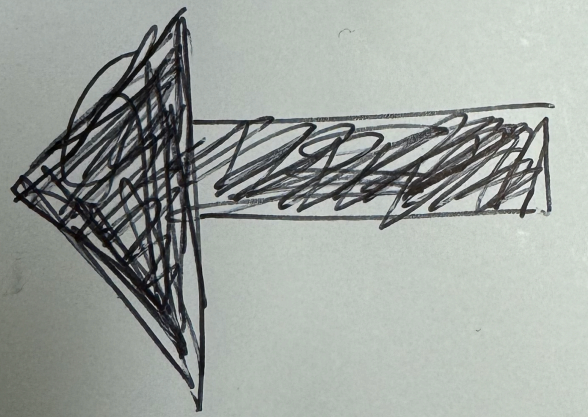
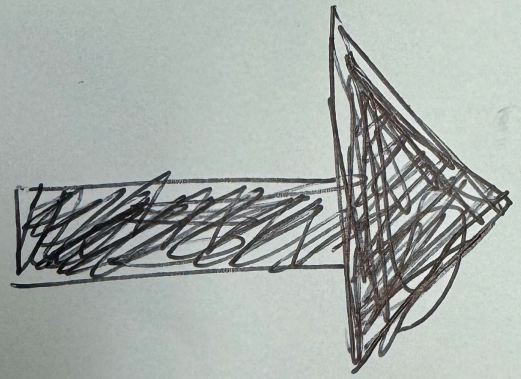
Softmax regression





Softmax regression as a generalization of logistic regression

	Logistic regression	Softmax regression
Output	Binary	Multiclass
Activation function	Sigmoid	Softmax
Prediction	Threshold	Argmax
Loss function	Binary cross-entropy	Cross-entropy

1. **Modeling**
2. **Prediction (forward propagation)**
3. Loss & cost function
4. Gradient descent (backward propagation)

From binary to multiclass

Logistic regression: `2` possible outcomes

- $a_1 = g(z) = \frac{1}{1+e^{-z}} = P(y = 1|x)$
- $a_2 = 1 - a_1 = P(y = 0|x)$

Softmax regression: `K` possible outcomes $(1, \ldots, K)$

- $a_1 = \text{softmax}(z_1) = P(y = 1|x)$
- $a_2 = \text{softmax}(z_2) = P(y = 2|x)$
- $\vdots$
- $a_K = \text{softmax}(z_K) = P(y = K|x)$

Softmax function

$$a_k = \text{softmax}(z_k) = \frac{e^{z_k}}{\sum_{k=1}^{K} e^{z_k}} = P(y = k|x)$$

For class $k = 1, 2, \ldots, K$

$$a_1 = \text{softmax}(z_1) = \frac{e^{z_1}}{e^{z_1} + e^{z_2} + \ldots + e^{z_K}} = P(y = 1|x)$$

