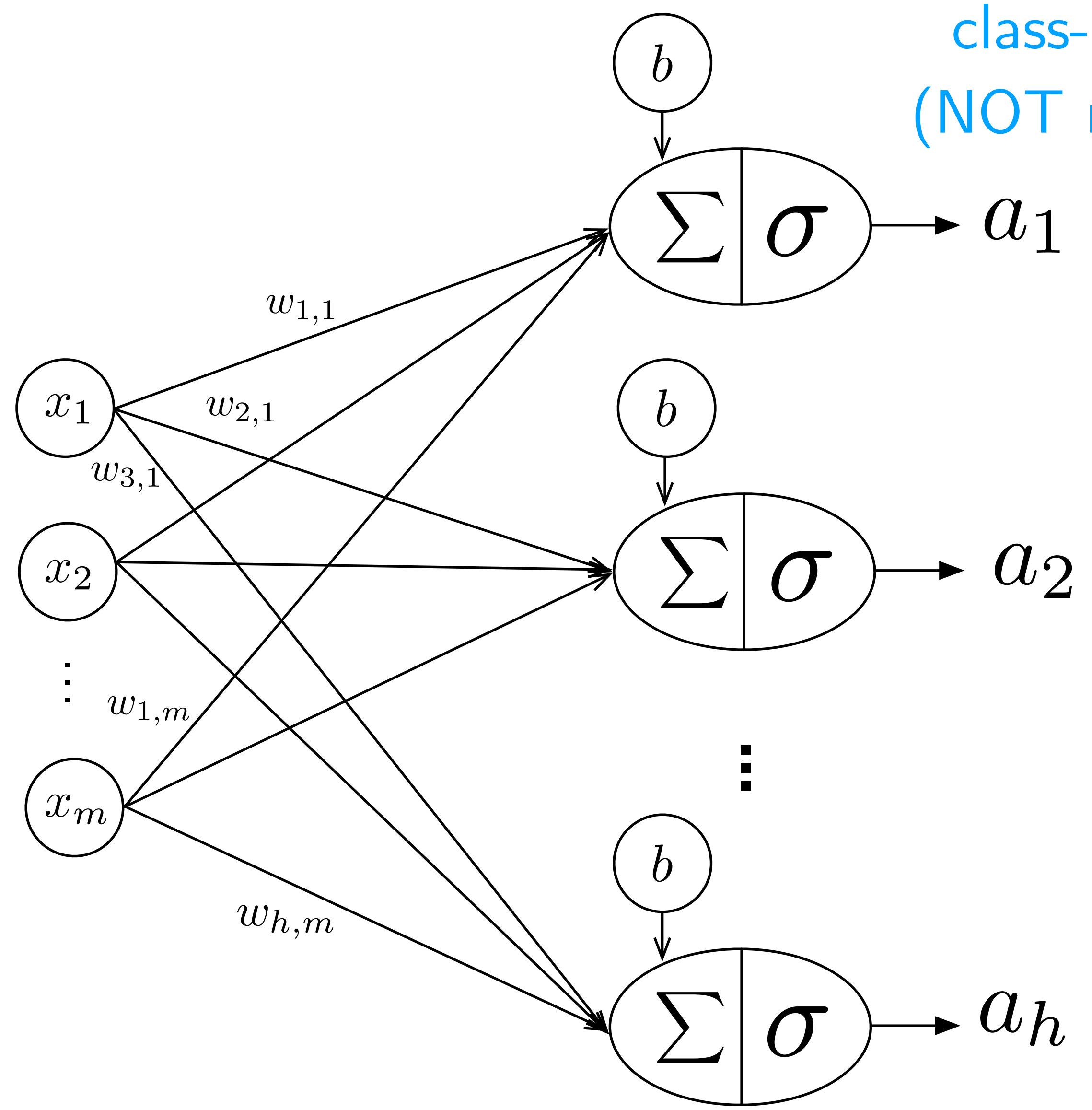
Number of classifiers needed:

num_classes x (num_classes - 1) / 2

Then, select the class by majority vote (and use confidence score in case of ties)

