機器學習

Lecture 4 Logistic Regression

Logistic Regression

- 二元分類
  - 癌症的診斷: 是(1) v.s. 否(0)
  - 購買商品的意願：會購買(1) v.s. 不想購買(0)

- 屬於某類的機率
  - e.x. 根據今天的溫度^{X_1}、濕度^{X_2}、風向^{X_3}來預測明天的降雨(1)的機率

Logistic Regression

- Logistic regression is a learning algorithm used in a supervised learning problem when the output $y \in \{0,1\}$
- Given a feature vector X, the algorithm will evaluate the probability of y = 1:

$$\hat{y} = P(y = 1 \mid x) \in [0,1]$$

複回歸

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

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

where

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

Logistic Regression

$$h_\theta(x_1, x_2, x_3) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3$$
$$= \overrightarrow{\theta} \cdot \overrightarrow{x}$$

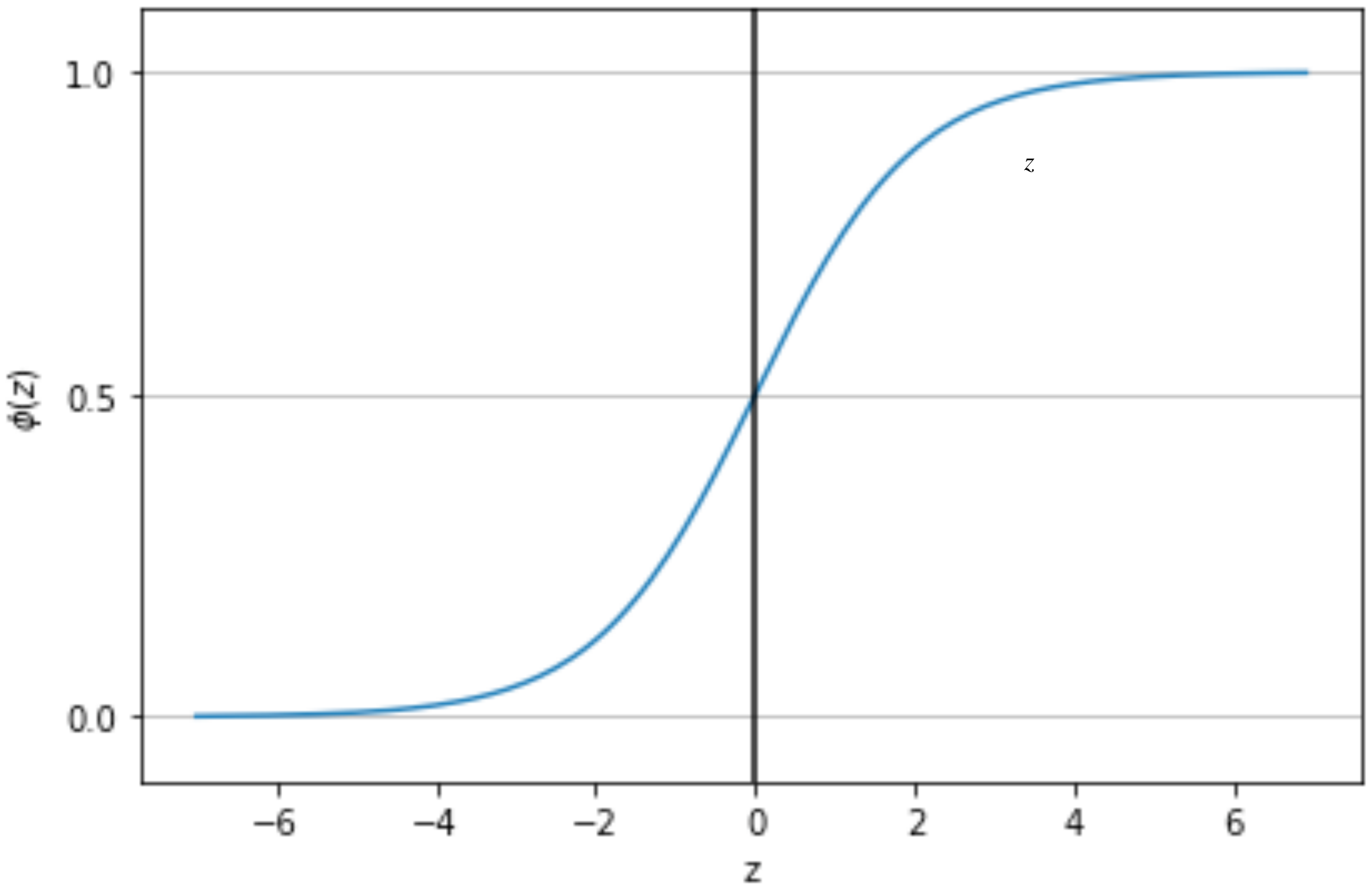
Logistic Regression:

$$\hat{y} = \frac{1}{1 + \exp\left(-\overrightarrow{\theta} \cdot \overrightarrow{x}\right)}$$

Sigmoid function

$$\phi(z) = \frac{1}{1+\exp(-z)}$$

$$\exp(-z) = e^{-z}$$



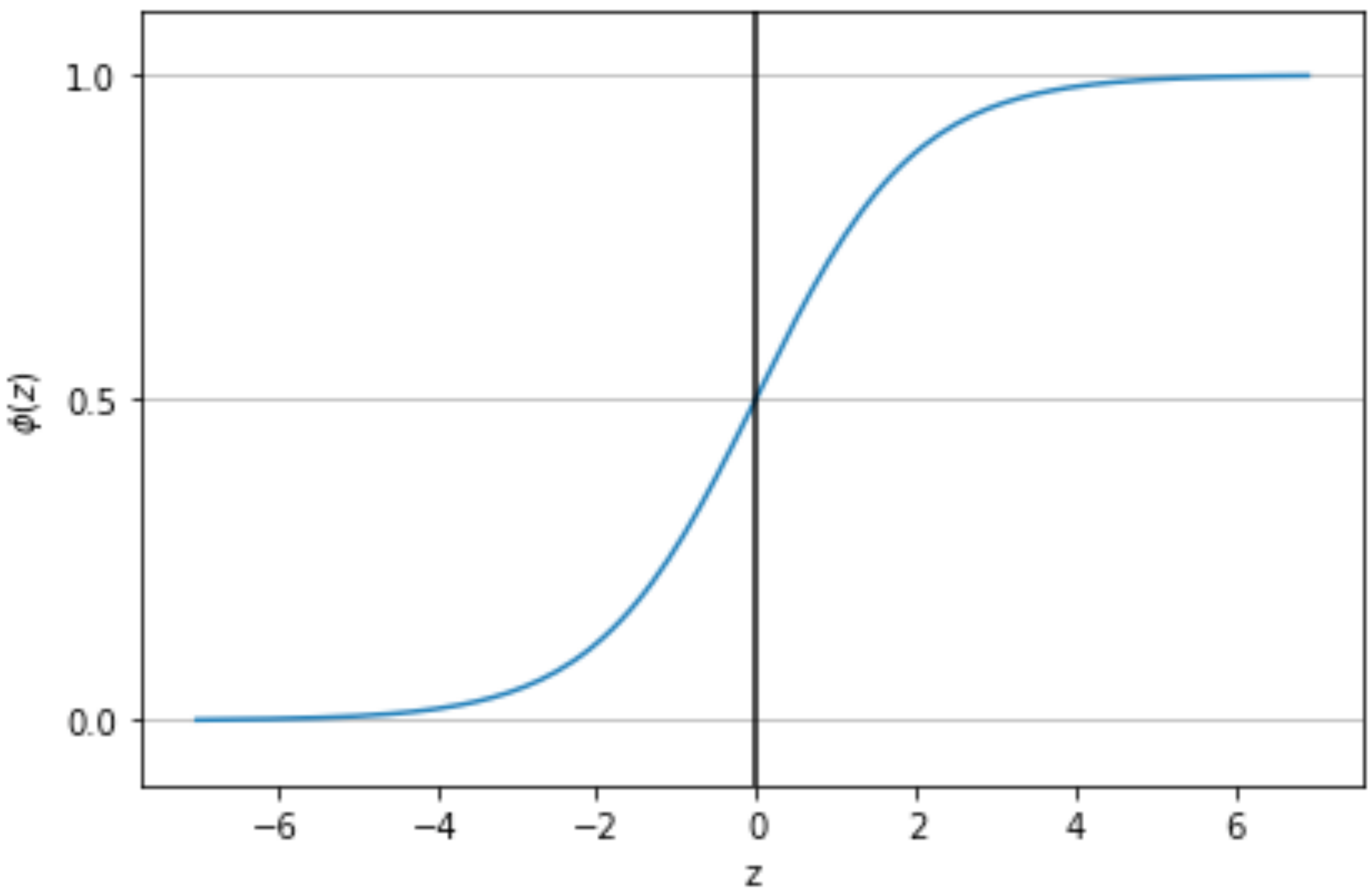
-Some observations

- If z is a large positive number, then $\phi(z) = 1$
- If z is small or a large negative number, then $\phi(z) = 0$
- If z = 0, then $\phi(z) = 0.5$

Decision Boundary (決策邊界)

$\hat{y} = P(y = 1 \mid x) = 0.8$ 降雨機率＝80% 雨天 (1)

$\hat{y} = P(y = 1 \mid x) = 0.2$ 降雨機率＝20% 晴天 (0)

