GENERAL ASSEMBLY

INTRO TO DATA SCIENCE
LECTURE 3: KNN CLASSIFICATION

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LAST TIME:

- INTRO TO MACHINE LEARNING & TYPICAL PROBLEMS
- MULTIPLE REGRESSION
- FEATURE SELECTION VIA BACKWARDS ELIMINATION

QUESTIONS?

I. CLASSIFICATION PROBLEMS
II. BUILDING EFFECTIVE CLASSIFIERS

EXERCISES:
III. THE KNN CLASSIFICATION MODEL

I. CLASSIFICATION PROBLEMS

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

	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*
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independent variables

class labels *(qualitative)*

Q: What does “supervised” mean?

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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?

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A: Data in, predicted labels out.

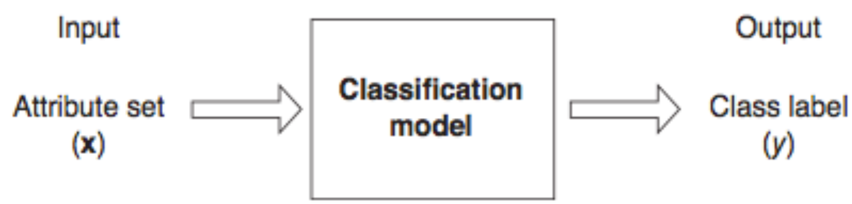
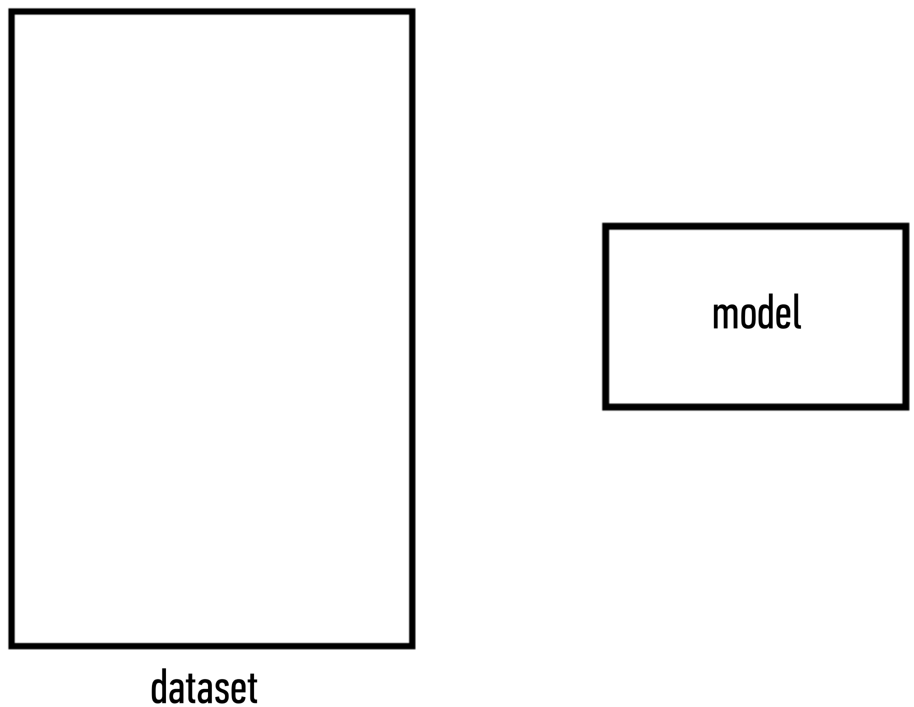


Figure 4.2. Classification as the task of mapping an input attribute set $\mathbf{x}$ into its class label y.

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

Q: What steps does a classification problem require?



