

INTRO to DATA SCIENCE

LECTURE 5: MACHINE LEARNING

I. WHAT IS MACHINE LEARNING?

II. MACHINE LEARNING PROBLEMS

III. CLASSIFICATION PROBLEMS

IV. KNN CLASSIFICATION

V. BUILDING EFFECTIVE CLASSIFIERS

I. WHAT IS MACHINE LEARNING?

WHAT IS MACHINE LEARNING?

4

from Wikipedia:

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

source: http://en.wikipedia.org/wiki/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...”

source: http://en.wikipedia.org/wiki/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

source: http://en.wikipedia.org/wiki/Machine_learning

WHAT IS MACHINE LEARNING?

7

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

source: http://en.wikipedia.org/wiki/Machine_learning

II. MACHINE LEARNING PROBLEMS

<i>supervised</i>	
<i>unsupervised</i>	

<i>supervised</i>	<i>making predictions</i>
<i>unsupervised</i>	<i>discovering patterns</i>

<i>supervised</i>	<i>labeled examples</i>
<i>unsupervised</i>	<i>no labeled examples</i>

continuous

categorical

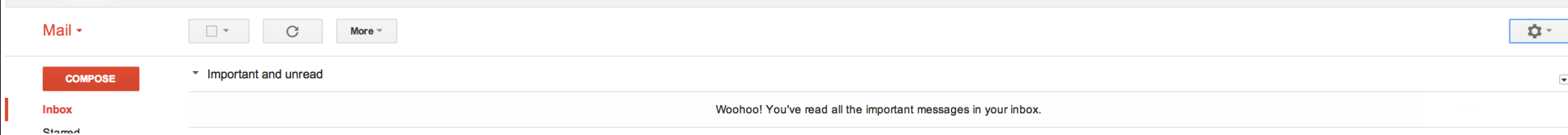
quantitative

qualitative

	<i>continuous</i>	<i>categorical</i>
<i>supervised</i>	<i>regression</i>	<i>classification</i>
<i>unsupervised</i>	<i>dimension reduction</i>	<i>clustering</i>

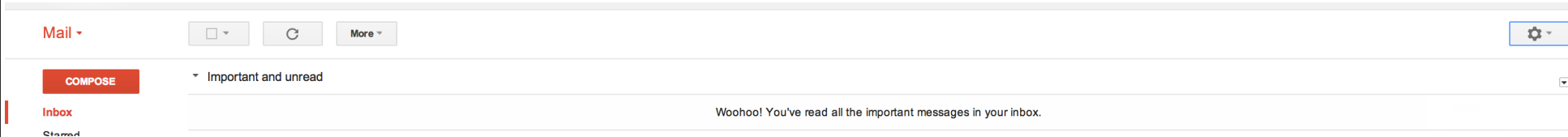
What type of problem is this?

Priority Inbox

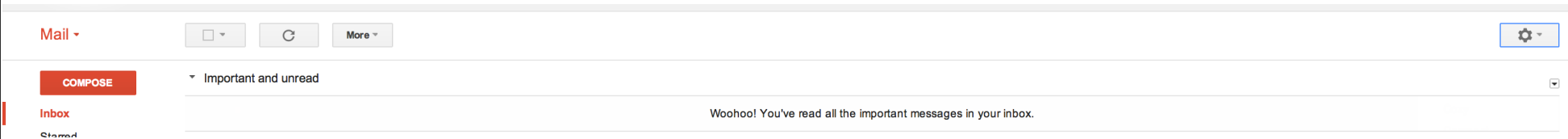


What type of problem is this?

Priority Inbox

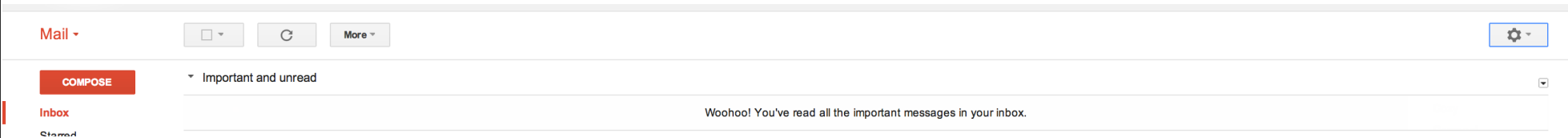


Probably either.



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



QUESTION

***HOW
DO YOU
DETERMINE
THE RIGHT
APPROACH?***

	<i>continuous</i>	<i>categorical</i>
<i>supervised</i>	<i>regression</i>	<i>classification</i>
<i>unsupervised</i>	<i>dimension reduction</i>	<i>clustering</i>

ANSWER

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

QUESTION

HOW
DO YOU
REPRESENT
YOUR
DATA?

continuous

categorical

quantitative

qualitative

	<i>continuous</i>	<i>categorical</i>
<i>color</i>	<i>RGB-values</i>	<i>{red, blue}</i>
<i>ratings</i>	<i>1 – 10 rating</i>	<i>1-5 star rating</i>

QUESTION

***HOW
DO YOU
MEASURE
QUALITY?***

<i>supervised</i> <i>unsupervised</i>	<i>making predictions</i> <i>extracting structure</i>
------------------------------------------	----------------------------------------------------------

<i>supervised</i> <i>unsupervised</i>	<i>test out your predictions</i> <i>...</i>
------------------------------------------	------------------------------------------------

QUESTION

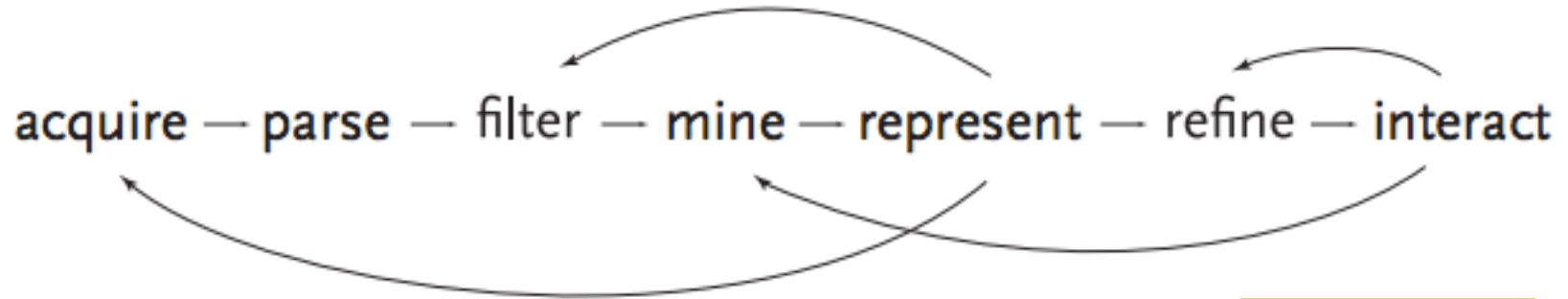
WHAT

DO YOU

DO

WITH YOUR

RESULTS?