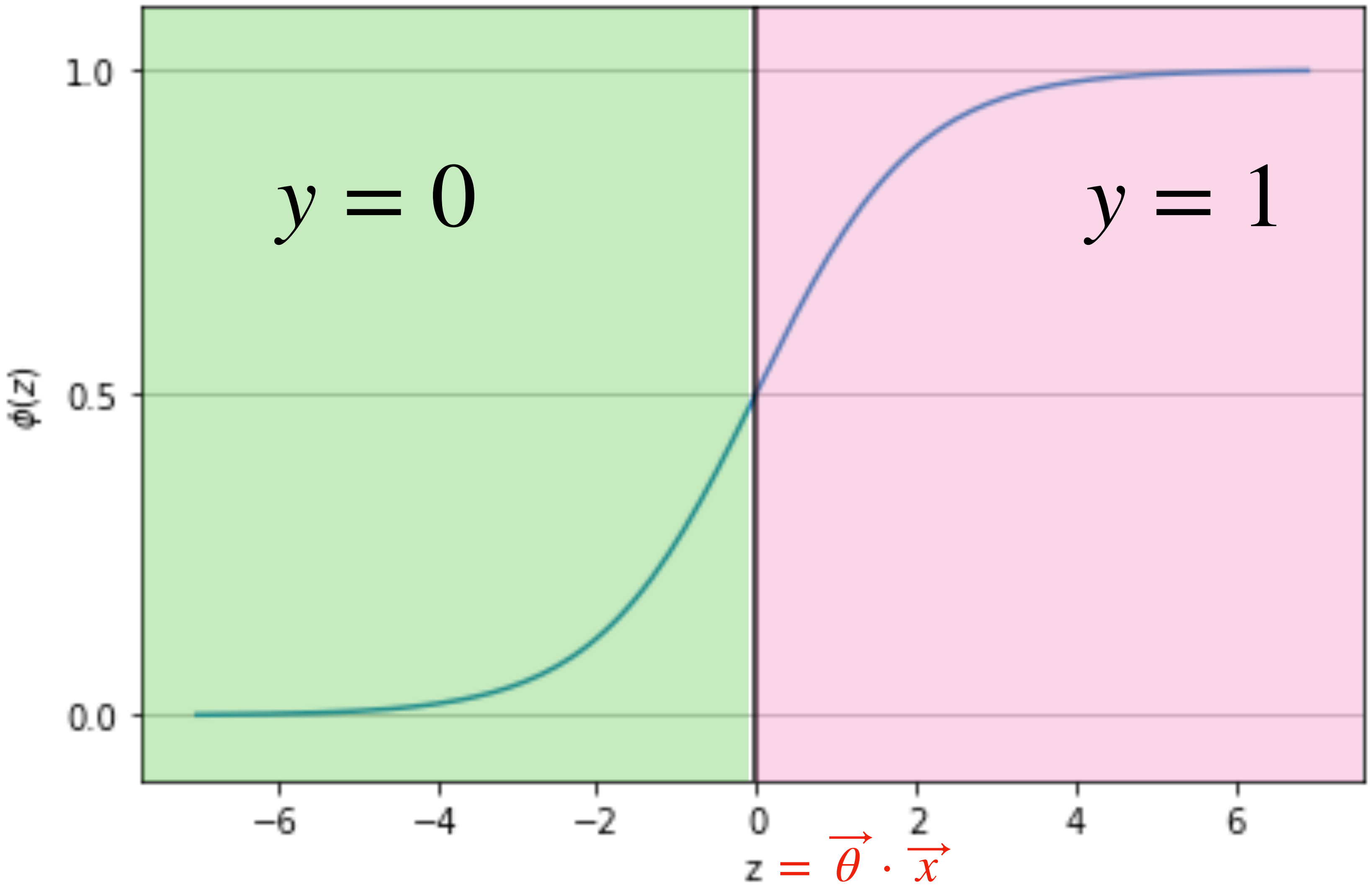


Decision Boundary (決策邊界)

$$\hat{y} = P(y=1|x) \geq 0.5 \Rightarrow y = 1$$

$$\hat{y} = P(y=1|x) < 0.5 \Rightarrow y = 0$$

$\vec{\theta} \cdot \vec{x} < 0$ $\vec{\theta} \cdot \vec{x} \geq 0$



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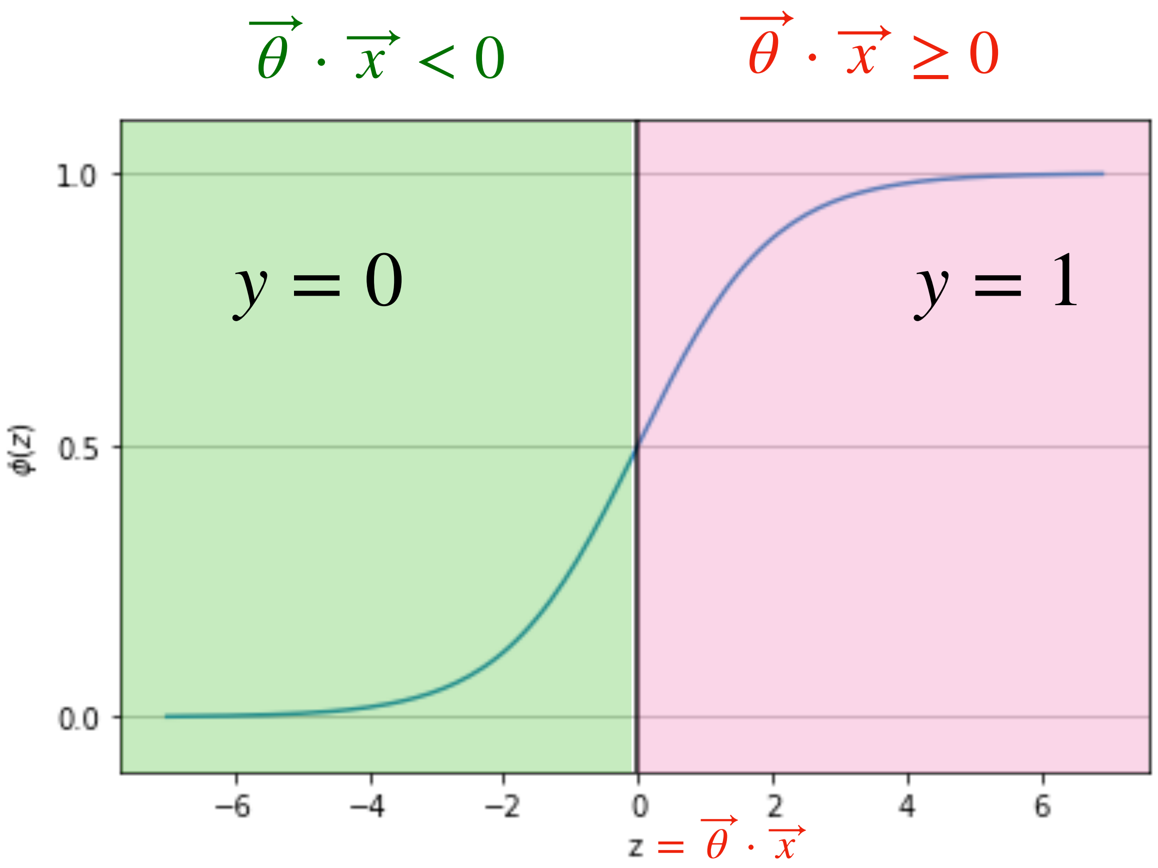
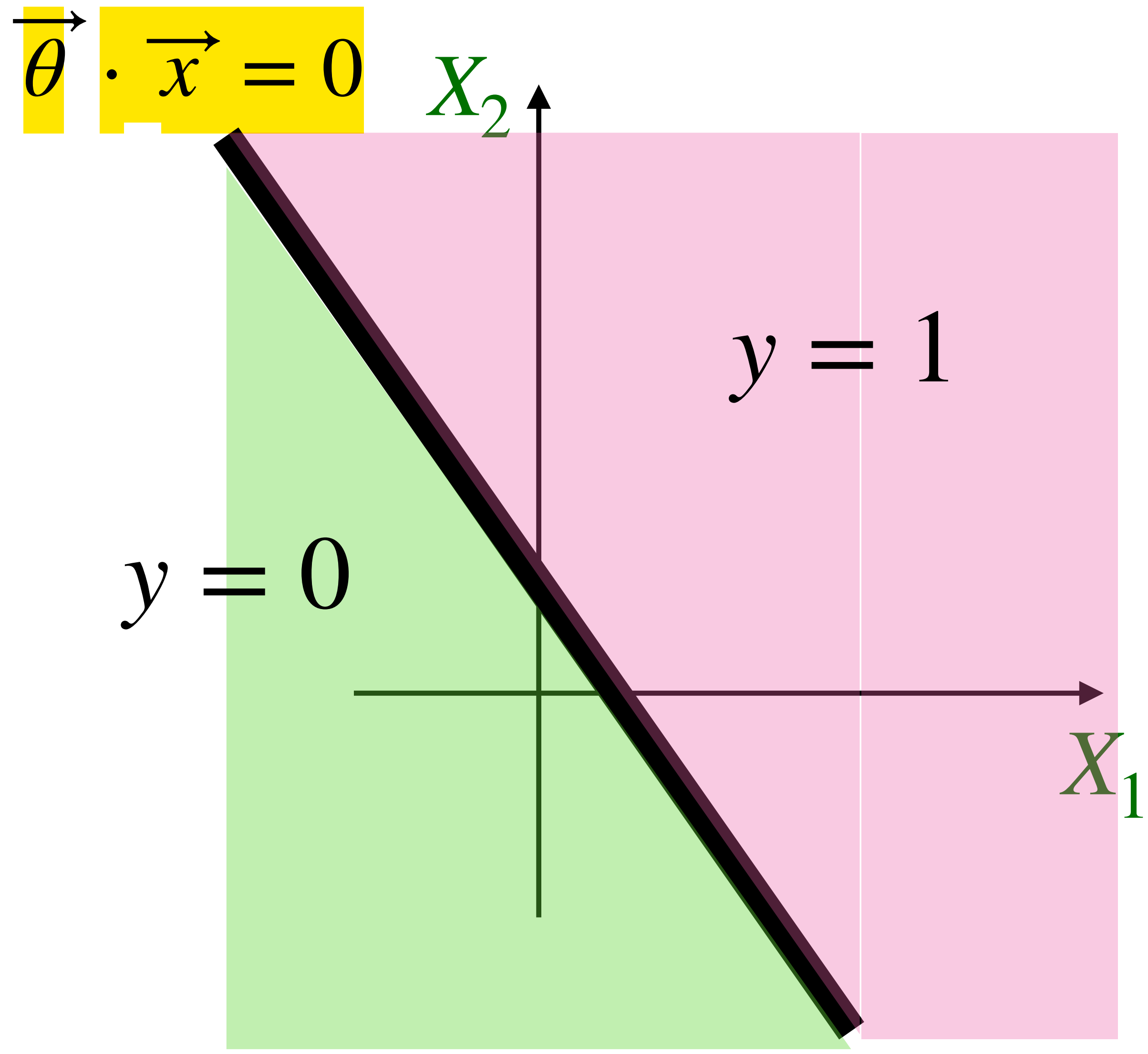
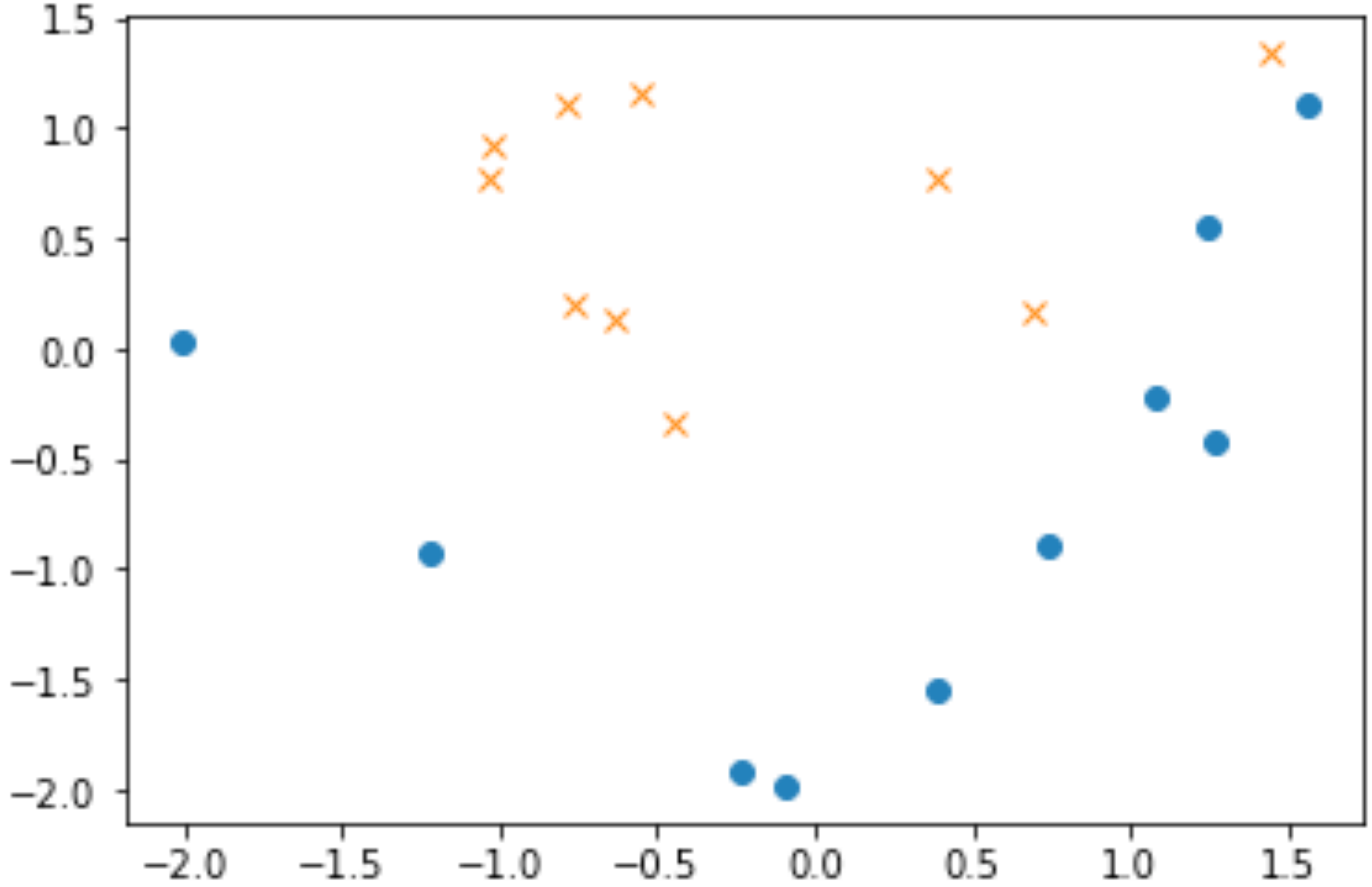