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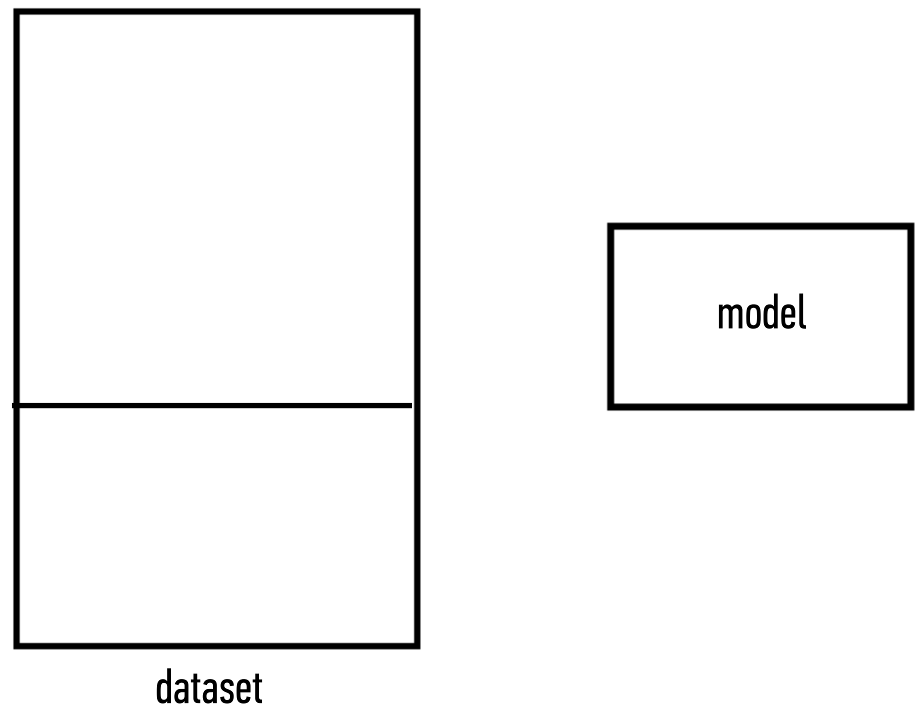
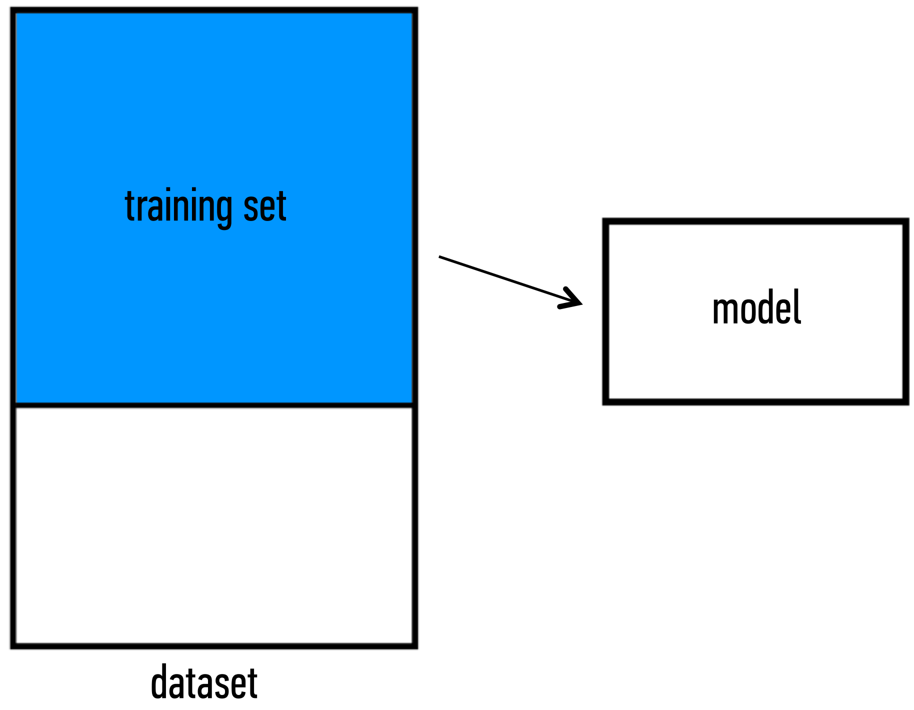
1) split dataset



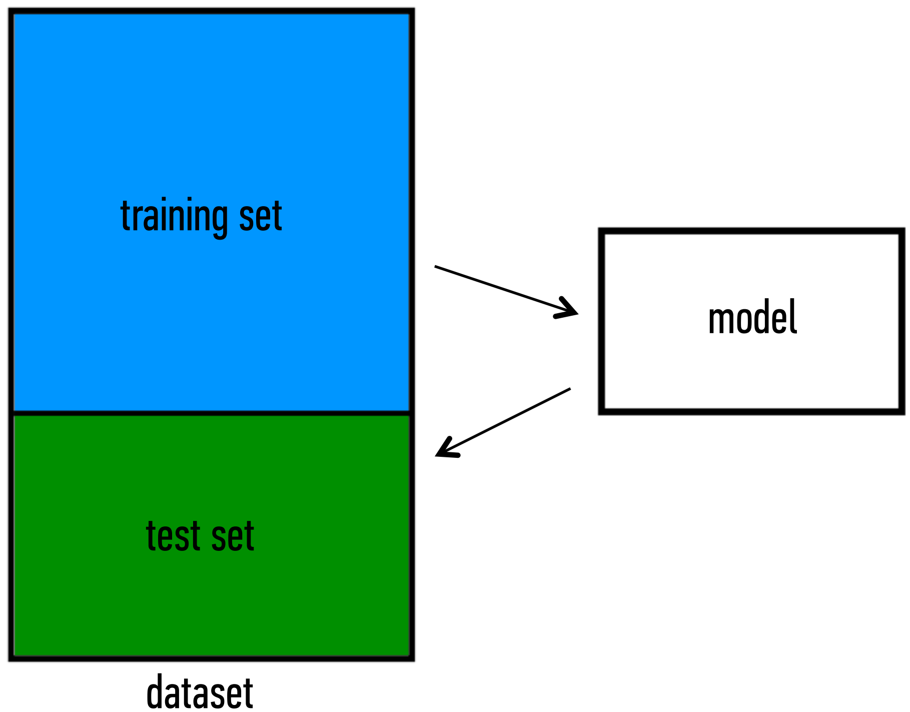
Q: What steps does a classification problem require?

1) split dataset
2) train model



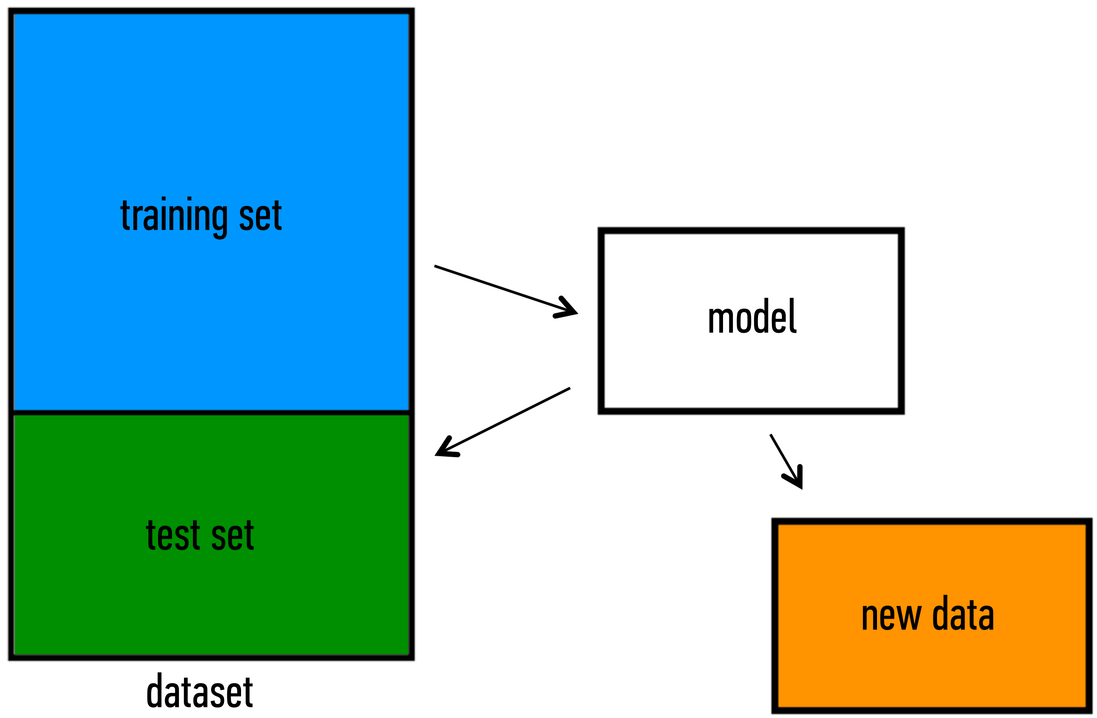
Q: What steps does a classification problem require?

