Applied Machine Learning

Model Evaluation & Selection

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Learning objectives

- Understand why accuracy only gives a partial picture of a classifier's performance.

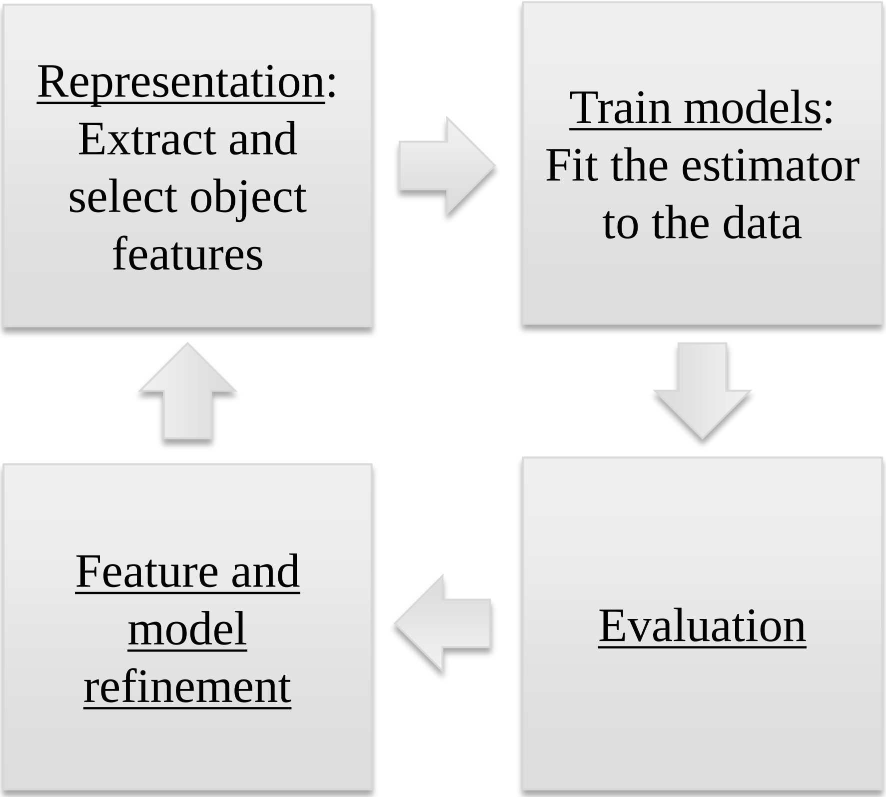
- Understand the motivation and definition of important evaluation metrics in machine learning.

Learning objectives

- Learn how to use a variety of evaluation metrics to evaluate supervised machine learning models.

- Learn about choosing the right metric for selecting between models or for doing parameter tuning.

Represent / Train / Evaluate / Refine Cycle



Evaluation

- Different applications have very different goals
- Accuracy is widely used, but many others are possible, e.g.:
  - User satisfaction (Web search)
  - Amount of revenue (e-commerce)
  - Increase in patient survival rates (medical)

Evaluation

- It's very important to choose evaluation methods that match the goal of your application.
- Compute your selected evaluation metric for multiple different models.
- Then select the model with 'best' value of evaluation metric.

Accuracy with imbalanced classes

- Suppose you have two classes:
  - Relevant (R): the positive class
  - Not_Relevant (N): the negative class
- Out of 1000 randomly selected items, on average
  - One item is relevant and has an R label
  - The rest of the items (999 of them) are not relevant and labelled N.
- Recall that:

$$\text{Accuracy} = \frac{\#\text{correct predictions}}{\#\text{total instances}}$$

Accuracy with imbalanced classes

- You build a classifier to predict relevant items, and see that its accuracy on a test set is **99.9**%.
- Wow! Amazingly good, right?
- For comparison, suppose we had a "dummy" classifier that didn't look at the features at all, and always just blindly predicted the most frequent class (i.e. the negative N class).

Accuracy with imbalanced classes

- Assuming a test set of 1000 instances, what would this dummy classifier's accuracy be?
- Answer:

$$\text{Accuracy}_{\text{DUMMY}} = 999 / 1000 = 99.9\%$$

Dummy classifiers completely ignore the input data!

- Dummy classifiers serve as a sanity check on your classifier's performance.
- They provide a null metric (e.g. null accuracy) baseline.
- Dummy classifiers should not be used for real problems.

Dummy classifiers completely ignore the input data!

