GENERAL ASSEMBLY

INTRO TO DATA SCIENCE

LECTURE 3: KNN CLASSIFICATION

LAST TIME:

- REGRESSION AND ASSUMPTIONS OF LINEAR MODELING
- MULTIPLE REGRESSION
- FEATURE SELECTION VIA BACKWARDS ELIMINATION
- INTRO TO MACHINE LEARNING & TYPICAL PROBLEMS

QUESTIONS?

I. CLASSIFICATION PROBLEMS
II. BUILDING EFFECTIVE CLASSIFIERS

EXERCISES:
III. THE KNN CLASSIFICATION MODEL

I. CLASSIFICATION PROBLEMS

	continuous	*categorical*
supervised	regression	classification
unsupervised	dimension reduction	clustering

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

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*

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. 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*

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: How does a classification problem work?

Q: How does a classification problem work?

A: Data in, predicted labels out.

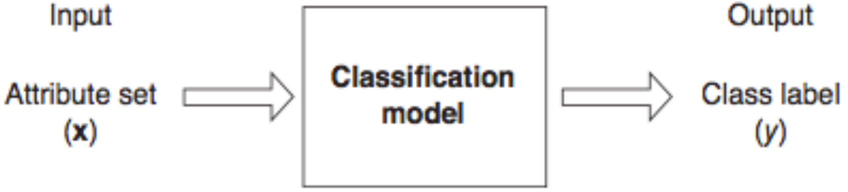
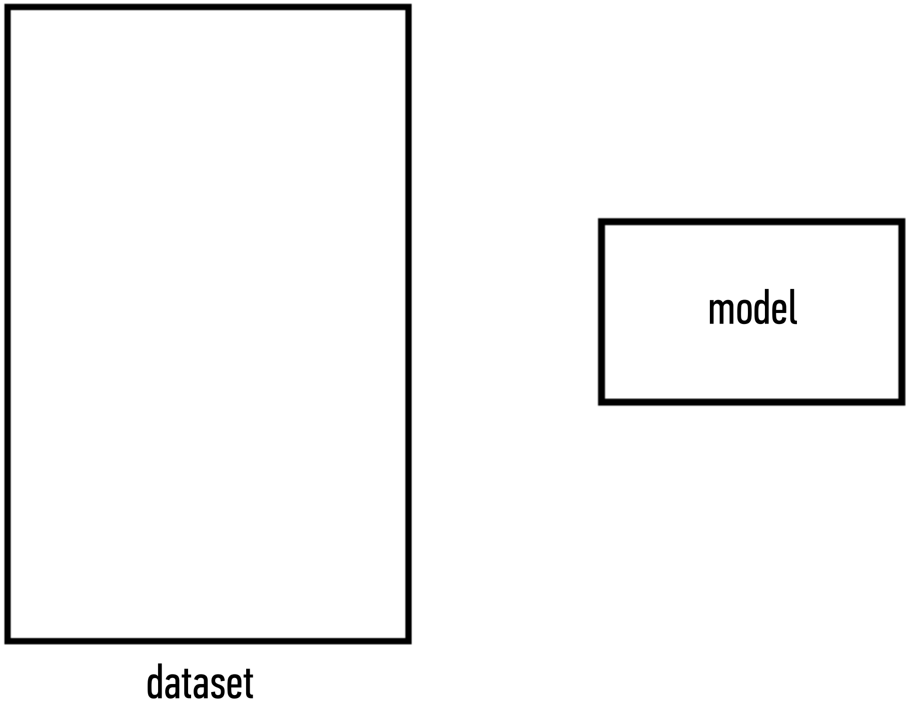


Figure 4.2. Classification as the task of mapping an input attribute set $\mathbf{x}$ into its class label y.

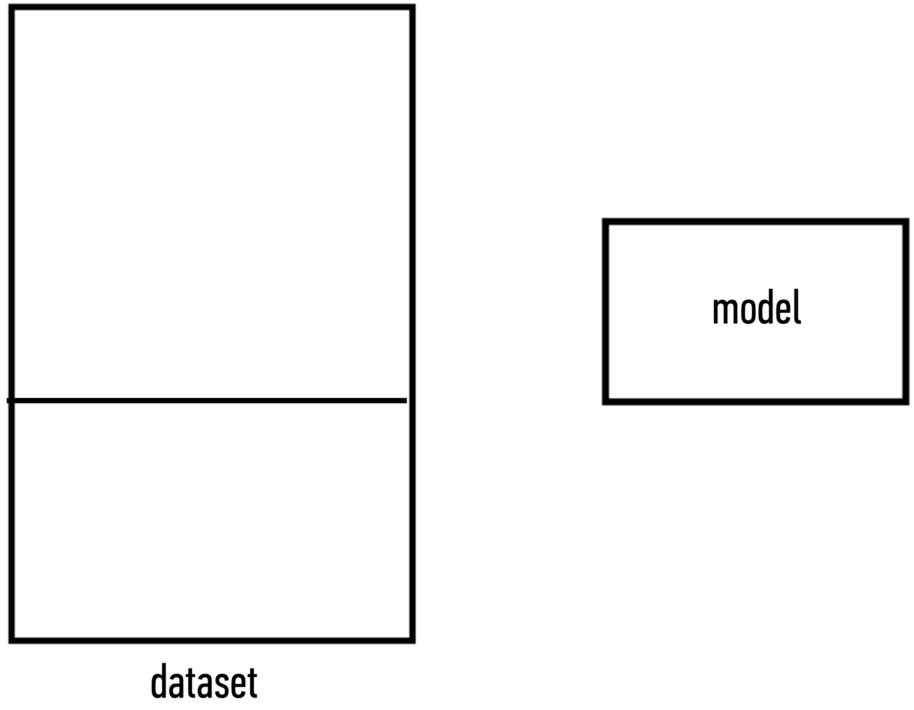
source: http://www-users.cs.umn.edu/~kumar/dmbook/ch4.pdf

Q: What steps does a classification problem require?



