

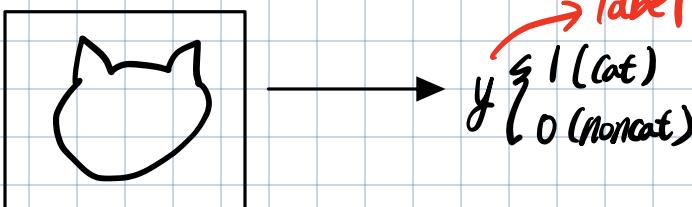
Week 2. Neural Network Basics

Essential Techniques for Neural Network

- ① Do not explicit for-loops to loop over your entire training set.
- ② Computation of neural network can be organized as Forward & backward propagation

1. Logistic Regression as a Neural Network

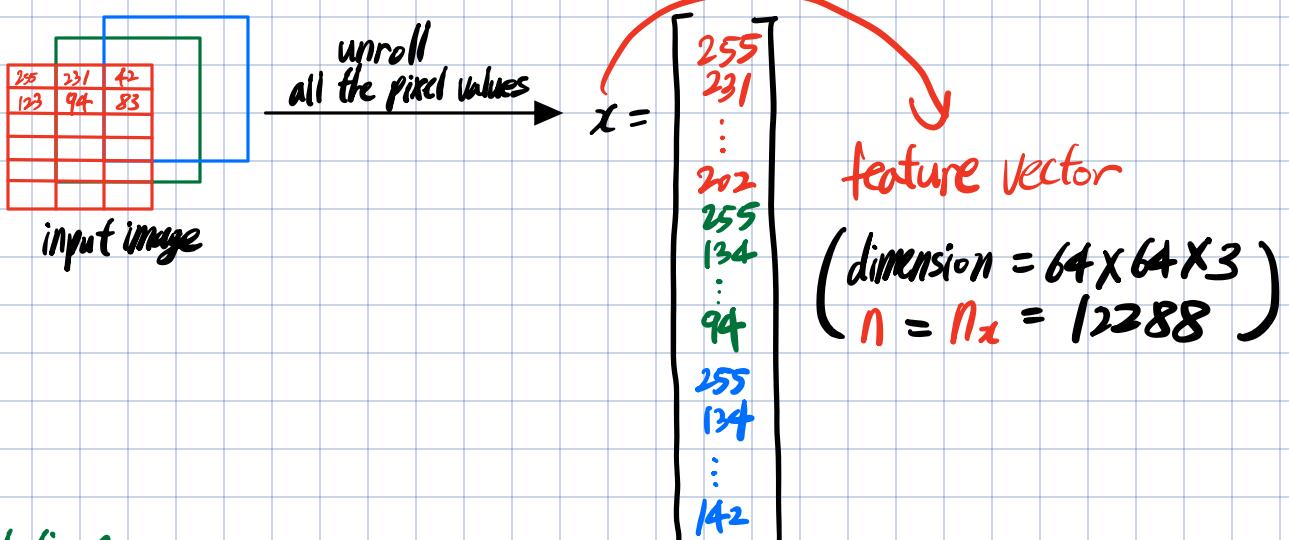
• Binary Classification



- how an image is represented in computer

⇒ computer stores image as **3 separate matrices (red, green, blue)**

∴ if image is $64 \times 64 \text{ px} \Rightarrow 64 \times 64 \text{ matrix } \times 3$



* Notation

(x, y) : a single training sample

x : feature vector, $x \in \mathbb{R}^m$

y : label, $y \in \{0, 1\}$

training set: $\{(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \dots, (x^{(m)}, y^{(m)})\}$

stack
training inputs $x^{(1)}, x^{(2)}, \dots$

m training samples

in columns

$$X = \begin{bmatrix} | & | & | \\ x^{(1)} & x^{(2)} & \dots & x^{(m)} \\ | & | & | \end{bmatrix}_{M \times n_x}$$

$Y = [y^{(1)}, y^{(2)}, y^{(3)}, \dots, y^{(m)}]$
 $Y = \mathbb{R}^{1 \times m} \Rightarrow Y.\text{shape} = (1, m)$

height of feature vector
of training samples

$\Rightarrow X.\text{shape} = (n_x, m)$

• Logistic Regression

— Algorithm for *binary classification*

Given $x, x \in \mathbb{R}^{n_x}$ e.g. cat vs noncat picture

Want $\hat{y} = P(y=1|x) \approx y$ e.g. probability of given image is a cat picture

