

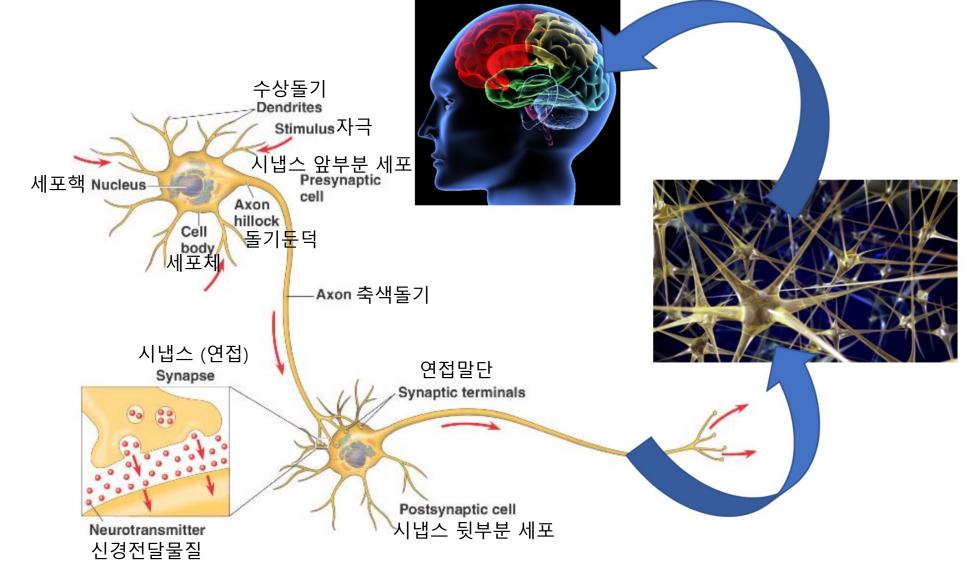
# Learning & Autograd

Sept. 2023

http://link.koreatech.ac.kr

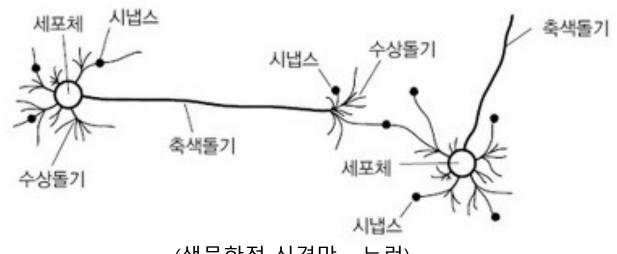
### **Human Brain**

# ◈Neuron (신경 세포)

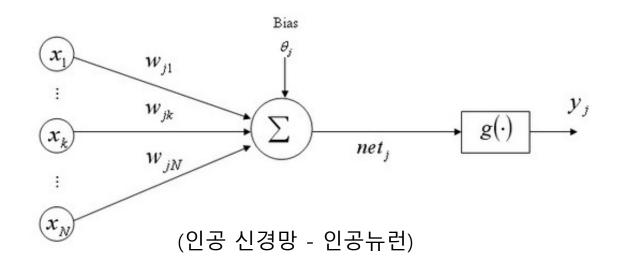


### **Human Brain**

### **♦**Neuron



— —.		
(생물학적	시겨마	느러기
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생물학적 신경망	인공 신경망
Dendrites (수상돌기)	Inputs
Cell Body (세포체)	Neuron
Axon (축색돌기)	Outputs

### **♦** Simple data representation

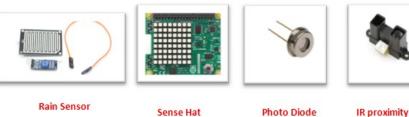
- Measurements by new two sensors
  - X = [[0.5, 0.9], [14.0, 12.0], [15.0, 13.6],[28.0, 22.8], [11.0, 8.1], [8.0, 7.1], [3.0, 2.9], [-4.0, 0.1], [6.0, 5.3], [13.0, 12.0], [21.0, 19.9], [-1.0, 1.5]]
  - Dataset shape:  $N \times F = 12 \times 2 \rightarrow (12, 2)$



#### Different types of Sensors



**Proximity Sensor** 







- Temperatures (measured at the same times of X measurement)

- y = [35.7, 55.9, 58.2, 81.9, 56.3, 48.9, 33.9, 21.8, 48.4, 60.4, 68.4, 29.1]
- This is a kind of target 'LABEL'
- Target dataset shape: (12,)



Sensor

 $\odot$  Simple data representation  $\rightarrow$  Simple Dataset (1/2)

```
class SimpleDataset(Dataset):
 def init (self, *args, **kwargs):
   super().__init__(*args, **kwargs)
   X = [[0.5, 0.9], [14.0, 12.0], [15.0, 13.6],
        [28.0, 22.8], [11.0, 8.1], [8.0, 7.1],
        [3.0, 2.9], [4.0, 0.1], [6.0, 5.3],
        [13.0, 12.0], [21.0, 19.9], [-1.0, 1.5]
   y = [35.7, 55.9, 58.2, 81.9, 56.3, 48.9, 33.9, 21.8, 48.4, 60.4, 68.4, 29.1]
   self.X = torch.tensor(X, dtype=torch.float, device=device)
   self.y = torch.tensor(y, dtype=torch.float, device=device)
   self.y = self.y * 0.01
```

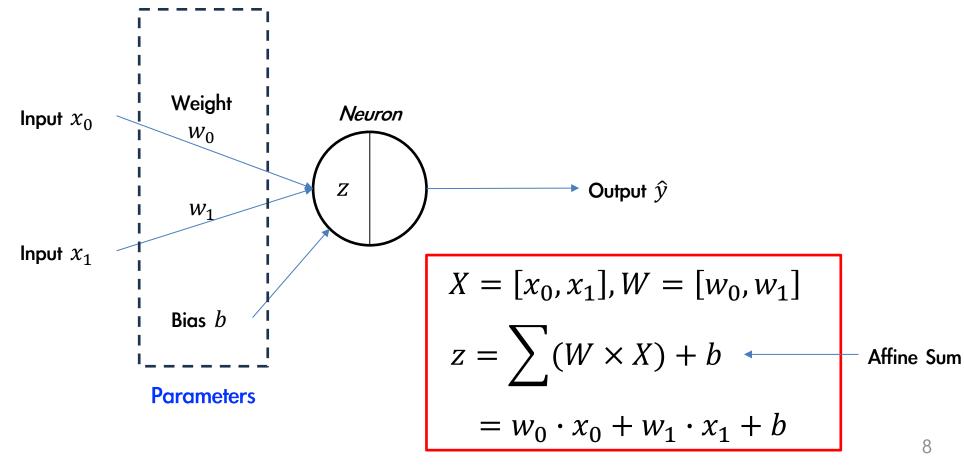
 $\odot$  Simple data representation  $\rightarrow$  Simple Dataset (2/2)

```
class SimpleDataset(Dataset):
 def len (self):
   return len(self.X)
 def getitem (self, idx):
   return {'input': self.X[idx], 'target': self.y[idx]}
 def str (self):
   str = "Data Size: {0}, Input Shape: {1}, Target Shape: {2}".format(
     len(self.X), self.X.shape, self.y.shape
   return str
```

### **Artificial Neuron**

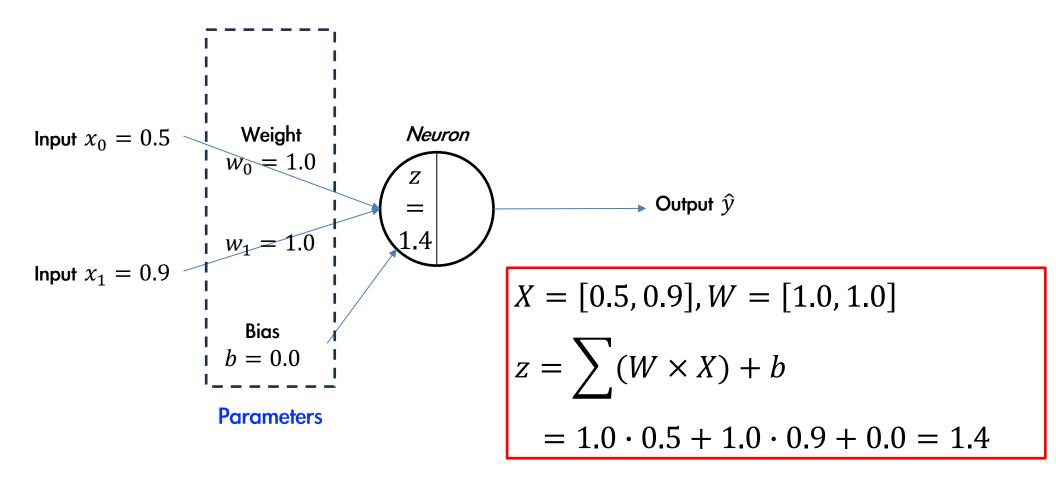
- A mathematical function conceived as a model of biological neurons

