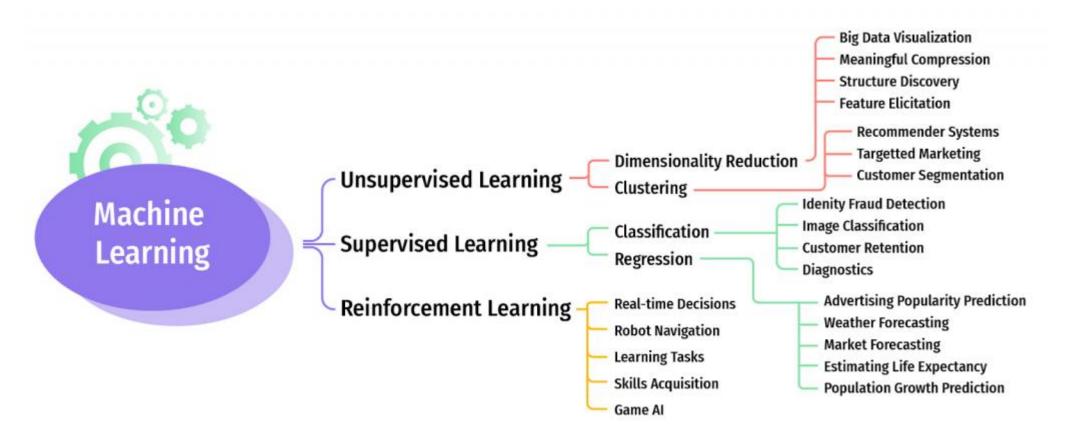
Computational Graph and Linear Regression

Quang-Vinh Dinh Ph.D. in Computer Science

Outline

- > Machine Learning
- > Derivative/Gradient
- > Linear Regression
- > Computational Graph
- > Generalized formulae

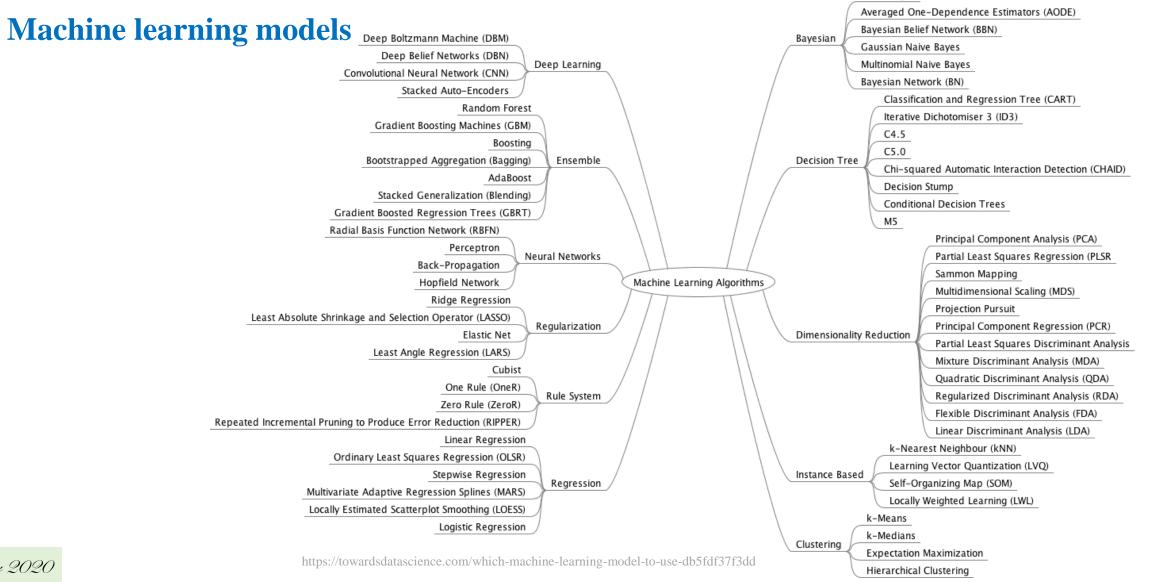
Overview



https://idapgroup.com/blog/types-of-machine-learning-out-there/

Year 2020

Naive Bayes





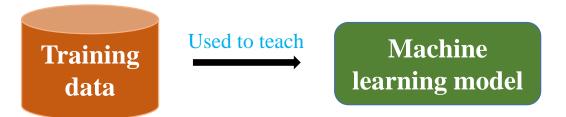
Supervised learning

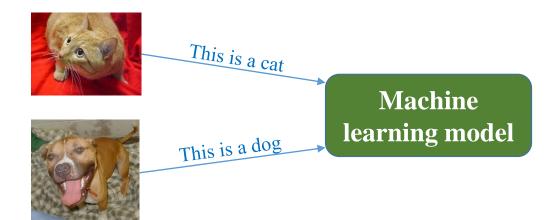
Input and output data is provided

- Training data
- Cats
- Dogs



Supervised learning





From Cat-Dog dataset



Testing data (≠ training data)



Training phase

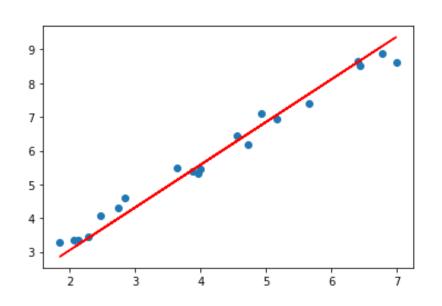
Testing phase

- **Supervised learning**
 - **Regression** (prediction)

Linear regression models ← Linear equations

Linear equation = $w_1x_1 + w_2x_2 + \cdots + w_nx_n + b$

where **w** is a weight vector and **x** is feature vector



- **Supervised learning**
 - ***** Linear Regression: Data processing

Feat	ure	Label	
a	rea	price	
	5.7	9.1	
4	4.6	5.9	
	3.5	4.6	
	5.5	6.7	

House price data

Model:
$$y = w_1x_1 + b$$

price = $a * area + b$

	Featur	es	Label
TV	+ Radio	Newspaper	\$ Sales
230.1	37.8	69.2	22.1
44.5	39.3	45.1	10.4
17.2	45.9	69.3	12
151.5	41.3	58.5	16.5
180.8	10.8	58.4	17.9

Advertising data

T abal

Model:
$$y = w_1x_1 + w_2x_2 + w_3x_3 + b$$

Sale = $w_1 * TV + w_2 * Radio + w_3 * Newspaper + b$

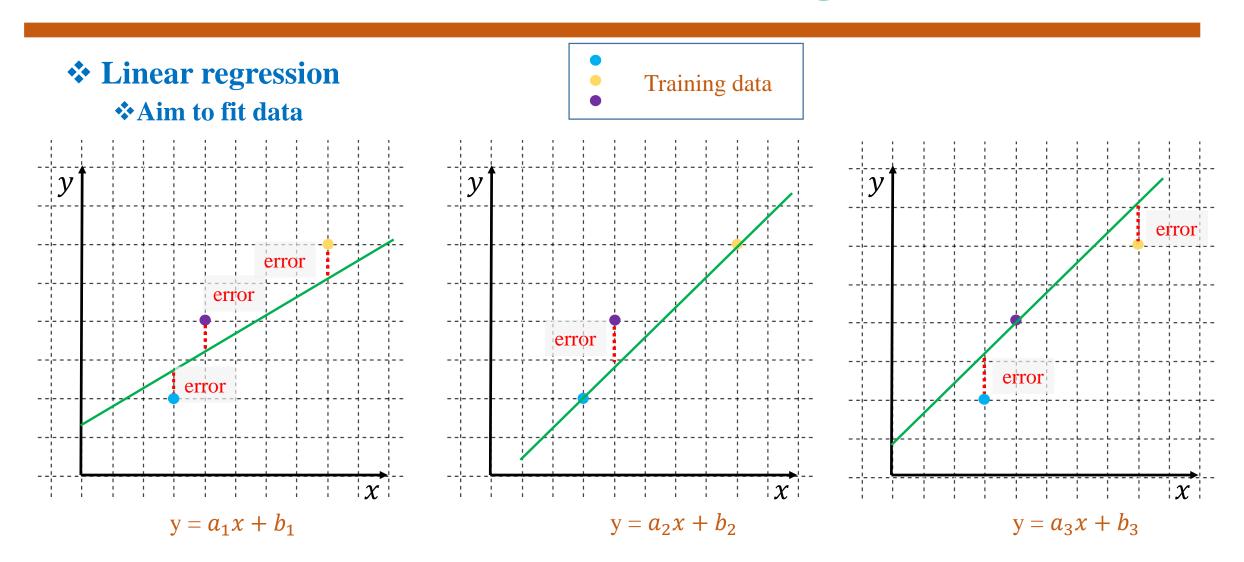
- **Supervised learning**
 - ***** Linear Regression: Data processing

