## INTRO TO DATA SCIENCE LECTURE 6: MACHINE LEARNING

#### **AGENDA**

I. WHAT IS MACHINE LEARNING?
II. MACHINE LEARNING PROBLEMS
III. SUPERVISED LEARNING PROBLEMS
IV. KNN CLASSIFICATION

## LEARNING?

#### WHAT IS MACHINE LEARNING?

#### from Wikipedia:

"Machine learning, a branch of artificial intelligence, is about the construction and study of systems that can *learn from data*."

#### from Wikipedia:

"Machine learning, a branch of artificial intelligence, is about the construction and study of systems that can *learn from data*."

"The core of machine learning deals with representation and generalization..."

#### WHAT IS MACHINE LEARNING?

#### from Wikipedia:

"Machine learning, a branch of artificial intelligence, is about the construction and study of systems that can *learn from data*."

"The core of machine learning deals with representation and generalization..."

representation – extracting structure from data

#### WHAT IS MACHINE LEARNING?

#### from Wikipedia:

"Machine learning, a branch of artificial intelligence, is about the construction and study of systems that can  $learn\ from\ data$ ."

"The core of machine learning deals with representation and generalization..."

- representation extracting structure from data
- generalization making predictions from data

## II. MACHINE LEARNING PROBLEMS

making predictions discovering patterns

labeled examples no labeled examples

#### **TYPES OF DATA**

### categorical continuous qualitative quantitative

	continuous	categorical
supervised unsupervised	regression dimension reduction	classification clustering

#### What type of problem is this?

#### **Priority Inbox**



#### What type of problem is this?

#### **Priority Inbox**



Probably either.



#### **Priority Inbox: Supervised Learning**

Predict which mails users are most likely to star



#### **Priority Inbox: Unsupervised Learning**

Group mails into groups and decide which group represents important mails

What type of problem is this?

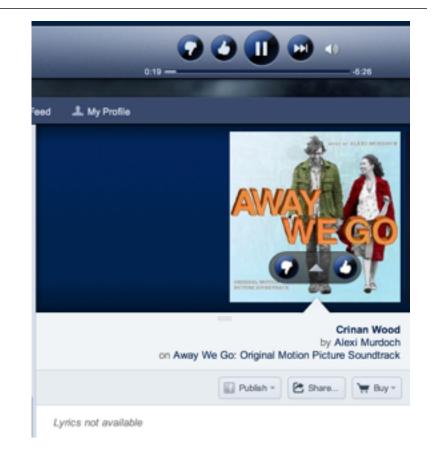
**Music Recommendation** 



What type of problem is this?

**Music Recommendation** 

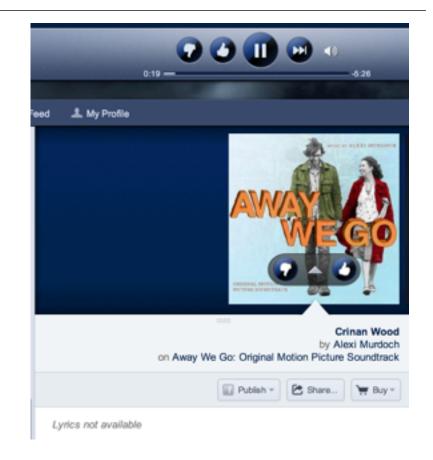
Probably either.



What type of problem is this?

**Music Recommendation** as Supervised Learning

Predict which songs a user will 'thumbs-up'



What type of problem is this?

**Music Recommendation As Unsupervised Learning** 

Cluster songs based on attributes and recommend songs in the same group



# HOW DO YOU DETERMINE

THE RIGHT
APPROACH?

#### continuous

### regression dimension reduction

### classification clustering

categorical

#### **ANSWER**

The right approach is determined by the desired solution and the data available.

# HOW DO YOU REPRESENT

YOUR
DATA?

