

# Introduction to Machine Learning

## Lecture 01: Supervised Learning I – Linear Regression

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Machine Intelligence Research and Applications Lab



# Contents

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- **An Example: The ETA Problem**
- **Linear Regression by Least Squares**
- **Linear Regression by Maximum Likelihood**

Some materials are from ESL, PRML, and RG.

- **An Example: The ETA Problem**
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# The ETA Problem

The **ETA** (**E**stimated **T**ime of **A**rrival) problem:

- Suppose that you are an engineer working at DiDi/Gaode/.... Your supervisor ask you to develop an algorithm to estimate the time of arrival for each customer. For the good of the customers' experience, the ETA given by your algorithm should be as accurate as possible.



Time of Wait

ETA

Time on the Road

$$\text{ETA} = \text{Time of Wait} + \text{Time on the Road}$$

# The ETA Problem

The **ETA** (**E**stimated **T**ime of **A**rrival) problem:

- Suppose that you are an engineer working at DiDi/Gaode/.... Your supervisor ask you to develop an algorithm to estimate the time of arrival for each customer. For the good of the customers' experience, the ETA given by your algorithm should be as accurate as possible.



Time of Wait

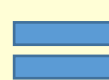
ETA

Time on the Road

How to solve this problem?



ETA

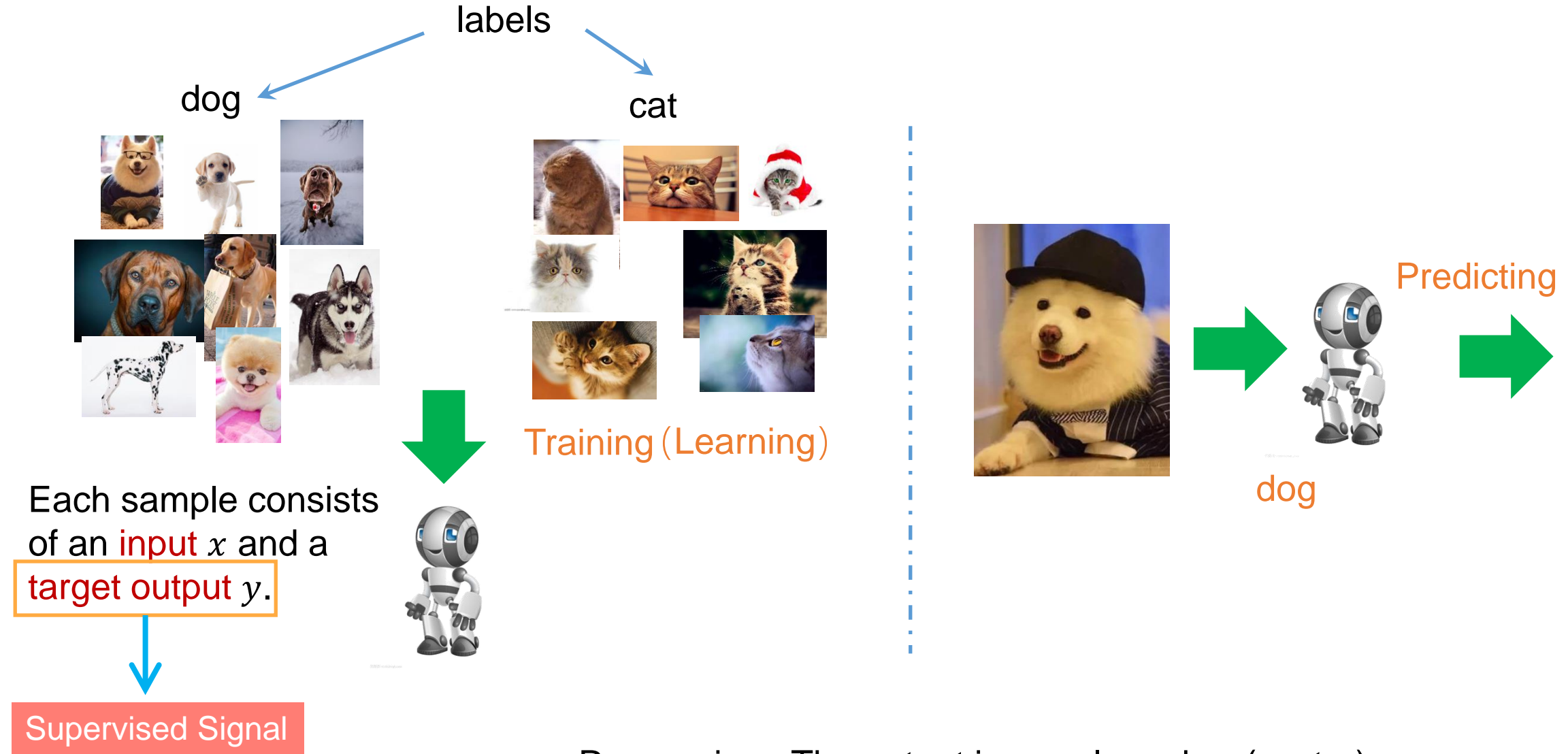


Time of Wait



Time on the Road

# Supervised Learning (Recall from Lec00)



- Regression : The output is a real number (vector)
- Classification : The output is a class label.

