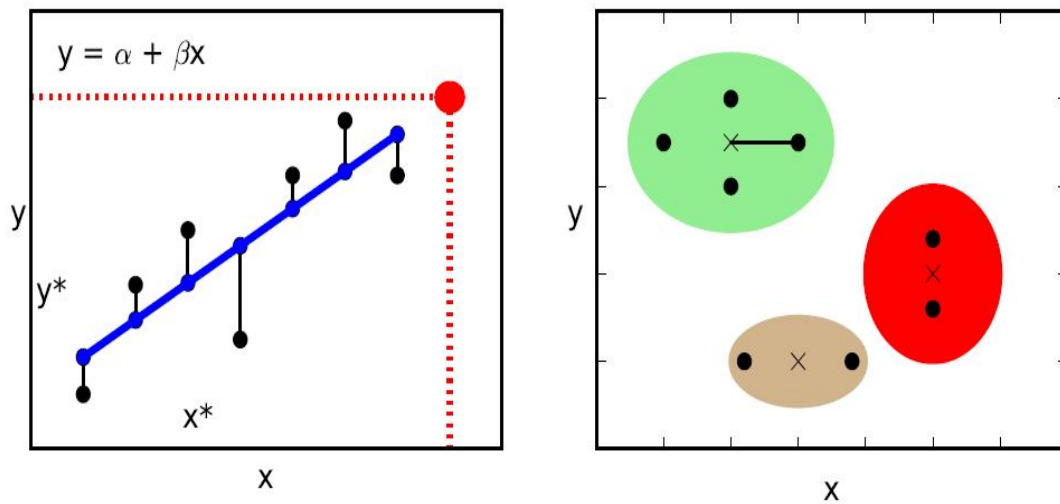


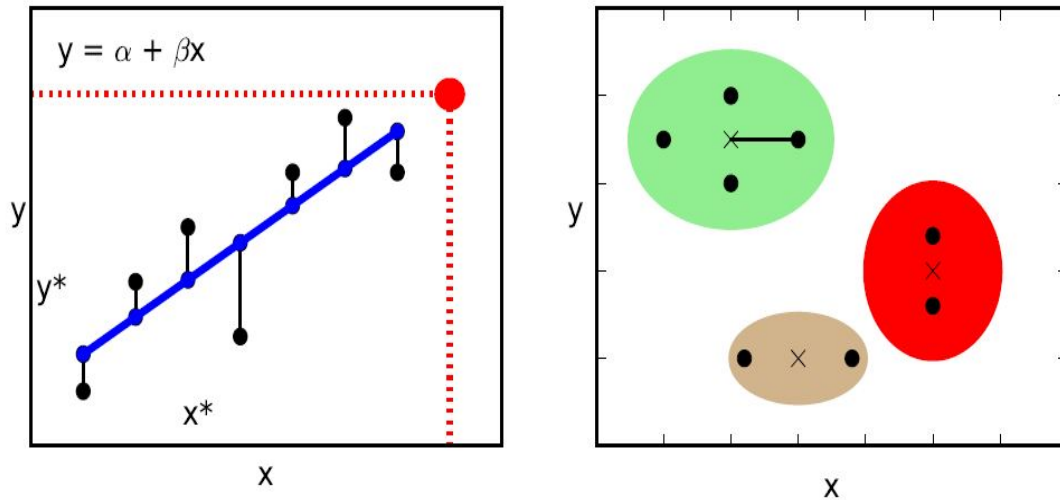
# CONCEPTS AND DEFINITIONS

# Prediction vs. Classification



- two main goals in machine learning

# Examples



- stock price prediction
- spam/no spam email classification

# A Numerical Dataset

object $x_i$	Height (H)	Weight (W)	Foot (F)	Label (L)
$x_1$	5.00	100	6	green
$x_2$	5.50	150	8	green
$x_3$	5.33	130	7	green
$x_4$	5.75	150	9	green
$x_5$	6.00	180	13	red
$x_6$	5.92	190	11	red
$x_7$	5.58	170	12	red
$x_8$	5.92	165	10	red

