STAT 453: Introduction to Deep Learning and Generative Models

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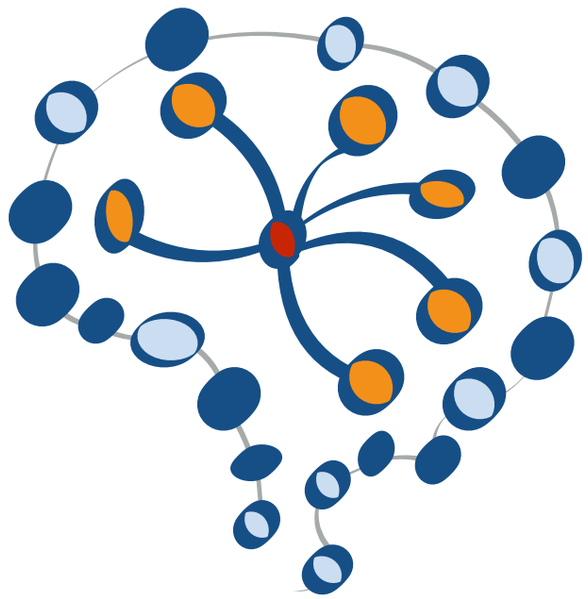
http://stat.wisc.edu/~sraschka/teaching

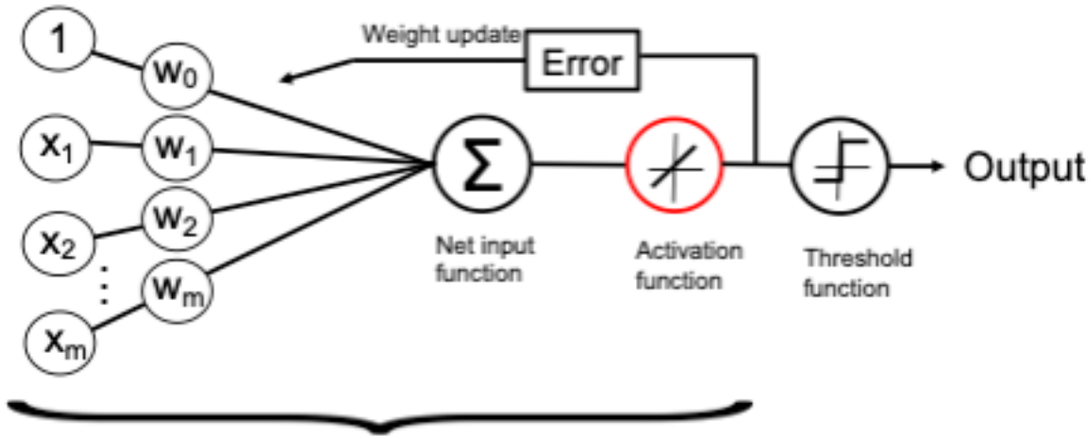


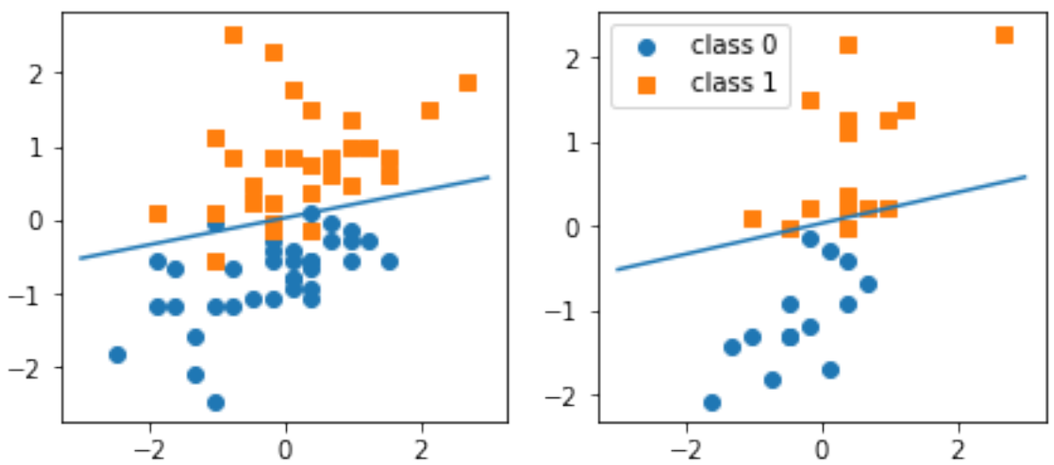
Lecture 08

Logistic Regression and Multi-class classification

Previous Lecture(s):

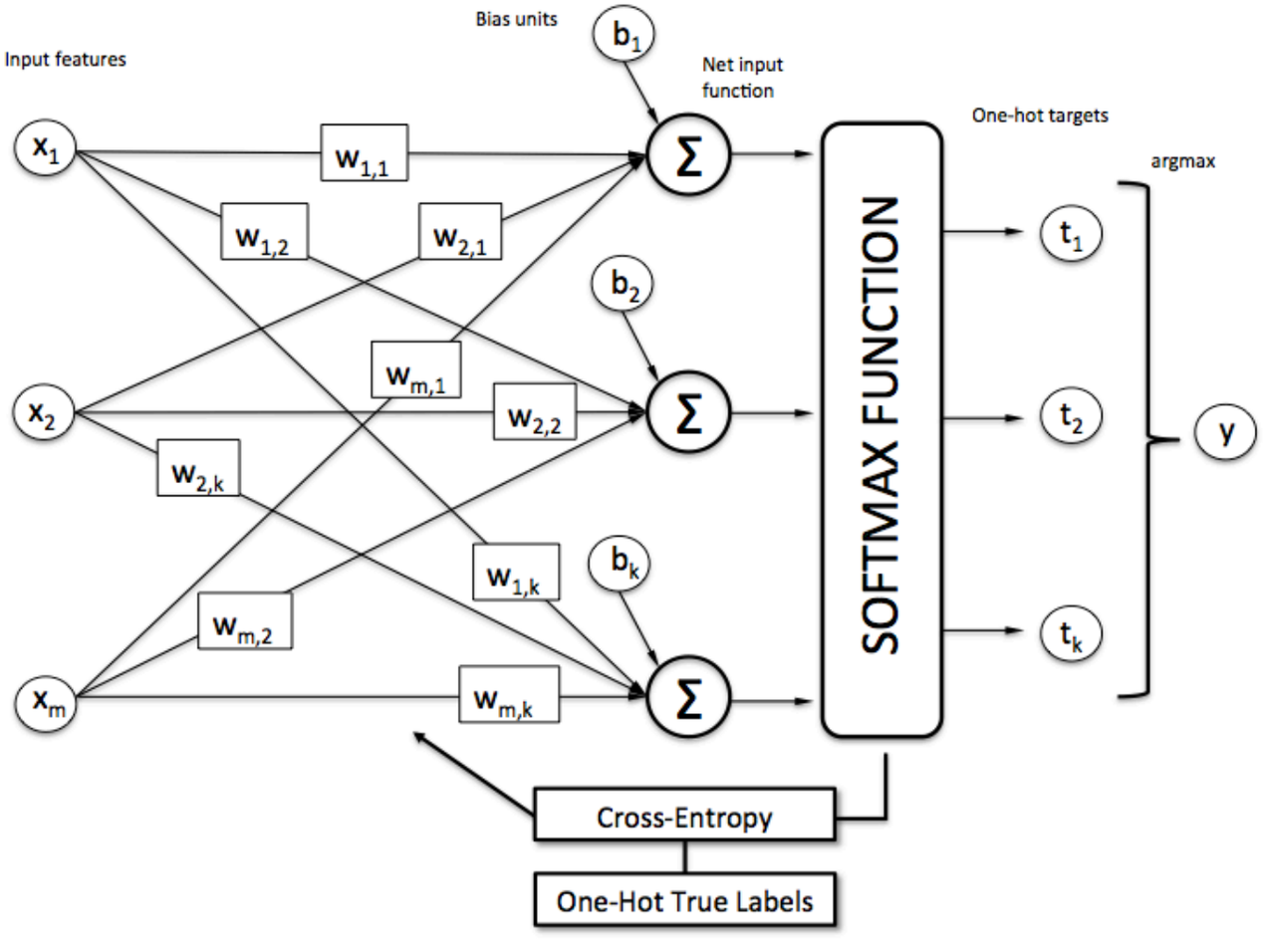
- Solved convergence issue of Perceptron via Adaline
- Conceptualized gradient descent via computation graphs



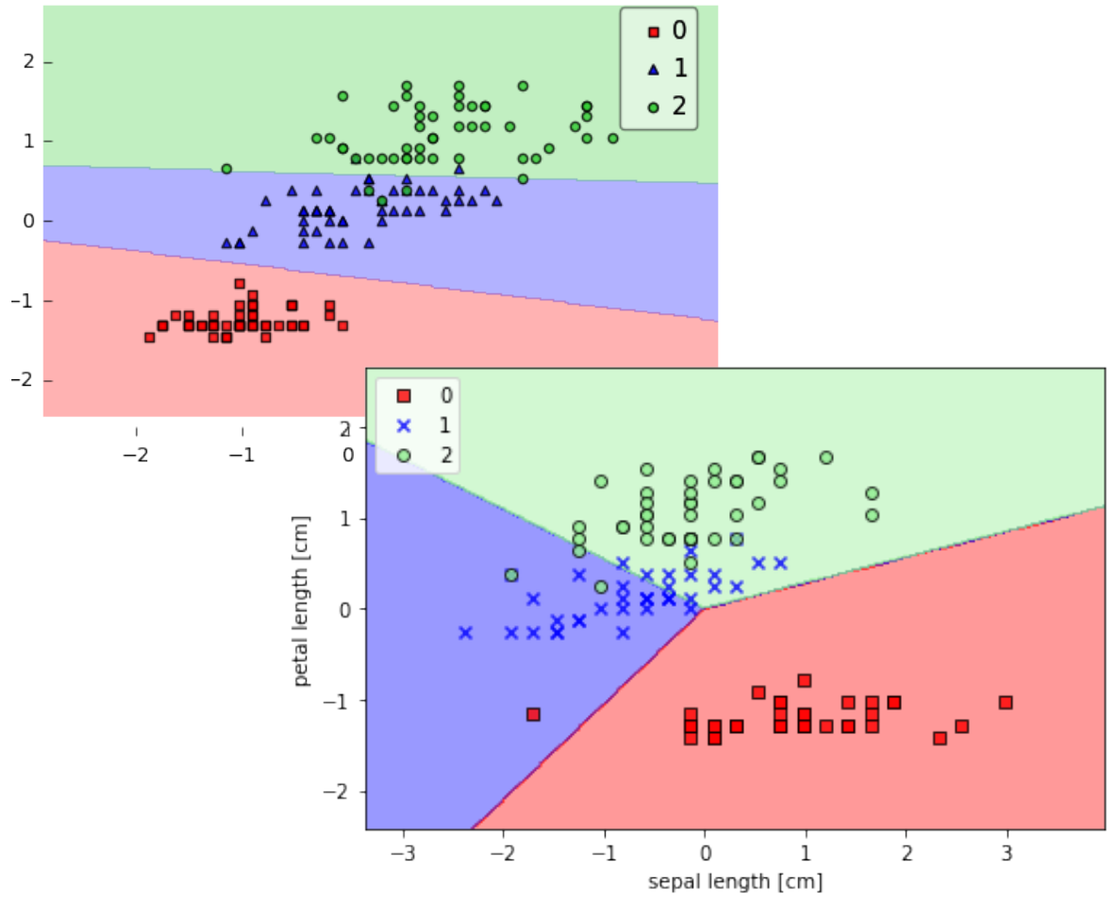


This Lecture:

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



Softmax Regression - Gradient Descent



Topics

1. Logistic Regression as an Artificial Neuron
2. Negative Log-Likelihood Loss
3. Logistic Regression Learning Rule
4. Logits and Cross Entropy
5. Logistic Regression Code Example
6. Generalizing to Multiple Classes: Softmax Regression
7. OneHot Encoding and Multi-category Cross Entropy
8. Softmax Regression Learning Rule
9. Softmax Regression Code Example

Viewing Logistic Regression as a Single Layer Neural Network

1. **Logistic Regression as an Artificial Neuron**
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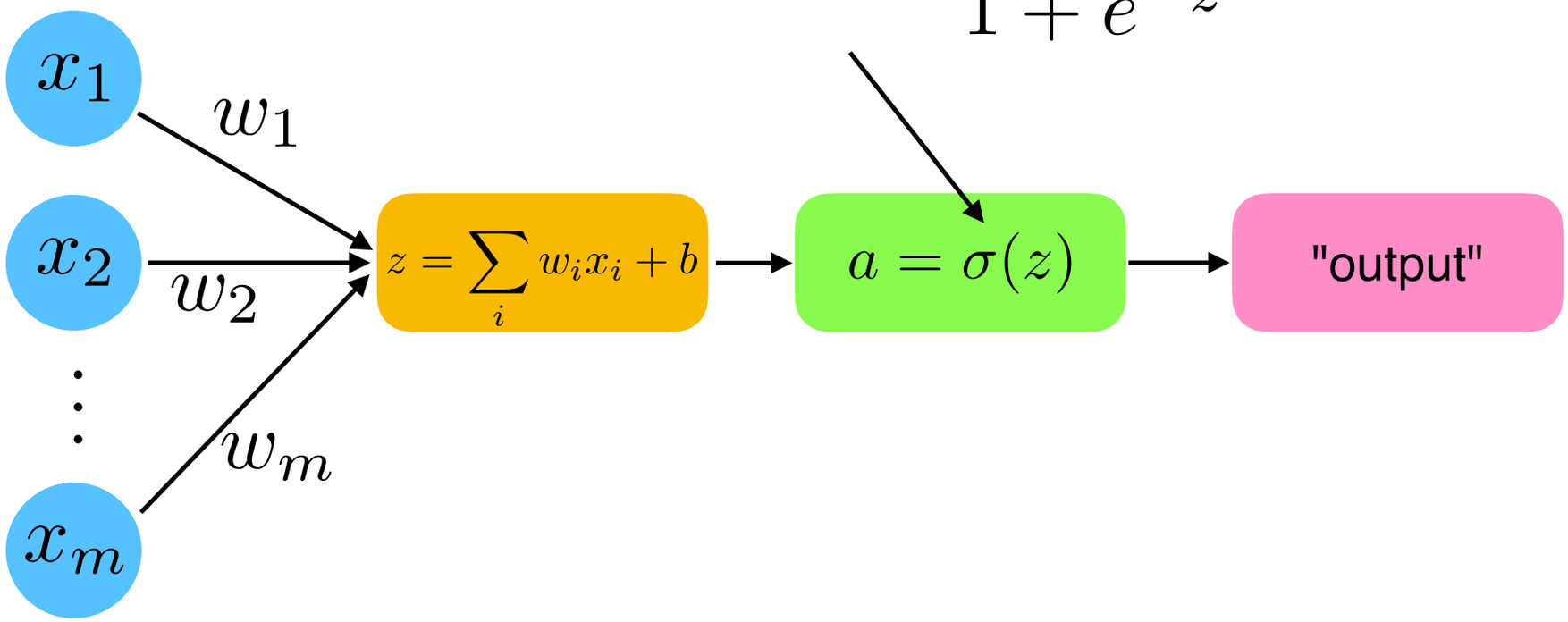
Logistic Regression Neuron

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

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

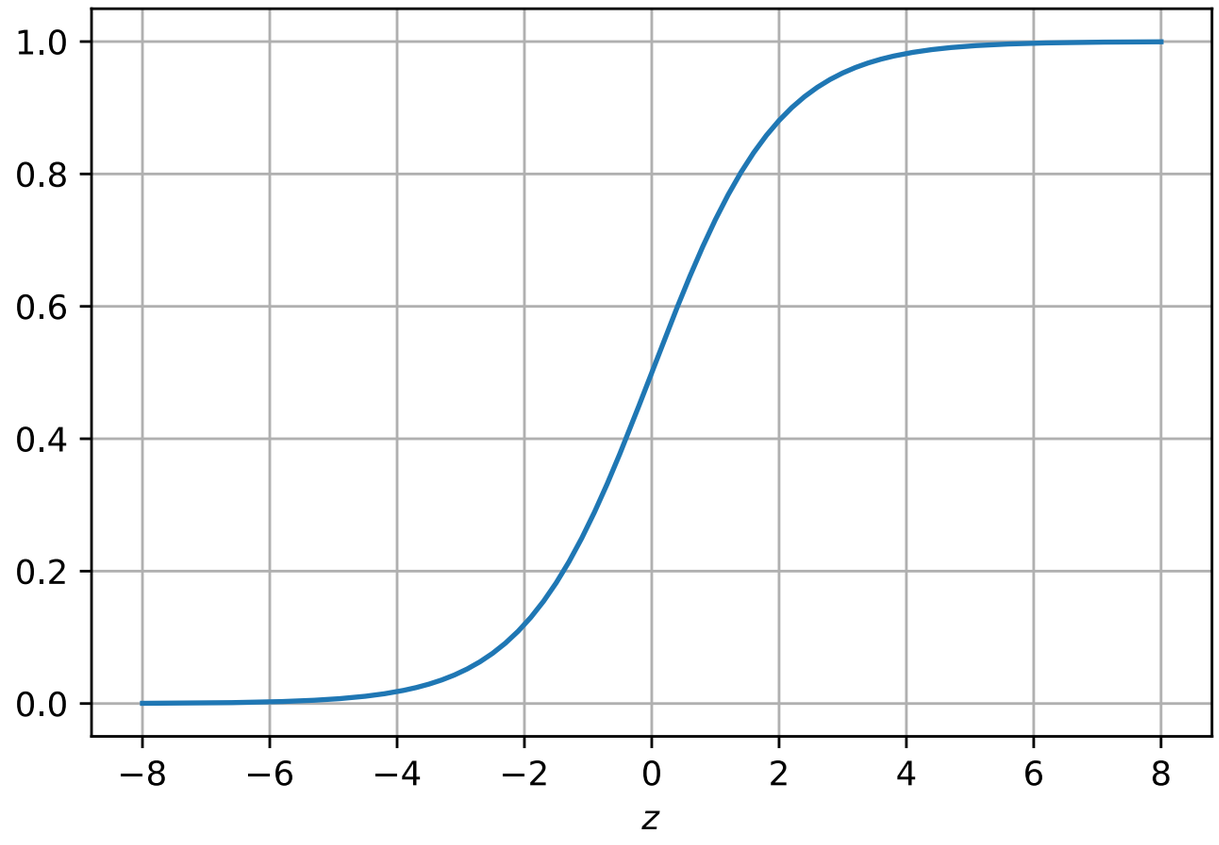


- In ADALINE, the activation function was an identity function, $\sigma(z) = z$
- ADALINE we used MSE as loss function: $\text{MSE} = \dfrac{1}{n} \sum_i (a^{[i]} - y^{[i]})^2$
- We will use a different loss function for logistic regression

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's Loss Function

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Logistic Regression

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rewrite more compactly

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

Logistic Regression

And for multiple training examples, we want to maximize:

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

by finding *good/optimal* parameters

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

Likelihood "Loss"

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

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

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

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, 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 a Logistic Regression Model

1. Logistic Regression as an Artificial Neuron
2. Negative Log-Likelihood Loss
3. **Logistic Regression Learning Rule**
4. Logits and Cross Entropy
5. Logistic Regression Code Example
6. Generalizing to Multiple Classes: Softmax Regression
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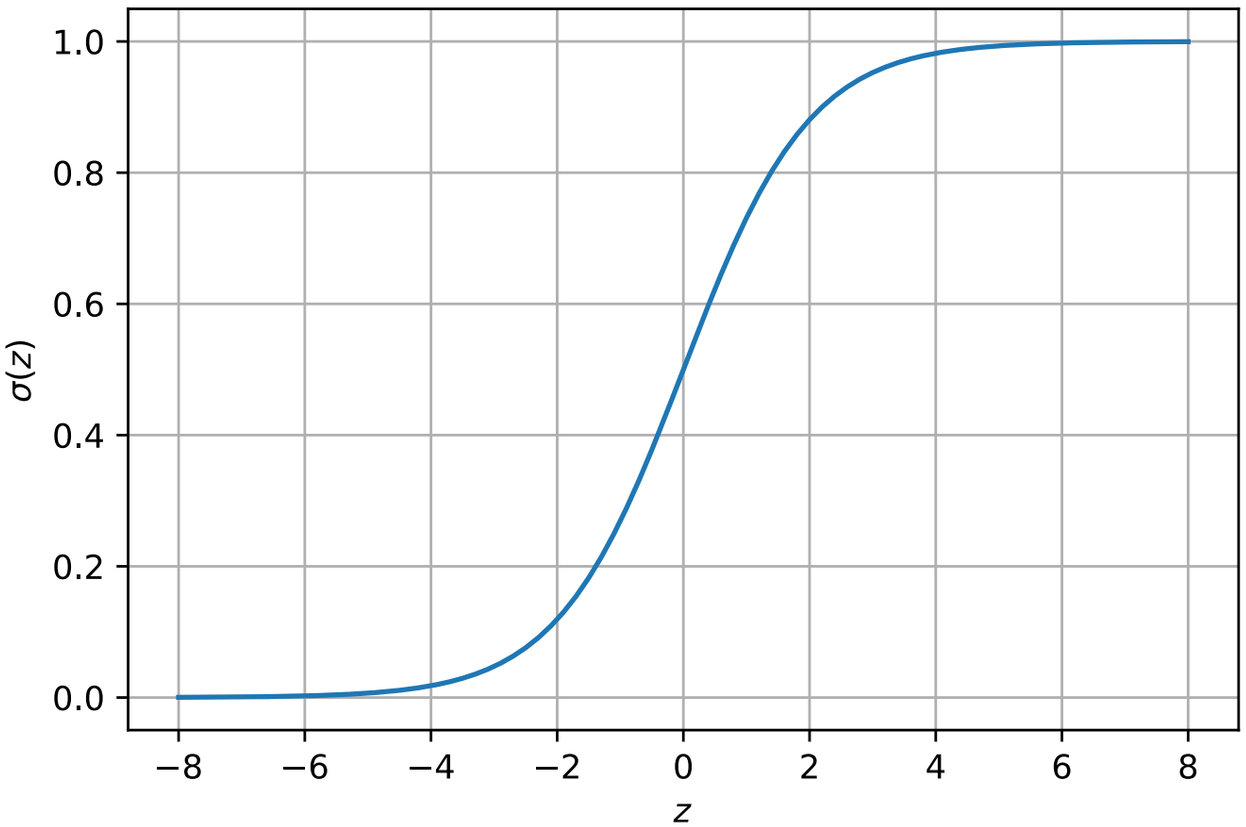
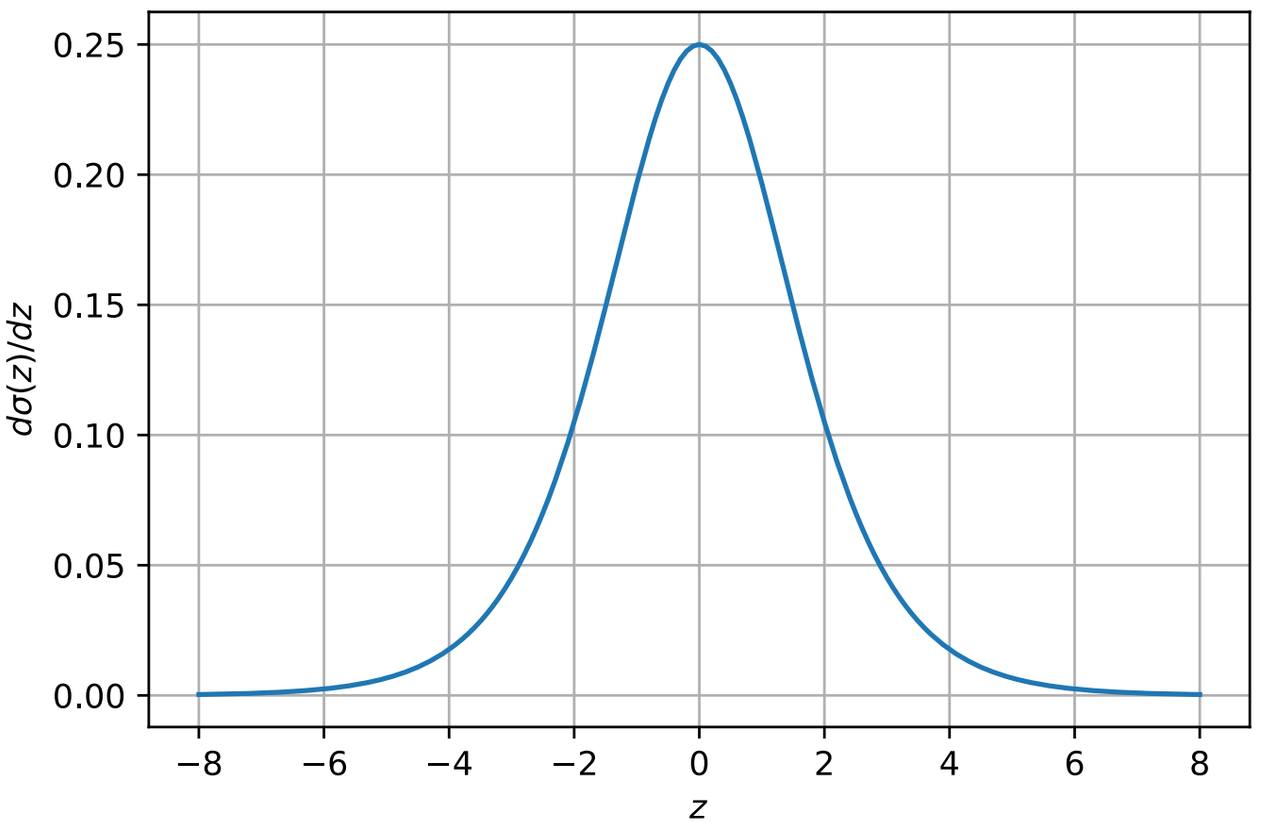
Logistic Sigmoid Derivative