[Weight Multiply & Bias Sum]



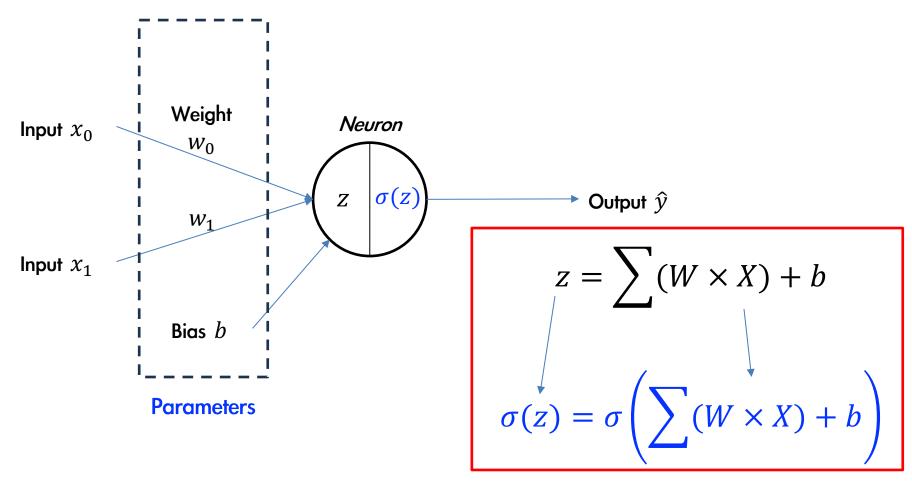
### **Artificial Neuron**

#### [Weight Multiply & Bias Sum]



### **Artificial Neuron**

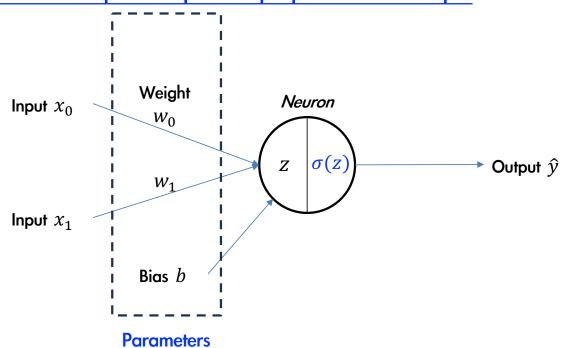
#### [Activation function $(\sigma)$ ]



#### **Artificial Neuron**

#### [Activation function $(\sigma)$ ]

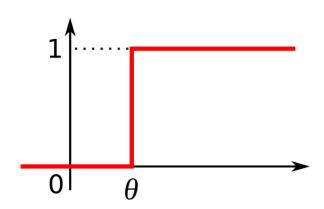
- A function that transforms input signals into output signals
- It transforms or squashes input signals
- The main goal of it is to introduce non-linear properties into the neural network
  - Non-linear mappings applied to inputs can capture important properties of the input
- Activation function examples
  - > Sigmoid
  - > Tanh
  - **➢** ReLU
  - **►** LeakyReLU
  - > ELU
  - >...



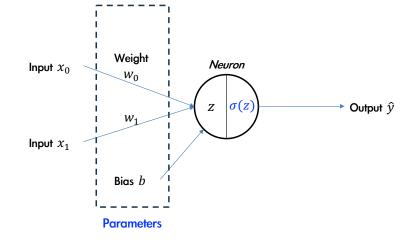


[Activation function  $(\sigma)$ ]

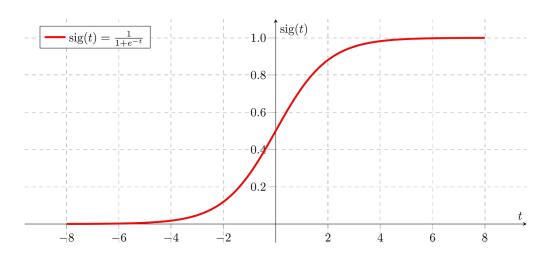




$$\sigma(z) = \begin{cases} 1 & \text{if } z \ge \theta \\ 0 & \text{otherwise} \end{cases}$$



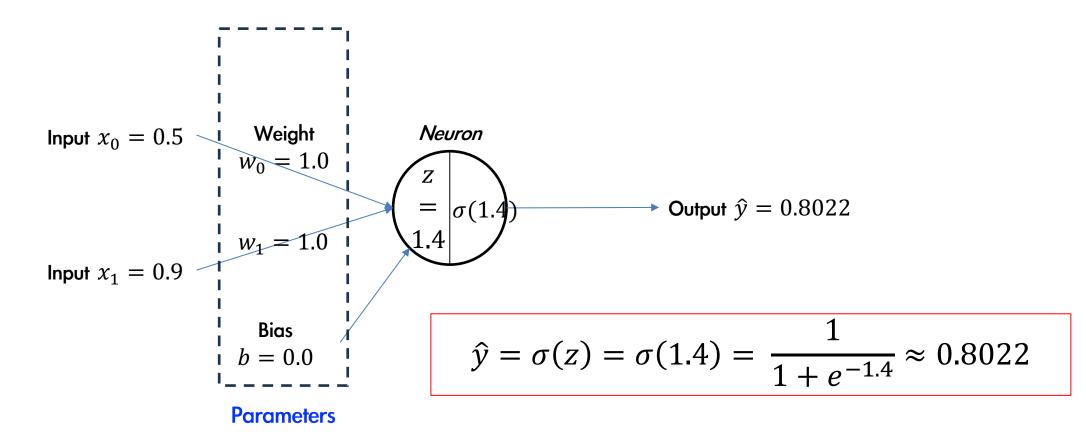
#### Sigmoid (or Logistic Activation)



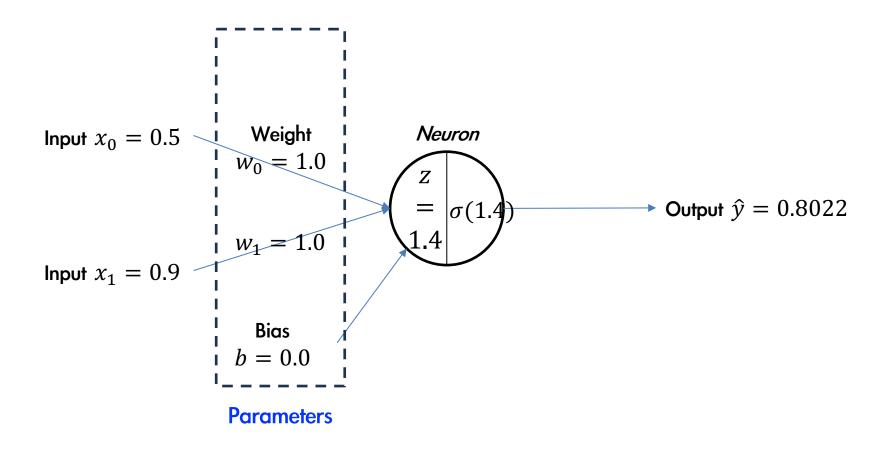
$$\sigma(z) = \frac{1}{1 + e^{-z}}$$

### **Artificial Neuron**

#### [Activation function $(\sigma)$ ]



$$\hat{y} = \sigma(z) = \sigma\left(\sum (W \times X) + b\right) = \frac{1}{1 + e^{-(\sum (W \times X) + b)}}$$



```
def model(X, W, b):
     print(X.shape) # >>> torch.Size([12, 2])
     print(W.shape) # >>> torch.Size([2])
                                                                              Weight
                                                                                             Neuron
                                                                 Input x_0
     print(b.shape) # >>> torch.Size([1])
                                                                                                \sigma(z)
                                                                                                                  lacktriangle Output \widehat{\mathcal{V}}
     u = torch.sum(X * W, dim=1) + b
     # u.shape: torch.Size([12])
                                                                 Input \chi_1
                                                                              Bias b
     z = activate(u)
                                                                            Parameters
     return z
                                                               X = [x_0, x_1], W = [w_0, w_1]z = \sum (W \times X) + b= w_0 \cdot x_0 + w_1 \cdot x_1 + b
def activate(u):
     return torch.sigmoid(u)
                                                                                                                   Affine Sum
```

```
def main():
   W = torch.ones((2,))
    b = torch.zeros((1,))
    simple_dataset = SimpleDataset()
   train_data_loader = DataLoader(dataset=simple_dataset, batch_size=len(simple_dataset))
    batch = next(iter(train_data_loader))
   y pred = model(batch["input"], W, b)
    print(y_pred.shape) # >>> torch.Size([12])
    print(y_pred) # >>> tensor([0.8022, 1.0000, 1.0000, 1.0000, 1.0000, 1.0000,
                       #
                                      0.9973, 0.0198, 1.0000, 1.0000, 1.0000, 0.6225])
if __name__ == "__main__":
   main()
```

