GENERAL ASSEMBLY

INTRO TO DATA SCIENCE

LECTURE 3: INTRO TO ML & KNN CLASSIFICATION

Rob Hall

DAT9 SF // August 12, 2014

LAST TIME:

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

QUESTIONS?

What's big data?

The practical viewpoint:

1. $O(n^2)$ algorithm feasible: small data
2. Fits on one machine: medium data
3. Doesn't fit on one machine: big data

source: http://people.cs.umass.edu/~mcgregor/stocworkshop/langford.pdf

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?

"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.”

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

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“The core of machine learning deals with representation and generalization…”

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WHAT IS MACHINE LEARNING?

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"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

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WHAT IS MACHINE LEARNING?

from Wikipedia:

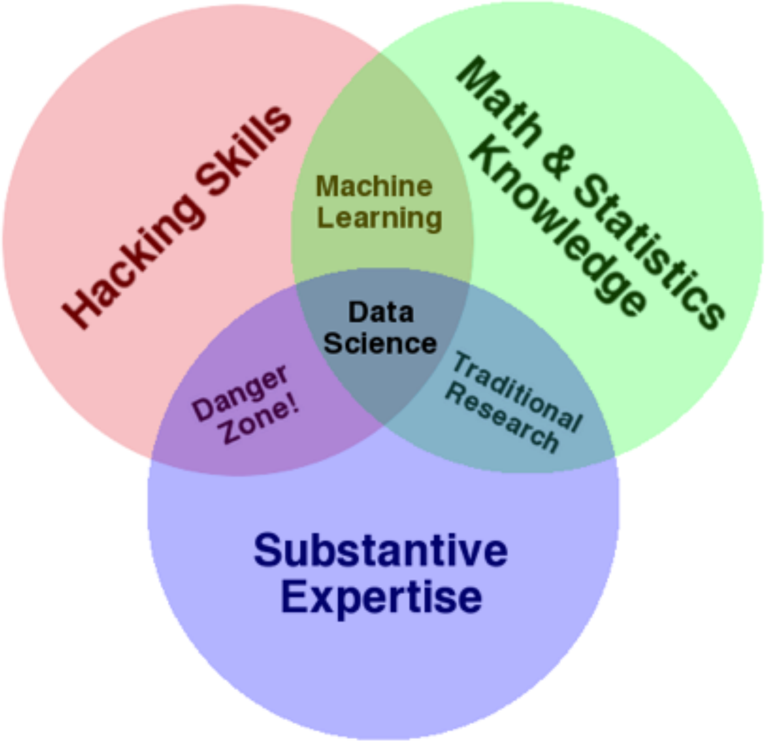
"Machine learning, a branch of artificial intelligence, is about the construction and study of systems that can learn from data."

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

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

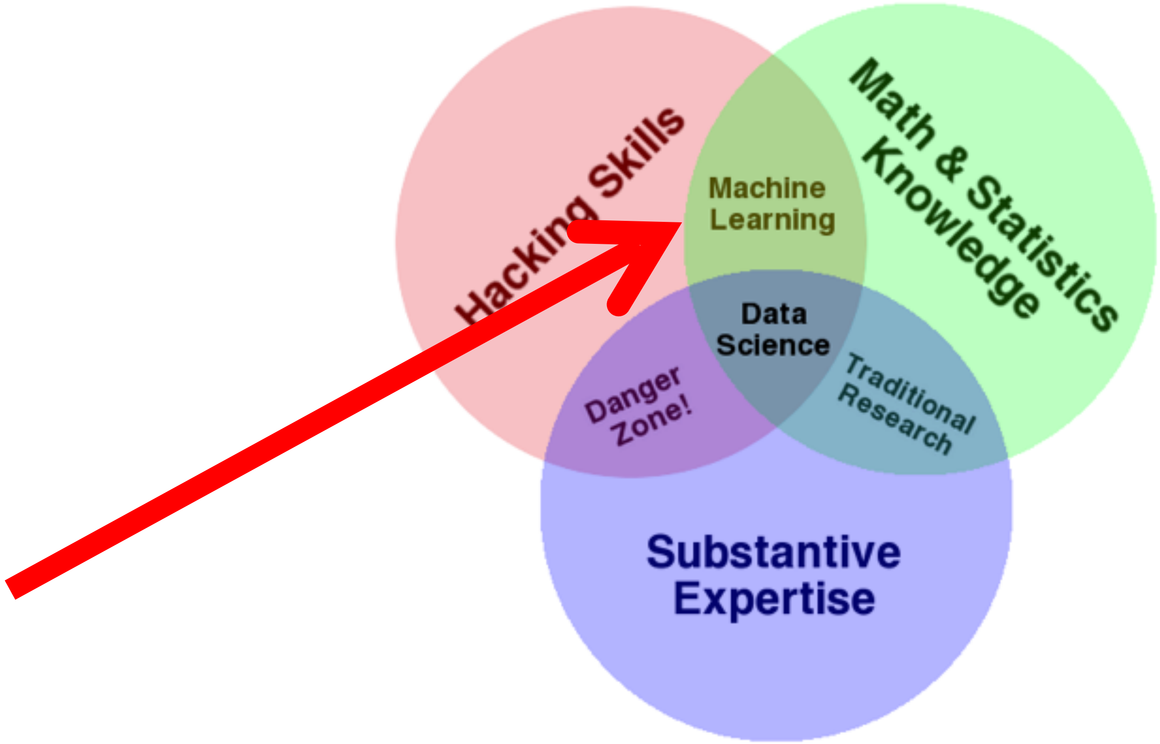
source: http://en.wikipedia.org/wiki/Machine_learning

REMEMBER THIS?



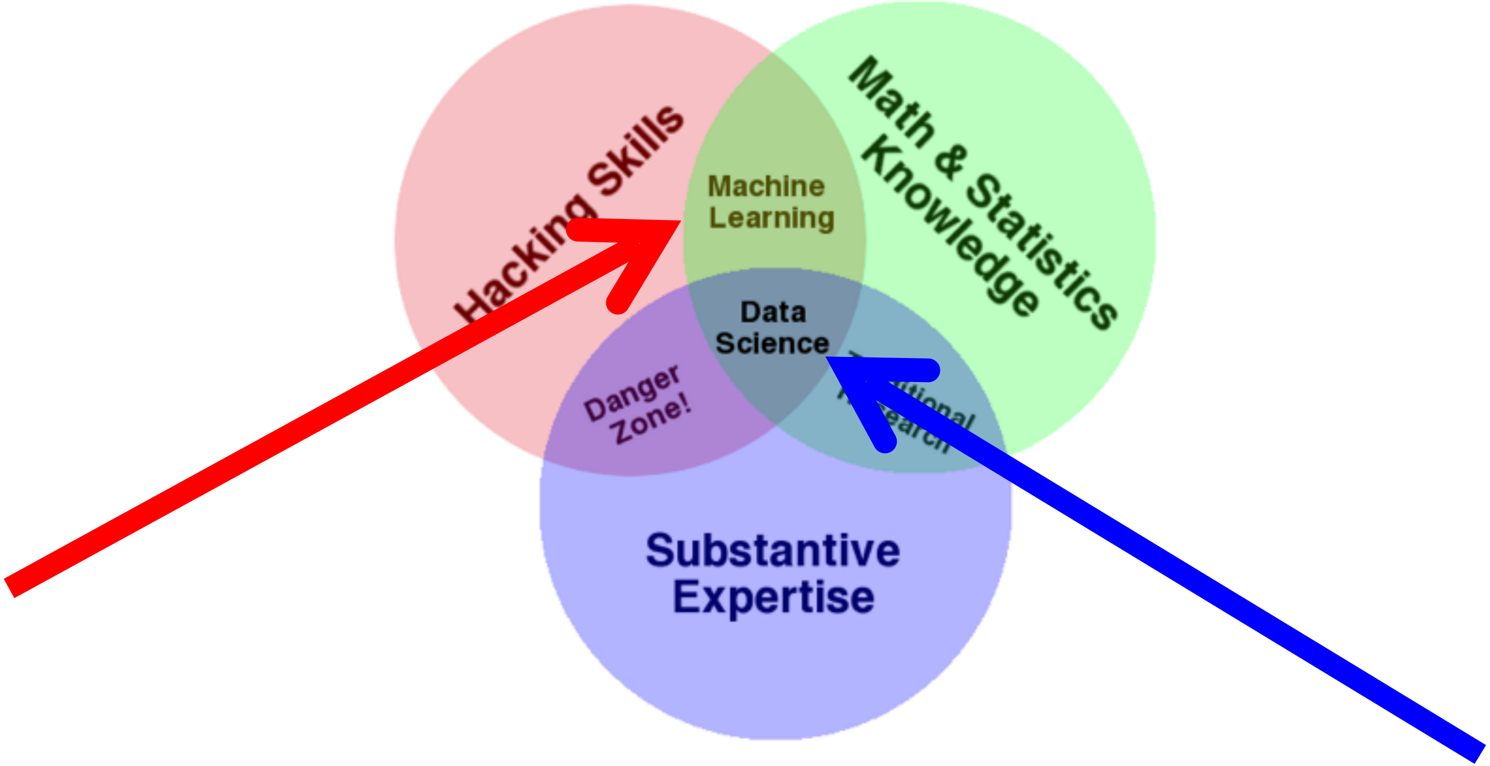
source: http://www.dataists.com/2010/09/the-data-science-venn-diagram/