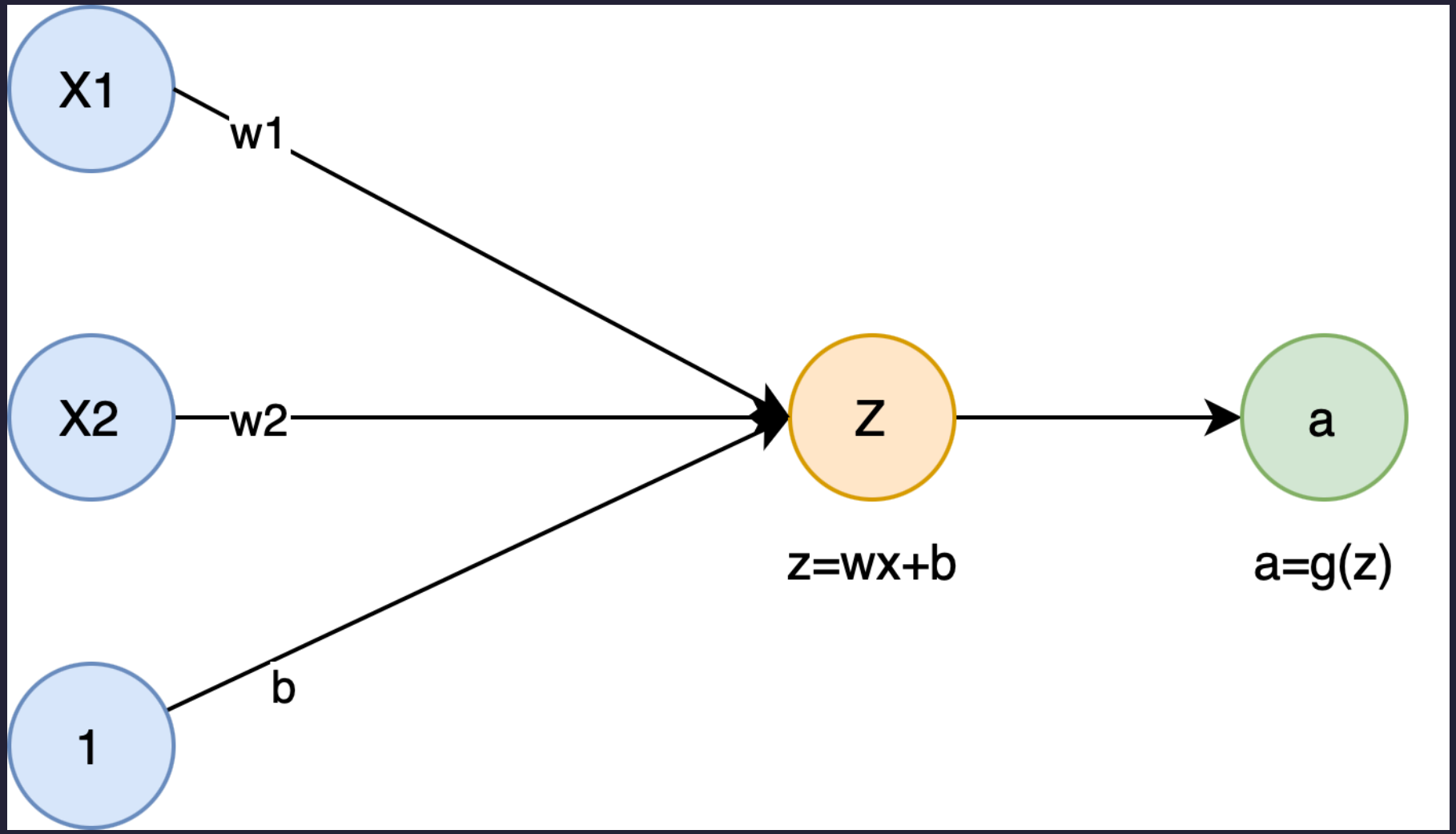
$$a_2 = \text{softmax}(z_2) = \frac{e^{z_2}}{e^{z_1} + e^{z_2} + \ldots + e^{z_K}} = P(y = 2|x)$$