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

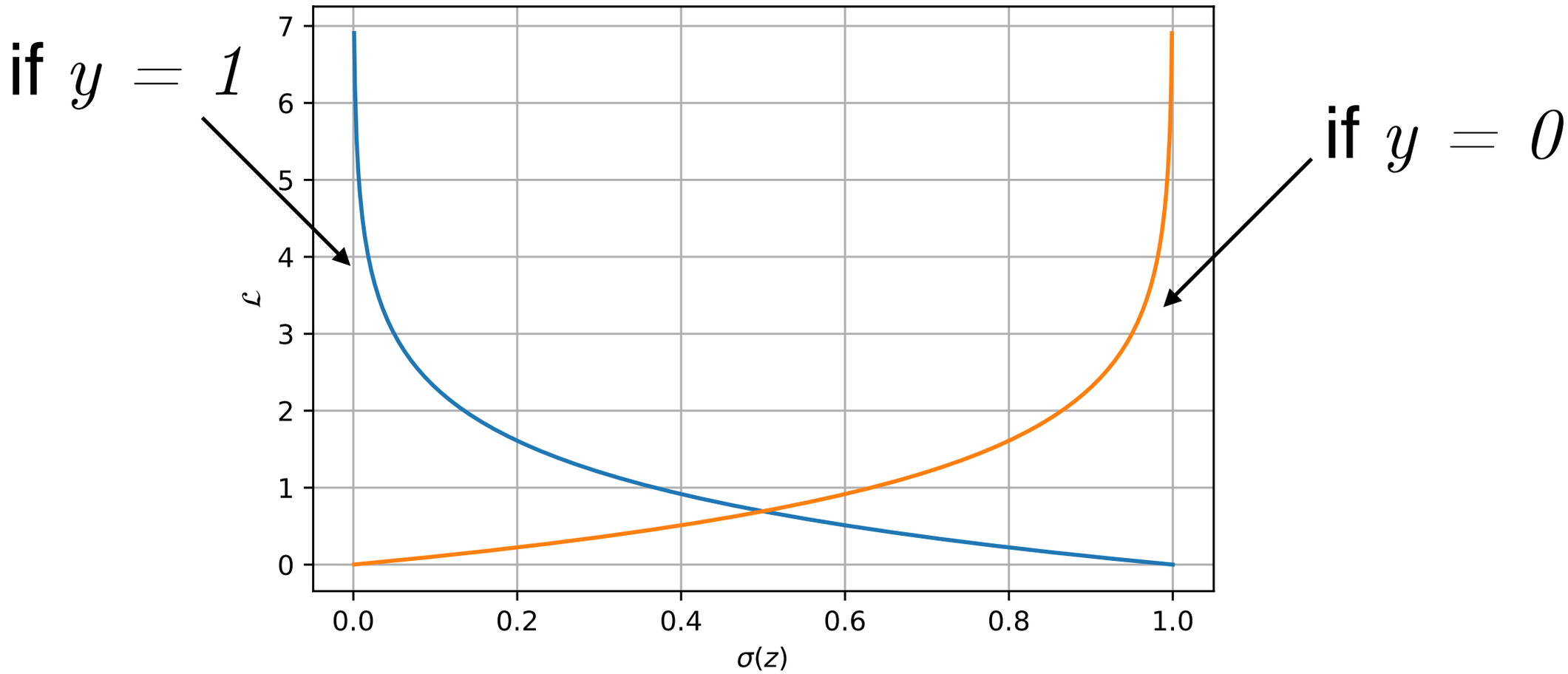
$$\sigma(z) = \frac{1}{1 + e^{-z}}$$

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





Loss for a Single Training Example



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

Learning Rule

Same gradient descent rule as before, for which we need

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

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

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

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

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

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

Learning Rule for Logistic Regression

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

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

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

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

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

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

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

Learning Rule for Logistic Regression

Remember the Linear Regression & ADALINE Lectures?

Stochastic gradient descent

1. Initialize $\mathbf{w} := \mathbf{0} \in \mathbb{R}^m$, $\mathbf{b} := 0$
2. For every training epoch:
   A. For every $\langle \mathbf{x}^{[i]}, y^{[i]} \rangle \in \mathcal{D}$
   (a) $\hat{y}^{[i]} := \sigma\left(\mathbf{x}^{[i]T}\mathbf{w} + b\right)$
   (b) $\nabla_{\mathbf{w}}\mathcal{L} = -\left(y^{[i]} - \hat{y}^{[i]}\right)\mathbf{x}^{[i]}$
   $\nabla_b\mathcal{L} = -\left(y^{[i]} - \hat{y}^{[i]}\right)$
   (c) $\mathbf{w} := \mathbf{w} + \eta \times (-\nabla_{\mathbf{w}}\mathcal{L})$
   $b := b + \eta \times (-\nabla_b\mathcal{L})$

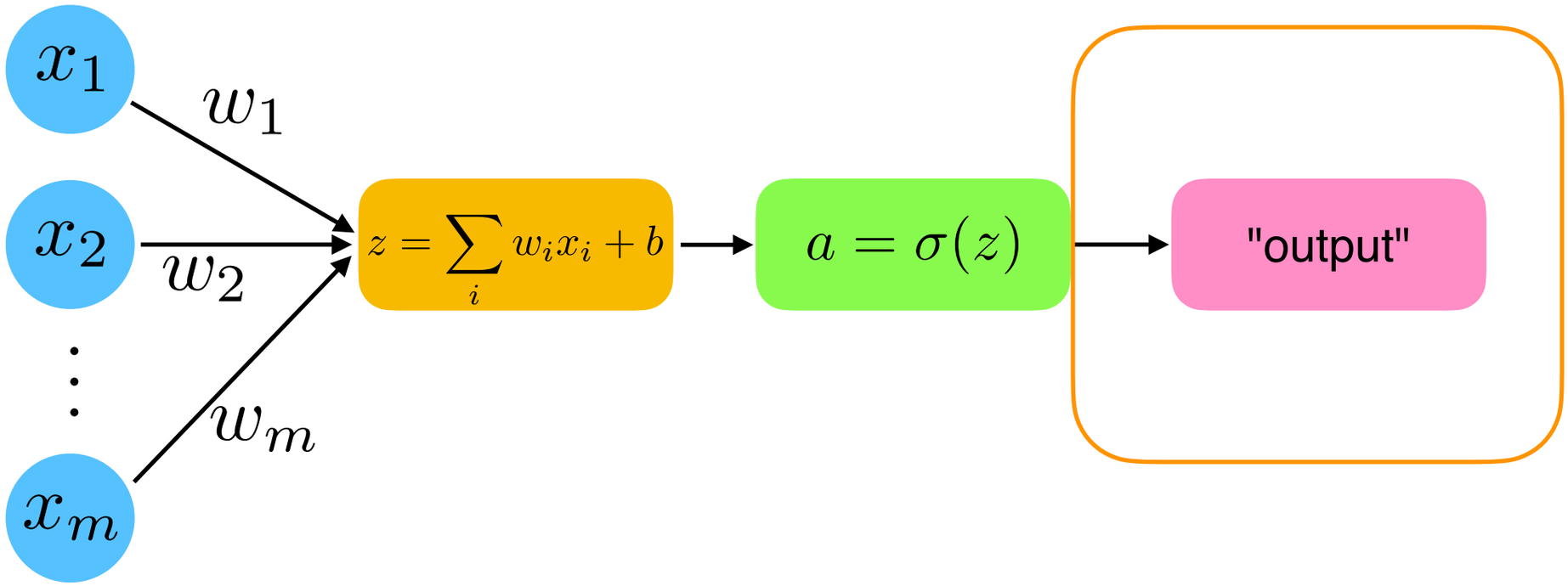
learning rate

negative gradient

Note

$a - y \Leftrightarrow -\left(y^{[i]} - \hat{y}^{[i]}\right)$

Class Label Predictions with Logistic Regression



In logistic regression, we can use

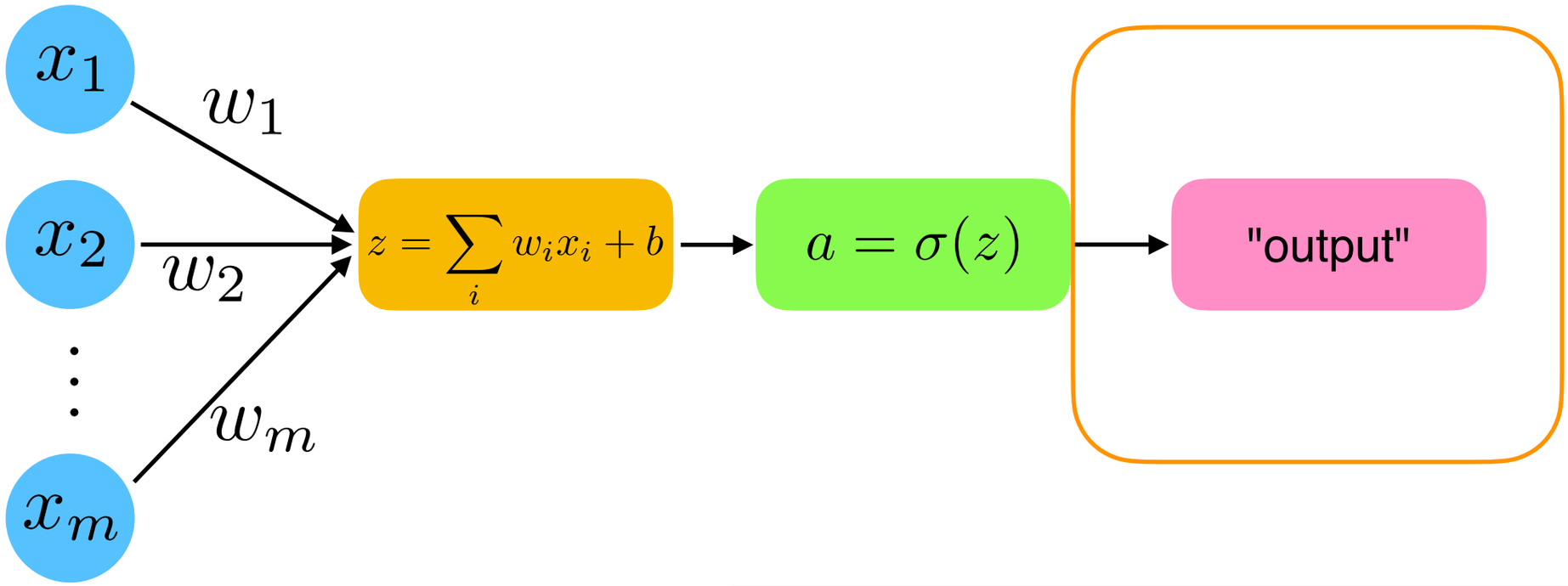
$$\hat{y} := \begin{cases} 1 & \text{if } \sigma(z) > 0.5 \\ 0 & \text{otherwise} \end{cases}$$