WE ARE NOW HERE



source: http://www.dataists.com/2010/09/the-data-science-venn-diagram/

WE WANT TO GO HERE



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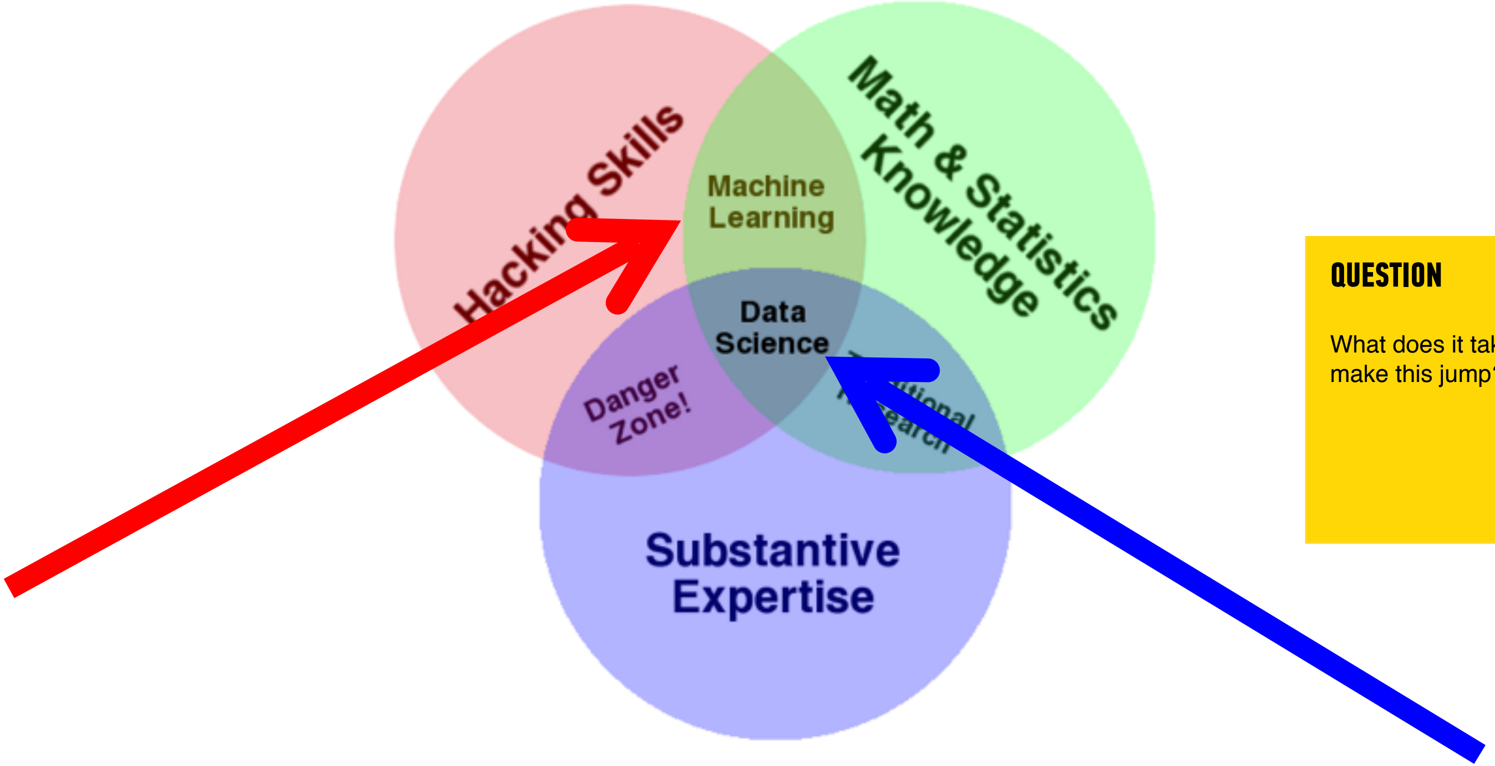
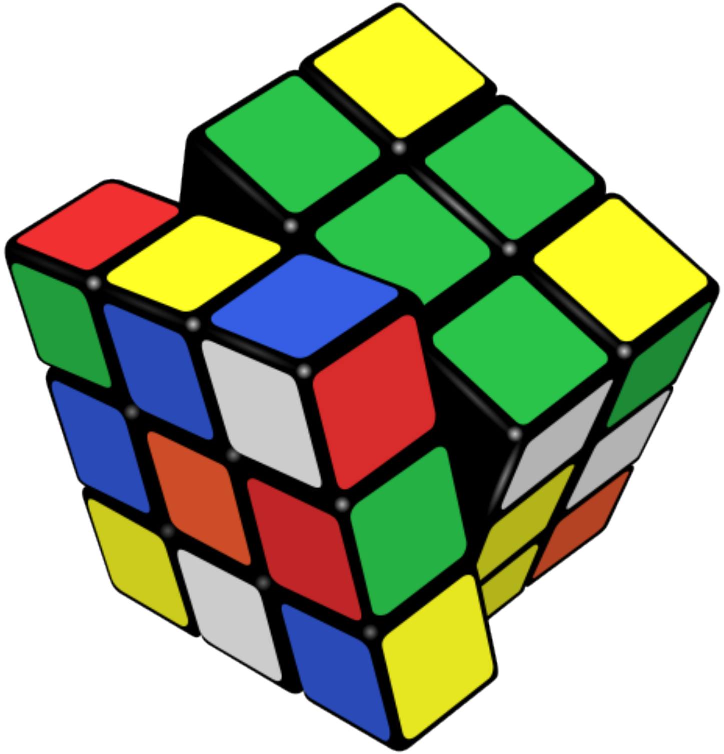


QUESTION

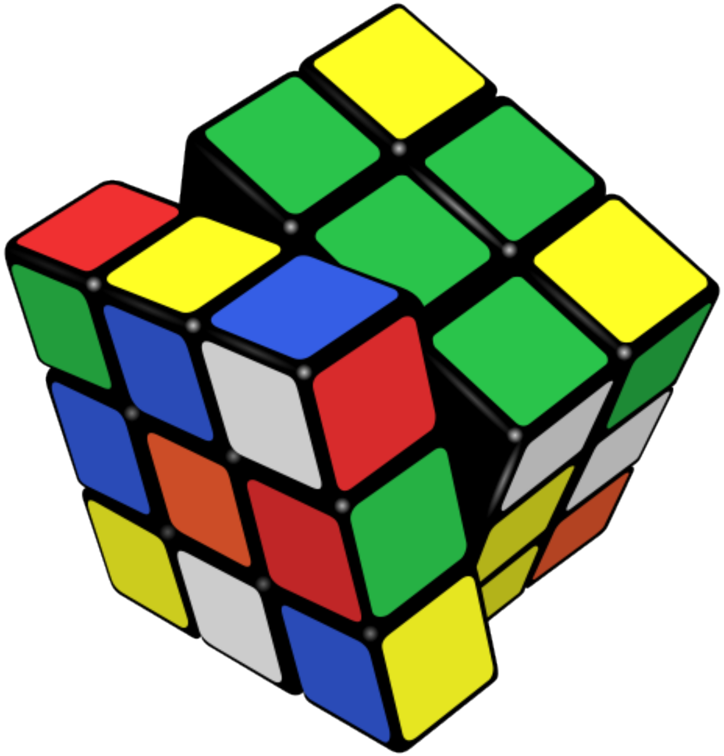
What does it take to make this jump?

source: http://www.dataists.com/2010/09/the-data-science-venn-diagram/

ANSWER: PROBLEM SOLVING!



ANSWER: PROBLEM SOLVING!



NOTE

Implementing solutions to ML problems is the focus of this course!