# Learning with Gradient Descent

### Predicted Output & Target Output

- Feature Data
  - X = [[0.5, 0.9], [14.0, 12.0], [15.0, 13.6], [28.0, 22.8], [11.0, 8.1], [8.0, 7.1], [3.0, 2.9], [-4.0, 0.1], [6.0, 5.3], [13.0, 12.0], [21.0, 19.9], [-1.0, 1.5]]
  - Target output (label)
    - y = [35.7, 55.9, 58.2, 81.9, 56.3, 48.9, 33.9, 21.8, 48.4, 60.4, 68.4, 29.1]

b = 0.0

- Predicted output (by artificial neuron)
  - $\hat{y} = [0.8022, 1.0000, 1.0000, 1.0000, 1.0000, 1.0000, 0.9973, 0.0198, 1.0000, 1.0000, 1.0000, 0.6225]$

### lacktriangleLoss (or Error) for m data samples

MSE (Mean Square Error)

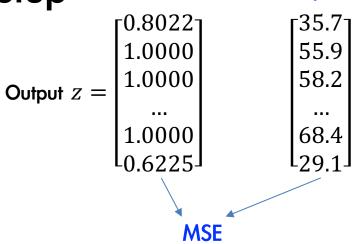
$$L(W,b) = \frac{1}{m} \sum_{x} (\hat{y} - y)^2 = \frac{1}{m} \sum_{x} \left( \sigma \left( \sum_{x} (W \times X) + b \right) - y \right)^2$$

RMSE (Root Mean Square Error)

$$L(W,b) = \sqrt{\frac{1}{m}\sum (\hat{y} - y)^2} = \sqrt{\frac{1}{m}\sum \left(\sigma\left(\sum (W \times X) + b\right) - y\right)^2}$$

MAE (Mean Absolute Error)

$$L(W,b) = \frac{1}{m} \sum |\hat{y} - y| = \frac{1}{m} \sum \left| \sigma \left( \sum (W \times X) + b \right) - y \right|$$



$$L(W,b) = \frac{1}{m} \sum_{i} (\hat{y} - y)^{2}$$

$$= \frac{1}{12} \sum_{i=1}^{n} \left[ \begin{bmatrix} 0.8022 \\ 1.0000 \\ 1.0000 \\ ... \\ 1.0000 \\ 0.6225 \end{bmatrix} - \begin{bmatrix} 35.7 \\ 55.9 \\ 58.2 \\ ... \\ 68.4 \\ 29.1 \end{bmatrix} \right]^{2}$$

$$= 2673.9028$$

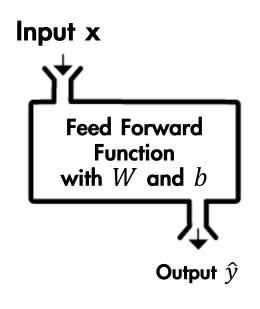
y

lacktriangleLoss (or Error) for m data samples

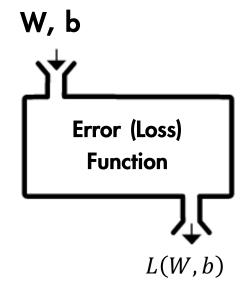
```
def loss_fn(y_pred, y):
   loss = torch.square(y_pred - y).mean()
   assert loss.shape == () or loss.shape == (1,)
   return loss
def main():
   W = torch.ones((2,))
   b = torch.zeros((1,))
   simple_dataset = SimpleDataset()
   train_data_loader = DataLoader(dataset=simple_dataset, batch_size=len(simple_dataset))
   batch = next(iter(train data loader))
   y_pred = model(batch["input"], W, b)
   print(y pred.shape) # >>> torch.Size([12])
   print(y_pred) # >>> tensor([0.8022, 1.0000, 1.0000, 1.0000, 1.0000, 1.0000,
                                     0.9973, 0.0198, 1.0000, 1.0000, 1.0000, 0.6225])
   loss = loss_fn(y_pred, batch["target"])
   print(loss) # >>> tensor(0.2254)
if name__ == "__main__":
   main()
```

### **♦**Our goal

Find  $W^*$  and  $b^*$  such that  $W^*, b^* = argmin_{W,b}L(W,b) = argmin_{W,b}\frac{1}{m}\sum_{i}(\hat{y} - y)^2$ 



$$\hat{y} = \sigma(z) = \sigma\left(\sum (W \times X) + b\right)$$



$$L(W,b) = \frac{1}{m} \sum_{i} (\hat{y} - y)^2$$

$$L(W,b) = \frac{1}{m} \sum_{i} (\hat{y} - y)^{2}$$
Our Goal
$$W^{*}, b^{*} = argmin_{W,b} L(W,b)$$

## ◈Derivative (도함수) of a function

$$f'(x) = \frac{df}{dx} =$$
 Derivative of a function  $f$ 

$$f'(x) = \frac{df}{dx} = \lim_{\Delta x \to 0} \frac{f(x + \Delta x) - f(x)}{\Delta x}$$

$$f'(x_0) = \frac{df}{dx} \bigg|_{x=x_0} = \lim_{\Delta x \to 0} \frac{f(x_0 + \Delta x) - f(x_0)}{\Delta x}$$

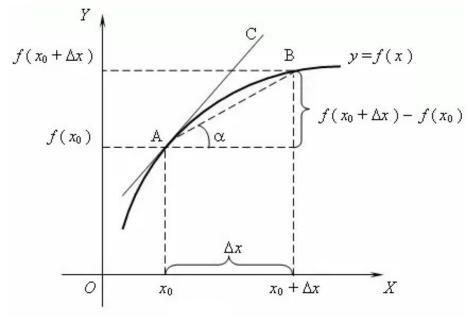
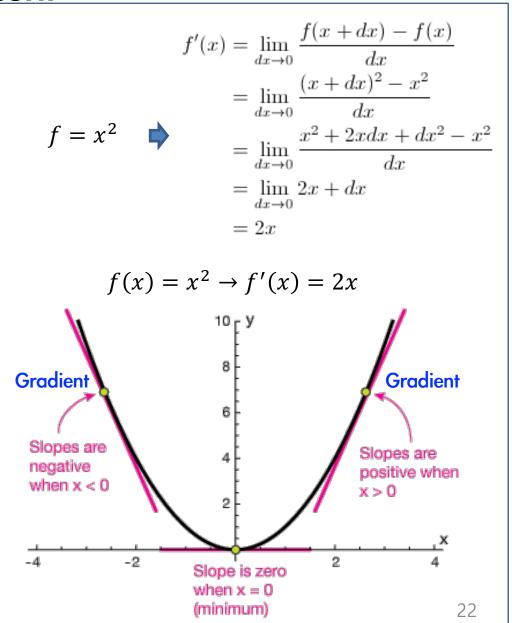


Fig. 1



- **Partial derivative** of a multi-variable function f(x, y, ...)
  - For a multi-variable function, like  $f(x,y) = x^2y$ , partial derivatives are as follows:

$$rac{\partial f}{\partial x} = rac{\partial}{\partial x} x^2 y = 2xy$$
Treat  $y$  as constant; take derivative.

$$f_x = \frac{\partial f}{\partial x} = \lim_{h \to 0} \frac{f(x+h,y) - f(x,y)}{h}$$

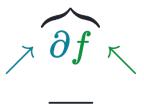
$$f_y = \frac{\partial f}{\partial y} = \lim_{h \to 0} \frac{f(x, y+h) - f(x, y)}{h}$$

$$rac{\partial f}{\partial x} = rac{\partial}{\partial x} x^2 y = 2xy \qquad \qquad rac{\partial f}{\partial y} = rac{\partial}{\partial y} x^2 y = x^2 \cdot 1$$

Treat x as constant; take derivative.

> Can be thought of as "a tiny change in the function's output"

Used instead of "d" in usual  $\frac{df}{dx}$  notation to emphasize that this is a partial derivative.



Multivariable function

Indicates which input variable is changed slightly.