### categorical continuous quantitative qualitative

	continuous	categorical	•
color	RGB-values	{red, blue}	
ratings	1 — 10 rating	1-5 star rating	

# HOW DO YOU MEASURE

OF QUALITY?

making predictions extracting structure

test out your predictions

--

#### supervised

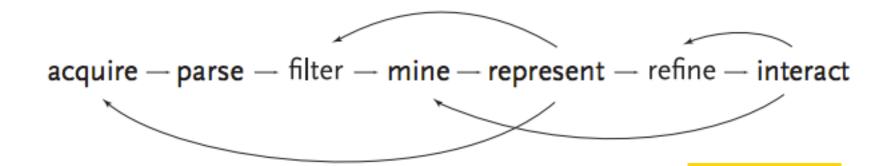
test out your predictions

#### QUESTION

### NHAT DO YOU WITH YOUR RESULTS?

**ANSWER** 

Interpret them and react accordingly.



source: http://benfry.com/phd/dissertation-110323c.pdf

### III. SUPERVISED LEARNING

### Q: How does a classification problem work? A: Data in, predicted labels out.

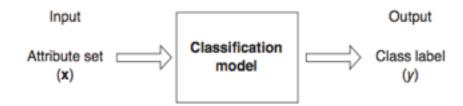
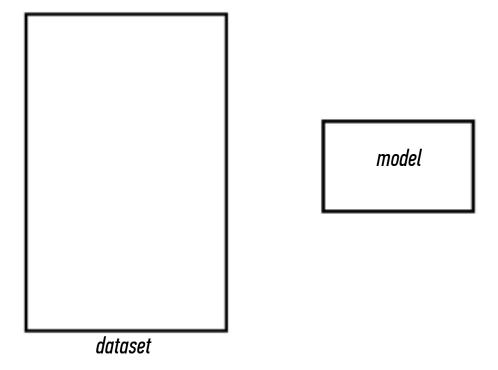


Figure 4.2. Classification as the task of mapping an input attribute set x into its class label y.

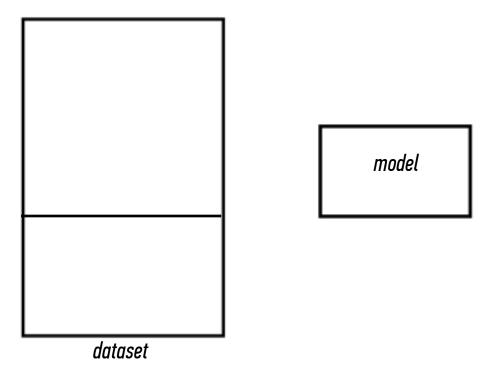
#### **SUPERVISED LEARNING PROBLEMS**

Q: What steps does a classification problem require?



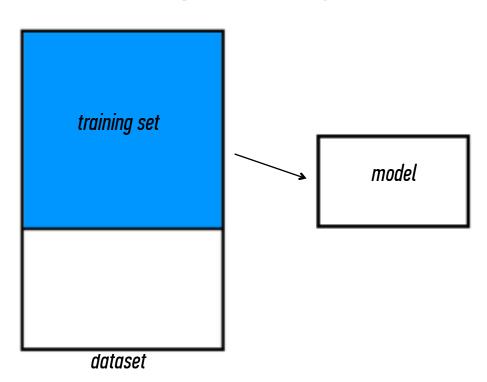
Q: What steps does a classification problem require?

