機器學習

Lecture 3　Regression

相關關係

- 某汽車公司 8 個分公司汽車銷售額與廣告支出數額的資料。

分公司名稱	廣告支出X	年銷售額Y
A	300	9,500
B	400	10,300
C	500	11,000
D	500	12,000
E	800	12,400
F	1,000	13,400
G	1,000	14,500
H	1,300	15,300

相關關係

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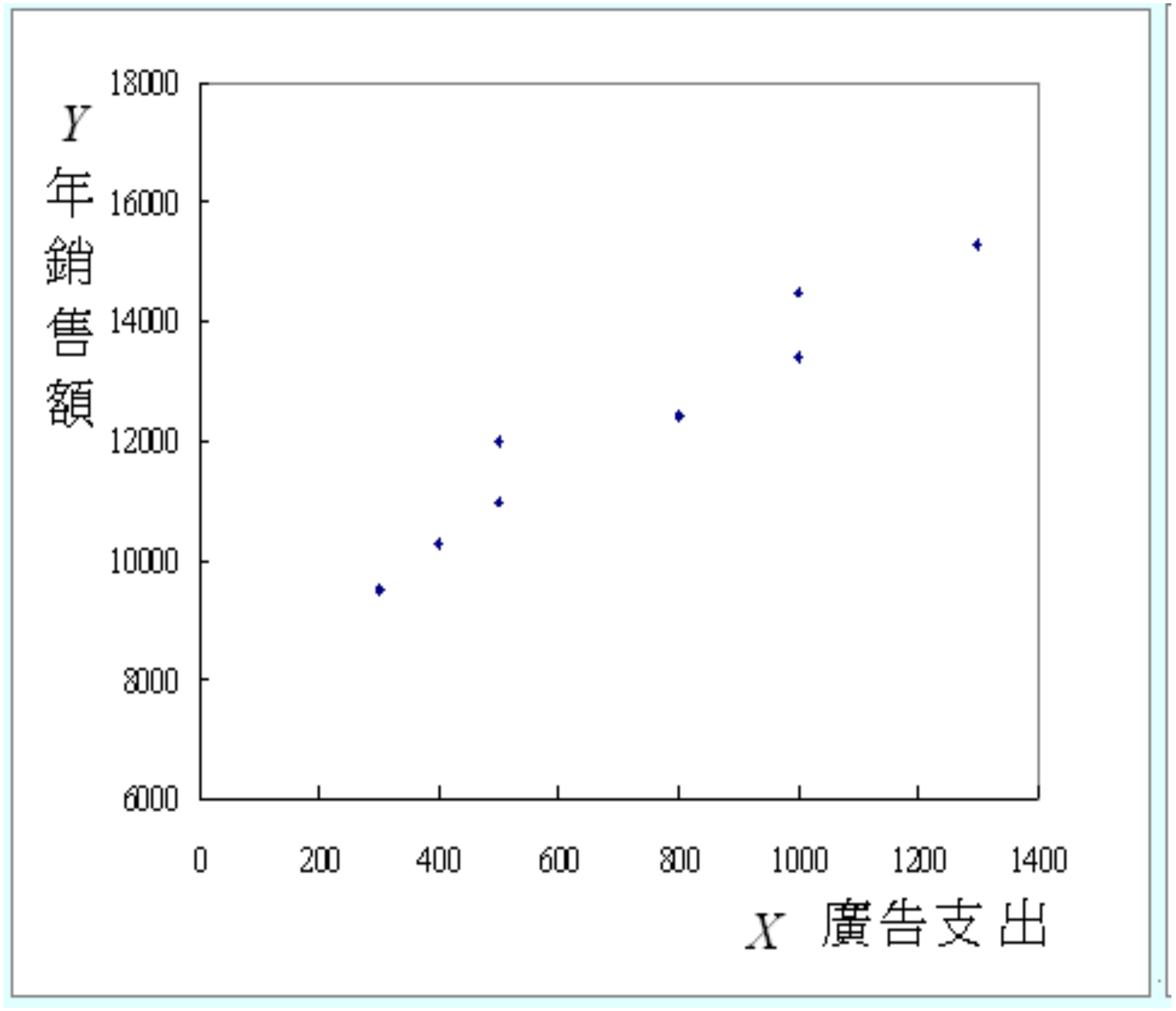

相關係數

$$r_{xy} = \frac{S_{xy}}{S_x S_y} = \frac{\sum (x-\bar{x})(y-\bar{y})}{\sqrt{\sum (x-\bar{x})^2}\sqrt{\sum (x-\bar{x})^2}} \in [-1,1]$$

其中，$S_{xy} = \dfrac{\sum (x-\bar{x})(y-\bar{y})}{n-1}$

$$S_x = \sqrt{\frac{\sum (x-\bar{x})^2}{n-1}}$$

$$S_y = \sqrt{\frac{\sum (y-\bar{y})^2}{n-1}}$$

相關係數

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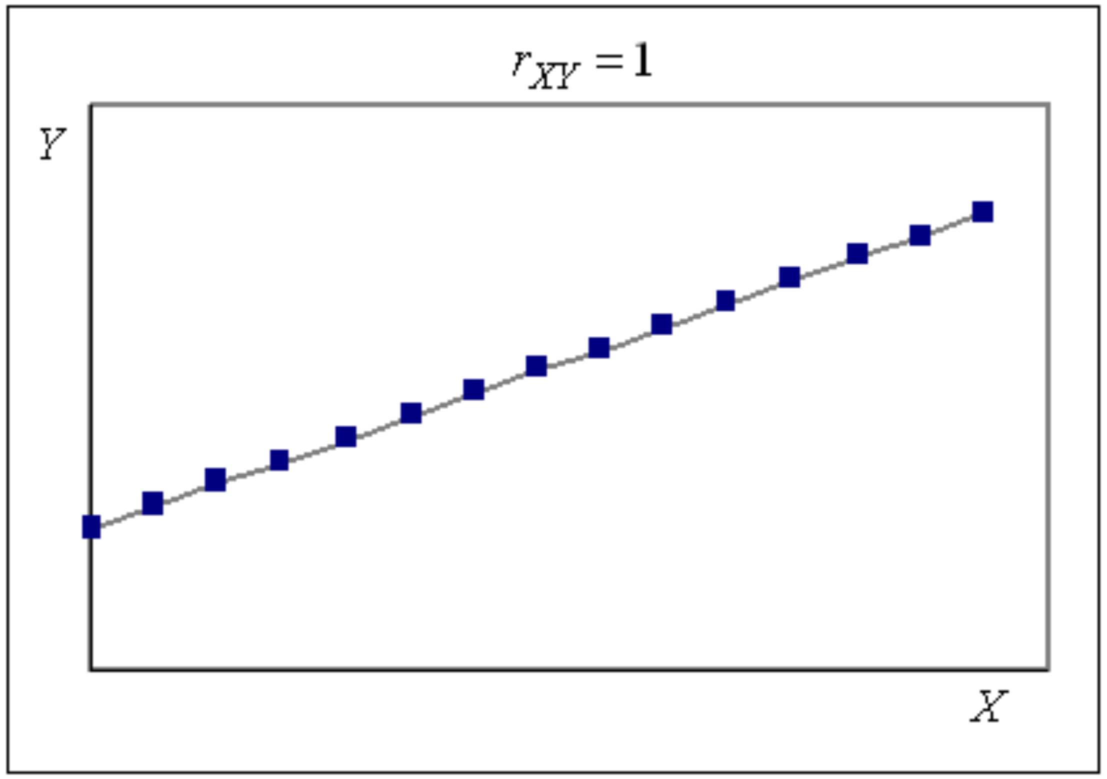
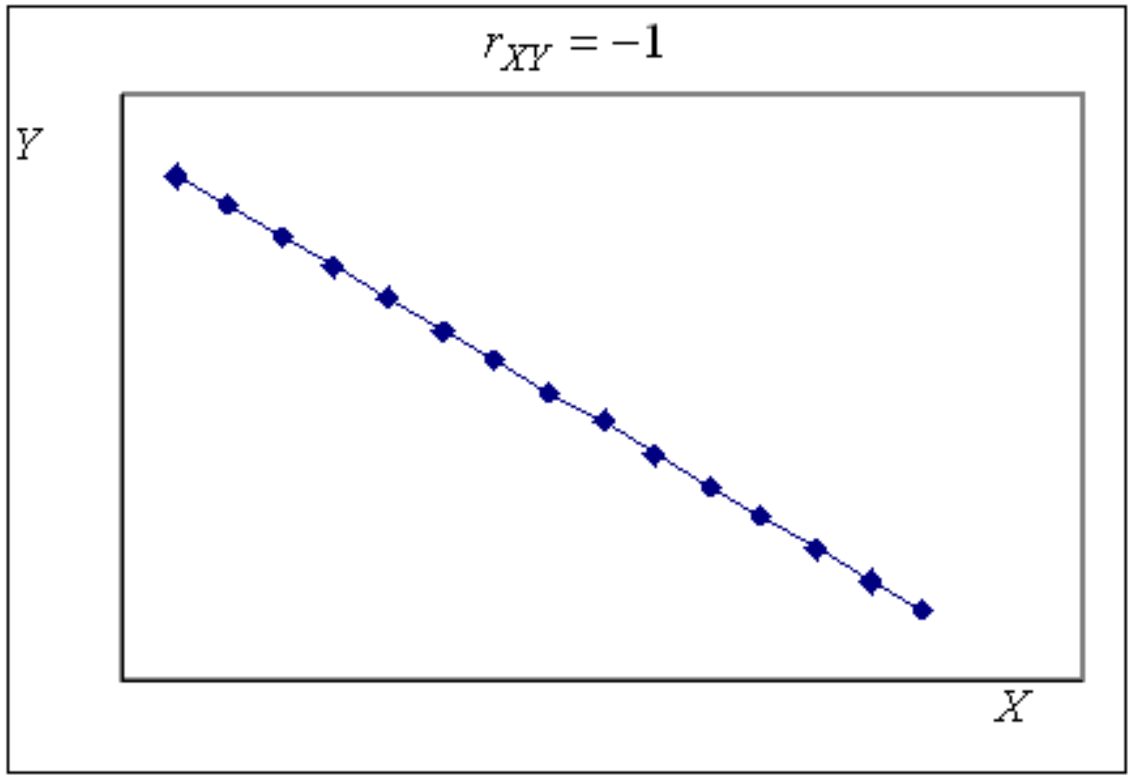
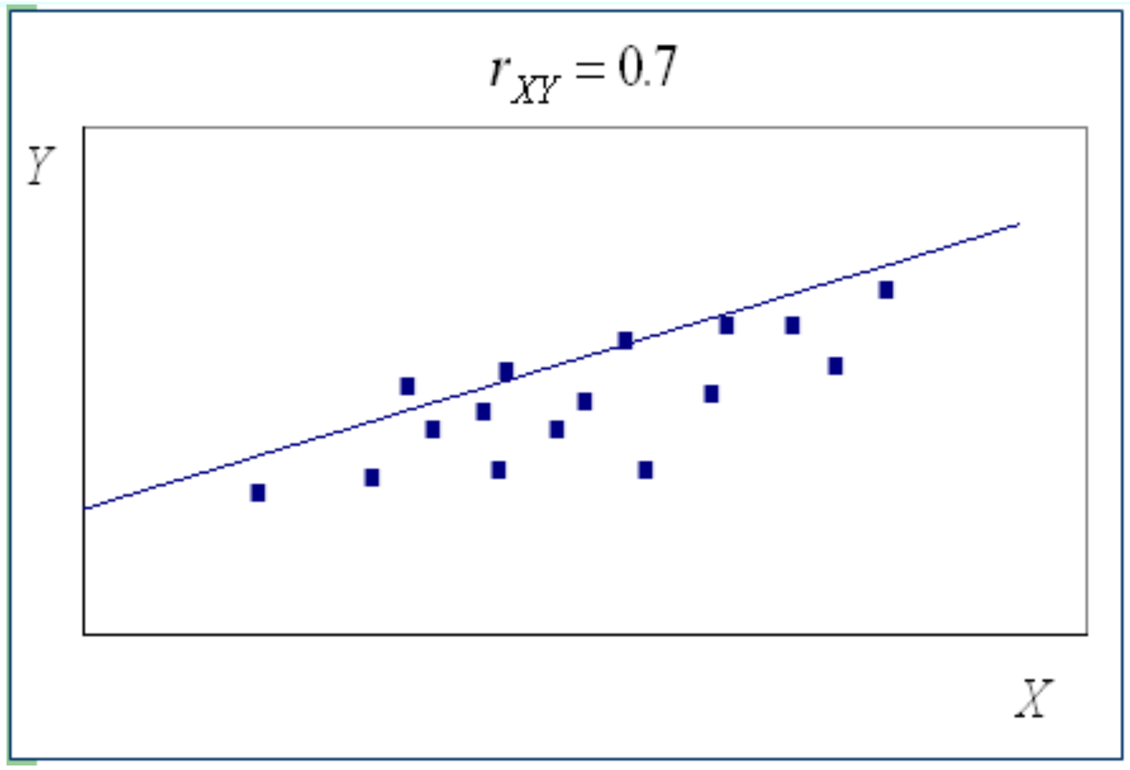
$$r_{XY} = \frac{\sum (X-\bar{X})(Y-\bar{Y})}{\sqrt{\sum (X-\bar{X})^2}\sqrt{\sum (Y-\bar{Y})^2}} = \frac{4{,}840{,}000}{\sqrt{875{,}000}\sqrt{28{,}680{,}000}} = 0.966$$