Can be thought of as "a tiny change in x"

- **The Stradient** by partial derivative of a multi-variable function f(x, y, ...)
  - Gradient of a (scalar-valued) multi-variable function f(x, y, ...), denoted  $\nabla f$ , is the collection of all its partial derivatives into a vector

$$abla f = \left[ egin{array}{c} rac{\partial f}{\partial x} \ rac{\partial f}{\partial y} \ dots \end{array} 
ight]$$

— this means  $\nabla f$  is a vector-valued function

- **The Stradient** by partial derivative of a multi-variable function f(x, y, ...)
  - Example differential operators

Name	Symbol	Example
Derivative	$rac{d}{dx}$	$rac{d}{dx}(x^2)=2x$
Partial derivative	$rac{\partial}{\partial x}$	$rac{\partial}{\partial x}(x^2-xy)=2x-y$
Gradient	$\nabla$	$ abla(x^2-xy)=\left[egin{array}{c}2x-y\-x\end{array} ight]$

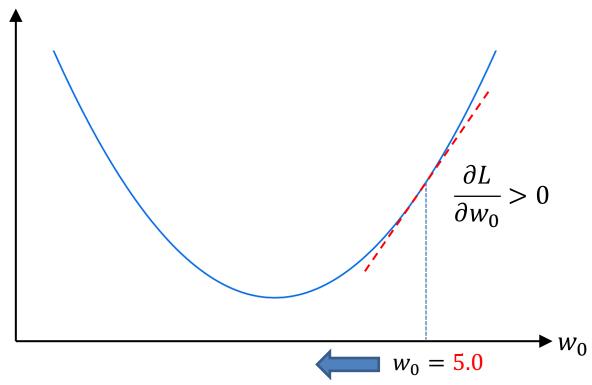
# $w_0^*, w_1^*, b^*$ = $argmin_{w_0, w_1, b} L(w_0, w_1, b)$

# ◈Gradient Descent Method (경사하강법)

$$L(W,b) = \frac{1}{m} \sum (\hat{y} - y)^2$$

$$= \frac{1}{m} \sum \left( \sigma \left( \sum (W \times X) + b \right) - y \right)^2$$

$$= \frac{1}{m} \sum (\sigma(x_0 \cdot w_0 + x_1 \cdot w_1 + b) - y)^2$$



$$w_0 = w_0 - \alpha \frac{\partial L}{\partial w_0}$$

**Using Partial Derivative** 

where  $\alpha$  is the learning rate

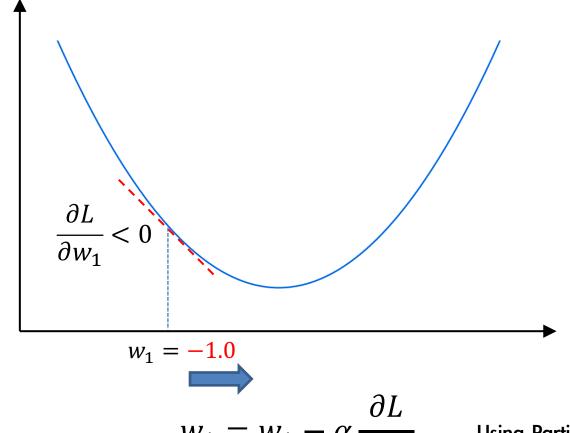
# $w_0^*, w_1^*, b^*$ = $argmin_{w_0, w_1, b} L(w_0, w_1, b)$

#### Gradient Descent Method

$$L(W,b) = \frac{1}{m} \sum (\hat{y} - y)^2$$

$$= \frac{1}{m} \sum \left( \sigma \left( \sum (W \times X) + b \right) - y \right)^2$$

$$= \frac{1}{m} \sum (\sigma(x_0 \cdot w_0 + x_1 \cdot w_1 + b) - y)^2$$



 $w_1 = w_1 - \alpha \frac{\partial L}{\partial w_1}$ 

**Using Partial Derivative** 

where  $\alpha$  is the learning rate

#### Gradient Descent Method

Find  $W^*$  and  $b^*$  such that

$$W^*, b^* = argmin_{W,b}L(W,b) = argmin_{W,b}\frac{1}{m}\sum_{k}(\hat{y} - y)^2$$

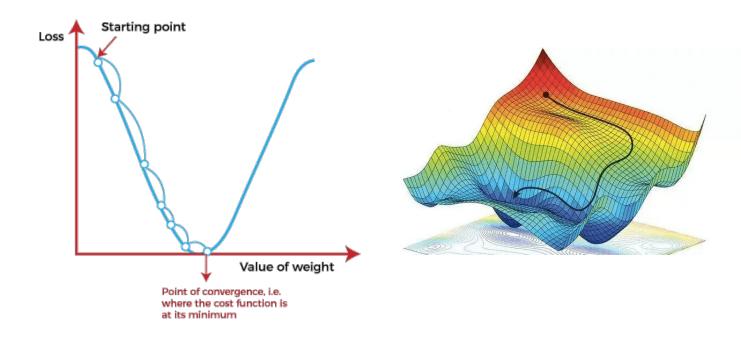
#### Solution:

$$w_0 = w_0 - \alpha \frac{\partial L}{\partial w_0}$$

$$w_1 = w_1 - \alpha \frac{\partial L}{\partial w_1}$$

$$b = b - \alpha \frac{\partial L}{\partial b}$$

where  $\alpha$  is the learning rate



#### Gradient Descent Method

Find  $W^*$  and  $b^*$  such that

$$W^*, b^* = argmin_{W,b}L(W,b) = argmin_{W,b}\frac{1}{m}\sum_{w}(\hat{y} - y)^2$$

The magnitude of each component of  $\nabla L$  is telling you that

"how sensitive the loss function 
$$L$$
 is to the current weight and bias"

$$VL = \begin{bmatrix} \frac{\partial L}{\partial w_0} \\ \frac{\partial L}{\partial w_1} \\ \frac{\partial L}{\partial b} \end{bmatrix} \qquad \begin{bmatrix} w_0 \\ w_1 \\ b \end{bmatrix} = \begin{bmatrix} w_0 \\ w_1 \\ b \end{bmatrix} - \alpha \begin{bmatrix} \frac{\partial L}{\partial w_0} \\ \frac{\partial L}{\partial w_1} \\ \frac{\partial L}{\partial b} \end{bmatrix} \qquad w_1 = w_1 - \alpha \frac{\partial L}{\partial w_1} \\ b = b - \alpha \frac{\partial L}{\partial b}$$

### **♦** Gradient Descent Method - Pseudo Code

#### Gradient descent

**Input**: Function *f* to minimize.

**Initialization**: initial weight vector  $w^{(0)}$  Weights & Bias

**Parameters**: step size  $\eta > 0$ . Learning Rate

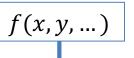
While not converge do

• 
$$\mathbf{w}^{(k+1)} \leftarrow \mathbf{w}^{(k)} - \eta \nabla f(\mathbf{w}^{(k)})$$

• 
$$k \leftarrow k + 1$$
.

Output:  $w^{(k)}$ .

### How to calculate gradient for a multi-variable function



#### Numerical Differentiation

$$f'(x) = \frac{\partial f}{\partial x} \approx \frac{f(x + \Delta x) - f(x)}{\Delta x}$$
$$= \frac{a(x + \Delta x)^n - a(x)^n}{\Delta x}$$

$$f'(x) = \frac{\partial f}{\partial x} \approx \frac{f(x + \Delta x) - f(x - \Delta x)}{2 \times \Delta x}$$
$$= \frac{a(x + \Delta x)^n - a(x - \Delta x)^n}{2 \times \Delta x}$$

$$f_x = \frac{\partial f}{\partial x} = \lim_{h \to 0} \frac{f(x+h,y) - f(x,y)}{h}$$

$$f_y = \frac{\partial f}{\partial y} = \lim_{h \to 0} \frac{f(x, y+h) - f(x, y)}{h}$$

#### Differentiation Formulas

$$\frac{d}{dx}k = 0$$

$$\frac{d}{dx}[f(x) \pm g(x)] = f'(x) \pm g'(x)$$

$$\frac{d}{dx}[k \cdot f(x)] = k \cdot f'(x)$$

$$\frac{d}{dx}[f(x)g(x)] = f(x)g'(x) + g(x)f'(x)$$

$$\frac{d}{dx}\left(\frac{f(x)}{g(x)}\right) = \frac{g(x)f'(x) - f(x)g'(x)}{[g(x)]^2}$$

$$\frac{d}{dx}f(g(x)) = f'(g(x)) \cdot g'(x)$$

$$\frac{d}{dx}x^n = nx^{n-1}$$

Chain Rule & Backpropagation

$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial g} \cdot \frac{\partial g}{\partial x}$$

$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial g} \cdot \frac{\partial g}{\partial h} \cdot \frac{\partial h}{\partial x}$$

$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial g} \cdot \frac{\partial g}{\partial h} \cdot \frac{\partial h}{\partial i} \cdot \frac{\partial i}{\partial x}$$

- **Differentiation formulas of a multi-variable function** f(x, y, ...)
  - Multiplication function of two numbers

$$f(x,y) = xy \longrightarrow \frac{\partial f}{\partial x} = y, \ \frac{\partial f}{\partial y} = x \longrightarrow \Delta f = \left[\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}\right] = [y,x]$$

• For example,

$$\Rightarrow x = 4, y = -3 \text{ then } f(x, y) = -12$$

The derivative on 
$$x$$
 and  $y$ :  $\frac{\partial f}{\partial x} = -3$   $\frac{\partial f}{\partial y} = 4$ 

- ➤ Interpretation
  - » If we increase the value of x by a tiny amount, the effect on the output would be to decrease it by -3
  - » If we increase the value of y by a tiny amount, the effect on the output would be to increase it by 4