# Code for the Dataset

```
import pandas as pd
data = pd.DataFrame(
    {"id": [ 1,2,3,4,5,6,7,8] ,
     "Label": ["green", "green",
               "green", "green",
               "red", "red",
               "red", "red"] ,
     "Height": [5, 5.5, 5.33, 5.75,
                6.00, 5.92, 5.58, 5.92] ,
     "Weight": [100, 150, 130, 150,
                180, 190, 170, 165] ,
     "Foot": [6, 8, 7, 9,
              13, 11, 12, 10]} ,
    columns = ["id", "Height",
               "Weight", "Foot",
               "Label"] )
```

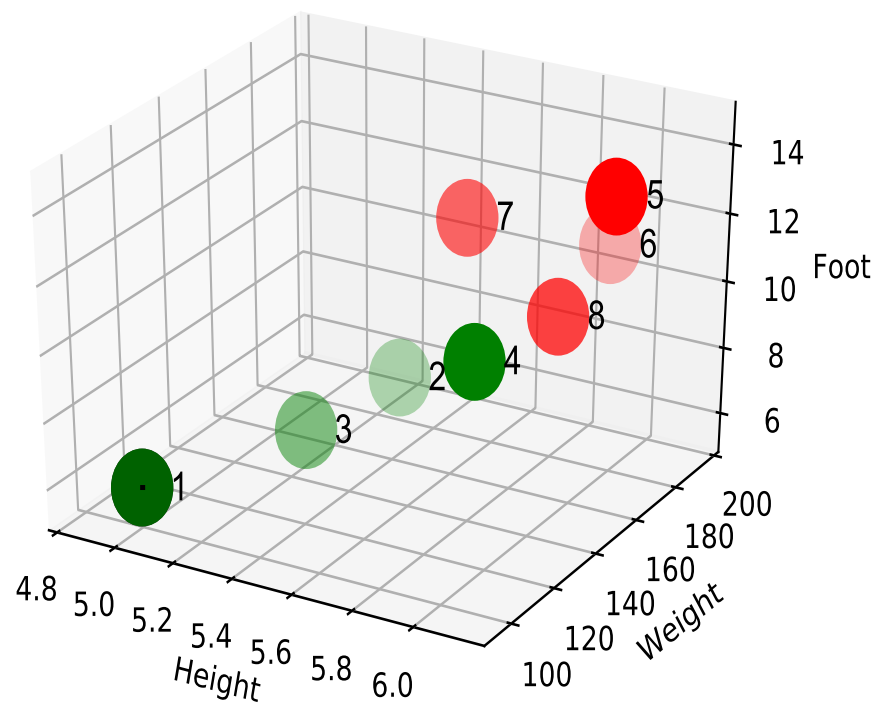
# Code for the Dataset

## (cont'd)

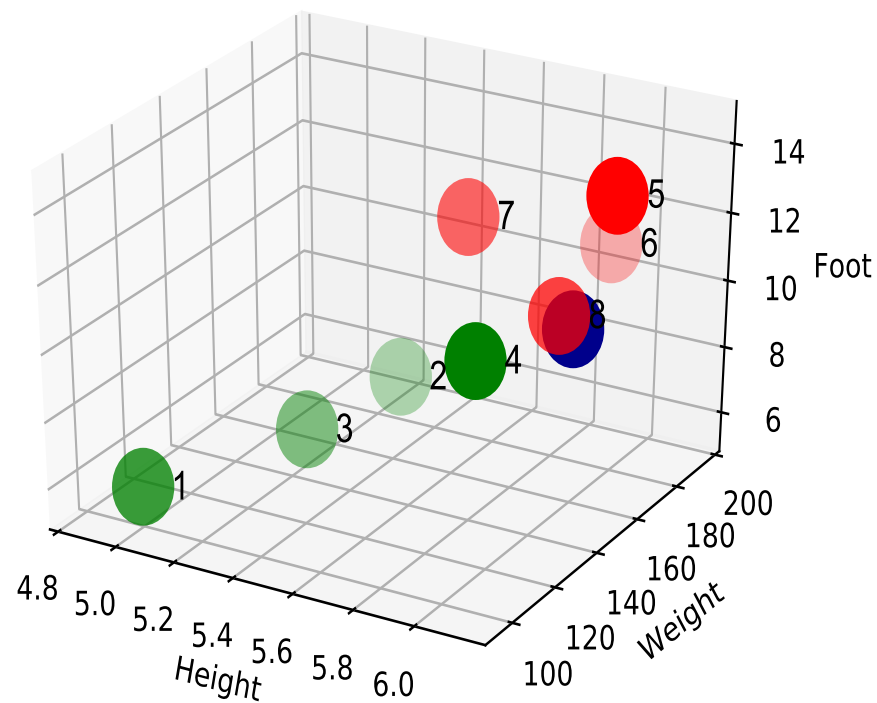
```
ipdb> data
```

	id	Height	Weight	Foot	Label
0	1	5.00	100	6	green
1	2	5.50	150	8	green
2	3	5.33	130	7	green
3	4	5.75	150	9	green
4	5	6.00	180	13	red
5	6	5.92	190	11	red
6	7	5.58	170	12	red
7	8	5.92	165	10	red

# A Dataset Illustration



# A New Instance



$(H=6, W=160, F=10) \mapsto ?$



# Categorical Dataset

Day	Weather	Temperature	Wind	Play
1	sunny	hot	low	<b>no</b>
2	rainy	mild	high	<b>yes</b>
3	sunny	cold	low	<b>yes</b>
4	rainy	cold	high	<b>no</b>
5	sunny	cold	high	<b>yes</b>
6	overcast	mild	low	<b>yes</b>
7	sunny	hot	low	<b>yes</b>
8	overcast	hot	high	<b>yes</b>
9	rainy	hot	high	<b>no</b>
10	rainy	mild	low	<b>yes</b>

- $x^* = (\text{sunny}, \text{cold}, \text{low}) \mapsto ?$
- need numeric values for attributes

# Python Code

```
import pandas as pd

data = pd.DataFrame(
