

Softmax Regression

Quang-Vinh Dinh
Ph.D. in Computer Science

Objectives

Motivation

Feature	Label
Petal_Length	Petal_Width
1.4	0.2
1.4	0.2
1.3	0.2
4.5	1.5
4.9	1.5
4	1.3
4.5	1.7
6.3	1.8
5.8	1.8
	Label
0	
0	
0	
1	
1	
1	
2	
2	
2	

#class=3
#feature=2

Feature is with two dimensions

→ Need two nodes for input

Three categories

→ Need three nodes for output

Softmax Regression

1. Forward computation

$$\mathbf{z} = \boldsymbol{\theta}^T \mathbf{x}$$
$$\hat{\mathbf{y}} = \frac{e^{\mathbf{z}}}{\sum_{j=0}^1 e^{z_j}}$$

2. Loss function

$$L(\boldsymbol{\theta}) = -\mathbf{y}^T \log \hat{\mathbf{y}}$$

3. Derivative

$$\frac{\partial L}{\partial w_i} = \mathbf{x}(\hat{\mathbf{y}}_i - \mathbf{y}_i)$$
$$\frac{\partial L}{\partial b_i} = \hat{\mathbf{y}}_i - \mathbf{y}_i$$

$$\nabla_{\boldsymbol{\theta}} L = \mathbf{x}(\hat{\mathbf{y}} - \mathbf{y})^T$$

4. Update

$$\boldsymbol{\theta} = \boldsymbol{\theta} - \eta \nabla_{\boldsymbol{\theta}} L$$

η is learning rate

Implementation

```
# compute z
z = theta.T.dot(xi)

# compute y_hat
exp_z = np.exp(z)
y_hat = exp_z / np.sum(exp_z, axis=0)

# compute the loss
loss = -yi.T.dot(np.log(y_hat))
losses.append(loss[0])

# compute the gradient dz
dz = y_hat - yi

# compute dtheta
dtheta = xi.dot(dz.T)

# update
theta = theta - learning_rate*dtheta
```

Outline

SECTION 1

Model Construction

SECTION 2

Cross-entropy Loss

SECTION 3

Implementation

Feature	Label	
Petal_Length	Petal_Width	Label
1.4	0.2	0
1.4	0.2	0
1.3	0.2	0
4.5	1.5	1
4.9	1.5	1
4	1.3	1
4.5	1.7	2
6.3	1.8	2
5.8	1.8	2

#class=3

#feature=2

Feature is with two dimensions

→ Need two nodes for input

Three categories

→ Need three nodes for output

Linear Regression

❖ Prediction

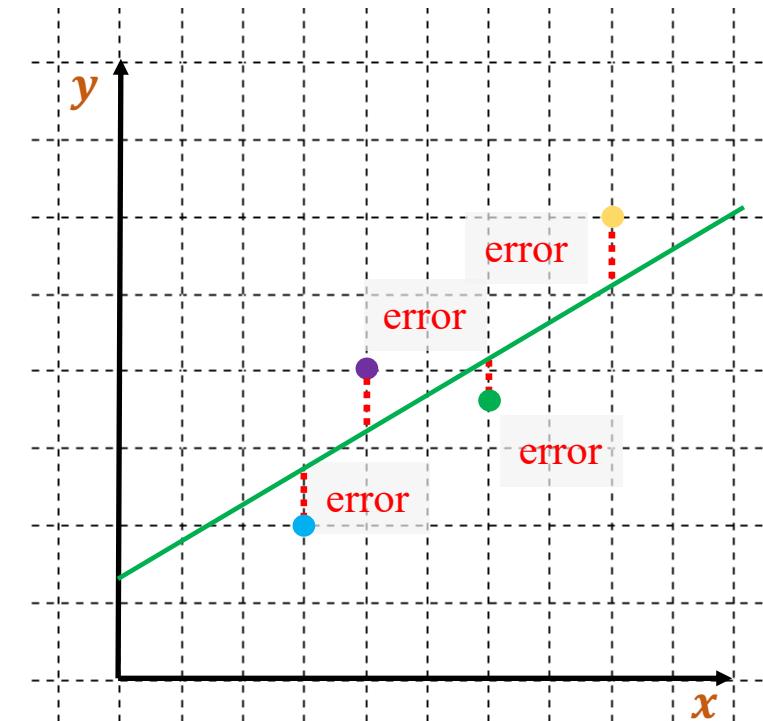
Area-based House Price Data	
Feature	Label
area	price
6.7	9.1
4.6	5.9
3.5	4.6
5.5	6.7

Training data

construct

$$\hat{y} = \theta^T x = wx + b$$
$$\hat{y} \in (-\infty, +\infty)$$

Model



Find the line $\hat{y} = \theta^T x$ that is best fitting to given data, then use \hat{y} to predict for new data

Logistic Regression

❖ Binary Classification

Feature	Label
Petal_Length	Category
1.4	Flower A
1	Flower A
1.5	Flower A
3	Flower B
3.8	Flower B
4.1	Flower B

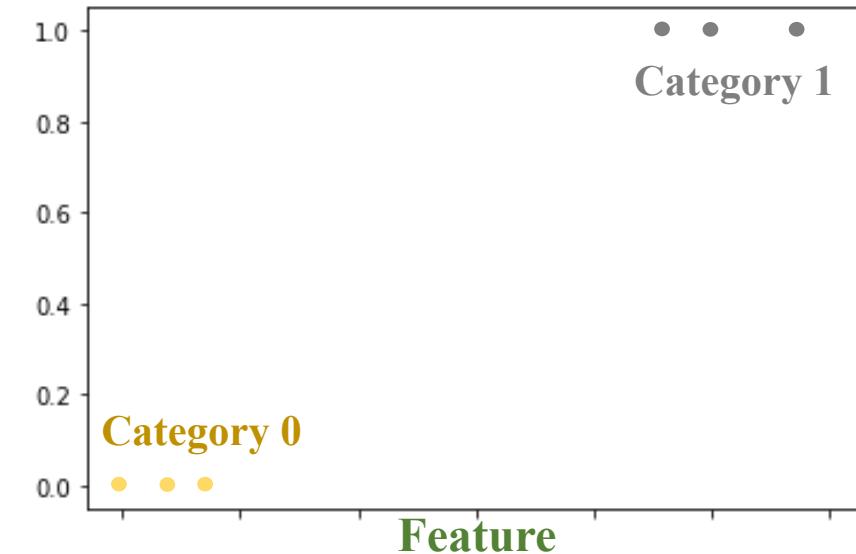
Category 0 Category 1

Assign numbers
to categories

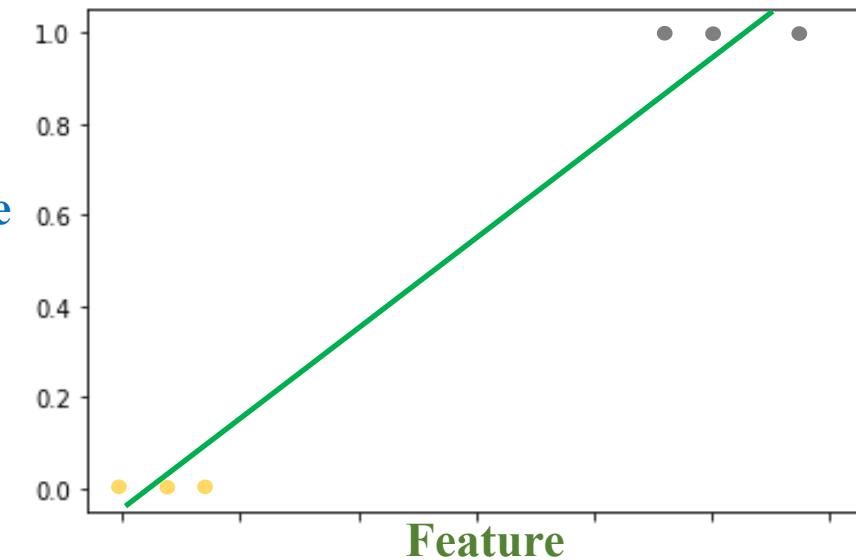
Feature	Label
Petal_Length	Category
1.4	0
1	0
1.5	0
3	1
3.8	1
4.1	1

Category 0 Category 1

Plot data



A line is not suitable
for this data



Idea of Logistic Regression

❖ Binary Classification

Feature	Label
Petal_Length	Category
1.4	Flower A
1	Flower A
1.5	Flower A
3	Flower B
3.8	Flower B
4.1	Flower B

Category 0 Category 1

↓ Assign numbers to categories

Feature	Label
Petal_Length	Category
1.4	0
1	0
1.5	0
3	1
3.8	1
4.1	1

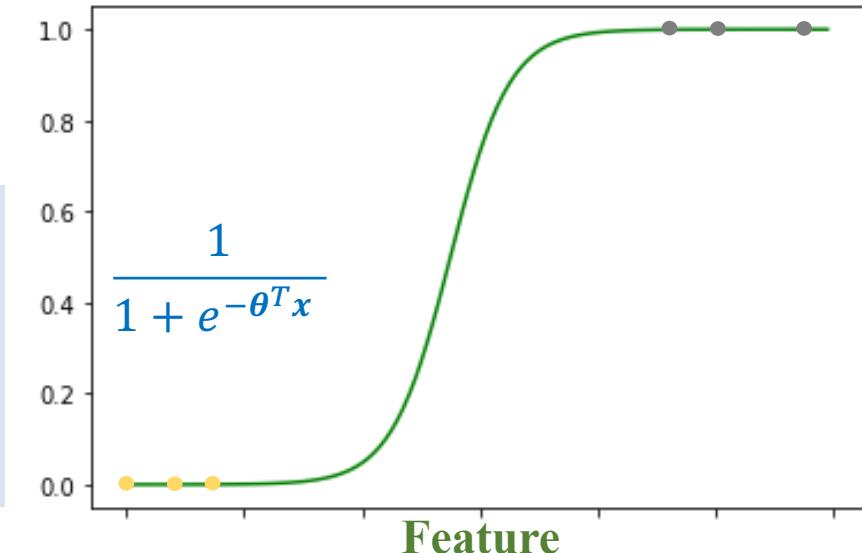
Category 0 Category 1

Sigmoid function could fit the data

$$z = \theta^T x = x^T \theta$$

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

$$\hat{y} \in (0 \quad 1)$$

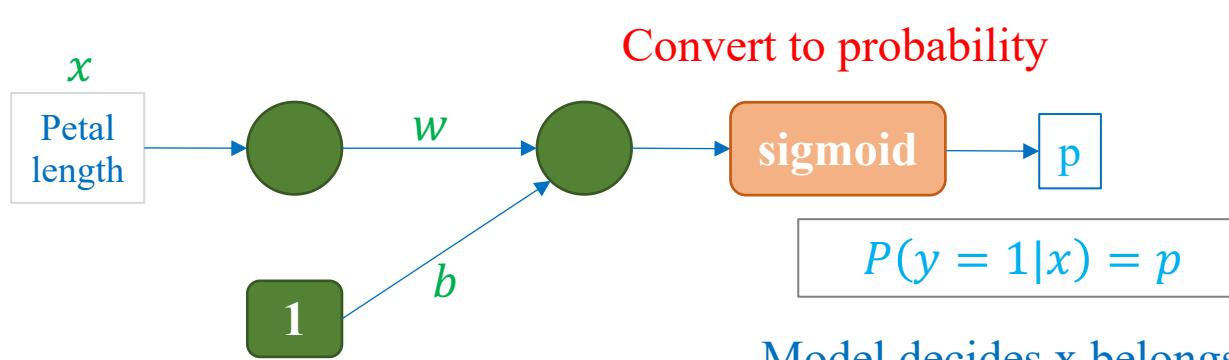


Binary cross-entropy

$$L = -y \log \hat{y} - (1 - y) \log(1 - \hat{y})$$

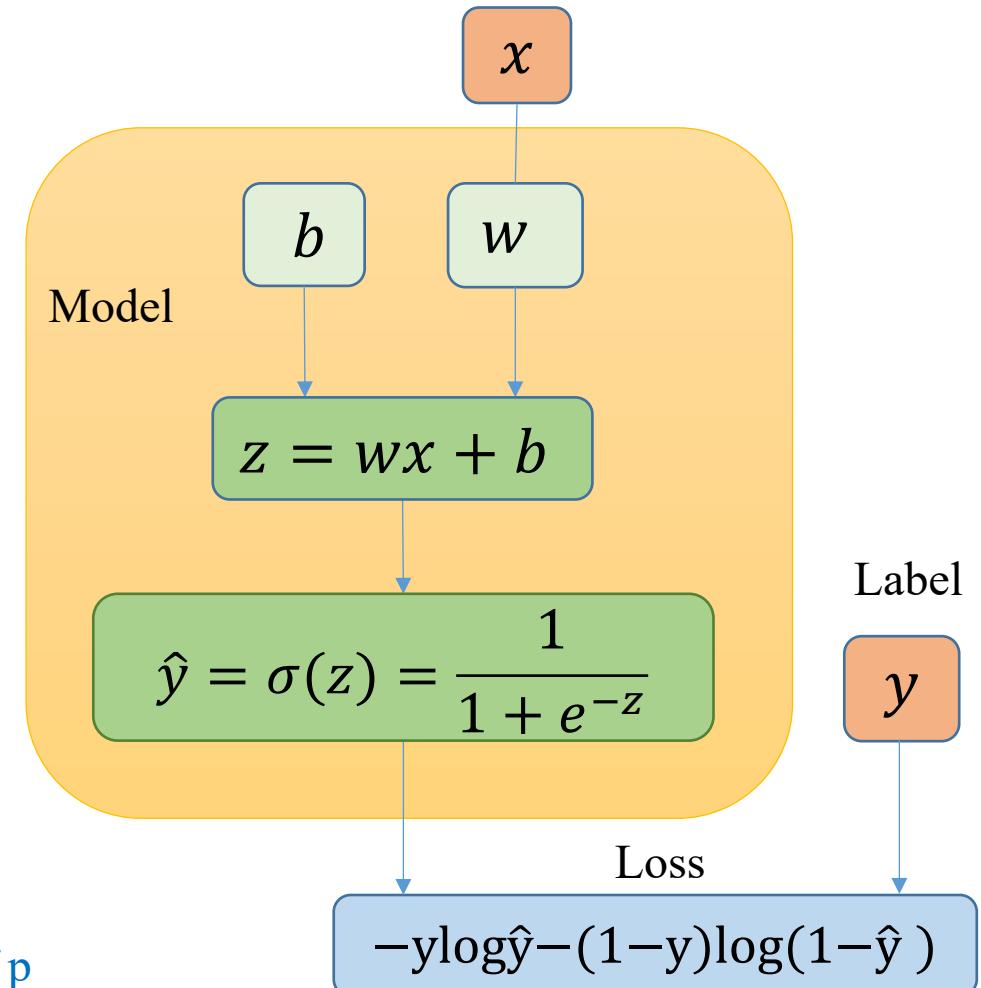
Motivation

Feature	Label
Petal_Length	Label
1.4	0
1.3	0
1.5	0
4.5	1
4.1	1
4.6	1



Model decides x belongs to the category (label=1) with the belief of p

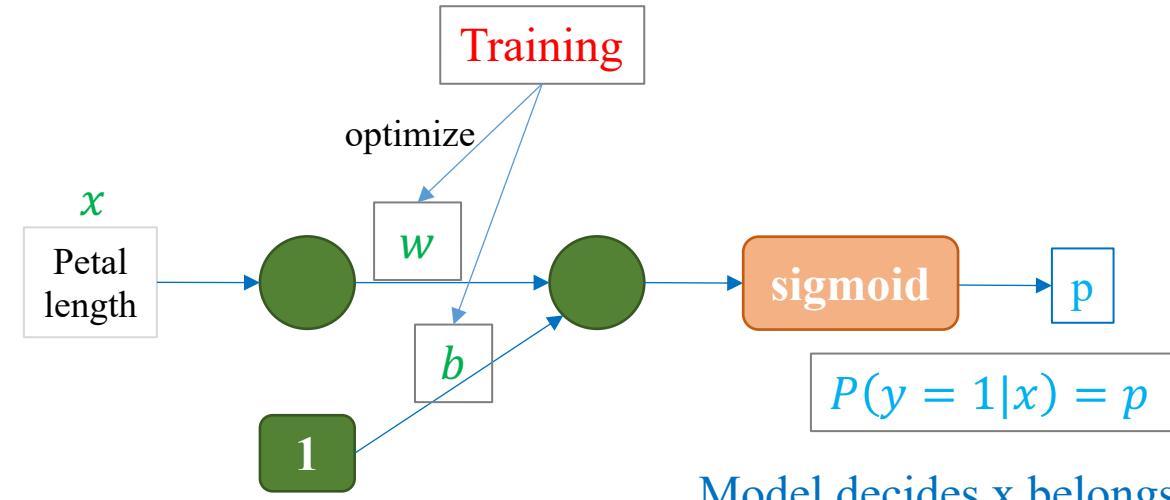
Implicitly conclude that $P(y = 0|x) = 1 - p$



Motivation

❖ Problem!

Feature	Label
Petal Length	Label
1.4	0
1.3	0
1.5	0
4.5	1
4.1	1
4.6	1



Model decides x belongs to category
($y=1$) with the belief of p

Implicitly extract that $P(\text{label} = 0|x) = 1 - p$

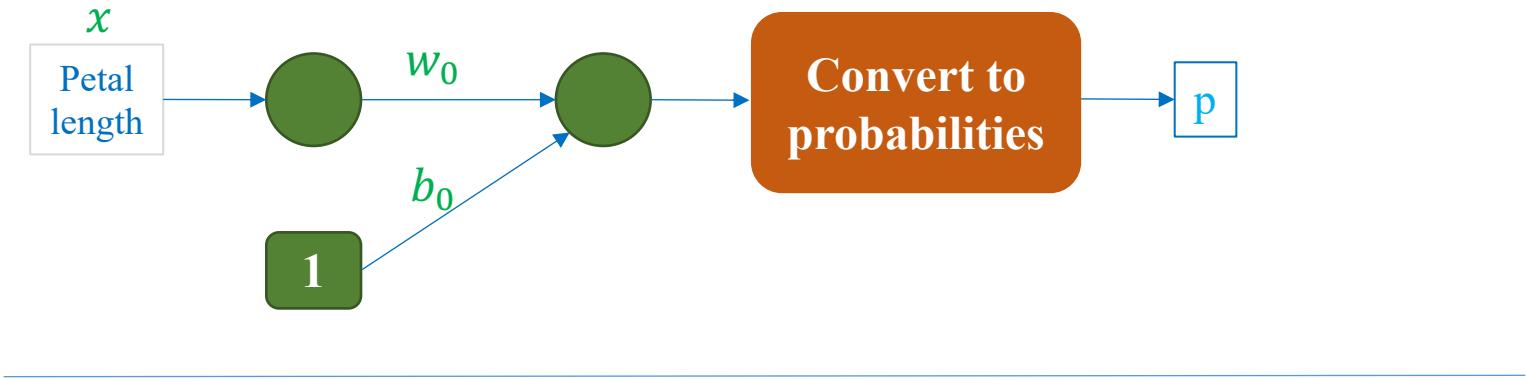
Optimize w and b for $P(\text{label} = 1|x)$ affects $P(\text{label} = 0|x)$ and vice versa

How to have explicitly $P(y = 0|x)$?

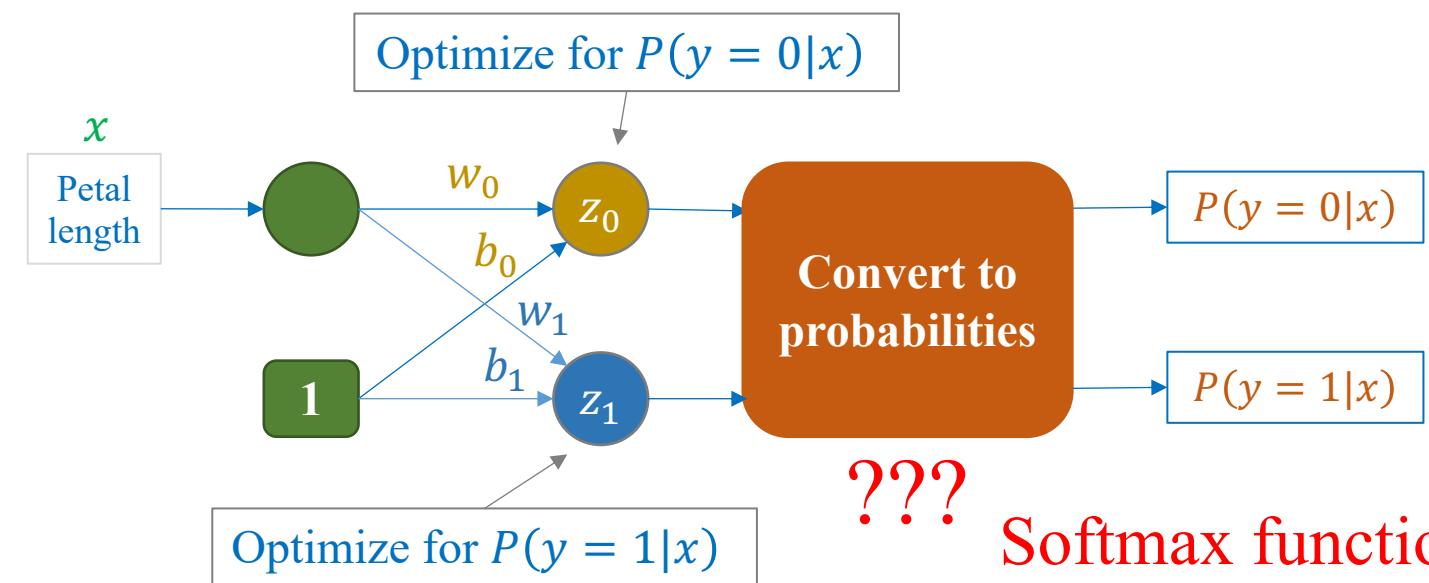
Motivation

❖ Problem!

