GENERAL ASSEMBLY

INTRO TO DATA SCIENCE

SESSION 3: INTRO TO MACHINE LEARNING WITH KNN

Rob Hall

DAT13 SF // March 16, 2015

LAST TIME:

- INTRO TO PYTHON
- LAB: INTRO TO NUMPY & PANDAS

QUESTIONS?

AGENDA

I. WHAT IS MACHINE LEARNING?
II. CLASSIFICATION PROBLEMS
III. BUILDING EFFECTIVE CLASSIFIERS
IV. THE KNN CLASSIFICATION MODEL

EXERCISES:
IV. LAB: KNN CLASSIFICATION IN PYTHON
V. BONUS LAB: VISUALIZATION WITH MATPLOTLIB (IF TIME ALLOWS)

I. WHAT IS MACHINE LEARNING?

- *Types of machine learning problems / algorithms*
- *Generalization*
- *Types of error (training, generalization, OOS)*
- *Over-fitting and under-fitting*
- *Cross-validation*

"A field of study that gives computers the ability to learn without being explicitly programmed." (1959)

Arthur Samuel, AI pioneer
Source: Stanford

WHAT IS MACHINE LEARNING?

"A computer program is said to learn from experience *E* with respect to some set of tasks *T* and performance measure *P*, if its performance at tasks in *T*, as measured by *P*, improves with experience *E*". (1989)

Tom Mitchell, Professor, CMU
(Source: CMU)

"A computer program is said to learn from experience E with respect to some set of tasks T and performance measure P, if its performance at tasks in T, as measured by P, improves with experience E".

A person is said to learn from a college course E with respect to some set of readings and midterms T and grades P, if its performance at tasks in T, as measured by P, improves with E.

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

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

WHAT IS MACHINE LEARNING?

- **Machine learning** *is an area in computer science that studies and develops algorithms that can learn from data.*

- **Machine learning** *is a set of methods that can automatically detect patterns in data and use the discovered patterns to predict future data or perform other kinds of decision making*

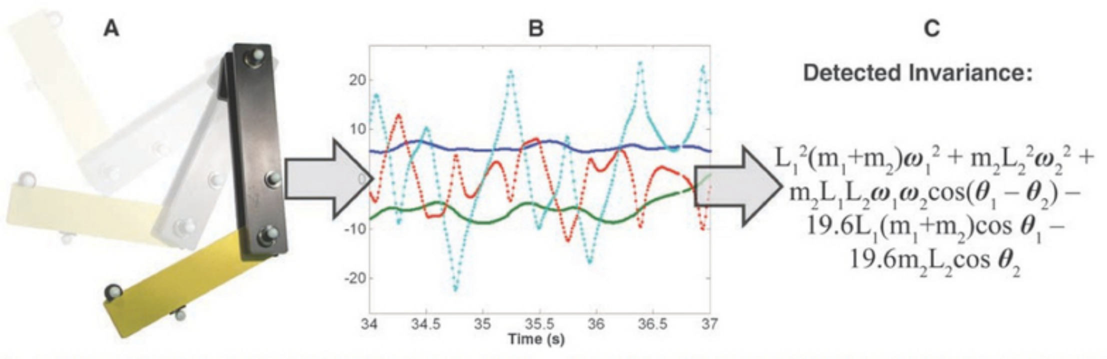
- *Statistical learning theory, Pattern recognition*

WHEN DO WE NEED MACHINE LEARNING?

Where we need it:

- *Some observable patterns exist*
- *There no explicitly known equations or dependencies (formulas)*
- *We have data on it*

Example: Newton's second law of motion, conservation of mechanical energy, pendulum motion



From "Distilling Free-Form Natural Laws from Experimental Data." M. Schmidt and H.Lipson. Science, 2009.

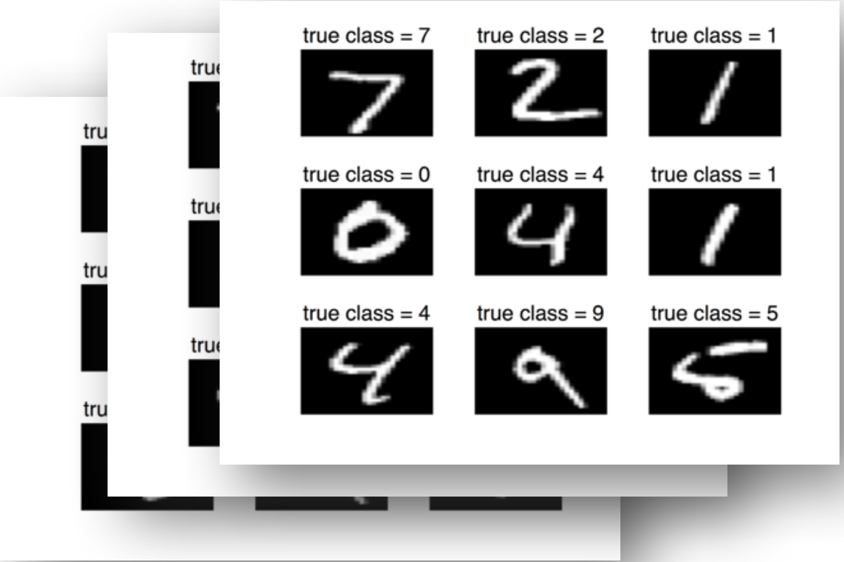
WHAT IS LEARNING?

Learning is not about memorizing and being able to recall, it is about generalizing the conclusions to previously unseen examples

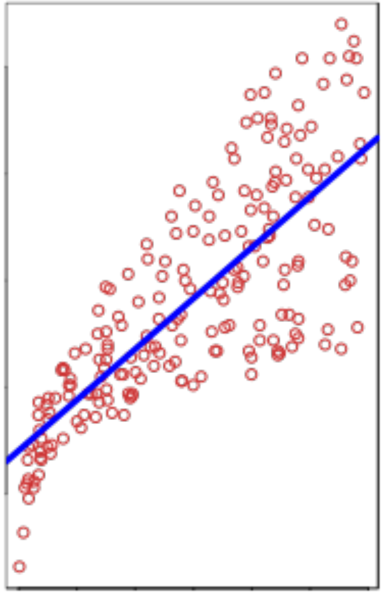
TYPES OF LEARNING?

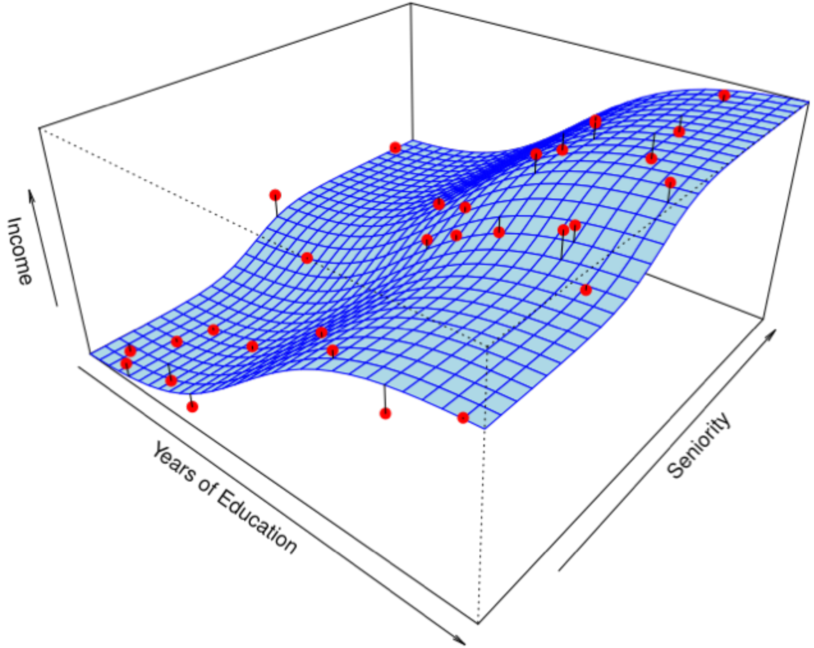
- **Supervised learning:** the goal is to learn mapping from given inputs x to outputs y, given a labeled set of input-output pairs (when the training set contains explicit examples of what correct output should be for given input
- **Unsupervised learning:** the goal is to learn interesting patterns and structure in data given only inputs (no output information given at all)

SUPERVISED LEARNING: CLASSIFICATION



SUPERVISED LEARNING: REGRESSION





SUPERVISED LEARNING: EXAMPLE

Credit Scoring

	Client 1	*Client 2*	*Client 3*
Age	*23*	*30*	*19*
Gender	*M*	*F*	*M*
Annual salary	*$30,000*	*$45,000*	*$15,000*
Years in residence	*3 years*	*1 year*	*3 month*
Years in job	*1 year*	*1 year*	*1 month*
Current debt	*$5,000*	*$1,000*	*$10,000*
Paid off credit	*Yes*	*Yes*	*No*