$$\vdots$$

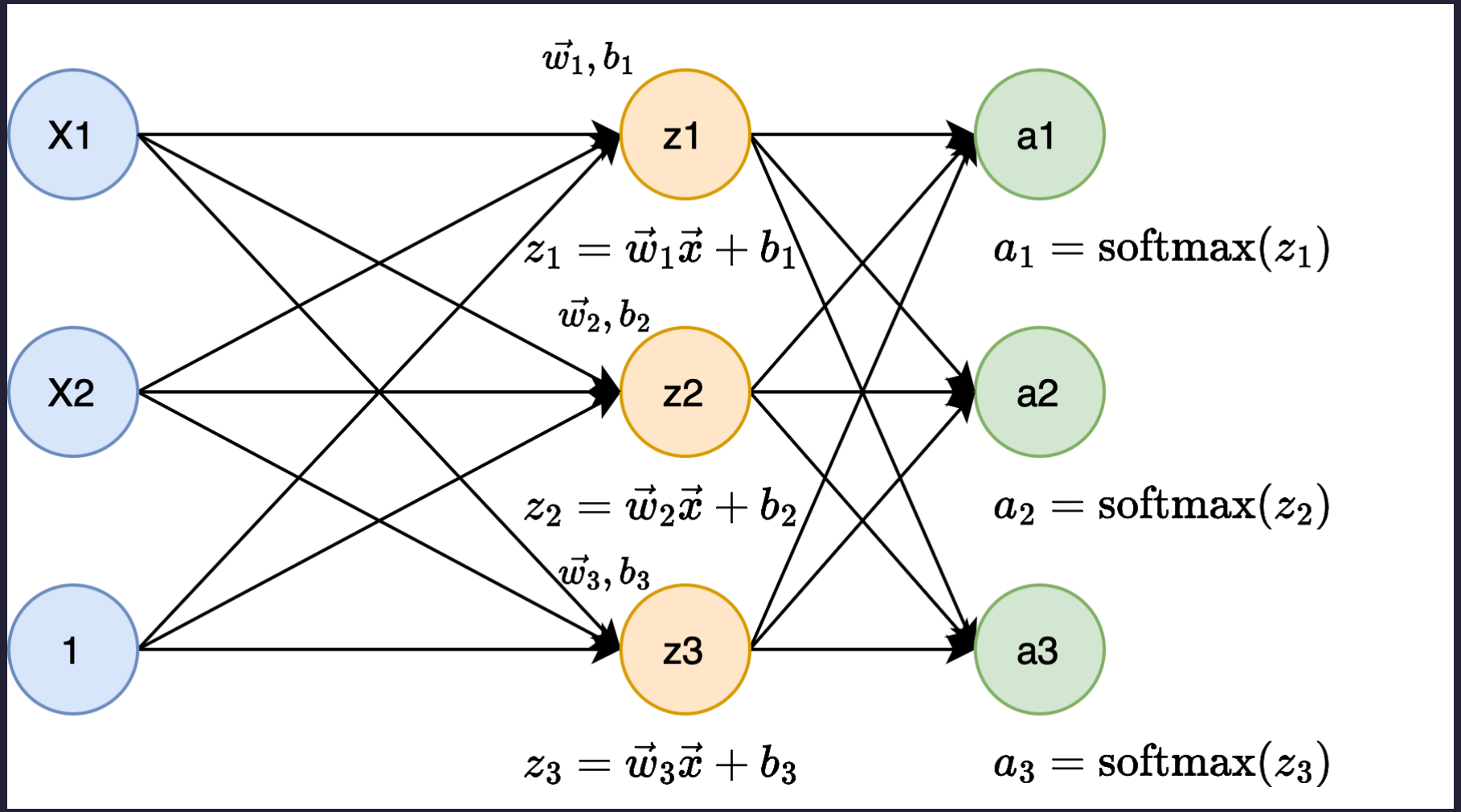
$$a_K = \text{softmax}(z_K) = \frac{e^{z_K}}{e^{z_1} + e^{z_2} + \ldots + e^{z_K}} = P(y = N|x)$$

logistic(sigmoid) function is a special case of softmax function. See page 23.