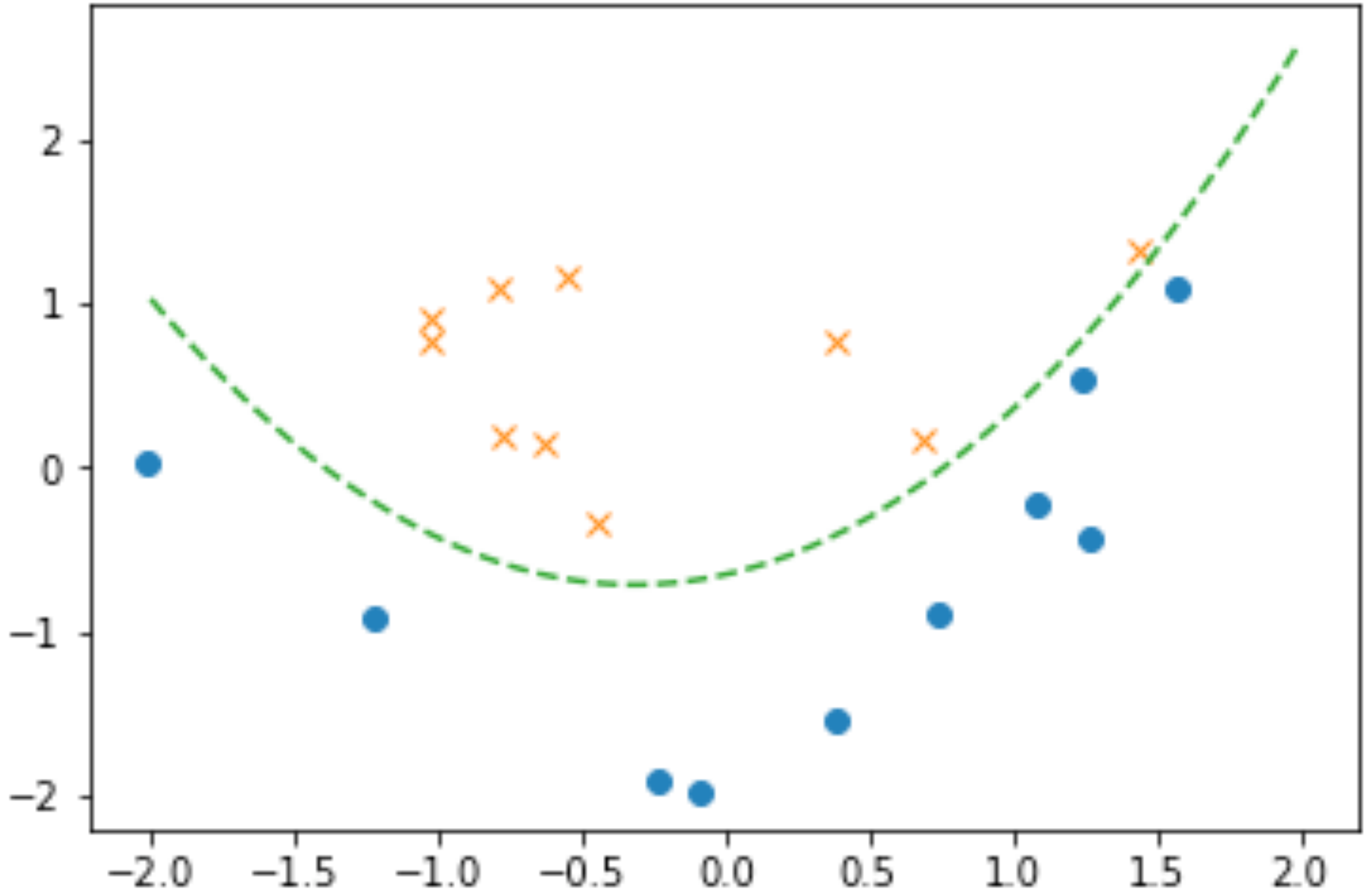


線性不可分離



Decision Boundary (決策邊界)

$$\overrightarrow{\theta} \cdot \overrightarrow{x} = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_1^2$$



Logistic Regression: Cost Function

- 觀察 $\hat{y} = P(y = 1 | x)$
  - 若 y = 1: 希望 $P(y = 1 | x)$ 越大越好
  - 若 y = 0: 希望 $P(y = 0 | x)$ 越大越好

x	y	機率
(80, 150)	0	希望 $P(y = 0 \| x)$ 越大越好
(35, 130)	0	希望 $P(y = 0 \| x)$ 越大越好
(160, 20)	1	希望 $P(y = 1 \| x)$ 越大越好
(125, 30)	1	希望 $P(y = 1 \| x)$ 越大越好

Goal: Maximize

$$P(y^{(1)} = 0 | x^{(1)}) P(y^{(2)} = 0 | x^{(2)}) P(y^{(3)} = 1 | x^{(3)}) P(y^{(4)} = 1 | x^{(4)})$$