Another Approach Could be ...

activations are
class-membership probabilities
(NOT mutually exclusive classes)

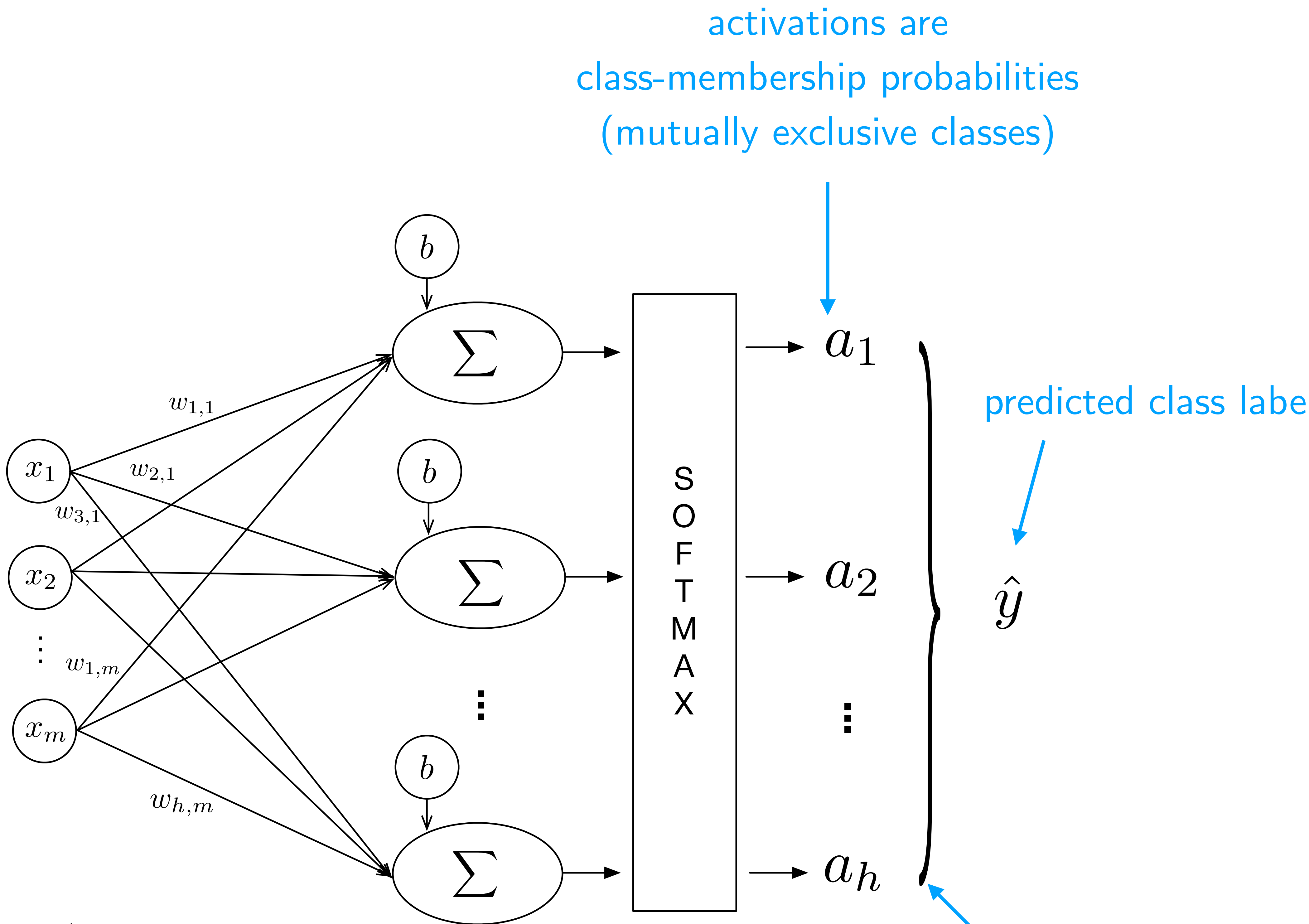


$$\sigma\left(\mathbf{W}\mathbf{x} + \mathbf{b}\right) = \sigma(\mathbf{z}) = \mathbf{a}$$

$$\mathbf{W} \in \mathbb{R}^{k \times m}$$

where k is the number of classes

Multinomial Logistic Regression / Softmax Regression



$$\sigma\big(\mathbf{W}\mathbf{x} + \mathbf{b}\big) = \sigma(\mathbf{z}) = \mathbf{a}$$