1) split dataset



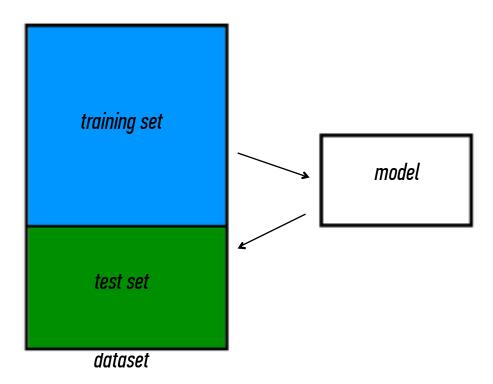
#### **SUPERVISED LEARNING PROBLEMS**

- Q: What steps does a classification problem require?
  - 1) split dataset
- 2) train model



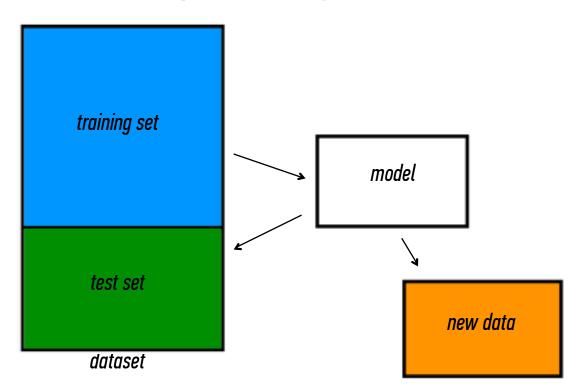
#### **SUPERVISED LEARNING PROBLEMS**

- 1) split dataset
- 2) train model
- 3) test model



#### **SUPERVISED LEARNING PROBLEMS**

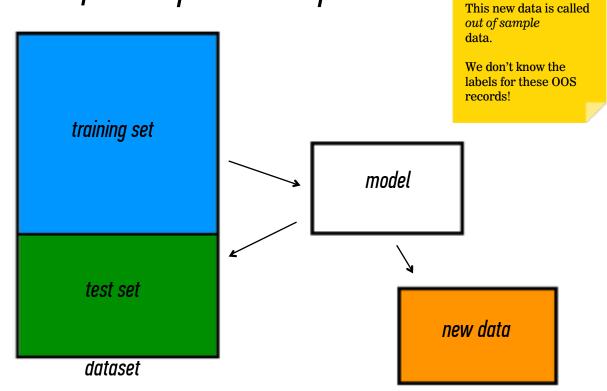
- 1) split dataset
- 2) train model
- 3) test model
- 4) make predictions



NOTE

#### **SUPERVISED LEARNING PROBLEMS**

- 1) split dataset
- 2) train model
- 3) test model
- 4) make predictions



	continuous	categorical
supervised	???	???
unsupervised	???	???

# continuouscategoricalsupervisedregressionclassificationunsuperviseddimension reductionclustering

# Here's (part of) an example dataset:

#### Fisher's Iris Data

Sepal length ¢	Sepal width ¢	Petal length ¢	Petal width ¢	Species ¢
5.1	3.5	1.4	0.2	I. setosa
4.9	3.0	1.4	0.2	I. setosa
4.7	3.2	1.3	0.2	I. setosa
4.6	3.1	1.5	0.2	I. setosa
5.0	3.6	1.4	0.2	I. setosa
5.4	3.9	1.7	0.4	I. setosa
4.6	3.4	1.4	0.3	I. setosa
5.0	3.4	1.5	0.2	I. setosa

# Here's (part of) an example dataset:

#### Fisher's Iris Data

# independent variables

Sepal length ¢	Sepal width ¢	Petal length ¢	Petal width ¢	Species ¢
5.1	3.5	1.4	0.2	I. setosa
4.9	3.0	1.4	0.2	I. setosa
4.7	3.2	1.3	0.2	I. setosa
4.6	3.1	1.5	0.2	I. setosa
5.0	3.6	1.4	0.2	I. setosa
5.4	3.9	1.7	0.4	I. setosa
4.6	3.4	1.4	0.3	I. setosa
5.0	3.4	1.5	0.2	I. setosa