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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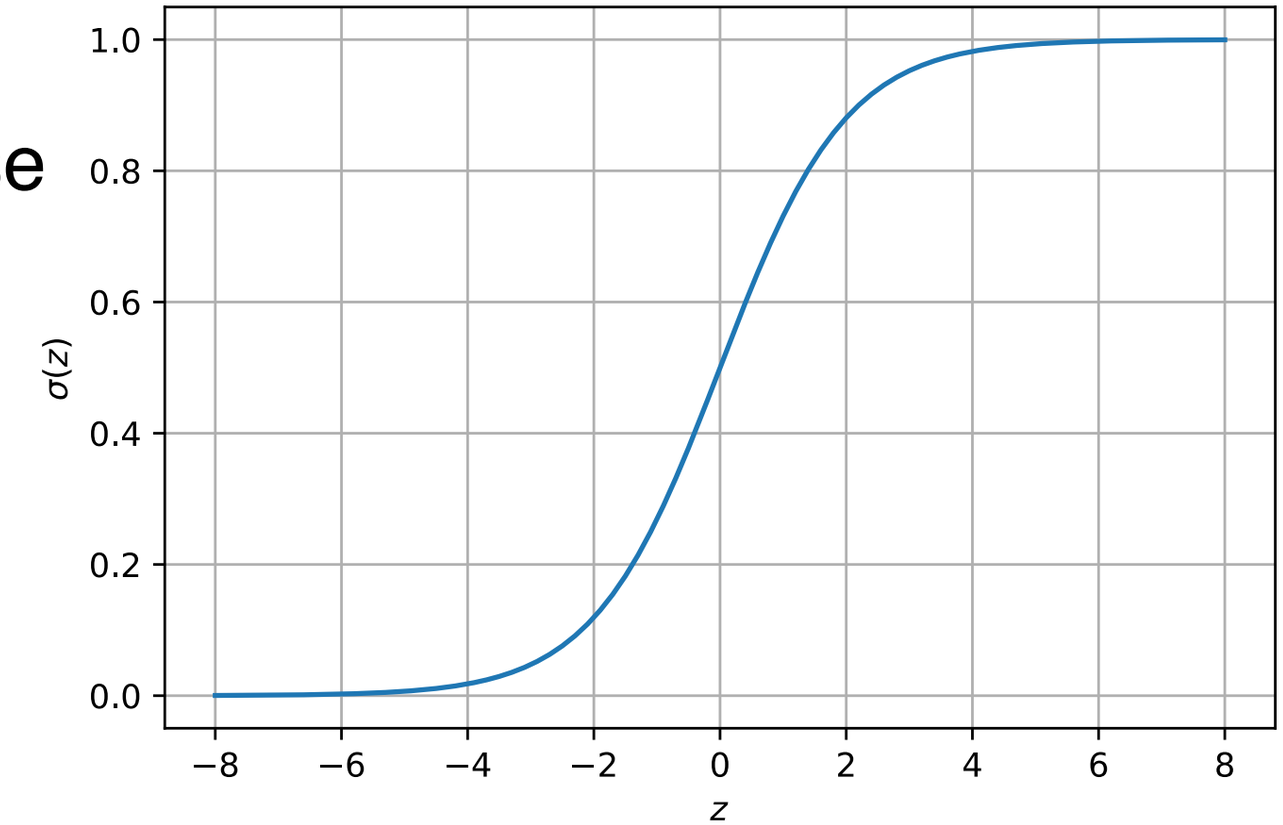

Logits and Cross Entropy

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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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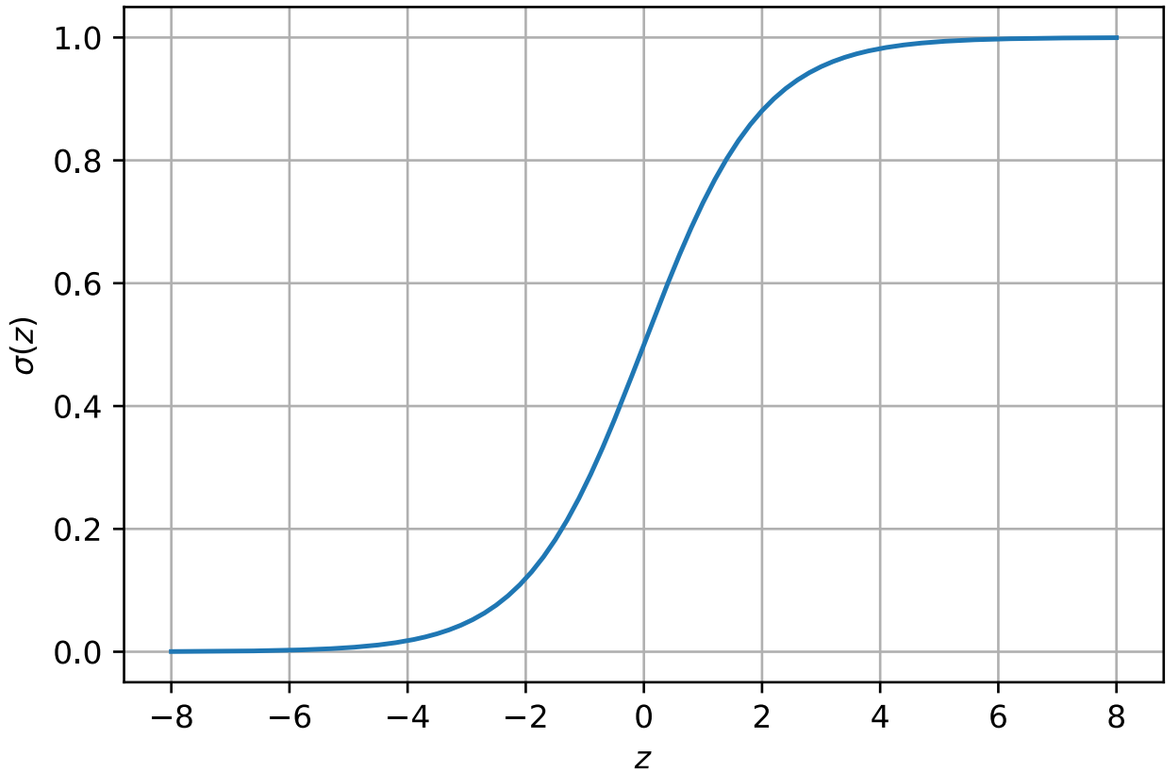

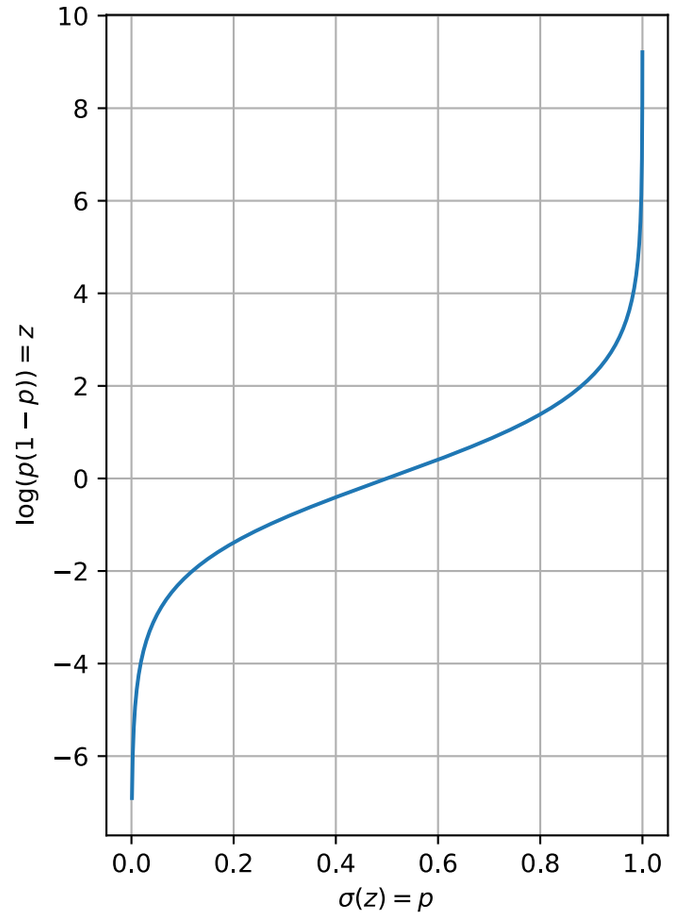

$$\sigma(z) = \frac{1}{1 + \exp(-z)}$$

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

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 STAT451: 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)

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

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

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Binary Cross Entropy

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

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

Logistic Regression Code Example

Logits and Cross Entropy

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Logistic Regression Coding Example

https://github.com/rasbt/stat453-deep-learning-ss21/blob/master/L08/code/logistic-regression.ipynb

Multinomial Logistic Regression / Softmax Regression

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MNIST - 60k Handwritten Digits

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

Balanced dataset:

- 10 classes (digits 0-9)
- 6k 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