Logistic Regression: Cost Function

- Goal: Maximize

$$\prod_{i=1}^{m} P(y^{(i)} = 1 \mid x^{(1)})^{y^{(i)}} P(y^{(i)} = 0 \mid x^{(i)})^{1-y^{(i)}}$$

- 觀察
  - 若 $y^{(i)} = 1$

$$P(y^{(i)} = 1 \mid x^{(1)})^{y^{(i)}} P(y^{(i)} = 0 \mid x^{(i)})^{1-y^{(i)}} = P(y^{(i)} = 1 \mid x^{(1)})$$

  - 若 $y^{(i)} = 0$

$$P(y^{(i)} = 1 \mid x^{(1)})^{y^{(i)}} P(y^{(i)} = 0 \mid x^{(i)})^{1-y^{(i)}} = P(y^{(i)} = 0 \mid x^{(1)})$$

Logistic Regression: log-likelihood Function

- Goal: Maximize

$$\prod_{i=1}^{m} P(y^{(i)} = 1 \mid x^{(1)})^{y^{(i)}} P(y^{(i)} = 0 \mid x^{(i)})^{1-y^{(i)}}$$

- 因為機率越乘越小，所以目標改為 Maximum

$$\log\left(\prod_{i=1}^{m} P(y^{(i)} = 1 \mid x^{(1)})^{y^{(i)}} P(y^{(i)} = 0 \mid x^{(i)})^{1-y^{(i)}}\right)$$

$$= \sum_{i=1}^{m} y^{(i)} \log\left(P(y^{(i)} = 1 \mid x^{(1)})\right) + \left(1 - y^{(i)}\right) \log\left(P(y^{(i)} = 0 \mid x^{(i)})\right)$$

$$= \sum_{i=1}^{m} y^{(i)} \log\left(\hat{y}^{(i)}\right) + \left(1 - y^{(i)}\right) \log\left(1 - \hat{y}^{(i)}\right)$$

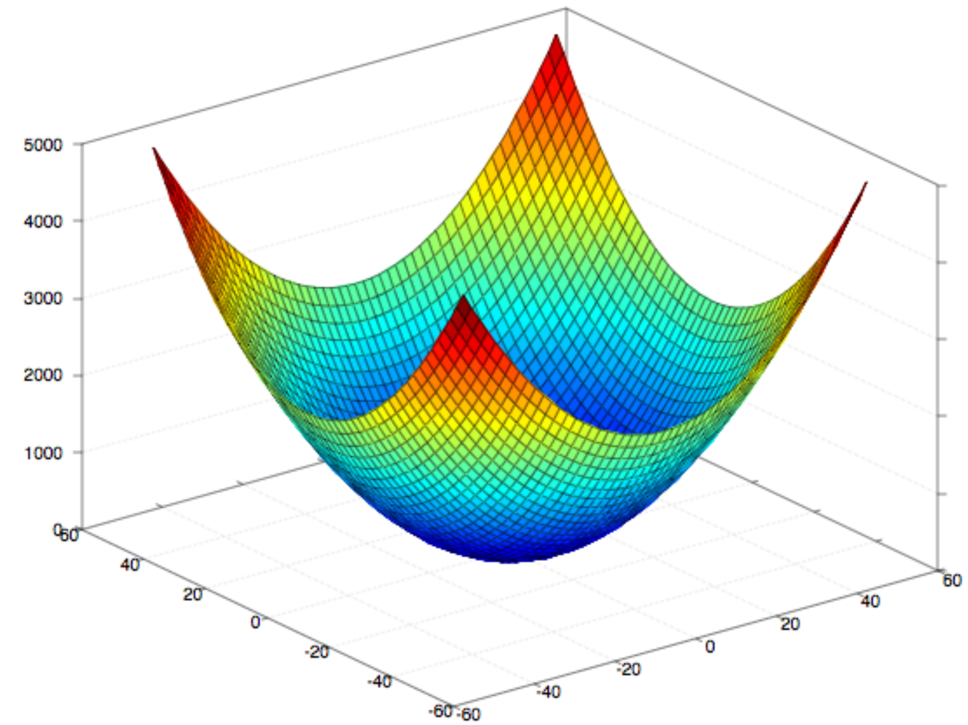
Logistic Regression: log-likelihood Function

- Goal: Maximize

$$\sum_{i=1}^{m} y^{(i)} \log\left(\hat{y}^{(i)}\right) + \left(1 - y^{(i)}\right) \log\left(1 - \hat{y}^{(i)}\right)$$

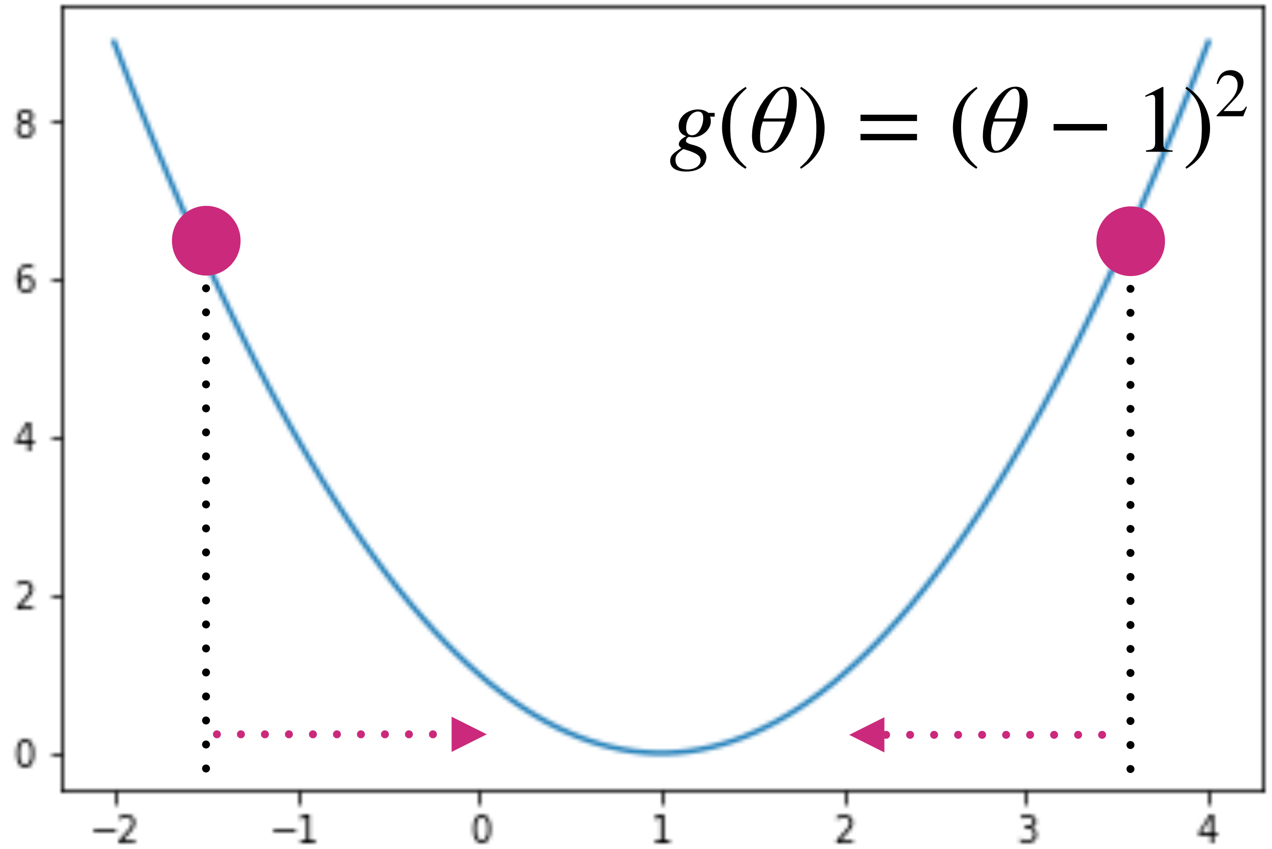
- Goal: Minimize Cost function

$$-\sum_{i=1}^{m} \left[y^{(i)} \log\left(\hat{y}^{(i)}\right) + \left(1 - y^{(i)}\right) \log\left(1 - \hat{y}^{(i)}\right)\right]$$



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

Logistic Regression: Algorithm

- Gradient descent (梯度下降法)

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

- Algorithm

$$\theta_j := \theta_j + \eta \sum_{i=1}^{m} \left(y^{(i)} - \hat{y}^{(i)} \right) x_j^{(i)}$$

Logistic Regression: regularization

- Goal: Minimize Cost function

$$\sum_{i=1}^{m}\left[-y^{(i)}\log\left(\hat{y}^{(i)}\right)-\left(1-y^{(i)}\right)\log\left(1-\hat{y}^{(i)}\right)\right]+\lambda\sum_{i=1}^{n}\theta_i^2$$

λ ：regularization parameter (正規化參數)

Iris Data Set (鳶尾花卉數據集)