Onehot Encoding Needed

class labels
0
1
3
2

→

class_0	class_1	class_2	class_3
1	0	0	0
0	1	0	0
0	0	0	1
0	0	1	0

Softmax Activation

$$P(y = t \mid z_t^{(i)}) = \sigma_{\text{softmax}}(z_t^{(i)}) = \frac{e^{z_t^{(i)}}}{\sum_{j=1}^{k} e^{z_j^{(i)}}}$$

$t \in \{j ... k\}$

k is the number of class labels

(Basically, softmax is just an exponential function that normalizes the activations so that they sum up to 1)

Loss Function

$$\mathcal{L} = \sum_{i=1}^{n} \sum_{j=1}^{k} -y_j^{[i]} \log \left(a_k^{[i]} \right)$$

(Multi-category) Cross Entropy
for k different class labels

This assumes one-hot encoded labels!

Loss Function

$$\mathcal{L}_{\text{binary}} = -\sum_{i=1}^{n} \Big(y^{[i]} \log(a^{[i]}) + (1 - y^{[i]}) \log(1 - a^{[i]}) \Big)$$

This assumes one-hot encoded labels!

$$\mathcal{L}_{\text{multiclass}} = \sum_{i=1}^{n} \sum_{j=1}^{k} -y_j^{[i]} \log \left(a_k^{[i]} \right)$$

(Multi-category) Cross Entropy for k different class labels

Loss Function

$$\mathcal{L}_{\text{binary}} = -\sum_{i=1}^{n} \left(y^{[i]} \log(a^{[i]}) + (1 - y^{[i]}) \log(1 - a^{[i]}) \right)$$

This assumes one-hot encoded labels!

$$\mathcal{L}_{\text{multiclass}} = \sum_{i=1}^{n} \sum_{j=1}^{k} -y_j^{[i]} \log \left(a_k^{[i]} \right)$$

(Multi-category) Cross Entropy for k different class labels

Cross Entropy Loss Function Example

$$\mathbf{Y}_{\text{onehot}} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \end{bmatrix} \qquad \mathbf{A}_{\text{softmax outputs}} = \begin{bmatrix} 0.3792 & 0.3104 & 0.3104 \\ 0.3072 & 0.4147 & 0.2780 \\ 0.4263 & 0.2248 & 0.3490 \\ 0.2668 & 0.2978 & 0.4354 \end{bmatrix}$$

(4 training examples, 3 classes)

Cross Entropy Loss Function Example

1 training example

$$\mathbf{Y}_{\text{onehot}} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \end{bmatrix} \qquad \mathbf{A}_{\text{softmax outputs}} = \begin{bmatrix} 0.3792 & 0.3104 & 0.3104 \\ 0.3072 & 0.4147 & 0.2780 \\ 0.4263 & 0.2248 & 0.3490 \\ 0.2668 & 0.2978 & 0.4354 \end{bmatrix}$$

(4 training examples, 3 classes)

$$\mathcal{L}_{\text{multiclass}} = \sum_{i=1}^{n} \sum_{j=1}^{k} -y_j^{[i]} \log\left(a_k^{[i]}\right)$$

$$\begin{aligned} \mathcal{L}^{[1]} &= [(-1) \cdot \log(0.3792)] \\ &+ [(-0) \cdot \log(0.3104)] \\ &+ [(-0) \cdot \log(0.3104)] \\ &= 0.969692... \end{aligned}$$

