Foundations of Data Science & Analytics: Evaluation and Testing

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Introduction to Data Mining, 2nd Edition
by
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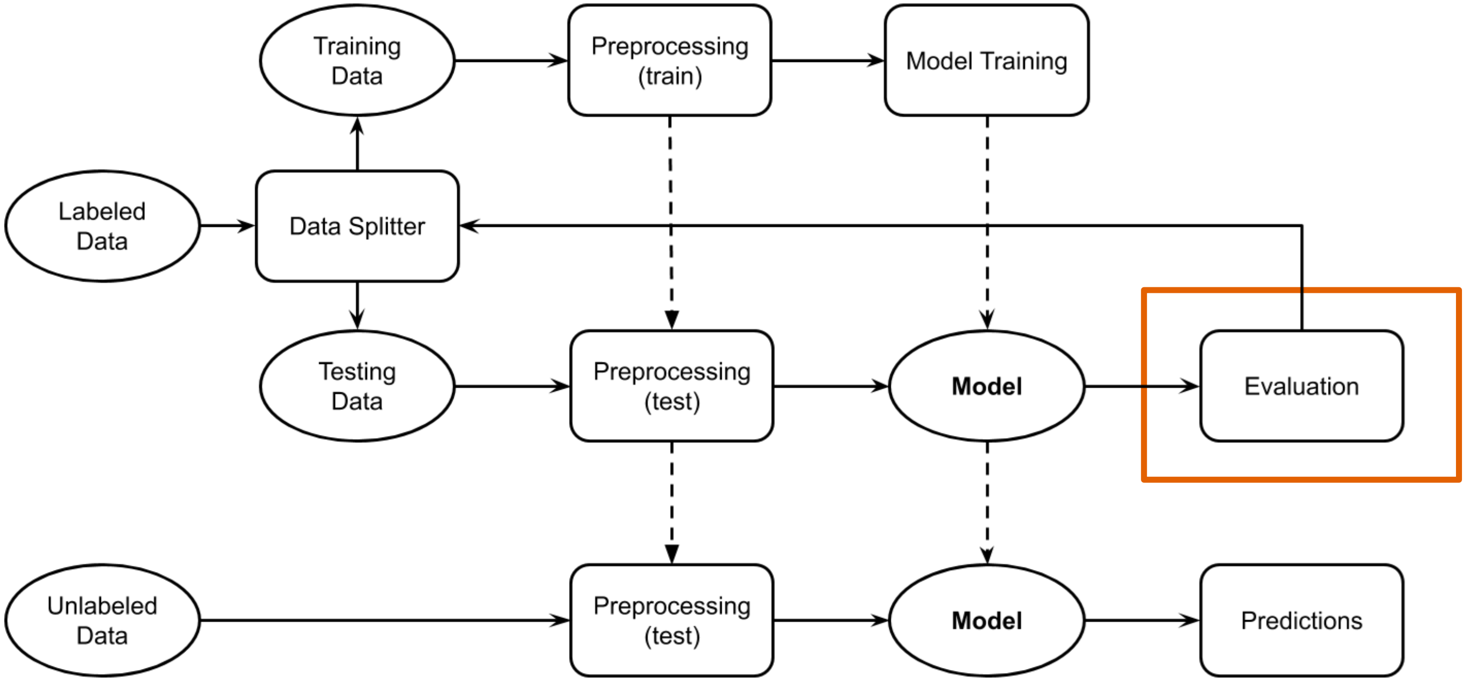
Evaluation


Training
Data
Preprocessing
(train)
Model Training
Labeled
Data
Data Splitter
Testing
Data
Preprocessing
(test)
Model
Evaluation
Unlabeled
Data
Preprocessing
(test)
Model
Predictions