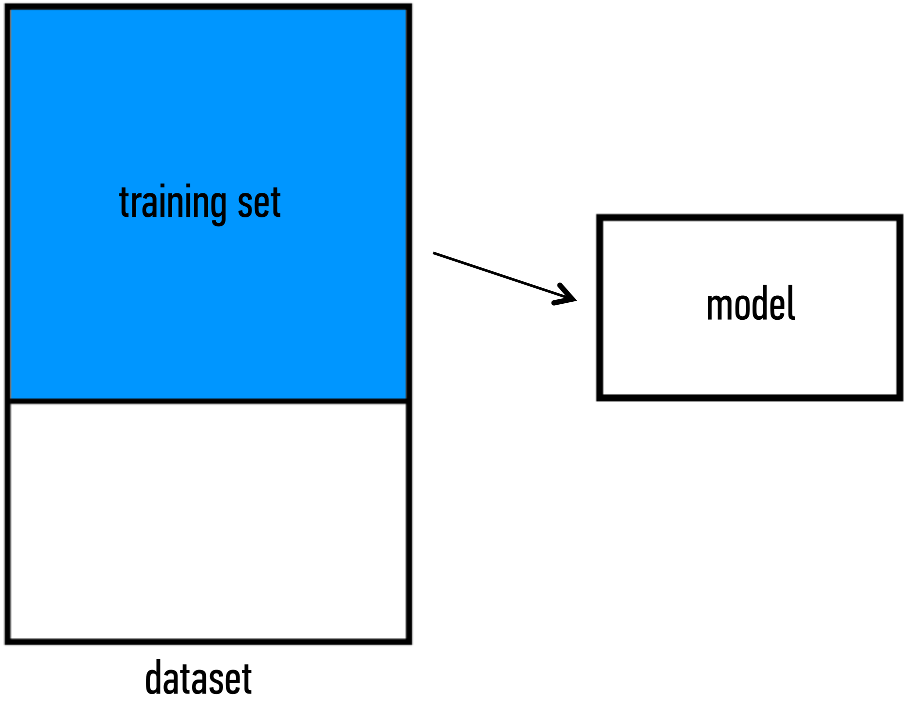
Q: What steps does a classification problem require?

1) split dataset



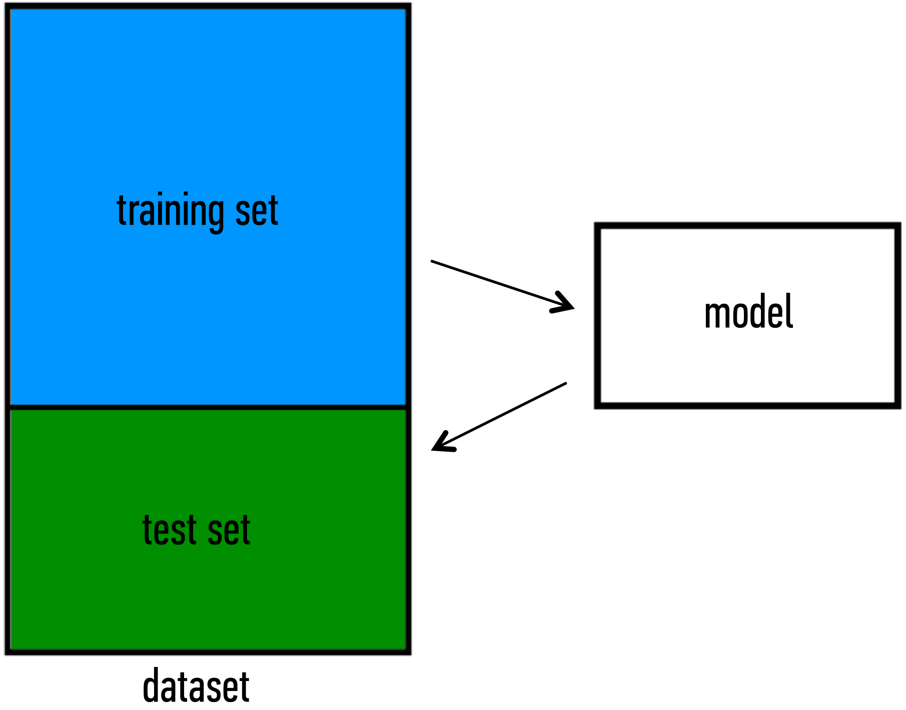
Q: What steps does a classification problem require?

1) split dataset
2) train model



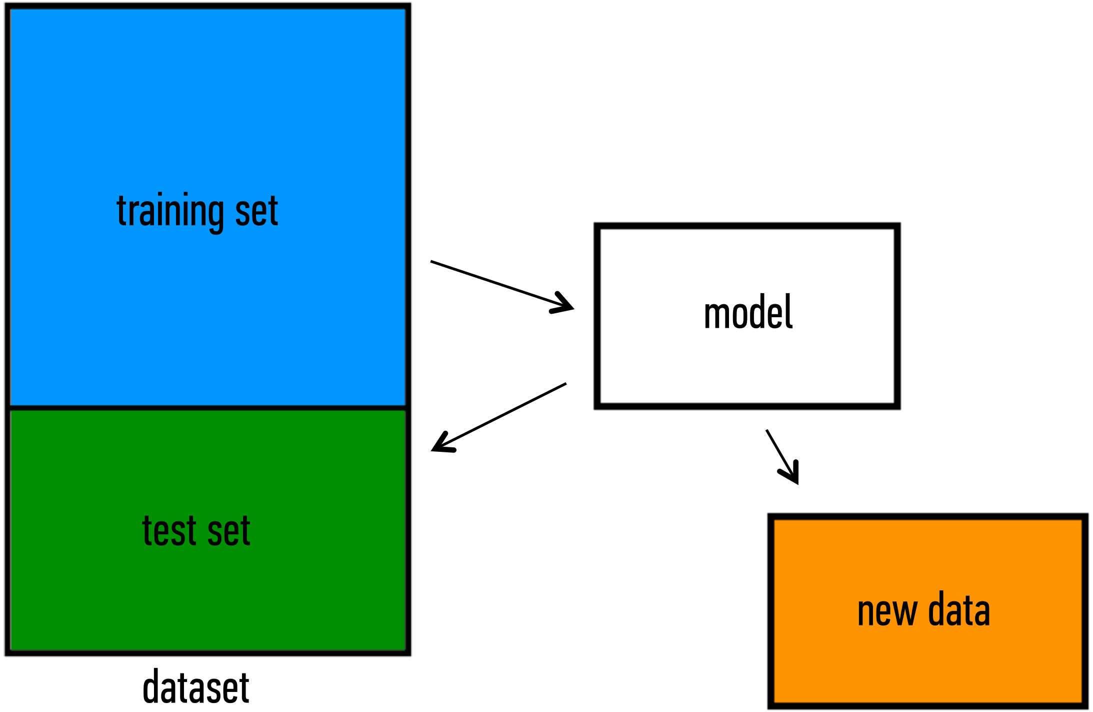
Q: What steps does a classification problem require?

