

# Logistic Regression

Kanokkorn Pimcharoen

# Speaker



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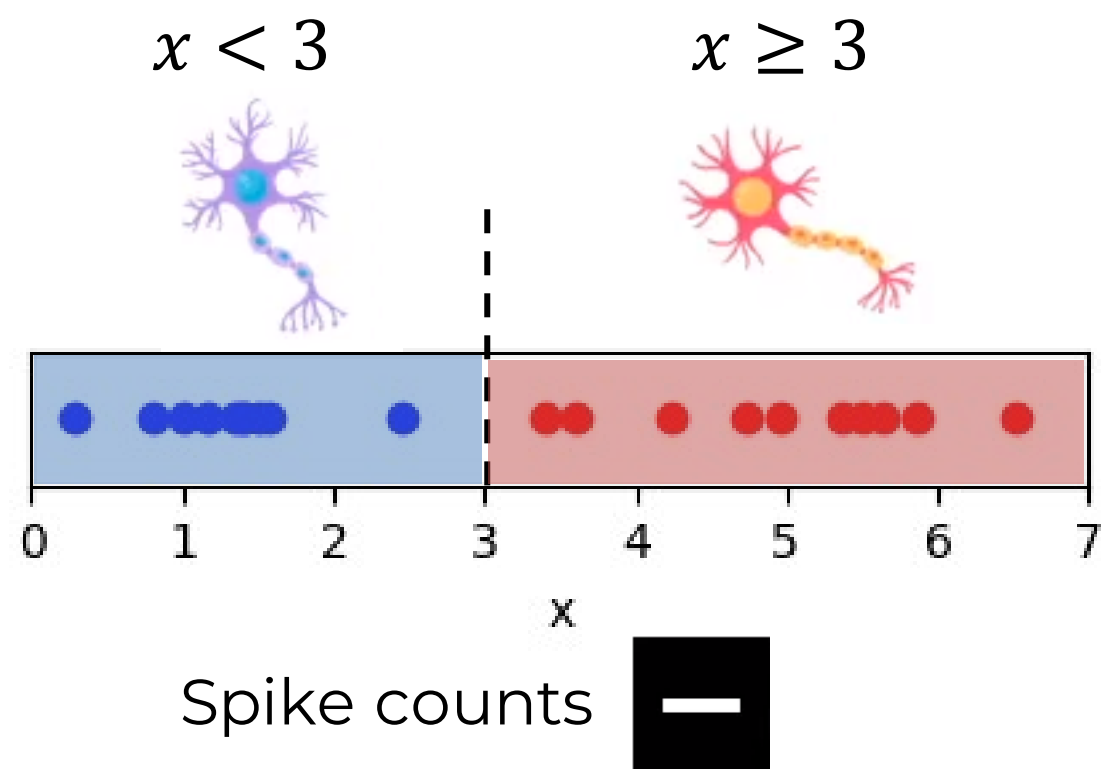
Researcher, Computational Physics and AI

Nanoinformatics and Artificial Intelligence

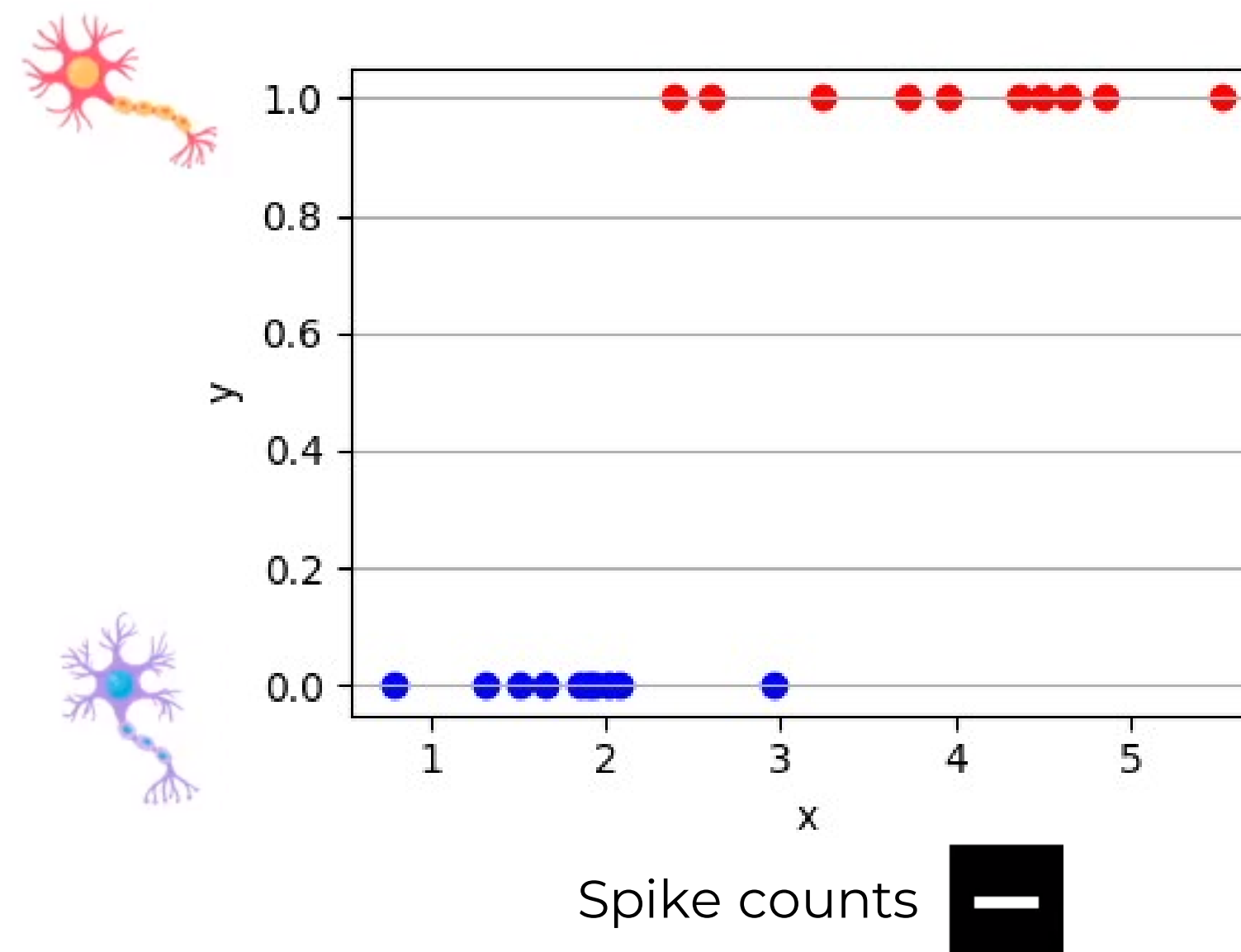
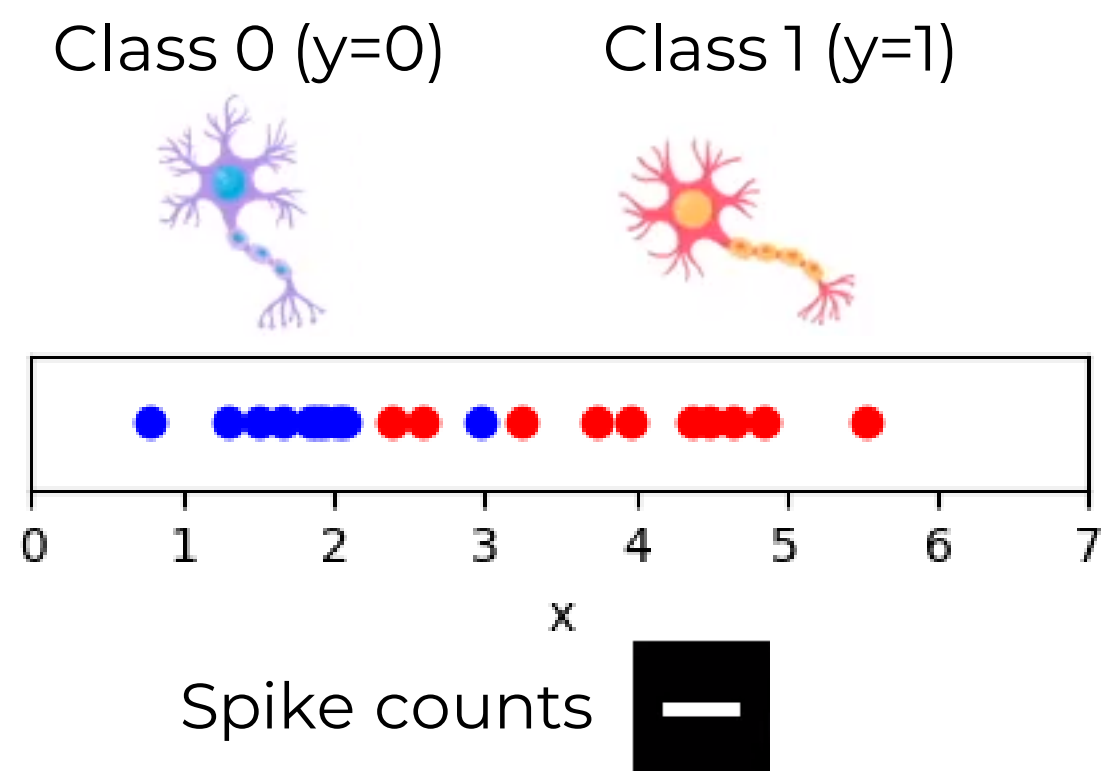
Research Team, NANOTEC, NSTDA