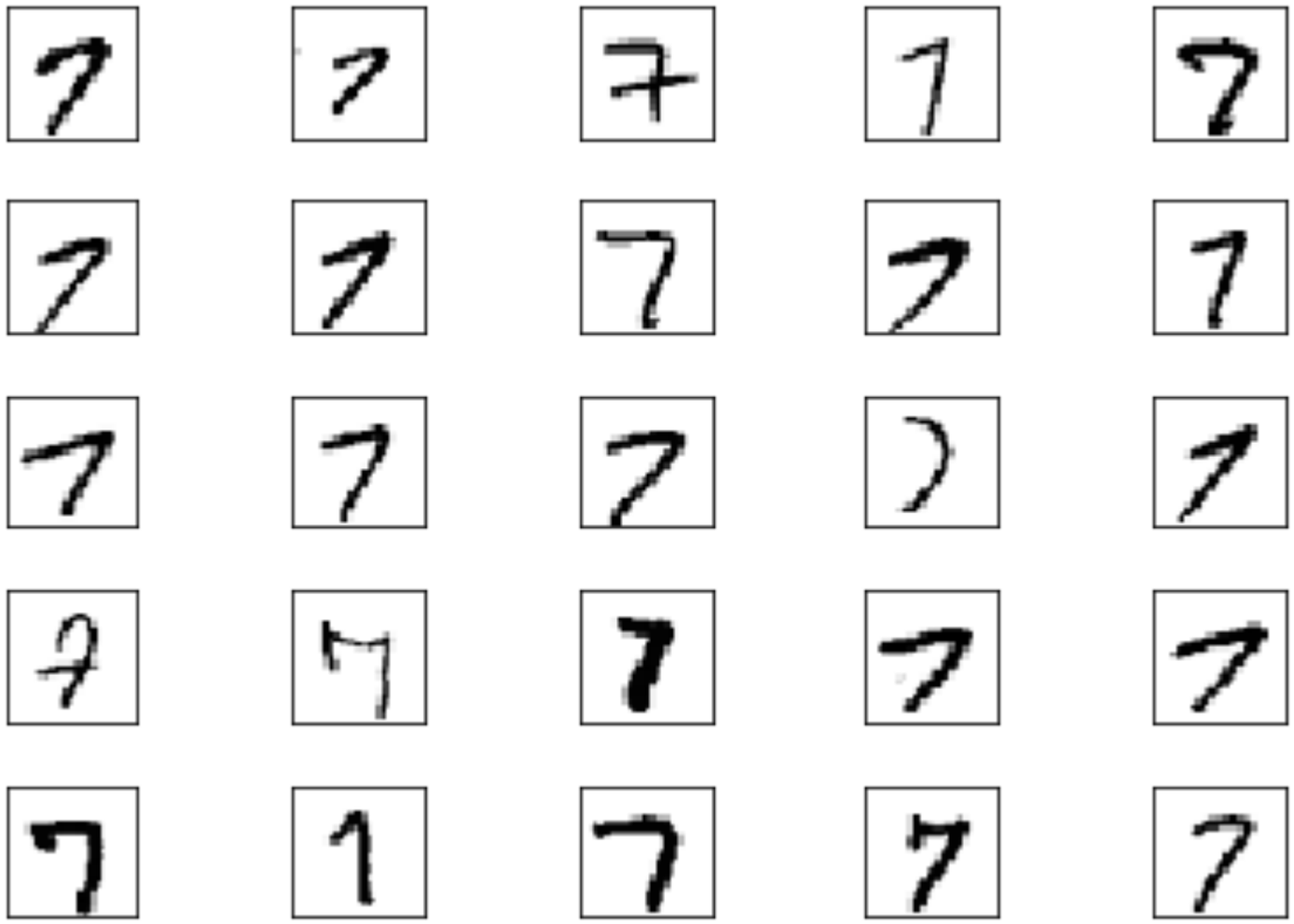

Illustration of different "7"s

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

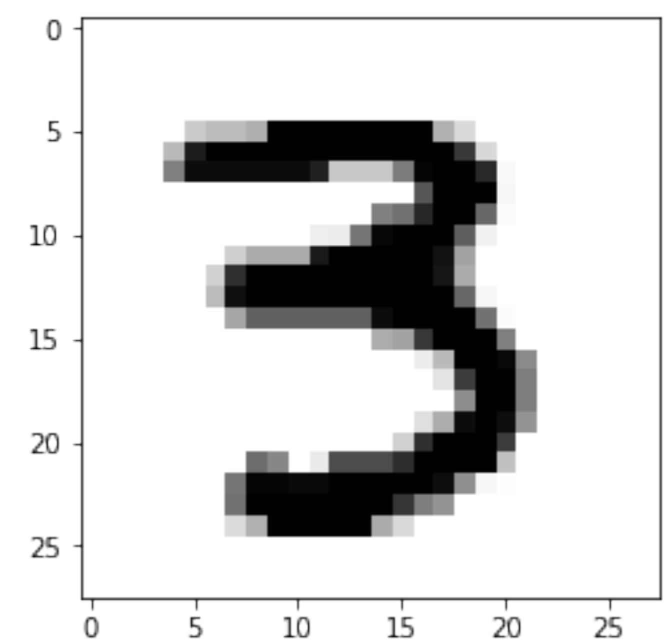

Note that I normalized pixels by factor 1/255 here

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,
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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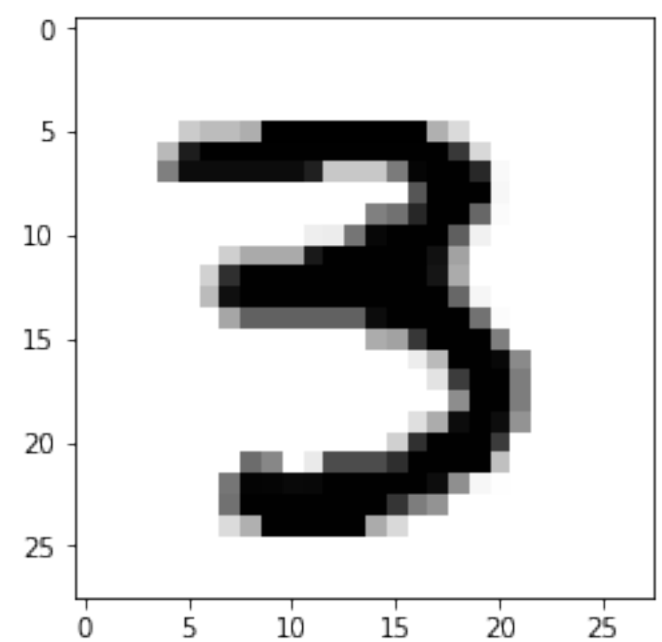
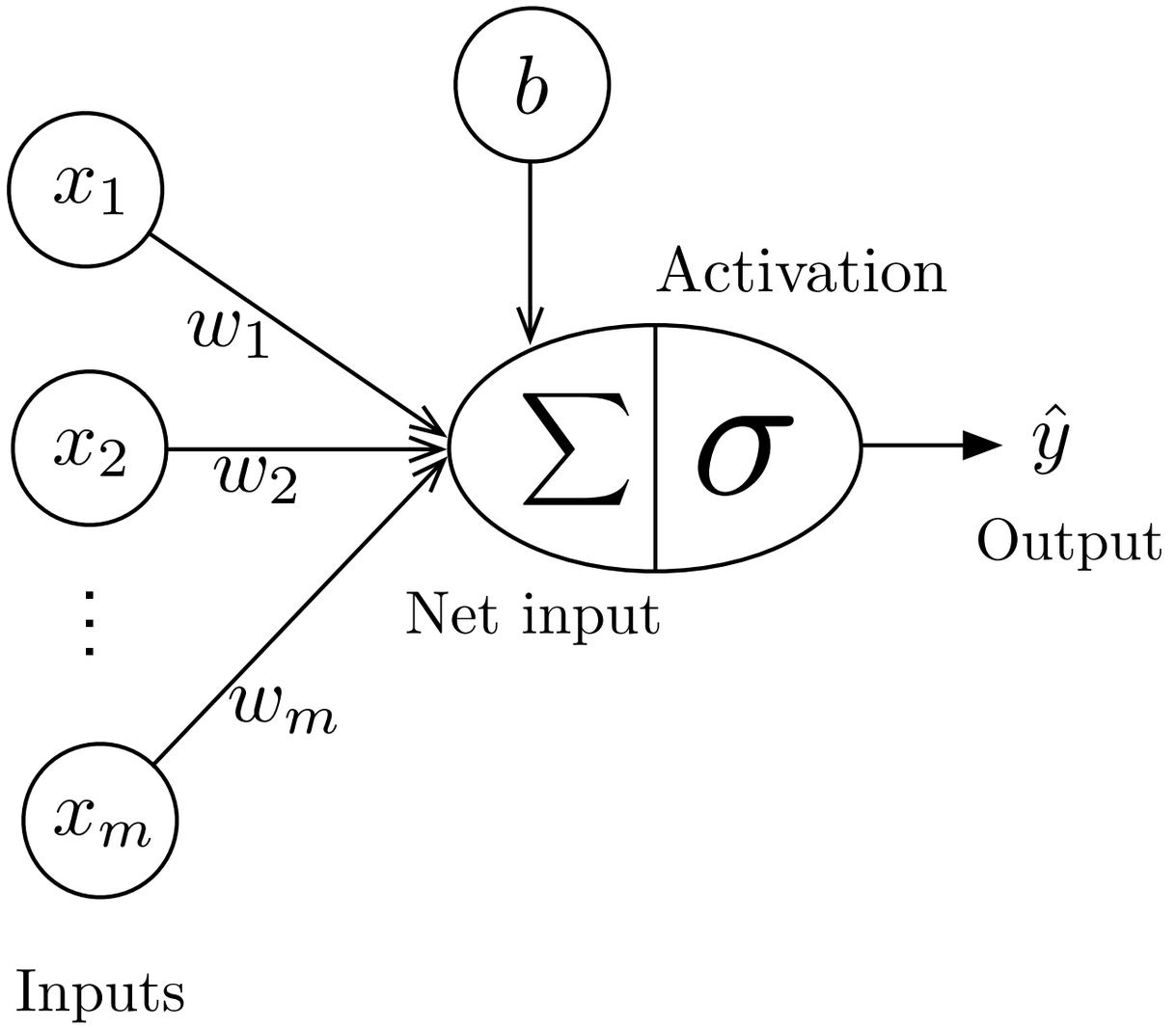
, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0]

Represent digit as a long vector of pixels



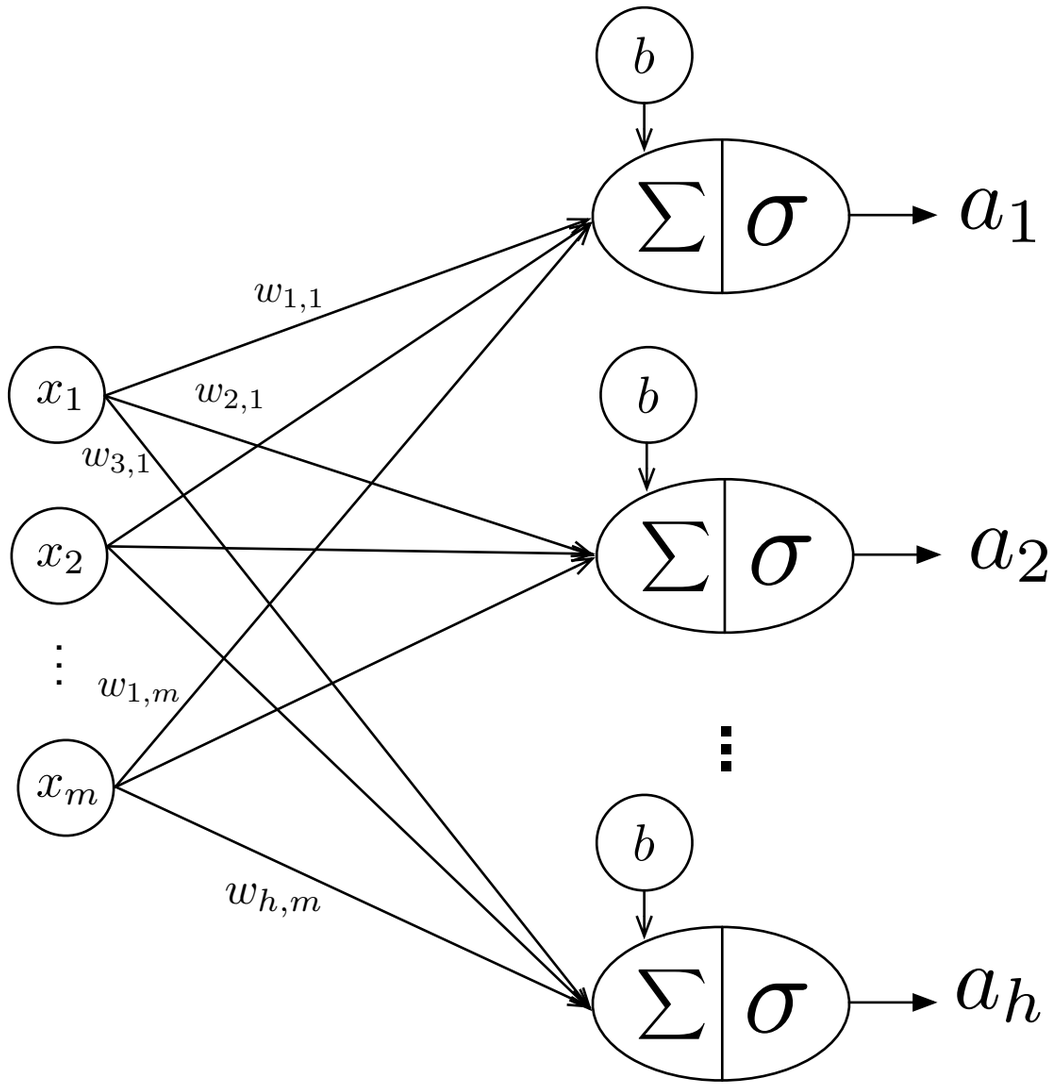
Note that I normalized pixels by factor 1/255 here

Previous Approach for Binary Classes



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

Another Approach Could be ...