- **Differentiation formulas of a multi-variable function** f(x, y, ...)
  - Addition function of two numbers

$$f(x,y) = x + y \longrightarrow \frac{\partial f}{\partial x} = 1, \ \frac{\partial f}{\partial y} = 1 \longrightarrow \Delta f = \left[\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}\right] = [1,1]$$

• For example,

$$> x = 4, y = -3$$
 then  $f(x, y) = 1$ 

The derivative on 
$$x$$
 and  $y$ :  $\frac{\partial f}{\partial x} = 1$   $\frac{\partial f}{\partial y} = 1$ 

- ➤ Interpretation
  - » This makes sense, since increasing either x, y would increase the output by the same amount, and the rate of that increase would be independent of what the actual values of x, y

- **Differentiation formulas of a multi-variable function** f(x, y, ...)
  - 'Max' function of two numbers

$$f(x,y) = \max(x,y) \longrightarrow \Delta f = \left[\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}\right] = [1,0] \text{ if } x \ge y$$
$$\Delta f = \left[\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}\right] = [0,1] \text{ if } x < y$$

- For example,
  - $\triangleright x = 4$ , y = 2 then f(x, y) = 4 and it is not sensitive of y
  - From the derivative on x and y:  $\frac{\partial f}{\partial x} = 1$   $\frac{\partial f}{\partial y} = 0$
  - ➤ Interpretation
    - » if we increase x by a tiny amount, the function would increase the output by the same amount
    - > if we increase y by a tiny amount, the function would keep outputting 4, and therefore the gradient is zero: there is no effect

### ◆Chain Rule (연쇄 법칙)

### 연쇄 법칙

위키백과, 우리 모두의 백과사전.

연쇄법칙은 두 함수를 합성한 합성 함수의 도함수에 관한 공식이다.

$$(f \circ g)'(x) = (f(g(x)))' = f'(g(x))g'(x)$$

라이프니츠 표기를 쓰면 다음과 같다.

$$\frac{df}{dx} = \frac{df}{dg} \cdot \frac{dg}{dx}$$

$$(f \circ g)'(x) = f'(g(x)) \times g'(x)$$

$$(f \circ g \circ h)'(x) = f'(g(h(x))) \times g'(h(x)) \times h'(x)$$

$$(f \circ g \circ h \circ i)'(x) = f'(g(h(i(x)))) \times g'(h(i(x))) \times h'(i(x)) \times i'(x)$$

$$f(x) = (x^{3} + x^{2} + x + 1)^{3}$$

$$g(x) = x^{3} + x^{2} + x + 1$$

$$f(g(x)) = g(x)^{3}$$

$$f(g(x))' = f'(g(x))g'(x)$$

$$\frac{df}{dx} = \frac{df}{dg} \cdot \frac{dg}{dx} = f'(g(x))g'(x)$$

$$= 3g(x)^{2} \cdot (3x^{2} + 2x + 1)$$

$$= 3(x^{3} + x^{2} + x + 1)^{2}(3x^{2} + 2x + 1)$$

$$\frac{df}{dx} = \frac{df}{dg} \cdot \frac{dg}{dx}$$

$$\frac{df}{dx} = \frac{df}{dg} \cdot \frac{dg}{dh} \cdot \frac{dh}{dx}$$

$$\frac{df}{dx} = \frac{df}{dg} \cdot \frac{dg}{dh} \cdot \frac{dh}{di} \cdot \frac{di}{dx}$$

$$f(x) = \frac{1}{x} \Rightarrow f'(x) = -\frac{1}{x^2}$$

### **♦**Chain Rule

### - Derivative of sigmoid function

$$\sigma(z) = \frac{1}{k(z)} \quad \text{where} \quad k(z) = 1 + e^{-z}$$

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

Weighted sum

by chain rule 
$$\frac{d\sigma}{dz} = \frac{d\sigma}{dk} \cdot \frac{dk}{dz} = -\frac{1}{k(z)^2} (-e^{-z})$$

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

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

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

Derivative of sigmoid function

$$\frac{d\sigma}{dz} = \sigma(z)(1 - \sigma(z))$$

### **♦**Chain Rule

$$L = \frac{1}{m} \sum l(w_0, w_1, b)$$



$$\frac{dL}{dx} = \frac{1}{m} \sum \frac{dl(w_0, w_1, b)}{dx}$$

$$l(w_0, w_1, b) = (\hat{y} - y)^2 \qquad \text{where} \qquad \hat{y} = \sigma(z)$$

$$= (\sigma(z) - y)^2 \qquad \text{where} \qquad \sigma(z) = \frac{1}{1 + e^{-z}}$$

$$= \left(\frac{1}{1 + e^{-z}} - y\right)^2 \qquad \text{where} \qquad z = x_0 \cdot w_0 + x_1 \cdot w_1 + b$$

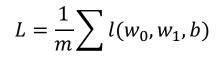
$$= \left(\frac{1}{1 + e^{-z}} - y\right)^2$$

$$\frac{\partial l}{\partial w_0} = \frac{\partial l}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial \sigma} \cdot \frac{\partial \sigma}{\partial z} \cdot \frac{\partial z}{\partial w_0} = 2(\hat{y} - y) \cdot 1.0 \cdot \sigma(z)(1 - \sigma(z)) \cdot x_0$$

$$\frac{\partial l}{\partial w_1} = \frac{\partial l}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial \sigma} \cdot \frac{\partial \sigma}{\partial z} \cdot \frac{\partial z}{\partial w_1} = 2(\hat{y} - y) \cdot 1.0 \cdot \sigma(z)(1 - \sigma(z)) \cdot x_1$$

$$\frac{\partial l}{\partial b} = \frac{\partial l}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial \sigma} \cdot \frac{\partial \sigma}{\partial z} \cdot \frac{\partial z}{\partial b} = 2(\hat{y} - y) \cdot 1.0 \cdot \sigma(z)(1 - \sigma(z)) \cdot 1.0$$

## **♦** Backpropgation





$$\frac{dL}{dx} = \frac{1}{m} \sum \frac{dl(w_0, w_1, b)}{dx}$$

Input 
$$x_0$$
  $w_0$   $\partial z$   $\partial w_0$   $\partial w_0$   $\partial w_0$   $\partial w_0$   $\partial w_1$   $\partial w_$ 

$$\frac{\partial l}{\partial w_0} = \frac{\partial l}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial \sigma} \cdot \frac{\partial \sigma}{\partial z} \cdot \frac{\partial z}{\partial w_0} = 2(\hat{y} - y) \cdot 1.0 \cdot \sigma(z)(1 - \sigma(z)) \cdot x_0$$

$$\frac{\partial l}{\partial w_1} = \frac{\partial l}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial \sigma} \cdot \frac{\partial \sigma}{\partial z} \cdot \frac{\partial z}{\partial w_1} = 2(\hat{y} - y) \cdot 1.0 \cdot \sigma(z)(1 - \sigma(z)) \cdot x_1$$

$$\frac{\partial l}{\partial b} = \frac{\partial l}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial \sigma} \cdot \frac{\partial \sigma}{\partial z} \cdot \frac{\partial z}{\partial b} = 2(\hat{y} - y) \cdot 1.0 \cdot \sigma(z)(1 - \sigma(z)) \cdot 1.0$$

### Backpropagation Implementation

$$f(x, y, z) = (x + y)z$$



- Chain Rule 
$$f(x, y, z) = (x + y)z$$
  $\Rightarrow$   $f = qz$  where  $q = x + y$ 

$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial q} \cdot \frac{\partial q}{\partial x} = z \cdot 1 = z$$

$$\frac{\partial f}{\partial y} = \frac{\partial f}{\partial q} \cdot \frac{\partial q}{\partial y} = z \cdot 1 = z$$

$$\frac{\partial f}{\partial z} = q = x + y$$

 $\left[\frac{\partial f}{\partial x'}, \frac{\partial f}{\partial v'}, \frac{\partial f}{\partial z}\right]$  is the sensitivity of the variables x, y, z on f

```
def backward(x, y, z):
   q = x + y
   f = q * z
   df_dq = z # -4
   df_dz = q # 3
   df_dx = z * 1.0 # -4
   df_dy = z * 1.0 # -4
   return df_dx, df_dy, df_dz
df_dx, df_dy, df_dz = \
   backward(x=-2, y=5, z=-4)
```