SUPERVISED LEARNING: EXAMPLE

Credit Scoring

	Applicant
Age	*25*
Gender	*M*
Annual salary	*$25,000*
Years in residence	*1 year*
Years in job	*2 year3*
Current debt	*$15,000*
Credit decision/ score	*???*

THE STRUCTURE OF MACHINE LEARNING PROBLEMS

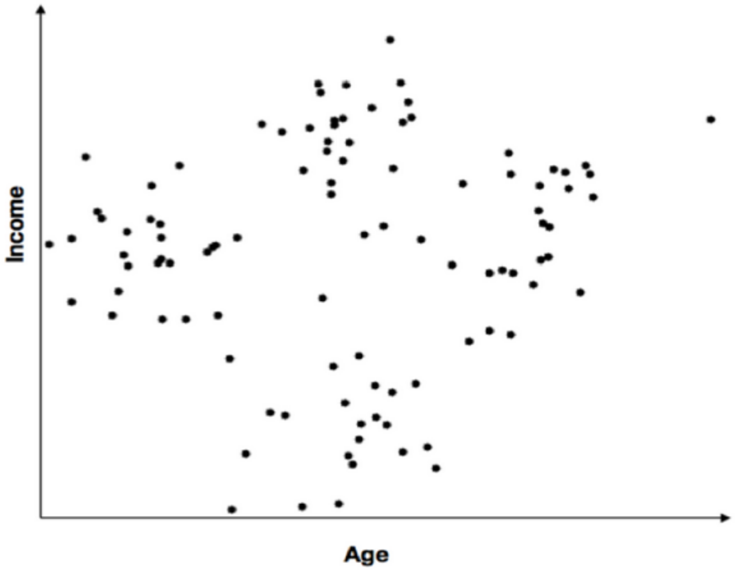
supervised	*making predictions*
unsupervised	*extracting structure*

generalization

supervised	*making predictions*
unsupervised	*extracting structure*

representation

Unsupervised Learning - Can we find structure to unlabeled data?



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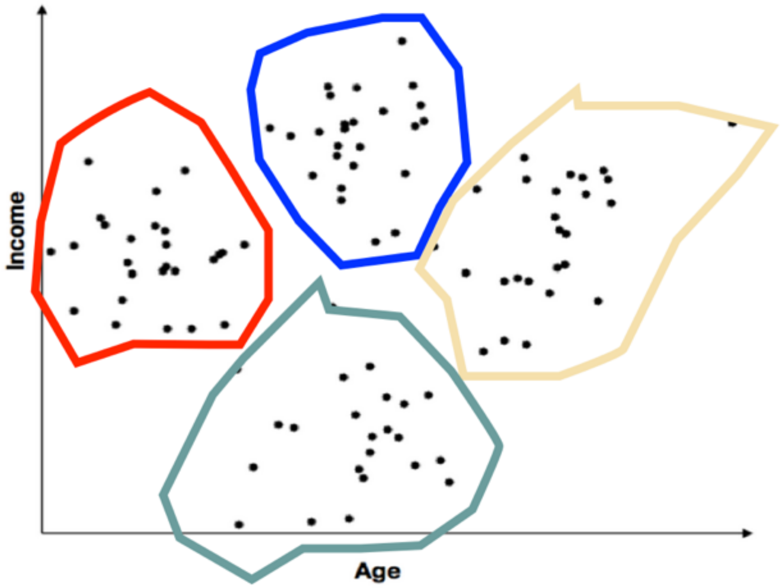

	continuous	**categorical**
	quantitative	*qualitative*

	continuous	categorical
	quantitative	qualitative

NOTE

The space where data live is called the *feature space.*

Each point in this space is called a *record*.

	continuous	categorical
supervised	regression	classification
unsupervised	dimension reduction	clustering

	continuous	*categorical*
supervised	*regression*	*classification*
unsupervised	*dimension reduction*	*clustering*

NOTE

We will implement solutions using *models* and *algorithms.*

Each will fall into one of these four buckets.

	continuous	categorical
supervised	regression	classification
unsupervised	dimension reduction	clustering

ANSWER

The right approach is determined by the desired solution.

	continuous	categorical
supervised	regression	classification
unsupervised	dimension reduction	clustering

ANSWER

The
is d
des

NOTE

All of this depends on your data!

II. 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.

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class labels

(qualitative)

Q: How does a classification problem work?

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A: Data in, predicted labels out.

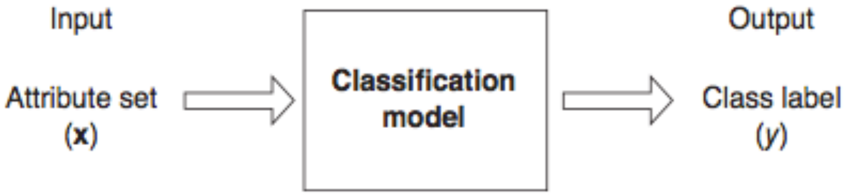
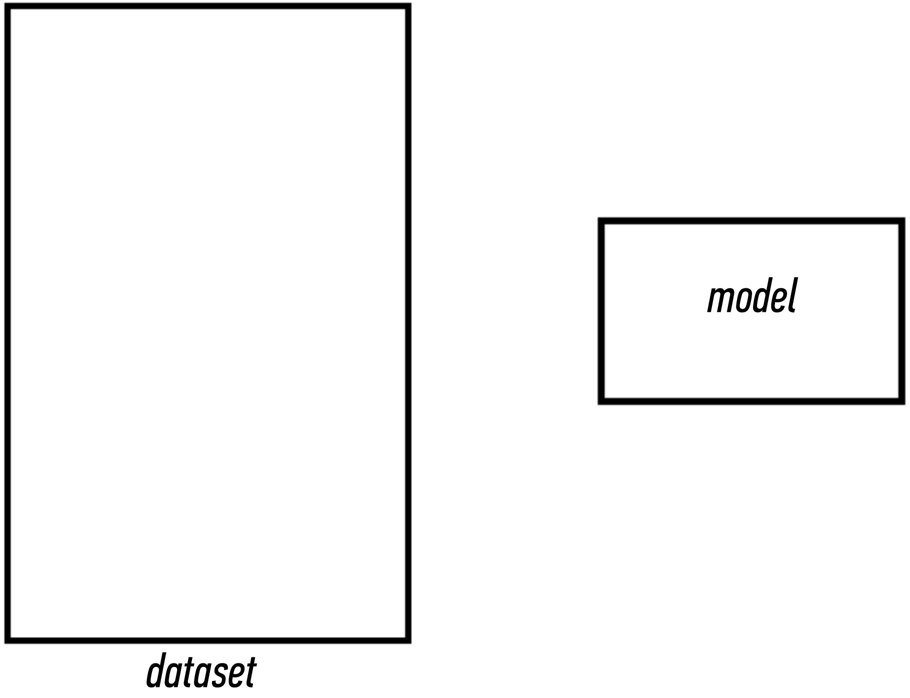


Figure 4.2. Classification as the task of mapping an input attribute set $\mathbf{x}$ into its class label y.

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

Q: What steps does a classification problem require?



