

# Polynomial Regression

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# **Warm-up: Linear Regression**

# Linear Regression (Task)


**Input:** vectors  $\mathbf{x}_1, \dots, \mathbf{x}_n \in \mathbb{R}^d$  and labels  $y_1, \dots, y_n \in \mathbb{R}$

**Output:** a vector  $\mathbf{w} \in \mathbb{R}^d$  and scalar  $b \in \mathbb{R}$  such that  $\mathbf{x}_i^T \mathbf{w} + b \approx y_i$ .

Tasks

Linear  
Regression

Inherently assume  $y_i$  is a linear function of  $\mathbf{x}_i$ .



# Least Squares Regression (Method)

**Input:** vectors  $\mathbf{x}_1, \dots, \mathbf{x}_n \in \mathbb{R}^d$  and labels  $y_1, \dots, y_n \in \mathbb{R}$

1. Add one dimension to  $\mathbf{x} \in \mathbb{R}^d$ :  $\bar{\mathbf{x}}_j = [\mathbf{x}_j; 1] \in \mathbb{R}^{d+1}$ .
2. Solve least squares regression:  $\min_{\mathbf{w} \in \mathbb{R}^{d+1}} \|\bar{\mathbf{X}} \mathbf{w} - \mathbf{y}\|_2^2$ .

Tasks

Methods

Linear  
Regression

Least Squares Regression

# Least Squares Regression (Method)

**Input:** vectors  $\mathbf{x}_1, \dots, \mathbf{x}_n \in \mathbb{R}^d$  and labels  $y_1, \dots, y_n \in \mathbb{R}$

1. Add one dimension to  $\mathbf{x} \in \mathbb{R}^d$ :  $\bar{\mathbf{x}}_j = [\mathbf{x}_j; 1] \in \mathbb{R}^{d+1}$ .
2. Solve least squares regression:  $\min_{\mathbf{w} \in \mathbb{R}^{d+1}} \|\bar{\mathbf{X}} \mathbf{w} - \mathbf{y}\|_2^2$ .

Tasks

Linear  
Regression

Methods

Least Squares Regression

Algorithms

Analytical Solution

Gradient Descent (GD)

Conjugate Gradient

# Polynomial Regression

# The Regression Task

**Input:** vectors  $\mathbf{x}_1, \dots, \mathbf{x}_n \in \mathbb{R}^d$  and labels  $y_1, \dots, y_n \in \mathbb{R}$ .

**Output:** a function  $f: \mathbb{R}^d \mapsto \mathbb{R}$  such that  $f(\mathbf{x}) \approx y$ .

**Question:**  $f$  is unknown! So how to learn  $f$ ?

**Answer:** polynomial approximation;  $f$  is a polynomial function.

# Polynomial Regression: 1D Example

**Input:** scalars  $x_1, \dots, x_n \in \mathbb{R}$  and labels  $y_1, \dots, y_n \in \mathbb{R}$ .

**Output:** a function  $f: \mathbb{R} \mapsto \mathbb{R}$  such that  $f(x) \approx y$ .

**One-dimensional example:**  $f(x) = w_0 + w_1x + w_2x^2 + \dots + w_px^p$ .

**Polynomial regression:**

1. Define a feature map  $\boldsymbol{\phi}(x) = [1, x, x^2, x^3, \dots, x^p]$ .
2. For  $j = 1$  to  $n$ , do the mapping  $x_j \mapsto \boldsymbol{\phi}(x_j)$ .
  - Let  $\boldsymbol{\Phi} = [\boldsymbol{\phi}(x_1); \dots, \boldsymbol{\phi}(x_n)]^T \in \mathbb{R}^{n \times (p+1)}$
3. Solve the least squares regression  $\min_{\mathbf{w} \in \mathbb{R}^{p+1}} \|\boldsymbol{\Phi} \mathbf{w} - \mathbf{y}\|_2^2$ .



# Polynomial Regression: 2D Example

**Input:** vectors  $\mathbf{x}_1, \dots, \mathbf{x}_n \in \mathbb{R}^2$  and labels  $y_1, \dots, y_n \in \mathbb{R}$ .

**Output:** a function  $f: \mathbb{R}^2 \mapsto \mathbb{R}$  such that  $f(\mathbf{x}_i) \approx y_i$ .

**Two-dimensional example:** how to do feature mapping?

**Polynomial features:**

$$\Phi(\mathbf{x}) = [1, \underbrace{x_1, x_2}_{\text{degree-1}}, \underbrace{x_1^2, x_2^2, x_1 x_2}_{\text{degree-2}}, \underbrace{x_1^3, x_2^3, x_1 x_2^2, x_1^2 x_2}_{\text{degree-3}}].$$

degree-0      degree-1      degree-2      degree-3

# Polynomial Regression

```
import numpy
X = numpy.arange(6).reshape(3, 2)
print('X = ')
print(X)
```

```
X =
[[0 1]
 [2 3]
 [4 5]]
```

```
from sklearn.preprocessing import PolynomialFeatures
poly = PolynomialFeatures(degree=3)
Phi = poly.fit_transform(X)
print('Phi = ')
print(Phi)
```

```
Phi =
[[ 1.  0.  1.  0.  0.  1.  0.  0.  0.  1.]
 [ 1.  2.  3.  4.  6.  9.  8. 12. 18. 27.]
 [ 1.  4.  5. 16. 20. 25. 64. 80. 100. 125.]]
```

degree-0      degree-1      degree-2      degree-3

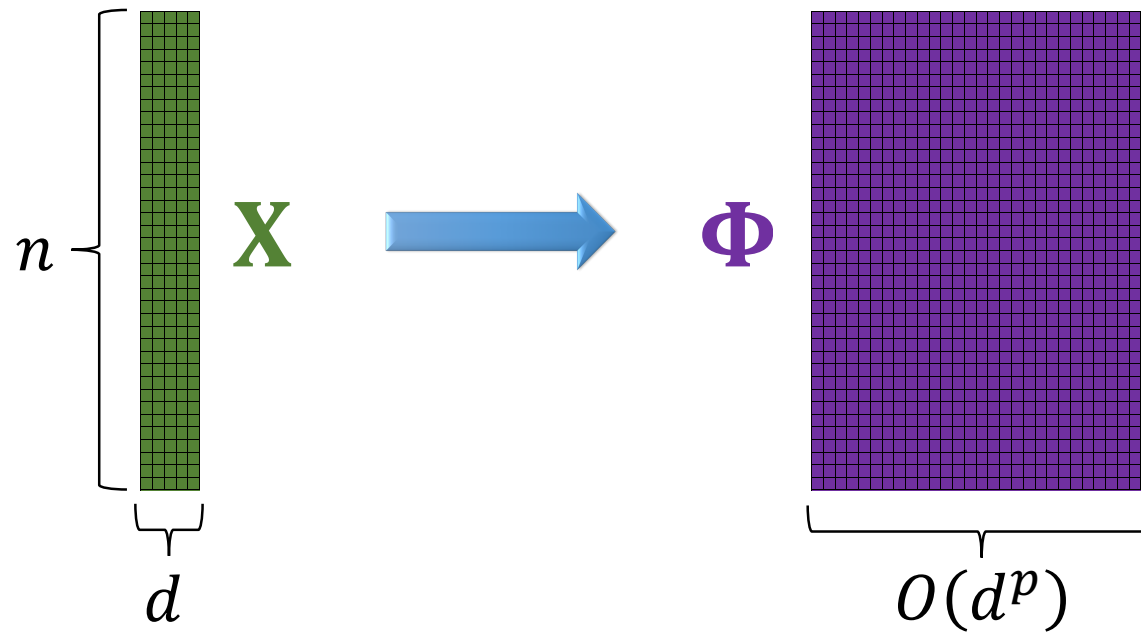
# Polynomial Regression

- $\mathbf{x}$ :  $d$ -dimensional
- $\Phi(\mathbf{x})$ :  $p$ -degree polynomial
- The dimension of  $\Phi(\mathbf{x})$  is  $O(d^p)$