- Some commonly-used settings for the `strategy` parameter for DummyClassifier in scikit-learn:
  - ***most_frequent*** : predicts the most frequent label in the training set.
  - ***stratified*** : random predictions based on training set class distribution.
  - ***uniform*** : generates predictions uniformly at random.
  - ***constant*** : always predicts a constant label provided by the user.
    - A major motivation of this method is F1-scoring, when the positive class is in the minority.

What if my classifier accuracy is close to the null accuracy baseline?

This could be a sign of:

- Ineffective, erroneous or missing features
- Poor choice of kernel or hyperparameter
- Large class imbalance

Dummy regressors

`strategy` parameter options:

- *mean* : predicts the mean of the training targets.
- *median* : predicts the median of the training targets.
- *quantile* : predicts a user-provided quantile of the training targets.
- *constant* : predicts a constant user-provided value.

Binary prediction outcomes

	Predicted negative	**Predicted** positive
True negative	TN	FP
True positive	FN	TP

Label 1 = positive class
(class of interest)

Label 0 = negative class
(everything else)

TP = true positive
FP = false positive (Type I error)
TN = true negative
FN = false negative (Type II error)

Confusion matrix for binary prediction task

	Predicted negative	Predicted positive
True negative	TN = 356	FP = 51
True positive	FN = 38	TP = 5

N = 450

- Every test instance is in exactly one box (integer counts).
- Breaks down classifier results by error type.
- Thus, provides more information than simple accuracy.
- Helps you choose an evaluation metric that matches project goals.
- Not a single number like accuracy.. but there are many possible metrics that can be derived from the confusion matrix.

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Confusion Matrices & Basic Evaluation Metrics

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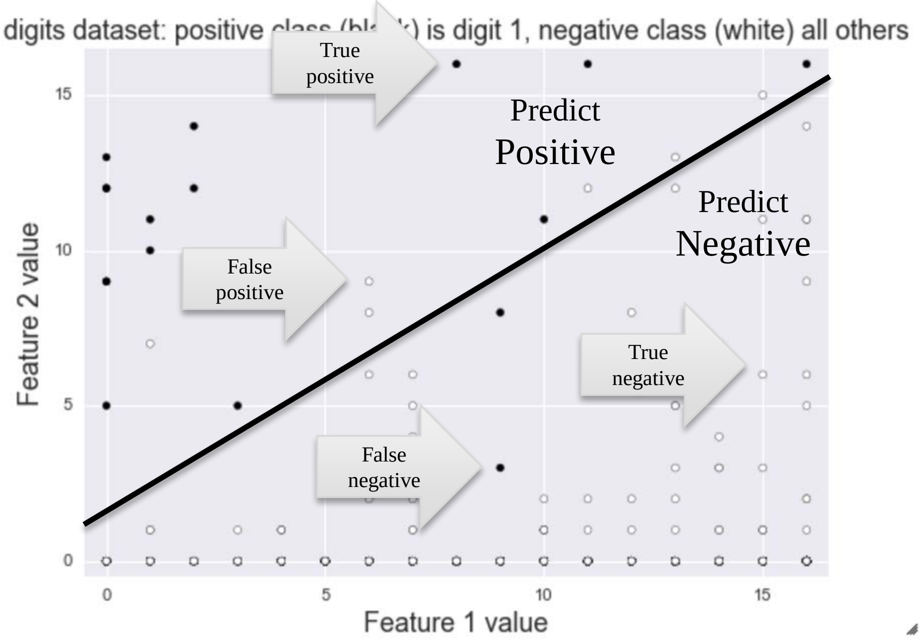
Confusion Matrix for Binary Prediction Task

	Predicted negative	Predicted positive	
True negative	TN = 400	FP = 7	
True positive	FN = 17	TP = 26	
			N = 450

Always look at the confusion matrix for your classifier.

Visualization of Different Error Types



TN = 429	FP = 6
FN = 2	TP = 13

Accuracy: for what fraction of all instances is the classifier's prediction correct (for either positive or negative class)?

	Predicted negative	Predicted positive	
True negative	TN = 400	FP = 7	
True positive	FN = 17	TP = 26	
			$N = 450$

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

$$= \frac{400+26}{400+26+17+7}$$

$$= 0.95$$

Classification error (1 – Accuracy): for what fraction of all instances is the classifier's prediction incorrect?

	Predicted negative	Predicted positive	
True negative	TN = 400	FP = 7	
True positive	FN = 17	TP = 26	
			$N = 450$

$$\text{ClassificationError} = \frac{FP + FN}{TN + TP + FN + FP}$$

$$= \frac{7+17}{400+26+17+7}$$

$$= 0.060$$

Recall, or True Positive Rate (TPR): what fraction of all positive instances does the classifier correctly identify as positive?