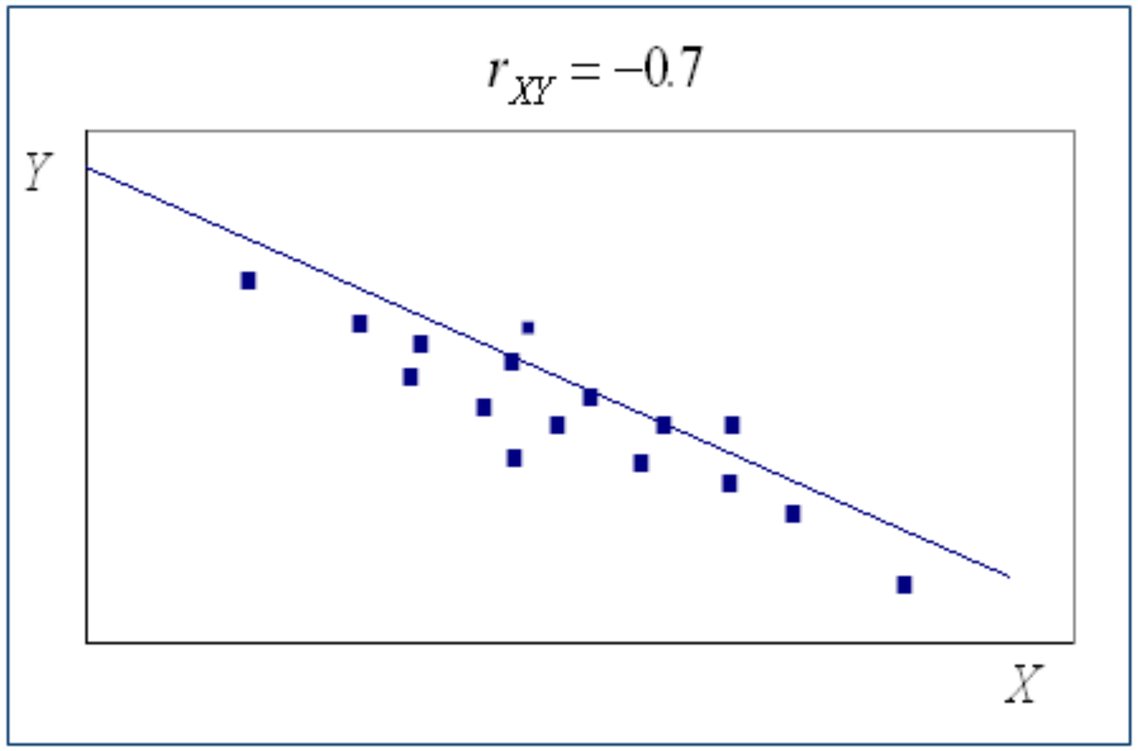
相關係數

正相關　　　　　　　　負相關



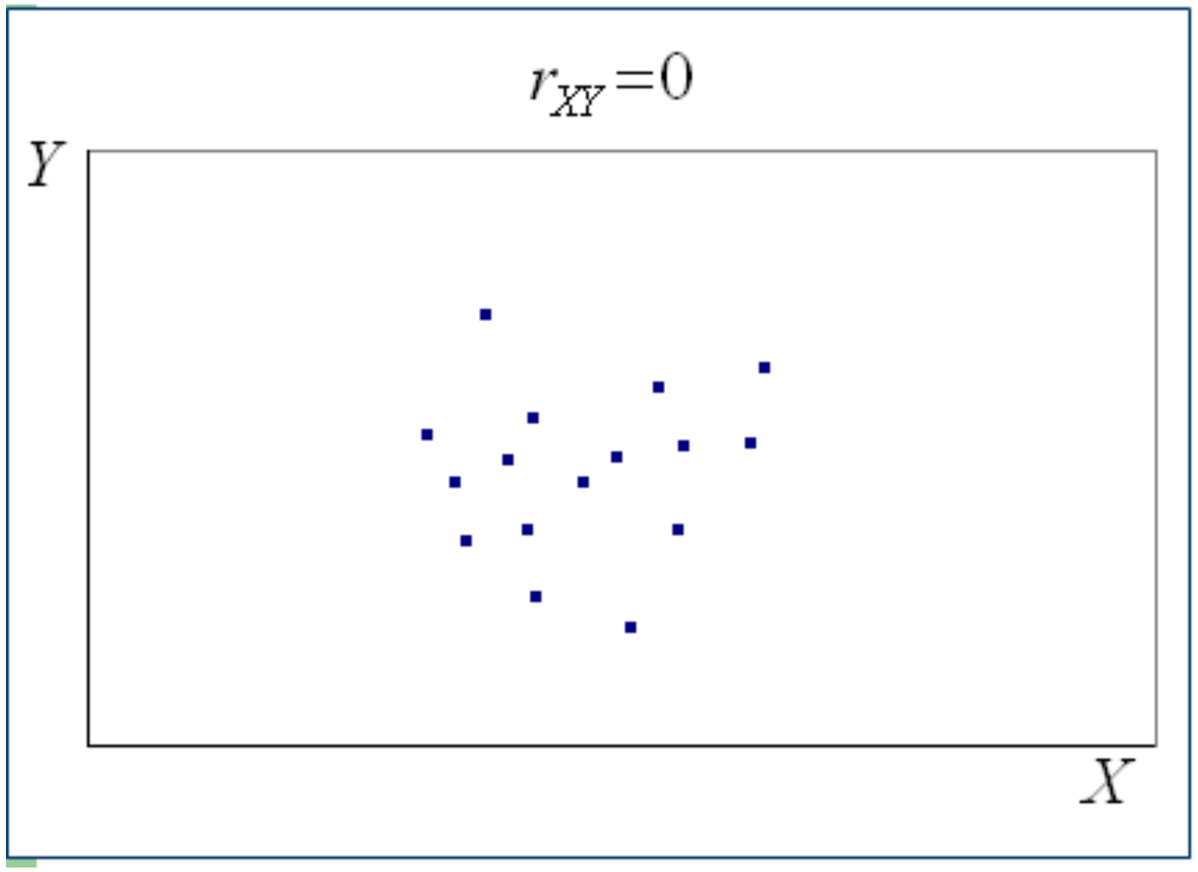


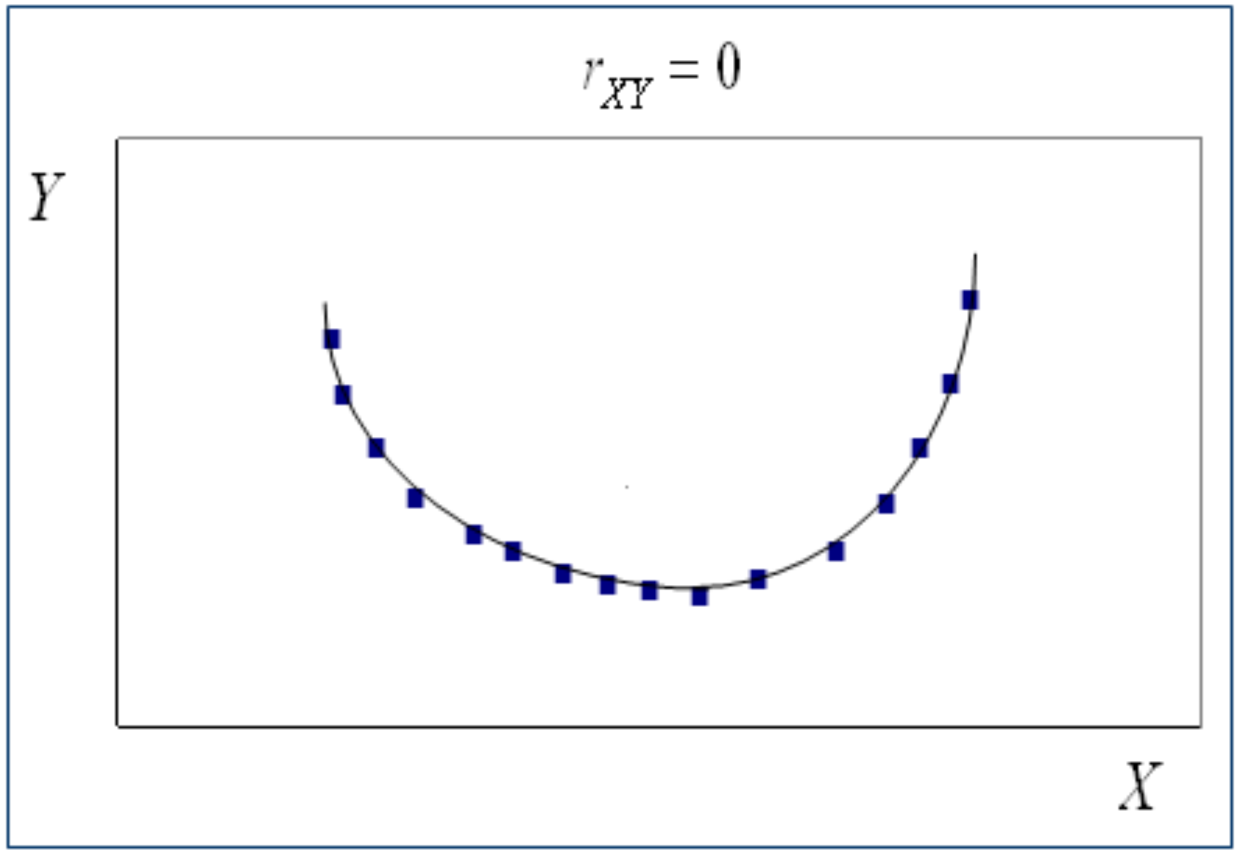




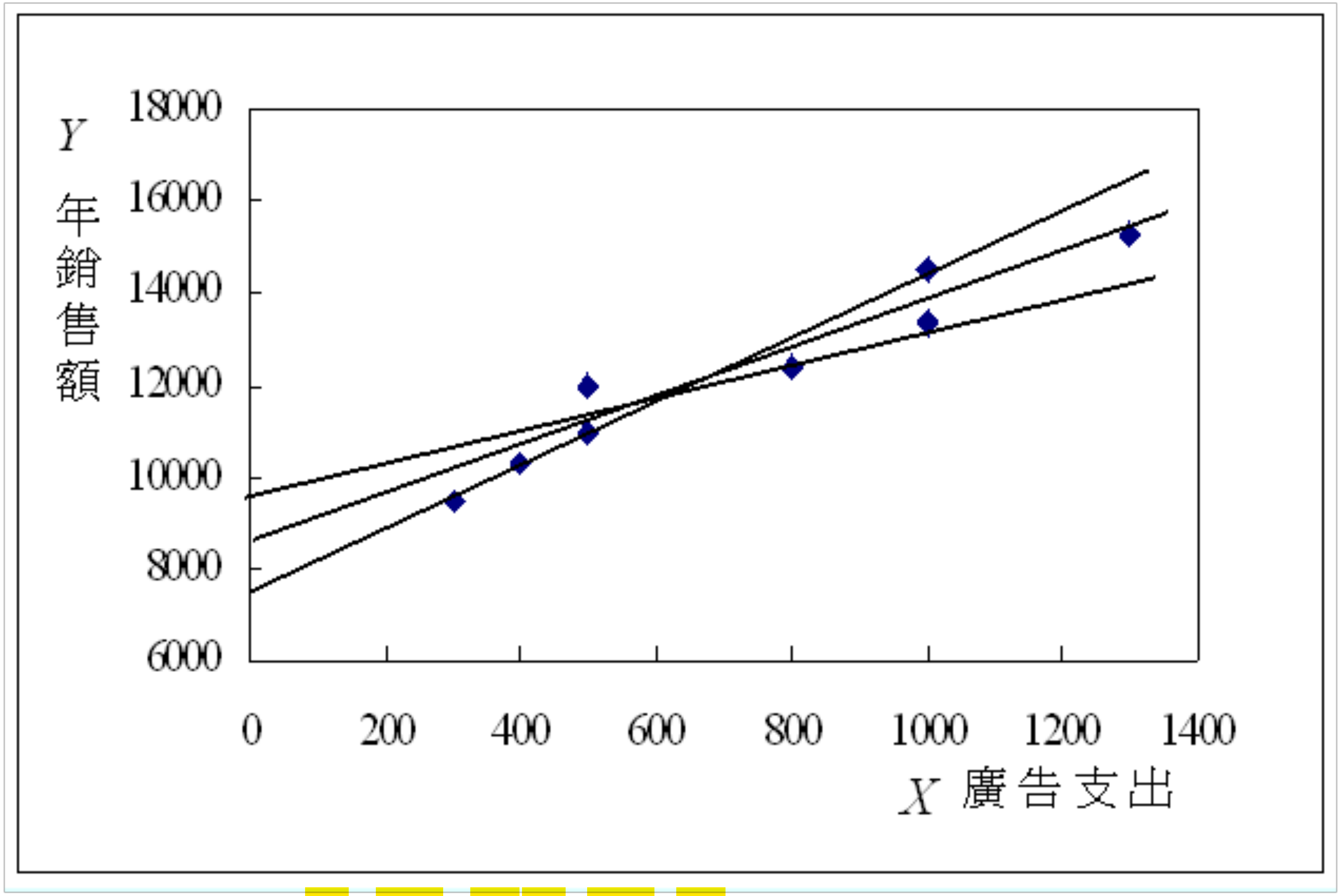
相關係數

不存在線性相關



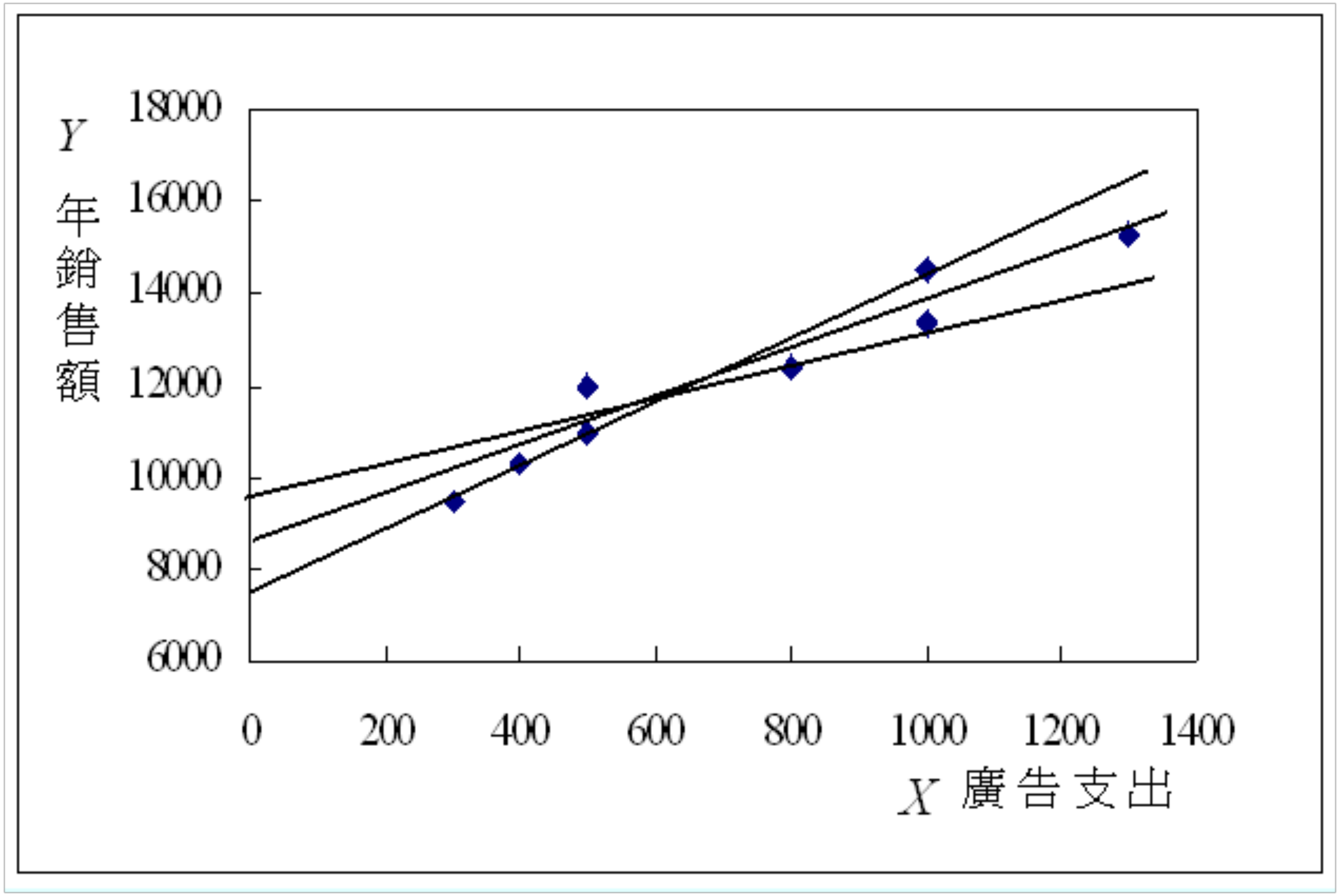


Regression



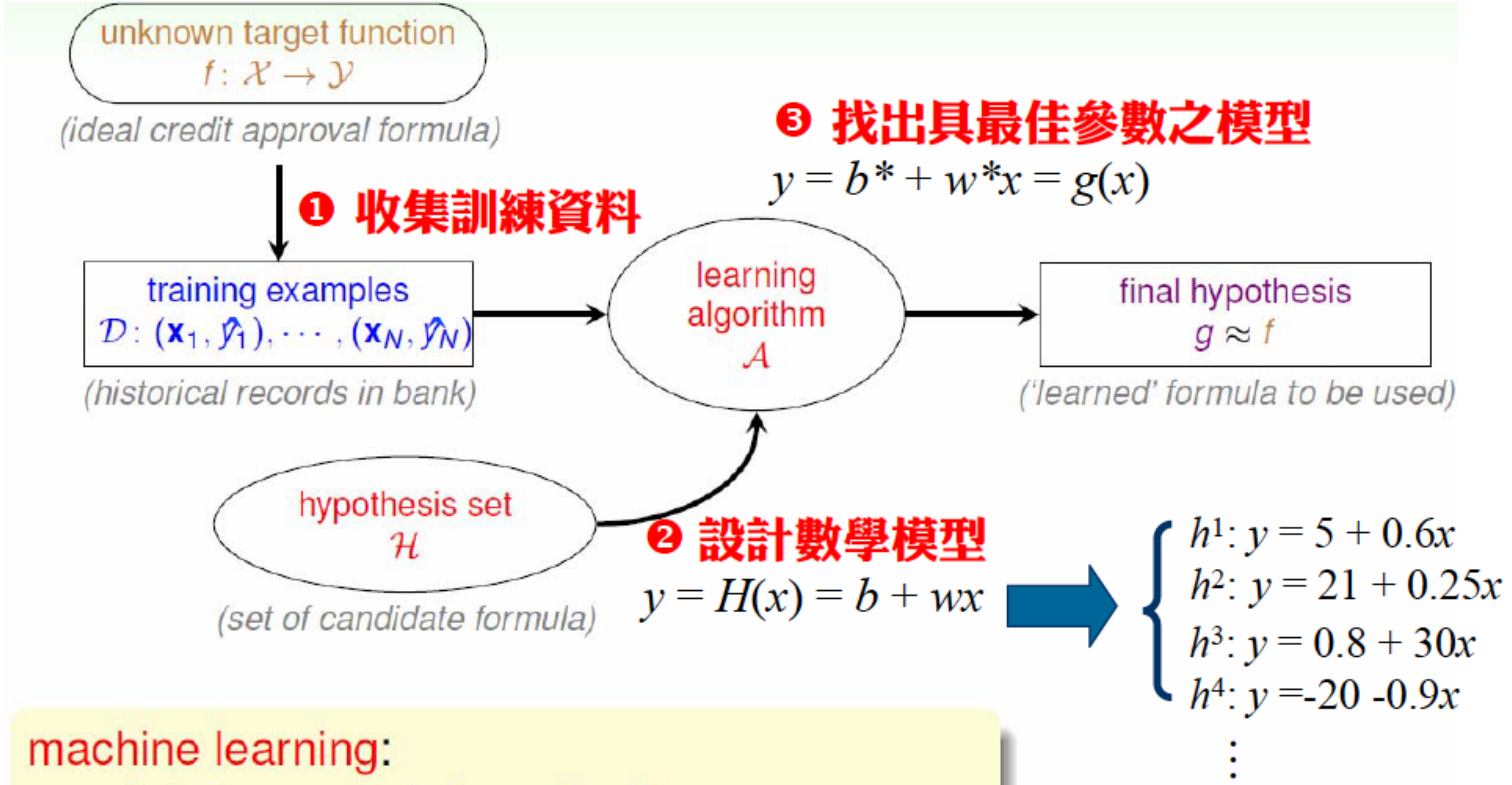
線性模型 $y = ax + b$

Regression



線性模型 $h_\theta(x) = \theta_0 + \theta_1 x$

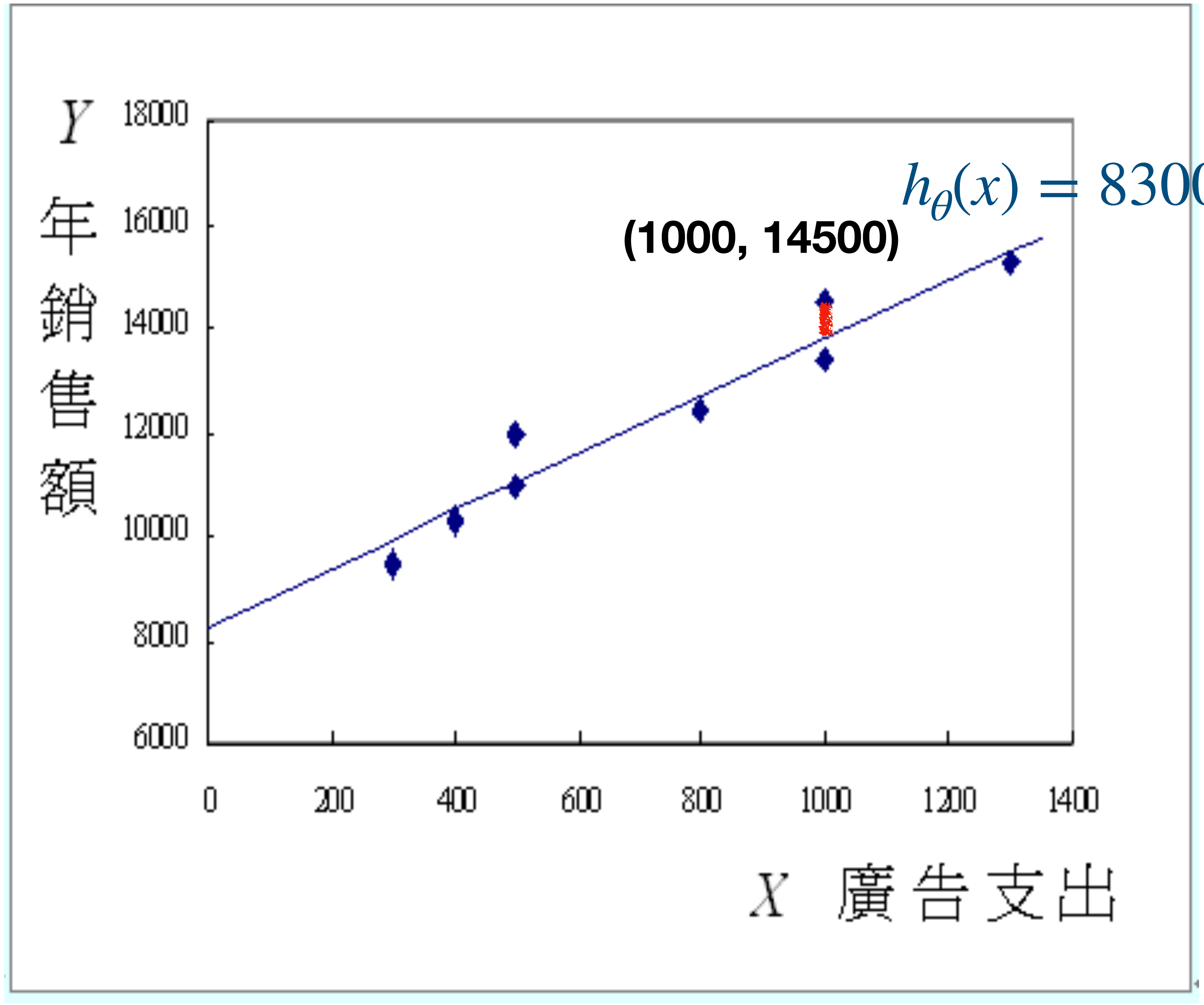
Regression



machine learning:
use data to compute hypothesis *g*
that approximates target *f*

台大資工：林軒田 教授

Regression

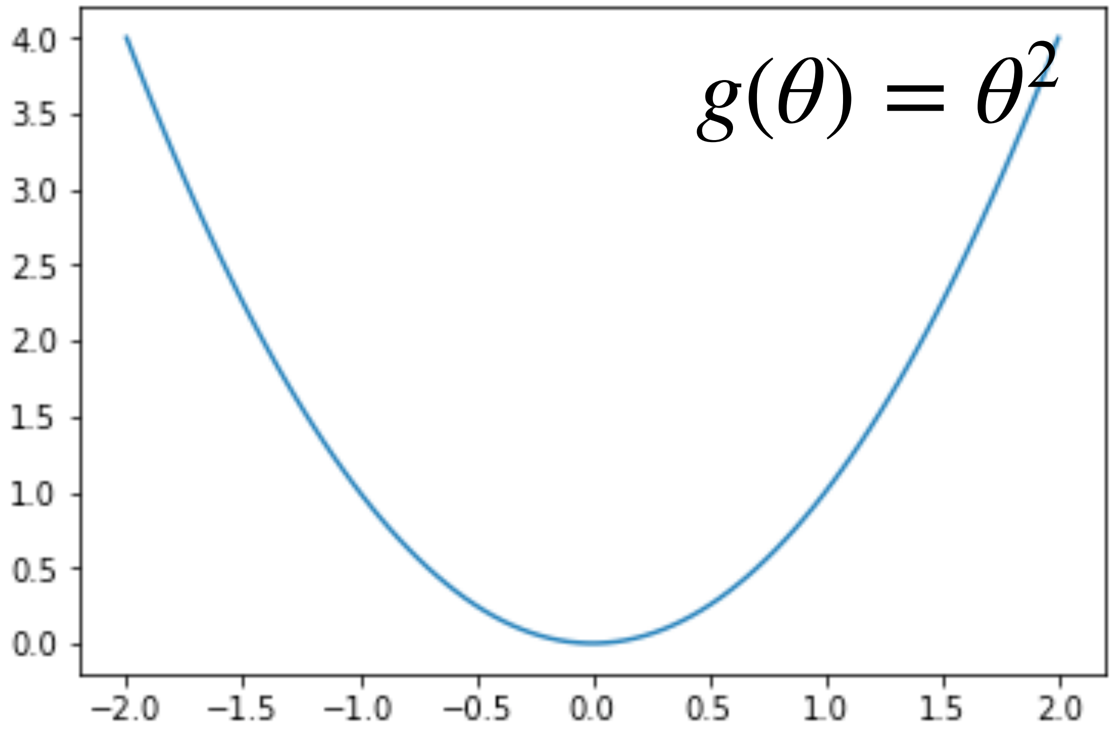


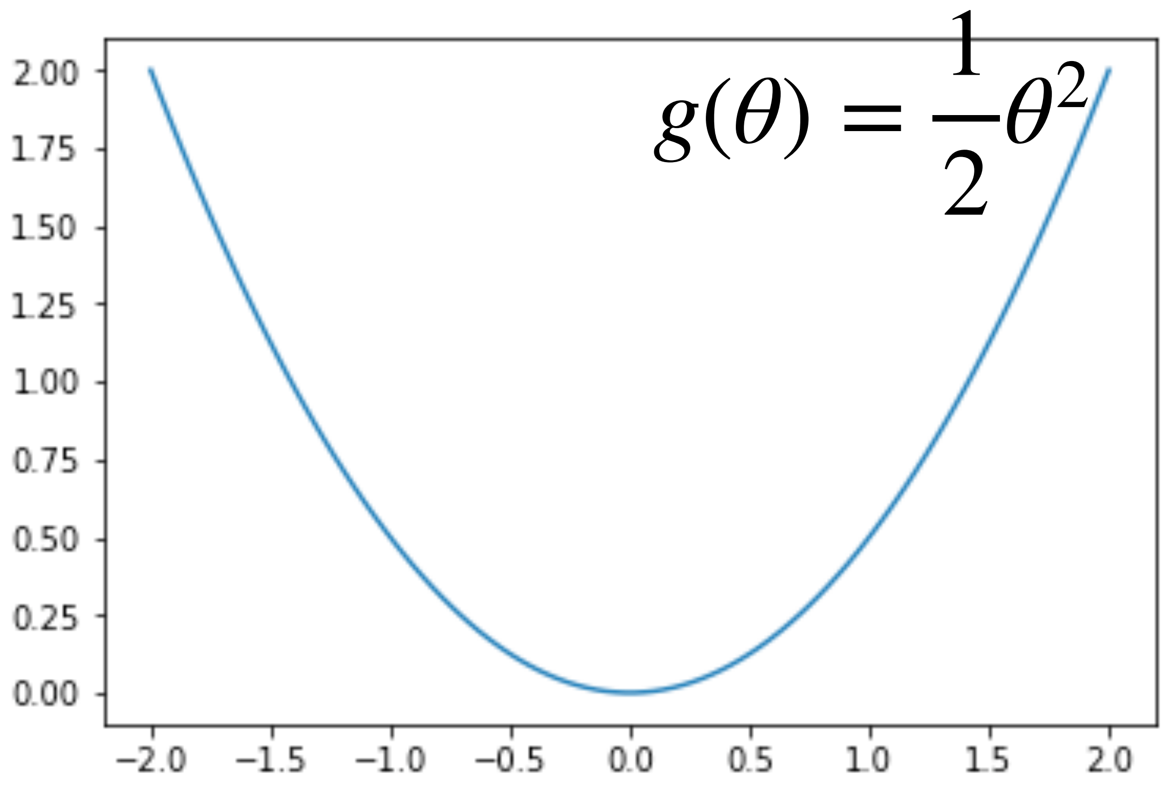
$$h_\theta(x) = 8300 + 5.5x$$

最小平方法 (Least square Method)

- Goal: minimize the cost function

$$min_{\theta_0,\theta_1} \boxed{\frac{1}{2}} \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)}\right)^2$$





最小平方法 (Least square Method)

- Cost function

$$E(\theta_0, \theta_1) = \frac{1}{2}\sum_{i=1}^{m}\left(h_\theta(x^{(i)}) - y^{(i)}\right)^2$$

- 找一組 θ_0, θ_1 使 $E(\theta_0, \theta_1)$ 最小

$$\frac{\partial E(\theta_0, \theta_1)}{\partial \theta_0} = \sum\left(\theta_0 + \theta_1 x^{(i)} - y^{(i)}\right) \equiv 0$$

$$\frac{\partial E(\theta_0, \theta_1)}{\partial \theta_1} = \sum\left(\theta_0 + \theta_1 x^{(i)} - y^{(i)}\right) \cdot x^{(i)} \equiv 0$$

最小平方法 (Least square Method)

- 解方程組得

$$\theta_1 = \frac{n\sum x^{(i)}y^{(i)} - \sum x^{(i)}\sum y^{(i)}}{n\sum (x^{(i)})^2 - \left(\sum x^{(i)}\right)^2} = \frac{\sum \left(x^{(i)} - \bar{x}\right)\left(y^{(i)} - \bar{y}\right)}{\sum \left(x^{(i)} - \bar{x}\right)^2}$$

$$\theta_0 = \bar{y} - \theta_1 \bar{x}$$

$$\theta_1 = r_{xy} \cdot \frac{S_y}{S_x}$$

Regression

- Cost function

$$E(\theta_0, \theta_1) = \frac{1}{2}\sum_{i=1}^{m}\left(h_\theta(x^{(i)}) - y^{(i)}\right)^2$$

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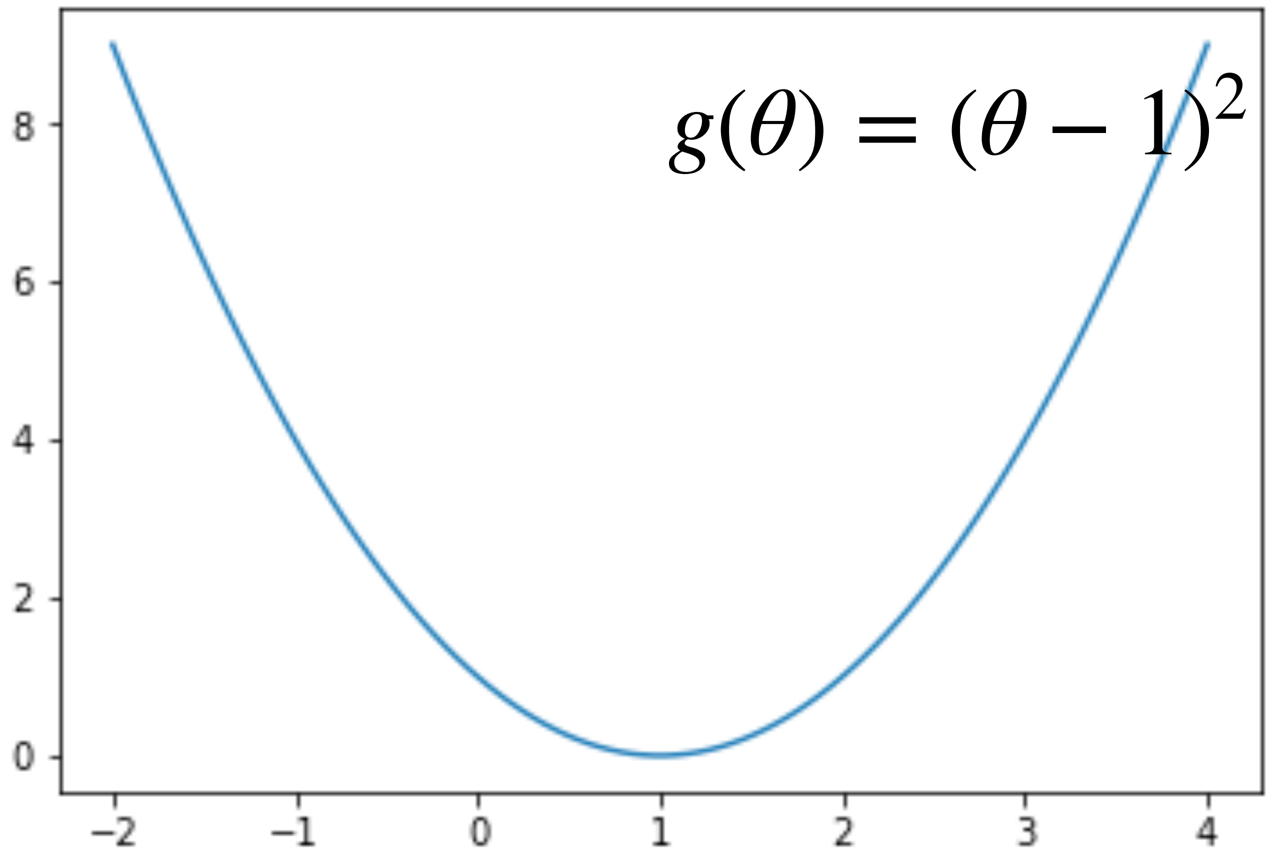
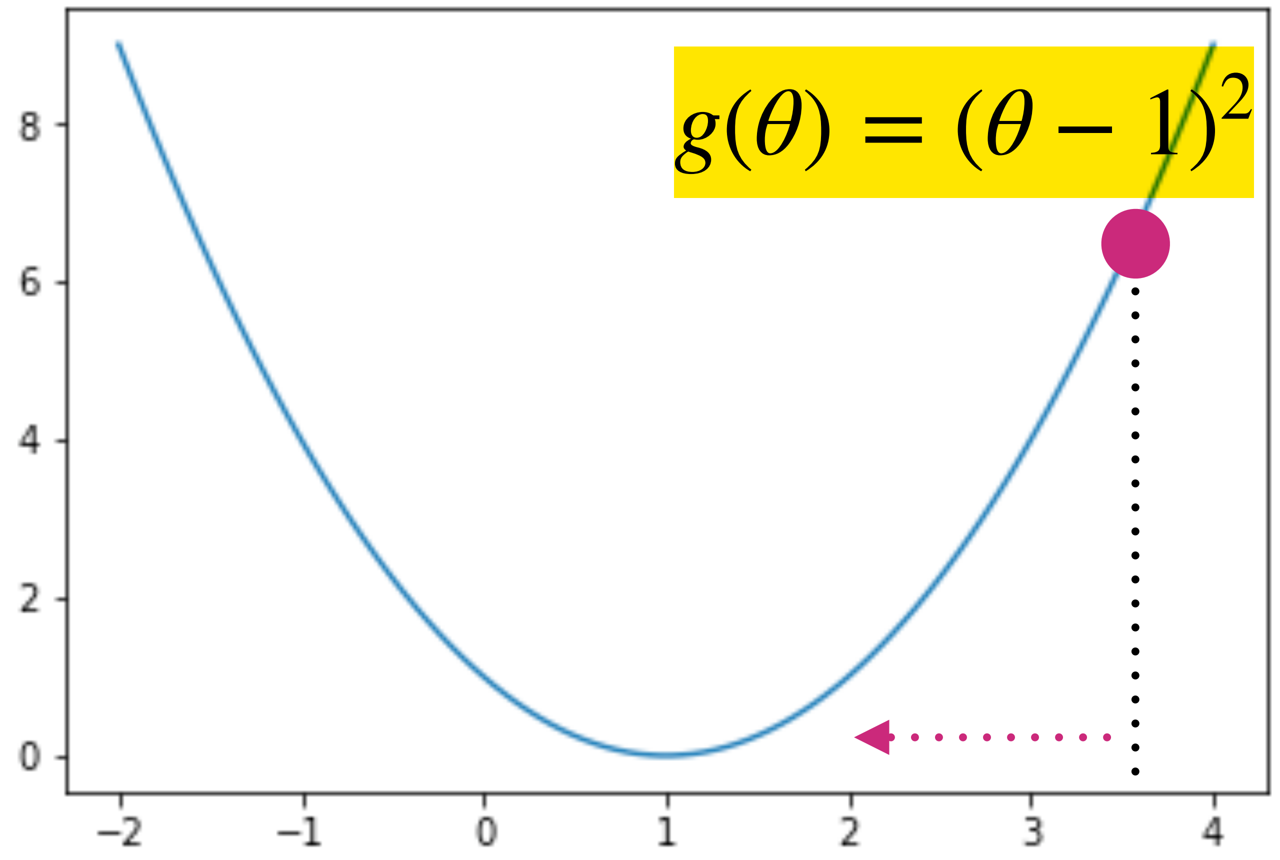
増減表