# Supervised Learning (Recall from Lec00)

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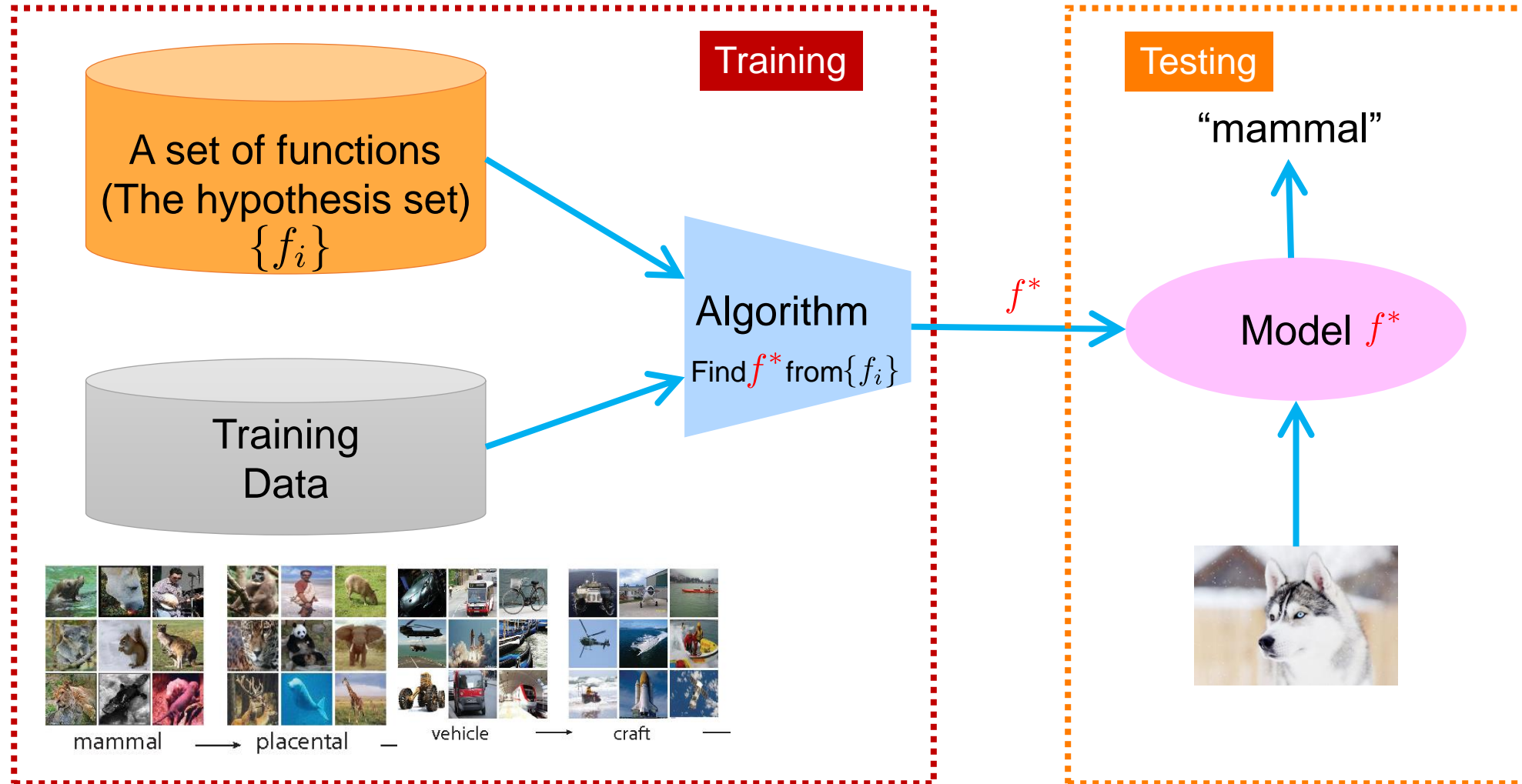
We are indeed looking for a mapping (function).