	Predicted negative	Predicted positive	
True negative	TN = 400	FP = 7	
True positive	FN = 17	TP = 26	
			$N = 450$

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

$$= \frac{26}{26+17}$$

$$= 0.60$$

Recall is also known as:

- True Positive Rate (TPR)
- Sensitivity
- Probability of detection

Precision: what fraction of positive predictions are correct?

	Predicted negative	Predicted positive	
True negative	TN = 400	FP = 7	
True positive	FN = 17	TP = 26	
			$N = 450$

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

$$= \frac{26}{26+7}$$

$$= 0.79$$

False positive rate (FPR): what fraction of all negative instances does the classifier <u>incorrectly</u> identify as positive?

True negative	TN = 400	FP = 7	
True positive	FN = 17	TP = 26	
	Predicted negative	Predicted positive	$N = 450$

$$FPR = \frac{FP}{TN+FP}$$

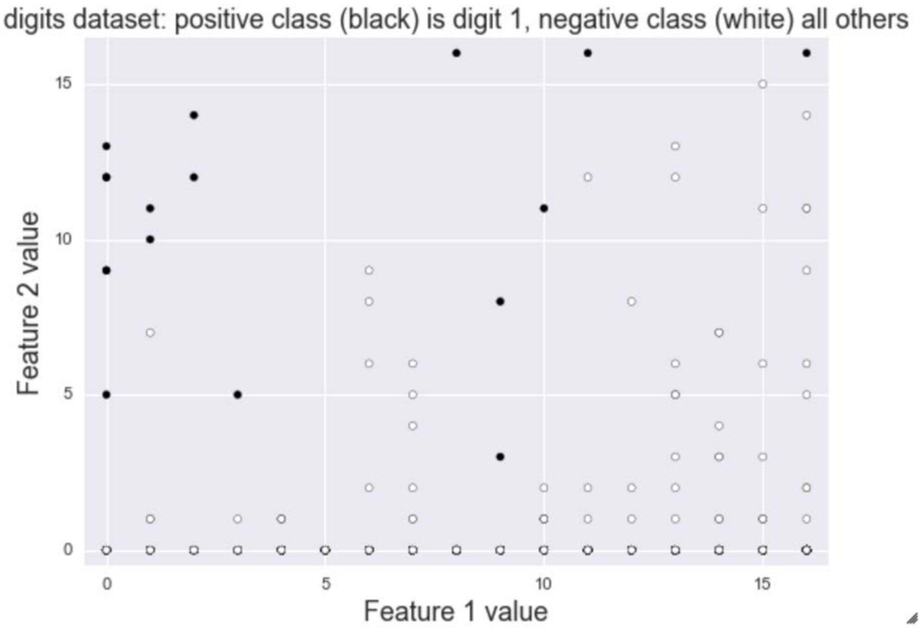
$$= \frac{7}{400+7}$$

$$= 0.02$$

False Positive Rate is also known as:

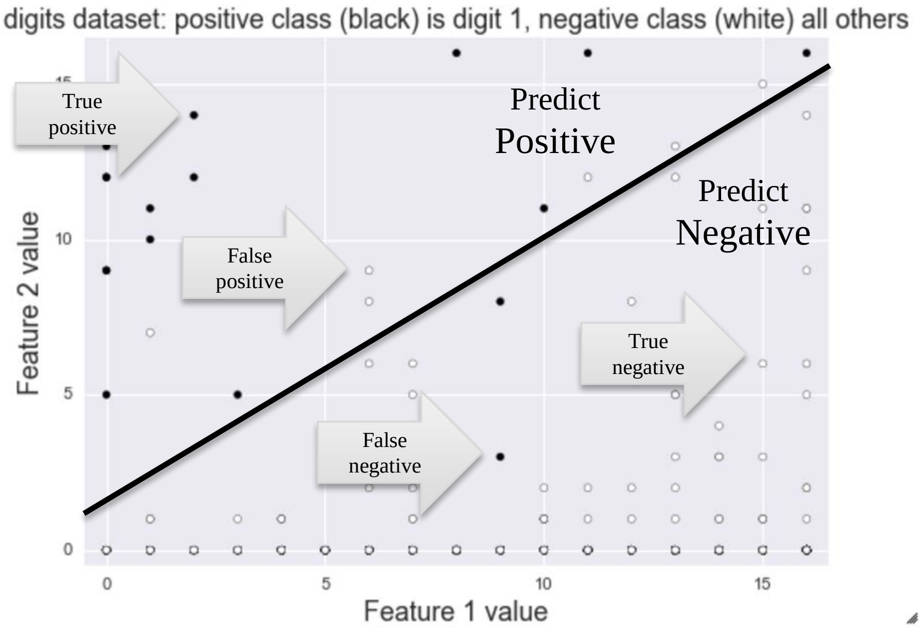
- Specificity

A Graphical Illustration of Precision & Recall



TN =	FP =
FN =	TP =

The Precision-Recall Tradeoff

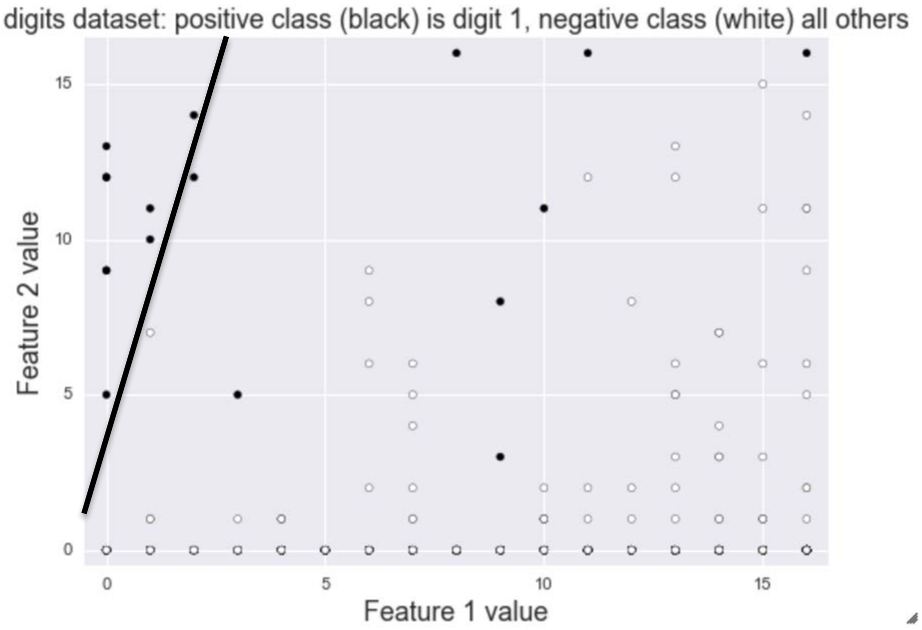


TN = 429	FP = 6
FN = 2	TP = 13

$$\text{Precision} = \frac{TP}{TP+FP} = \frac{13}{19} = 0.68$$

$$\text{Recall} = \frac{TP}{TP+FN} = \frac{13}{15} = 0.87$$

High Precision, Lower Recall

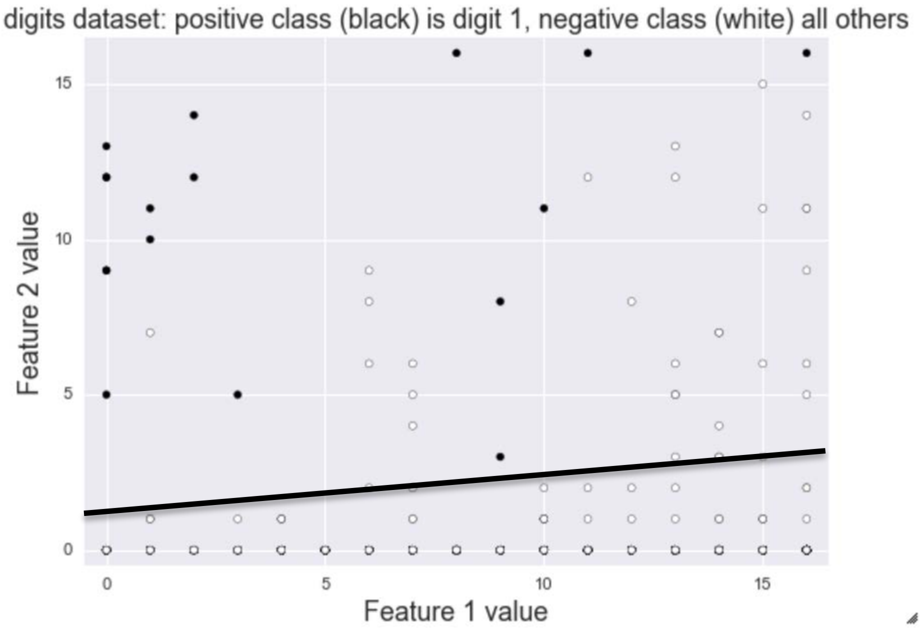


TN = 435	FP = 0
FN = 8	TP = 7

$$\text{Precision} = \frac{TP}{TP+FP} = \frac{7}{7} = 1.00$$

$$\text{Recall} = \frac{TP}{TP+FN} = \frac{7}{15} = 0.47$$

Low Precision, High Recall



TN = 408	FP = 27
FN = 0	TP = 15

$$\text{Precision} = \frac{TP}{TP+FP} = \frac{15}{42} = 0.36$$

$$\text{Recall} = \frac{TP}{TP+FN} = \frac{15}{15} = 1.00$$

There is often a tradeoff between precision and recall

- Recall-oriented machine learning tasks:
  - Search and information extraction in legal discovery
  - Tumor detection
  - Often paired with a human expert to filter out false positives
- Precision-oriented machine learning tasks:
  - Search engine ranking, query suggestion
  - Document classification
  - Many customer-facing tasks (users remember failures!)

F1-score: combining precision & recall into a single number

$$F_1 = 2 \cdot \frac{Precision \cdot Recall}{Precision + Recall} = \frac{2 \cdot TP}{2 \cdot TP + FN + FP}$$

F-score: generalizes F1-score for combining precision & recall into a single number

$$F_1 = 2 \cdot \frac{Precision \cdot Recall}{Precision + Recall} = \frac{2 \cdot TP}{2 \cdot TP + FN + FP}$$

$$F_\beta = (1 + \beta^2) \cdot \frac{Precision \cdot Recall}{(\beta^2 \cdot Precision) + Recall} = \frac{(1 + \beta^2) \cdot TP}{(1 + \beta^2) \cdot TP + \beta \cdot FN + FP}$$

