GENERAL ASSEMBLY

INTRO TO DATA SCIENCE

CLASS 5: MODEL EVALUATION

LAST TIME:

- INTRO TO MACHINE LEARNING
- OVERVIEW OF K NEAREST NEIGHBORS

QUESTIONS?

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WHAT WAS THE MOST INTERESTING THING YOU LEARNED?

WHAT WAS THE HARDEST TO GRASP?

AGENDA

I. QUICK REVIEW OF CLASSIFICATION PROBLEMS
II. ERRORS, UNDERFITTING & OVERFITTING
III. CROSS VALIDATION

IV. LAB: CROSS VALIDATION IN SCIKIT-LEARN

I. QUICK REVIEW OF 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*
4.6	3.4	1.4	0.3	*I. setosa*
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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?

A: Data in, predicted labels out.

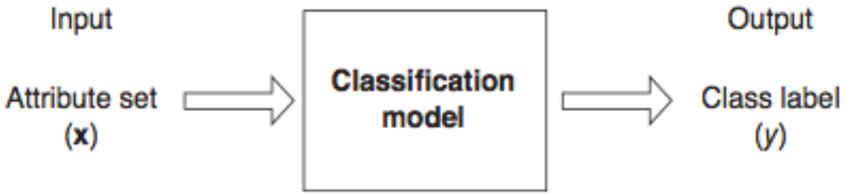
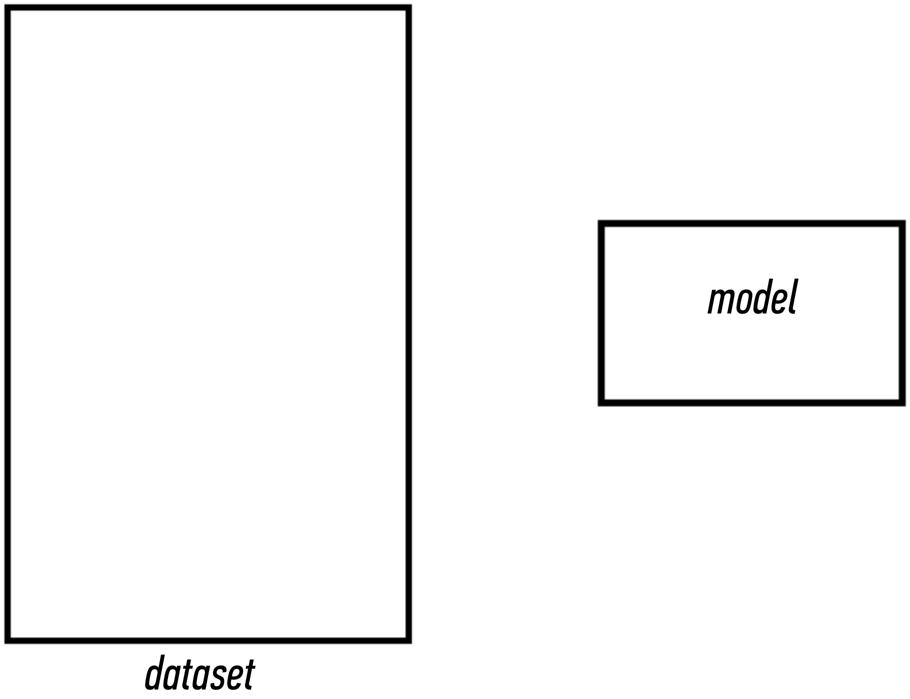


Figure 4.2. Classification as the task of mapping an input attribute set $\mathbf{x}$ into its class label y.

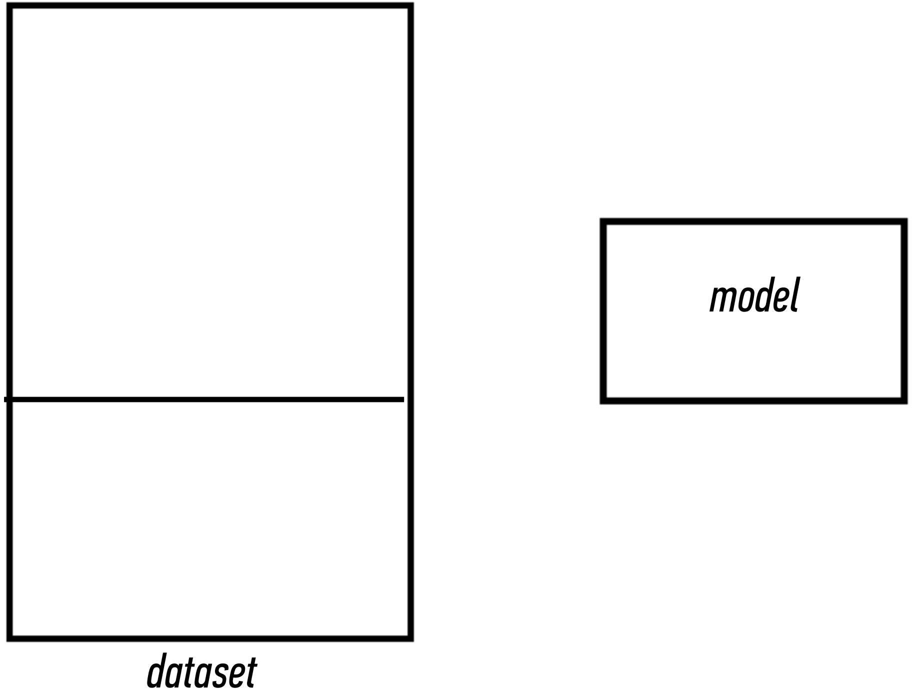
source: http://www-users.cs.umn.edu/~kumar/dmbook/ch4.pdf

Q: What steps does a classification problem require?