# Polynomial Regression

**Input:** vectors  $\mathbf{x}_1, \dots, \mathbf{x}_n \in \mathbb{R}^d$  and labels  $y_1, \dots, y_n \in \mathbb{R}$ .

**Output:** a function  $f: \mathbb{R}^d \mapsto \mathbb{R}$  such that  $f(\mathbf{x}_i) \approx y_i$ .



# Training, Test, and Overfitting

# Polynomial Regression: Training

**Input:** vectors  $\mathbf{x}_1, \dots, \mathbf{x}_n \in \mathbb{R}^d$  and labels  $y_1, \dots, y_n \in \mathbb{R}$ .

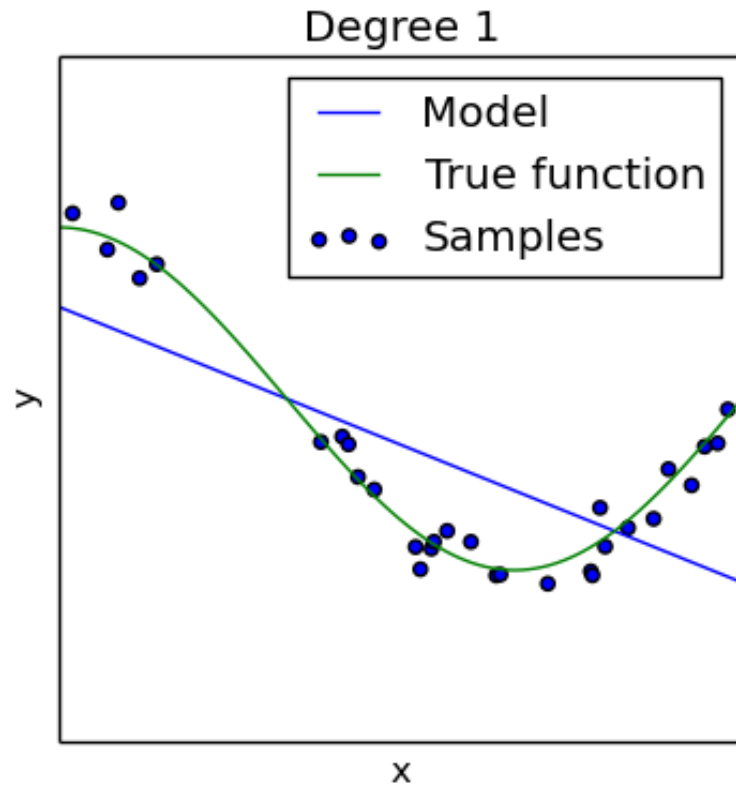
**Feature map:**  $\phi(\mathbf{x}) = \bigotimes^p \bar{\mathbf{x}}$ . Its dimension is  $O(d^p)$ .

**Least squares:**  $\min_{\mathbf{w}} \|\Phi \mathbf{w} - \mathbf{y}\|_2^2$ .

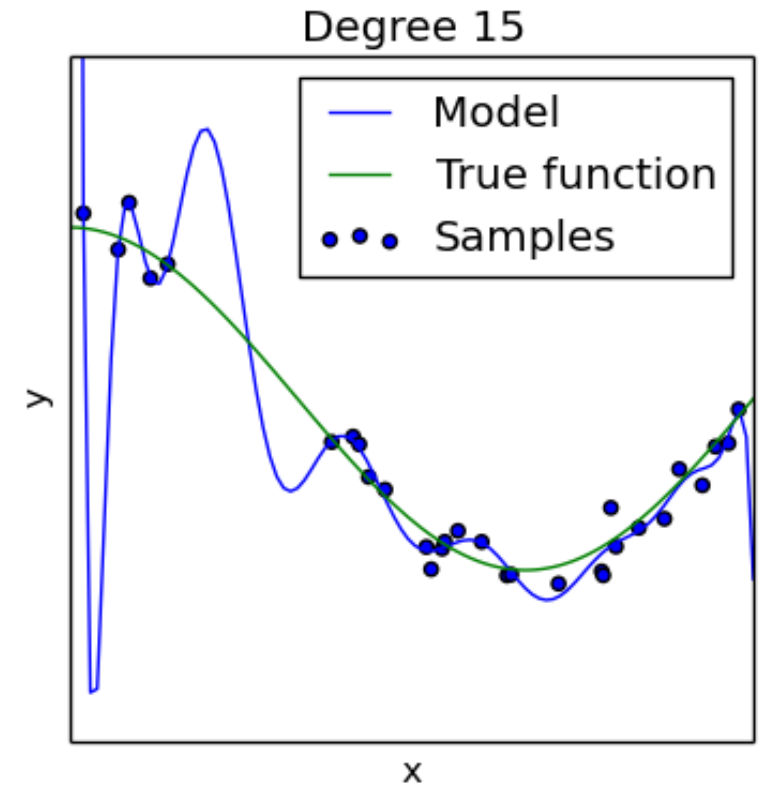
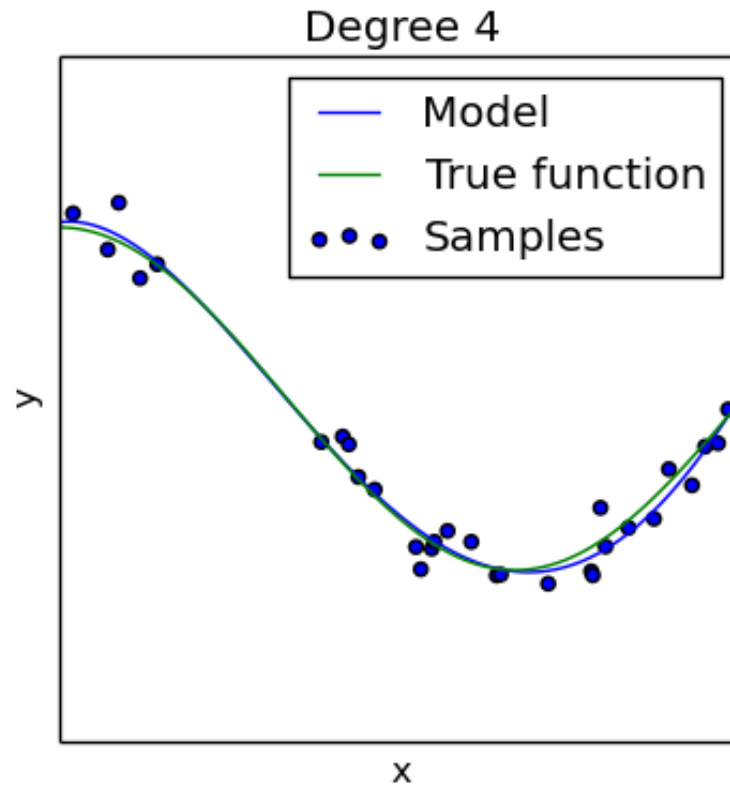
**Question:** what will happen as  $p$  grows?