- Image classification



$f(\cdot)$  → “Dog”

# Framework of Supervised Learning (Recall from Lec00)





# Framework of Supervised Learning

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# Step 1: Data Preparation

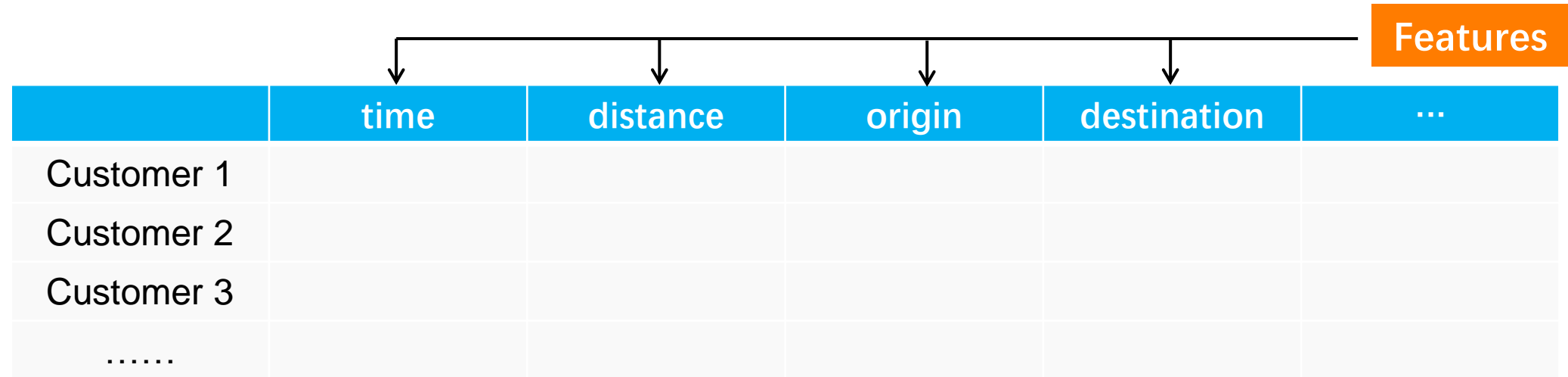
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What kind of data you would like to collect?

# Step 1: Data Preparation

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- What kind of data you would like to collect?



The diagram illustrates the data collection process. A horizontal line with four downward-pointing arrows is positioned above the table headers. An orange box labeled 'Features' is located to the right of this line. The table below has five columns: 'time', 'distance', 'origin', 'destination', and '...'. The first column is labeled with customer names: 'Customer 1', 'Customer 2', 'Customer 3', and '.....'.

	time	distance	origin	destination	...
Customer 1					
Customer 2					
Customer 3					
.....					

# Step 1: Data Preparation

- What kind of data you would like to collect?

	Features				
	time	distance	origin	destination	...
Customer 1					
Customer 2					
Customer 3					
.....					



The data determines the upper bound of the performance that can be achieved by your model.



In real world applications, you need to determine which kind of data can be helpful to your task and collect them by yourself.



The knowledge that can help you to determine which kind of data to collect is the so-called **domain knowledge**.

# Step 1: Data Preparation

- Data cleaning

	time	distance	origin	destination	...
Customer 1					
Customer 2		?			
Customer 3				?	
.....					

Missing values

# Step 1: Data Preparation

- Data cleaning

	time	distance	origin	destination	...
Customer 1					
Customer 2					
Customer 3		800 km	中科大西校区	合肥南站	
.....					

An error?



```
graph TD; A[800 km] --> D[An error?]; B[中科大西校区] --> D; C[合肥南站] --> D;
```

# Step 1: Data Preparation

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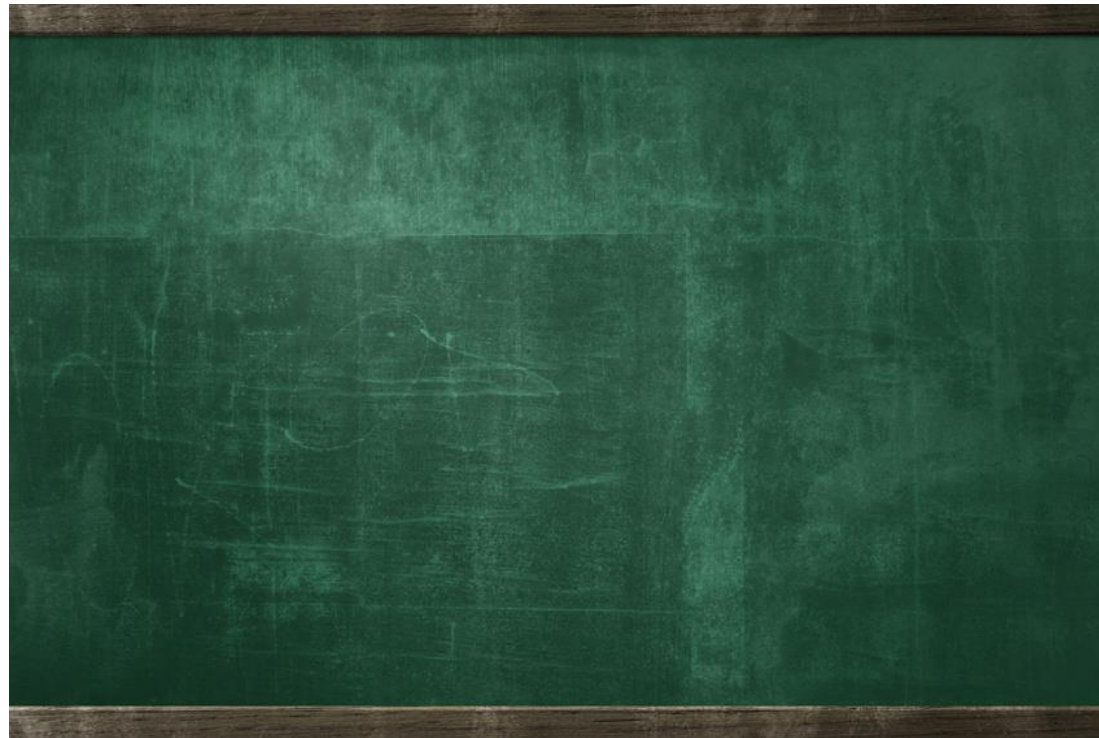