Features	Label
1 Catales	Laber

Boston House Price Data

crim \$	zn ÷	indus \$	chas \$	nox \$	rm 💠	age \$	dis	≑ rad ≎	tax \$	ptratio \$	black \$	Istat \$	medv \$
0.00632	18	2.31	0	0.538	6.575	65.2	4.09	1	296	15.3	396.9	4.98	24
0.02731	0	7.07	0	0.469	6.421	78.9	4.9671	2	242	17.8	396.9	9.14	21.6
0.03237	0	2.18	0	0.458	6.998	45.8	6.0622	3	222	18.7	394.63	2.94	33.4
0.06905	0	2.18	0	0.458	7.147	54.2	6.0622	3	222	18.7	396.9	5.33	36.2
0.08829	12.5	7.87	0	0.524	6.012	66.6	5.5605	5 5	311	15.2	395.6	12.43	22.9

$$medv = w_1 * x_1 + \dots + w_{13} * x_{13} + b$$

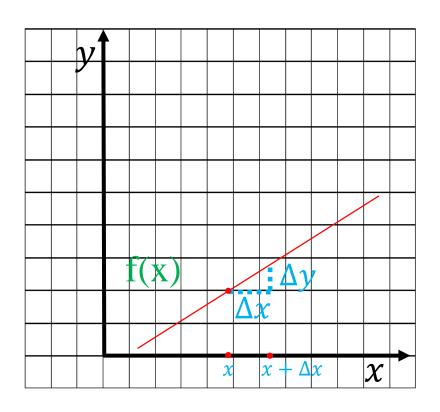


Outline

- > Machine Learning
- > Derivative/Gradient
- > Linear Regression
- > Computational Graph
- > Generalized formulae

Derivative/Gradient

A cue to optimize a function



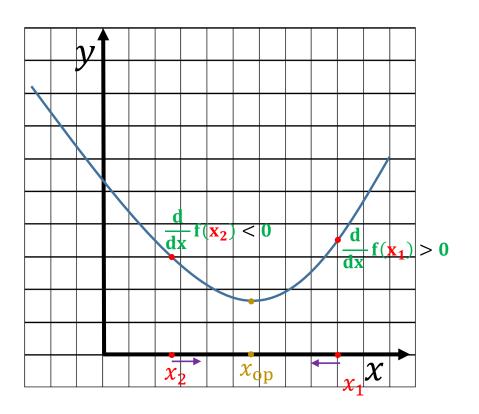
Đạo hàm =
$$\frac{Thay \, \text{đổi theo } y}{Thay \, \text{đổi theo } x} = \frac{\Delta y}{\Delta x}$$

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

Δx cần tiến về 0 để đường tiếp tuyến tiến về hàm f(x) trong vùng lân cận tại x

Derivative/Gradient

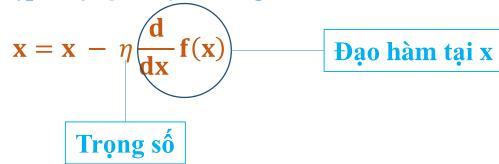
A cue to optimize a function



Quan sát: x_{op} ở vị trí ngược hướng đạo hàm tại x_1 và x_2

Cách xử lý việc di chuyển ngược hướng đạo hàm cho $\mathbf{x_1}$ và $\mathbf{x_2}$ (để tìm $\mathbf{x_{op}}$) khác nhau hình thành các thuật toán tối ưu hóa khác nhau

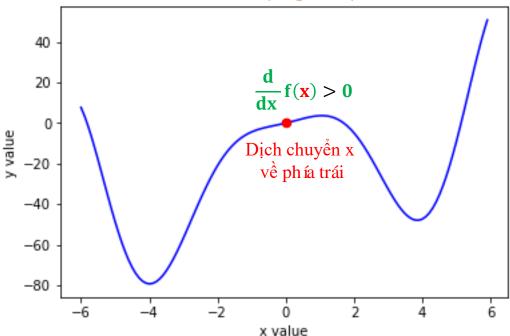
Cách cập nhật giá trị x đơn giản

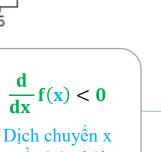


Derivative/Gradient

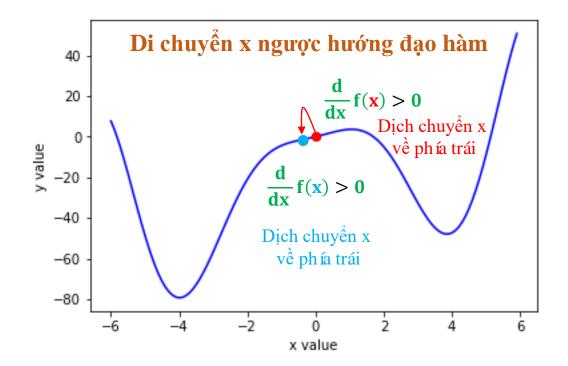
A cue to optimize a function

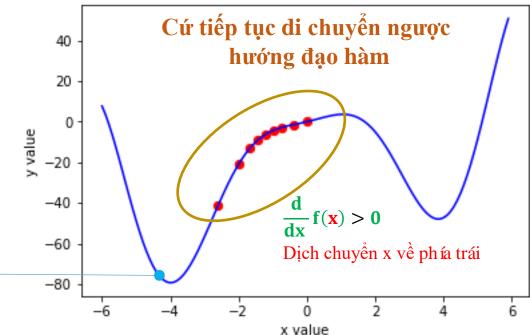






về phía phải

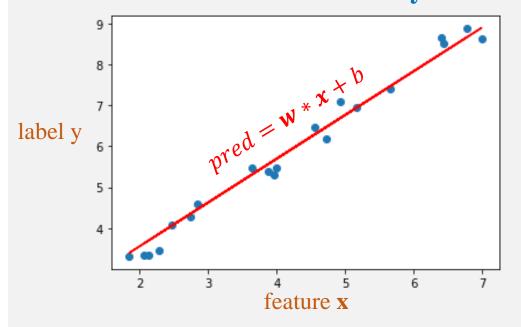




Outline

- > Machine Learning
- > Derivative/Gradient
- > Linear Regression
- > Computational Graph
- > Generalized formulae

Model the relationship between feature x and label y



Using a linear equation to fit data
Samples (x, y) are given in advance

Linear equation

$$o = w_1 x_1 + w_2 x_2 + \dots + w_n x_n + b$$

where o is a predicted value, $w_1, w_2, ..., w_n$ and b are parameters and $\mathbf{x} = [x_1 \ x_2 \ ... \ x_n]^T$ is feature vector.

Error (loss) computation

Idea: compare predicted values **o** and label values **y** Squared loss

$$L(\mathbf{w}, \mathbf{b}) = (o - y)^2$$

Linear equation

$$0 = w_1 x_1 + w_2 x_2 + \dots + w_n x_n + b$$

where o is a predicted value, $w_1, w_2, ..., w_n$ and b are parameters and $\mathbf{x} = [x_1 \ x_2 \ ... \ x_n]^T$ is feature vector.

Error (loss) computation

Idea: compare predicted values **o** and label values **y** Squared loss

$$L(\mathbf{w}, \mathbf{b}) = (o - y)^2$$

How to find optimal w and b?