Types of Classification Problems

- Binary Classification
- Multi-Class Classification

Binary Classification

Confusion Matrix		Predicted	
		Yes	**No**
Actual	**Yes**	TP	FN
	No	FP	TN

Binary Classification

Confusion Matrix		Predicted	
		Yes	**No**
Actual	**Yes**	5	2
	No	40	1000

Binary Classification

Confusion Matrix		Predicted	
		Yes	**No**
Actual	**Yes**	TP	FN
	No	FP	TN

$$Accuracy = \frac{TP+TN}{TP+TN+FP+FN}$$

$$Error\ Rate = \frac{FP+FN}{TP+TN+FP+FN}$$

$$= 1 - Accuracy$$

- Pros:
  - Can apply to multi-class
  - A general evaluation
- Cons:
  - Tends to ignore minority classes
  - Need to decide a threshold

Binary Classification

Confusion Matrix		Predicted	
		Yes	**No**
Actual	**Yes**	TP	FN
	No	FP	TN

$$Recall = \frac{TP}{TP+FN}$$

$$Precision = \frac{TP}{TP+FP}$$

$$F_1 = 2 \times \frac{precision \times recall}{precision + recall}$$

- Pros:
  - Good indicator for imbalanced classes
- Cons:
  - **Must be used together (precision + recall)**
  - Cannot directly apply to multi-class

Binary Classification

$$Precision = \frac{TP}{TP+FP}$$

$$Recall = \frac{TP}{TP+FN}$$

$$F_1 = 2 \times \frac{precision \times recall}{precision + recall}$$

Confusion Matrix		Predicted	
		Yes	**No**
Actual	**Yes**	5	2
	No	40	1000

Accuracy = 1005/1047 = 0.960

Precision = 5/45 = 0.111

Recall = 5/7 = 0.714

F1 score = 0.192

Multi-Class Classification

$$Accuracy = \frac{correct\ predictions}{all\ data}$$

$$Error\ Rate = \frac{incorrect\ predictions}{all\ data}$$
$$= 1 - Accuracy$$

- Pros:
  - A general evaluation
- Cons:
  - Tend to ignore minority classes
  - Need to decide a threshold

Multi-Class Classification

<table>
<tr><td colspan="2" rowspan="2">One vs. Rest</td><td colspan="2">Predicted</td></tr>
<tr><td>Yes (Ci)</td><td>No (Not Ci)</td></tr>
<tr><td rowspan="2">Actual</td><td>Yes (Ci)</td><td>TP(Ci)</td><td>FN(Ci)</td></tr>
<tr><td>No (Not Ci)</td><td>FP(Ci)</td><td>TN(Ci)</td></tr>
</table>

Multi-Class Classification

$$Precision(C_i) = \frac{TP(C_i)}{TP(C_i)+FP(C_i)}$$

$$Recall(C_i) = \frac{TP(C_i)}{TP(C_i)+FN(C_i)}$$

$$F_1(Ci) = 2 \times \frac{precision(Ci) \times recall(Ci)}{precision(Ci)+recall(Ci)}$$

Multi-Class Classification

		True/Actual		
		Cat (🐱)	Fish (🐠)	Hen (🐔)
Predicted	Cat (🐱)	4	6	3
	Fish (🐠)	1	2	0
	Hen (🐔)	1	2	6

Multi-Class Classification

Class	Precision	Recall	F1-score
Cat	30.8%	66.7%	42.1%
Fish	66.7%	20.0%	30.8%
Hen	66.7%	66.7%	66.7%

Macro-precision = (31% + 67% + 67%) / 3 = 54.7%

Macro-recall = (67% + 20% + 67%) / 3 = 51.1%

Macro-F1 = (42.1% + 30.8% + 66.7%) / 3 = 46.5%

Minority Classes are represented equally in Macro-metrics

Multi-Class Classification

		True/Actual		
		Cat (🐱)	Fish (🐠)	Hen (🐔)
Predicted	Cat (🐱)	4	6	3
	Fish (🐠)	1	2	0
	Hen (🐔)	1	2	6