1. For sufficiently large  $p$ , the dimension of the feature  $\phi(\mathbf{x})$  exceeds  $n$ .
2. Then you can find  $\mathbf{w}$  such that  $\Phi \mathbf{w} = \mathbf{y}$ . (Zero training error!)

# Training and Testing



**Underfitting**



**Overfitting**

# Training and Testing

**Train:**

**Input:** vectors  $\mathbf{x}_1, \dots, \mathbf{x}_n \in \mathbb{R}^d$  and labels  $y_1, \dots, y_n \in \mathbb{R}$ .

**Output:** a function  $f: \mathbb{R}^d \mapsto \mathbb{R}$  such that  $f(\mathbf{x}_i) \approx y_i$ .

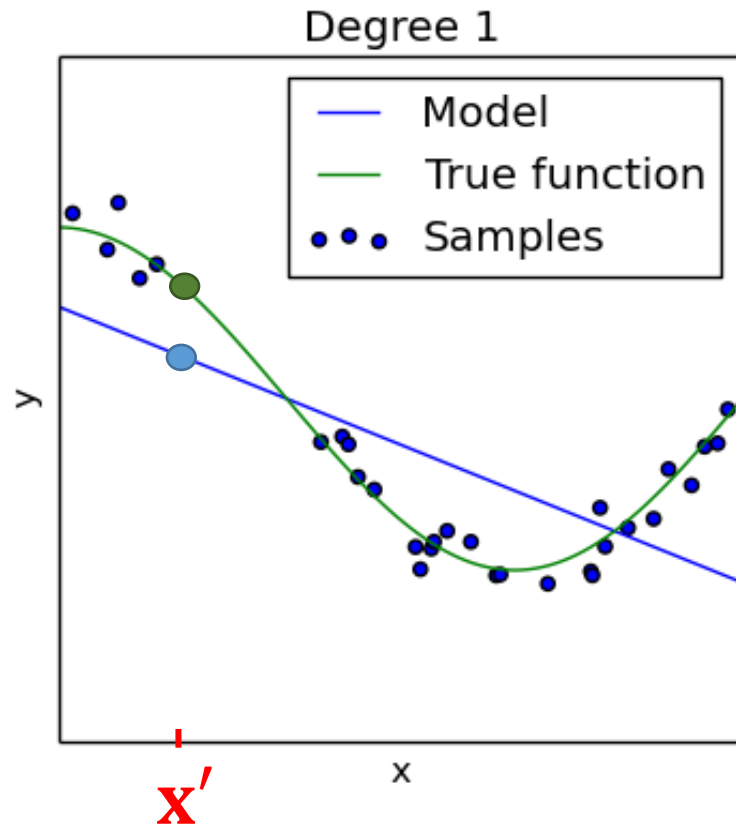
**Test:**

**Input:** a *never-seen-before* feature vectors  $\mathbf{x}' \in \mathbb{R}^d$ .

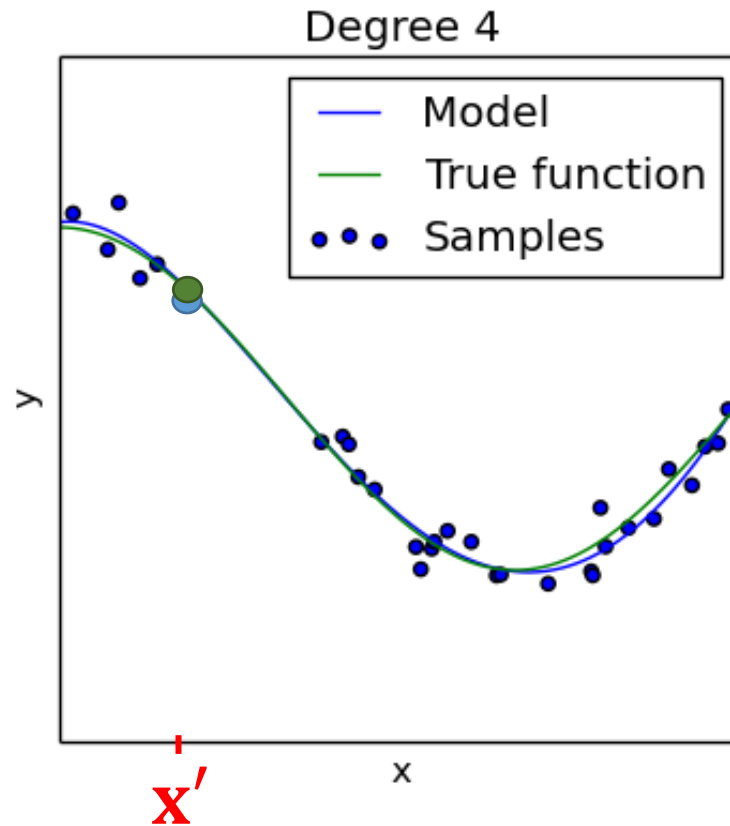
**Input:** predict its label by  $f(\mathbf{x}')$ .



