Lecture 07

Logistic Regression and Multi-class Classification

STAT 453: Deep Learning, Spring 2020

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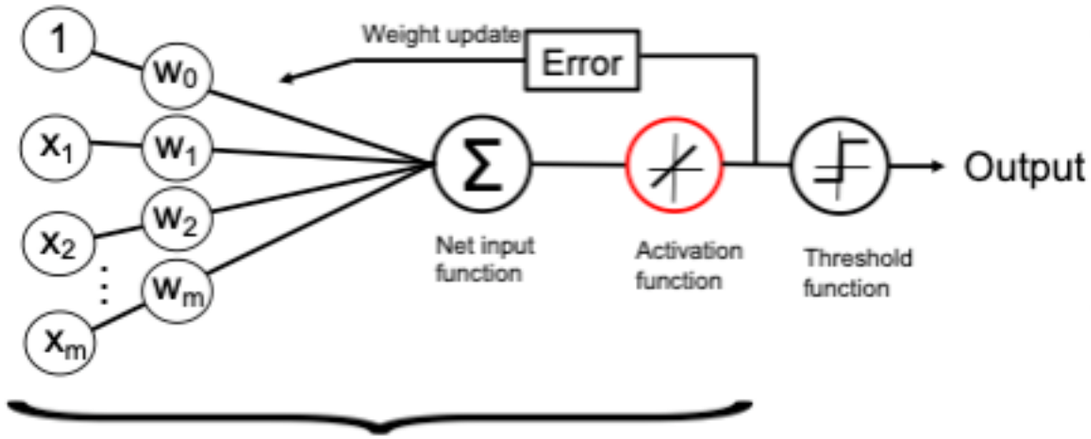
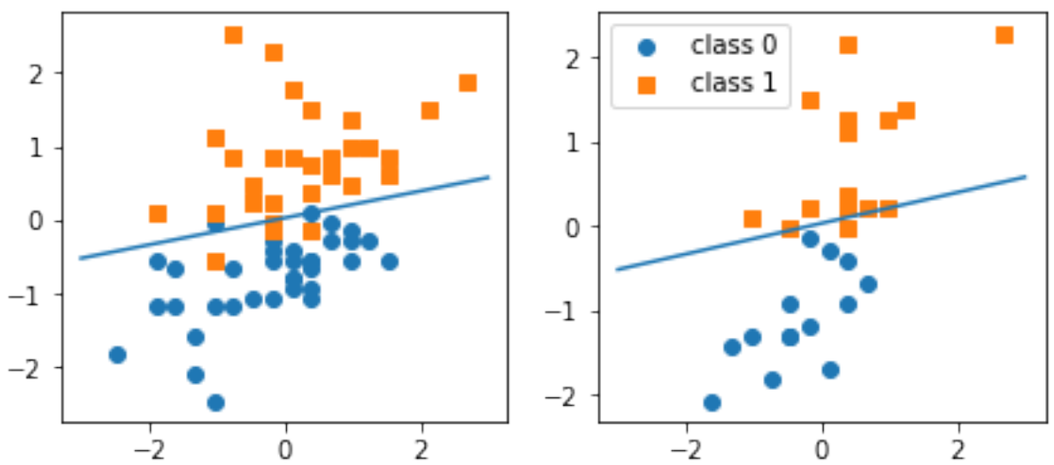
pages.stat.wisc.edu/~sraschka/teaching/stat453-ss2020/

Last Lecture(s):

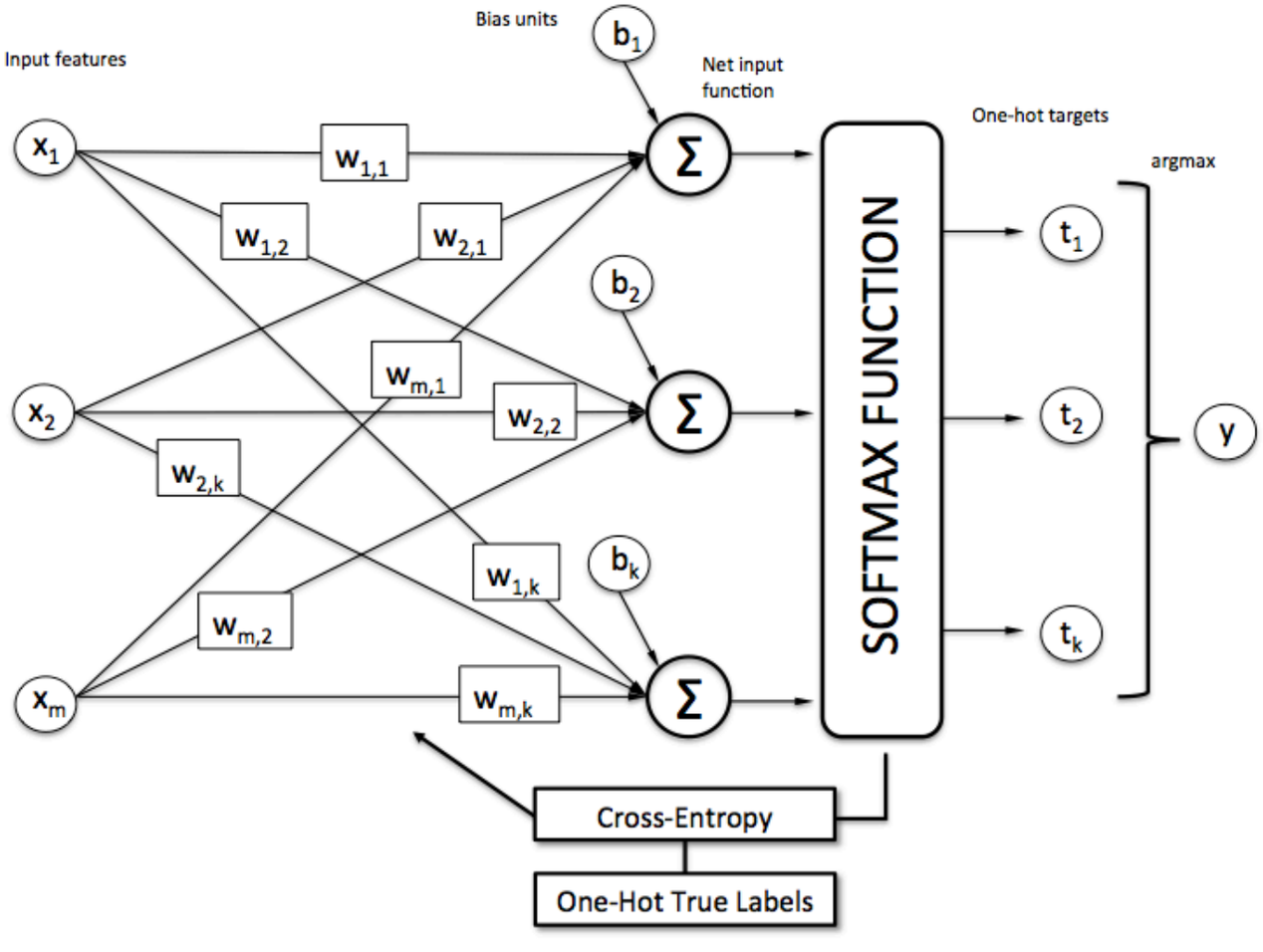
- Solved convergence issue of Perceptron via Adaline
- Conceptualized gradient descent via computation graphs

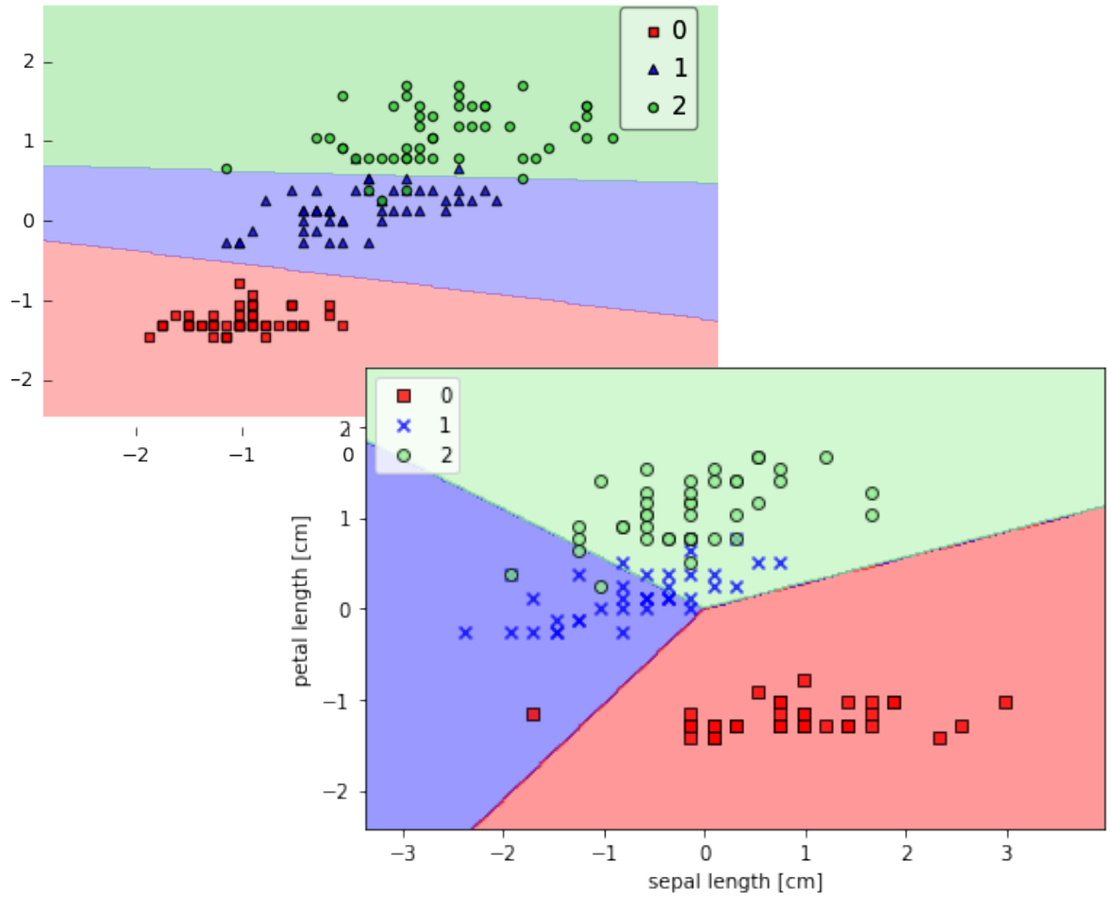




This Lecture:

- A better loss function for classification (cross-entropy instead of MSE)
- Extending neurons to multi-class classification (multiple output notes + softmax)