ANSWER

Interpret them and react accordingly.

III. CLASSIFICATION PROBLEMS

Q: How does a classification problem work?

Q: How does a classification problem work?

A: Data in, predicted labels out.

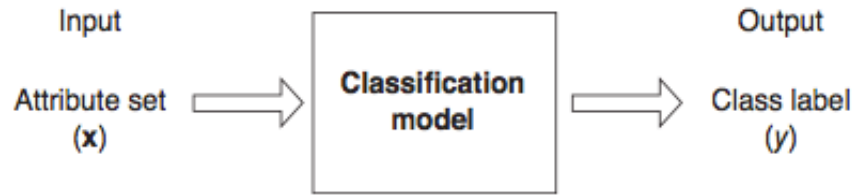


Figure 4.2. Classification as the task of mapping an input attribute set x into its class label y .

	<i>continuous</i>	<i>categorical</i>
<i>supervised</i>	???	???
<i>unsupervised</i>	???	???

	<i>continuous</i>	<i>categorical</i>
<i>supervised</i>	<i>regression</i>	<i>classification</i>
<i>unsupervised</i>	<i>dimension reduction</i>	<i>clustering</i>

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>I. setosa</i>
4.9	3.0	1.4	0.2	<i>I. setosa</i>
4.7	3.2	1.3	0.2	<i>I. setosa</i>
4.6	3.1	1.5	0.2	<i>I. setosa</i>
5.0	3.6	1.4	0.2	<i>I. setosa</i>
5.4	3.9	1.7	0.4	<i>I. setosa</i>
4.6	3.4	1.4	0.3	<i>I. setosa</i>
5.0	3.4	1.5	0.2	<i>I. setosa</i>

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>I. setosa</i>
4.9	3.0	1.4	0.2	<i>I. setosa</i>
4.7	3.2	1.3	0.2	<i>I. setosa</i>
4.6	3.1	1.5	0.2	<i>I. setosa</i>
5.0	3.6	1.4	0.2	<i>I. setosa</i>
5.4	3.9	1.7	0.4	<i>I. setosa</i>
4.6	3.4	1.4	0.3	<i>I. setosa</i>
5.0	3.4	1.5	0.2	<i>I. setosa</i>

*independent
variables*



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>I. setosa</i>
4.9	3.0	1.4	0.2	<i>I. setosa</i>
4.7	3.2	1.3	0.2	<i>I. setosa</i>
4.6	3.1	1.5	0.2	<i>I. setosa</i>
5.0	3.6	1.4	0.2	<i>I. setosa</i>
5.4	3.9	1.7	0.4	<i>I. setosa</i>
4.6	3.4	1.4	0.3	<i>I. setosa</i>
5.0	3.4	1.5	0.2	<i>I. setosa</i>

*independent
variables*

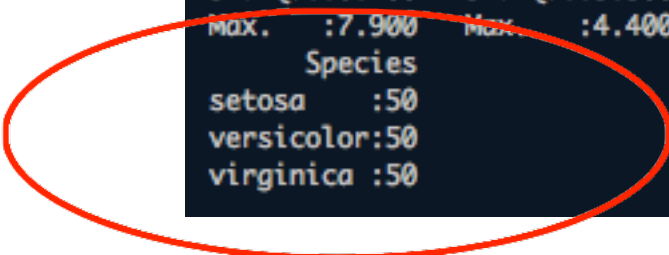
*class
labels
(qualitative)*

Q: What does “supervised” mean?

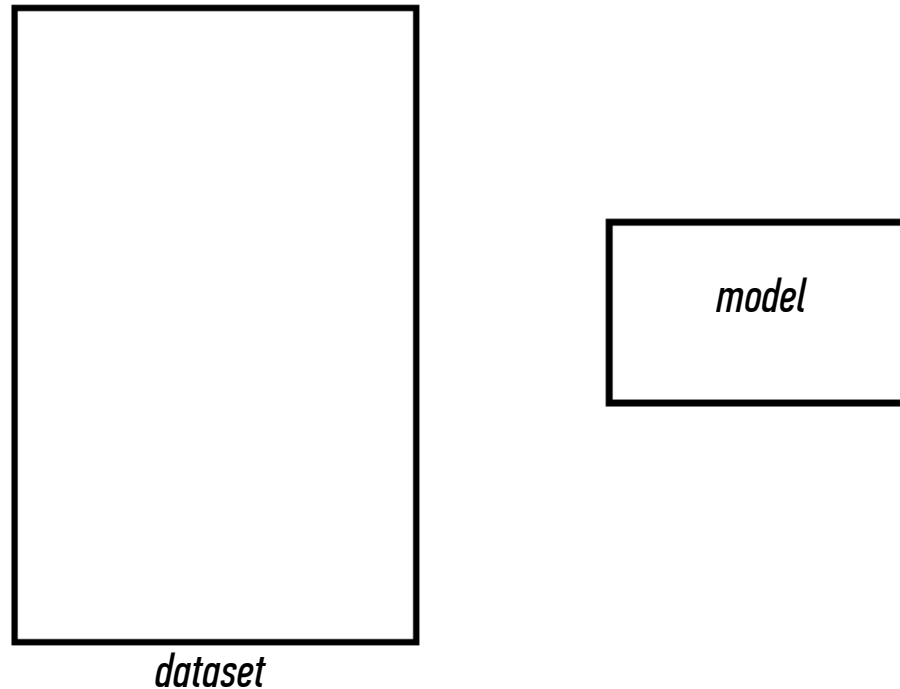
Q: What does “supervised” mean?

