Machine Learning

Logistic Regression

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克明峻德，格物致知

Service records show year-3 car owners going quiet. The clocks tick past the warranty period.

The budget can't cover everyone. We focus on the likely leavers and send a "stay" bundle voucher.

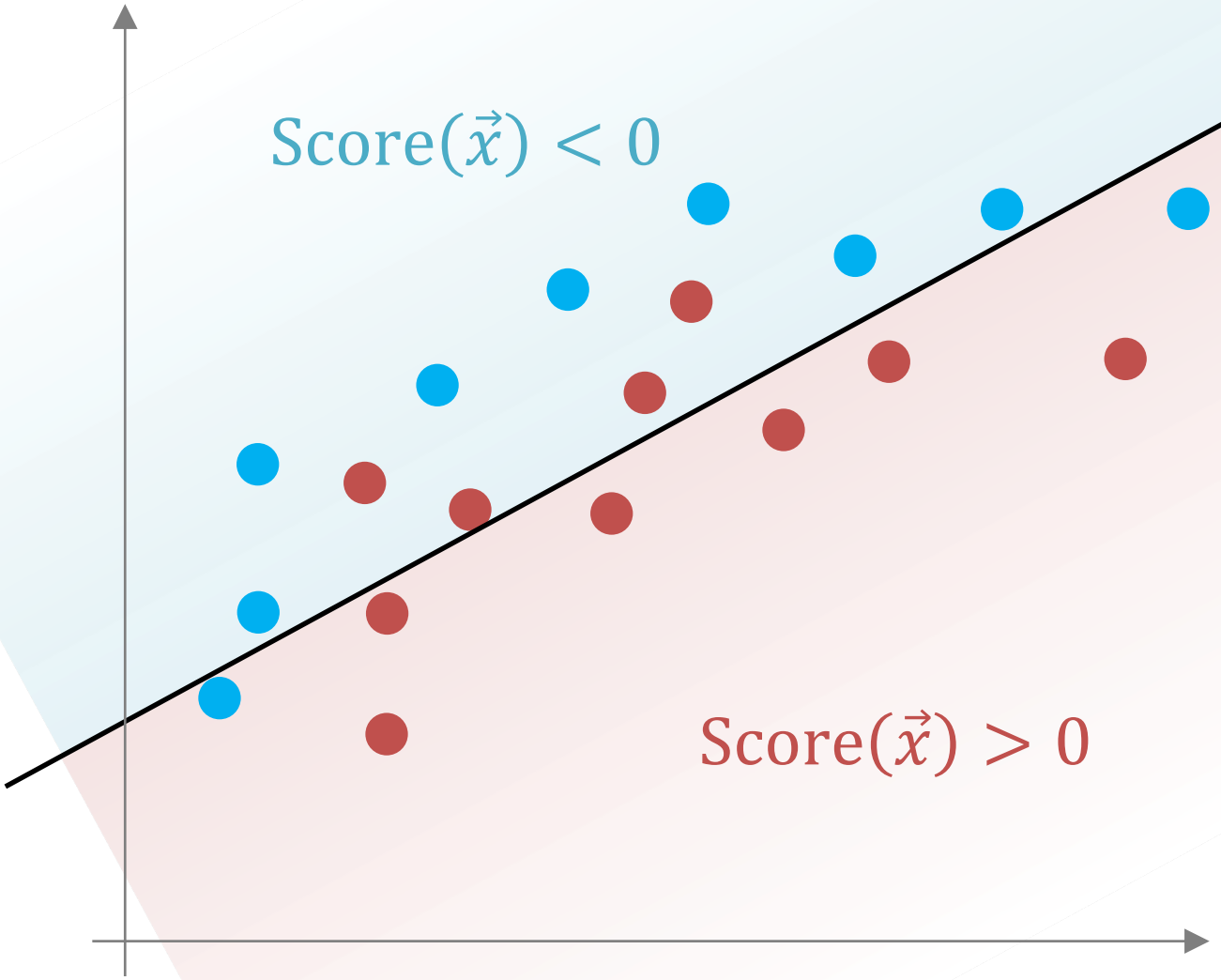
We maximise our ROI with we have.

Q: How is this like for an ML classifier?

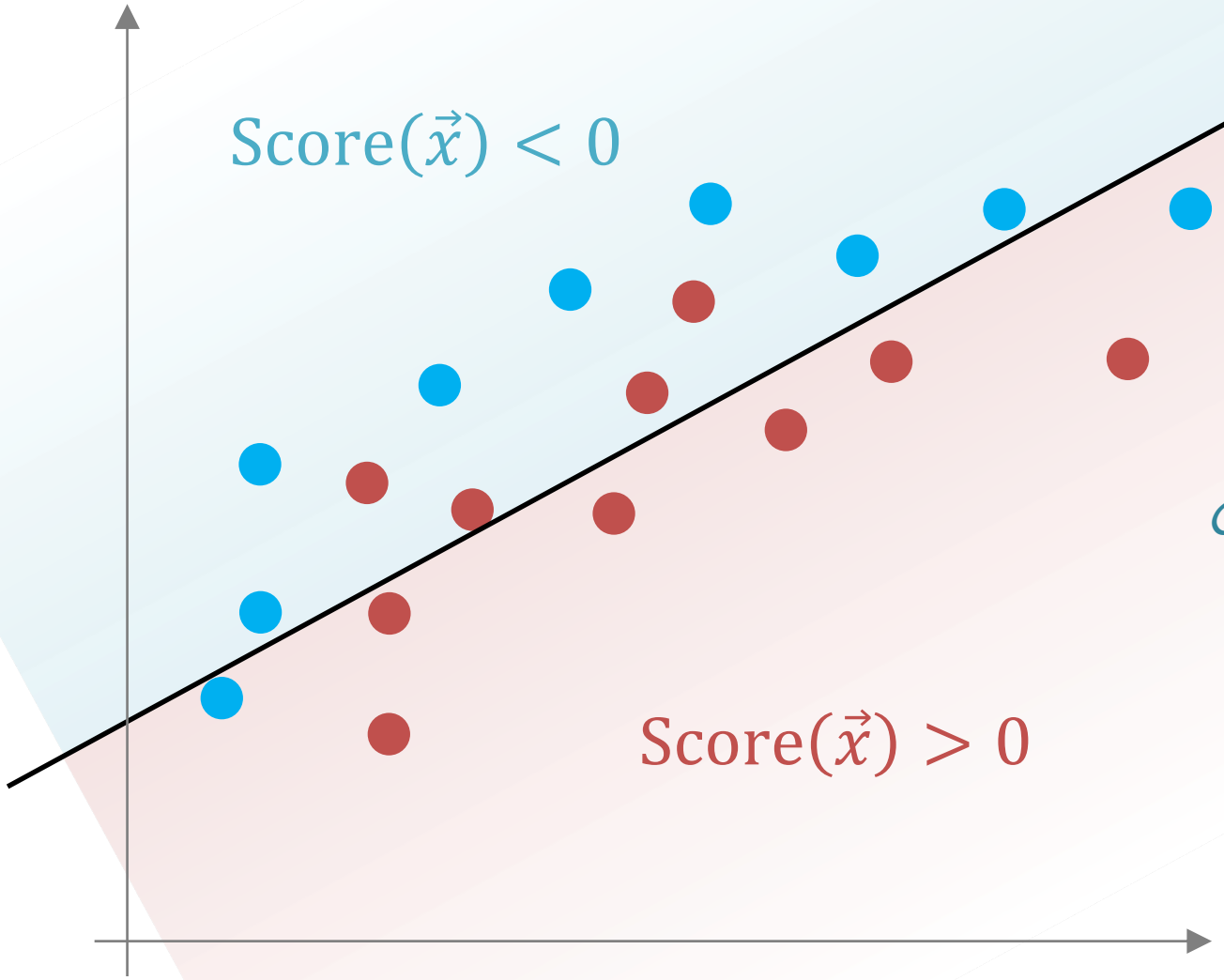
A: Logistic Regression outputs a likelihood, instead of a hard yes-or-no decision.

Not all mistakes cost the same.

Linear Classifier



Recap: Accuracy



$$\vec{x}^T \times \vec{w} = 0$$

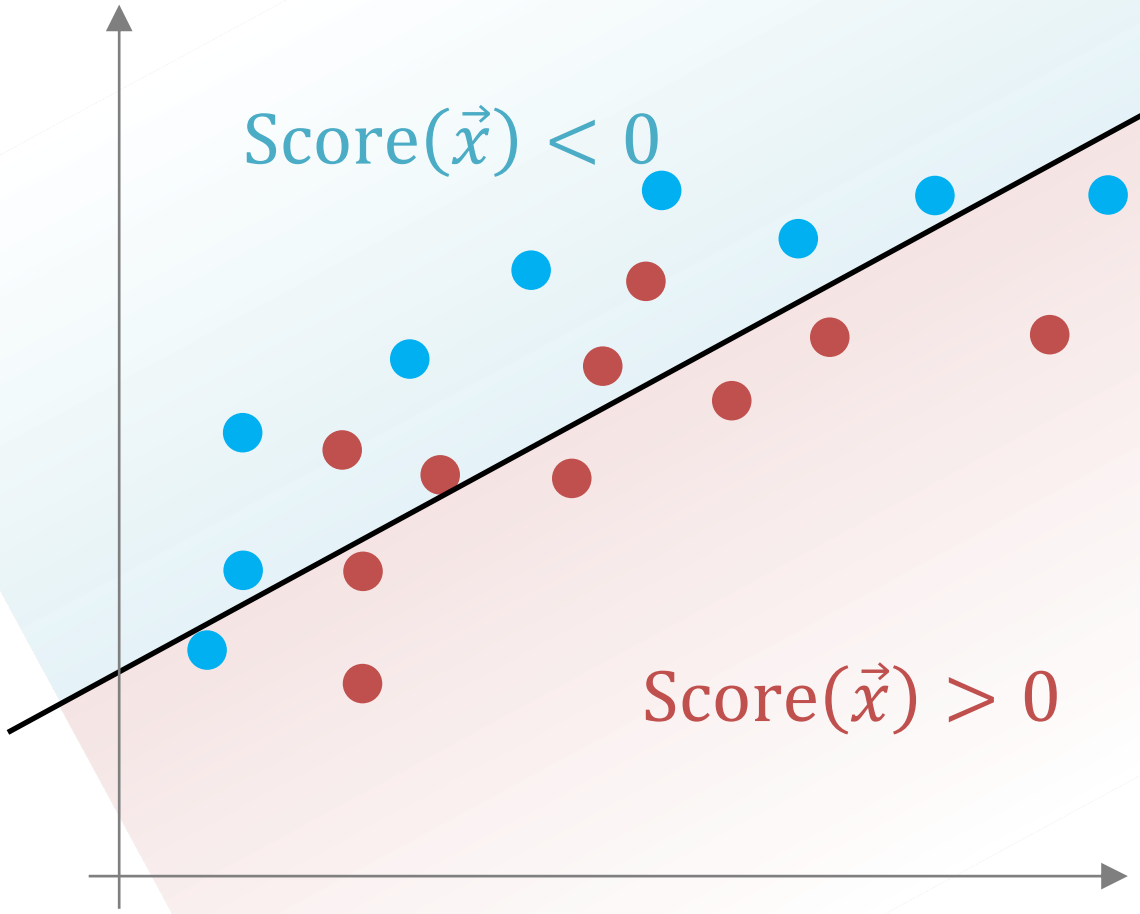
(Decision Boundary)

Q: How many did we classify it correctly?

$$\text{Accuracy} = \frac{6+7}{19}$$

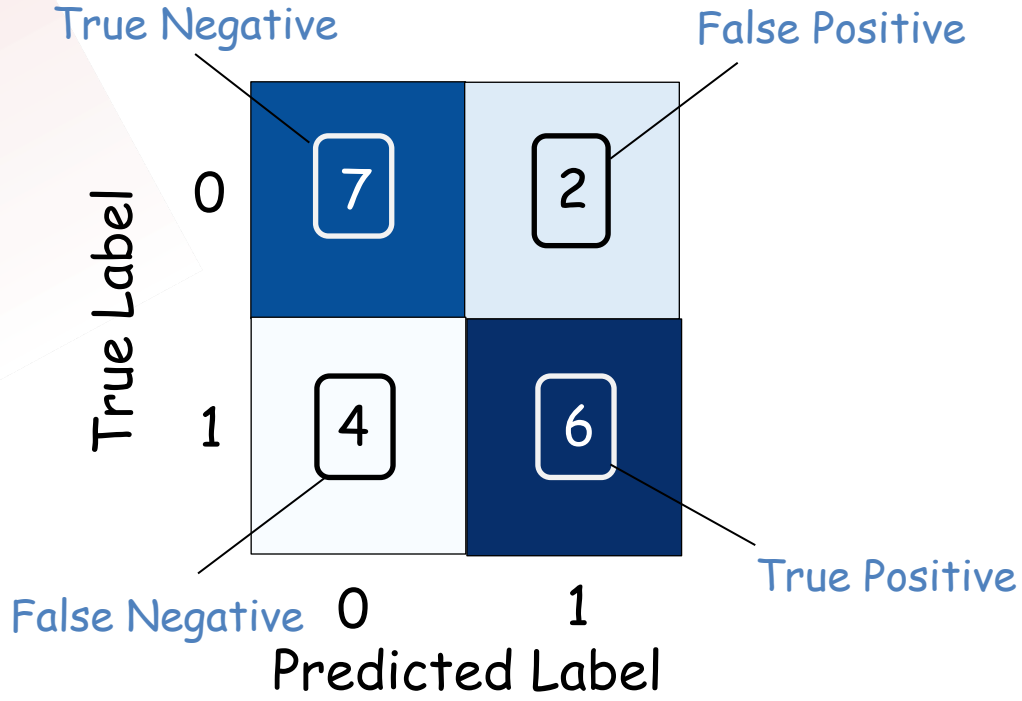
$$\approx 0.68$$

Recap: Confusion Matrix



$\vec{x}^T \times \vec{w} = 0$

(Decision Boundary)



Prediction Confidence

The ramen & everything else were awesome!

Definitely Positive

$$P\left(y = 1 \,\middle|\, \vec{x} = \text{"The ramen \& everything else were awesome!"}\right) = 0.99$$

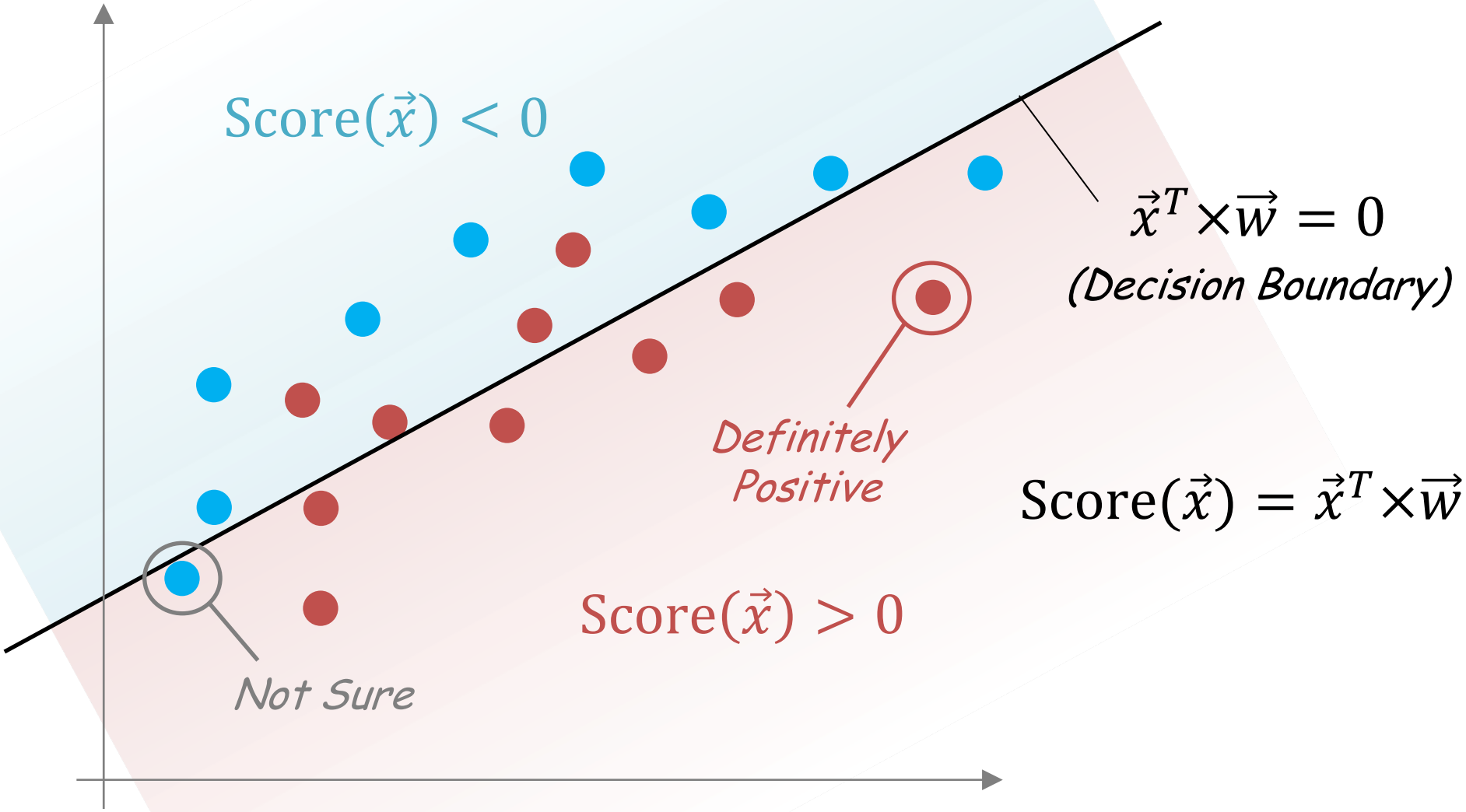
The ramen was good, the service was OK.

Not Sure

$$P\left(y = 1 \,\middle|\, \vec{x} = \text{"The ramen was good, the service was OK."}\right) = 0.55$$

We read the conditional probability $P(y|\vec{x})$ as "the probability of y given $\vec{x}$".

How Confidence?