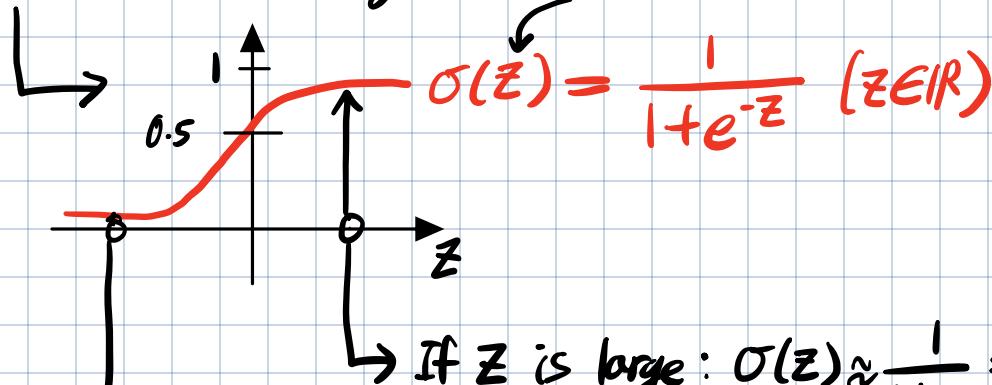
Parameters: $w \in \mathbb{R}^{n_x}, b \in \mathbb{R}$ (real number)

⇒ Given an input x and the parameters w and b ,
how do we generate output \hat{y} ?

① linear function of the input x : $\hat{y} = w^T x + b$

But, \hat{y} should be $0 \leq \hat{y} \leq 1$

② Apply Sigmoid function: $\hat{y} = \sigma(w^T x + b)$



If z is large: $\sigma(z) \approx \frac{1}{1+0} = 1$
If z is small: $\sigma(z) = \frac{1}{1+\text{big num}} \approx 0$
(large negative)

∴ Goal: Learn parameters w & $b \rightarrow \hat{y}$ becomes a good estimate

* Notation (Alternative notation)

$$x_0 = 1, x \in \mathbb{R}^{n+1}$$

$$g = \sigma(\theta^T x), \theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \vdots \\ \theta_{n+1} \end{bmatrix} \begin{matrix} b \\ \\ \\ \\ w \end{matrix}$$

of the chance of $y=1$

how to know
best parameters $w & b$?

• Logistic Regression

- $\hat{y}^{(i)} = \sigma(w^T x^{(i)} + b)$, where $\sigma(z^{(i)}) = \frac{1}{1 + e^{-z^{(i)}}}$

Given $\{(x^{(i)}, y^{(i)})\}, \dots, (x^{(m)}, y^{(m)})\}$, want $\hat{y}^{(i)} \approx y^{(i)}$

* $A^{(i)}$: i -th sample

- Loss (error) function: measure how well algorithm is doing on
 - ↳ cost of a single training sample
 - = how good output \hat{y} is close to true label y
 - = minimize the loss (error) function!

① Squared Error: $L(\hat{y}, y) = \frac{1}{2}(\hat{y} - y)^2$

\Rightarrow it's non-convex: have many local optima so the algorithm cannot find global optimum

\Rightarrow it makes gradient descent not work well

② $L(\hat{y}, y) = -(y \log \hat{y} + (1-y) \log(1-\hat{y}))$

intuitive look

$$\left[\begin{array}{l} y=1: L(\hat{y}, y) = -\log \hat{y} \\ y=0: L(\hat{y}, y) = -\log(1-\hat{y}) \end{array} \right]$$

want large $\log \hat{y} \Rightarrow$ want large $\hat{y} \Rightarrow \hat{y} \approx 1 (0 \leq \hat{y} \leq 1)$

want large $\log(1-\hat{y}) \Rightarrow$ want small $\hat{y} \Rightarrow \hat{y} \approx 0 (0 \leq \hat{y} \leq 1)$

- Cost function: measure how well algorithm is doing on

↳ cost of parameters entire training set

= average of loss function applied to each of m training samples

⇒ find best parameters $w & b$ that minimizes cost function J .

$$J(w, b) = \frac{1}{m} \sum_{i=1}^m L(\hat{y}^{(i)}, y^{(i)}) = -\frac{1}{m} \sum_{i=1}^m y^{(i)} \log \hat{y}^{(i)} - (1-y^{(i)}) \log (1-\hat{y}^{(i)})$$

• Logistic Regression Cost function

- Why do we use $L(y, \hat{y}) = -(y \log \hat{y} + (1-y) \log (1-\hat{y}))$ as a cost function?

Given $x, x \in \mathbb{R}^{n_x}$

Want $\hat{y} = P(y=1|x) \approx y \Rightarrow \hat{y} = y \text{ if } 1 \leq \hat{y} \leq 1$

Parameters: $w \in \mathbb{R}^{n_x}$, $b \in \mathbb{R}$ (real number)

binary classification

$$\text{If } y=1 : P(y|x) = \hat{y}$$

$$\text{If } y=0 : P(y|x) = 1-\hat{y}$$

⇒ Let's summarize these 2 equations into a single equation.