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.:5.100   1st Qu.:2.800   1st Qu.:1.600   1st Qu.:0.300
Median :5.800   Median :3.000   Median :4.350   Median :1.300
Mean   :5.843   Mean   :3.057   Mean   :3.758   Mean   :1.199
3rd Qu.:6.400   3rd Qu.:3.300   3rd Qu.:5.100   3rd Qu.:1.800
Max.   :7.900   Max.   :4.400   Max.   :6.900   Max.   :2.500
   Species
setosa   :50
versicolor:50
virginica :50
```

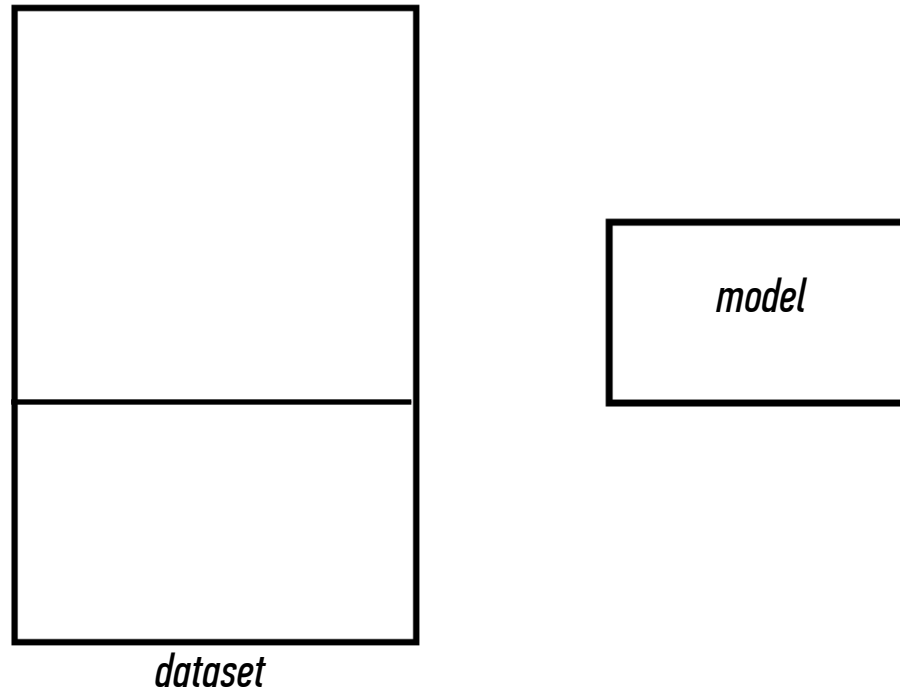


Q: What steps does a classification problem require?



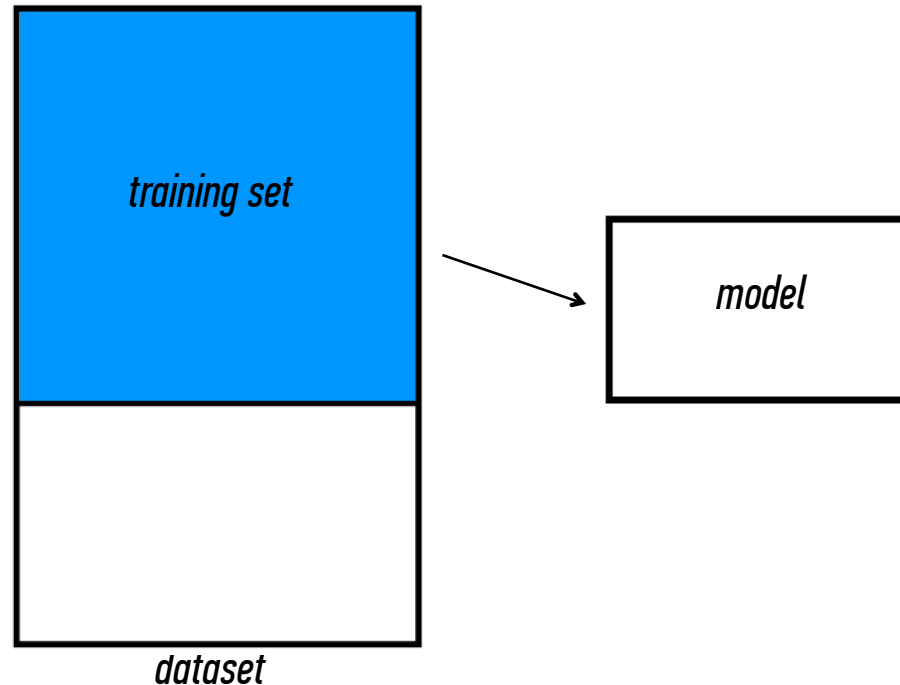
Q: What steps does a classification problem require?

1) split dataset



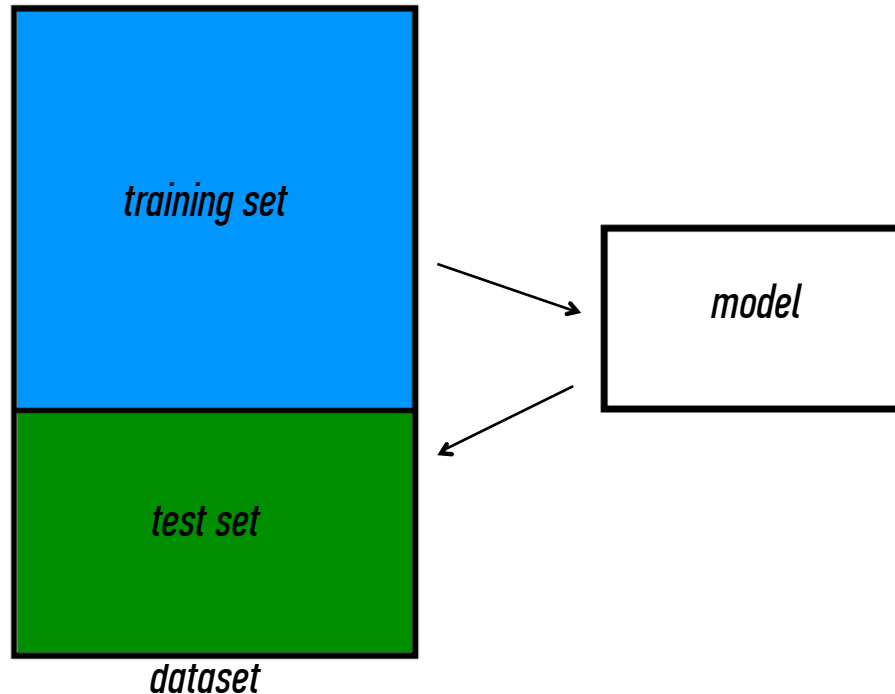
Q: What steps does a classification problem require?

- 1) split dataset*
- 2) train model*



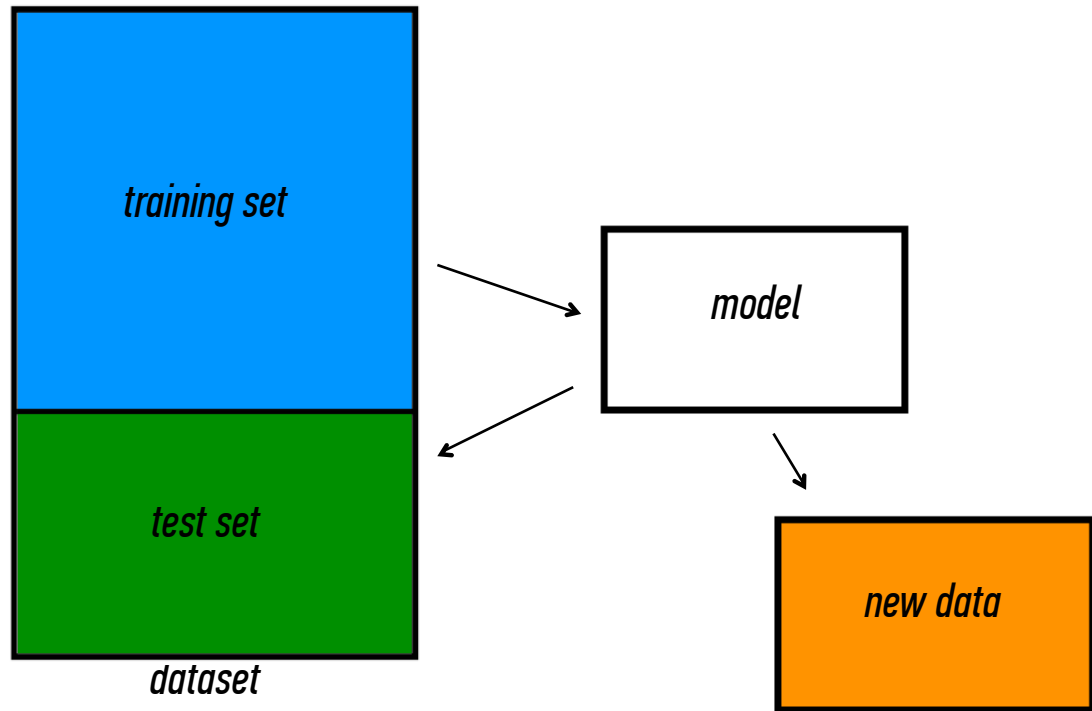
Q: What steps does a classification problem require?