Scoring Interpretation

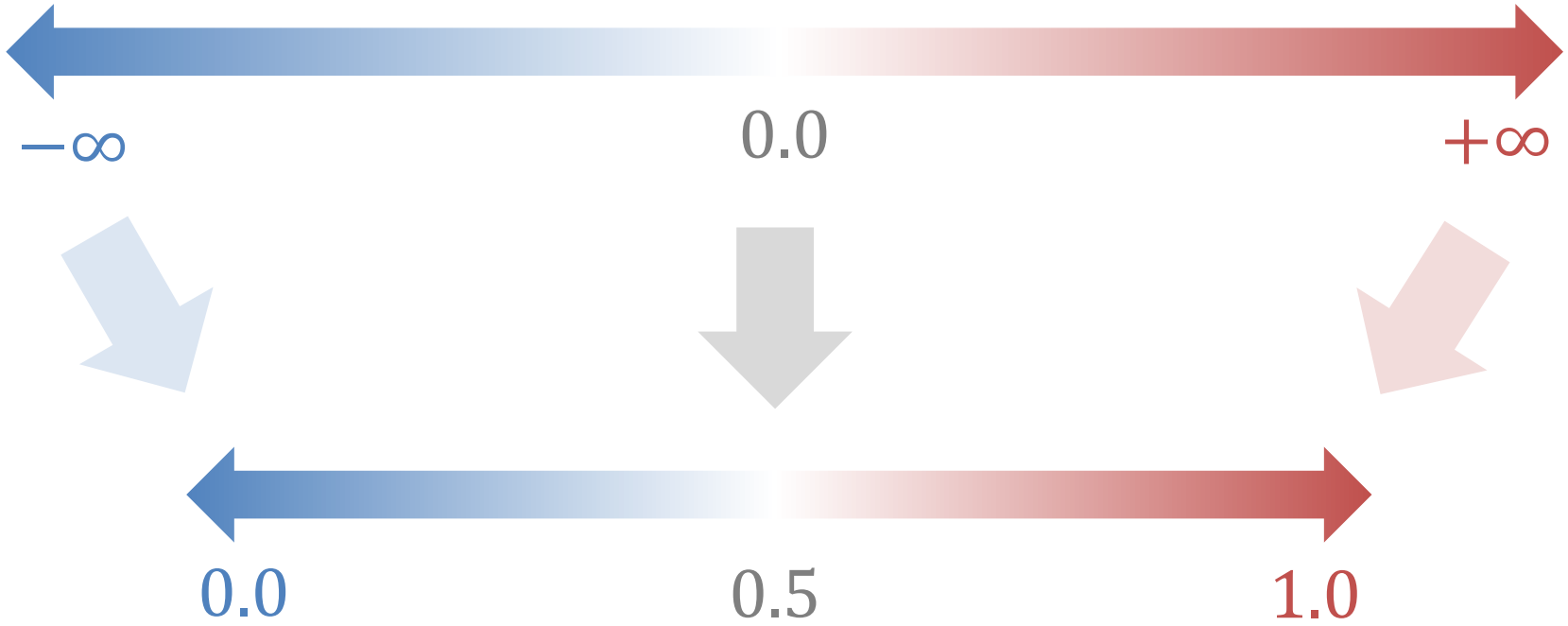
$$\text{Score}(\vec{x}^{(i)}) = \left(\vec{x}^{(i)}\right)^T \times \vec{w}$$

$-\infty$ $\quad \hat{y}^{(i)} = 0 \quad$ 0.0 $\quad \hat{y}^{(i)} = 1 \quad$ $+\infty$

Very Sure	*Not Sure If*	*Very Sure*
$\hat{y}^{(i)} = 0$	$\hat{y}^{(i)} = 0 \; or \; 1$	$\hat{y}^{(i)} = 1$
$P\left(y = 1 \middle\| \vec{x}^{(i)}, \vec{w}\right) = 0$	$P\left(y = 1 \middle\| \vec{x}^{(i)}, \vec{w}\right) = 0.5$	$P\left(y = 1 \middle\| \vec{x}^{(i)}, \vec{w}\right) = 1$

Scoring Interpretation

$$\text{Score}(\vec{x}^{(i)}) = \left(\vec{x}^{(i)}\right)^T \times \vec{w}$$



$$P\left(y = 1 \,\middle|\, \vec{x}^{(i)}\right)$$

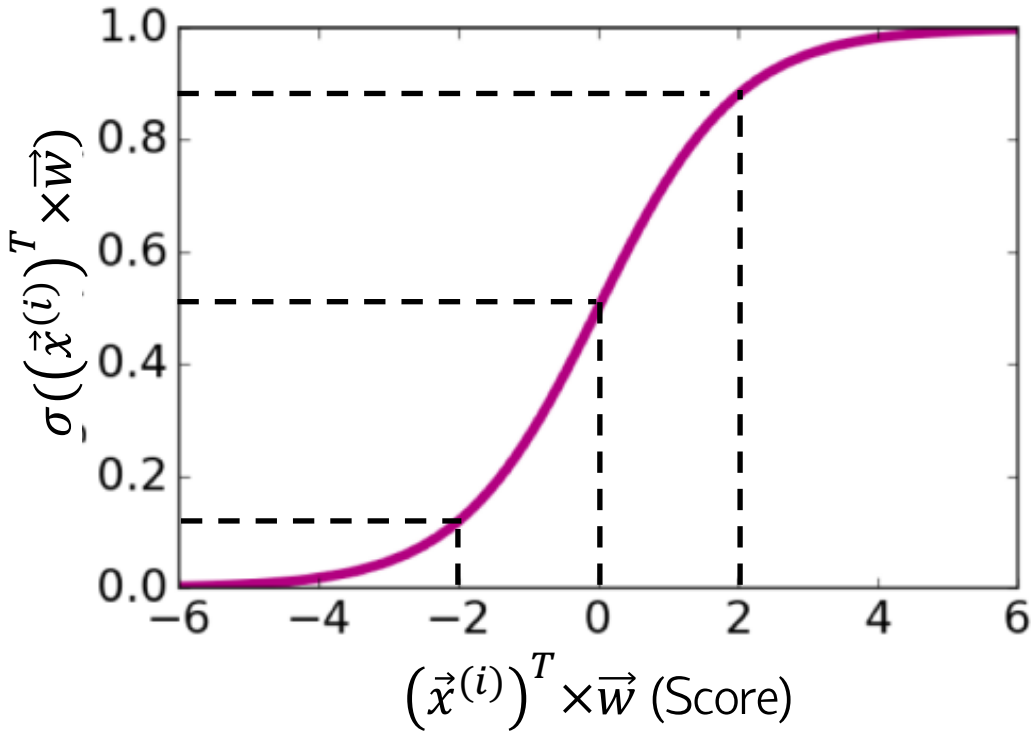
Q: How do we map (-∞, +∞) to [0.0, 1.0]?

Sigmoid (or Logistic) Function

Sigmoid Function:

$$\sigma\left(\left(\vec{x}^{(i)}\right)^T \times \vec{w}\right) = \frac{1}{1 + e^{-\left(\vec{x}^{(i)}\right)^T \times \vec{w}}}$$

$(\vec{x}^{(i)})^T \times \vec{w}$ (Score)	$\sigma\left(\left(\vec{x}^{(i)}\right)^T \times \vec{w}\right)$
$-\infty$	0.0
-2.0	0.12
0.0	0.5
$+2.0$	0.88
$+\infty$	1.0



Logistic Regression Model

$$\text{Score}(\vec{x}^{(i)}) = \left(\vec{x}^{(i)}\right)^T \times \vec{w}$$

$$P\left(y = 1 \,\middle|\, \vec{x}^{(i)}, \vec{w}\right) = \frac{1}{1+e^{-\left(\vec{x}^{(i)}\right)^T \times \vec{w}}}$$

Understand Logistic Regression

Probabilistic Score:

$$P\left(y=1 \mid \vec{x}^{(i)}, \vec{w}\right) = \frac{1}{1+e^{-\left(\vec{x}^{(i)}\right)^T \times \vec{w}}}$$

$\left(\vec{x}^{(i)}\right)^T \times \vec{w}$ (Score)	$P\left(y=1 \mid \vec{x}^{(i)}, \vec{w}\right)$
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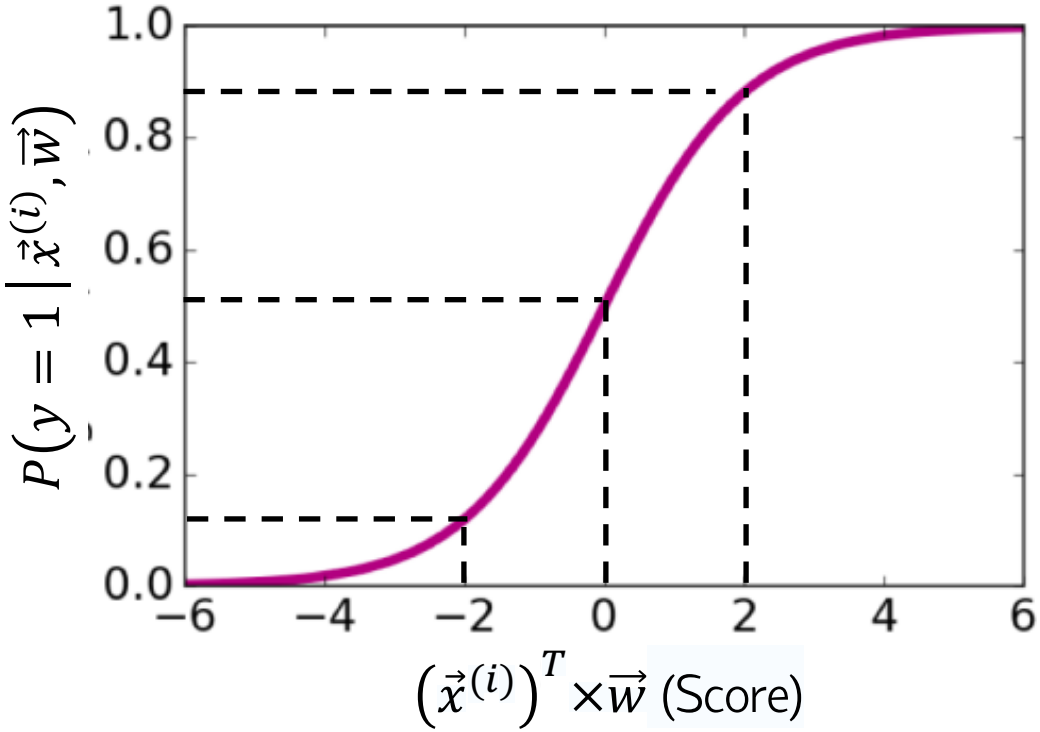
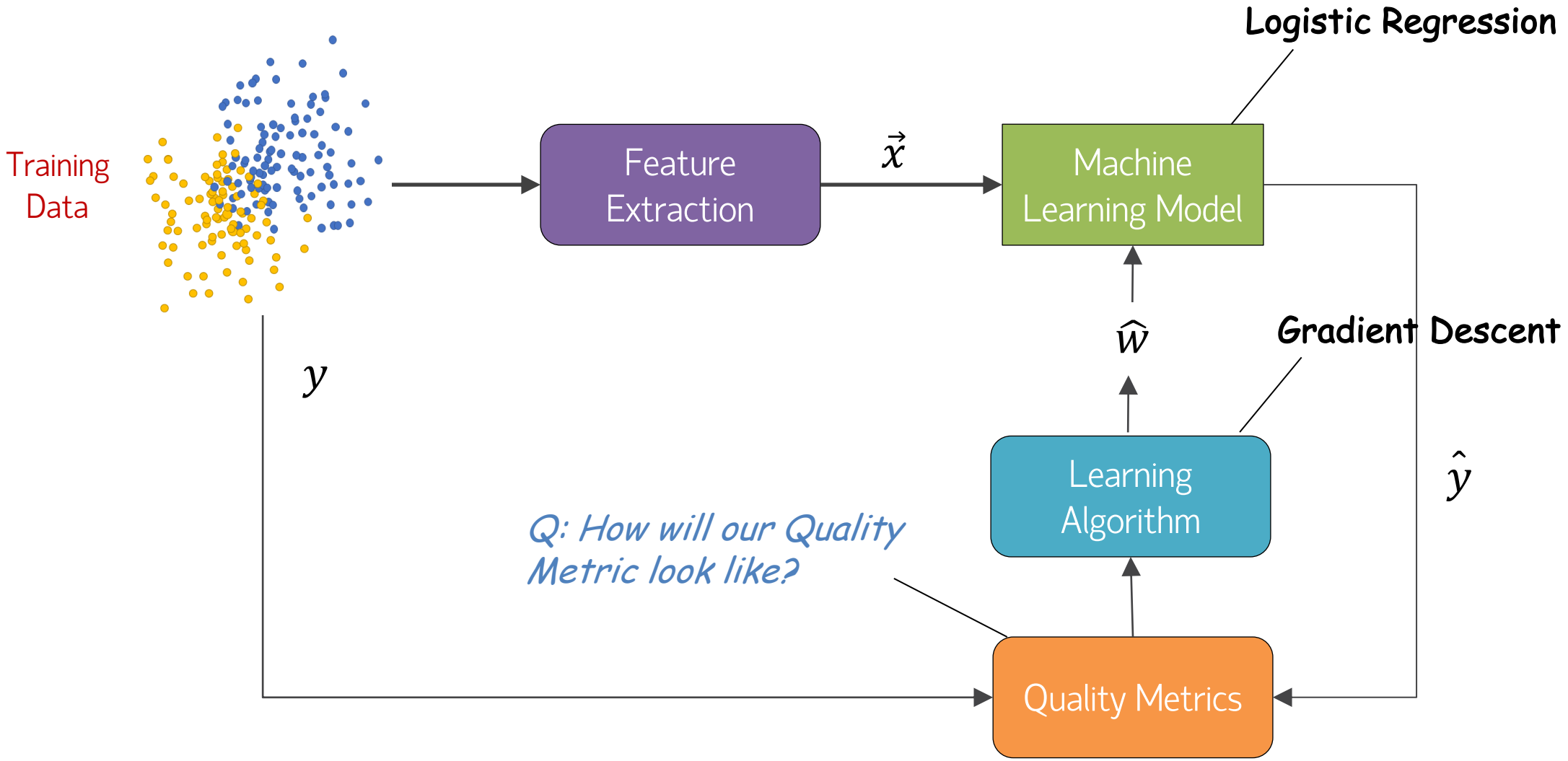


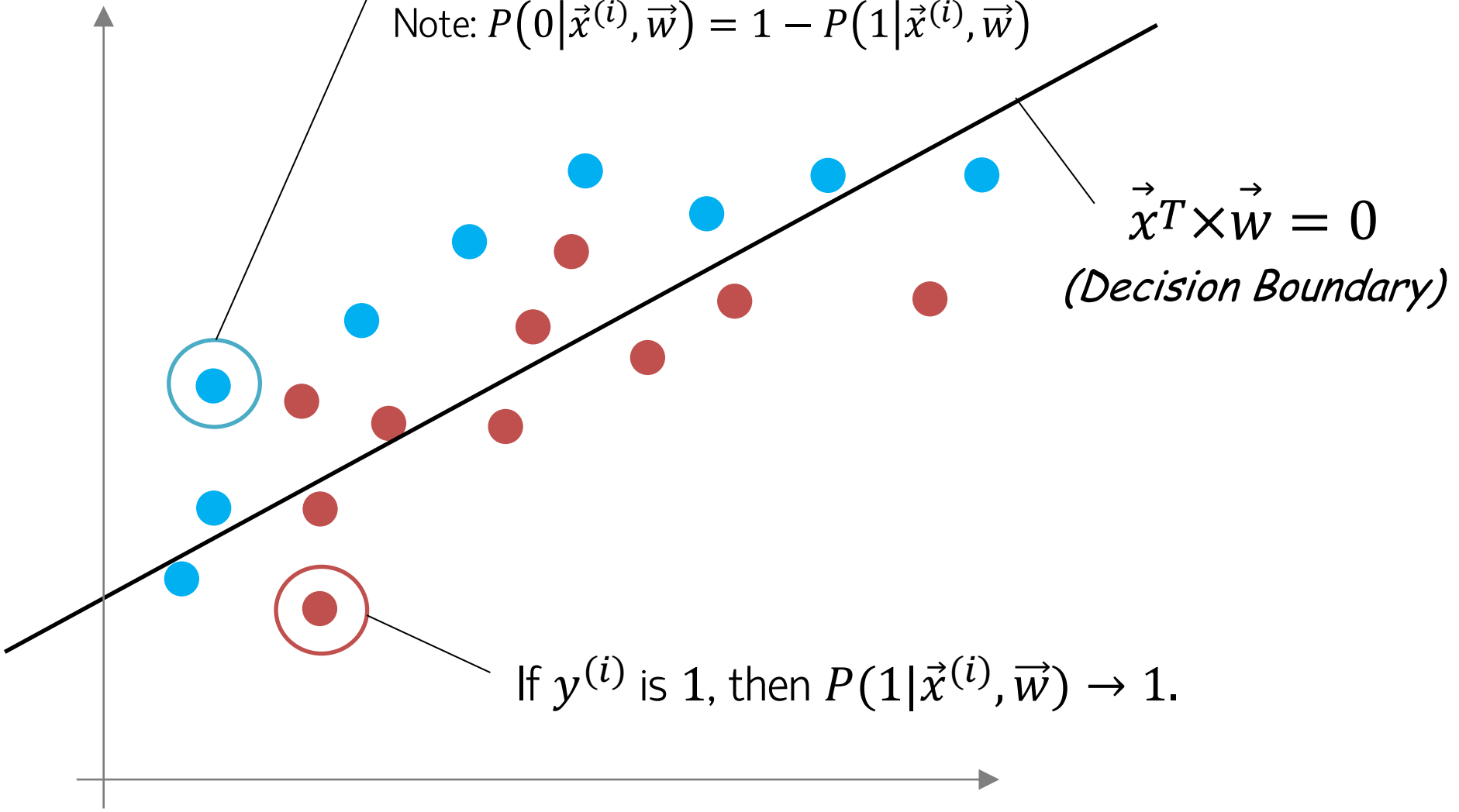
Workflow: Logistic Regression



What We Are Optimising

If $y^{(i)}$ is 0, then $P\left(0\middle|\vec{x}^{(i)},\vec{w}\right) \rightarrow 1$ (or $P\left(1\middle|\vec{x}^{(i)},\vec{w}\right) \rightarrow 0$).

Note: $P\left(0\middle|\vec{x}^{(i)},\vec{w}\right) = 1 - P\left(1\middle|\vec{x}^{(i)},\vec{w}\right)$



$\vec{x}^T \times \vec{w} = 0$

(Decision Boundary)

If $y^{(i)}$ is 1, then $P(1|\vec{x}^{(i)},\vec{w}) \rightarrow 1$.

Recall: Joint Probability

Q: What is the probability (or likelihood) of rolling a six on both dice?

A: $\frac{1}{6} \times \frac{1}{6} = \frac{1}{36}$

$$P(A,B) = P(A) \times P(B)$$

Probability of Rolling a Six on Dice A

Probability of Rolling a Six on Dice B

Quality Metric: Likelihood Function

Likelihood Function:

If y_i is 1, then $P(1|\vec{x}_i, \vec{w}) \rightarrow 1$.

$$L(\vec{w}) = \prod_{i=1}^{N} P(1|\vec{x}^{(i)}, \vec{w})^{y^{(i)}} \times [1 - P(1|\vec{x}^{(i)}, \vec{w})]^{(1-y^{(i)})}$$

≈ 1 if $y^{(i)} = 0$

≈ 1 if $y^{(i)} = 1$

If y_i is 0, then $P(1|\vec{x}^{(i)}, \vec{w}) \rightarrow 0$ (or $P(0|\vec{x}^{(i)}, \vec{w}) \rightarrow 1$).