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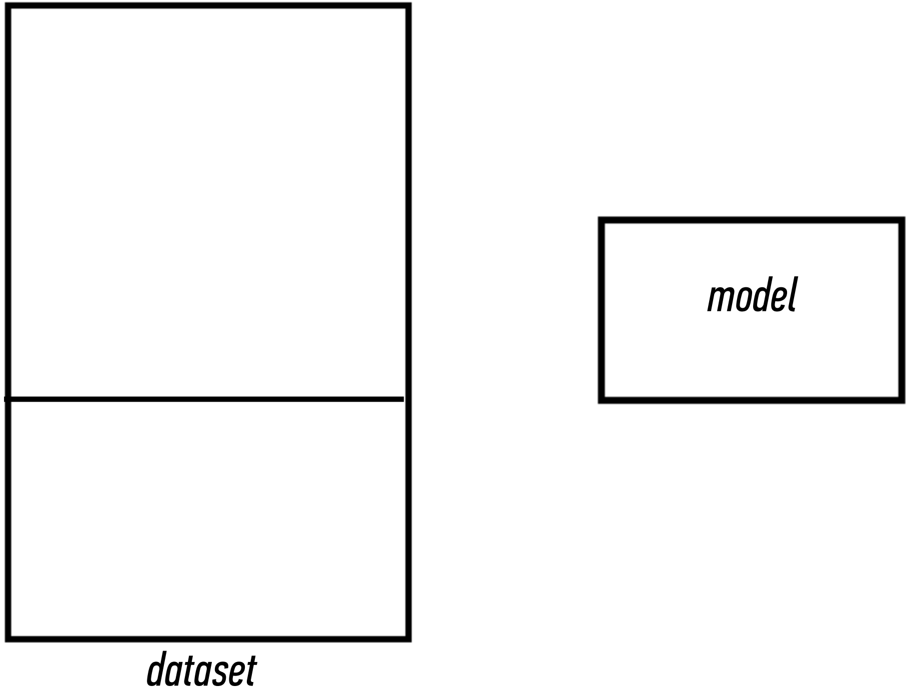
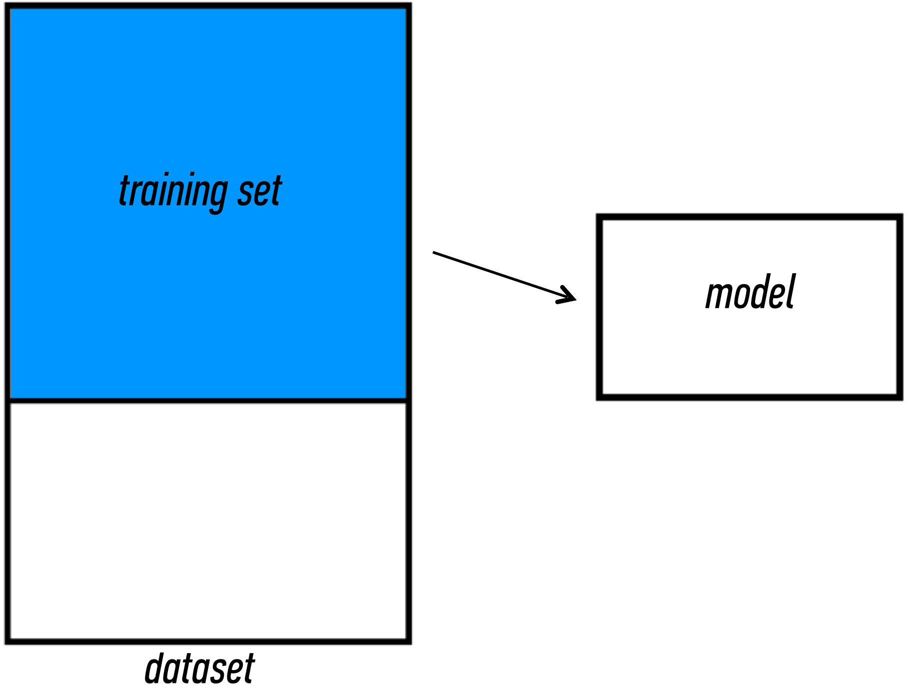


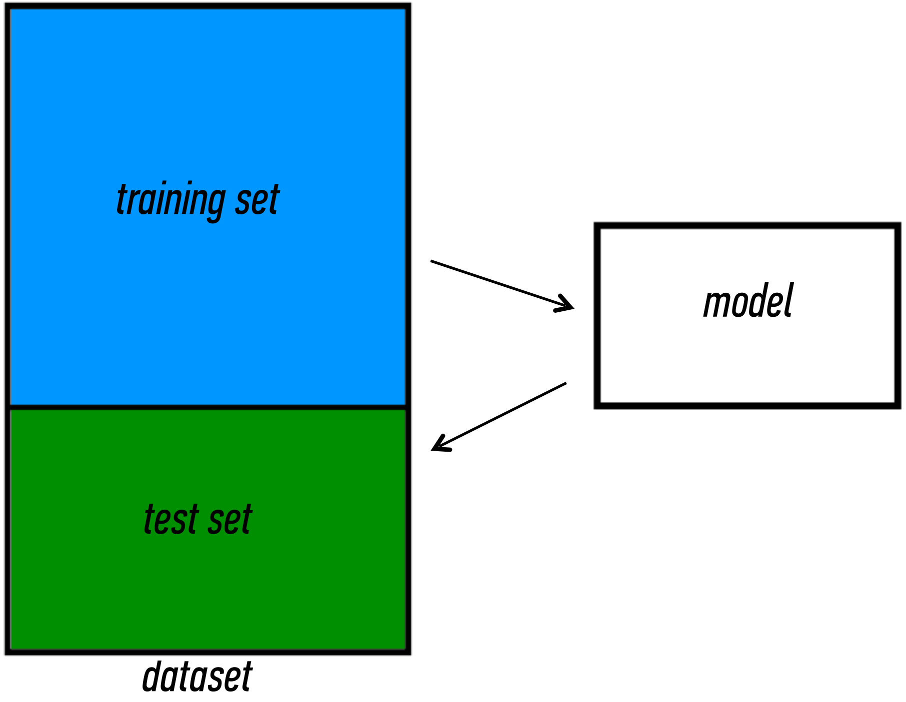
Q: What steps does a classification problem require?

1) split dataset
2) train model



Q: What steps does a classification problem require?

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



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1) split dataset
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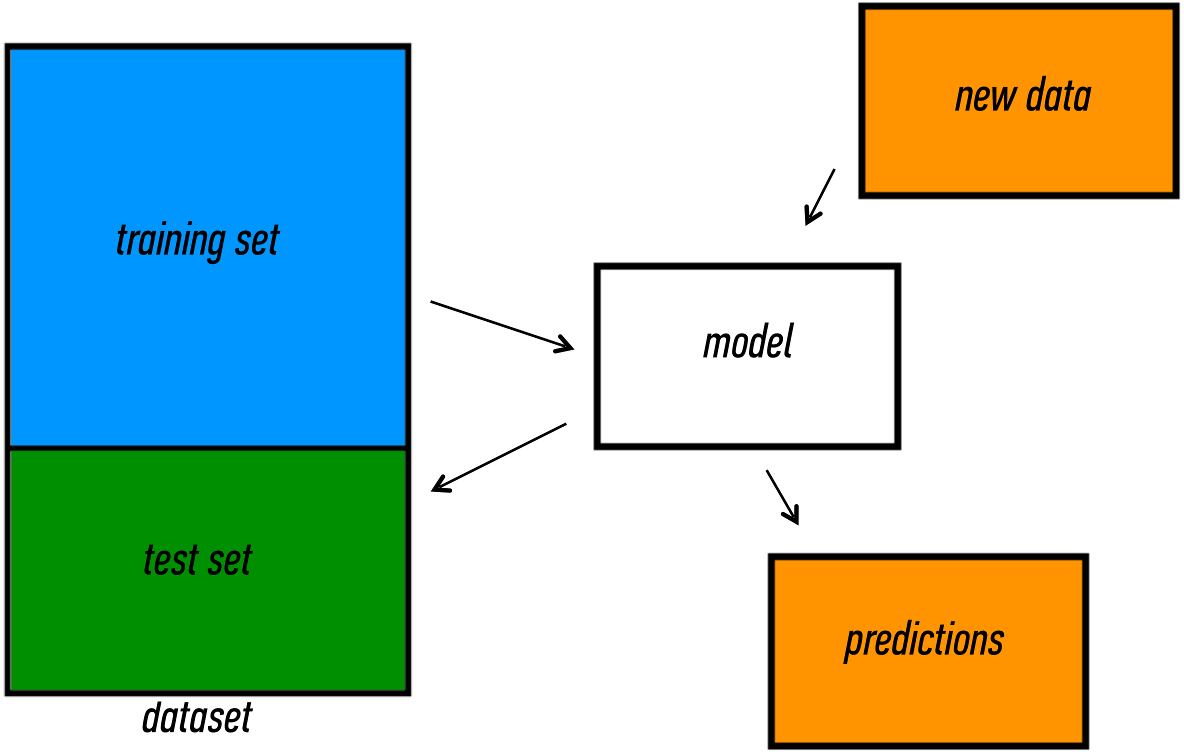
4) make predictions