Topics

Logistic Regression

Negative Log-Likelihood Loss

Logistic Regression Learning Rule

Softmax Regression

Softmax Loss Gradients

Logistic Regression for Binary Classification

Logistic Regression

Negative Log-Likelihood Loss

Logistic Regression Learning Rule

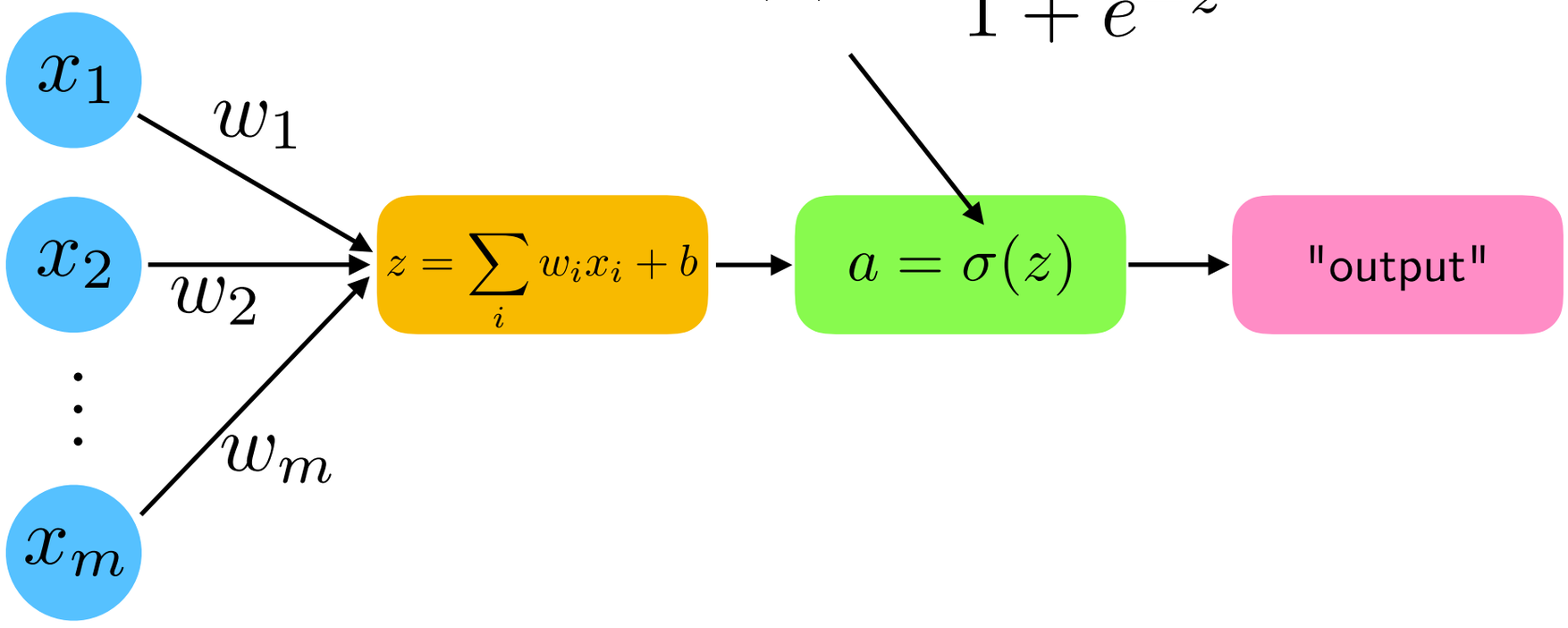
Softmax Regression

Softmax Loss Gradients

Logistic Regression Neuron

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

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

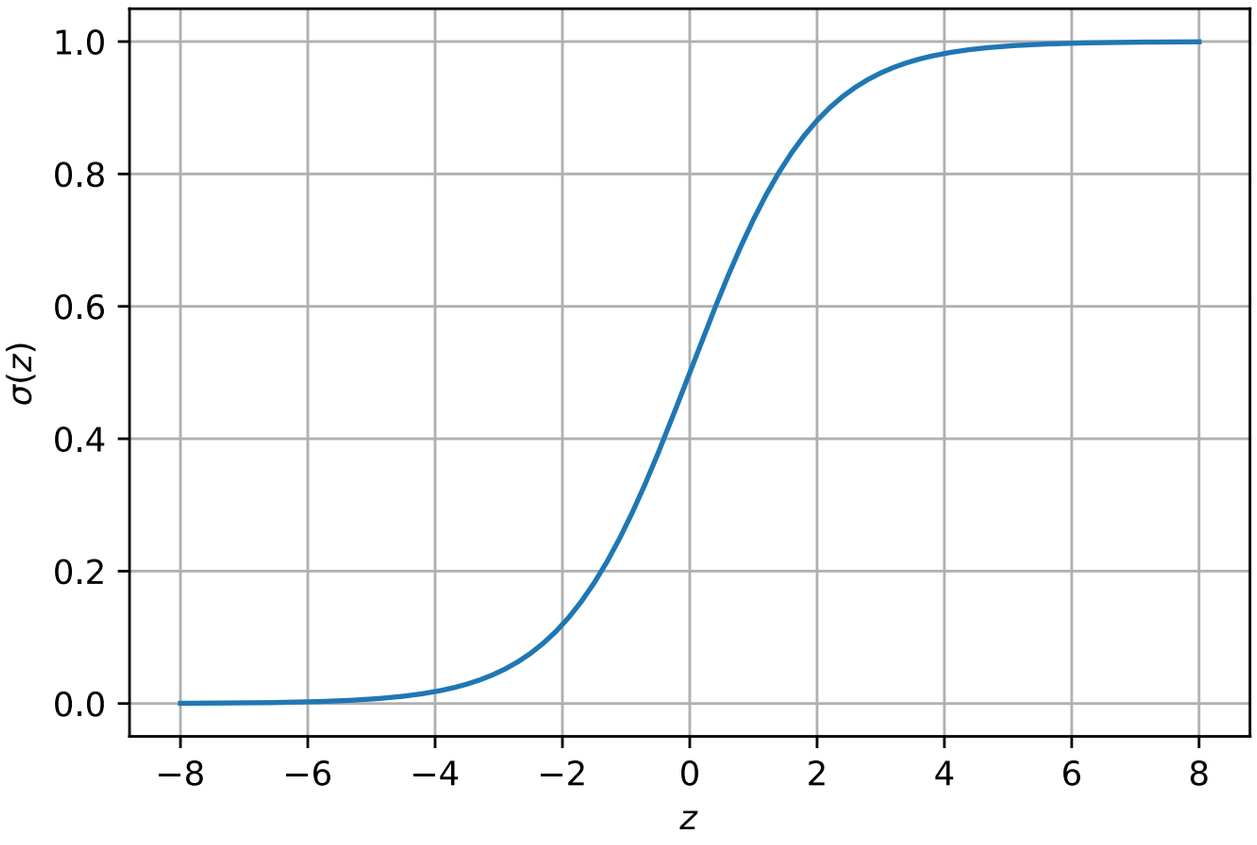


- In ADALINE, the activation function was an identity function, $\sigma(z) = z$
- In HW2, the activation function was different sigmoid function, $\sigma(z) = (e^z - e^{-z})/(e^z + e^{-z})$
- In both cases, ADALINE & HW2, we used MSE as loss function: $\text{MSE} = \dfrac{1}{n} \sum_i (a^{[i]} - y^{[i]})^2$

Logistic Sigmoid Function

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

activation



net input

Logistic Regression

Given the output:

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

here, the "hypothesis" is just our activation function output

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

We compute the posterior as:

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

For a binary class problem (0 and 1), we want these probabilities to be:

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

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

Logistic Regression

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

here, the "hypothesis" is just our activation function output

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

We compute the posterior as:

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

rewrite more compactly

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

Logistic Regression

And for multiple training examples, we want to maximize:

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

by finding *good/optimal* parameters

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

Logistic Regression Loss Function

Likelihood "Loss"

$$L(\mathbf{w}) = P(\mathbf{y} \mid \mathbf{x}; \mathbf{w})$$

$$= \prod_{i=1}^{n} P\big(y^{(i)} \mid x^{(i)}; \mathbf{w}\big)$$

$$= \prod_{i=1}^{n} \Big(\sigma\big(z^{(i)}\big)\Big)^{y^{(i)}} \Big(1 - \sigma\big(z^{(i)}\big)\Big)^{1-y^{(i)}}$$

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:

$$\mathcal{L}(\mathbf{w}) = -l(\mathbf{w})$$

$$= -\sum_{i=1}^{n} \left[y^{(i)} \log \left(\sigma\left(z^{(i)}\right) \right) + \left(1 - y^{(i)}\right) \log \left(1 - \sigma\left(z^{(i)}\right)\right) \right]$$

(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)