Note: $P(0|\vec{x}^{(i)}, \vec{w}) = 1 - P(1|\vec{x}^{(i)}, \vec{w})$

Log Likelihood Function

Likelihood Function:

$$L(\vec{w}) = \prod_{i=1}^{N} P(1|\vec{x}^{(i)}, \vec{w})^{y^{(i)}} \times [1 - P(1|\vec{x}^{(i)}, \vec{w})]^{(1-y^{(i)})}$$

Log Likelihood Function:

$$\log L(\vec{w}) = \sum_{i=1}^{N} [y^{(i)} \log P(1|\vec{x}^{(i)}, \vec{w}) + (1 - y^{(i)}) \log(1 - P(1|\vec{x}^{(i)}, \vec{w}))]$$

Relevant Logarithmic Rules:

$$\log(A \times B) = \log A + \log B \qquad \log A^N = N \log A$$

Numerical Underflow

$P(1|\vec{x}^{(i)}, \vec{w})$ and $1 - P\left(1\middle|\vec{x}^{(i)}, \vec{w}\right)$ are less than 1. Hence, $L(\vec{w}) \to 0$.

This could lead to numerical underflow. *Try: 0.1**1000 (i.e. 1.0×10^{-1000}) in Python.*

Moreover, our gradients would be vanishing as $L(\vec{w}_k) \approx 0$. *Consequently, if no gradient, then gradient descent will not work.*

Q: How can we handle very very small numbers?

A: We take Log. 1000xLog(0.1) = 1,000x(-1) = -1,000.

Likelihood Function as an On/Off Switch

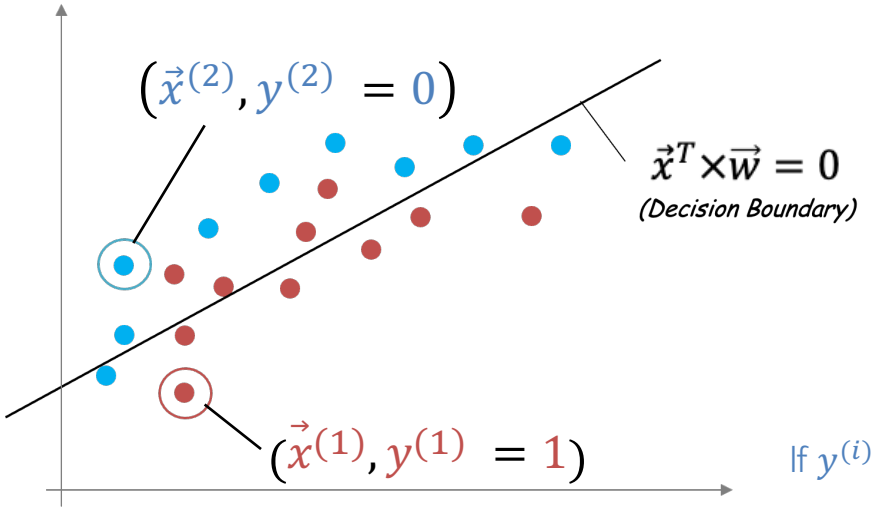
Likelihood Function:

0 (OFF) if $y^{(i)} = 0$ // 0 (OFF) if $y^{(i)} = 1$ //

$$L(\vec{w}, b) = -\sum_{i=1}^{N} \left[y^{(i)} \log P(1|\vec{x}^{(i)}, \vec{w}, b) + (1 - y^{(i)}) \log(1 - P(1|\vec{x}^{(i)}, \vec{w}, b)) \right]$$

Related Properties:

$P(y = 1\|\vec{x}, \vec{w}, b) \in (0,1)$	$P(y = 1\|\vec{x}, \vec{w}, b) \to 1^-$
$\log P(y = 1\|\vec{x}, \vec{w}, b) \in (-\infty, 0)$	$\log P(y = 1\|\vec{x}, \vec{w}, b) \to 0^-$
$-\log P(y = 1\|\vec{x}, \vec{w}, b) \in (0, +\infty)$	$-\log P(y = 1\|\vec{x}, \vec{w}, b) \to 0^+$



If $y^{(i)}$ is 1, then $-\log P(1|\vec{x}^{(i)}, \vec{w}) \to 0^+$.

$$\begin{aligned} L(\vec{x}^{(1)}, \vec{w}, b) &= -\left[y^{(1)} \log P(1|\vec{x}^{(1)}, \vec{w}, b) + (1 - y^{(1)}) \log\left(1 - P(1|\vec{x}^{(1)}, \vec{w}, b)\right) \right] \\ &= -\left[1 \times \log P(1|\vec{x}^{(1)}, \vec{w}, b) + (1 - 1) \log\left(1 - P(1|\vec{x}^{(1)}, \vec{w}, b)\right) \right] \\ &= -\log P(1|\vec{x}^{(1)}, \vec{w}, b) \end{aligned}$$

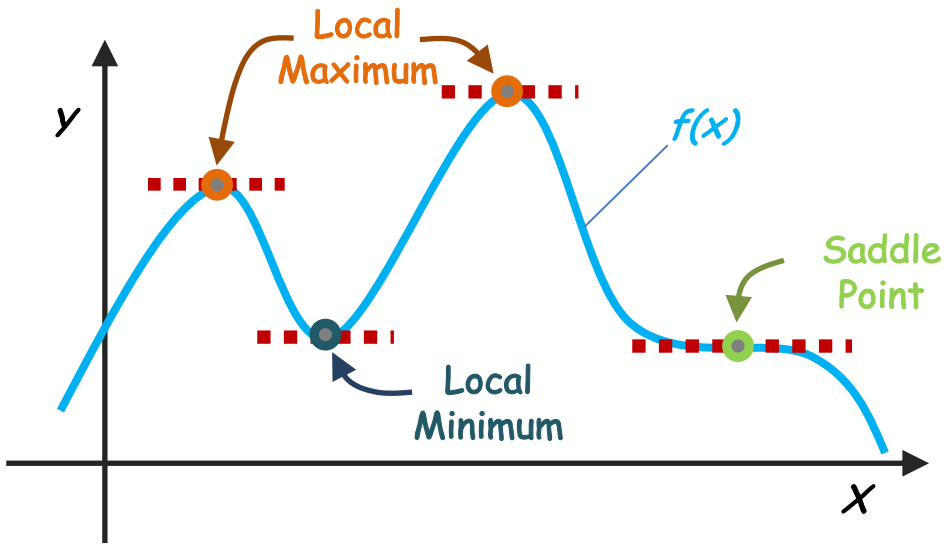
$$\begin{aligned} L(\vec{x}^{(2)}, \vec{w}, b) &= -\left[y^{(2)} \log P(1|\vec{x}^{(2)}, \vec{w}, b) + (1 - y^{(2)}) \log\left(1 - P(1|\vec{x}^{(2)}, \vec{w}, b)\right) \right] \\ &= -\left[0 \times \log P(1|\vec{x}^{(2)}, \vec{w}, b) + (1 - 0) \log\left(1 - P(1|\vec{x}^{(2)}, \vec{w}, b)\right) \right] \\ &= -\log\left(1 - P(1|\vec{x}^{(2)}, \vec{w}, b)\right) \\ &= -\log P(0|\vec{x}^{(2)}, \vec{w}, b) \end{aligned}$$

If $y^{(i)}$ is 0, then $-\log\left(1 - P(1|\vec{x}^{(2)}, \vec{w}, b)\right) \to 0^+$ (or $-\log P(0|\vec{x}^{(i)}, \vec{w}, b) \to 0^+$).

Best Decision Boundary

Maximising Log Likelihood:

$$\max_{\vec{w}} \sum_{i=1}^{N} \left[y^{(i)} \log P(1|\vec{x}^{(i)}, \vec{w}) + (1 - y^{(i)}) \log(1 - P\left(1\middle|\vec{x}^{(i)}, \vec{w}\right)) \right]$$



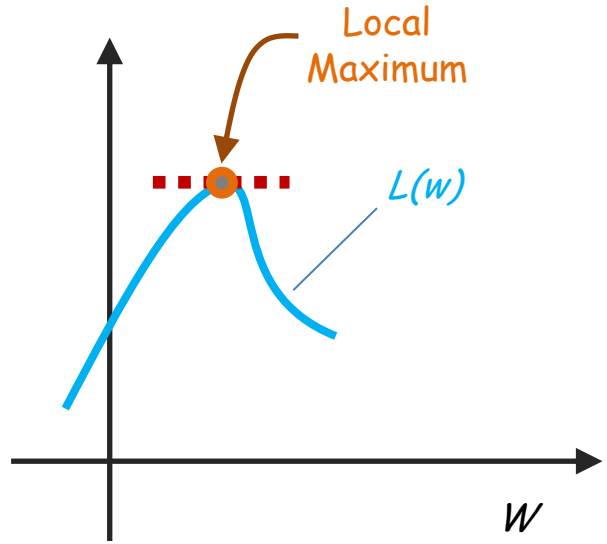
Q: Which value of x will f(x) be maximum?

A: … Slope (or Gradient) = 0 …

Gradient Descent: Minimisation

Maximising Log Likelihood:

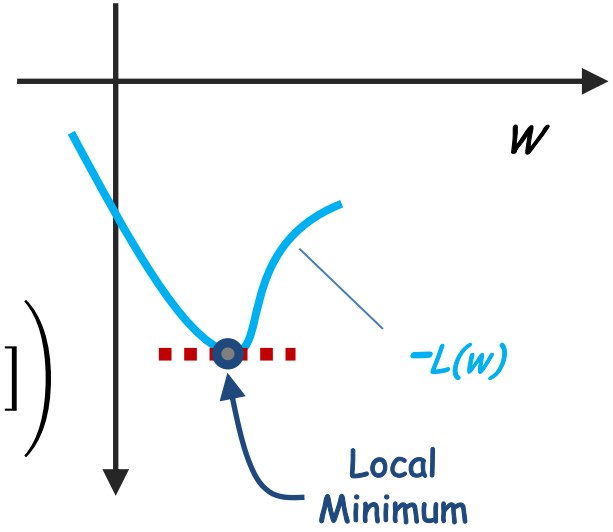
$$\max_{\vec{w}} \sum_{i=1}^{N} [y^{(i)} \log P(1|\vec{x}^{(i)}, \vec{w}) + (1 - y^{(i)}) \log(1 - P(1|\vec{x}^{(i)}, \vec{w}))]$$



equivalent to

Minimising Negative Log Likelihood:

$$\min_{\vec{w}} -\left(\sum_{i=1}^{N} [y^{(i)} \log P(1|\vec{x}^{(i)}, \vec{w}) + (1 - y^{(i)}) \log(1 - P(1|\vec{x}^{(i)}, \vec{w}))]\right)$$



Gradient Vector

Negative Log Likelihood:

$$J(\vec{w}) = -\sum_{i=1}^{N}\left[y^{(i)}\log P(1|\vec{x}^{(i)},\vec{w}) + (1-y^{(i)})\log(1-P\left(1\middle|\vec{x}^{(i)},\vec{w}\right))\right]$$

Derivative of Log Likelihood:

$$\frac{\partial J(\vec{w})}{\partial w_j} = -\sum_{i=1}^{N}\left(y^{(i)} - \log P(1|\vec{x}^{(i)},\vec{w})\right)x_j^{(i)}$$

Gradient Vector:

$$\nabla_{\vec{w}} J(\vec{w}) = -X^T(Y - P(1|X,\vec{w}))$$

Pseudocode for Logistic Regression

```
# Logistic Regression — Gradient Descent on NLL

# Inputs
#  data     ← (X, y) with y ∈ {0,1}
#  n        ← learning rate
#  max_iter ← maximum iterations
#  tol      ← stop when ‖∇L(w)‖ ≤ tol
#  X_query  ← examples to predict

# ----- fit -----
Φ ← concat_column(ones(N), X)                  # design matrix with bias
w ← zeros(columns(Φ))                          # initialize
# NLL: L(w) = - Σ [ y log p + (1-y) log(1-p) ],  p = σ(Φw)
FOR t = 1 TO max_iter DO
  z ← Φ · w
  p ← 1 / (1 + exp(-z))                        # sigmoid
  g ← transpose(Φ) · (p - y)          # ∇L(w)
  IF norm(g) ≤ tol THEN BREAK
  w ← w - n · g                                # GD step
END FOR

# ----- predict -----
Φ* ← concat_column(ones(|X_query|), X_query)
p* ← 1 / (1 + exp(-Φ* · w))
ŷ  ← 1 if p* ≥ 0.5 else 0

RETURN p*, ŷ
```

Logistic Regression from Scratch

```
from sklearn.base import BaseEstimator, ClassifierMixin
import numpy as np
from scipy.special import expit  # ← stable sigmoid

class MyLogisticRegression(BaseEstimator, ClassifierMixin):
    def __init__(self, eta=1e-3, max_iter=2000, tol=1e-6):
        self.eta, self.max_iter, self.tol = eta, max_iter, tol

    def fit(self, X, y):
        Phi = np.c_[np.ones(X.shape[0]), X]          # [1 | X]
        N, D = Phi.shape

        def grad(w):                                  # ∇(avg NLL)
            p = expit(Phi @ w)
            return Phi.T @ (p - y)

        w0 = np.zeros(D)
        w, n_iter, gn = gradient_descent(
            grad, w0, eta=self.eta, max_iter=self.max_iter, tol=self.tol
        )

        self.weights_, self.n_iter_, self.grad_norm_ = w, n_iter, gn
        return self

    def predict_proba(self, X):
        Xs = np.c_[np.ones(X.shape[0]), X]
        z  = Xs @ self.weights_
        p1 = expit(z)
        return np.column_stack([1 - p1, p1])

    def predict(self, X):
        return (self.predict_proba(X)[:, 1] ≥ 0.5).astype(int)
```

Gradient Descent from Scratch

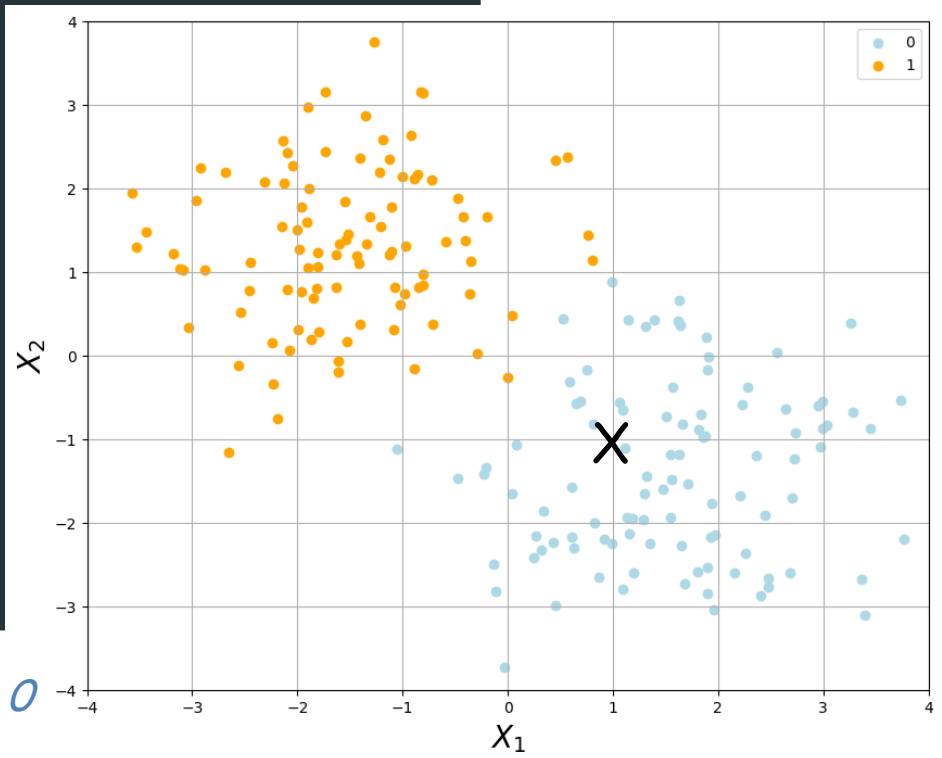
```
from typing import Callable, Tuple
import numpy as np

def gradient_descent(
    grad: Callable[[np.ndarray], np.ndarray],
    w0: np.ndarray,
    eta: float = 0.05,
    max_iter: int = 1000,
    tol: float = 1e-6,
) → Tuple[np.ndarray, int, float]:
    w = np.asarray(w0, dtype=float).ravel()
    n_iter = 0

    for t in range(max_iter):
        g = grad(w)
        gn = float(np.linalg.norm(g))
        if gn ⩽ tol:
            n_iter = t
            break
        w = w - eta * g
        n_iter = t + 1
    else:
        # loop exhausted without break → recompute final grad norm
        gn = float(np.linalg.norm(grad(w)))

    return w, n_iter, gn
```