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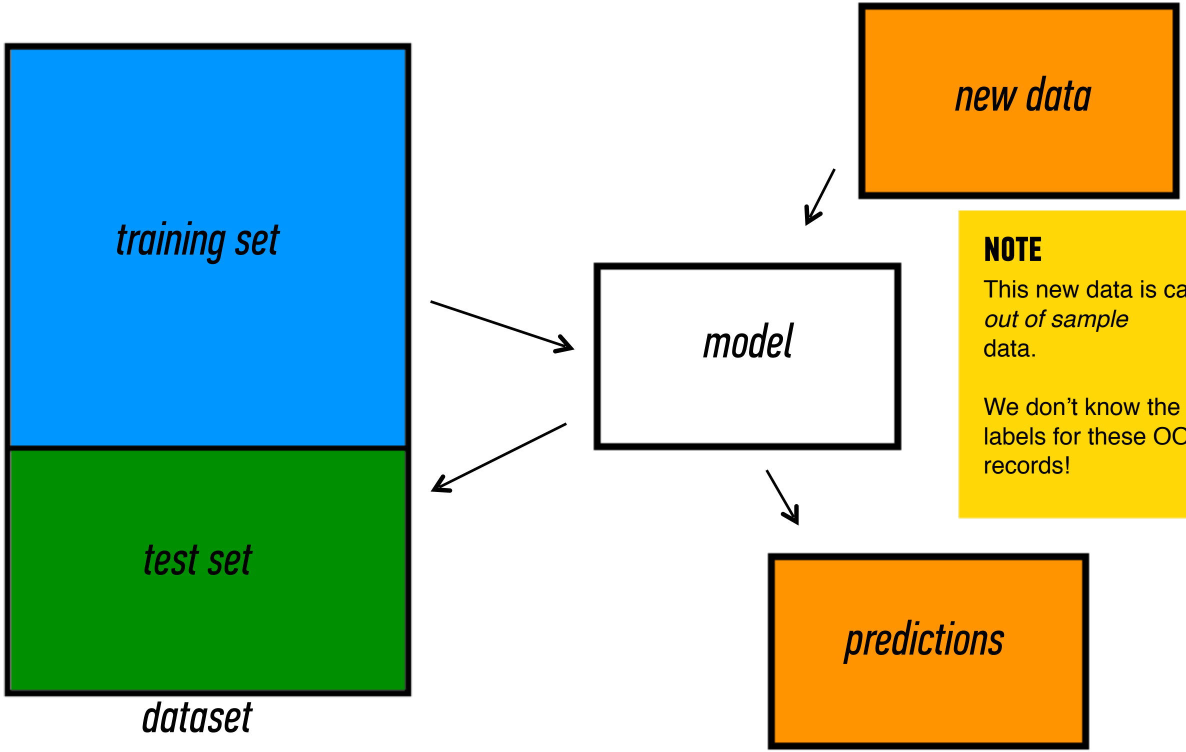
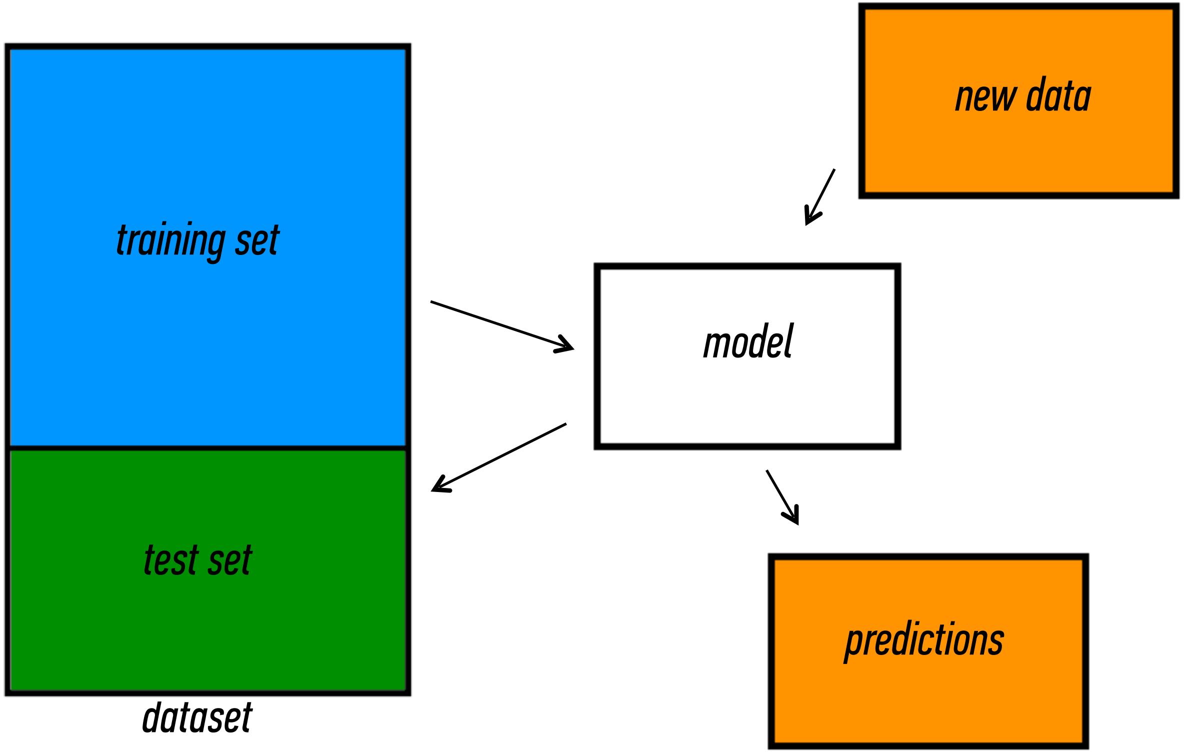


NOTE
This new data is called *out of sample* data.

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

III. BUILDING EFFECTIVE CLASSIFIERS

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



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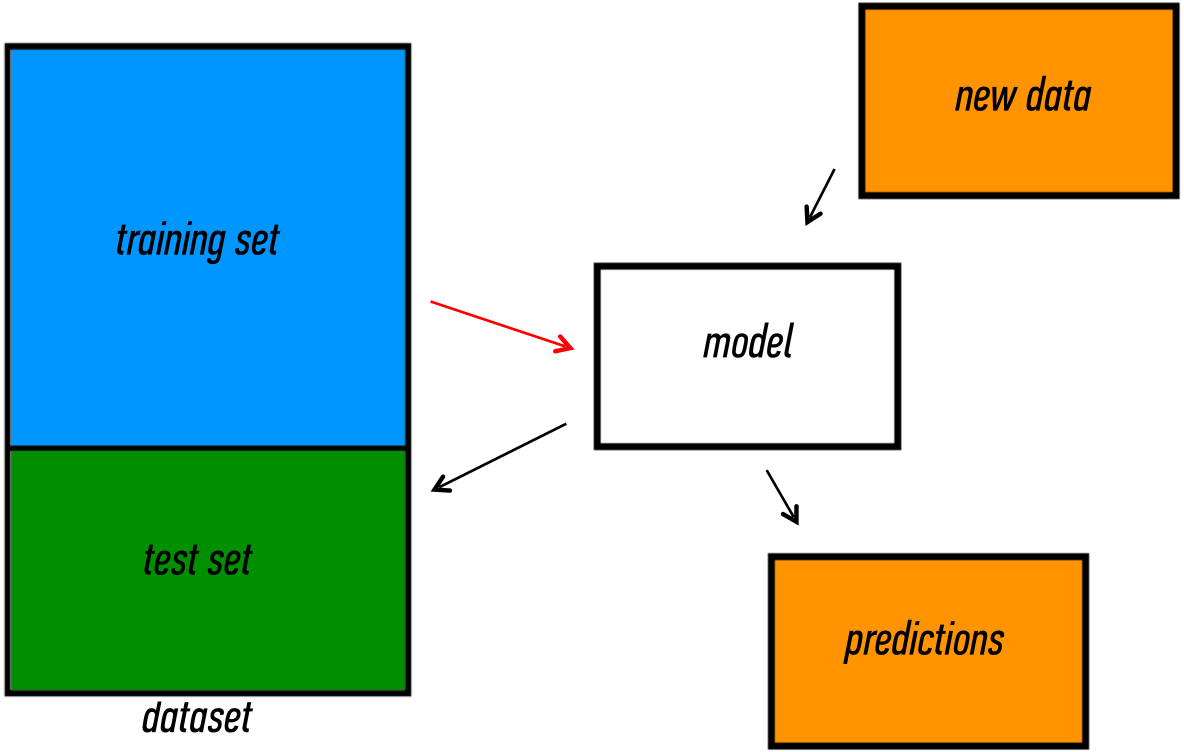
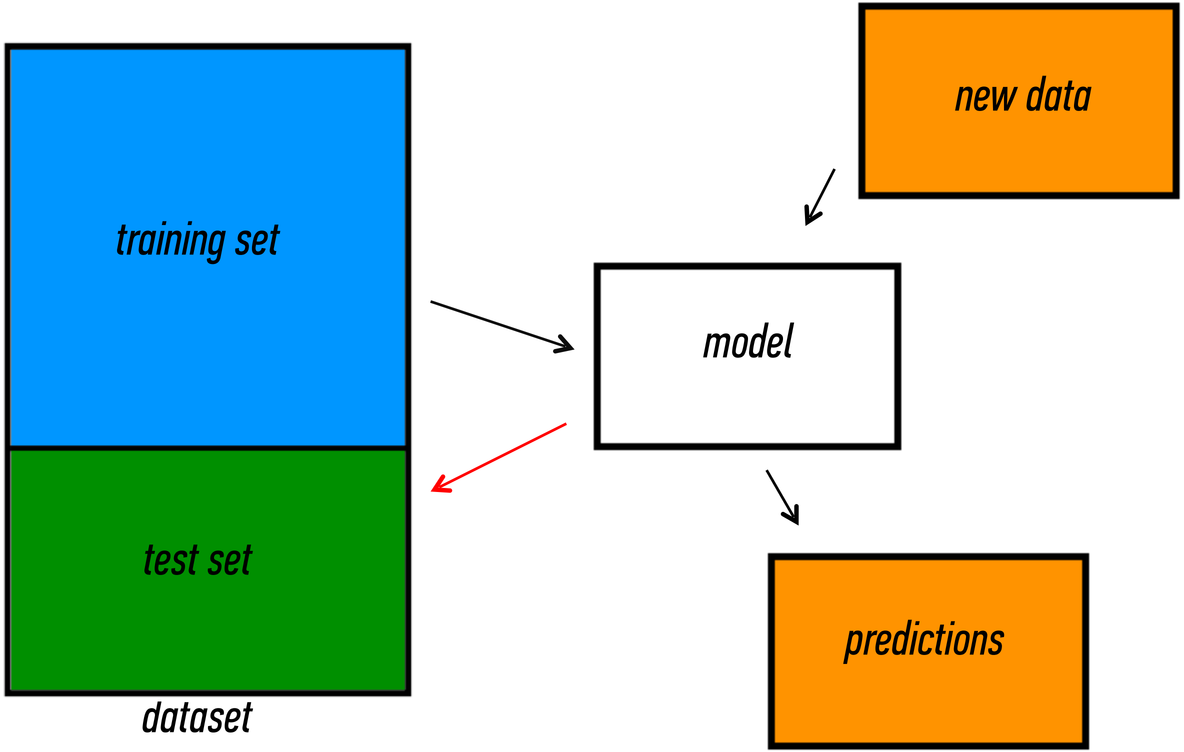
1) training error