Cross Entropy Loss Function Example

$$\mathbf{Y}_{\text{onehot}} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \end{bmatrix} \qquad \mathbf{A}_{\text{softmax outputs}} = \begin{bmatrix} 0.3792 & 0.3104 & 0.3104 \\ 0.3072 & 0.4147 & 0.2780 \\ 0.4263 & 0.2248 & 0.3490 \\ 0.2668 & 0.2978 & 0.4354 \end{bmatrix}$$

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$$\begin{aligned} \mathcal{L}^{[2]} &= [(-0) \cdot \log(0.3072)] \\ &+ [(-1) \cdot \log(0.4147)] \\ &+ [(-0) \cdot \log(0.2780)] \\ &= 0.880200... \end{aligned}$$

$$\begin{aligned} \mathcal{L}^{[3]} &= [(-0) \cdot \log(0.4263)] \\ &+ [(-0) \cdot \log(0.2248)] \\ &+ [(-1) \cdot \log(0.3490)] \\ &= 1.05268... \end{aligned}$$

$$\begin{aligned} \mathcal{L}^{[4]} &= [(-0) \cdot \log(0.2668)] \\ &+ [(-0) \cdot \log(0.2978)] \\ &+ [(-1) \cdot \log(0.4354)] \\ &= 0.831490... \end{aligned}$$

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$$\mathcal{L}_{\text{multiclass}} = \sum_{i=1}^{n} \sum_{j=1}^{k} -y_j^{[i]} \log \left(a_k^{[i]} \right)$$

$$\approx 0.9335$$

Cross Entropy Hands-On Example

https://github.com/rasbt/stat479-deep-learning-ss19/blob/master/L08_logistic/code/cross-entropy-pytorch.ipynb

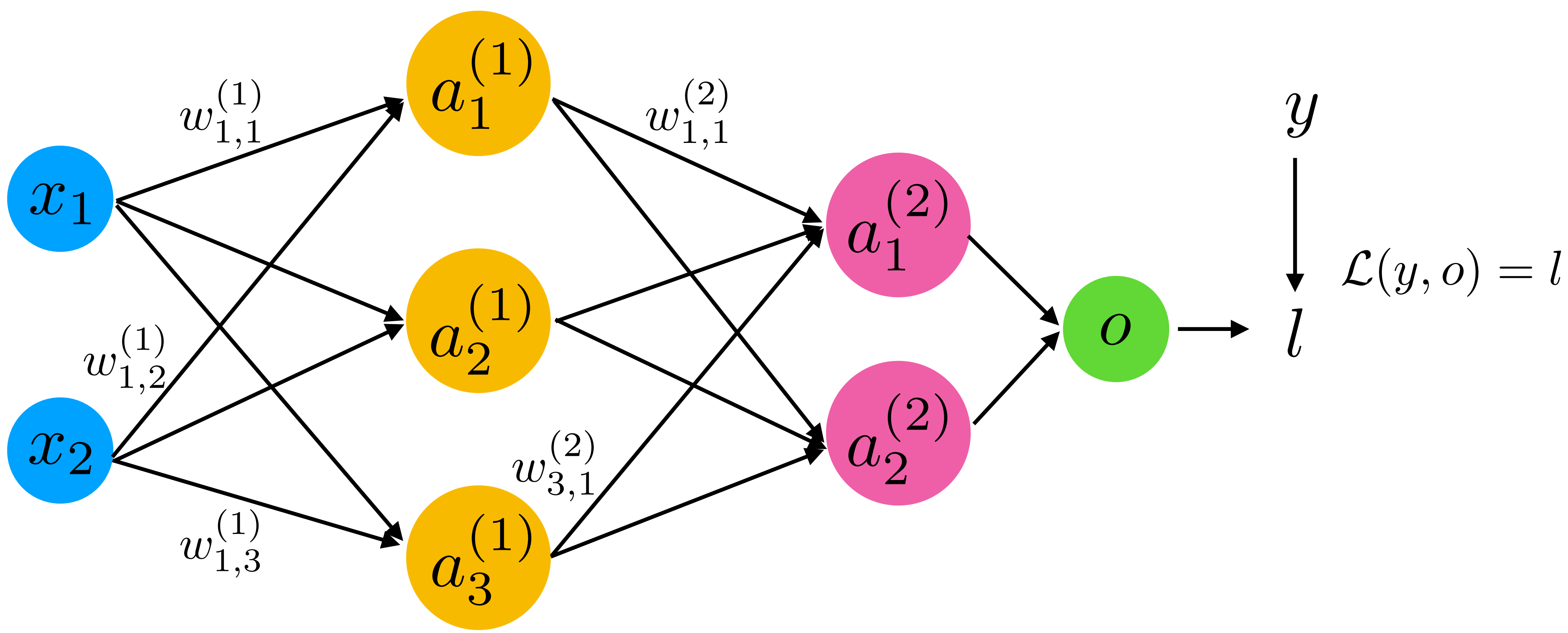
The Same Overall Concept Applies ...