Usage Example

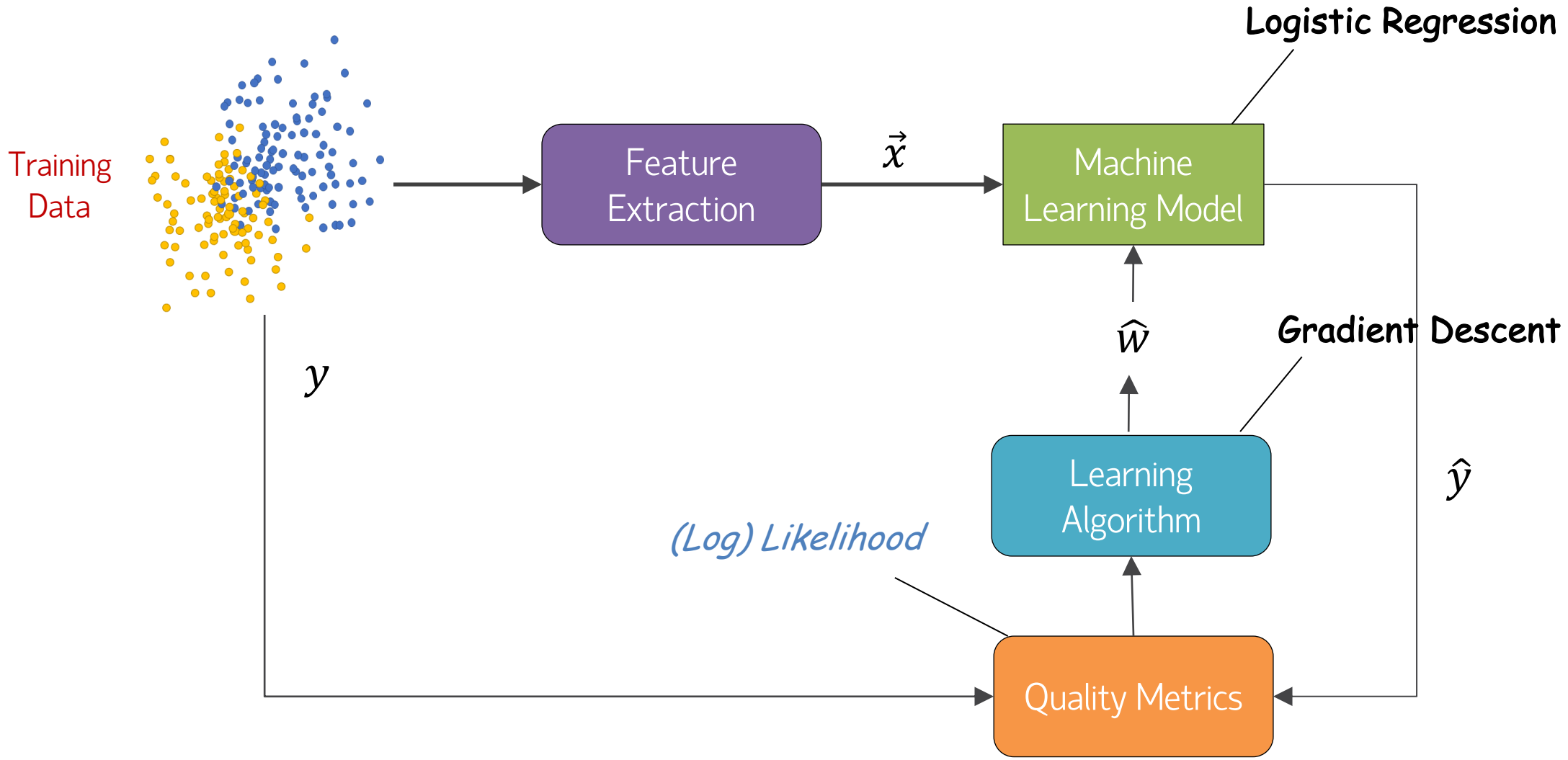
```
import numpy as np
# from your_module import MyLogisticRegression  # class already defined earlier

# ----- data generation -----
m, n = 100, 2
np.random.seed(0)

class_0 = np.hstack((1.5 + np.random.randn(m, 1), -1.5 + np.random.randn(m, 1)))
class_1 = np.hstack((-1.5 + np.random.randn(m, 1),  1.5 + np.random.randn(m, 1)))

X_train = np.vstack((class_0, class_1))          # shape (2m, 2)
y_train = np.concatenate([np.zeros(m), np.ones(m)])  # shape (2m,)

# one (or more) test points (no bias term needed; the model adds it)
X_test = np.array([[1.0, -1.0]])                 # shape (1, 2)

# ----- train -----
eta, max_iter, tol = 0.1, 1000, 1e-6
model = MyLogisticRegression(eta=eta, max_iter=max_iter, tol=tol)
model.fit(X_train, y_train)

# ----- predict on X_test -----
proba = model.predict_proba(X_test)[:, 1]        # P(y=1 | x)

print(f"Predicted probability for X_test: {proba[0]:.4f}")
```

```
Predicted probability for X_test: 0.0069173]
```

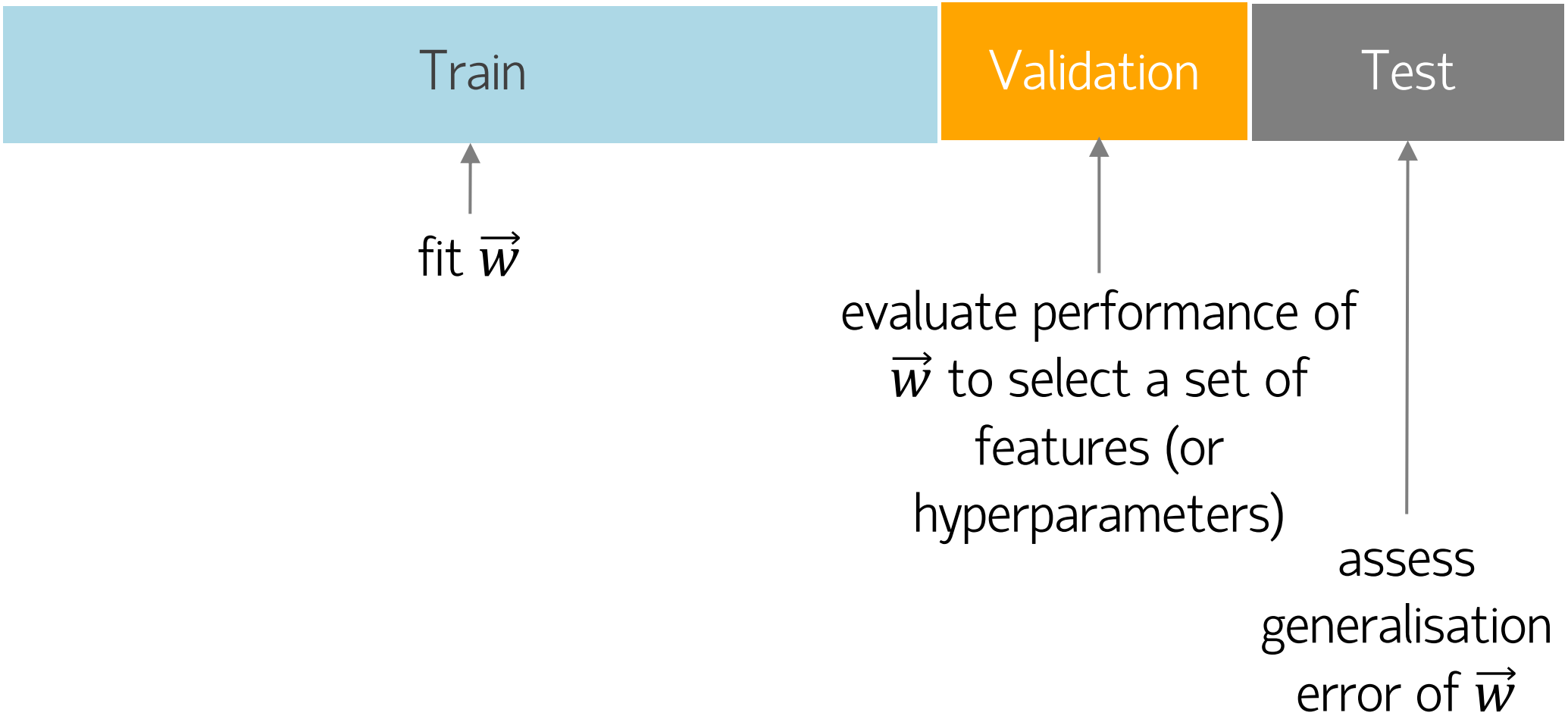
~0.007 → Class 0



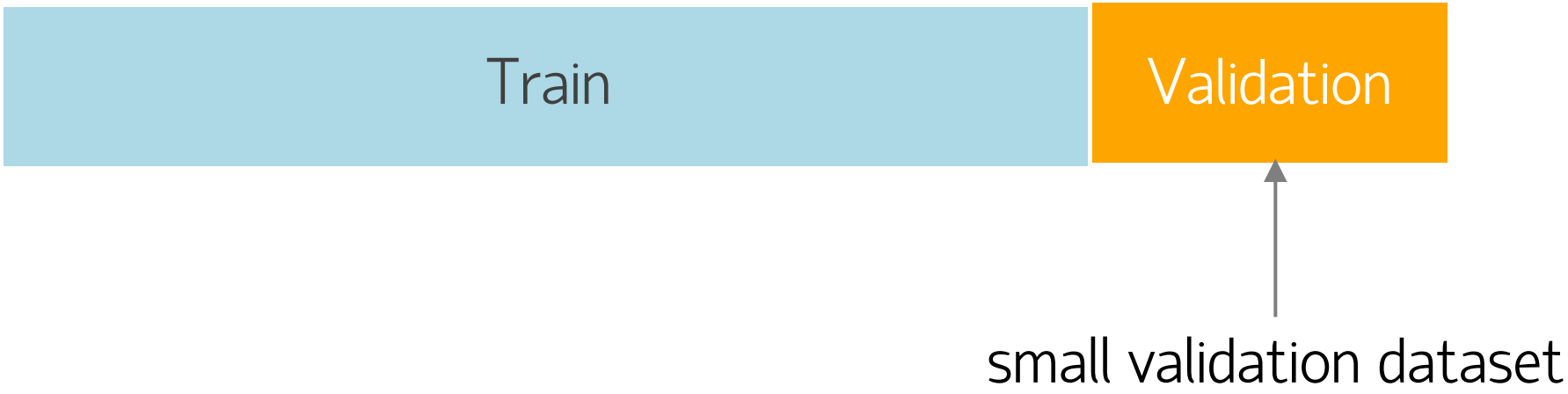
Workflow: Logistic Regression



Large Dataset



Small Dataset



Q: Is validation set enough to compare performance of $\vec{w}$ across a set of features (or hyperparameters)?

A: No.

Choosing Validation Dataset

Q: Which subset should we use?

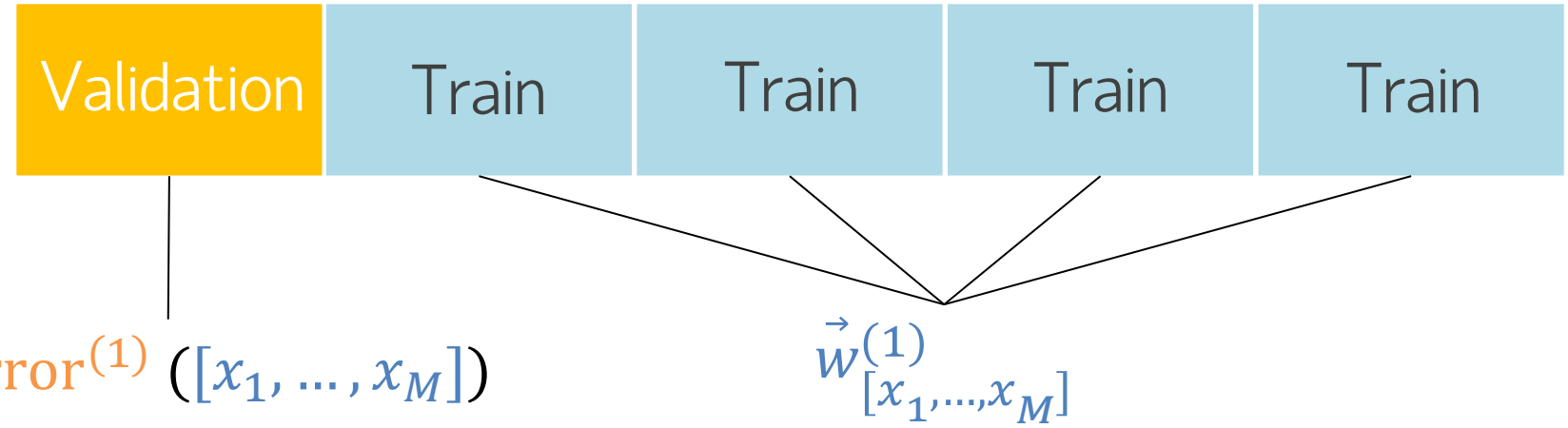
A: All. We can average performance over all choices.

K-Fold Cross Validation

k = 5

We commonly use either 70% or 80% of the overall data for training. For K-fold, we randomly split the data into K groups (or folds), where K is typically either 3, 5 or 10.

K-Fold Cross Validation



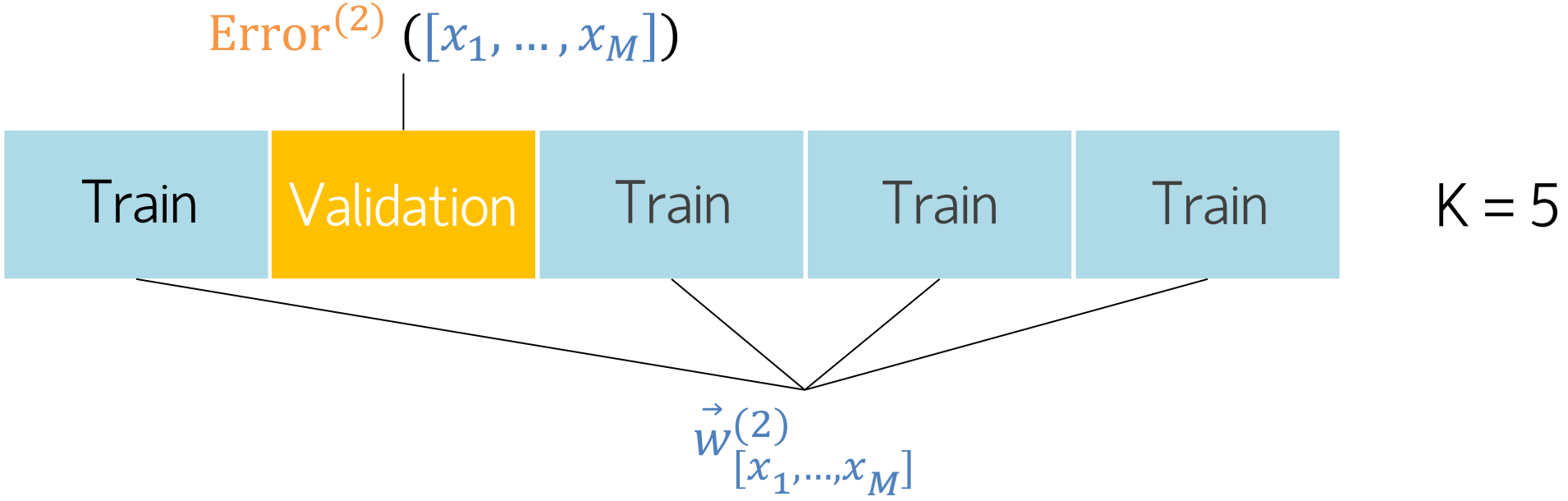
$[x_1, \ldots, x_M]$ is a set of features.

For k = 1, ..., K

Step 1: Estimate $\vec{w}^{(k)}_{[x_1,\ldots,x_M]}$ on the training blocks.

Step 2: Compute error on Validation Block: $\text{Error}^{(k)}([x_1, \ldots, x_M])$.

K-Fold Cross Validation

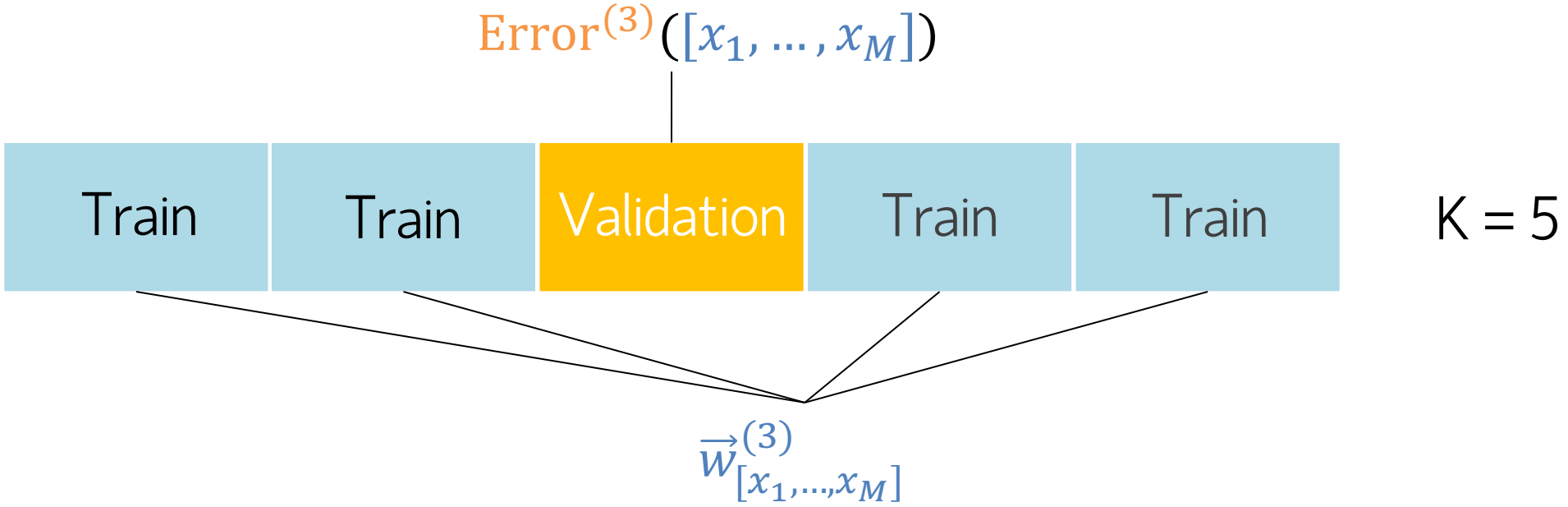


For k = 1, ..., K

Step 1: Estimate $\vec{w}^{(k)}_{[x_1,\ldots,x_M]}$ on the training blocks.

Step 2: Compute error on Validation Block: $\text{Error}^{(k)}([x_1, \ldots, x_M])$.

K-Fold Cross Validation

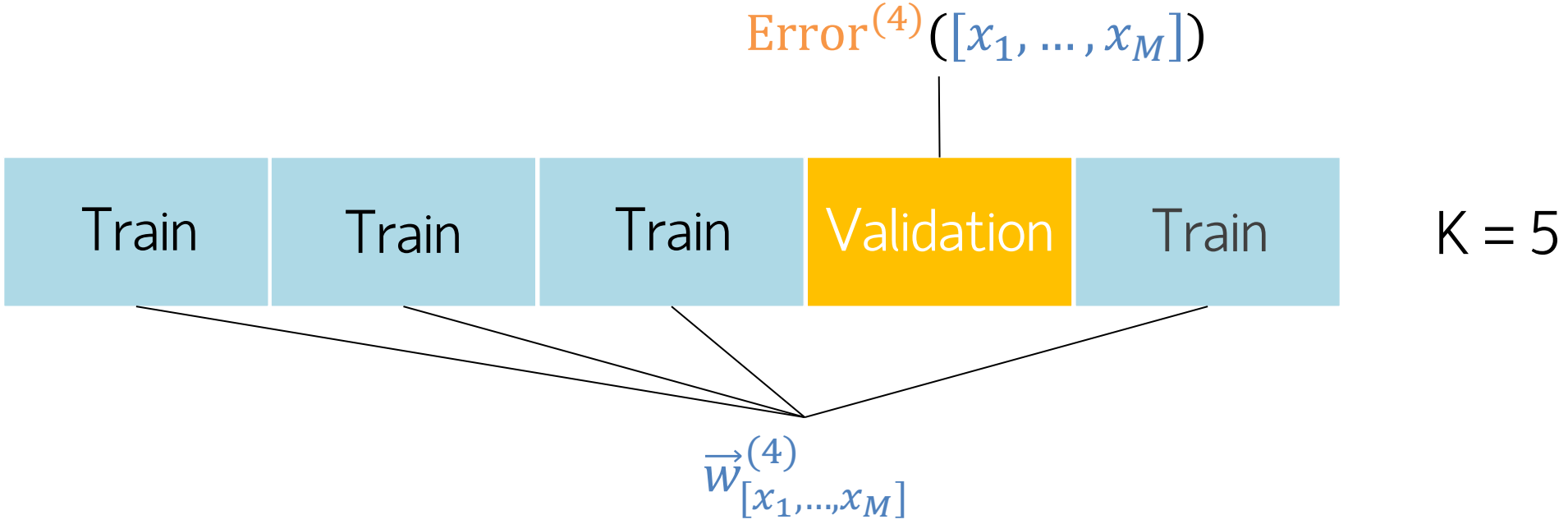


For k = 1, ..., K

Step 1: Estimate $\vec{w}^{(k)}_{[x_1,\ldots,x_M]}$ on the training blocks.