In real world applications, data preparation (cleaning) often takes up to **80%** (even **90%**) of the entire project lifecycle.

# Step 2: Picking a hypothesis space

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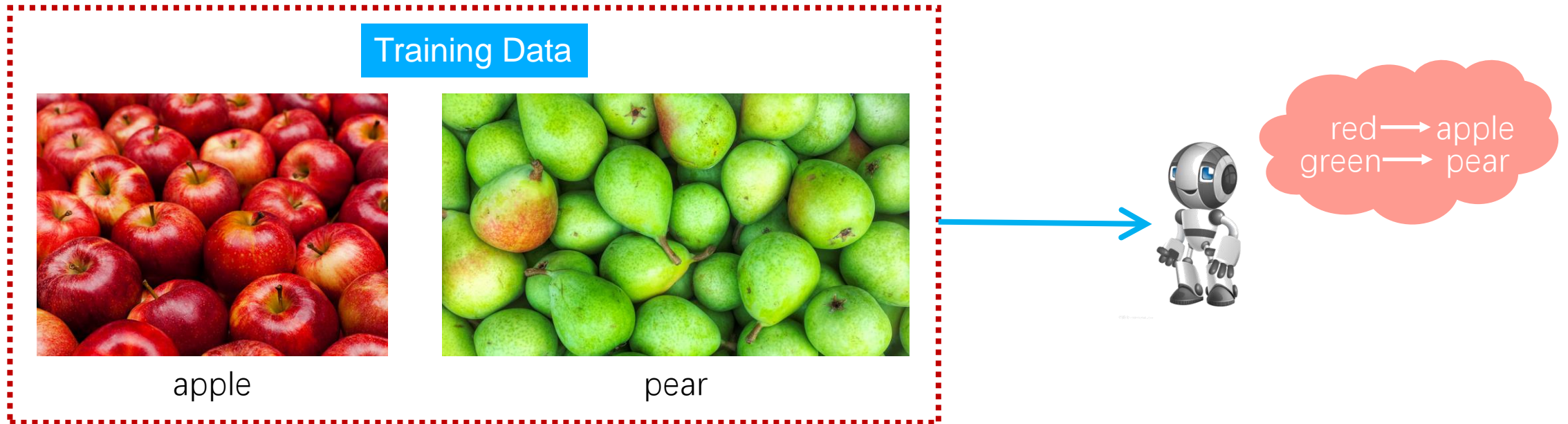
- Linear regression
  - Least squares