Want: $\frac{\partial \mathcal{L}}{\partial w_i}$ and $\frac{\partial \mathcal{L}}{\partial b}$

$$\frac{\partial \mathcal{L}}{\partial w_i} = \frac{\partial \mathcal{L}}{\partial a} \frac{da}{dz} \frac{\partial z}{\partial w_i}$$

$$\frac{\partial \mathcal{L}}{\partial b} = \frac{\partial \mathcal{L}}{\partial a} \frac{da}{dz} \frac{\partial z}{\partial b}$$

Graph with Fully-Connected Layers (later in this course)



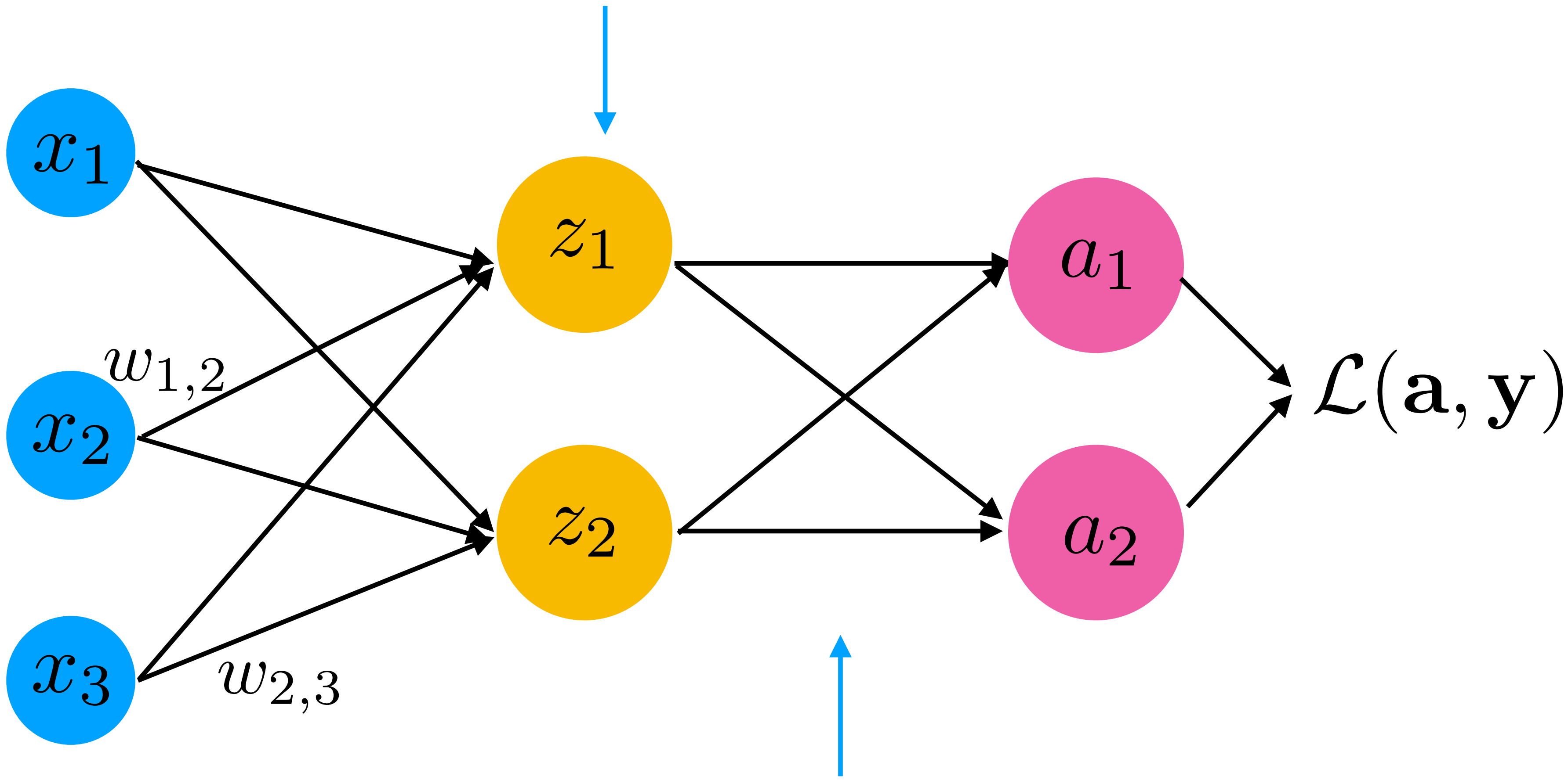
$$\frac{\partial l}{\partial w_{1,1}^{(1)}} = \frac{\partial l}{\partial o} \cdot \frac{\partial o}{\partial a_1^{(2)}} \cdot \frac{\partial a_1^{(2)}}{\partial a_1^{(1)}} \cdot \frac{\partial a_1^{(1)}}{\partial w_{1,1}^{(1)}} + \frac{\partial l}{\partial o} \cdot \frac{\partial o}{\partial a_2^{(2)}} \cdot \frac{\partial a_2^{(2)}}{\partial a_1^{(1)}} \cdot \frac{\partial a_1^{(1)}}{\partial w_{1,1}^{(1)}}$$