β allows adjustment of the metric to control the emphasis on recall vs precision:

- **Precision-oriented users: $\boldsymbol{\beta}$ = 0.5 (false positives hurt performance more than false negatives)**
- **Recall-oriented users: $\boldsymbol{\beta}$ = 2 (false negatives hurt performance more than false positives)**

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Classifier Decision Functions

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Decision Functions (decision_function)

- Each classifier score value per test point indicates how confidently the classifier predicts the positive class (large-magnitude positive values) or the negative class (large-magnitude negative values).
- Choosing a fixed decision threshold gives a classification rule.
- By sweeping the decision threshold through the entire range of possible score values, we get a series of classification outcomes that form a curve.

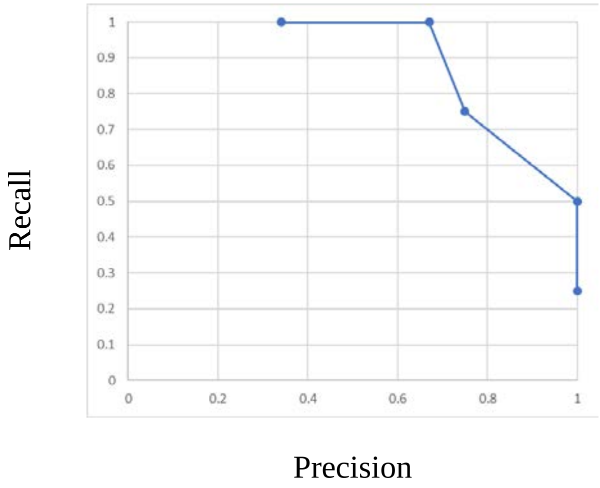
Predicted Probability of Class Membership (predict_proba)

- Typical rule: choose most likely class
  - e.g class 1 if threshold > 0.50.
- Adjusting threshold affects predictions of classifier.
- Higher threshold results in a more conservative classifier
  - e.g. only predict Class 1 if estimated probability of class 1 is above 70%
  - This increases precision. Doesn't predict class 1 as often, but when it does, it gets high proportion of class 1 instances correct.
- Not all models provide realistic probability estimates

Varying the Decision Threshold

True Label	Classifier score
0	-27.6457
0	-25.8486
0	-25.1011
0	-24.1511
0	-23.1765
0	-22.575
0	-21.8271
0	-21.7226
0	-19.7361
0	-19.5768
0	-19.3071
0	-18.9077
0	-13.5411
0	-12.8594
1	-3.9128
0	-1.9798
1	1.824
0	4.74931
1	15.234624
1	21.20597