# Here's (part of) an example dataset:

#### Fisher's Iris Data

independent variables

Sepal length ¢	Sepal width ¢	Petal length ¢	Petal width ¢	Species ¢
5.1	3.5	1.4	0.2	I. setosa
4.9	3.0	1.4	0.2	I. setosa
4.7	3.2	1.3	0.2	I. setosa
4.6	3.1	1.5	0.2	I. setosa
5.0	3.6	1.4	0.2	I. setosa
5.4	3.9	1.7	0.4	I. setosa
4.6	3.4	1.4	0.3	I. setosa
5.0	3.4	1.5	0.2	I. setosa

class labels (qualitative)

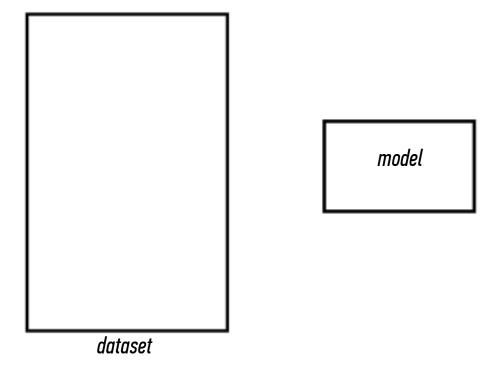
Q: What does "supervised" mean?

# Q: What does "supervised" mean?

A: We know the labels.

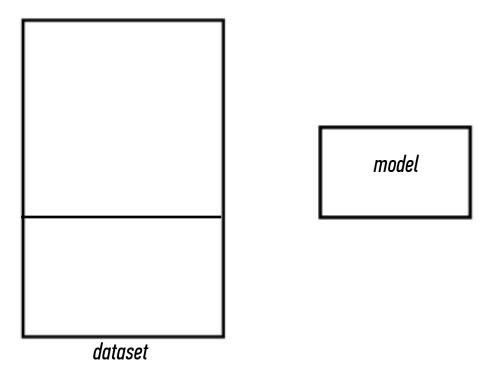
```
Welcome to R! Thu Feb 28 13:07:25 2013
> summary(iris)
 Sepal.Length
                Sepal.Width
                                Petal.Length
                                                 Petal.Width
Min.
       :4.300
                Min.
                       :2.000
                                Min.
                                       :1.000
                                                Min.
                                                       :0.100
                1st Qu.:2.800
                                1st Qu.:1.600
                                                1st Qu.:0.300
 1st Qu.:5.100
                Median :3.000
Median :5.800
                                Median :4.350
                                                Median :1.300
       :5.843
                       :3.057
                                       :3.758
                                                       :1.199
 Mean
                Mean
                                Mean
                                                Mean
 3rd Qu.:6.400
                3rd Qu.:3.300
                                3rd Qu.:5.100
                                                3rd Qu.:1.800
        :7.900 MgX
                        :4.400
                                        :6.900
                                                        :2.500
                                Max.
                                                Max.
 Max.
      Species
           :50
 setosa
versicolor:50
 virginica:50
```

Q: How does a classification problem work?

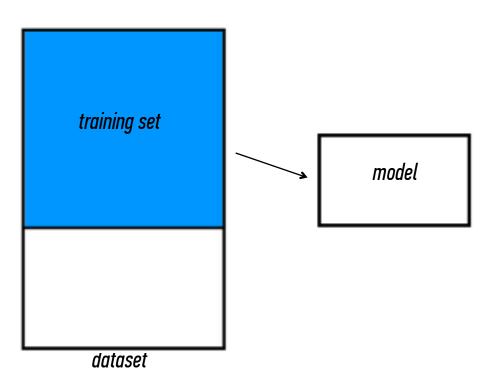


Q: What steps does a classification problem require?