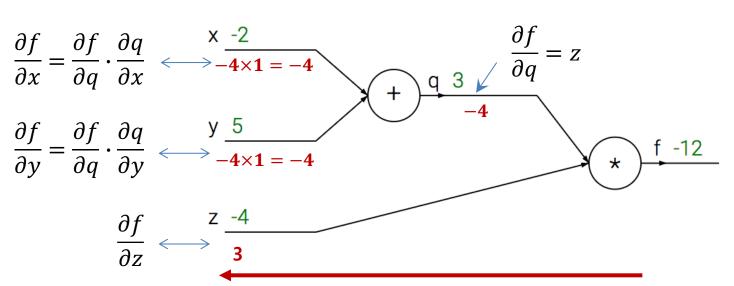
### Backpropagation Implementation

Computational graph (Visual representation of the computation)

$$f(x, y, z) = (x + y)z$$



$$f(x, y, z) = (x + y)z$$
  $\Rightarrow$   $f = qz$  where  $q = x + y$ 



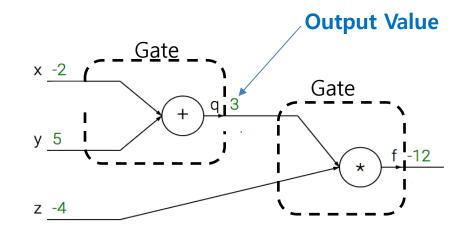
- Backward pass via computational graph
  - right performs backpropagation which starts at the end and recursively applies the chain rule to compute the gradients all the way to the inputs of the graph

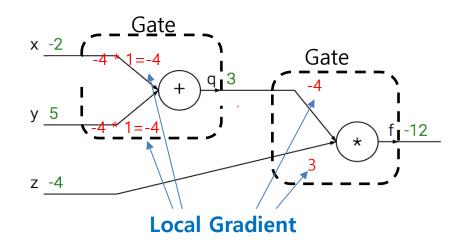
```
def backward(x, y, z):
   q = x + y
   f = q * z
   df dq = z
                    # -4
   df_dz = q # 3
   df_dx = z * 1.0 # -4
   df dy = z * 1.0
                      # -4
   return df_dx, df_dy, df_dz
df_dx, df_dy, df_dz = \
   backward(x=-2, y=5, z=-4)
```

Backpropagation Implementation

### Backpropagation is a beautifully local process!

Each gate produce its output and local gradient completely independently without being aware of any of the details of the full graph





### **♦**Training with Backpropagation (1/3)

```
def gradient(W, b, X, y):
       # W.shape: (2,), b.shape: (1,), X.shape: (12, 2), y.shape: (12)
       y pred = model(X, W, b)
       dl_dy = 2 * (y_pred - y)
       dl dy = dl dy.unsqueeze(dim=-1)
                                                                                                                                 # dl dy.shape: (12, 1)
       dy df = 1.0
       z = torch.sum(X * W, dim=-1) + b
                                                                                                                                 # z.shape: (12,)
       ds dz = activate(z) * (1.0 - activate(z))
       ds dz = ds dz.unsqueeze(dim=-1)
                                                                                                                                 # ds dz.shape: (12, 1)
       W_grad = torch.mean(dl_dy * dy_df * ds_dz * X, dim=0) # W_grad.shape: (2,)
       \frac{\partial l}{\partial w_0} = \frac{\partial l}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial \sigma} \cdot \frac{\partial \sigma}{\partial z} \cdot \frac{\partial z}{\partial w_0} = 2(\hat{y} - y) \cdot 1.0 \cdot \sigma(z)(1 - \sigma(z)) \cdot x_0
       return W grad, b grad
                                                                                            \frac{\partial l}{\partial \mathbf{w_1}} = \frac{\partial l}{\partial \hat{\mathbf{y}}} \cdot \frac{\partial \hat{\mathbf{y}}}{\partial \sigma} \cdot \frac{\partial \sigma}{\partial z} \cdot \frac{\partial z}{\partial \mathbf{w_1}} = 2(\hat{\mathbf{y}} - \mathbf{y}) \cdot 1.0 \cdot \sigma(z)(1 - \sigma(z)) \cdot \mathbf{x_1}
                                                                                                \frac{\partial l}{\partial b} = \frac{\partial l}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial \sigma} \cdot \frac{\partial \sigma}{\partial z} \cdot \frac{\partial z}{\partial b} = 2(\hat{y} - y) \cdot 1.0 \cdot \sigma(z)(1 - \sigma(z)) \cdot 1.0
```

**♦**Training with Backpropgation (2/3)

```
def learn(W, b, train data loader):
 MAX EPOCHS = 20 000
 LEARNING RATE = 0.01
 for epoch in range(0, MAX_EPOCHS):
    batch = next(iter(train data loader))
   y pred = model(batch["input"], W, b)
    loss = loss_fn(y_pred, batch["target"])
   W_grad, b_grad = gradient(W, b, batch["input"], batch["target"])
    if epoch % 100 == 0:
      print("[Epoch:{0:6,}] loss:{1:8.5f}, w0:{2:6.3f}, w1:{3:6.3f}, b:{4:6.3f}".format(
        epoch, loss.item(), W[0].item(), W[1].item(), b.item()
      ), end=", ")
      print("W.grad: {0}, b.grad:{1}".format(W_grad, b_grad))
   W = W - LEARNING_RATE * W_grad
    b = b - LEARNING RATE * b grad
```

**♦**Training with Backpropgation (3/3)

```
def main():
   W = torch.ones((2,))
   b = torch.zeros((1,))
    simple_dataset = SimpleDataset()
   train_data_loader = DataLoader(dataset=simple_dataset, batch_size=len(simple_dataset))
   batch = next(iter(train data loader))
   y pred = model(batch["input"], W, b)
   print(y_pred.shape) # >>> torch.Size([12])
   print(y_pred) # >>> tensor([0.8022, 1.0000, 1.0000, 1.0000, 1.0000, 1.0000,
                                     0.9973, 0.0198, 1.0000, 1.0000, 1.0000, 0.6225])
   loss = loss_fn(y_pred, batch["target"])
   print(loss) # >>> tensor(2673.9028)
   learn(W, b, train_data_loader)
if __name__ == "__main__":
   main()
```

# Backpropagation with PyTorch Autograd

link\_dl/\_01\_code/\_04\_learning\_and\_autograd/b\_autograd\_1.py

# **Autograd**

## Pytorch Autograd

- Creating Tensors with requires\_grad=True enables autograd
- Operations on Tensors with
   requires\_grad=True cause PyTorch to build
   a computational graph
- grad attribute is created, but it is None
- Since w is created by the user, its grad\_fn is None
- We will not want gradients (of loss) with respect to just constant (or gathered data)
- x was created as a result of an operation, so it has grad & grad\_fn attributes
- grad\_fn references a Function that has created the Tensor

```
w = torch.ones(3, requires_grad=True)
print(w)
# >>> tensor([1., 1., 1.], requires_grad=True)
print(w.grad, w.grad_fn)
# >>> None None
c = torch.tensor([2])
X = W + C
print(x)
# >>> tensor([3., 3., 3.], grad_fn=<AddBackward0>)
print(x.grad_fn)
# >>> <AddBackward0 object at 0x11b082ef0>
# Do more operations on x
y = x * 3
print(y)
# >>> tensor([27., 27., 27.], grad_fn=<MulBackward0>)
print(y.grad_fn)
# >>> <AddBackward0 object at 0x11b082ef0>
z = y.mean() # Make the output scalar
print(z) # >>> tensor(27., grad_fn=<MeanBackward0>)
print(z.shape) # >>> torch.Size([])
print(z.grad_fn)
# >>> <AddBackward0 object at 0x11b082ef0>
```

link\_dl/\_01\_code/\_04\_learning\_and\_autograd/b\_autograd\_1.py

# **Autograd**

♦ Pytorch Autograd

y was created as a result of an operation, so it has grad & grad\_fn attributes.

z was once more created as a result of 'mean' operator, so it still keeps grad & grad\_fn attributes.

```
w = torch.ones(3, requires_grad=True)
print(w)
# >>> tensor([1., 1., 1.], requires_grad=True)
print(w.grad, w.grad_fn)
# >>> None None
c = torch.tensor([2])
X = W + C
print(x)
# >>> tensor([3., 3., 3.], grad_fn=<AddBackward0>)
print(x.grad_fn)
# >>> <AddBackward0 object at 0x11b082ef0>
# Do more operations on x
y = x * 3
print(y)
# >>> tensor([27., 27., 27.], grad_fn=<MulBackward0>)
print(y.grad_fn)
# >>> <AddBackward0 object at 0x11b082ef0>
z = y.mean()  # Make the output scalar
          # >>> tensor(27., grad_fn=<MeanBackward0>)
print(z.shape) # >>> torch.Size([])
print(z.grad_fn)
# >>> <AddBackward0 object at 0x11b082ef0>
```

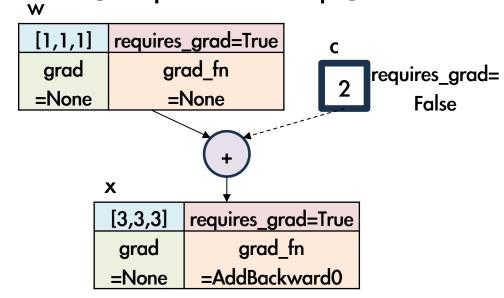
link\_dl/\_01\_code/\_04\_learning\_and\_autograd/b\_autograd\_1.py