THE STRUCTURE OF MACHINE LEARNING PROBLEMS

supervised	*making predictions*
unsupervised	*extracting structure*

REMEMBER WHAT WE SAID BEFORE?

generalization

supervised	*making predictions*
unsupervised	*extracting structure*

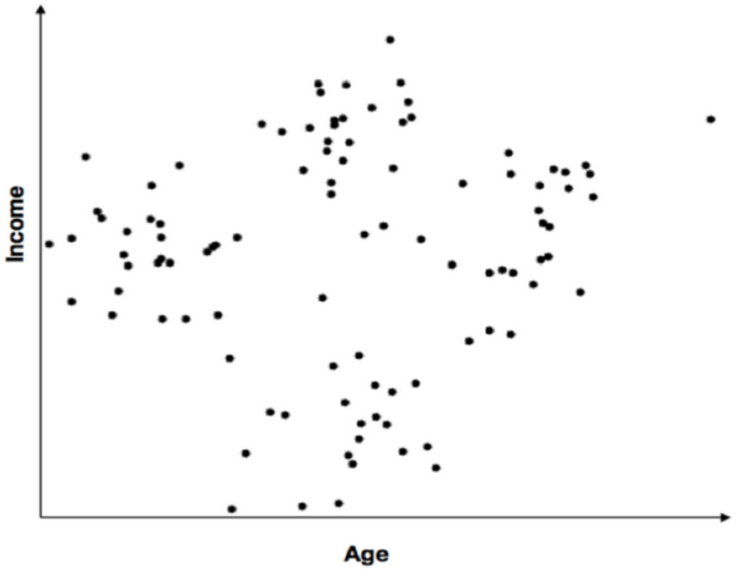
representation

Supervised Learning - Can we create a function that predicts a value based on labeled training data?

Regression example: Alan is 30 years old and can eat *four donuts an hour*. Betty is 60 years old, and can eat *two donuts an hour*. Cameron is 15 years old--how many donuts an hour eaten would be a good guess? This prediction is a regression model.

Classification example: Let' s use the same data above. What is the probability that Cameron will eat eight donuts? Here, we have an answer and am now calculating the probability that an outcome has occurred.

Unsupervised Learning - Can we find structure to unlabeled data?



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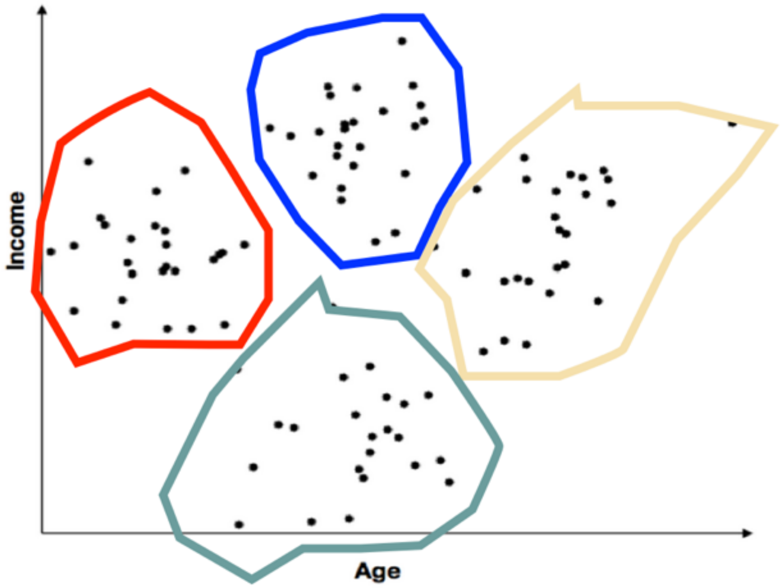

	continuous	categorical
	quantitative	qualitative

	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.

QUESTION

WHAT
IS THE
GOAL
OF
MACHINE LEARNING?

supervised	*making predictions*
unsupervised	*extracting structure*

ANSWER

The goal is determined by the type of problem.

QUESTION

HOW
DO YOU
DETERMINE
THE RIGHT
APPROACH?

	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
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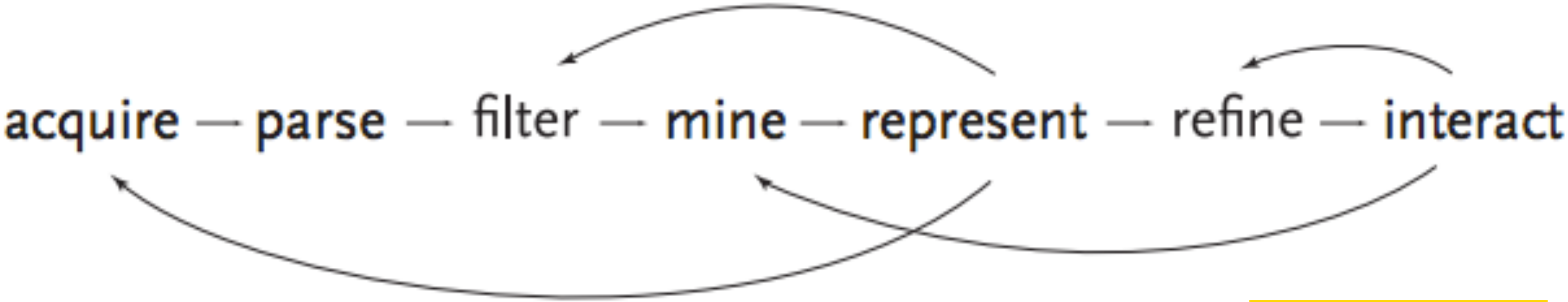
NOTE

All of this depends on your data!

QUESTION

WHAT DO YOU DO WITH YOUR RESULTS?

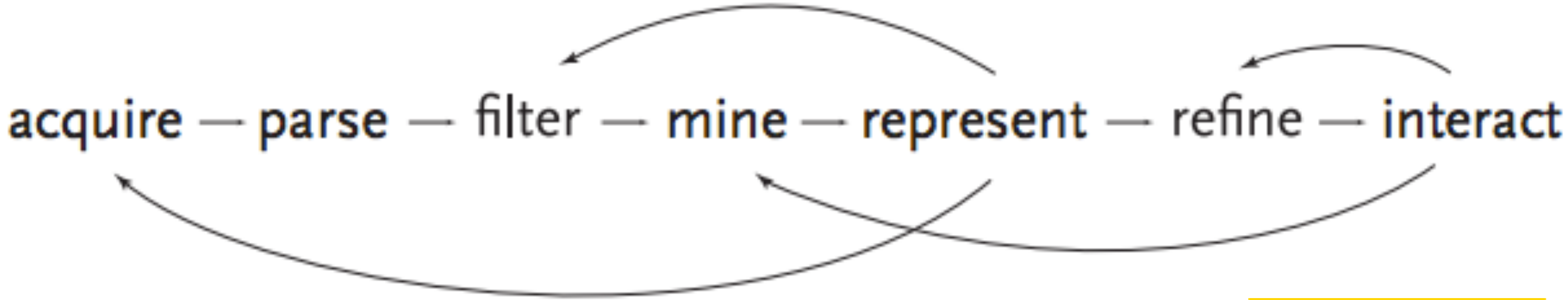


ANSWER

Interpret them and react accordingly.

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

THE DATA SCIENCE WORKFLOW



ANSWER

Int
re

NOTE

This also relies on your problem solving skills!

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

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?

Q: How does a classification problem work?

A: Data in, predicted labels out.

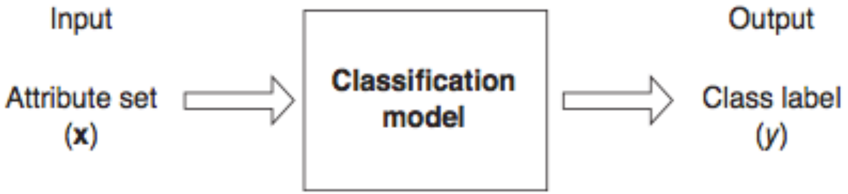
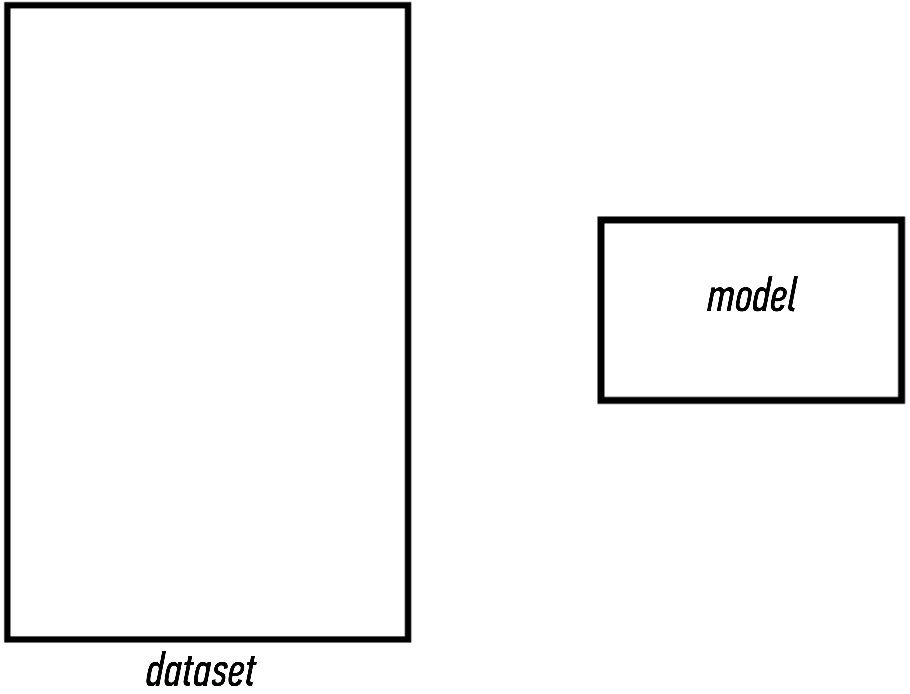


Figure 4.2. Classification as the task of mapping an input attribute set $\mathbf{x}$ into its class label y.