Remember when I introduced the multivariable chain rule earlier in this course? Now, we need it!

Softmax Regression Sketch

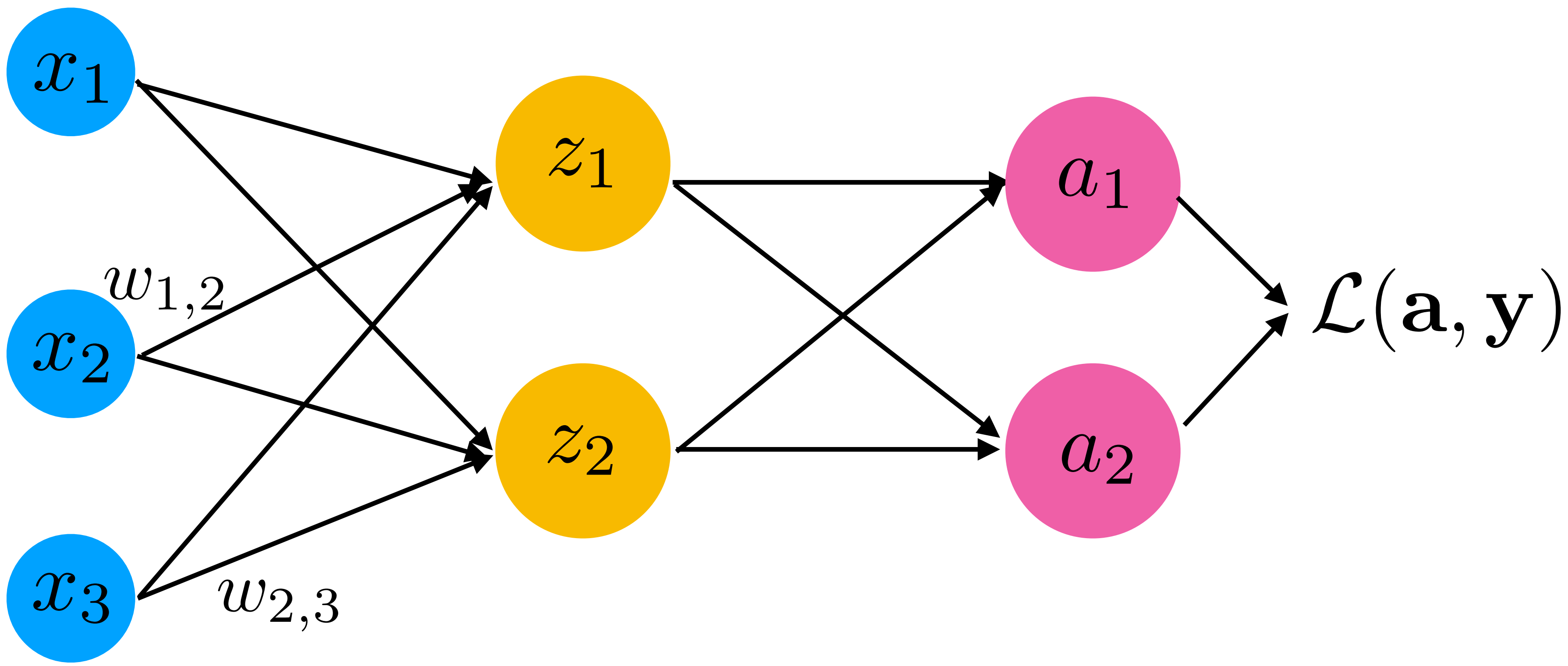
(This is NOT a multi-layer neural network; still 1-layer, no hidden layer)

Note that I put the logits (net inputs) as the intermediate step



The activation function (softmax) would be applied here to obtain the activations

Softmax Regression Sketch



Multivariable chain rule

$$\frac{\partial L}{\partial w_{1,2}} = \frac{\partial L}{\partial a_1}\frac{\partial a_1}{\partial z_1}\frac{\partial z_1}{\partial w_{1,2}} + \frac{\partial L}{\partial a_2}\frac{\partial a_2}{\partial z_1}\frac{\partial z_1}{\partial w_{1,2}}$$

