# — Machine Learning —

July 20, 2016

#### Example machine learning problem: Decide whether to play tennis at a given day.

Day	Outlook	Temperature	Humidity	Wind	PlayTennis
D1	Sunny	$\operatorname{Hot}$	High	Weak	No
D2	Sunny	$\operatorname{Hot}$	High	Strong	No
D3	Overcast	$\operatorname{Hot}$	High	Weak	Yes
D4	Rain	Mild	High	Weak	Yes
D5	Rain	Cool	Normal	Weak	Yes
D6	Rain	Cool	Normal	Strong	No
D7	Overcast	Cool	Normal	Strong	Yes
D8	Sunny	Mild	High	Weak	No
D9	Sunny	Cool	Normal	Weak	Yes
D10	Rain	Mild	Normal	Weak	Yes
D11	Sunny	Mild	Normal	Strong	Yes
D12	Overcast	Mild	High	Strong	Yes
D13	Overcast	$\operatorname{Hot}$	Normal	Weak	Yes
D14	Rain	Mild	High	Strong	No

#### Example machine learning problem: Decide whether to play tennis at a given day.

	Day	Outlook	Temperature	Humidity	Wind	PlayTennis
	D1	Sunny	$\operatorname{Hot}$	High	Weak	No
	D2	Sunny	$\operatorname{Hot}$	High	Strong	No
Input Attributes	D3	Overcast	$\operatorname{Hot}$	High	Weak	Yes
- or -	D4	Rain	Mild	High	Weak	Yes
Input Variables	D5	Rain	Cool	Normal	Weak	Yes
- or -	D6	Rain	Cool	Normal	Strong	No
Features	D7	Overcast	Cool	Normal	Strong	Yes
- or -	D8	Sunny	Mild	High	Weak	No
Attributes	D9	Sunny	Cool	Normal	Weak	Yes
	D10	Rain	Mild	Normal	Weak	Yes
	D11	Sunny	Mild	Normal	Strong	Yes
	D12	Overcast	Mild	High	Strong	Yes
	D13	Overcast	$\operatorname{Hot}$	Normal	Weak	Yes
	D14	Rain	Mild	High	Strong	No

#### Example machine learning problem: Decide whether to play tennis at a given day.

Day	Outlook	Temperature	Humidity	Wind	PlayTennis	L	
D1	$\operatorname{Sunny}$	$\operatorname{Hot}$	High	Weak	No	L	
D2	Sunny	$\operatorname{Hot}$	High	Strong	No	L	Target Variable
D3	Overcast	$\operatorname{Hot}$	High	Weak	Yes	L	- or -
D4	Rain	Mild	High	Weak	Yes	L	Class Label
D5	Rain	Cool	Normal	Weak	Yes	L	- or -
D6	Rain	$\operatorname{Cool}$	Normal	Strong	No		Goal
D7	Overcast	$\operatorname{Cool}$	Normal	Strong	Yes	Y	- or -
D8	Sunny	Mild	High	Weak	No	L	Output Variable
D9	Sunny	Cool	Normal	Weak	Yes	L	
D10	Rain	Mild	Normal	Weak	Yes	L	
D11	Sunny	Mild	Normal	Strong	Yes	L	
D12	Overcast	Mild	High	Strong	Yes	L	
D13	Overcast	$\operatorname{Hot}$	Normal	Weak	Yes	L	
D14	Rain	Mild	High	Strong	No	L	

#### **Supervised Learning:**

- Output variables (class labels) are given.
- The relationship between input and output is known.

#### **Reinforced Learning:**

- Output variables are not known, but actions are rewarded or punished.

#### **Unsupervised Learning:**

- Learn patterns from data without output variable or feedback.

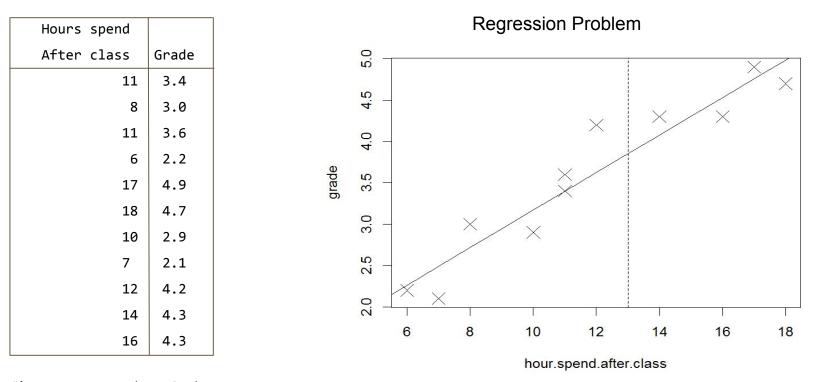
#### (Semi-supervised Learning:)

- Only a small amount of data is labeled.