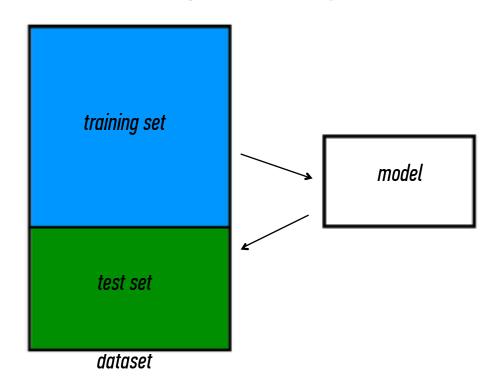
1) split dataset



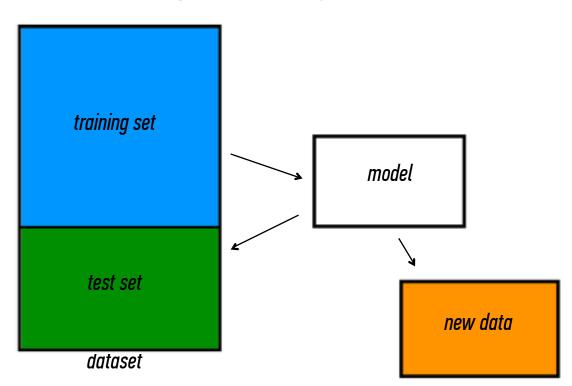
- 1) split dataset
- 2) train model



- 1) split dataset
- 2) train model
- 3) test model

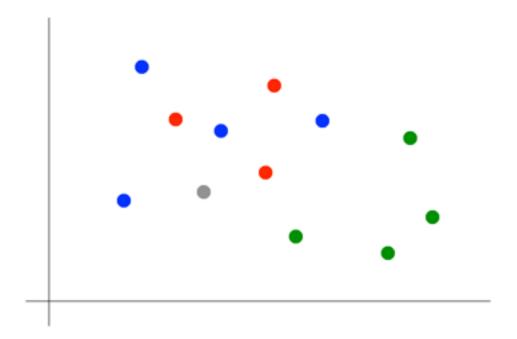


- 1) split dataset
- 2) train model
- 3) test model
- 4) make predictions



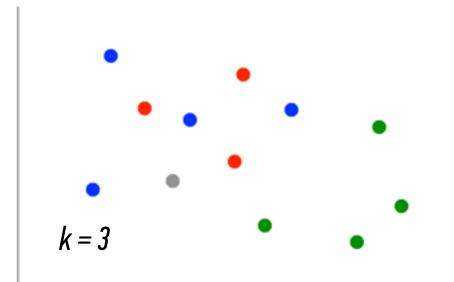
# KNN CLASSIFICATION

Suppose we want to predict the color of the grey dot.



Suppose we want to predict the color of the grey dot.

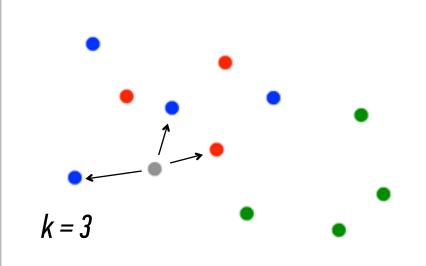
1) Pick a value for k.



#### KNN CLASSIFICATION

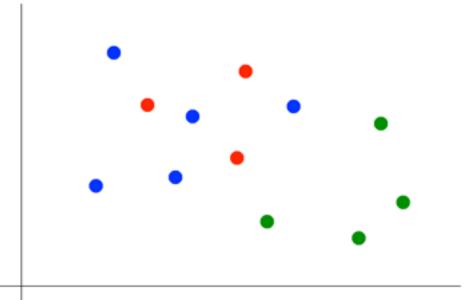
# Suppose we want to predict the color of the grey dot.

- 1) Pick a value for k.
- 2) Find colors of k nearest neighbors.



# Suppose we want to predict the color of the grey dot.

- 1) Pick a value for k.
- 2) Find colors of k nearest neighbors.
- 3) Assign the most common color to the grey dot.