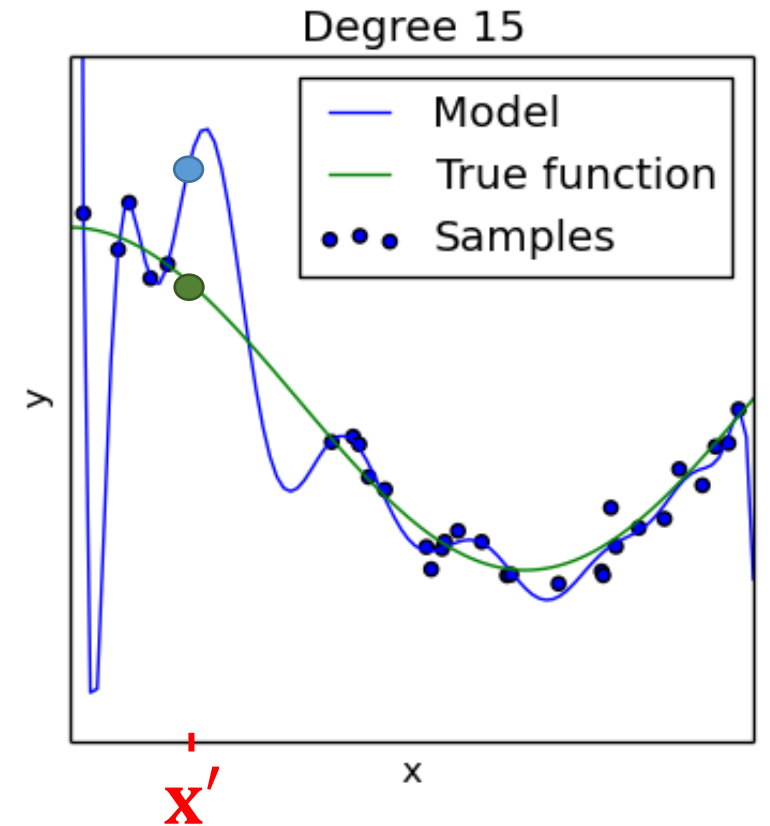
# Training and Testing



**BAD**

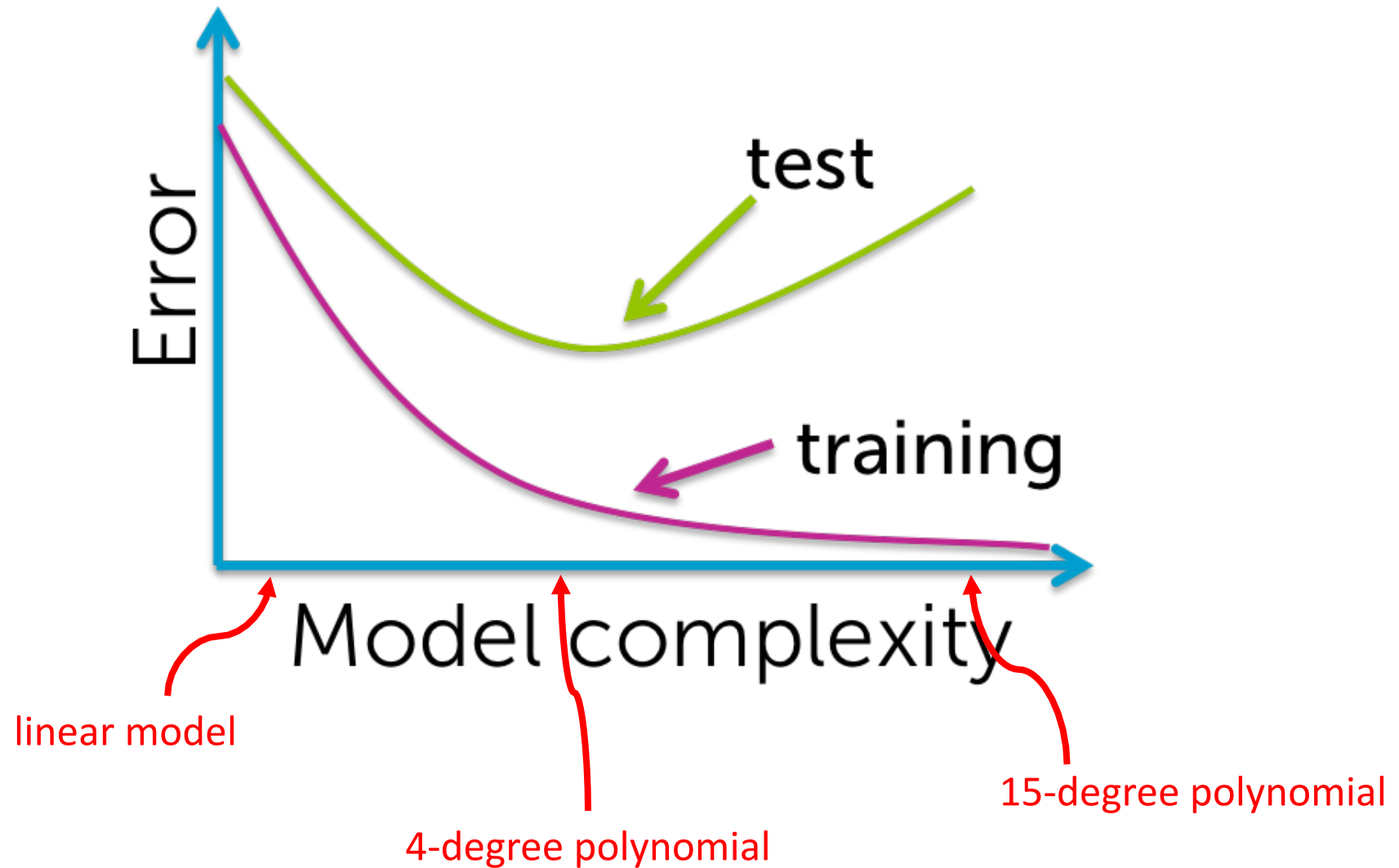


**GOOD**



**BAD**

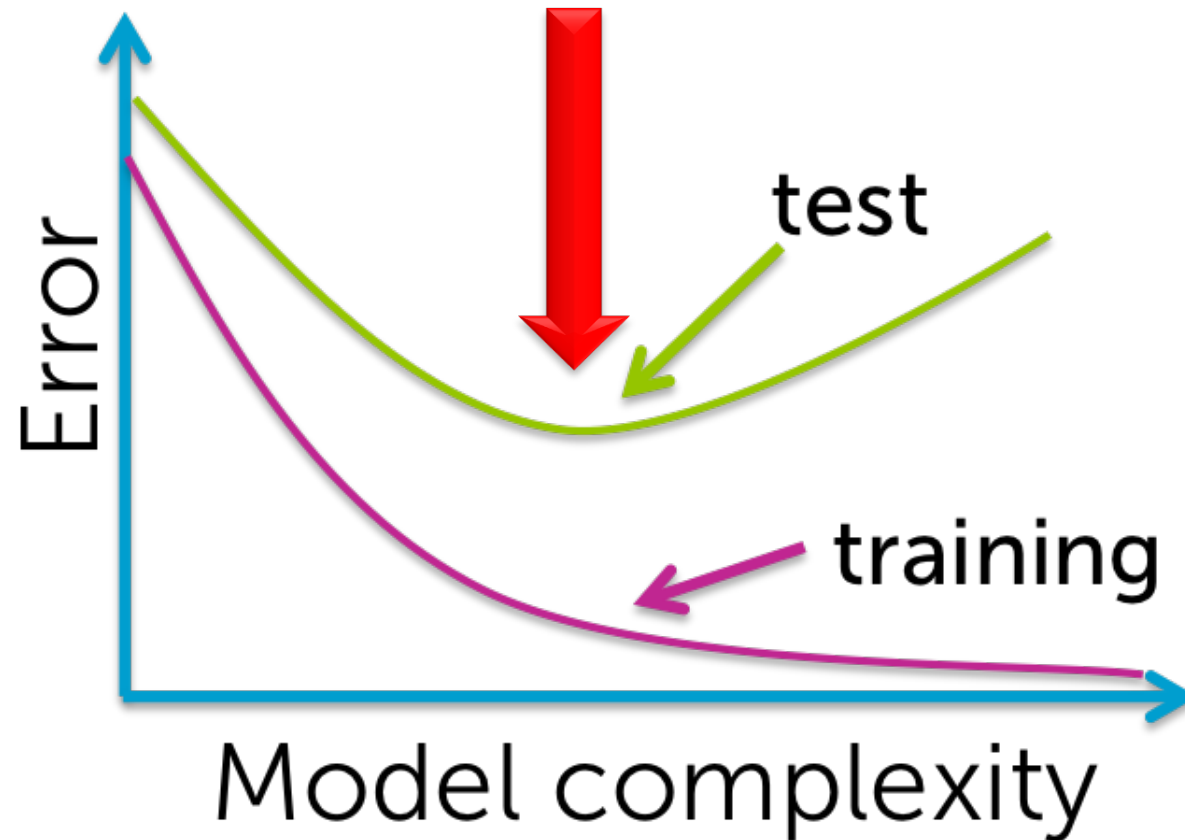
# Training and Testing



# Hyper-Parameter Tuning

**Question:** for the polynomial regression model, how to determine the degree  $p$ ?

**Answer:** the degree  $p$  leads to the smallest test error.



# Hyper-Parameter Tuning

## Training Set

## Test Set

Train a 1-degree polynomial regression



Test MSE = 23.2

Train a 2-degree polynomial regression



Test MSE = 19.0

Train a 3-degree polynomial regression



Test MSE = 16.7

Train a 4-degree polynomial regression



Test MSE = 12.2

Train a 5-degree polynomial regression



Test MSE = 14.8

Train a 6-degree polynomial regression



Test MSE = 25.1

Train a 7-degree polynomial regression



Test MSE = 39.4

Train a 8-degree polynomial regression



Test MSE = 53.0

# Hyper-Parameter Tuning

## Training Set

## Test Set

Train a 1-degree polynomial regression



Test MSE = 23.2

Train a 2-degree polynomial regression