- In Supervised Learning:
  - Classification: Output variable takes a finite set of values (Categorical Variable).
  - Regression: Output variable is numeric (Continuous Variable).

- In Unsupervised Learning:
  - Clustering is a common approach.

### **Classification vs Regression**



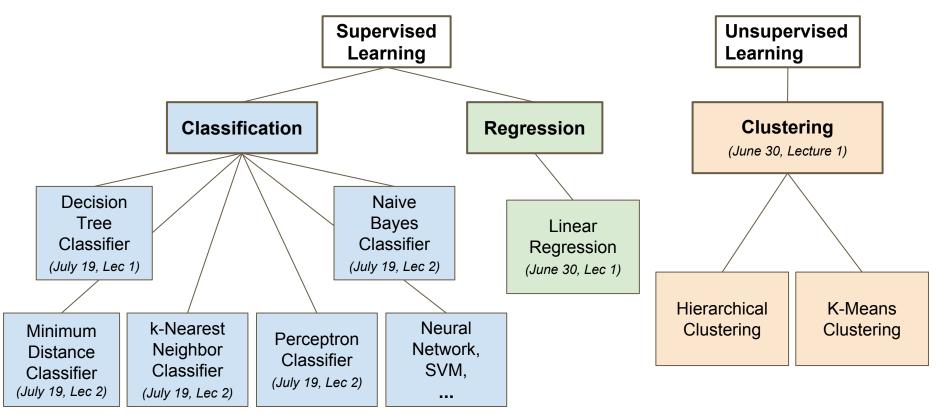
Given a new student S who spend 13 hours, what is the best guess of his/her grade?

#### **Classification vs Regression**

Hours spend		Classification Problem				
After class	Grade	- · · · · · · · · · · · · · · · · · · ·				
11	Y					
8	Y	0.8				
11	Y					
6	N					
17	Y	is.pass				
18	Y	. 0 –				
10	Ν	- 0				
7	N	0				
12	N					
14	N	6 8 10 12 14 16 18	-			
16	N					
		hour.spend.after.class				

Given a new student S who spend 13 hours, how likely will he/she pass the class?

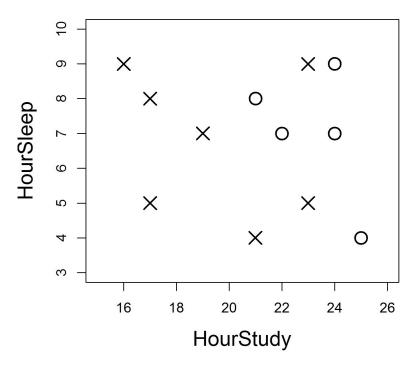
# In CS171, we learned:



Note: Most classification methods can be applied to regression problems.

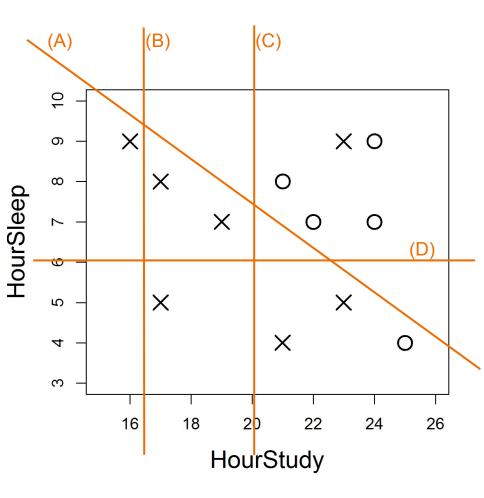
Consider the following set of training examples. There are two features: Number of hours a student spent studying (HourStudy), and the number of hours a student spent sleeping the night before the exam (HourSleep). The target variable is whether the student pass the class (Grade). The data is plotted on the right.

Grade	HourSleep	HourStudy
F	9	16
F	5	17
F	8	17
F	7	19
F	4	21
F	9	23
F	5	23
P	8	21
P	7	22
P	7	24
P	9	24
P	4	25



Use **Decision Tree Classifier**, which line best split the data as the first split?