	$\theta < 1$	$\theta = 1$	$\theta > 1$
$g'(\theta)$	$-$	0	$+$
	↘	minimum	↗

$$\frac{d}{d\theta} g(\theta) = 2\theta - 2$$

增減表



	$\theta < 1$	$\theta = 1$	$\theta > 1$
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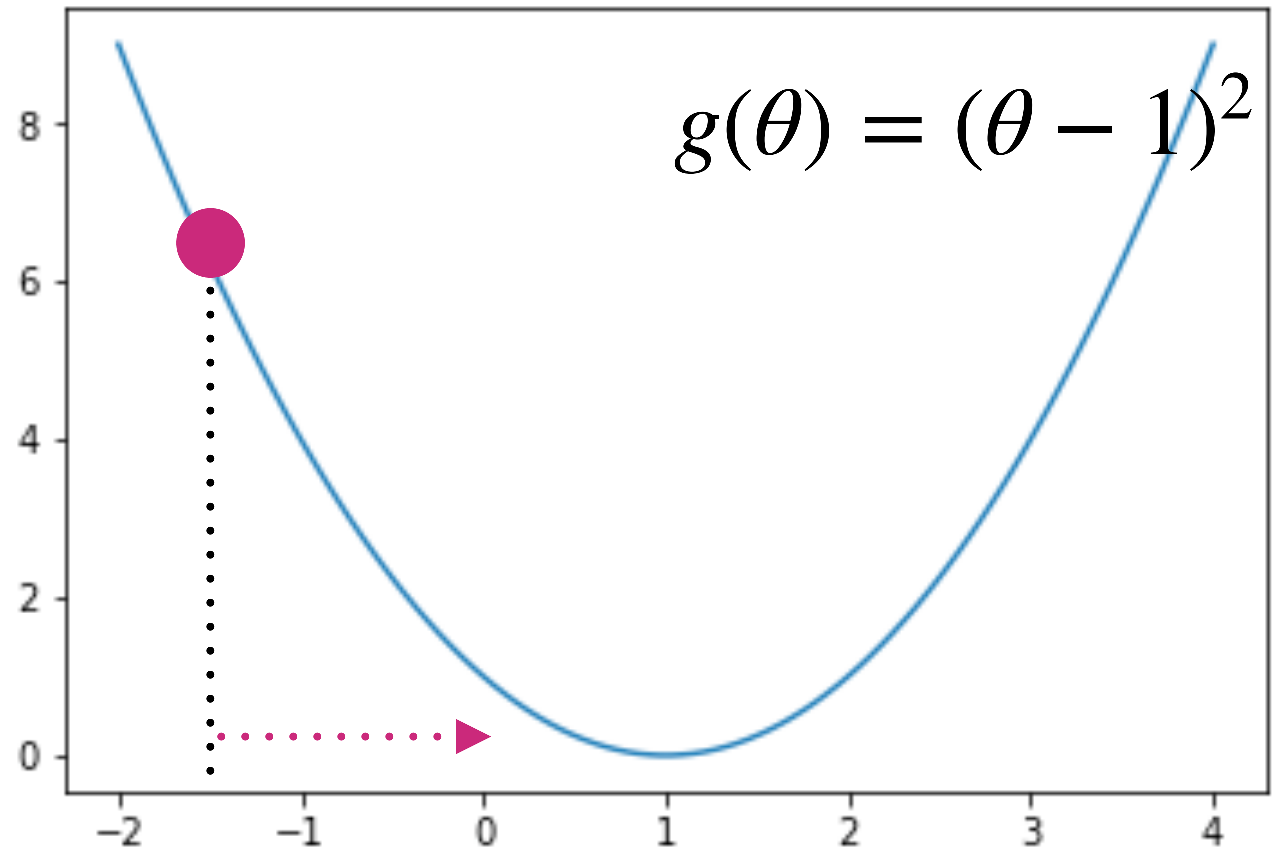
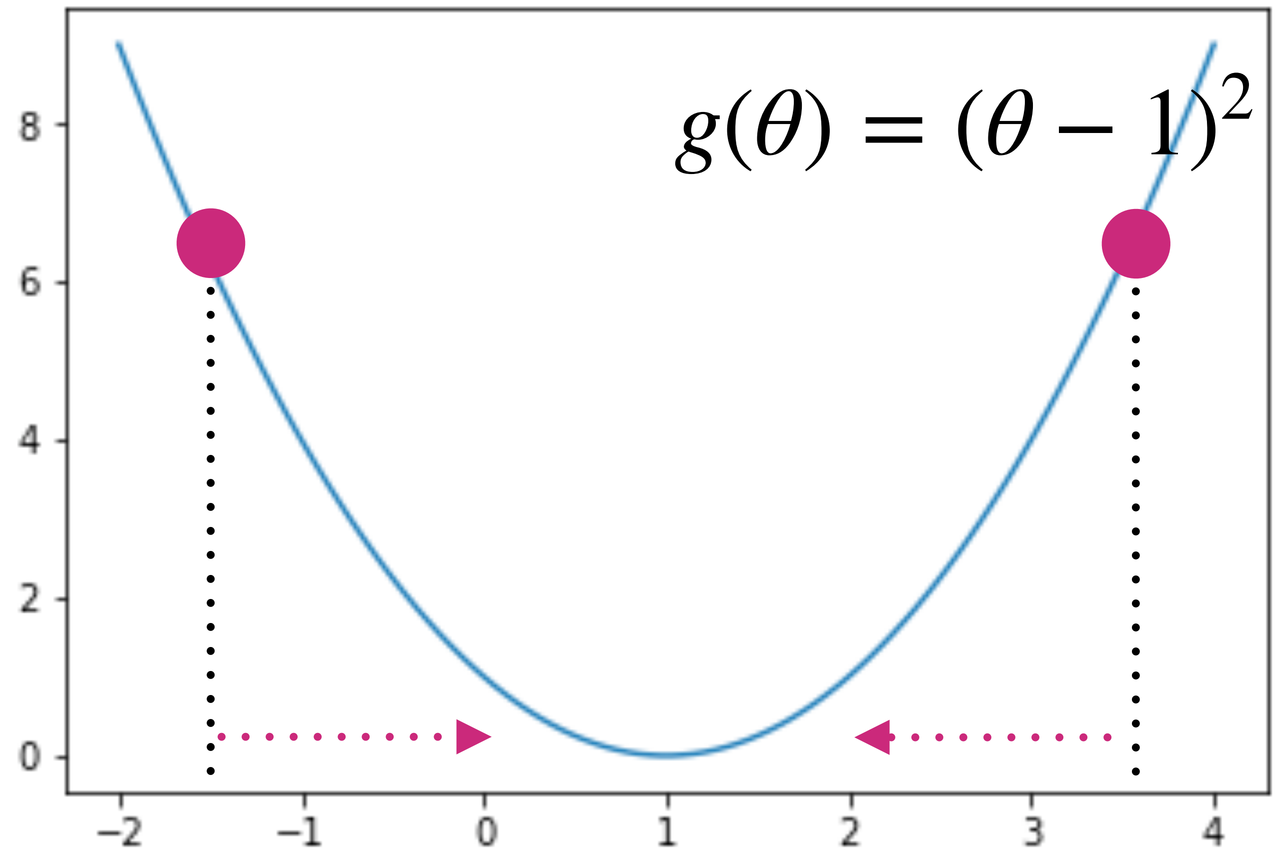


$$\frac{d}{d\theta} g(\theta) = 2\theta - 2$$

	$\theta < 1$	$\theta = 1$	$\theta > 1$
$g'(\theta)$	$-$	0	$+$
	↘	minimum	↗

Gradient descent（梯度下降法)

往與導函數相反的方向移動，就會往最小值的方向移動



Gradient descent（梯度下降法)

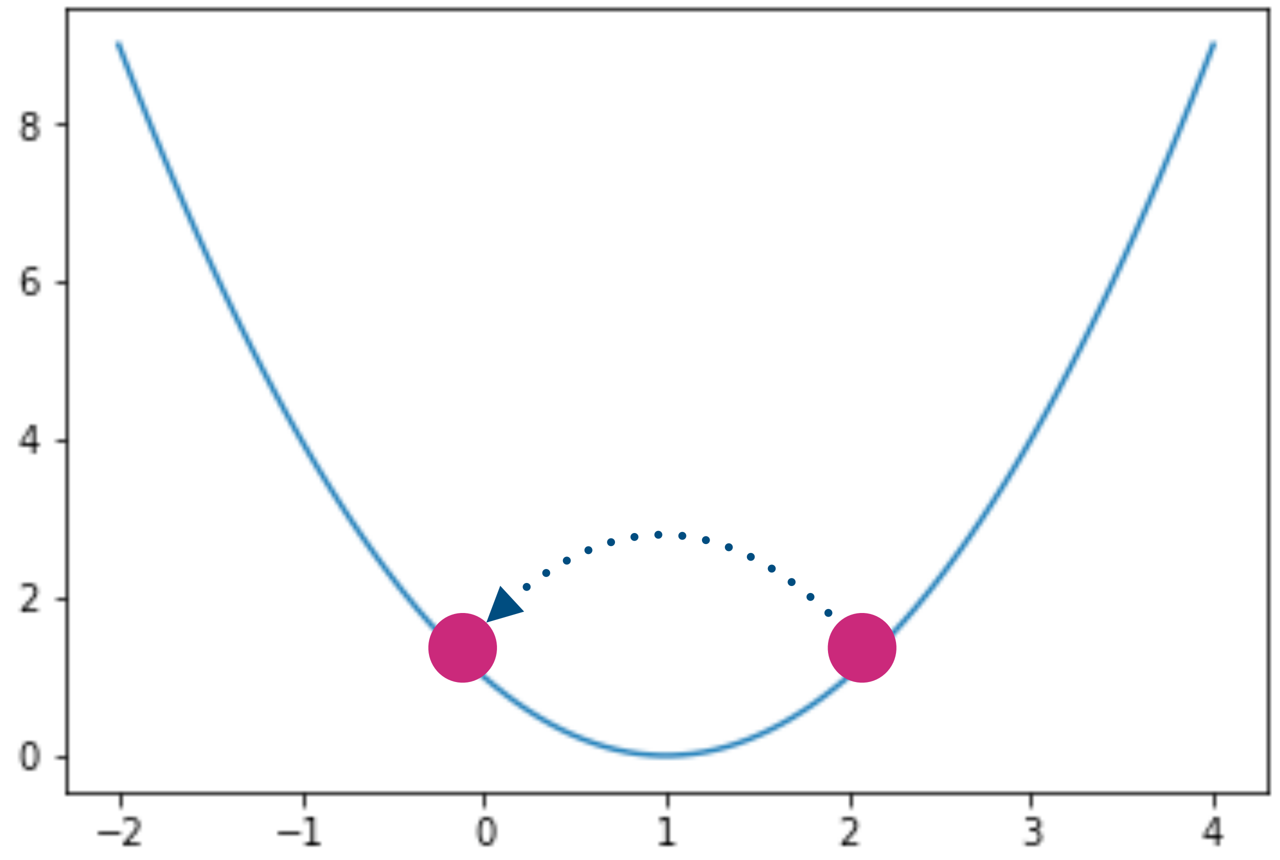
$$\theta := \theta - \eta \frac{d}{d\theta} g(\theta)$$

η : learning rate

Gradient descent (梯度下降法)

Suppose $\eta = 1$

$$g(\theta) = (\theta - 1)^2$$



$$\frac{d}{d\theta} g(\theta) = 2\theta - 2$$

Gradient descent (梯度下降法)

$$\theta := \theta - \eta \frac{d}{d\theta} g(\theta)$$

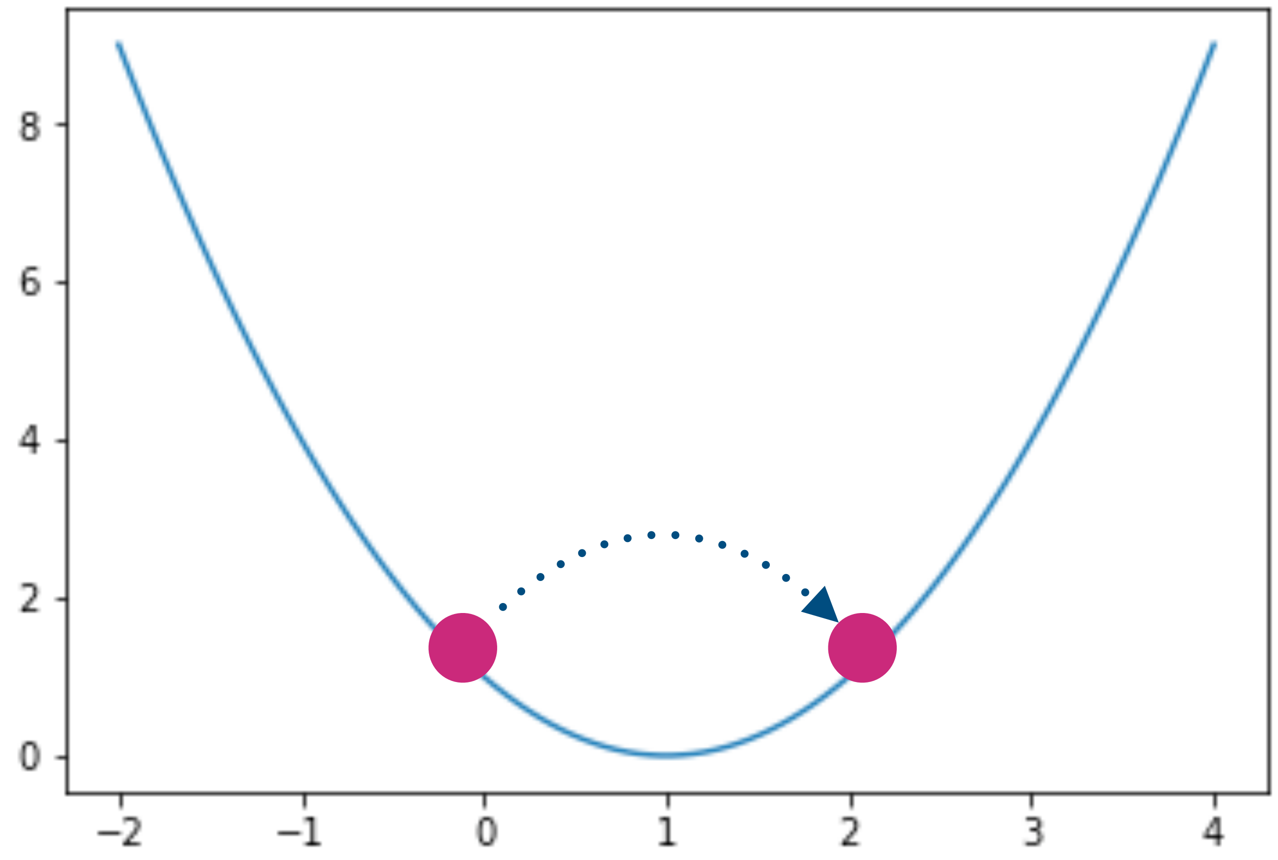
$$= \theta - \eta(2\theta - 2)$$

$$\theta := 2 - 1(2 \cdot 2 - 2) = 2 - 2 = 0$$

Gradient descent（梯度下降法)

Suppose $\eta = 1$

$$g(\theta) = (\theta - 1)^2$$



$$\frac{d}{d\theta} g(\theta) = 2\theta - 2$$

Gradient descent（梯度下降法)

$$\theta := \theta - \eta \frac{d}{d\theta} g(\theta)$$

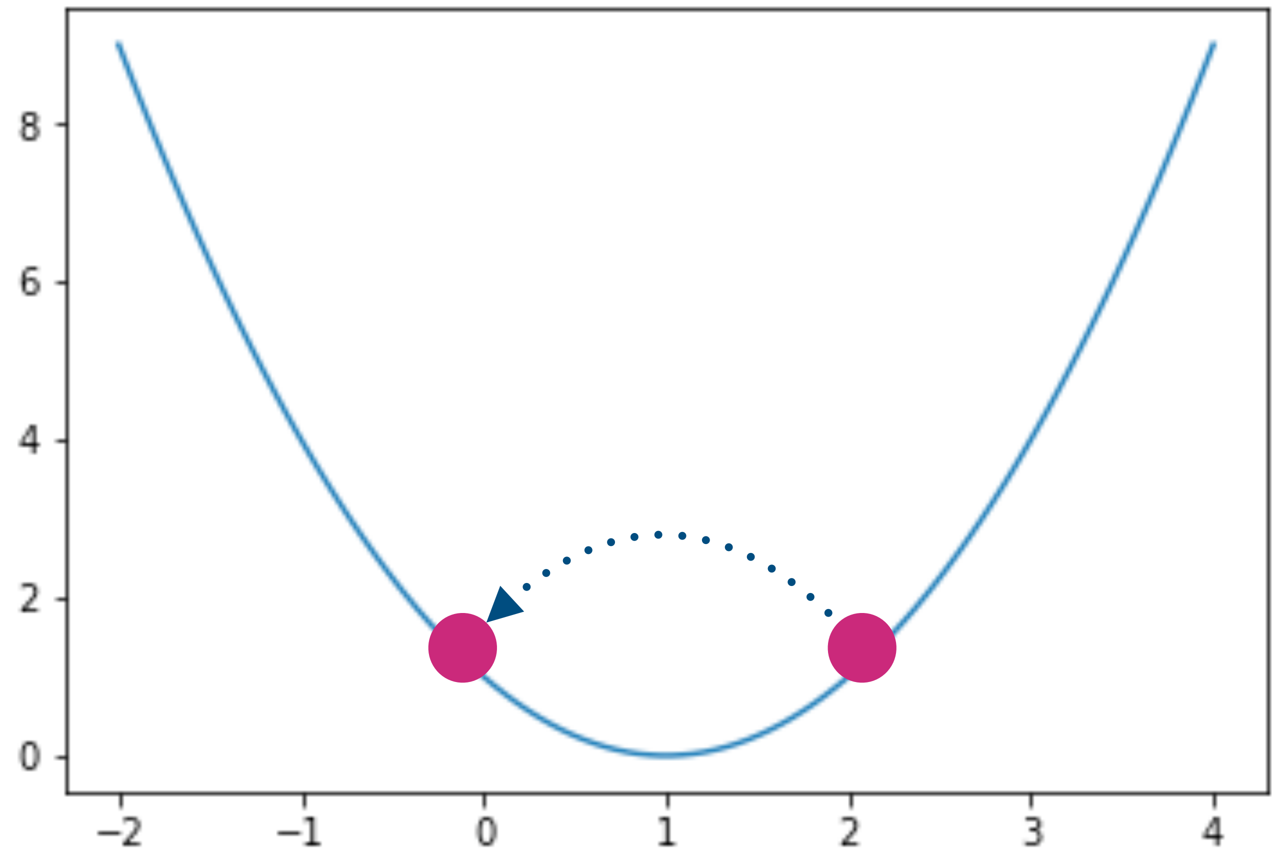
$$= \theta - \eta(2\theta - 2)$$

$$\theta := 0 - 1(2 \cdot 0 - 2) = 0 + 2 = 2$$

Gradient descent (梯度下降法)

Suppose $\eta = 1$

$$g(\theta) = (\theta - 1)^2$$



$$\frac{d}{d\theta} g(\theta) = 2\theta - 2$$

Gradient descent (梯度下降法)

$$\theta := \theta - \eta \frac{d}{d\theta} g(\theta)$$

$$= \theta - \eta(2\theta - 2)$$

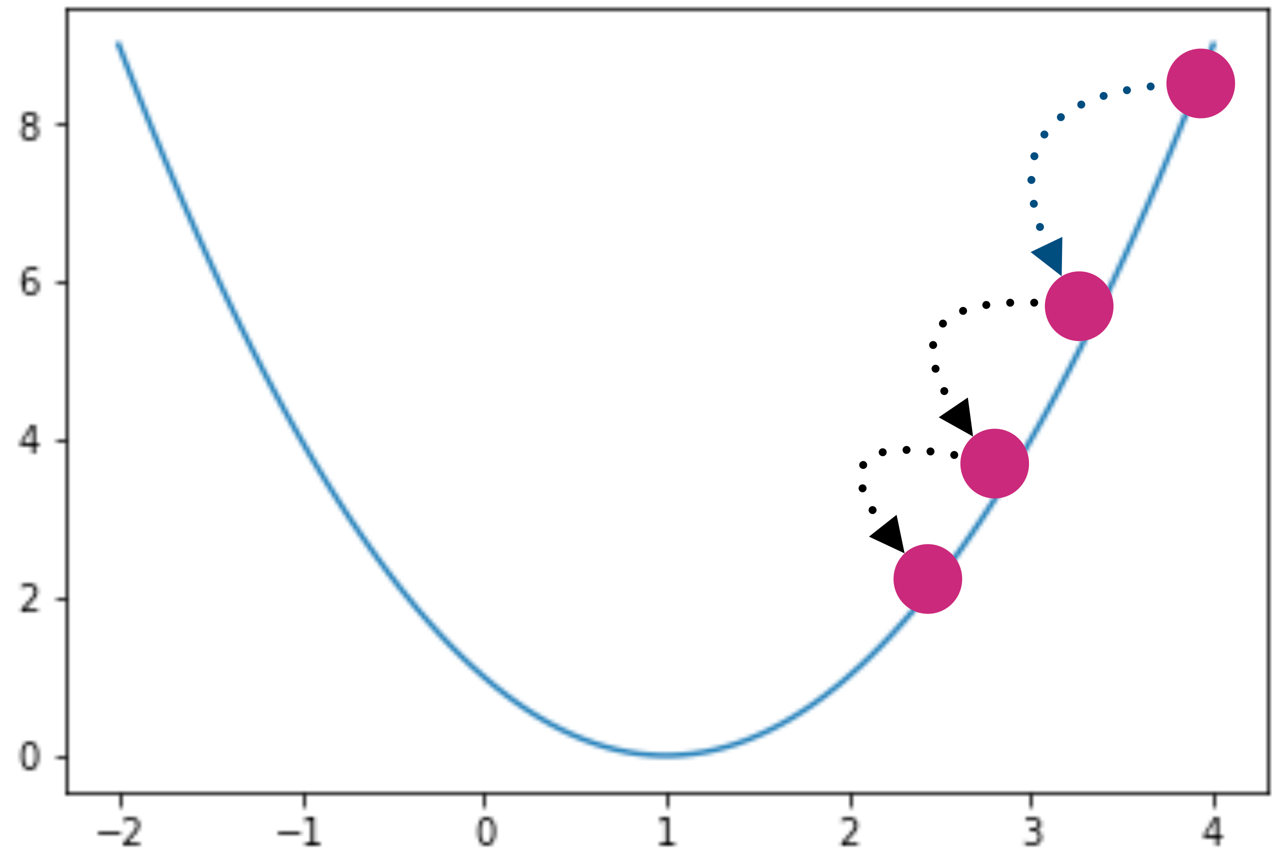
$$\theta := 2 - 1(2 \cdot 2 - 2) = 2 - 2 = 0$$