Step 2: Compute error on Validation Block: $\text{Error}^{(k)}([x_1, \ldots, x_M])$.

K-Fold Cross Validation

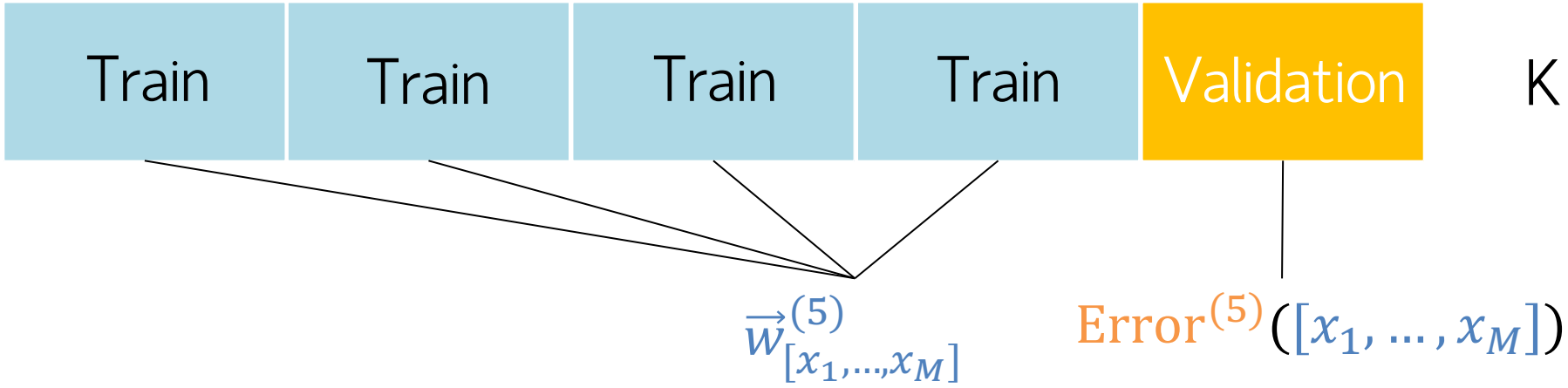


For k = 1, ..., K

Step 1: Estimate $\vec{w}^{(k)}_{[x_1,\ldots,x_M]}$ on the training blocks.

Step 2: Compute error on Validation Block: $\text{Error}^{(k)}([x_1, \ldots, x_M])$.

K-Fold Cross Validation



For k = 1, ..., K

Step 1: Estimate $\vec{w}^{(k)}_{[x_1,\ldots,x_M]}$ on the training blocks.

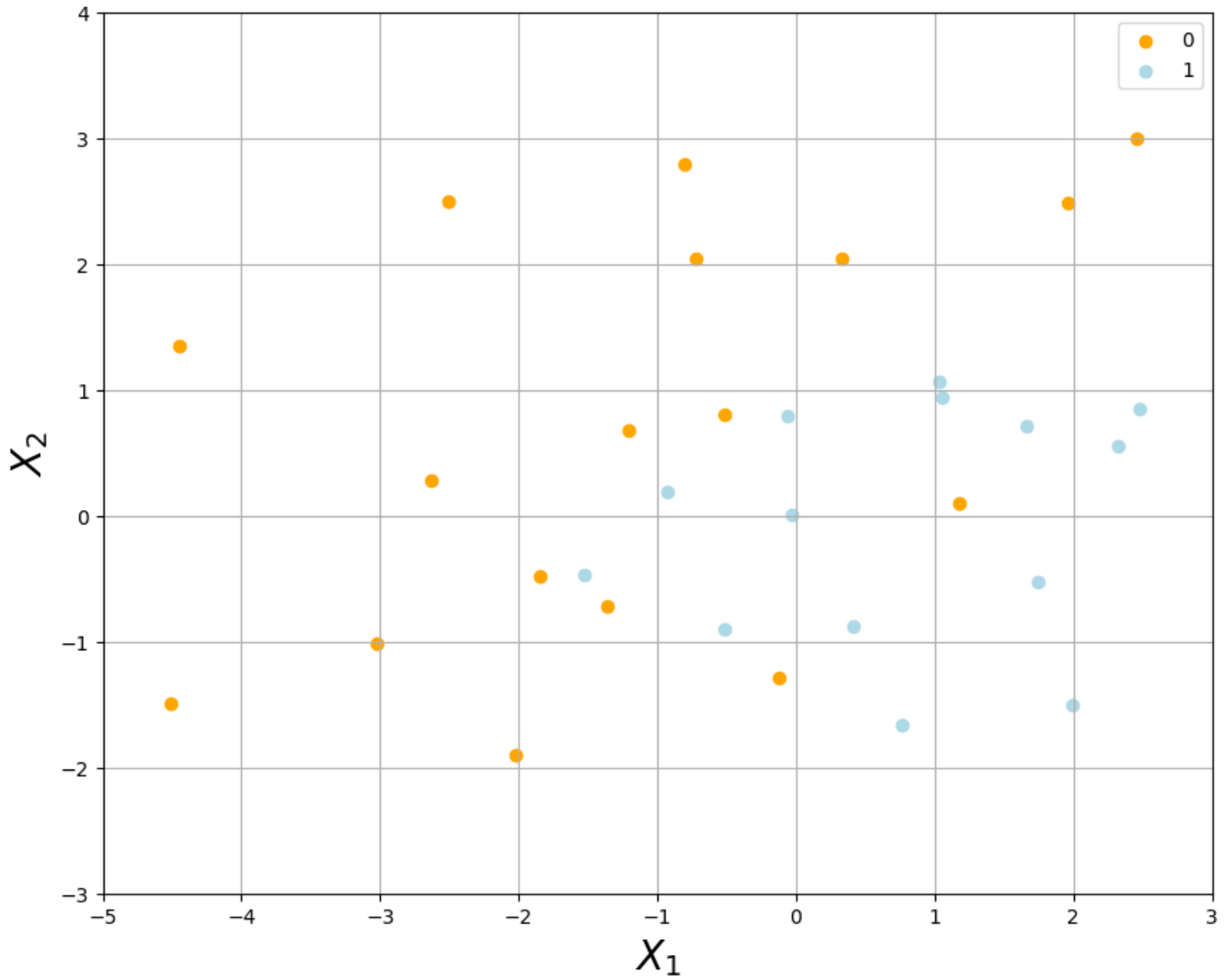
Step 2: Compute error on Validation Block: $\text{Error}^{(k)}([x_1, \ldots, x_M])$.

Compute Average Error: $\text{CV}([x_1, \ldots, x_M]) = \frac{1}{K}\sum_{k=1}^{K} \text{Error}^{(k)}([x_1, \ldots, x_M])$.

Pseudocode for Cross-Validation

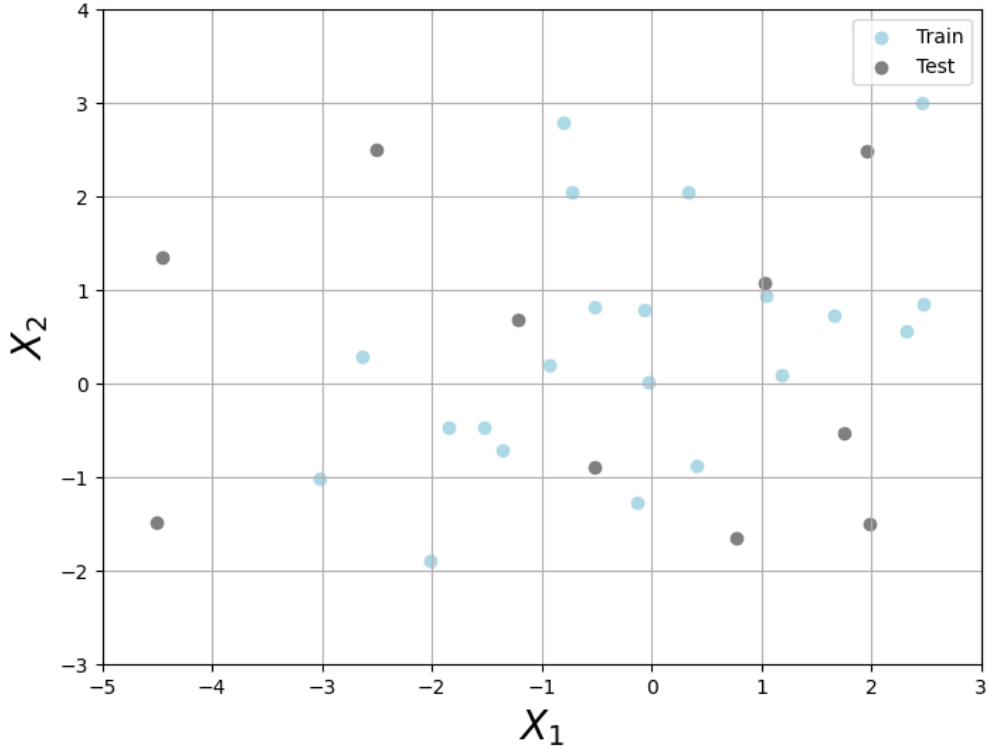
```
# Inputs
#  model    ← untrained estimator (cloneable)
#  X, y     ← dataset
#  cv       ← splitter yielding (train_idx, val_idx)  e.g., KFold
#  scoring  ← string name or callable scorer(est, X, y)

# ----- evaluate across folds -----
scores ← empty list

FOR (train_idx, val_idx) IN cv.split(X, y) DO
  est ← clone(model)                              # fresh copy per fold

  X_tr ← X[train_idx]    ;  y_tr ← y[train_idx]
  X_va ← X[val_idx]      ;  y_va ← y[val_idx]

  fit est on (X_tr, y_tr)

  IF is_callable(scoring) THEN
      s ← scoring(est, X_va, y_va)
  ELSE
      s ← LOOKUP_SCORER(scoring)(est, X_va, y_va)
  END IF

  append s to scores
END FOR

RETURN scores                                      # like sklearn's cross_val_score
# (optional) mean_score ← mean(scores)
```

Example Dataset



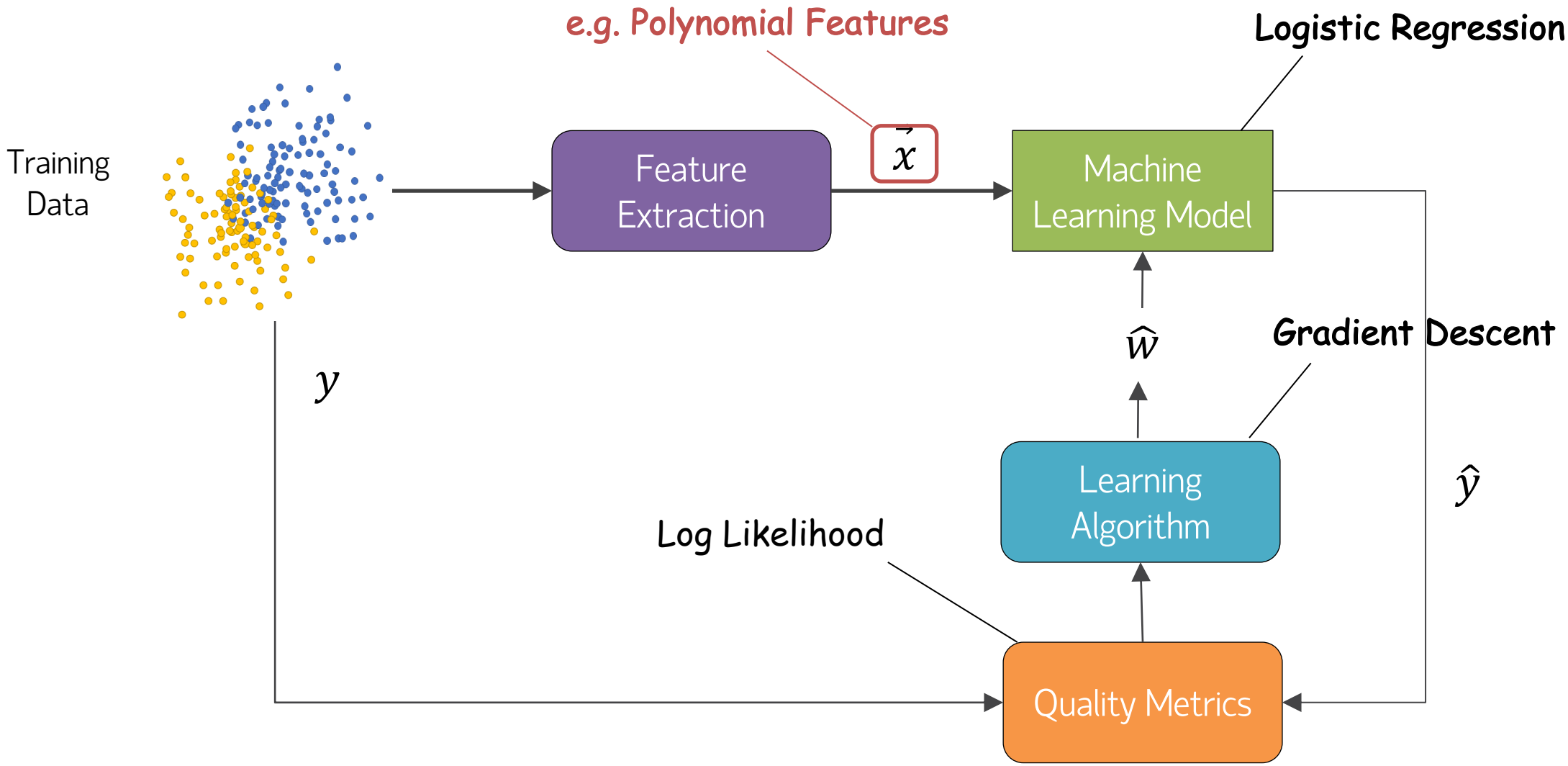
Train, Validation and Test Datasets

```
from sklearn.model_selection import train_test_split

# First, split the data into train (70%) and test (30%)
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.3, random_state=42, stratify=y)
```



- Train:Test is typicaly either 0.8:0.2 or 0.7:0.3.
- **Test** dataset is a proxy of unseen data, and it will only be used in the final evaluation.
- **Train** dataset is further divided into k folds (e.g., 5 or 10).For each fold, the model is trained on k-1 folds and validated on the remaining fold.
- We use **K-Fold Cross-Validation** to fine-tune or optimize the ML model. Here, we find a set of hyper-parameters (or features) based on the average performance across folds.

Workflow: Logistic Regression

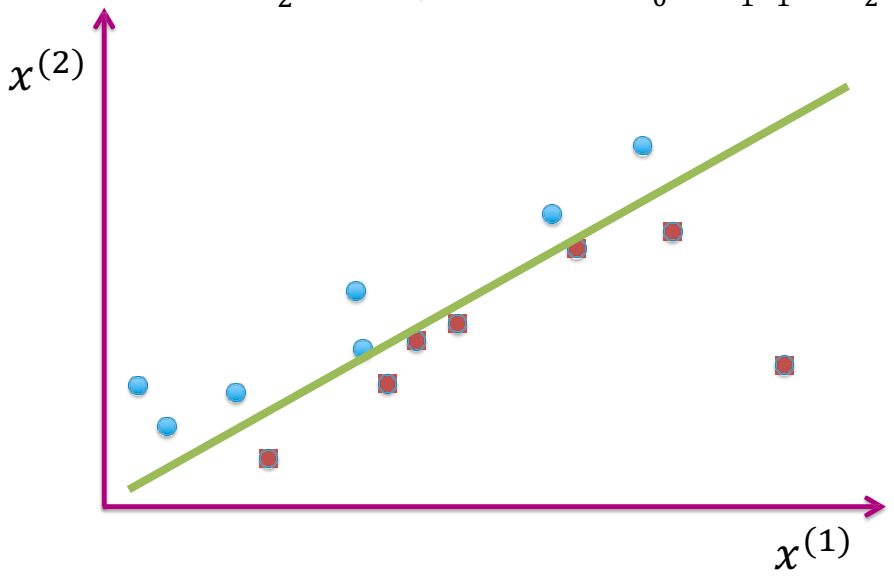


Feature Extraction: Polynomial Features

$$\vec{x} = \begin{bmatrix} 1 \\ x_1 \\ x_2 \end{bmatrix}$$

$$0 = \vec{x}^T \times \vec{w}$$

$$0 = w_0 + w_1 x_1 + w_2 x_2$$



1st Degree: $\vec{x} = [1 \quad x_1 \quad x_2]^T$

2nd Degree: $\vec{x} = [1 \quad x_1 \quad x_2 \quad (x_1)^2 \quad (x_2)^2]^T$

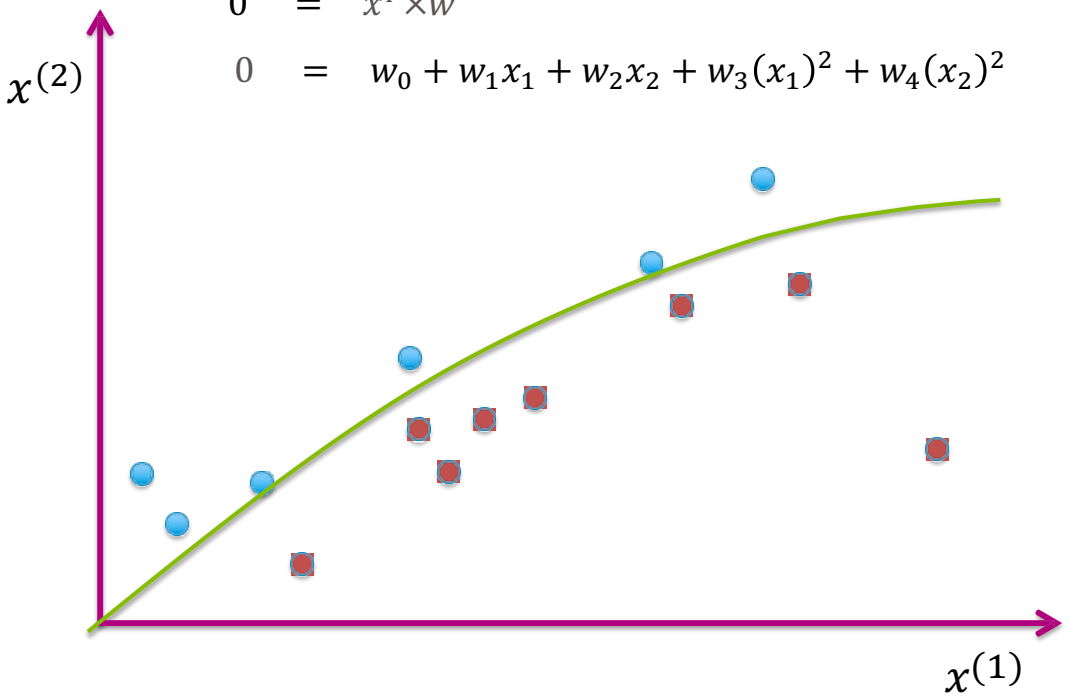
3rd Degree: $\vec{x} = [1 \quad x_1 \quad x_2 \quad (x_1)^2 \quad (x_2)^2 \quad (x_1)^3 \quad (x_2)^3]^T$