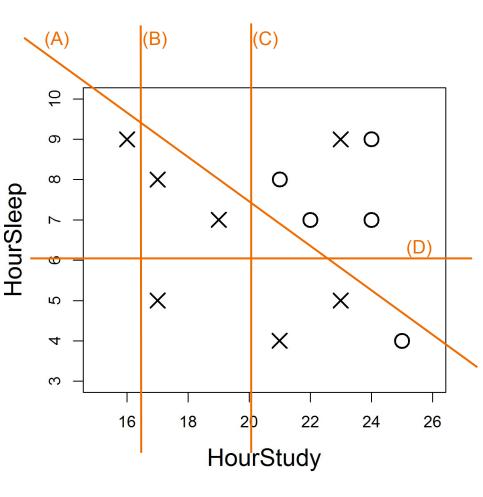
HourStudy	HourSleep	Grade
16	9	F
17	5	F
17	8	F
19	7	F
21	4	F
23	9	F
23	5	F
21	8	Р
22	7	P
24	7	Р
24	9	P
25	4	Р



Use **Decision Tree Classifier**, which line best split the data as the first split?

HourStudy	HourSleep	Grade
16	9	F
17	5	F
17	8	F
19	7	F
21	4	F
23	9	F
23	5	F
21	8	P
22	7	P
24	7	P
24	9	Р
25	4	Р

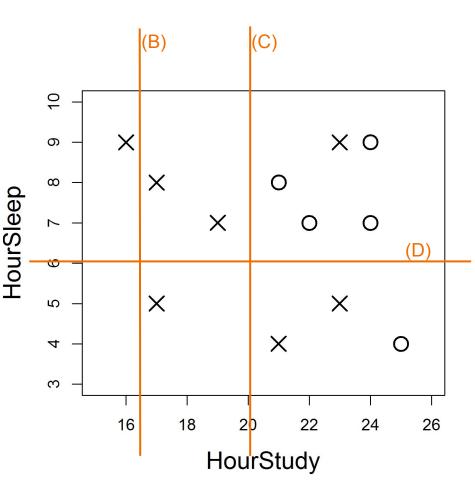
(A) is incorrect because when using decision tree we are splitting 1 variable at a time. Decision boundaries have to be perpendicular to x or y axis.



Use **Decision Tree Classifier**, which line best split the data as the first split?

HourStudy	HourSleep	Grade	
16	9	F	
17	5	F	
17	8	F	
19	7	F	
21	4	F	
23	9	F	
23	5	F	
21	8	P	
22	7	Р	
24	7	Р	
24	9	P	
25	4	Р	

(B) is not a good split because it clearly doesn't differentiate the dataset.



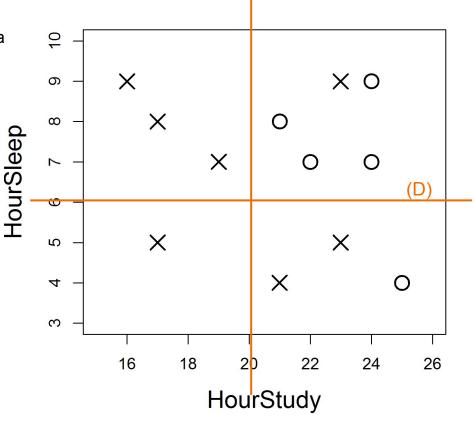
Use **Decision Tree Classifier**, which line best split the da as the first split?

HourStudy	HourSleep	Grade
16	9	F
17	5	F
17	8	F
19	7	F
21	4	F
23	9	F
23	5	F
21	8	P
22	7	P
24	7	Р
24	9	P
25	4	Р

(C) and (D) **can** both be reasonable splits. We have to examine their **entropy** values after the split.

In binary case,  $H(p) = -p \log p - (1-p) \log (1-p)$ 

Smaller entropy after splits  $\implies$  Greater information gain

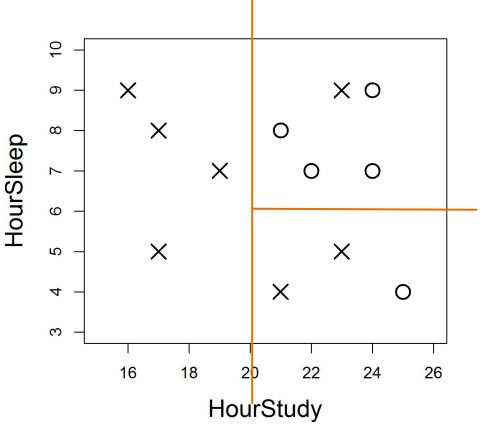


(C)