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

Q: What steps does a classification problem require?



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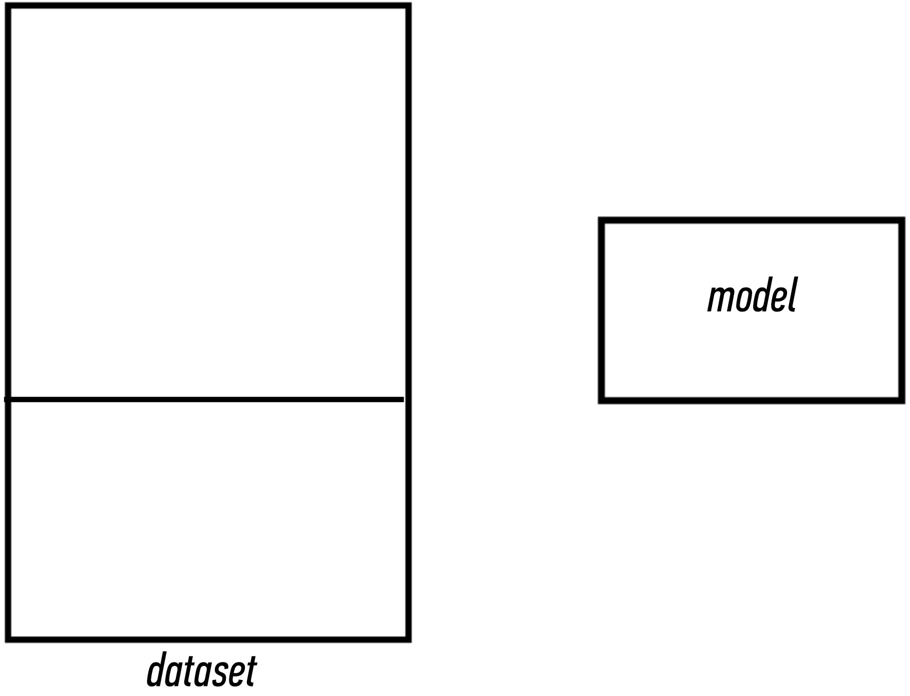
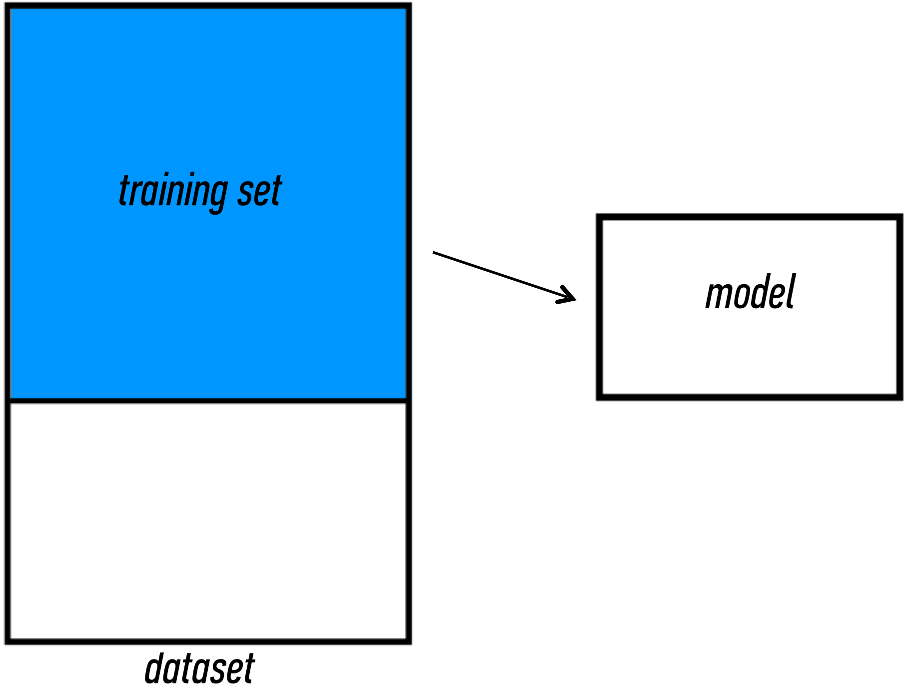


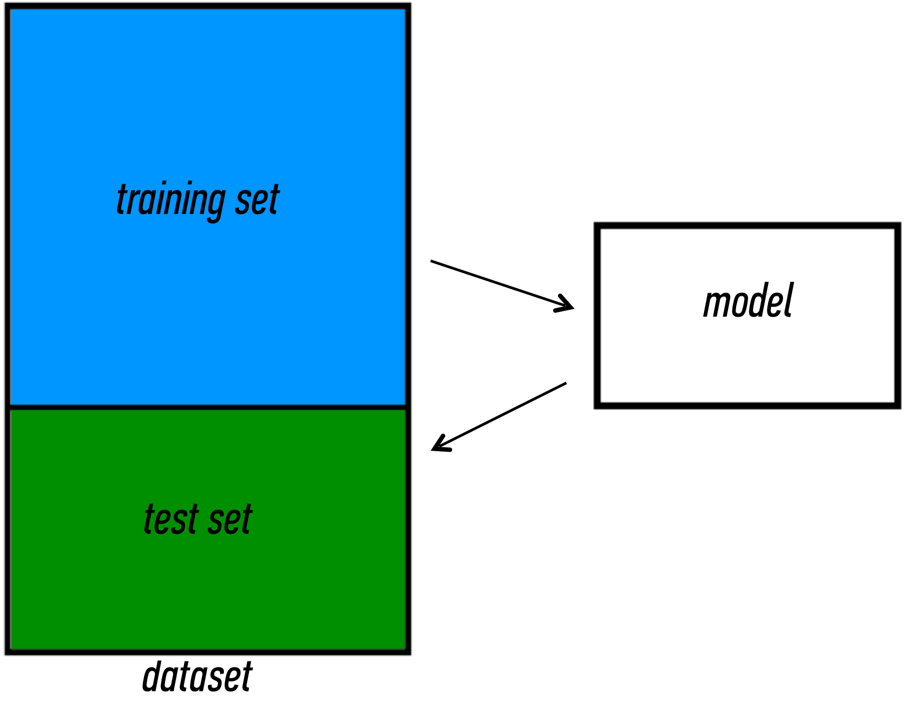
Q: What steps does a classification problem require?

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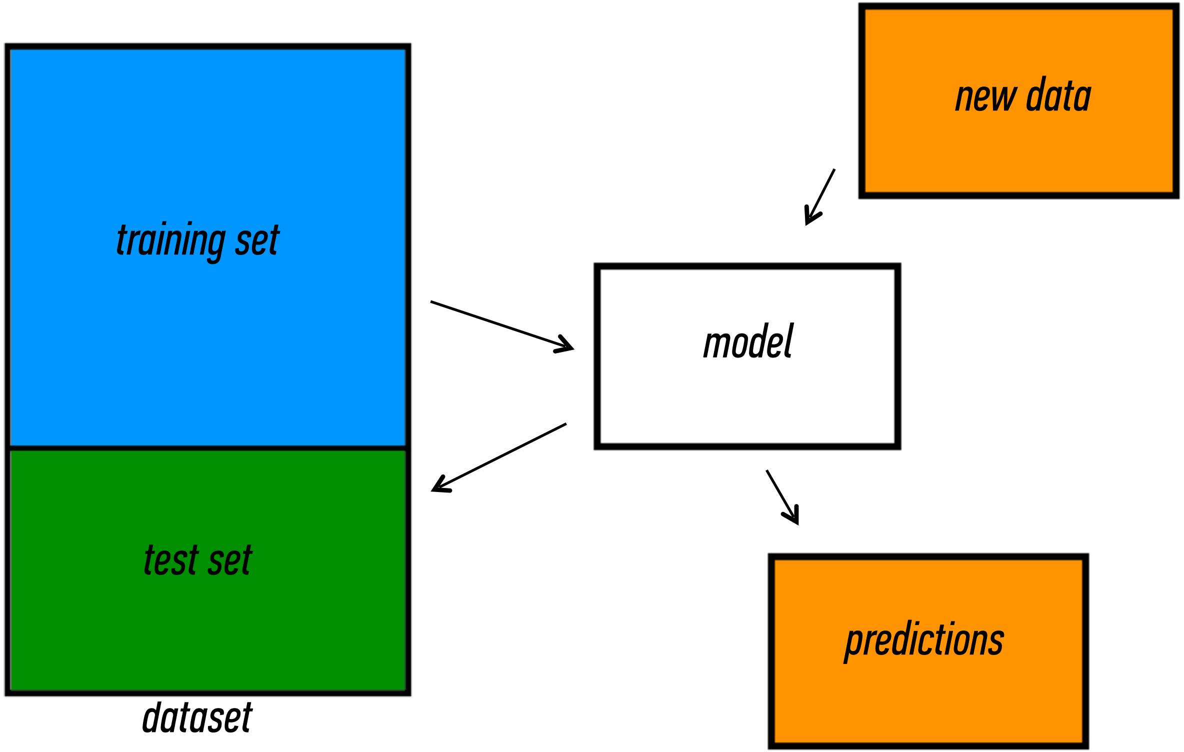
1) split dataset
2) train model
3) test model
4) make predictions