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



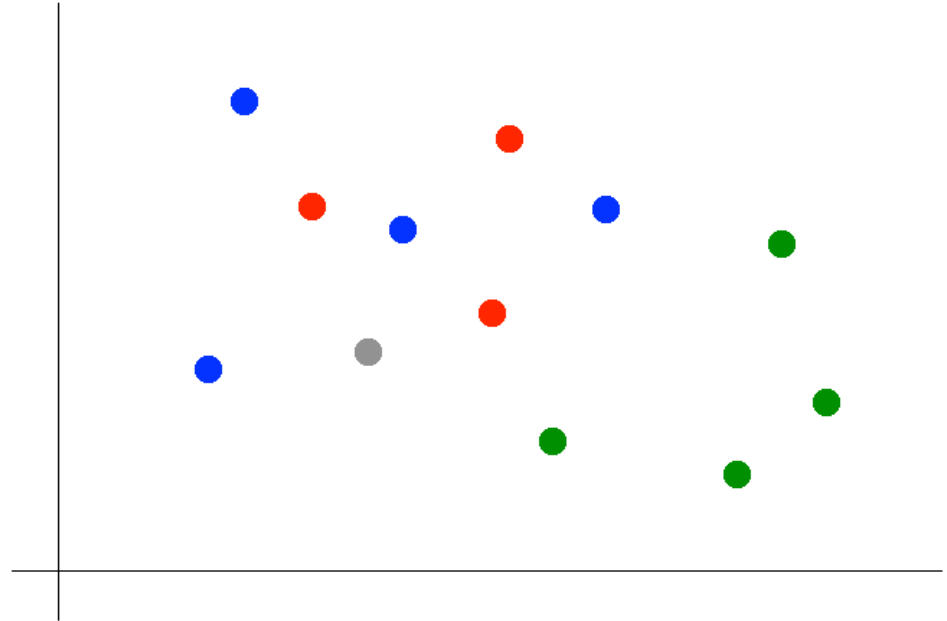
Q: What steps does a classification problem require?

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



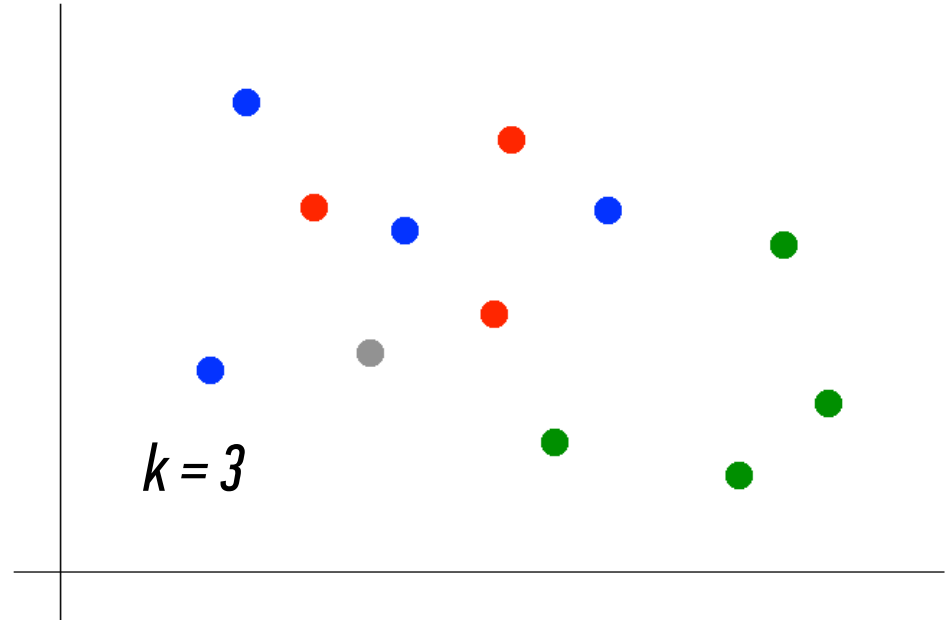
IV. KNN CLASSIFICATION

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



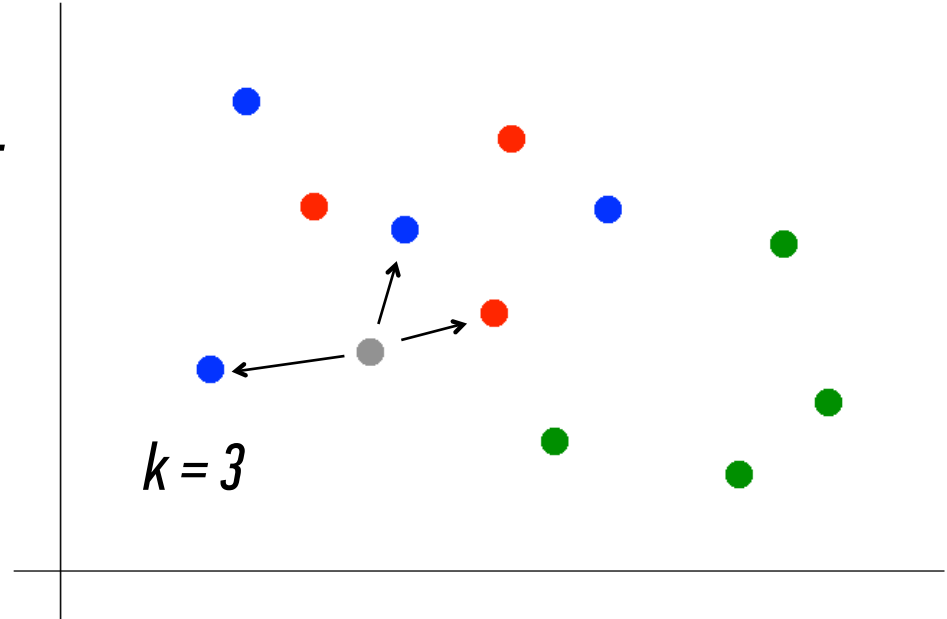
Suppose we want to predict the color of the grey dot.

1) Pick a value for k .



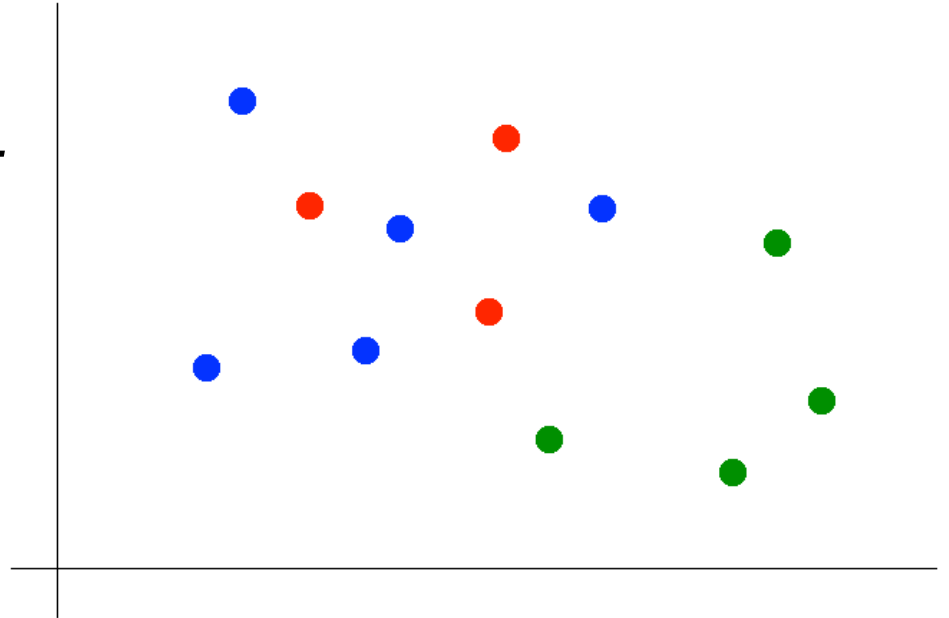
Suppose we want to predict the color of the grey dot.

- 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.*

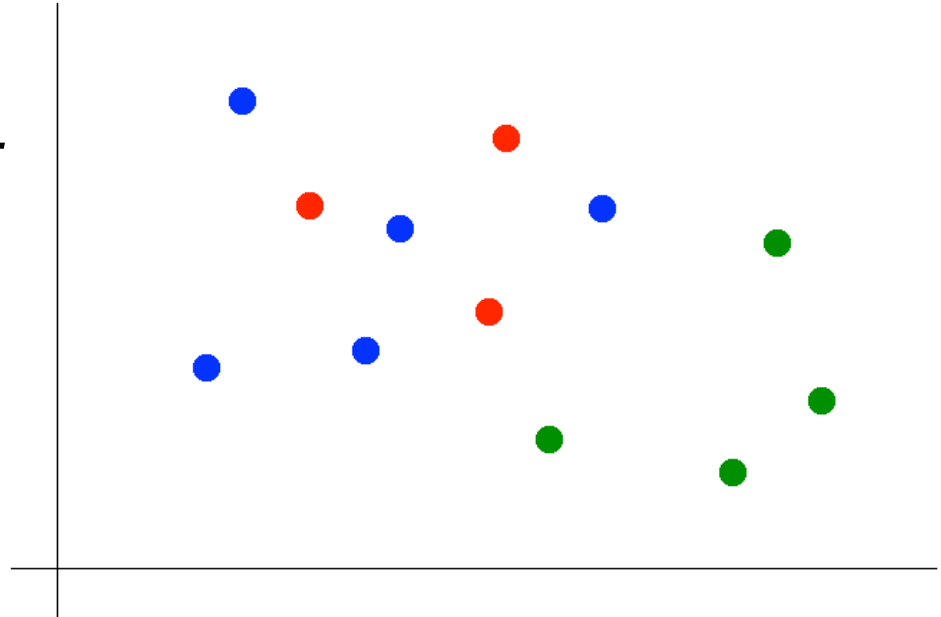


Suppose we want to predict the color of the grey dot.

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

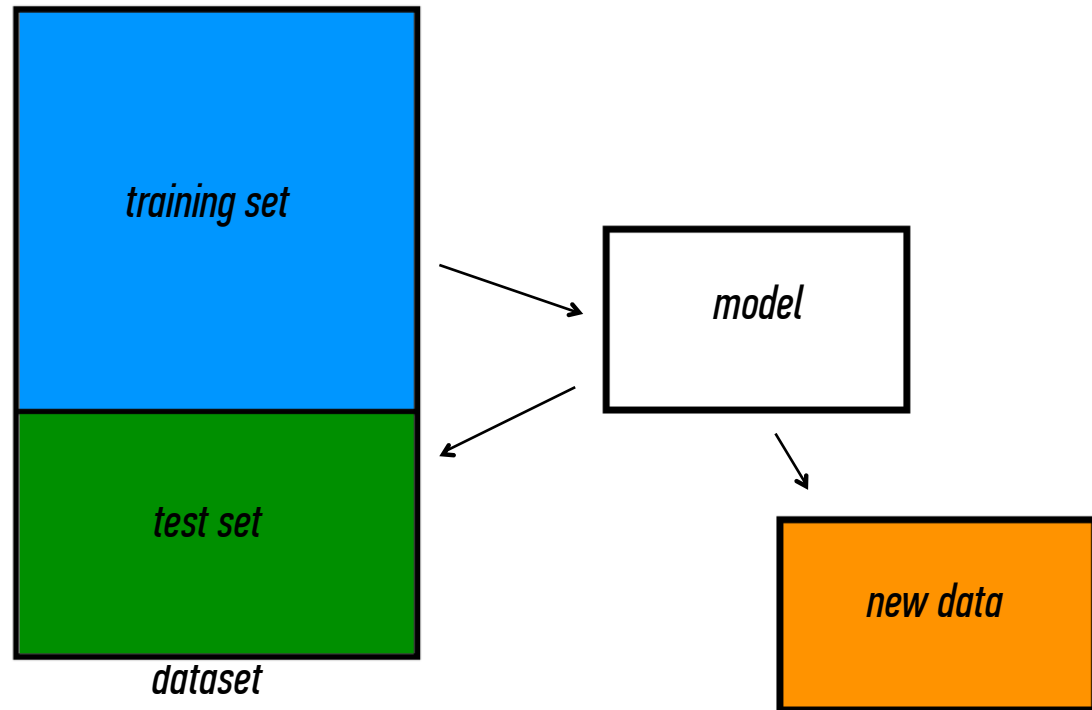
OPTIONAL NOTE

Our definition of “nearest” implicitly uses the Euclidean distance function.