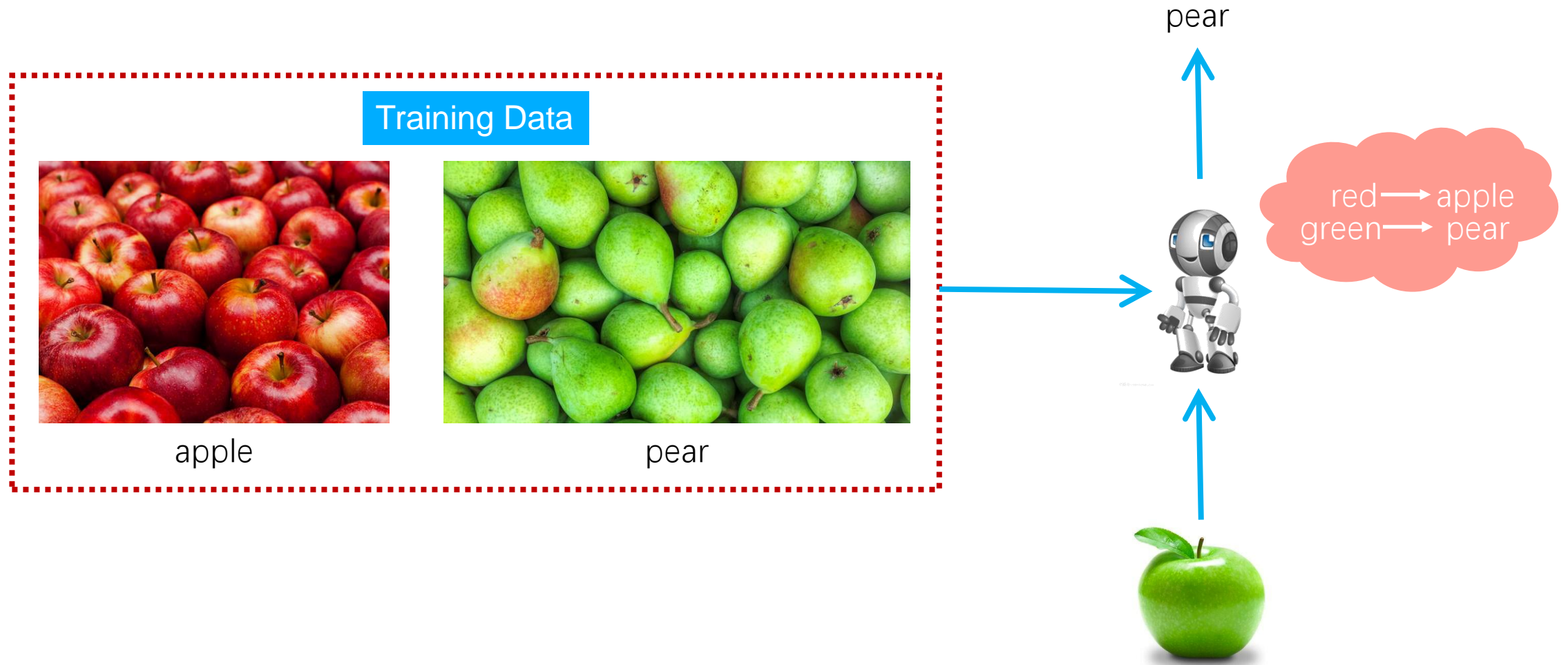
# Step 2: Picking a hypothesis space

- Linear regression
  - Overfitting



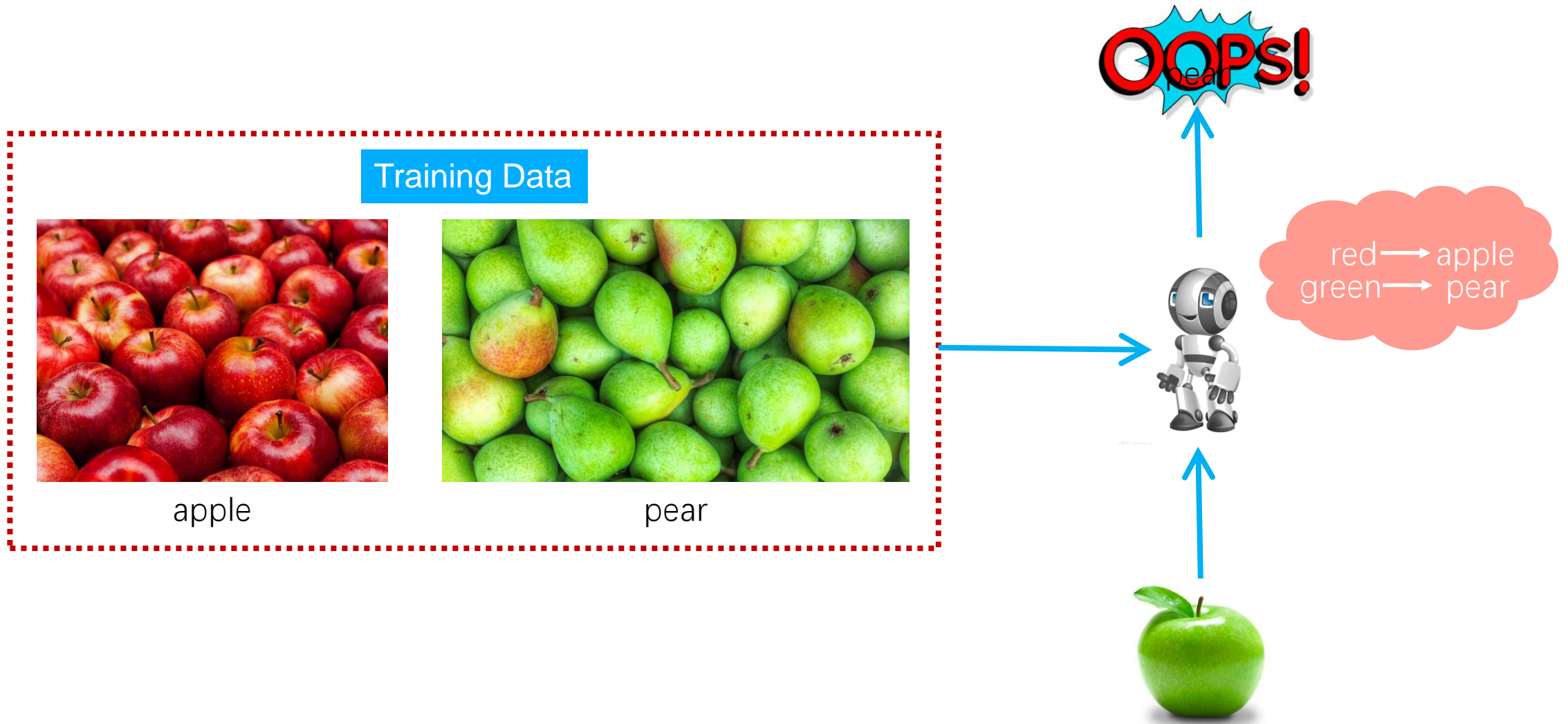
# Step 2: Picking a hypothesis space

- Linear regression
  - Overfitting



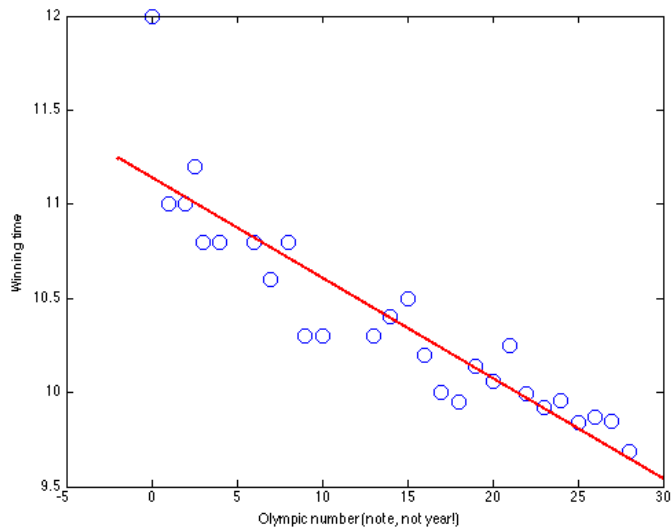
# Step 2: Picking a hypothesis space

- Linear regression
  - Overfitting

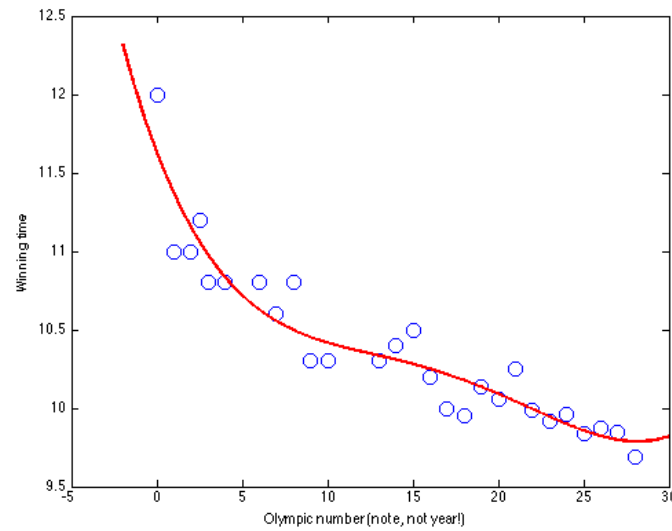


# Step 2: Picking a hypothesis space

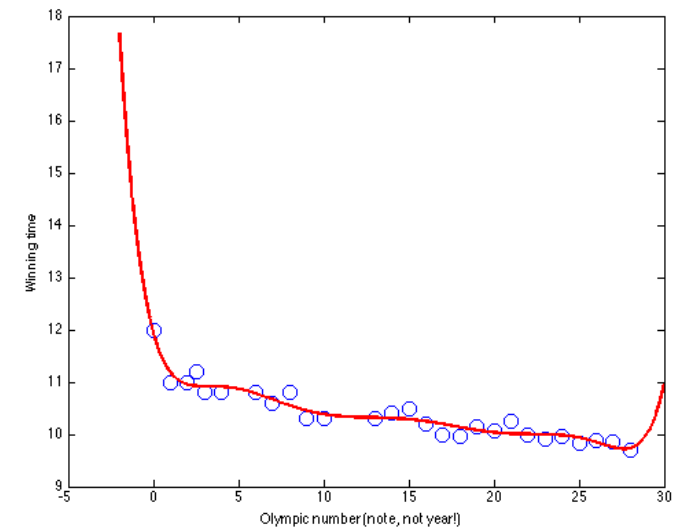