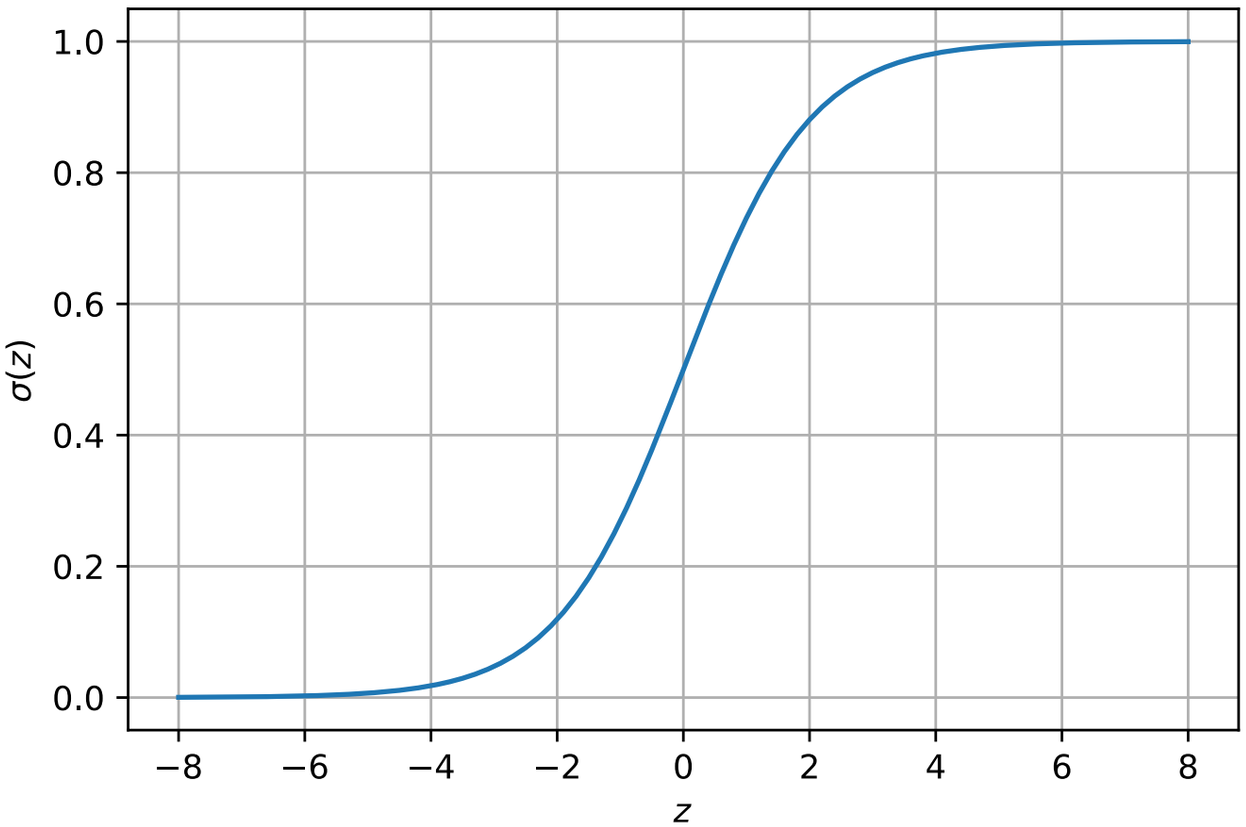
Training Logistic Regression

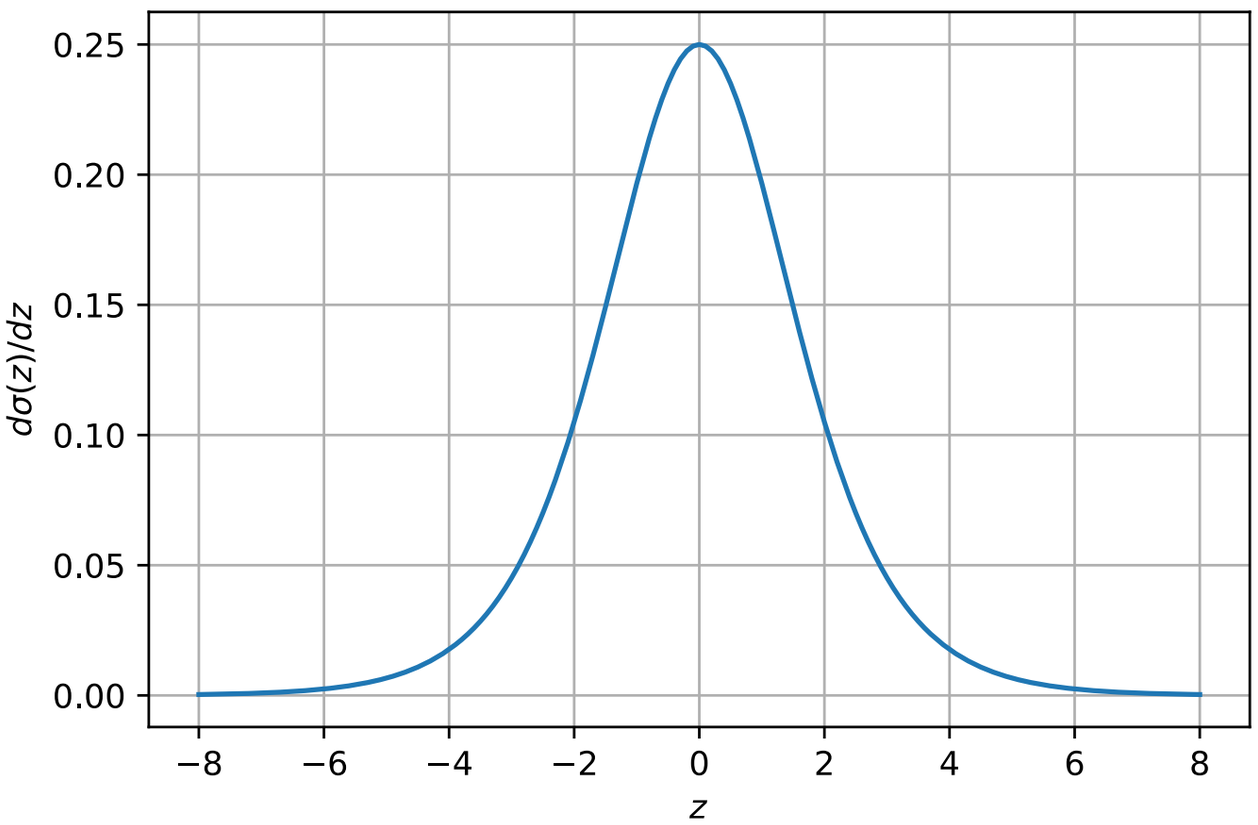
Logistic Sigmoid Derivative

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

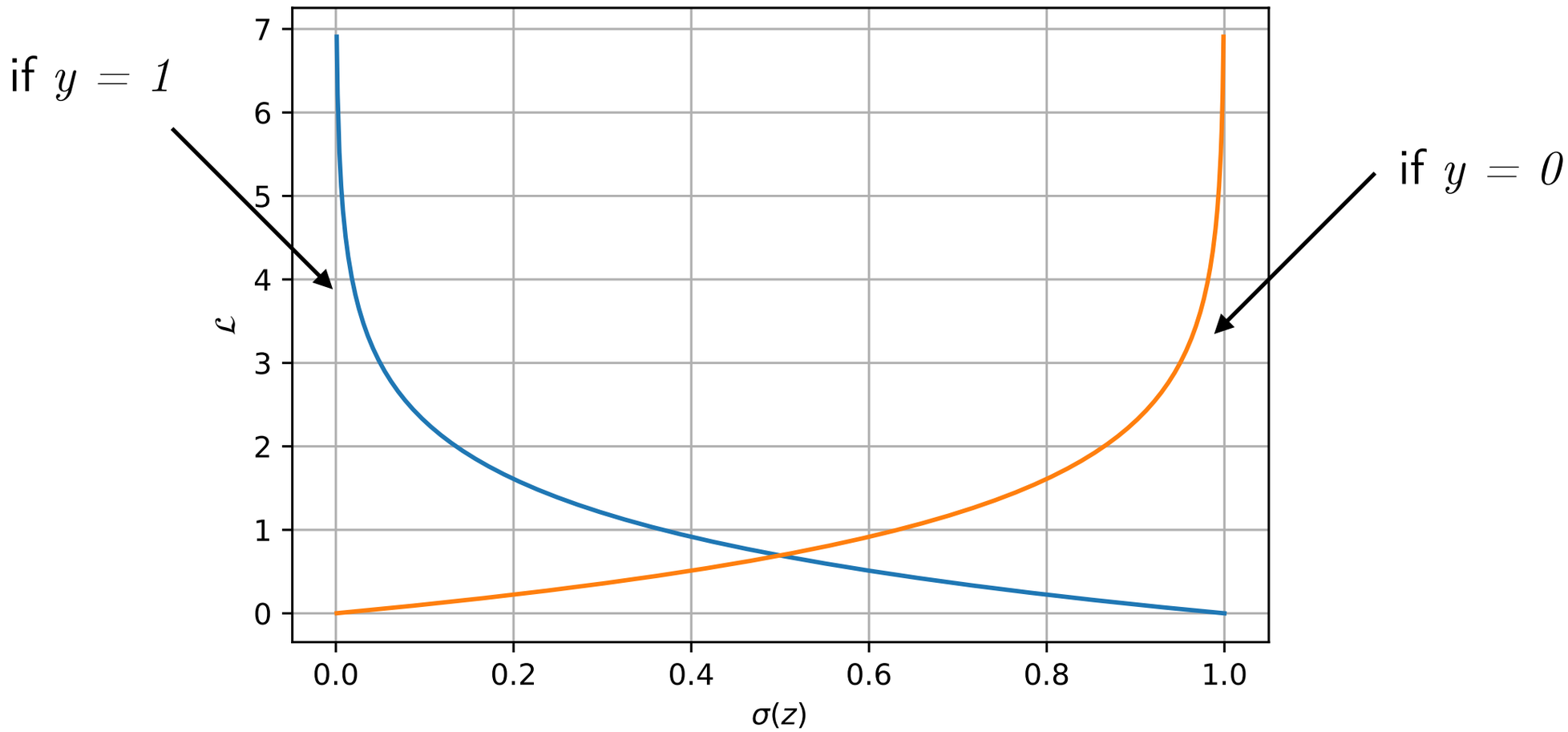
$$\sigma(z) = \frac{1}{1 + e^{-z}}$$

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





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

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

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

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

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

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

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

Learning Rule for Logistic Regression

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

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

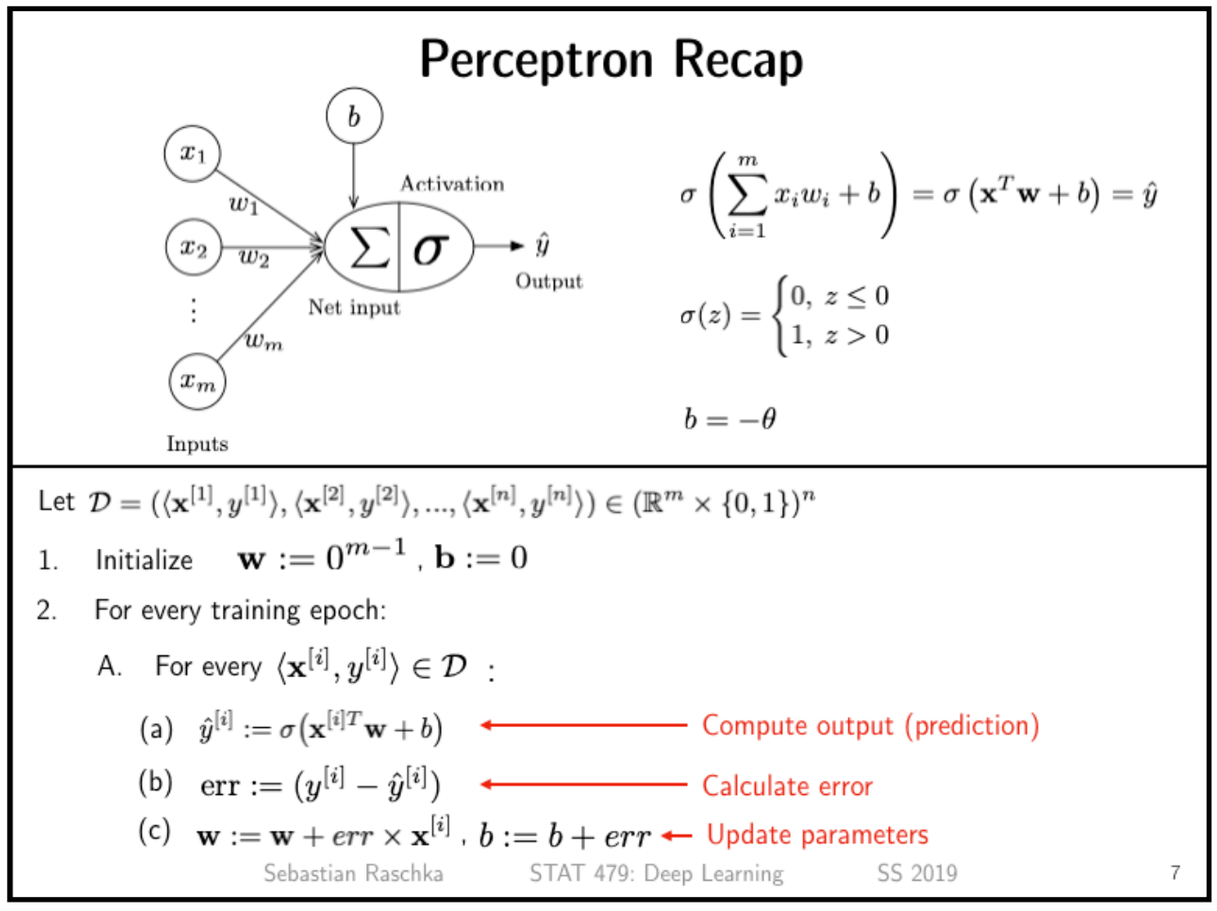
$$\frac{\partial \mathcal{L}}{\partial a} = -\left(y \frac{1}{a} - (1-y) \frac{1}{1-a} \right)$$

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

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

Learning Rule for Logistic Regression

Remember the Perceptron & ADALINE Lectures?



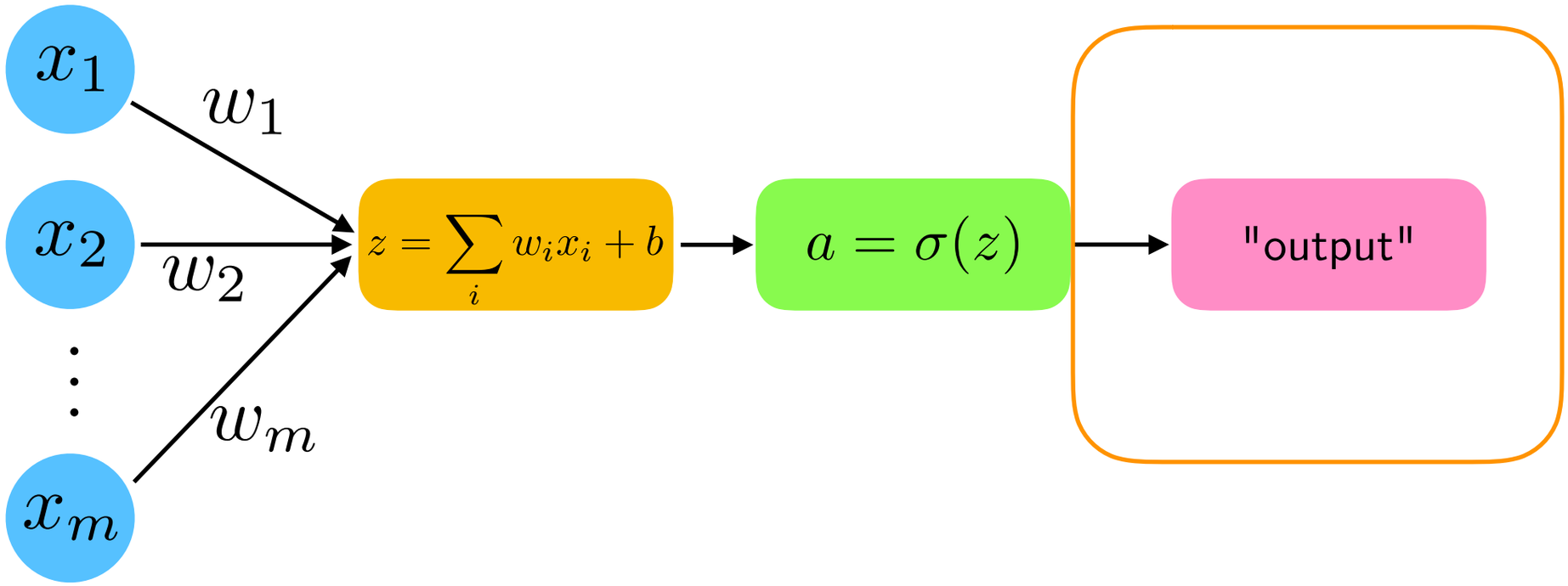
$$\frac{\partial \mathcal{L}}{\partial w_j} = (y - a)x_j$$