Hobbies: Travel and Coffee

# Classification Problem

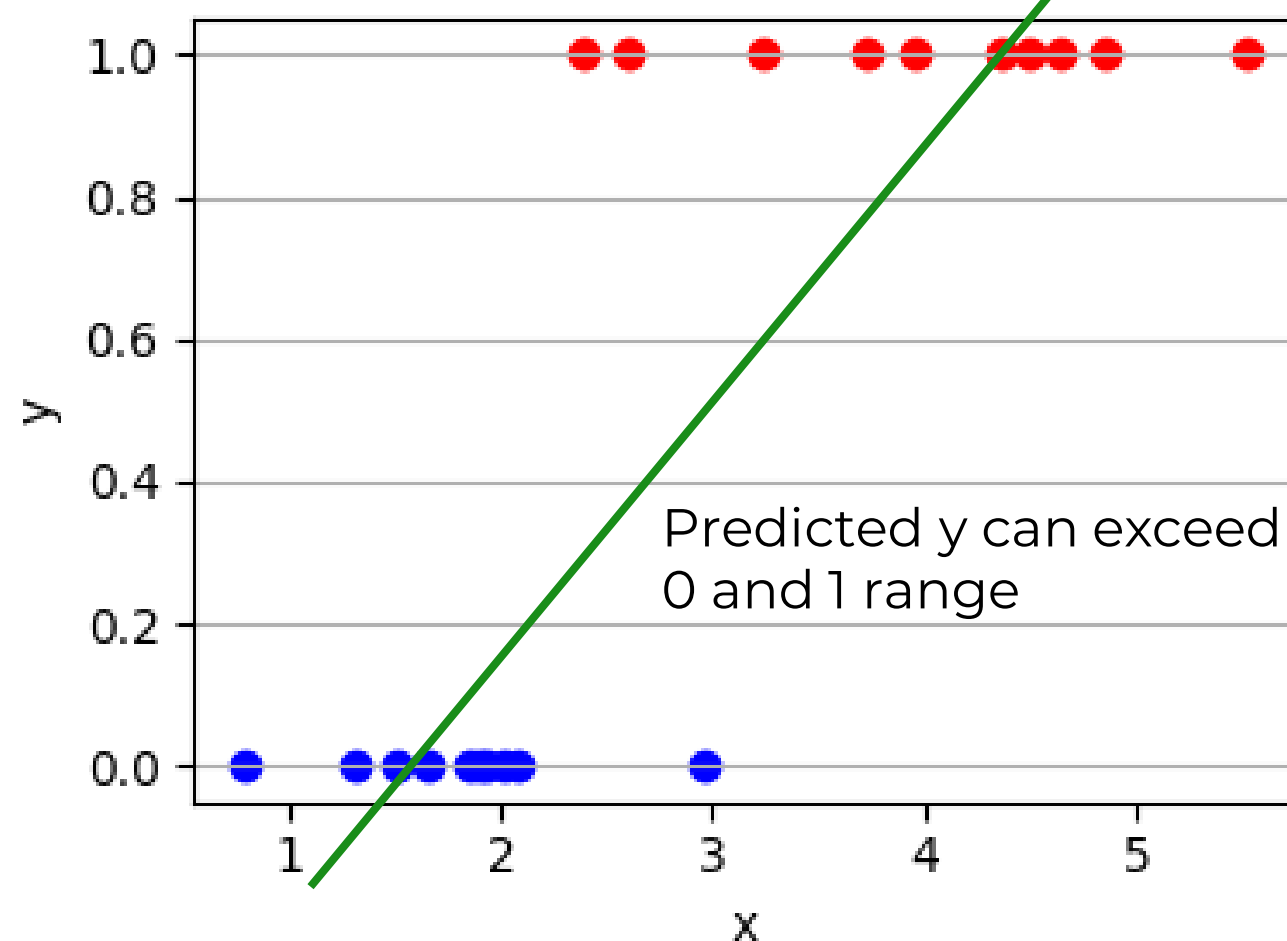


# Classification Problem



# Generalized Linear Models

## Linear Regression

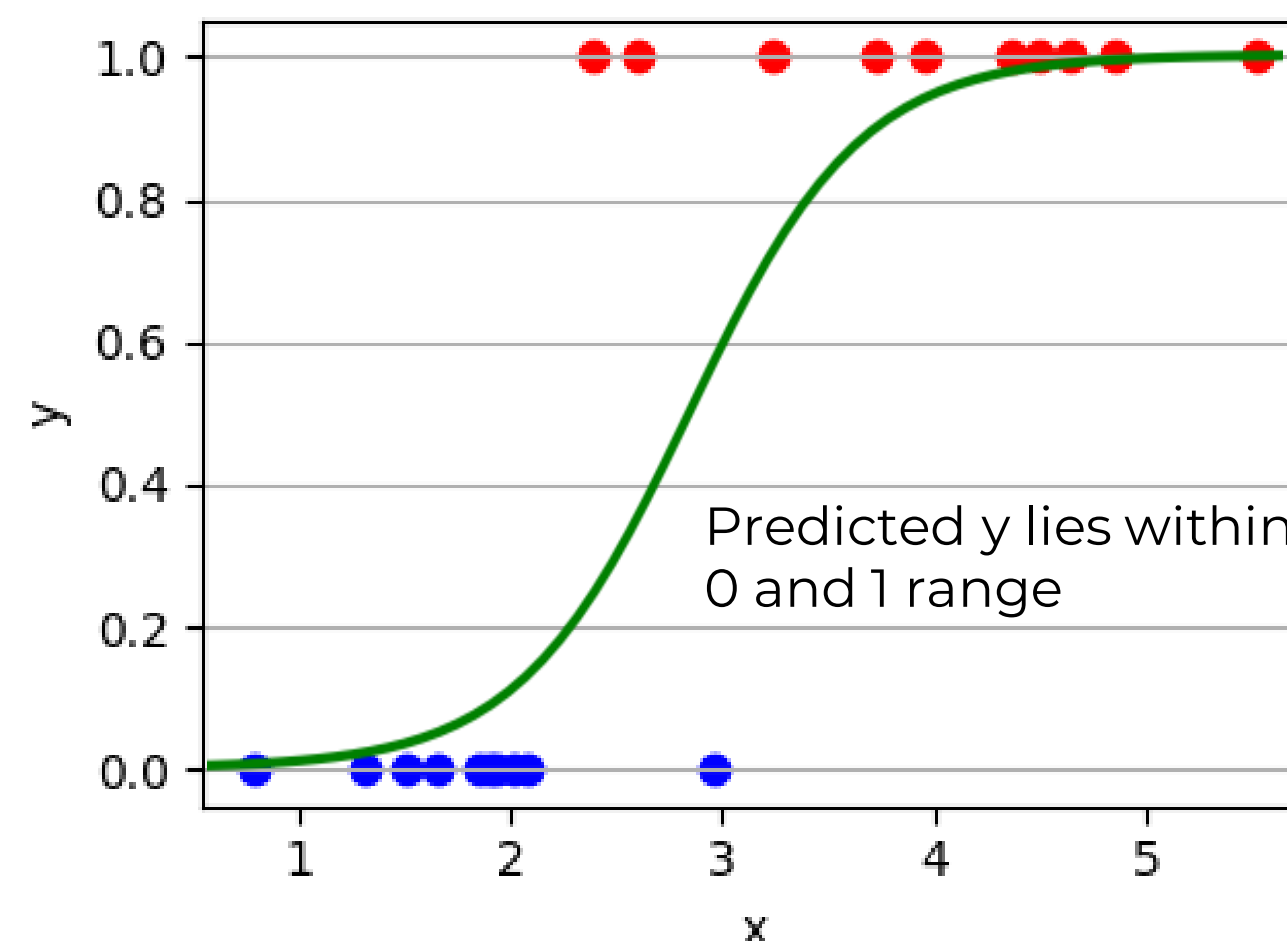


$$y = w_0 + w_1 x$$

$w_1$ : slope

$w_0$ : y-intercept

## Logistic Regression

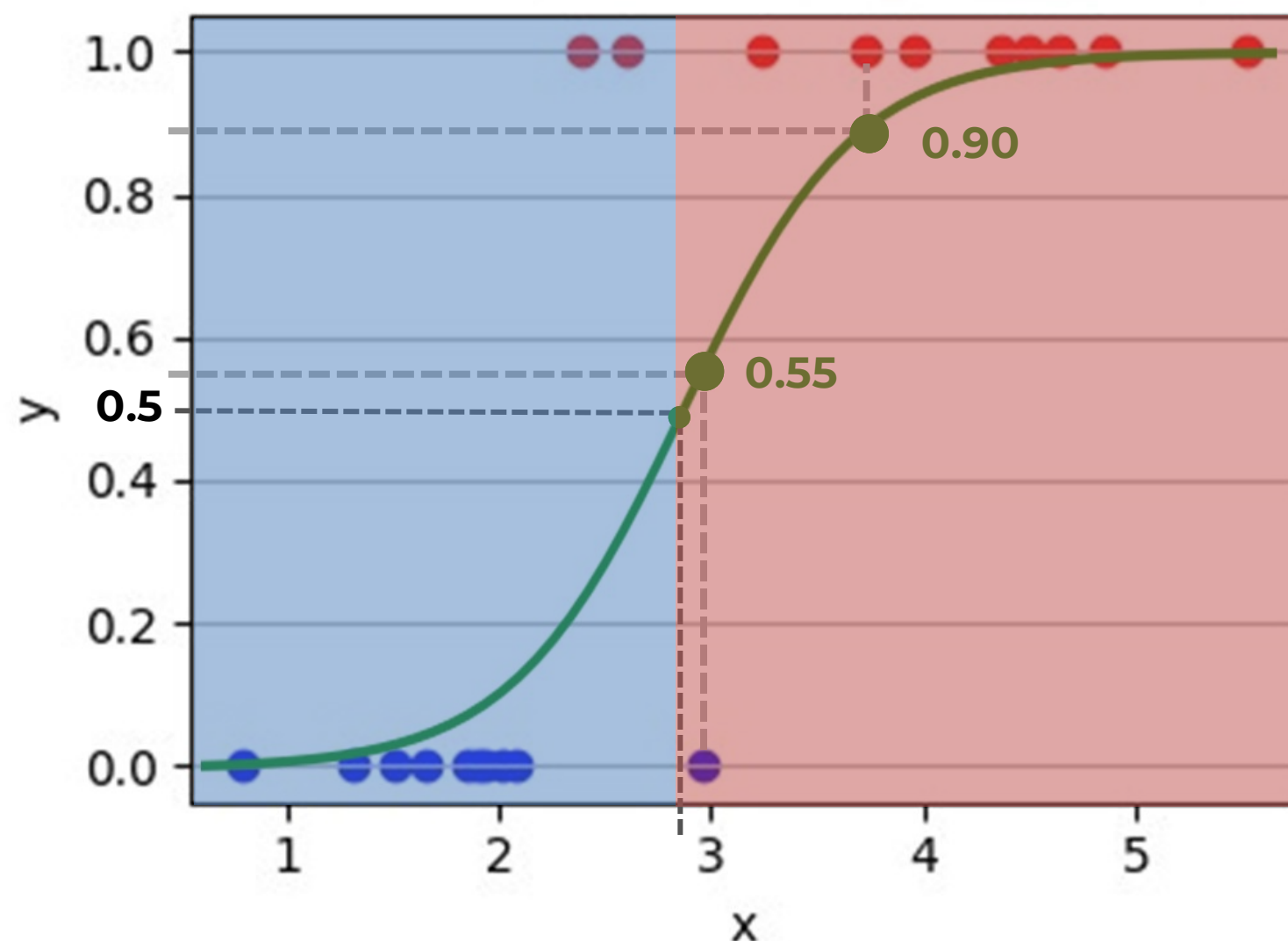