- Linear regression
  - Overfitting



Linear function



4<sup>th</sup> order polynomial



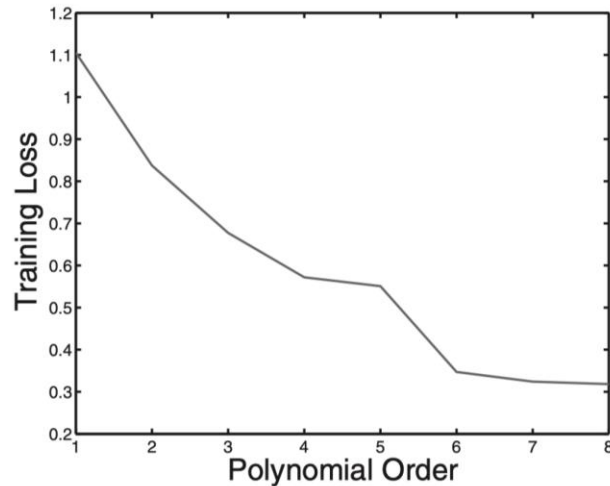
8<sup>th</sup> order polynomial

# Step 2: Picking a hypothesis space

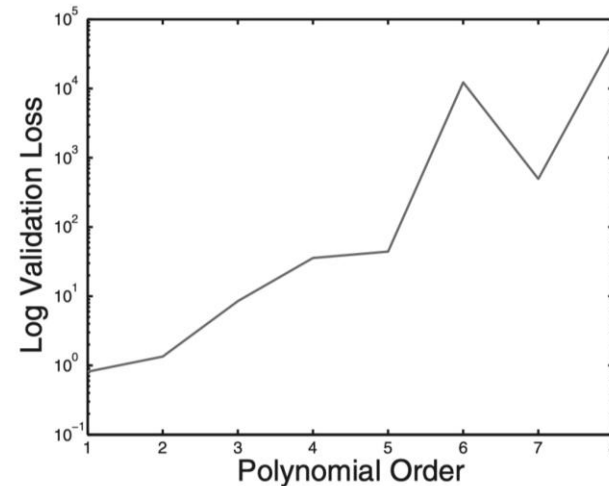
- Linear regression
  - How to alleviate overfitting?

Validation data

Either provided separately or can be created by splitting the original data