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Train a 7-degree polynomial regression



Test MSE = 39.4

Train a 8-degree polynomial regression



Test MSE = 53.0

# Hyper-Parameter Tuning

## Training Set

## Test Set

Train a 1-degree polynomial regression



Test MSE = 23.2

Train a 2-degree polynomial regression



Test MSE = 18.2

Train a 3-degree polynomial regression



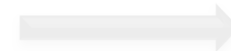
Test MSE = 16.7

Train a 4-degree polynomial regression



Test MSE = 12.2

Train a 5-degree polynomial regression



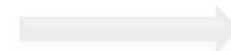
Test MSE = 14.8

Train a 6-degree polynomial regression



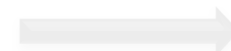
Test MSE = 25.1

Train a 7-degree polynomial regression



Test MSE = 39.4

Train a 8-degree polynomial regression



Test MSE = 53.0

**Wrong! The test labels are unavailable!**

- Even if you have the test labels, never do this!
- An established researcher got fired because of this stupid mistake.

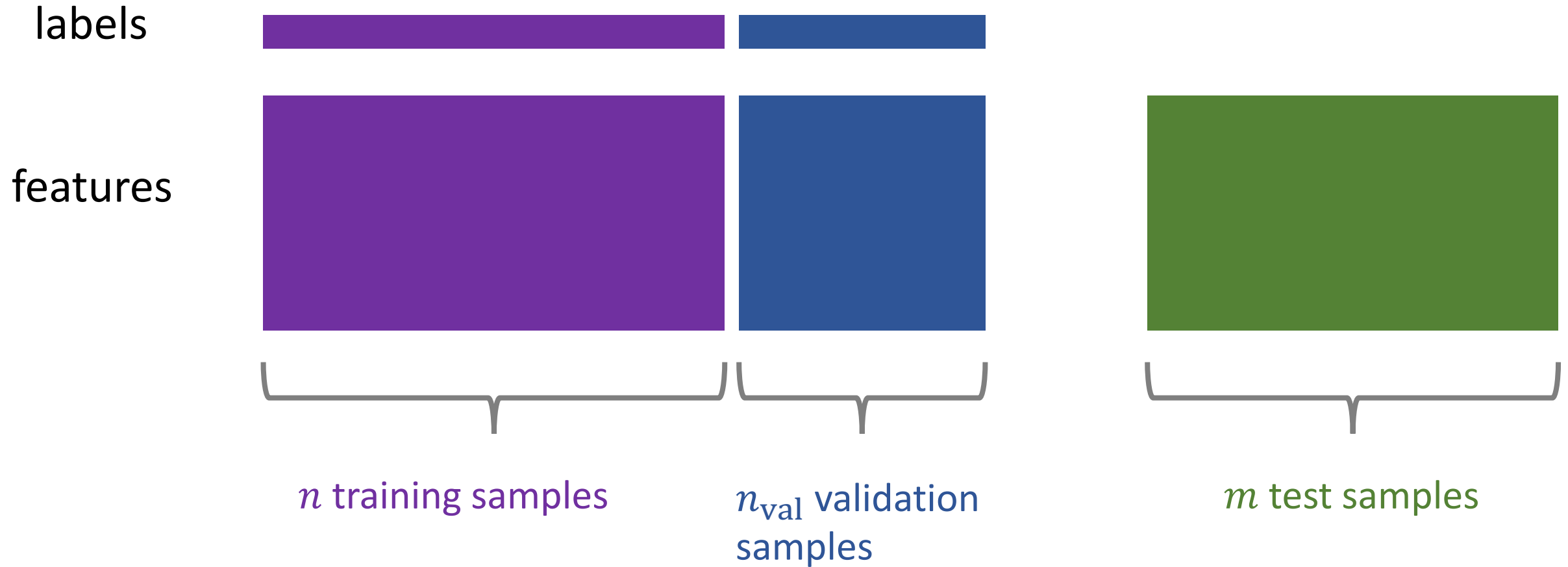
# **Cross-Validation (Naïve Approach) for Hyper-Parameter Tuning**