    {"Day": [1, 2, 3, 4, 5, 6, 7, 8, 9, 10],
     "Weather": ["sunny", "rainy", "sunny",
                  "rainy", "sunny", "overcast",
                  "sunny", "overcast",
                  "rainy", "rainy"],
     "Temperature": ["hot", "mild",
                     "cold", "cold", "cold",
                     "mild", "hot", "hot",
                     "hot", "mild"],
     "Wind": ["low", "high", "low",
              "high", "high", "low",
              "low", "high", "high", "low"],
     "Play": ["no", "yes", "yes", "no", "yes",
              "yes", "yes", "yes", "no", "yes"]},
    columns=["Day", "Weather",
             "Temperature", "Wind", "Play"])
```

# Basic Definitions

- eight objects:  $x_1, \dots, x_8$
- three features: height  $H$ , weight  $W$ , foot  $F$
- for input  $x$ , its feature vector  $\phi(x) = [H(x), W(x), F(x)]$
- $\phi(x)$  is a point in 3-dimensional space  $R^3$

# Examples of Objectives

1. binary classification: compute label (green or red) on new instance

$$x \mapsto \phi(\cdot) \mapsto y \in \{0, 1\}$$

2. regression: predict foot size given height and weight

$$x \mapsto \phi(\cdot) \mapsto y \in R$$

- how do we compute  $\phi(\cdot)$ ?

# Computing Prediction

- choose a class of functions (e.g. linear, polynomial)
- choose hyper-parameters to:
  1. minimize training loss
  2. generalize to unseen data
- example: in linear regression we choose slope and intercept (hyper-parameters) to minimize sum of squared residuals