Feature	Label
Petal Length	Label
1.4	0
1.3	0
1.5	0
4.5	1
4.1	1
4.6	1



Explicitly output $P(y = 0|x)$ and $P(y = 1|x)$



??? Softmax function

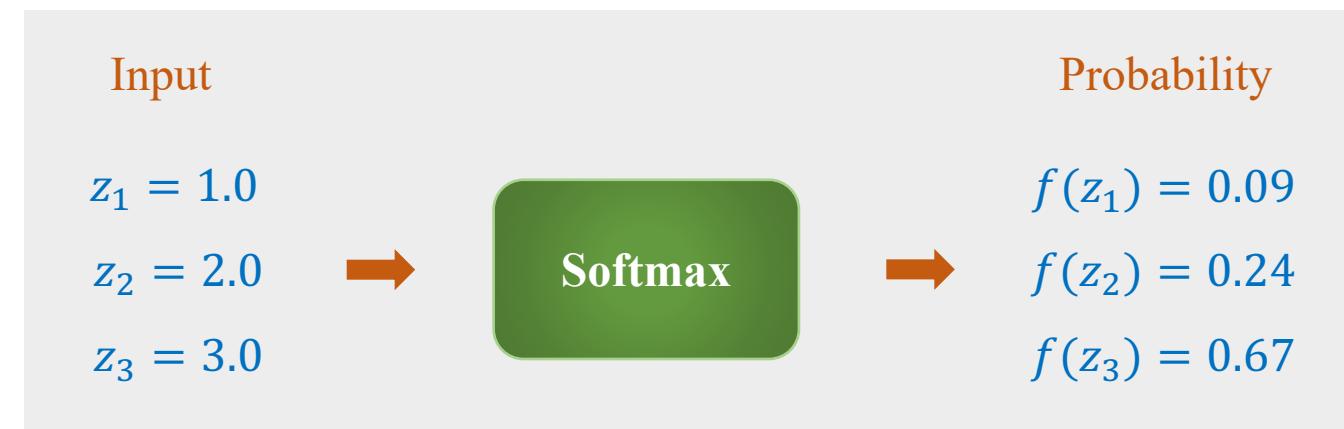
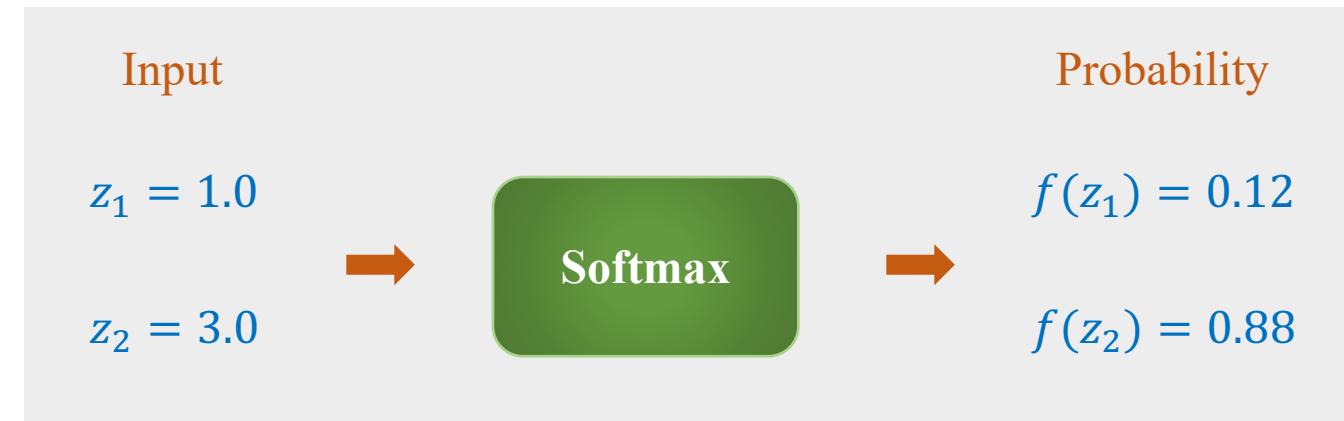
Motivation

Softmax function

$$P_i = f(z_i) = \frac{e^{z_i}}{\sum_j e^{z_j}}$$

$$0 \leq f(z_i) \leq 1$$

$$\sum_i f(z_i) = 1$$



Softmax function

Chuyển các giá trị của một vector thành các giá trị xác suất

Formula

$$f(x_i) = \frac{e^{x_i}}{\sum_j e^{x_j}}$$

$$0 \leq f(x_i) \leq 1$$

$$\sum_i f(x_i) = 1$$

Input

$$x_1 = 1.0$$

$$x_2 = 2.0$$

$$x_3 = 3.0$$

Softmax

Probability

$$f(x_1) = 0.09$$

$$f(x_2) = 0.24$$

$$f(x_3) = 0.67$$

```

1 import numpy as np
2
3 def softmax(X):
4     exps = np.exp(X)
5     return exps / np.sum(exps)

```

```

1 X = np.array([1.0, 2.0, 3.0])
2 f = softmax(X)
3 print(f)

```

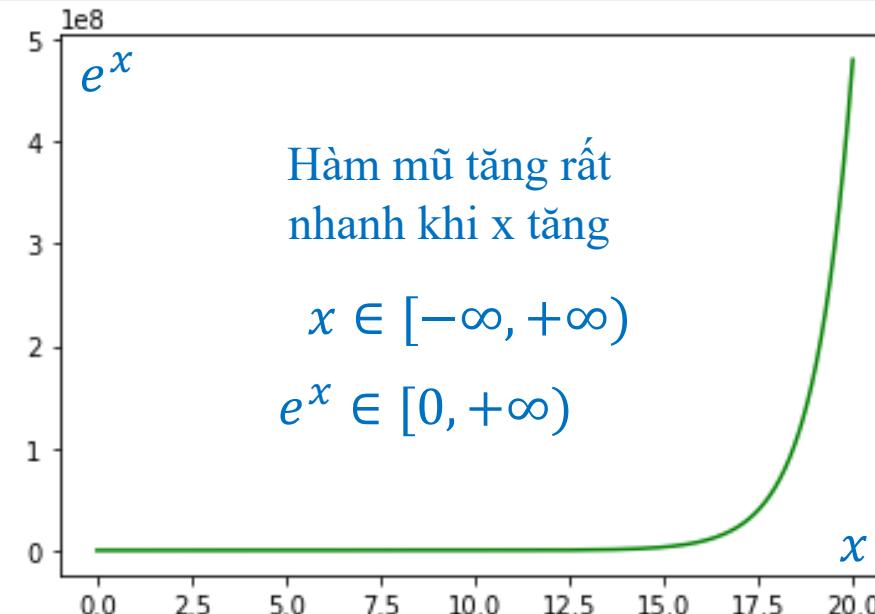
[0.09003057 0.24472847 0.66524096]

```

1 X = np.array([1000.0, 1001.0, 1002.0])
2 f = softmax(X)
3 print(f)

```

[nan nan nan]



Giá trị nan vì e^x vượt giới hạn lưu trữ của biến

Softmax function (stable)

(Stable) Formula

$$m = \max(x)$$

$$f(x_i) = \frac{e^{(x_i-m)}}{\sum_j e^{(x_j-m)}}$$

X

$$x_1 = 1.0$$

$$x_2 = 2.0$$

$$x_3 = 3.0$$

X-m

$$x_1 = -2.0$$

$$x_2 = -1.0$$

$$x_3 = 0$$

Probability

$$f(x_1) = 0.09$$

$$f(x_2) = 0.24$$

$$f(x_3) = 0.67$$

Softmax

```

1 import numpy as np
2
3 def stable_softmax(X):
4     exps = np.exp(X-np.max(X))
5     return exps / np.sum(exps)

```

```

1 X = np.array([1.0, 2.0, 3.0])
2 f = stable_softmax(X)
3 print(f)

```

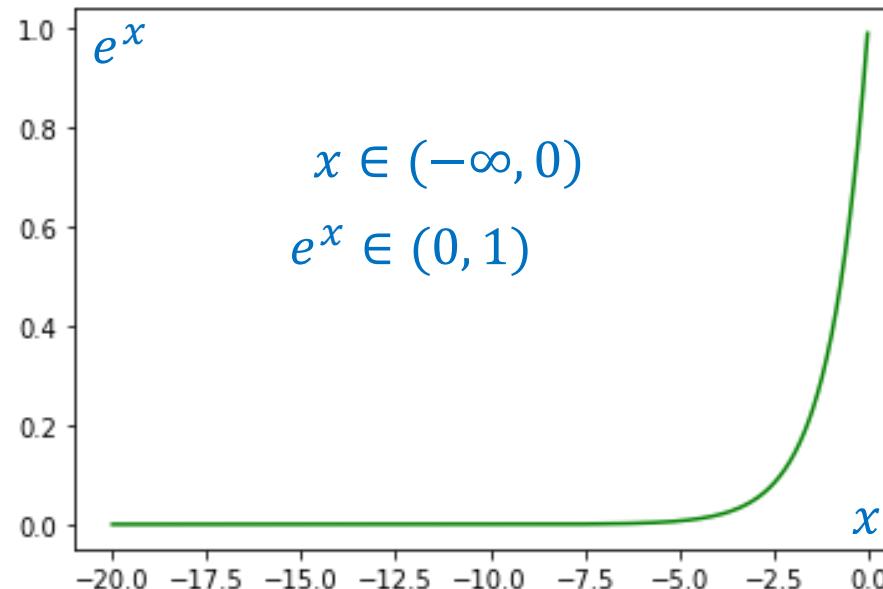
[0.09003057 0.24472847 0.66524096]

```

1 X = np.array([1000.0, 1001.0, 1002.0])
2 f = stable_softmax(X)
3 print(f)

```

[0.09003057 0.24472847 0.66524096]



```

1 X = np.array([1.0, 1001.0, 1002.0])
2 f = stable_softmax(X)
3 print(f)

```

[0.09003057 0.24472847 0.66524096]

Motivation

Feature	Label
Petal_Length	Label
1.4	0
1.3	0
1.5	0
4.5	1
4.1	1
4.6	1

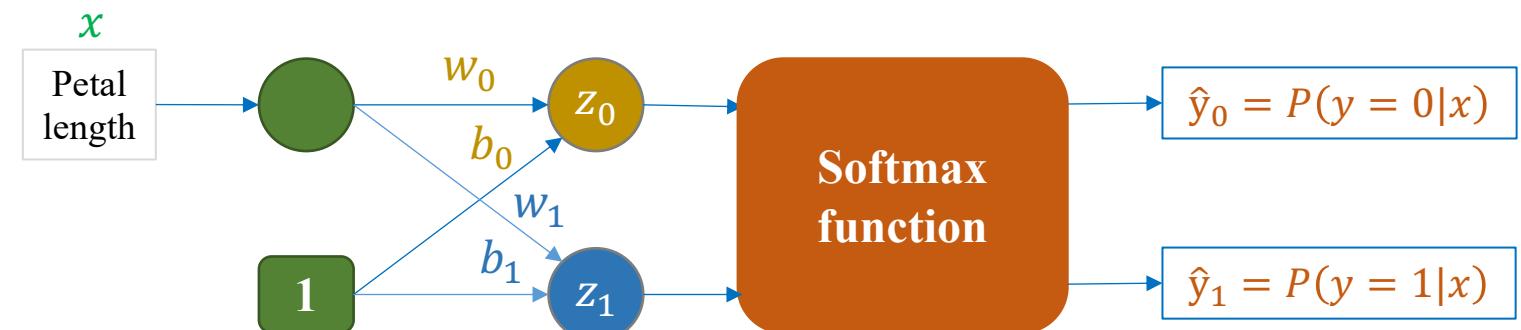
Softmax function

$$P_i = f(z_i) = \frac{e^{z_i}}{\sum_j e^{z_j}}$$

$$0 \leq f(z_i) \leq 1$$

$$\sum_i f(z_i) = 1$$

Explicitly output $P(y = 1|x)$ and $P(y = 0|x)$



How about loss function?

$$L(\theta) = -y \log \hat{y}_1 - (1-y) \log (\hat{y}_0)$$

Model Construction

❖ 1-D Feature and two classes

Feature	Label
Petal_Length	Label
1.4	0
1.3	0
1.5	0
4.5	1
4.1	1
4.6	1

#class=2

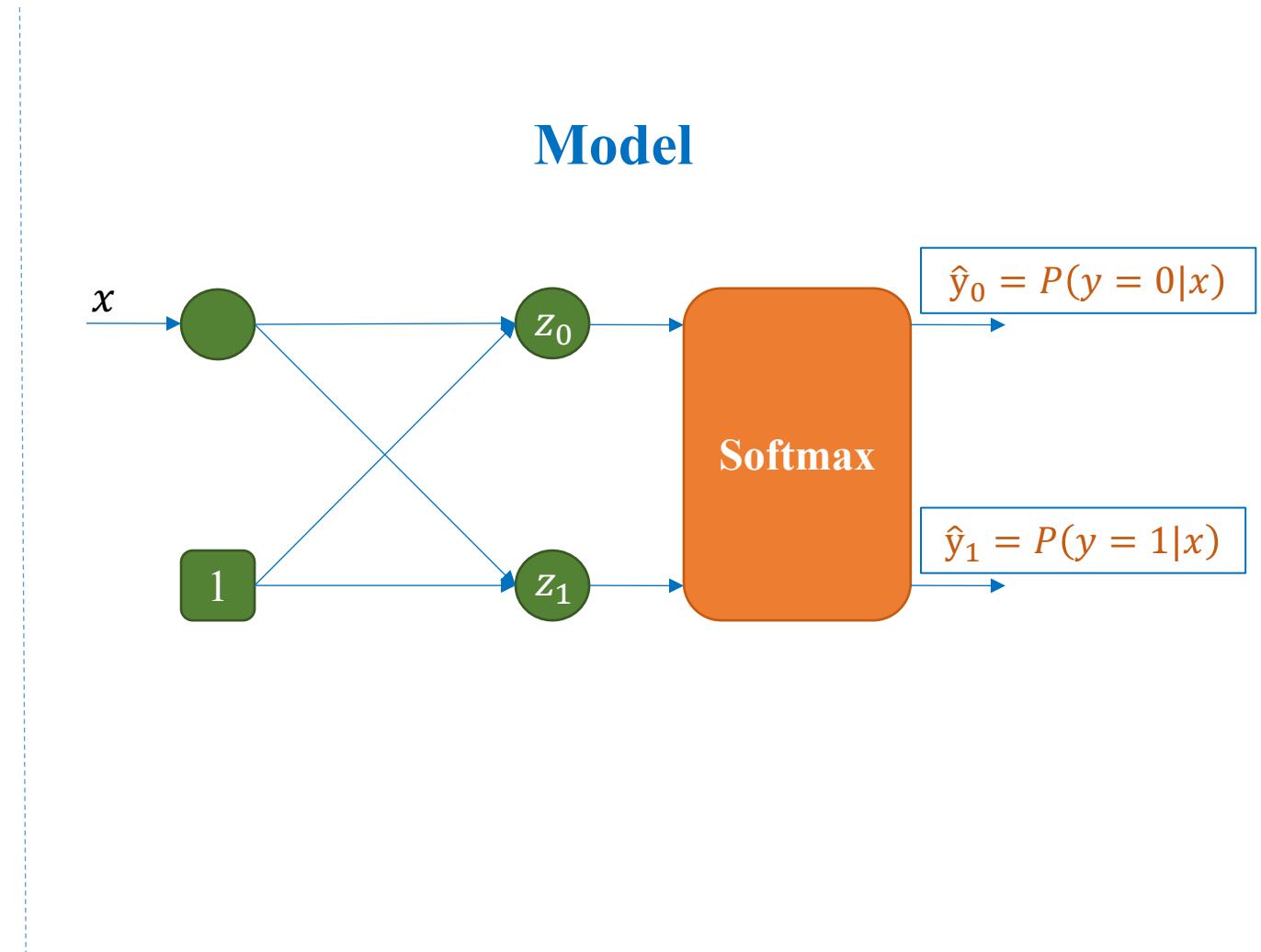
#feature=1

Feature is with one dimension

→ Need one node for input

Two categories

→ Need two node for output



Model Construction

❖ 1-D Feature and three classes

Feature	Label
Petal_Length	Label
1.4	0
1.3	0
1.5	0
4.5	1
4.1	1
4.6	1
5.2	2
5.6	2
5.9	2

#class=3

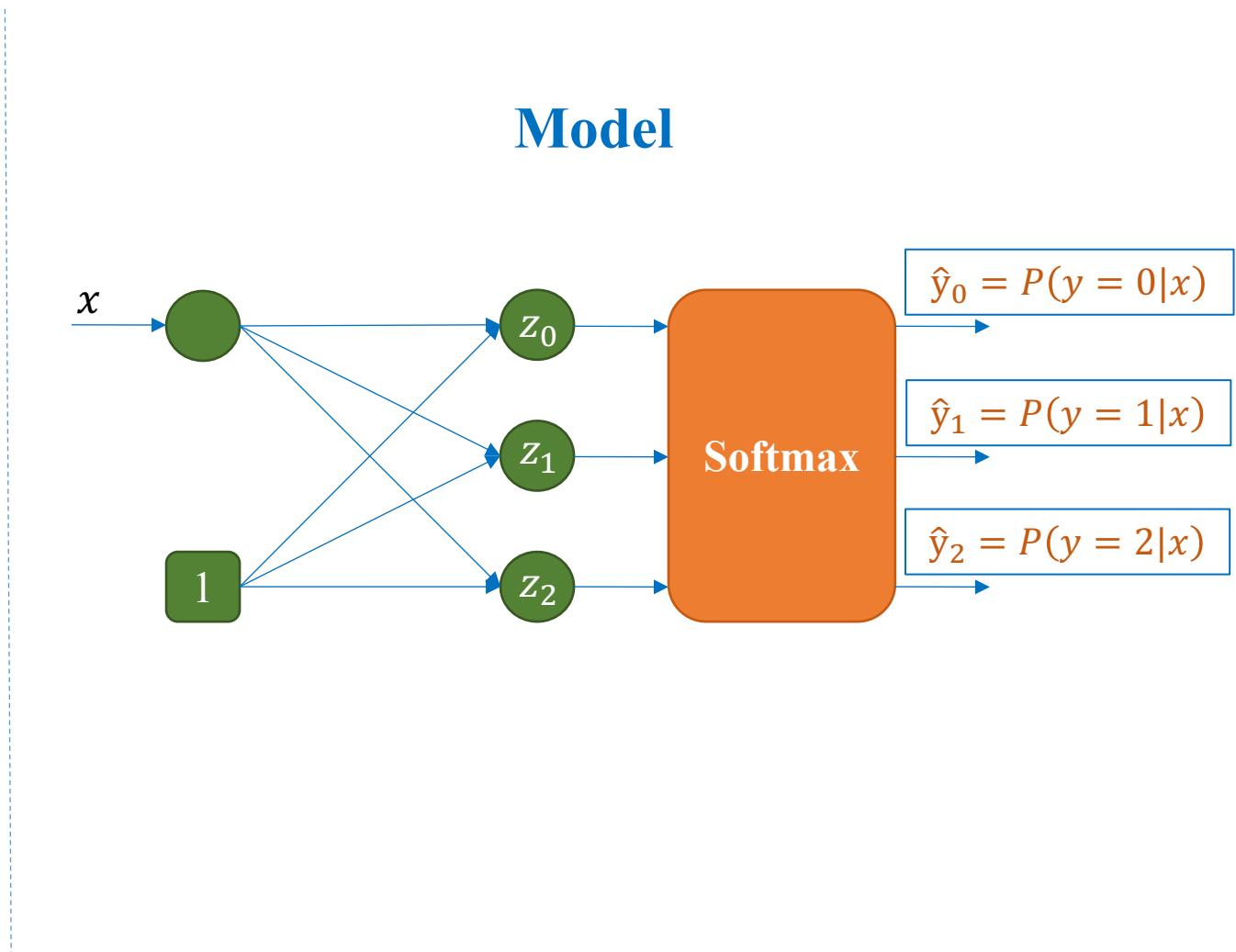
#feature=1

Feature is with one dimension

→ Need one node for input

Three categories

→ Need three nodes for output



Model Construction

❖ 4-D Feature and three classes

Feature	Label	
Petal_Length	Petal_Width	
1.4	0.2	0
1.4	0.2	0
1.3	0.2	0
4.5	1.5	1
4.9	1.5	1
4	1.3	1
4.5	1.7	2
6.3	1.8	2
5.8	1.8	2

#class=3

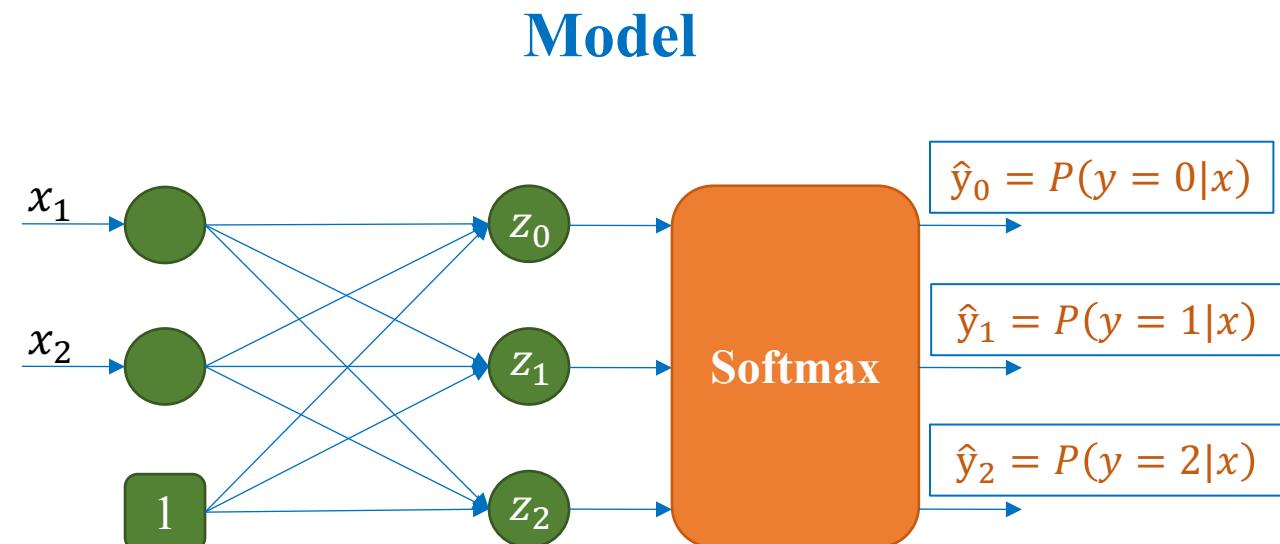
#feature=2

Feature is with two dimensions

→ Need two nodes for input

Three categories

→ Need three nodes for output



Model Construction

❖ 4-D Feature and three classes

Feature				Label
Sepal_Length	Sepal_Width	Petal_Length	Petal_Width	Label
5.1	3.5	1.4	0.2	0
4.9	3	1.4	0.2	0
4.7	3.2	1.3	0.2	0
6.4	3.2	4.5	1.5	1
6.9	3.1	4.9	1.5	1
5.5	2.3	4	1.3	1
4.9	2.5	4.5	1.7	2
7.3	2.9	6.3	1.8	2
6.7	2.5	5.8	1.8	2