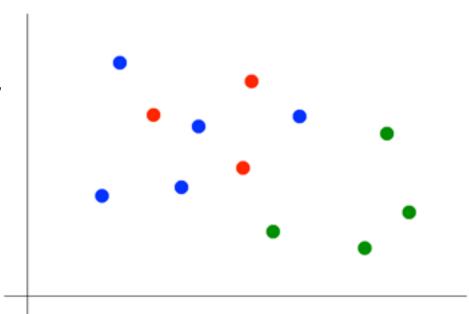
#### KNN CLASSIFICATION

# Suppose we want to predict the color of the grey dot.

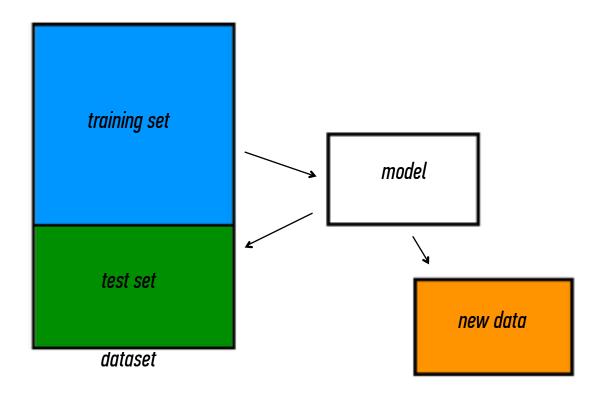
- 1) Pick a value for k.
- 2) Find colors of k nearest neighbors.
- 3) Assign the most common color to the grey dot.

#### **OPTIONAL NOTE**

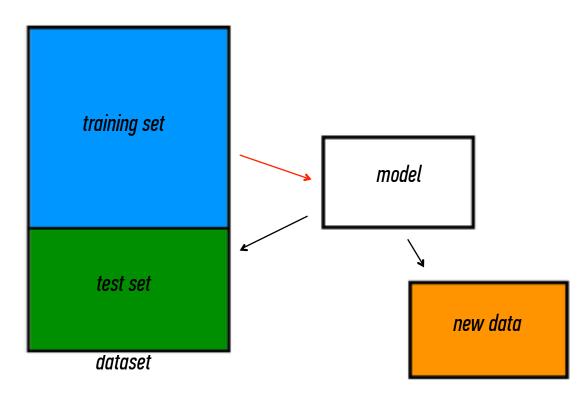
Our definition of "nearest" implicitly uses the Euclidean distance function.