# **Autograd**

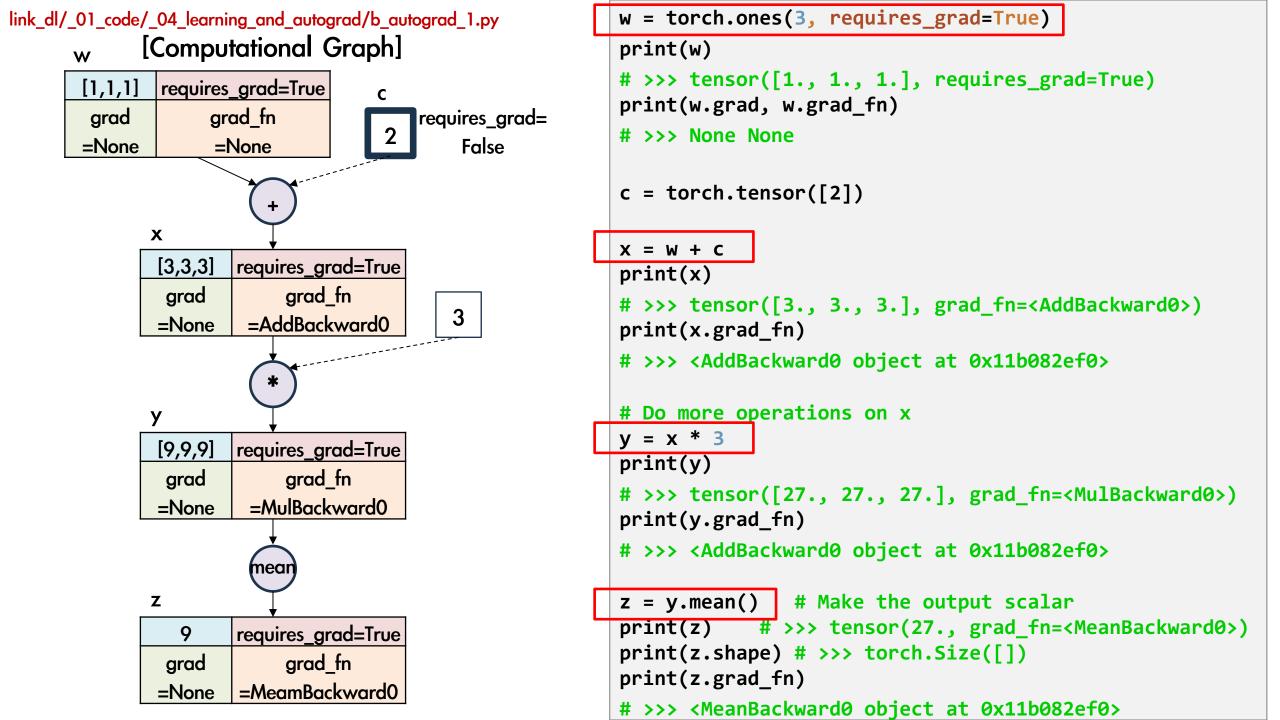
### **♦** Computational Graph

Every operation on a tensor with requires\_grad=True will add to the computational graph, and the resulting tensors will also have requires\_grad=True

### [Computational Graph]



```
w = torch.ones(3, requires_grad=True)
print(w)
# >>> tensor([1., 1., 1.], requires_grad=True)
print(w.grad, w.grad_fn)
# >>> None None
c = torch.tensor([2])
X = W + C
print(x)
# >>> tensor([3., 3., 3.], grad_fn=<AddBackward0>)
print(x.grad_fn)
# >>> <AddBackward0 object at 0x11b082ef0>
# Do more operations on x
V = X * 3
print(y)
# >>> tensor([27., 27., 27.], grad_fn=<MulBackward0>)
print(y.grad fn)
# >>> <AddBackward0 object at 0x11b082ef0>
z = y.mean() # Make the output scalar
          # >>> tensor(27., grad_fn=<MeanBackward0>)
print(z.shape) # >>> torch.Size([])
print(z.grad_fn)
# >>> <AddBackward0 object at 0x11b082ef0>
```



### [Computational Graph] W [1,1,1] requires\_grad=True C grad fn grad =[1,1,1] =None X [3,3,3] requires\_grad=True grad\_fn grad =AddBackward0 =[1,1,1] Backpropagation [9,9,9] requires\_grad=True grad\_fn grad [.3,.3,.3] =MulBackward0 Z requires\_grad=True

grad

=[1]

grad fn

=MeanBackward0

# Autograd

- ♦ tensor.backward()
  - Backpropate to all tensors with requires\_grad=True
  - After backward finishes, gradients are accumulated into w.grad, x.grad, y.grad and z.grad and the graph is destroyed

```
...
z.backward()

print(w.grad)
# >>> tensor([1., 1., 1.])
```

### W

[1,1,1]	requires_grad=True
grad	grad_fn
=[1,1,1]	=None

X

[3,3,3]	requires_grad=True
grad	grad_fn
=[1,1,1]	=AddBackward0

У

[9,9,9]	requires_grad=True
grad	grad_fn
=[.3,.3,.3]	=MulBackward0

Z

9	requires_grad=True
grad	grad_fn
=[1]	=MulBackward0

# **Autograd**

- **♦** tensor.backward()
  - By default, you're not allowed to print the gradients for intermediate tensors

```
. . .
z.backward()
print(z.grad)
# >>> UserWarning: The .grad attribute of a Tensor tha
t is not a leaf Tensor is being accessed.
print(y.grad)
# >>> UserWarning: The .grad attribute of a Tensor tha
t is not a leaf Tensor is being accessed.
print(x.grad)
# >>> UserWarning: The .grad attribute of a Tensor
that is not a leaf Tensor is being accessed.
print(w.grad)
# >>> tensor([1., 1., 1.])
```

### W

[1,1,1]	requires_grad=True
grad	grad_fn
=[1,1,1]	=None

X

[3,3,3]	requires_grad=True
grad	grad_fn
=[1,1,1]	=AddBackward0

У

[9,9,9]	requires_grad=True
grad	grad_fn
=[.3,.3,.3]	=MulBackward0

Z

9	requires_grad=True
grad	grad_fn
=[1]	=MulBackward0

# **Autograd**

- ♦ tensor.backward()
  - If you indeed want the Tensor.grad field to be populated for a non-leaf Tensor, use Tensor.retain\_grad() on the non-leaf Tensor

```
y.retain_grad()
z = y.mean() # Make the output scalar
print(z) # >>> tensor(27., grad_fn=<MeanBackward0>)
print(z.shape) # >>> torch.Size([])
print(z.grad_fn)
# >>> <MeanBackward0 object at 0x11b082ef0>
z.backward()
print(y.grad) # dz/dy
# >>> tensor([0.3333, 0.3333, 0.3333])
```

## ♦ Stop a tensor from tracking history

- Tensor.requires\_grad\_()
  - changes a tensor's gradient requirement
    - > .requires\_grad\_(True)
    - .requires\_grad\_(False)

```
a = torch.randn(2, 2)
print(a.requires grad) # >>> False
b = ((a * 3) / (a - 1))
print(b.grad_fn) # >>> None
#b.backward()
# >>> RuntimeError: element 0 of tensors does not
require grad and does not have a grad_fn
a.requires_grad_(True)
print(a.requires_grad) # >>> True
c = (a * a).sum()
print(c.grad_fn)
# >>> <SumBackward0 object at 0x116773d60>
c.backward()
print(a.grad)
# >>>
tensor([[3.9463, 0.2887],
        [0.5109, 3.0314]])
```

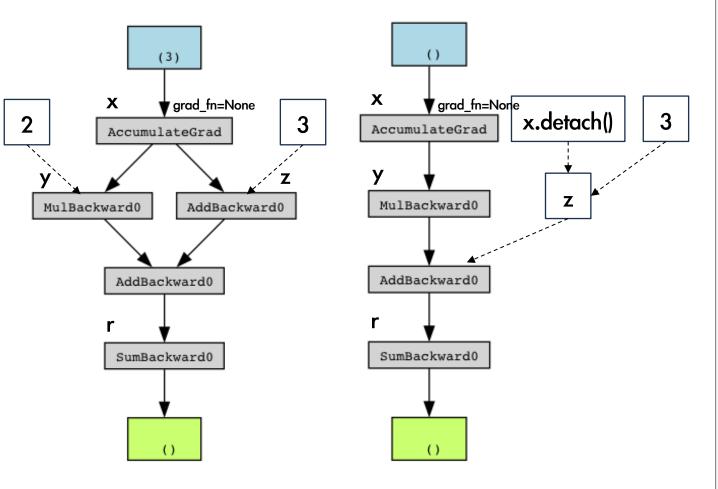
## ♦ Stop a tensor from tracking history