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



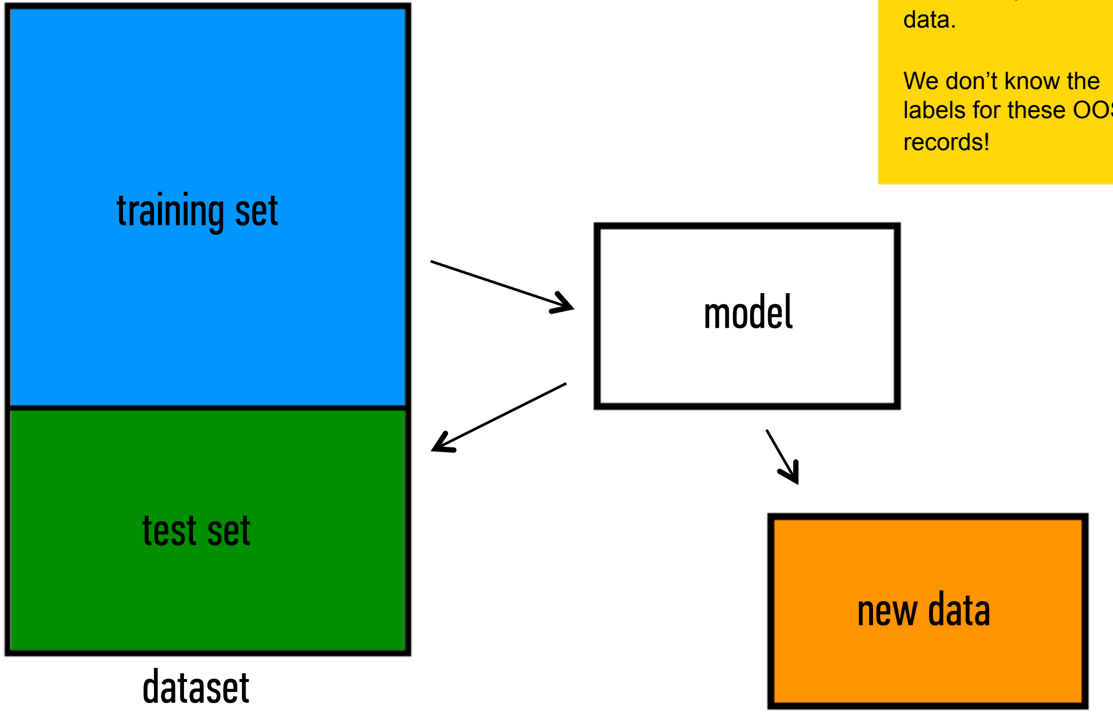
Q: What steps does a classification problem require?

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



Q: What steps does a classification problem require?

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



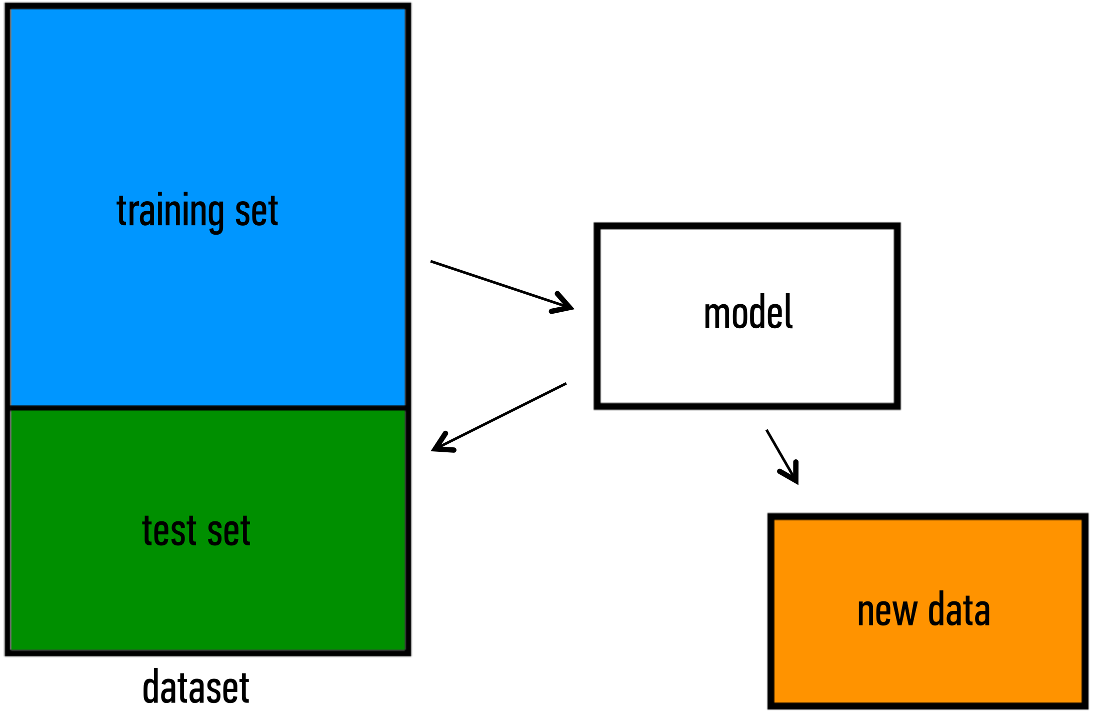
NOTE

This new data is called *out of sample* data.

We don't know the labels for these OOS records!