▪UCI

https://archive.ics.uci.edu/ml/datasets/Iris

https://www.kaggle.com/uciml/iris

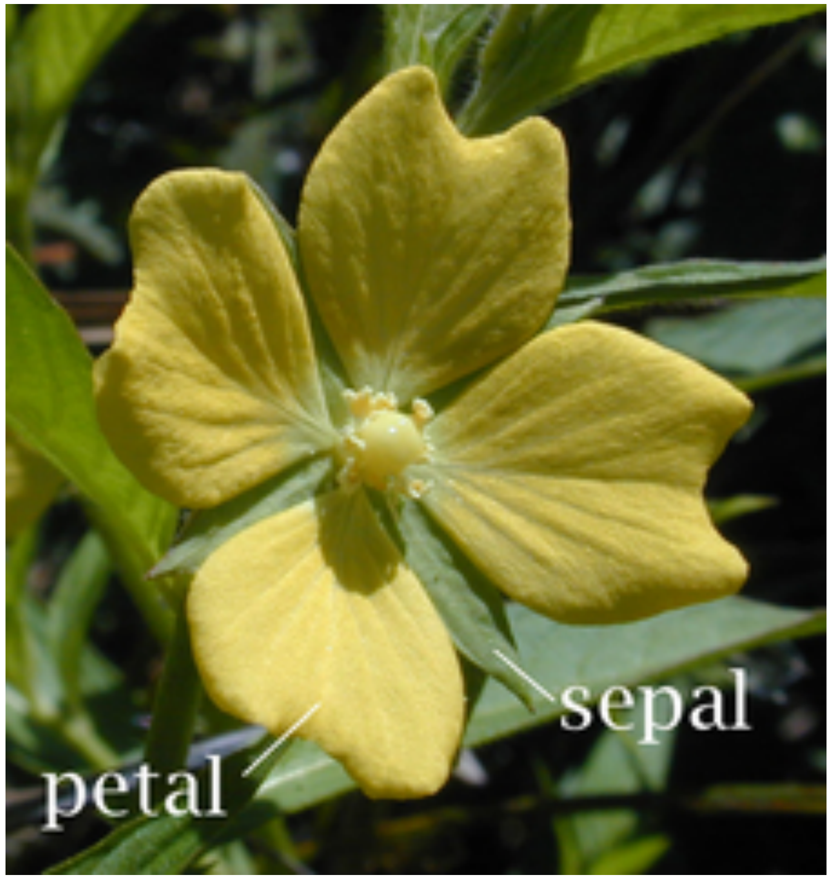
setosa

- 150個樣本，都屬於鳶尾屬下的三個亞屬，分別是山鳶尾、變色鳶尾和維吉尼亞鳶尾。

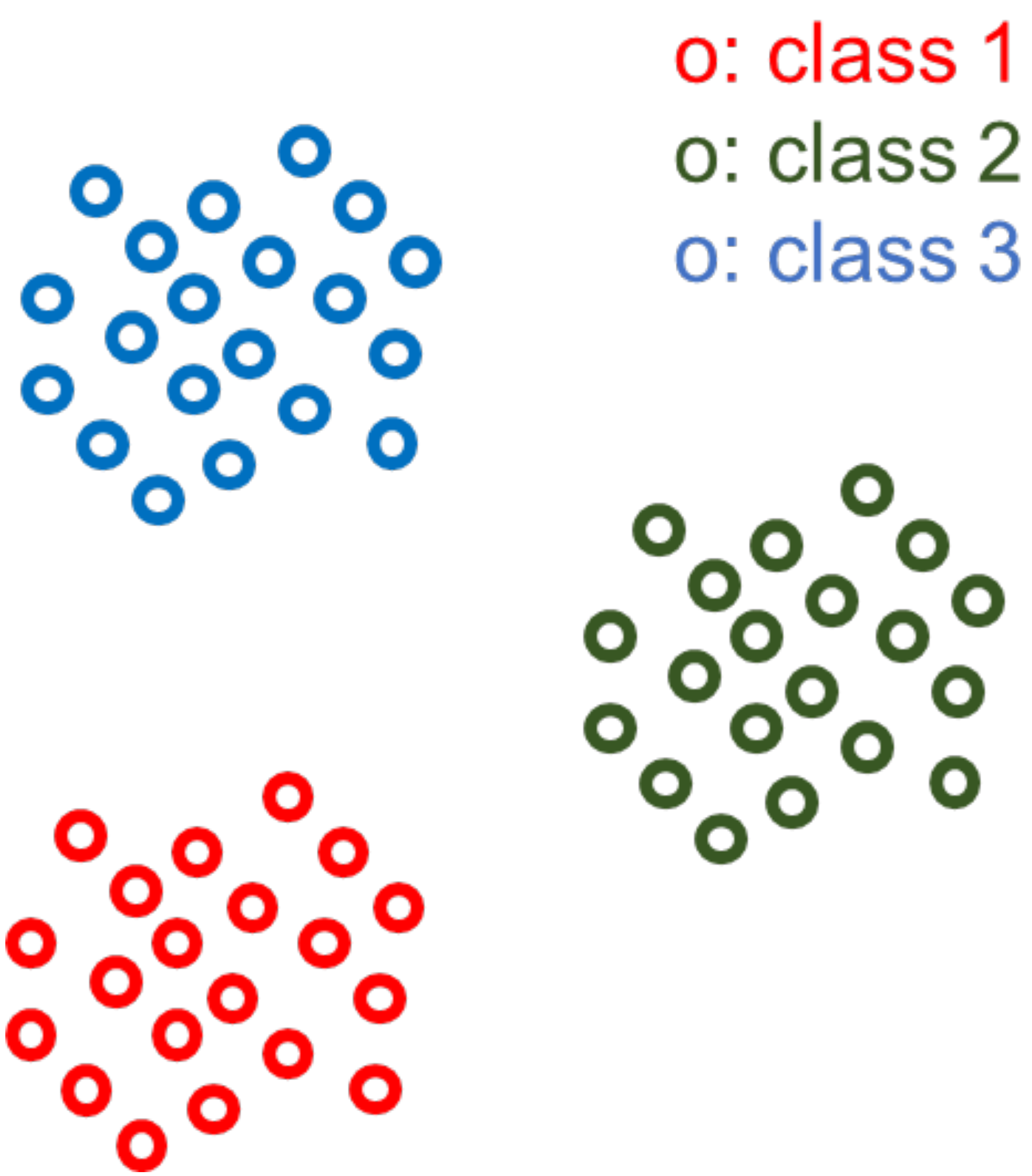
  versicolor virginica

- 四個特徵: 花萼和花瓣的長度和寬度

  Sepal Petal



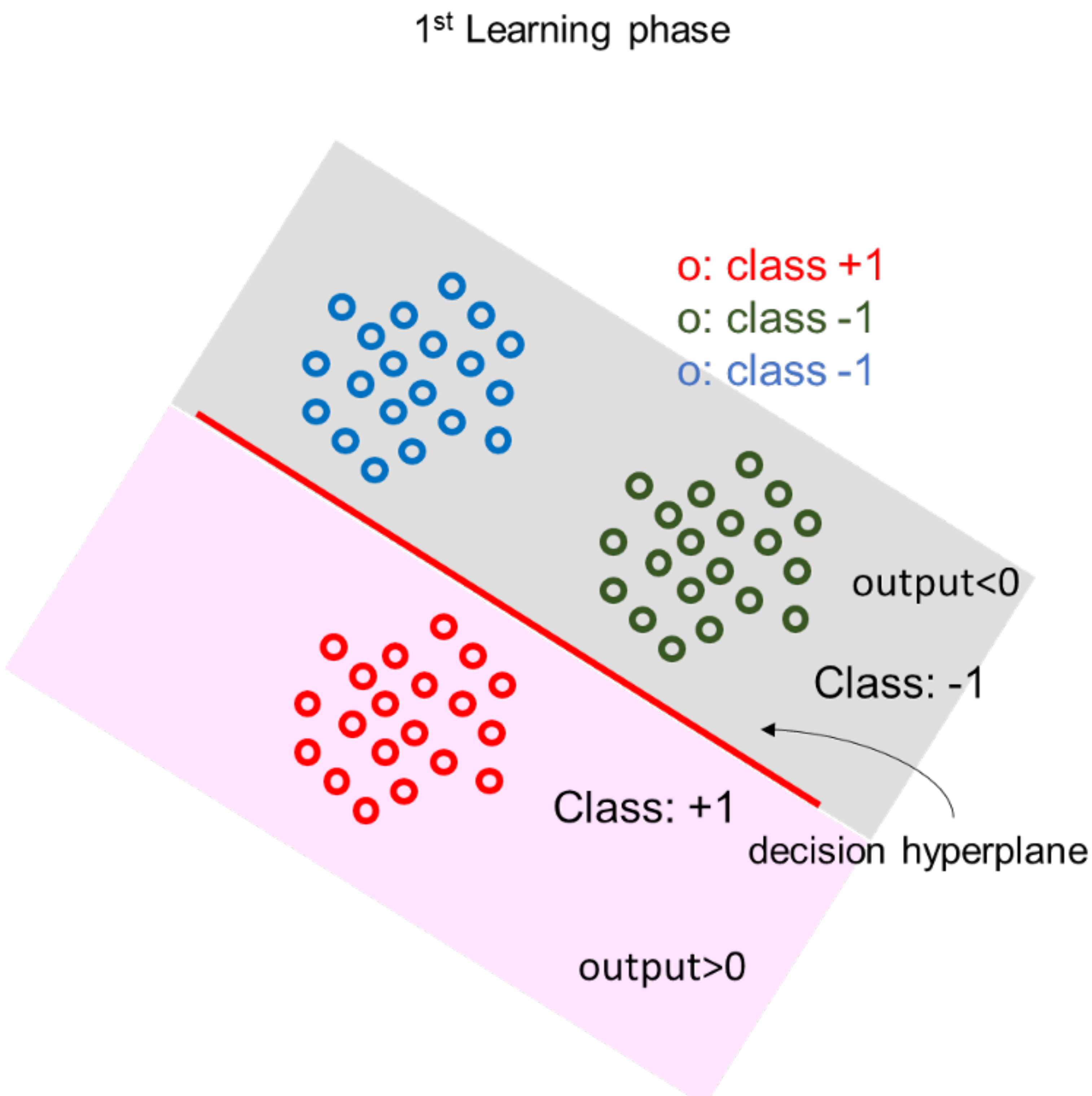
Multiple Classification



Source: https://medium.com/@chih.sheng.huang821/機器學習-如何在多類別分類問題上使用用二元分類器進行分類-multiclass-strategy-for-binary-classifier-b4e5017202ff

Multiple Classification

OvR
(One-vs.-Rest)