- Tensor.detach()
  - Returns a <u>new Tensor</u>, detached from the current computational graph
    - pet a new Tensor with the same content but no gradient computation

```
a = torch.randn(2, 2, requires_grad=True)
print(a.requires_grad) # >>> True
# b is a new tensor detached from the current
# computational graph
b = a.detach()
print(b.requires_grad) # >>> False
print(b is a)
                        # >>> False
```

## ♦ Stop a tensor from tracking history

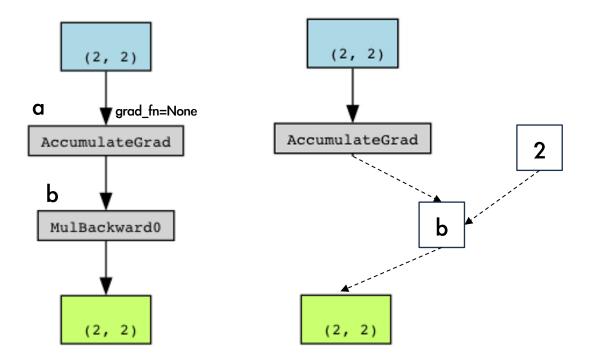
— Tensor.detach()



```
# pip install graphviz
# pip install torchviz
from torchviz import make_dot
x = torch.ones(3, requires_grad=True)
V = 2 * X
z = 3 + x
r = (y + z).sum()
make_dot(r).render("torchviz_1", format="png")
# Detach
x = torch.ones(3, requires_grad=True)
V = 2 * X
z = 3 + x.detach()
r = (y + z).sum()
make_dot(r).render("torchviz_2", format="png")
```

## **♦**Stop a tensor from tracking history

- wrap in with torch.no\_grad()
  - prevent gradient calculations for the wrapped parts of code to save memory and computational resources
  - or using the @torch.no\_grad on function def.



```
a = torch.randn(2, 2, requires_grad=True)
b = a * 2
make_dot(b).render("torchviz_3", format="png")
a = torch.randn(2, 2, requires_grad=True)
print(a.requires_grad) # >>> True
# Tell PyTorch not to build a graph
# for the wrapped operations
with torch.no_grad():
    print(a.requires grad) # >>> True
    b = a * 2
print(a.requires_grad) # >>> True
print(b.requires_grad) # >>> False
make_dot(b).render("torchviz_4", format="png")
```

```
weights = torch.ones(4, requires_grad=True)
for epoch in range(3):
   # just a dummy example
    output = (weights * 3).sum()
    print("[output {0}]:".format(epoch), output)
    output.backward()
    print("weights.grad:", weights.grad)
   # optimize model by gradient descent method
    with torch.no grad():
        weights -= 0.1 * weights.grad
        # 'empty gradients' is important!
        # It affects the final weights & output
        weights.grad.zero_()
    print("weights:", weights)
output = (weights * 3).sum()
print("\n[output final]:", output)
```

### **Empty** gradients

- Tensor.backward() <u>accumulates the</u>
   <u>gradient</u> for this tensor into the <u>.grad</u> attribute
  - We need to be careful during optimization!!!
- Tensor.grad.zero\_() empty the gradients before a new optimization step!

Tell PyTorch not to build a graph for these operations

Make gradient step on weights

Set gradients to zero

```
weights = torch.ones(4, requires_grad=True)
for epoch in range(3):
   # just a dummy example
    output = (weights * 3).sum()
    print("[output {0}]:".format(epoch), output)
    output.backward()
    print("weights.grad:", weights.grad)
    # optimize model by gradient descent method
    with torch.no_grad():
        weights -= 0.1 * weights.grad
        # 'empty gradients' is important!
        # It affects the final weights & output
        weights.grad.zero_()
    print("weights:", weights)
output = (weights * 3).sum()
print("\n[output final]:", output)
```

### **Empty** gradients

- Tensor.backward() <u>accumulates the</u>
   <u>gradient</u> for this tensor into the .grad attribute
  - We need to be careful during optimization !!!
- Tensor.grad.zero\_() empty the gradients before a new optimization step!

```
# >>>
[output 0]: tensor(12., grad_fn=<SumBackward0>)
weights.grad: tensor([3., 3., 3., 3.])
weights: tensor([0.7000, 0.7000, 0.7000], requires g
rad=True)
[output 1]: tensor(8.4000, grad fn=<SumBackward0>)
weights.grad: tensor([3., 3., 3., 3.])
weights: tensor([0.4000, 0.4000, 0.4000, 0.4000], requires_g
rad=True)
[output 2]: tensor(4.8000, grad_fn=<SumBackward0>)
weights.grad: tensor([3., 3., 3., 3.])
weights: tensor([0.1000, 0.1000, 0.1000], requires g
rad=True)
[output final]: tensor(1.2000, grad fn=<SumBackward0>)
```

```
weights = torch.ones(4, requires_grad=True)
for epoch in range(3):
    # just a dummy example
    output = (weights * 3).sum()
    print("[output {0}]:".format(epoch), output)
    output.backward()
    print("weights.grad:", weights.grad)
    # optimize model by gradient descent method
    with torch.no grad():
        weights -= 0.1 * weights.grad
        # 'empty gradients' is important!
        # It affects the final weights & output
        weights.grad.zero ()
    print("weights:", weights)
output = (weights * 3).sum()
print("\n[output final]:", output)
```

```
weights = torch.ones(4, requires grad=True)
optimizer = torch.optim.SGD([weights], lr=0.1)
for epoch in range(3):
    # just a dummy example
    output = (weights * 3).sum()
    print("[output {0}]:".format(epoch), output)
    output.backward()
    print("weights.grad:", weights.grad)
    # optimize model by gradient descent method
    optimizer.step()
    optimizer.zero_grad() # empty gradients
    print("weights:", weights)
output = (weights * 3).sum()
print("\n[output final]:", output)
```

```
weights = torch.ones(4, requires_grad=True)
optimizer = torch.optim.SGD([weights], lr=0.1)
for epoch in range(3):
   # just a dummy example
    output = (weights * 3).sum()
    print("[output {0}]:".format(epoch), output)
    output.backward()
    print("weights.grad:", weights.grad)
    # optimize model by gradient descent method
    optimizer.step()
    optimizer.zero grad() # empty gradients
    print("weights:", weights)
output = (weights * 3).sum()
print("\n[output final]:", output)
```

### **Output** Update the tensors

- torch.optim.Optimizer
  - It helps in updating the parameters during performing the gradient descent

```
    torch.optim.Optimizer.SGD
    torch.optim.Optimizer.RMSprop
    ...
```

- torch.optim.Optimizer.step()
  - This is called <u>after computing gradients</u> using backpropagation
  - This updates the parameters of a neural network model using gradient descent during training
- torch.optim.Optimizer.zero\_grad()
  - empty the gradients

```
# >>>
(Same output! As the previous run)
```

**Example of Autograd at Gradient Descent** 

```
def learn(W, b, train_data_loader):
 MAX EPOCHS = 20 000
 LEARNING_RATE = 0.01
 for epoch in range(0, MAX EPOCHS):
    batch = next(iter(train_data_loader))
   y pred = model(batch["input"], W, b)
    loss = loss_fn(y_pred, batch["target"])
    loss.backward()
    if epoch % 100 == 0:
      print("[Epoch:{0:6,}] loss:{1:8.5f}, w0:{2:6.3f}, w1:{3:6.3f}, b:{4:6.3f}".format(
        epoch, loss.item(), W[0].item(), W[1].item(), b.item()
      ), end=", ")
      print("W.grad: {0}, b.grad:{1}".format(W.grad, b.grad))
   with torch.no_grad():
      W -= LEARNING_RATE * W.grad
      b -= LEARNING RATE * b.grad
      W.grad = None
      b.grad = None
```

Example of Autograd with Step() at Gradient Descent

```
def learn(W, b, train_data_loader):
 MAX EPOCHS = 20 000
 LEARNING_RATE = 0.01
 from torch import optim
  optimizer = optim.SGD([W, b], lr=LEARNING_RATE)
  for epoch in range(0, MAX_EPOCHS):
    batch = next(iter(train data loader))
   y_pred = model(batch["input"], W, b)
    loss = loss_fn(y_pred, batch["target"])
    loss.backward()
    if epoch % 100 == 0:
      print("[Epoch:{0:6,}] loss:{1:8.5f}, w0:{2:6.3f}, w1:{3:6.3f}, b:{4:6.3f}".format(
        epoch, loss.item(), W[0].item(), W[1].item(), b.item()
      ), end=", ")
      print("W.grad: {0}, b.grad:{1}".format(W.grad, b.grad))
    optimizer.step()
    optimizer.zero grad()
```

### **♦** Example of Autograd main()

```
def main():
    W = torch.ones((2,), requires_grad=True)
    b = torch.zeros((1,), requires_grad=True)

    simple_dataset = SimpleDataset()
    train_data_loader = DataLoader(dataset=simple_dataset, batch_size=len(simple_dataset))

    learn(W, b, train_data_loader)

if __name__ == "__main__":
    main()
```