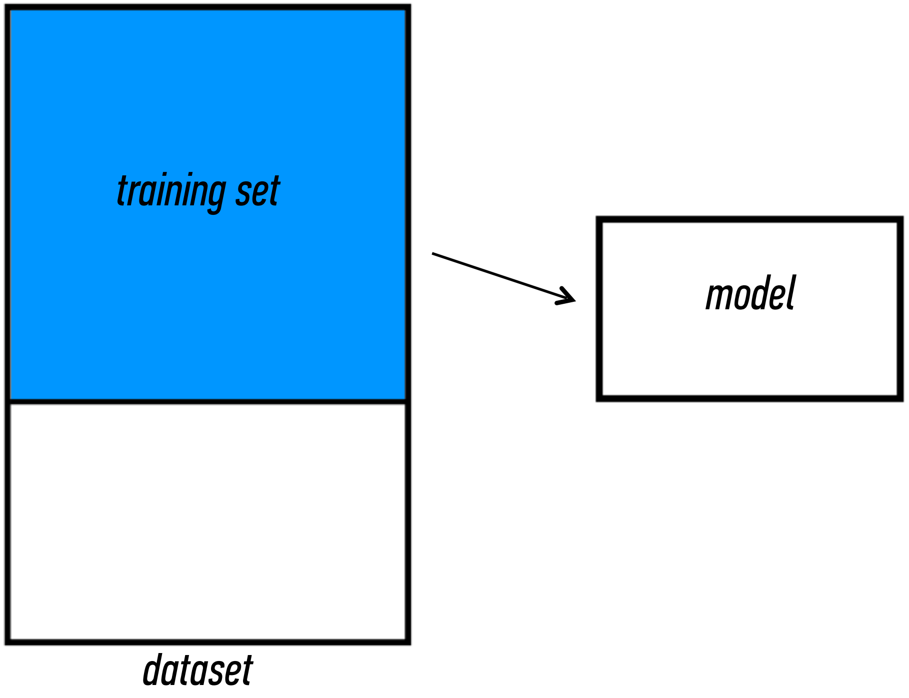
Q: What steps does a classification problem require?

1) *split dataset*



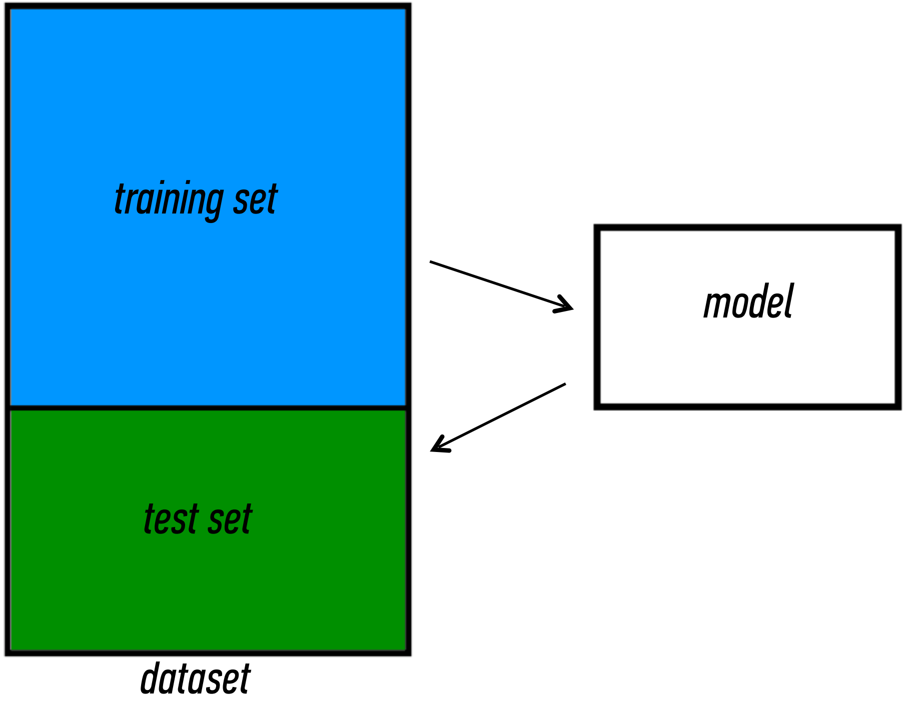
Q: What steps does a classification problem require?

1) split dataset
2) train model



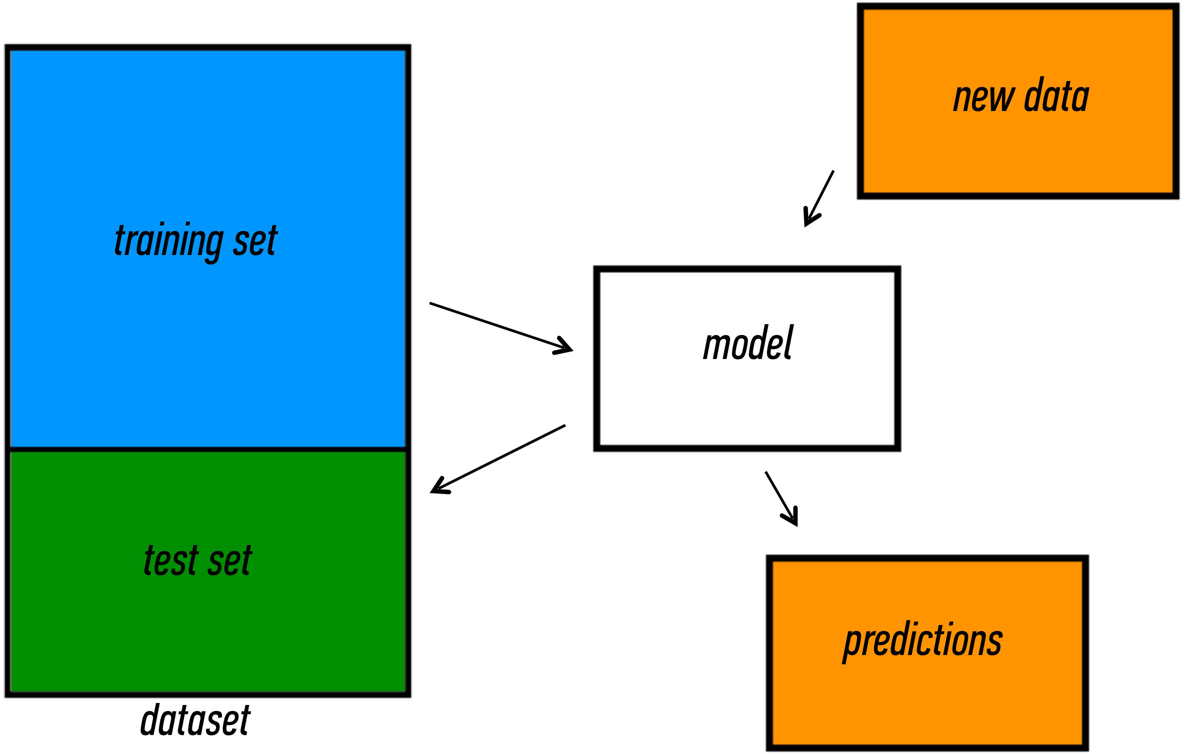
Q: What steps does a classification problem require?