$$y = \frac{1}{1 + e^{-(w_0 + w_1 x)}} \quad \text{or} \quad \log\left(\frac{y}{1-y}\right) = w_0 + w_1 x$$

*Probability*

*log - odds*

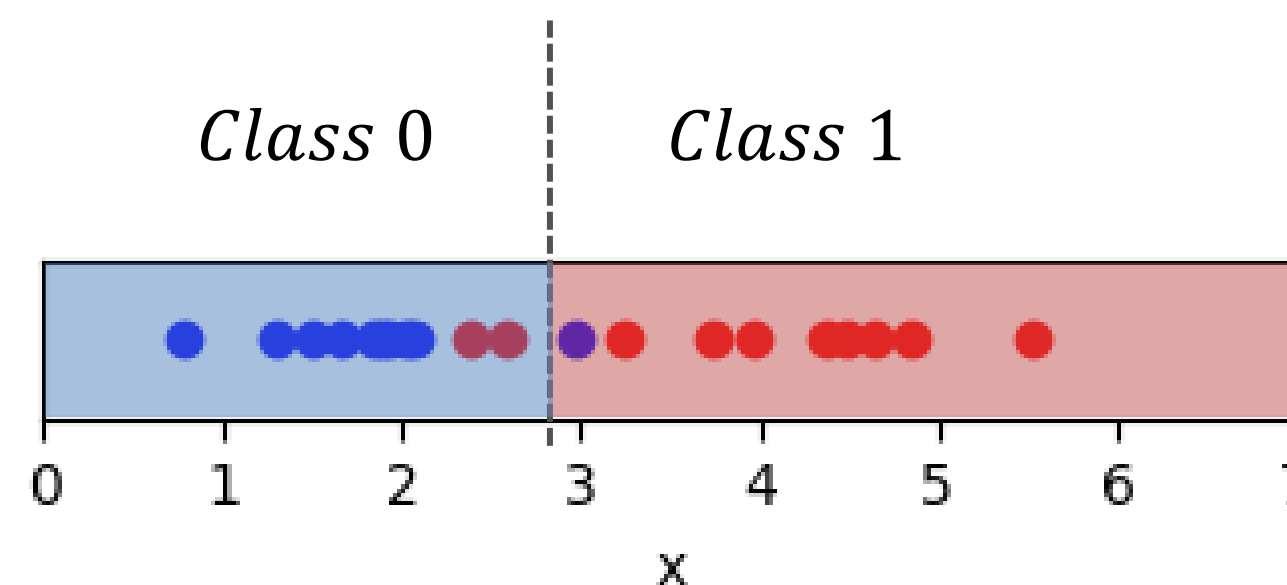
# Logistic Regression



$y = \text{Probability of class 1}$

$y \geq 0.5 \rightarrow \text{Class 1} \leftarrow x \geq 2.8$

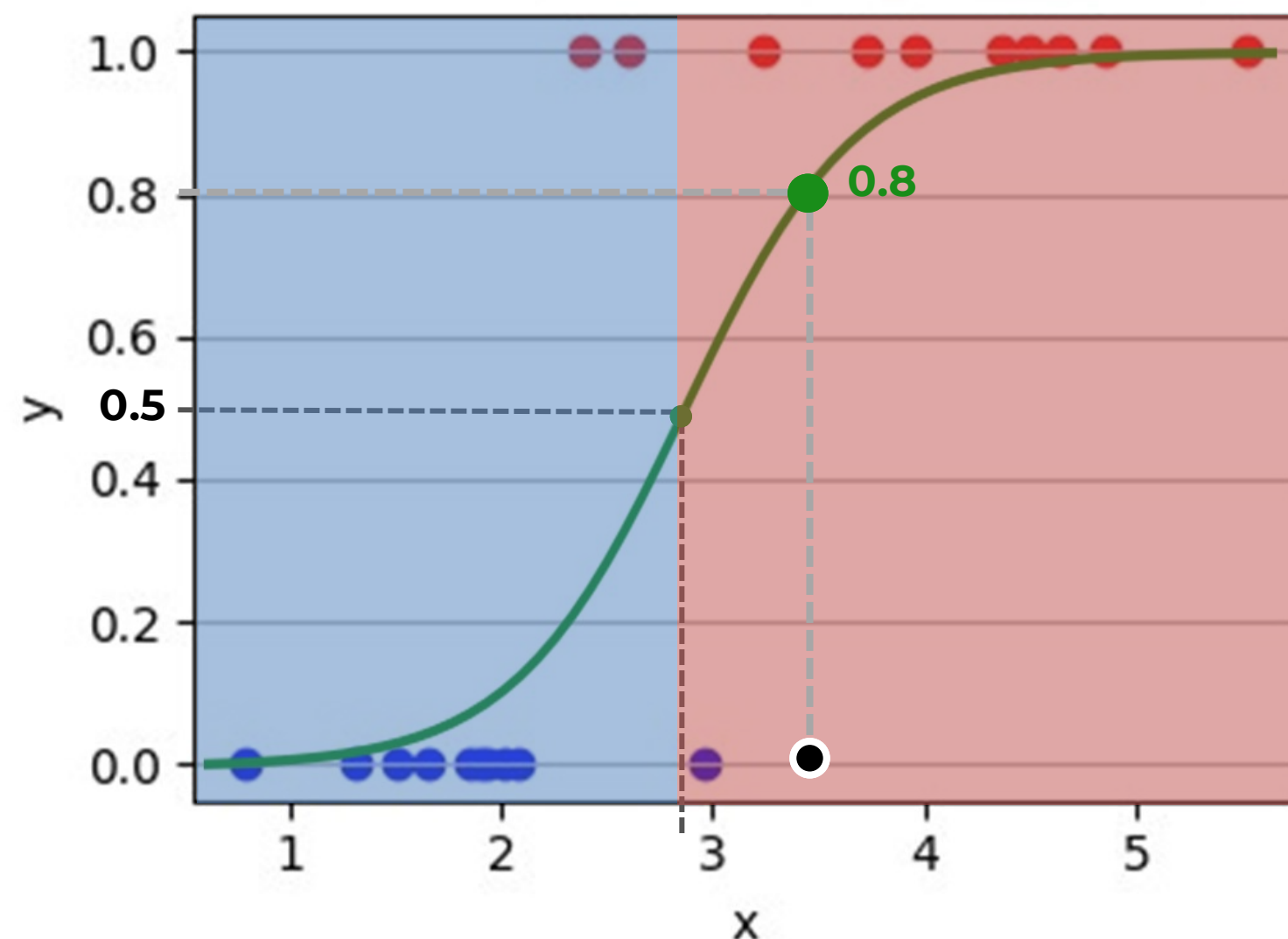
$y < 0.5 \rightarrow \text{Class 0} \leftarrow x < 2.8$