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

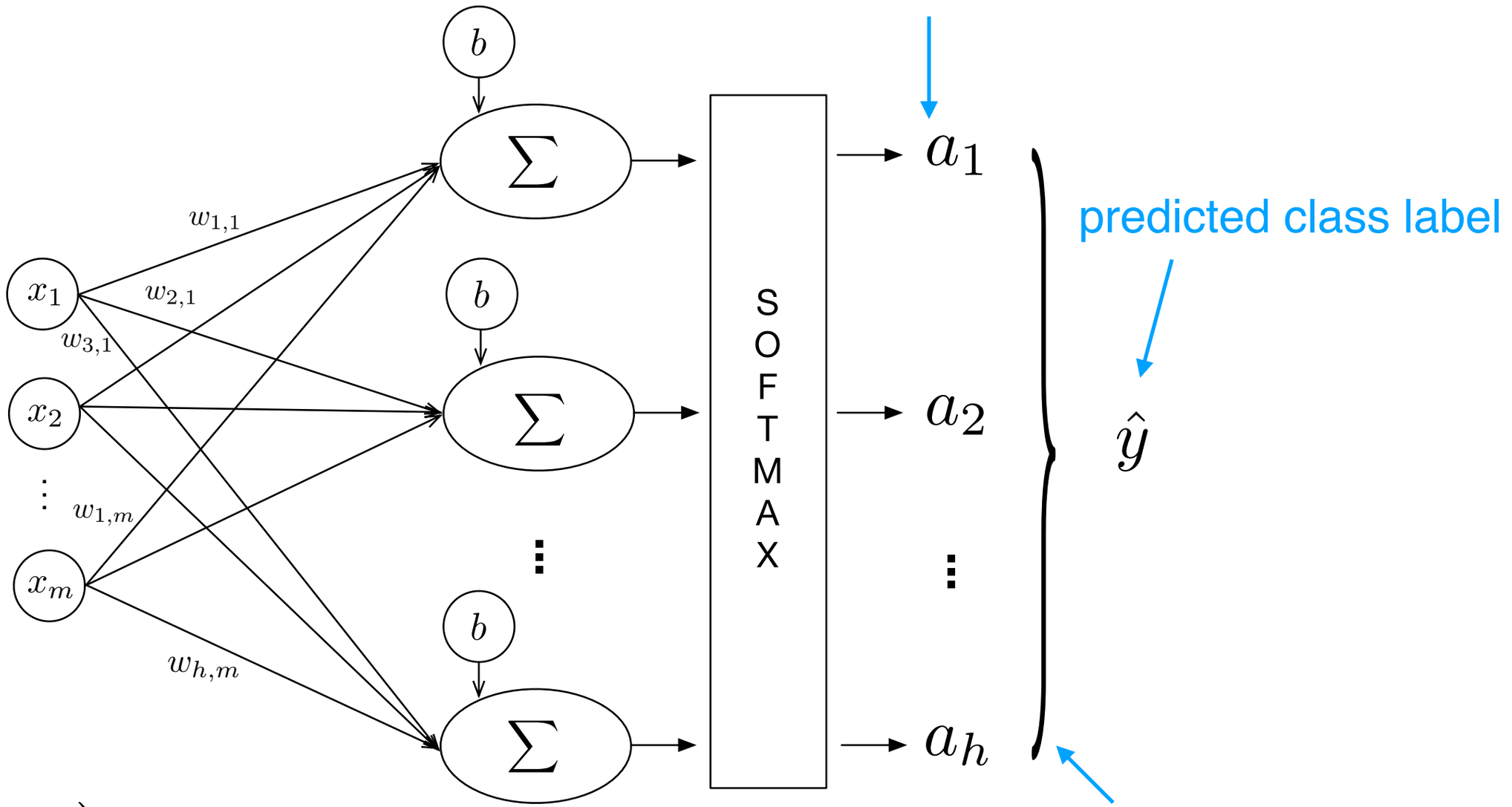
$$\sigma\left(\mathbf{W}\mathbf{x} + \mathbf{b}\right) = \sigma(\mathbf{z}) = \mathbf{a}$$

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

where h is the number of classes

Multinomial Logistic Regression / Softmax Regression

activations are
class-membership probabilities
(mutually exclusive classes)



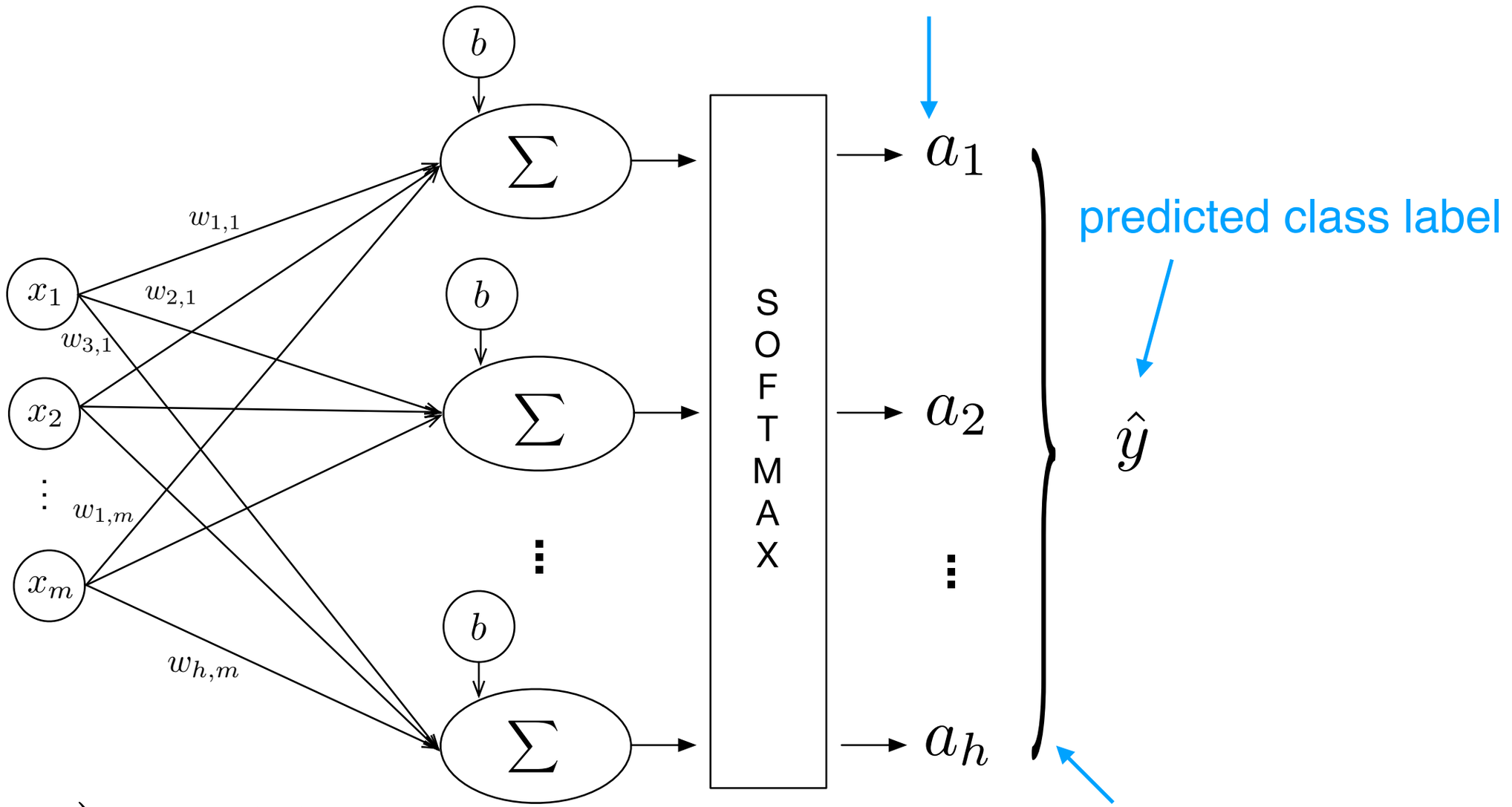
$$\sigma\left(\mathbf{W}\mathbf{x} + \mathbf{b}\right) = \sigma(\mathbf{z}) = \mathbf{a}$$

Representing Class Labels via Onehot Encoding for the Multi-category Cross Entropy Loss

1. Logistic Regression as an Artificial Neuron
2. Negative Log-Likelihood Loss
3. Logistic Regression Learning Rule
4. Logits and Cross Entropy
5. Logistic Regression Code Example
6. Generalizing to Multiple Classes: Softmax Regression
7. **OneHot Encoding and Multi-category Cross Entropy**
8. Softmax Regression Learning Rule
9. Softmax Regression Code Example

Multinomial Logistic Regression / Softmax Regression

activations are
class-membership probabilities
(mutually exclusive classes)



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

Softmax Activation

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

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

h is the number of class labels

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

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

Loss Function

(Multi-category) Cross Entropy

for h different class labels

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

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!

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

for h different class labels

(Multi-category) Cross Entropy

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)

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

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

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

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

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

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

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

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

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

$$\approx 0.9335$$

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-ss21/blob/master/L07/code/cross-entropy-pytorch.ipynb

Softmax Regression Derivatives for Gradient Descent

1. Logistic Regression as an Artificial Neuron
2. Negative Log-Likelihood Loss
3. Logistic Regression Learning Rule
4. Logits and Cross Entropy
5. Logistic Regression Code Example
6. Generalizing to Multiple Classes: Softmax Regression
7. OneHot Encoding and Multi-category Cross Entropy
8. **Softmax Regression Learning Rule**
9. Softmax Regression Code Example

The Same Overall Concept Applies ...