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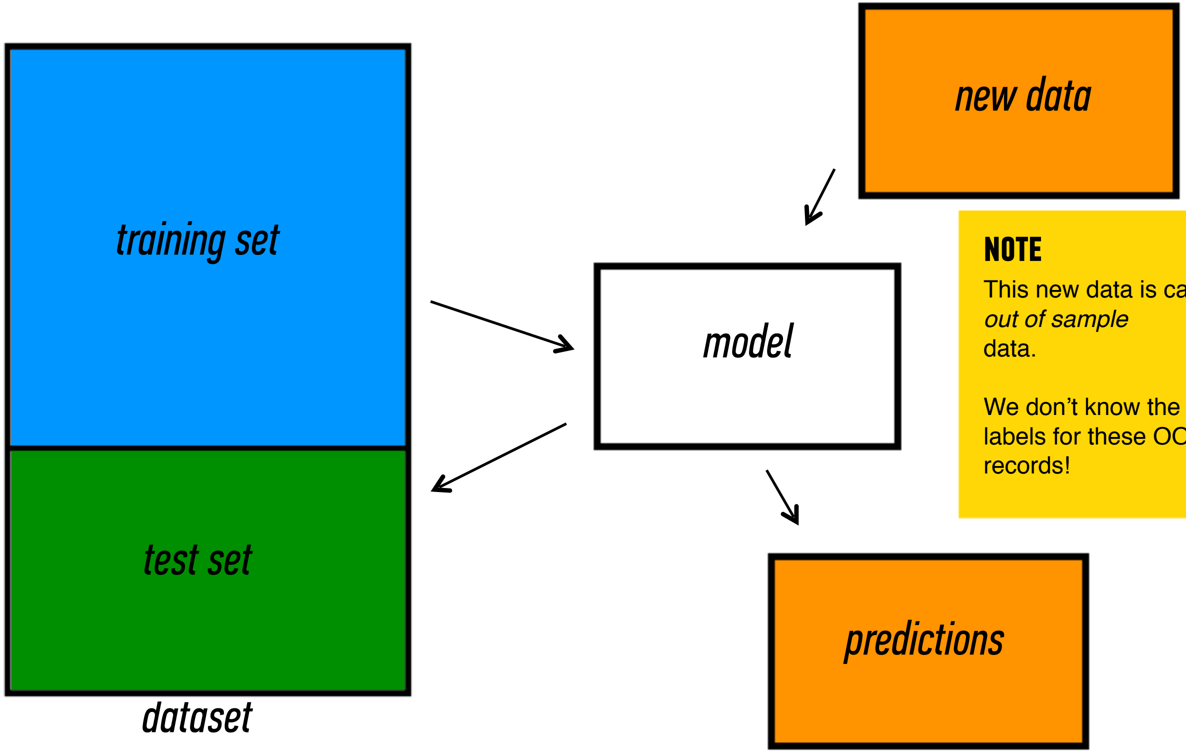
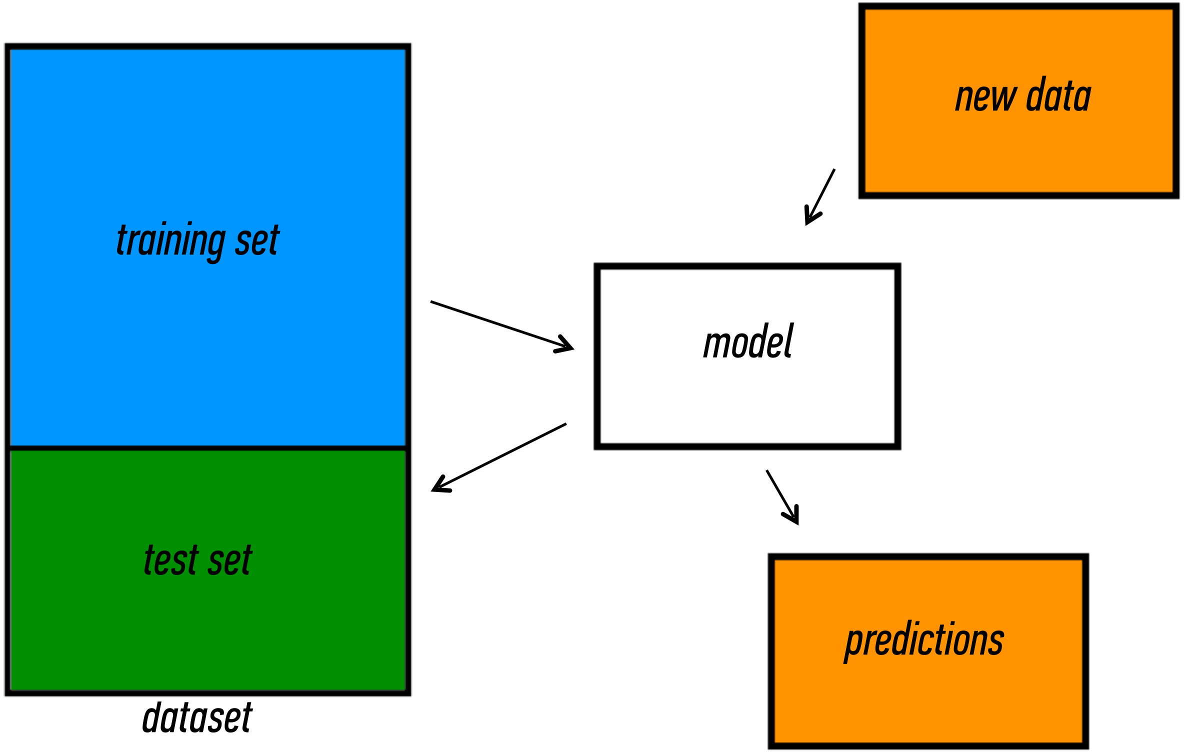


NOTE
This new data is called *out of sample* data.

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

III. BUILDING EFFECTIVE CLASSIFIERS

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



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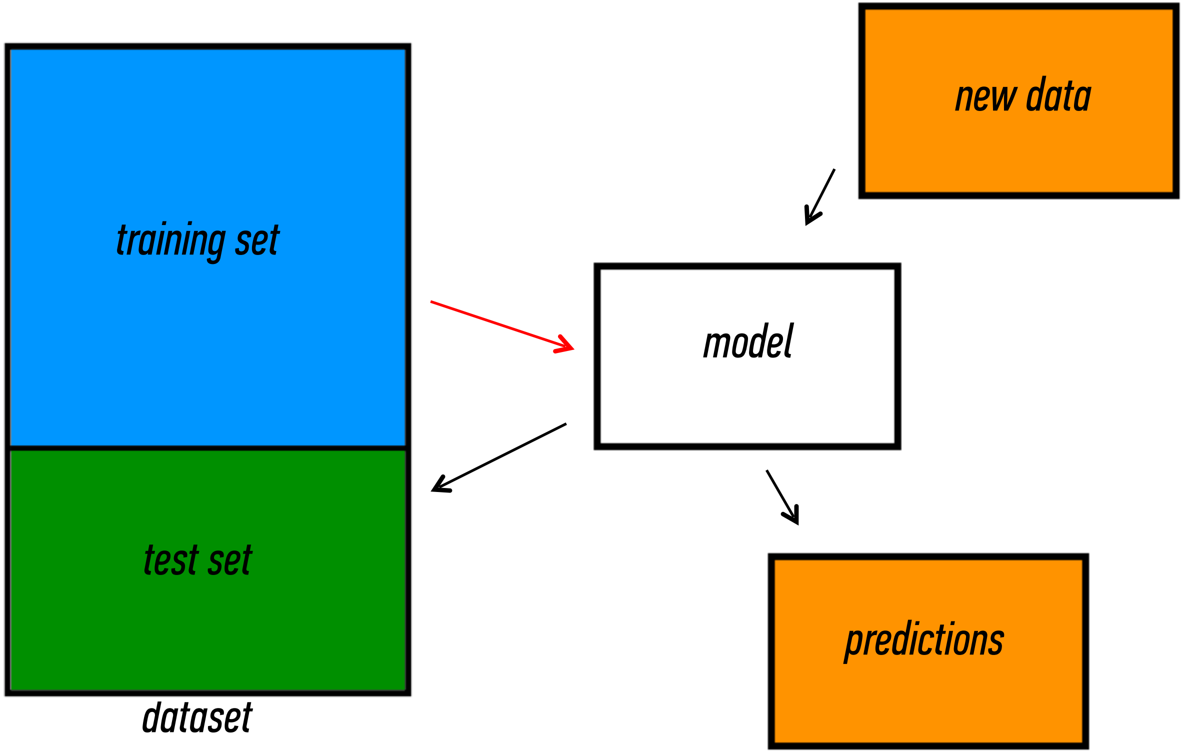