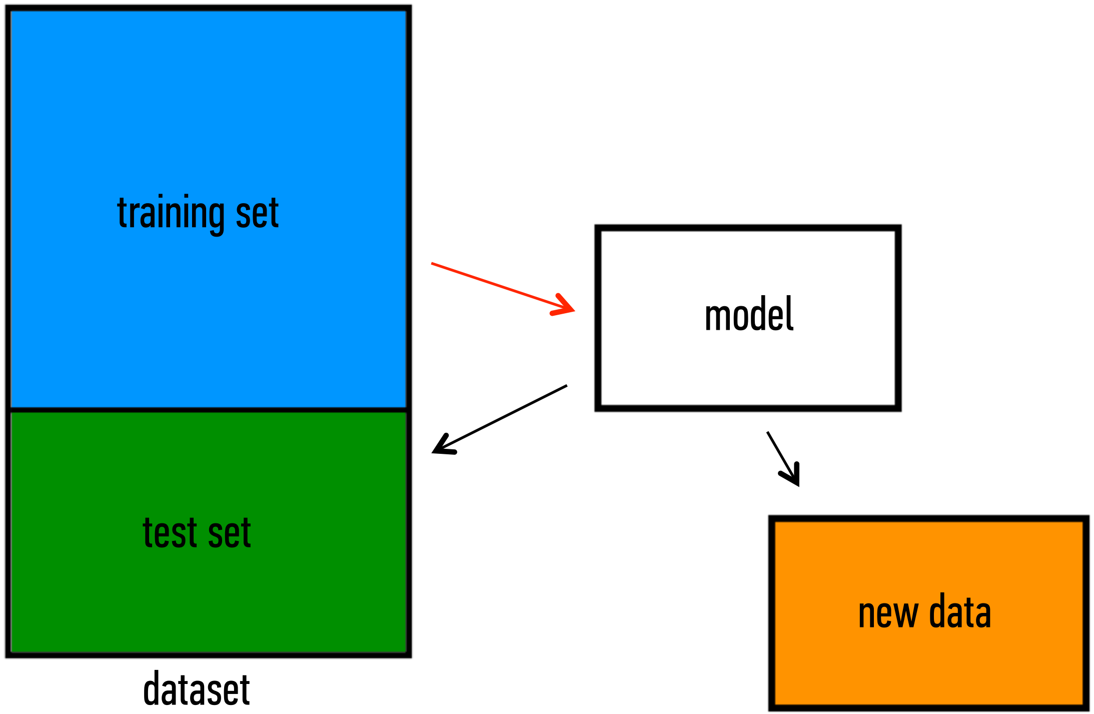
II. BUILDING EFFECTIVE CLASSIFIERS

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



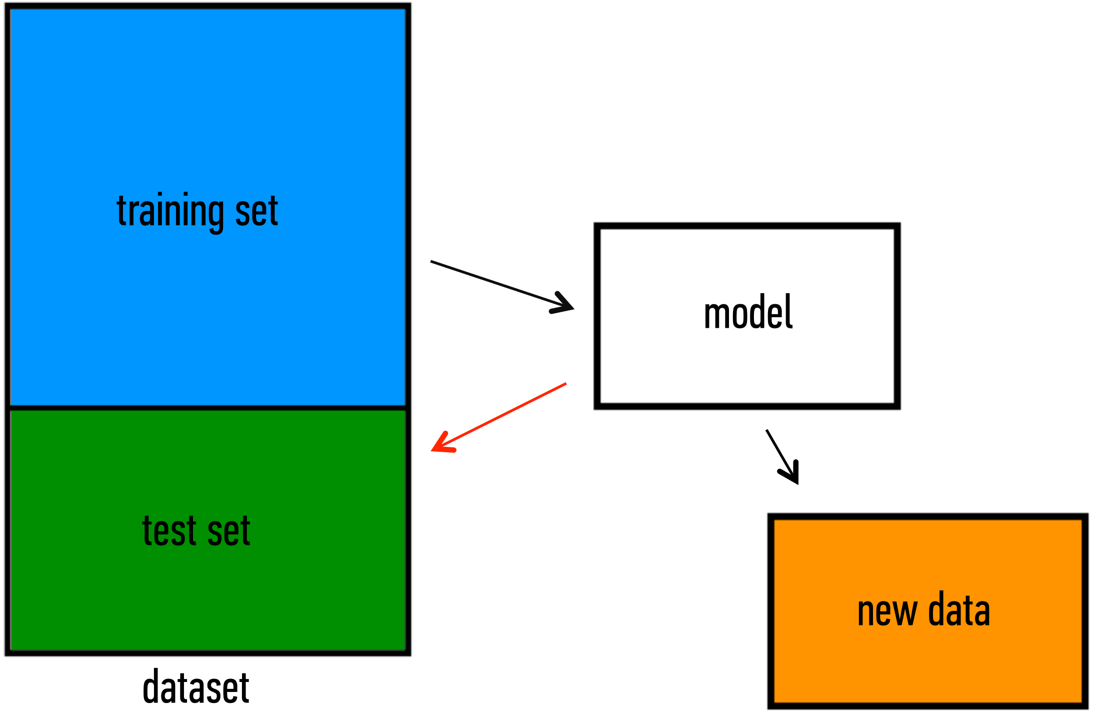
Q: What types of prediction error will we run into?

1) training error



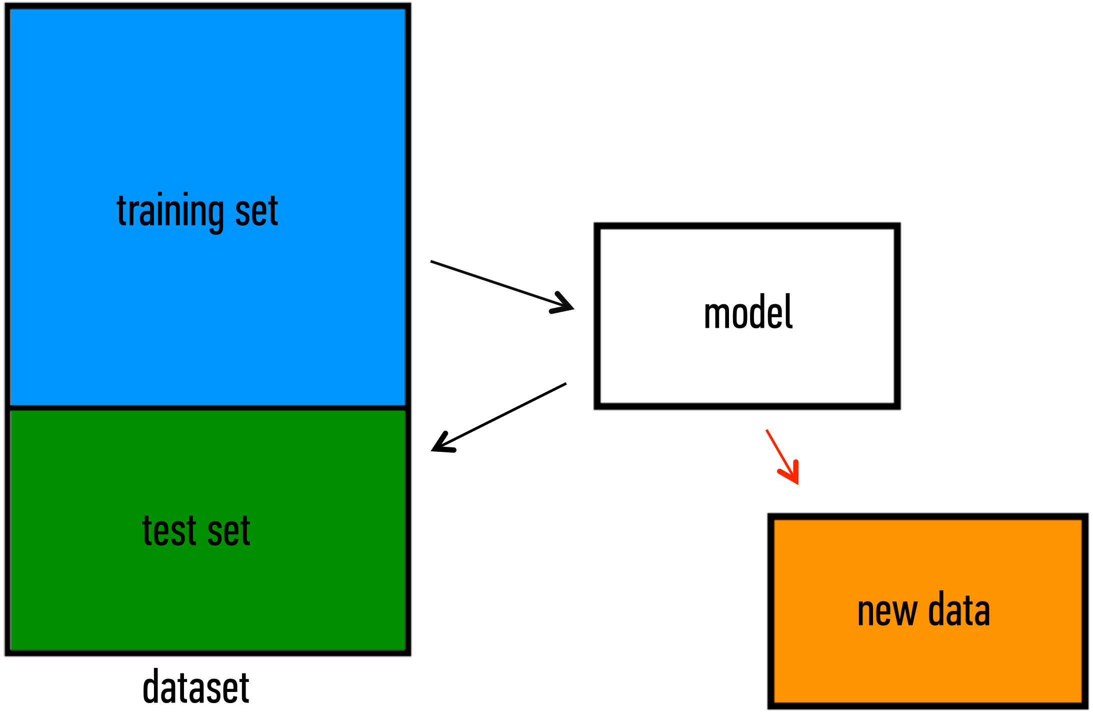
Q: What types of prediction error will we run into?