Gradient descent（梯度下降法)

Suppose $\eta = 0.1$

$$g(\theta) = (\theta - 1)^2$$

$$\frac{d}{d\theta} g(\theta) = 2\theta - 2$$



Gradient descent（梯度下降法)

$$\theta := \theta - \eta \frac{d}{d\theta} g(\theta)$$

$$= \theta - \eta(2\theta - 2)$$

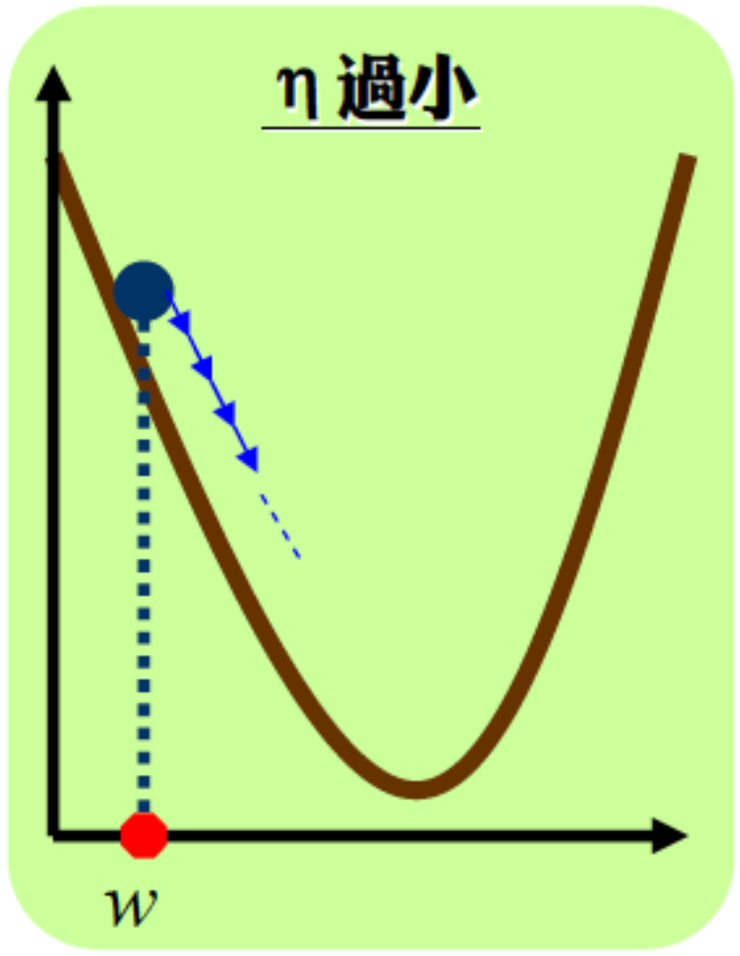
$$\theta := 4 - 0.1(2 \cdot 4 - 2) = 4 - 0.6 = 3.4$$

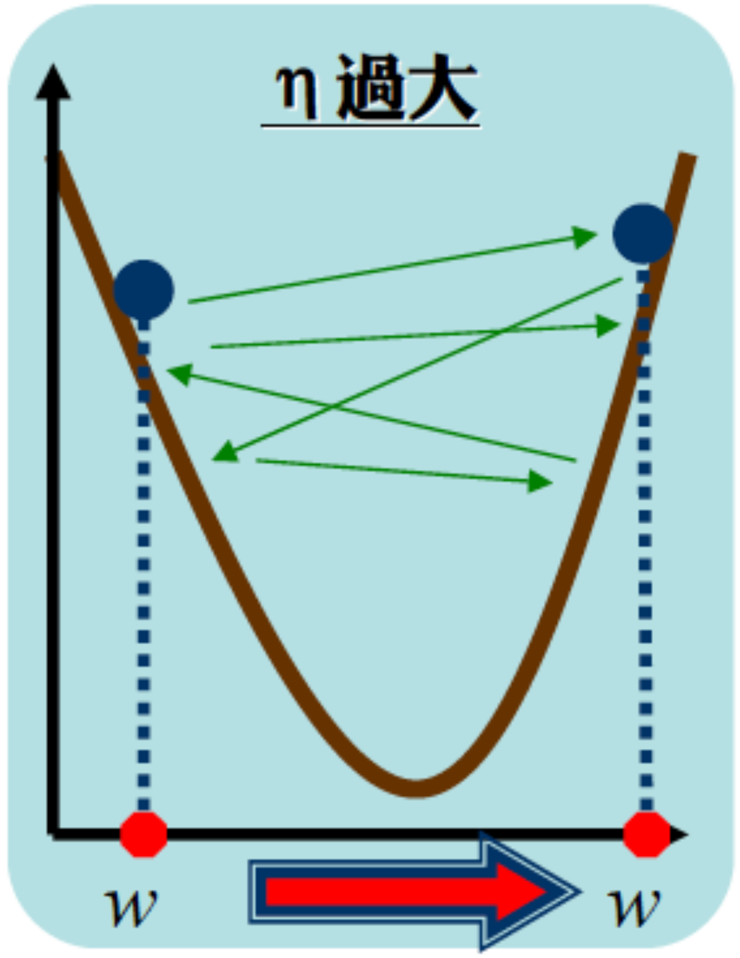
$$\theta := 3.4 - 0.1(2 \cdot 3.4 - 2) = 3.4 - 0.48 = 2.92$$

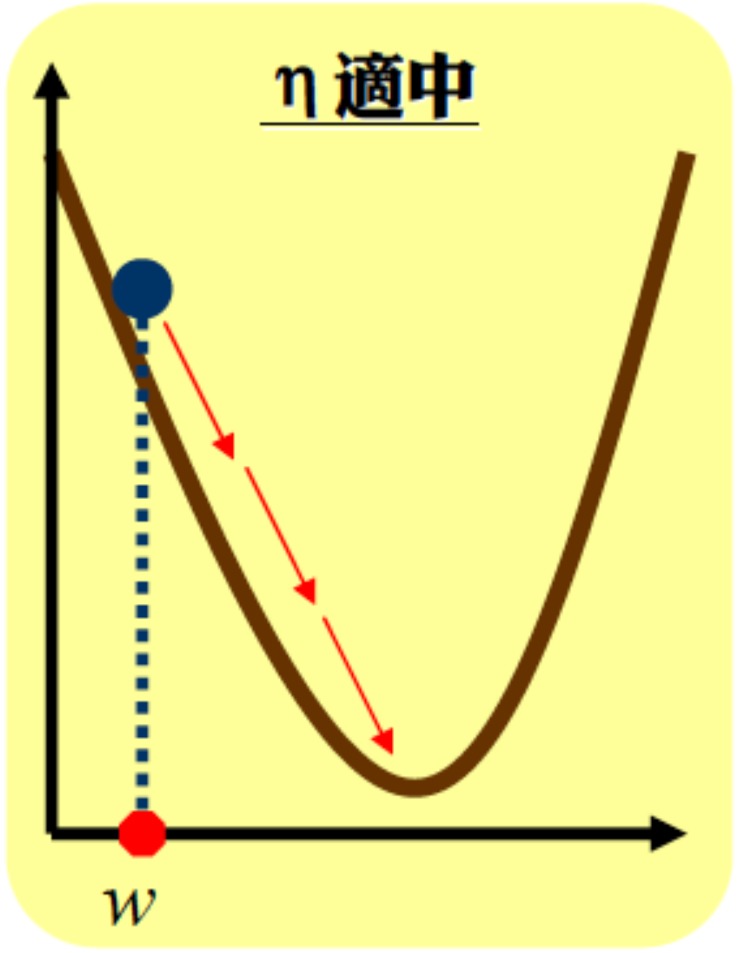
$$\theta := 2.92 - 0.1(2 \cdot 2.92 - 2) = 2.92 - 0.384 = 2.536$$

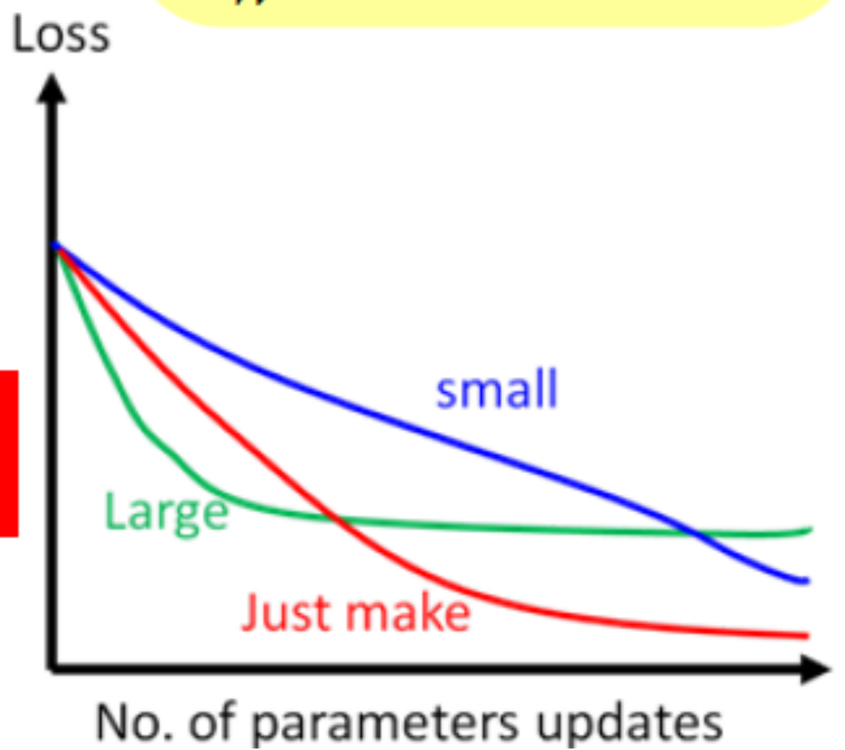
Gradient descent (梯度下降法)

- η的設定，過大過小都不適宜…









要找到一個固定且適合的η不容易

Gradient descent（梯度下降法)

- Cost function

$$E(\theta_0, \theta_1) = \frac{1}{2}\sum_{i=1}^{m}\left(h_\theta(x^{(i)}) - y^{(i)}\right)^2$$

- Gradient descent

$$\theta_0 := \theta_0 - \eta\frac{\partial E}{\partial \theta_0}$$

$$\theta_1 := \theta_1 - \eta\frac{\partial E}{\partial \theta_1}$$

Gradient descent（梯度下降法)

- Cost function

$$E(\theta_0, \theta_1) = \frac{1}{2}\sum_{i=1}^{m}\left(h_\theta(x^{(i)}) - y^{(i)}\right)^2$$

- Gradient descent

Simultaneous update

$$\theta_0 := \theta_0 - \eta\sum_{i=1}^{m}\left(h_\theta(x^{(i)}) - y^{(i)}\right)$$

$$\theta_1 := \theta_1 - \eta\sum_{i=1}^{m}\left(h_\theta(x^{(i)}) - y^{(i)}\right)x^{(i)}$$

Exercise

- 假設 $\theta_0 = 0, \theta_1 = 0$，請完成下列表格，並算出一次梯度下降法的更新 ($\eta = 0.01$)

x	y	$h_\theta(x) = \theta_0 + \theta_1 x$	$h_\theta(x) - y$	$\left(h_\theta(x) - y\right) \cdot x$
-3	6			
-1	4			
0	2			
1	0			
4	-8			

Exercise

$\theta_0 = 0, \theta_1 = 0 \qquad \eta = 0.01$

x	y	$h_\theta(x) = \theta_0 + \theta_1 x$	$h_\theta(x) - y$	$\left(h_\theta(x) - y\right) \cdot x$
-3	6	0	-6	18
-1	4	0	-4	4
0	2	0	-2	0
1	0	0	0	0
4	-8	0	8	32

$$\theta_0 := \theta_0 - \eta \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)}\right) = 0 - 0.01 * (-4) = 0.04$$

$$\theta_1 := \theta_1 - \eta \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)}\right) x^{(i)} = 0 - 0.01 * 54 = -0.54$$

$$h_\theta(x) = \theta_0 + \theta_1 x = 0.04 - 0.54x$$

Gradient descent（梯度下降法)

- Cost function

$$E(\theta_0, \theta_1) = \frac{1}{2}\sum_{i=1}^{m}\left(h_\theta(x^{(i)}) - y^{(i)}\right)^2$$

- Gradient descent

$$\theta_0 := \theta_0 - \eta\frac{\partial E}{\partial \theta_0}$$

$$\theta_1 := \theta_1 - \eta\frac{\partial E}{\partial \theta_1}$$

Simultaneous update

Gradient descent（梯度下降法)

- Gradient descent (Simultaneous update)

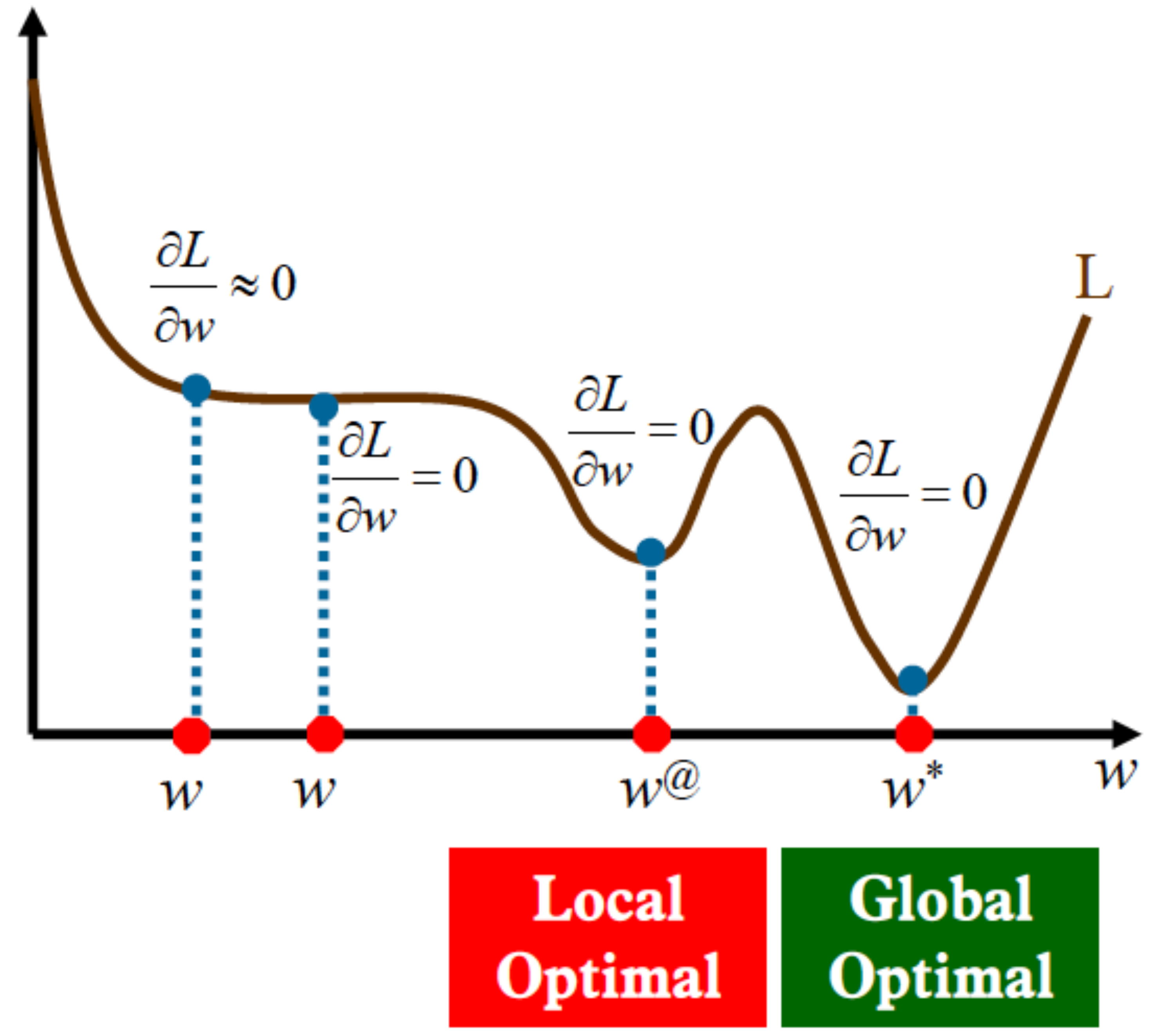
$$temp0 := \theta_0 - \eta \frac{\partial E}{\partial \theta_0}$$

$$temp1 := \theta_1 - \eta \frac{\partial E}{\partial \theta_1}$$

$$\theta_0 := temp0$$

$$\theta_1 := temp1$$

Gradient descent（梯度下降法)

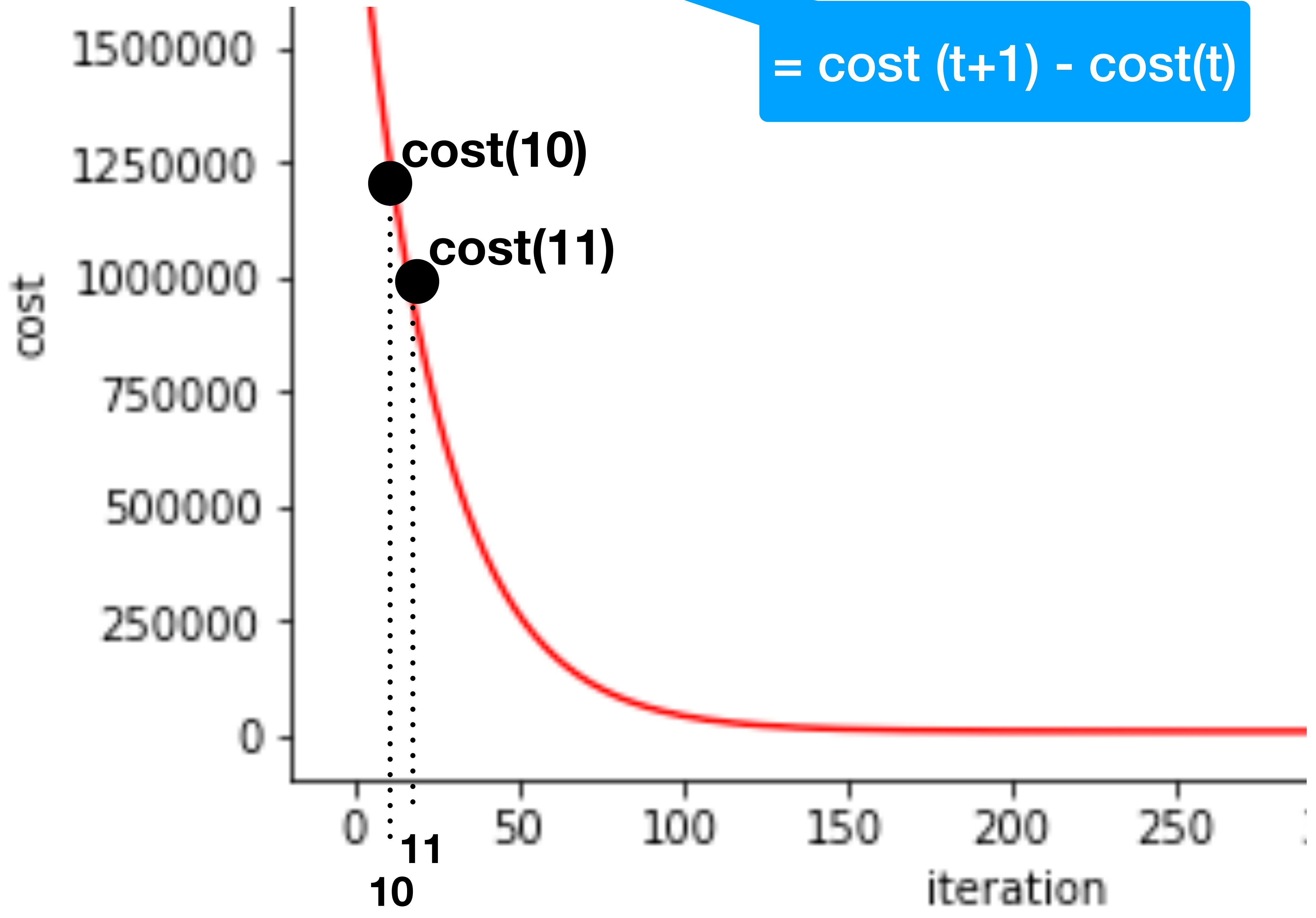


$\frac{\partial L}{\partial w} \approx 0$
$\frac{\partial L}{\partial w} = 0$
$\frac{\partial L}{\partial w} = 0$
$\frac{\partial L}{\partial w} = 0$
L
w
w
$w@$
w^*
w
Local Optimal
Global Optimal

When to stop?

