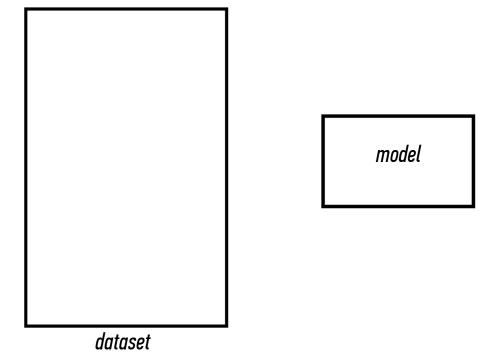
# INTRO TO DATA SCIENCE CROSS-VALIDATION

# Q: What steps does a classification problem require?



Q: What steps does a classification problem require?

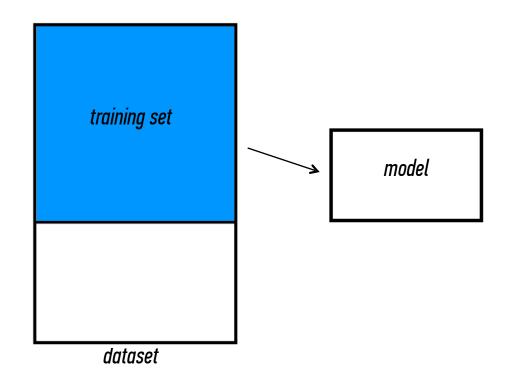
1) split dataset



model

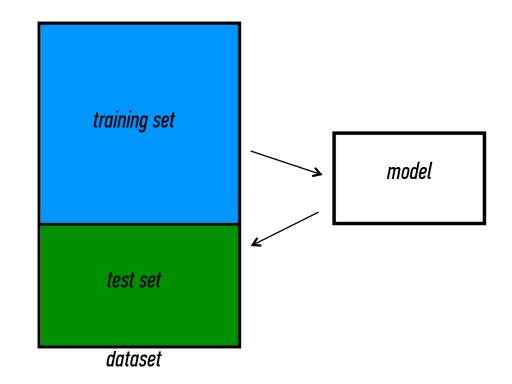
dataset

- Q: What steps does a classification problem require?
  - 1) split dataset
- 2) train model



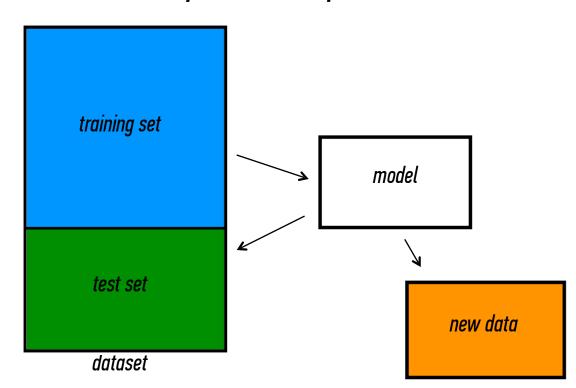
## Q: What steps does a classification problem require?

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



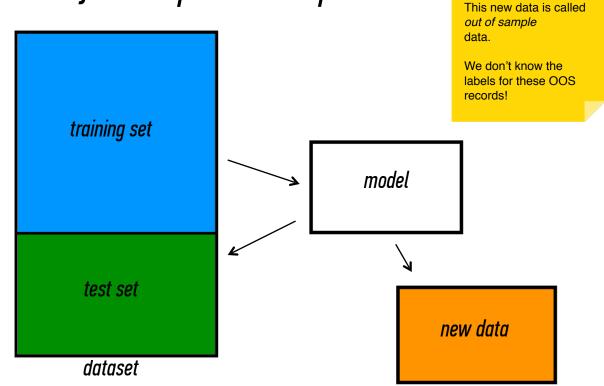
## Q: What steps does a classification problem require?

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



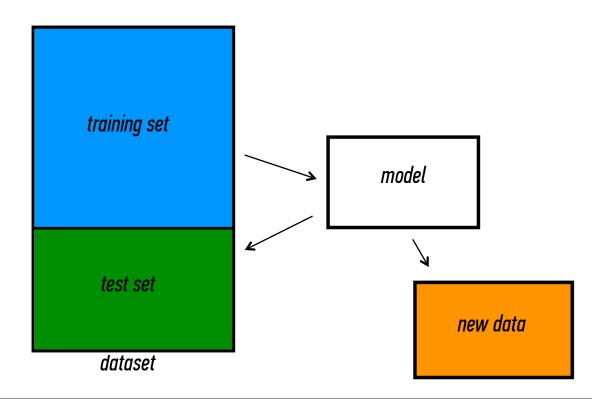
# Q: What steps does a classification problem require?

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



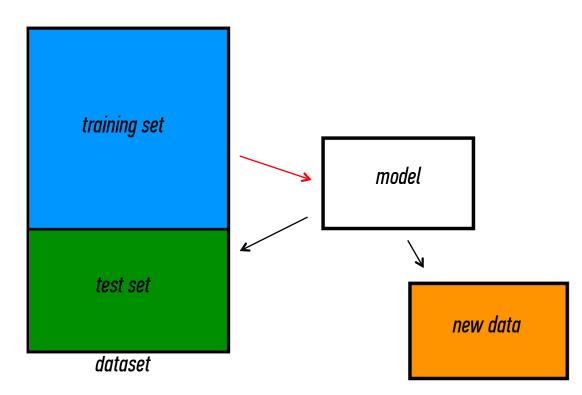
NOTE

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

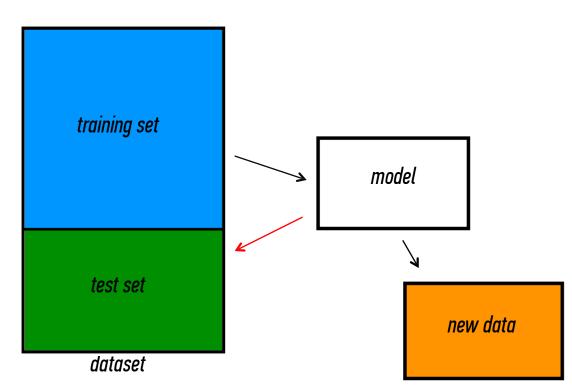


Q: What types of prediction error will we run into?