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



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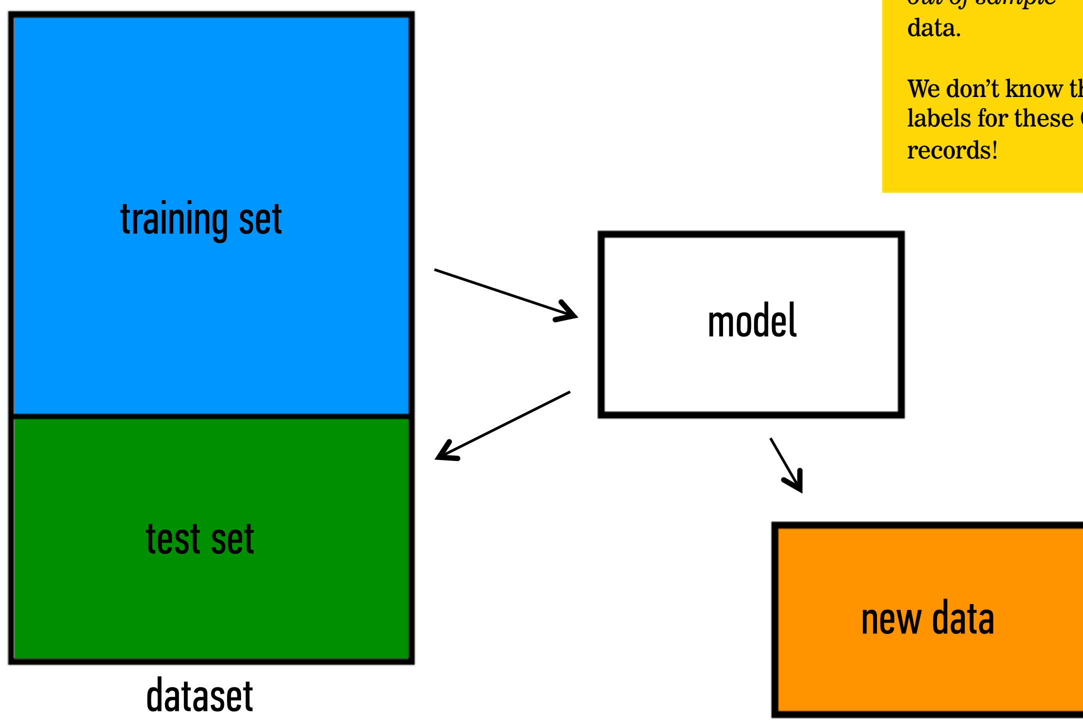


NOTE

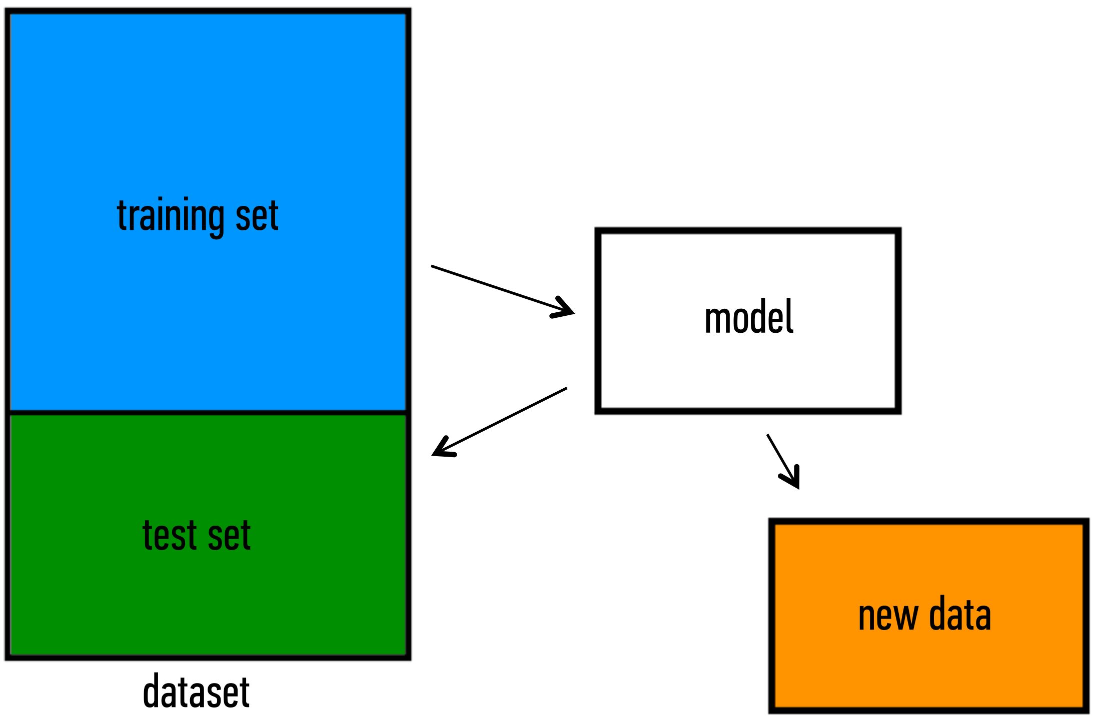
This new data is called *out of sample* data.