- Stop when the diff is small (ex. <0.01)

= cost (t+1) - cost(t)

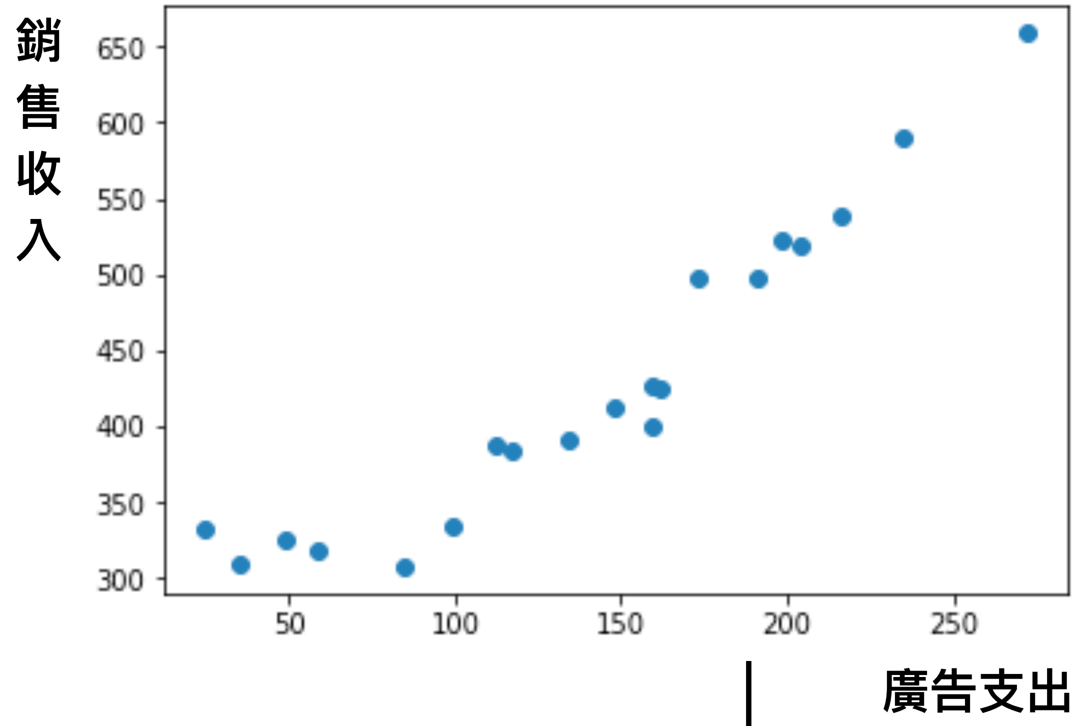


Linear regression
- using sklearn

Linear regression

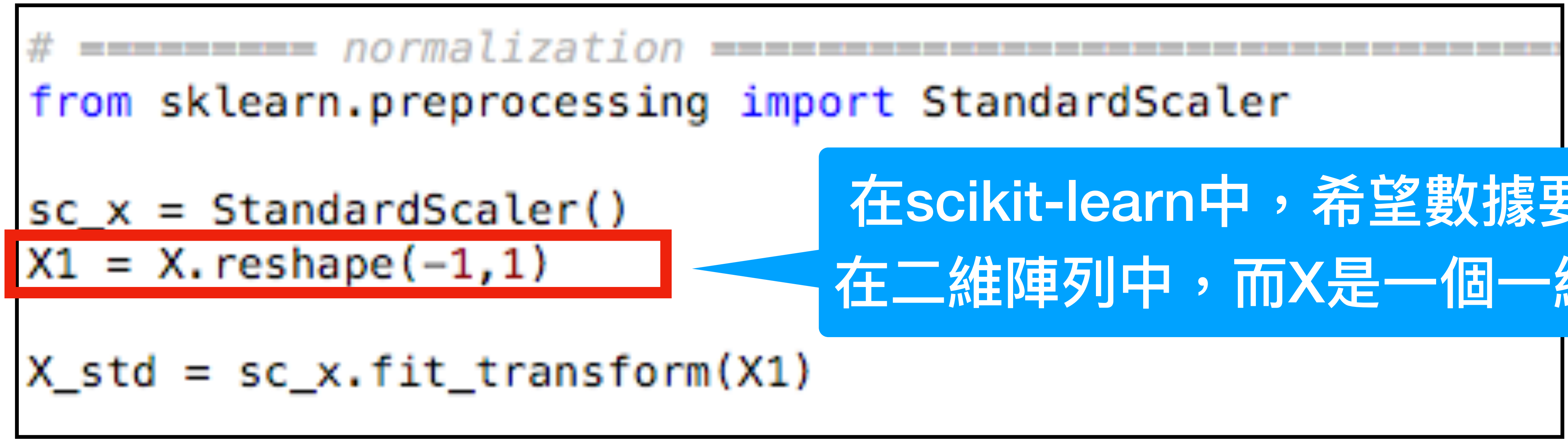
- Loading data set and normalization

```
# loading libraries
import pandas as pd
import matplotlib.pyplot as plt
import numpy as np

# loading training data
data = pd.read_csv('regression1.csv')
X = data.iloc[:,0].values
y = data.iloc[:,-1].values

# ========== normalization ========================================
from sklearn.preprocessing import StandardScaler

sc_x = StandardScaler()
X_std = sc_x.fit_transform(X)
```



Linear regression

- Linear Regression

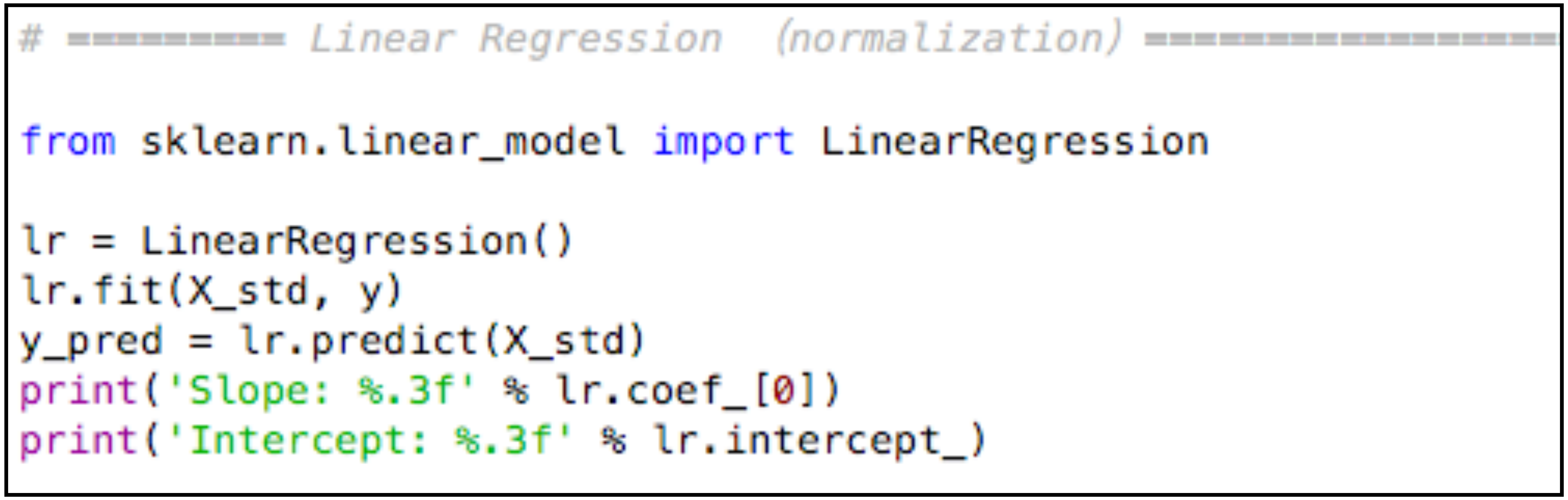


```
# ========== normalization ========================================
from sklearn.preprocessing import StandardScaler

sc_x = StandardScaler()
X1 = X.reshape(-1,1)

X_std = sc_x.fit_transform(X1)
```

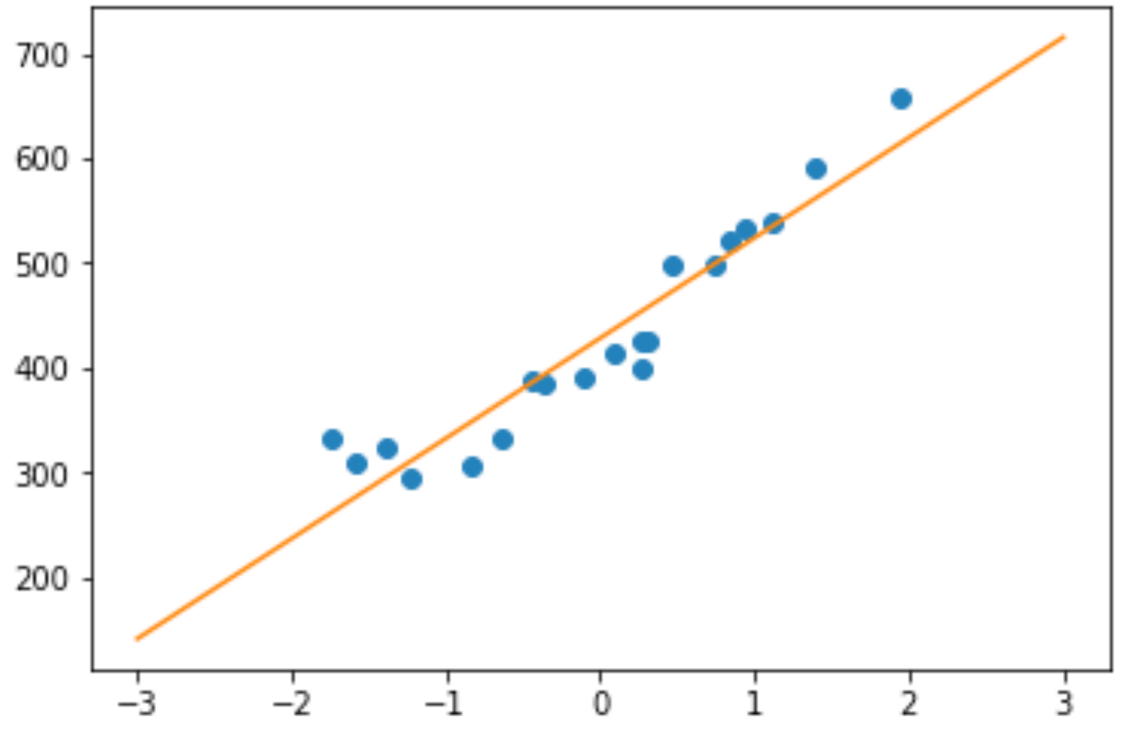
在scikit-learn中，希望數據要儲存在二維陣列中，而X是一個一維陣列

Linear regression

- Linear Regression



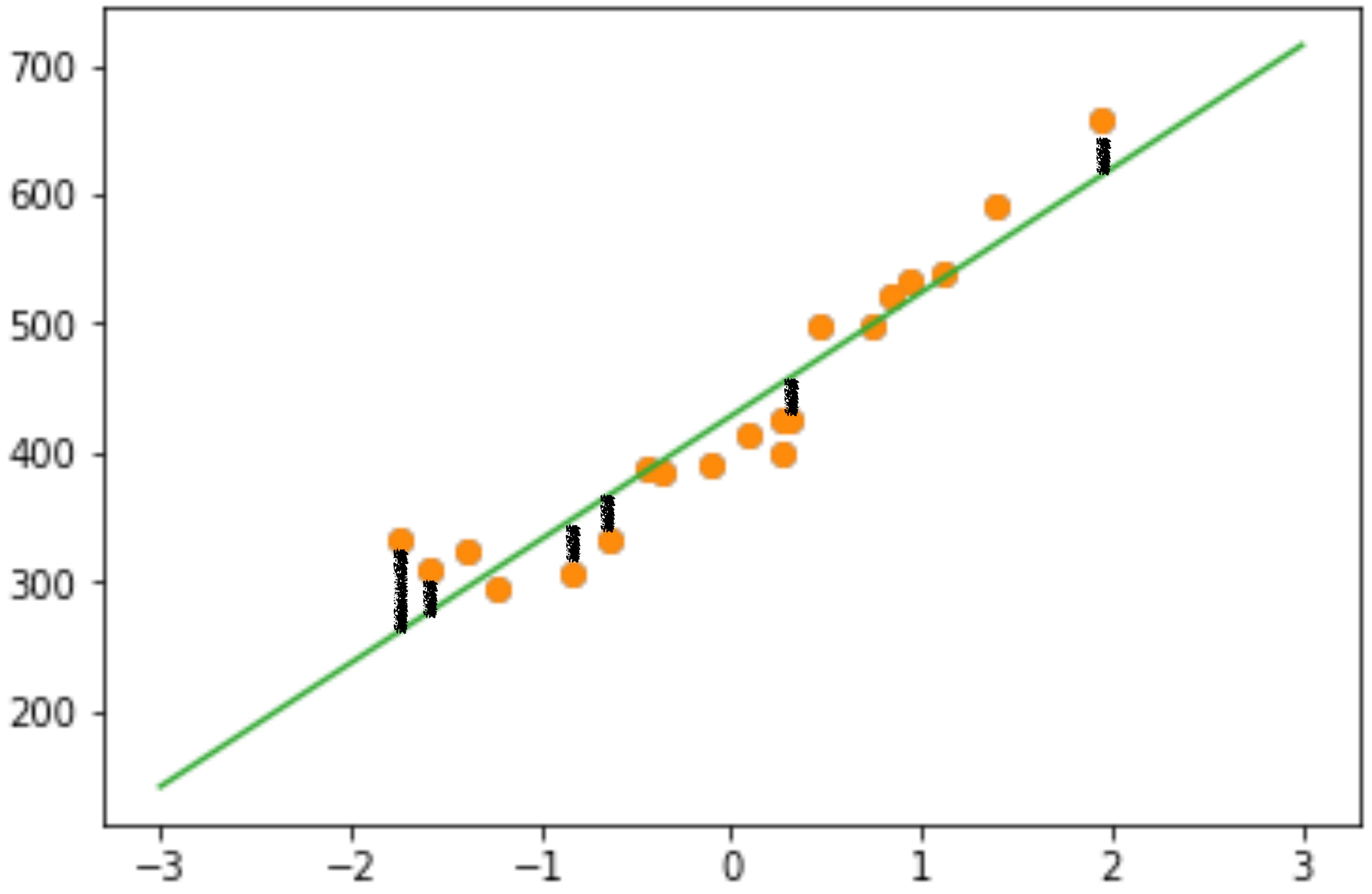
```python
# ========= Linear Regression  (normalization) ==================

from sklearn.linear_model import LinearRegression

lr = LinearRegression()
lr.fit(X_std, y)
y_pred = lr.predict(X_std)
print('Slope: %.3f' % lr.coef_[0])
print('Intercept: %.3f' % lr.intercept_)
```



Linear regression - 評估模型的效能

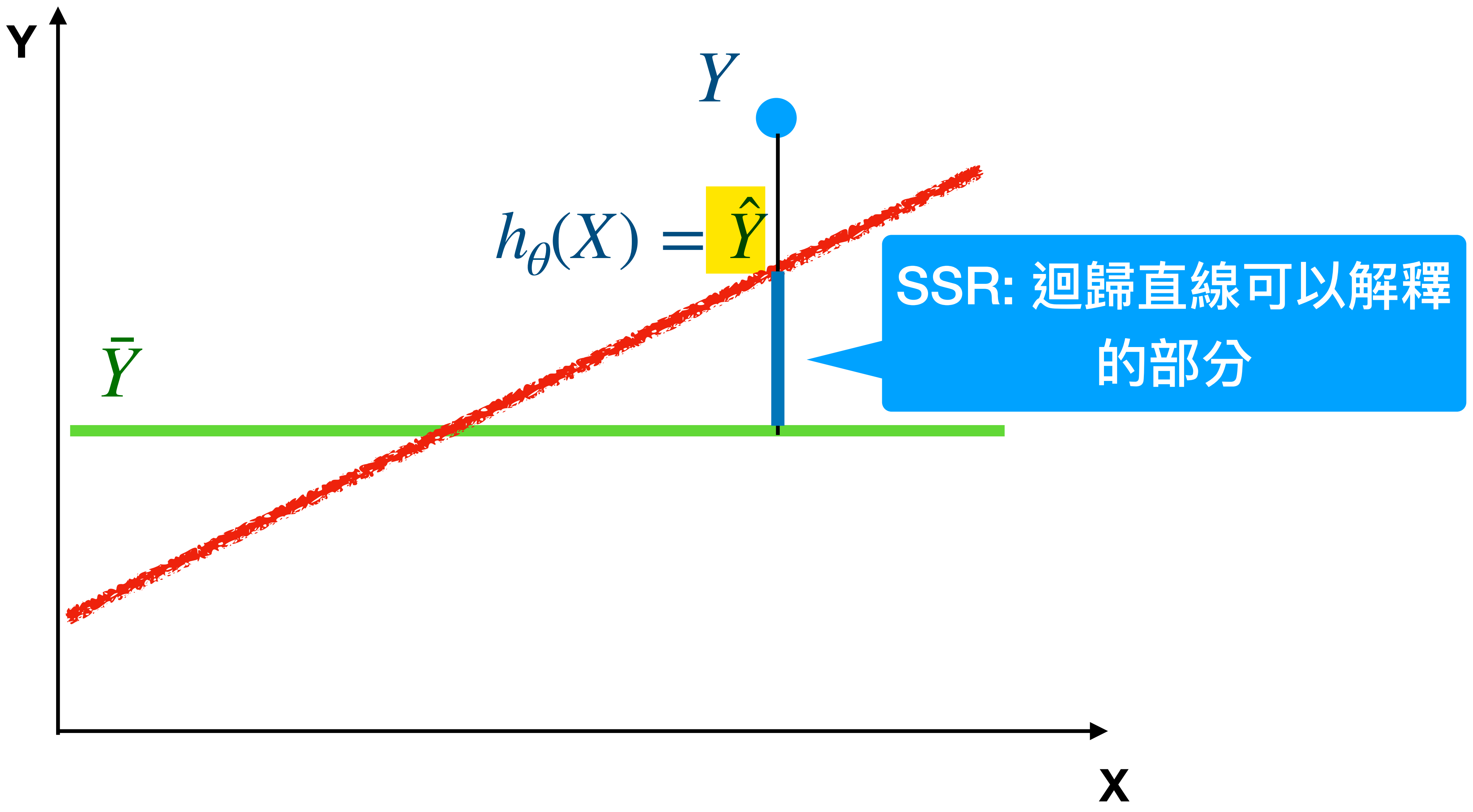
- MSE (Mean Squared Error, 均方誤差)

$$\frac{1}{m}\sum_{i=1}^{m}\left(h_\theta(x^{(i)}) - y^{(i)}\right)^2$$



決定係數(Coefficient of Determination)

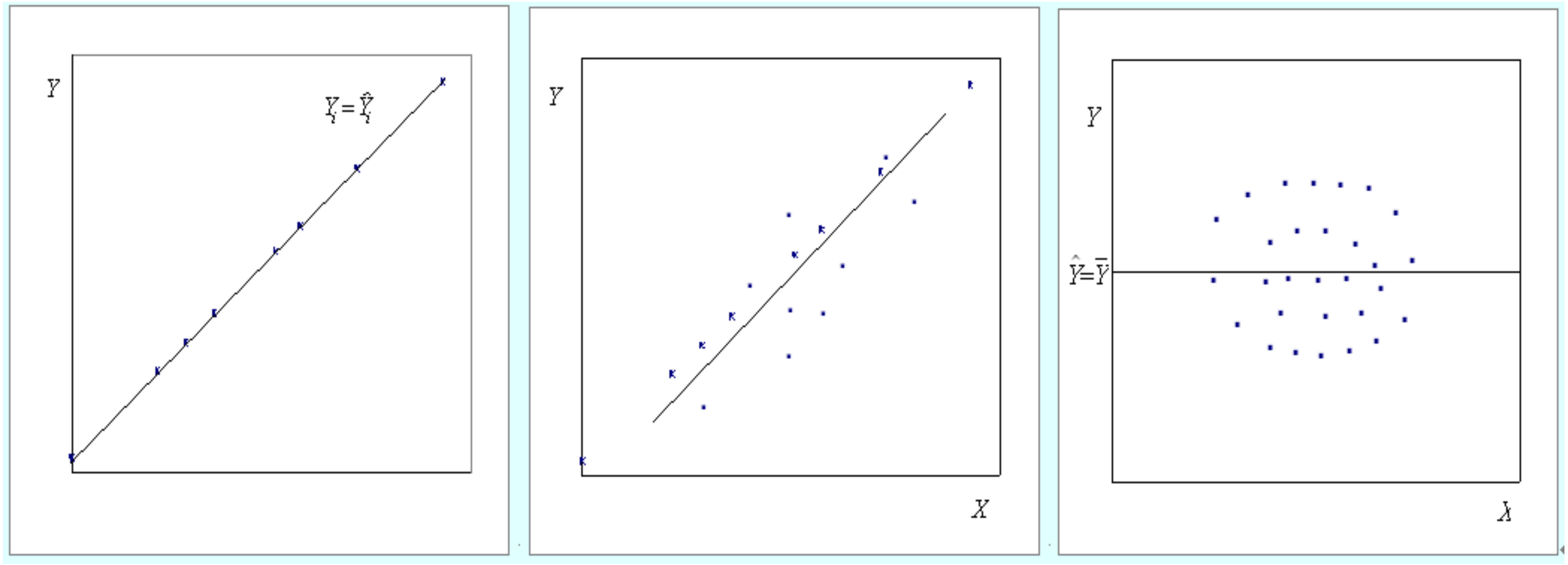
$$\underbrace{\sum_{i=1}^{n}(Y_i - \bar{Y})^2}_{\text{SST}} = \underbrace{\sum_{i=1}^{n}(\hat{Y} - \bar{Y})^2}_{\text{SSR}} + \underbrace{\sum_{i=1}^{n}(Y_i - \hat{Y}_i)^2}_{\text{SSE}}$$



決定係數(Coefficient of Determination)

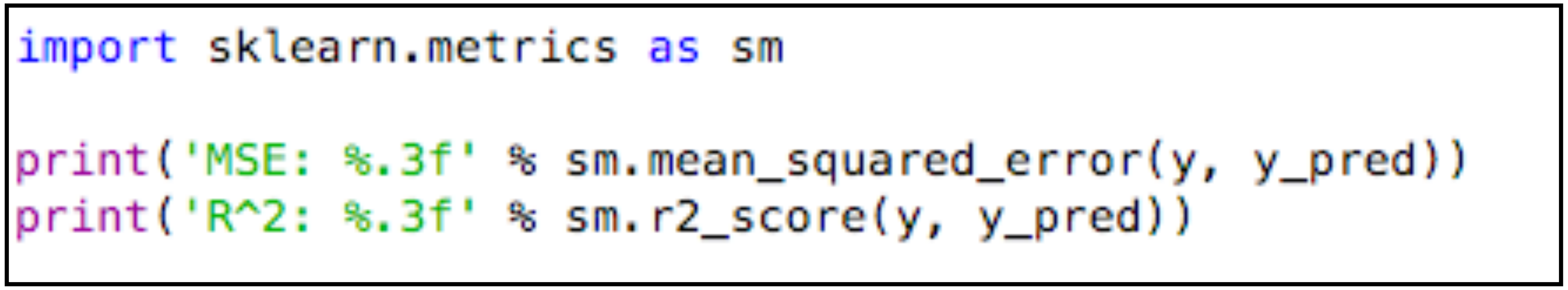
$$R^2 = \frac{\text{SSR}}{\text{SST}} = \frac{\sum(\hat{Y}_i - \overline{Y})^2}{\sum(Y_i - \overline{Y})^2}$$

可以理解為標準化的MSE



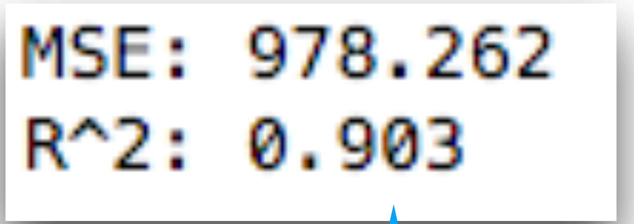
Linear regression

- Computing MSE 和 判定係數



```
import sklearn.metrics as sm

print('MSE: %.3f' % sm.mean_squared_error(y, y_pred))
print('R^2: %.3f' % sm.r2_score(y, y_pred))
```