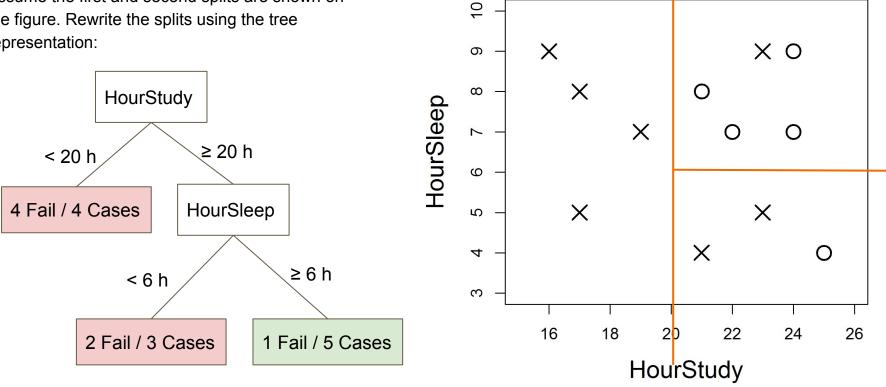
In binary case,  $H(p) = -p \log p - (1-p) \log (1-p)$ 10 X хо 0  $H(C_{\text{left}}) = 0$ Pick (C) Х Ο 8 HourSleep  $H(C_{\text{right}}) = -\frac{5}{8}\log_2 \frac{5}{8} - \frac{3}{8}\log_2 \frac{3}{8} = 0.95$ Х  $\cap$ 0 7 (D) 0  $H(C) = \frac{4}{12}H(C_{\text{left}}) + \frac{8}{12}H(C_{\text{right}}) = 0.63$ Х Х **Ω** -Х 0 4  $H(D_{top}) = -\frac{4}{8}\log_2\frac{4}{8} - \frac{4}{8}\log_2\frac{4}{8} = 1$ 3  $H(D_{\text{bottom}}) = -\frac{1}{4}\log_2\frac{1}{4} - \frac{3}{4}\log_2\frac{3}{4} = 0.81$ 16 18 22 24 20 26 HourStudy  $H(D) = \frac{8}{12}H(D_{\text{top}}) + \frac{4}{12}H(D_{\text{bottom}}) = 0.94$ 

(C)

Assume the first and second splits are shown on the figure. Rewrite the splits using the tree representation:

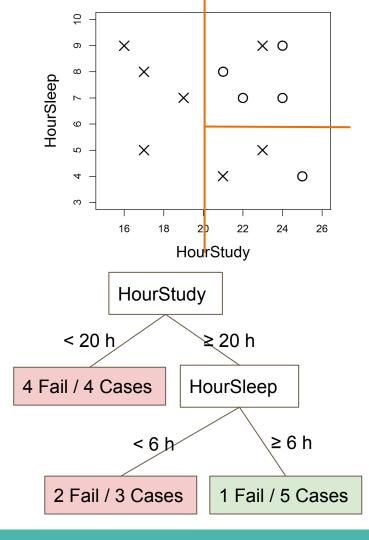


Assume the first and second splits are shown on the figure. Rewrite the splits using the tree representation:



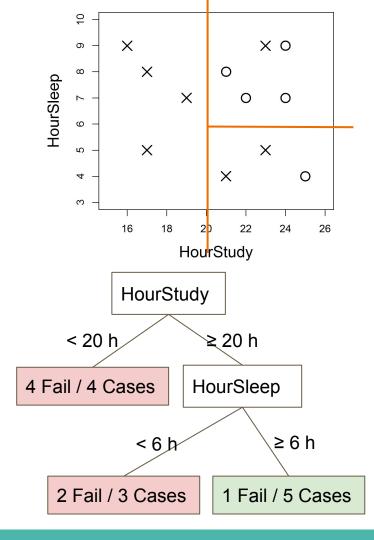
Classify the following test data cases. You should be able to obtain the predictions using either representation.

Student	HourStudy	HourSleep	Pass?
Alice	16	9	
Bob	26	5	
Charlie	21	8	



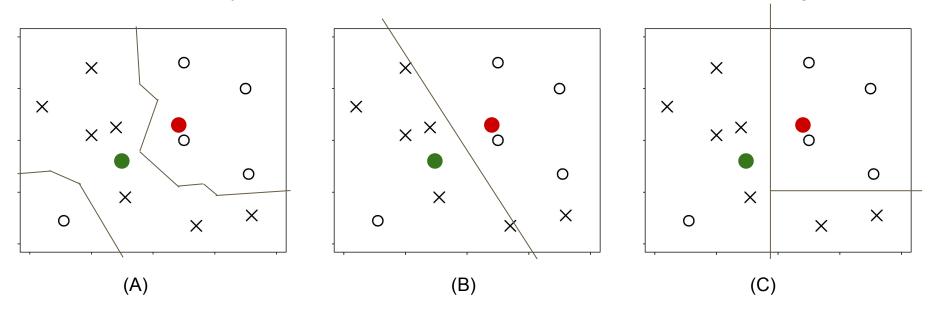
Classify the following test data cases. You should be able to obtain the predictions using either representation.