Use gradient descent to minimize the loss function

Tính đạo hàm

$$\frac{\partial L}{\partial w_j} = \frac{\partial L}{\partial o} \frac{\partial o}{\partial w_j} = 2x_j(o - y)$$

$$\frac{\partial L}{\partial b} = \frac{\partial L}{\partial o} \frac{\partial o}{\partial w_i} = 2(o - y)$$

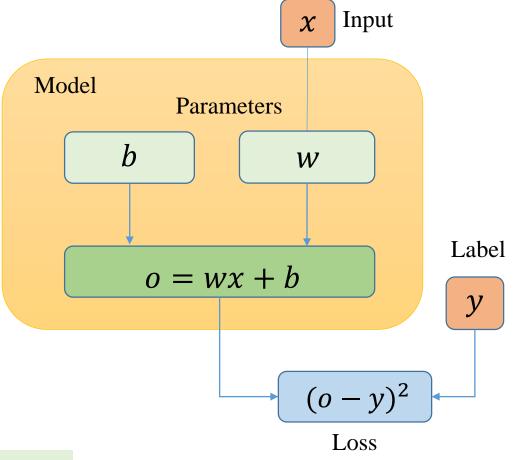
Cập nhật tham số

$$w_{j} = w_{j} - \eta L'_{w_{j}}$$

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

$$\eta \text{ is learning rate}$$

Diagram



Cheat sheet

Tính output o

$$o = wx + b$$

Tính Loss

$$L = (o - y)^2$$

Tính đạo hàm

$$L'_{w_j} = 2x_j(o - y)$$
 $w_j = w_j - \eta L'_{w_j}$
 $L'_b = 2(o - y)$ $b = b - \eta L'_b$

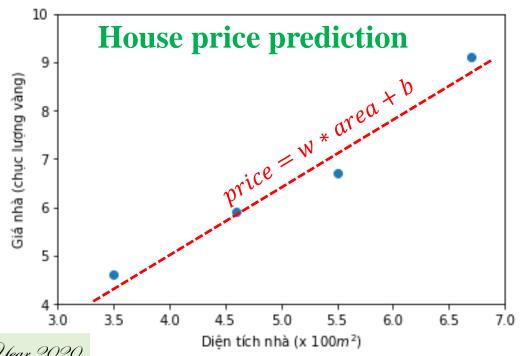
$$L_b' = 2(o - y)$$

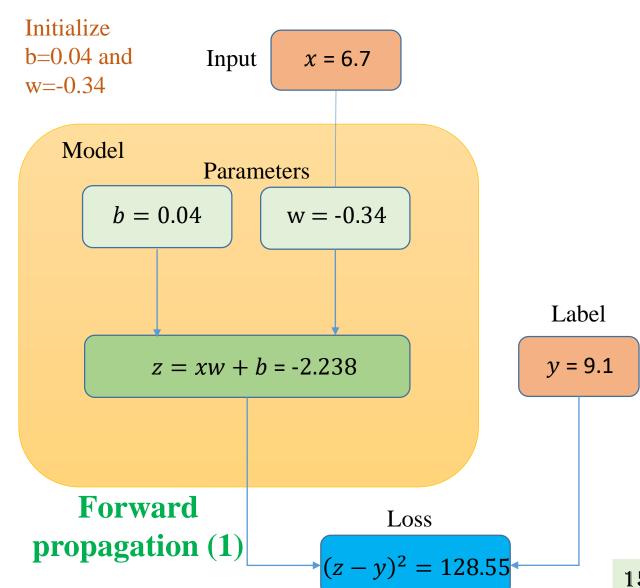
Cập nhật tham số

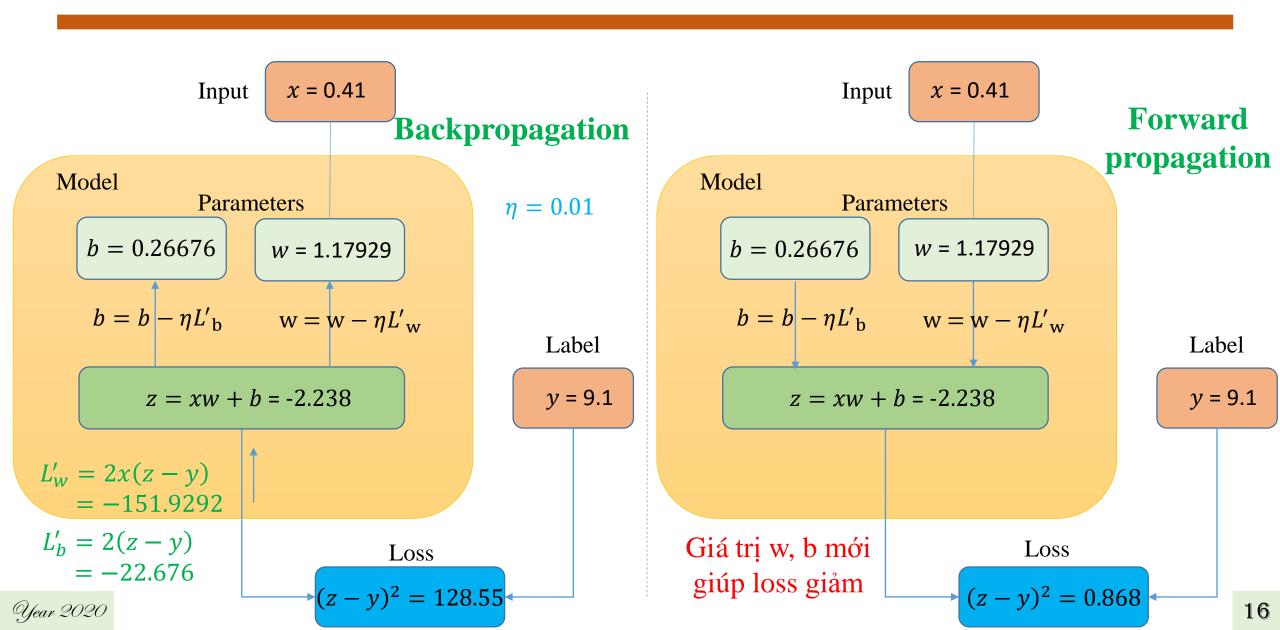
$$w_j = w_j - \eta L'_{w_j}$$

$$b = b - \eta L_b'$$

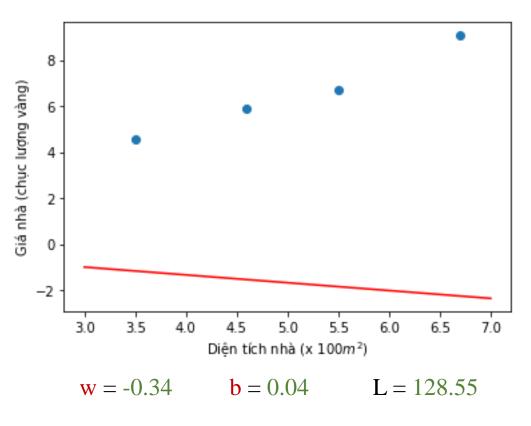


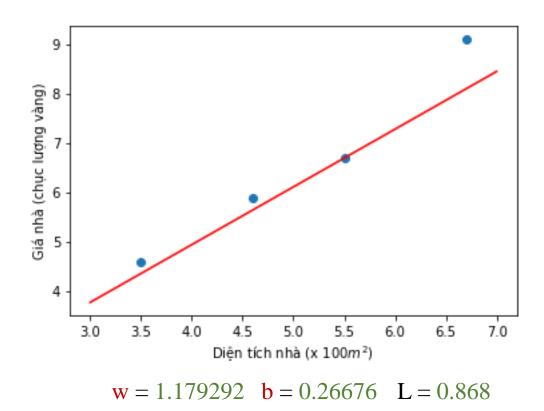






Model prediction before and after the first update





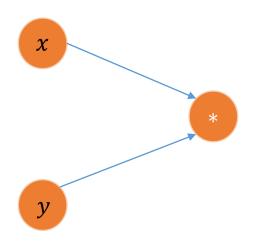
Before updating

After updating

Outline

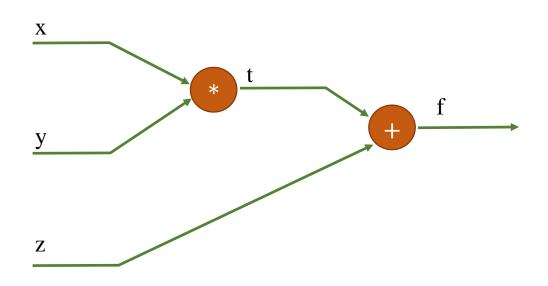
- > Machine Learning
- > Derivative/Gradient
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- > Computational Graph
- > Generalized formulae