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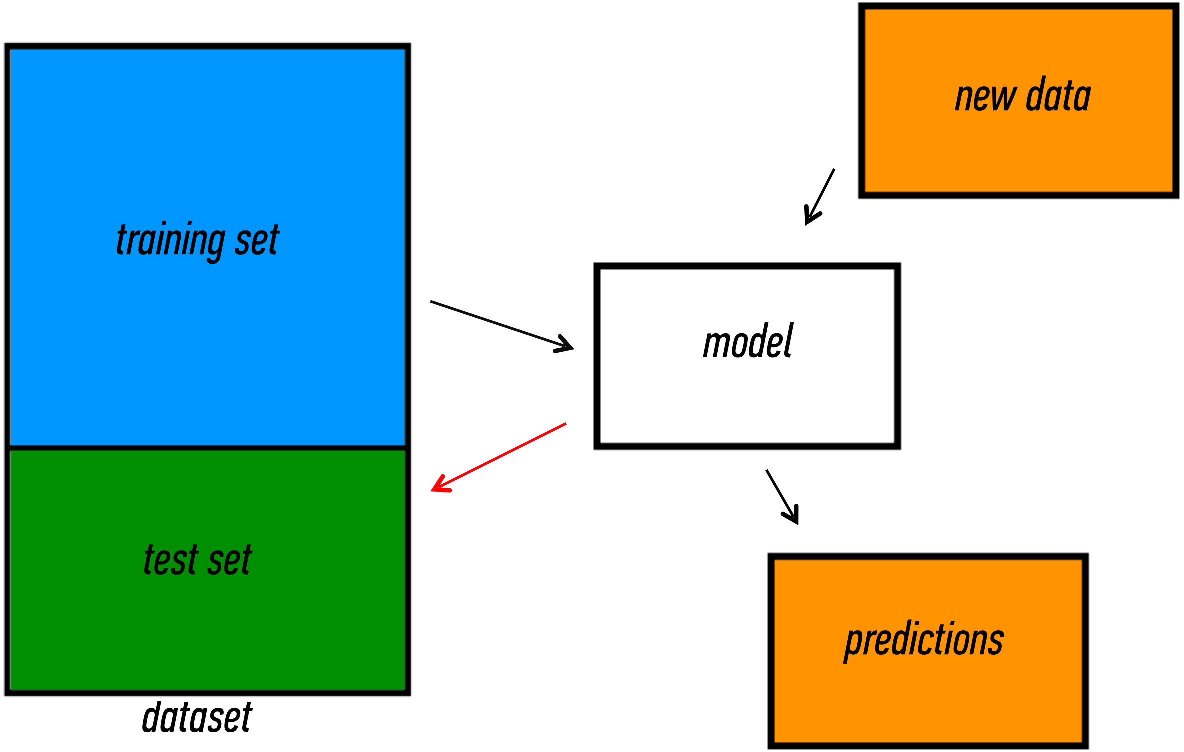
1) training error
2) generalization error



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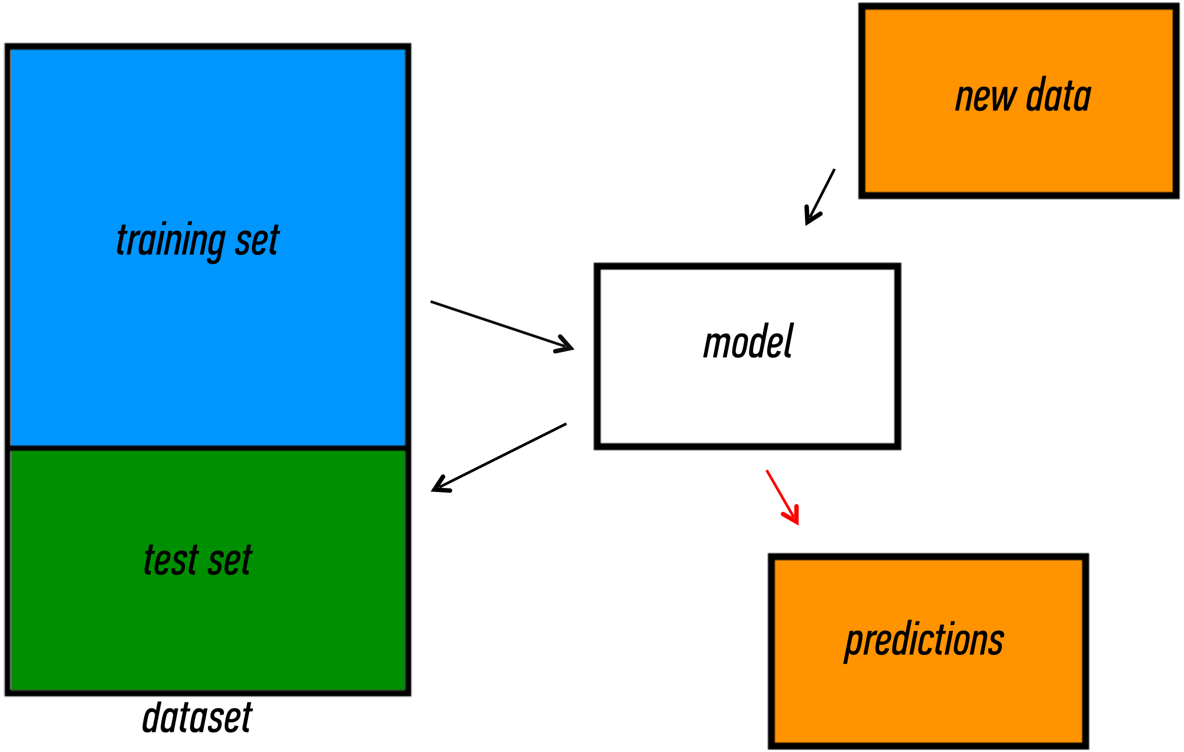
3) OOS error



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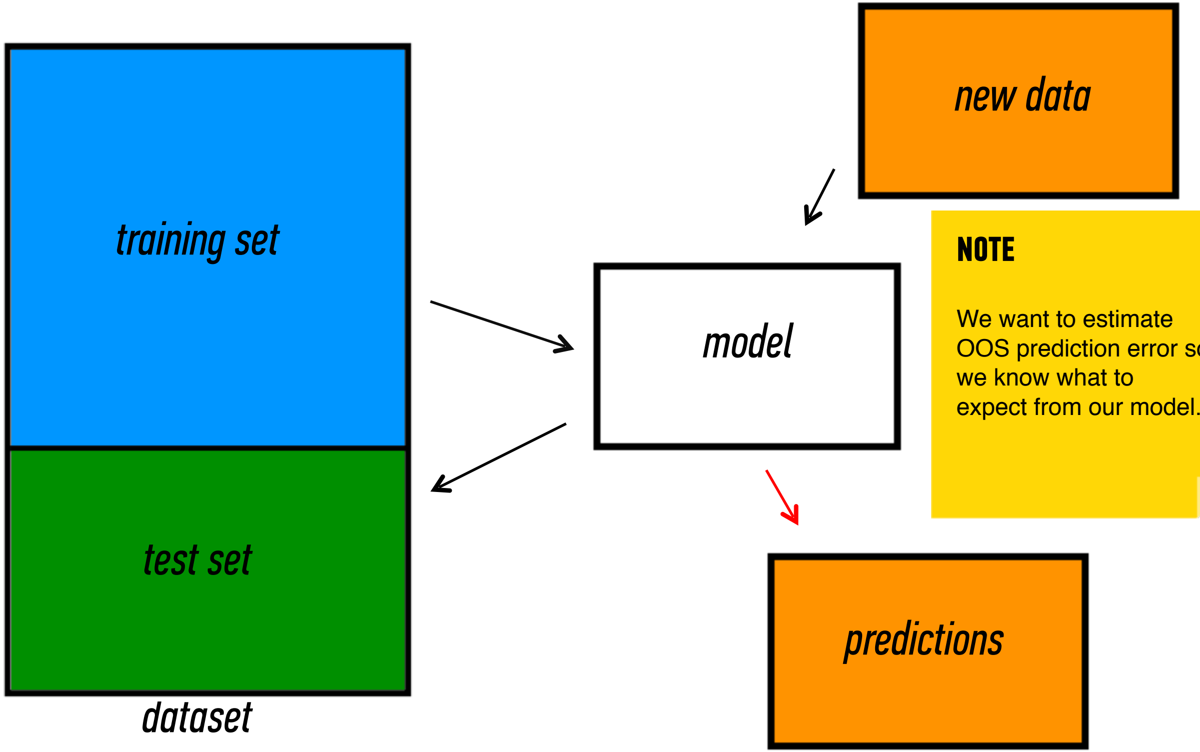

NOTE

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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NOTE

This phenomenon is called *overfitting*.