N^{th} Degree: $\vec{x} = [1 \quad x_1 \quad x_2 \quad \cdots \quad (x_1)^N \quad (x_2)^N]^T$

$$\vec{x} = [1 \quad x_1 \quad x_2 \quad (x_1)^2 \quad (x_2)^2]^T$$

$$0 = \vec{x}^T \times \vec{w}$$

$$0 = w_0 + w_1 x_1 + w_2 x_2 + w_3 (x_1)^2 + w_4 (x_2)^2$$



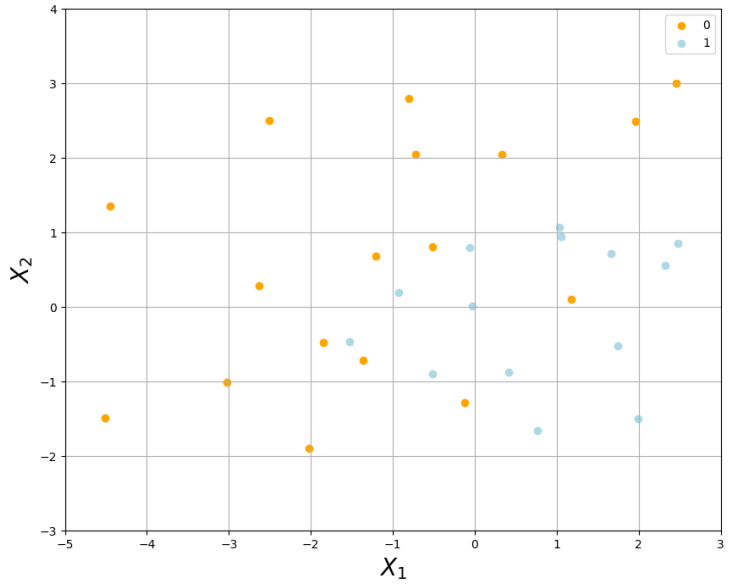
scikit-learn: Logistic Regression

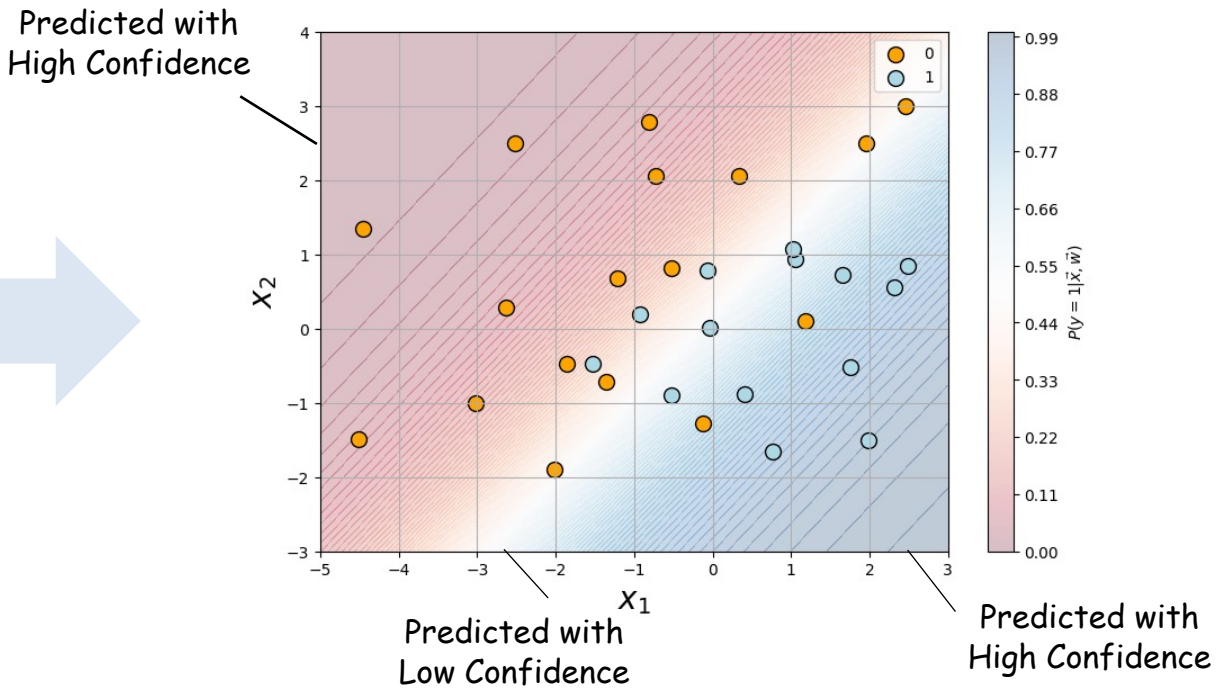
```
import numpy as np
from sklearn.linear_model import LogisticRegression
from sklearn.model_selection import KFold, cross_val_score

# Step 1: Create an instance of LogisticRegression
model = LogisticRegression(penalty=None)

# Step 2: Define cross-validation strategy
k = 5
kf = KFold(n_splits=k, shuffle=True, random_state=42)

# Step 3: Perform cross-validation on the training data
cv_scores = cross_val_score(model, X_train, y_train, cv=kf, scoring='accuracy')
print("Mean Cross-Validation Accuracy: {:.2f}".format(np.mean(cv_scores)))
# optional: print per-fold scores
# print("Per-fold:", cv_scores)
```


```
Mean Cross-Validation Accuracy: 0.781
```

Learned Decision Boundary

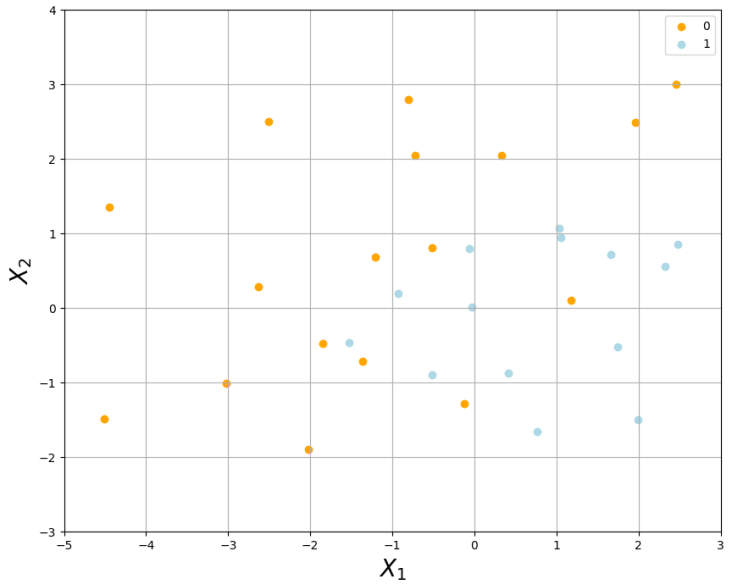
Feature	Coefficient
1	0.246
x_1	1.113
x_2	-1.062

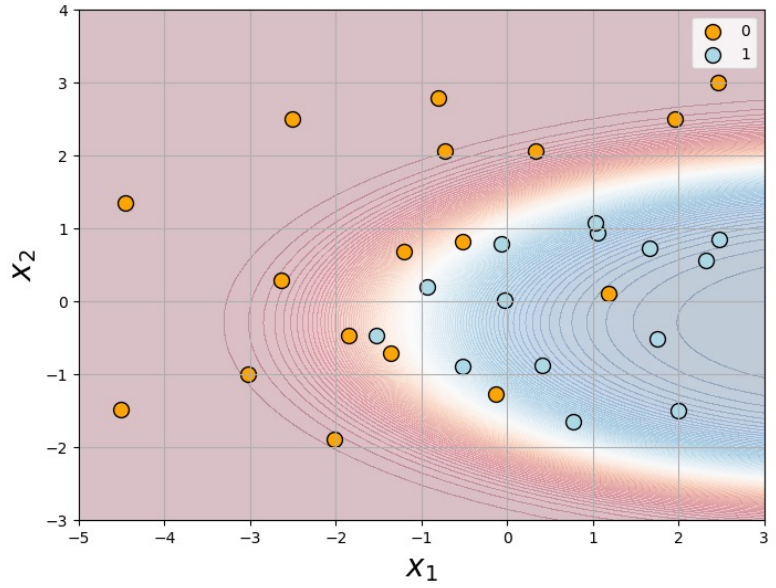




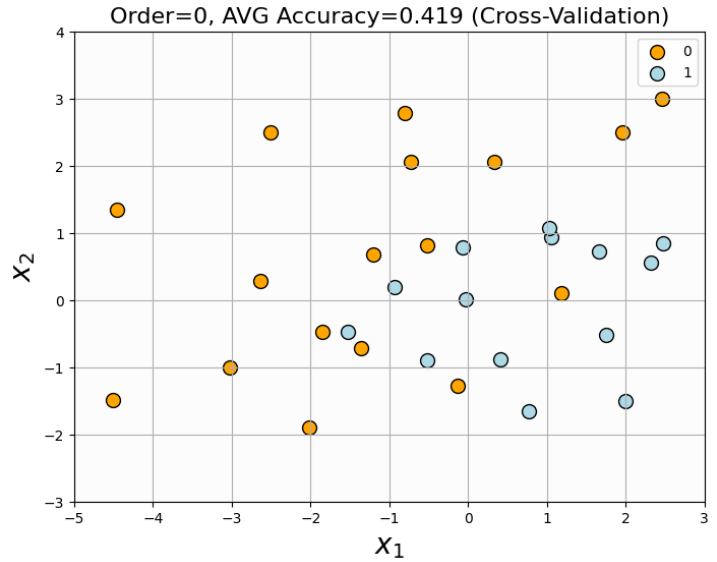
Learned Decision Boundary (2nd Order)

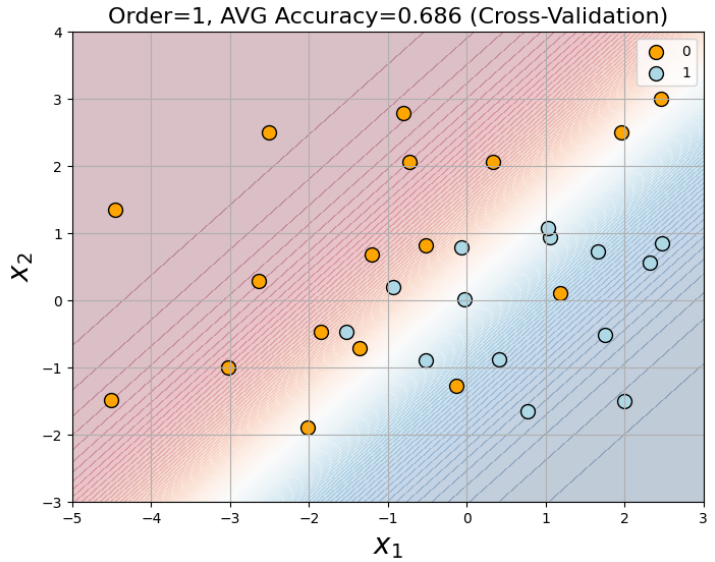
Feature	Coefficient
1	1.717
x_1	1.385
x_2	-0.579
x_1^2	-0.167
x_2^2	0.978

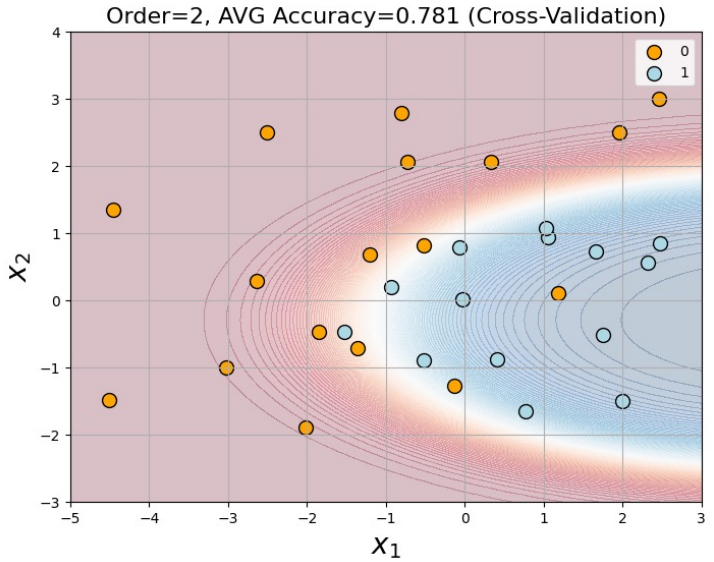


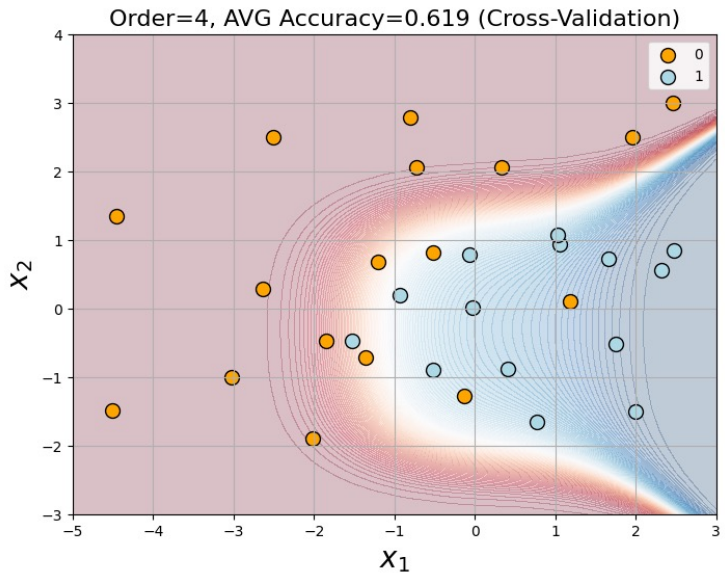


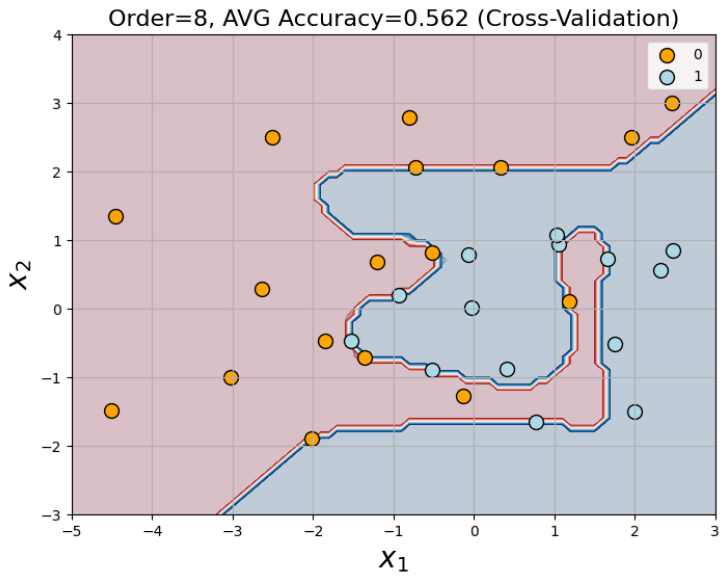
Model Complexity

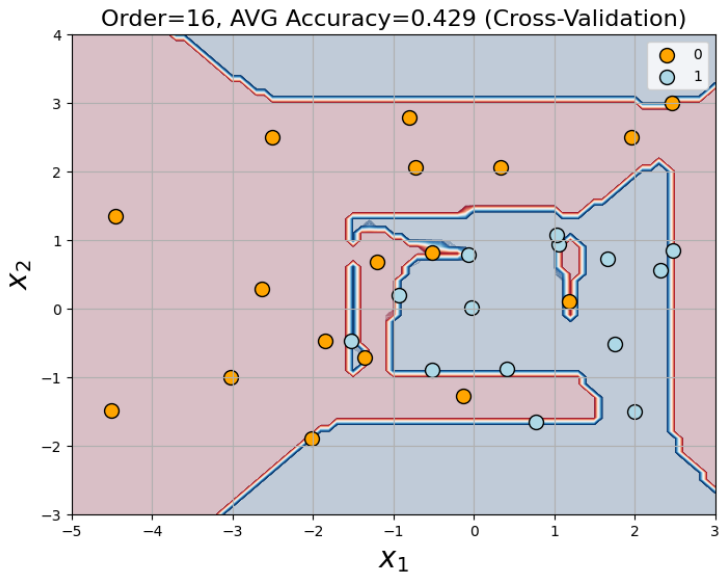








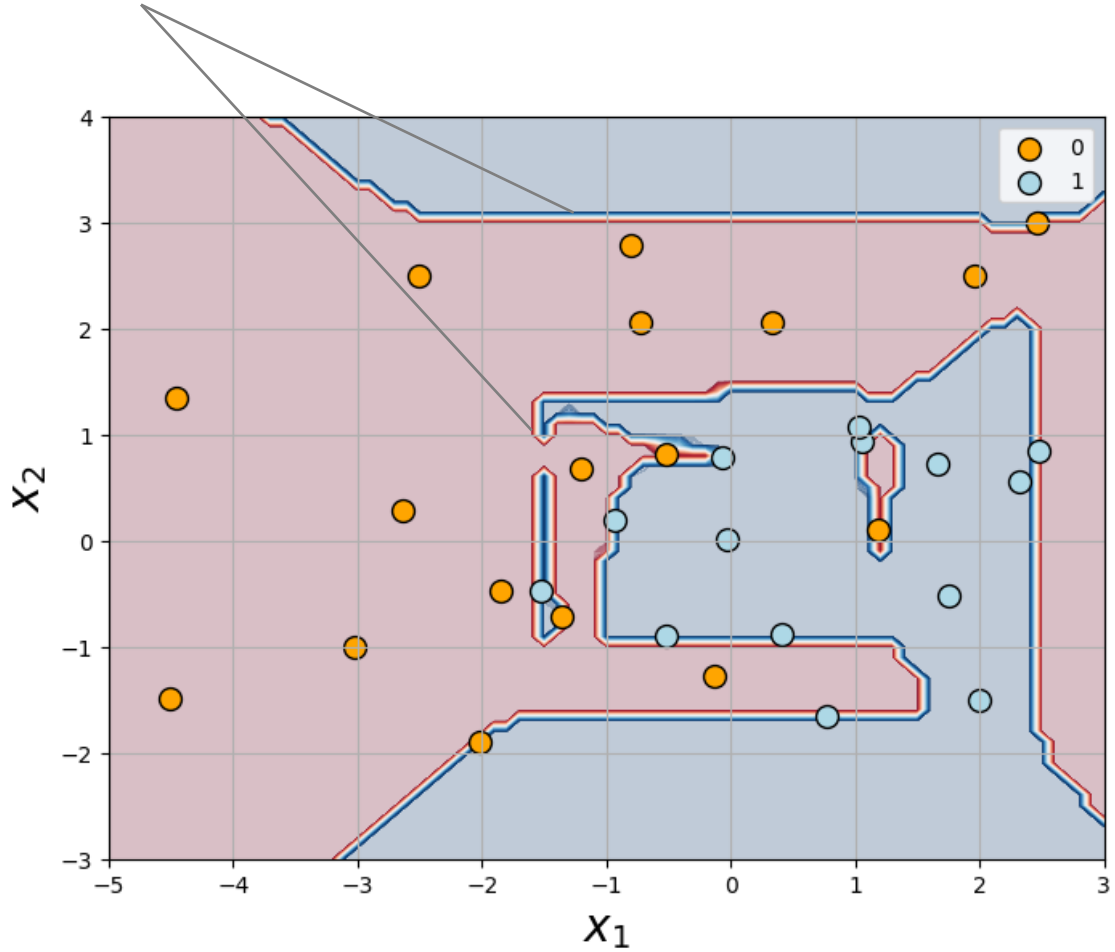




Over-Confident Predictions

Tiny Uncertain Regions → Overfitting & Over-Confident Predictions

We are sure we are right, when we are surely wrong.