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

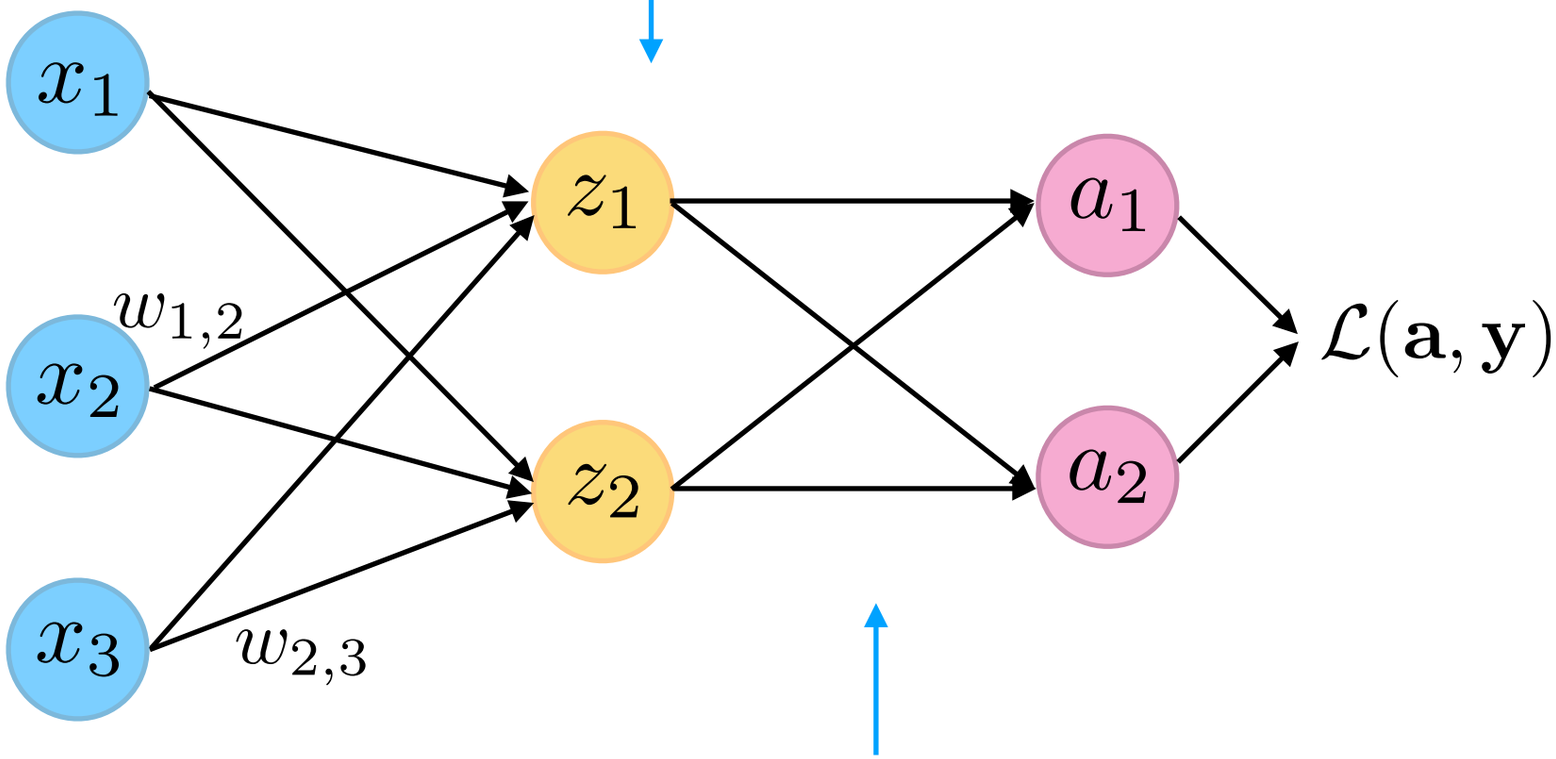
$$\frac{\partial \mathcal{L}}{\partial w_i} = \frac{\partial \mathcal{L}}{\partial a} \frac{da}{dz} \frac{\partial z}{\partial w_i}$$

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

Softmax Regression Sketch

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

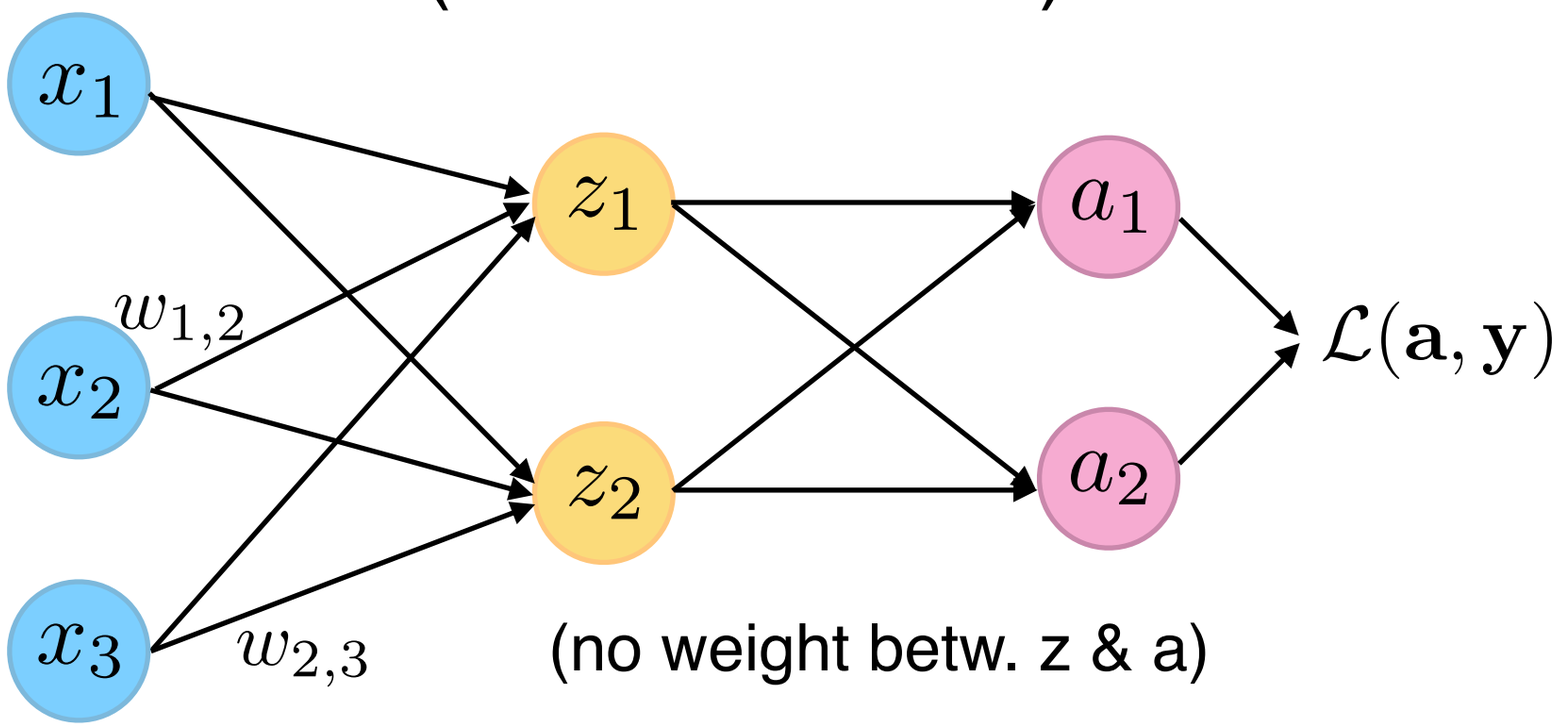
Note that I put the logits (net inputs) as the intermediate step



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

Softmax Regression Sketch

(bias not shown)



Multivariable chain rule

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

$$-\frac{y_1}{a_1} \quad a_1(1-a_1) \quad x_2 \qquad -\frac{y_2}{a_2} \quad -a_2 a_1 \quad x_2$$

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

$$-\frac{y_1}{a_1}$$

$$\frac{\partial L}{\partial a_1} = \frac{\partial}{\partial a_1}\left[\sum_{j=1}^{h} -y_j \log\left(a_j\right)\right]$$

$$= \frac{\partial}{\partial a_1}\left[-y_1 \log\left(a_1\right)\right]$$

$$= -\frac{y_1}{a_1}$$

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

$$\downarrow$$

$$a_1(1 - a_1)$$

$$\frac{\partial a_1}{\partial z_1} = \frac{\partial}{\partial z_1}\left[\frac{e^{z_1}}{\sum_{j=1}^{h} e^{z_j}}\right]$$

$$= \frac{\left[\sum_{j=1}^{h} e^{z_j}\right]\frac{\partial}{\partial z_1}e^{z_1} - e^{z_1}\frac{\partial}{\partial z_1}\left[\sum_{j=1}^{h} e^{z_j}\right]}{\left[\sum_{j=1}^{h} e^{z_j}\right]^2}$$

$$= \frac{\left[\sum_{j=1}^{h} e^{z_j}\right]e^{z_1} - e^{z_1}e^{z_1}}{\left[\sum_{j=1}^{h} e^{z_j}\right]^2}$$

$$= \frac{e^{z_1}\left(\left[\sum_{j=1}^{h} e^{z_1}\right] - e^{z_1}\right)}{\left[\sum_{j=1}^{h} e^{z_j}\right]^2} = \frac{e^{z_1}}{\left[\sum_{j=1}^{h} e^{z_j}\right]} \cdot \frac{\left[\sum_{j=1}^{h} e^{z_j}\right] - e^{z_1}}{\left[\sum_{j=1}^{h} e^{z_j}\right]} = a_1(1 - a_1)$$

	Function	Derivative
Sum Rule	$f(x) + g(x)$	$f'(x) + g'(x)$
Difference Rule	$f(x) - g(x)$	$f'(x) - g'(x)$
Product Rule	$f(x)g(x)$	$f'(x)g(x) + f(x)g'(x)$
Quotient Rule	$f(x)/g(x)$	$[g(x)f'(x) - f(x)g'(x)]/[g(x)]^2$
Reciprocal Rule	$1/f(x)$	$-[f'(x)]/[f(x)]^2$
Chain Rule	$f(g(x))$	$f'(g(x))g'(x)$

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

$$\downarrow$$

$$-a_2 a_1$$

$$\frac{\partial a_2}{\partial z_1} = \frac{\partial}{\partial z_1}\left[\frac{e^{z_2}}{\sum_{j=1}^{h} e^{z_j}}\right]$$

	Function	Derivative
Sum Rule	$f(x) + g(x)$	$f'(x) + g'(x)$
Difference Rule	$f(x) - g(x)$	$f'(x) - g'(x)$
Product Rule	$f(x)g(x)$	$f'(x)g(x) + f(x)g'(x)$
Quotient Rule	$f(x)/g(x)$	$[g(x)f'(x) - f(x)g'(x)]/[g(x)]^2$
Reciprocal Rule	$1/f(x)$	$-[f'(x)]/[f(x)]^2$
Chain Rule	$f(g(x))$	$f'(g(x))g'(x)$

$$= \frac{\left[\sum_{j=1}^{h} e^{z_j}\right]\frac{\partial}{\partial z_1}e^{z_2} - e^{z_2}\frac{\partial}{\partial z_1}\left[\sum_{j=1}^{h} e^{z_j}\right]}{\left[\sum_{j=1}^{h} e^{z_j}\right]^2}$$

$$= \frac{0 - e^{z_2}e^{z_1}}{\left[\sum_{j=1}^{h} e^{z_j}\right]^2}$$

$$= \frac{-e^{z_2}}{\left[\sum_{j=1}^{h} e^{z_j}\right]} \cdot \frac{e^{z_1}}{\left[\sum_{j=1}^{h} e^{z_j}\right]} \quad = -a_2 a_1$$