- **A** directed graph
- Nodes represent variables or operations



- **Construct computational graph for** f(x, y, z) = x * y + z
- ightharpoonup Rewrite f(x, y, z) as

$$f(t,z) = t + z$$
 where $t = x * y$

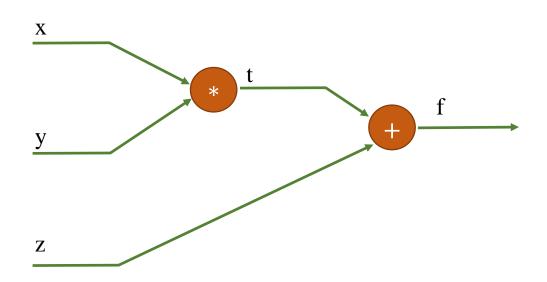


Construct computational graph for

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

ightharpoonup Rewrite f(x, y, z) as

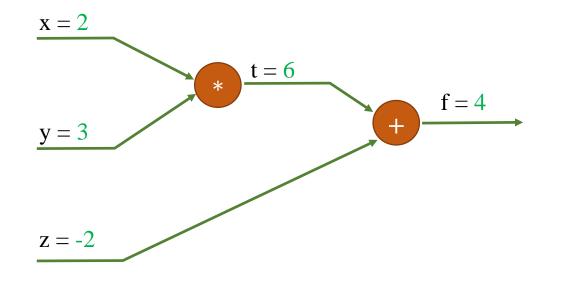
$$f(t,z) = t + z$$
 where $t = x * y$



$$\frac{\partial t}{\partial x} = y \qquad \qquad \frac{\partial f}{\partial z} = 1 \qquad \qquad \frac{\partial f}{\partial x} = 3$$

$$\frac{\partial t}{\partial y} = x \qquad \qquad \frac{\partial f}{\partial t} = 1 \qquad \qquad \frac{\partial f}{\partial y} = 3$$

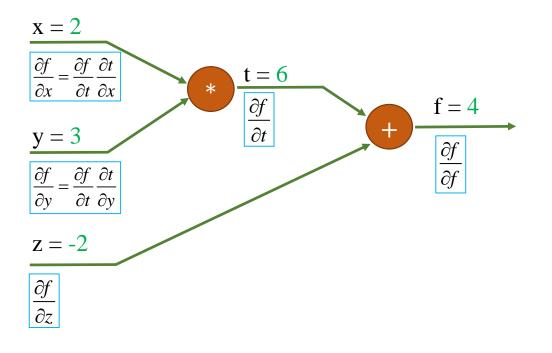
Compute f(x, y, z) **vói** x = 2, y = 3 **và** z = -2.



$$\frac{\partial t}{\partial x} = y \qquad \qquad \frac{\partial f}{\partial z} = 1 \qquad \qquad \frac{\partial f}{\partial x} = y$$

$$\frac{\partial t}{\partial y} = x \qquad \qquad \frac{\partial f}{\partial t} = 1 \qquad \qquad \frac{\partial f}{\partial y} = x$$

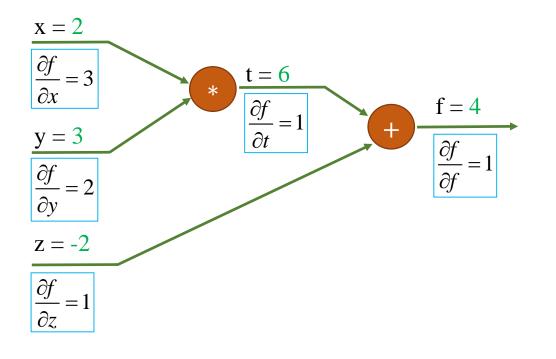
Compute f(x, y, z) **vói** x = 2, y = 3 **và** z = -2.



$$\frac{\partial t}{\partial x} = y \qquad \qquad \frac{\partial f}{\partial z} = 1 \qquad \qquad \frac{\partial f}{\partial x} = y$$

$$\frac{\partial t}{\partial y} = x \qquad \qquad \frac{\partial f}{\partial t} = 1 \qquad \qquad \frac{\partial f}{\partial y} = x$$

Compute f(x, y, z) **vói** x = 2, y = 3 **và** z = -2.



$$\frac{\partial t}{\partial x} = y \qquad \qquad \frac{\partial f}{\partial z} = 1 \qquad \qquad \frac{\partial f}{\partial x} = y$$

$$\frac{\partial t}{\partial y} = x \qquad \qquad \frac{\partial f}{\partial t} = 1 \qquad \qquad \frac{\partial f}{\partial y} = x$$

Outline

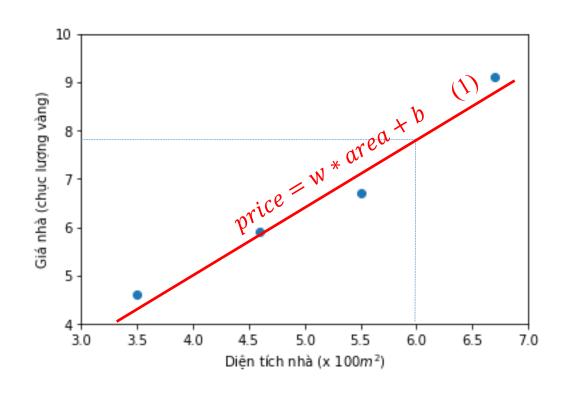
- > Machine Learning
- > Derivative/Gradient
- > Linear Regression
- > Computational Graph
 - > 1-sample training
- > Generalized formulae

***** House price predictions

\clubsuit How much for a 600- m^2 house?

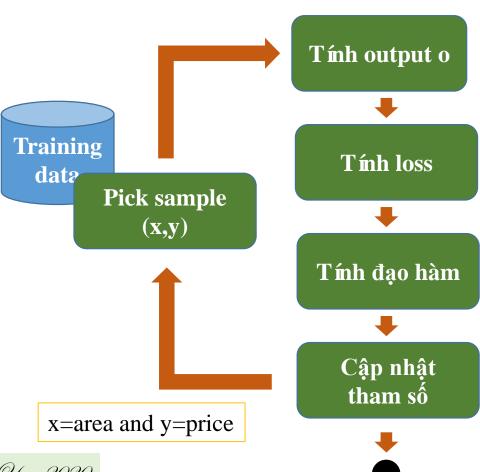
area	price	
6.7	9.1	
4.6	5.9	
3.5	4.6	
5.5	6.7	

Given sample data



How to compute (1) using computational graph

- ***** House price prediction
 - **❖** One-sample training



- 1) Pick a sample (x, y) from training data
- 2) Tính output o

$$o = wx + b$$

3) Tính loss

$$L = (o - y)^2$$

4) Tính đạo hàm

$$L'_w = 2x(o - y)$$

$$L'_h = 2(o - y)$$

5) Cập nhật tham số

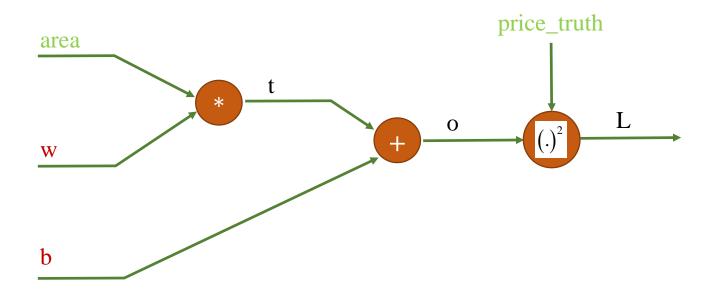
$$w = w - \eta L'_{w}$$

$$b = b - \eta L'_{h}$$
Learning rate η

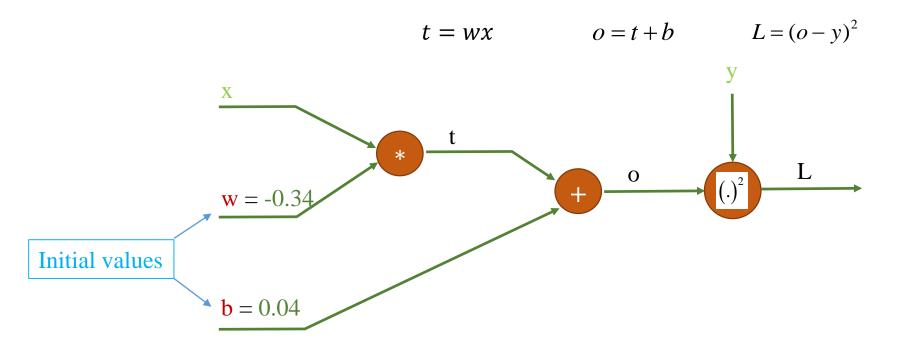
- ***** House price prediction
 - ***** One-sample training