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



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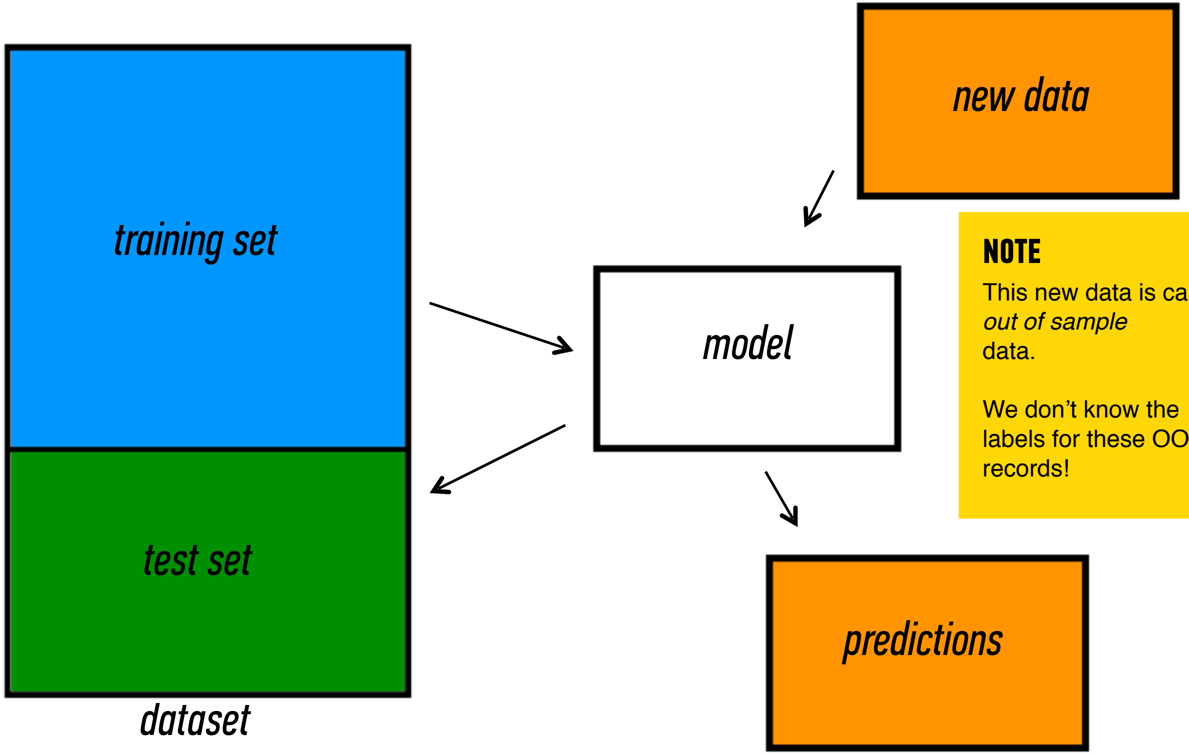
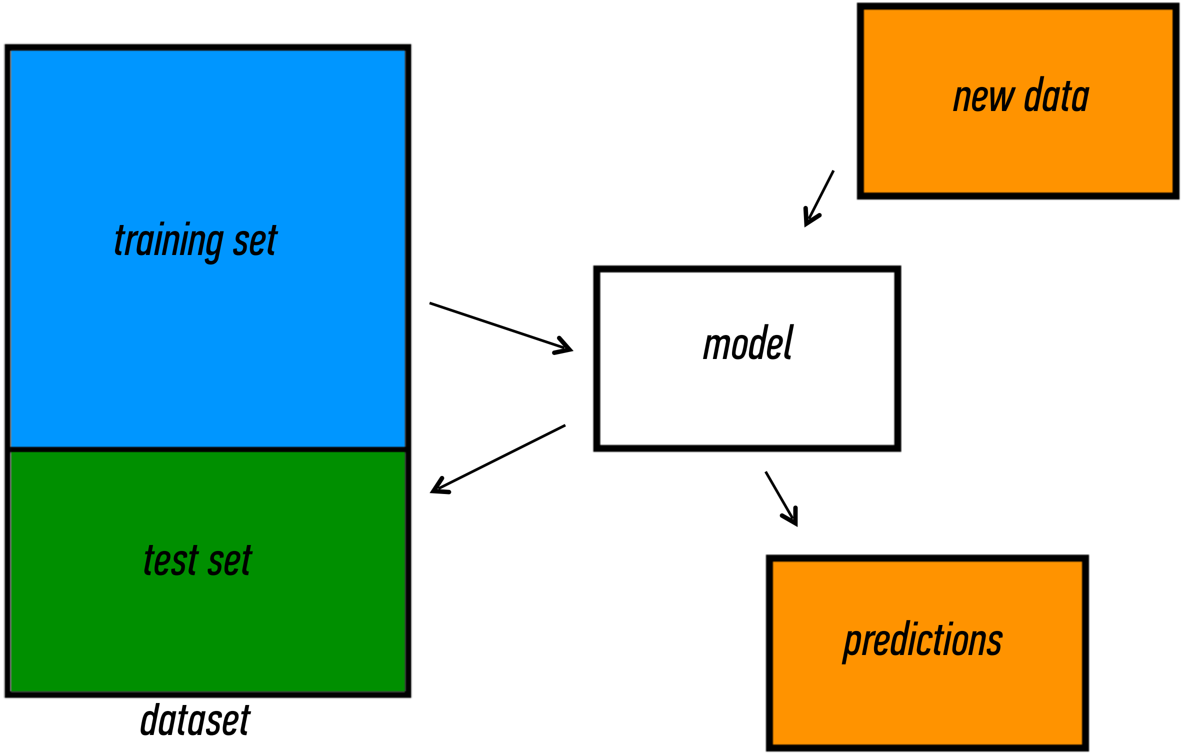