$$y = \frac{1}{1 + e^{-(w_0 + w_1 x)}} \quad \text{or} \quad \log\left(\frac{y}{1-y}\right) = w_0 + w_1 x$$

Decision Boundary

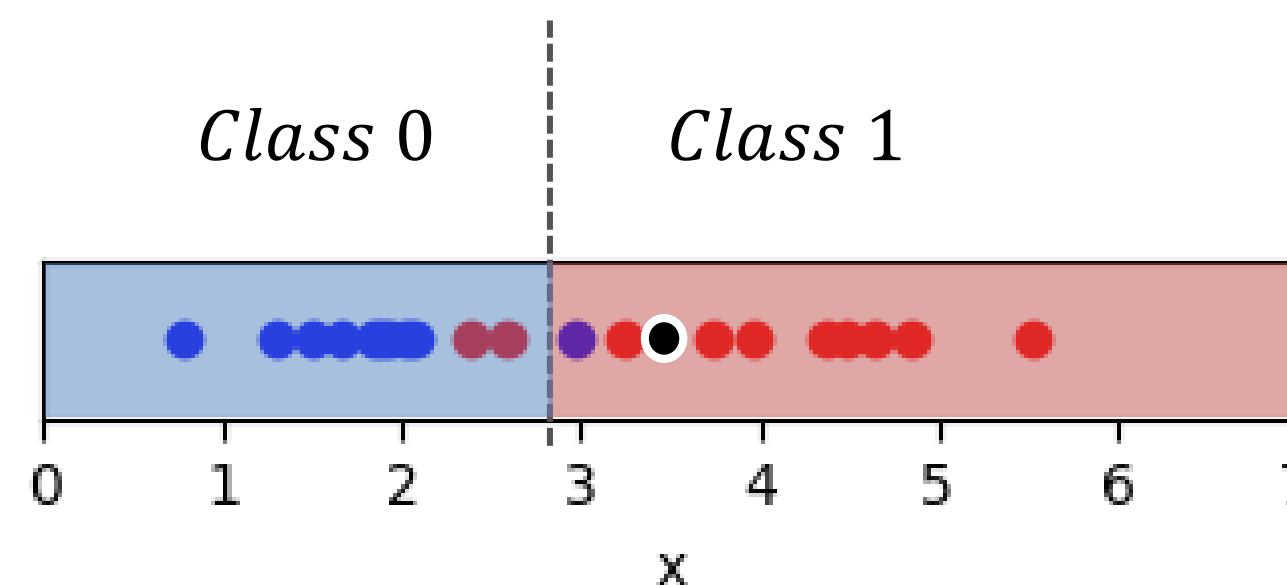
# Logistic Regression



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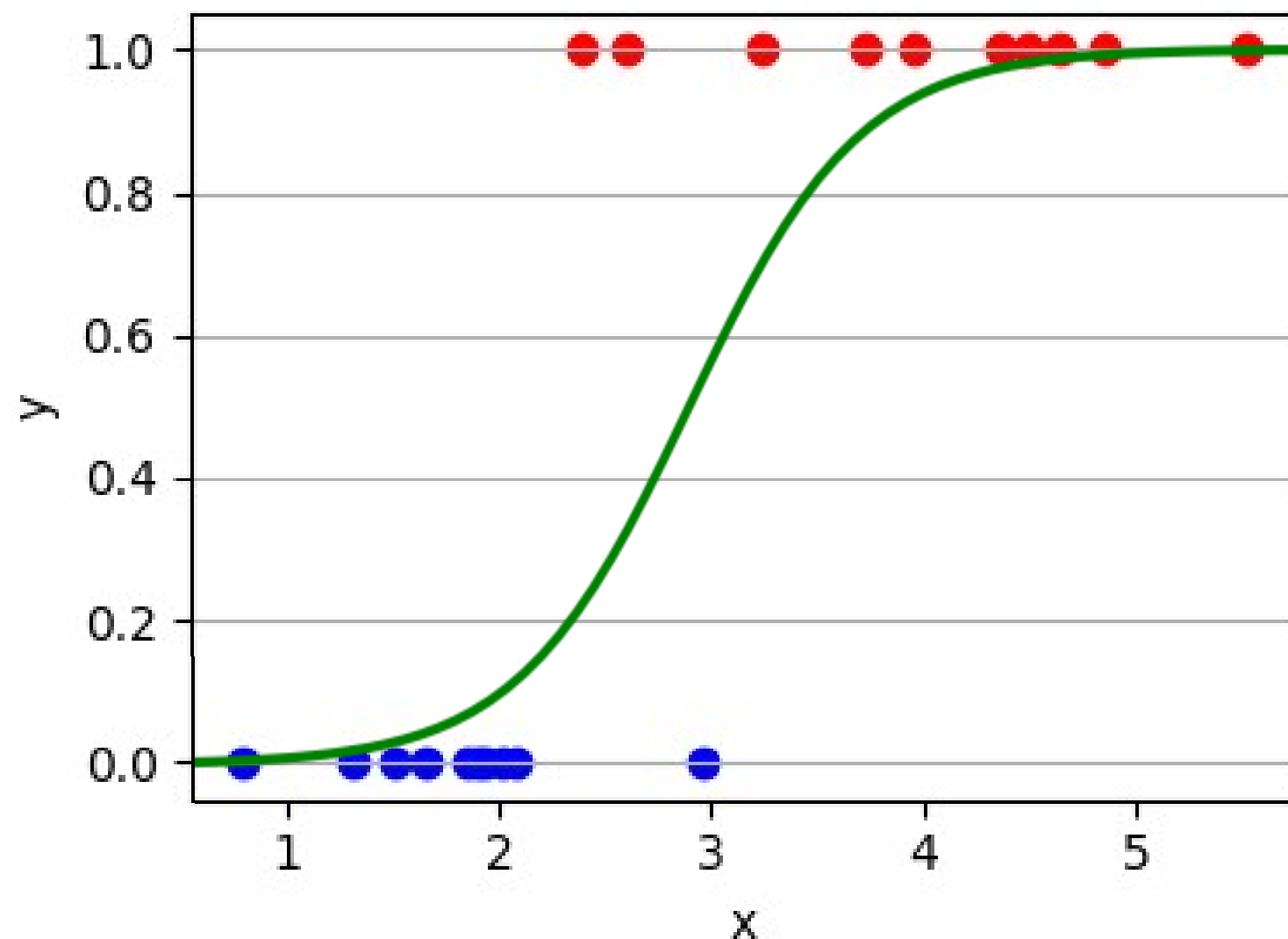
$y < 0.5 \rightarrow \text{Class 0} \leftarrow x < 2.8$



$$y = \frac{1}{1 + e^{-(w_0 + w_1 x)}} \quad \text{or} \quad \log\left(\frac{y}{1-y}\right) = w_0 + w_1 x$$