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

INTRO TO DATA SCIENCE

II. BUILDING EFFECTIVE CLASSIFIERS

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



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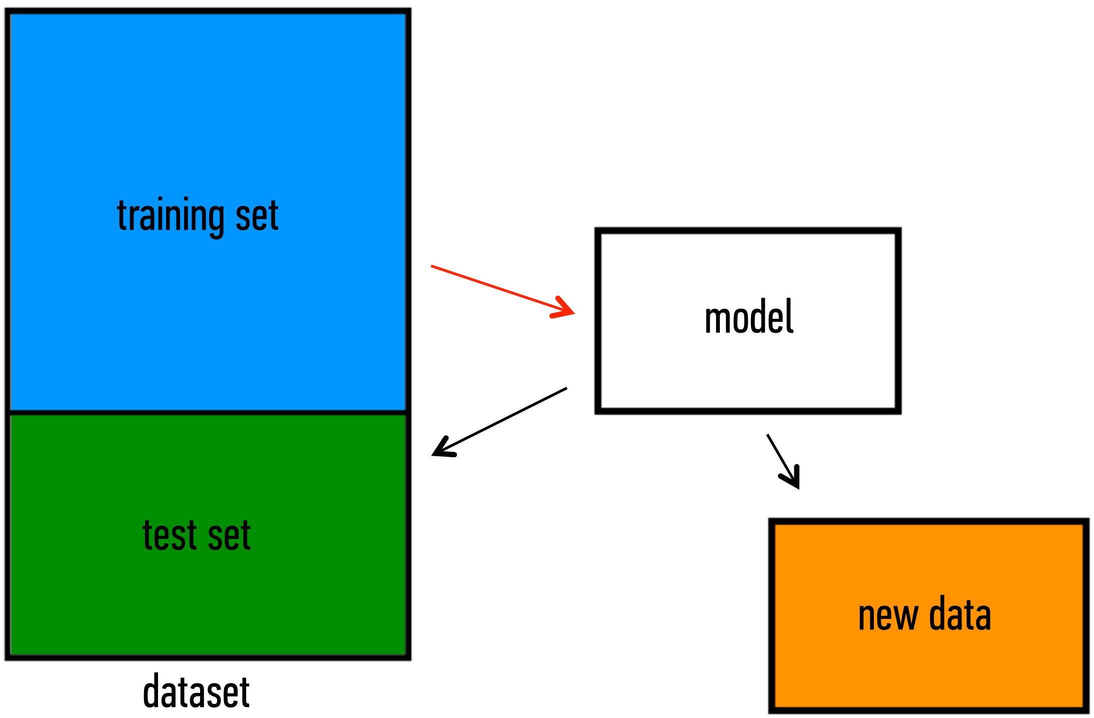

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1) training error
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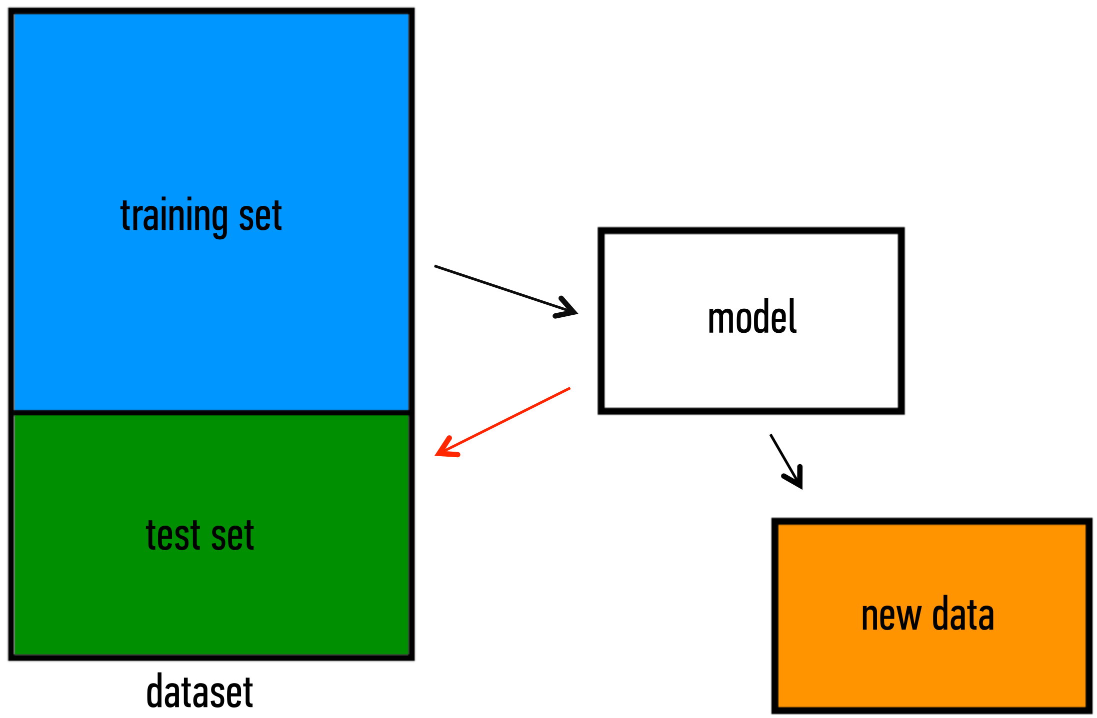