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

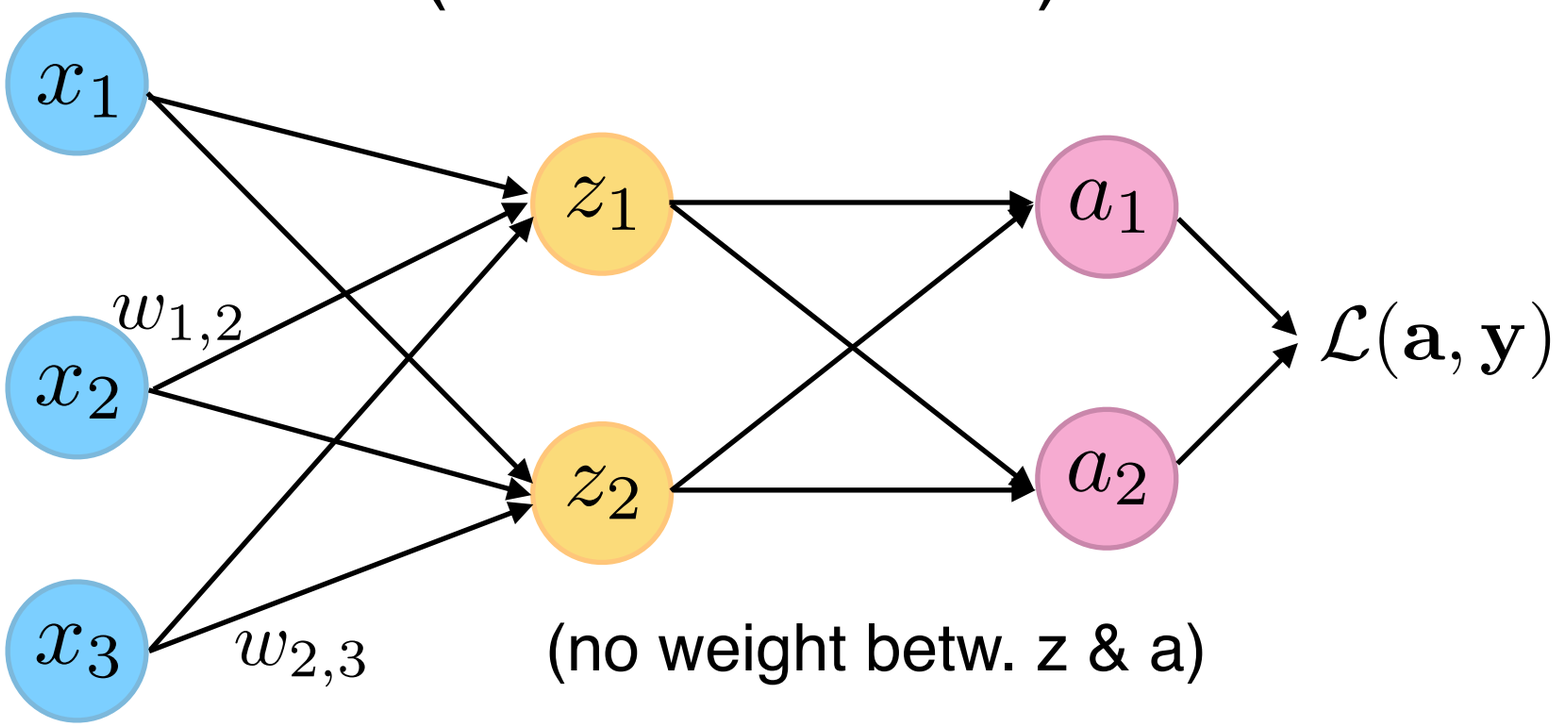
x_2

$$= \frac{\partial}{\partial w_{1,2}}\left[w_{1,2} \cdot x_2 + b\right]$$

$$= x_2$$

Softmax Regression Sketch

(bias not shown)



Multivariable chain rule

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

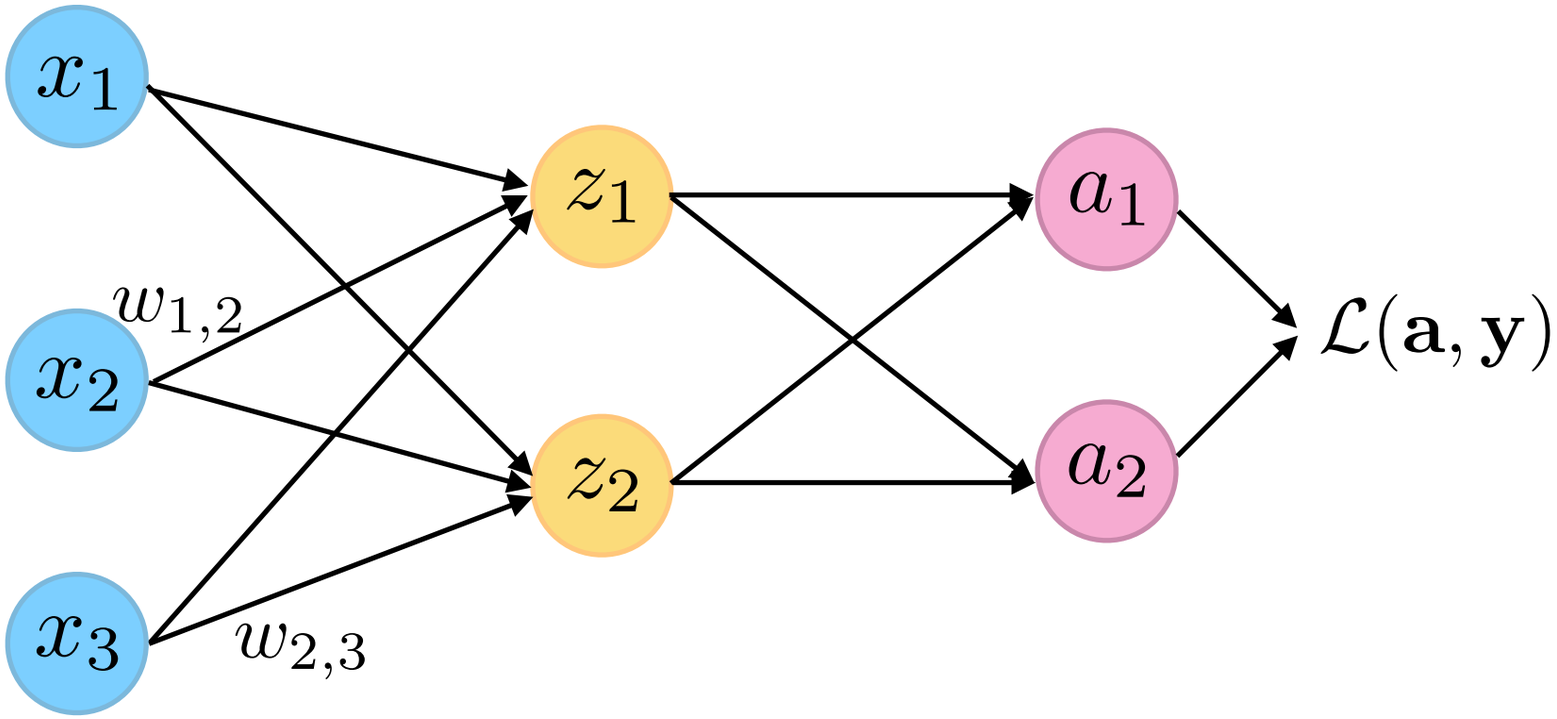
$$= \frac{-y_1}{a_1}[a_1(1-a_1)]x_2 + \frac{-y_2}{a_2}(-a_2 a_1)x_2$$

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

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

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

Softmax Regression Sketch



Vectorized Form:

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

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

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

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

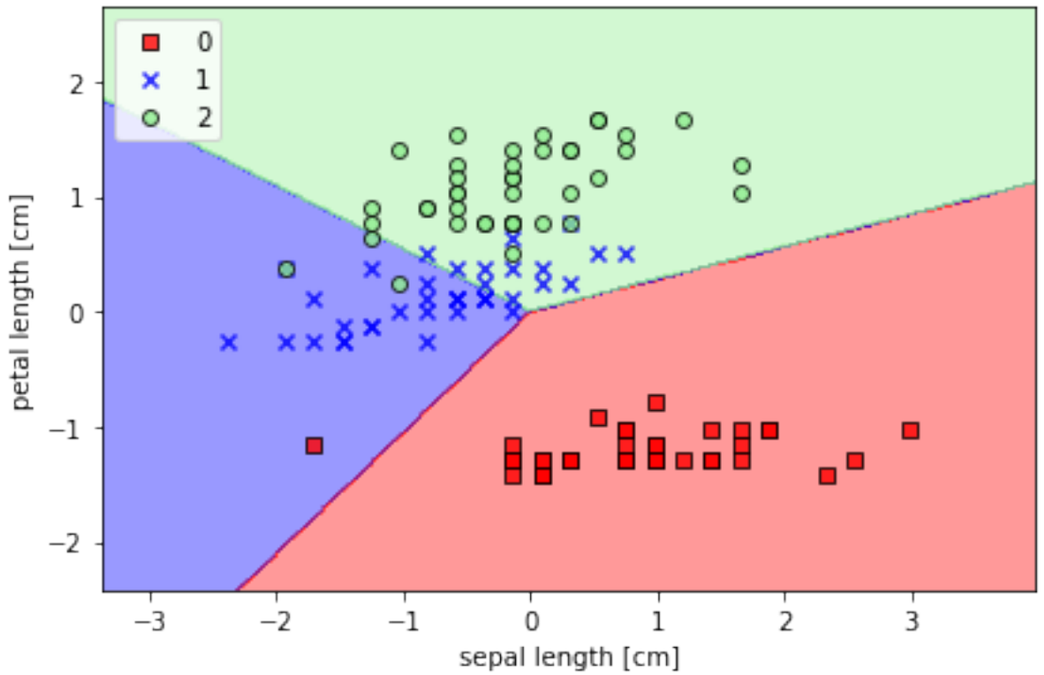
$\mathbf{A} \in \mathbb{R}^{n \times h}$

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

Softmax Regression Code Example

1. Logistic Regression as an Artificial Neuron
2. Negative Log-Likelihood Loss
3. Logistic Regression Learning Rule
4. Logits and Cross Entropy
5. Logistic Regression Code Example
6. Generalizing to Multiple Classes: Softmax Regression
7. OneHot Encoding and Multi-category Cross Entropy
8. Softmax Regression Learning Rule
9. **Softmax Regression Code Example**

Softmax Regression Hands-On Example (Iris)

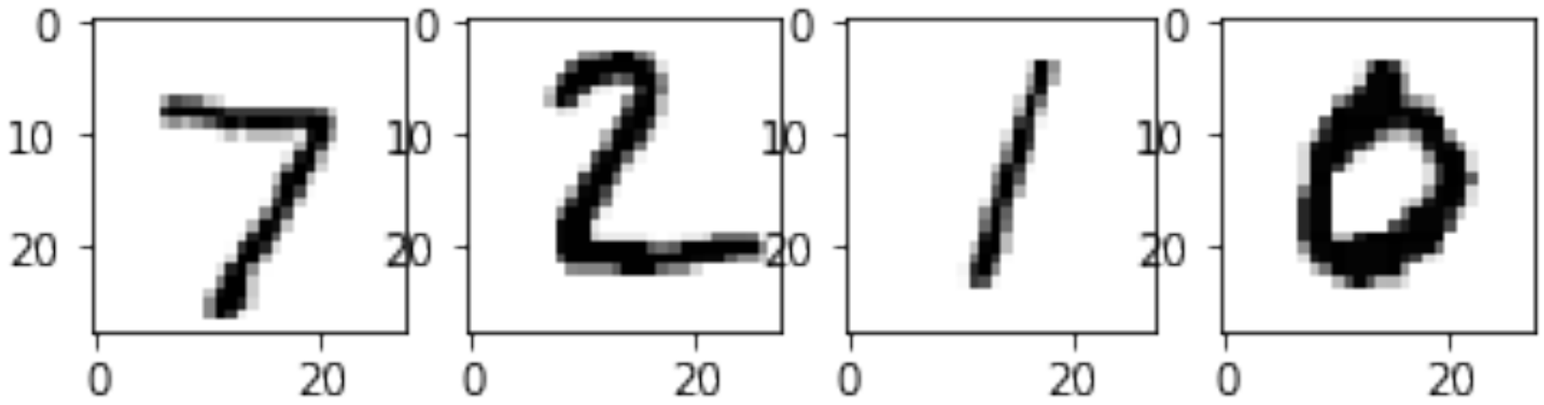


"From scratch" implementation & PyTorch autodiff implementation

https://github.com/rasbt/stat453-deep-learning-ss21/blob/master/L08/code/softmax-regression_scratch.ipynb

Softmax Regression Hands-On (MNIST)

Using PyTorch (with autodiff an nn.Module)



https://github.com/rasbt/stat453-deep-learning-ss21/blob/master/L08/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