OVERFITTING

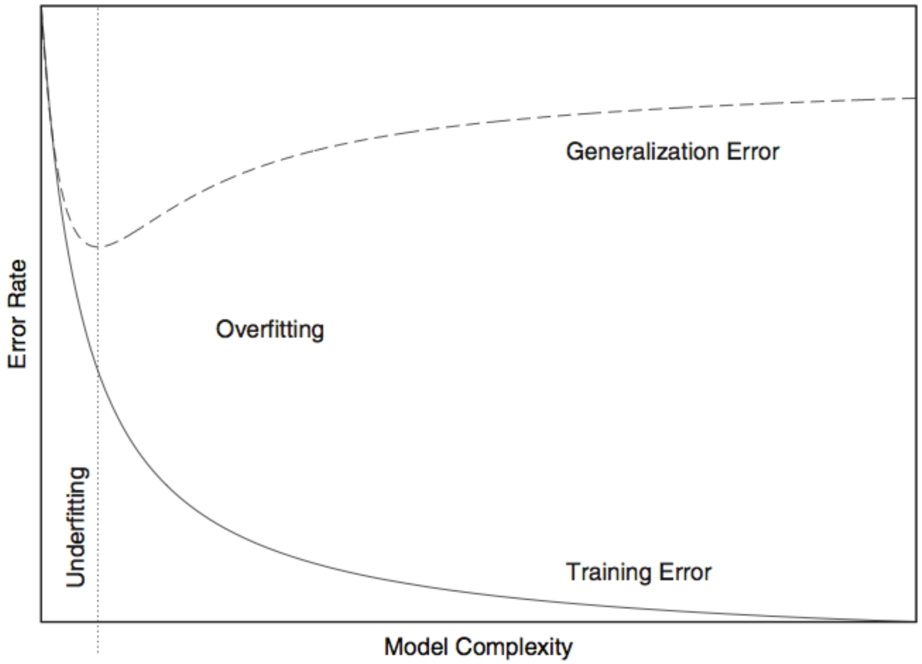
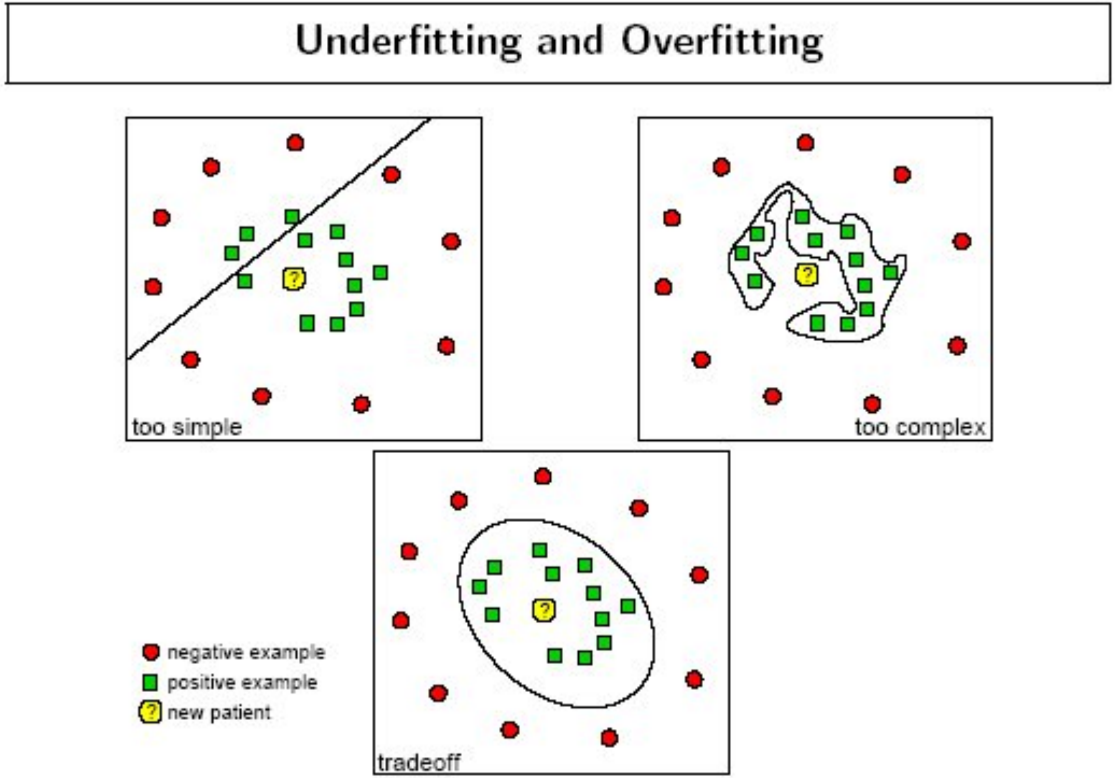


FIGURE 18-1. Overfitting: as a model becomes more complex, it becomes increasingly able to represent the training data. However, such a model is overfitted and will not generalize well to data that was not used during training.

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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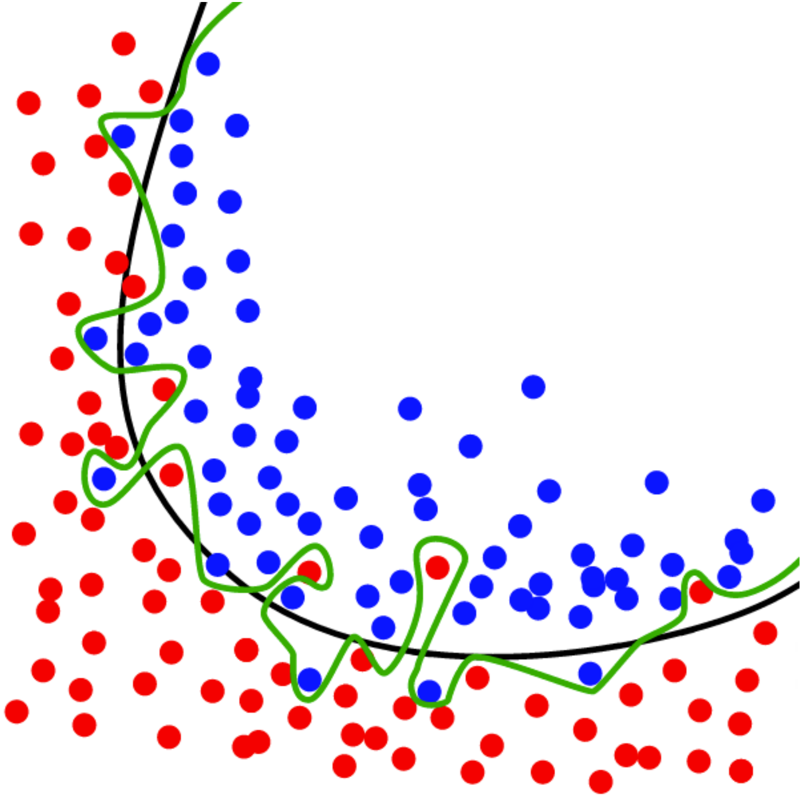

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This phenomenon is called *overfitting*.

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: On its own, not very well.

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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!

Something is still missing!

Q: How can we do better?

Something is still missing!

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Thought experiment:

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

Something is still missing!

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A: Now you're talking!

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A: Cross-validation.

Steps for n-fold cross-validation:

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1) *Randomly split the dataset into n equal partitions.*

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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:

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1) *More accurate estimate of OOS prediction error.*

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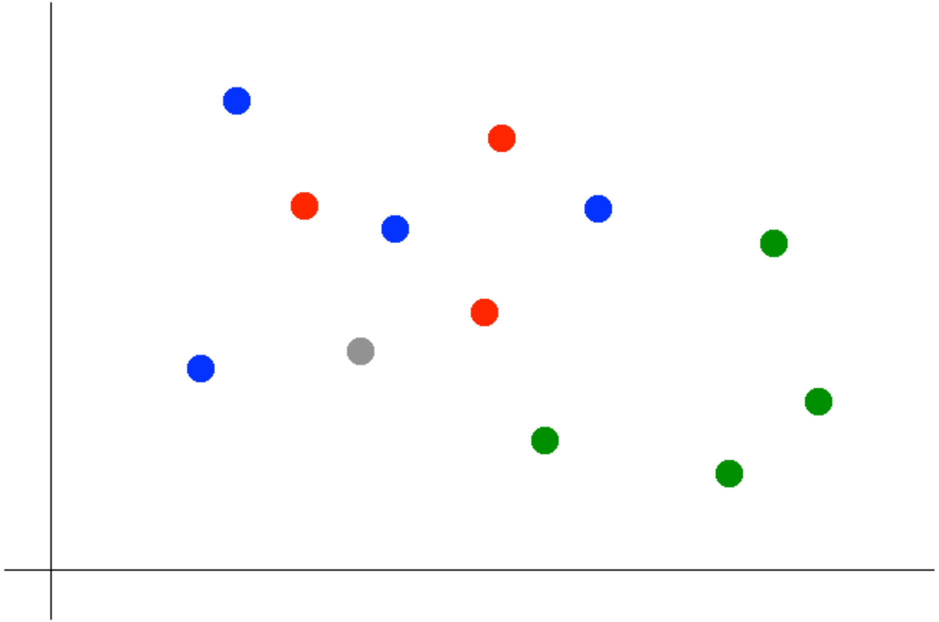
   - *Each record in our dataset is used for both training and testing.*
3) *Presents tradeoff between efficiency and computational expense.*
   - *10-fold CV is 10x more expensive than a single train/test split*
4) *Can be used for model selection.*