Code (4/6)



```
MSE: 978.262
R^2: 0.903
```

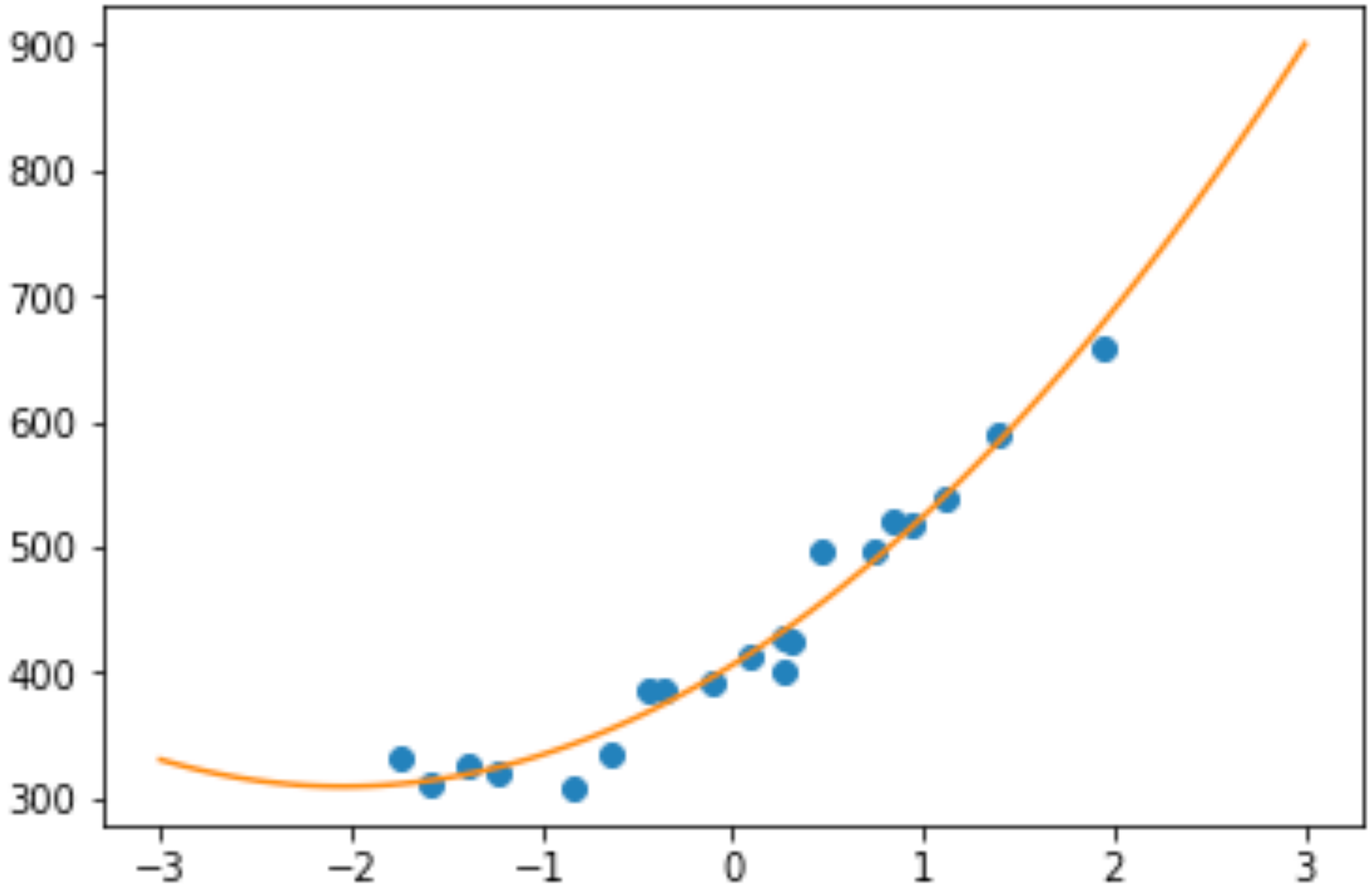
此公式只能解釋 90.3% 銷售收入變因

多項式回歸

- using sklearn

Example

$$h_\theta(x) = \theta_0 + \theta_1 x + \theta_2 x^2$$

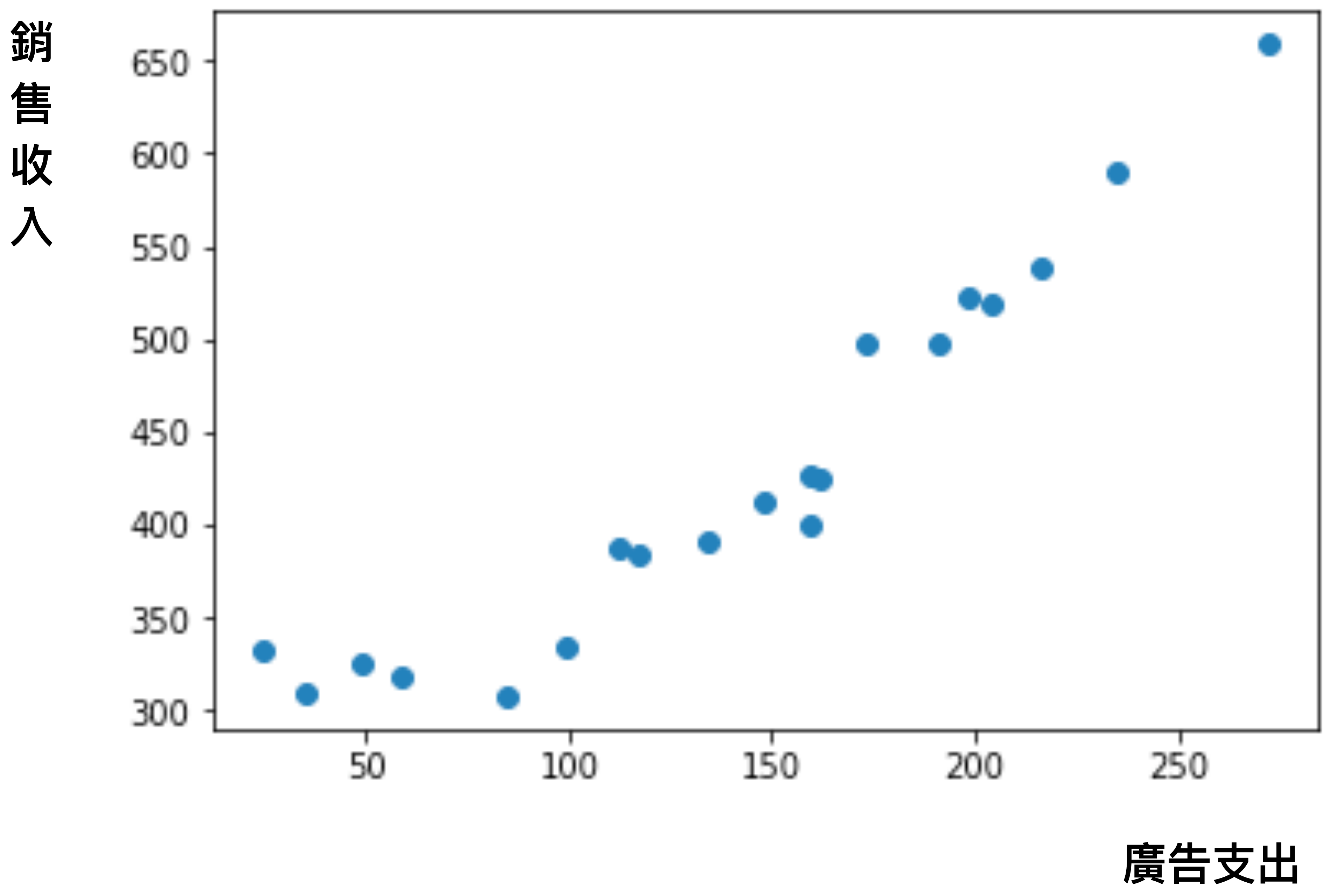


Question

Overfitting

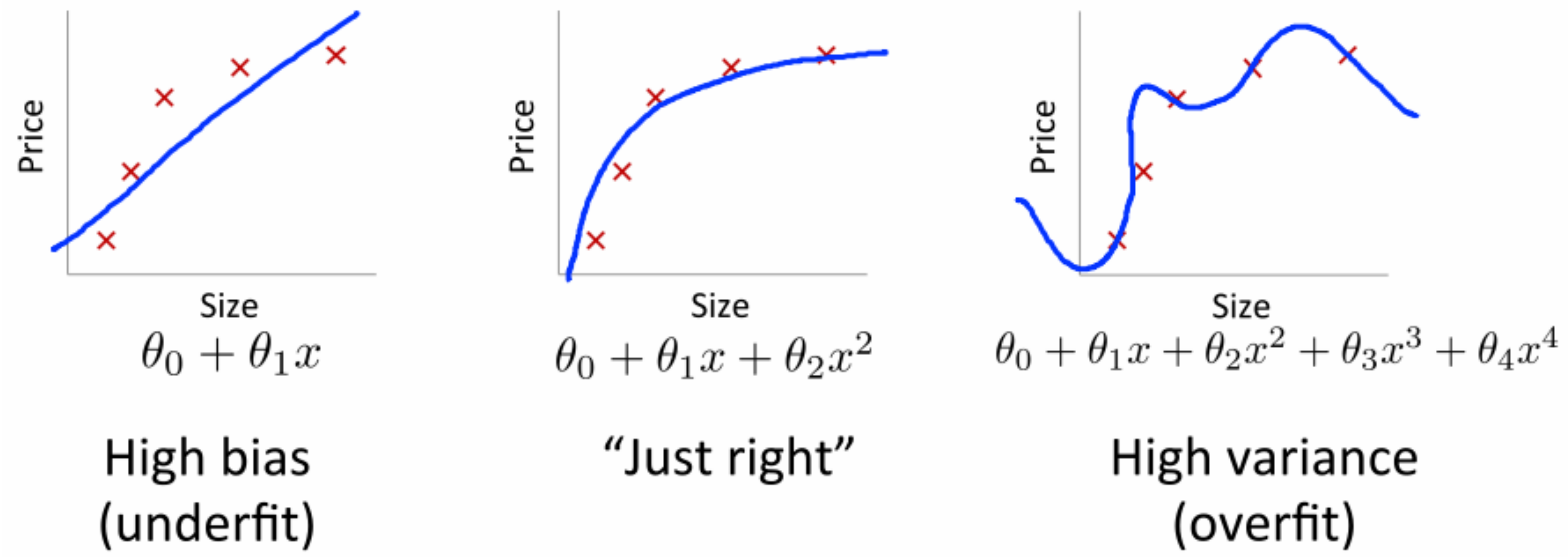
- How about

$$h_\theta(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \cdots + \theta_n x^n$$



Overfitting v.s. underfitting

Source: http://murphymind.blogspot.com/2017/06/machine-learning-advice-for-applying.html



$\theta_0 + \theta_1 x$

High bias (underfit)

$\theta_0 + \theta_1 x + \theta_2 x^2$

"Just right"

$\theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$

High variance (overfit)

Gradient descent（梯度下降法)

- Cost function

$$E(\theta_0, \theta_1, \theta_2) = \frac{1}{2}\sum_{i=1}^{m}\left(h_\theta(x^{(i)}) - y^{(i)}\right)^2$$

- Gradient descent

$$\theta_0 := \theta_0 - \eta\frac{\partial E}{\partial \theta_0}$$

$$\theta_1 := \theta_1 - \eta\frac{\partial E}{\partial \theta_1}$$

$$\theta_2 := \theta_2 - \eta\frac{\partial E}{\partial \theta_2}$$

Gradient descent（梯度下降法)

repeat until convergence

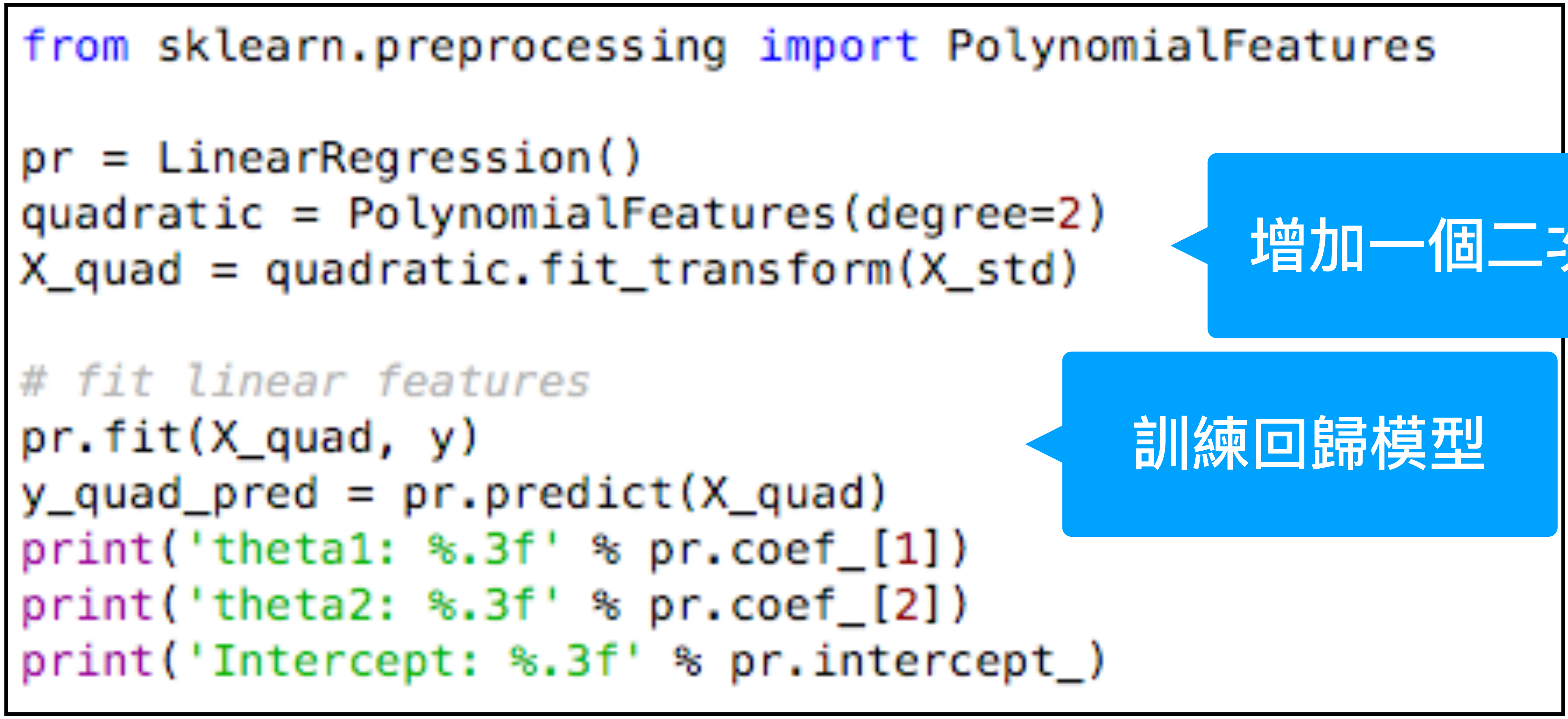
$$\theta_0 := \theta_0 - \eta \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)} \right)$$

$$\theta_1 := \theta_1 - \eta \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)} \right) x^{(i)}$$

$$\theta_2 := \theta_2 - \eta \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)} \right) (x^{(i)})^2$$

Polynomial regression

- Polynomial Regression



```
from sklearn.preprocessing import PolynomialFeatures

pr = LinearRegression()
quadratic = PolynomialFeatures(degree=2)
X_quad = quadratic.fit_transform(X_std)

# fit linear features
pr.fit(X_quad, y)
y_quad_pred = pr.predict(X_quad)
print('theta1: %.3f' % pr.coef_[1])
print('theta2: %.3f' % pr.coef_[2])
print('Intercept: %.3f' % pr.intercept_)
```

增加一個二次項

訓練回歸模型

Code (5/6)

練習

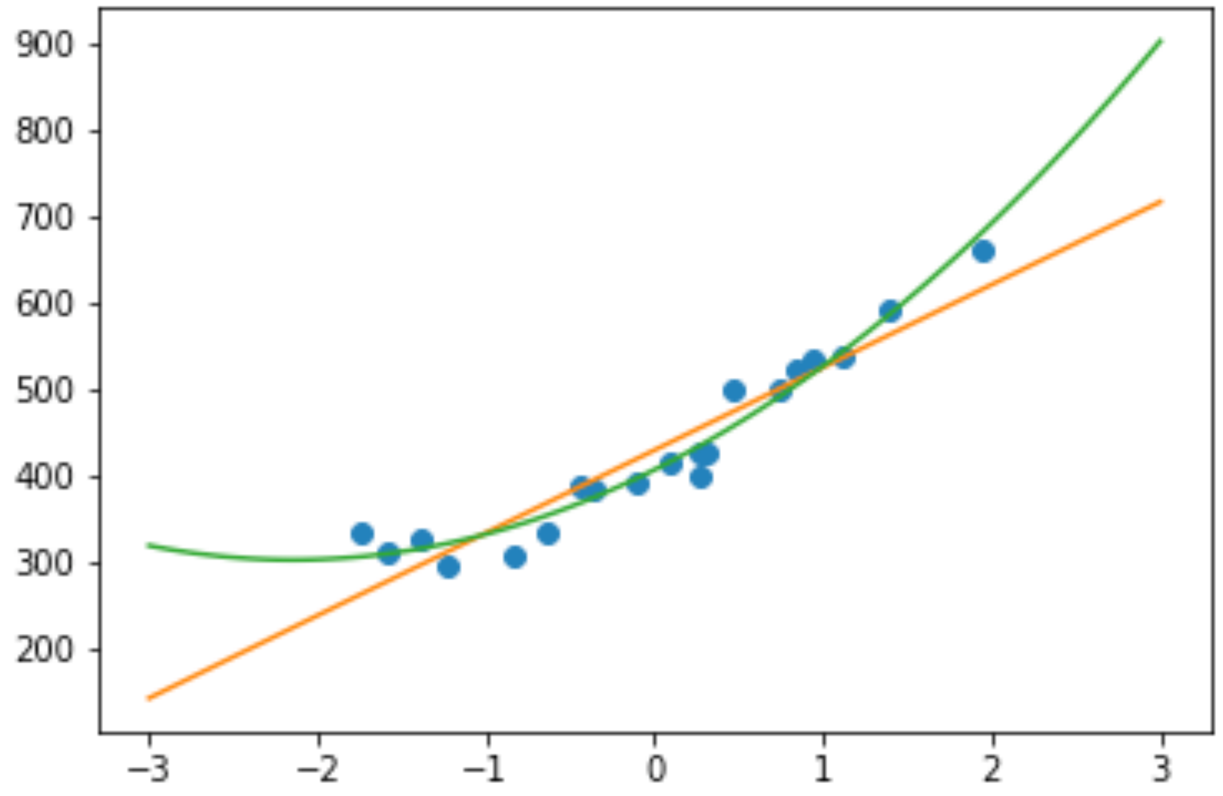
- 在散點圖上，畫出線性回歸線及多項式(二次式)回歸線，並比較其優劣

Polynomial regression

- Graph and MSE

Code (6/6)

```
x=np.linspace(-3, 3, 100)

plt.plot(X_std, y, 'o')
plt.plot(x, lr.intercept_+lr.coef_[0]*x)
plt.plot(x, pr.intercept_+pr.coef_[1]*x+pr.coef_[2]*x**2)
plt.show()
```

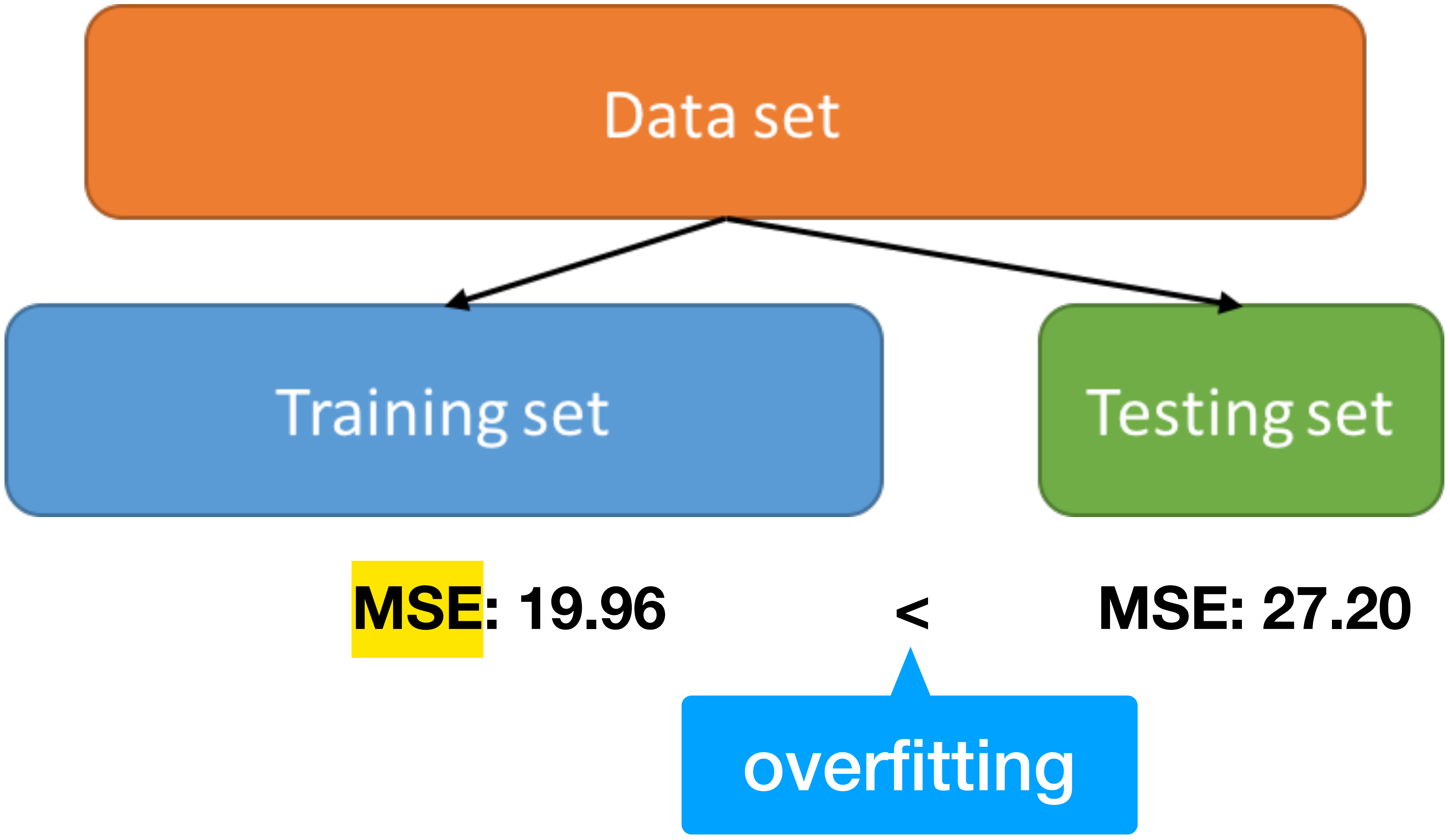


$$h_\theta(x) = 405.977 + 97.133x + 22.623x^2$$

$$h_\theta(x) = 428.6 + 95.564x$$

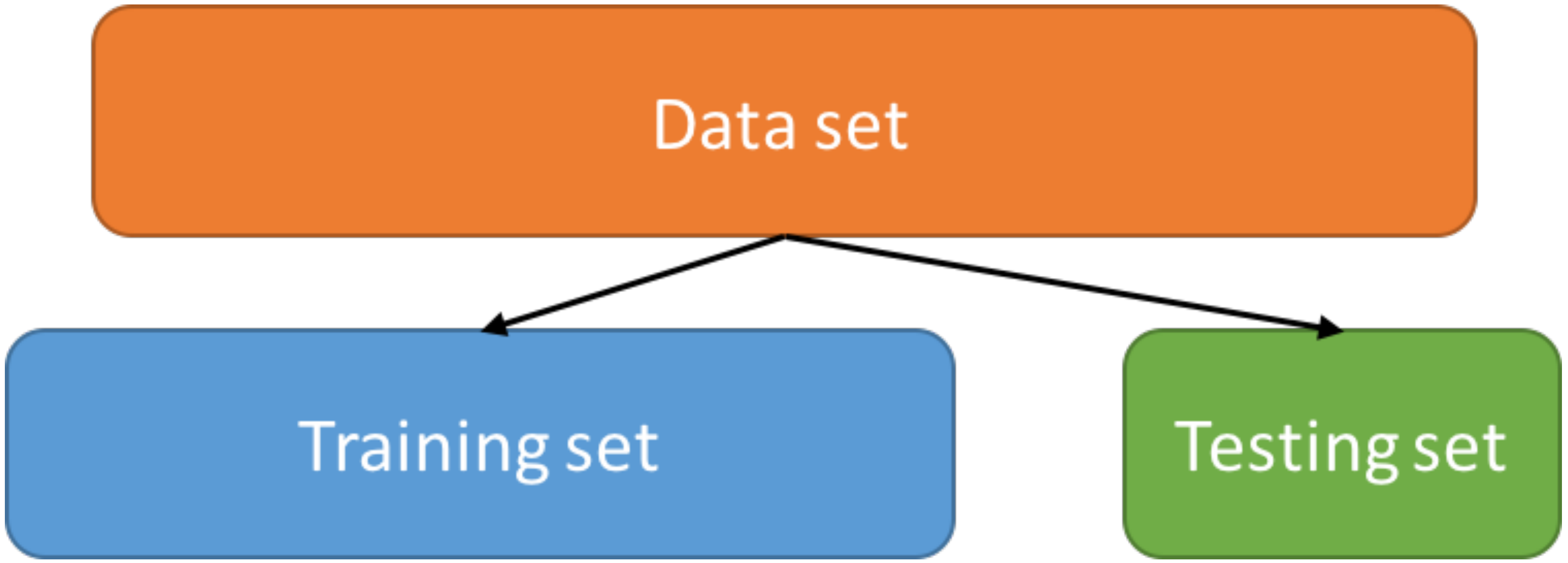
Overfitting v.s. underfitting

Source: https://aldro61.github.io/microbiome-summer-school-2017/sections/basics/



Overfitting v.s. underfitting

Source: https://aldro61.github.io/microbiome-summer-school-2017/sections/basics/

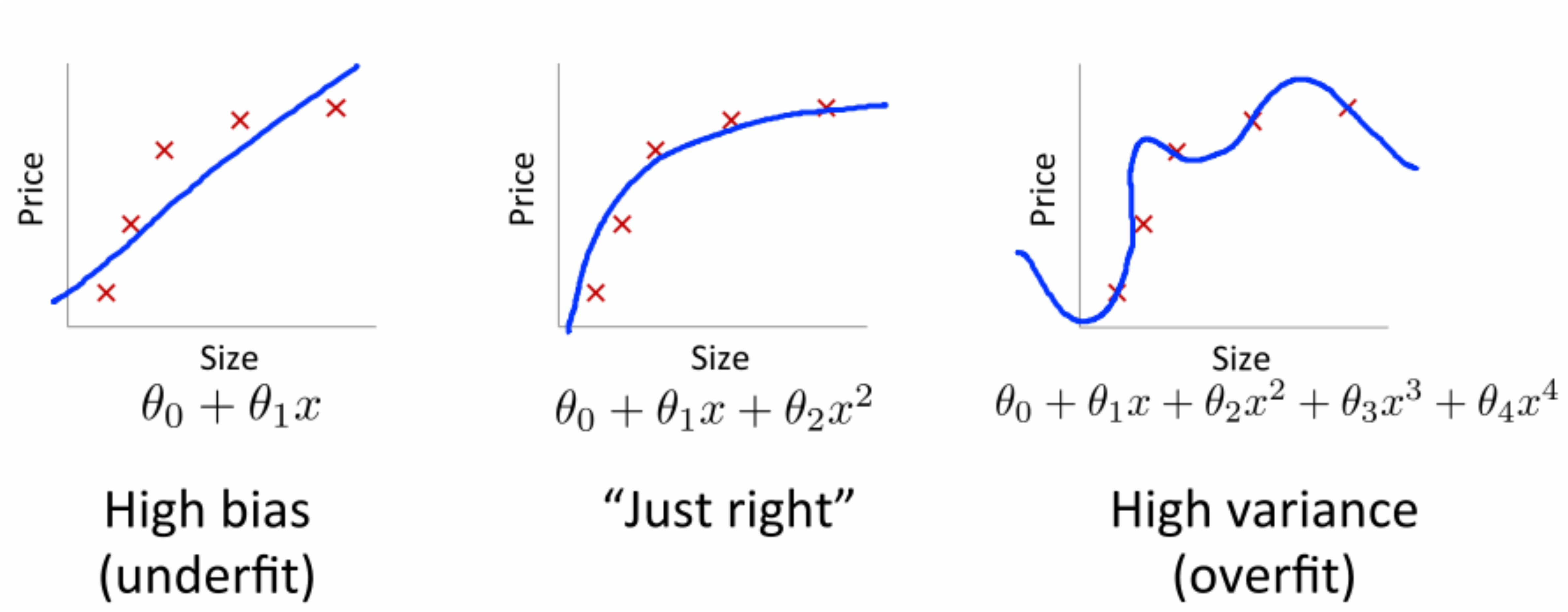


$R^2 = 0.765$ > $R^2 = 0.673$

overfitting

Overfitting v.s. underfitting

Source: http://murphymind.blogspot.com/2017/06/machine-learning-advice-for-applying.html



$$E(\theta) = \frac{1}{2}\sum_{i=1}^{m}\left(h_\theta(x^{(i)}) - y^{(i)}\right)^2 + \boxed{1000 \cdot \theta_3^2 + 1000 \cdot \theta_4^2}$$