# Loss Minimization

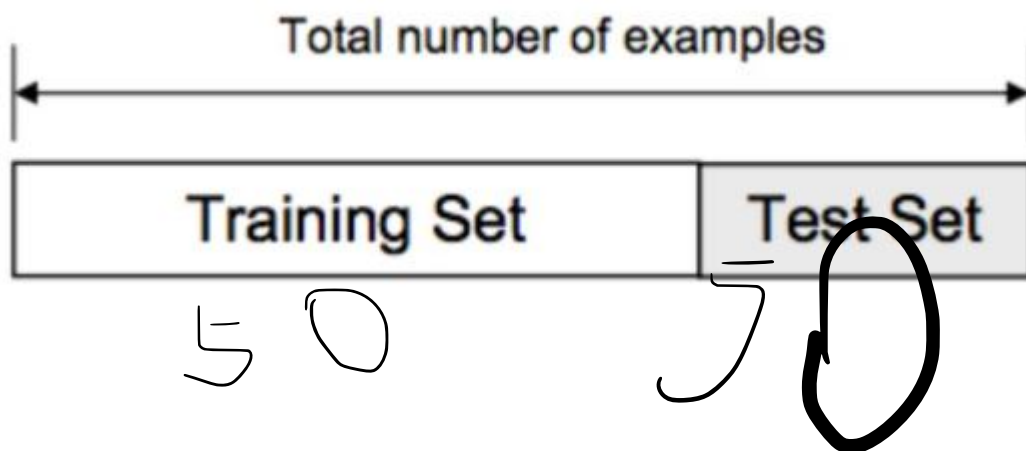
- compute parameters to minimize loss
- learning is optimization
- solution depends on the loss function
- examples of loss functions:
  1. squared loss  $(y - \phi(x))^2$
  2. absolute loss  $|y - \phi(x)|$
- use gradient descent to compute hyper-parameters

# Testing/Training Sets

- Q: how do we compute model parameters?
- Q: how do we estimate accuracy?
- A: split known objects into two subsets
  1.  $X_{\text{train}}$ : for parameters
  2.  $X_{\text{testing}}$ : for accuracy

# Testing/Training Sets

(cont'd)



- need to minimize any biases in the data



# Bias in Training Data

```
import pandas as pd
data = pd.DataFrame(
    {"id": [ 1,2,3,4,5,6,7,8] ,
     "Label": ["green", "green",
               "green", "green",
               "red", "red",
               "red", "red"] ,
     "Height": [5, 5.5, 5.33, 5.75,
                6.00, 5.92, 5.58, 5.92] ,
     "Weight": [100, 150, 130, 150,
                180, 190, 170, 165] ,
     "Foot": [6, 8, 7, 9,
              13, 11, 12, 10]} ,
    columns = ["id", "Height",
               "Weight", "Foot",
               "Label"] )
X = data[["Height", "Weight", "Foot"]]
X_train = X[ : 4]
X_test  = X[ 4 : ]
```

# Bias in Training Data

## (cont'd)

```
ipdb> X_train
```

0	5.00	100	6	green
1	5.50	150	8	green
2	5.33	130	7	green
3	5.75	150	9	green

```
ipdb> X_test
```

	Height	Weight	Foot	Label
4	6.00	180	13	red
5	5.92	190	11	red
6	5.58	170	12	red
7	5.92	165	10	red

```
ipdb> X_test
```

- need to randomize data

# Eliminating Bias

```
import pandas as pd
from sklearn.model_selection \
    import train_test_split

data = pd.DataFrame(
    {"id": [ 1,2,3,4,5,6,7,8],
     "Label":["green","green","green","green",
              "red","red","red","red"],
     "Height":[5, 5.5, 5.33,5.75,
               6.00,5.92,5.58,5.92],
     "Weight":[100, 150, 130, 150,
               180, 190, 170, 165],
     "Foot":[6, 8, 7, 9, 13, 11, 12, 10]},
    columns = ["id", "Height",
               "Weight", "Foot","Label"] )

X = data[["Height","Weight","Foot"]]
y = data["Label"]

X_train,X_test,y_train,y_test=\
    train_test_split(X, y, train_size=0.5)
```

# Eliminating Bias

```
ipdb> X_train
```

	Height	Weight	Foot	Label
3	5.75	150	9	green
1	5.50	150	8	green
4	6.00	180	13	red
5	5.92	190	11	red

```
ipdb> X_test
```

	Height	Weight	Foot	Label
2	5.33	130	7	green
0	5.00	100	6	green
7	5.92	165	10	red
6	5.58	170	12	red

```
ipdb> X_test
```

- data is now "shuffled"