Feature is with four dimensions

→ Need four nodes for input

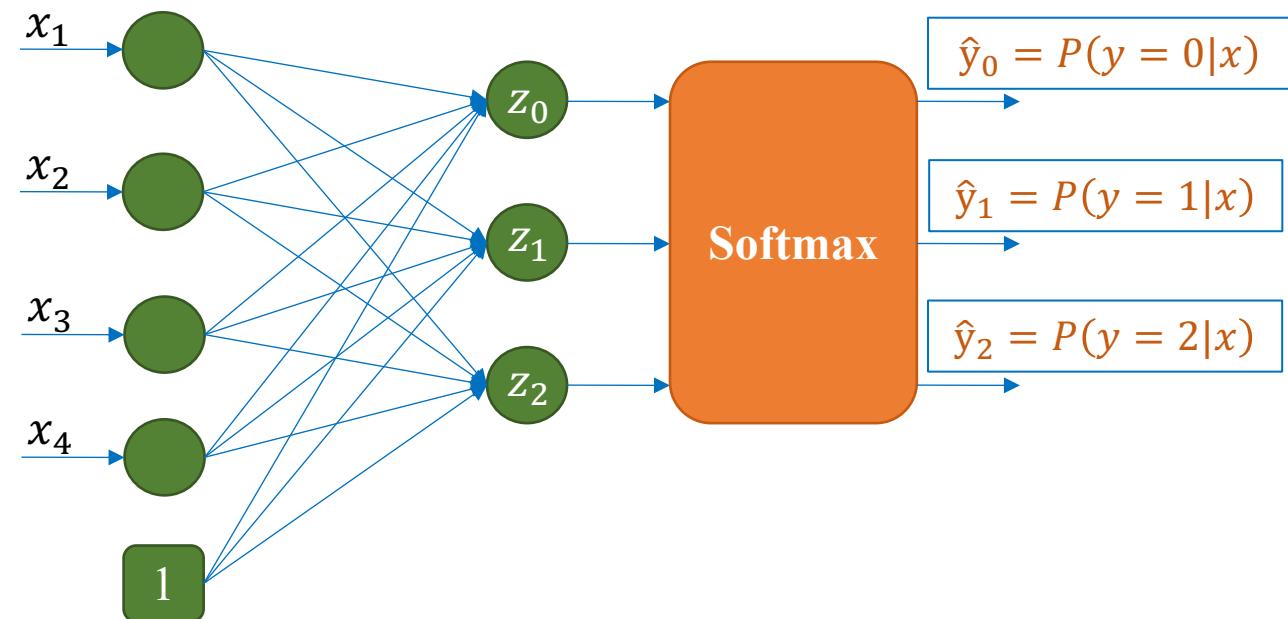
Three categories

→ Need three nodes for output

#class=3

#feature=4

Model



Outline

SECTION 1

Model Construction

SECTION 2

Cross-entropy Loss

SECTION 3

Implementation

1. Forward computation

$$\begin{aligned}\mathbf{z} &= \boldsymbol{\theta}^T \mathbf{x} \\ \hat{\mathbf{y}} &= \frac{e^{\mathbf{z}}}{\sum_{j=0}^1 e^{z_j}}\end{aligned}$$

2. Loss function

$$L(\boldsymbol{\theta}) = -\mathbf{y}^T \log \hat{\mathbf{y}}$$

3. Derivative

$$\begin{aligned}\frac{\partial L}{\partial w_i} &= \mathbf{x}(\hat{y}_i - y_i) & \frac{\partial L}{\partial b_i} &= \hat{y}_i - y_i\end{aligned}$$

$$\nabla_{\boldsymbol{\theta}} L = \mathbf{x}(\hat{\mathbf{y}} - \mathbf{y})^T$$

4. Update

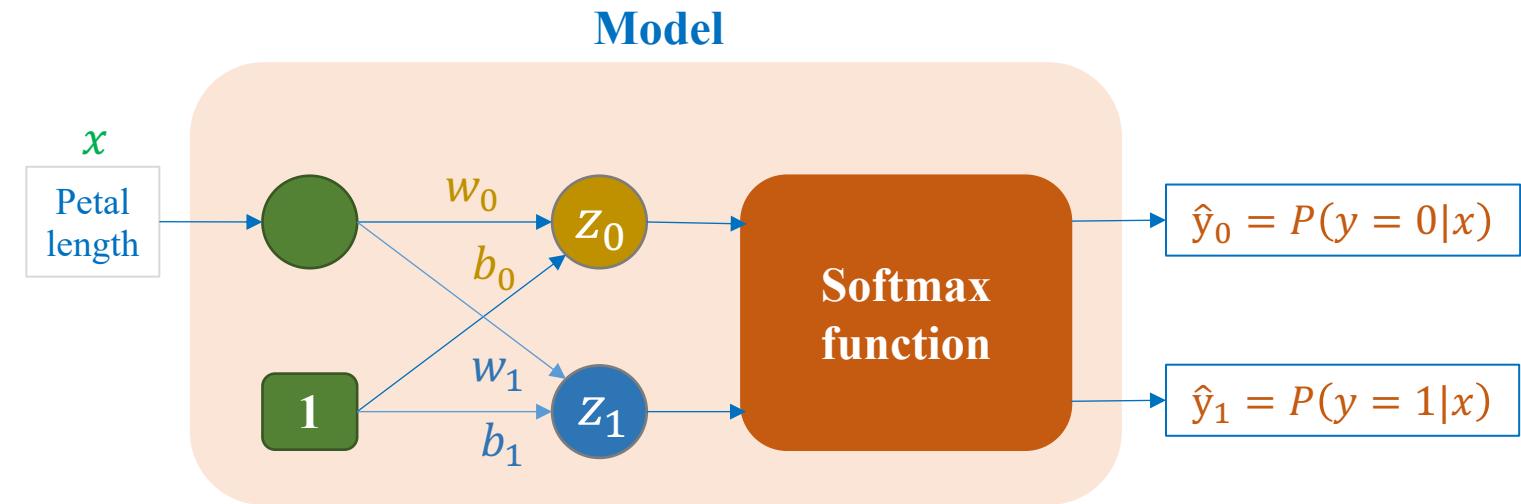
$$\boldsymbol{\theta} = \boldsymbol{\theta} - \eta \nabla_{\boldsymbol{\theta}} L$$

η is learning rate

Loss function

❖ Simple illustration

Feature	Label
Petal_Length	Category
1.4	0
1	0
1.5	0
3	1
3.8	1
4.1	1



One-hot encoding for label

$$y = 0 \rightarrow \mathbf{y} = [1 \quad 0]$$

$$y = 1 \rightarrow \mathbf{y} = [0 \quad 1]$$

scalar

vector

$$z_0 = xw_0 + b_0$$

$$z_1 = xw_1 + b_1$$

$$\hat{y}_0 = \frac{e^{z_0}}{\sum_{j=0}^1 e^{z_j}}$$

$$\hat{y}_1 = \frac{e^{z_1}}{\sum_{j=0}^1 e^{z_j}}$$

$$\mathbf{z} = \begin{bmatrix} z_0 \\ z_1 \end{bmatrix} = \begin{bmatrix} b_0 & w_0 \\ b_1 & w_1 \end{bmatrix} \begin{bmatrix} 1 \\ x \end{bmatrix} = \begin{bmatrix} \theta_0^T \\ \theta_1^T \end{bmatrix} \begin{bmatrix} 1 \\ x \end{bmatrix} = \boldsymbol{\theta}^T \mathbf{x}$$

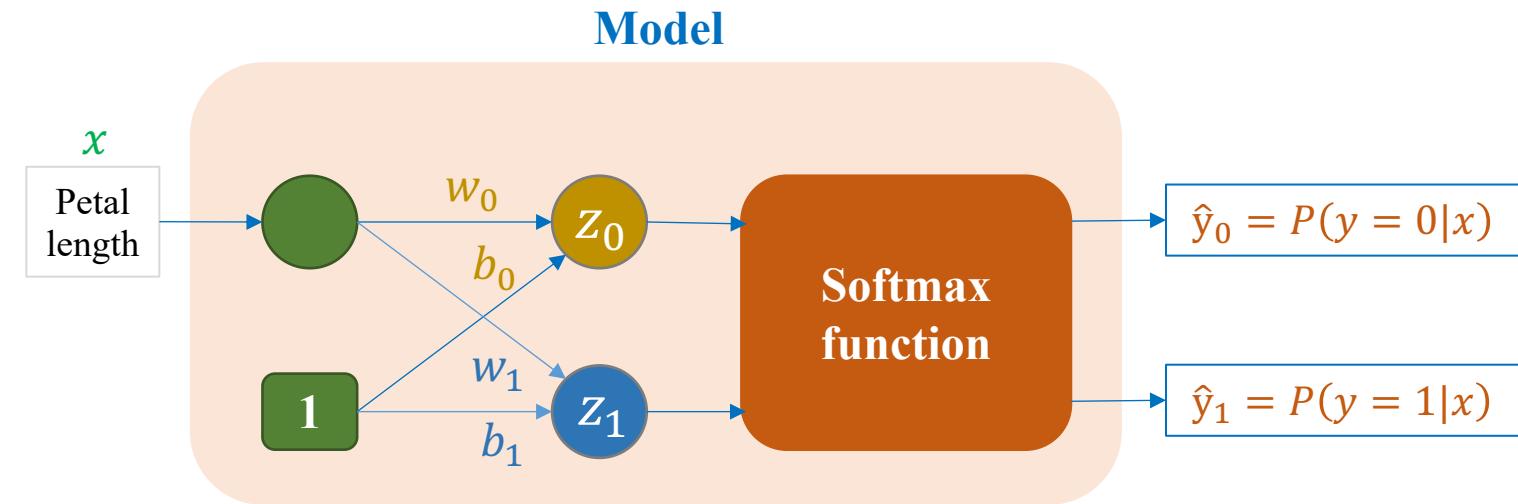
$$\hat{\mathbf{y}} = \begin{bmatrix} \hat{y}_0 \\ \hat{y}_1 \end{bmatrix} = \frac{1}{\sum_{j=0}^1 e^{z_j}} \begin{bmatrix} e^{z_0} \\ e^{z_1} \end{bmatrix} = \frac{e^{\mathbf{z}}}{\sum_{j=0}^1 e^{z_j}}$$

A vector is by default a column vector $\boldsymbol{\theta}_0 = \begin{bmatrix} b_0 \\ w_0 \end{bmatrix}$
 vector transpose $\boldsymbol{\theta}_0^T = [b_0 \quad w_0]$

Loss function

❖ Simple illustration

Feature	Label
Petal_Length	Category
1.4	0
1	0
1.5	0
3	1
3.8	1
4.1	1



One-hot encoding for label

$$y = 0 \rightarrow \mathbf{y} = [1 \ 0]$$

$$y = 1 \rightarrow \mathbf{y} = [0 \ 1]$$

scalar

vector

$$z_0 = xw_0 + b_0$$

$$z_1 = xw_1 + b_1$$

$$\hat{y}_0 = \frac{e^{z_0}}{\sum_{j=0}^1 e^{z_j}}$$

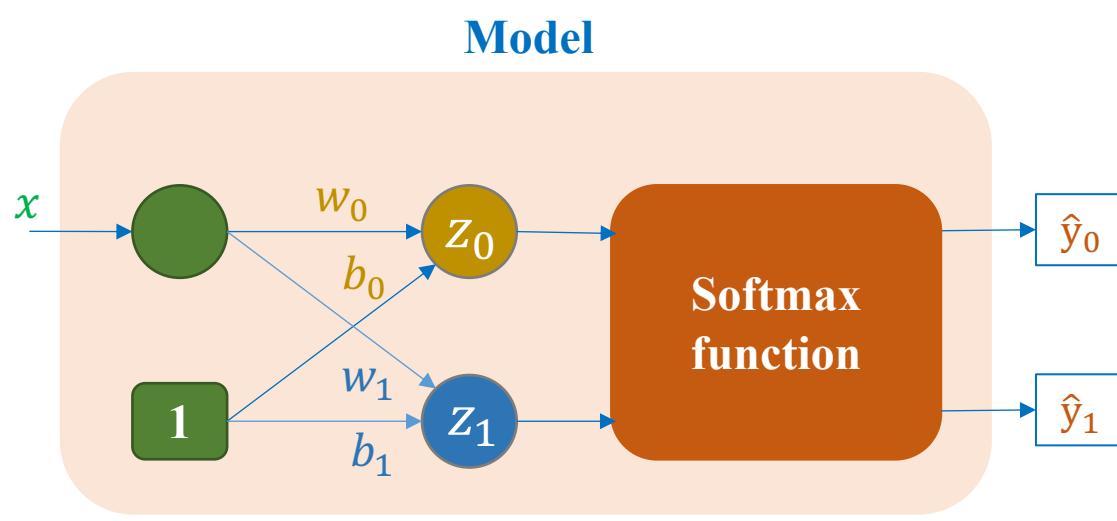
$$\hat{y}_1 = \frac{e^{z_1}}{\sum_{j=0}^1 e^{z_j}}$$

$$\mathbf{z} = \begin{bmatrix} z_0 \\ z_1 \end{bmatrix} = \begin{bmatrix} b_0 & w_0 \\ b_1 & w_1 \end{bmatrix} \begin{bmatrix} 1 \\ x \end{bmatrix} = \begin{bmatrix} \theta_0^T \\ \theta_1^T \end{bmatrix} \begin{bmatrix} 1 \\ x \end{bmatrix} = \boldsymbol{\theta}^T \mathbf{x}$$

$$\hat{\mathbf{y}} = \begin{bmatrix} \hat{y}_0 \\ \hat{y}_1 \end{bmatrix} = \frac{1}{\sum_{j=0}^1 e^{z_j}} \begin{bmatrix} e^{z_0} \\ e^{z_1} \end{bmatrix} = \frac{e^{\mathbf{z}}}{\sum_{j=0}^1 e^{z_j}}$$

$$L(\boldsymbol{\theta}) = -y_0 \log \hat{y}_0 - y_1 \log \hat{y}_1 = - \sum_{i=0}^1 y_i \log \hat{y}_i = -\mathbf{y}^T \log \hat{\mathbf{y}}$$

Loss function



$$L(\theta) = -y_0 \log \hat{y}_0 - y_1 \log \hat{y}_1 = -\sum_{i=0}^1 y_i \log \hat{y}_i = -\mathbf{y}^T \log \hat{\mathbf{y}}$$

$$\hat{y}_0 = \frac{e^{z_0}}{\sum_{j=0}^1 e^{z_j}}$$

$$\hat{y}_1 = \frac{e^{z_1}}{\sum_{j=0}^1 e^{z_j}}$$

Derivative

$$\frac{\partial \hat{y}_i}{\partial z_j} = \begin{cases} \hat{y}_i(1 - \hat{y}_i) & \text{if } i = j \\ -\hat{y}_i \hat{y}_j & \text{if } i \neq j \end{cases}$$

$$\begin{aligned} \frac{\partial L}{\partial z_i} &= -\sum_k y_k \frac{\partial \log(\hat{y}_k)}{\partial z_i} \\ &= -\sum_k y_k \frac{\partial \log(\hat{y}_k)}{\partial \hat{y}_k} \frac{\partial \hat{y}_k}{\partial z_i} \\ &= -\sum_k y_k \frac{1}{\hat{y}_k} \frac{\partial \hat{y}_k}{\partial z_i} \\ \\ \frac{\partial L}{\partial z_i} &= -y_i(1 - \hat{y}_i) - \sum_{k \neq i} y_k \frac{1}{\hat{y}_k} (-\hat{y}_k \hat{y}_i) \\ &= -y_i(1 - \hat{y}_i) + \sum_{k \neq i} y_k \hat{y}_i \\ &= -y_i + y_i \hat{y}_i + \sum_{k \neq i} y_k \hat{y}_i \\ &= \hat{y}_i \left(y_i + \sum_{k \neq i} y_k \right) - y_i \\ &= \hat{y}_i - y_i \end{aligned}$$

$$L(\theta) = -y_0 \log \hat{y}_0 - y_1 \log \hat{y}_1 = -\sum_{i=0}^1 y_i \log \hat{y}_i = -\mathbf{y}^T \log \hat{\mathbf{y}}$$

$$\hat{y}_0 = \frac{e^{z_0}}{\sum_{j=0}^1 e^{z_j}} \qquad \hat{y}_1 = \frac{e^{z_1}}{\sum_{j=0}^1 e^{z_j}}$$

$$L(\theta) = -y_0 \log \hat{y}_0 - y_1 \log \hat{y}_1 = -\sum_{i=0}^1 y_i \log \hat{y}_i = -\mathbf{y}^T \log \hat{\mathbf{y}}$$

$$\frac{\partial \hat{y}_i}{\partial z_j} = \begin{cases} \hat{y}_i(1-\hat{y}_i) & if \; i=j \\ -\hat{y}_i\hat{y}_j & if \; i \neq j \end{cases}$$

Loss function

One-hot encoding for label

$$y = 0 \rightarrow \mathbf{y}^T = [1 \ 0]$$

$$y = 1 \rightarrow \mathbf{y}^T = [0 \ 1]$$

↑ scalar ↑ vector

$$z_0 = xw_0 + b_0$$

$$z_1 = xw_1 + b_1$$

$$\hat{y}_0 = \frac{e^{z_0}}{\sum_{j=0}^1 e^{z_j}}$$

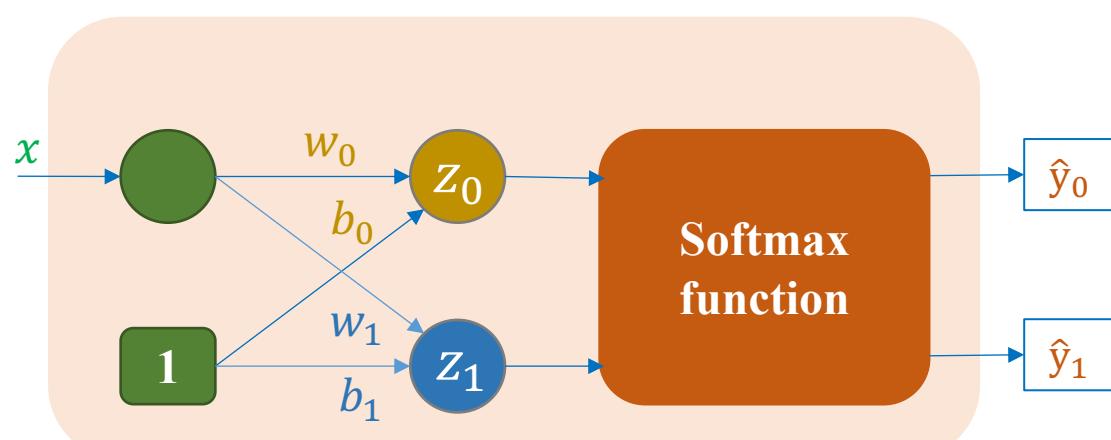
$$\hat{y}_1 = \frac{e^{z_1}}{\sum_{j=0}^1 e^{z_j}}$$

$$\mathbf{z} = \begin{bmatrix} z_0 \\ z_1 \end{bmatrix} = \begin{bmatrix} b_0 & w_0 \\ b_1 & w_1 \end{bmatrix} \begin{bmatrix} 1 \\ x \end{bmatrix} = \begin{bmatrix} \boldsymbol{\theta}_0^T \\ \boldsymbol{\theta}_1^T \end{bmatrix} \begin{bmatrix} 1 \\ x \end{bmatrix} = \boldsymbol{\theta}^T \mathbf{x}$$

$$\hat{\mathbf{y}} = \begin{bmatrix} \hat{y}_0 \\ \hat{y}_1 \end{bmatrix} = \frac{1}{\sum_{j=0}^1 e^{z_j}} \begin{bmatrix} e^{z_0} \\ e^{z_1} \end{bmatrix} = \frac{e^{\mathbf{z}}}{\sum_{j=0}^1 e^{z_j}}$$

$$L(\boldsymbol{\theta}) = - \sum_{i=0}^1 y_i \log \hat{y}_i = -\mathbf{y}^T \log \hat{\mathbf{y}}$$

Model



$$\frac{\partial L}{\partial \hat{y}_i} = -\frac{y_i}{\hat{y}_i}$$

$$\frac{\partial \hat{y}_i}{\partial z_j} = \begin{cases} \hat{y}_i(1 - \hat{y}_i) & \text{if } i = j \\ -\hat{y}_i \hat{y}_j & \text{if } i \neq j \end{cases}$$

$$\frac{\partial L}{\partial z_i} = \hat{y}_i - y_i$$

Derivative

$$\frac{\partial L}{\partial w_i} = x(\hat{y}_i - y_i)$$

$$\frac{\partial L}{\partial b_i} = \hat{y}_i - y_i$$

Simple Illustration - Summary

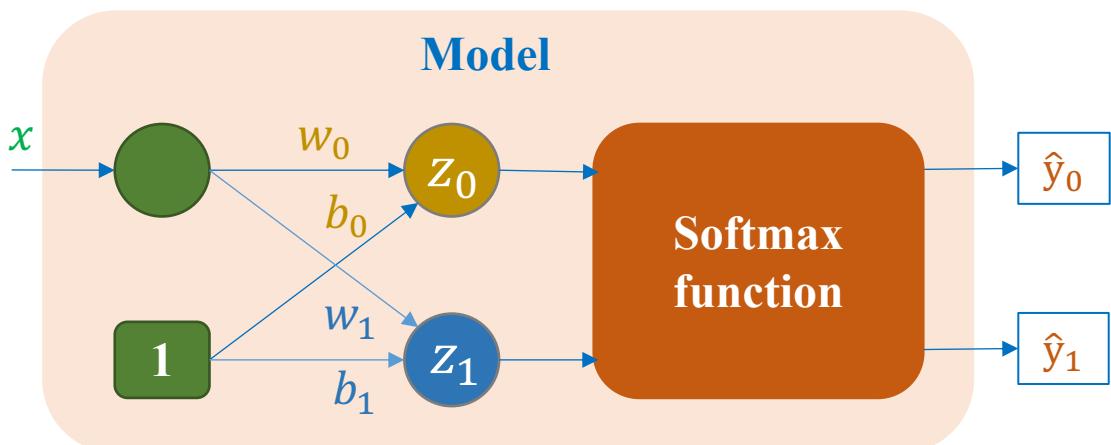
Feature	Label
Petal_Length	Category
1.4	0
1	0
1.5	0
3	1
3.8	1
4.1	1