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

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

Update for each batch/minibatch with learning rate

Class Label Predictions with Logistic Regression



In logistic regression, we can use

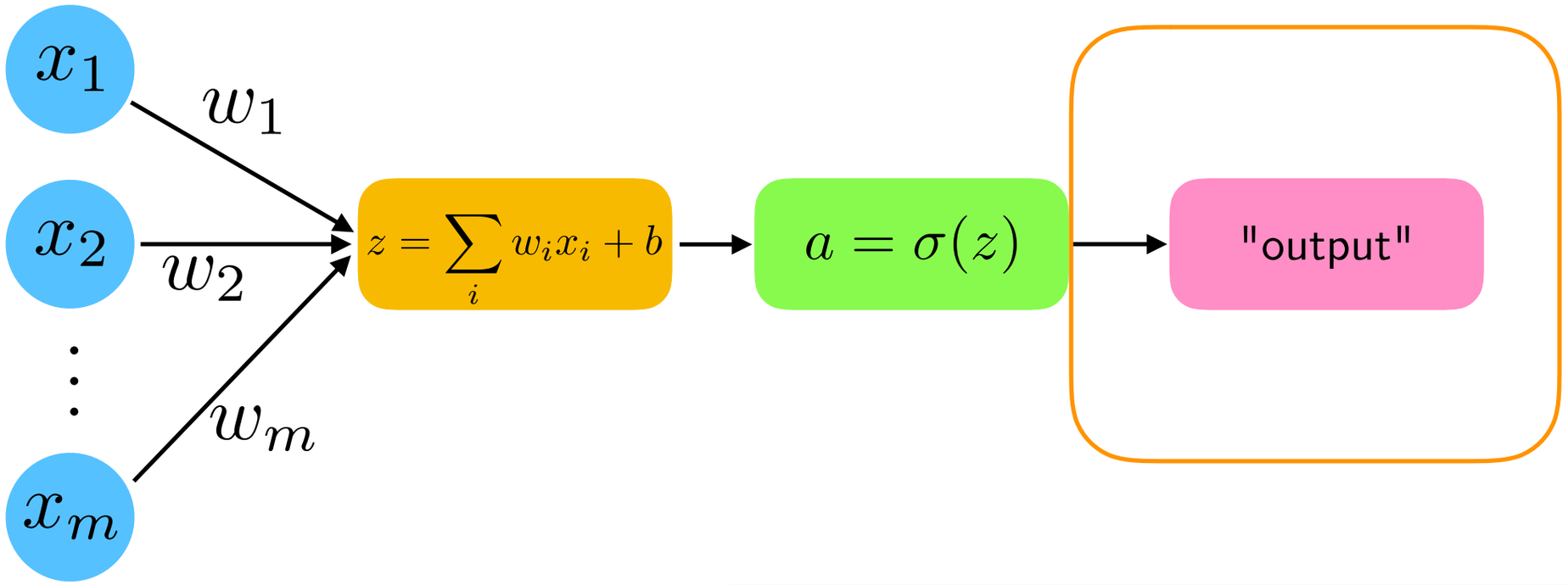
$$\hat{y} := \begin{cases} 1 & \text{if } \sigma(z) > 0.5 \\ 0 & \text{otherwise} \end{cases}$$

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

Class Label Predictions with Logistic Regression



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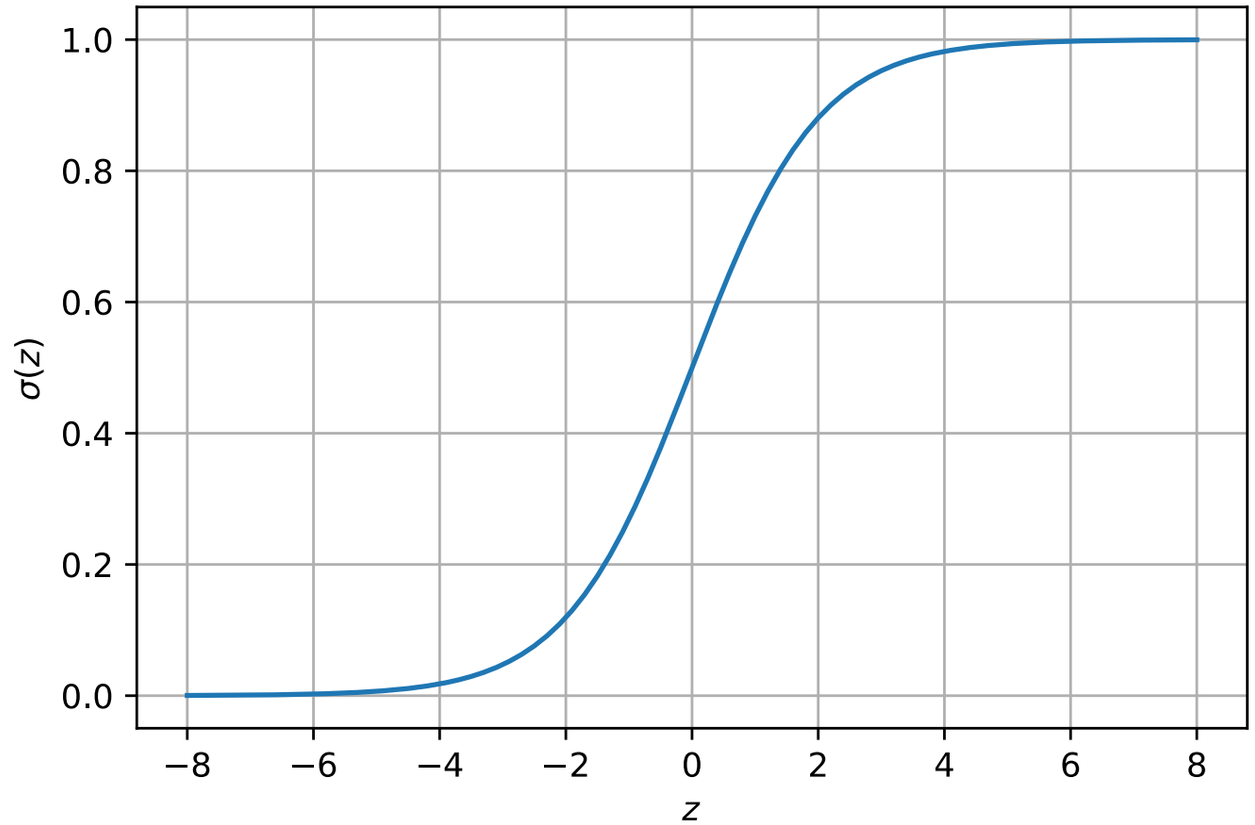

About the Term "Logits"

"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

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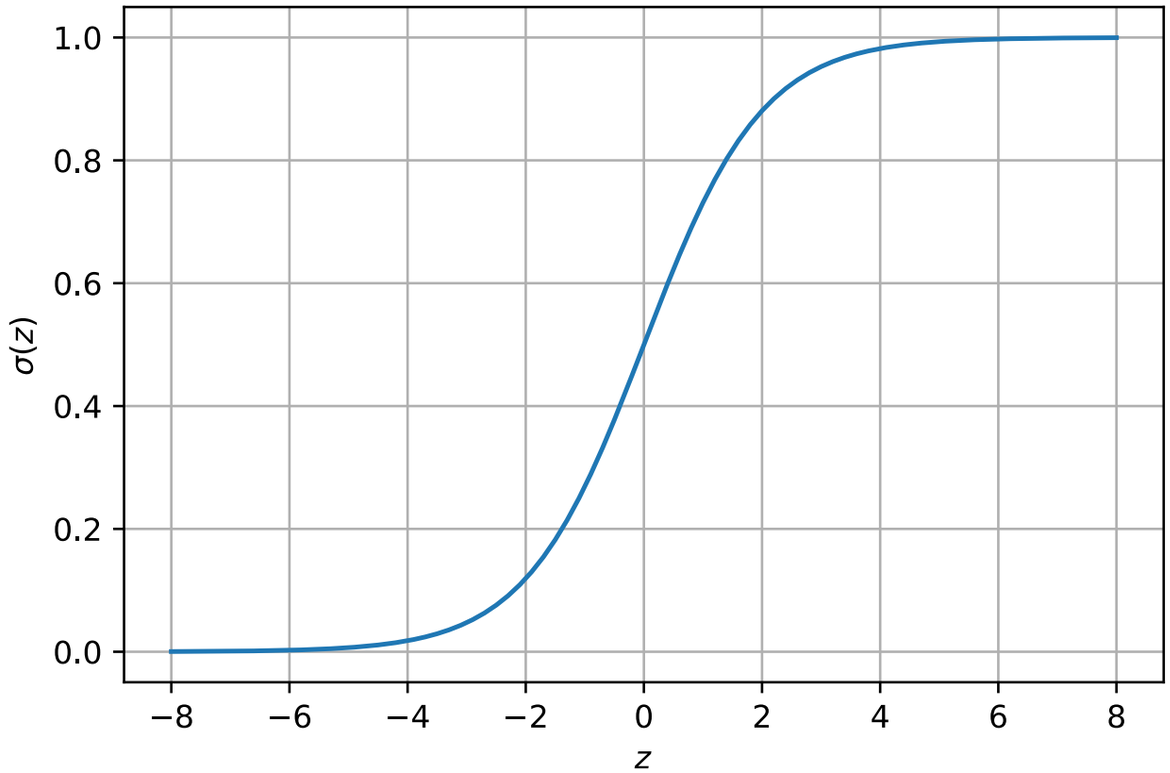

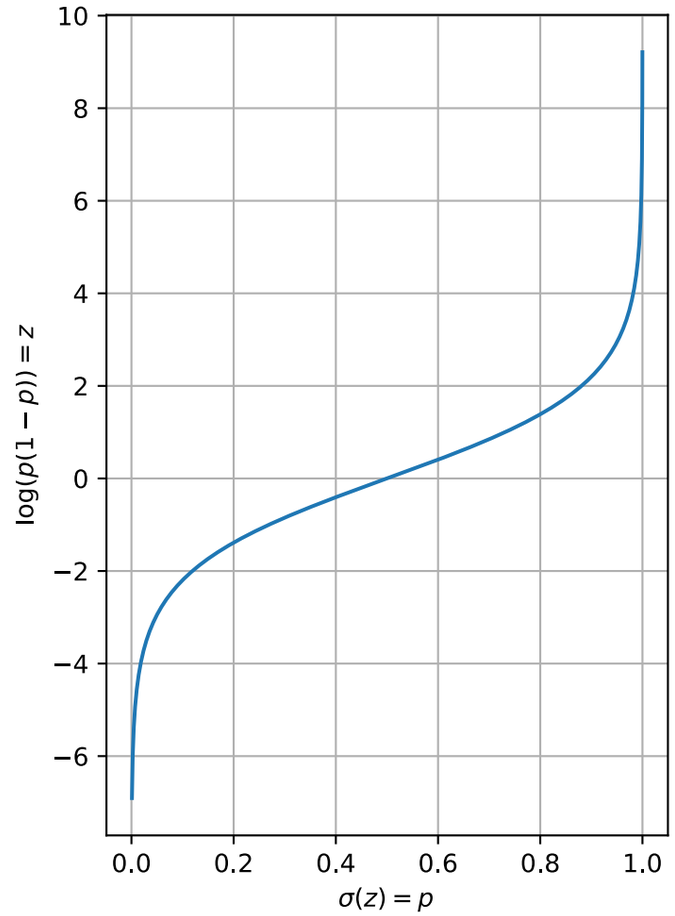

$$\sigma(z) = \frac{1}{1 + \exp(-z)}$$

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

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 entropy (not-cross entropy though) in the context of decision trees (but with $\log_2$ instead of the natural log)

https://github.com/rasbt/stat479-machine-learning-fs19/blob/master/06_trees/06-trees__notes.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