# Stratifying Classes

```
import pandas as pd
from sklearn.model_selection \
    import train_test_split

data = pd.DataFrame(
    {"id": [ 1,2,3,4,5,6,7,8],
     "Label":["green","green","green","green",
              "red","red","red","red"],
     "Height":[5, 5.5, 5.33,5.75,
               6.00,5.92,5.58,5.92],
     "Weight":[100, 150, 130, 150,
               180, 190, 170, 165],
     "Foot":[6, 8, 7, 9, 13, 11, 12, 10]},
    columns = ["id", "Height",
               "Weight", "Foot","Label"] )

X = data[["Height","Weight","Foot"]]
y = data["Label"]

X_train,X_test,y_train,y_test=\
    train_test_split(X, y, train_size=0.75)
```

# Stratifying Classes

```
ipdb> X_train
```

	Height	Weight	Foot	Label
6	5.58	170	12	red
2	5.33	130	7	green
3	5.75	150	9	green
0	5.00	100	6	green
1	5.50	150	8	green
4	6.00	180	13	red

```
ipdb> X_test
```

	Height	Weight	Foot	Label
7	5.92	165	10	red
5	5.92	190	11	red

- label counts are not evenly distributed

# Split and Stratify

```
import pandas as pd
from sklearn.model_selection \
    import train_test_split

data = pd.DataFrame(
    {"id": [ 1,2,3,4,5,6,7,8],
     "Label":["green","green","green","green",
              "red","red","red","red"],
     "Height":[5, 5.5, 5.33,5.75,
               6.00,5.92,5.58,5.92],
     "Weight":[100, 150, 130, 150,
               180, 190, 170, 165],
     "Foot":[6, 8, 7, 9, 13, 11, 12, 10]},
    columns = ["id", "Height",
               "Weight", "Foot","Label"] )

X = data[["Height","Weight","Foot"]]
y = data["Label"]

X_train,X_test,y_train,y_test=\
    train_test_split(X, y,
                     train_size=0.75,stratify=y)
```

# Stratifying Classes

```
ipdb> X_train
```

1	5.50	150	8	green
6	5.58	170	12	red
3	5.75	150	9	green
5	5.92	190	11	red
2	5.33	130	7	green
7	5.92	165	10	red

```
ipdb> X_test
```

	Height	Weight	Foot	Label
0	5.0	100	6	green
4	6.0	180	13	red

- label counts are now evenly distributed



# Cross Validation

- we use only a portion of data for testing and training
- can use more with  $n$ -fold cross validation
  1. split data randomly into  $n$  parts
  2. use  $n - 1$  for training
  3. use 1 part for testing
  4. repeat  $n$  times using different part for testing
  5. average results

# $k$ -fold Validation



- expensive for large  $n$

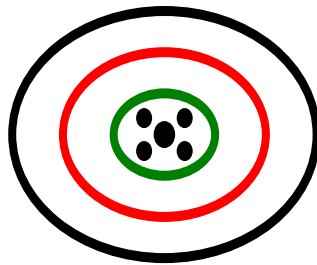
# Bias-Variance Decomposition

- bias - average difference between prediction and correct value
- variance - variability of prediction for a given point

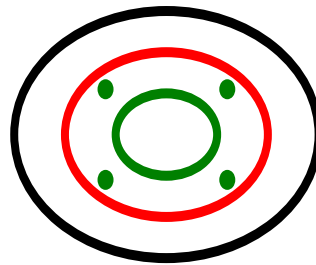
$$\text{Error} = \text{Bias}^2 + \text{Variance} + \text{Irreducible Error}$$