Decision Boundary

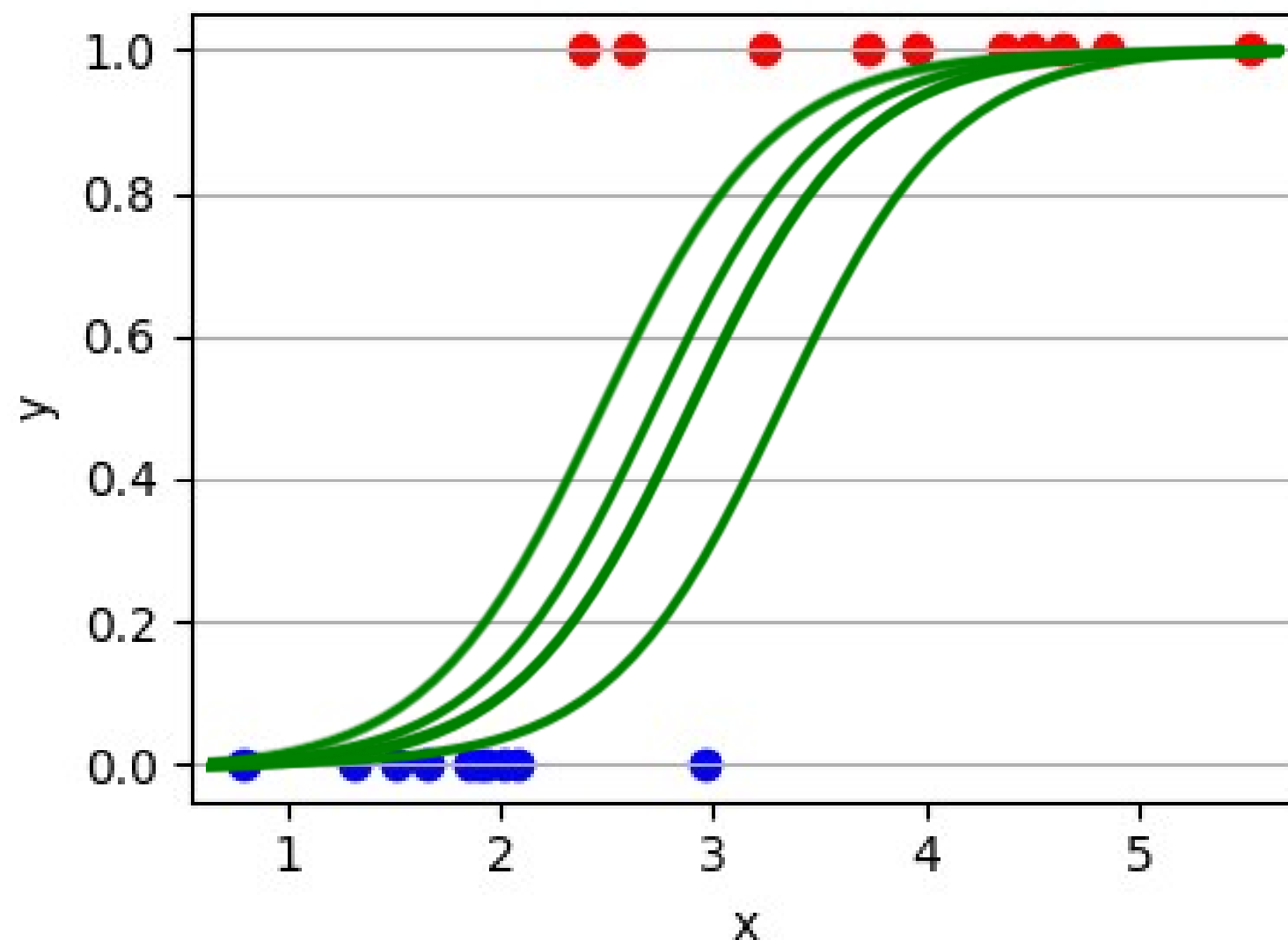
# Logistic Regression: Optional



$$y = \frac{1}{1 + e^{-(w_0 + w_1 x)}} \quad \text{or} \quad \log\left(\frac{y}{1-y}\right) = w_0 + w_1 x$$



# Logistic Regression: Optional



$$y = \frac{1}{1 + e^{-(w_0 + w_1 x)}} \quad \text{or} \quad \log\left(\frac{y}{1-y}\right) = w_0 + w_1 x$$

## Maximum Likelihood Estimation

$$\mathcal{L}(x) = \prod_i \left[ \frac{1}{1 + e^{-(w_0 + w_1 x_i)}} \right] \times \prod_j \left[ 1 - \frac{1}{1 + e^{-(w_0 + w_1 x_j)}} \right]$$

To obtain the values of  $w_0$  and  $w_1$  that maximize  $\mathcal{L}(x)$ , an iterative solver is applied.

When the difference of  $\mathcal{L}(x)$  between two consecutive iterations becomes lower than **tolerance**, the solver is converged and yielded the optimal parameters  $w_0$  and  $w_1$ .

# sklearn.linear\_model.LogisticRegression

```
class sklearn.linear_model.LogisticRegression(penalty='l2', *, dual=False, tol=0.0001, C=1.0,
fit_intercept=True, intercept_scaling=1, class_weight=None, random_state=None, solver='lbfgs', max_iter=100,
multi_class='auto', verbose=0, warm_start=False, n_jobs=None, l1_ratio=None) \[source\]
```

## Parameters:

**solver** : {'lbfgs', 'liblinear', 'newton-cg', 'newton-cholesky', 'sag', 'saga'}, default='lbfgs'

**'lbfgs'** :

- Small-to-medium dataset
- Support L2 regularization only

**'liblinear'** :

- Small dataset
- Support both L1 and L2 regularizations

**'newton-cg'** :

- Large dataset
- The computation time grows with increasing number of features
- Support L2 regularization only

**tol** : float, default=1e-4

Tolerance for stopping criteria.

**max\_iter** : int, default=100

Maximum number of iterations taken for the solvers to converge.

# sklearn.linear\_model.LogisticRegression

```
class sklearn.linear_model.LogisticRegression(penalty='l2', *, dual=False, tol=0.0001, C=1.0,
fit_intercept=True, intercept_scaling=1, class_weight=None, random_state=None, solver='lbfgs', max_iter=100,
multi_class='auto', verbose=0, warm_start=False, n_jobs=None, l1_ratio=None) \[source\]
```

## Parameters:

**penalty** : {'l1', 'l2', 'elasticnet', None}, default='l2'

Specify the norm of the penalty:

- **None**: no penalty is added;
- **'l2'**: add a L2 penalty term and it is the default choice;
- **'l1'**: add a L1 penalty term;
- **'elasticnet'**: both L1 and L2 penalty terms are added.

**C** : float, default=1.0

Inverse of regularization strength; must be a positive float.

$$\mathcal{L}(x, y) + \lambda R(w) \longrightarrow C \mathcal{L}(x, y) + R(w)$$

Setting C to high value will reduce the effect of regularization.

**Warning:** The choice of the algorithm depends on the penalty chosen. Supported penalties by solver:

- 'lbfgs' - ['l2', None]
- 'liblinear' - ['l1', 'l2']
- 'newton-cg' - ['l2', None]
- 'newton-cholesky' - ['l2', None]
- 'sag' - ['l2', None]
- 'saga' - ['elasticnet', 'l1', 'l2', None]

# sklearn.linear\_model.LogisticRegression

```
class sklearn.linear_model.LogisticRegression(penalty='l2', *, dual=False, tol=0.0001, C=1.0,
fit_intercept=True, intercept_scaling=1, class_weight=None, random_state=None, solver='lbfgs', max_iter=100,
multi_class='auto', verbose=0, warm_start=False, n_jobs=None, l1_ratio=None) \[source\]
```

## Attributes:

**classes\_ : ndarray of shape (n\_classes,)**

A list of class labels known to the classifier.

**coef\_ : ndarray of shape (1, n\_features) or (n\_classes, n\_features)**

Coefficient of the features in the decision function.

coef\_ is of shape (1, n\_features) when the given problem is binary. In particular, when multi\_class='multinomial', coef\_ corresponds to outcome 1 (True) and -coef\_ corresponds to outcome 0 (False).

**intercept\_ : ndarray of shape (1,) or (n\_classes,)**

Intercept (a.k.a. bias) added to the decision function.