1) training error
2) generalization error



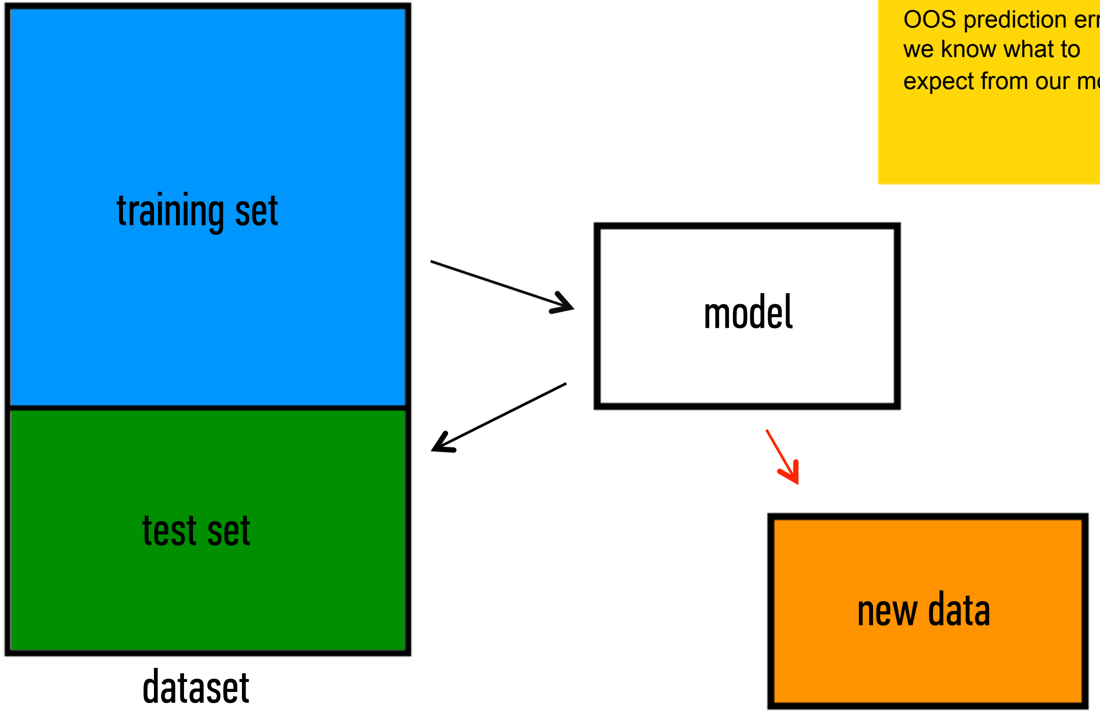
Q: What types of prediction error will we run into?

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?

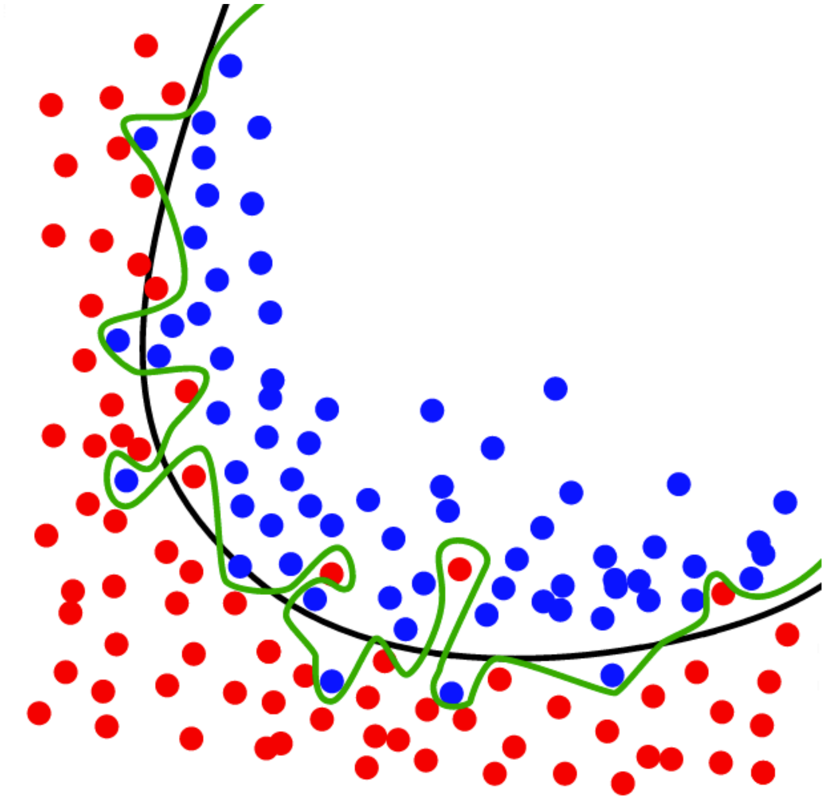
- *We can make the model arbitrarily complex (effectively "memorizing" the entire training set).*

A: Down to zero!

NOTE

This phenomenon is called *overfitting*.