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

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



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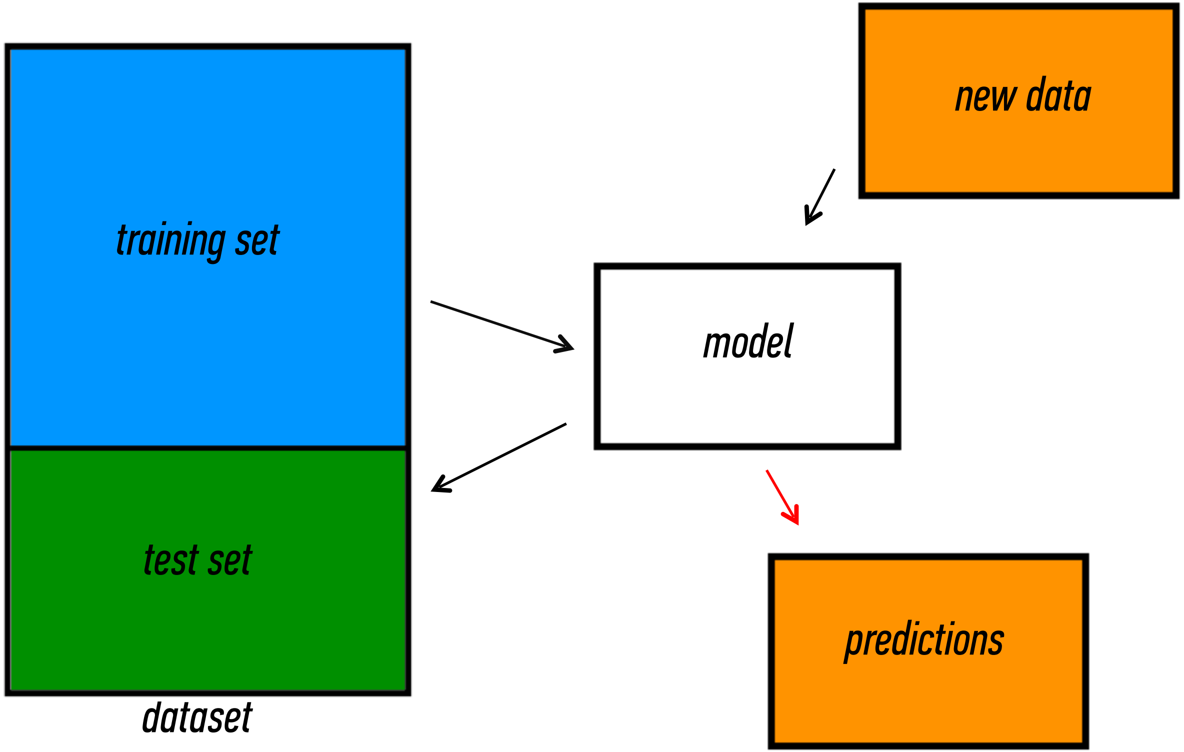

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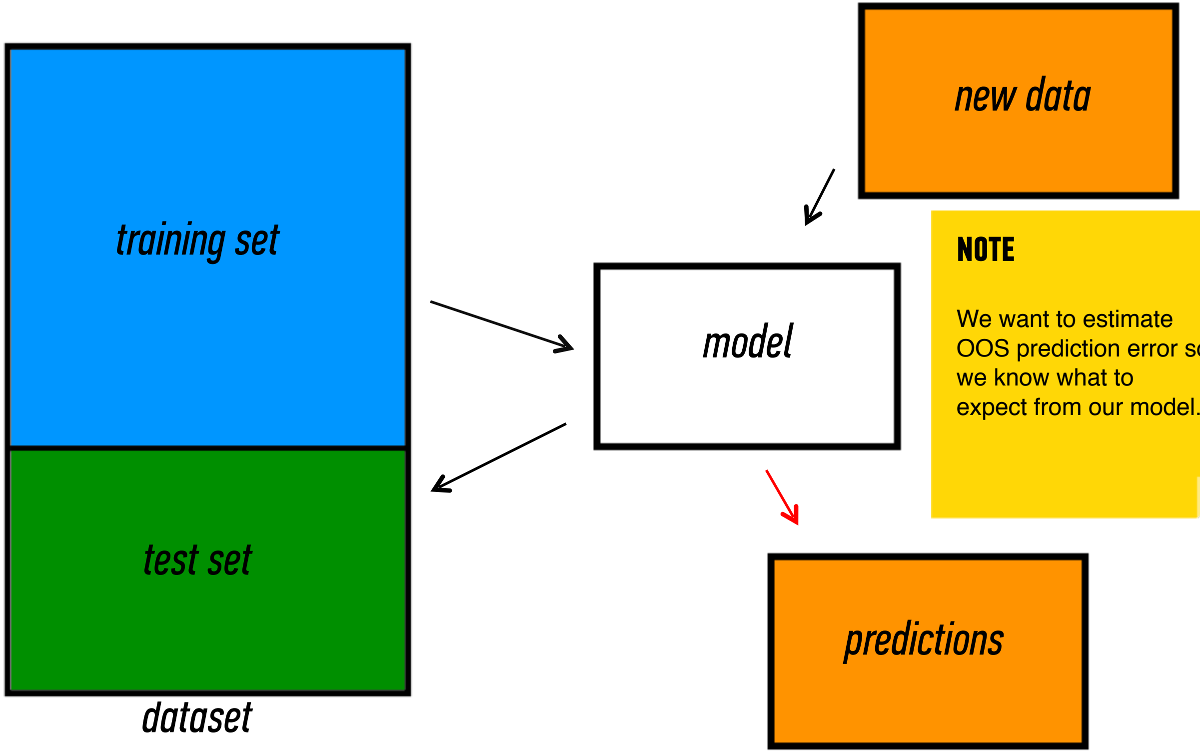

NOTE

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

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A: Down to zero!

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NOTE

This phenomenon is called *overfitting*.