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

↳ how? because this equation returns exactly what we wanted!

$$\text{If } y=1 : P(y|x) = \hat{y}$$

$$\text{If } y=0 : P(y|x) = (1-\hat{y})$$

⇒ What about log?

∴ log function is strictly monotonically increasing function,

Maximizing $\log p(y|x)$ gives you similar result of maximizing $p(y|x)$

$$\log P(y|x) = y \log \hat{y} - (1-y) \log(1-\hat{y}) = -L(\hat{y}, y)$$

minimize loss function
= maximize log of probability

↳ increasing probability ↑
in other algorithms, but
logistic algorithm wants to
minimize the loss function

- Overall cost function on the m training samples

$$P(\text{Labels in training set}) = \prod_{i=1}^m p(y^{(i)}|x^{(i)})$$

↳ samples are iid

⇒ to carry out maximum likelihood estimation, find out parameter that maximizes
chance of observations of training set

$$\log(P(\text{Labels in training set})) = \log\left(\prod_{i=1}^m p(y^{(i)}|x^{(i)})\right)$$

$$= \sum_{i=1}^m \log(p(y^{(i)}|x^{(i)}))$$

$-L(\hat{y}^{(i)}, y^{(i)})$

$$= - \sum_{i=1}^m L(\hat{y}^{(i)}, y^{(i)})$$

We want to minimize the cost,

as maximize the likelihood

⇒ removed (-) sign)

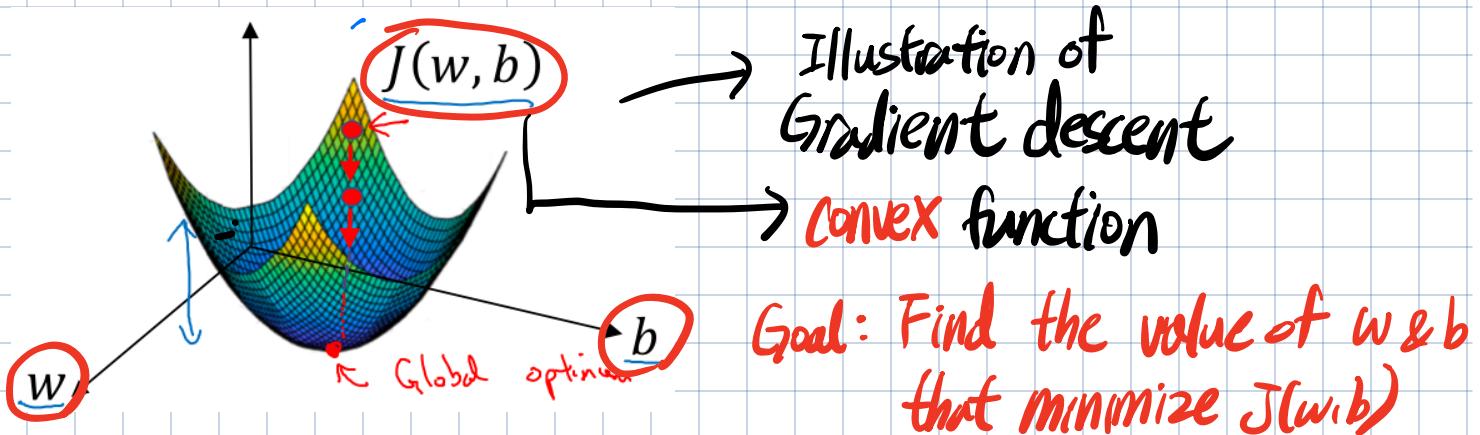
and $\frac{1}{m}$ for better scale

$$\Rightarrow \text{Cost: } J(w, b) = \frac{1}{m} \sum_{i=1}^m L(\hat{y}^{(i)}, y^{(i)})$$

⇒ By minimizing $J(w, b)$, carry out maximum likelihood estimation
over the regression model (under assumption training samples are iid)

• Gradient descent

- how to train (learn) w and b on the training set?

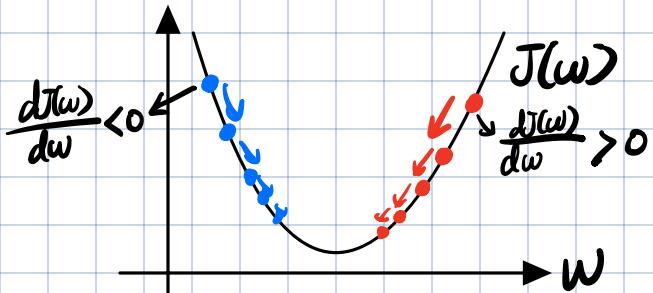


① Set initial value to $(0, 0)$ → [Random value effect]

② Take a step to the steepest direction

③ Iterate step ② until it converges to the global optimum

- Let's simplify $J(w, b) \rightarrow J(w)$ ($3D \rightarrow 2D$)



∴ Repeat $\left\{ \begin{array}{l} w := w - \alpha \frac{dJ(w)}{dw} \\ \end{array} \right.$

↗ dw in Python

⇒ In cost function...