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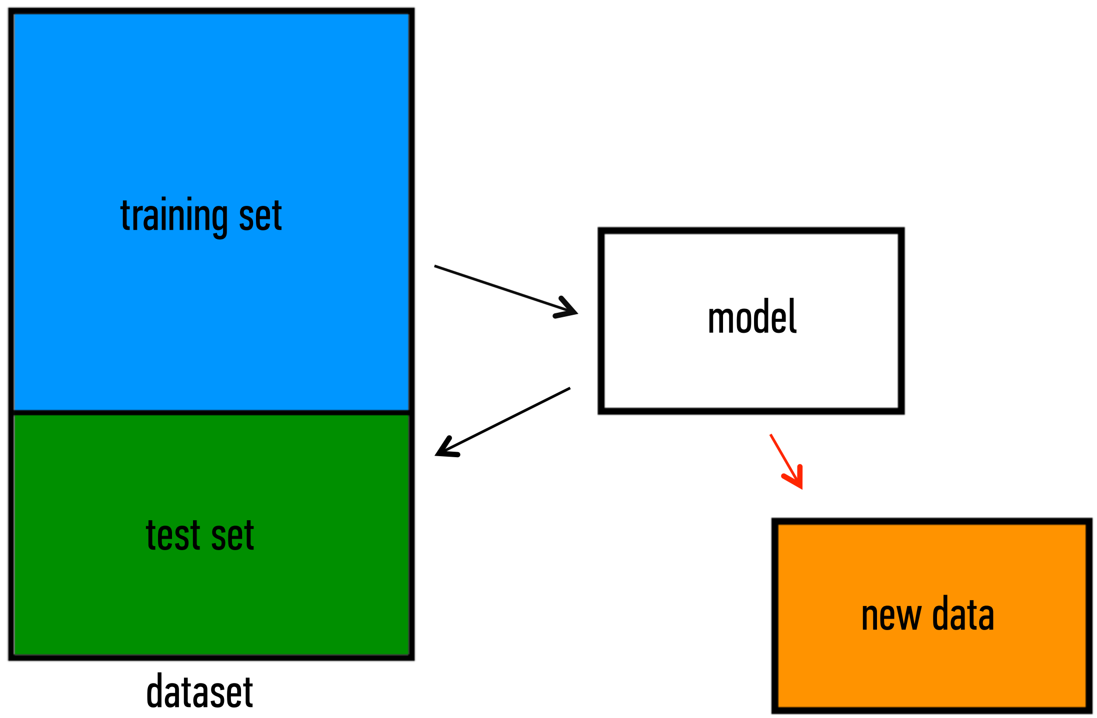

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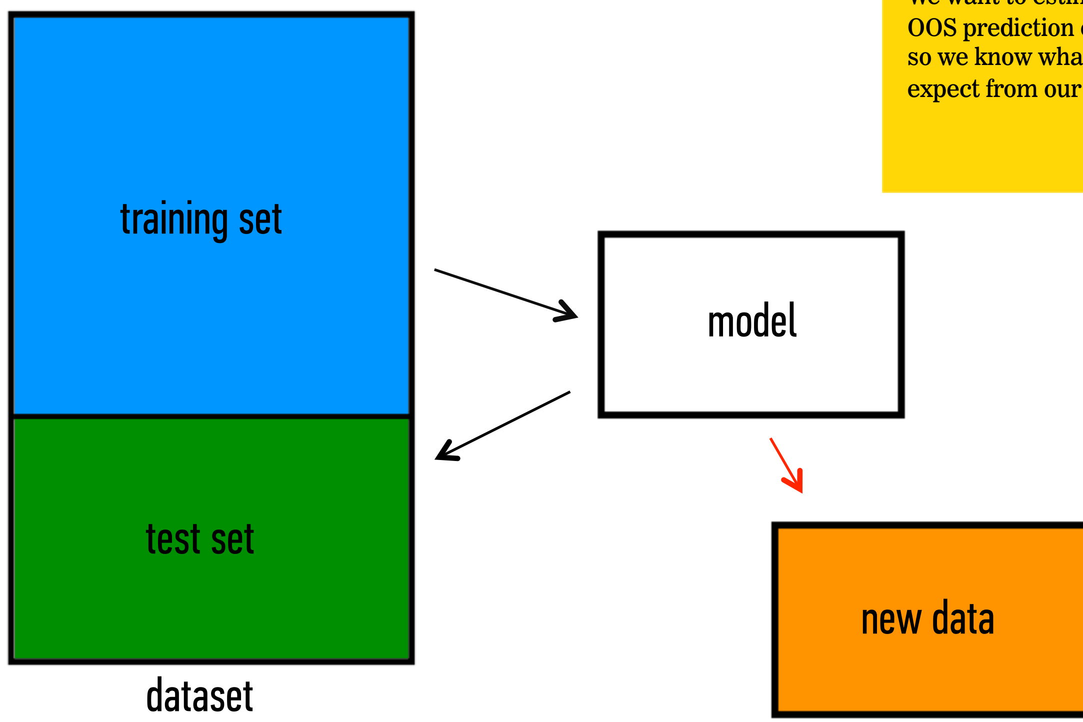

NOTE

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

Q: Why should we use training & test sets?

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Thought experiment:
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NOTE

This phenomenon is called *overfitting*.