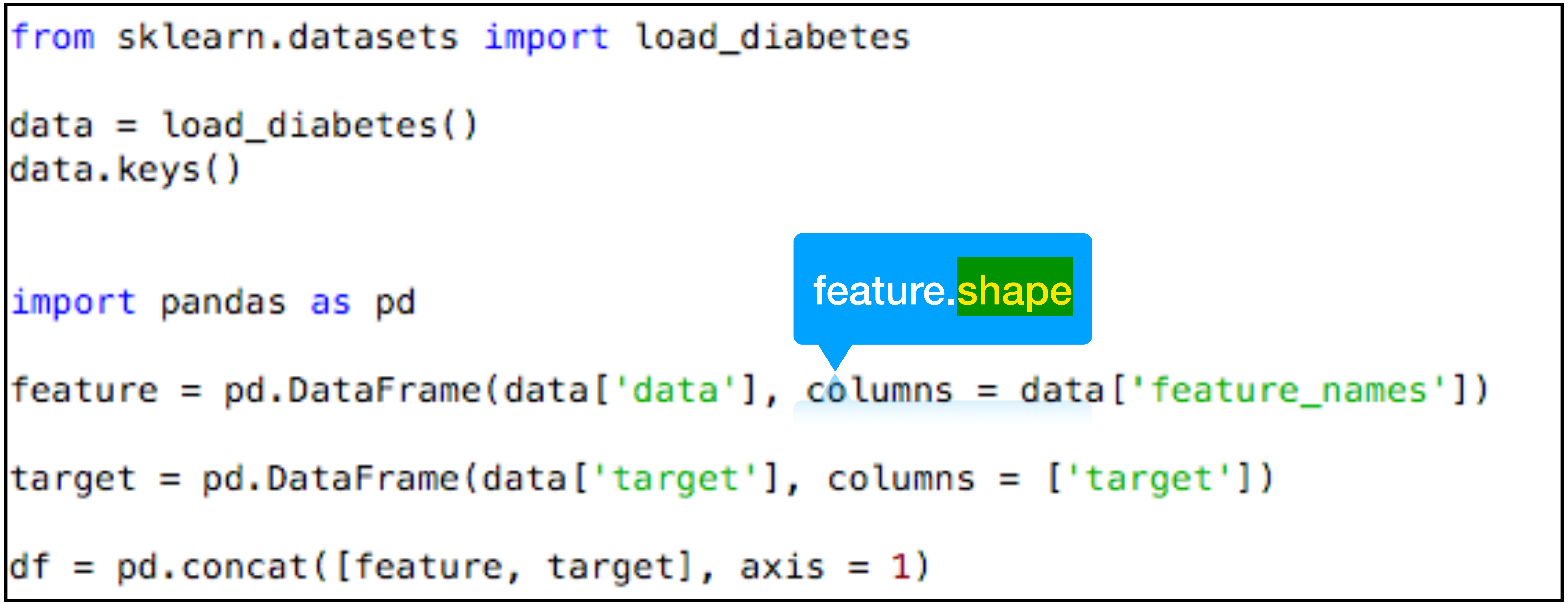
複迴歸

糖尿病數據集

- Diabetes dataset
- 10 feature variables （已標準化）
  - Age
  - Sex
  - Body mass index (BMI)
  - Average blood pressure (平均血壓)
  - S1 ~ S6 : 6 種生理數據
- 目標變數：一年後病情發展的狀況

糖尿病數據集

- 載入數據集



```
from sklearn.datasets import load_diabetes

data = load_diabetes()
data.keys()


import pandas as pd

feature = pd.DataFrame(data['data'], columns = data['feature_names'])

target = pd.DataFrame(data['target'], columns = ['target'])

df = pd.concat([feature, target], axis = 1)
```

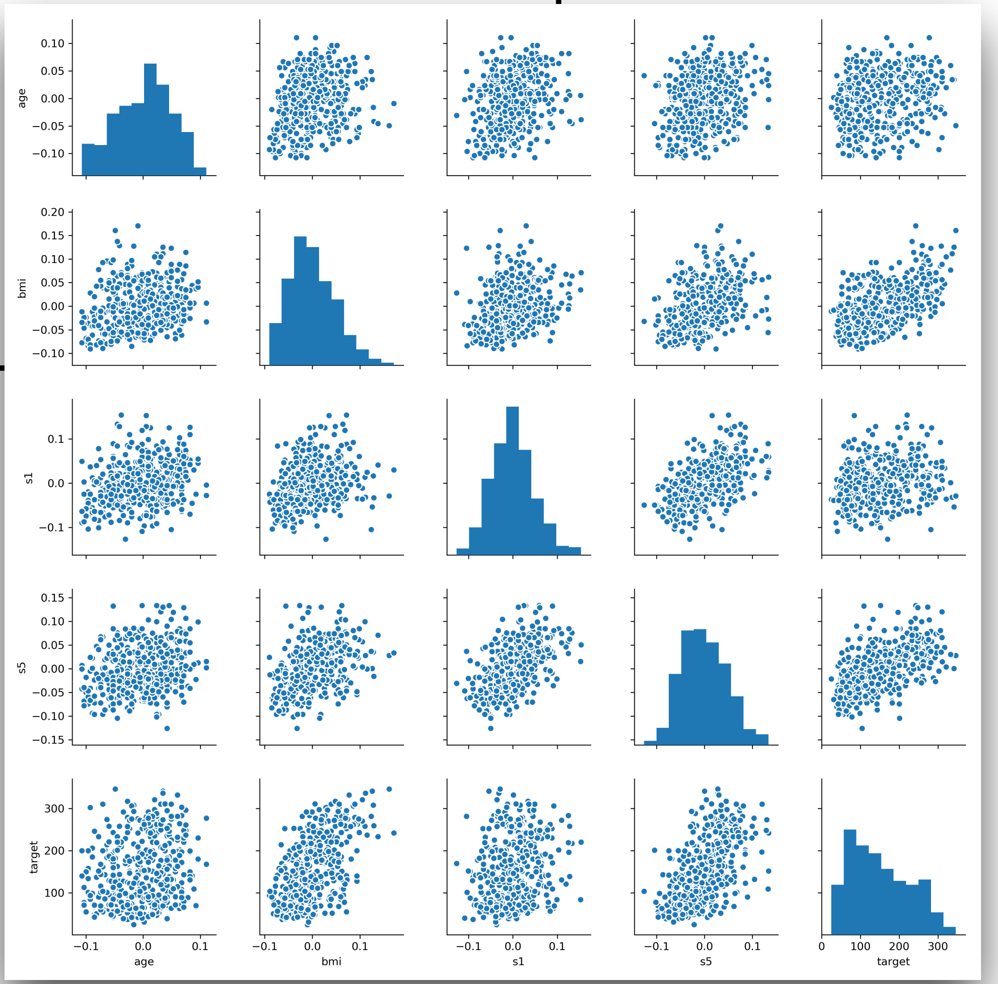
Code (1/8)

糖尿病數據集

- 畫出散點圖

Code (2/8)

```
import matplotlib.pyplot as plt
import seaborn as sns

cols = ['age', 'bmi', 's1', 's5', 'target']

sns.pairplot(df[cols])
plt.tight_layout()
plt.savefig('scatterplot.png', dpi=300)
plt.show()
```

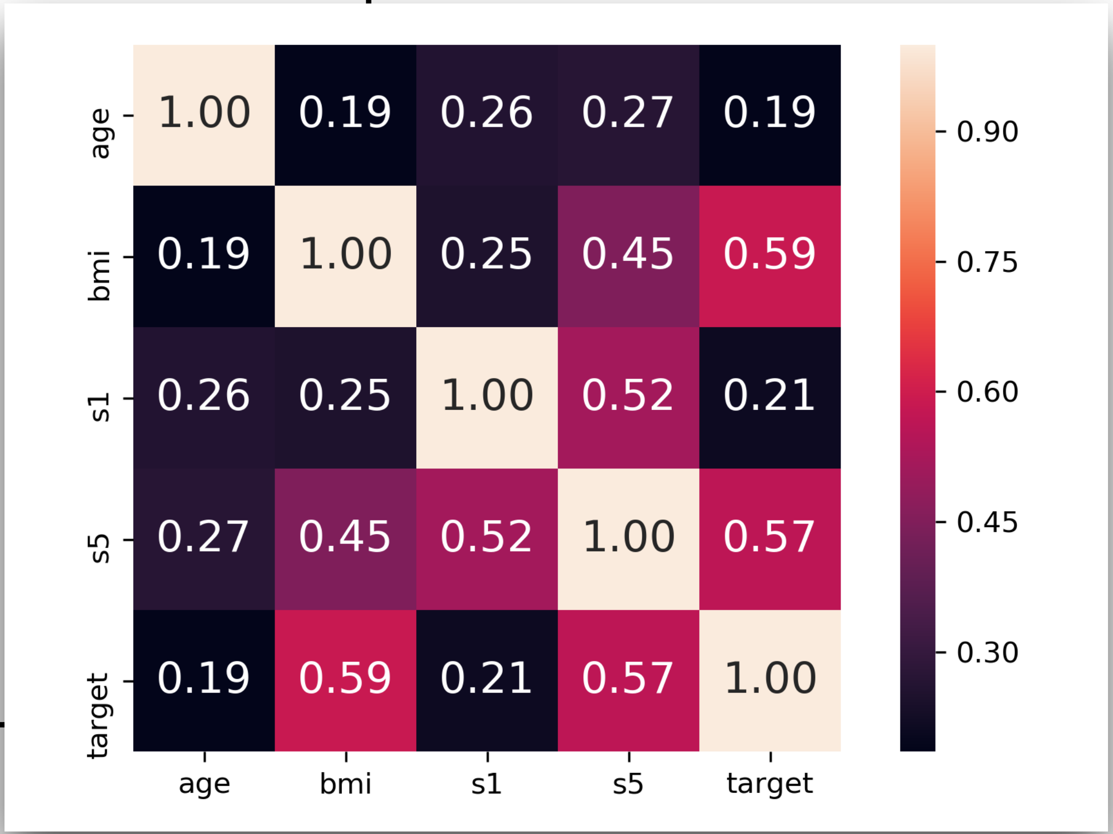


糖尿病數據集

- 以熱度圖（heat map）畫出相關係數矩陣 (correlation matrix)

Code (3/8)

```
import numpy as np

cm = np.corrcoef(df[cols].values.T)
#sns.set(font_scale=1.5)
hm = sns.heatmap(cm,
                 cbar=True,
                 annot=True,
                 square=True,
                 fmt='.2f',
                 annot_kws={'size': 15},
                 yticklabels=cols,
                 xticklabels=cols)

plt.tight_layout()
plt.savefig('correlation.png', dpi=300)
plt.show()
```



	age	bmi	s1	s5	target
age	1.00	0.19	0.26	0.27	0.19
bmi	0.19	1.00	0.25	0.45	0.59
s1	0.26	0.25	1.00	0.52	0.21
s5	0.27	0.45	0.52	1.00	0.57
target	0.19	0.59	0.21	0.57	1.00

複迴歸

$$h_\theta(x_1, x_2, x_3) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3$$

$$= \overrightarrow{\theta} \cdot \overrightarrow{x}$$

where

$$\overrightarrow{\theta} = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_n \end{bmatrix} \qquad \overrightarrow{x} = \begin{bmatrix} 1 \\ x_1 \\ \vdots \\ x_n \end{bmatrix}$$

Normal equation

$$h_\theta(x) = \overrightarrow{\theta} \cdot \overrightarrow{x}$$

$$X = \begin{bmatrix} - - x^{(1)} - - \\ \vdots \\ - - x^{(n)} - - \end{bmatrix} \quad y = \begin{bmatrix} y^{(1)} \\ \vdots \\ y^{(n)} \end{bmatrix}$$

- Cost function

$$E(\theta) = \frac{1}{2}\sum_{i=1}^{m}\left(h_\theta(x^{(i)}) - y^{(i)}\right)^2$$

$$= \frac{1}{2}\|X\overrightarrow{\theta} - \overrightarrow{y}\|^2$$

$$= \frac{1}{2}\left(\overrightarrow{\theta}^T X^T X \overrightarrow{\theta} - 2\overrightarrow{\theta}^T X^T \overrightarrow{y} + \overrightarrow{y}^T \overrightarrow{y}\right)$$

Normal equation

$$h_\theta(x) = \overrightarrow{\theta} \cdot \overrightarrow{x}$$

- Cost function

$$E(\theta) = \frac{1}{2}\sum_{i=1}^{m}\left(h_\theta(x^{(i)}) - y^{(i)}\right)^2$$

$$\Rightarrow \nabla E(\theta) = X^T X \overrightarrow{\theta} - X^T \overrightarrow{y} \equiv \overrightarrow{0}$$

$$\Rightarrow \overrightarrow{\theta} = \left(X^T X\right)^{-1} X^T \overrightarrow{y}$$

Gradient descent（梯度下降法)

- Cost function

$$E(\theta) = \frac{1}{2}\sum_{i=1}^{m}\left(h_\theta(x^{(i)}) - y^{(i)}\right)^2$$

- Gradient descent

$$\theta_j := \theta_j - \eta\frac{\partial E}{\partial \theta_j}$$ **for j = 0, 1, …, n**

$$\Rightarrow \theta_j := \theta_j - \eta\sum_{i=1}^{m}\left(h_\theta(x^{(i)}) - y^{(i)}\right)x_j^{(i)}$$

Normalization

Why normalize inputs?

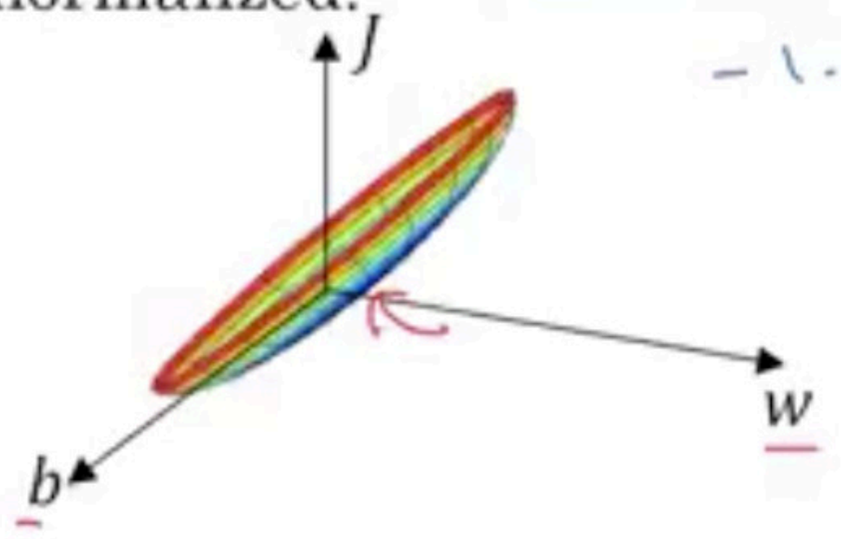
$$J(w,b) = \frac{1}{m}\sum_{i=1}^{m}\mathcal{L}(\hat{y}^{(i)}, y^{(i)})$$

w_1 x_1 : $\underline{1 \dots 1000}$

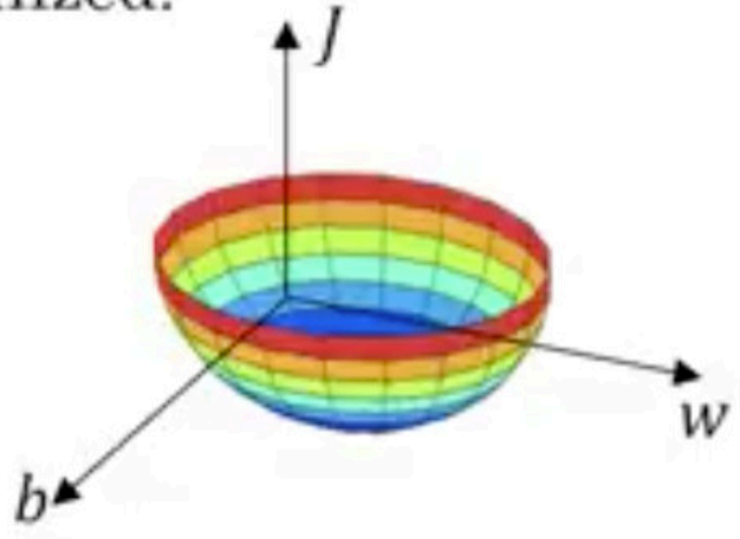
w_2 x_2 : $\underline{0 \dots 1}$

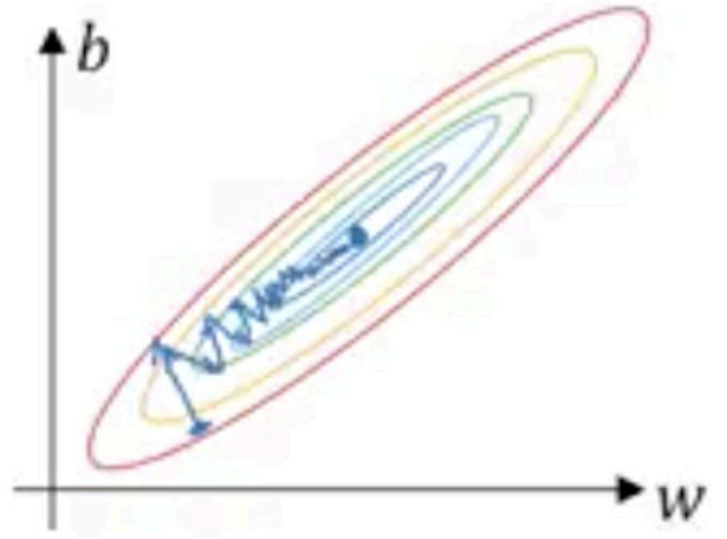
$-1 \dots 1$

Unnormalized:



Normalized:

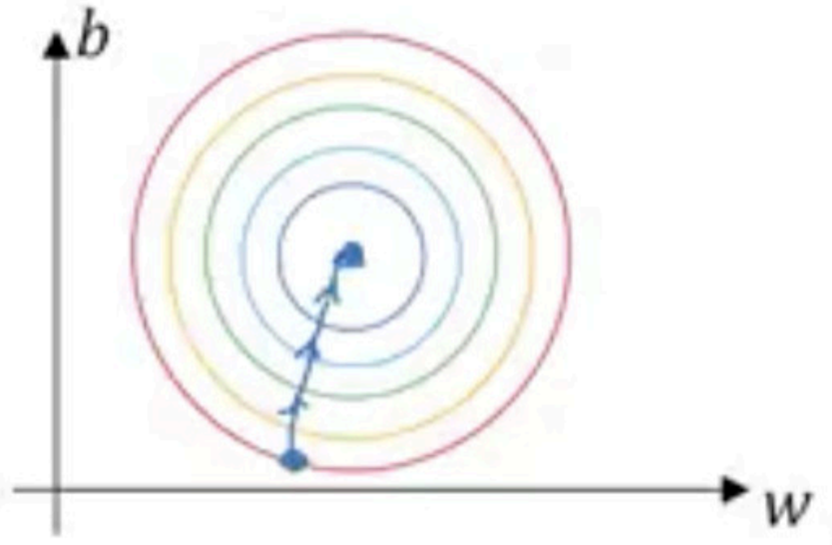




x_1 : $0 \dots 1$

x_2 : $-1 \dots 1$

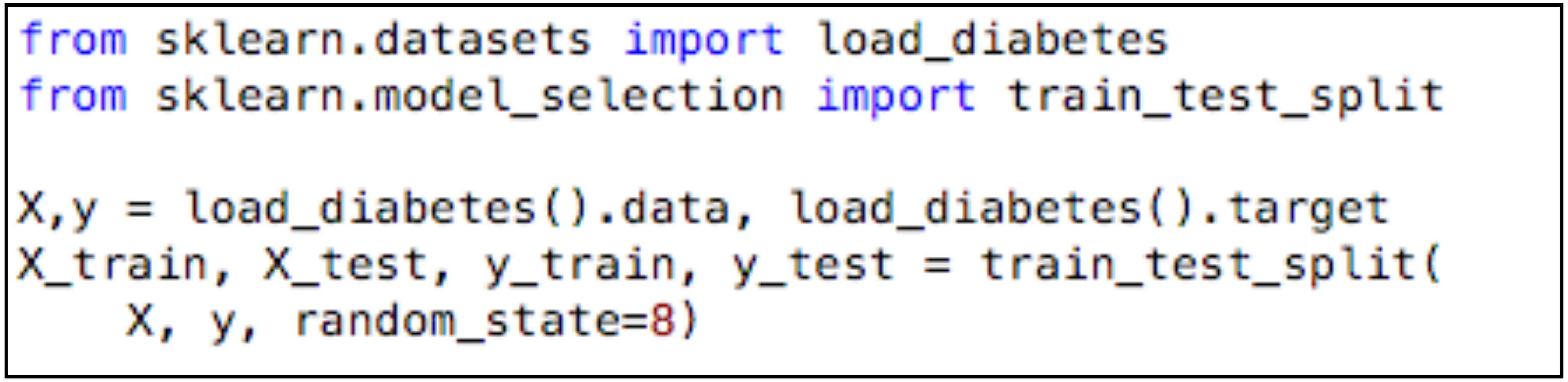
x_3 : $1 \dots 2$



Andrew Ng

糖尿病數據集

- 將糖尿病數據集分成training set 及 test set

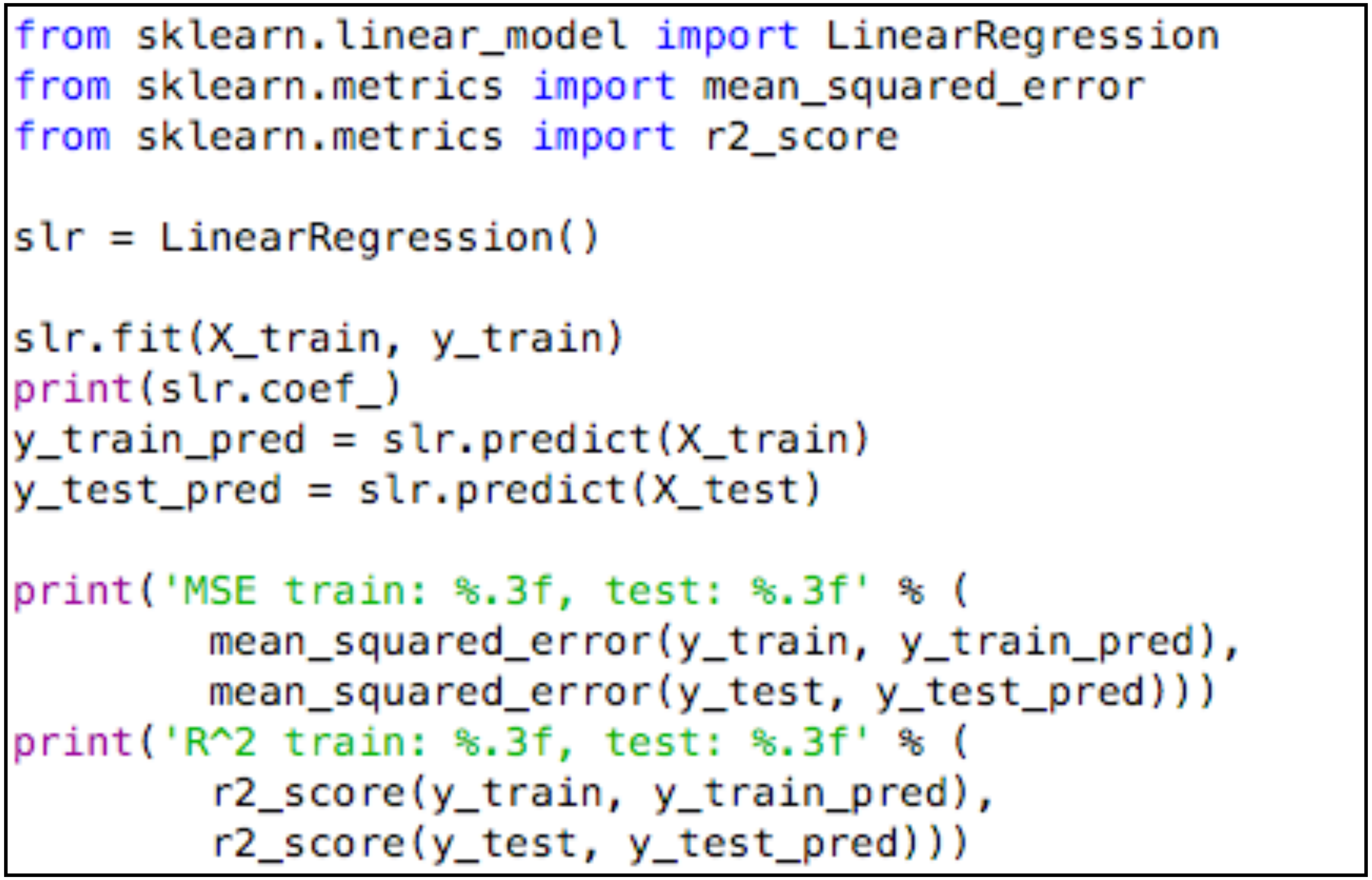


```python
from sklearn.datasets import load_diabetes
from sklearn.model_selection import train_test_split

X,y = load_diabetes().data, load_diabetes().target
X_train, X_test, y_train, y_test = train_test_split(
    X, y, random_state=8)
```