OVERFITTING – EXAMPLE



source: http://www.dtreg.com

OVERFITTING

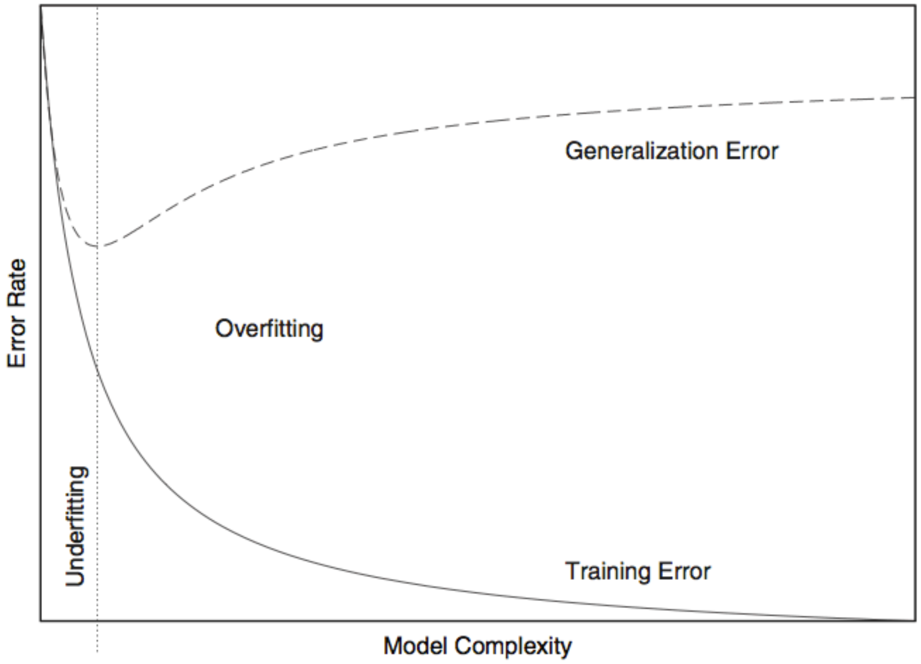
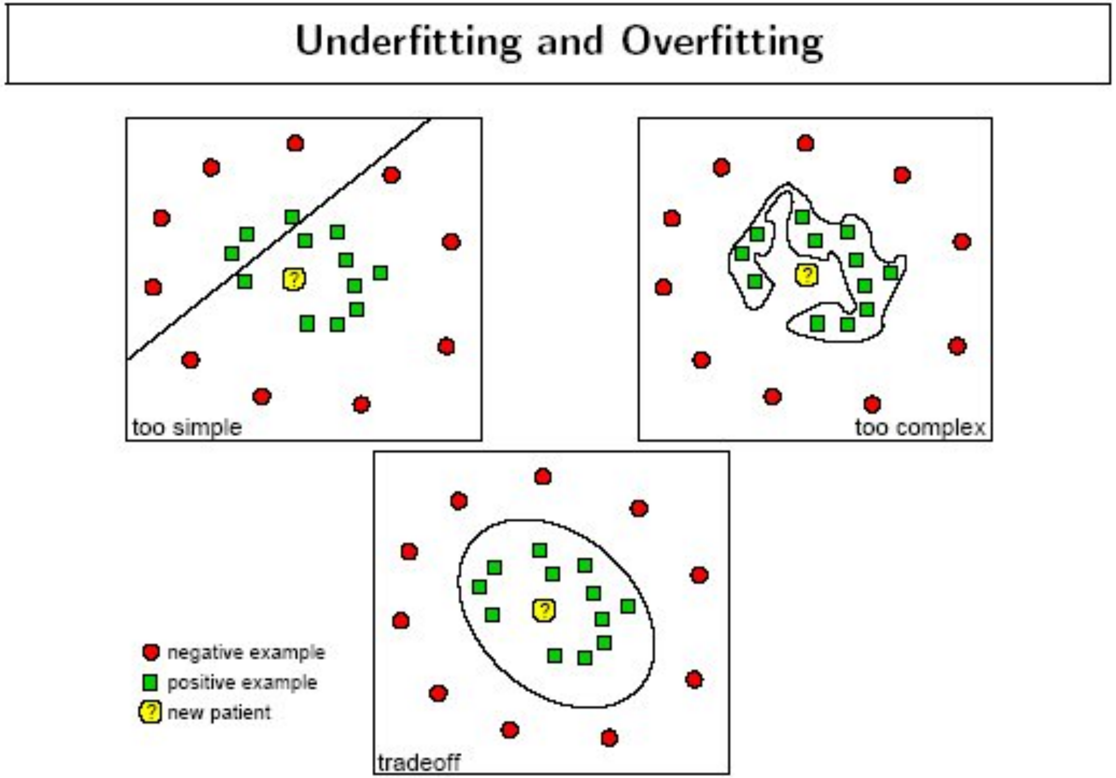


FIGURE 18-1. Overfitting: as a model becomes more complex, it becomes increasingly able to represent the training data. However, such a model is overfitted and will not generalize well to data that was not used during training.

source: Data Analysis with Open Source Tools, by Philipp K. Janert. O'Reilly Media, 2011.

OVERFITTING – EXAMPLE



source: http://www.dtreg.com

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 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.

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.

NOTE

The generalization error gives a *high-variance estimate* of OOS accuracy.

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!