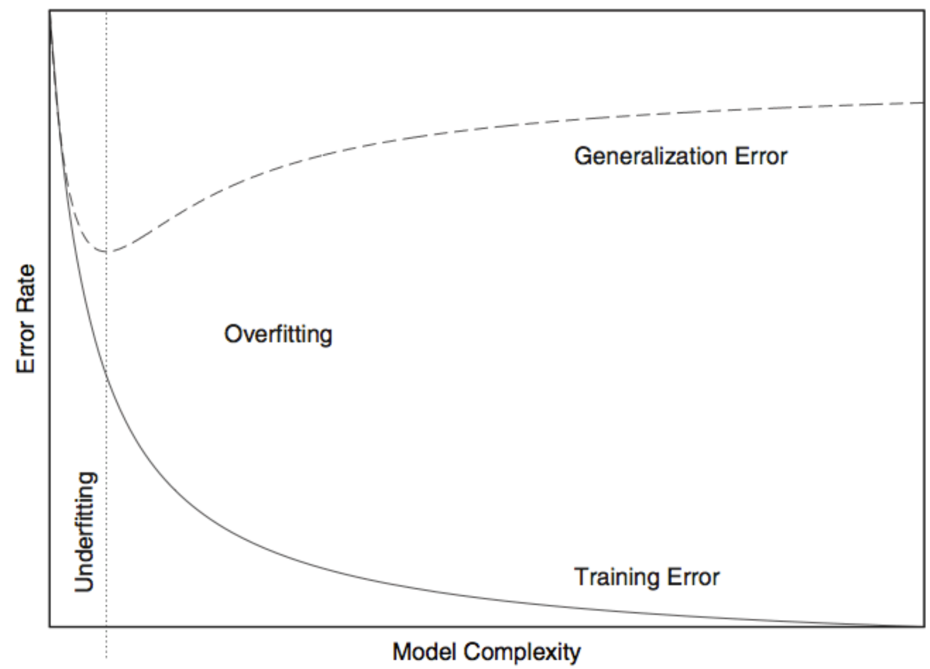
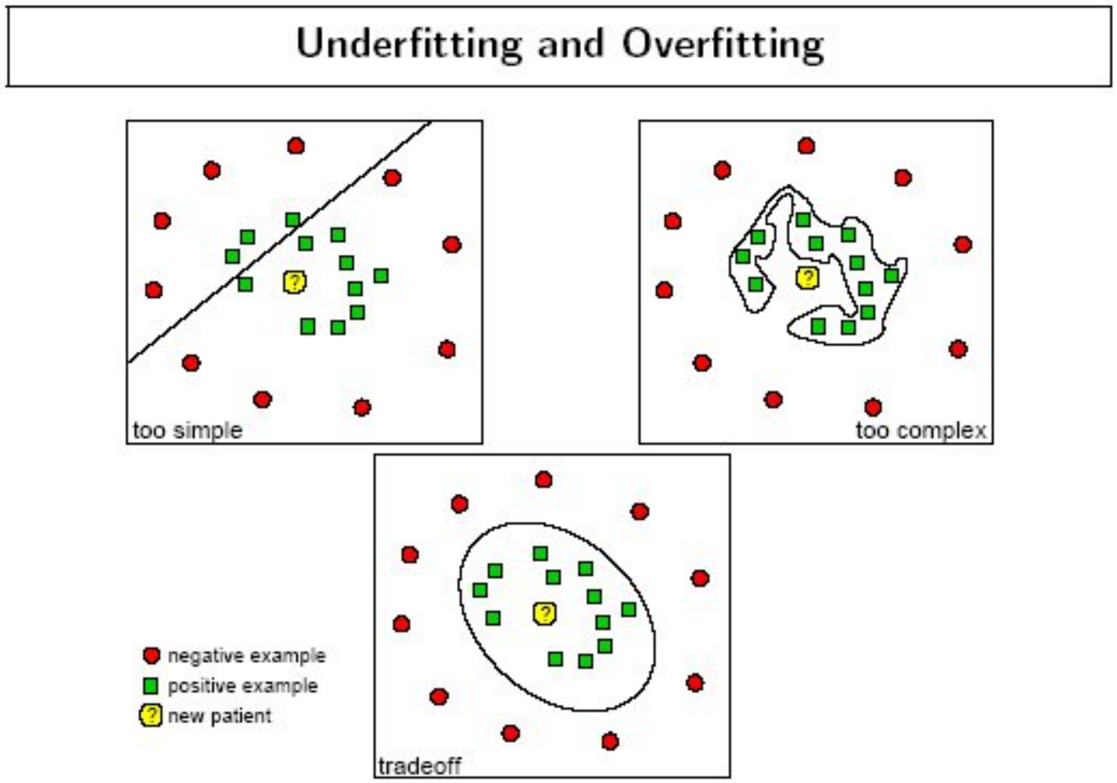


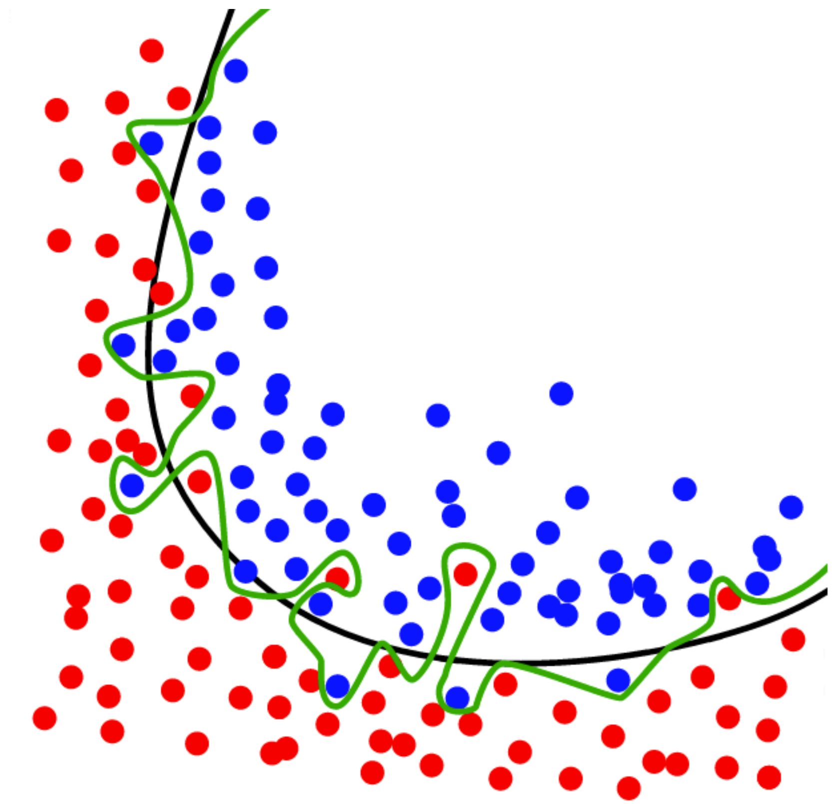
FIGURE 18-1. Overfitting: as a model becomes more complex, it becomes increasingly able to represent the training data. However, such a model is overfitted and will not generalize well to data that was not used during training.