$J(w, b)$

$$w := w - \alpha \frac{dJ(w, b)}{dw}$$

$$b := b - \alpha \frac{dJ(w, b)}{db}$$

Implementation

$J(w, b)$

$$w := w - \alpha dw$$

$$b := b - \alpha db$$

* Notation

$:=$:update

α : learning rate (step size)

$\frac{dJ(w)}{dw}$: derivative = slope of the function, used for update of the change of w

$\partial(\partial)$: used for derivative of function with 2 or more variables

• Computation Graph

- Computation of neural network [forward propagation \rightarrow computes output.

[back propagation \rightarrow compute gradients (derivatives)]

- Try compute

$$J(a, b, c) = 3(a + bc) \Rightarrow \text{In LR, } J \text{ is cost function to minimize}$$

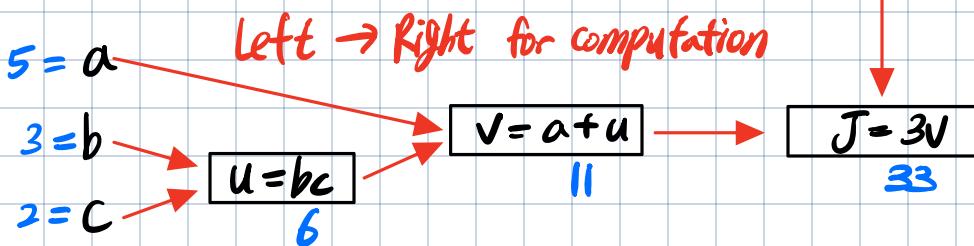
① Compute U , $U = bc$

Computation graph

② Compute V , $V = a + U$

\Rightarrow distinguish specific output
that you want to optimize

③ Compute J , $J = 3V$



• Derivatives with a computation graph

- let's compute derivative of J with respect to V

\Rightarrow How would the value of J change if we change the value of V ?

$$b = 3 \rightarrow 3.001$$

$$U = b \cdot c = 6 \rightarrow 6.002$$

$$\therefore \frac{dJ}{db} = \frac{dJ}{du} \cdot \frac{du}{db} = 6$$

3 2

$$J = 3V$$

$$a = 5 \rightarrow 5.001$$

$$V = 11 \rightarrow 11.001$$

$$J = 33 \rightarrow 33.003$$

$$\therefore \frac{dJ}{da} = 3$$

$$J = 3V$$

$$V = 11 \rightarrow 11.001$$

$$J = 33 \rightarrow 33.003$$

$$\therefore \frac{dJ}{dv} = 3$$

$$\frac{dJ}{db}$$

$$5 = a$$

$$\therefore \frac{dJ}{da} = 3 \rightarrow da$$

$$\frac{dJ}{dv} = 3 \rightarrow dv$$

$$\begin{array}{c}
 \frac{\partial J}{\partial b} = 6 \quad 3 = b \\
 \frac{\partial J}{\partial c} = 9 \quad 2 = c \\
 \frac{\partial J}{\partial u} = 3 \quad 11 \\
 \frac{\partial J}{\partial v} = 3 \quad 33 \\
 \end{array}$$

$$\frac{dJ}{dc} = \frac{dJ}{du} \cdot \frac{du}{dc} = 9$$

$$\therefore \frac{du}{db} = 2$$

$$\begin{aligned}
 u &= 6 \rightarrow 6.001 \\
 v &= 11 \rightarrow 11.001 \\
 J &= 33 \rightarrow 33.003
 \end{aligned}$$

$$\therefore \frac{dJ}{du} = 3 = \frac{dJ}{dv} \cdot \frac{dv}{du}$$

- Chain rule

\Rightarrow if you change $a \rightarrow$ change $v \rightarrow$ change J

a 를 바꿧을 때 J 의 변화량 = a 를 바꿧을 때 v 의 변화량 \times v 를 바꿧을 때 J 의 변화량

$$\frac{dJ}{da} = \frac{dJ}{dv} \times \frac{dv}{da}$$

* Notation

$\frac{d\text{final output var}}{d\text{var}}$ \Rightarrow dvar : derivative of the final output with respect to intermediate quantities.