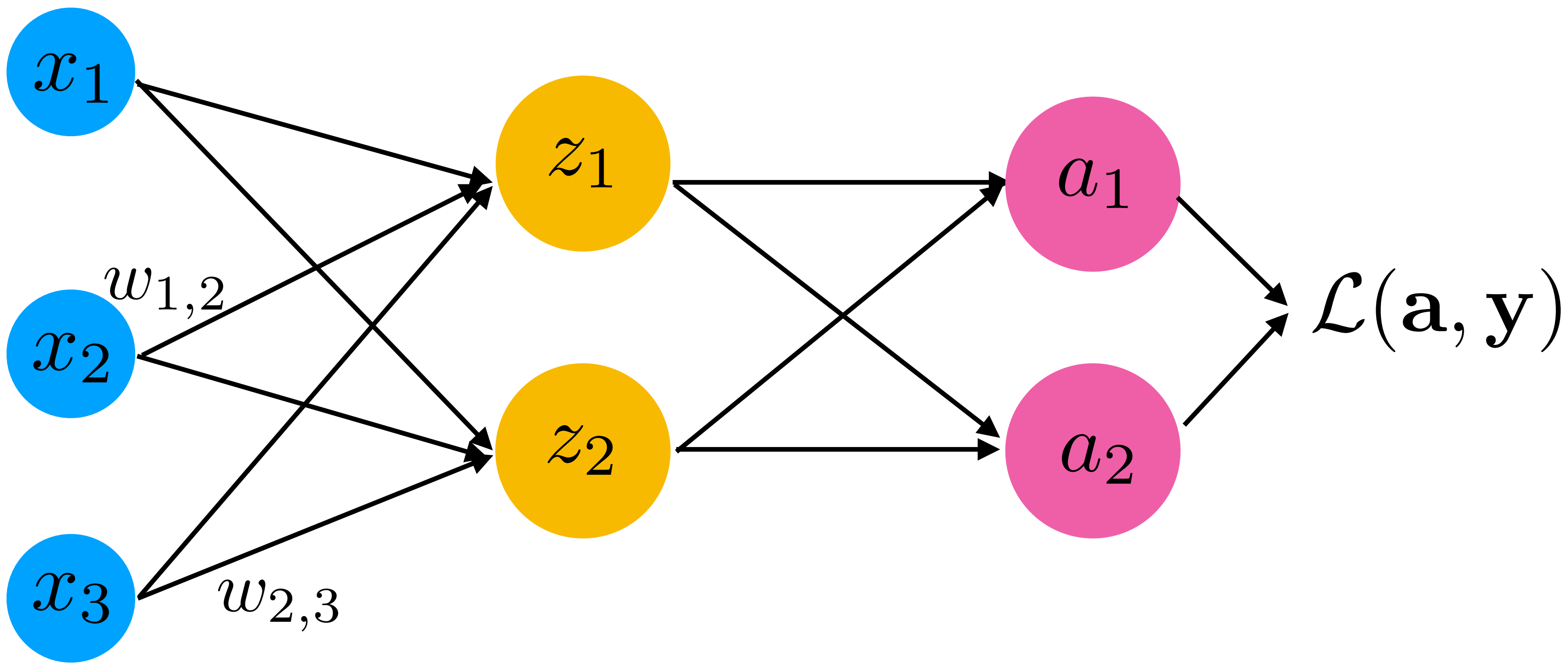
$$= \frac{-y_1}{a_1}[a_1(1-a_1)]x_2 + \frac{-y_2}{a_2}(-a_2 a_1)x_2$$

$$= (y_2 a_1 - y_1 + y_1 a_1)x_2$$

$$= (a_1(y_1 + y_2) - y_1)x_2$$

$$= -(y_1 - a_1)x_2$$

Softmax Regression Sketch



$$
\begin{aligned}
\frac{\partial L}{\partial w_{1,2}} &= \frac{\partial L}{\partial a_1} \frac{\partial a_1}{\partial z_1} \frac{\partial z_1}{\partial w_{1,2}} + \frac{\partial L}{\partial a_2} \frac{\partial a_2}{\partial z_1} \frac{\partial z_1}{\partial w_{1,2}} \\
&= \frac{-y_1}{a_1}[a_1(1-a_1)]x_2 + \frac{-y_2}{a_2}(-a_2 a_1)x_2 \\
&= (y_2 a_1 - y_1 + y_1 a_1)x_2 \\
&= (a_1(y_1 + y_2) - y_1)x_2 \\
&= -(y_1 - a_1)x_2
\end{aligned}
$$

Vectorized Form:

$$\nabla_{\mathbf{W}} \mathcal{L} = -(\mathbf{X}^\top (\mathbf{Y} - \mathbf{A}))^\top$$

where $\mathbf{W} \in \mathbb{R}^{k \times m}$

$\mathbf{X} \in \mathbb{R}^{n \times m}$

$\mathbf{A} \in \mathbb{R}^{n \times k}$

$\mathbf{Y} \in \mathbb{R}^{n \times k}$

Softmax Regression Hands-On Example (Iris)

From Scratch + PyTorch

https://github.com/rasbt/stat479-deep-learning-ss19/blob/master/L08_logistic/code/softmax-regression_scratch.ipynb

Softmax Regression Hands-On (MNIST)

Using PyTorch

https://github.com/rasbt/stat479-deep-learning-ss19/blob/master/L08_logistic/code/softmax-regression-mnist.ipynb

Reading Assignments

Softmax regression tutorial:
http://ufldl.stanford.edu/wiki/index.php/Softmax_Regression