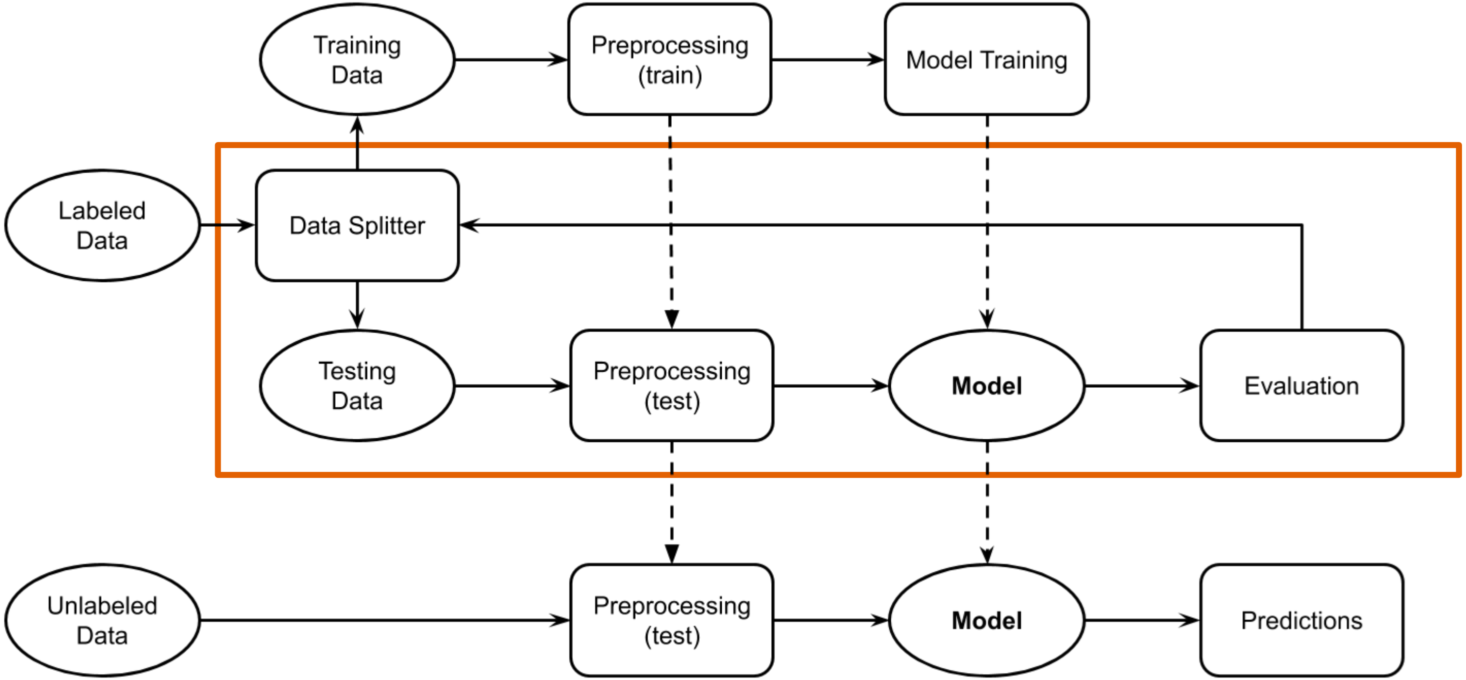
Weighted-F1 = (6 × 42.1% + 10 × 30.8% + 9 × 66.7%) / 25 = 46.4%