Student	HourStudy	HourSleep	Pass?
Alice	16	9	F
Bob	26	5	F
Charlie	21	8	Т



#### **Decision Boundary: Exercise**

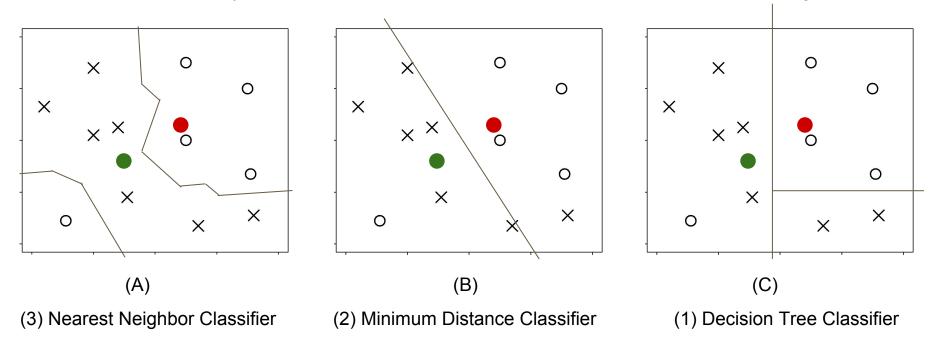
Match the decision boundary with the most probable classifiers. (Mean for each class is shown as red/green circle)



(1) Decision Tree Classifier; (2) Minimum Distance Classifier; (3) Nearest Neighbor Classifier.

#### **Decision Boundary: Exercise**

Match the decision boundary with the most probable classifiers. (Mean for each class is shown as red/green circle)



#### **Naive Bayes Classifier: Example**

Consider the following set of training examples. A and B are features and Y is the target variable. Each row indicates the values observed, and how many times that set of values was observed. For example, (t, t, 1) was observed 3 times, while (t, t, 0) was never observed.

А	В	Y	Count
t	t	1	3
t	f	1	2
f	t	1	1
f	f	1	2
t	t	0	0
t	f	0	1
f	t	0	1
f	f	0	2

In general:

$$P(Y|X_1, X_2, ...) = \frac{P(X_1, X_2, ..., Y)}{P(X_1, X_2, ...)} = \frac{P(X_1, X_2, ...|Y)P(Y)}{P(X_1, X_2, ...)}$$
(Bayes' rule)  
=  $\alpha P(X_1, X_2, ...|Y)P(Y)$  (let  $\alpha = \frac{1}{P(X_1, X_2, ...)}$ ).  
=  $\alpha P(Y)P(X_1|Y)P(X_2|P)...$  (Features are independent given the class)

Apply to this problem:

 $P(Y|A,B) = \alpha \ P(A|Y)P(B|Y)P(Y)$ 

We just need to calculate P(A|Y) P(B|Y) and P(Y)

This is a variation of problem 1 in http://www.cs.cmu.edu/afs/andrew/course/15/381f08/www/homework/hw5-sol.pdf

#### **Naive Bayes Classifier: Example**

Consider the following set of training examples. A and B are features and Y is the target variable. Each row indicates the values observed, and how many times that set of values was observed. For example, (t, t, 1) was observed 3 times, while (t, t, 0) was never observed.

А	В	Y	Count
t	t	1	3
t	f	1	2
f	t	1	1
f	f	1	2
t	t	0	0
t	f	0	1
f	t	0	1
f	f	0	2

 $P(Y|A, B) = \alpha \ P(A|Y)P(B|Y)P(Y)$ 

Eg.  $P(A = f | Y = 1) = \alpha 3/8$ ;  $P(B = t | Y = 1) = \alpha 4/8$  $P(Y = 1) = \alpha 8/12$ 

Given a test data case (f, t, ?), what is the most probable Y value?

This is a variation of problem 1 in http://www.cs.cmu.edu/afs/andrew/course/15/381-f08/www/homework/hw5-sol.pdf

#### **Naive Bayes Classifier: Example**

Consider the following set of training examples. A and B are features and Y is the target variable. Each row indicates the values observed, and how many times that set of values was observed. For example, (t, t, 1) was observed 3 times, while (t, t, 0) was never observed.