Logistic regression for two classes



Softmax regression for three classes



Compute sigmoid probability for two classes

Model: $w = 2, b = 1$

Input: $x = 1$

$$z = wx + b = 2 \cdot 1 + 1 = 3$$

$$a = g(z) = \frac{1}{1 + e^{-z}} = \frac{1}{1 + e^{-3}} = 0.9526$$

$$1 - a = 1 - 0.9526 = 0.0474$$

Compute softmax probability for three classes

Model: $\vec{w} = [2, 3, 5], \vec{b} = [1, 1, 1]$

Input: $x = 1$

$$z_1 = 2 \cdot 1 + 1 = 3$$
$$z_2 = 3 \cdot 1 + 1 = 4$$
$$z_3 = 5 \cdot 1 + 1 = 6$$

$$a_1 = \text{softmax}(z_1) = \frac{e^{z_1}}{e^{z_1} + e^{z_2} + e^{z_3}} = \frac{e^3}{e^3 + e^4 + e^6} = 0.0420$$

$$a_2 = \text{softmax}(z_2) = \frac{e^4}{e^3 + e^4 + e^6} = 0.1141$$

$$a_3 = \text{softmax}(z_3) = \frac{e^6}{e^3 + e^4 + e^6} = 0.8437$$

Prediction

Select the class with the highest probability

$$\begin{aligned}\hat{y} &= \text{argmax}_k P(y = k|x) \\ &= \text{argmax}_k a_k\end{aligned}$$

- a_k: predicted probability of class k
- k: class index $(1, 2, \ldots, K)$
- e.g., $\hat{y} = 3$ if $a_1 = 0.0420, a_2 = 0.1141, a_3 = 0.8437$

1. Modeling
2. Prediction (forward propagation)
3. **Loss & cost function**
4. Gradient descent (backward propagation)

Loss function: cross-entropy loss

Logistic regression: binary cross-entropy loss

$$L = \begin{cases} -\log(a_1) & \text{if } y = 1 \\ -\log(1 - a_1) = -\log(a_2) & \text{if } y = 0 \end{cases}$$

$$= -y \log(a_1) - (1 - y) \log(1 - a_1) = -y_1 \log(a_1) - y_2 \log(a_2) = -\sum_{k=1}^{2} y_k \log(a_k)$$

Softmax regression: cross-entropy loss

$$L = \begin{cases} -\log(a_1) & \text{if } y = 1 \\ -\log(a_2) & \text{if } y = 2 \\ \vdots & \\ -\log(a_K) & \text{if } y = K \end{cases}$$

$$= -y_1 \log(a_1) - y_2 \log(a_2) - \cdots - y_N \log(a_K) \qquad = -\sum_{k=1}^{K} y_k \log(a_k)$$

Cost function: average loss over all samples

Logistic regression

$$J = -\frac{1}{m}\sum_{i=1}^{m}\left[\sum_{k=1}^{2} y_k^{(i)} \log(a_k^{(i)})\right]$$

Softmax regression

$$J = -\frac{1}{m}\sum_{i=1}^{m}\left[\sum_{k=1}^{K} y_k^{(i)} \log(a_k^{(i)})\right]$$

- $y_k^{(i)}$: output label of class k for sample i
- $a_k^{(i)}$: predicted probability of class k for sample i
- m: number of samples
- K: number of classes