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



source: http://www.dtreg.com

OVERFITTING – EXAMPLE



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This phenomenon is called *overfitting*.

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

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A: On its own, not very well.

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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!

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

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A: Cross-validation.

Steps for n-fold cross-validation:

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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.

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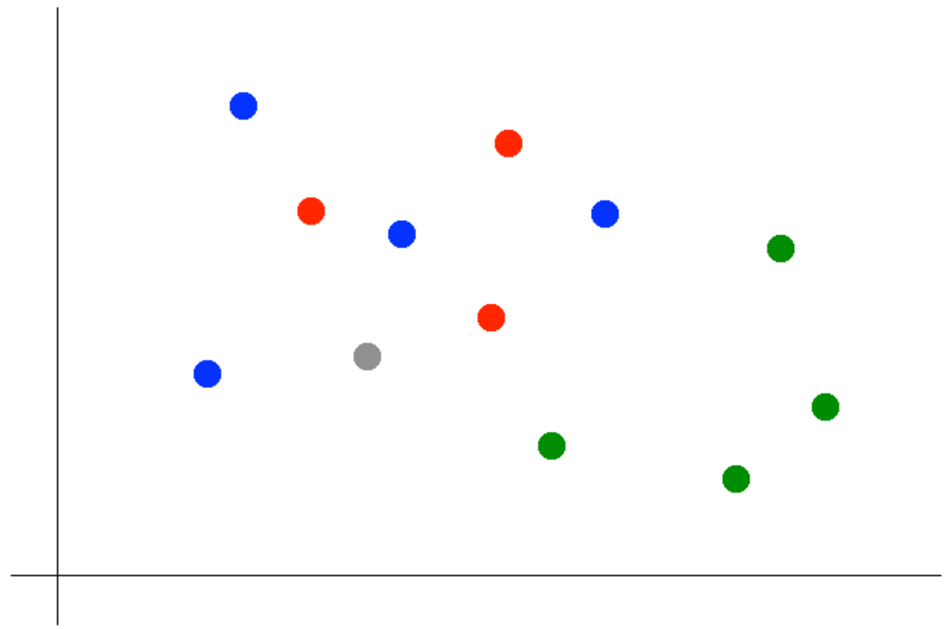
    - Each record in our dataset is used for both training and testing.
3) Presents tradeoff between efficiency and computational expense.
    - 10-fold CV is 10x more expensive than a single train/test split
4) Can be used for model selection.