Classifier score threshold	Precision	Recall
-20	4/12=0.34	4/4=1.00
-10	4/6=0.67	4/4=1.00
0	3/4=0.75	3/4=0.75
10	2/2=1.0	2/4=0.50
20	1/1=1.0	1/4 = 0.25



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Precision-Recall and ROC curves

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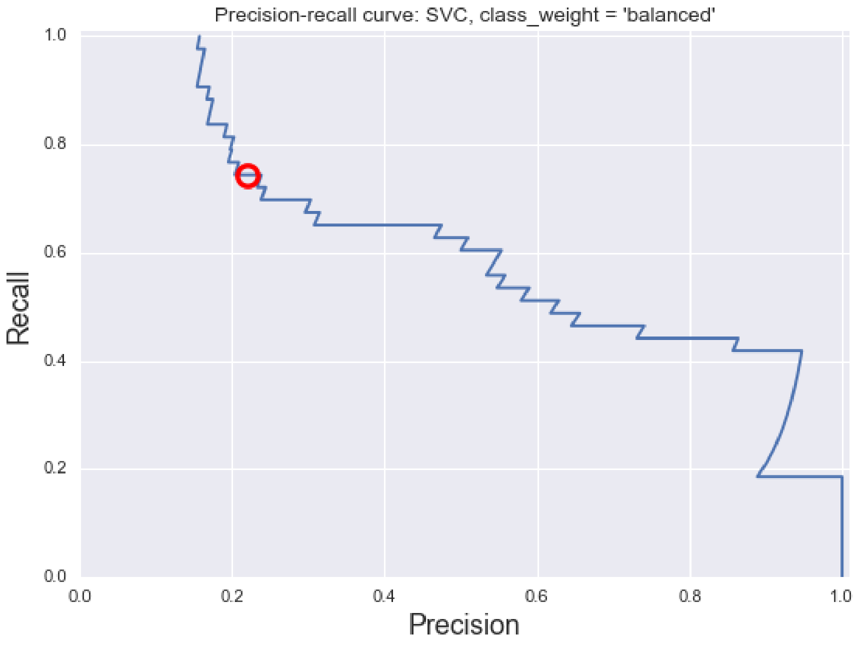
Precision-Recall Curves

X-axis: Precision
Y-axis: Recall

Top right corner:
- **The "ideal" point**
- **Precision = 1.0**
- **Recall = 1.0**

"Steepness" of P-R curves is important:
- **Maximize precision**
- **while maximizing recall**