Credit Card Fraud

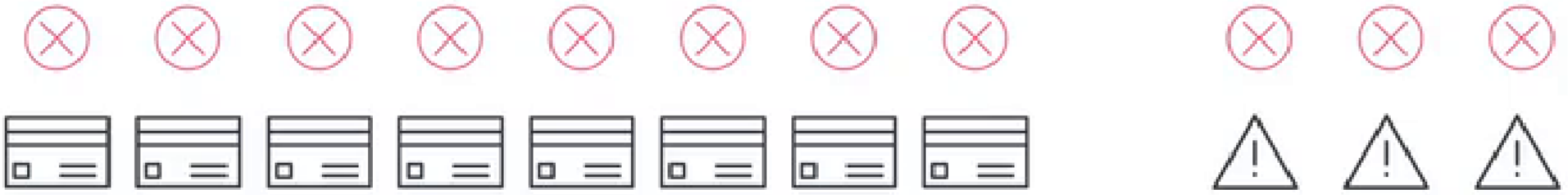
Our model predicted all transaction are good.

$$\text{Accuracy} = \frac{284{,}335}{284{,}887}$$

$$= 99.83\%$$

Problem: We're not catching any of the bad ones.

Credit Card Fraud

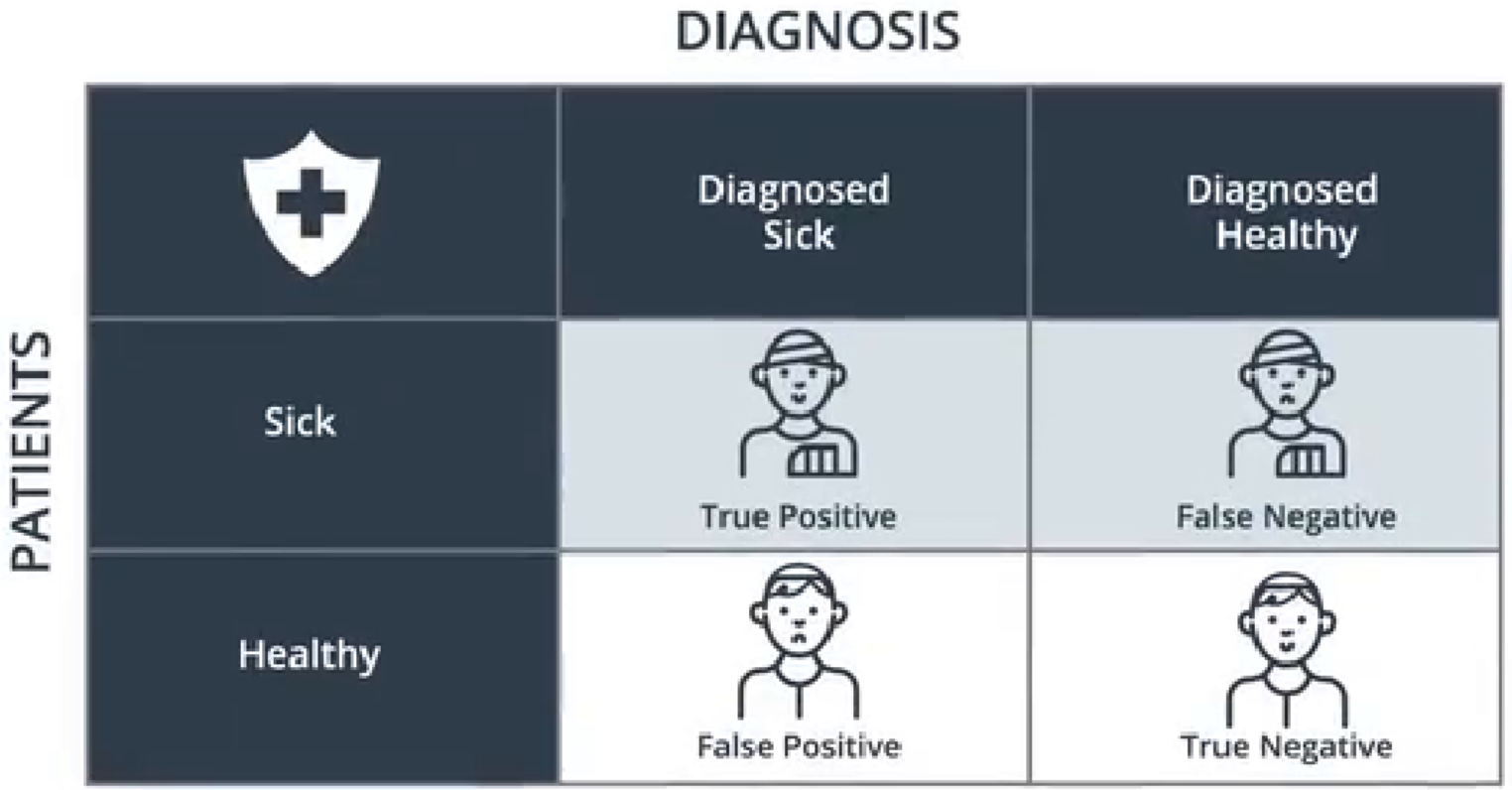


Our model predicted all transactions are fraudulent.

Great! Now, we're catching all of the fraudulent transactions.

Problem: We're accidentally catching all of the good ones.

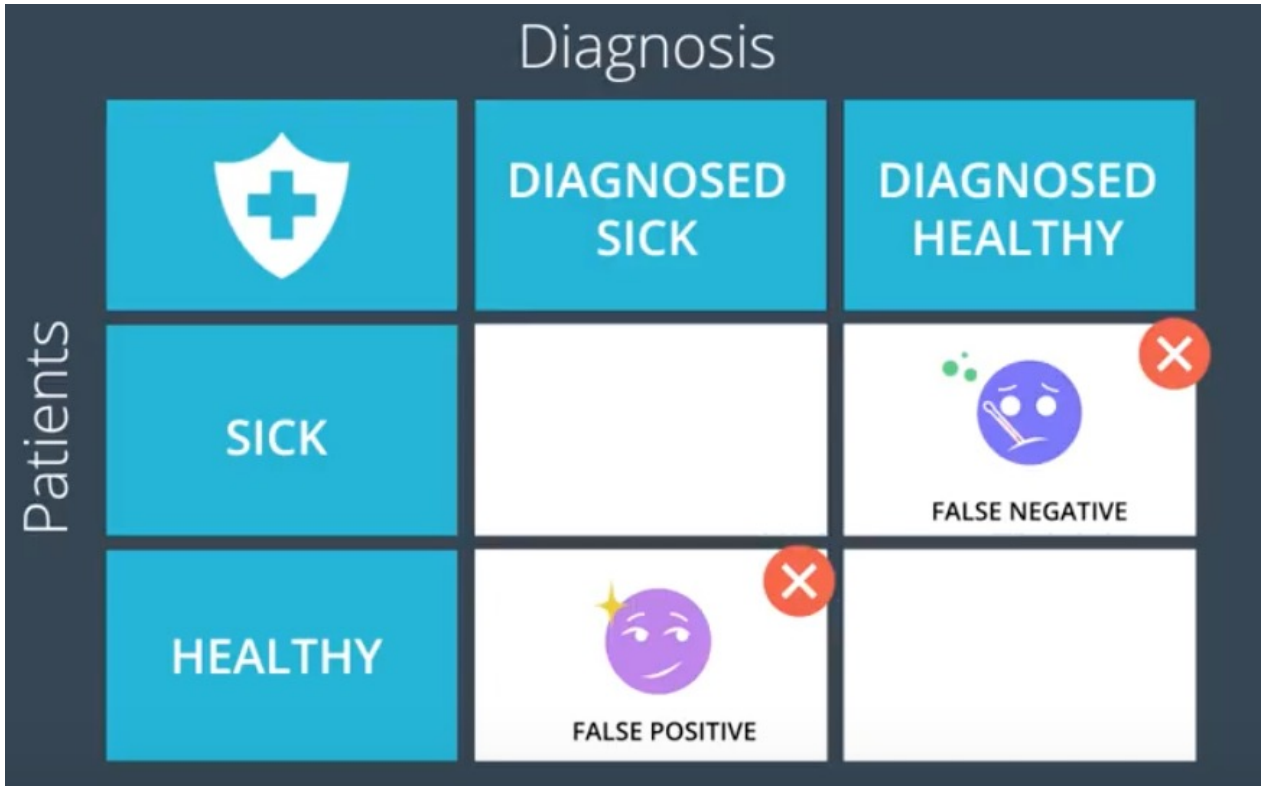
Quiz: False Positives and Negatives



Quiz: False Positives and Negatives

Which one do you think is worse, a false positive or a false negative? In other words, what is the worst mistake, to misdiagnose a healthy patient as sick or a sick patient as healthy?

- ☐ False Positive
- ☐ False Negative



Quiz: False Positives and Negatives

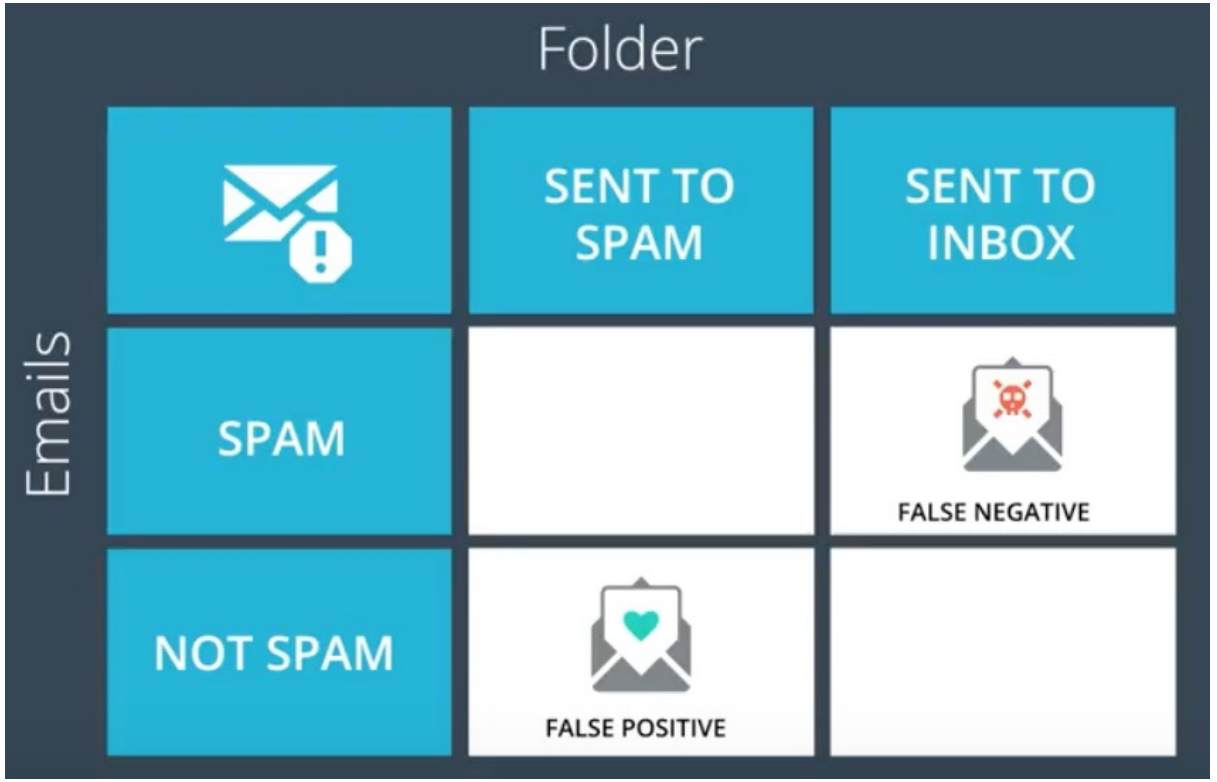
FOLDER

EMAIL	Sent to Spam Folder	Sent to Inbox
Spam	True Positive	False Negative
Not Spam	False Positive	True Negative

Quiz: False Positives and Negatives

Which one do you think is worse, a false positive or a false negative? In other words, what is the worst mistake, to accidentally send your grandma's email to the spam folder or to accidentally send the spam email into your inbox?

- ☐ False Positive
- ☐ False Negative

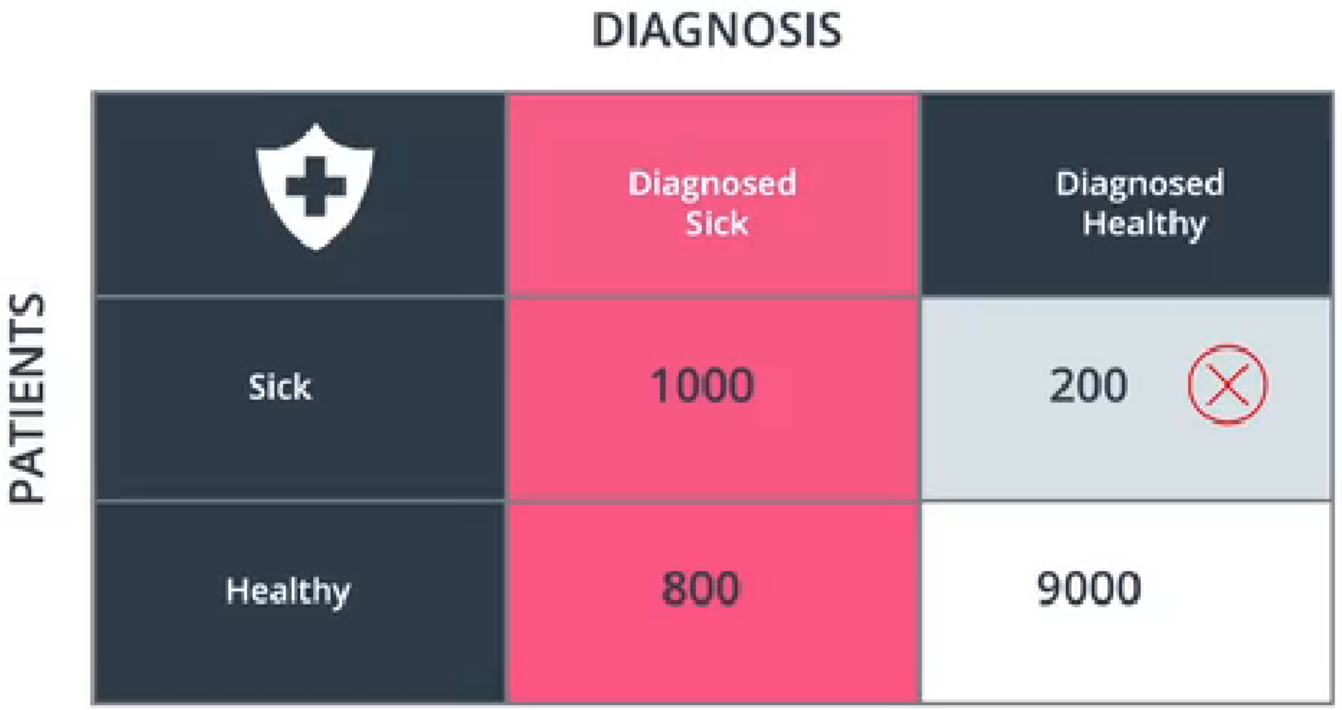


Solution: False Positives and Negatives

High Recall

High Precision

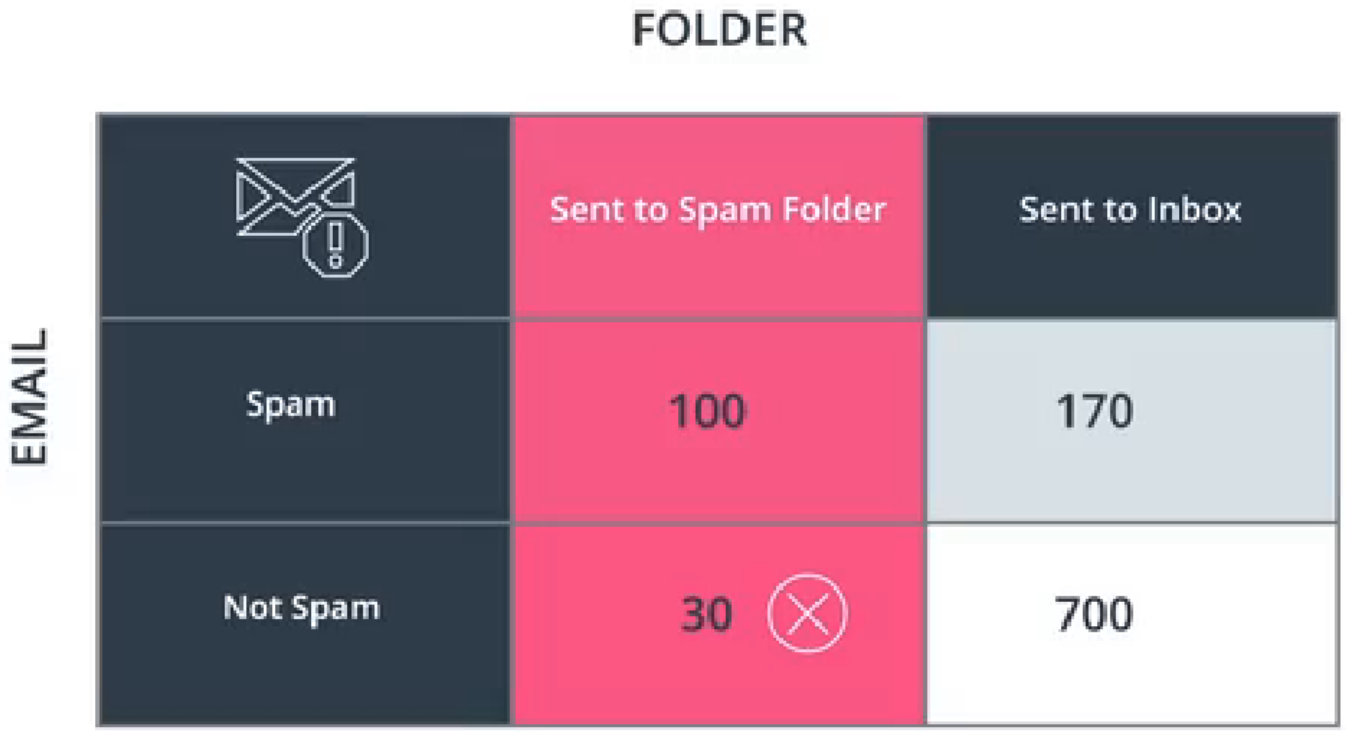
Precision



PRECISION: OUT OF THE PATIENTS WE DIAGNOSED WITH AN ILLNESS, HOW MANY DID WE CLASSIFY CORRECTLY?