# Cross-Validation (Naïve Approach)





# Cross-Validation (Naïve Approach)



# Cross-Validation (Naïve Approach)

## Training Set

## Test~~Set~~

Train a 1-degree polynomial regression



Test MSE~~X~~ = 23.2

Train a 2-degree polynomial regression



Test MSE~~X~~ = 19.0

Train a 3-degree polynomial regression



Test MSE~~X~~ = 16.7

Train a 4-degree polynomial regression



Test MSE~~X~~ = 12.2

Train a 5-degree polynomial regression



Test MSE~~X~~ = 14.8

Train a 6-degree polynomial regression



Test MSE~~X~~ = 25.1

Train a 7-degree polynomial regression



Test MSE~~X~~ = 39.4

Train a 8-degree polynomial regression



Test MSE~~X~~ = 53.0

# Cross-Validation (Naïve Approach)

## Training Set

## Validation Set

~~Test Set~~

Train a 1-degree polynomial regression



Valid. MSE = 23.1

Train a 2-degree polynomial regression



Valid. MSE = 19.2

Train a 3-degree polynomial regression



Valid. MSE = 16.3

Train a 4-degree polynomial regression



Valid. MSE = 12.5

Train a 5-degree polynomial regression



Valid. MSE = 14.4

Train a 6-degree polynomial regression



Valid. MSE = 25.0

Train a 7-degree polynomial regression



Valid. MSE = 39.1

Train a 8-degree polynomial regression

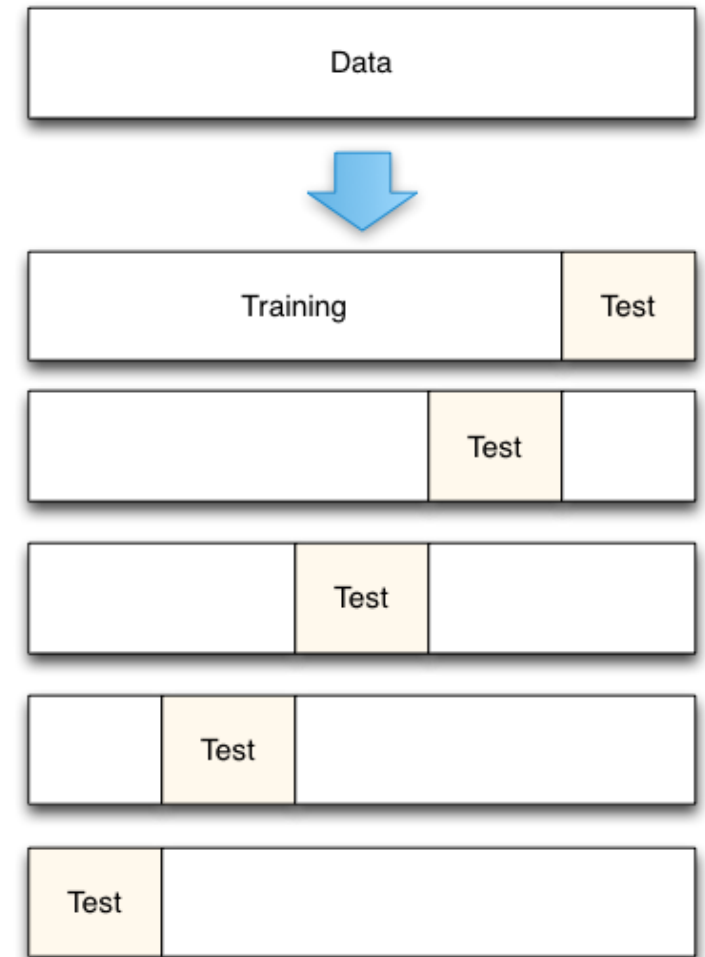


Valid. MSE = 53.5

# **$k$ -Fold Cross-Validation**

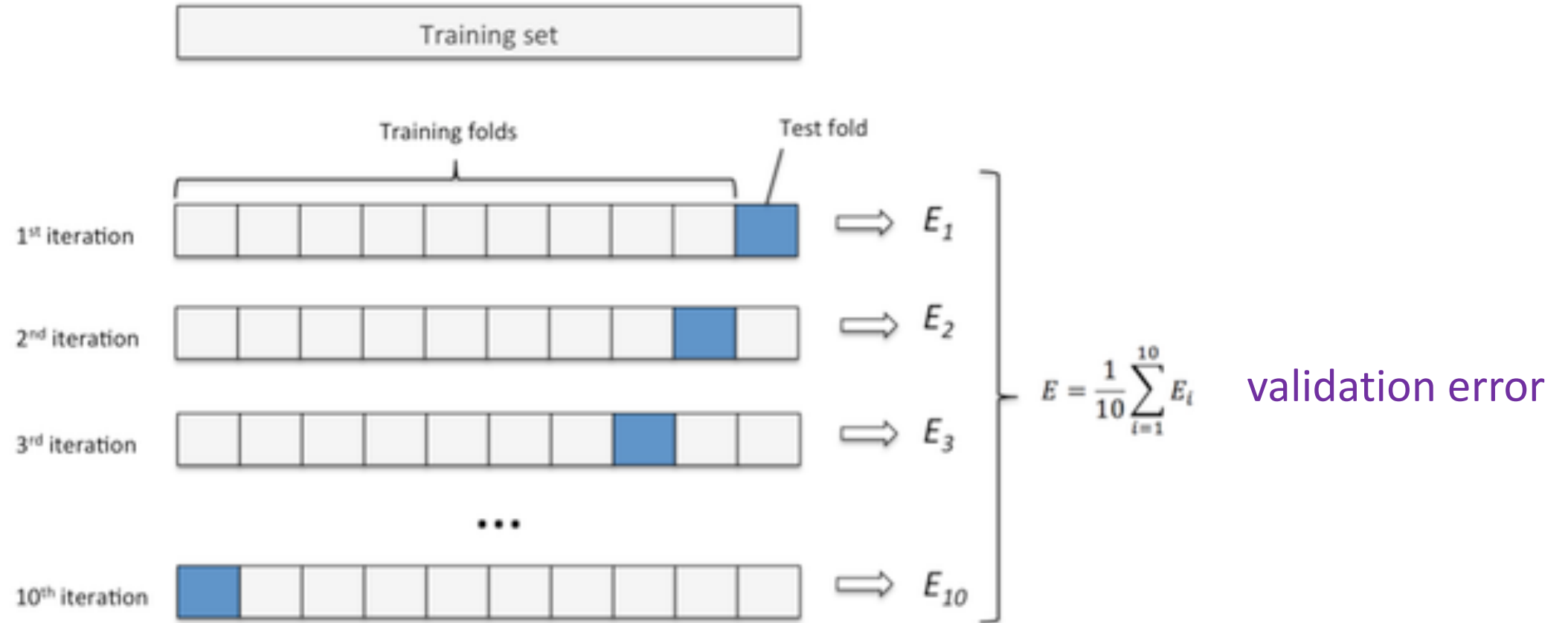
# $k$ -Fold Cross-Validation

1. Propose a grid of hyper-parameters.
  - E.g.  $p \in \{1, 2, 3, 4, 5\}$ .
2. Randomly partition the training samples to  $k$  parts.
  - $k - 1$  parts for training.
  - One part for test.
3. Compute the averaged test errors of the  $k$  repeats.
  - The average is called the **validation error**.
4. Choose the hyper-parameter  $p$  that leads to the smallest **validation error**.