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:

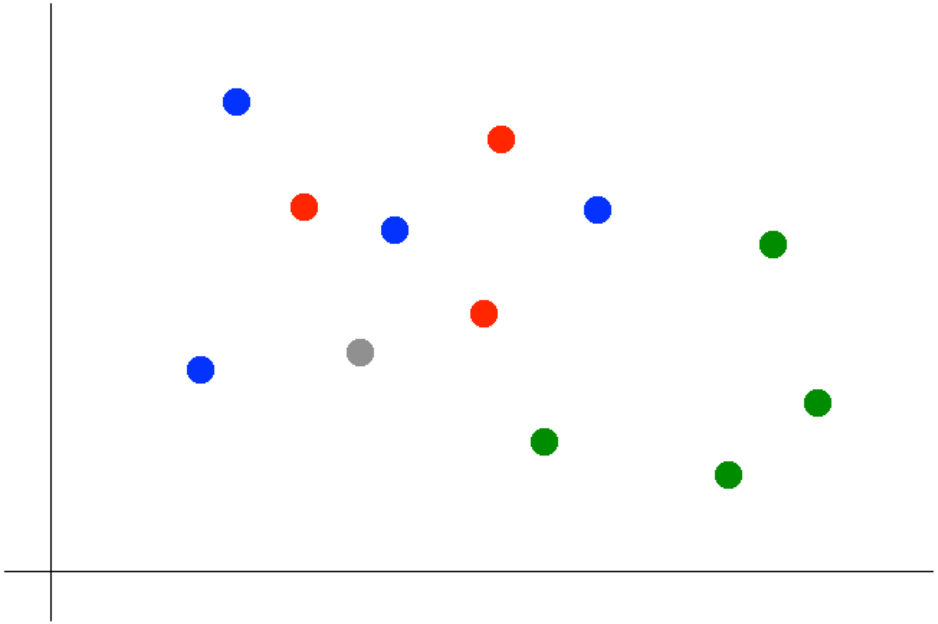
1) More accurate estimate of OOS prediction error.
2) More efficient use of data than single train/test split.
   - Each record in our dataset is used for both training and testing.
3) Presents tradeoff between efficiency and computational expense.
   - 10-fold CV is 10x more expensive than a single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

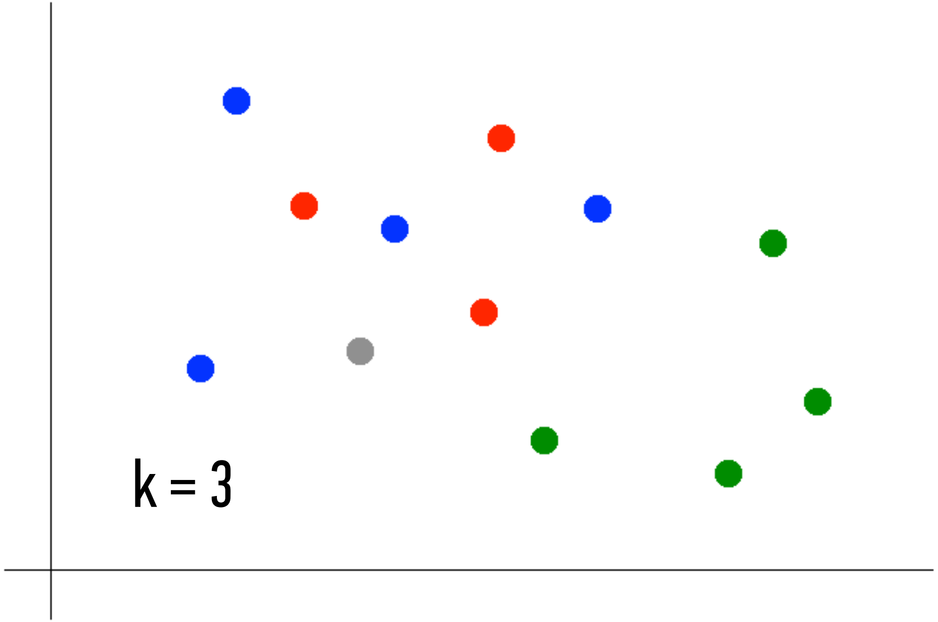
III. KNN CLASSIFICATION

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



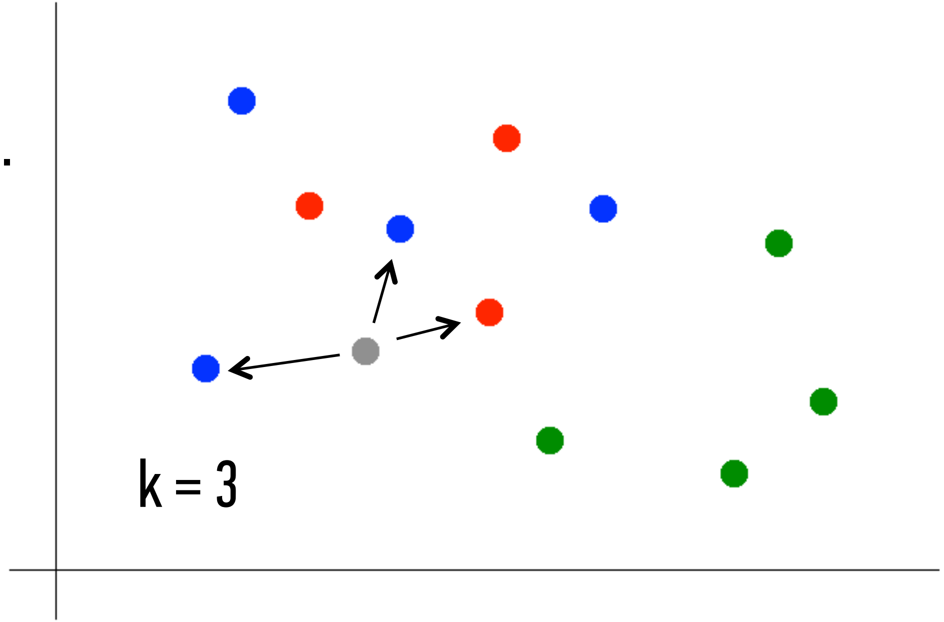
Suppose we want to predict the color of the grey dot.

1) Pick a value for k.