$$price = o = w * area + b$$

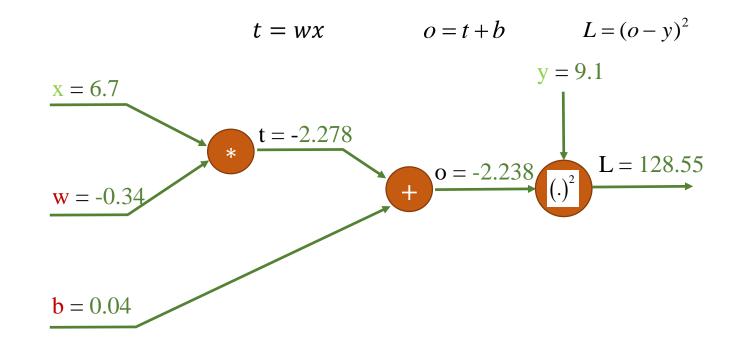
 $t = w * area$



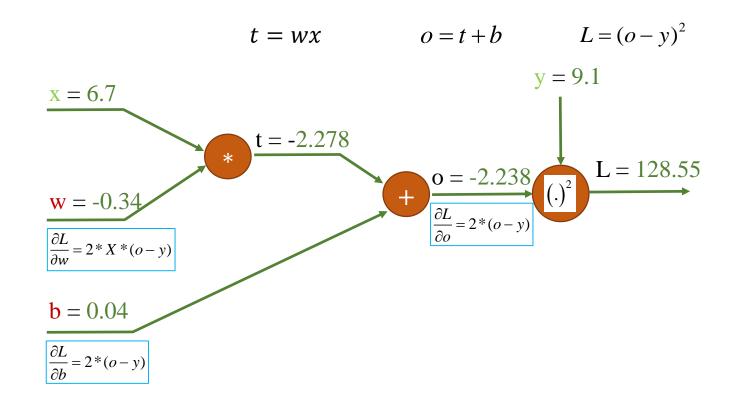
- ***** House price prediction
 - ***** One-sample training



- ***** House price prediction
 - ***** One-sample training



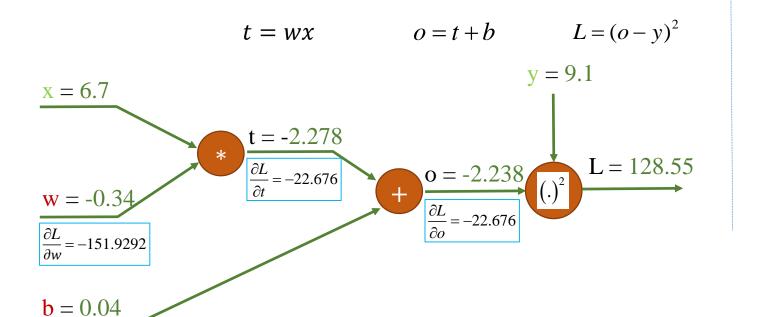
- ***** House price prediction
 - ***** One-sample training



***** House price prediction

 $\frac{\partial L}{\partial b} = -22.676$

❖ One-sample training



Cách cập nhật a và b

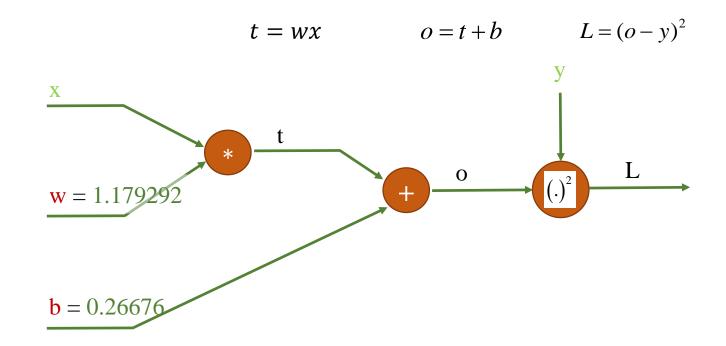
$$w = w - \eta * \frac{\partial L}{\partial w}$$
$$b = b - \eta * \frac{\partial L}{\partial b}$$

Learning rate $\eta = 0.01$

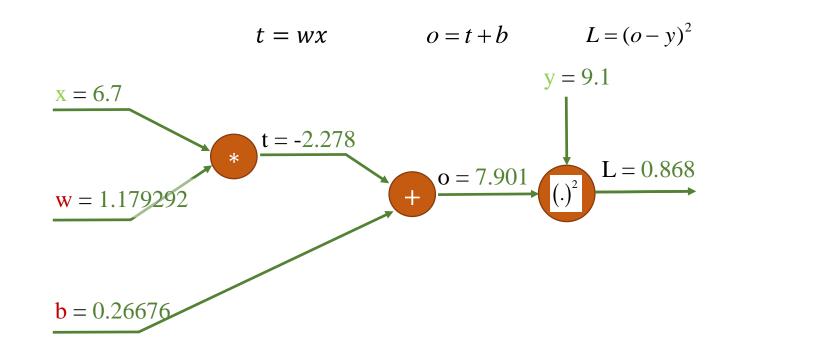
$$w = -0.34 - (0.01 * (-151.9)) = 1.179$$