1. Modeling
2. Prediction (forward propagation)
3. Loss & cost function
4. **Gradient descent (backward propagation)**

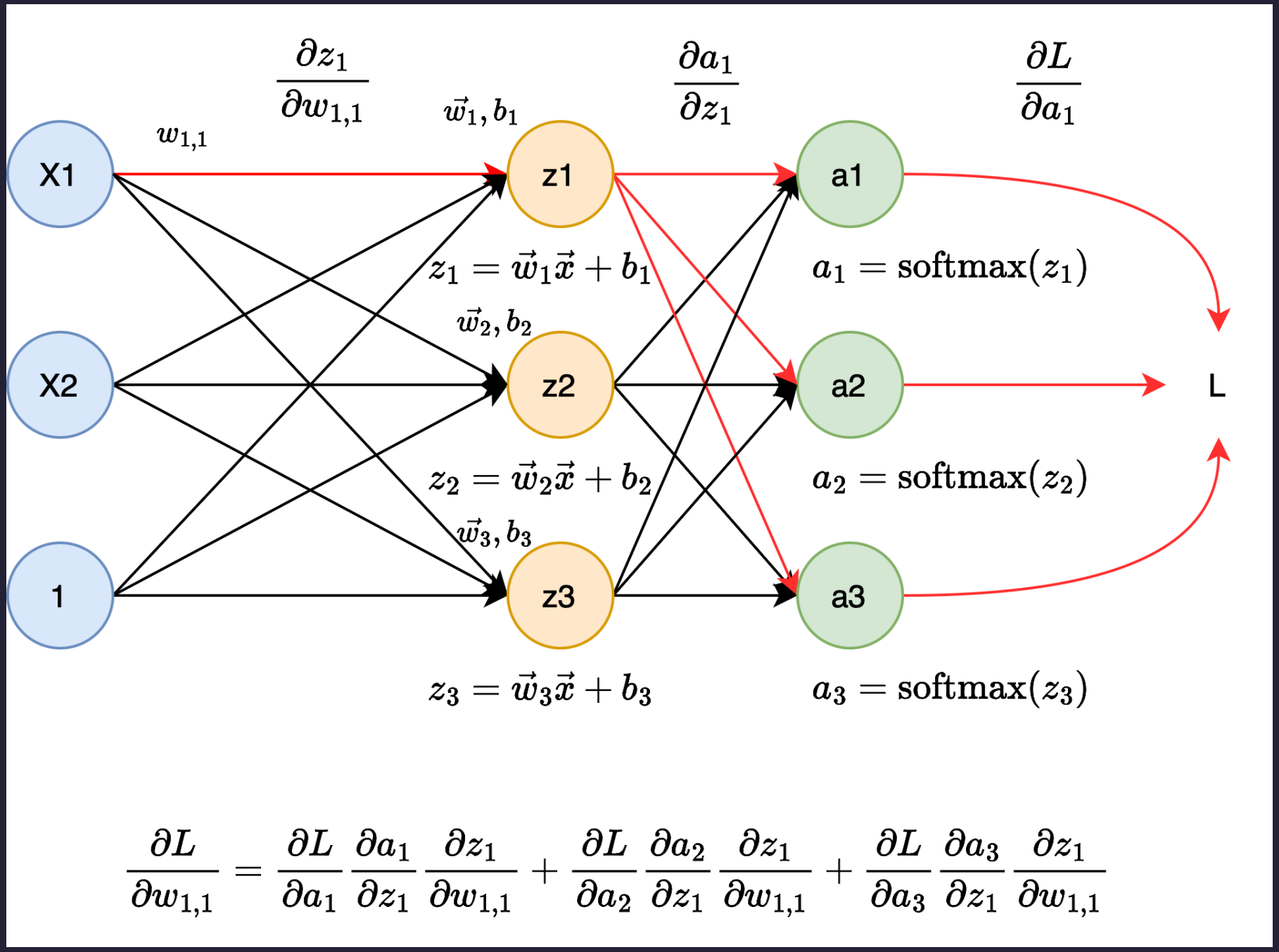
Gradient descent

Repeat until convergence

$$w_{k,j} = w_{k,j} - \alpha \frac{\partial J(\vec{w}, b)}{\partial w_{k,j}}$$

$$b_k = b_k - \alpha \frac{\partial J(\vec{w}, b)}{\partial b_k}$$

- k: class index $(1, 2, \ldots, K)$
- j: feature index $(1, 2, \ldots, N)$



$$\frac{\partial L}{\partial w_{1,1}} = \frac{\partial L}{\partial a_1}\frac{\partial a_1}{\partial z_1}\frac{\partial z_1}{\partial w_{1,1}} + \frac{\partial L}{\partial a_2}\frac{\partial a_2}{\partial z_1}\frac{\partial z_1}{\partial w_{1,1}} + \frac{\partial L}{\partial a_3}\frac{\partial a_3}{\partial z_1}\frac{\partial z_1}{\partial w_{1,1}}$$