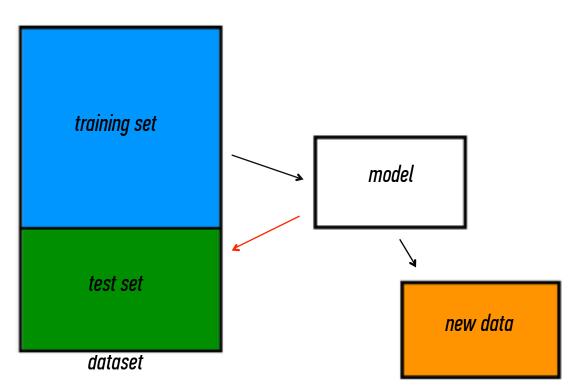
# BUILDING EFFECTIVE CLASSIFIERS



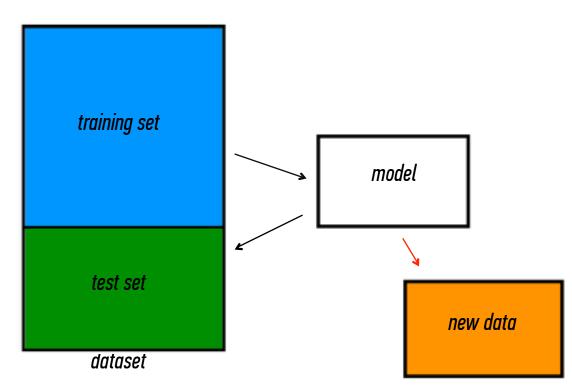
1) training error



- 1) training error
- 2) generalization error



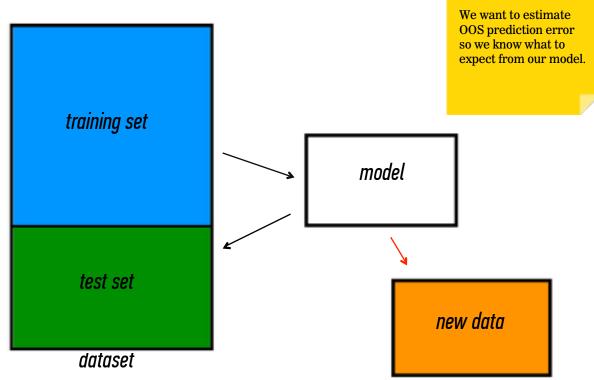
- 1) training error
- 2) generalization error
- *3) 00S error*



NOTE

#### **BUILDING EFFECTIVE CLASSIFIERS**

- Q: What types of prediction error will we run into?
- 1) training error
- 2) generalization error
- *3) 00S error*



#### **TRAINING ERROR**

Q: Why should we use training & test sets?

#### TRAINING ERROR

Q: Why should we use training & test sets?

Thought experiment:

Suppose instead, we train our model using the entire dataset.

Thought experiment:

Suppose instead, we train our model using the entire dataset.

Q: How low can we push the training error?

Thought experiment:

Suppose instead, we train our model using the entire dataset.

- Q: How low can we push the training error?
- We can make the model arbitrarily complex (effectively "memorizing" the entire training set).

Thought experiment:

Suppose instead, we train our model using the entire dataset.

Q: How low can we push the training error?

- We can make the model arbitrarily complex (effectively "memorizing" the entire training set).

A: Down to zero!

#### Thought experiment:

Suppose instead, we train our model using the entire dataset.

Q: How low can we push the training error?

 We can make the model arbitrarily complex (effectively "memorizing" the entire training set).

A: Down to zero!

#### NOTE

This phenomenon is called *overfitting*.

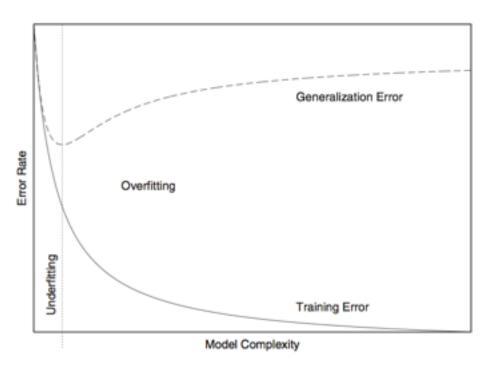
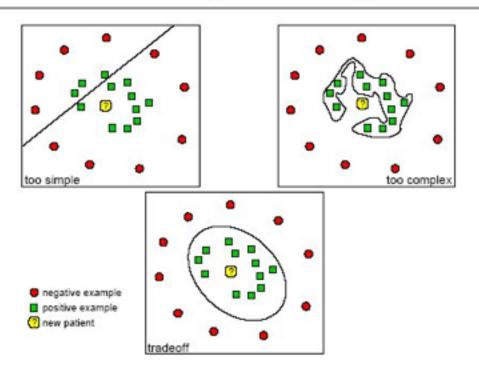


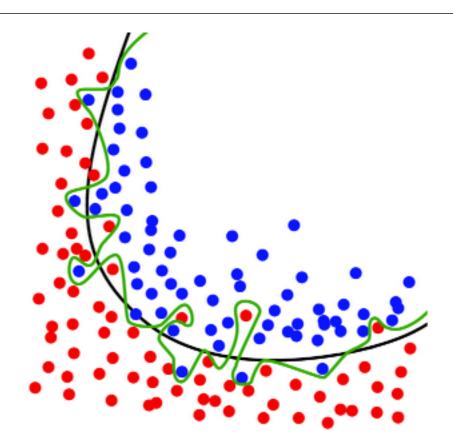
FIGURE 18-1. Overfitting: as a model becomes more complex, it becomes increasingly able to represent the training data. However, such a model is overfitted and will not generalize well to data that was not used during training.