NOTE
This new data is called *out of sample* data.

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

II. ERRORS, UNDERFITTING & OVERFITTING

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



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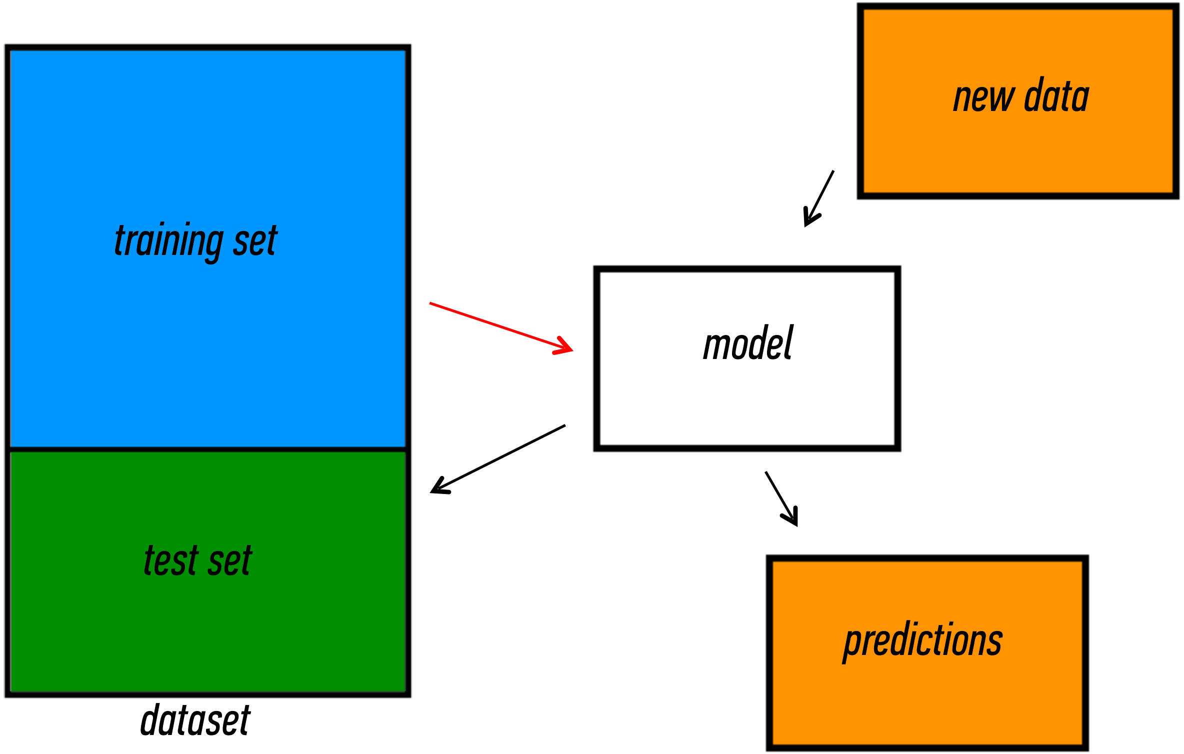