Gradient with respect to weight $w_{1,1}$

$w_{1,1}$: weight for class 1 and feature 1

$$z_1 = w_{1,1}x_1 + w_{1,2}x_2 + b_1$$

$$a_k = \frac{e^{z_k}}{\sum_{k=1}^{3} e^{z_k}}$$

$$L = -y_1 \log(a_1) - y_2 \log(a_2) - y_3 \log(a_3)$$

$$\frac{\partial L}{\partial w_{1,1}} = \frac{\partial L}{\partial a_1}\frac{\partial a_1}{\partial z_1}\frac{\partial z_1}{\partial w_{1,1}} + \frac{\partial L}{\partial a_2}\frac{\partial a_2}{\partial z_1}\frac{\partial z_1}{\partial w_{1,1}} + \frac{\partial L}{\partial a_3}\frac{\partial a_3}{\partial z_1}\frac{\partial z_1}{\partial w_{1,1}}$$

$$= (a_1 - y_1)x_1$$

See page 20 for the derivation

Gradient with respect to bias b_1

$$L = -y_1 \log(a_1) - y_2 \log(a_2) - y_3 \log(a_3)$$

$$a_k = \frac{e^{z_k}}{\sum_{k=1}^{3} e^{z_k}}$$

$$z_1 = w_{1,1}x_1 + w_{1,2}x_2 + b_1$$

$$\frac{\partial L}{\partial b_1} = \frac{\partial L}{\partial a_1}\frac{\partial a_1}{\partial z_1}\frac{\partial z_1}{\partial b_1} + \frac{\partial L}{\partial a_2}\frac{\partial a_2}{\partial z_1}\frac{\partial z_1}{\partial b_1} + \frac{\partial L}{\partial a_3}\frac{\partial a_3}{\partial z_1}\frac{\partial z_1}{\partial b_1}$$

$$= (a_1 - y_1)$$

See page 21 for the derivation

Gradient of the cost function

$w_{k,j}$: weight for class k and feature j
b_k: bias for class k

Partial derivative of the cost function with respect to $w_{k,j}$

$$\frac{\partial J(\vec{w}, \vec{b})}{\partial w_{k,j}} = \frac{1}{m} \sum_{i=1}^{m} (a_k^{(i)} - y_k^{(i)}) x_j^{(i)}$$

Partial derivative of the cost function with respect to b_k

$$\frac{\partial J(\vec{w}, \vec{b})}{\partial b_k} = \frac{1}{m} \sum_{i=1}^{m} (a_k^{(i)} - y_k^{(i)})$$

Comparison of gradients for different models

Linear regression

$$\frac{\partial J(\vec{w},b)}{\partial w_j} = \frac{2}{m}\sum_{i=1}^{m}(a^{(i)} - y^{(i)})x_j^{(i)}$$

Logistic regression

$$\frac{\partial J(\vec{w},b)}{\partial w_j} = \frac{1}{m}\sum_{i=1}^{m}(a^{(i)} - y^{(i)})x_j^{(i)}$$

Softmax regression

$$\frac{\partial J(\vec{w},\vec{b})}{\partial w_{k,j}} = \frac{1}{m}\sum_{i=1}^{m}(a_k^{(i)} - y_k^{(i)})x_j^{(i)}$$