OVERFITTING

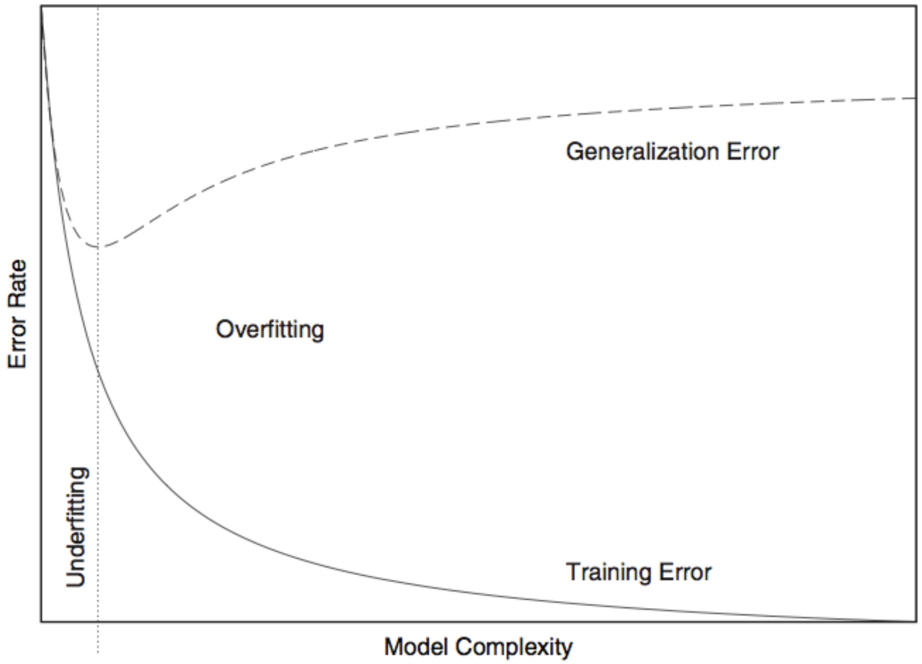
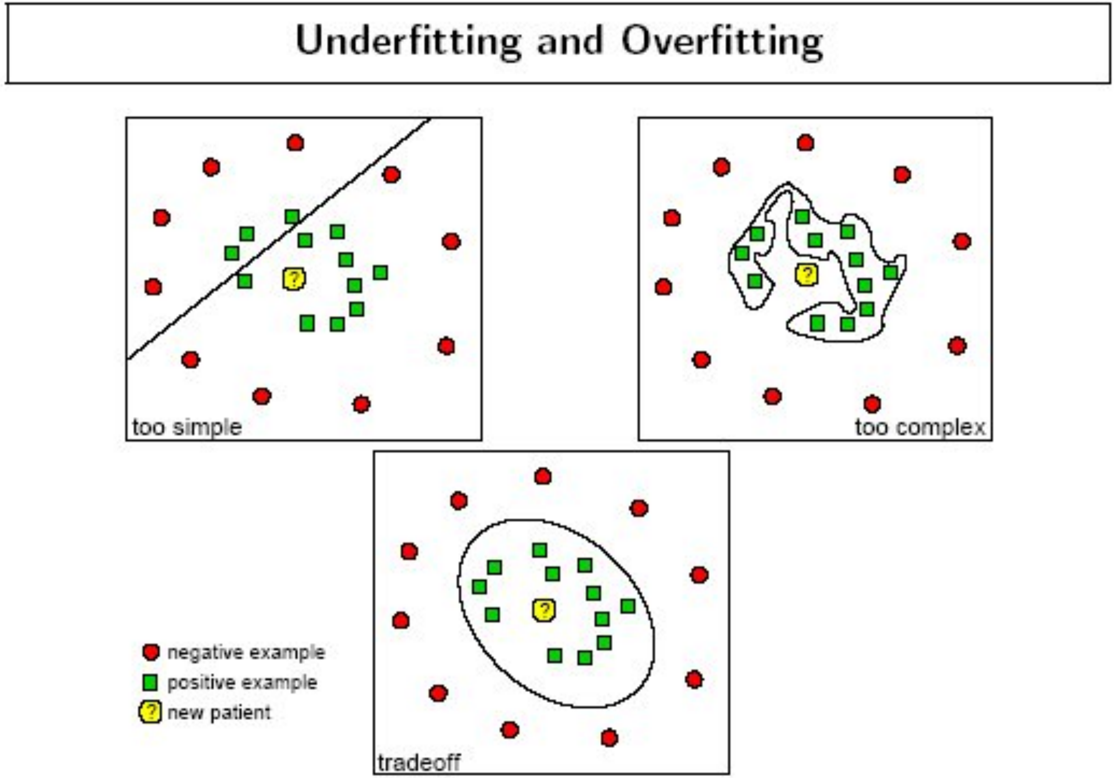


FIGURE 18-1. Overfitting: as a model becomes more complex, it becomes increasingly able to represent the training data. However, such a model is overfitted and will not generalize well to data that was not used during training.

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

OVERFITTING - EXAMPLE



source: http://www.dtreg.com

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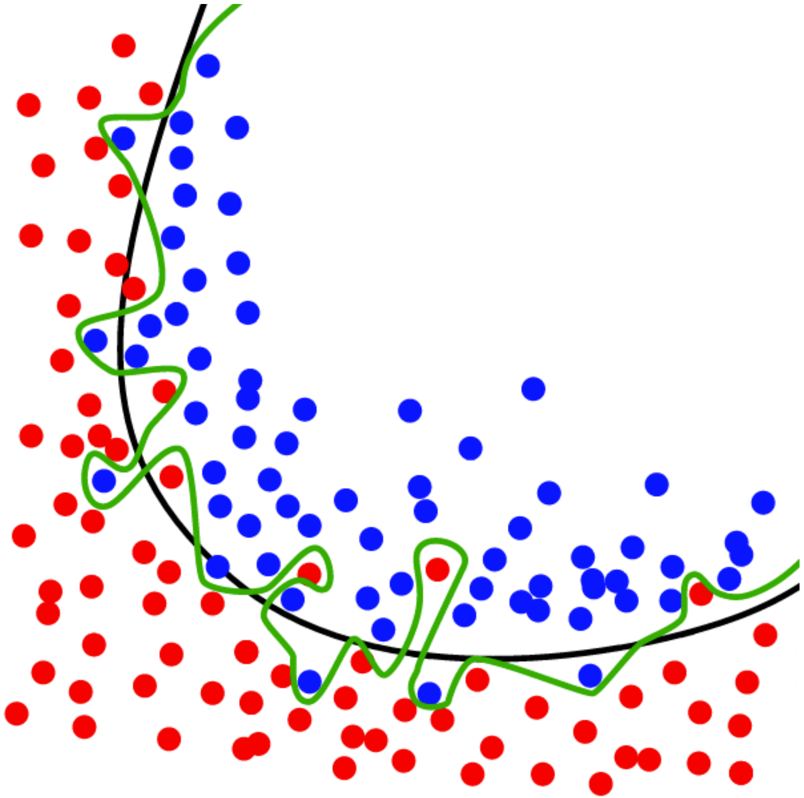

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NOTE

This phenomenon is called *overfitting*.

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

Suppose we do the train/test split.

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Q: How well does generalization error predict OOS accuracy?

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A: Of course not!

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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.

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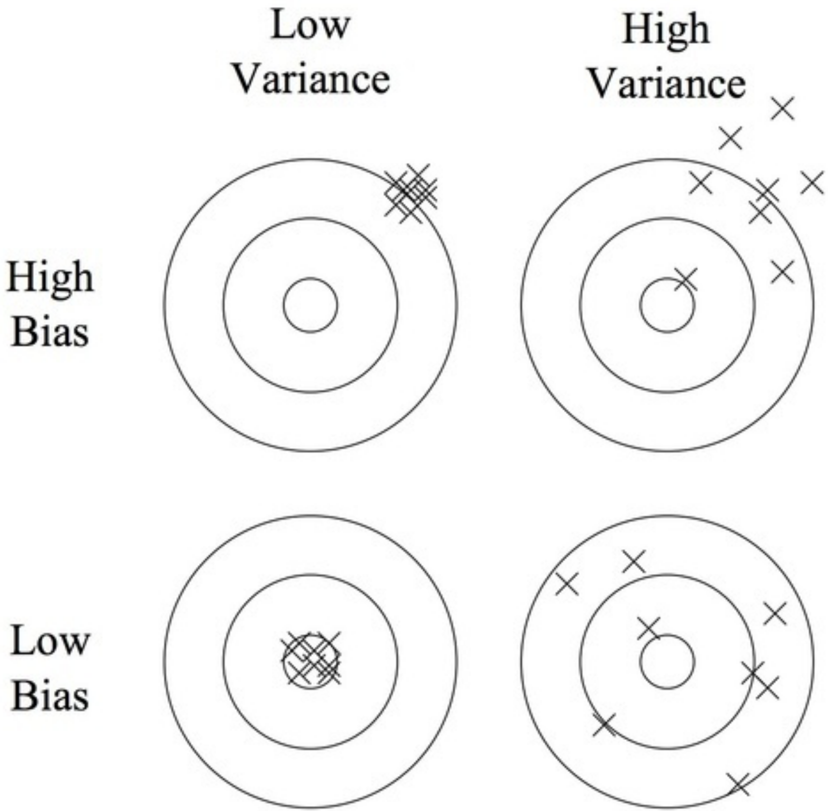
NOTE

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

BIAS-VARIANCE



Something is still missing!

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Q: How can we do better?

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Thought experiment:

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

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A: Now you're talking!

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A: Cross-validation.