• Logistic Regression Gradient Descent

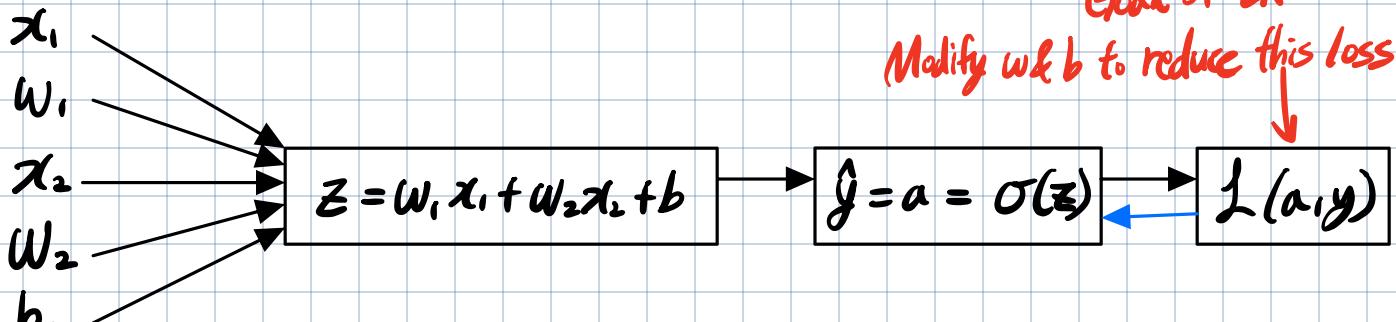
- logistic Regression Recap

$$z = w^T x + b$$

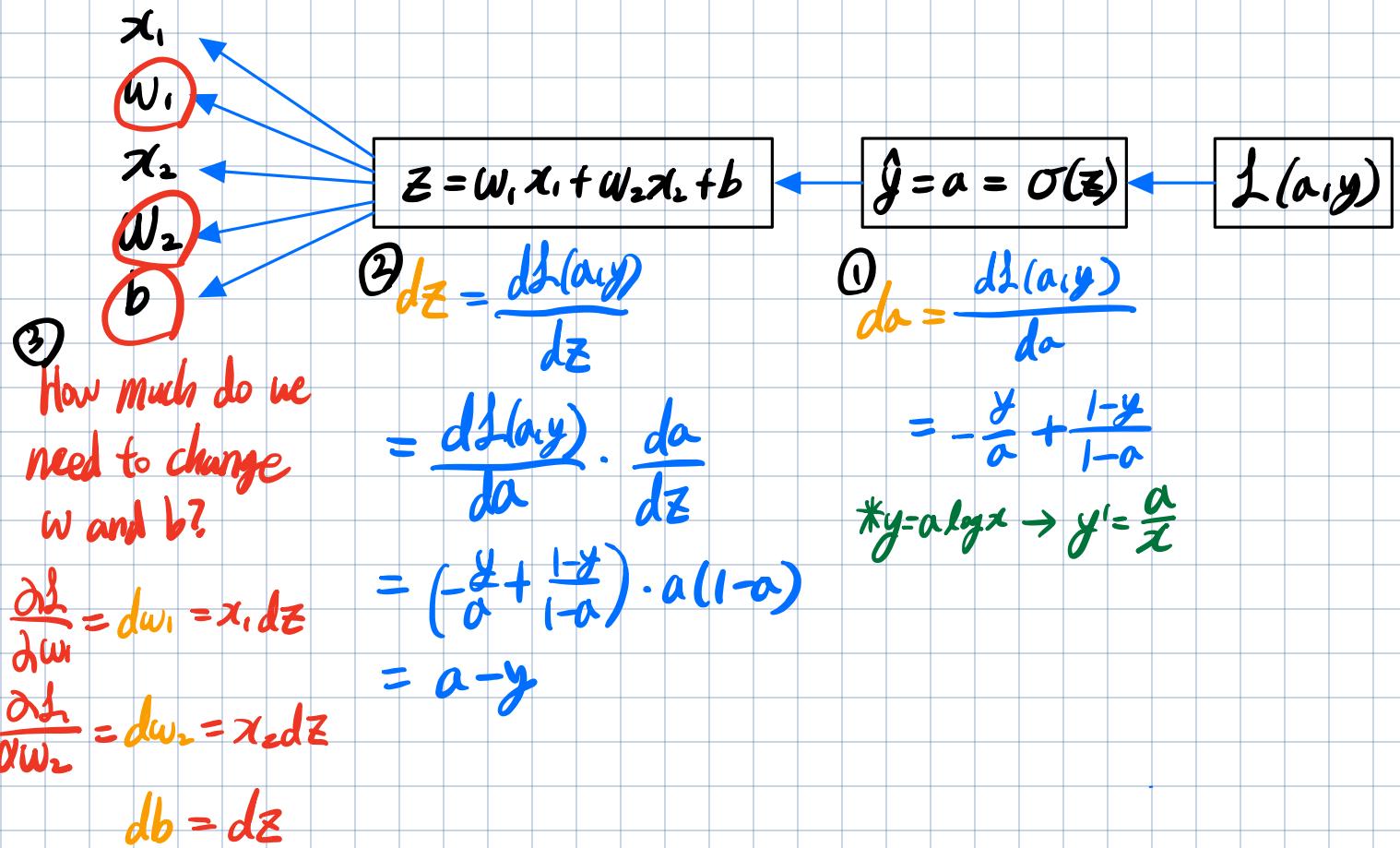
$$\hat{y} = a = \sigma(z)$$

$$L(a, y) = -(y \log(a) + (1-y) \log(1-a))$$

- Computation graph of LR (with 2 features)



- Backpropagation of LR
 \Rightarrow Compute derivative of $L(a, y)$



- Perform gradient descent to a single training sample..

① Compute $dz \rightarrow dw_1, dw_2, db$

② Update the values

$$w_1 := cw_1 - \alpha dw_1$$

$$w_2 := cw_2 - \alpha dw_2$$

$$b := b - \alpha db$$

\Rightarrow What about m training samples?

• Gradient descent on m example

- Cost function

$$J(w, b) = \frac{1}{m} \sum_{i=1}^m L(a^{(i)}, y^{(i)}) \rightarrow \text{average of individual losses}$$

$$a^{(i)} = \hat{y}^{(i)} = \sigma(Z^{(i)}) = \sigma(W^T x^{(i)} + b)$$

$$\frac{d}{dw_i} J(w, b) = \frac{1}{m} \sum_{i=1}^m \frac{\partial}{\partial w_i} \underbrace{L(a^{(i)}, y^{(i)})}_{dw_i^{(i)} - (x^{(i)}, y^{(i)})} \rightarrow \text{average of individual derivatives}$$

↳ overall gradient

- Let's implement algorithm

① Initialization

$$J=0, dw_1=0, dw_2=0, db=0 \quad \begin{matrix} \xrightarrow{\text{accumulative}} \\ \text{Var} \\ \therefore \text{no } (i) \end{matrix} \quad dw_i = \frac{\partial J}{\partial w_i}$$

② Calculate derivatives

For $i=1$ to m

$$Z^{(i)} = W^T x^{(i)} + b$$

$$a^{(i)} = \sigma(Z^{(i)})$$

$$J += -[y^{(i)} \log a^{(i)} - (1-y^{(i)}) \log (1-a^{(i)})]$$

\nwarrow i-th training sample

$$dz^{(i)} = a^{(i)} - y^{(i)}$$

$$dw_1 += x_1^{(i)} dz^{(i)} \quad] \quad 2 \text{ features}$$

$$dw_2 += x_2^{(i)} dz^{(i)}$$

$$db += dz^{(i)}$$

$$J/m$$