One-hot encoding for label

$$y = 0 \rightarrow \mathbf{y}^T = [1 \ 0]$$

$$y = 1 \rightarrow \mathbf{y}^T = [0 \ 1]$$

scalar vector



$$\boldsymbol{\theta} = \begin{bmatrix} b_0 & b_1 \\ w_0 & w_1 \end{bmatrix}$$

$$\mathbf{x} = \begin{bmatrix} 1 \\ x \end{bmatrix}$$

1. Forward computation

$$\mathbf{z} = \boldsymbol{\theta}^T \mathbf{x}$$

$$\hat{\mathbf{y}} = \frac{e^{\mathbf{z}}}{\sum_{j=0}^1 e^{z_j}}$$

2. Loss function

$$L(\boldsymbol{\theta}) = -\mathbf{y}^T \log \hat{\mathbf{y}}$$

3. Derivative

$$\frac{\partial L}{\partial w_i} = \mathbf{x}(\hat{y}_i - y_i)$$

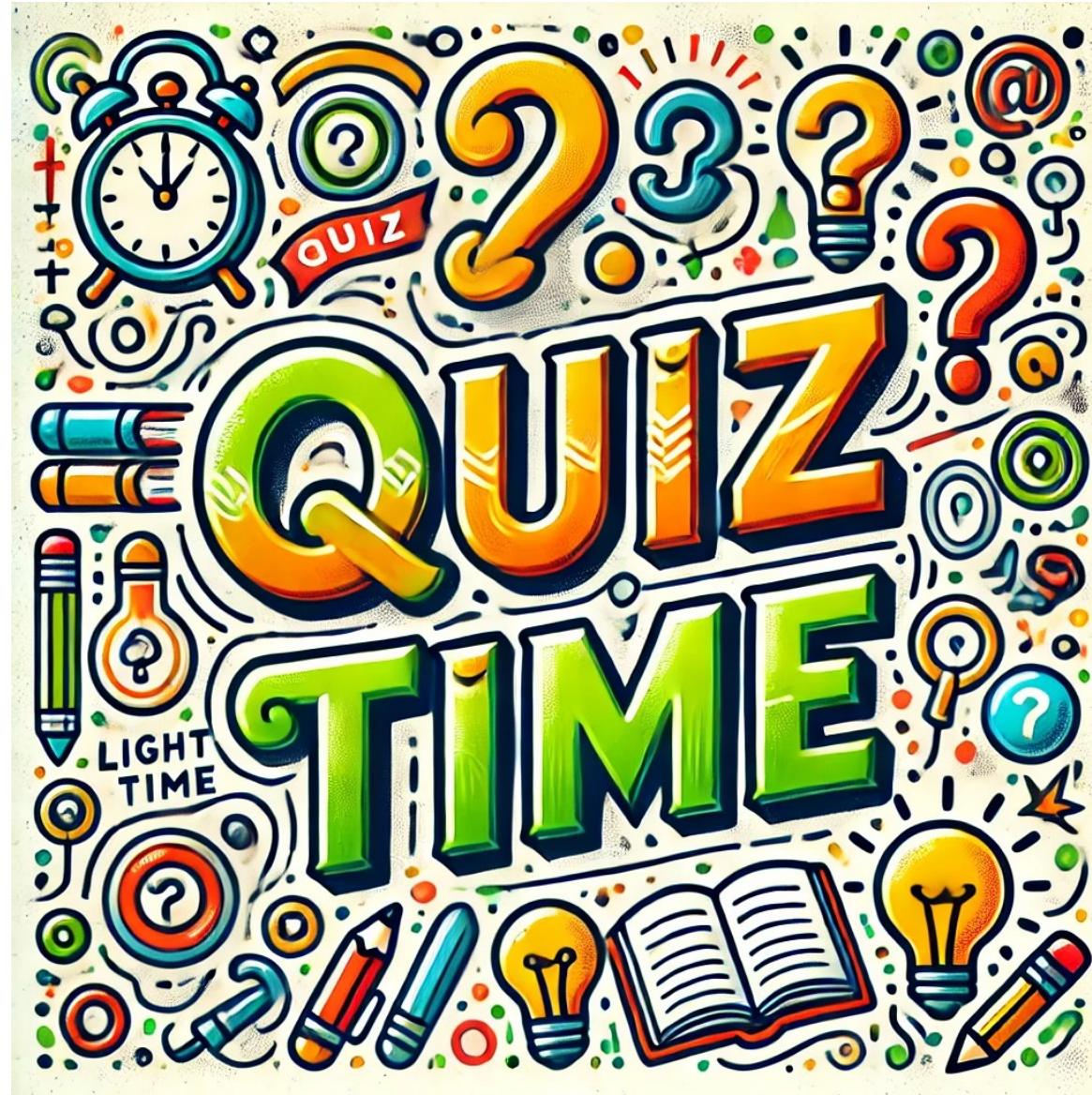
$$\frac{\partial L}{\partial b_i} = \hat{y}_i - y_i$$

$$\nabla_{\boldsymbol{\theta}} L = \mathbf{x}(\hat{\mathbf{y}} - \mathbf{y})^T$$

4. Update

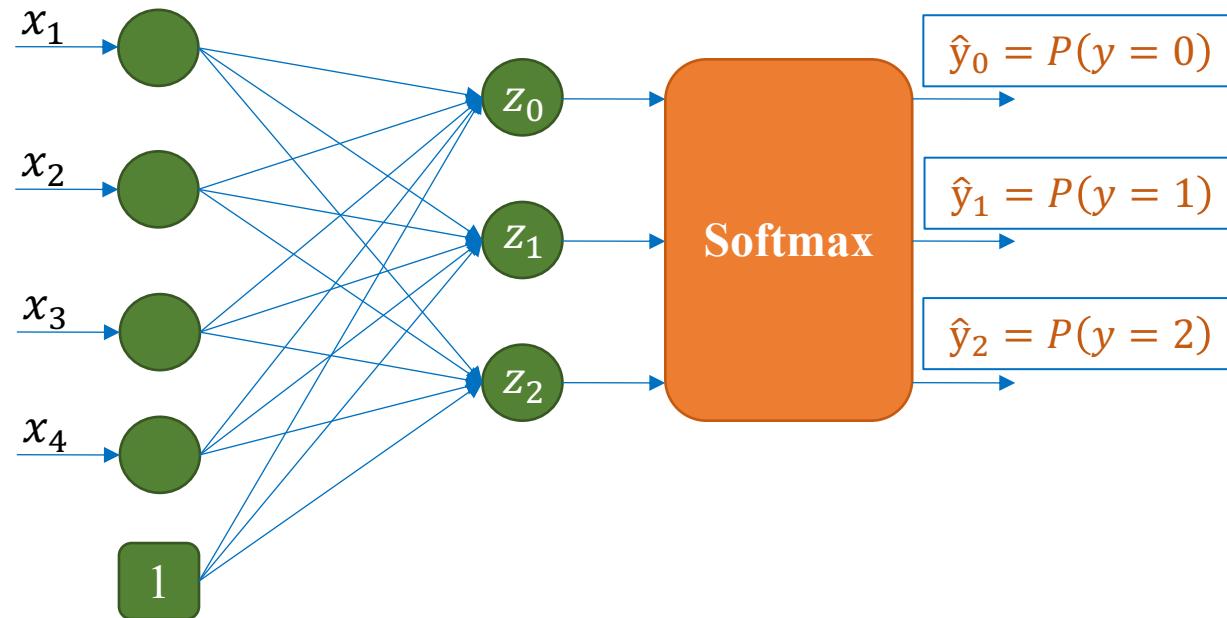
$$\boldsymbol{\theta} = \boldsymbol{\theta} - \eta \nabla_{\boldsymbol{\theta}} L$$

η is learning rate



Question 1

❖ Mô hình sau có bao nhiêu tham số (tham số của model)?



- a) 3 tham số
- b) 5 tham số
- c) 12 tham số
- d) 15 tham số

Question 2

❖ Độ dài của vector y (vector label sau khi thực thi(en) bước one-hot encoding) là bao nhiêu?

Feature	Label
Petal_Length	
1.4	0
1.3	0
1.5	0
4.5	1
4.1	1
4.6	1
5.2	2
5.6	2
5.9	2

a) length=1

b) length=2

c) length=3

d) length=4

Question 3

- ❖ Hàm loss sau là tổng của 10 thành phần (phân loại cho 10 category). Với sample thuộc category thứ 3, hàm loss này thực chất sẽ là tổng của bao nhiêu thành phần?

$$L(\theta) = - \sum_{i=0}^9 y_i \log \hat{y}_i$$

Hàm loss trên là tổng của 10 thành phần (phân loại cho 10 category)

- a) Của 1 thành phần
- b) Của 2 thành phần
- c) Của 3 thành phần
- d) Không xác định

Question 4

❖ Shape của biến result là gì?

```
data1 = np.array([1, 2]).reshape(2, 1)
data2 = np.array([3, 4]).reshape(2, 1)
result = data1.dot(data2.T)
print(result)
```

- a) shape=(2, 1)
- b) shape=(1, 2)
- c) shape=(2, 2)
- d) Chương trình báo lỗi

Question 5

❖ Hàm delta được định nghĩa thế nào để hai hàm loss sau tương đồng?

$$L(\boldsymbol{\theta}) = - \sum_{i=1}^2 \delta(i, y) \log \hat{y}_i \quad L(\boldsymbol{\theta}) = - \sum_{i=0}^1 y_i \log \hat{y}_i$$

W1

$$\delta(i, j) = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}$$

W2

$$\delta(i, j) = \begin{cases} 0 & \text{if } i = j \\ 1 & \text{if } i \neq j \end{cases}$$

- a) Chỉ W1 đúng
- b) Chỉ W2 đúng
- c) Cả W1 và W2 đều đúng
- d) Cả W1 và W2 đều sai

Question 6

❖ Cài đặt nào chạy cho kết quả đúng cho hàm loss sau?

$$L(.) = -\mathbf{y}^T \log \hat{\mathbf{y}}$$

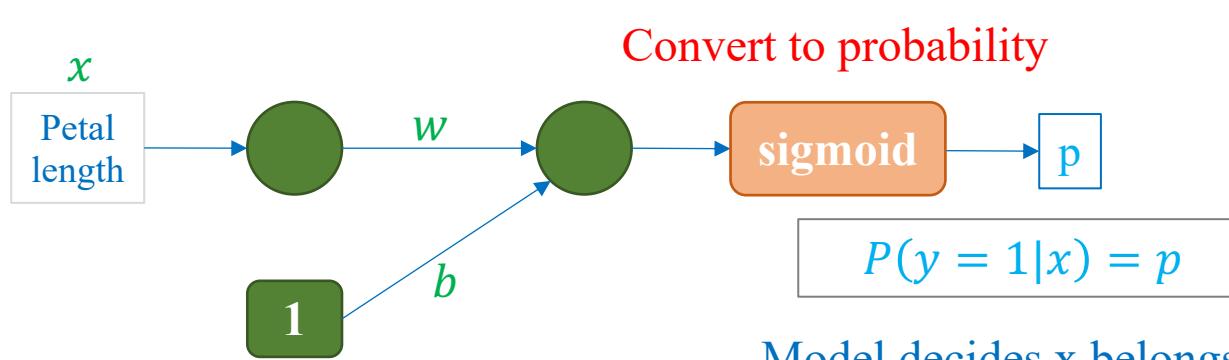
```
L1 = -y.T.dot(np.log(y_hat))  
L2 = -np.log(y.T.dot(y_hat))
```

- a) Chỉ L1 đúng
- b) Chỉ L2 đúng
- c) Cả L1 và L2 đều đúng
- d) Cả L1 và L2 đều sai

Different viewpoint of Cross-entropy

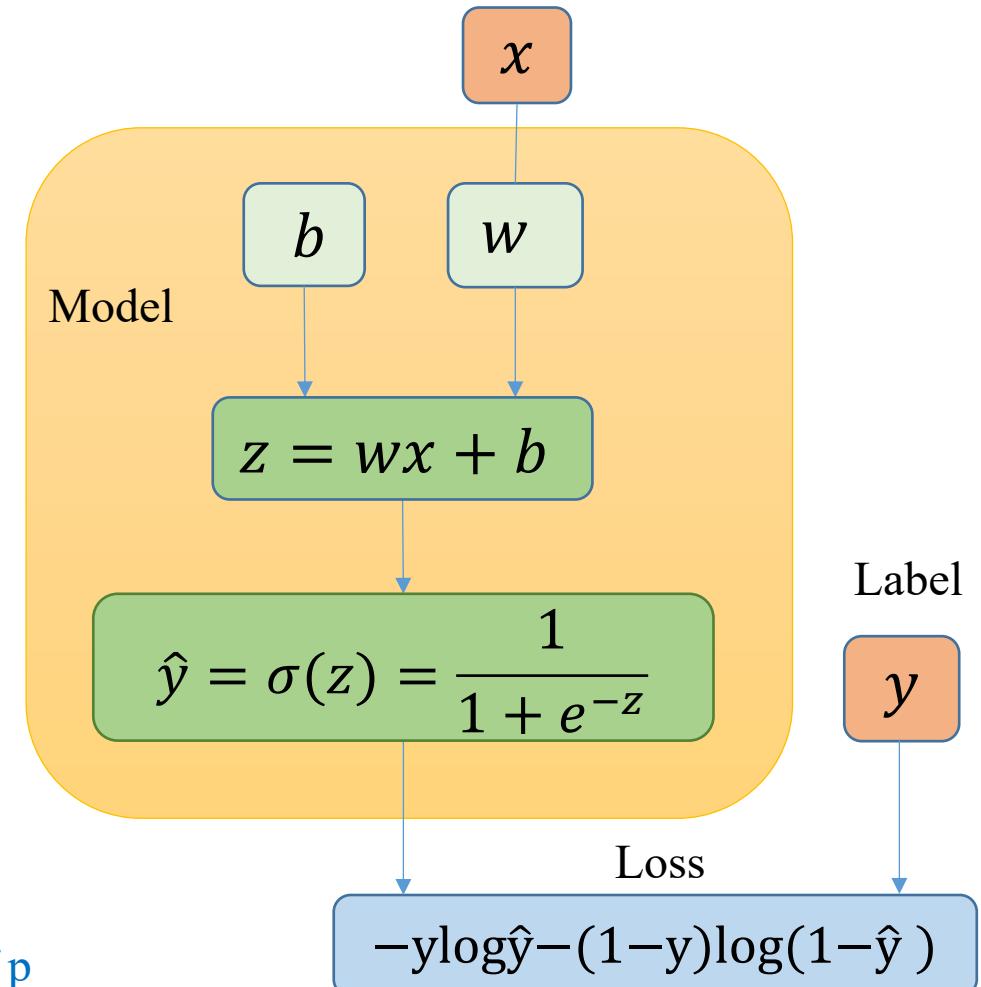
Motivation

Feature	Label
Petal_Length	Label
1.4	0
1.3	0
1.5	0
4.5	1
4.1	1
4.6	1



Model decides x belongs to the category (label=1) with the belief of p

Implicitly conclude that $P(y = 0|x) = 1 - p$



Outputs of Model

Feature Label

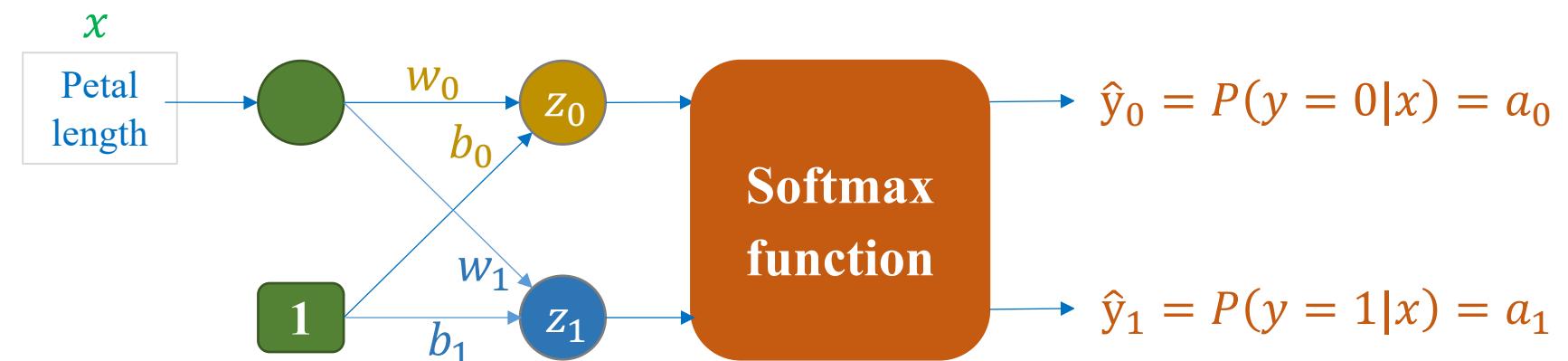
Petal_Length	Label
1.4	0
1.3	0
1.5	0
4.5	1
4.1	1
4.6	1

Softmax function

$$\hat{y}_i = \frac{e^{z_i}}{\sum_j e^{z_j}}$$

$$0 \leq f(z_i) \leq 1$$

$$\sum_i f(z_i) = 1$$



Explicitly output $P(y = 1|x)$ and $P(y = 0|x)$

For a Given Sample

Feature	Label
Petal_Length	Label
1.4	0
1.3	0
1.5	0
4.5	1
4.1	1
4.6	1

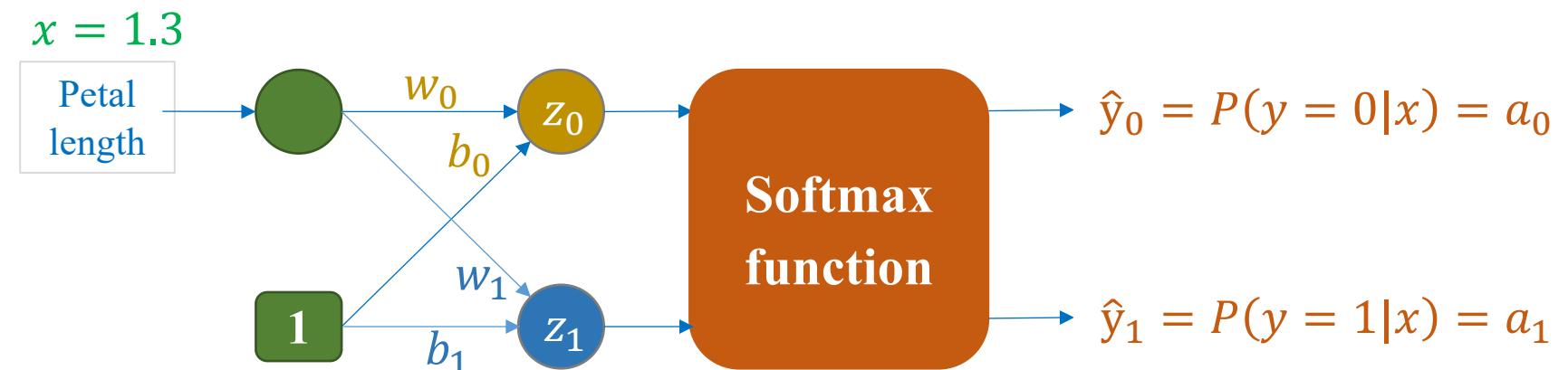
Softmax function

$$\hat{y}_i = \frac{e^{z_i}}{\sum_j e^{z_j}}$$

$$0 \leq f(z_i) \leq 1$$

$$\sum_i f(z_i) = 1$$

Given a sample ($x = 1.3, y = 0$)

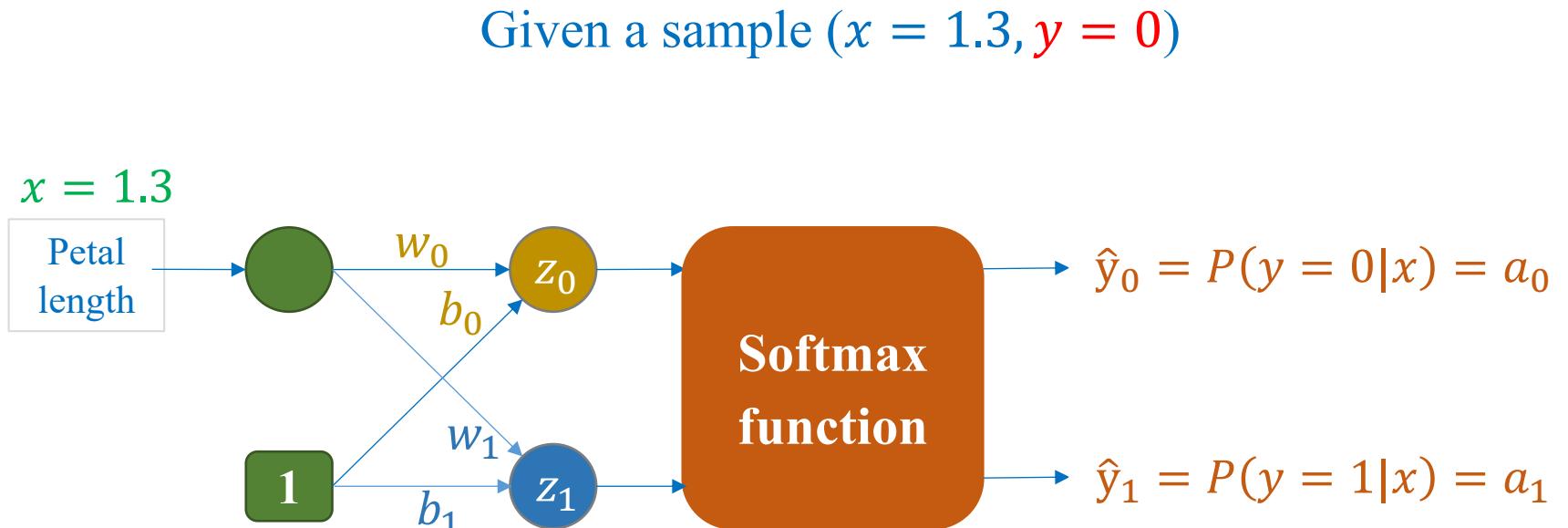


With $(x = 1.3, y = 0)$, model becomes better when a_0 increases and a_1 decreases

Differences between increasing a_0 and decreasing a_1 ?