CROSS-VALIDATION

Steps for n-fold cross-validation:

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3) *Find generalization error.*

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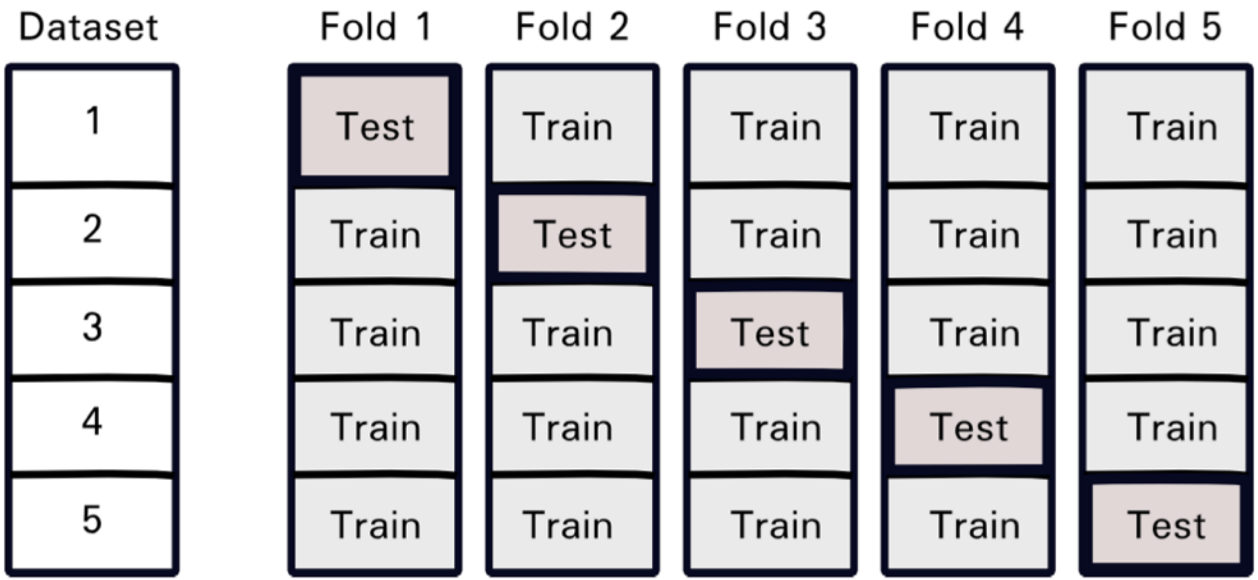
4) *Repeat steps 2-3 using a different partition as the test set at each iteration.*

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.

CROSS-VALIDATION: 5-FOLD EXAMPLE



Accuracy

k_1 %

k_2 %

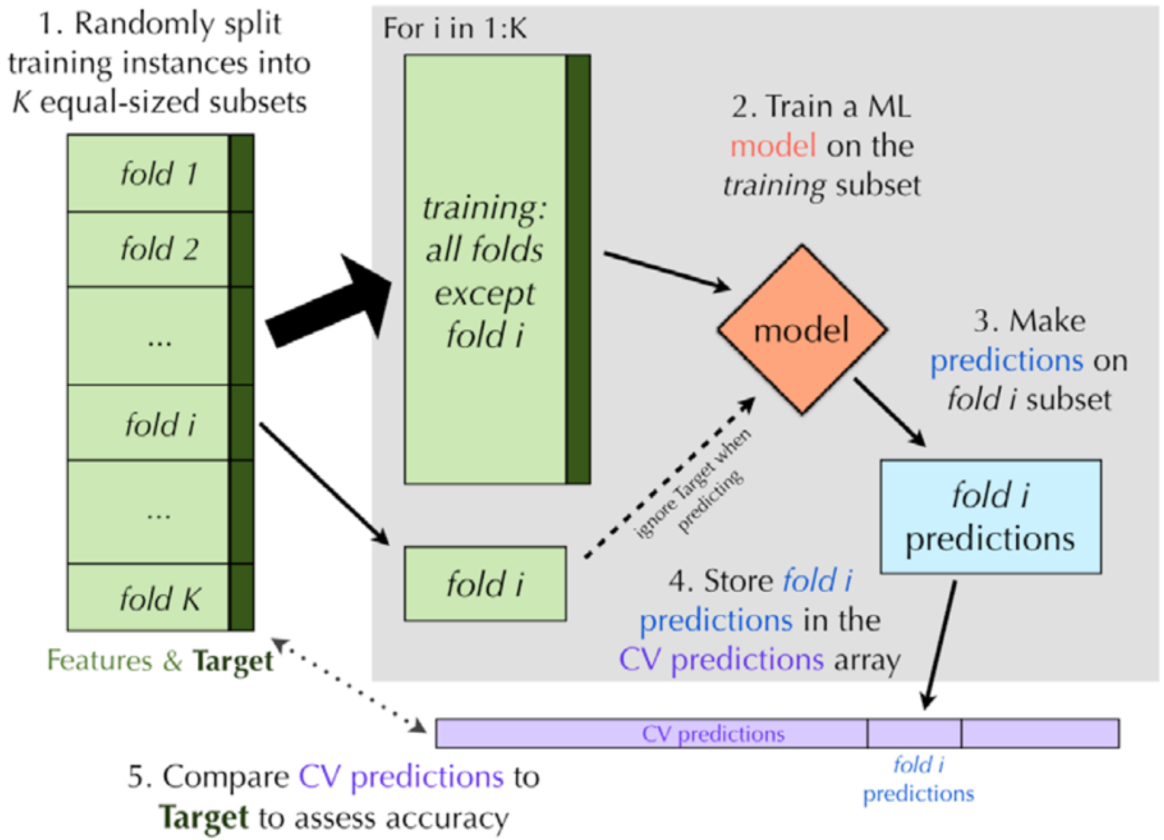
k_3 %

k_4 %

k_5 %

5-Fold Generalization Error $= (k_1 + k_2 + k_3 + k_4 + k_5) / 5$

CROSS-VALIDATION



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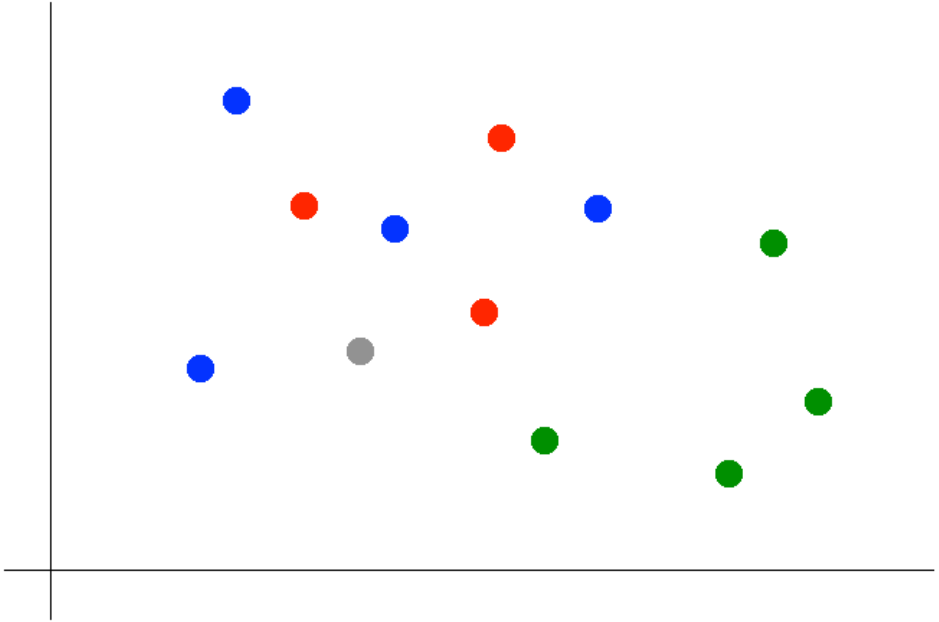
   - *Each record in our dataset is used for both training and testing.*
3) *Presents tradeoff between efficiency and computational expense.*
   - *10-fold CV is 10x more expensive than a single train/test split*
4) *Can be used for model selection.*