$$dw_1/m; dw_2/m, db/m$$

③ Implement 1 step of gradient descent

$$w_1 := w_1 - \alpha dw_1$$

$$w_2 := w_2 - \alpha dw_2$$

$$b := b - \alpha db$$

④ Repeat multiple steps of gradient descent

- Weakness of this implement: 2 for loops over m training samples & n features
 \Rightarrow efficiency ↓

⇒ Use vectorization for deep learning with large data set.

• Vectorization

— to avoid expliciting **for loops**

— what is vectorization?

$$z = \underline{w^T x + b} \Rightarrow w = \begin{bmatrix} \vdots \\ \vdots \end{bmatrix}, w \in \mathbb{R}^{n_x} \quad x = \begin{bmatrix} \vdots \\ \text{y} \\ \vdots \end{bmatrix}, x \in \mathbb{R}^{n_x}$$

↓

Non-vectorized

$$z = 0$$

for i in range(n_x):

$$z += w[i] * x[i]$$

$$z += b$$

→ Slow

Vectorized

$$z = \underbrace{\text{np. dot}(w, x)}_{w^T x} + b$$

→ Just compute $w^T x$ directly (Fast)

→ Single Instruction Multiple Data

— CPU & GPU have parallelized command (SIMD)

→ built-in function like np.dot can compute much faster

• More Vectorization Examples

— Whenever possible, avoid explicit for-loops.

e.g. $u = A v$
 Vector ↘ Vector
 Matrix ↘ Matrix multiply

$$u_i = \sum_j A_{ij} v_j$$

Non-vectorized

for-loops [for i ...
 2 for j ...
 $u[i] += A[i][j] * v[j]$

Vectorized

$$u = \text{np. dot}(A, v)$$

- Say you need to apply the exponential operation on every element of a Matrix/vector

$$v = \begin{bmatrix} v_1 \\ \vdots \\ v_n \end{bmatrix} \quad u = \begin{bmatrix} e^{v_1} \\ \vdots \\ e^{v_n} \end{bmatrix}$$

Non-vectorized

$$u = np.zeros((n, 1))$$

for i in range(n):

$$u[i] = \text{math.exp}(v[i])$$

Vectorized

$$u = np.exp(v)$$

- Let's apply to gradient descent to remove a for-loop.