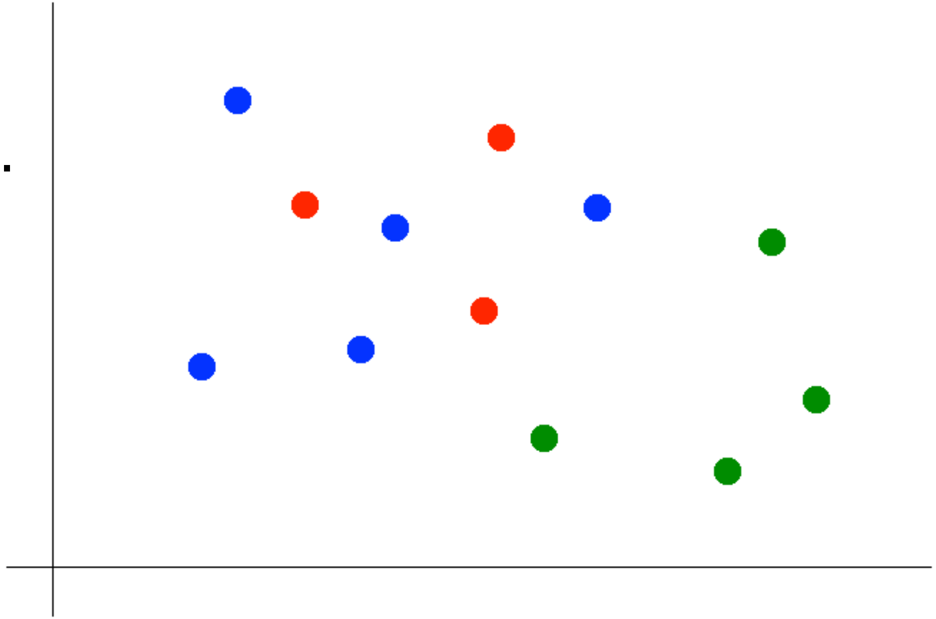
Suppose we want to predict the color of the grey dot.

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



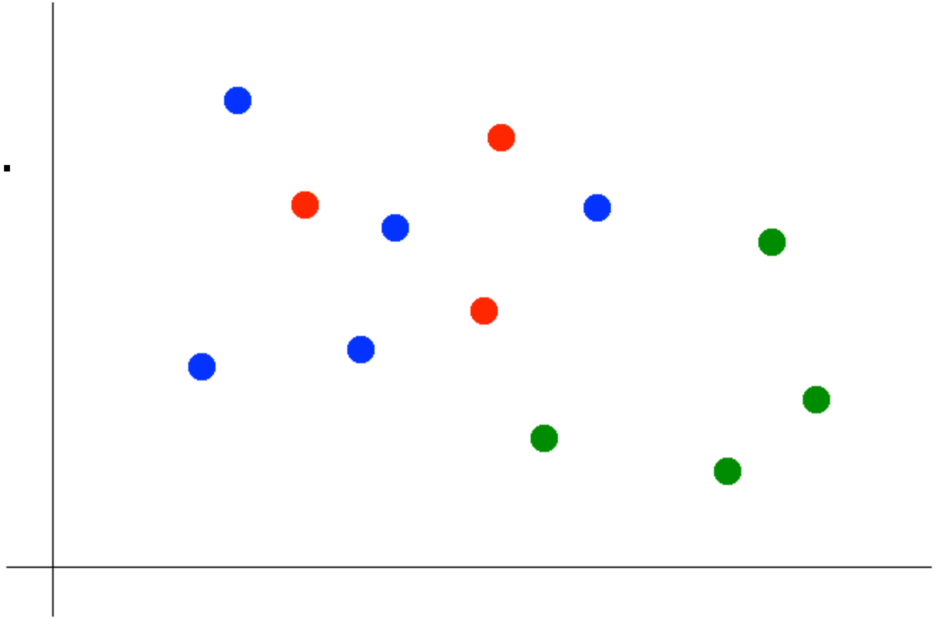
Suppose we want to predict the color of the grey dot.

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.*

EXERCISE – K NEAREST NEIGHBORS CLASSIFICATION IN R

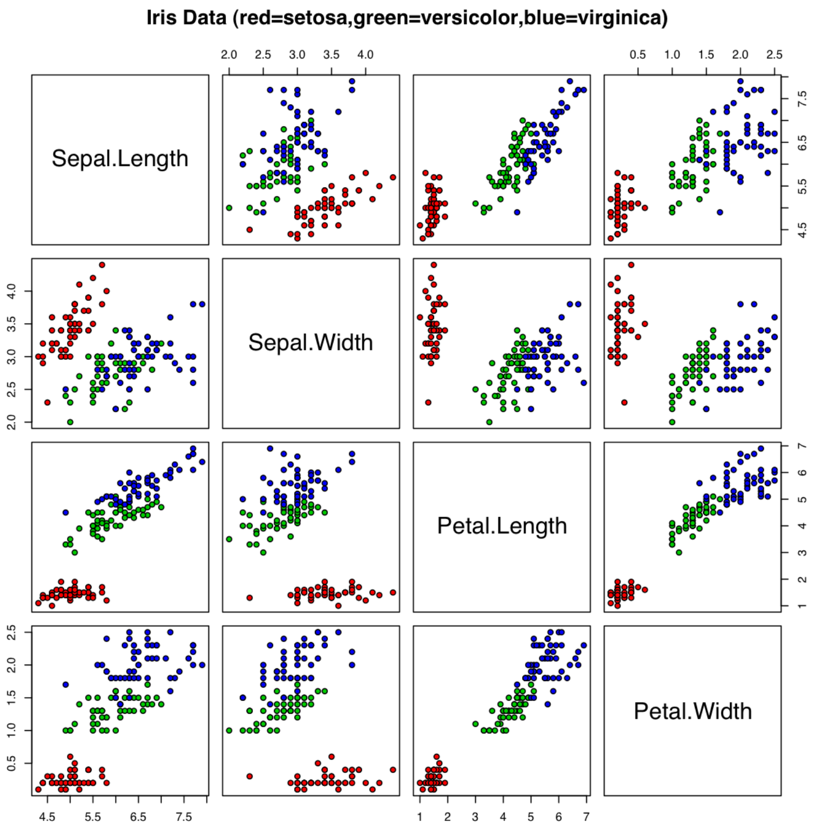
KEY OBJECTIVES

- knn classification using train/test sets

R FUNCTIONS

- knn {class}

IRIS DATA


Iris Data (red=setosa,green=versicolor,blue=virginica)
Sepal.Length
Sepal.Width
Petal.Length
Petal.Width
2.0 2.5 3.0 3.5 4.0
0.5 1.0 1.5 2.0 2.5
4.5 5.5 6.5 7.5
1 2 3 4 5 6 7

ASSIGNMENT – KNN WITH N-FOLD CROSS-VALIDATION

KEY OBJECTIVES

Extend the script we used in class to implement knn classification on the iris dataset using n-fold cross-validation.

(Bonus: split code into functions)

for example:

```
knn.nfold <- function(n, … ) {
   # create n-fold partition of dataset
   # perform knn classification n times
   # n-fold generalization error = average over all iterations
}
```

DISCUSSION