Example: 5-fold cross-validation

# Example: 10-Fold Cross-Validation



# Example: 10-Fold Cross-Validation

parameter

validation error

p=1

23.19

p=2

21.00

p=3

18.54

p=4

24.36

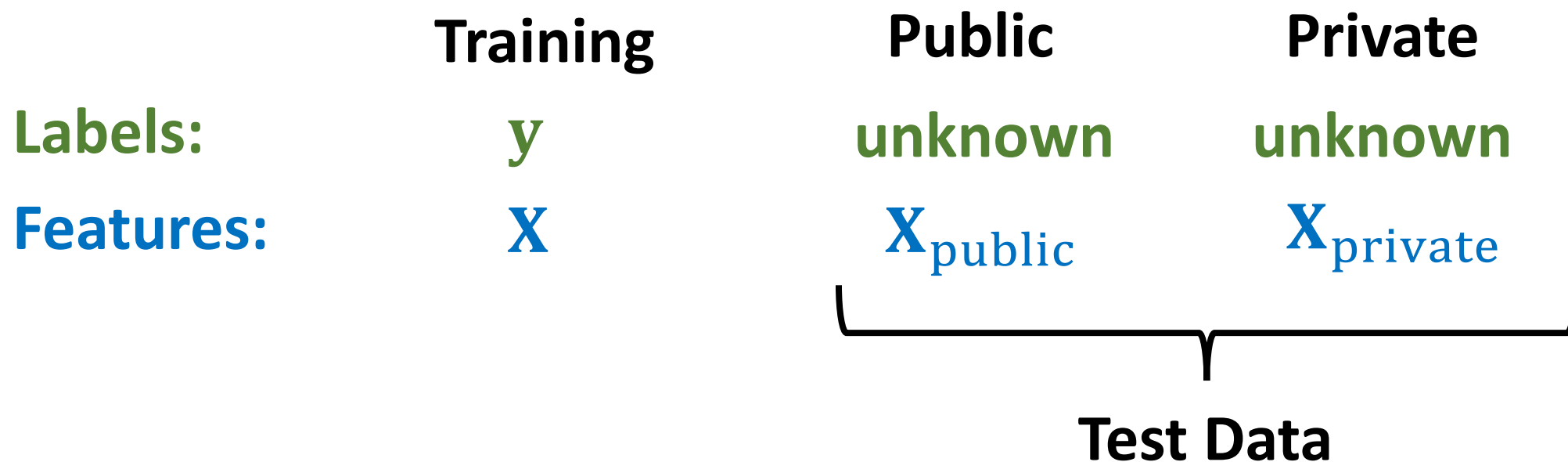
p=5

27.96

# **Real-World Machine Learning Competition**

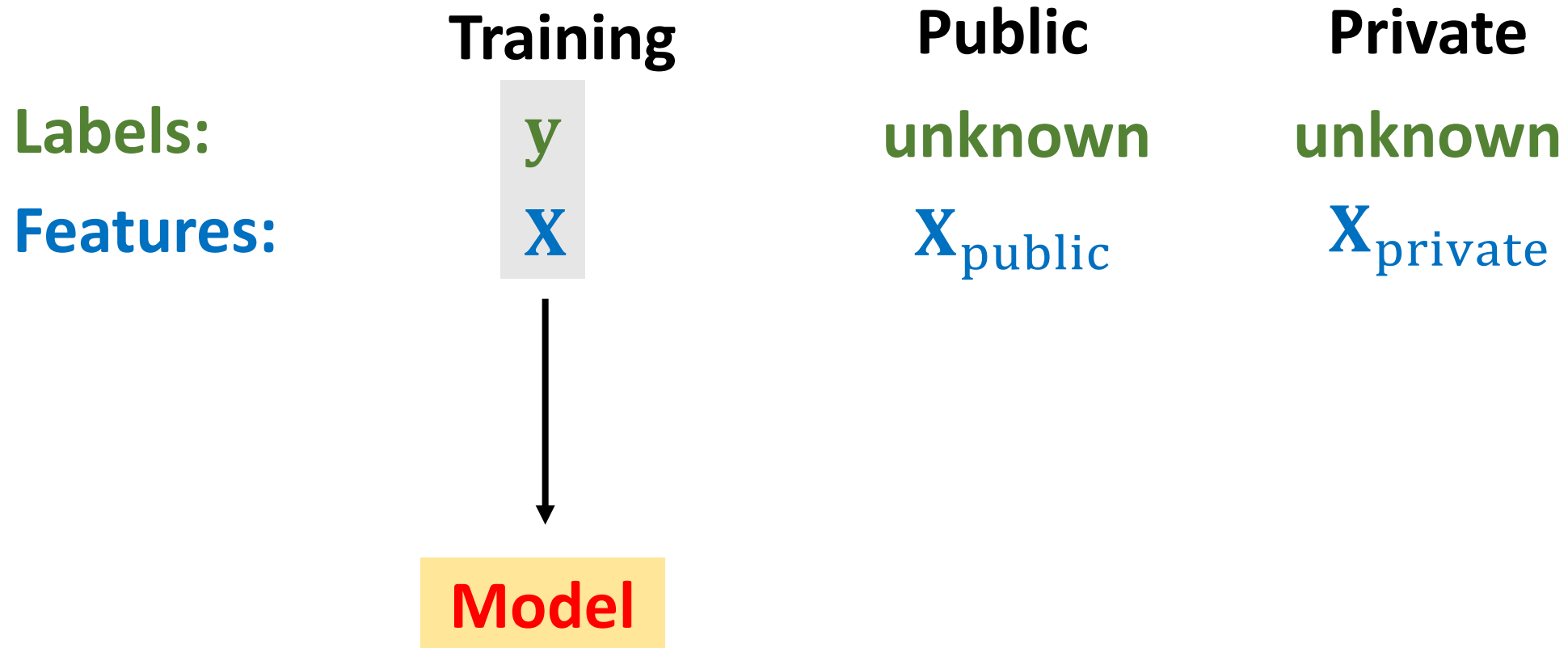


# The Available Data

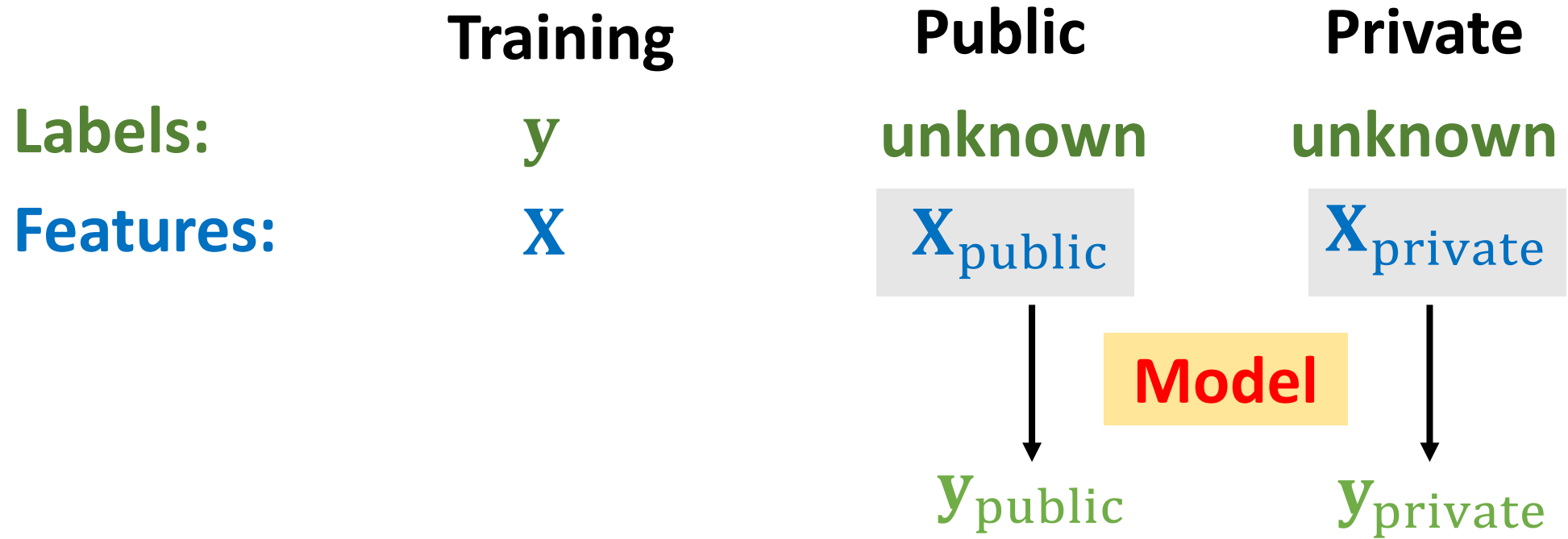


The public and private are mixed;  
Participants cannot distinguish them.