⇒ Remove one for-loop (②)

<Non-Vectorized>

$$J=0, [dw_1=0, dw_2=0], db=0$$

① For i=1 to m

$$z^{(i)} = w^T x^{(i)} + b$$

$$a^{(i)} = \sigma(z^{(i)})$$

$$J += -[y^{(i)} \log a^{(i)} - (1-y^{(i)}) \log (1-a^{(i)})]$$

$$dz^{(i)} = a^{(i)} - y^{(i)}$$

② $\begin{aligned} &\text{for } j=1 \dots n \\ &dw_j += \dots \end{aligned}$

$$\begin{aligned} \text{②} \quad dw_1 &+= x_1^{(i)} dz^{(i)} \\ dw_2 &+= x_2^{(i)} dz^{(i)} \end{aligned}$$

$$\text{③ } db += dz^{(i)}$$

$$J /= m, [dw_1 /= m, dw_2 /= m, db /= m]$$

<Vectorized>

$$dw = np.zeros((n_x, 1))$$

$$dw = x^{(i)} dz^{(i)}$$

$$dw / m$$

• Vectorizing Logistic Regression

- Forward Propagation

$$z^{(1)} = w^T x^{(1)} + b$$

$$a^{(1)} = \sigma(z^{(1)})$$

$$z^{(2)} = w^T x^{(2)} + b$$

$$a^{(2)} = \sigma(z^{(2)})$$

$$z^{(3)} = w^T x^{(3)} + b$$

$$a^{(3)} = \sigma(z^{(3)})$$

$$\begin{bmatrix} 1 & 1 & 1 & 1 \end{bmatrix}$$

$$X = \begin{bmatrix} | & | & | \\ x^{(1)} & x^{(2)} & \dots & x^{(m)} \\ | & | & | \end{bmatrix}, X \in \mathbb{R}^{n_x \times m}$$

← Stack feature vector x horizontally

⇒ how to compute $z^{(1)}, z^{(2)}, z^{(3)}, \dots$ all in one-line code?

Make a row vector...

$$\begin{aligned} [z^{(1)} \ z^{(2)} \ \dots \ z^{(m)}] &= w^T X + [b \ b \ \dots \ b] \Rightarrow w^T \begin{bmatrix} | & | & | \\ x^{(1)} & x^{(2)} & \dots & x^{(m)} \\ | & | & | \end{bmatrix} \\ &= [w^T x^{(1)} + b \ \dots \ w^T x^{(m)} + b] \end{aligned}$$

$\underbrace{\quad \quad \quad}_{(1,m) \text{ vector}}$

⇒ Just as X was obtained by stacking training samples **horizontally**,

Define Z as...

$$\begin{aligned} Z &= [z^{(1)} \ z^{(2)} \ \dots \ z^{(m)}] = w^T X + [b \ b \ \dots \ b] \\ &\quad (1,m) \\ &= np.\text{dot}(w^T, X) + b \end{aligned}$$

* broadcasting

$- b \in \mathbb{R} \Rightarrow [b, b, b, \dots, b]$: python automatically change real number b into a vector/matrix when real num + vector/matrix

⇒ how to compute $a^{(1)}, a^{(2)}, a^{(3)}, \dots, a^{(m)}$ all in one-line code?

stack $a^{(i)}$ horizontally and define as A

$$A = [a^{(1)}, a^{(2)}, \dots, a^{(m)}] = \sigma(Z)$$

• Vectorizing Logistic Regression's Gradient Computation

- Back propagation

$$dz^{(1)} = a^{(1)} - y^{(1)} \quad dz^{(2)} = a^{(2)} - y^{(2)}$$

$$dZ = [dz^{(1)} \ dz^{(2)} \ \dots \ dz^{(m)}] = [a^{(1)} - y^{(1)} \ \dots \ a^{(m)} - y^{(m)}] = A - Y \quad (1 \times m)$$

$$A = [a^{(1)} \ \dots \ a^{(m)}]$$

$$Y = [y^{(1)} \ \dots \ y^{(m)}]$$

- Vectorizing db

$$\begin{cases} \sum db = 0 \\ db_1 += dz^{(1)} \\ db_2 += dz^{(2)} \\ \vdots \\ db_m += dz^{(m)} \\ db / = m \end{cases}$$