For a Given Sample

Feature	Label
Petal_Length	Label
1.4	0
1.3	0
1.5	0
4.5	1
4.1	1
4.6	1



With ($x = 1.3, y = 0$), model becomes better when a_0 increases and a_1 decreases

Softmax function

$$\hat{y}_i = \frac{e^{z_i}}{\sum_j e^{z_j}}$$

$$0 \leq f(z_i) \leq 1$$

$$\sum_i f(z_i) = 1$$

Increasing a_0 : $\hat{y}_0 = \frac{e^{z_0}}{e^{z_0} + e^{z_1}} \rightarrow$

increasing z_0
decreasing z_1

Decreasing a_1 : $\hat{y}_1 = \frac{e^{z_1}}{e^{z_0} + e^{z_1}} \rightarrow$

increasing z_0
decreasing z_1

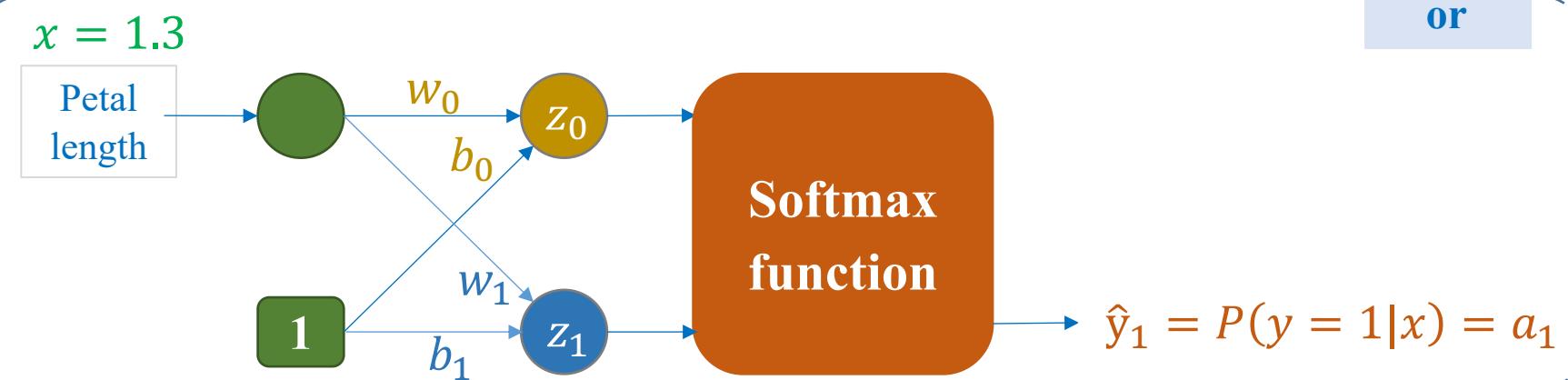
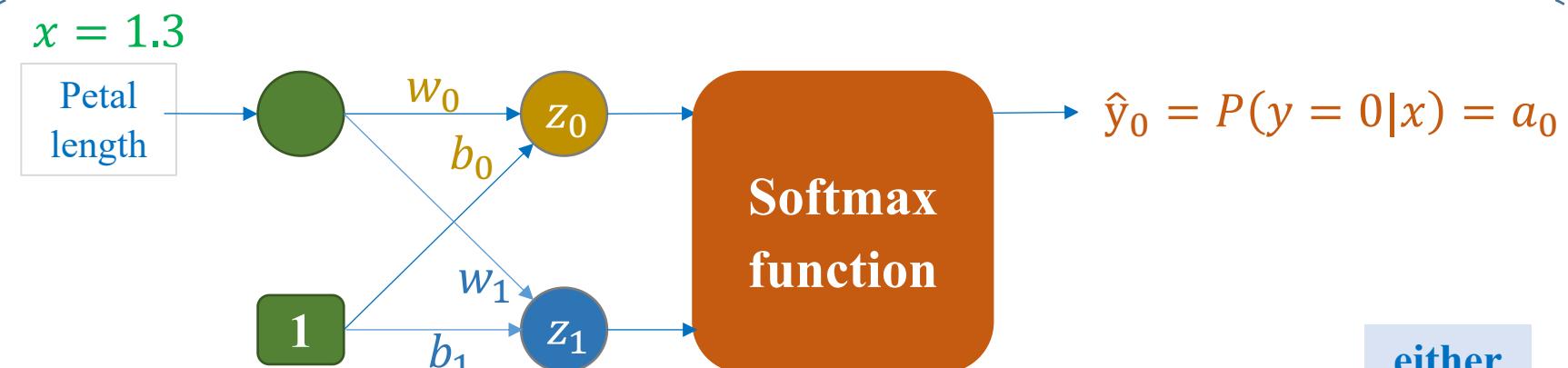
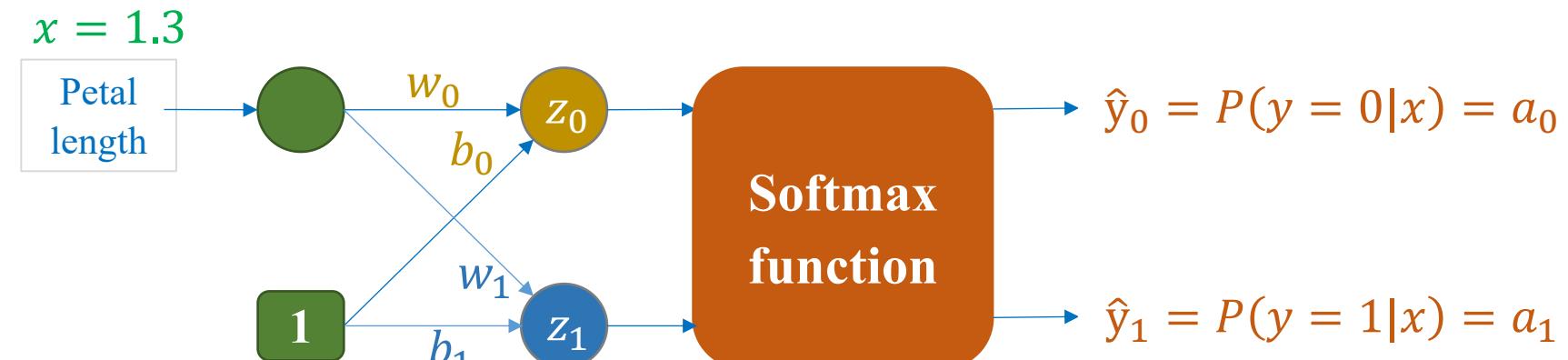
Observation

Feature Label

Petal_Length	Label
1.4	0
1.3	0
1.5	0
4.5	1
4.1	1
4.6	1

With $(x = 1.3, y = 0)$, model becomes better when a_0 increases and a_1 decreases

→ increasing z_0
decreasing z_1



either

or

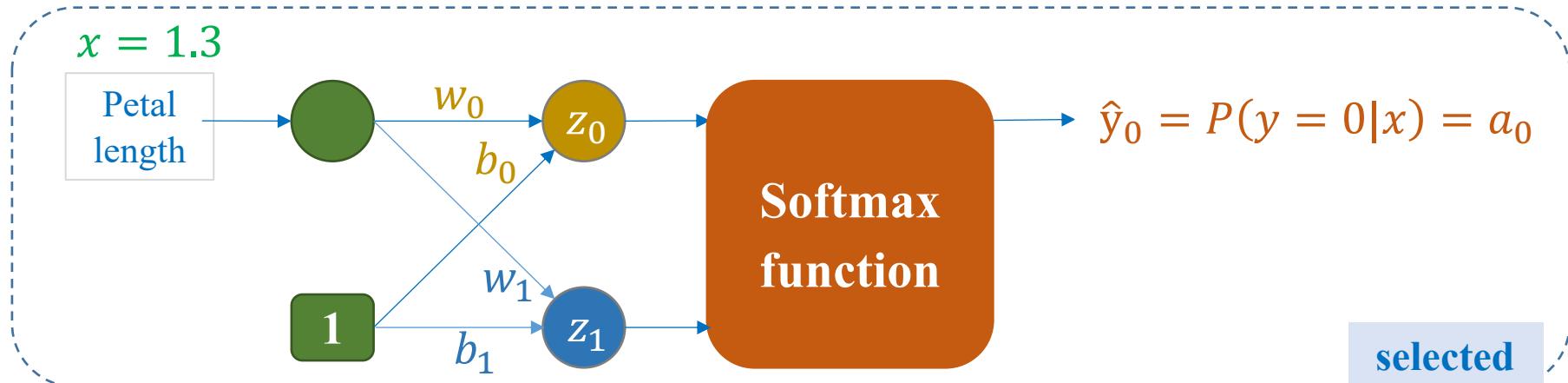
Loss Computation

Feature Label

Petal_Length	Label
1.4	0
1.3	0
1.5	0
4.5	1
4.1	1
4.6	1

With $(x = 1.3, y = 0)$, model becomes better when a_0 increases and a_1 decreases

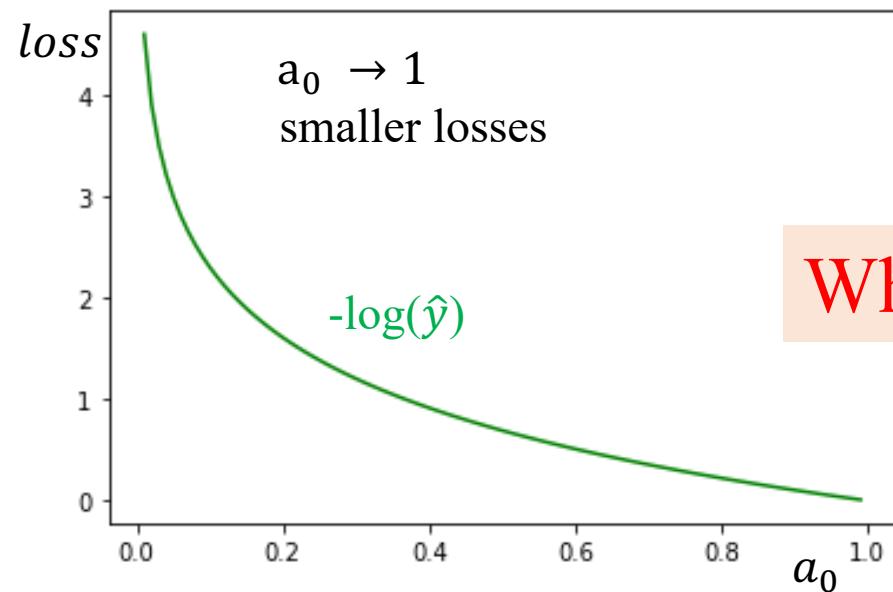
→ increasing z_0
decreasing z_1



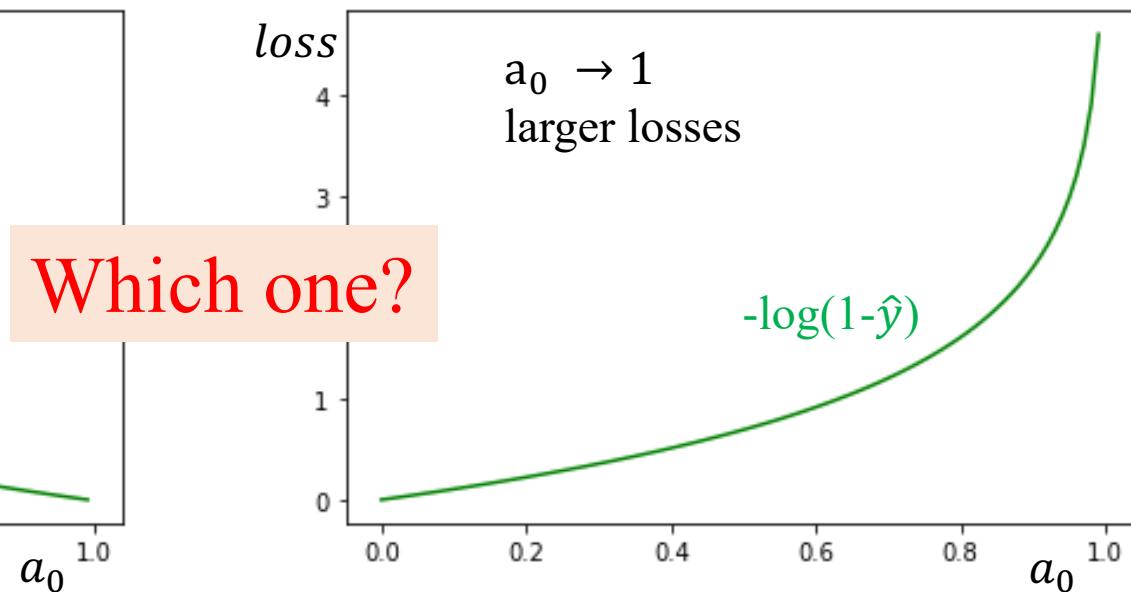
$$a_0 \in [0,1]$$

When $a_0 = 0$, the model (or θ) is worst

When $a_0 = 1$, the model (or θ) is perfect



Which one?



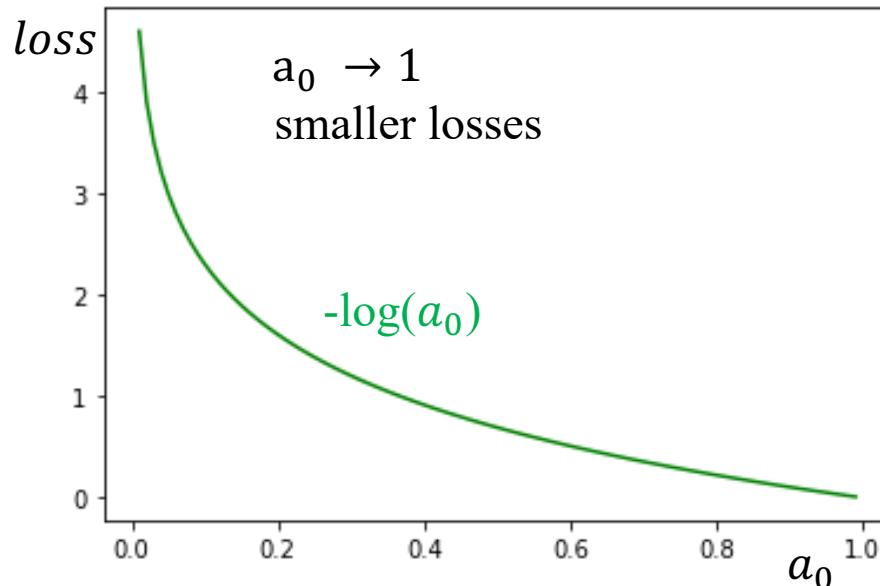
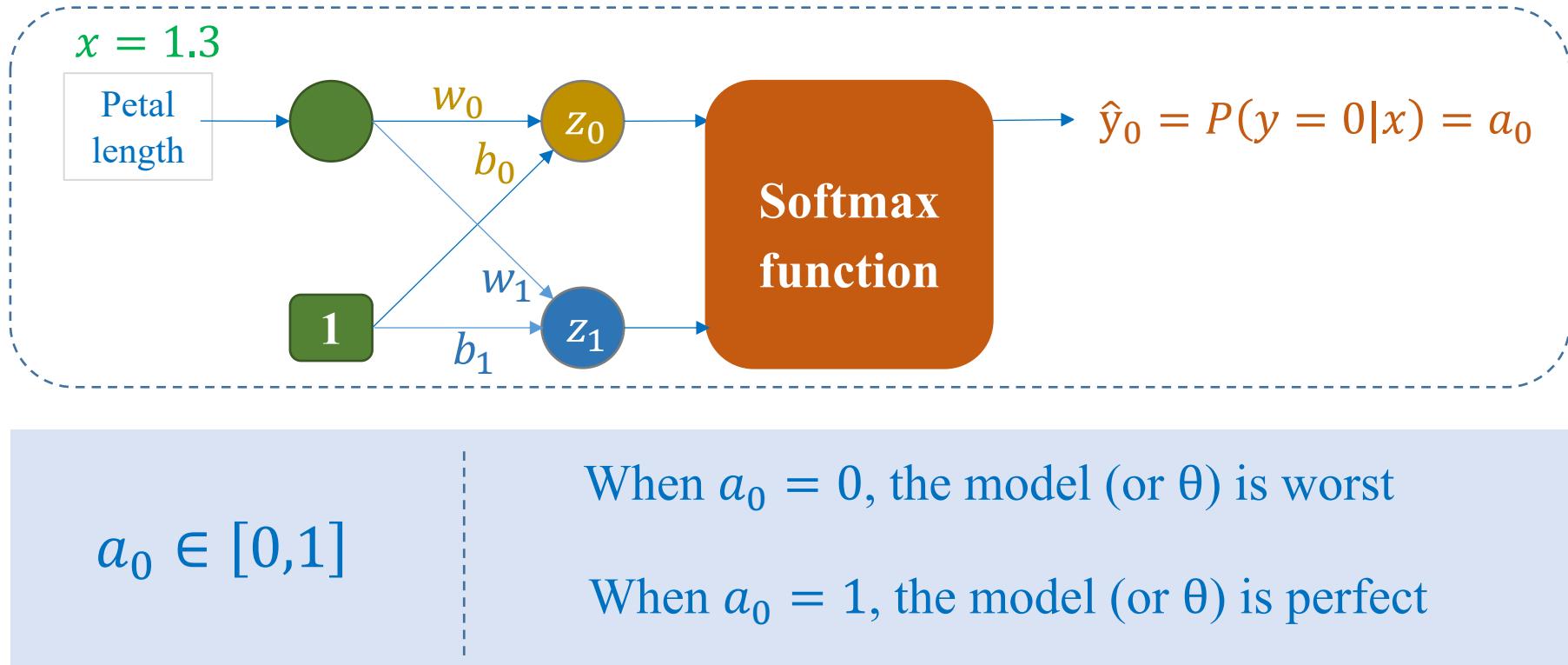
Loss Computation

Feature Label

Petal_Length	Label
1.4	0
1.3	0
1.5	0
4.5	1
4.1	1
4.6	1

With $(x = 1.3, y = 0)$, model becomes better when a_0 increases and a_1 decreases

→ increasing z_0
decreasing z_1



Loss function

$$L(\theta) = -\log(\hat{y}_0)$$

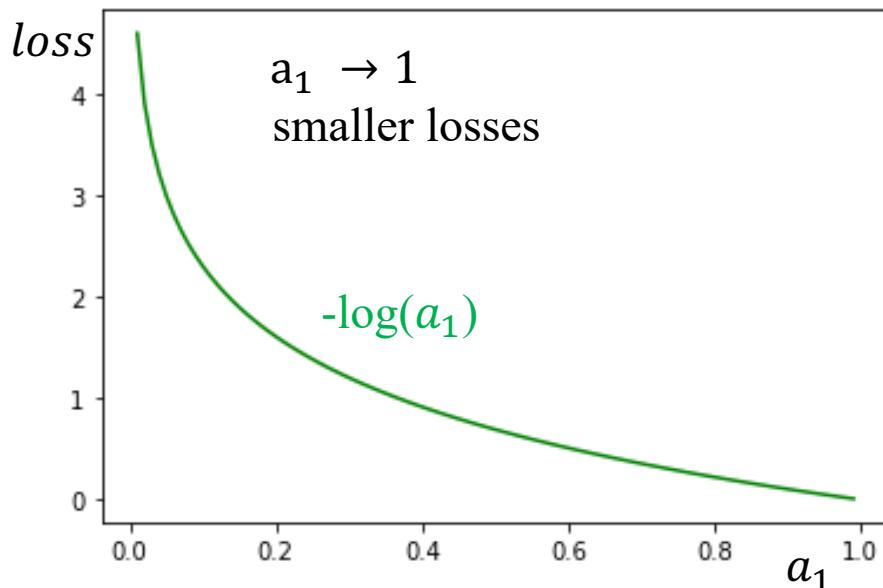
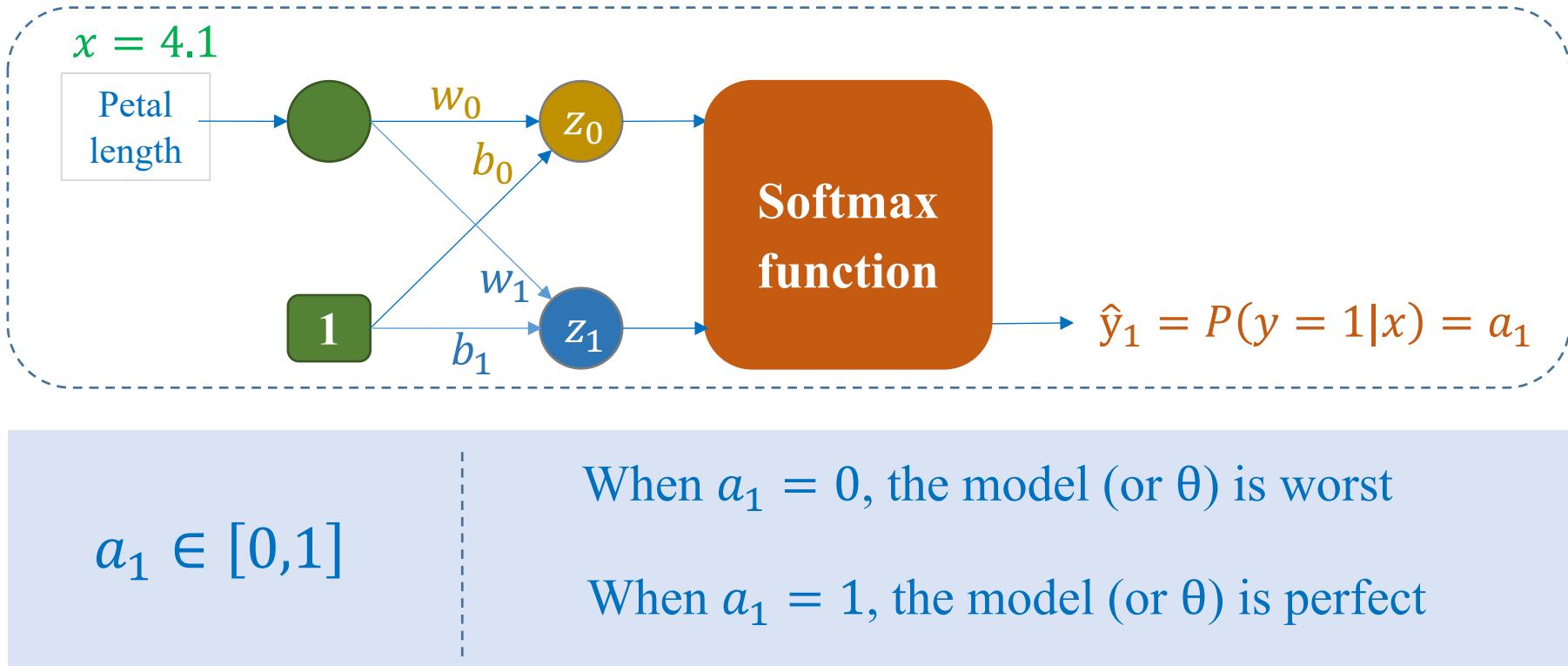
Another Sample

Feature Label

Petal_Length	Label
1.4	0
1.3	0
1.5	0
4.5	1
4.1	1
4.6	1

With $(x = 4.1, y = 1)$, model becomes better when a_1 increases and a_0 decreases