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This assumes one-hot encoding where the y's are either 0 or 1

$$H_{\mathbf{a}}(\mathbf{y}) = -\sum_i \left(y^{[i]} \log(a^{[i]}) + (1 - y^{[i]}) \log(1 - a^{[i]}) \right)$$

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

Logistic Regression Coding Example

https://github.com/rasbt/stat453-deep-learning-ss20/blob/master/L07-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

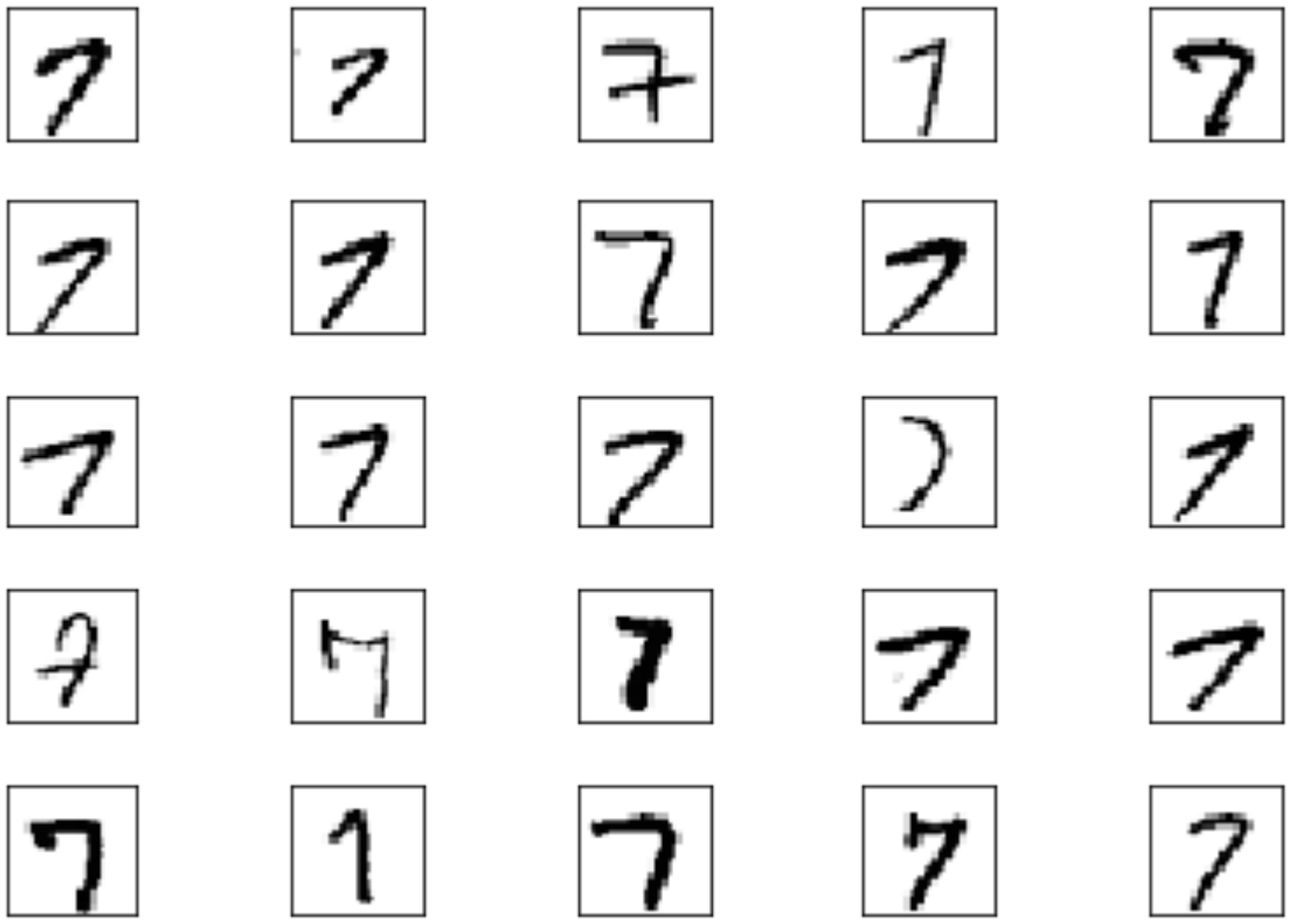

Illustration of different "7"s

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,
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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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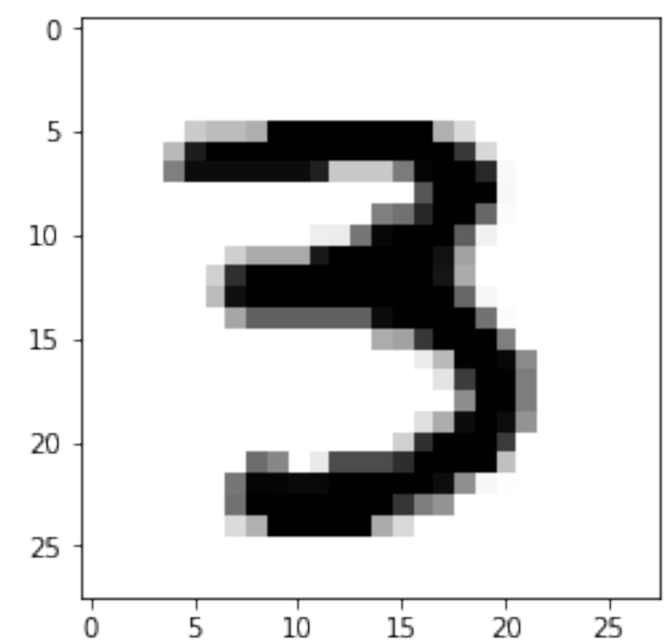