$$\Rightarrow db = \frac{1}{m} \sum_{i=1}^m dz^{(i)} = \frac{1}{m} np.sum(dz)$$

row vector

- Vectorizing $d\omega$

$$\begin{cases} \sum d\omega = 0 \\ d\omega_1 += x^{(1)} dz^{(1)} \\ d\omega_2 += x^{(2)} dz^{(2)} \\ \vdots \\ d\omega_m += x^{(m)} dz^{(m)} \\ d\omega / = m \end{cases}$$

$$\begin{aligned} \Rightarrow d\omega &= \frac{1}{m} \begin{bmatrix} | & | \\ x^{(1)} & \dots & x^{(m)} \\ | & | \end{bmatrix} \begin{bmatrix} dz^{(1)} \\ \vdots \\ dz^{(m)} \end{bmatrix} \\ &= \frac{1}{m} [x^{(1)} dz^{(1)} + \dots + x^{(m)} dz^{(m)}]_{(m, 1)} \\ &= \frac{1}{m} X dz^T \end{aligned}$$

<Non-Vectorized>

$$J=0, d\omega_1=0, d\omega_2=0, db=0$$

For $i=1$ to m

$$Z^{(i)} = w^T x^{(i)} + b$$

$$a^{(i)} = \sigma(Z^{(i)})$$

$$J += -[y^{(i)} \log a^{(i)} - (1-y^{(i)}) \log(1-a^{(i)})]$$

$$dz^{(i)} = a^{(i)} - y^{(i)}$$

$$d\omega_1 += x_1^{(i)} dz^{(i)}$$

$$d\omega_2 += x_2^{(i)} dz^{(i)}$$

$$db += dz^{(i)}$$

$$J /= m, d\omega_1 /= m, d\omega_2 /= m, db /= m$$

<Vectorized>

$$J=0, db=0$$

$$d\omega = np.zeros((n_x, 1))$$

$$Z = np.dot(w.T, X) + b$$

$$dZ = A - Y$$

$$d\omega = \frac{1}{m} X dZ^T$$

$$db = \frac{1}{m} np.sum(dZ)$$

$$w := w - \alpha d\omega$$

$$b := b - \alpha db$$

→ a single step of gradient descent

→ you have to use for loop to specify # of iteration

• Broadcasting in Python

- Example: Calculate % of calories from carb, protein, and fat from each of the food without for-loop.

	Apples	Beef	Eggs	Potatoes	
Carb	56.0	0.0	4.4	68.0	
Protein	1.2	104.0	52.0	8.0	
Fat	1.8	135.0	99.0	0.9	

① Sum down the columns

$$\text{cal} = A.\text{sum}(\text{axis}=0) \quad ((1,4))$$

* np axis

0: column (1/3)

1: row (7/3)

② Divide each of the 4 columns by their corresponding sum

$$\text{percentage} = 100 * A / \text{cal}. \text{reshape}((1,4))$$

→ 행별로 100% 합산하기 | 단위 %

- how can you divide 3x4 matrix by 1x4 matrix?

⇒ python automatically expands 1x4 to 3x4

e.g.

$$\begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \end{bmatrix} + \frac{1}{100} \rightarrow \begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \end{bmatrix} + \begin{bmatrix} 100 \\ 100 \\ 100 \\ 100 \end{bmatrix} = \begin{bmatrix} 101 \\ 102 \\ 103 \\ 104 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix} + \begin{bmatrix} 100 \\ 200 \end{bmatrix} \rightarrow = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix} + \begin{bmatrix} 100 & 100 & 100 \\ 200 & 200 & 200 \end{bmatrix} = \begin{bmatrix} 101 & 102 & 103 \\ 104 & 105 & 106 \end{bmatrix}$$

- General Principle of broadcasting

(m, n) + -*/ (1, n) or (m, 1)

Matrix

\downarrow
(m,n)

\downarrow
(m,n)

⇒ element-wise calculation

, (m, 1) + -*/ Real#

⇒ element-wise calculation

$(1, n)$

↓ copying n times

$(m, 1)$ of Real num
 $(1, n)$

• A Note on python / numpy vectors

- When construct vectors **never use rank 1 array!**

$a = np.random.randn(5)$

$print(a.shape) \Rightarrow (5,)$ → rank 1 array (neither row/column vector)

⇒ $a.T$ does not change the shape

⇒ $np.dot(a, a)$ returns a real number

- Proper way to construct vectors

$a = np.random.randn(5, 1)$

$a.shape = (5, 1)$ → 5×1 matrix (Column Vector)

⇒ $a.T$ returns 1×5 matrix

⇒ $np.dot(a, a)$ returns outer product
(matrix)

- Tip:

[Use assert to ensure dimension of vectors

Assert ($a.shape == (5, 1)$)

] when you got rank 1 array, Use reshape

$a = a.reshape((5, 1))$