#### **OVERFITTING - EXAMPLE**

#### **Underfitting and Overfitting**



#### **OVERFITTING - EXAMPLE**



## Q: Why should we use training & test sets?

### Thought experiment:

Suppose instead, we train our model using the entire dataset.

Q: How low can we push the training error?

 We can make the model arbitrarily complex (effectively "memorizing" the entire training set).

A: Down to zero!

#### NOTE

This phenomenon is called overfitting.

A: Training error is not a good estimate of OOS accuracy.

## Suppose we do the train/test split.

Suppose we do the train/test split.

Q: How well does generalization error predict 00S accuracy?

Suppose we do the train/test split.

Q: How well does generalization error predict 00S accuracy?

Thought experiment:

Suppose we had done a different train/test split.

Suppose we do the train/test split.

Q: How well does generalization error predict 00S accuracy?

Thought experiment:

Suppose we had done a different train/test split.

Q: Would the generalization error remain the same?

Suppose we do the train/test split.

Q: How well does generalization error predict 00S accuracy?

Thought experiment:

Suppose we had done a different train/test split.

Q: Would the generalization error remain the same?

A: Of course not!

Suppose we do the train/test split.

Q: How well does generalization error predict 00S accuracy?

Thought experiment:

Suppose we had done a different train/test split.

Q: Would the generalization error remain the same?

A: Of course not!

A: On its own, not very well.

## Something is still missing!

Something is still missing!

Q: How can we do better?

Q: How can we do better?

Thought experiment:

Different train/test splits will give us different generalization errors.

Q: How can we do better?

Thought experiment:

Different train/test splits will give us different generalization errors.

Q: What if we did a bunch of these and took the average?

Q: How can we do better?

Thought experiment:

Different train/test splits will give us different generalization errors.

Q: What if we did a bunch of these and took the average?

A: Now you're talking!

Q: How can we do better?

Thought experiment:

Different train/test splits will give us different generalization errors.

Q: What if we did a bunch of these and took the average?

A: Now you're talking!

A: Cross-validation.

## Steps for n-fold cross-validation:

1) Randomly split the dataset into n equal partitions.

- 1) Randomly split the dataset into n equal partitions.
- 2) Use partition 1 as test set & union of other partitions as training set.

- 1) Randomly split the dataset into n equal partitions.
- 2) Use partition 1 as test set & union of other partitions as training set.
- 3) Find generalization error.

- 1) Randomly split the dataset into n equal partitions.
- 2) Use partition 1 as test set & union of other partitions as training set.
- 3) Find generalization error.
- 4) Repeat steps 2-3 using a different partition as the test set at each iteration.

- 1) Randomly split the dataset into n equal partitions.
- 2) Use partition 1 as test set & union of other partitions as training set.
- 3) Find generalization error.
- 4) Repeat steps 2-3 using a different partition as the test set at each iteration.
- 5) Take the average generalization error as the estimate of OOS accuracy.

## Features of n-fold cross-validation:

1) More accurate estimate of 00S prediction error.

- 1) More accurate estimate of 00S prediction error.
- 2) More efficient use of data than single train/test split.
  - Each record in our dataset is used for both training and testing.

- 1) More accurate estimate of OOS prediction error.
- 2) More efficient use of data than single train/test split.
  - Each record in our dataset is used for both training and testing.
- 3) Presents tradeoff between efficiency and computational expense.
  - 10-fold CV is 10x more expensive than a single train/test split

- 1) More accurate estimate of OOS prediction error.
- 2) More efficient use of data than single train/test split.
  - Each record in our dataset is used for both training and testing.
- 3) Presents tradeoff between efficiency and computational expense.
  - 10-fold CV is 10x more expensive than a single train/test split
- 4) Can be used for model selection.

#### INTRO TO DATA SCIENCE

# DISCUSSION