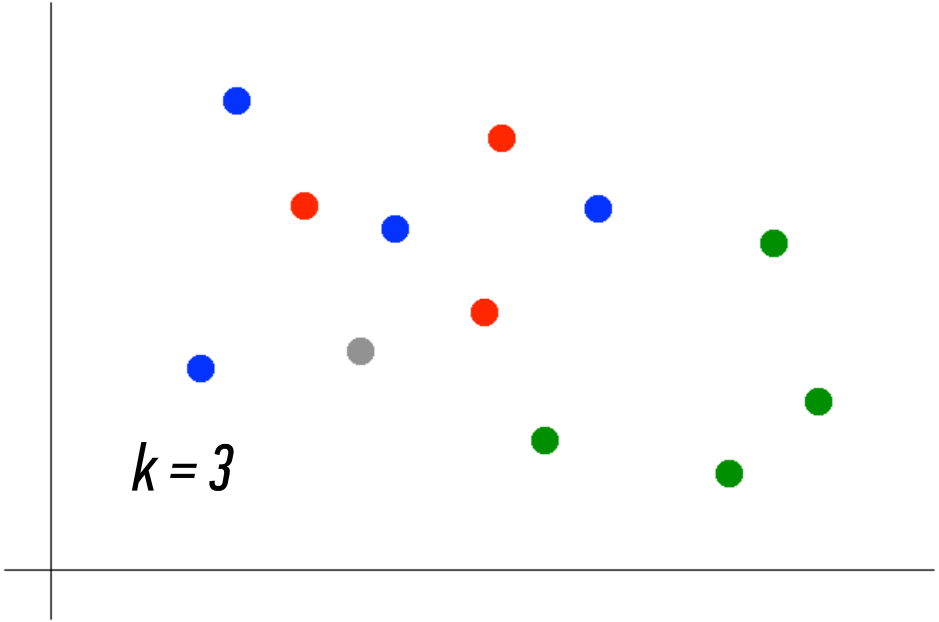
IV. KNN CLASSIFICATION

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



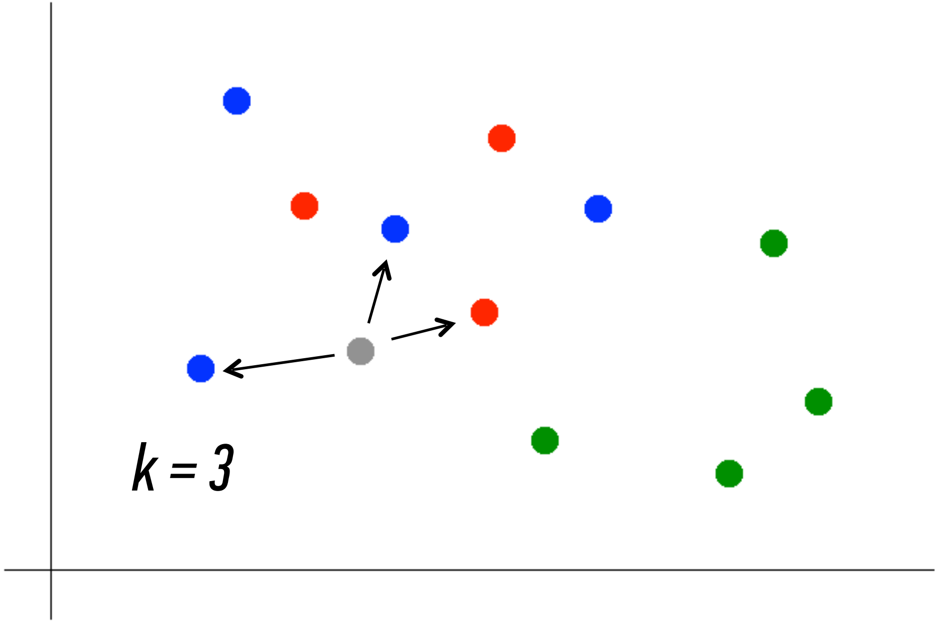
Suppose we want to predict the color of the grey dot.

1) *Pick a value for k.*



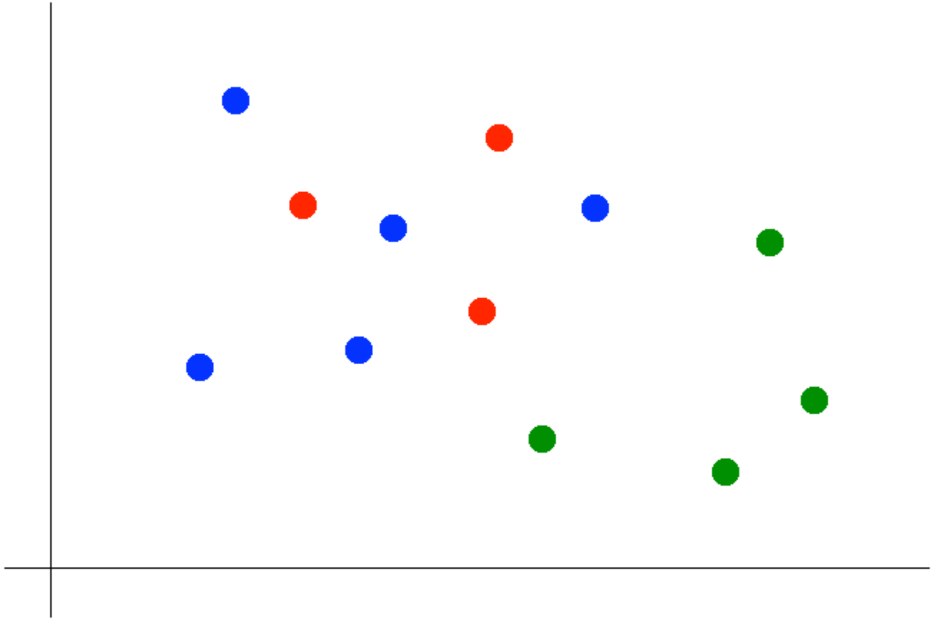
Suppose we want to predict the color of the grey dot.

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.

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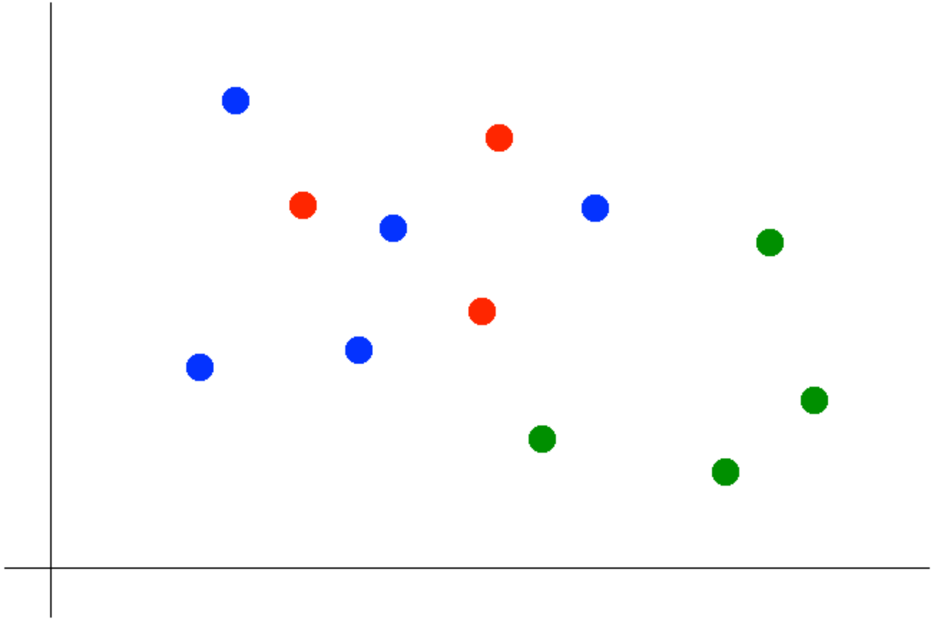
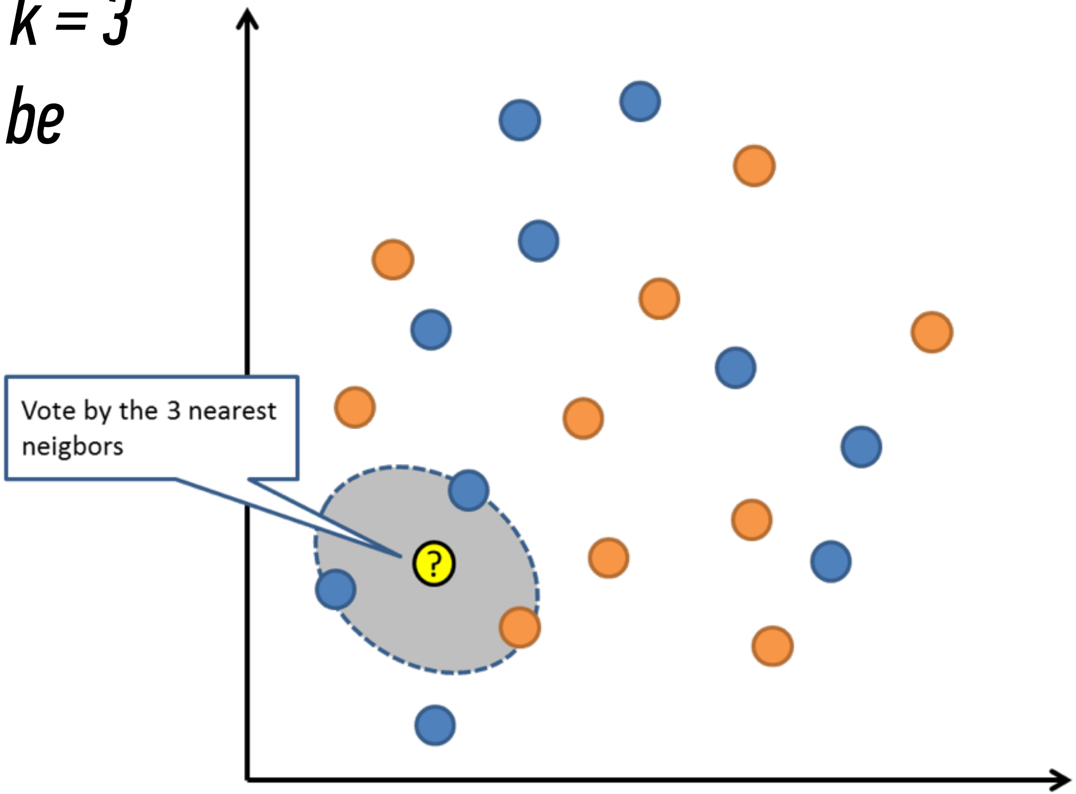


OPTIONAL NOTE

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

Another example with k = 3
Will our new example be blue or orange?



- *Types of machine learning problems / algorithms*
- *Generalization*
- *Types of error (training, generalization, OOS)*
- *Over-fitting and under-fitting*
- *Cross-validation*

LABS