A	В	Y	Count
t	t	1	3
t	f	1	2
f	t	1	1
f	f	1	2
t	t	0	0
t	f	0	1
f	t	0	1
f	f	0	2

 $P(Y|A, B) = \alpha \ P(A|Y)P(B|Y)P(Y)$ 

Eg.  $P(A = f | Y = 1) = \alpha 3/8$ ;  $P(B = t | Y = 1) = \alpha 4/8$  $P(Y = 1) = \alpha 8/12$ 

Given a test data case (f, t, ?), what is the most probable Y value?

$$\begin{split} \mathsf{P}(\mathsf{Y} = 1 | \mathsf{A} = \mathsf{f}, \, \mathsf{B} = \mathsf{t}) &= \alpha \, \mathsf{P}(\mathsf{A} = \mathsf{f} \mid \mathsf{Y} = 1) \, \mathsf{P}(\mathsf{B} = \mathsf{t} \mid \mathsf{Y} = 1) \, \mathsf{P}(\mathsf{Y} = 1) = \alpha \, 3/8^* 4/8^* 8/12 \\ &= \alpha \, 1/8 \\ \mathsf{P}(\mathsf{Y} = 0 | \mathsf{A} = \mathsf{f}, \, \mathsf{B} = \mathsf{t}) = \alpha \, \mathsf{P}(\mathsf{A} = \mathsf{f} \mid \mathsf{Y} = 0) \, \mathsf{P}(\mathsf{B} = \mathsf{t} \mid \mathsf{Y} = 0) \, \mathsf{P}(\mathsf{Y} = 0) = \alpha \, 3/4^* 1/4^* 4/12 \\ &= \alpha \, 1/16 \end{split}$$

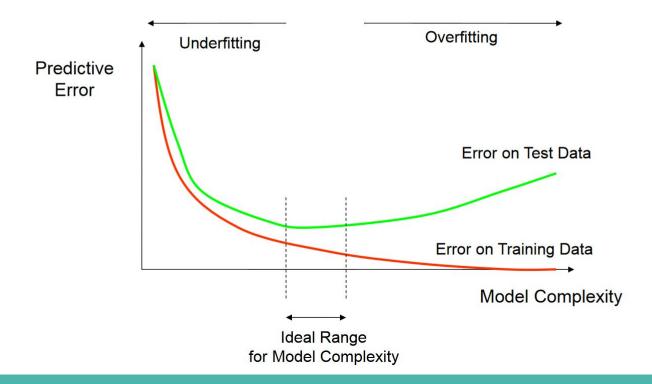
P(Y = 1|A = f, B = t) > P(Y = 0|A = f, B = t); The prediction is Y = 1.

This is a variation of problem 1 in http://www.cs.cmu.edu/afs/andrew/course/15/381f08/www/homework/hw5-sol.pdf

# Bias vs. Variance (Underfitting vs. Overfitting): Review

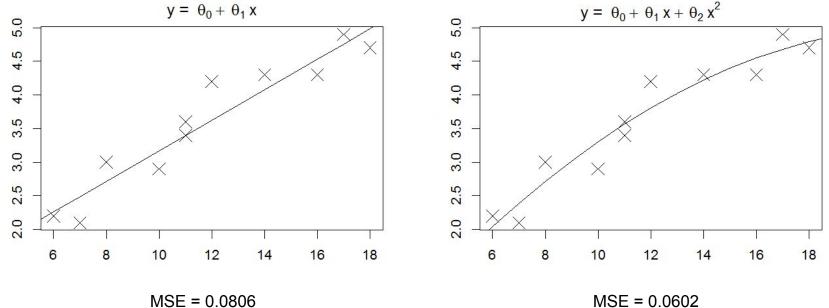
Underfitting: Error is caused by model bias.

Overfitting: Error is caused by data variance. (Slide 45-55, Lec1, July 19).



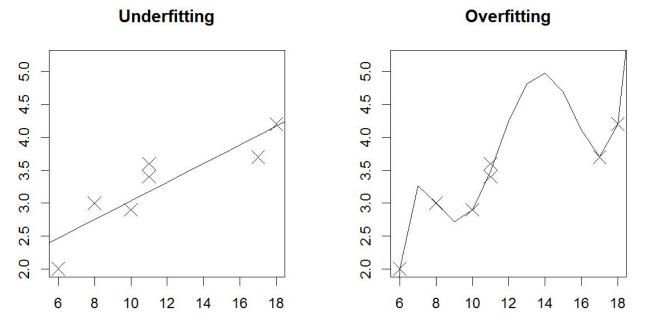
#### Bias vs. Variance (Underfitting vs. Overfitting): Review

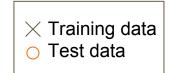
**Model complexity** in linear regression can be characterized by the number of parameters in the polynomial.