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1) training error
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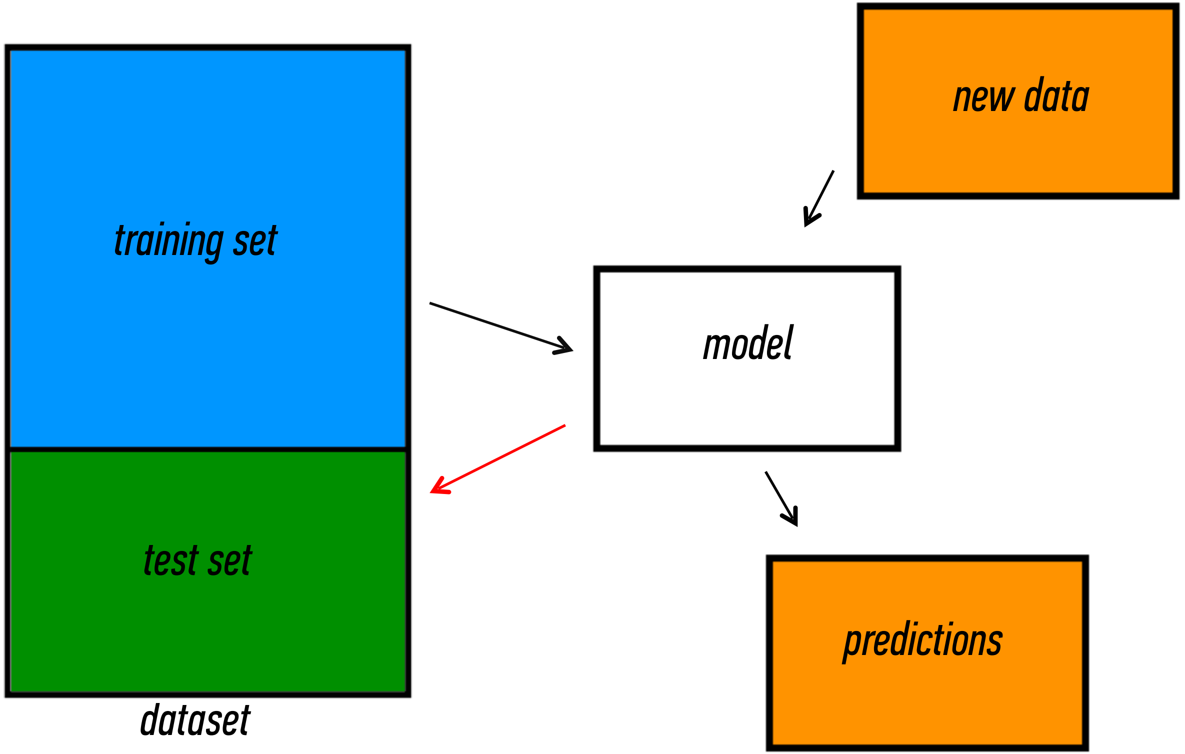
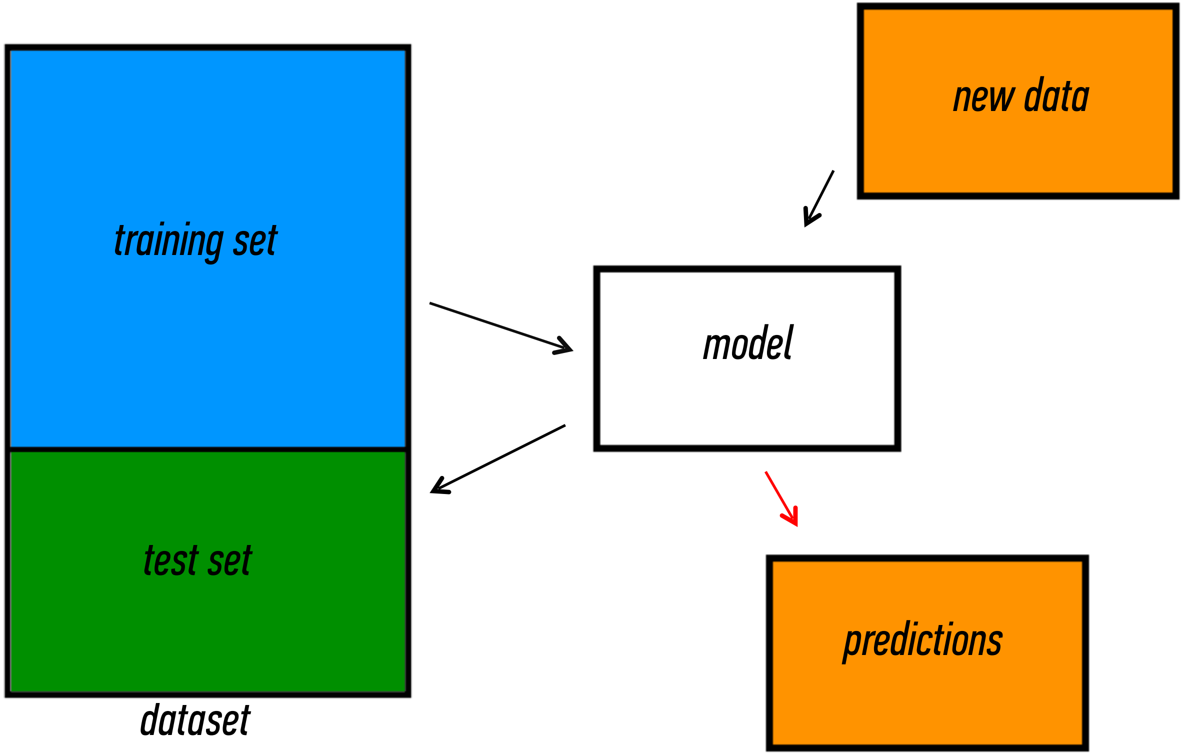


Q: What types of prediction error will we run into?

1) training error
2) generalization error
3) OOS error



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

1) *training error*
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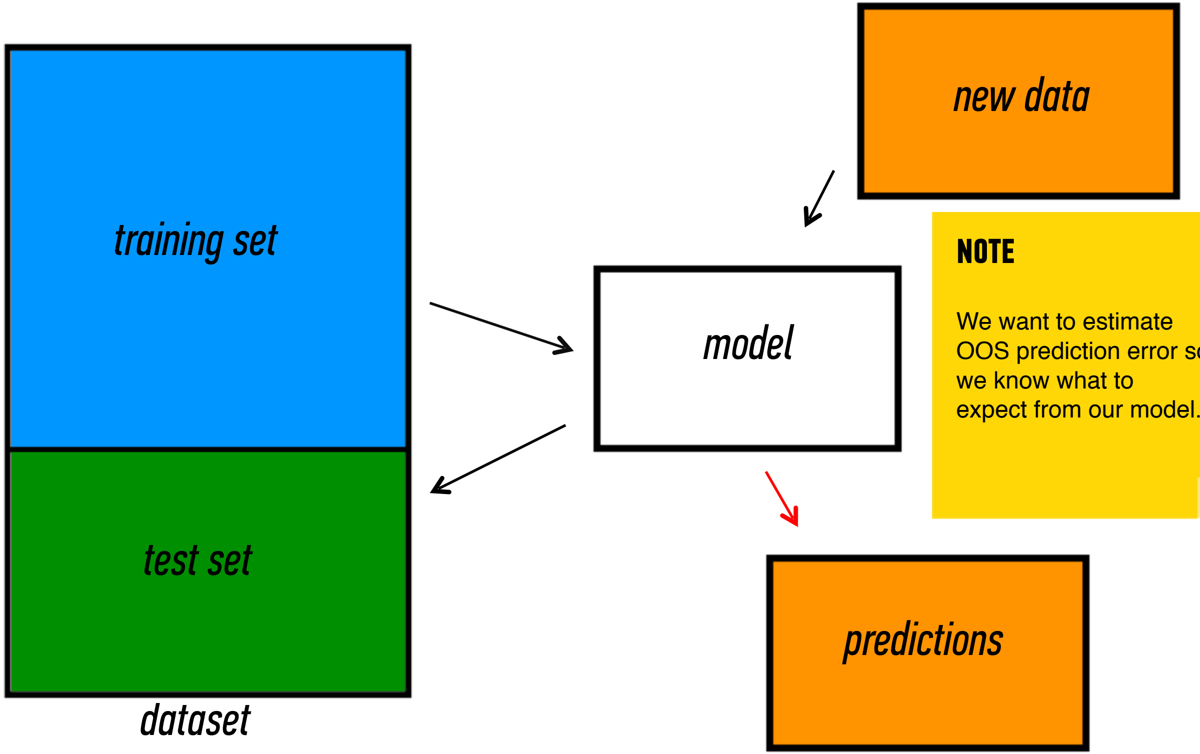
3) *OOS error*