Multi-Class Classification

		True/Actual		
		Cat	Fish	Hen
Predicted	Cat	4	6	3
	Fish	1	2	0
	Hen	1	2	6

Micro-F1 = Micro-Precision = Micro-Recall = Accuracy = Green/(Green+Red)=12/25

Testing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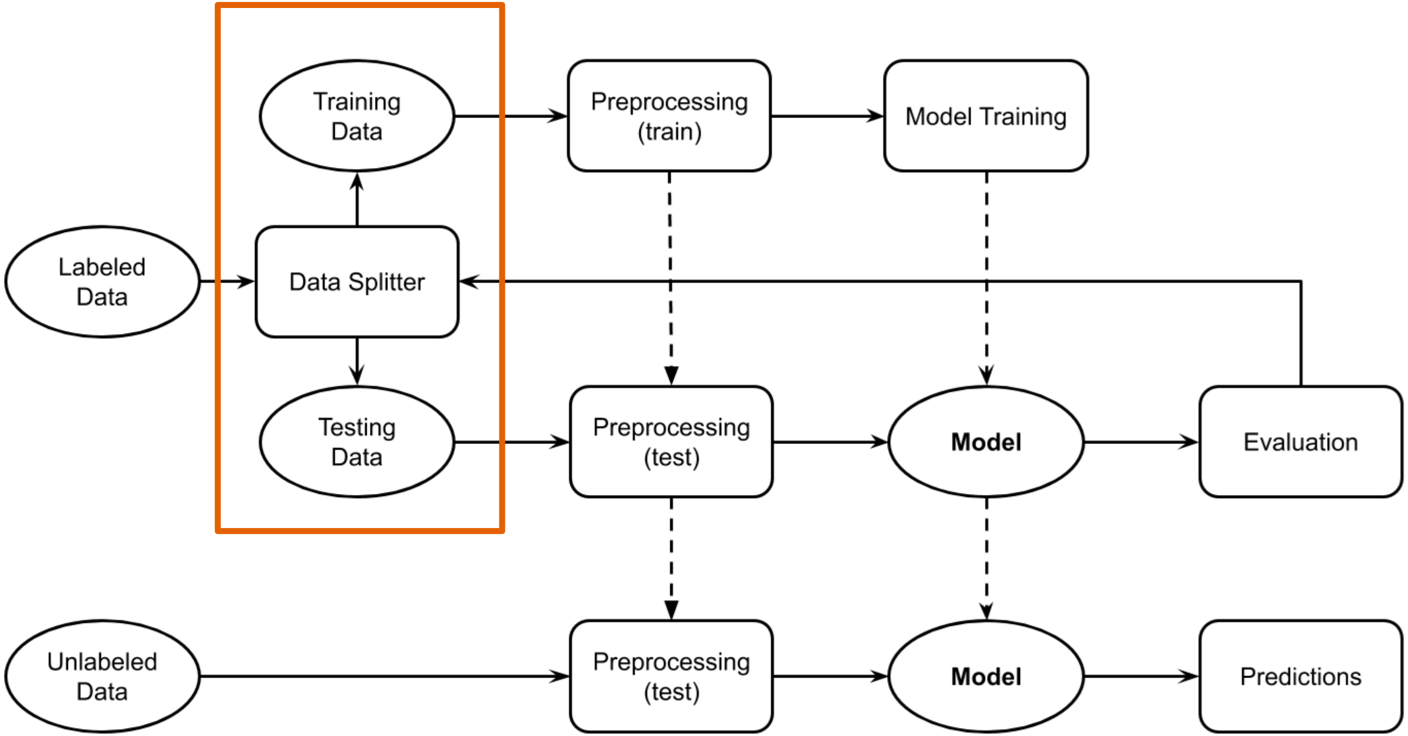
Why is Testing Needed?

- Compare the performance of different models
- Check if performance of a certain model is "good enough" on future (unseen) data

How?

- Reserve a subset of the full data set as the test set
- Train model on rest of the data, then evaluate model predictions on the test set.