# Bias-Variance Trade-Off

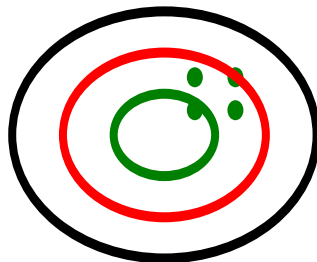
low bias, low variance



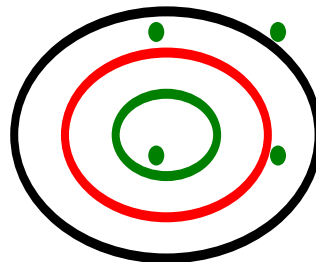
low bias, high variance



high bias, low variance

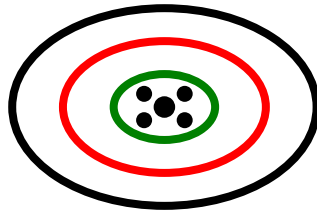


high bias, high variance

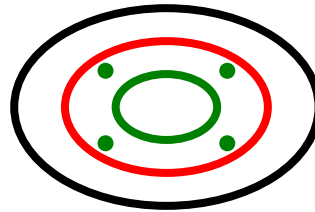


# Bias-Variance Trade-Off

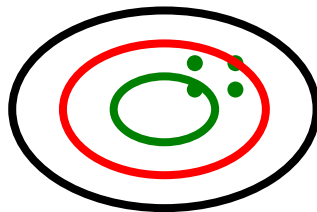
low bias, low variance



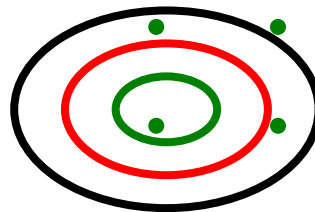
low bias, high variance



high bias, low variance

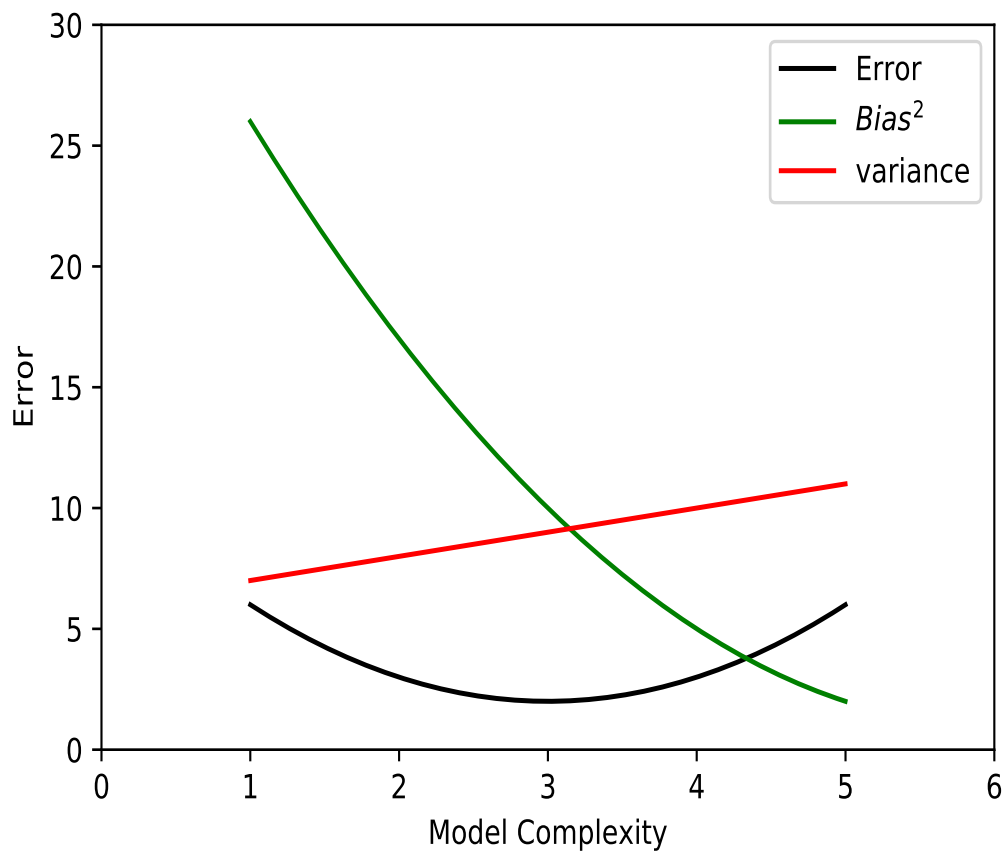


high bias, high variance



- "overfitting" - low bias, high variance
- "underfitting" - low variance, high bias

# Bias-Variance: Ideal Model



## Concepts Check:

- (a) prediction vs. classification
- (b) numerical vs. categorical data
- (c) loss function
- (d) testing and training data
- (e) bias elimination and stratification
- (f) cross and  $k$ -fold validation
- (g) bias vs. variance trade-offs