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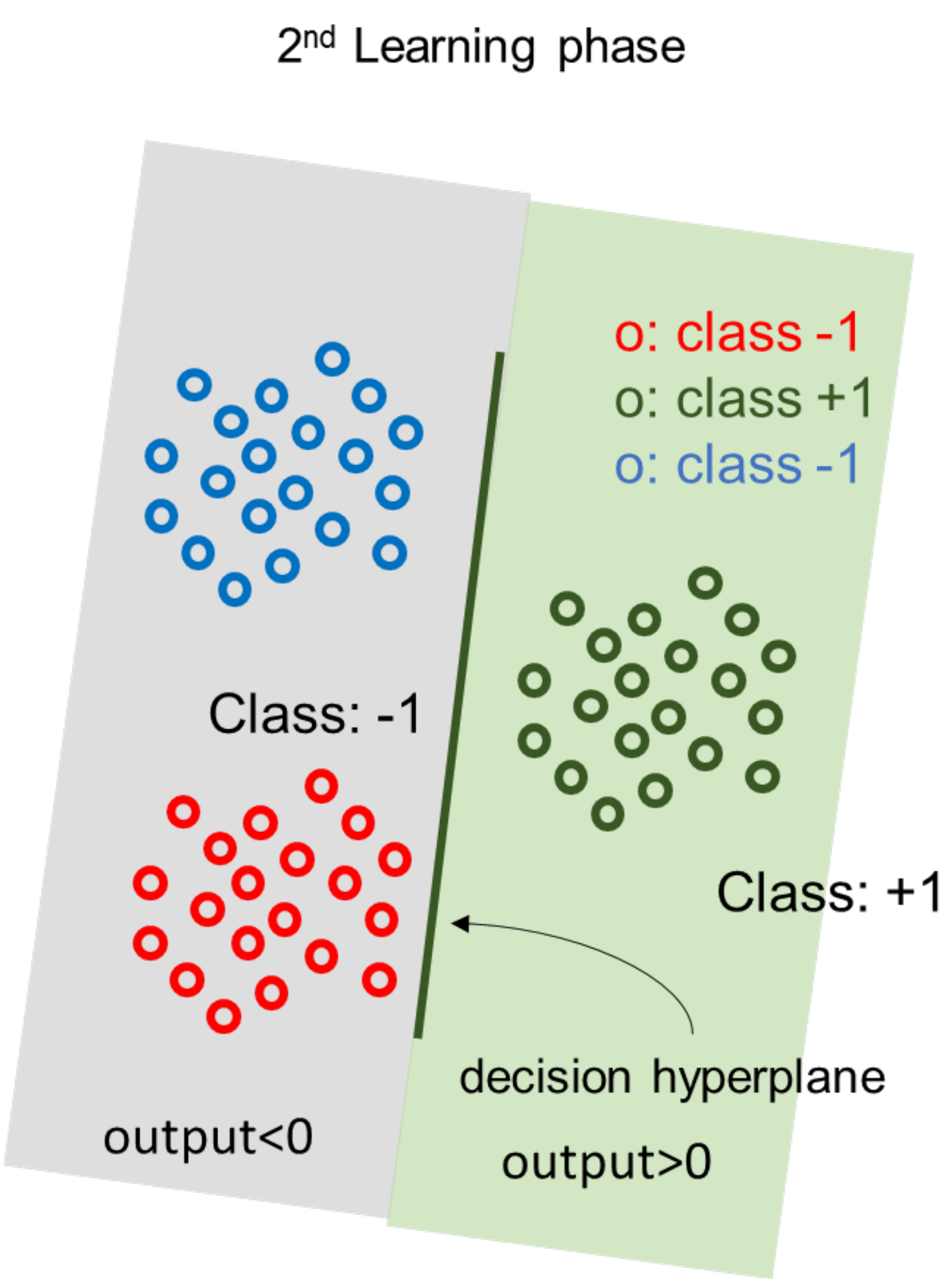
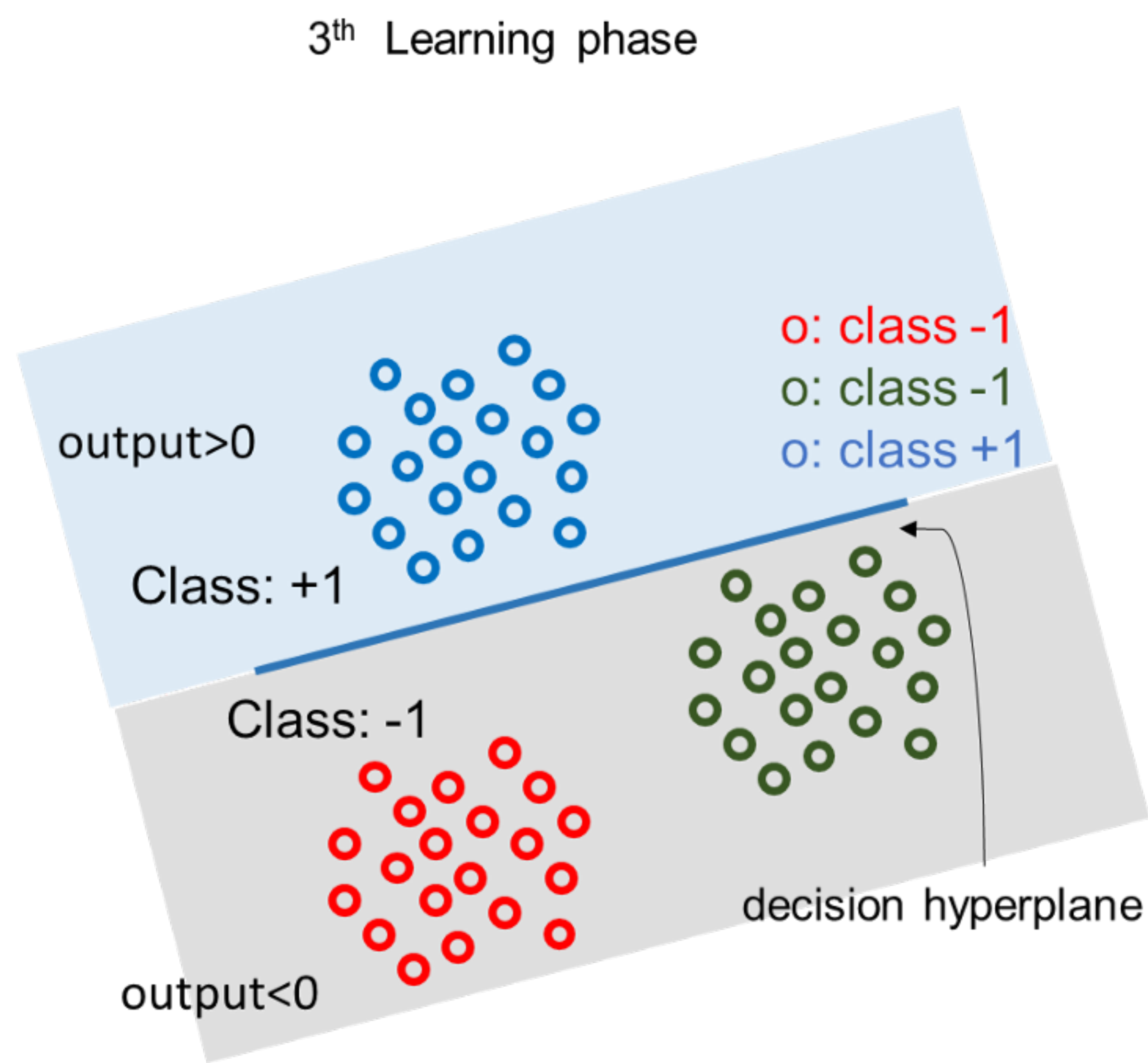
Multiple Classification





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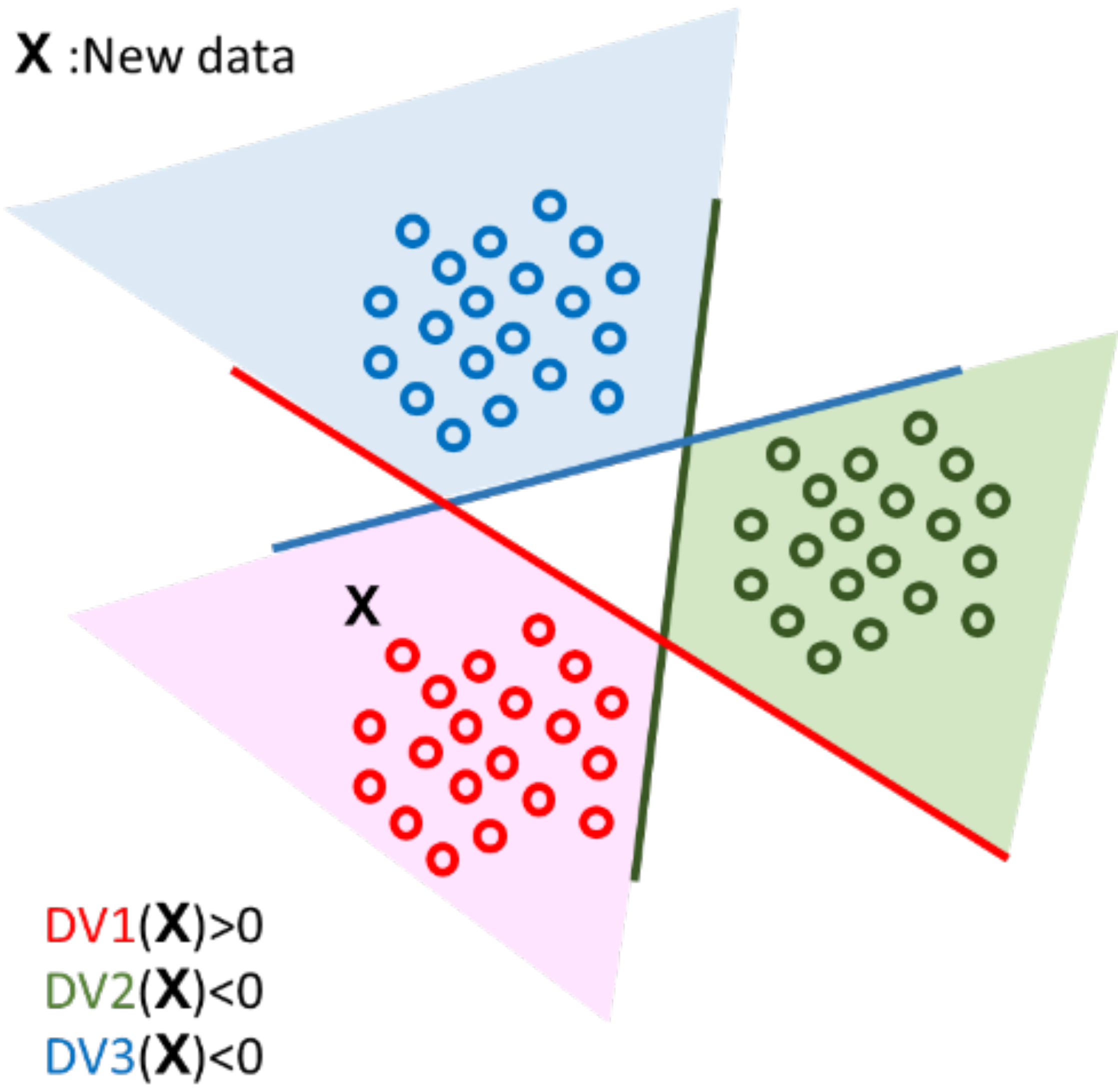
Multiple Classification