How?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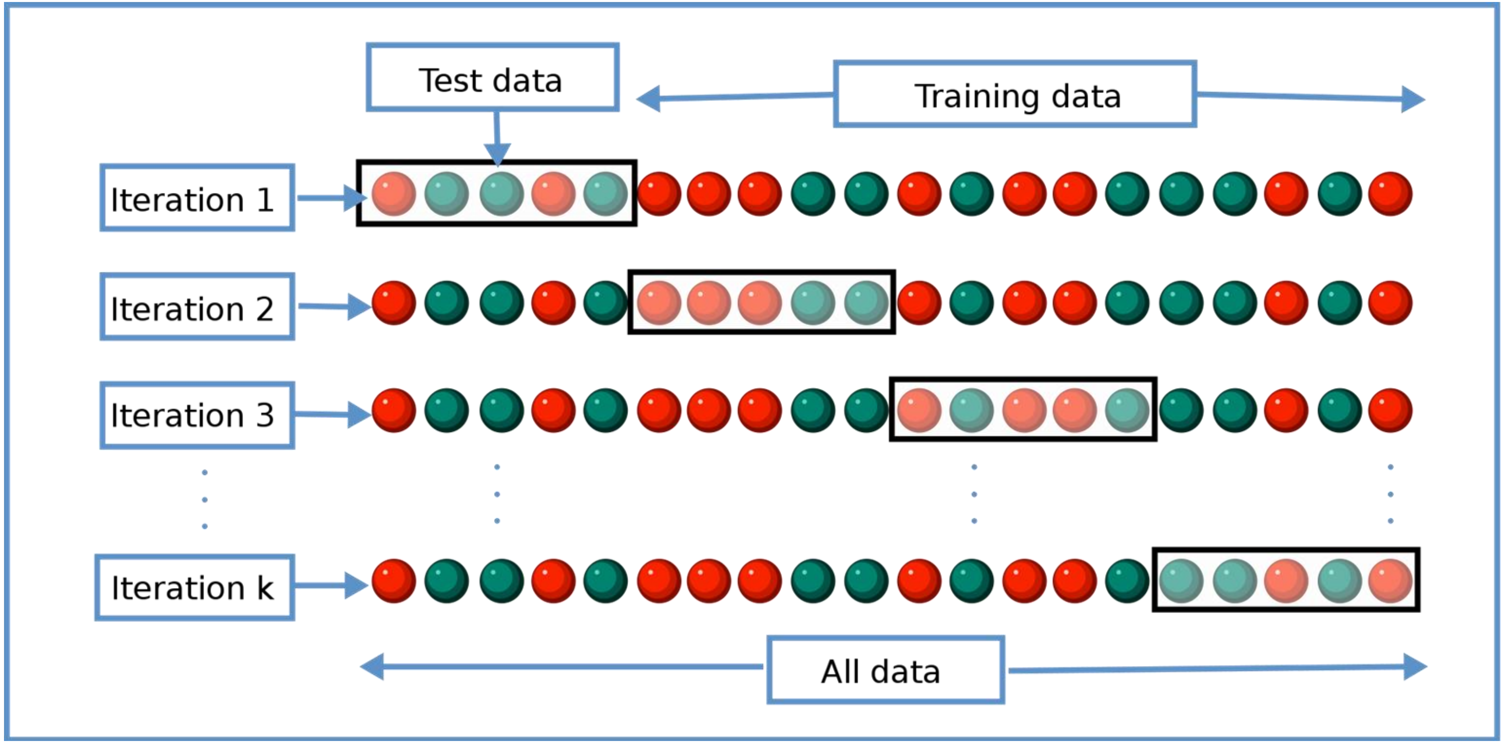
Holdout

- The most basic way to create a training and test set is to use “Holdout”
- Split the data using X% for training and Y% for testing
  - Typical splits tend to be 75/25, 80/20, 90/10
  - Splits should use stratified sampling, based upon the class distribution of the full data set
- This process should be repeated multiple times to mitigate the effects of “luck"