Note that I normalized pixels by factor 1/255 here

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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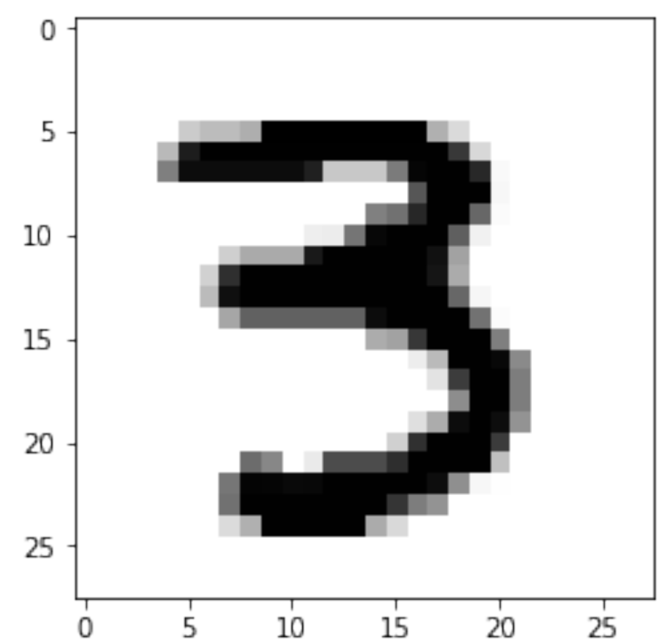
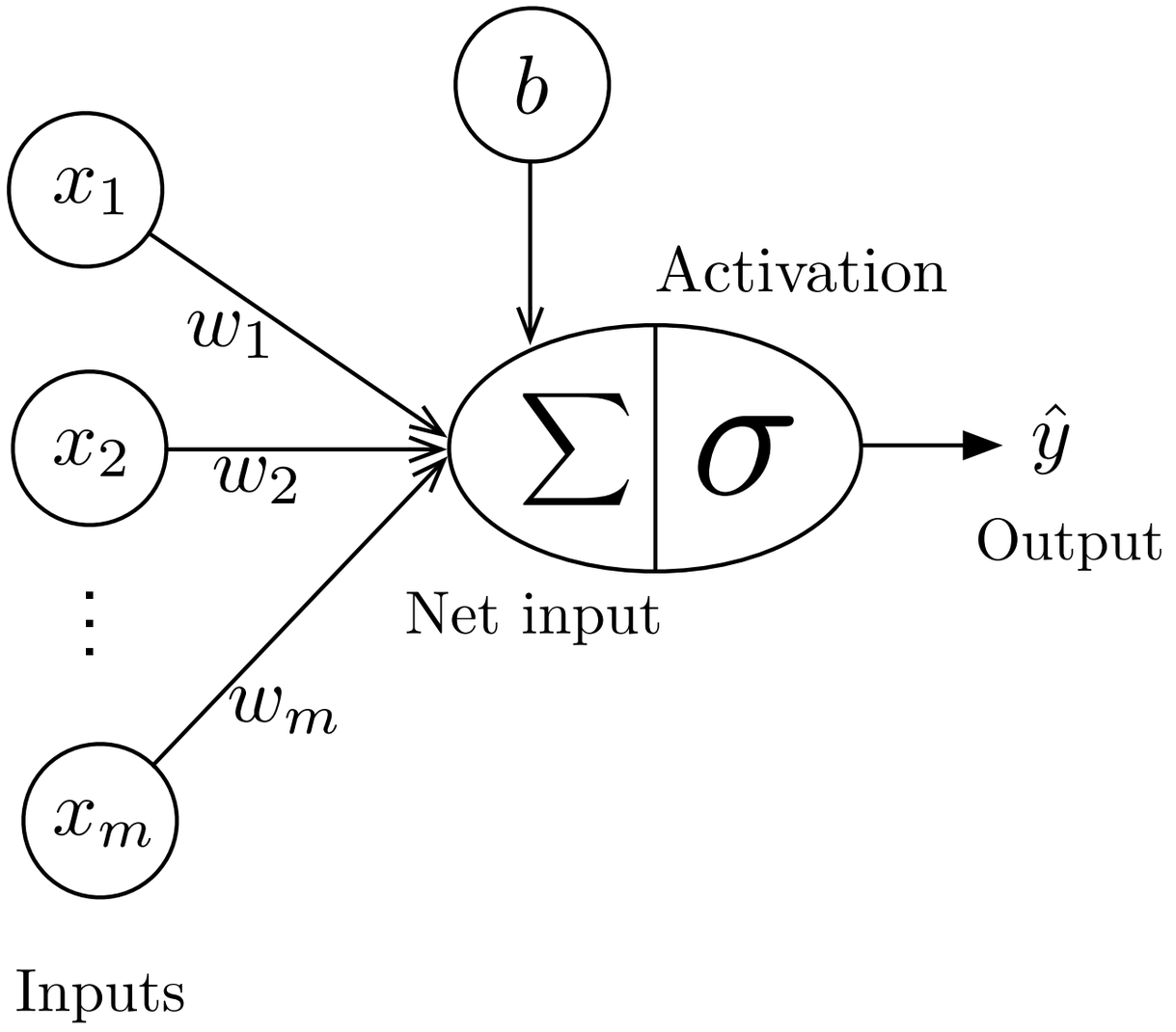
```

Represent digit as a long vector of pixels



Note that I normalized pixels by factor 1/255 here

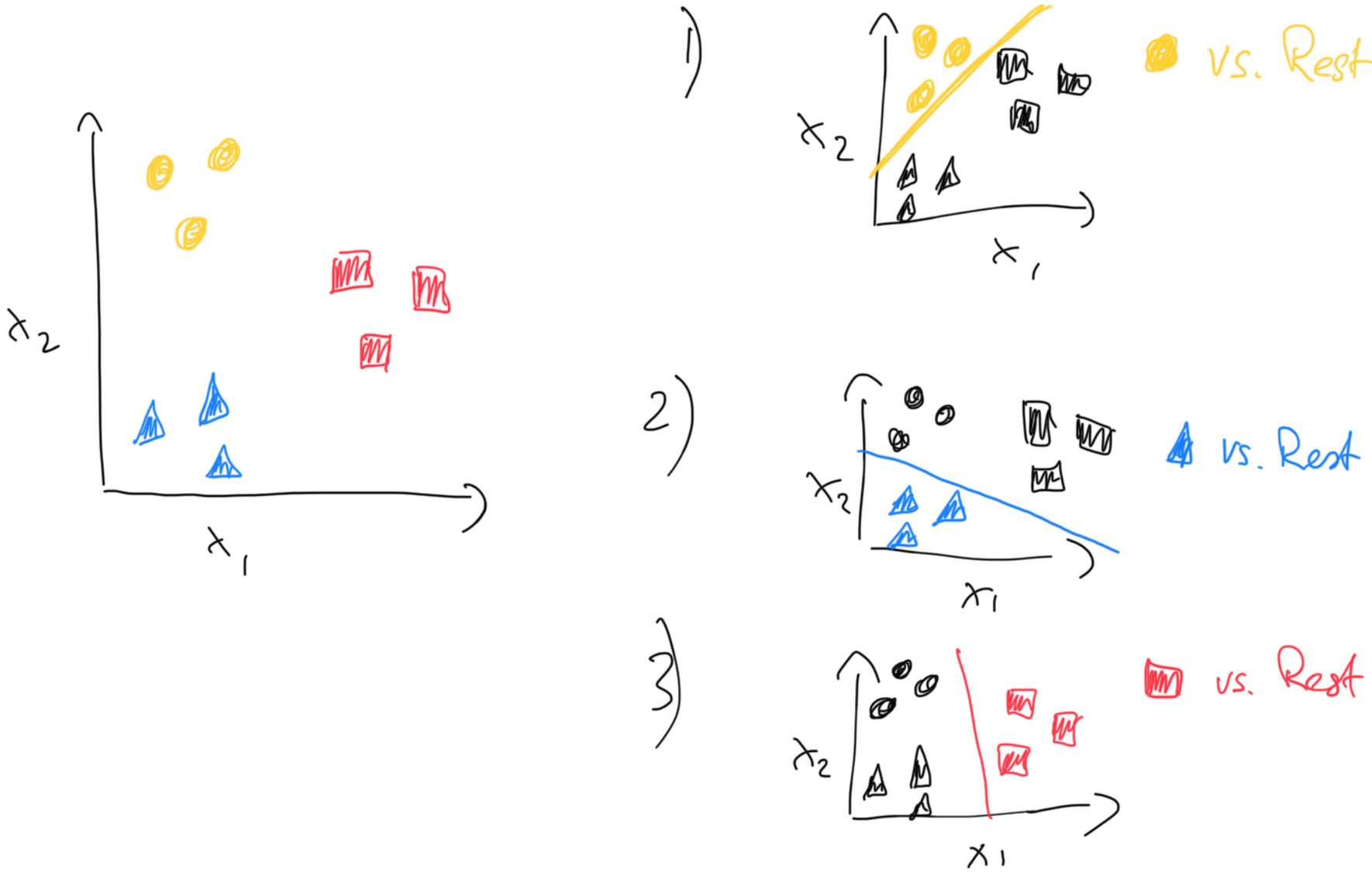
Previous Approach for Binary Classes



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

Multi-Class Classification with Multiple Binary Classifiers

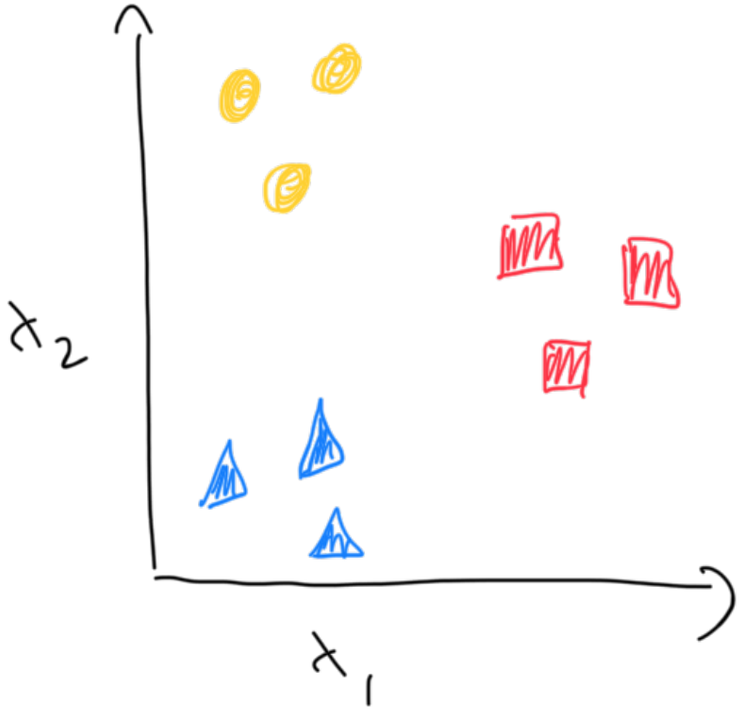
One-vs-Rest (OvR) / One-vs-All (OvA)

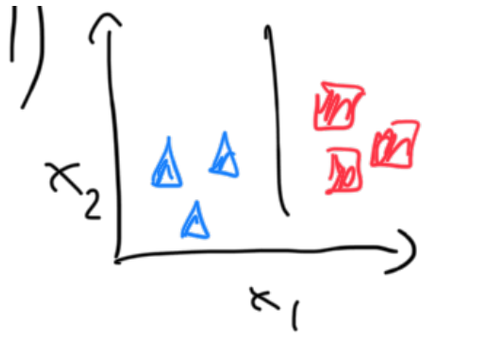


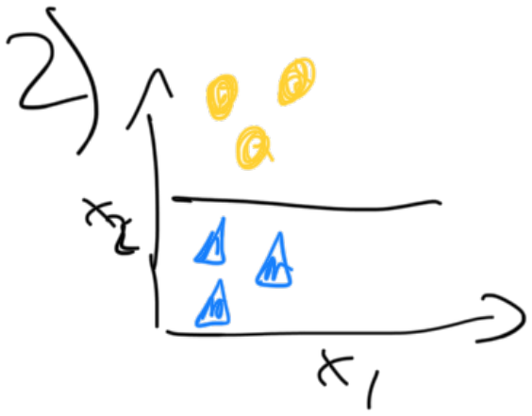
Then, choose the class with the highest confidence score

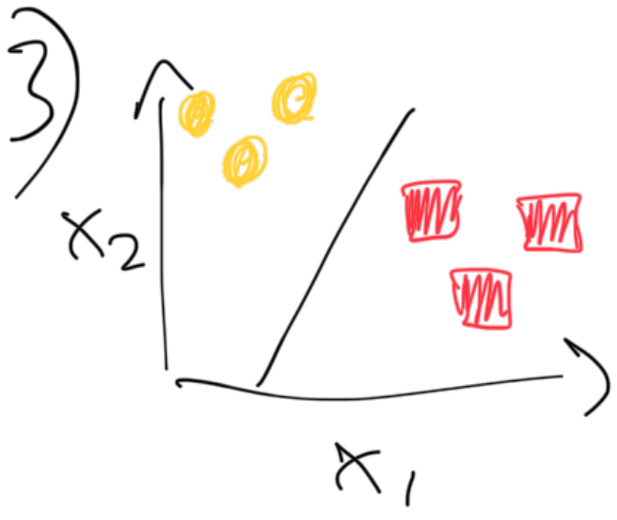
Multi-Class Classification with Multiple Binary Classifiers

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









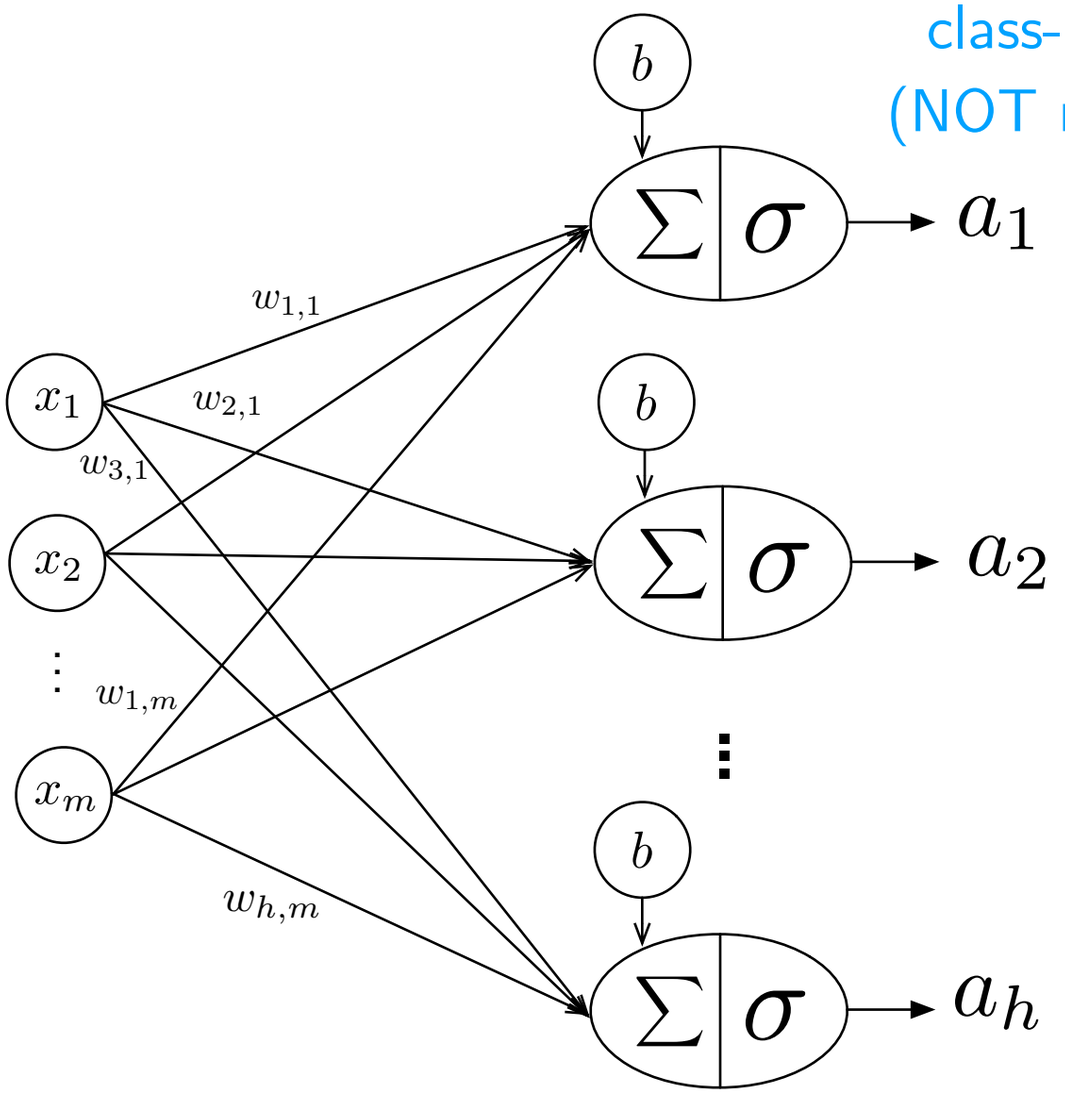
Number of classifiers needed:

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)

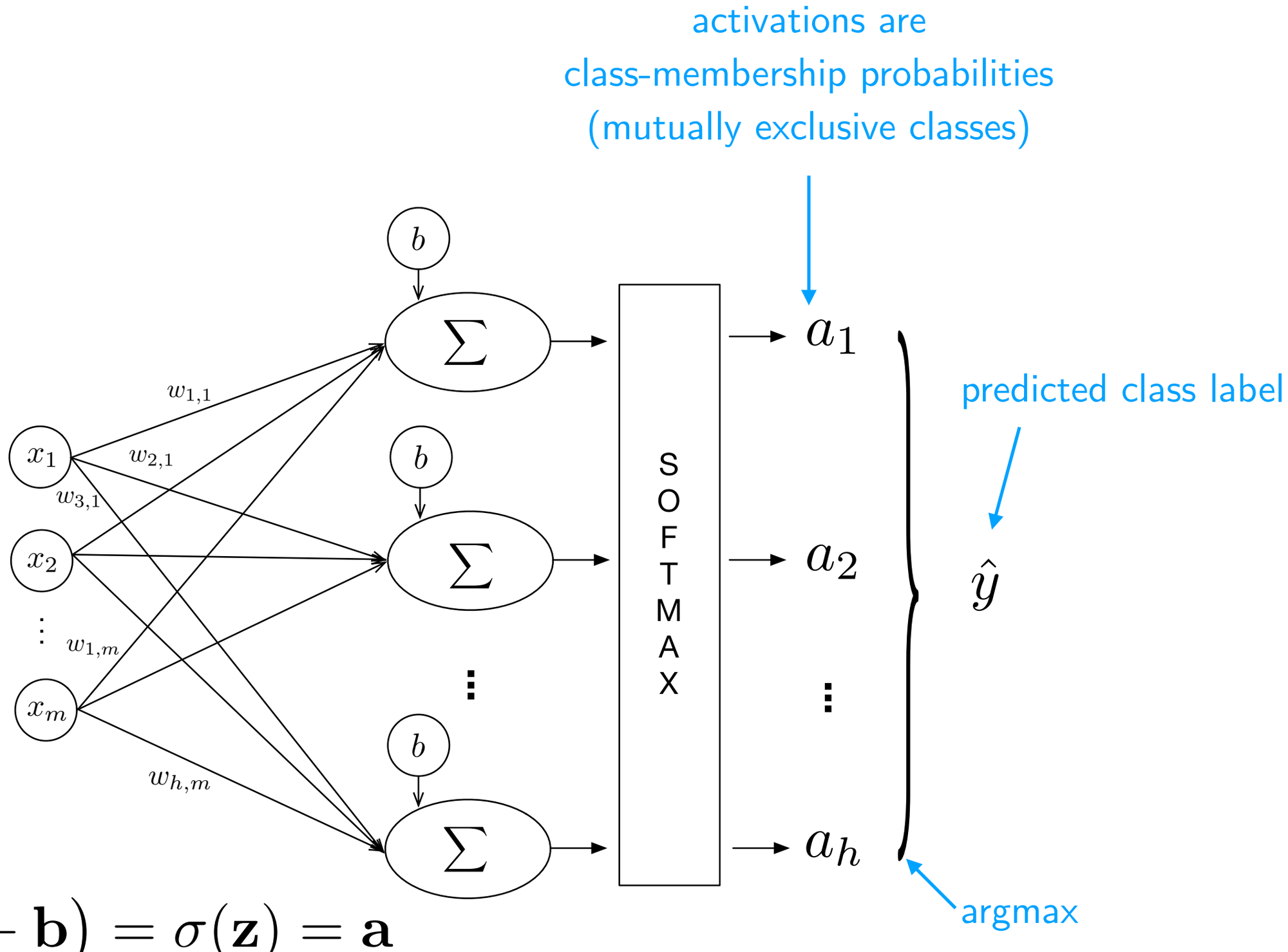


$$\sigma\big(\mathbf{W}\mathbf{x} + \mathbf{b}\big) = \sigma(\mathbf{z}) = \mathbf{a}$$

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

where k is the number of classes

Multinomial Logistic Regression / Softmax Regression



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

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

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)

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

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

Cross Entropy Loss Function Example

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

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

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

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

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

Cross Entropy Loss Function Example

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

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

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

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

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

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

$$\approx 0.9335$$

Cross Entropy Hands-On Example

Understanding Onehot Encoding and Cross Entropy in PyTorch