(a) Training loss for the Olympic men's 100 m data.



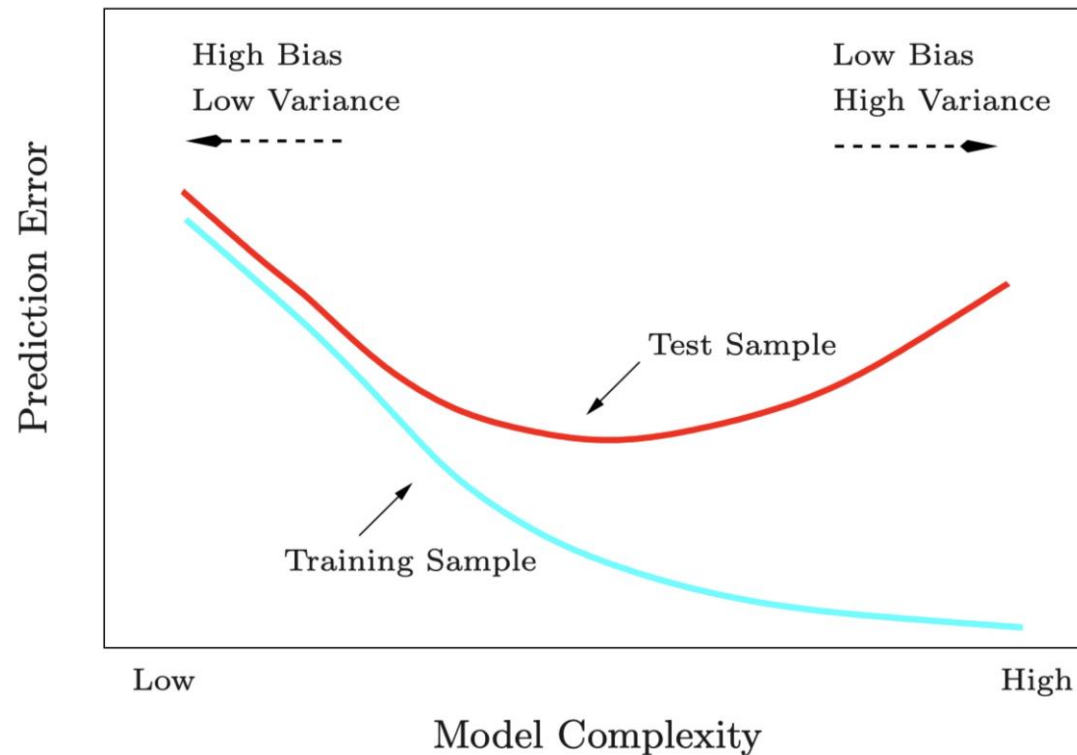
(b) Log validation loss for the Olympic men's 100 m data. When using the squared loss, this is also known as the squared predictive error and measures how close the predicted values are to the true values. Note that the log loss is plotted as the value increases so rapidly.

# Step 2: Picking a hypothesis space

- Linear regression
  - How to alleviate overfitting?