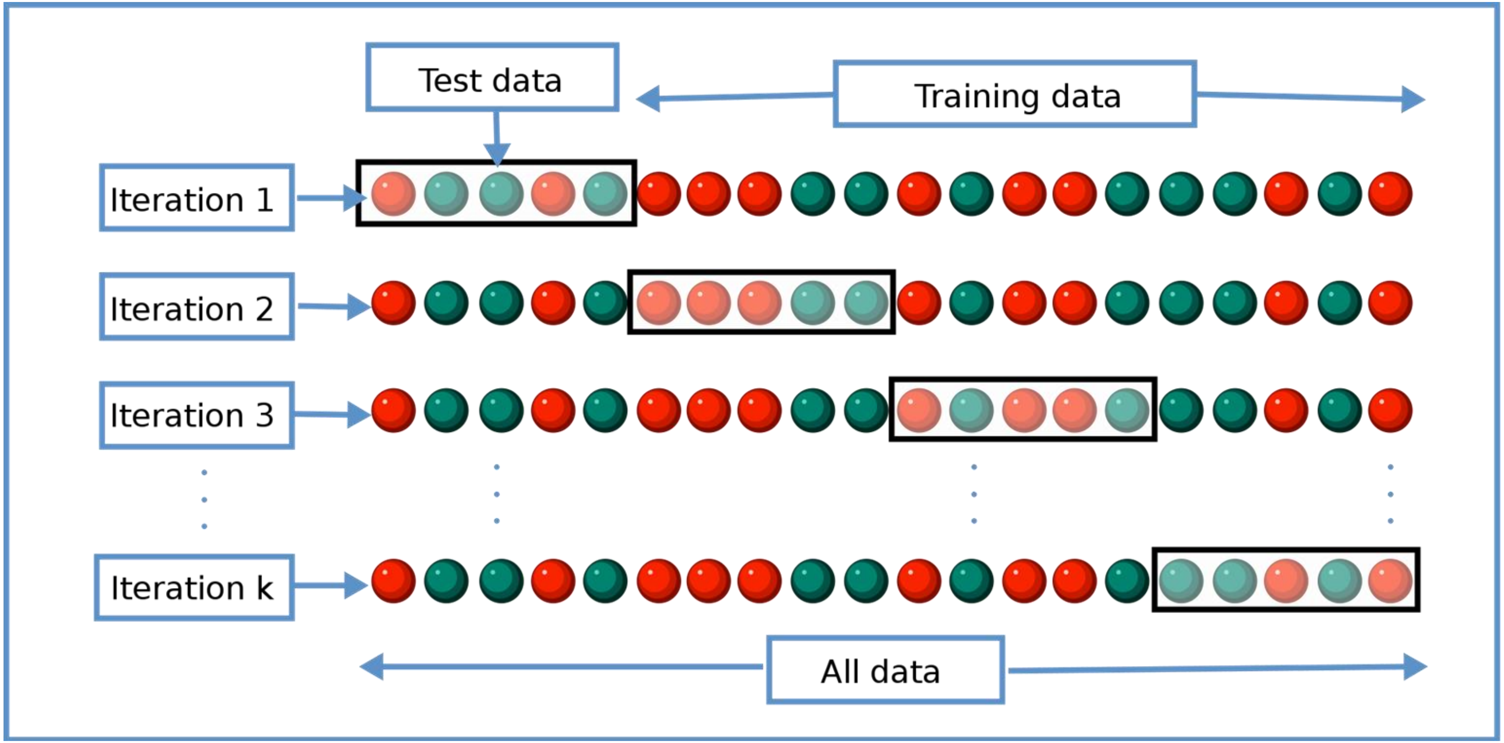
Cross-Validation

Use all data for testing



Cross-Validation

- **K-folds:**
  - split data into K subsets
  - each subset will be used as validation set once
  - performances are averaged across all K subsets



F1 = 0.6

F1 = 0.7

F1 = 0.6

F1 = 0.4

F1_cross = (0.6 + 0.7 + 0.6 + 0.4) / 4 = 0.575

Cross-Validation

- **L × K-fold:**
  - Shuffle data **L** times randomly
    - Each time perform a K-fold cross-validation
    - Collect performance
  - End up with **L** performance metrics

Avoid **lucky** wins

- **Compare the L metrics of each treatment to decide which is the best**