$$b = 0.04 - (0.01 * (-22.67)) = 0.266$$

- ***** House price prediction
 - ***** One-sample training



- ***** House price prediction
 - ***** One-sample training

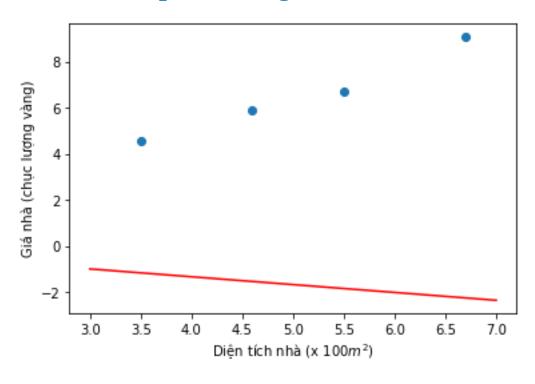


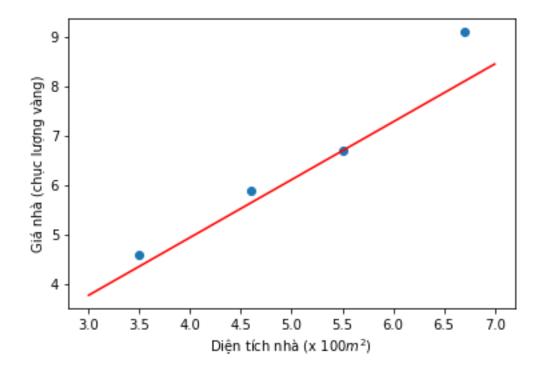
previous L = 128.55

Updated a and b values help to reduce the L value

***** House price prediction

***** One-sample training





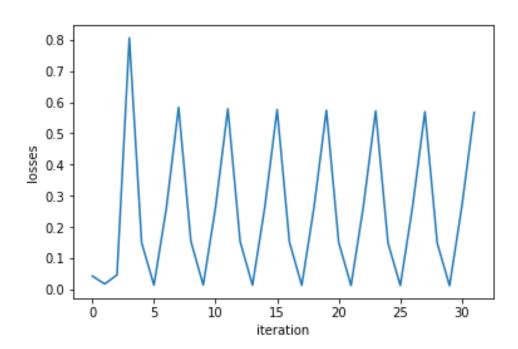
w = -0.34

b = 0.04

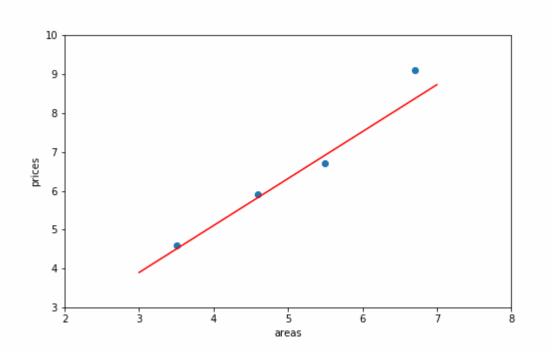
L = 128.55

 $\mathbf{w} = 1.179292$ $\mathbf{b} = 0.26676$ $\mathbf{L} = 0.868$

- ***** House price prediction
 - ***** One-sample training



Losses for 30 iterations

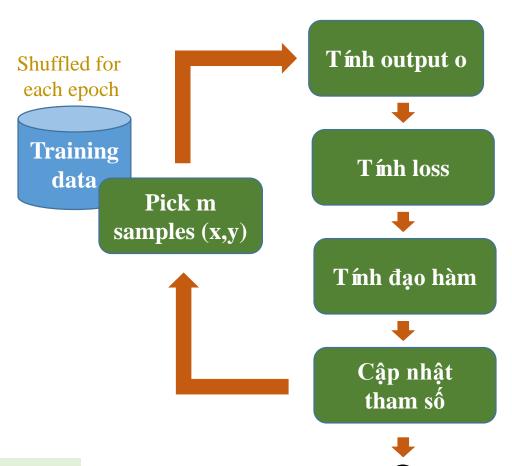


Model updating for different iterations

Outline

- > Machine Learning
- > Derivative/Gradient
- > Linear Regression
- > Computational Graph
 - > 1-sample training
 - m-sample training
- > Generalized formulae

- ***** House price prediction
 - **❖** m-sample training (1<m<N)



- 1) Pick m samples $(x^{(i)}, y^{(i)})$ from training data
- 2) Tính output o_i

$$o^{(i)} = wx^{(i)} + b \qquad \text{for } 0 \le i < m$$

3) Tính loss

$$L^{(i)} = (o^{(i)} - y^{(i)})^2$$
 for $0 \le i < m$

4) Tính đạo hàm

$$L_w^{\prime(i)} = 2x(o^{(i)} - y^{(i)})$$

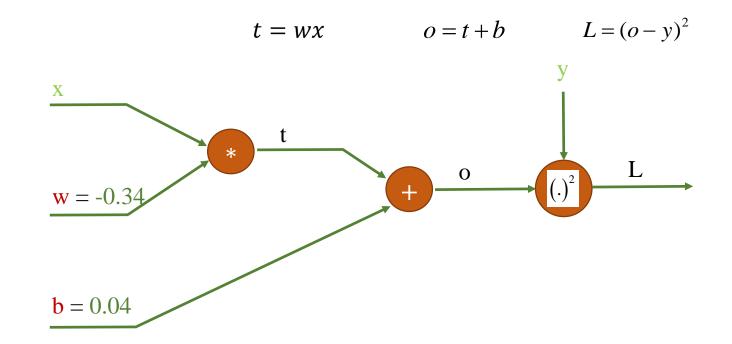
$$L_h^{\prime(i)} = 2(o^{(i)} - y^{(i)}) \text{ for } 0 \le i < m$$

5) Cập nhật tham số

$$w = w - \eta \frac{\sum_{i} L_{w}^{\prime(i)}}{m}$$

$$b = b - \eta \frac{\sum_{i} L_{b}^{\prime(i)}}{m}$$
Learning rate η

- ***** House price prediction
 - **❖** m-sample training (1<m<N)



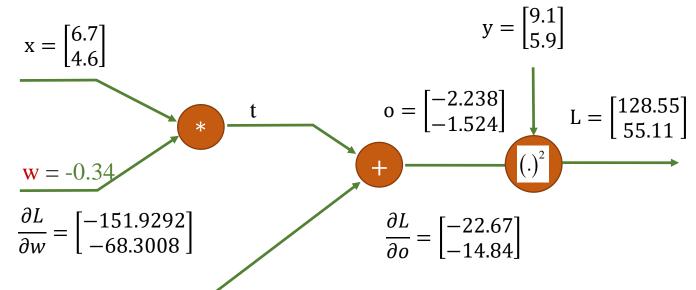
***** House price prediction

❖ m-sample training (1<m<N)

$$m = 2$$

$$\frac{sum(\frac{\partial L}{\partial w})}{m} = -110.115 \qquad \frac{\partial L}{\partial w} = \begin{bmatrix} -151.9292\\ -68.3008 \end{bmatrix}$$

$$\frac{sum(\frac{\partial L}{\partial b})}{m} = -18.762$$



$$\frac{\partial L}{\partial h} = \begin{bmatrix} -22.676 \\ 14.949 \end{bmatrix}$$

$$t = wx$$

$$o = t + b$$

$$o = t + b L = (o - y)^2$$

***** House price prediction

❖ m-sample training (1<m<N)

Cách cập nhật a và b

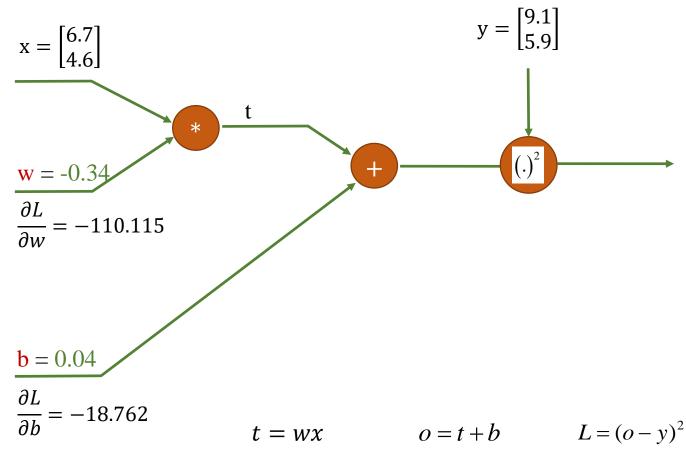
$$w = w - \eta * \frac{\partial L}{\partial w}$$

$$b = b - \eta * \frac{\partial L}{\partial b}$$

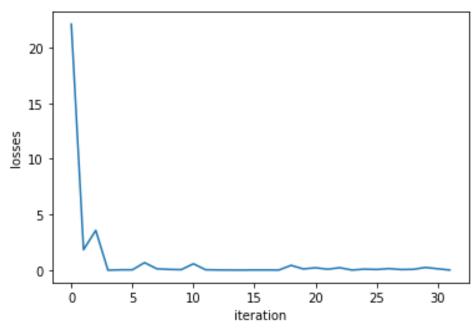
Learning rate $\eta = 0.01$

$$w = -0.34 - (0.01 * (-110.115)) = 0.761$$

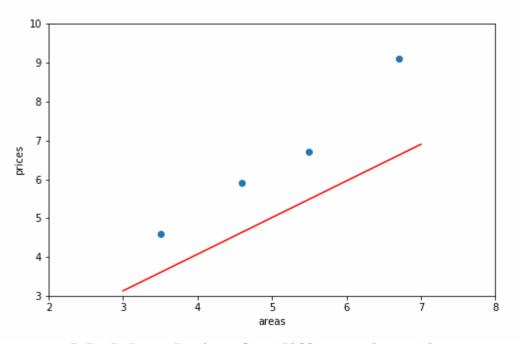
$$b = 0.04 - (0.01 * (-18.762)) = 0.227$$



- ***** House price prediction
 - **❖** m-sample training (1<m<N)