If fit\_intercept is set to False, the intercept is set to zero. intercept\_ is of shape (1,) when the given problem is binary. In particular, when multi\_class='multinomial', intercept\_ corresponds to outcome 1 (True) and -intercept\_ corresponds to outcome 0 (False).

$$y = \frac{1}{1 + e^{-(w_0 + w_1x_1 + w_2x_2 + \dots + w_mx_m)}}$$

$w_1, w_2, \dots, w_m$

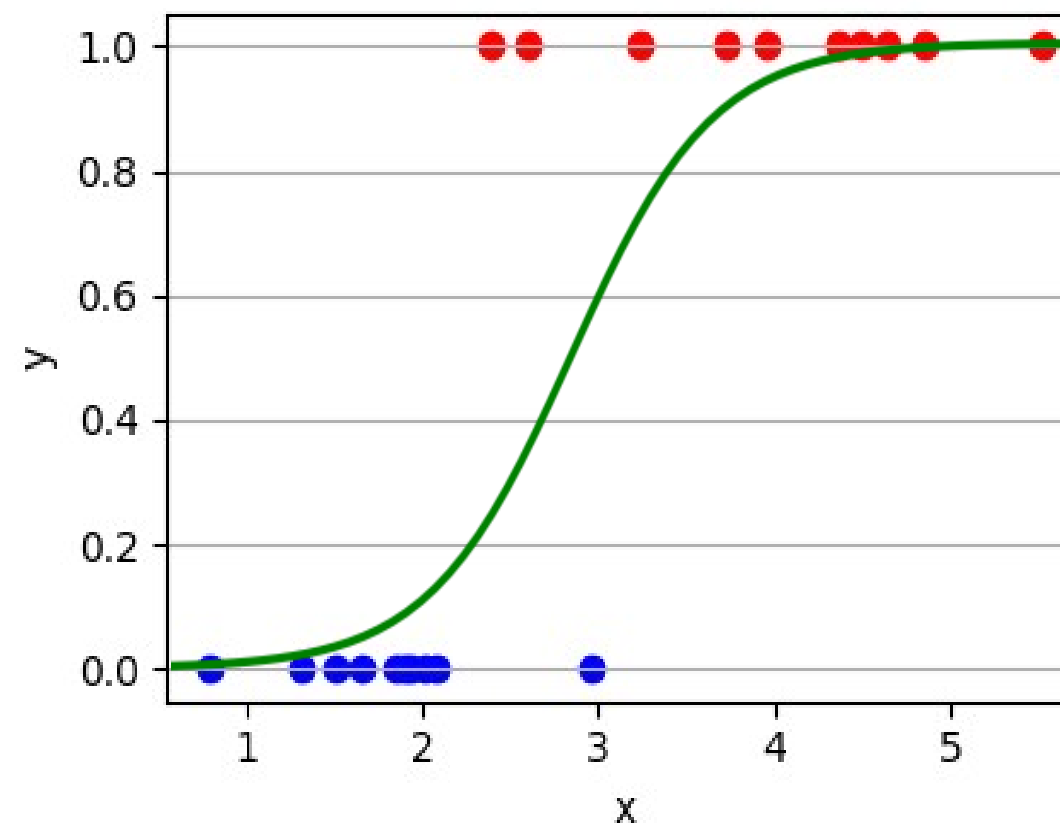
$w_0$

# Logistic Regression

Dataset

$(x_1, y_1), (x_2, y_2), (x_3, y_3), \dots, (x_n, y_n)$

Dataset for binary classification (n=20)



**x**

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix}$$

shape = (n, 1)

**y**

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_n \end{bmatrix}$$

shape = (n, 1)

```
# Import a necessary modules
from sklearn.linear_model import LogisticRegression

# Create the model
clf = LogisticRegression()

# Train the model
clf.fit(x, y)

# Obtain model parameters
w0 = clf.intercept_
w1 = clf.coef_

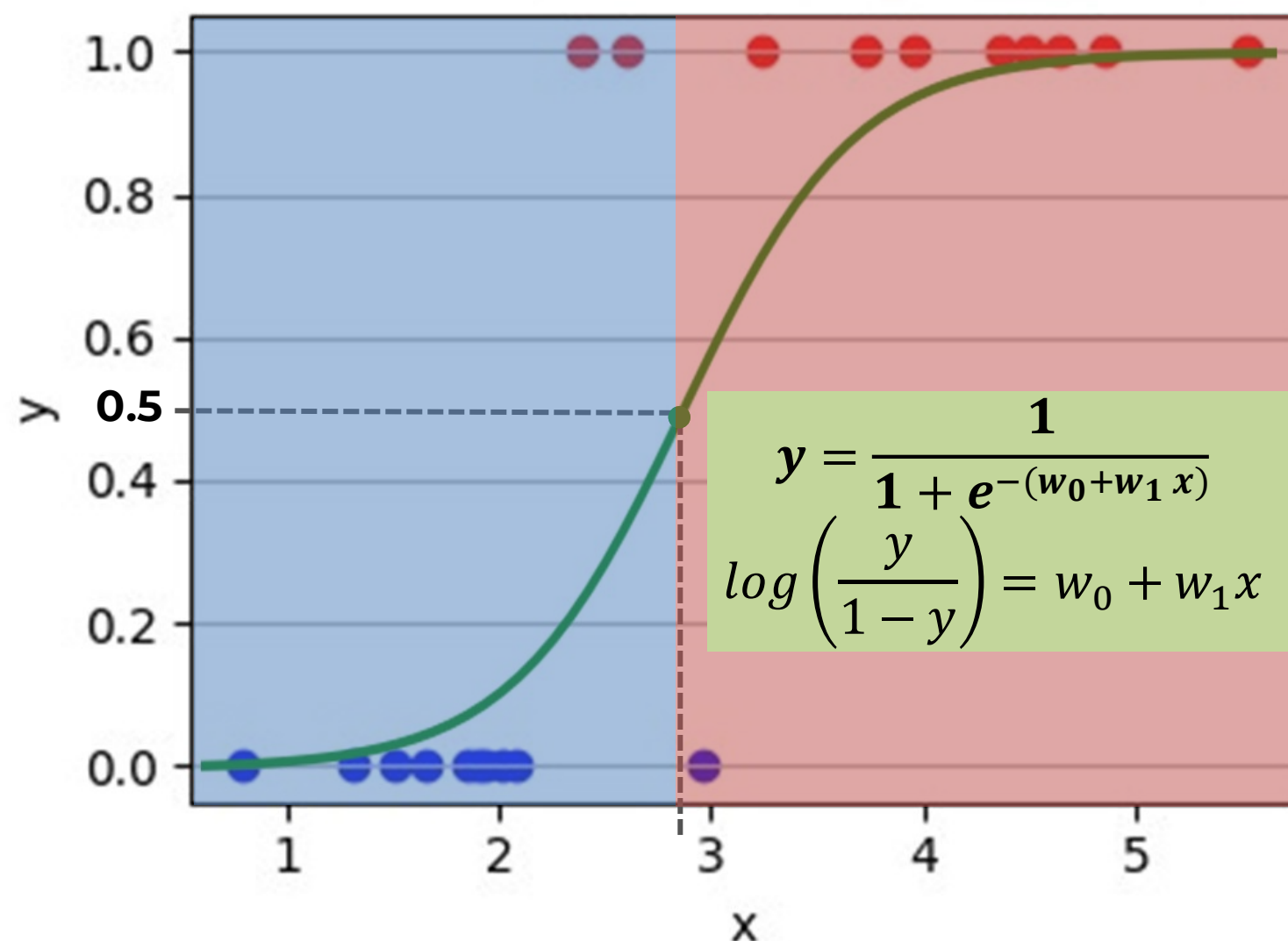
# Make prediction
y_pred = clf.predict(x_test)
```

$$y = \frac{1}{1 + e^{-(w_0 + w_1 x)}}$$

# Logistic Regression

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# Logistic Regression: Optional



$$y = \frac{1}{1 + e^{-(w_0 + w_1 x)}} \quad \text{or} \quad \log\left(\frac{y}{1-y}\right) = w_0 + w_1 x$$

$y = \text{Probability of class 1}$

$$\begin{aligned} y \geq 0.5 &\rightarrow \text{Class 1} \quad \longleftrightarrow \quad w_0 + w_1 x \geq 0 \\ y < 0.5 &\rightarrow \text{Class 0} \quad \longleftrightarrow \quad w_0 + w_1 x < 0 \end{aligned}$$