MSE = 0.0602

# Bias vs. Variance (Underfitting vs. Overfitting): Example

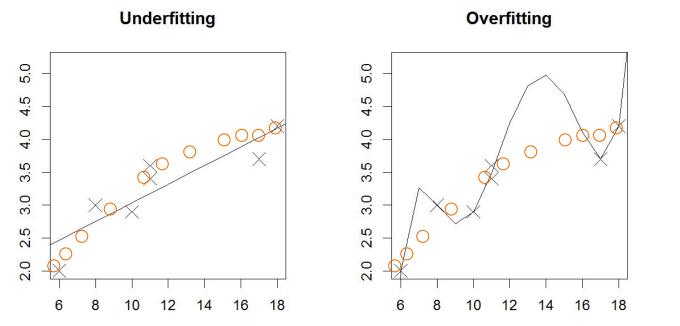




On the left: Linear regression (2 parameters). On the right: Polynomial regression (6 parameters).

Polynomial regression with 6 parameters is more complex than linear regression with 2 parameters, thus achieves smaller training error. (Assume the error measure is MSE = mean squared distance to the fitted line)

# Bias vs. Variance (Underfitting vs. Overfitting): Example



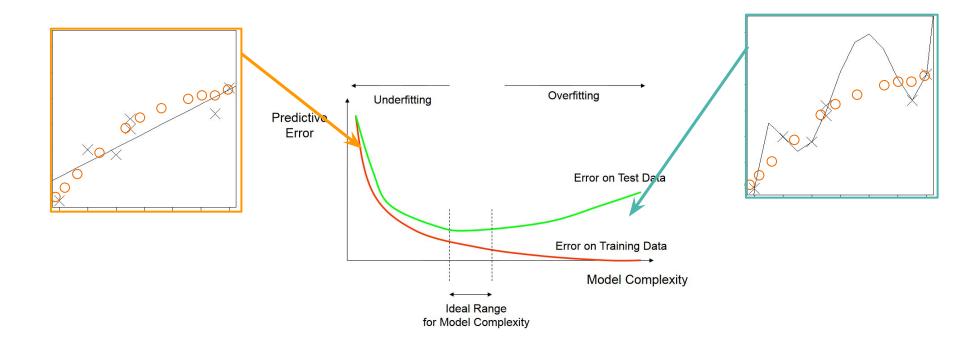
X Training data ○ Test data

However, when we used the fitted line to predict the values of the test data, polynomial model with 6 parameters suffers. It is because the model overfits the training data. Linear model suffers too (to a lesser extent) because it is too simple for the data.

# Bias vs. Variance (Underfitting vs. Overfitting): Review

Underfitting: Error is caused by model bias.

Overfitting: Error is caused by data variance. (Slide 45-55, Lec1, July 19).



Consider this training data set with 9 students' final scores and class grade. The single feature is **Final Score**, and class labels (**Grade**) are A, B, or C. (*This is a variation of Question 1, Final Exam, Fall 2014*).

Student	1	2	3	4	5	6	7	8	9
Final Score	53	59	70	79	84	87	91	93	99
Grade	В	С	В	В	А	В	А	A	А

Using 1-Nearest Neighbor, what class label would be assigned to a new student, who has Final Score = 86?

Using 3-Nearest Neighbor, what class label would be assigned to a new student, who has Final Score = 86?

Consider this training data set with 9 students' final scores and class grade. The single feature is **Final Score**, and class labels (**Grade**) are A, B, or C. (*This is a variation of Question 1, Final Exam, Fall 2014*).

Student	1	2	3	4	5	6	7	8	9
Final Score	53	59	70	79	84	87	91	93	99
Grade	В	С	В	В	А	В	A	A	А

Using 1-Nearest Neighbor, what class label would be assigned to a new student, who has Final Score = 86? B

Using 3-Nearest Neighbor, what class label would be assigned to a new student, who has Final Score = 86? A

Consider this training data set with 9 students' final scores and class grade. The single feature is **Final Score**, and class labels (**Grade**) are A, B, or C. (*This is a variation of Question 1, Final Exam, Fall 2014*).