💻 Softmax regression

Gradient for weight $w_{1,1}$

$$L = -y_1 \log(a_1) - y_2 \log(a_2) - y_3 \log(a_3)$$

$$a_k = \frac{e^{z_1}}{\sum_{k=1}^{3} e^{z_k}}$$

$$z_1 = w_{1,1}x_1 + w_{1,2}x_2 + b_1$$

$$\begin{aligned}
\frac{\partial L}{\partial w_{1,1}} &= \frac{\partial L}{\partial a_1}\frac{\partial a_1}{\partial z_1}\frac{\partial z_1}{\partial w_{1,1}} + \frac{\partial L}{\partial a_2}\frac{\partial a_2}{\partial z_1}\frac{\partial z_1}{\partial w_{1,1}} + \frac{\partial L}{\partial a_3}\frac{\partial a_3}{\partial z_1}\frac{\partial z_1}{\partial w_{1,1}} \\
&= -\frac{y_1}{a_1}a_1(1-a_1)x_1 - \frac{y_2}{a_2}(-a_1a_2)x_1 - \frac{y_3}{a_3}(-a_1a_3)x_1 \\
&= -y_1x_1 + a_1x_1(y_1+y_2+y_3) \\
&= -y_1x_1 + a_1x_1 \\
&= (a_1 - y_1)x_1
\end{aligned}$$

Gradient for bias b_1

$$L = -y_1 \log(a_1) - y_2 \log(a_2) - y_3 \log(a_3)$$

$$a_k = \frac{e^{z_1}}{\sum_{k=1}^{3} e^{z_k}}$$

$$z_1 = w_{1,1}x_1 + w_{1,2}x_2 + b_1$$

$$\begin{aligned}
\frac{\partial L}{\partial b_1} &= \frac{\partial L}{\partial a_1}\frac{\partial a_1}{\partial z_1}\frac{\partial z_1}{\partial b_1} + \frac{\partial L}{\partial a_2}\frac{\partial a_2}{\partial z_1}\frac{\partial z_1}{\partial b_1} + \frac{\partial L}{\partial a_3}\frac{\partial a_3}{\partial z_1}\frac{\partial z_1}{\partial b_1} \\
&= -\frac{y_1}{a_1}a_1(1-a_1) - \frac{y_2}{a_2}(-a_1a_2) - \frac{y_3}{a_3}(-a_1a_3) \\
&= -y_1 + a_1(y_1 + y_2 + y_3) \\
&= a_1 - y_1
\end{aligned}$$

$\partial a_1 / \partial z_1$

$$
\begin{aligned}
a_1 &= \frac{e^{z_1}}{\sum_{k=1}^{K} e^{z_k}} \\
\frac{\partial a_1}{\partial z_1} &= \frac{e^{z_1} \sum_{k=1}^{K} e^{z_k} - e^{z_1} e^{z_1}}{(\sum_{k=1}^{K} e^{z_k})^2} \\
&= \frac{e^{z_1} (\sum_{k=1}^{K} e^{z_k} - e^{z_1})}{(\sum_{k=1}^{K} e^{z_k})^2} \\
&= \frac{e^{z_1}}{\sum_{k=1}^{K} e^{z_k}} \left(1 - \frac{e^{z_1}}{\sum_{k=1}^{K} e^{z_k}} \right) \\
&= a_1 (1 - a_1)
\end{aligned}
$$

$\partial a_2 / \partial z_1$

$$
\begin{aligned}
a_2 &= \frac{e^{z_2}}{\sum_{k=1}^{K} e^{z_k}} \\
\frac{\partial a_2}{\partial z_1} &= \frac{0 \cdot \sum_{k=1}^{K} e^{z_k} - e^{z_2} e^{z_1}}{(\sum_{k=1}^{K} e^{z_k})^2} \\
&= -\frac{e^{z_2} e^{z_1}}{(\sum_{k=1}^{K} e^{z_k})^2} \\
&= -a_2 a_1
\end{aligned}
$$

Sigmoid function as a special case of softmax

$$
\begin{aligned}
a_1 &= \frac{e^{z_1}}{e^{z_1} + e^{z_2}} \\
&= \frac{\frac{e^{z_1}}{e^{z_1}}}{\frac{e^{z_1}}{e^{z_1}} + \frac{e^{z_2}}{e^{z_1}}} \\
&= \frac{1}{1 + e^{-(z_1 - z_2)}} \\
&= \frac{1}{1 + e^{-z'}}
\end{aligned}
$$