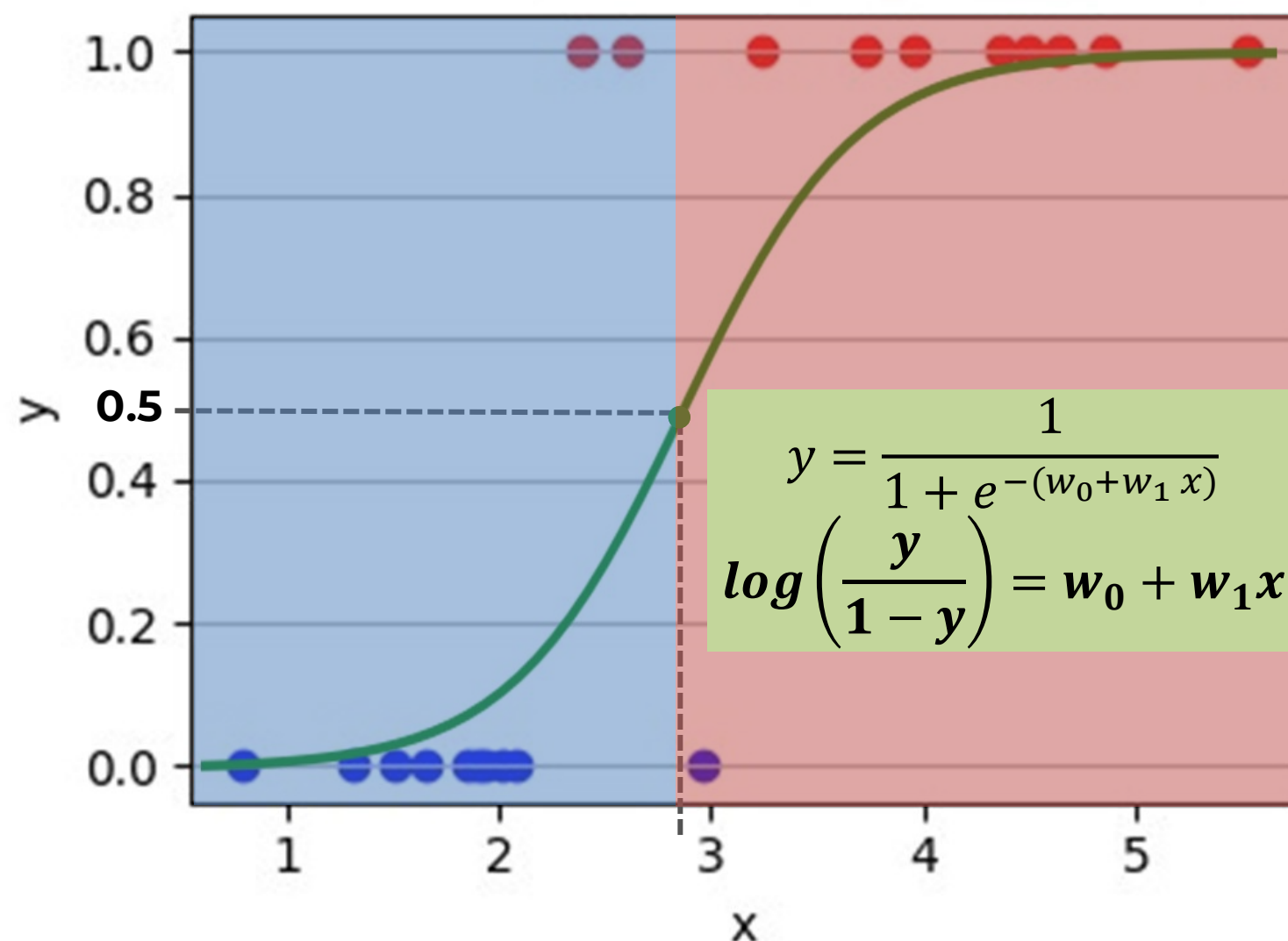
$$\begin{aligned} y &= \frac{1}{1 + e^{-(w_0 + w_1 x)}} \geq \frac{1}{2} \\ 2 &\geq 1 + e^{-(w_0 + w_1 x)} \\ 1 &\geq e^{-(w_0 + w_1 x)} \\ \ln 1 &\geq -(w_0 + w_1 x) \end{aligned}$$

$$w_0 + w_1 x \geq 0$$

Given  $y = 0.5$ , decision boundary (DB)?

$$w_0 + w_1 x_{DB} = 0 \rightarrow x_{DB} = -w_0 / w_1$$

# Logistic Regression: Optional



$$y = \frac{1}{1 + e^{-(w_0 + w_1 x)}} \quad \text{or} \quad \log\left(\frac{y}{1-y}\right) = w_0 + w_1 x$$

$w_1$ : slope     $w_0$ : log-odd-intercept

Probability of class 1  $\rightarrow$  0

Probability of class 1  $\rightarrow$  1

$$\lim_{y \rightarrow 0} \log\left(\frac{y}{1-y}\right) = -\infty \quad \text{and} \quad \lim_{y \rightarrow 1} \log\left(\frac{y}{1-y}\right) = +\infty$$

Log-odd has a range of  $-\infty$  to  $+\infty$

Given  $y = 0.5$ , decision boundary (DB)?

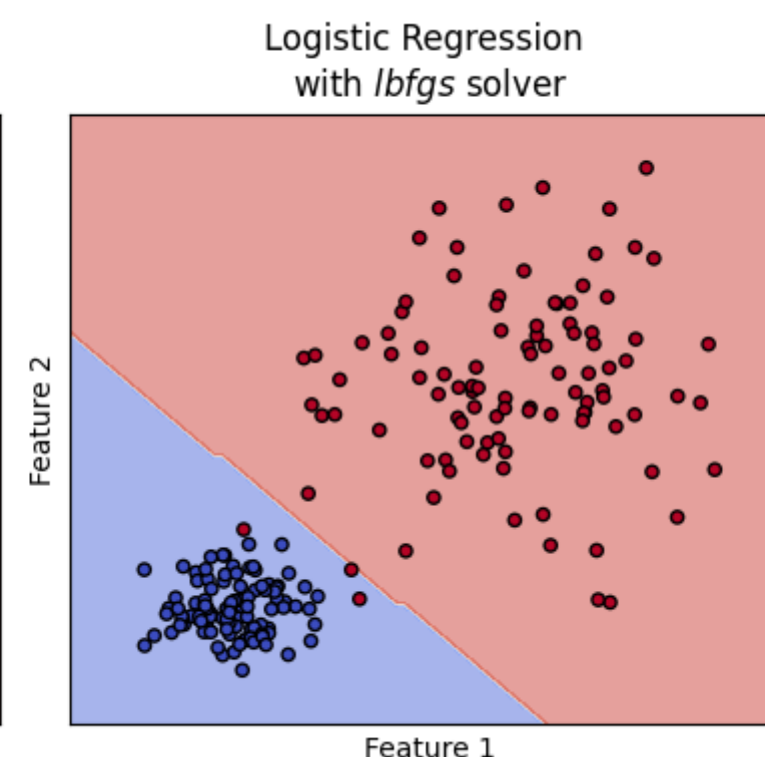
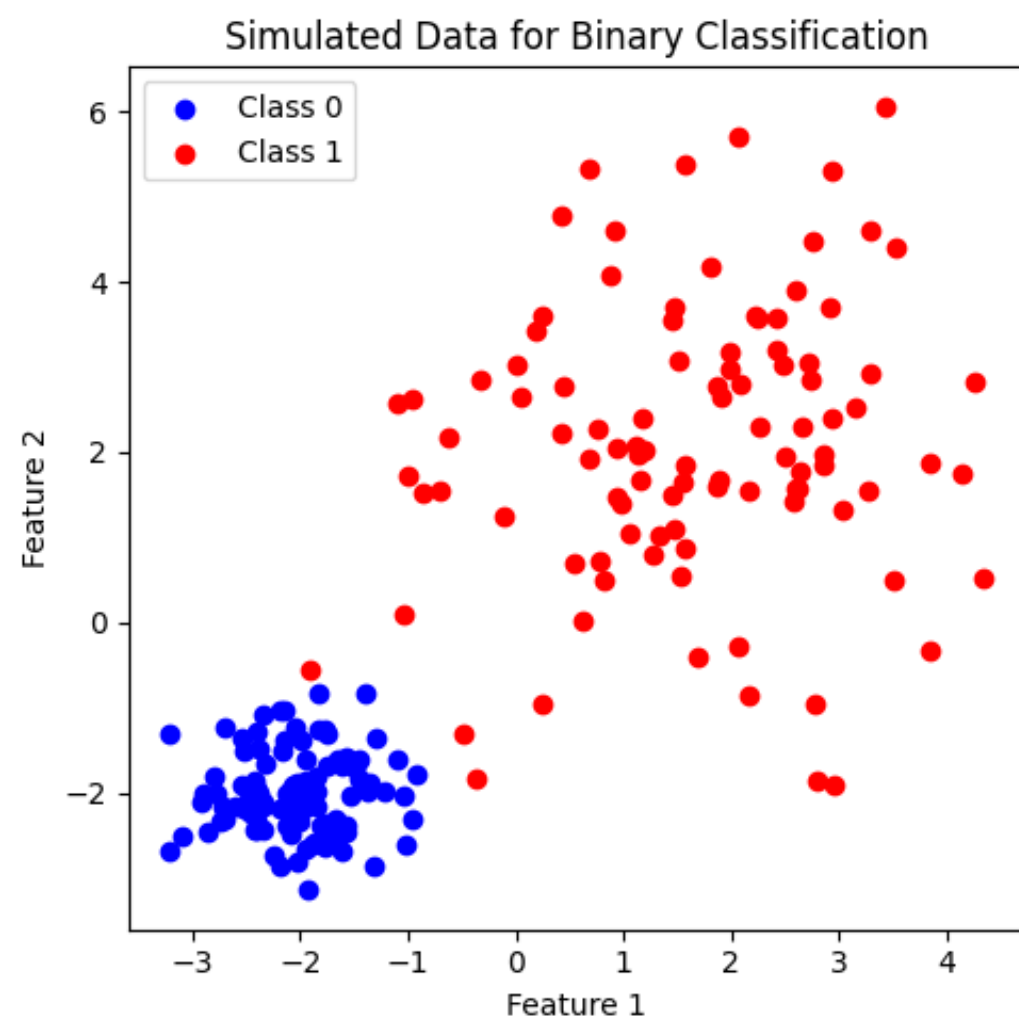
$$\log\left(\frac{0.5}{1-0.5}\right) = \log 1 = w_0 + w_1 x_{DB} \longleftrightarrow x_{DB} = -w_0/w_1$$