$$\text{PRECISION} = \frac{1{,}000}{1{,}000 + 800} = 55.6\%$$

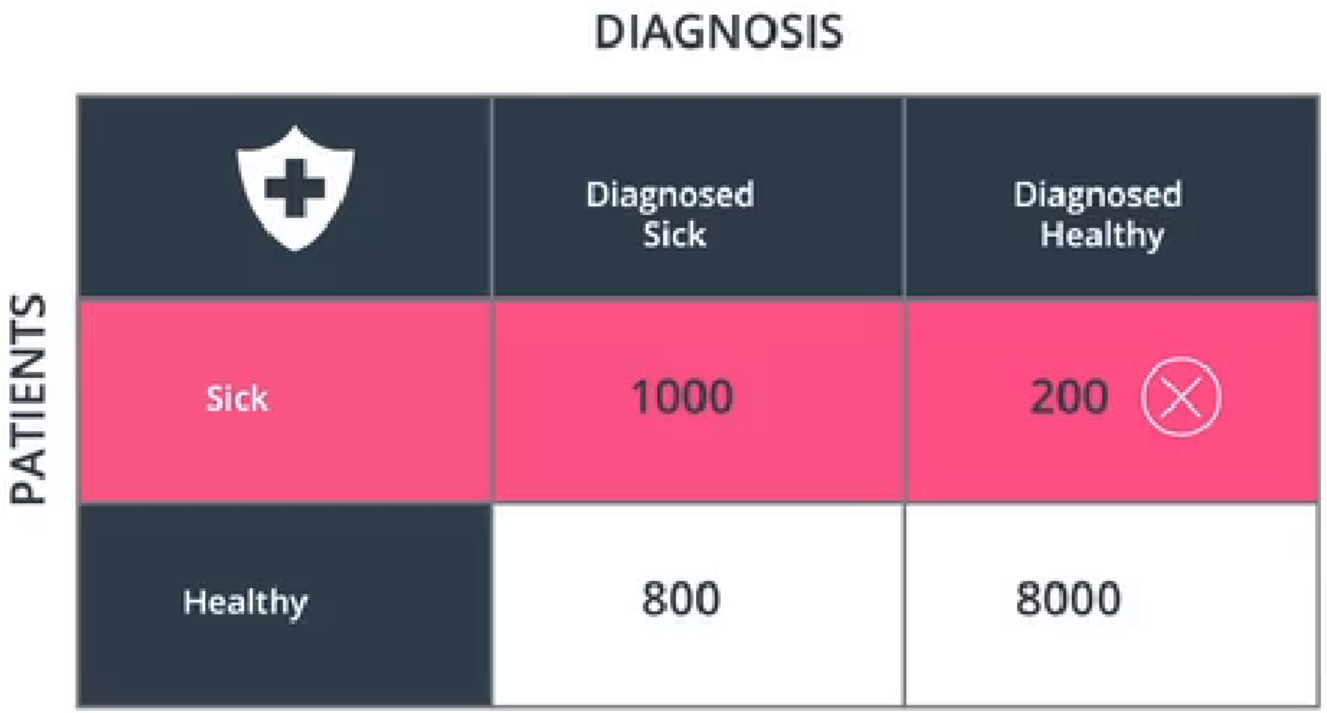
Precision



OUT OF ALL THE E-MAILS
SENT TO THE SPAM FOLDER,
HOW MANY WERE ACTUALLY SPAM?

$$\text{PRECISION} = \frac{100}{100 + 30}$$

Recall



OUT OF THE SICK PATIENTS, HOW MANY DID WE CORRECTLY DIAGNOSE AS SICK?

$$\text{RECALL} = \frac{1{,}000}{1{,}000 + 200} = 83.3\%$$

Recall

FOLDER

EMAIL

	Sent to Spam Folder	Sent to Inbox
Spam	100	170
Not Spam	30	700

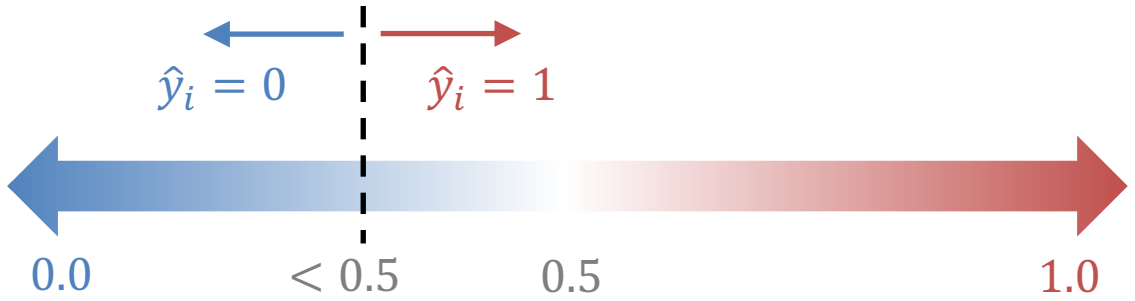
OUT OF ALL THE SPAM E-MAILS, HOW MANY WERE CORRECTLY SENT TO THE SPAM FOLDER?

$$\text{Recall} = \frac{100}{100 + 170} = 37\%$$

Output Probability and Recall Rate

Q: How can we improve recall?

A: We set the threshold, i.e. cut-off probability, to be lower than 0.5.



$$P\left(y = 1 \,|\, \vec{x}_i\right)$$

$$\text{Recall} = \frac{TP}{TP + FN}$$

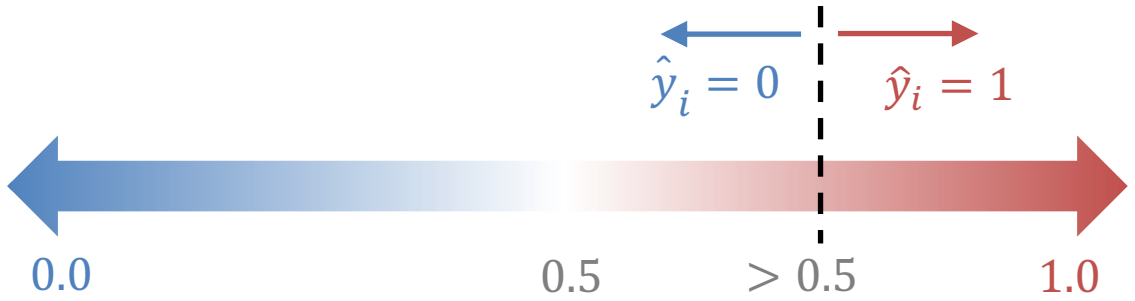
Lower Threshold → Higher TP → Higher Recall.

(also Higher FP)

Output Probability and Precision Rate

Q: How can we improve precision?

A: We set the threshold, i.e. cut-off probability, to be higher than 0.5.



$$P\left(y = 1 \,\middle|\, \vec{x}_i\right)$$

$$\text{Precision} = \frac{TP}{TP + FP}$$

Higher Threshold → Lower FP → Higher Precision.

(also Higher FN)

F_1 Score

MEDICAL MODEL

PRECISION: 55.7%

RECALL: 83.3%

One Score?

SPAM DETECTOR

PRECISION: 76.9%

RECALL: 37%

$$F_1 \text{ Score} = \frac{\text{Precision} \times \text{Recall}}{\text{Precision} + \text{Recall}}$$

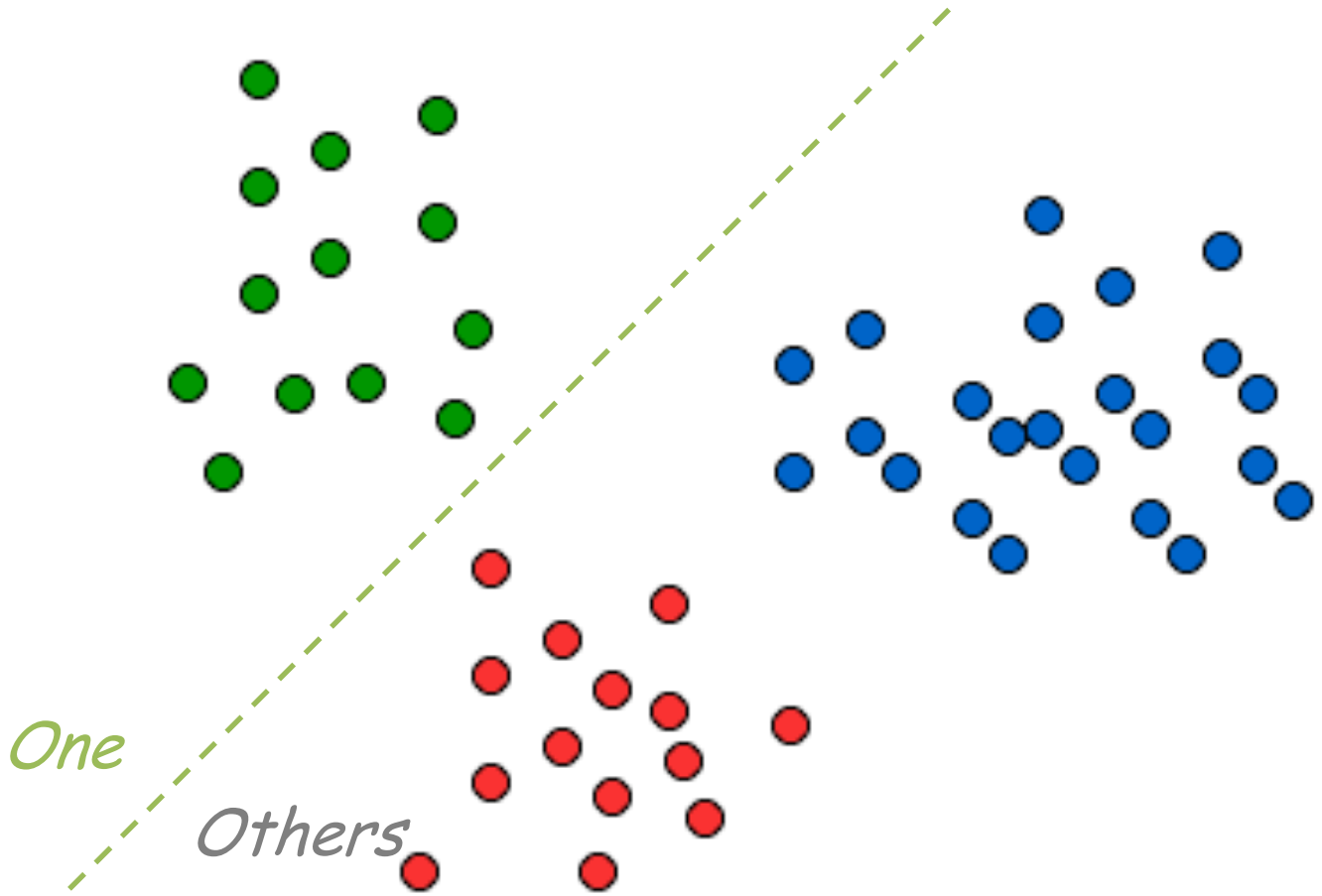
Geometric Mean

Credit Card Fraud

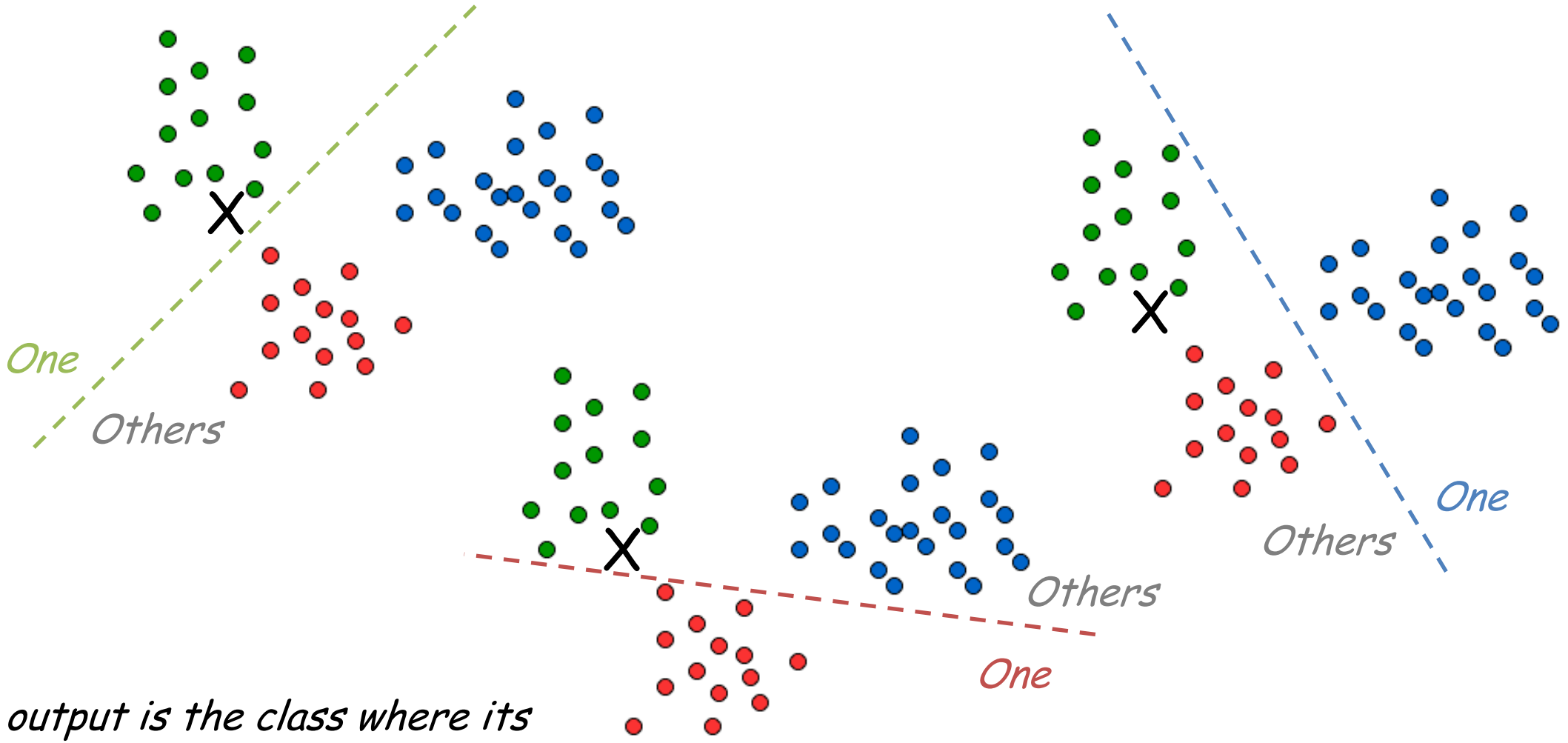
Our model predicted all transaction are good.

$$\text{Prediction} = 100\% \qquad F_1 \text{ Score} = 0 \qquad \text{Recall} = 0\%$$

Multiclass Classification



3 Logistic Classifiers



The output is the class where its output probability is the highest (among the 3 classifiers).

Ex. [0.6, 0.4, 0.1] → Green Class

Pseudocode for Multi-Class Classifiers

```
# Inputs
#  models  ← list of C trained binary classifiers (one per class)
#  C       ← number of classes (C = length(models))
#  X_query ← set of examples to predict

# ----- predict -----
ŷ     ← list of length |X_query|                # predicted class per example
P     ← matrix of size |X_query| × C            # per-class probabilities (optional)

FOR i = 1 TO |X_query| DO
  x* ← X_query[i]

  FOR c = 1 TO C DO
    P[i, c] ← models[c].predict_probability(x*)  # p(y = c | x*)
  END FOR

  ŷ[i] ← argmax_index(P[i, :])                  # class with highest prob (1..C)
END FOR

RETURN ŷ, P
```

Summary

- Logistic regression models the probability of a binary outcome by applying a logistic (sigmoid) function to a linear combination of features. This function ensures predicted probabilities are bounded between 0 and 1, making it suitable for classification tasks.
- The decision boundary in logistic regression is defined by a linear combination of features. Data points on either side of this boundary are assigned different class labels, making it useful in applications with linearly separable classes.
- Maximum likelihood estimation (MLE) is used to determine the optimal weights. By maximizing the likelihood (or equivalently, the log-likelihood) of the observed data, logistic regression finds parameters that best explain the class distribution. This is typically achieved through iterative optimization methods like gradient descent.
- Threshold tuning is critical for practical applications. Adjusting the decision threshold allows control over the sensitivity to false positives vs. false negatives. This adjustment makes logistic regression a versatile choice for tasks like fraud detection, medical diagnostics, and risk assessment.
- K-Fold Cross Validation enhances evaluation by splitting data into multiple folds, with each fold used once for validation and the rest for training. This method, often with K=5, maximizes data usage, making it ideal for small datasets. It provides a reliable performance measure by reducing overfitting and ensuring the model generalizes well to unseen data.