NOTE

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

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Thought experiment:
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NOTE

This phenomenon is called *overfitting*.

OVERFITTING

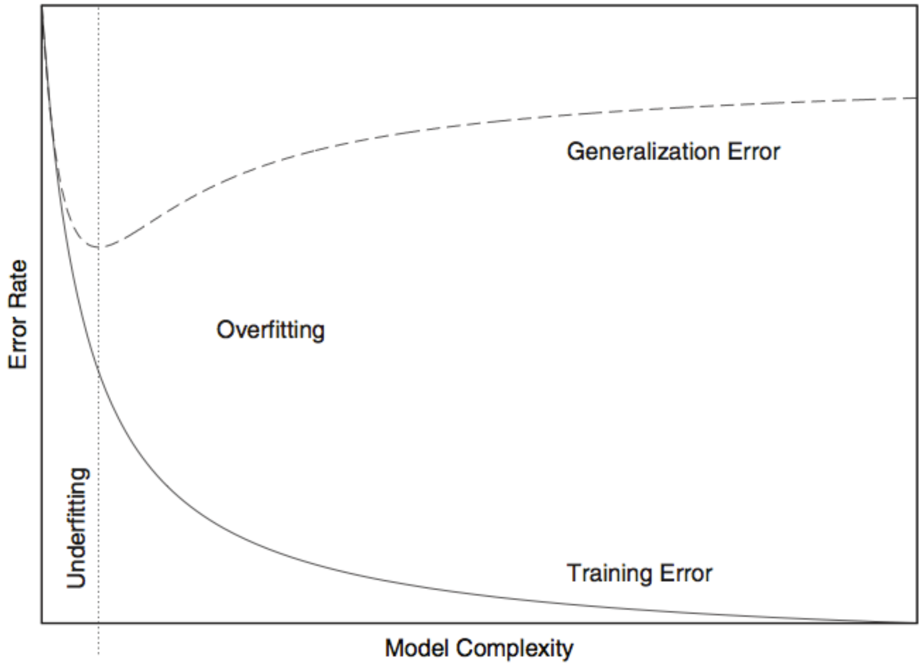
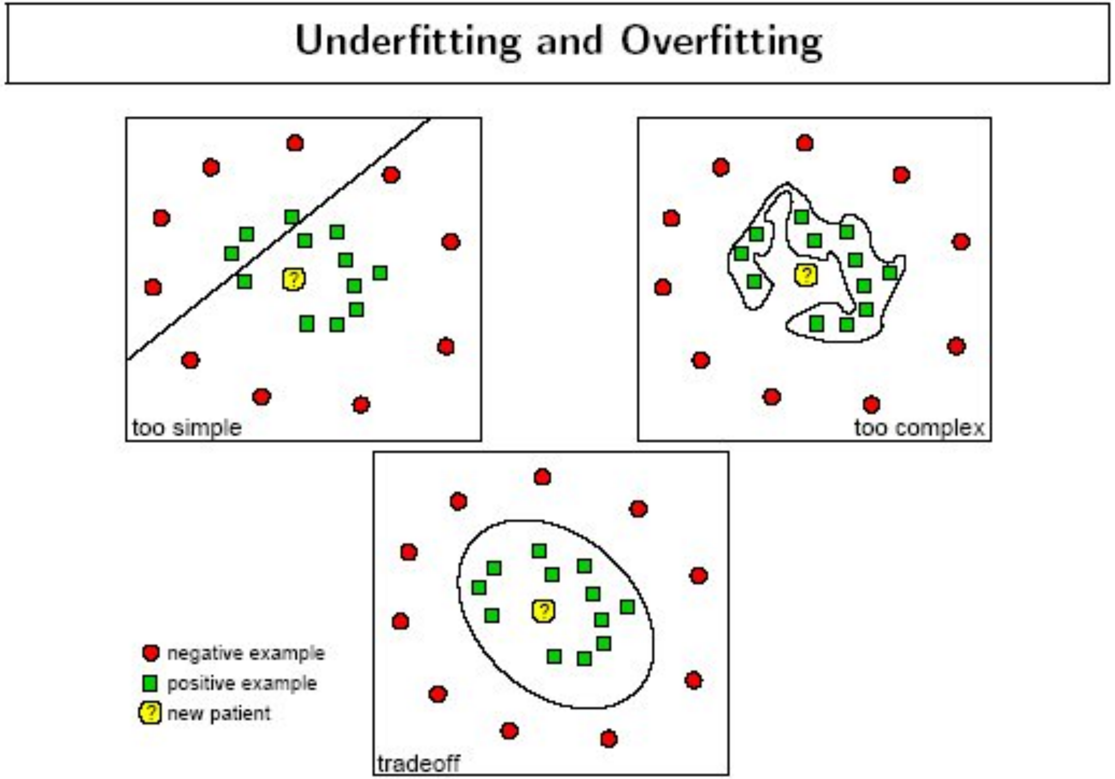


FIGURE 18-1. Overfitting: as a model becomes more complex, it becomes increasingly able to represent the training data. However, such a model is overfitted and will not generalize well to data that was not used during training.