Code (4/8)

糖尿病數據集

- 訓練線性迴歸模型，並計算MSE及 R^2



```
from sklearn.linear_model import LinearRegression
from sklearn.metrics import mean_squared_error
from sklearn.metrics import r2_score

slr = LinearRegression()

slr.fit(X_train, y_train)
print(slr.coef_)
y_train_pred = slr.predict(X_train)
y_test_pred = slr.predict(X_test)

print('MSE train: %.3f, test: %.3f' % (
        mean_squared_error(y_train, y_train_pred),
        mean_squared_error(y_test, y_test_pred)))
print('R^2 train: %.3f, test: %.3f' % (
        r2_score(y_train, y_train_pred),
        r2_score(y_test, y_test_pred)))
```

Code (5/8)

Linear regression 的結果

```
      Age            Sex            BMI            ABP             S1
[  11.5106203   -282.51347161  534.20455671  401.73142674  -1043.89718398
 634.92464089   186.43262636  204.93373199  762.47149733    91.9460394 ]
      S2             S3             S4             S5              S6
```

Target = 11.51 * age + … + 91.94 * S6

迴歸係數

小心共線性

當其他預測因子存在的情況下，該預測因子的強度

Note 1: X 要先標準化 （去除單位的影響）

Note 2: 回歸係數數值越大表示對 Y 的影響力越大

Note 3: 回歸係數為負表示負相關

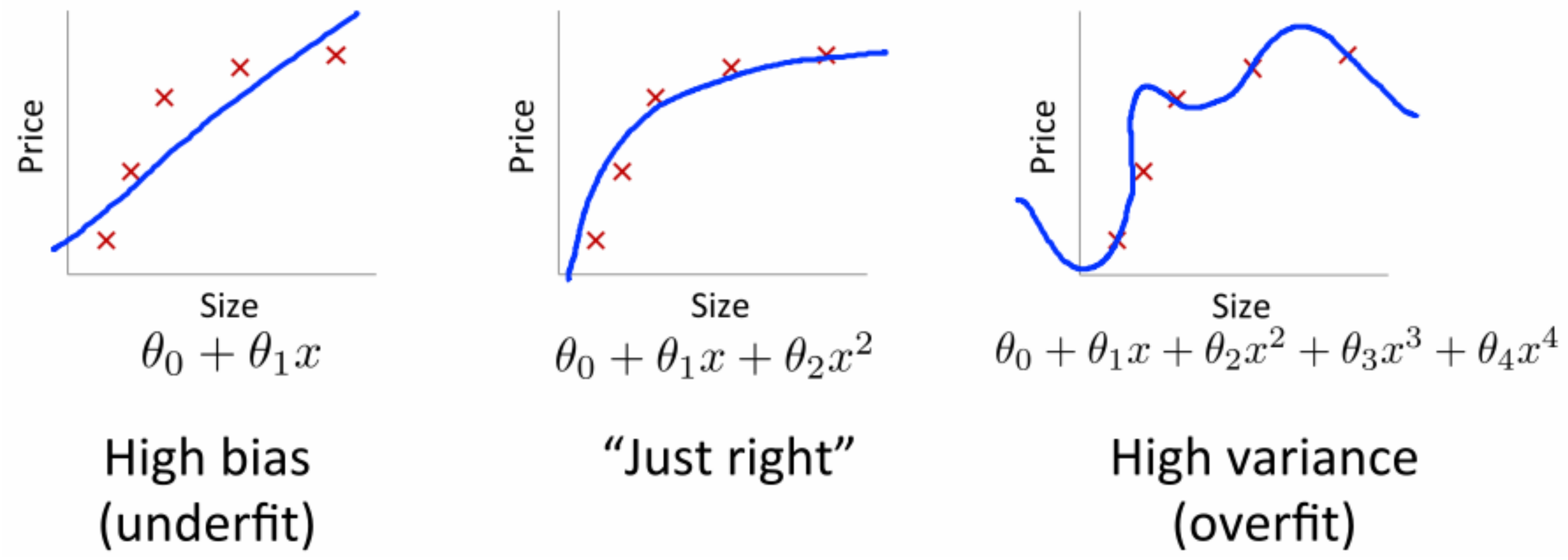
怎麼解決共線性

- 資料預處理
  - 資料轉換
  - 只留下獨立(不相關)的變數
- 脊迴歸（ridge regression）
- 主成分分析 (principal component analysis)

https://taweihuang.hpd.io/2016/09/12/讀者提問：多元迴歸分析的變數選擇/

Overfitting v.s. underfitting

Source: http://murphymind.blogspot.com/2017/06/machine-learning-advice-for-applying.html



$$E(\theta) = \frac{1}{2}\sum_{i=1}^{m}\left(h_\theta(x^{(i)}) - y^{(i)}\right)^2 + \boxed{1000 \cdot \theta_3^2 + 1000 \cdot \theta_4^2}$$

Regularization (正則化)

- 脊迴歸　(Ridge Regression)

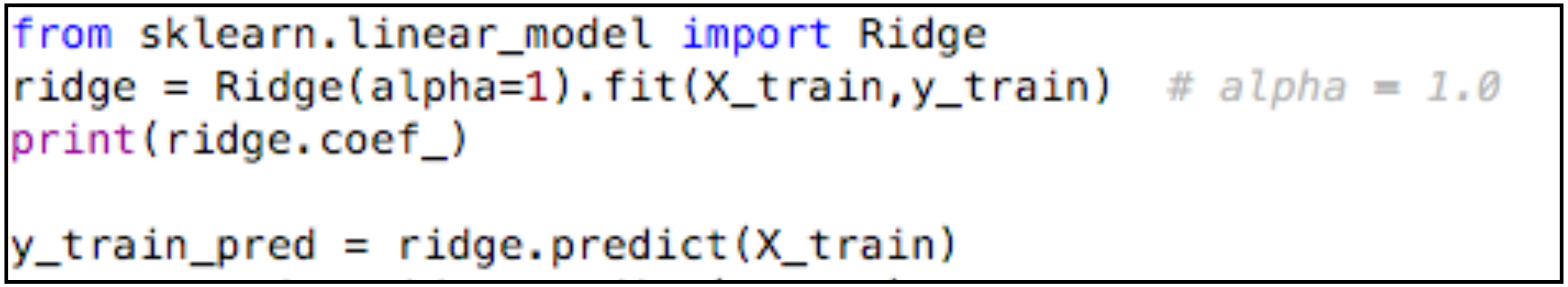
$$E(\theta) = \frac{1}{2}\sum_{i=1}^{m}\left(h_\theta(x^{(i)}) - y^{(i)}\right)^2 + \alpha \cdot \sum_{i=1}^{n}\theta_i^2$$

不考慮截距項

控制正則項的強度

糖尿病數據集

- 訓練Ridge模型，並計算MSE及 R^2



```
from sklearn.linear_model import Ridge
ridge = Ridge(alpha=1).fit(X_train,y_train)  # alpha = 1.0
print(ridge.coef_)

y_train_pred = ridge.predict(X_train)
```

Ridge 的參數

複雜度越低的模型在訓練集上的表現越差，但泛化的能力會更好

如果我們更在意模型在泛化方面的能力，應該選擇Ridge 而非線性迴歸

	Linear Regression		Ridge $\alpha = 1$	Ridge $\alpha = 10$	Ridge $\alpha = 0.1$
R^2 值 Train	0.530	>	0.433		
			=		
R^2 值 Test	0.459		0.433		

overfitting

Ridge 的參數

增加 α 後，模型的分數大幅降低，然而 test 分數 > train 分數

若模型出現overfitting，可以透過提高 α 值來降低 overfitting的程度

	Linear Regression	Ridge $\alpha = 1$	Ridge $\alpha = 10$	Ridge $\alpha = 0.1$
R^2 值 Train	0.530	0.433	0.151	
R^2 值 Test	0.459	0.433	$\wedge$ 0.162	

overfitting

Ridge 的參數

非常小的 α 值，會使結果很接近線性迴歸

	Linear Regression	Ridge $\alpha = 1$	Ridge $\alpha = 10$	Ridge $\alpha = 0.1$
R^2 值 Train	0.530	0.433	0.151	0.522
R^2 值 Test	0.459	0.433	0.162	0.473

overfitting

Ridge 的參數

參數的取值須視使用的數據集

增加α會降低係數，使其趨近於 0 ，降低訓練集的分數，但有助於泛化

	Linear Regression	Ridge $\alpha = 1$	Ridge $\alpha = 10$	Ridge $\alpha = 0.1$
R^2 值 Train	0.530	0.433	0.151	0.522
R^2 值 Test	0.459	0.433	0.162	0.473

overfitting

Regularization (正則化)

- 脊迴歸 (Ridge Regression)

不考慮截距項

$$E(\theta) = \frac{1}{2}\sum_{i=1}^{m}\left(h_\theta(x^{(i)}) - y^{(i)}\right)^2 + \alpha \cdot \sum_{i=1}^{n}\theta_i^2$$

控制正則項的強度

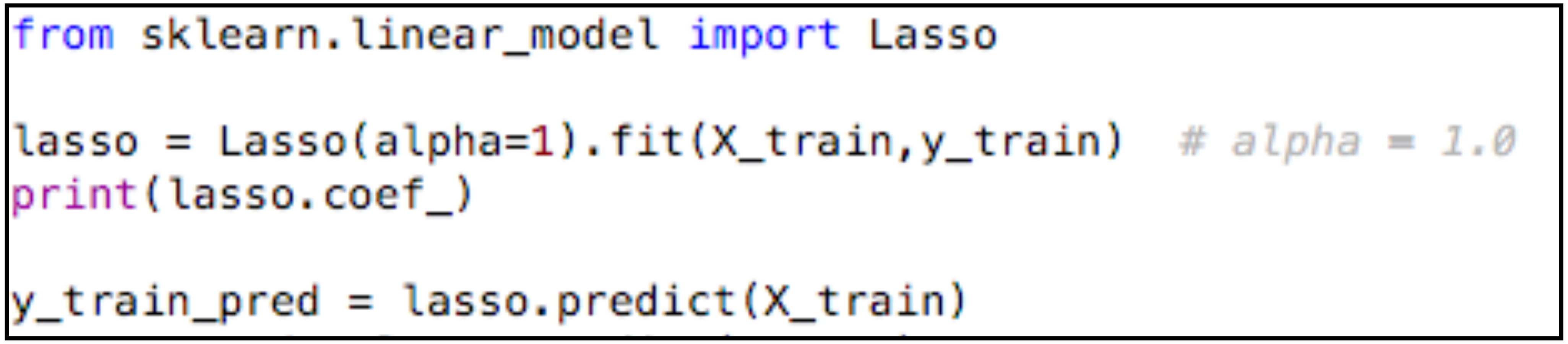
- 最小絕對壓縮挑選機制 (Least Absolute Shrinkage and Selection Operator, LASSO)

$$E(\theta) = \frac{1}{2}\sum_{i=1}^{m}\left(h_\theta(x^{(i)}) - y^{(i)}\right)^2 + \alpha \cdot \sum_{i=1}^{n}|\theta_i|$$

使某些係數變為 0

糖尿病數據集

- 訓練LASSO模型，並計算MSE及R^2



```
from sklearn.linear_model import Lasso

lasso = Lasso(alpha=1).fit(X_train,y_train)  # alpha = 1.0
print(lasso.coef_)

y_train_pred = lasso.predict(X_train)
```

LASSO 的參數

LASSO 的得分都很低，模型只使用 3 個特徵

```
[           0          0     384.73421807      72.69325545          0
            0          0          0          247.88881314          0      ]
```

	Linear Regression	LASSO $\alpha = 1$	LASSO $\alpha = 0.1$	LASSO $\alpha = 0.001$
R^2 值 Train	0.530	0.362		
R^2 值 Test	0.459	0.366		

overfitting

underfitting

LASSO 的參數

降低 α 後，模型的分數大幅增加，模型較複雜 （7 個特徵）

相對Ridge, LASSO表現稍好，且只用 7 個特徵，使模型較好理解

	Linear Regression	LASSO $\alpha = 1$	LASSO $\alpha = 0.1$	LASSO $\alpha = 0.001$
R^2 值 Train	0.530	0.362	0.519	
R^2 值 Test	0.459	0.366	0.480	

overfitting

LASSO 的參數

非常小的 α 值，使用了全部特徵，會使結果很接近線性迴歸

```
[   11.82931254   -281.06324599   534.59556593   401.25597128   -971.04936503
   579.28119134    151.83257187   191.85084436   736.83680063     91.17487055]
```

	Linear Regression	LASSO $\alpha = 1$	LASSO $\alpha = 0.1$	LASSO $\alpha = 0.001$
R^2 值 Train	0.530	0.362	0.519	0.530
R^2 值 Test	0.459	0.366	0.480	0.460

overfitting

Ridge v.s. LASSO

- 實作時，Ridge通常是首選，因為LASSO在移除變數的同時，會犧牲模型的正確性
- 但如果特徵太多，且只有一小部分是真正重要的，那應該選擇LASSO
- 如果須解釋模型，LASSO也更好理解，因為使用較少特徵

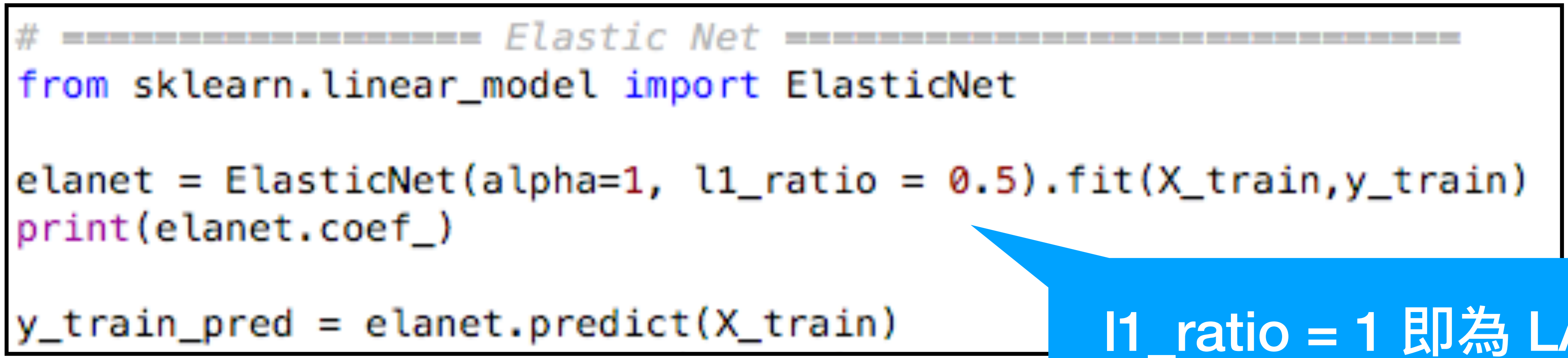
Regularization (正則化)

- 彈性網 (Elastic Net)

$$E(\theta) = \frac{1}{2}\sum_{i=1}^{m}\left(h_\theta(x^{(i)}) - y^{(i)}\right)^2 + a \cdot \sum_{i=1}^{n} |\theta_i| + b \cdot \sum_{i=1}^{n} \theta_i^2$$

糖尿病數據集

- 訓練Elastic Net模型，並計算MSE及R^2



```
# =================== Elastic Net ===============================
from sklearn.linear_model import ElasticNet

elanet = ElasticNet(alpha=1, l1_ratio = 0.5).fit(X_train,y_train)
print(elanet.coef_)

y_train_pred = elanet.predict(X_train)
```

l1_ratio = 1 即為 LASSO

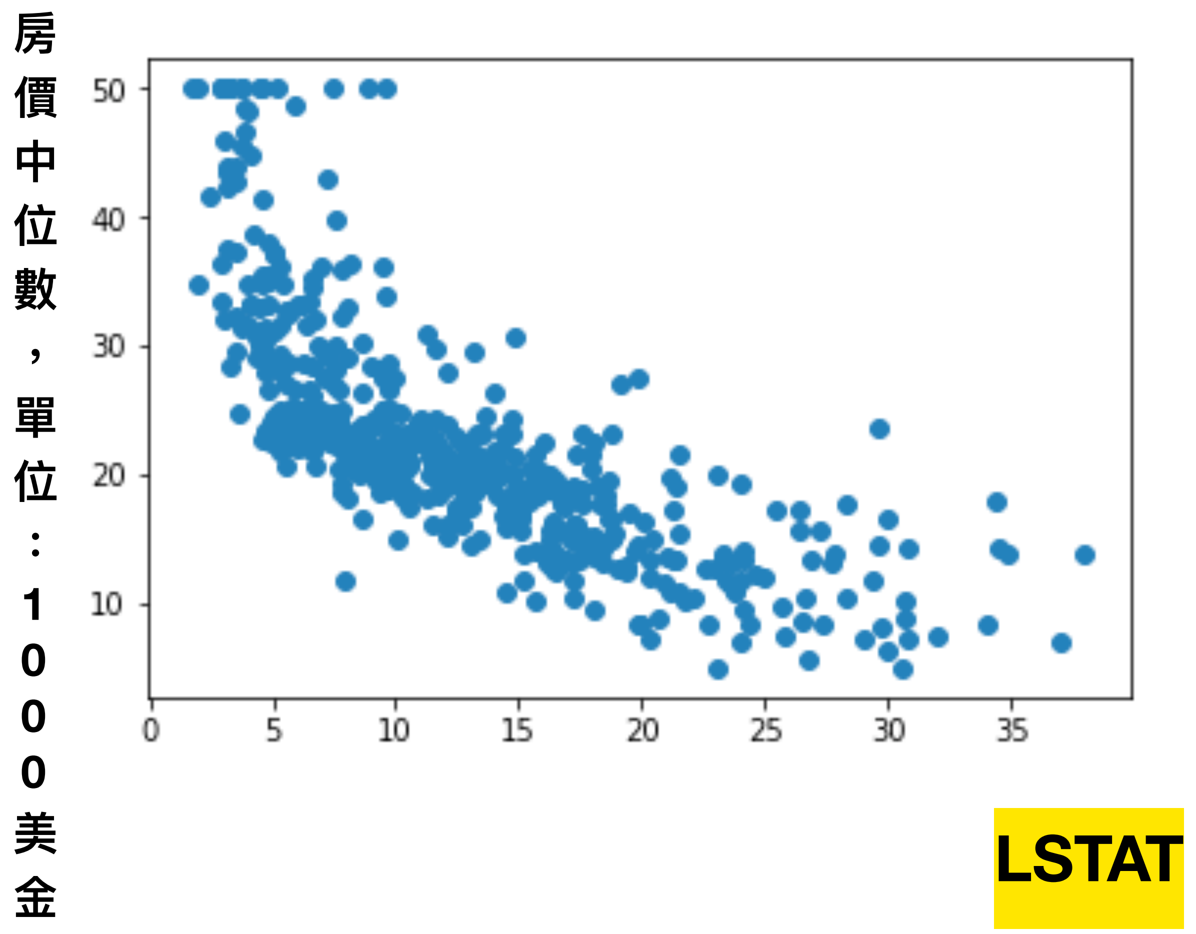
https://scikit-learn.org/stable/modules/generated/sklearn.linear_model.ElasticNet.html

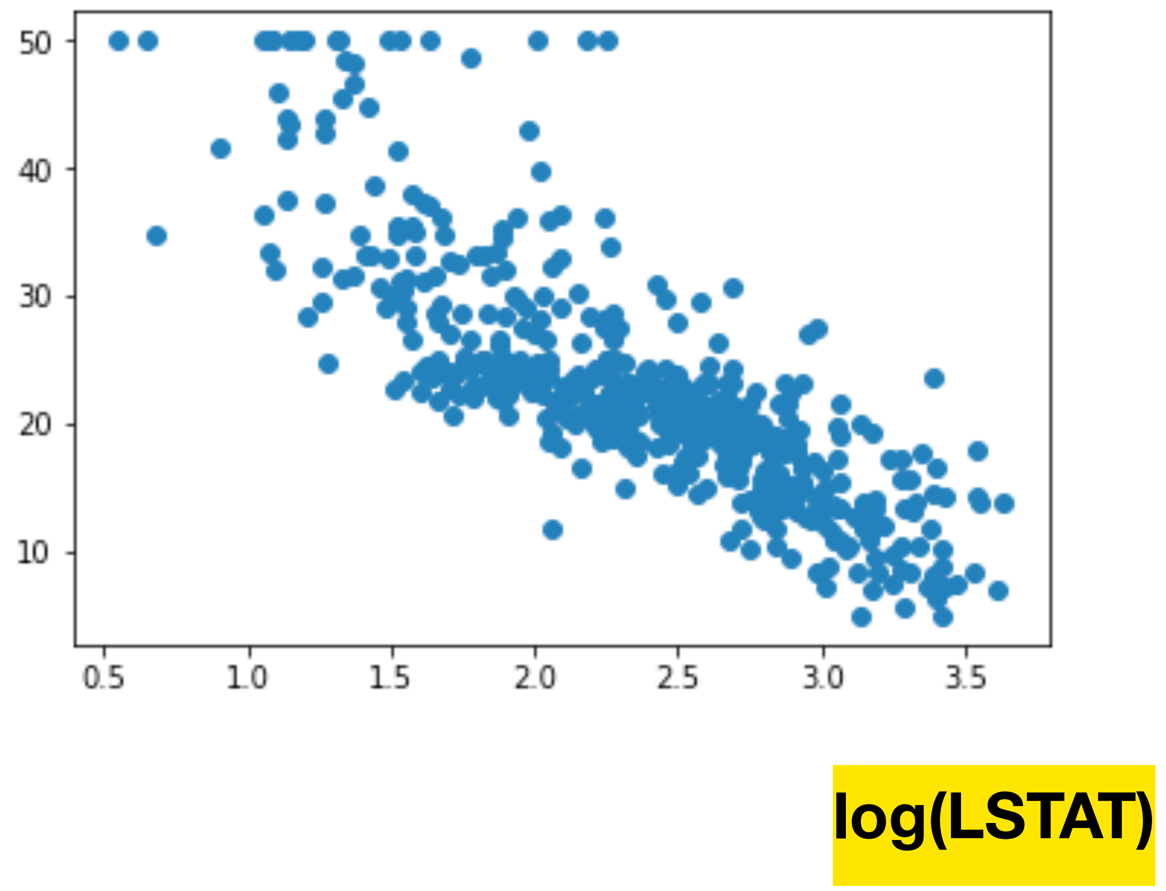
Pros & Cons

- Pros:
  - 簡單, 直覺, 易於運算
  - 迴歸係數能得到有用的訊息
- Cons:
  - 易受異常值影響
  - 相關預測因子的權重會被扭曲
  - 曲線趨勢

Example: 波士頓房價

- D . Harrison 與 D. L. Rubinfeld 在1978年收集的波士頓郊區的“房價數據集”，其中包含14個特徵，其中 LSTAT(低社經地位的人口比例)





Pros & Cons

- Pros:
  - 簡單, 直覺, 易於運算
  - 迴歸係數能得到有用的訊息

- Cons:
  - 易受異常值影響
  - 相關預測因子的權重會被扭曲
  - 曲線趨勢
  - 預測因子和結果並不暗示因果關係