→ increasing z_1
decreasing z_0

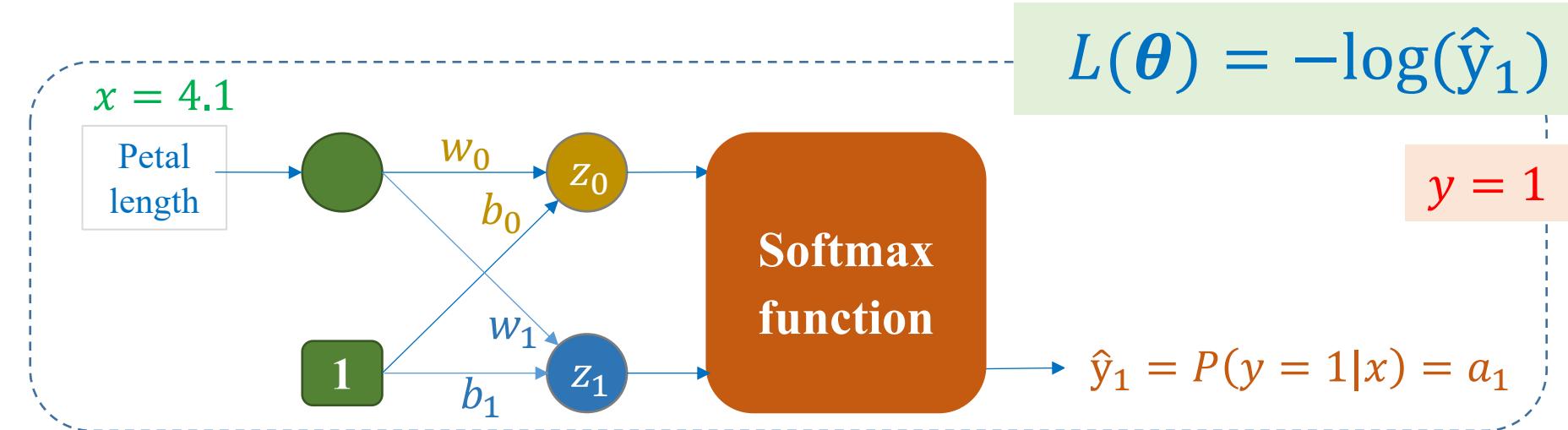
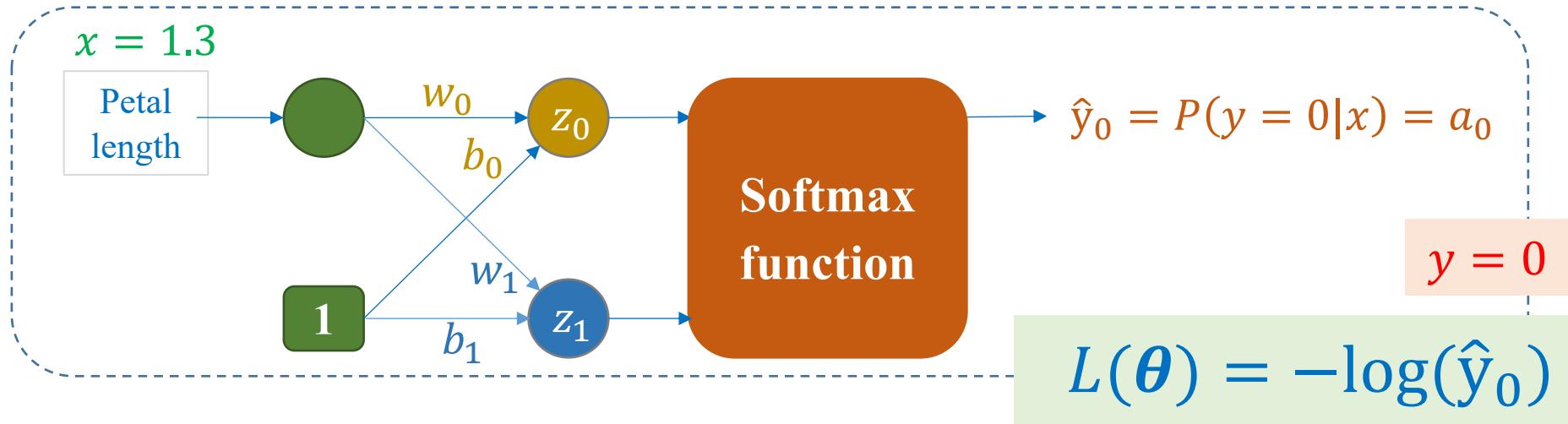


Loss function

$$L(\theta) = -\log(\hat{y}_1)$$

Observation

Feature	Label
Petal_Length	Label
1.4	0
1.3	0
1.5	0
4.5	1
4.1	1
4.6	1



With $(x = \dots, y = ?)$,
model becomes better
when $a_?$ increases

Loss function

$$L(\theta) = -y \log \hat{y}_1 - (1-y) \log \hat{y}_0$$

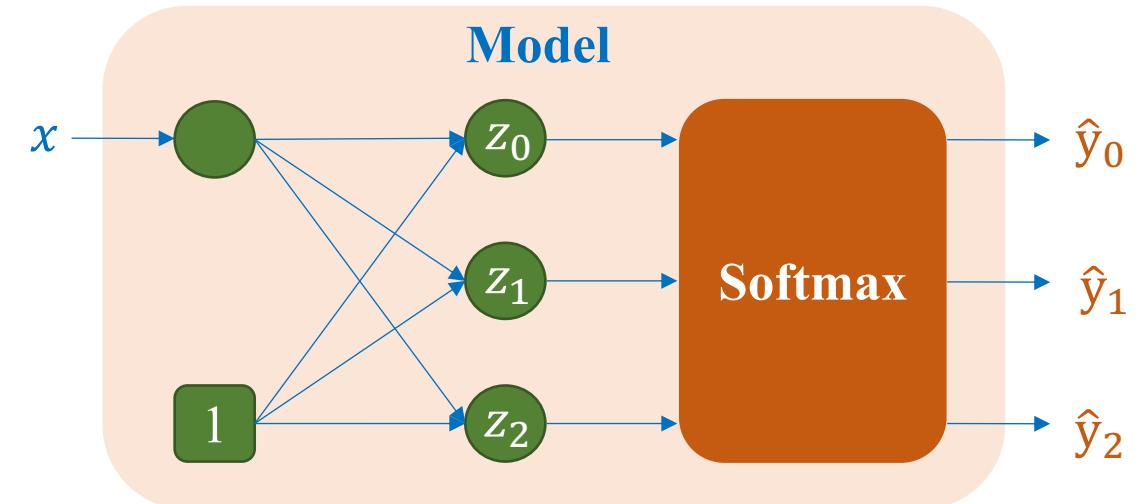
What about 3+ classes?

Feature	Label
Petal_Length	Label
1.4	0
1.3	0
1.5	0
4.5	1
4.1	1
4.6	1
5.2	2
5.6	2
5.9	2

#features = 1

#classes = 3

$y \in \{0,1,2\}$



$$y = 0 \rightarrow L(\theta) = -\log(\hat{y}_0)$$

$$y = 1 \rightarrow L(\theta) = -\log(\hat{y}_1)$$

$$y = 2 \rightarrow L(\theta) = -\log(\hat{y}_2)$$

How to convert into a single function?

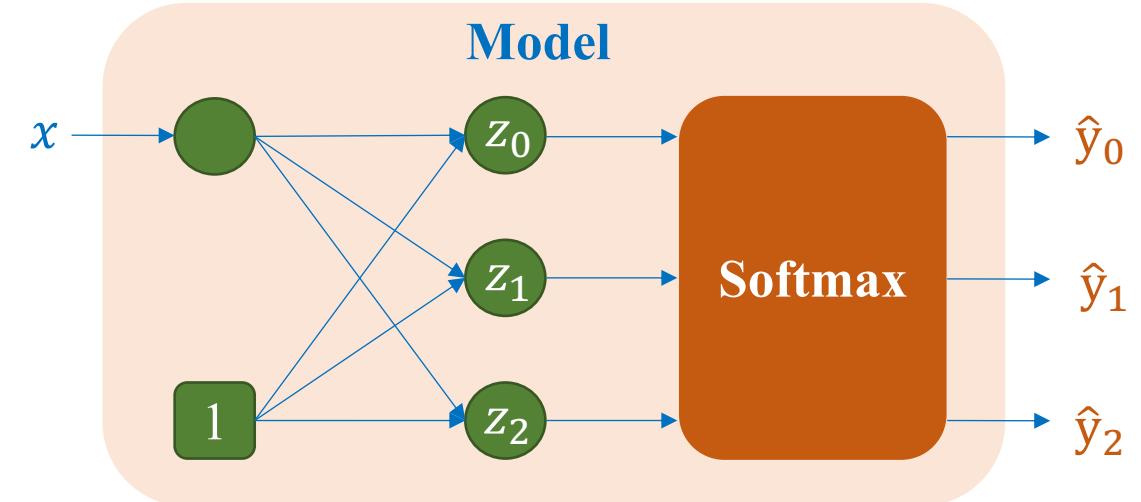
A Suggested Function

Feature	Label
Petal_Length	Label
1.4	0
1.3	0
1.5	0
4.5	1
4.1	1
4.6	1
5.2	2
5.6	2
5.9	2

#features = 1

#classes = 3

$y \in \{0,1,2\}$



$$L(\theta) = -\frac{y(1-y)}{-2} \log(\hat{y}_2) - y(2-y)\log(\hat{y}_1) - (1-y)\left(\frac{2-y}{2}\right)\log(\hat{y}_0)$$

$y = 2$ $y = 1$ $y = 0$

Ok! but awkward!!! ... and how to improve?

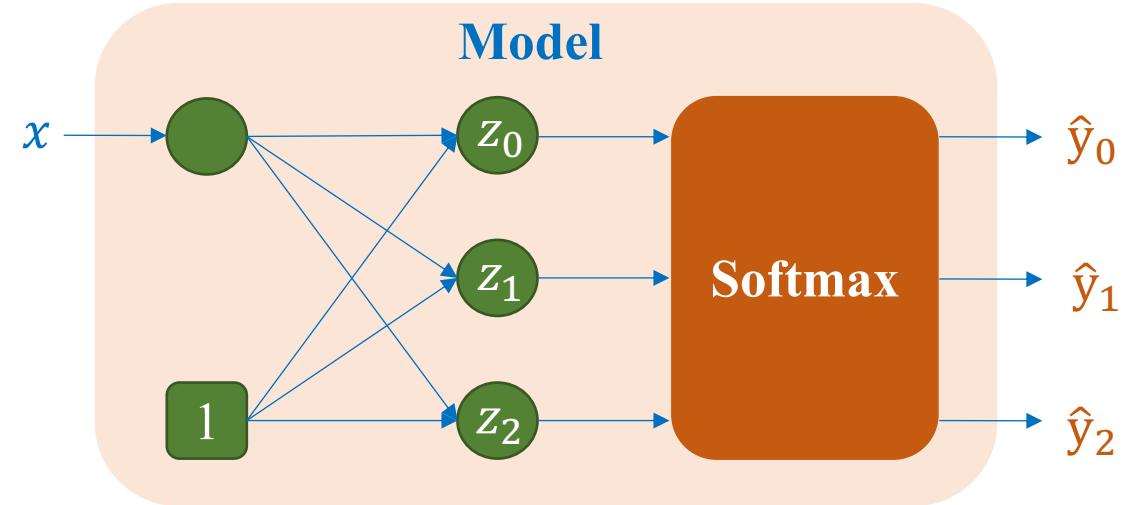
Using One-Hot Encoding

Feature	Label
Petal_Length	Label
1.4	0
1.3	0
1.5	0
4.5	1
4.1	1
4.6	1
5.2	2
5.6	2
5.9	2

#features = 1

#classes = 3

$$y \in \{0,1,2\}$$



One-hot encoding for label

$$\mathbf{y} = \begin{bmatrix} y_0 \\ y_1 \\ y_2 \end{bmatrix} \quad y_i \in \{0,1\} \quad \sum_i y_i = 1$$

$$y = 0 \rightarrow \mathbf{y} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \quad y = 1 \rightarrow \mathbf{y} = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \quad y = 2 \rightarrow \mathbf{y} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

Loss function

$$\begin{aligned} L(\boldsymbol{\theta}) &= -y_2 \log(\hat{y}_2) - y_1 \log(\hat{y}_1) - y_0 \log(\hat{y}_0) \\ &= - \sum_i y_i \log(\hat{y}_i) \end{aligned}$$

Petal_Length	Label
1.4	0
1.3	0
1.5	0
4.5	1
4.1	1
4.6	1

$$x = \begin{bmatrix} 1 \\ x \end{bmatrix}$$

$$\theta = \begin{bmatrix} b_0 & b_1 \\ w_0 & w_1 \end{bmatrix}$$

One-hot encoding for label

$$y = 0 \rightarrow \mathbf{y}^T = \begin{bmatrix} y_0 & y_1 \end{bmatrix} = [1 \ 0]$$

$$y = 1 \rightarrow \mathbf{y}^T = [0 \ 1]$$

scalar vector

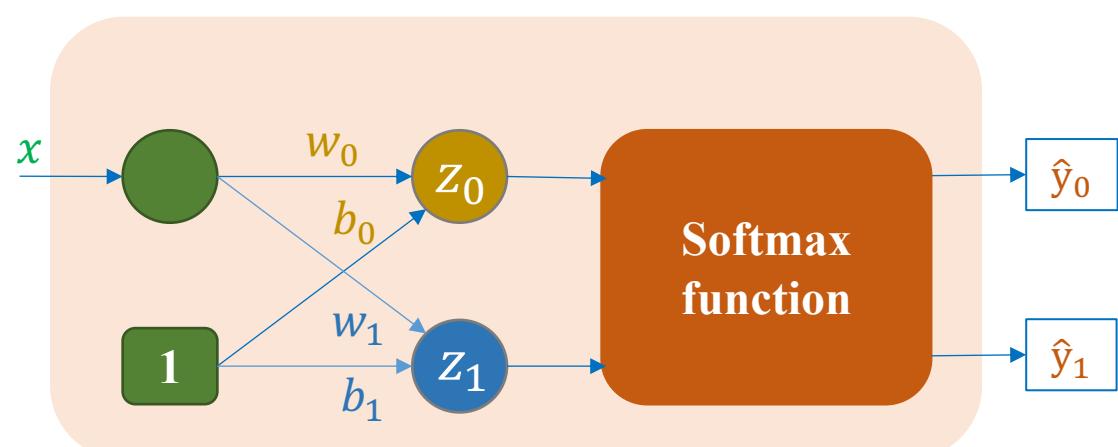
Summary

$$\mathbf{z} = \begin{bmatrix} z_0 \\ z_1 \end{bmatrix} = \begin{bmatrix} b_0 & w_0 \\ b_1 & w_1 \end{bmatrix} \begin{bmatrix} 1 \\ x \end{bmatrix} = \begin{bmatrix} \theta_0^T \\ \theta_1^T \end{bmatrix} \begin{bmatrix} 1 \\ x \end{bmatrix} = \theta^T x$$

$$\hat{\mathbf{y}} = \begin{bmatrix} \hat{y}_0 \\ \hat{y}_1 \end{bmatrix} = \frac{1}{\sum_{j=0}^1 e^{z_j}} \begin{bmatrix} e^{z_0} \\ e^{z_1} \end{bmatrix} = \frac{e^{\mathbf{z}}}{\sum_{j=0}^1 e^{z_j}}$$

$$L(\theta) = - \sum_{i=0}^1 y_i \log \hat{y}_i = -\mathbf{y}^T \log \hat{\mathbf{y}}$$

Model



$$\frac{\partial L}{\partial \hat{y}_i} = -\frac{y_i}{\hat{y}_i}$$

$$\frac{\partial \hat{y}_i}{\partial z_j} = \begin{cases} \hat{y}_i(1 - \hat{y}_i) & \text{if } i = j \\ -\hat{y}_i \hat{y}_j & \text{if } i \neq j \end{cases}$$

$$\frac{\partial L}{\partial z_i} = \hat{y}_i - y_i$$

Derivative

$$\frac{\partial L}{\partial w_i} = x(\hat{y}_i - y_i)$$

$$\frac{\partial L}{\partial b_i} = \hat{y}_i - y_i$$

Outline

SECTION 1

Model Construction

SECTION 2

Cross-entropy Loss

SECTION 3

Implementation

```
# compute z
z = theta.T.dot(xi)

# compute y_hat
exp_z = np.exp(z)
y_hat = exp_z / np.sum(exp_z, axis=0)

# compute the loss
loss = -yi.T.dot(np.log(y_hat))
losses.append(loss[0])

# compute the gradient dz
dz = y_hat - yi

# compute dtheta
dtheta = xi.dot(dz.T)

# update
theta = theta - learning_rate*dtheta
```

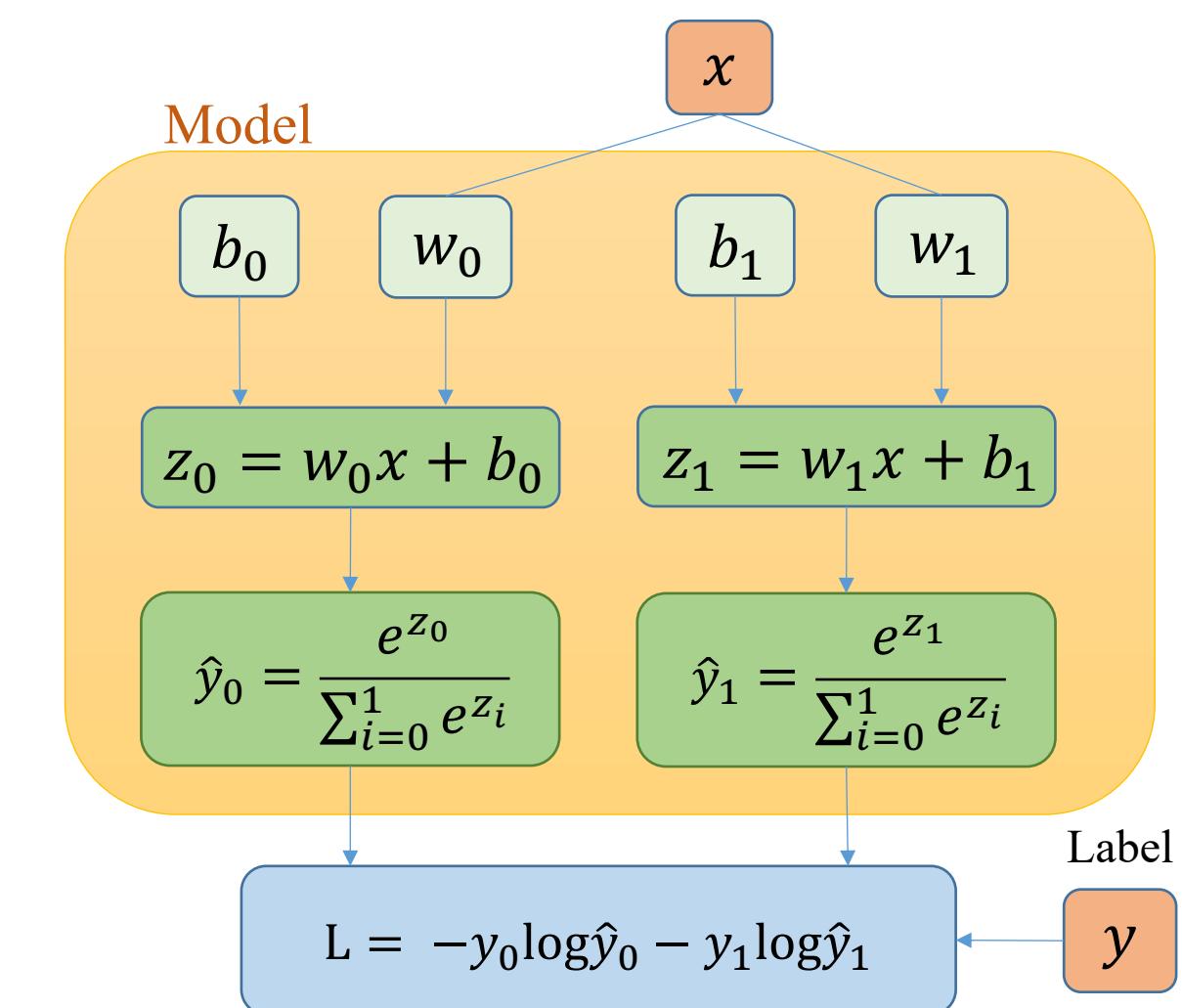
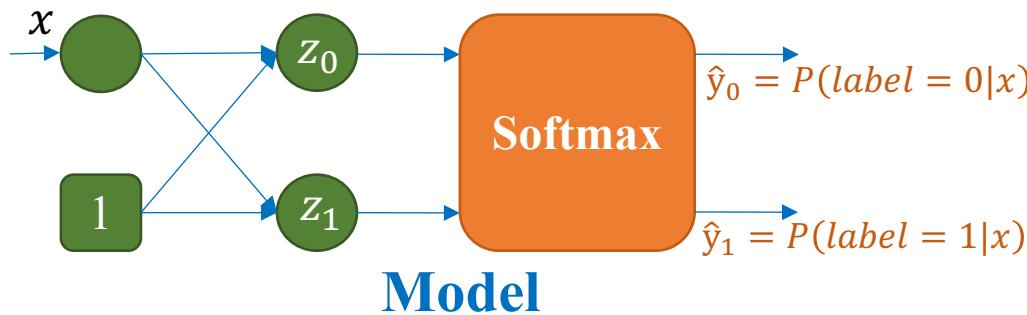
Softmax Regression – Naïve

Training data

Feature	Label	
Petal_Length	Label	
1.4	0	Category A
1.3	0	
1.5	0	
4.5	1	Category B
4.1	1	
4.6	1	

One-hot encoding for labels

$$\begin{aligned} y = 0 &\rightarrow \mathbf{y}^T = [1, 0] \\ y = 1 &\rightarrow \mathbf{y}^T = [0, 1] \end{aligned}$$