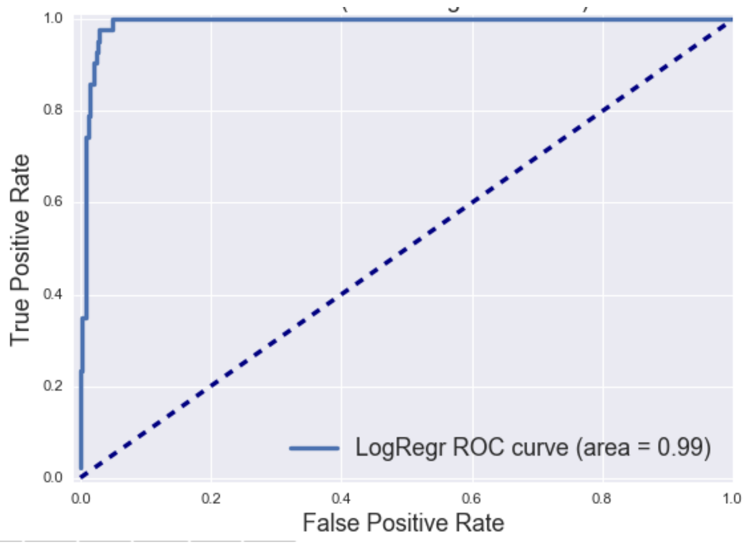


ROC Curves

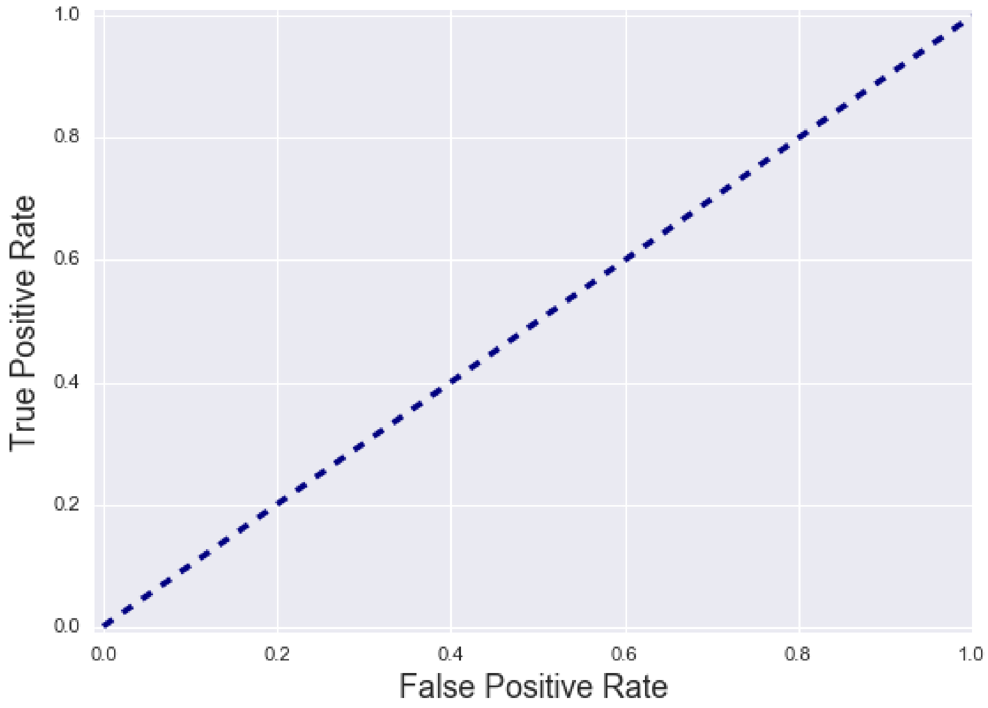
X-axis: False Positive Rate
Y-axis: True Positive Rate

Top left corner:
- **The "ideal" point**
- **False positive rate of zero**
- **True positive rate of one**

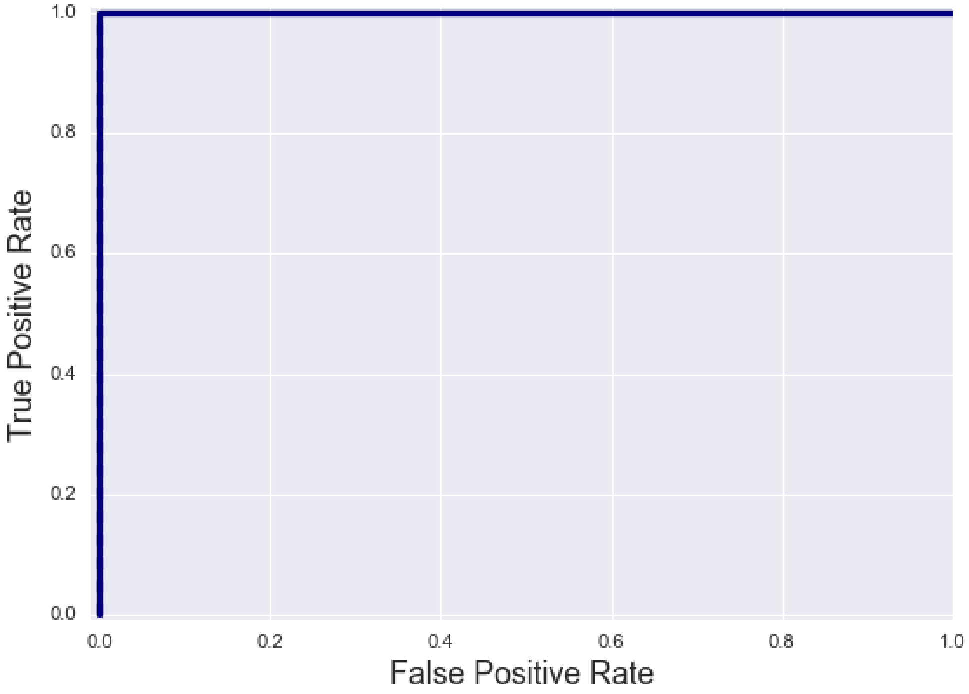
"Steepness" of ROC curves is important:
- **Maximize the true positive rate**
- **while minimizing the false positive rate**