Losses for 30 iterations

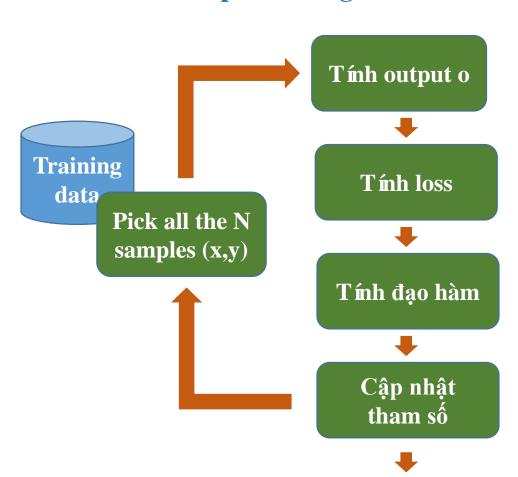


Model updating for different iterations

Outline

- > Machine Learning
- > Derivative/Gradient
- > Linear Regression
- > Computational Graph
 - > 1-sample training
 - m-sample training
 - > N-sample training
- > Generalized formulae

- ***** House price prediction
 - **❖** N-sample training



- 1) Pick all the N samples $(x^{(i)}, y^{(i)})$ from training data
- 2) Tính output o_i

$$o^{(i)} = wx^{(i)} + b \qquad \text{for } 0 \le i < N$$

3) Tính loss

$$L^{(i)} = (o^{(i)} - y^{(i)})^2$$
 for $0 \le i < N$

4) Tính đạo hàm

$$L_w^{\prime(i)} = 2x(o^{(i)} - y^{(i)})$$

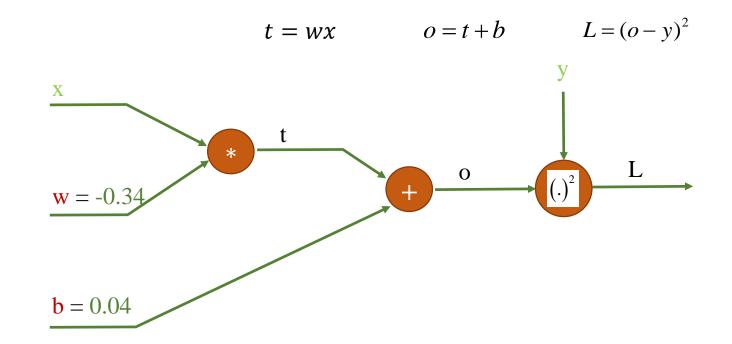
$$L_h^{\prime(i)} = 2(o^{(i)} - y^{(i)}) \text{ for } 0 \le i < N$$

5) Cập nhật tham số

$$w = w - \eta \frac{\sum_{i} L_{w}^{\prime(i)}}{N}$$

$$b = b - \eta \frac{\sum_{i} L_{b}^{\prime(i)}}{N}$$
Learning rate η

- ***** House price prediction
 - ***** N-sample training

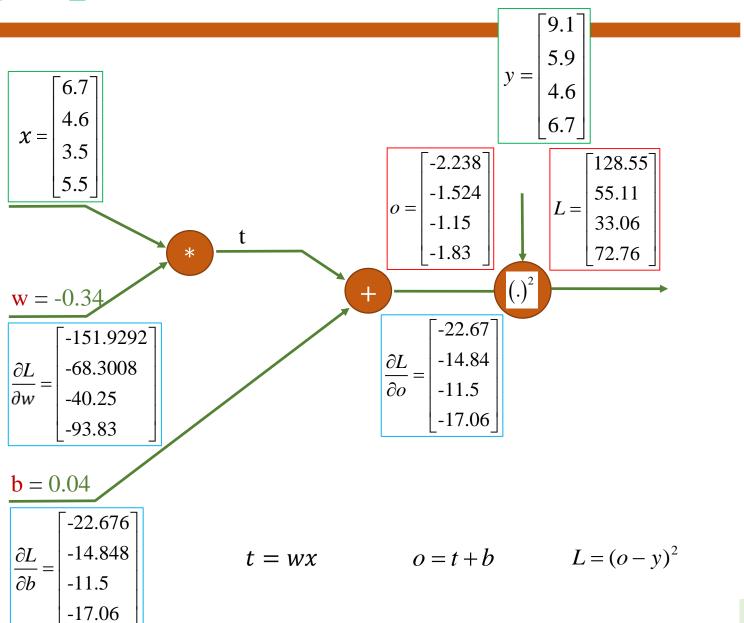


***** House price prediction

***** N-sample training

$$\frac{sum(\frac{\partial L}{\partial w})}{4} = -88.5775$$

$$\frac{sum(\frac{\partial L}{\partial b})}{4} = -16.521$$



***** House price prediction

***** N-sample training

Cách cập nhật a và b

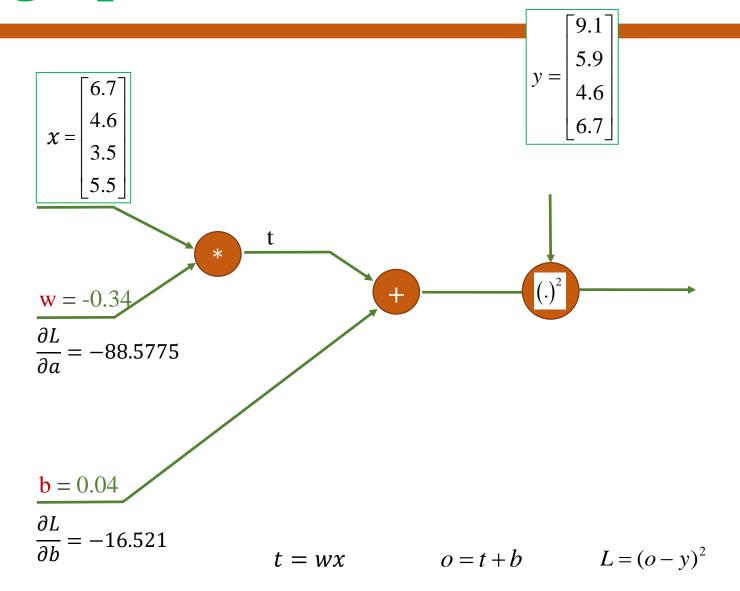
$$w = w - \eta * \frac{\partial L}{\partial w}$$

$$b = b - \eta * \frac{\partial L}{\partial b}$$

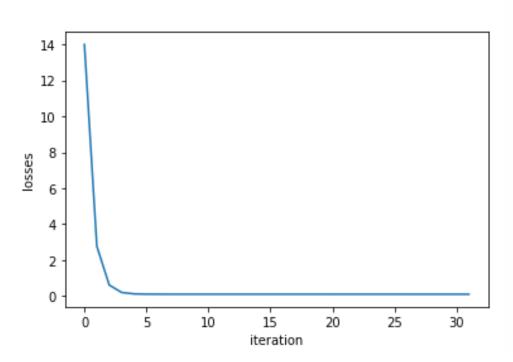
Learning rate $\eta = 0.01$

$$w = -0.34 - (0.01 * (-88.5775)) = 0.54$$

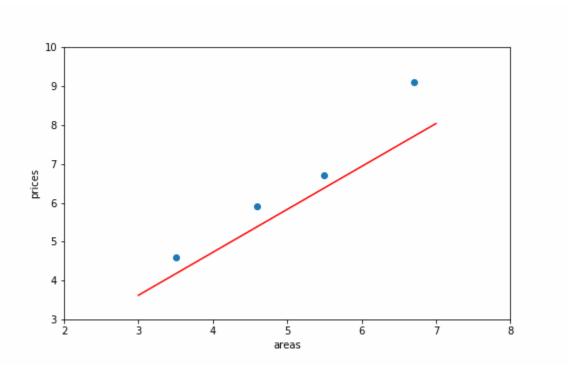
$$b = 0.04 - (0.01 * (-16.521)) = 0.205$$



- ***** House price prediction
 - ***** N-sample training



Losses for 30 iterations



Model updating for different iterations

Outline

- > Machine Learning
- > Derivative/Gradient
- > Linear Regression
- > Computational Graph
- > Generalized formulae