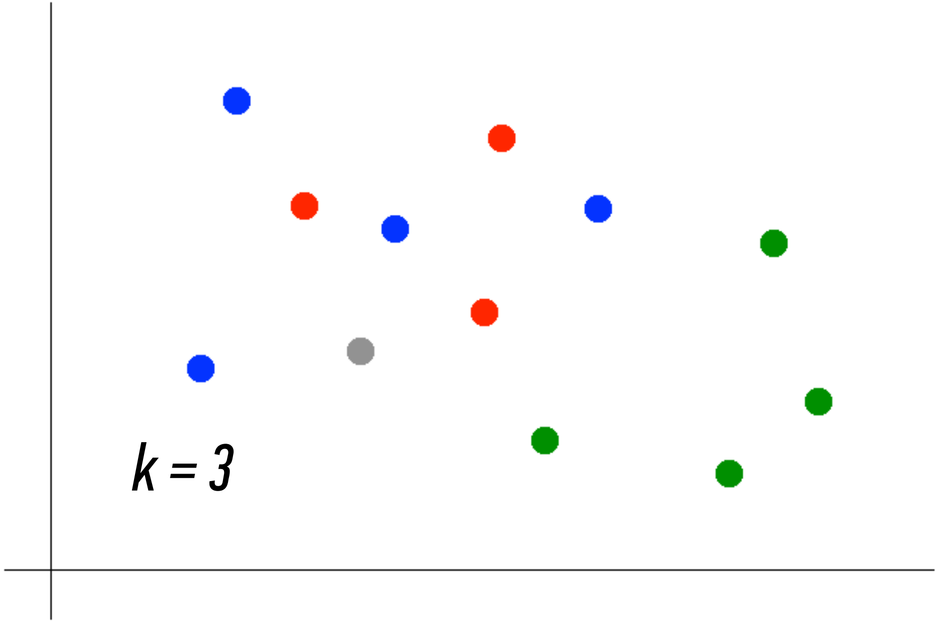
IV. KNN CLASSIFICATION

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



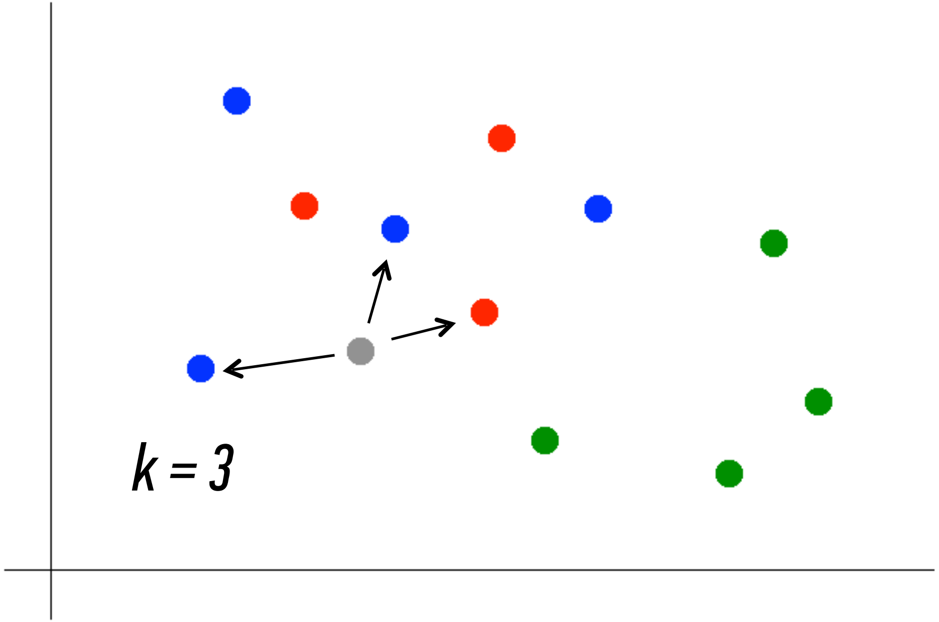
Suppose we want to predict the color of the grey dot.

1) *Pick a value for k.*



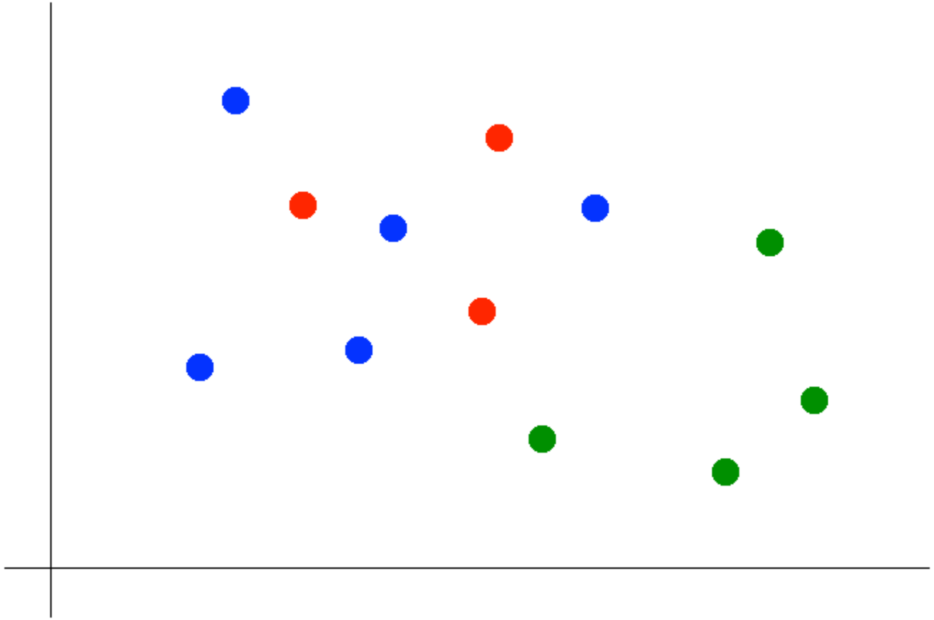
Suppose we want to predict the color of the grey dot.

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.*



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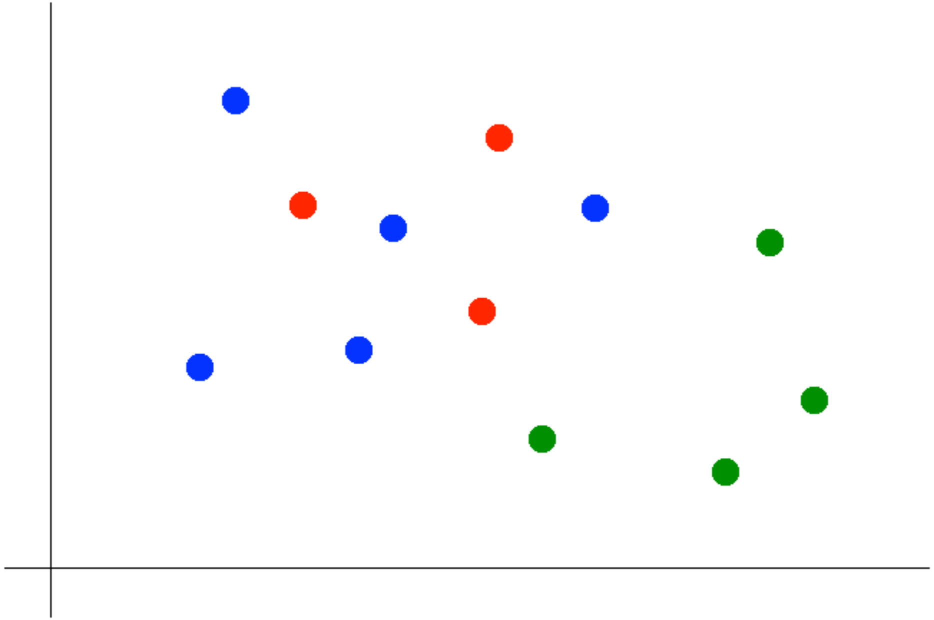
1) Pick a value for k.
2) Find colors of k nearest neighbors.
3) Assign the most common color to the grey dot.



OPTIONAL NOTE

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

LABS