Student	1	2	3	4	5	6	7	8	9
Final Score	53	59	70	79	84	87	91	93	99
Grade	В	С	В	В	А	В	A	A	А

Using 1-Nearest Neighbor and 3-fold Cross-Validation, what is the cross-validated accuracy of 1-Nearest Neighbor on this training set? (The validation partitions are given to you as Partition 1 =  $\{1,4,7\}$ ; Partition 2 =  $\{2,5,8\}$ ; Partition 3 =  $\{3,6,9\}$ )

Consider this training data set with 9 students' final scores and class grade. The single feature is **Final Score**, and class labels (**Grade**) are A, B, or C. (*This is a variation of Question 1, Final Exam, Fall 2014*).

Student	1	2	3	4	5	6	7	8	9	Color Labels
Final Score	53	59	70	79	84	87	91	93	99	"Training Set"
Grade	В	С	В	В	А	В	А	А	Α	Validation Set

Using 1-Nearest Neighbor and 3-fold Cross-Validation, what is the cross-validated accuracy of 1-Nearest Neighbor on this training set? (The validation partitions are given to you as Partition 1 =  $\{1,4,7\}$ ; Partition 2 =  $\{2,5,8\}$ ; Partition 3 =  $\{3,6,9\}$ )

Partition 1: Student 1's nearest neighbor is Student 2, predict C. - Incorrect. Student 4's nearest neighbor is Student 5, predict A. - Incorrect. Student 7's nearest neighbor is Student 8, predict A. - Correct. Accuracy of Partition 1 = 1/3

Consider this training data set with 9 students' final scores and class grade. The single feature is **Final Score**, and class labels (**Grade**) are A, B, or C. (*This is a variation of Question 1, Final Exam, Fall 2014*).

Student	1	2	3	4	5	6	7	8	9	Color Labels
Final Score	53	59	70	79	84	87	91	93	99	"Training Set"
Grade	В	С	В	В	А	В	А	А	А	Validation Set

Using 1-Nearest Neighbor and 3-fold Cross-Validation, what is the cross-validated accuracy of 1-Nearest Neighbor on this training set? (The validation partitions are given to you as Partition 1 =  $\{1,4,7\}$ ; Partition 2 =  $\{2,5,8\}$ ; Partition 3 =  $\{3,6,9\}$ )

Partition 2: Student 2's nearest neighbor is Student 1, predict B. - Incorrect. Student 5's nearest neighbor is Student 6, predict B. - Incorrect. Student 8's nearest neighbor is Student 7, predict A. - Correct. Accuracy of Partition 1 = 1/3 Accuracy of Partition 2 = 1/3

Consider this training data set with 9 students' final scores and class grade. The single feature is **Final Score**, and class labels (**Grade**) are A, B, or C. (*This is a variation of Question 1, Final Exam, Fall 2014*).

Student	1	2	3	4	5	6	7	8	9	Color Labels
Final Score	53	59	70	79	84	87	91	93	99	"Training Set"
Grade	В	С	В	В	А	В	А	А	A	Validation Set

Using 1-Nearest Neighbor and 3-fold Cross-Validation, what is the cross-validated accuracy of 1-Nearest Neighbor on this training set? (The validation partitions are given to you as Partition 1 =  $\{1,4,7\}$ ; Partition 2 =  $\{2,5,8\}$ ; Partition 3 =  $\{3,6,9\}$ )

Partition 3: Student 3's nearest neighbor is Student 4, predict B. - **Correct.** Student 6's nearest neighbor is Student 5, predict A. - **Incorrect.** Student 9's nearest neighbor is Student 8, predict A. - **Correct.**  Accuracy of Partition 1 = 1/3 Accuracy of Partition 2 = 1/3 Accuracy of Partition 3 = 2/3

Cross-validated Accuracy = 1/3 \* (1/3+1/3+2/3) = 4/9

# **Nearest Neighbor Classifier & Cross Validation : Verify at home**

Consider this training data set with 9 students' final scores and class grade. The single feature is **Final Score**, and class labels (**Grade**) are A, B, or C. (*This is a variation of Question 1, Final Exam, Fall 2014*).

Student	1	2	3	4	5	6	7	8	9
Final Score	58	59	70	79	84	87	91	93	99
Grade	В	С	В	В	A	В	А	А	А

Using **3-Nearest Neighbor** and 3-fold Cross-Validation, what is the cross-validated accuracy of 3-Nearest Neighbor on this training set? (The validation partitions are given to you as Partition  $1 = \{1,4,7\}$ ; Partition  $2 = \{2,5,8\}$ ; Partition  $3 = \{3,6,9\}$ )

Accuracy of Partition 1 (1,4,7 as validation set) = 1 Accuracy of Partition 2 (2,5,8 as validation set) = 1/3 Accuracy of Partition 3 (3,6,9 as validation set) = 2/3

Cross-validated Accuracy =1/3 \* (1+1/3+2/3) = 2/3