Softmax Regression - Naïve

Training data

Feature	Label
Petal_Length	Label
1.4	0
1.3	0
1.5	0
4.5	1
4.1	1
4.6	1

#class=2

#feature=1

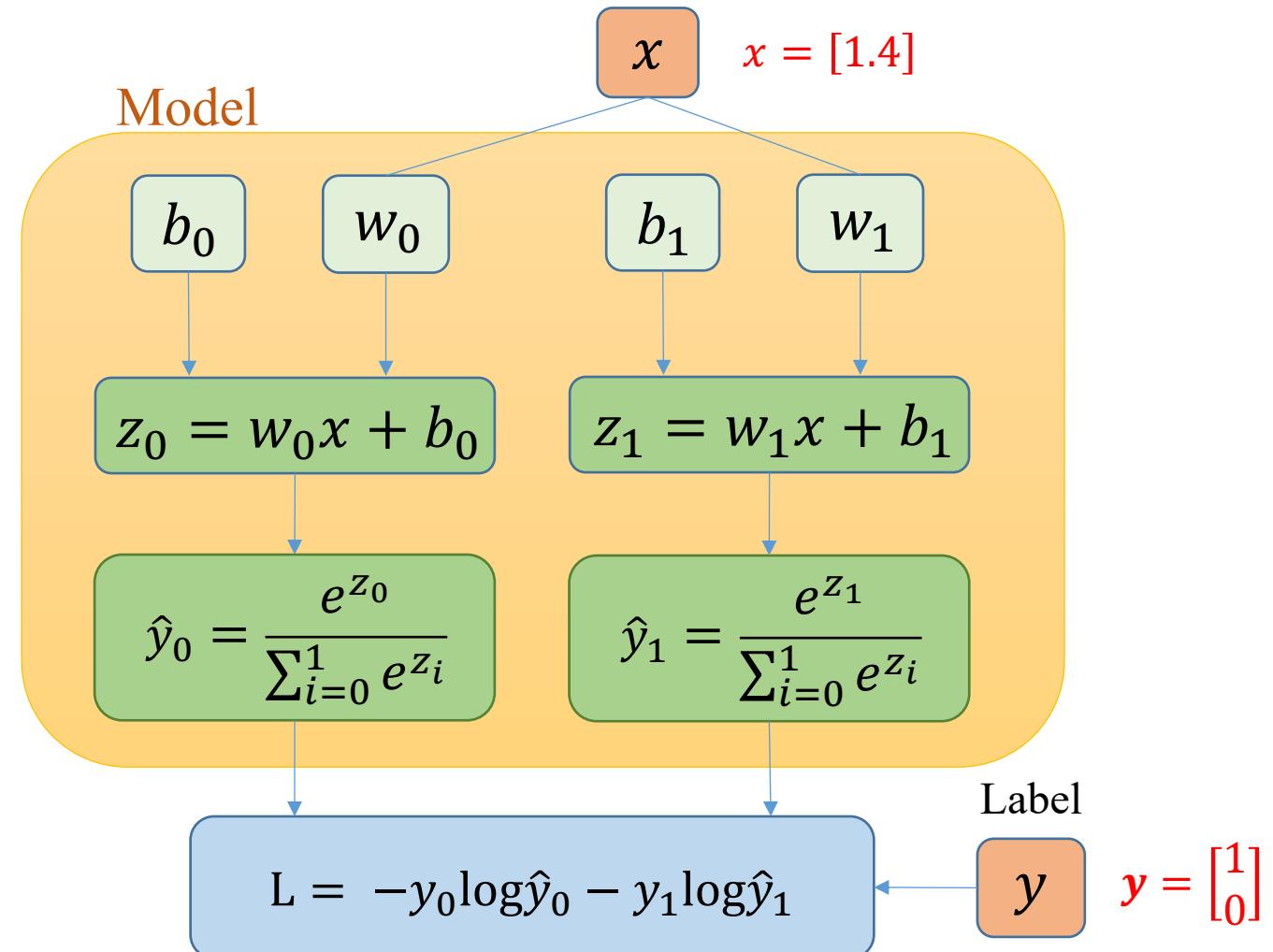
One-hot encoding for label

$$y = 0 \rightarrow \mathbf{y}^T = [y_0 \ y_1]$$

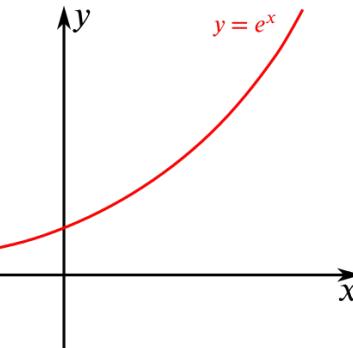
$$y = 1 \rightarrow \mathbf{y}^T = [0 \ 1]$$

Training example

$$(x, y) = (1.4, 0)$$



Softmax Regression Naïve



Training data

Feature	Label
Petal_Length	Label
1.4	0
1.3	0
1.5	0
4.5	1
4.1	1
4.6	1

#class=2

#feature=1

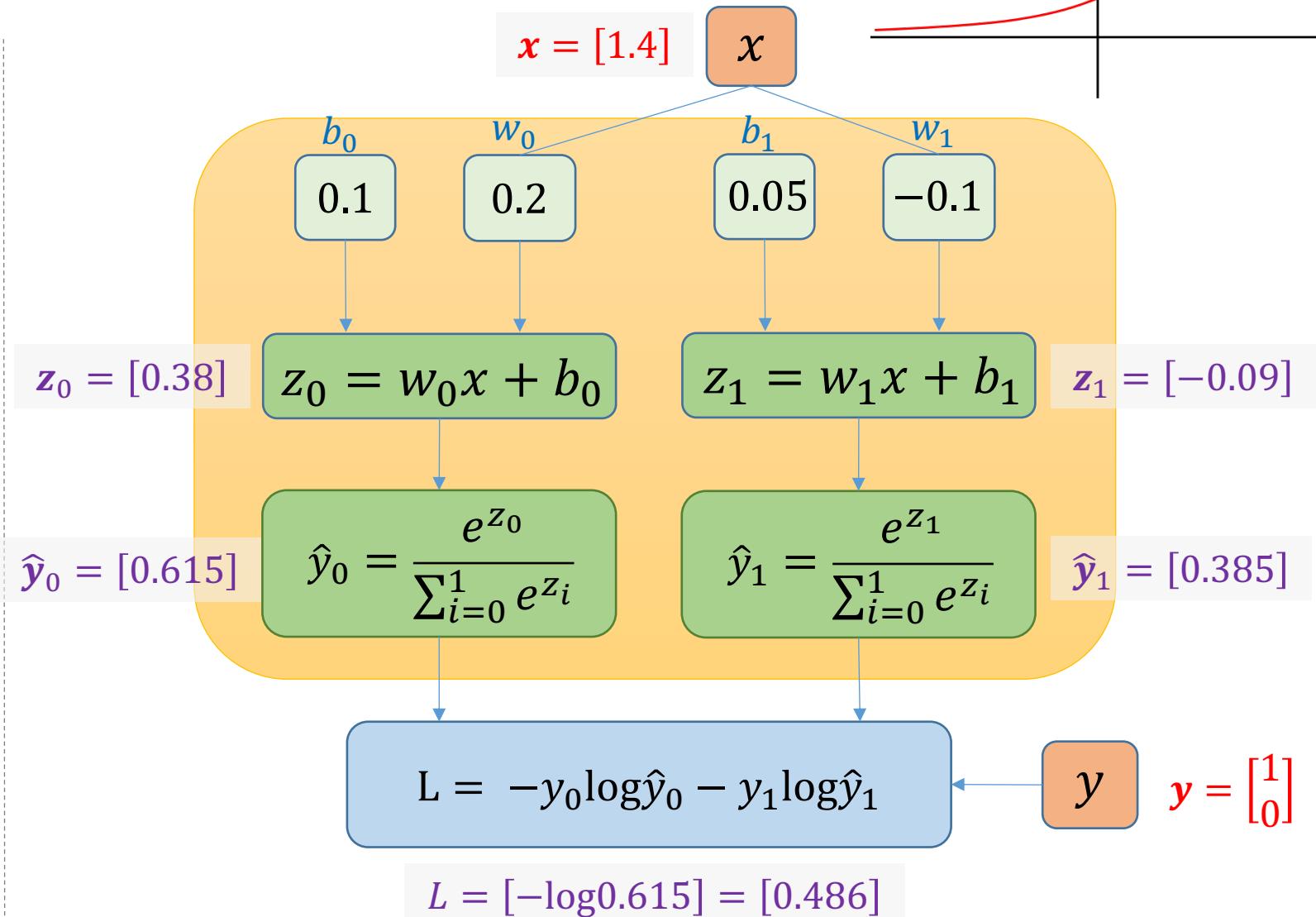
One-hot encoding for label

$$y = 0 \rightarrow \mathbf{y}^T = [1 \ 0]$$

$$y = 1 \rightarrow \mathbf{y}^T = [0 \ 1]$$

Training example

$$(x, y) = (1.4, 0)$$



Softmax Regression - Naïve

Derivative

$$\frac{\partial L}{\partial z_i} = \hat{y}_i - y_i$$

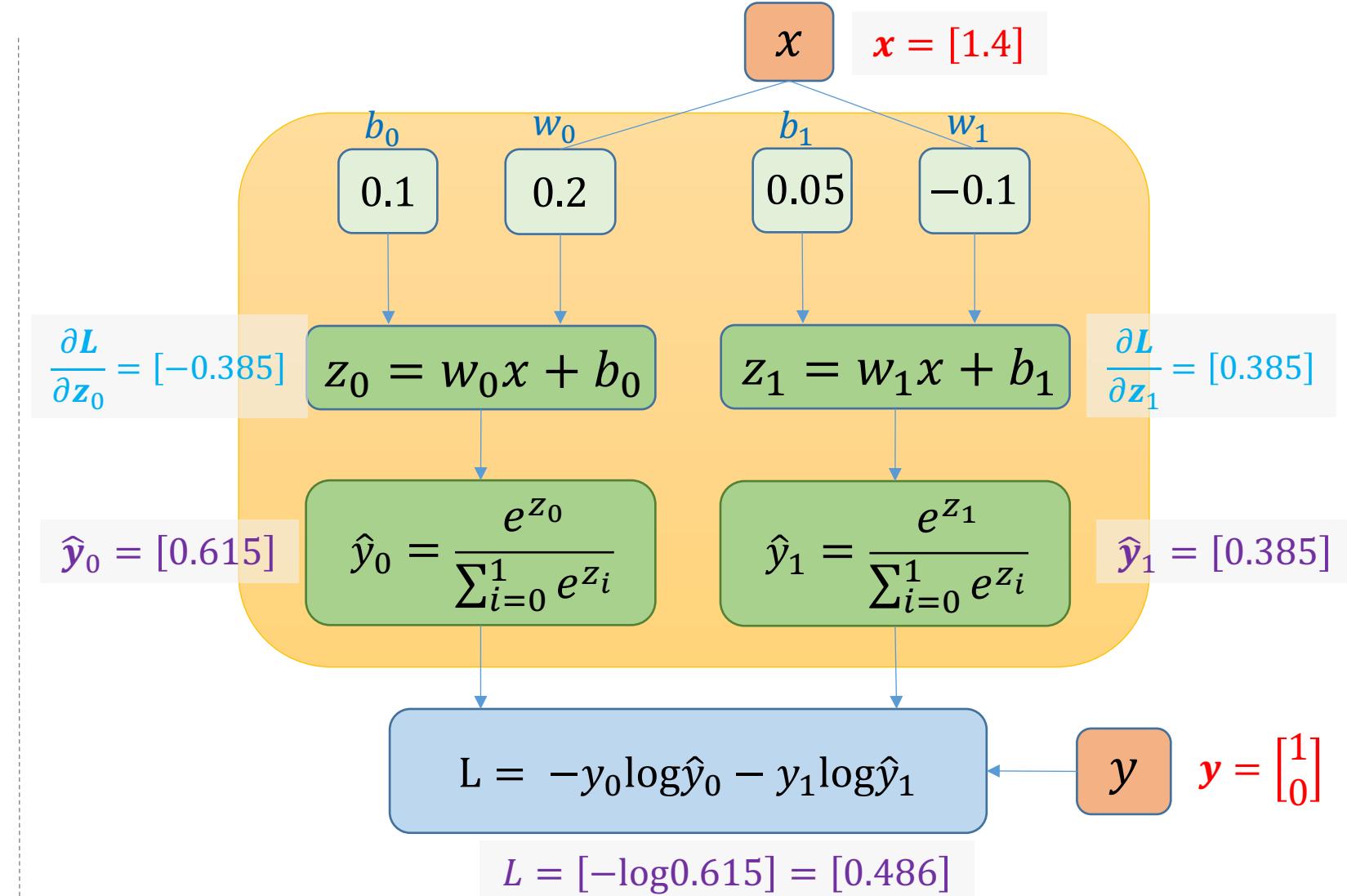
$$\frac{\partial L}{\partial w_i} = x(\hat{y}_i - y_i)$$

$$\frac{\partial L}{\partial b_i} = \hat{y}_i - y_i$$

$$y = 0 \rightarrow \mathbf{y}^T = [1 \quad 0]$$

$$y = 1 \rightarrow \mathbf{y}^T = [0 \quad 1]$$

$$\begin{aligned}\frac{\partial L}{\partial z_0} &= \hat{y}_0 - 1 \\ &= 0.615 - 1 = -0.385 \\ \frac{\partial L}{\partial z_1} &= \hat{y}_1 - 0 = 0.385\end{aligned}$$



Softmax Regression - Naïve

Derivative

$$\frac{\partial L}{\partial z_i} = \hat{y}_i - y_i$$

$$\frac{\partial L}{\partial w_i} = x(\hat{y}_i - y_i)$$

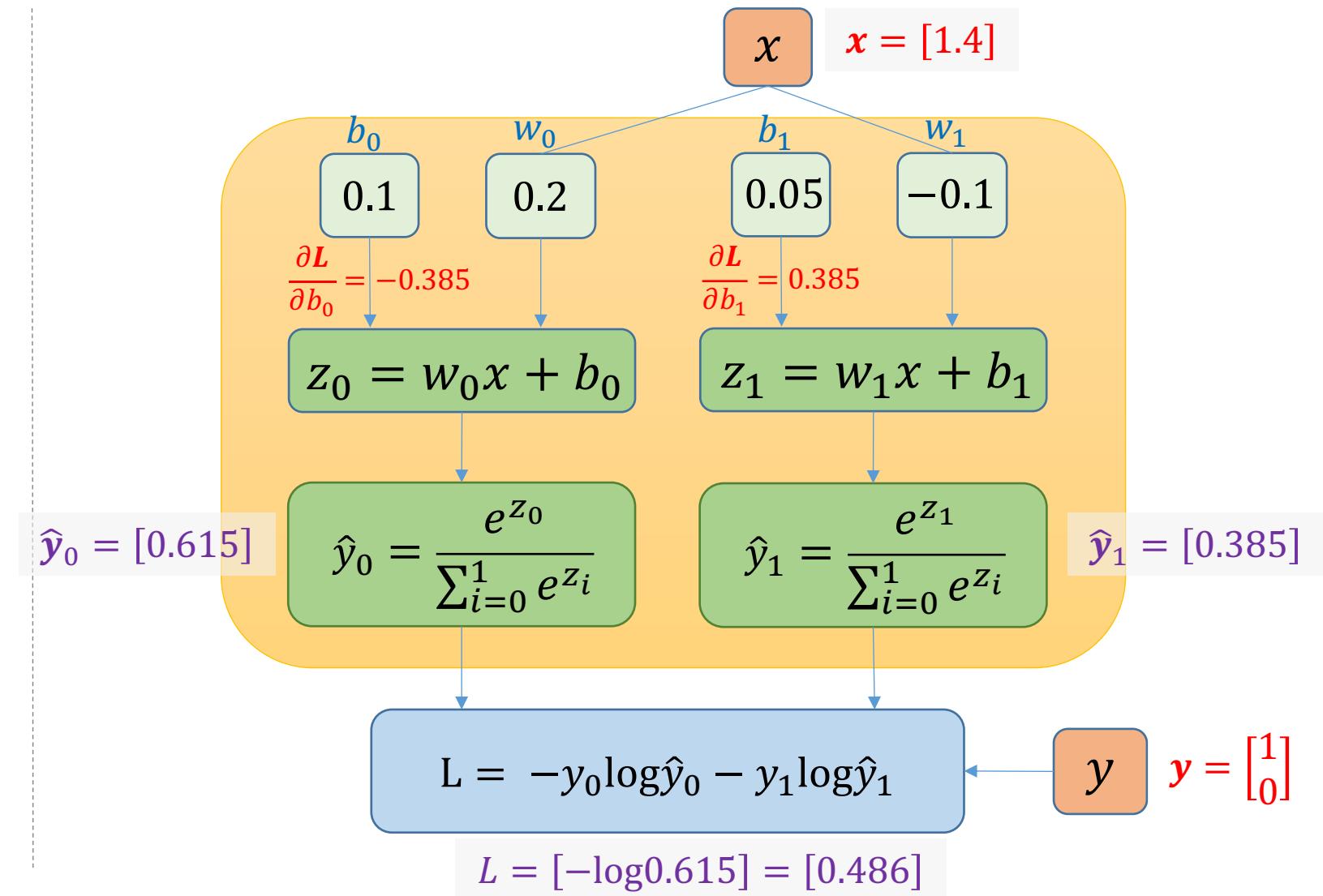
$$\frac{\partial L}{\partial b_i} = \hat{y}_i - y_i$$

$$y = 0 \rightarrow \mathbf{y}^T = [1 \quad 0]$$

$$y = 1 \rightarrow \mathbf{y}^T = [0 \quad 1]$$

$$\frac{\partial L}{\partial b_0} = (\hat{y}_0 - 1) = -0.385$$

$$\frac{\partial L}{\partial b_1} = (\hat{y}_1 - 0) = 0.385$$



Softmax Regression - Naïve

Derivative

$$\frac{\partial L}{\partial z_i} = \hat{y}_i - y_i$$

$$\frac{\partial L}{\partial w_i} = x(\hat{y}_i - y_i)$$

$$\frac{\partial L}{\partial b_i} = \hat{y}_i - y_i$$

$$y = 0 \rightarrow \mathbf{y}^T = [1 \quad 0]$$

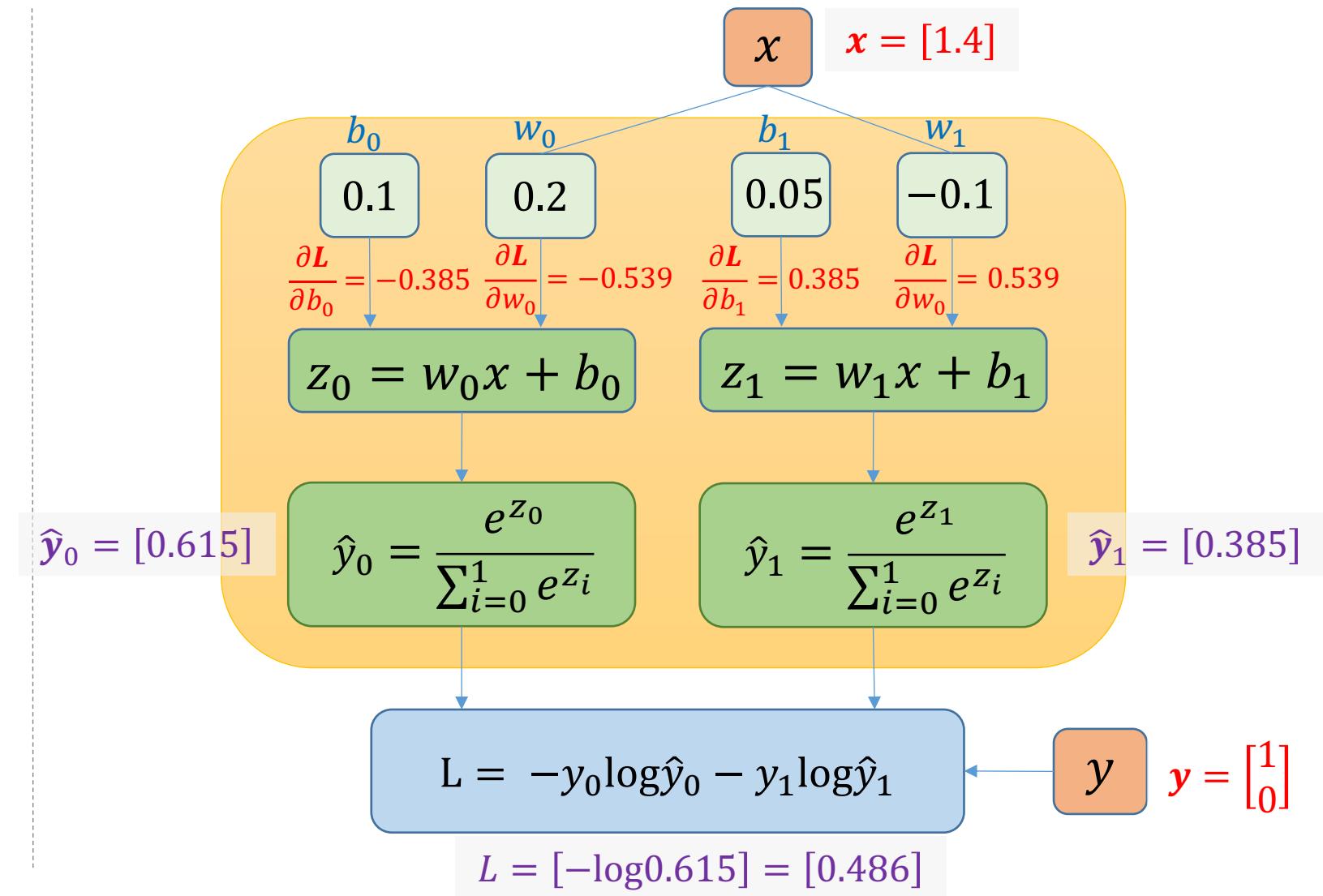
$$y = 1 \rightarrow \mathbf{y}^T = [0 \quad 1]$$

$$\frac{\partial L}{\partial w_0} = x(\hat{y}_0 - 1)$$

$$= -0.385 * 1.4 = -0.539$$

$$\frac{\partial L}{\partial w_1} = x(\hat{y}_1 - 0)$$

$$= 0.385 * 1.4 = 0.539$$



Softmax Regression - Naïve

Update parameters

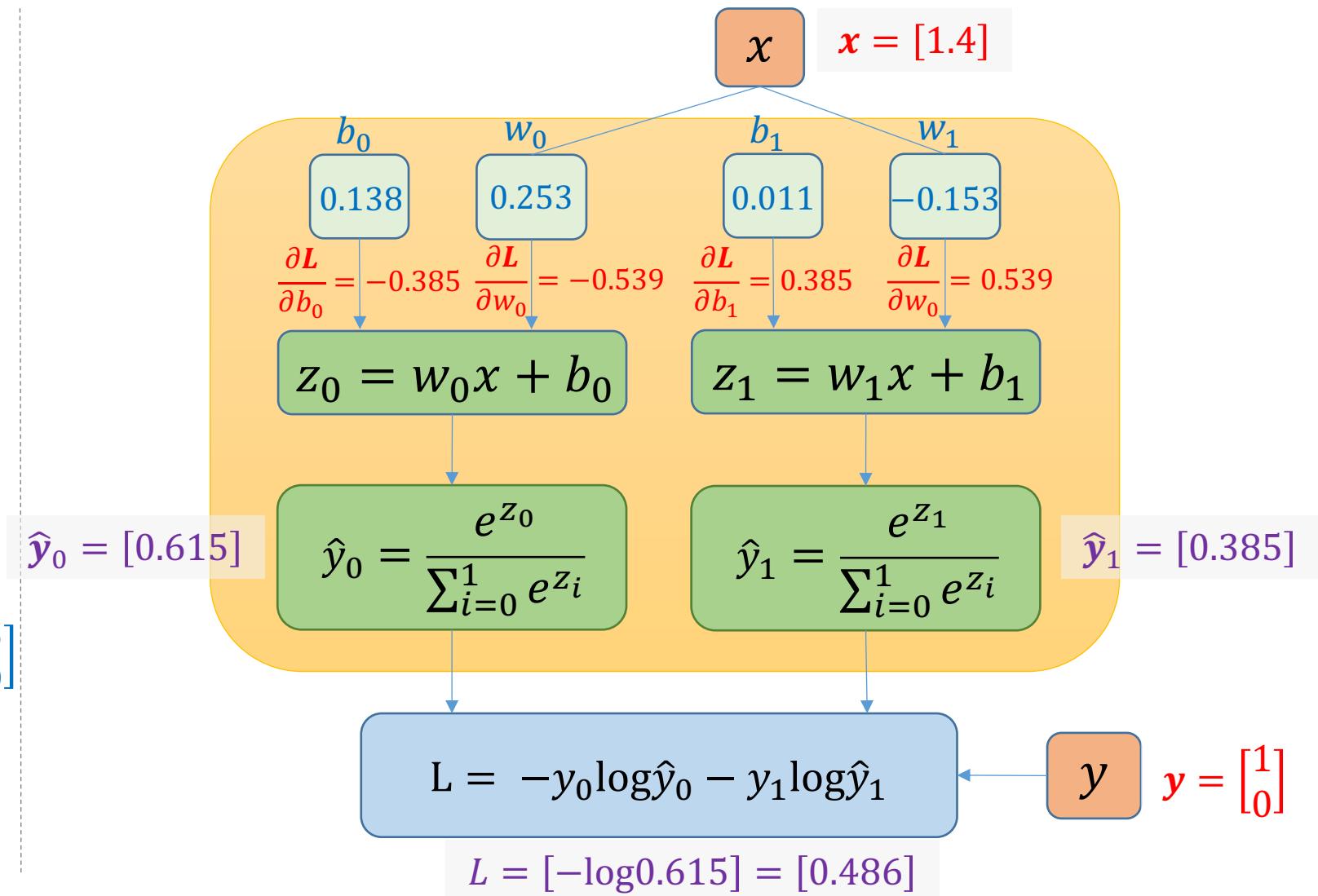
$$\theta = \theta - \eta L'_{\theta}$$

η is learning rate

$$\theta = \begin{bmatrix} b_0 & b_1 \\ w_0 & w_1 \end{bmatrix} \quad L'_{\theta} = \begin{bmatrix} \frac{\partial L}{\partial b_0} & \frac{\partial L}{\partial b_1} \\ \frac{\partial L}{\partial w_0} & \frac{\partial L}{\partial w_1} \end{bmatrix}$$