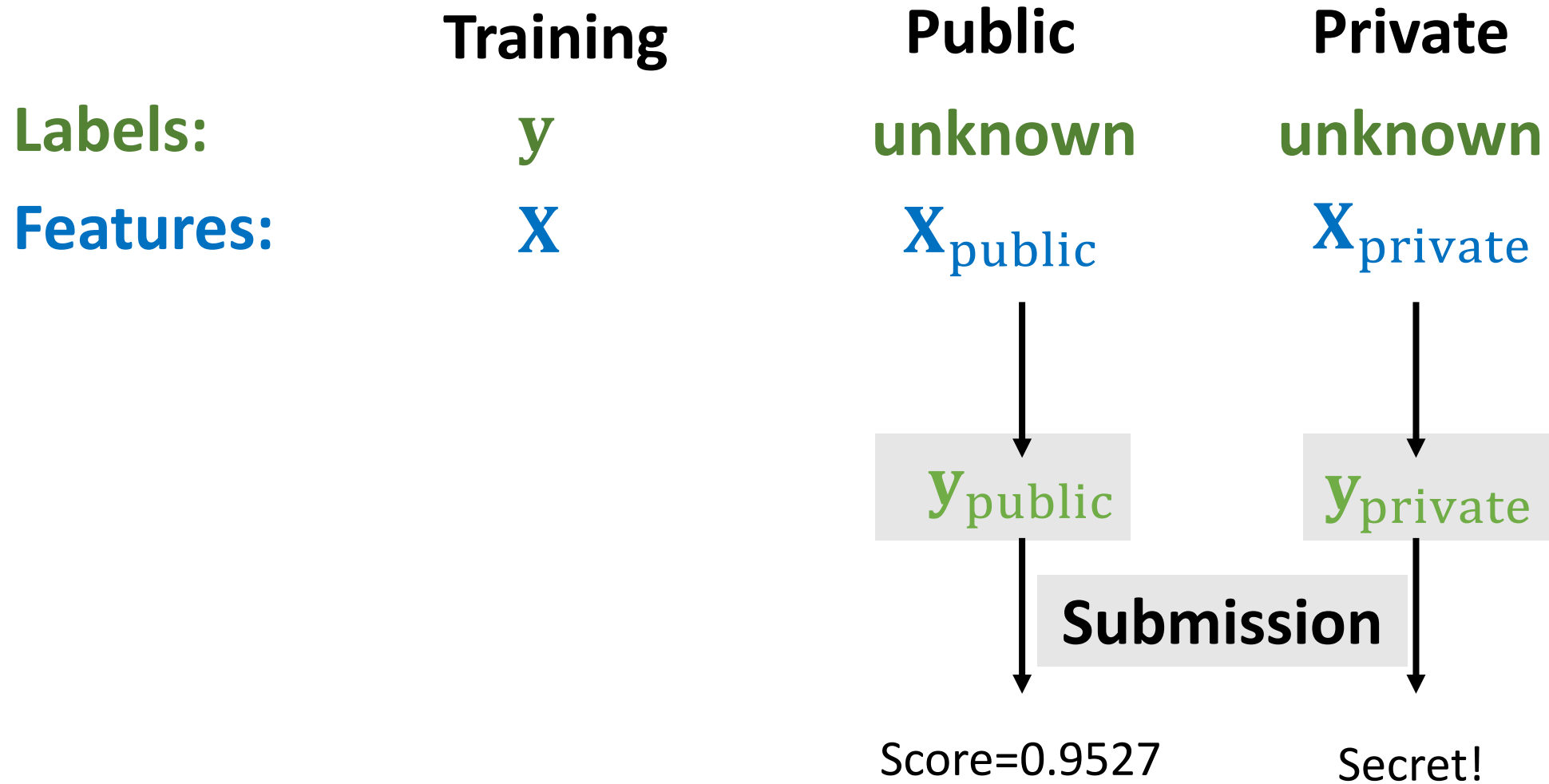
# Train A Model



# Prediction



# Submission to Leaderboard



# Submission to Leaderboard

Training

Labels:

$y$

Features:

$X$

Public

unknown

$X_{\text{public}}$

Private

unknown

$X_{\text{private}}$

**Question:** Why two leaderboards?

**Answer:** The score can be evilly used for hyper-parameter tuning (cheating).

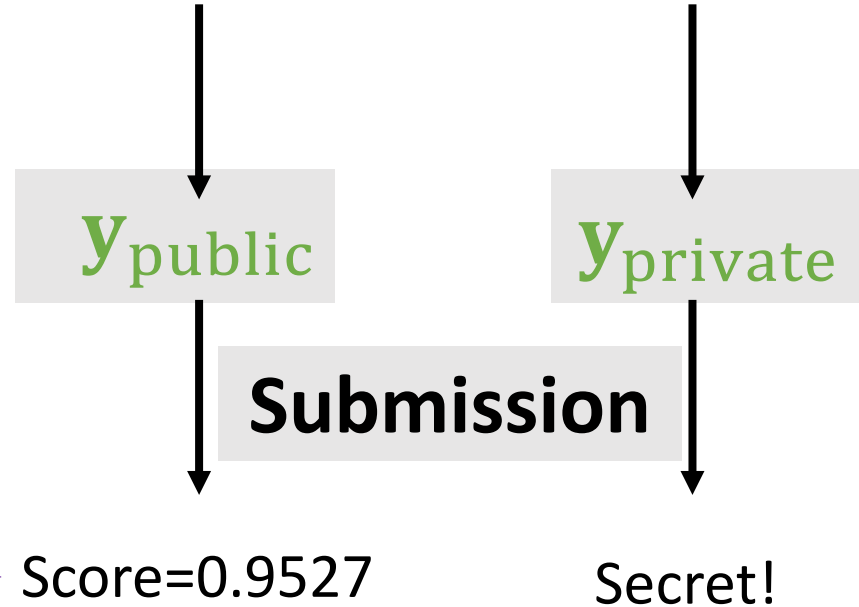
$y_{\text{public}}$

$y_{\text{private}}$

Submission

Score=0.9527

Secret!



# Summary

- Polynomial regression for non-linear problems.
- Polynomial regression has a **hyper-parameter**  $p$ .
- Tune the **hyper-parameters** using cross-validation.
- Make your model **parameters** and **hyper-parameters** independent of the test set!!!