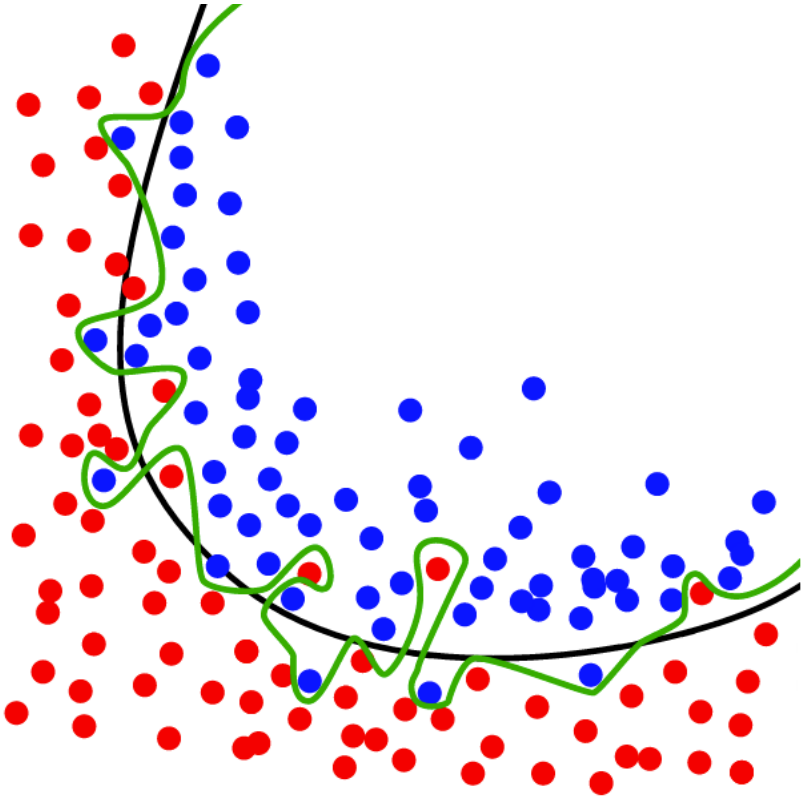
source: Data Analysis with Open Source Tools, by Philipp K. Janert. O'Reilly Media, 2011.

OVERFITTING - EXAMPLE



source: http://www.dtreg.com

OVERFITTING – EXAMPLE



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

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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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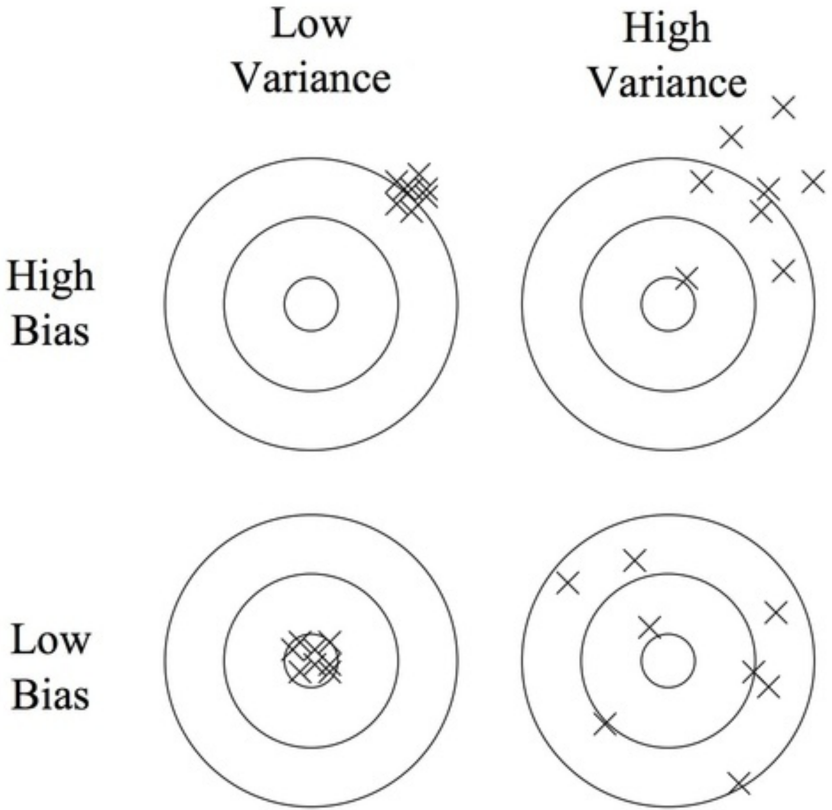
NOTE

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

BIAS-VARIANCE



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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.