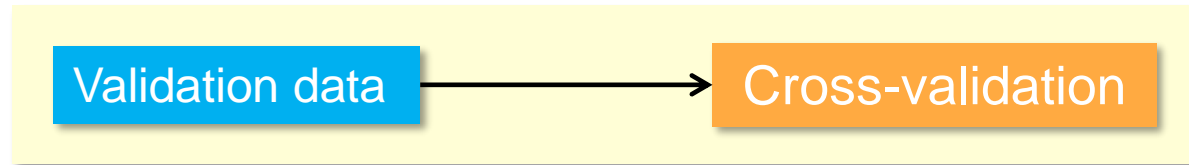
Validation data

Either provided separately or can be created by splitting the original data



# Step 2: Picking a hypothesis space

- Linear regression
  - How to alleviate overfitting?



validation	train	train	train	train
train	validation	train	train	train
train	train	validation	train	train
train	train	train	validation	train
train	train	train	train	validation

Five-fold cross-validation

Cross-validation

Choose the model with the smallest prediction error on the validation sets averaged over the five folds

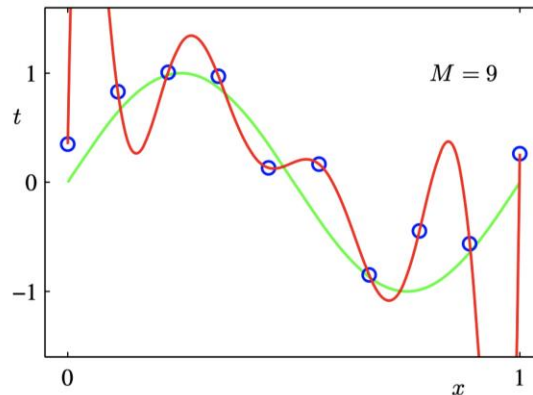
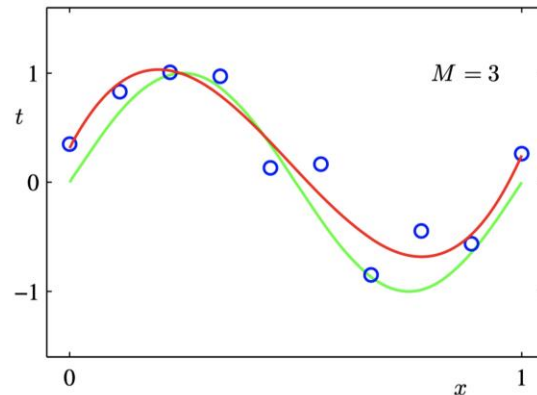
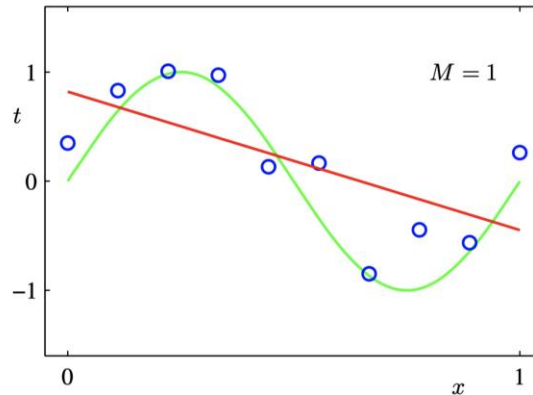
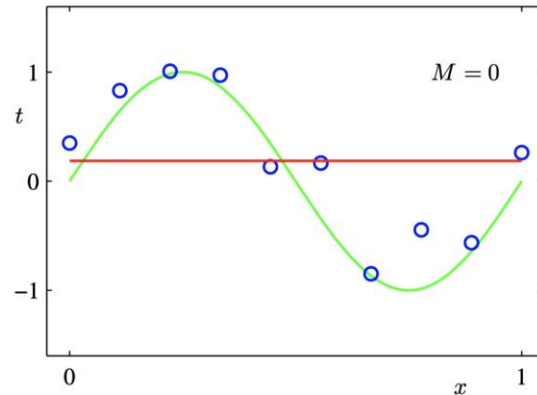


# Step 2: Picking a hypothesis space

- Linear regression
  - How to alleviate overfitting?

regularization

Stem the coefficients from exploding



	$M = 0$	$M = 1$	$M = 6$	$M = 9$
$w_0^*$	0.19	0.82	0.31	0.35
$w_1^*$		-1.27	7.99	232.37
$w_2^*$			-25.43	-5321.83
$w_3^*$			17.37	48568.31
$w_4^*$				-231639.30
$w_5^*$				640042.26
$w_6^*$				-1061800.52
$w_7^*$				1042400.18
$w_8^*$				-557682.99
$w_9^*$				125201.43



# Step 2: Picking a hypothesis space

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- Linear regression
  - How to alleviate overfitting?

regularization

Stem the coefficients from exploding