2 Features:  $0 = w_0 + w_1 x_{1,DB} + w_2 x_{2,DB}$

$$x_{2,DB} = \frac{w_0}{-w_2} + \frac{w_1}{-w_2} x_{1,DB}$$

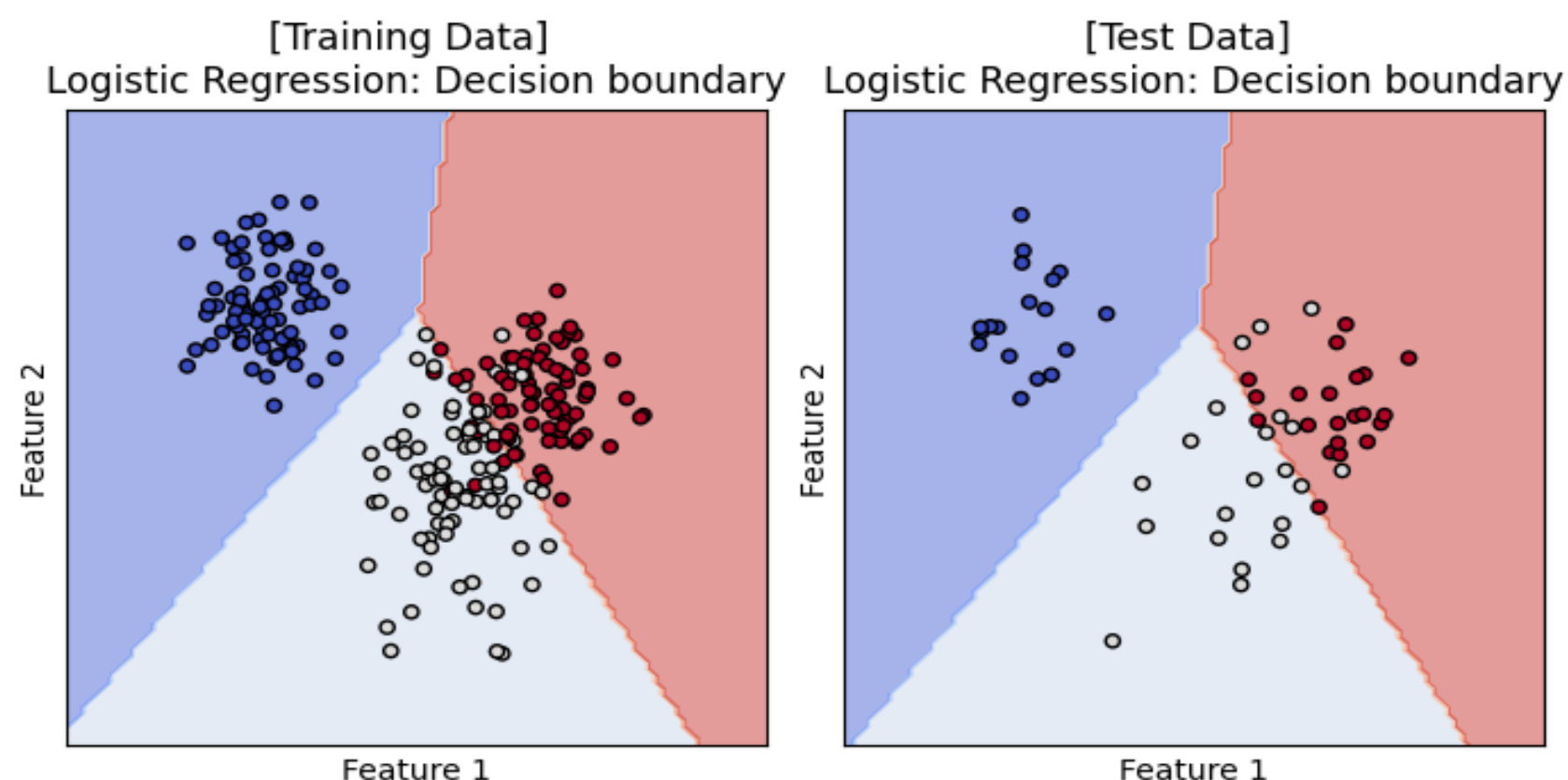
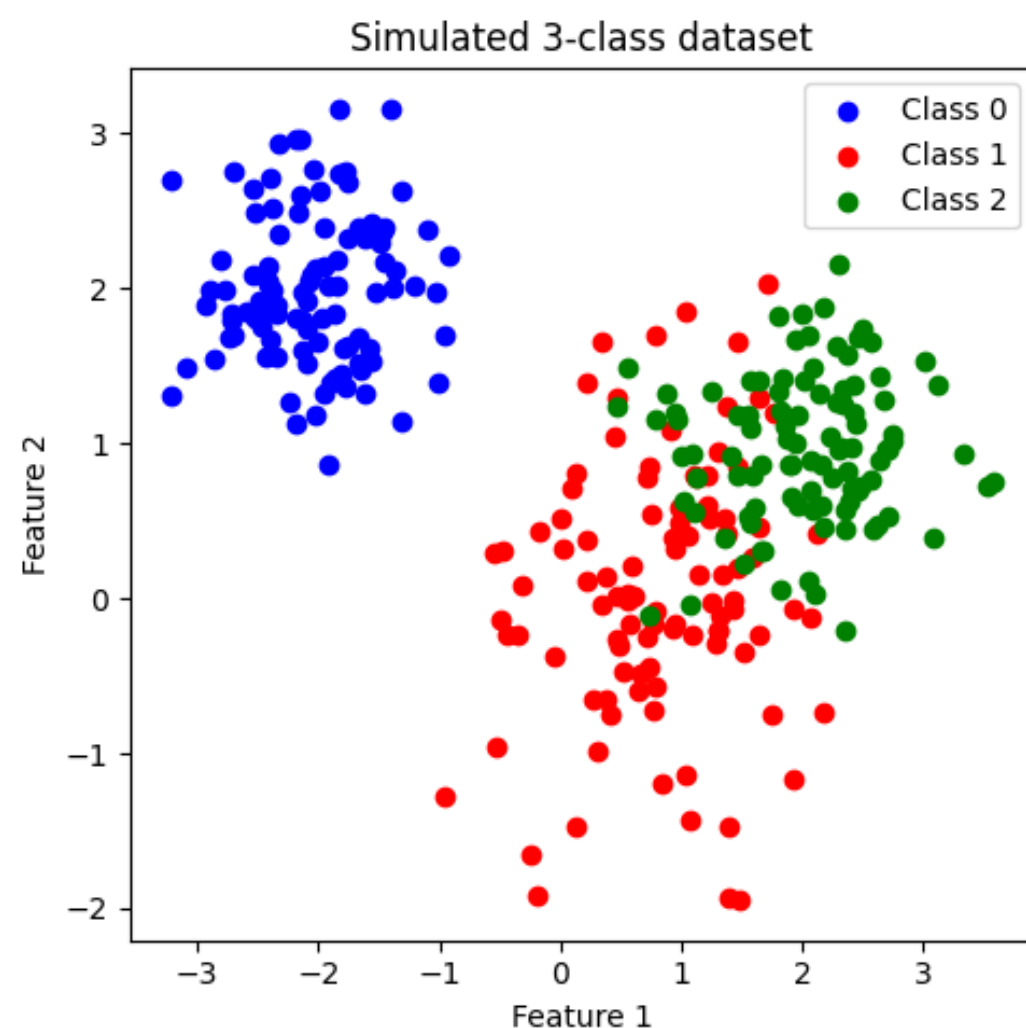


# Logistic Regression



Though the small variations of decision boundaries are observed when using different solvers, the decision boundary of logistic regression exhibits linear behavior, showing a straight line.

# Logistic Regression



Solvers = 'lbfgs'

Decision boundary of logistic regression is consisting of straight lines.