$$\theta = \begin{bmatrix} 0.1 & 0.05 \\ 0.2 & -0.1 \end{bmatrix} - 0.1 \begin{bmatrix} -0.385 & 0.385 \\ -0.539 & 0.539 \end{bmatrix}$$

$$= \begin{bmatrix} 0.138 & 0.011 \\ 0.253 & -0.153 \end{bmatrix}$$



Softmax Regression - Naïve

Training data

Feature	Label
Petal_Length	Label
1.4	0
1.3	0
1.5	0
4.5	1
4.1	1
4.6	1

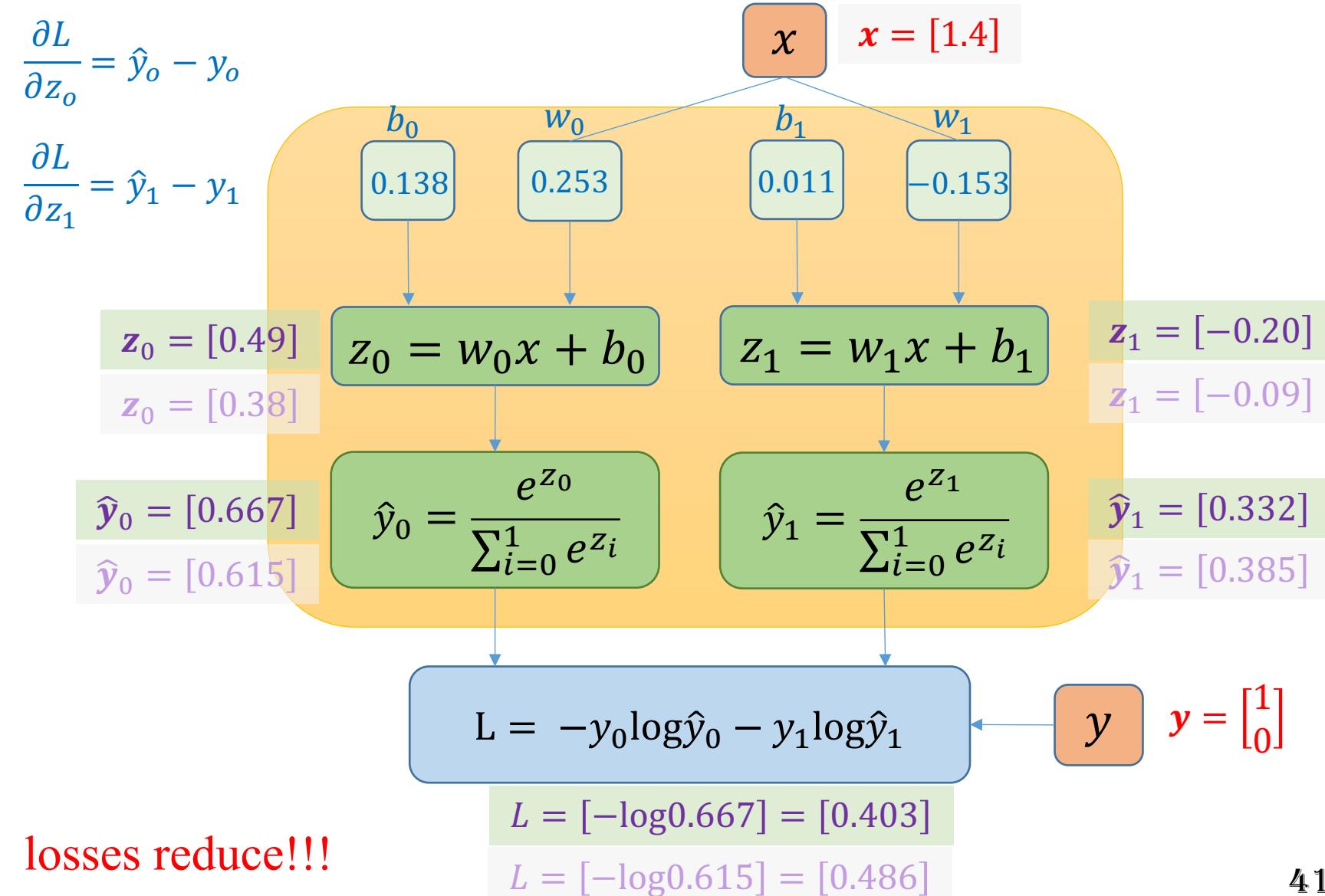
One-hot encoding for label

$$y = 0 \rightarrow \mathbf{y}^T = [1 \ 0]$$

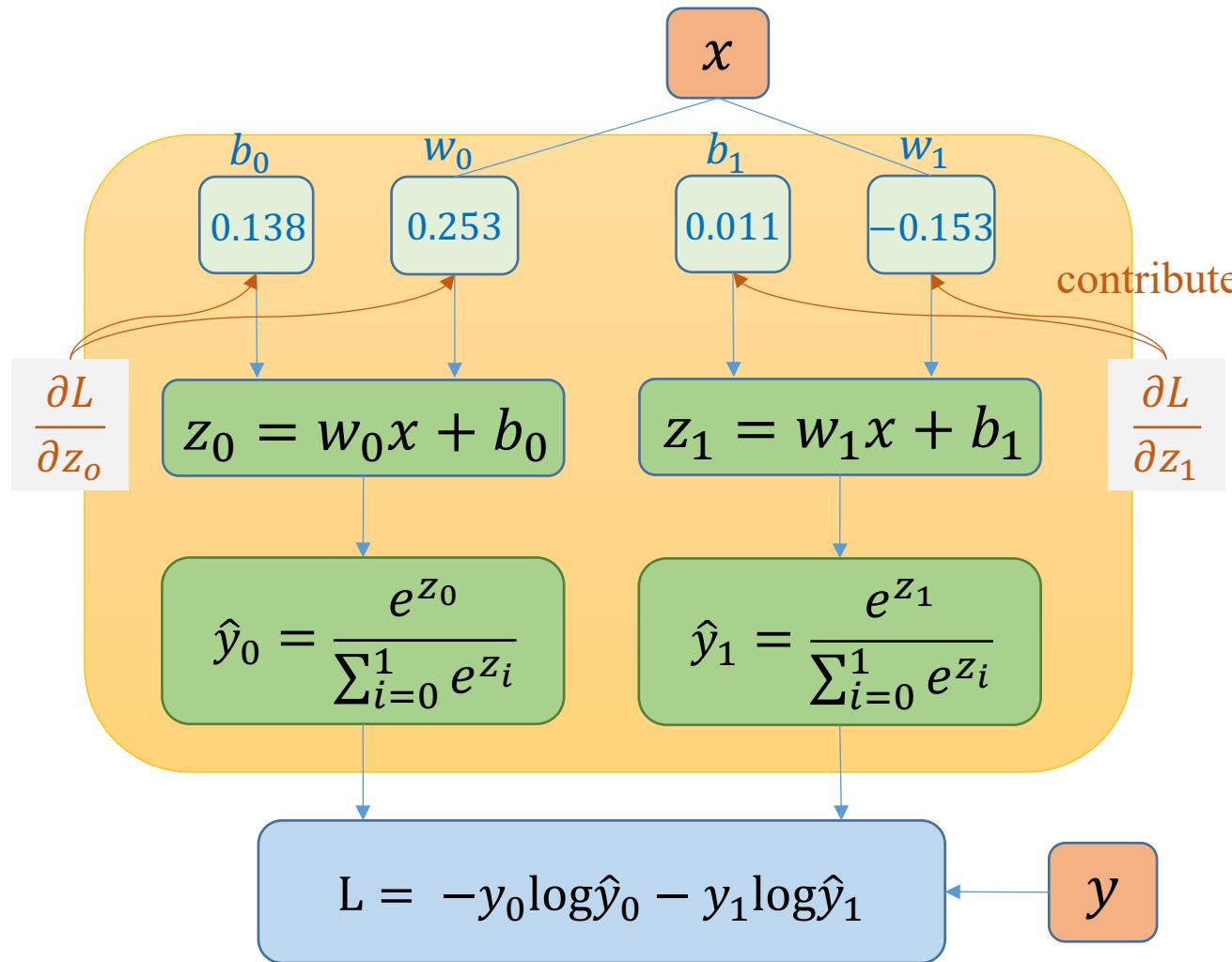
$$y = 1 \rightarrow \mathbf{y}^T = [0 \ 1]$$

Training example

$$(x, y) = (1.4, 0)$$



Softmax Regression - Naïve



$$\frac{\partial L}{\partial z_0} = \hat{y}_0 - y_0$$

$$\frac{\partial L}{\partial z_1} = \hat{y}_1 - y_1$$

$$\frac{\partial L}{\partial w_0} = x(\hat{y}_0 - y_0)$$

$$\frac{\partial L}{\partial w_1} = x(\hat{y}_1 - y_1)$$

$$\frac{\partial L}{\partial b_0} = \hat{y}_0 - y_0$$

$$\frac{\partial L}{\partial b_1} = \hat{y}_1 - y_1$$

Softmax Regression - Naïve

$$\frac{\partial L}{\partial z_o} = \hat{y}_o - y_o$$

$$\frac{\partial L}{\partial z_1} = \hat{y}_1 - y_1$$

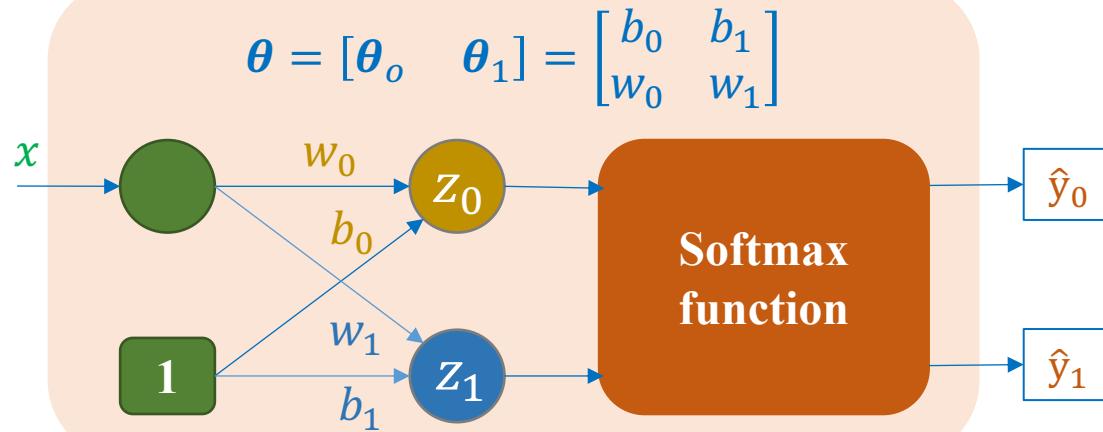
$$\frac{\partial L}{\partial w_0} = x(\hat{y}_0 - y_0)$$

$$\frac{\partial L}{\partial w_1} = x(\hat{y}_1 - y_1)$$

$$\frac{\partial L}{\partial b_0} = \hat{y}_0 - y_0$$

$$\frac{\partial L}{\partial b_1} = \hat{y}_1 - y_1$$

$$\theta = [\theta_o \quad \theta_1] = \begin{bmatrix} b_0 & b_1 \\ w_0 & w_1 \end{bmatrix}$$



$$\nabla_{\theta} L = x(\hat{y} - y)^T$$

$$L'_{\theta} = \begin{bmatrix} \frac{\partial L}{\partial b_0} & \frac{\partial L}{\partial b_1} \\ \frac{\partial L}{\partial w_0} & \frac{\partial L}{\partial w_1} \end{bmatrix} = \begin{bmatrix} 1 & \frac{\partial L}{\partial z_0} \\ x & \frac{\partial L}{\partial z_0} \end{bmatrix} \begin{bmatrix} 1 & \frac{\partial L}{\partial z_1} \\ x & \frac{\partial L}{\partial z_1} \end{bmatrix}$$

$$L'_{\theta} = \begin{bmatrix} \frac{\partial L}{\partial b_0} & \frac{\partial L}{\partial b_1} \\ \frac{\partial L}{\partial w_0} & \frac{\partial L}{\partial w_1} \end{bmatrix} = \begin{bmatrix} 1 & \frac{\partial L}{\partial z_0} \\ x & \frac{\partial L}{\partial z_0} \end{bmatrix} \begin{bmatrix} 1 & \frac{\partial L}{\partial z_1} \\ x & \frac{\partial L}{\partial z_1} \end{bmatrix} L'_{\mathbf{z}} = \begin{bmatrix} \frac{\partial L}{\partial z_0} \\ \frac{\partial L}{\partial z_1} \end{bmatrix}$$

Softmax Regression - Vectorization

$$\frac{\partial L}{\partial z_o} = \hat{y}_o - y_o$$

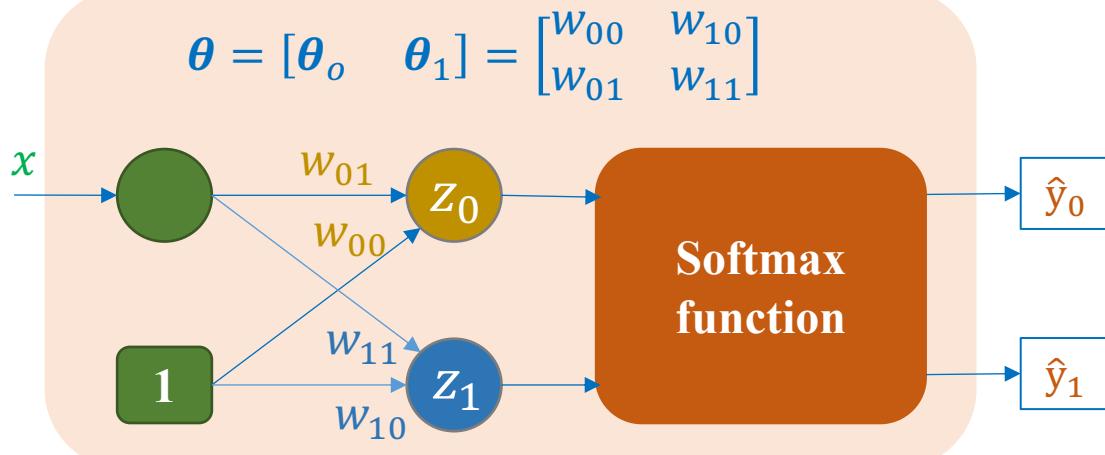
$$\frac{\partial L}{\partial z_1} = \hat{y}_1 - y_1$$

$$\frac{\partial L}{\partial w_0} = x \frac{\partial L}{\partial z_o}$$

$$\frac{\partial L}{\partial w_1} = x \frac{\partial L}{\partial z_1}$$

$$\frac{\partial L}{\partial b_0} = \frac{\partial L}{\partial z_o}$$

$$\frac{\partial L}{\partial b_1} = \frac{\partial L}{\partial z_1}$$



$$\nabla_{\theta} L = \mathbf{x}(\hat{\mathbf{y}} - \mathbf{y})^T$$

$$L'_{\theta} = \begin{bmatrix} \frac{\partial L}{\partial w_{00}} & \frac{\partial L}{\partial w_{10}} \\ \frac{\partial L}{\partial w_{01}} & \frac{\partial L}{\partial w_{11}} \end{bmatrix} = \begin{bmatrix} x_0 \frac{\partial L}{\partial z_o} & x_0 \frac{\partial L}{\partial z_1} \\ x_1 \frac{\partial L}{\partial z_o} & x_1 \frac{\partial L}{\partial z_1} \end{bmatrix}$$

$$L'_{\theta} = \begin{bmatrix} \frac{\partial L}{\partial w_{00}} & \frac{\partial L}{\partial w_{10}} \\ \frac{\partial L}{\partial w_{01}} & \frac{\partial L}{\partial w_{11}} \end{bmatrix} = \begin{bmatrix} x_0 \frac{\partial L}{\partial z_o} & x_0 \frac{\partial L}{\partial z_1} \\ x_1 \frac{\partial L}{\partial z_o} & x_1 \frac{\partial L}{\partial z_1} \end{bmatrix}$$

Softmax Regression - Vectorization

1) Pick a sample from training data

2) Tính output \hat{y}

$$z = \theta^T x$$

$$\hat{y} = \frac{e^z}{\sum_j e^{z_j}}$$

3) Tính loss (cross-entropy)

$$L(\theta) = -y^T \log \hat{y}$$

4) Tính đạo hàm

$$\nabla_{\theta} L = x(\hat{y} - y)^T$$

5) Cập nhật tham số

$$\theta = \theta - \eta L'_{\theta}$$

η is learning rate

$$x = \begin{bmatrix} x_0 \\ x_1 \end{bmatrix} \quad \theta = [\theta_0 \quad \theta_1] = \begin{bmatrix} w_{00} & w_{10} \\ w_{01} & w_{11} \end{bmatrix}$$

$$\hat{y} = \begin{bmatrix} \hat{y}_0 \\ \hat{y}_1 \end{bmatrix}$$

$$y = 0 \rightarrow y^T = [1 \ 0] \quad L(\theta) = -y^T \log \hat{y} = -\log \hat{y}_0$$

$$y = 1 \rightarrow y^T = [0 \ 1] \quad L(\theta) = -y^T \log \hat{y} = -\log \hat{y}_1$$

$$L'_{\theta} = \begin{bmatrix} x_0 \\ x_1 \end{bmatrix} \begin{bmatrix} \frac{\partial L}{\partial z_0} & \frac{\partial L}{\partial z_1} \end{bmatrix} = \begin{bmatrix} x_0 \frac{\partial L}{\partial z_0} & x_0 \frac{\partial L}{\partial z_1} \\ x_1 \frac{\partial L}{\partial z_0} & x_1 \frac{\partial L}{\partial z_1} \end{bmatrix}$$

$$\theta = \begin{bmatrix} w_{00} & w_{10} \\ w_{01} & w_{11} \end{bmatrix} - \eta \begin{bmatrix} x_0 \frac{\partial L}{\partial z_0} & x_0 \frac{\partial L}{\partial z_1} \\ x_1 \frac{\partial L}{\partial z_0} & x_1 \frac{\partial L}{\partial z_1} \end{bmatrix}$$

Summary

Motivation

Feature	Label
Petal_Length	Petal_Width
1.4	0.2
1.4	0.2
1.3	0.2
4.5	1.5
4.9	1.5
4	1.3
4.5	1.7
6.3	1.8
5.8	1.8
	Label
0	
0	
0	
1	
1	
1	
2	
2	
2	

#class=3
#feature=2

Feature is with two dimensions

→ Need two nodes for input

Three categories

→ Need three nodes for output

Softmax Regression

1. Forward computation

$$\mathbf{z} = \boldsymbol{\theta}^T \mathbf{x}$$
$$\hat{\mathbf{y}} = \frac{e^{\mathbf{z}}}{\sum_{j=0}^1 e^{z_j}}$$

2. Loss function

$$L(\boldsymbol{\theta}) = -\mathbf{y}^T \log \hat{\mathbf{y}}$$

3. Derivative

$$\frac{\partial L}{\partial w_i} = \mathbf{x}(\hat{\mathbf{y}}_i - \mathbf{y}_i)$$
$$\frac{\partial L}{\partial b_i} = \hat{\mathbf{y}}_i - \mathbf{y}_i$$

$$\nabla_{\boldsymbol{\theta}} L = \mathbf{x}(\hat{\mathbf{y}} - \mathbf{y})^T$$

4. Update

$$\boldsymbol{\theta} = \boldsymbol{\theta} - \eta \nabla_{\boldsymbol{\theta}} L$$

η is learning rate

Implementation

```
# compute z
z = theta.T.dot(xi)

# compute y_hat
exp_z = np.exp(z)
y_hat = exp_z / np.sum(exp_z, axis=0)

# compute the loss
loss = -yi.T.dot(np.log(y_hat))
losses.append(loss[0])

# compute the gradient dz
dz = y_hat - yi

# compute dtheta
dtheta = xi.dot(dz.T)

# update
theta = theta - learning_rate*dtheta
```

Friday - Pytorch



```
import numpy as np
import torch
import torch.nn as nn
import torch.optim as optim

# Load data
iris = np.genfromtxt('iris_1D_2c.csv', dtype=None,
                     delimiter=',', skip_header=1)
X = torch.tensor(iris[:, 0:1], dtype=torch.float32)
y = torch.tensor(iris[:, 1], dtype=torch.int64)
```

```
# create model
input_dim = X.shape[1]
output_dim = len(torch.unique(y))
model = nn.Linear(input_dim, output_dim)

# Loss and optimizer
criterion = nn.CrossEntropyLoss()
optimizer = optim.SGD(model.parameters(), lr=0.1)

# Training Loop
max_epoch = 100
for epoch in range(max_epoch):
    # Zero the gradients
    optimizer.zero_grad()

    # Forward pass
    outputs = model(X)
    loss = criterion(outputs, y)

    # Backward pass
    loss.backward()
    optimizer.step()
```