III. CROSS VALIDATION

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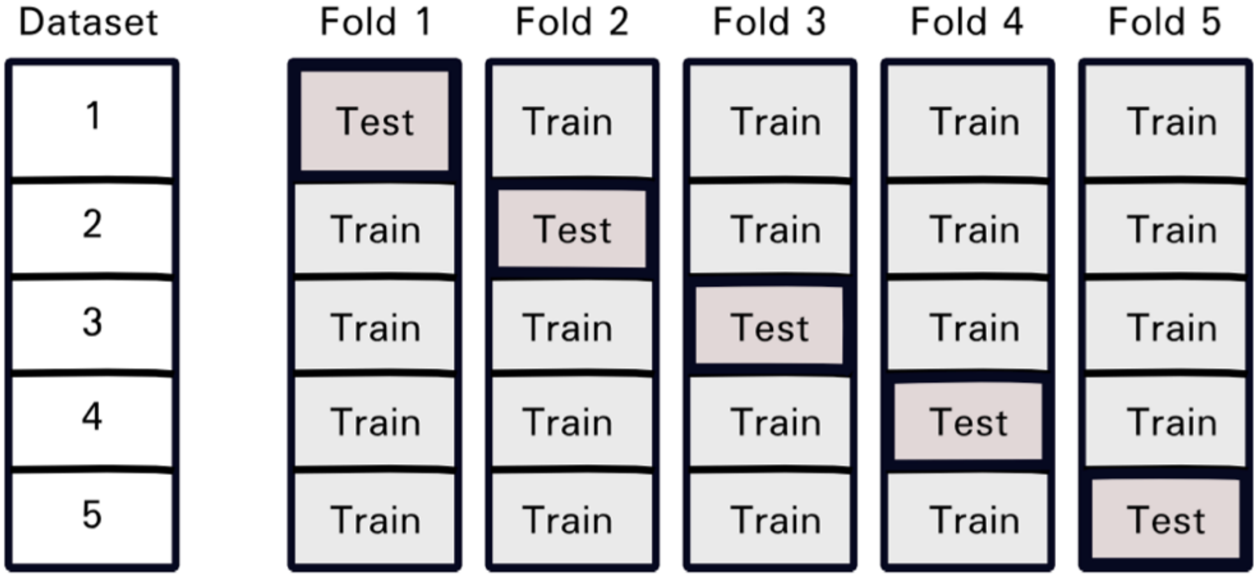
5) *Take the average generalization error as the estimate of OOS accuracy.*

CROSS-VALIDATION: 5-FOLD EXAMPLE



Accuracy

k_1 %

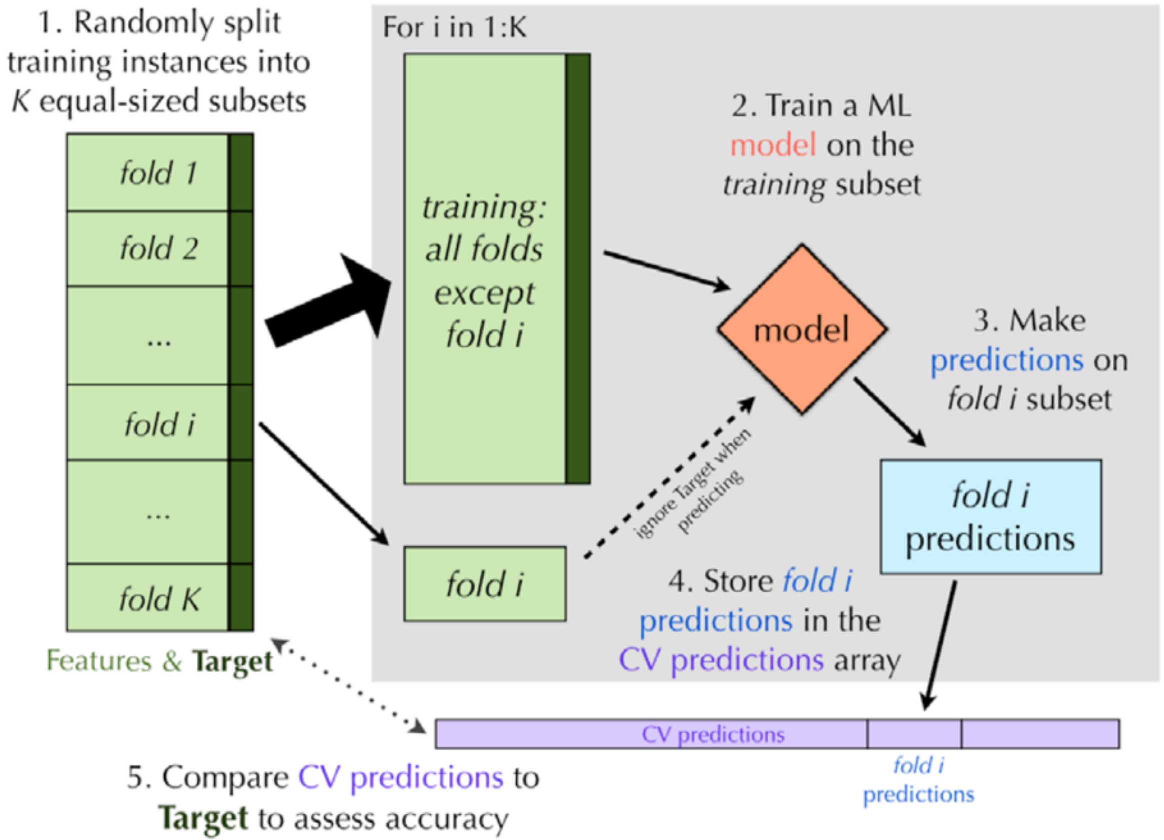
k_2 %

k_3 %

k_4 %

k_5 %

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


1. Randomly split training instances into K equal-sized subsets
fold 1
fold 2
...
fold i
...
fold K
Features & Target
For i in 1:K
training: all folds except fold i
2. Train a ML model on the training subset
model
3. Make predictions on fold i subset
ignore Target when predicting
fold i
fold i predictions
4. Store fold i predictions in the CV predictions array
CV predictions
fold i predictions
5. Compare CV predictions to Target to assess accuracy

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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.*

Last time:

- *Types of machine learning problems / algorithms*
- *Generalization*

This time:

- *Train / Test Split*
- *Errors, Overfitting and underfitting*
- *Cross validation*

LAB: CROSS VALIDATION WITH KIN