Case 1
If the new data locates at non-overlap area
(only one positive area)



This new data would be classified to class 1.

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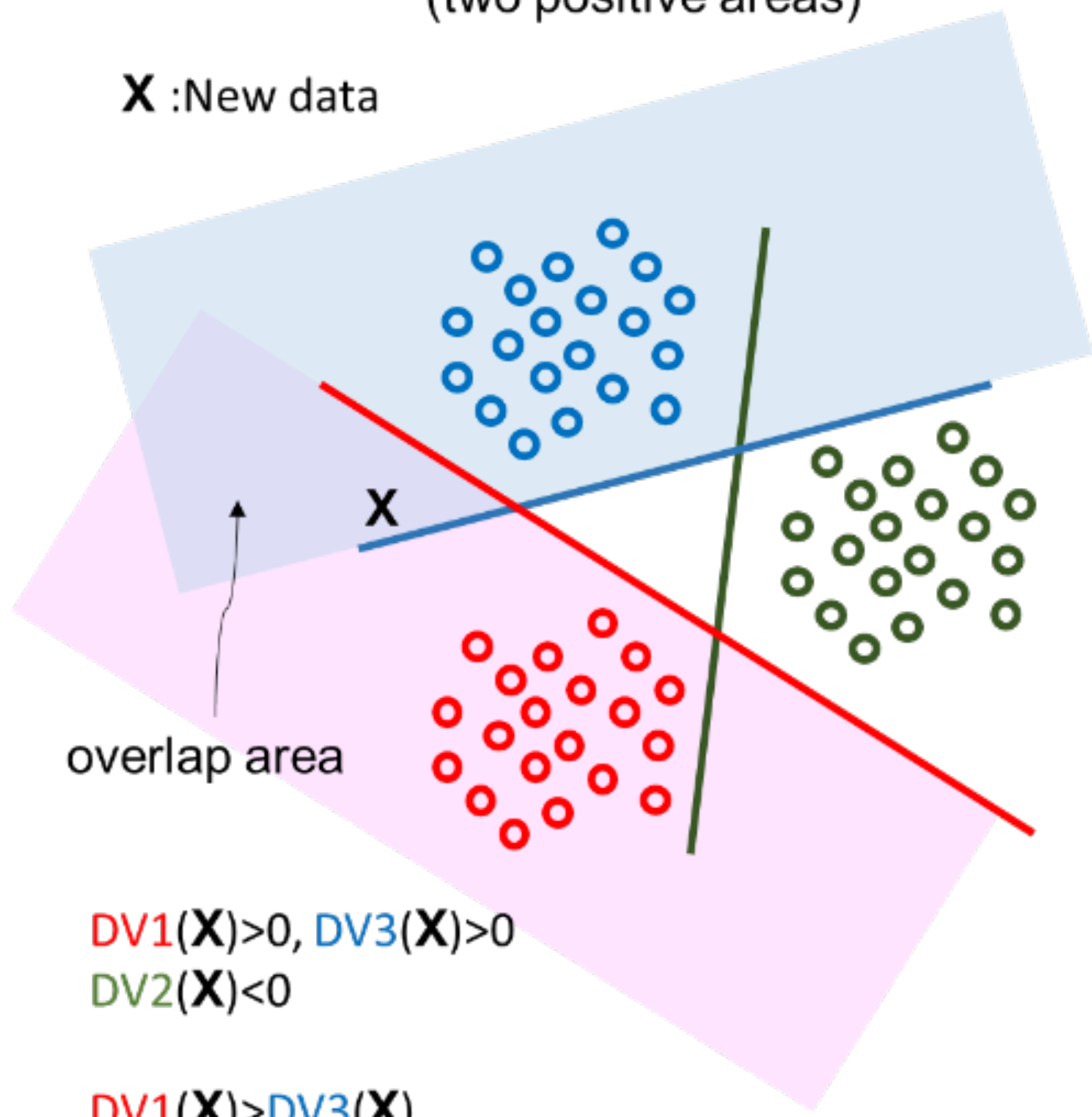
Multiple Classification

Case 2
If the new data locates at overlap area
(two positive areas)



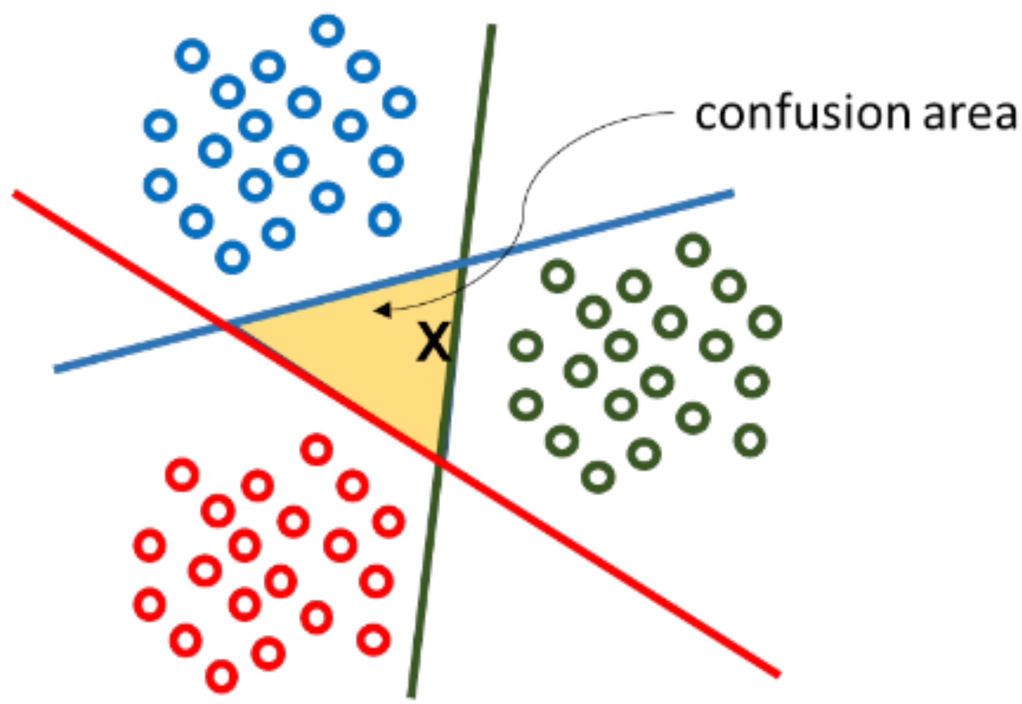
This new data would be classified to class 1.

Source: https://medium.com/@chih.sheng.huang821/機器學習-如何在多類別分類問題上使用用二元分類器進行分類-multiclass-strategy-for-binary-classifier-b4e5017202ff

Multiple Classification

Case 3
If the new data locates at confusion area
(three negative areas)

X :New data



DV1(**X**)<0, DV2(**X**)<0, DV3(**X**)<0

DV2(**X**)>DV3(**X**) > DV1(**X**)

This new data would be classified to class 2.