1) training error

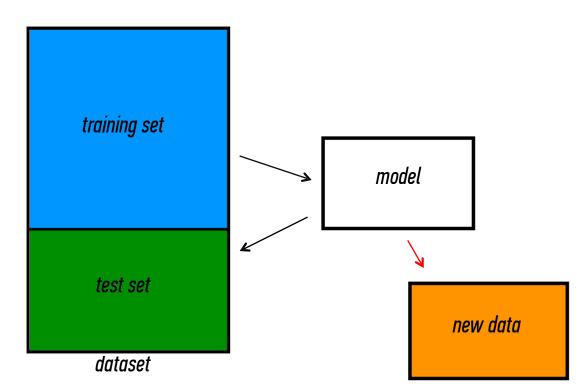


- Q: What types of prediction error will we run into?
  - 1) training error
- 2) generalization error



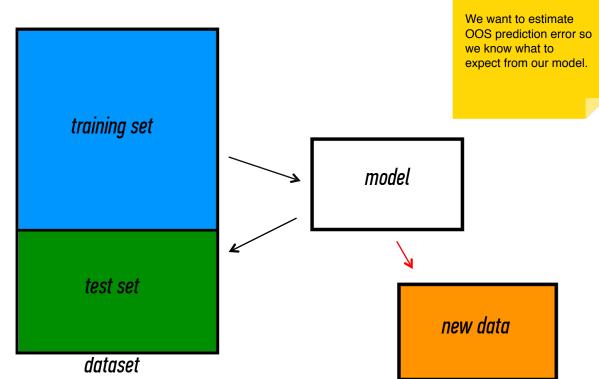
## Q: What types of prediction error will we run into?

- 1) training error
- 2) generalization error
- *3) 00S error*



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

- 1) training error
- 2) generalization error
- *3) 00S error*



NOTE

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**

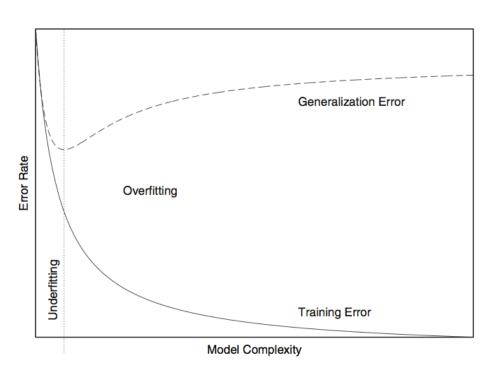
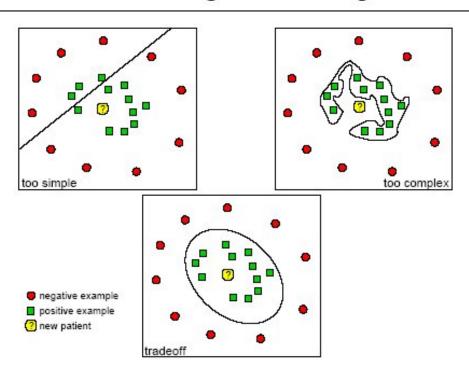


FIGURE 18-1. Overfitting: as a model becomes more complex, it becomes increasingly able to represent the training data. However, such a model is overfitted and will not generalize well to data that was not used during training.

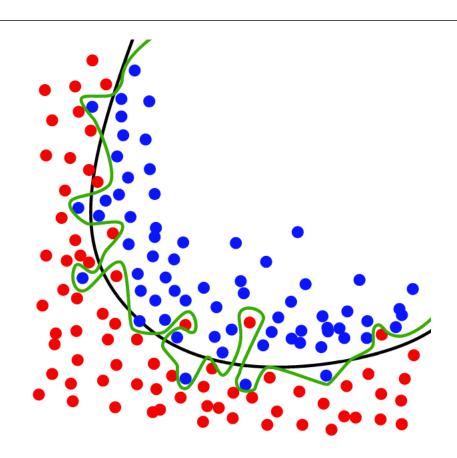
source: Data Analysis with Open Source Tools, by Philipp K. Janert. O'Reilly Media, 2011.

#### **OVERFITTING - EXAMPLE**

## **Underfitting and Overfitting**



#### **OVERFITTING - EXAMPLE**



# 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 phenomenor 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?

Q: How well does generalization error predict OOS accuracy? Thought experiment:

Suppose we had done a different train/test split.

Q: How well does generalization error predict 00S accuracy?

Thought experiment:

Suppose we had done a different train/test split.

Q: Would the generalization error remain the same?

Q: How well does generalization error predict 00S accuracy?

Thought experiment:

Suppose we had done a different train/test split.

Q: Would the generalization error remain the same?

A: Of course not!

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 00S 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!

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:

1) Randomly split the dataset into n equal partitions.

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

- 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.

- 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.

- 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:

1) More accurate estimate of 00S prediction error.

- 1) More accurate estimate of 00S 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.

- 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

- 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.