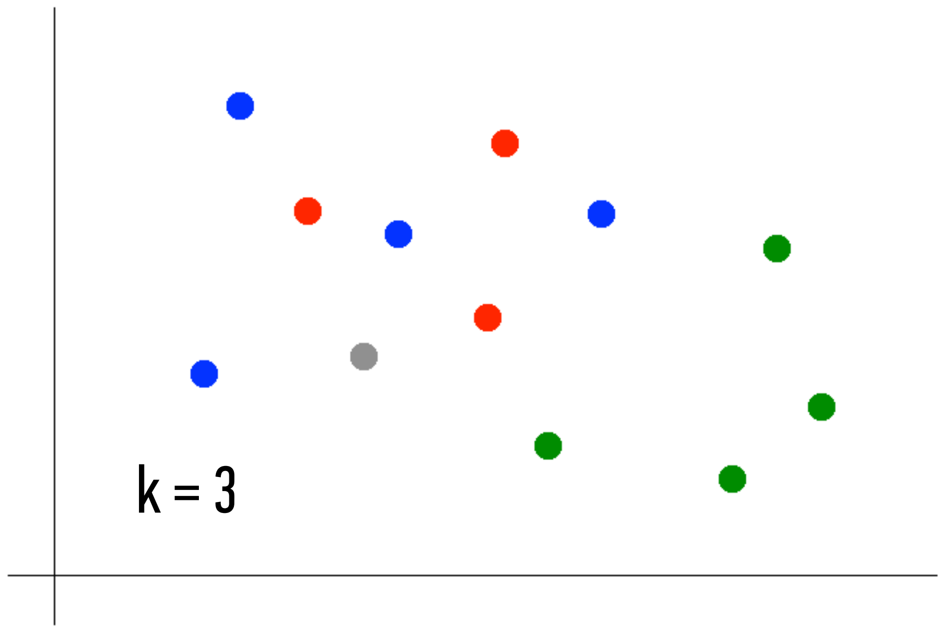
III. KNN CLASSIFICATION

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



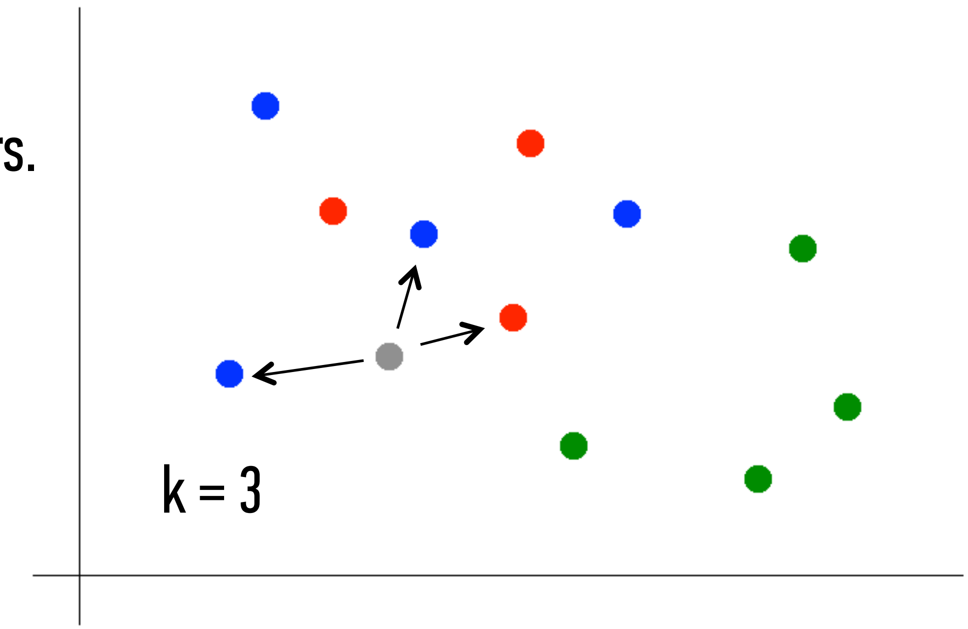
Suppose we want to predict the color of the grey dot.

1) Pick a value for k.



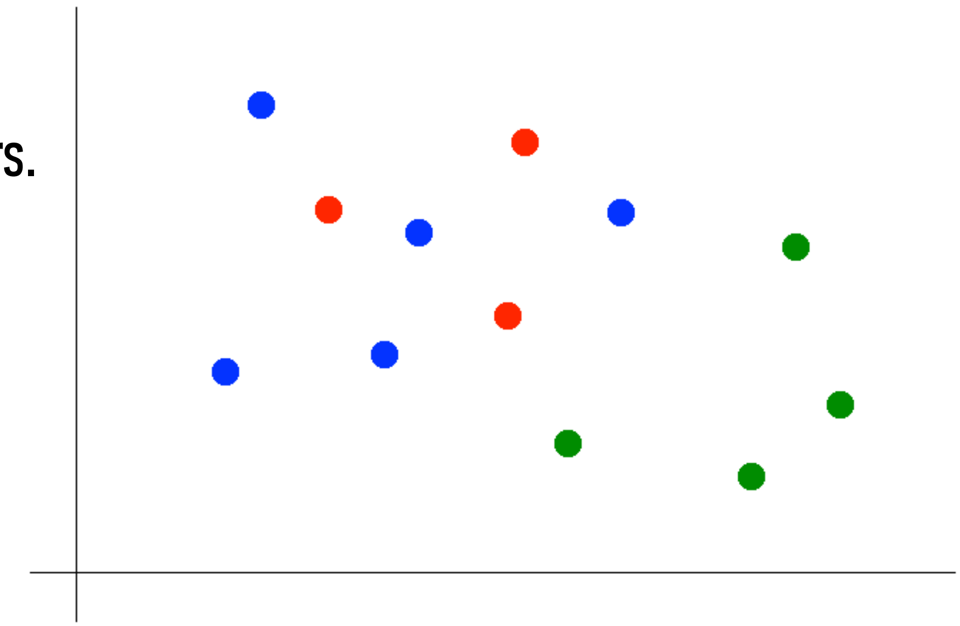
Suppose we want to predict the color of the grey dot.

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.



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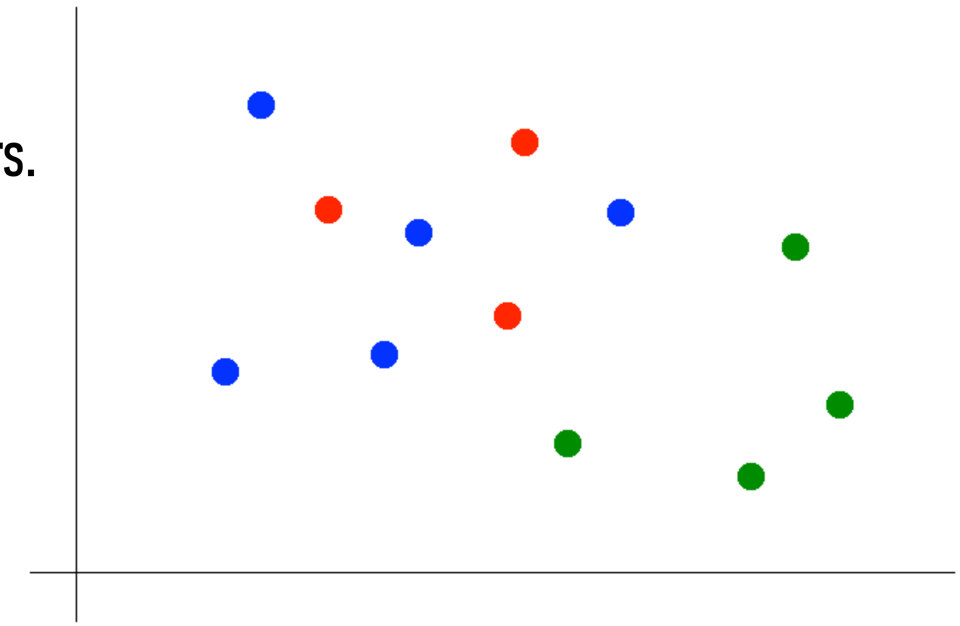
OPTIONAL NOTE

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}

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