Source: https://medium.com/@chih.sheng.huang821/機器學習-如何在多類別分類問題上使用用二元分類器進行分類-multiclass-strategy-for-binary-classifier-b4e5017202ff

Python

- 載入 Iris data set

(1/6)

```
import pandas as pd
import numpy as np
from sklearn.datasets import load_iris

iris = load_iris()

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

data = pd.concat([feature, target], axis = 1)
df = data[data['class'] != 2]
```

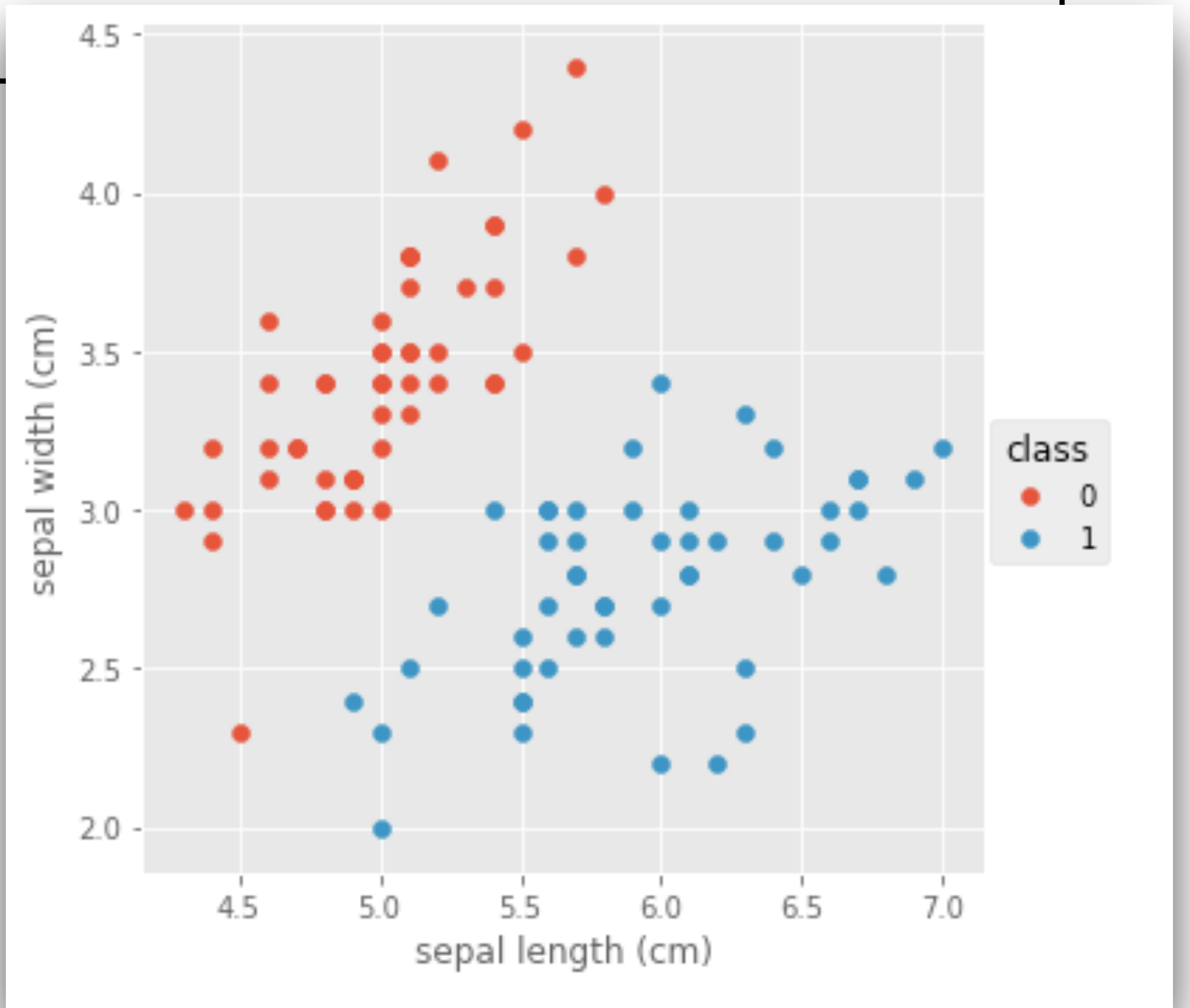
只考慮類別為 0 和 1 的資料

Python

- 畫散佈圖

(2/6)

```
import matplotlib.pyplot as plt
import seaborn as sns
plt.style.use('ggplot') # make plots look better
g = sns.FacetGrid(df, hue="class", size=5)
g.map(plt.scatter, "sepal length (cm)", "sepal width (cm)")
g.add_legend()
```



Python

- 標準化

```
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import StandardScaler

X = df.iloc[:,:2].values
y = df.iloc[:,4].values


sc = StandardScaler()
sc.fit(X)
X_std = sc.transform(X)
```

(3/6)

Python

- 訓練 logistic regression 模型

(4/6)

```
from sklearn.linear_model import LogisticRegression
from matplotlib.colors import ListedColormap

lr = LogisticRegression(C=100.0, random_state=1)
lr.fit(X_std, y)


print(lr.coef_)
print(lr.intercept_ )
```

$C = \frac{1}{\lambda}$

Output $\overrightarrow{\theta}$

Python

- 定義決策區域 (decision region)

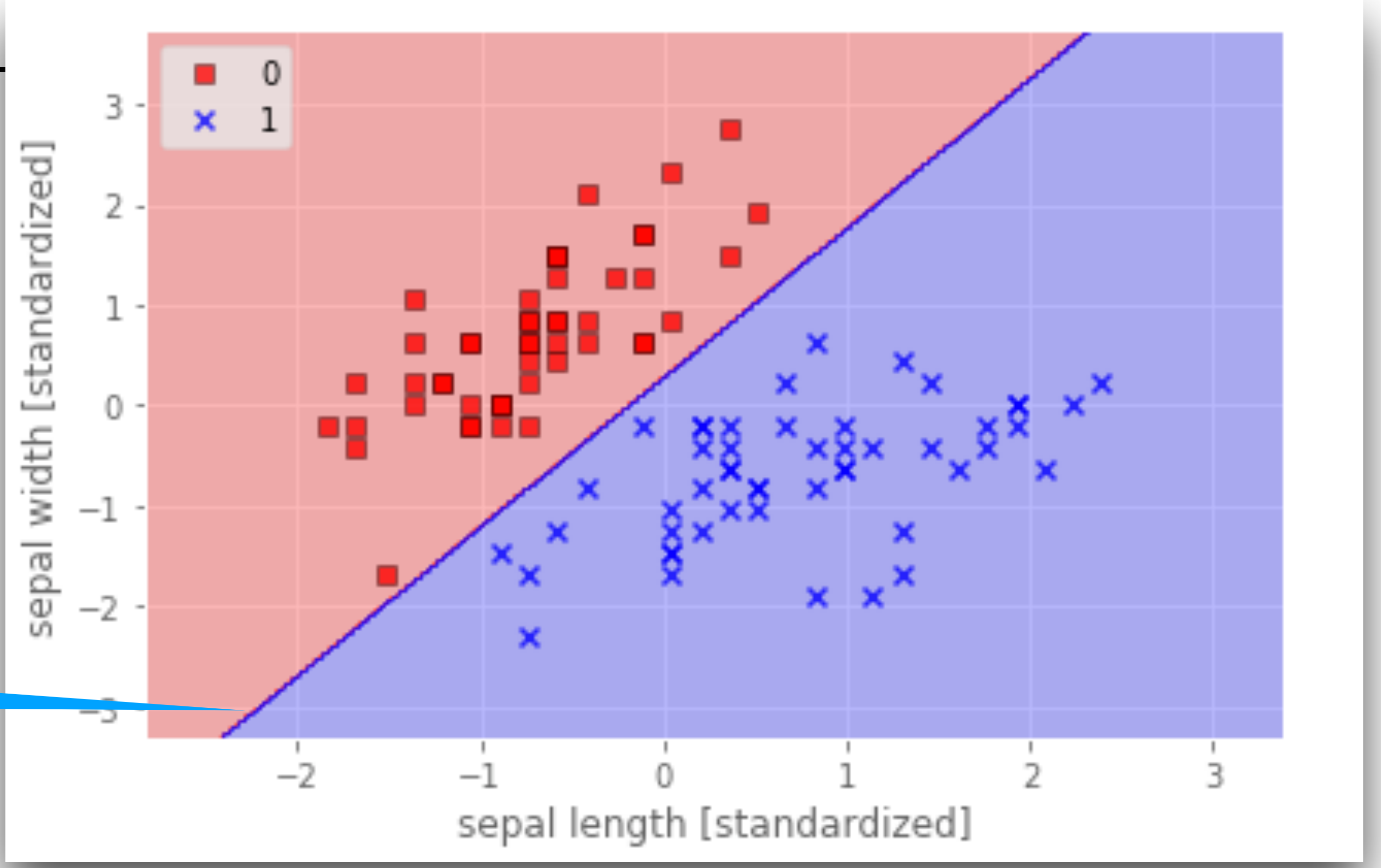
```python
def plot_decision_regions(X, y, classifier, test_idx=None, resolution=0.02):

    # setup marker generator and color map
    markers = ('s', 'x', 'o', '^', 'v')
    colors = ('red', 'blue', 'lightgreen', 'gray', 'cyan')
    cmap = ListedColormap(colors[:len(np.unique(y))])

    # plot the decision surface
    x1_min, x1_max = X[:, 0].min() - 1, X[:, 0].max() + 1
    x2_min, x2_max = X[:, 1].min() - 1, X[:, 1].max() + 1
    xx1, xx2 = np.meshgrid(np.arange(x1_min, x1_max, resolution),
                           np.arange(x2_min, x2_max, resolution))
    Z = classifier.predict(np.array([xx1.ravel(), xx2.ravel()]).T)
    Z = Z.reshape(xx1.shape)
    plt.contourf(xx1, xx2, Z, alpha=0.3, cmap=cmap)
    plt.xlim(xx1.min(), xx1.max())
    plt.ylim(xx2.min(), xx2.max())

    for idx, cl in enumerate(np.unique(y)):
        plt.scatter(x=X[y == cl, 0],
                    y=X[y == cl, 1],
                    alpha=0.8,
                    c=colors[idx],
                    marker=markers[idx],
                    label=cl,
                    edgecolor='black')

    # highlight test samples
    if test_idx:
        # plot all samples
        X_test, y_test = X[test_idx, :], y[test_idx]

        plt.scatter(X_test[:, 0],
                    X_test[:, 1],
                    c='',
                    edgecolor='black',
                    alpha=1.0,
                    linewidth=1,
                    marker='o',
                    s=100,
                    label='test set')
```

Python

- 畫出目前模型的決策邊界

(6/6)

```
plot_decision_regions(X_std, y, classifier=lr)
plt.xlabel('sepal length [standardized]')
plt.ylabel('sepal width [standardized]')
plt.legend(loc='upper left')
plt.tight_layout()
#plt.savefig('images.png', dpi=300)
plt.show()
```



決策邊界的方程式為何？