Generalized formula

Lahel

Feature

House price data

Catuic	Laber
area	price
6.7	9.1
4.6	5.9
3.5	4.6
5.5	6.7

Model

$$price = w * area + b$$
$$y = wx + b$$

Model (vectorization)

$$y = \boldsymbol{\theta}^T \boldsymbol{x}$$
 where $\boldsymbol{\theta}^T = [b \ w]^T$

$$\boldsymbol{x} = [x_0 \ area]^T$$

$$x_0 = 1$$

Features

Label

TV	Radio	Newspaper	\$ Sales
230.1	37.8	69.2	22.1
44.5	39.3	45.1	10.4
17.2	45.9	69.3	12
151.5	41.3	58.5	16.5
180.8	10.8	58.4	17.9

Advertising data

Model

Sale =
$$w_1 * TV + w_2 * Radio + w_3 * Newspaper + b$$

 $y = w_1x_1 + w_2x_2 + w_3x_3 + b$

Model (vectorization)

$$y = \boldsymbol{\theta}^T \boldsymbol{x}$$
 where $\boldsymbol{\theta}^T = [b \ w_1 \ w_2 \ w_3]^T$ $\boldsymbol{x} = [x_0 \ TV \ Radio \ Newspaper]^T$ $x_0 = 1$

& Generalized formula

Features	Label

Boston House Price Data

crim \$	zn ÷	indus \$	chas \$	nox ÷	rm 💠	age \$	dis	≑ rad ≑	tax ÷	ptratio \$	black \$	Istat \$	medv \$
0.00632	18	2.31	0	0.538	6.575	65.2	4.09	1	296	15.3	396.9	4.98	24
0.02731	0	7.07	0	0.469	6.421	78.9	4.9671	2	242	17.8	396.9	9.14	21.6
0.03237	0	2.18	0	0.458	6.998	45.8	6.0622	3	222	18.7	394.63	2.94	33.4
0.06905	0	2.18	0	0.458	7.147	54.2	6.0622	3	222	18.7	396.9	5.33	36.2
0.08829	12.5	7.87	0	0.524	6.012	66.6	5.5605	5 5	311	15.2	395.6	12.43	22.9

Model

$$medv = w_1 * x_1 + \dots + w_{13} * x_{13} + b$$

Model (vectorization)

$$y = \boldsymbol{\theta}^T \boldsymbol{x}$$
 where $\boldsymbol{\theta}^T = [b \quad w_1 \quad ... \quad w_{13}]^T$
 $\boldsymbol{x} = [x_0 \quad x_1 \quad ... \quad x_{13}]^T$
 $x_0 = 1$

Linear Regression (1-sample)

- 1) Pick a sample (x, y) from training data
- 2) Tính output o

$$o = wx + b$$

3) Tính loss

$$L = (o - y)^2$$

4) Tính đạo hàm

$$L'_w = 2x(o - y)$$

$$L'_b = 2(o - y)$$

5) Cập nhật tham số

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

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

$$\eta \text{ is learning rate}$$

- 1) Pick a sample (x, y) from training data
- 2) Tính output o

$$o = \boldsymbol{\theta}^T \boldsymbol{x}$$

3) Tính loss

$$L = (o - y)^2$$

4) Tính đạo hàm

$$L_{\boldsymbol{\theta}}' = 2\boldsymbol{x}(o - \boldsymbol{y})$$

5) Cập nhật tham số

$$\boldsymbol{\theta} = \boldsymbol{\theta} - \eta L_{\boldsymbol{\theta}}'$$

 η is learning rate

Linear Regression (m-samples)

- 1) Pick m samples $(x^{(i)}, y^{(i)})$ from training data
- 1.1) Tính output $o^{(i)}$

$$o^{(i)} = wx^{(i)} + b \qquad \text{for } 0 \le i < m$$

1.2) Tính loss

$$L^{(i)} = (o^{(i)} - y^{(i)})^2$$
 for $0 \le i < m$

1.3) Tính đao hàm

$$L_w^{\prime(i)} = 2x(o^{(i)} - y^{(i)})$$

$$L_h^{\prime(i)} = 2(o^{(i)} - y^{(i)}) \text{ for } 0 \le i < m$$

2) Cập nhật tham số
$$w = w - \eta \frac{\sum_{i} L'_{w}^{(i)}}{m}$$

$$b = b - \eta \frac{\sum_{i} L'_{b}^{(i)}}{m}$$
 η is learning rate

- 1) Pick m samples $(x^{(i)}, y^{(i)})$ from training data
- 1.1) Tính output $o^{(i)}$

$$o^{(i)} = \boldsymbol{\theta}^T \boldsymbol{x}^{(i)} \qquad \text{for } 0 \le i < m$$

1.2) Tính loss

$$L^{(i)} = (o^{(i)} - y^{(i)})^2$$
 for $0 \le i < m$

1.3) Tính đao hàm

$$L_{\theta}^{'(i)} = 2x(o^{(i)} - y^{(i)})$$
 for $0 \le i < m$

2) Cập nhật tham số

$$\boldsymbol{\theta} = \boldsymbol{\theta} - \eta \frac{\sum_{i} L_{\boldsymbol{\theta}}^{\prime(i)}}{m}$$
 η is learning rate

Linear Regression (N-samples)

- 1) Pick all the N samples from training data
- 2) Tính output $o^{(i)}$

$$o^{(i)} = wx^{(i)} + b \qquad \text{for } 0 \le i < N$$

3) Tính loss

$$L^{(i)} = (o^{(i)} - y^{(i)})^2$$
 for $0 \le i < N$

4) Tính đao hàm

$$L_w^{\prime(i)} = 2x(o^{(i)} - y^{(i)})$$

$$L_h^{\prime(i)} = 2(o^{(i)} - y^{(i)}) \text{ for } 0 \le i < N$$

5) Cập nhật tham số
$$w = w - \eta \frac{\sum_{i} L'_{w}^{(i)}}{N}$$

$$b = b - \eta \frac{\sum_{i} L'_{b}^{(i)}}{N}$$
 η is learning rate

- 1) Pick all the N samples from training data
- 2) Tính output $o^{(i)}$

$$o^{(i)} = \boldsymbol{\theta}^T \boldsymbol{x}^{(i)} \qquad \text{for } 0 \le i < N$$

3) Tính loss

$$L^{(i)} = (o^{(i)} - y^{(i)})^2$$
 for $0 \le i < N$

4) Tính đao hàm

$$L_{\theta}^{\prime(i)} = 2x(o^{(i)} - y^{(i)})$$
 for $0 \le i < N$

5) Cập nhật tham số

$$\boldsymbol{\theta} = \boldsymbol{\theta} - \eta \frac{\sum_{i} L_{\boldsymbol{\theta}}^{\prime(i)}}{N}$$
 η is learning rate

***** House price prediction

Demo

Year 2020

Advertising-based sale prediction

Demo

Uear 2020

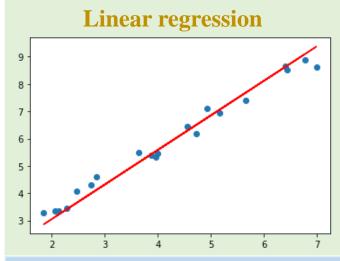
***** House price prediction

❖Boston data

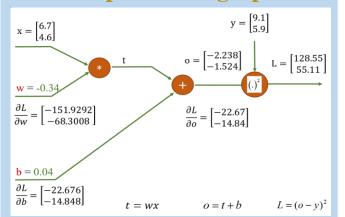
Demo

Year 2020

Summary



Computational graph



Formulae cheat sheet

- 1) Pick a sample (x, y) from training data
- 2) Tính output o

$$o = \boldsymbol{\theta}^T \boldsymbol{x}$$

3) Tính loss

$$L = (o - y)^2$$

4) Tính đạo hàm

$$L_{\boldsymbol{\theta}}' = 2\boldsymbol{x}(o-\boldsymbol{y})$$

5) Cập nhật tham số

$$\boldsymbol{\theta} = \boldsymbol{\theta} - \eta L_{\boldsymbol{\theta}}'$$

 η is learning rate