```
import torch
```

Onehot Encoding

```
def to_onehot(y, num_classes):
    y_onehot = torch.zeros(y.size(0), num_classes)
    y_onehot.scatter_(1, y.view(-1, 1).long(), 1).float()
    return y_onehot

y = torch.tensor([0, 1, 2, 2])

y_enc = to_onehot(y, 3)

print('one-hot encoding:\n', y_enc)
```

```
one-hot encoding:
 tensor([[1., 0., 0.],
        [0., 1., 0.],
        [0., 0., 1.],
        [0., 0., 1.]])
```

https://github.com/rasbt/stat453-deep-learning-ss20/blob/master/L07-logistic/code/cross-entropy-pytorch.ipynb

Training Softmax Regression

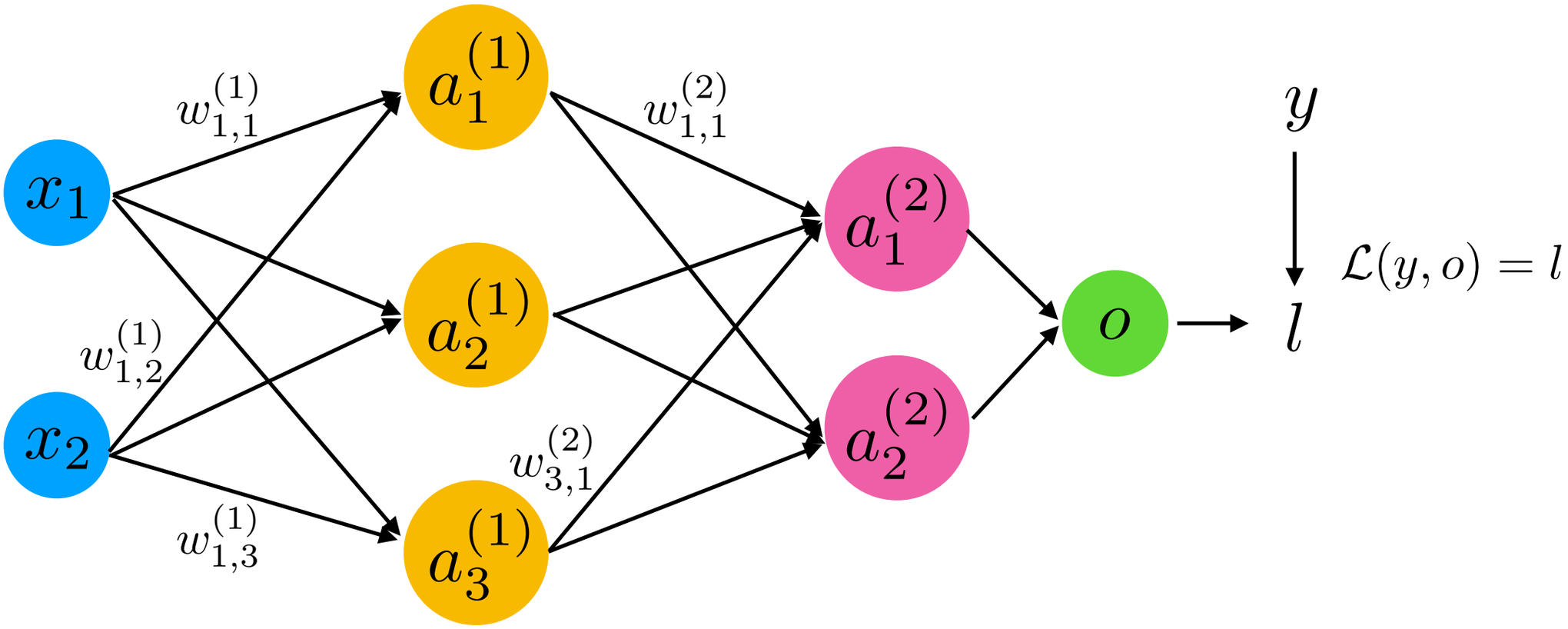
The Same Overall Concept Applies ...

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)



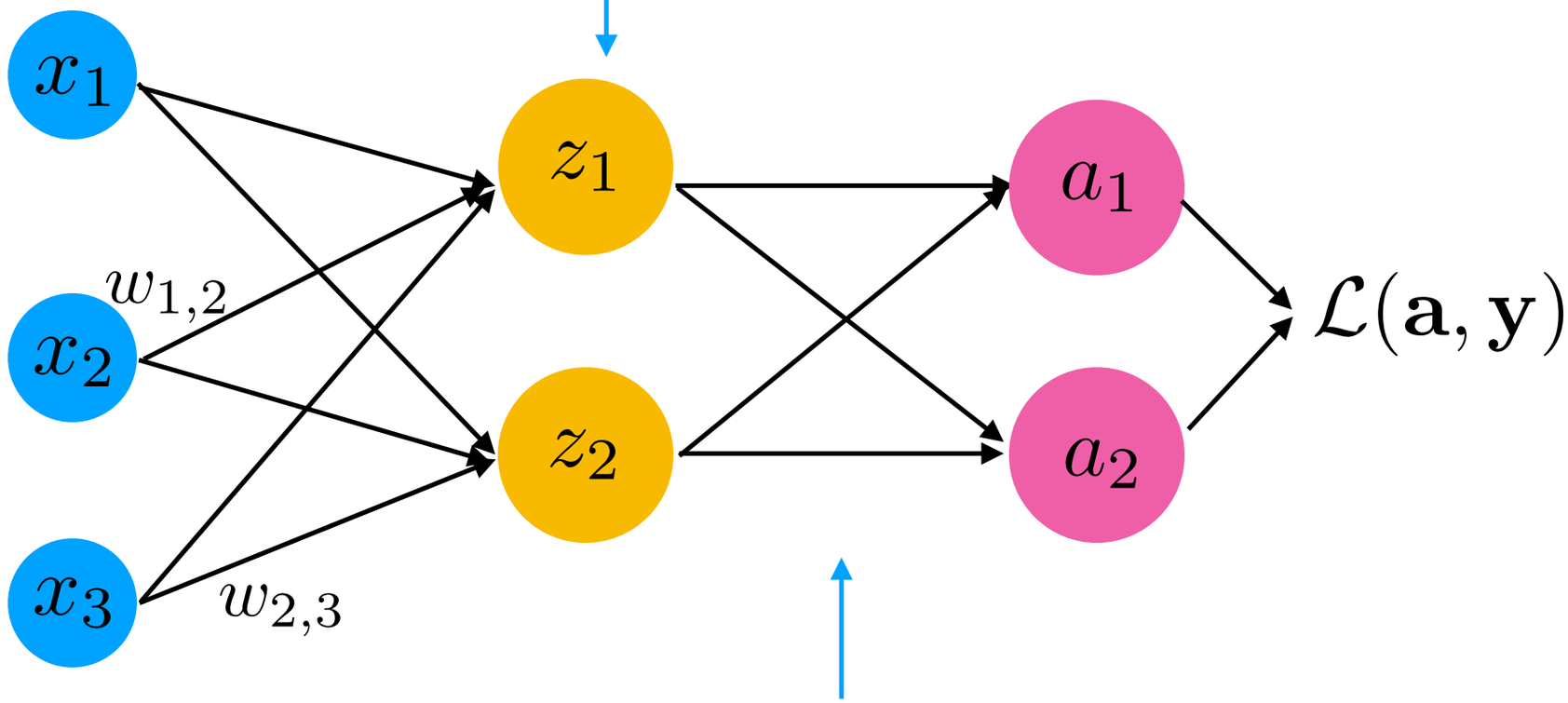
$$\frac{\partial l}{\partial w_{1,1}^{(1)}} = \frac{\partial l}{\partial o} \cdot \frac{\partial o}{\partial a_1^{(2)}} \cdot \frac{\partial a_1^{(2)}}{\partial a_1^{(1)}} \cdot \frac{\partial a_1^{(1)}}{\partial w_{1,1}^{(1)}}$$
$$+ \frac{\partial l}{\partial o} \cdot \frac{\partial o}{\partial a_2^{(2)}}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

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

Softmax Regression Sketch

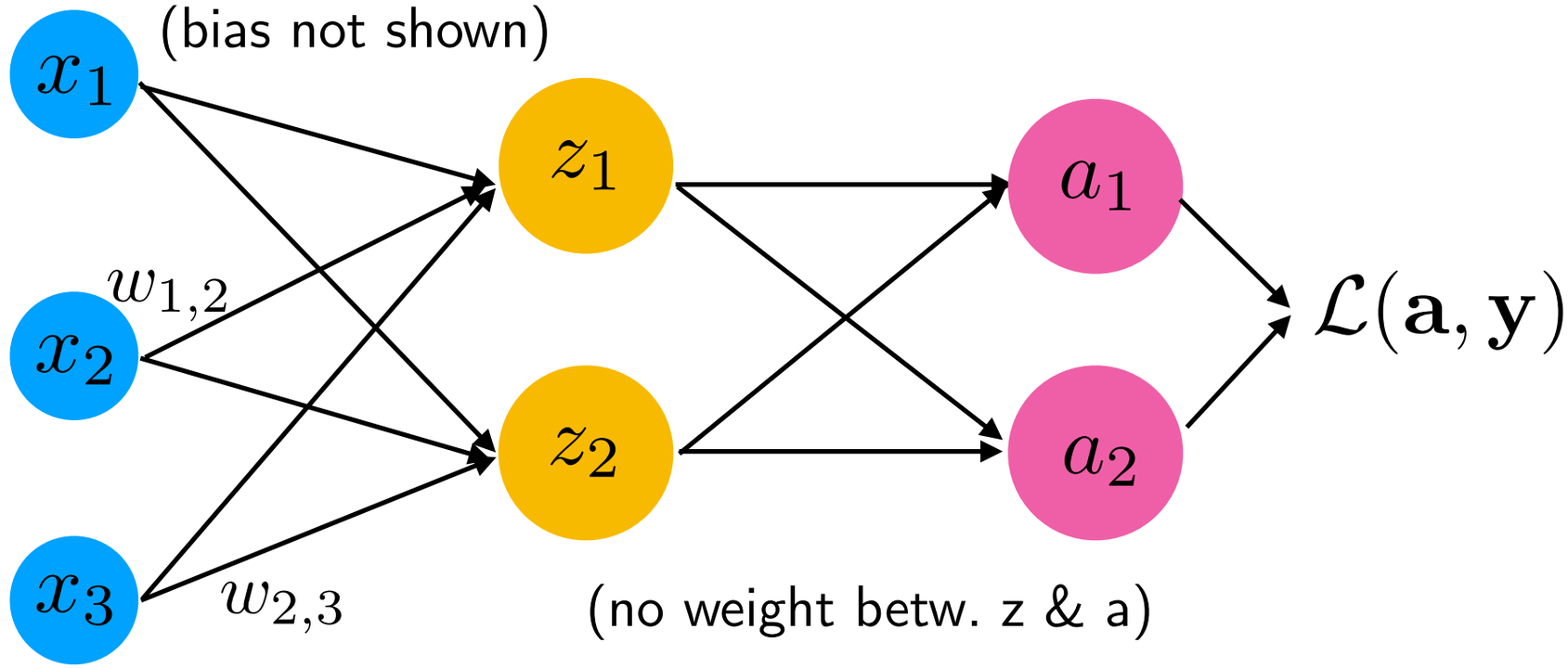
(This is NOT a multi-layer neural network; still 1-layer, no hidden layer)

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



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

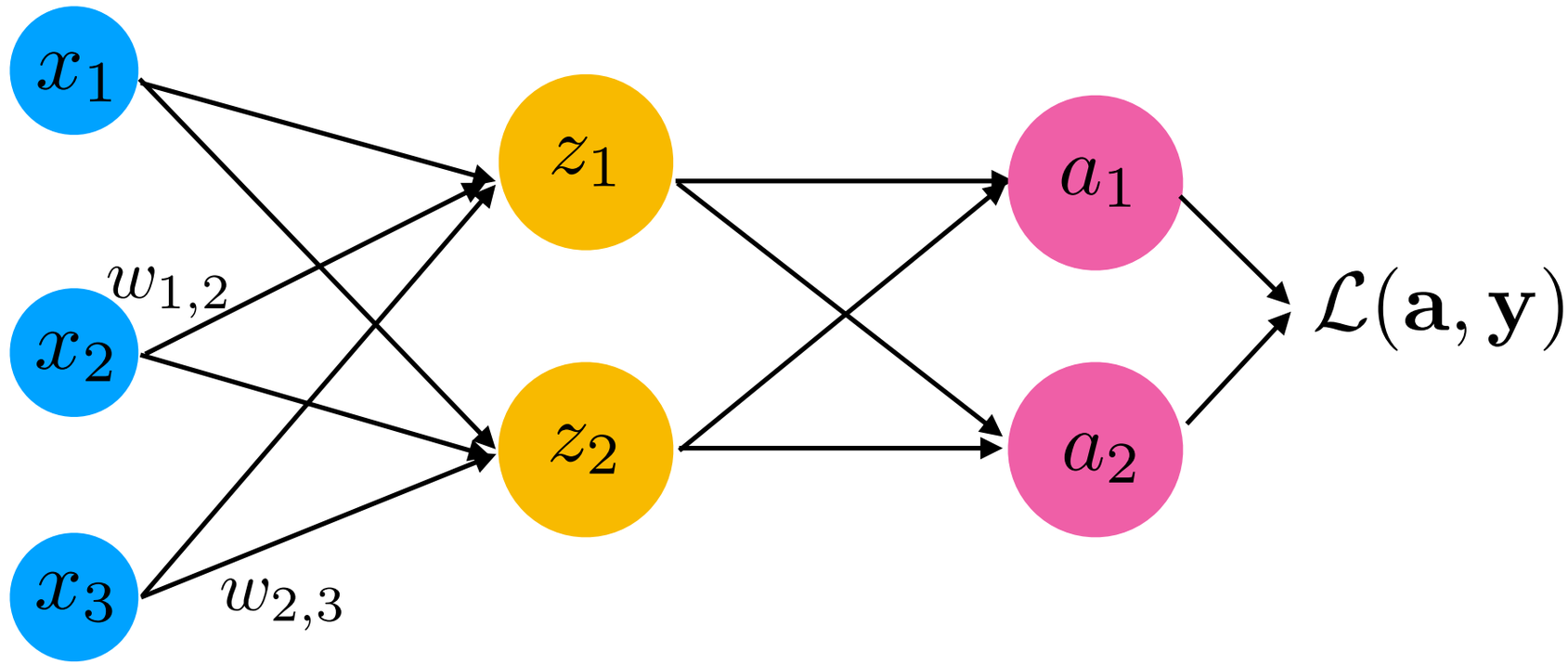
Softmax Regression Sketch



Multivariable chain rule

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

Softmax Regression Sketch



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

Vectorized Form:

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

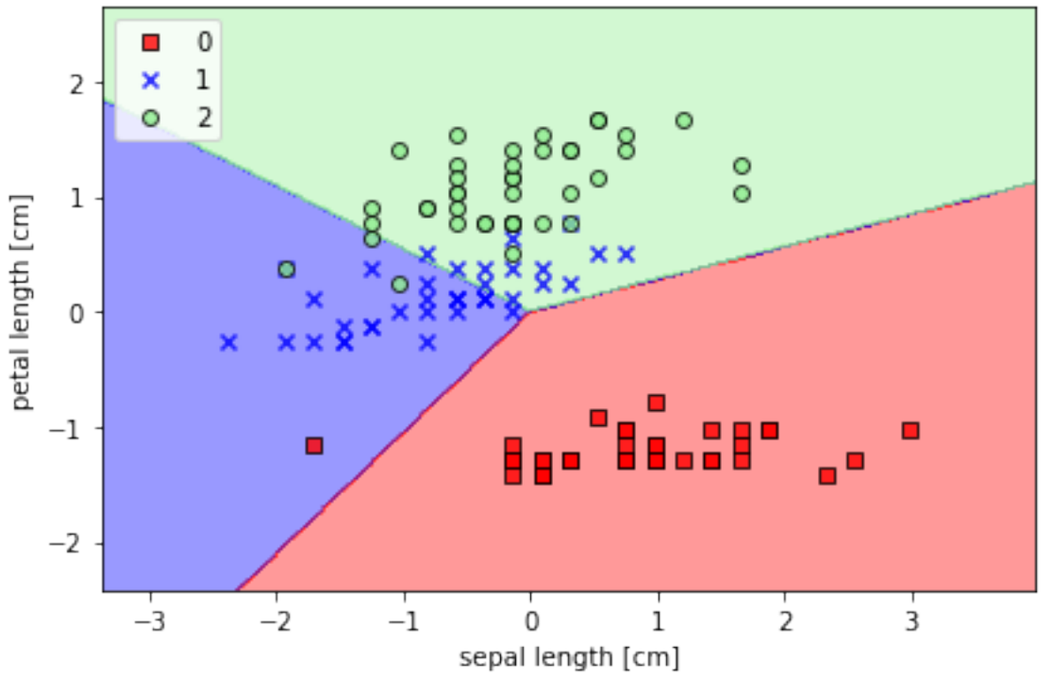
where $\mathbf{W} \in \mathbb{R}^{k \times m}$

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

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

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

Softmax Regression Hands-On Example (Iris)

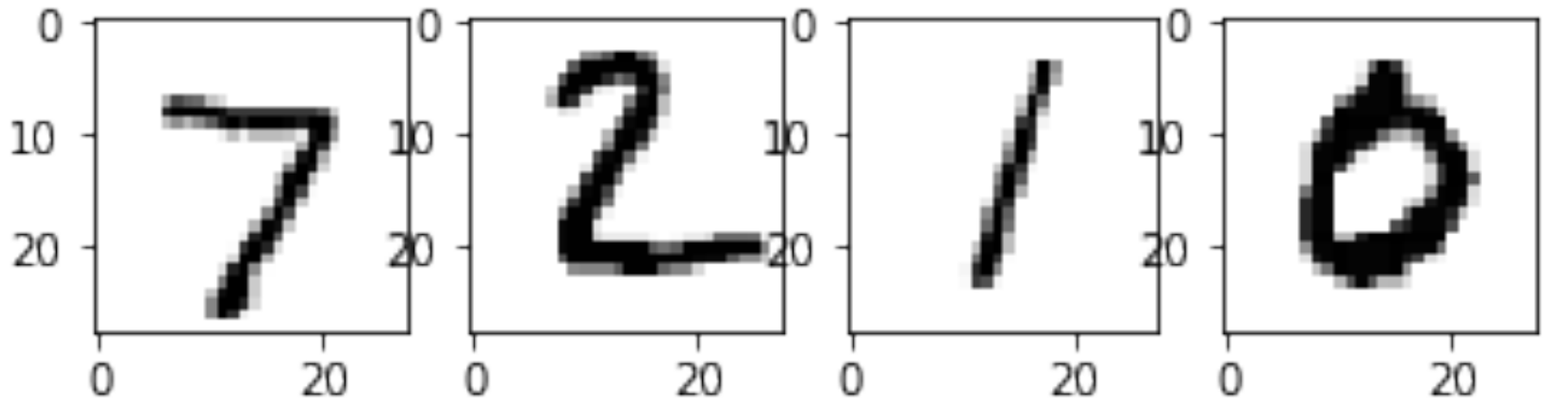


"From scratch" implementation & PyTorch autodiff implementation

https://github.com/rasbt/stat453-deep-learning-ss20/blob/master/L07-logistic/code/softmax-regression_scratch.ipynb

Softmax Regression Hands-On (MNIST)

Using PyTorch (with autodiff an nn.Module)



https://github.com/rasbt/stat453-deep-learning-ss20/blob/master/L07-logistic/code/softmax-regression-mnist.ipynb

PyTorch Loss-Input Confusion (Cheatsheet)

- `torch.nn.functional.binary_cross_entropy` takes logistic sigmoid values as inputs
- `torch.nn.functional.binary_cross_entropy_with_logits` takes logits as inputs
- `torch.nn.functional.cross_entropy` takes logits as inputs (performs `log_softmax` internally)
- `torch.nn.functional.nll_loss` is like `cross_entropy` but takes log-probabilities (log-softmax) values as inputs

Additional Reading Material

Softmax regression tutorial:
https://mccormickml.com/2014/06/13/deep-learning-tutorial-softmax-regression/