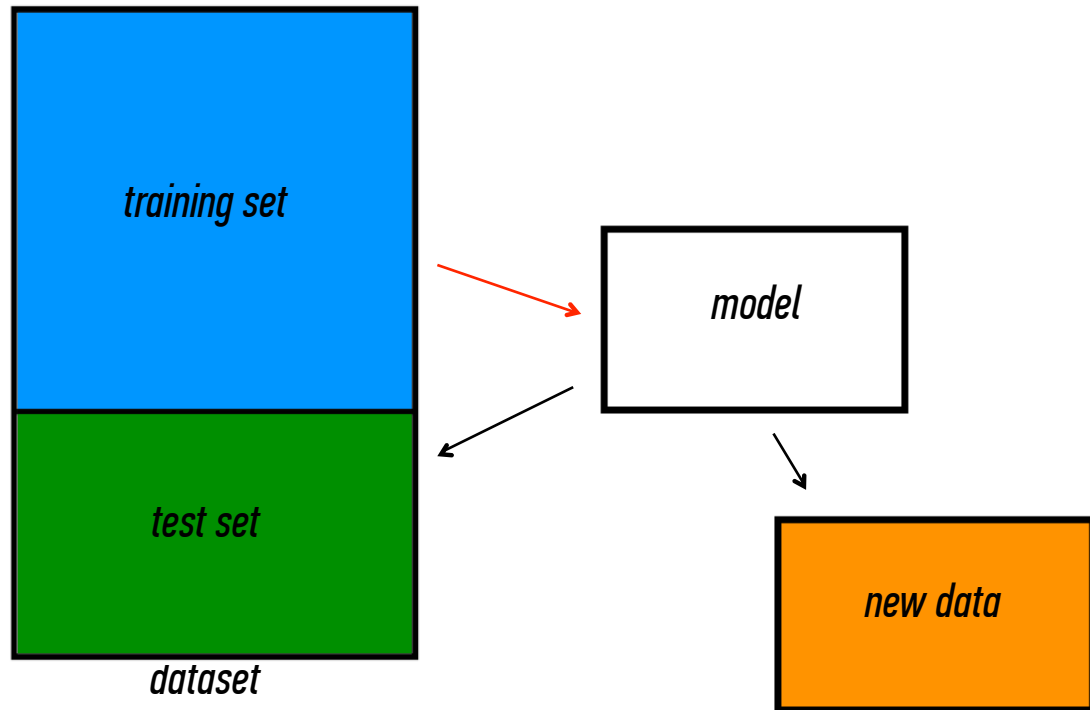
V. BUILDING EFFECTIVE CLASSIFIERS

Q: What types of prediction error will we run into?



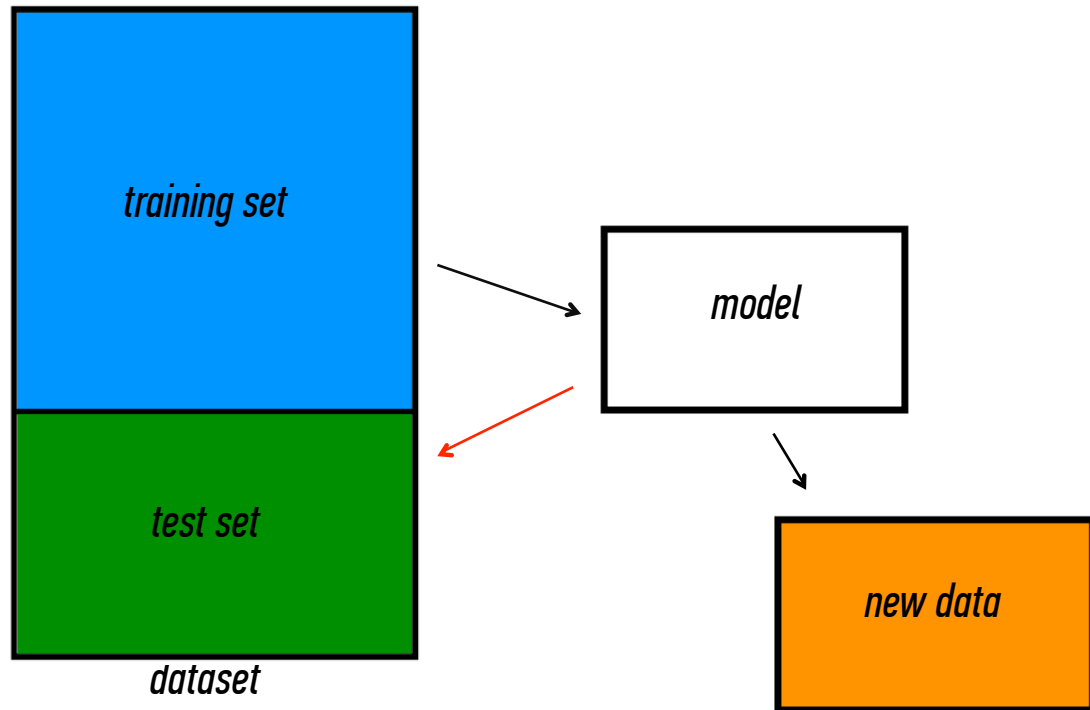
Q: What types of prediction error will we run into?

1) training error



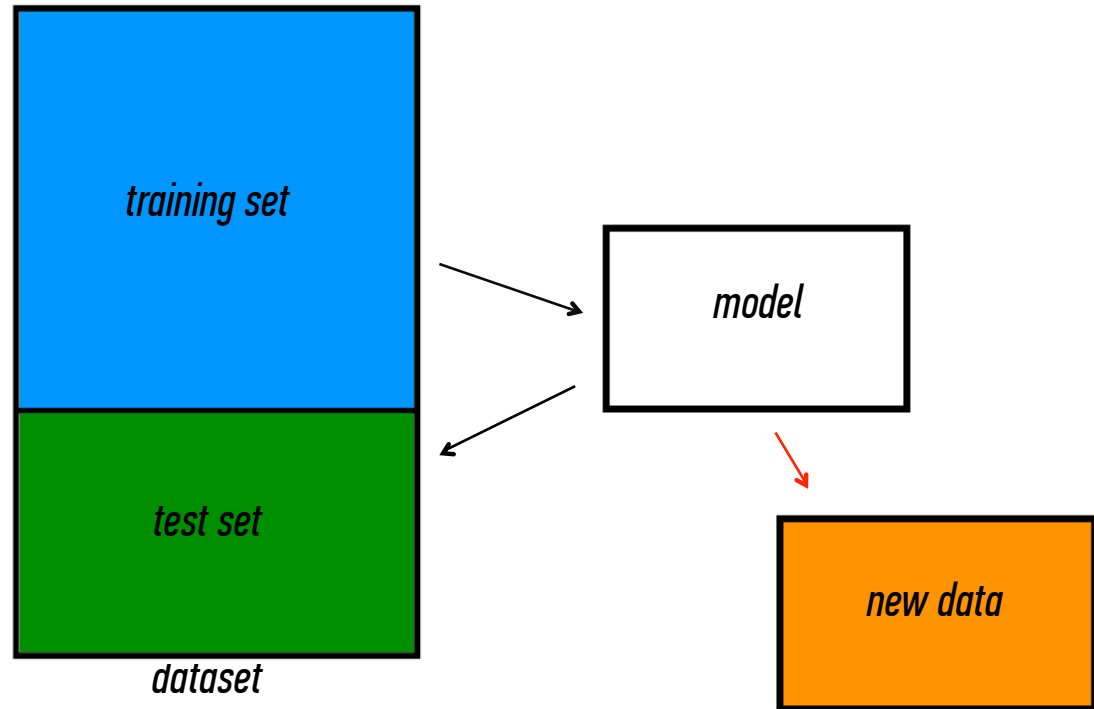
Q: What types of prediction error will we run into?

- 1) training error*
- 2) generalization error*



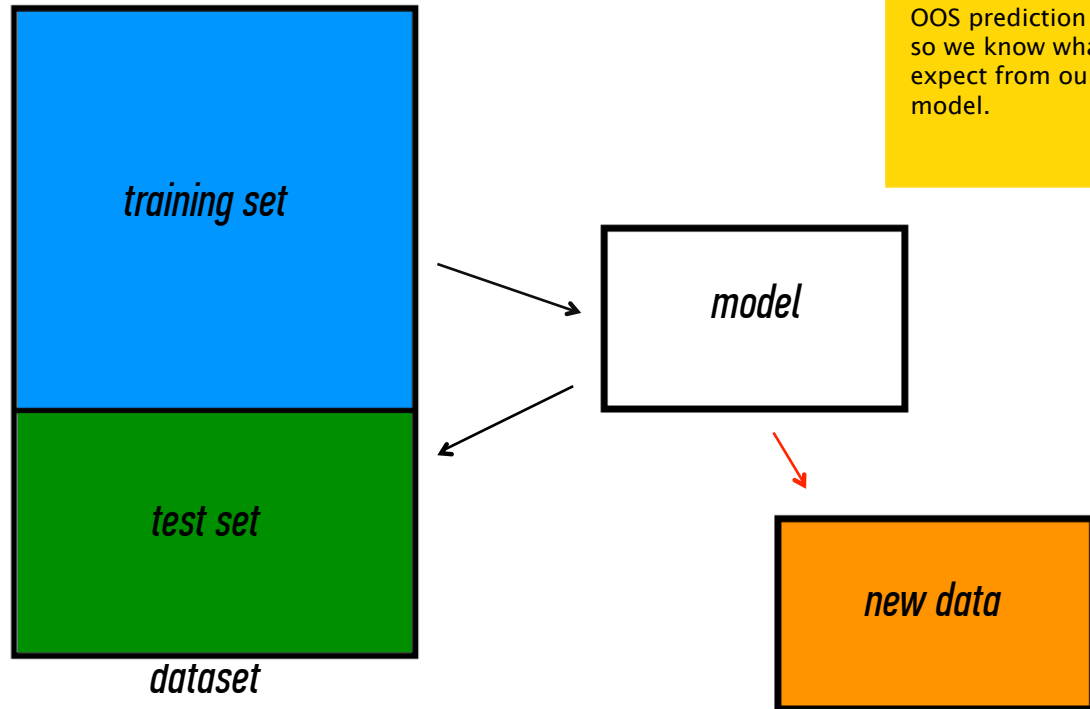
Q: What types of prediction error will we run into?

- 1) training error*
- 2) generalization error*
- 3) OOS error*



Q: What types of prediction error will we run into?

- 1) training error*
- 2) generalization error*
- 3) OOS error*



NOTE

We want to estimate OOS prediction error so we know what to expect from our model.

Q: Why should we use training & test sets?

Q: Why should we use training & test sets?

Thought experiment:

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

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?

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).*

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!

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.

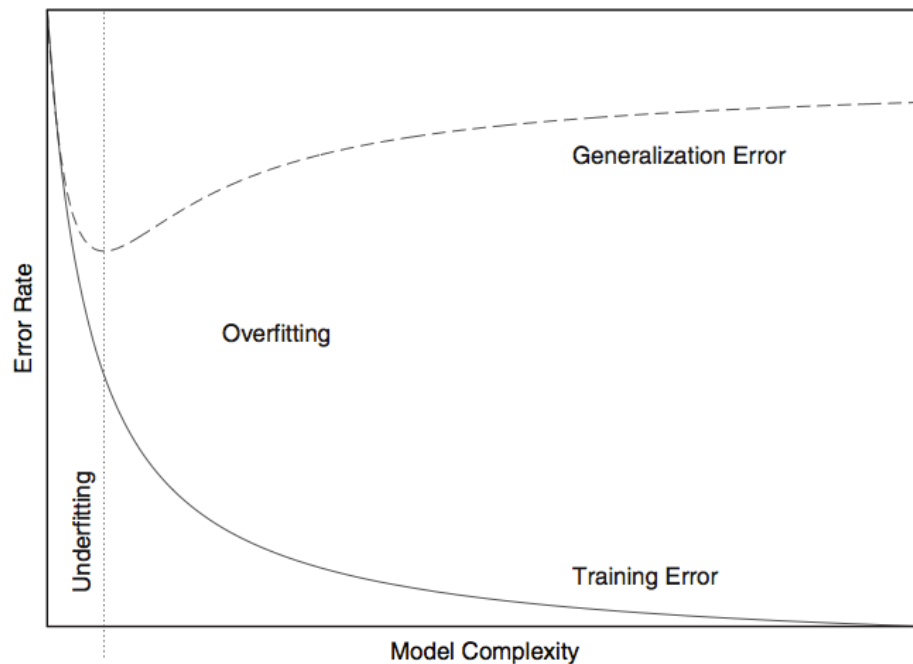
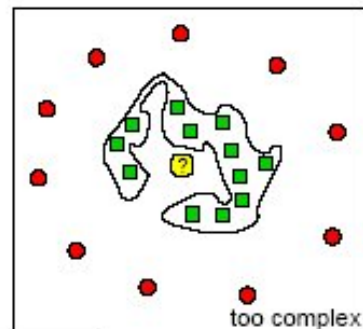
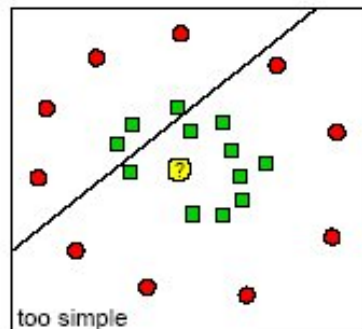
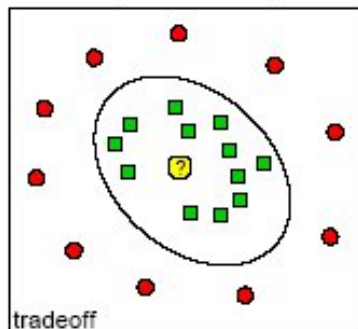


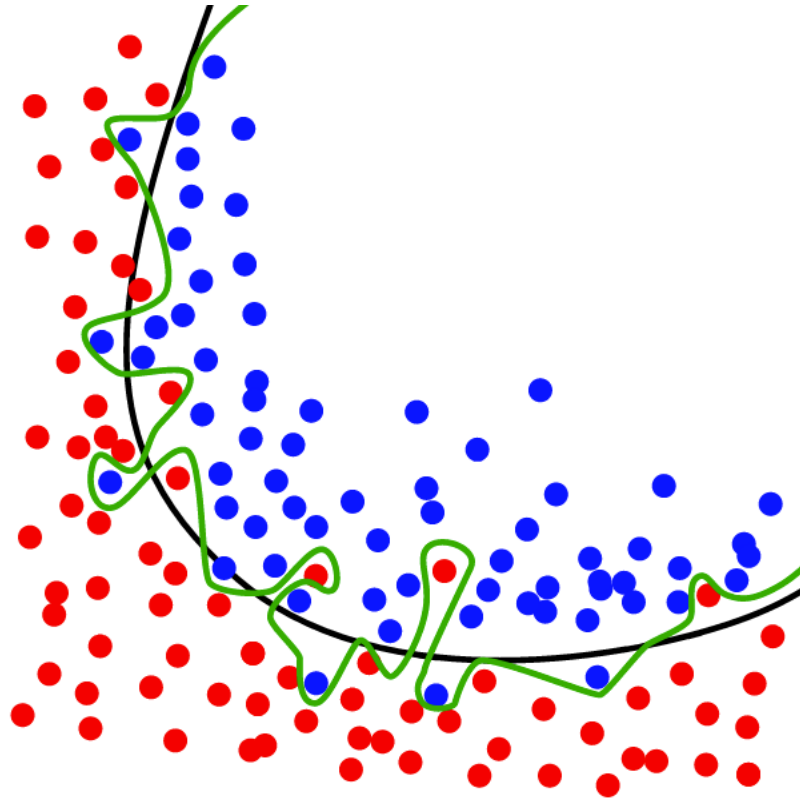
FIGURE 18-1. Overfitting: as a model becomes more complex, it becomes increasingly able to represent the training data. However, such a model is overfitted and will not generalize well to data that was not used during training.

Underfitting and Overfitting



- negative example
- positive example
- new patient





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!

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

NOTE

This phenomenon is called overfitting.

Suppose we do the train/test split.

Suppose we do the train/test split.

Q: How well does generalization error predict OOS accuracy?

Suppose we do the train/test split.

Q: How well does generalization error predict OOS 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 OOS 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 OOS 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 OOS 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?

Something is still missing!

Q: How can we do better?

Thought experiment:

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

Something is still missing!

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?

Something is still missing!

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!

Something is still missing!

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:

Steps for n -fold cross-validation:

1) Randomly split the dataset into n equal partitions.

Steps for n -fold cross-validation:

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

Steps for n -fold cross-validation:

- 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.*

Steps for n -fold cross-validation:

- 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.*

Steps for n -fold cross-validation:

- 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:

Features of n -fold cross-validation:

1) More accurate estimate of OOS prediction error.

Features of n -fold cross-validation:

- 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.*

Features of n-fold cross-validation:

- 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*

Features of n -fold cross-validation:

- 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