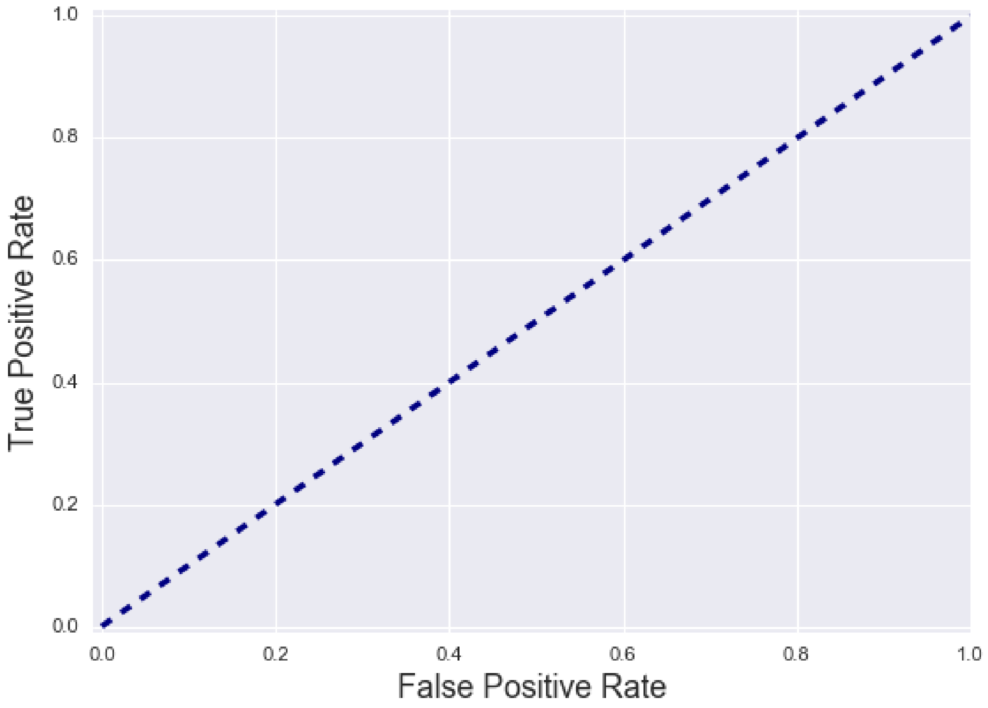
ROC curve examples: random guessing



ROC curve examples: perfect classifier

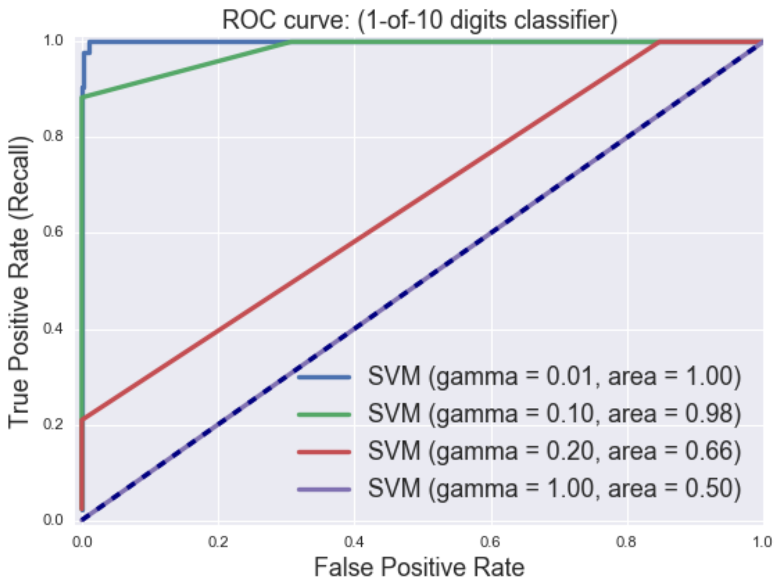


ROC curve examples: bad, okay,



Summarizing an ROC curve in one number: Area Under the Curve (AUC)

- AUC = 0 (worst) AUC = 1 (best)
- AUC can be interpreted as:
  1. The total area under the ROC curve.
  2. The probability that the classifier will assign a higher score to a randomly chosen positive example than to a randomly chosen negative example.
- Advantages:
  - Gives a single number for easy comparison.
  - Does not require specifying a decision threshold.
- Drawbacks:
  - As with other single-number metrics, AUC loses information, e.g. about tradeoffs and the shape of the ROC curve.
  - This may be a factor to consider when e.g. wanting to compare the performance of classifiers with overlapping ROC curves.



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Multi-Class Evaluation

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Multi-Class Evaluation

- Multi-class evaluation is an extension of the binary case.
  - A collection of true vs predicted binary outcomes, one per class
  - Confusion matrices are especially useful
  - Classification report
- Overall evaluation metrics are averages across classes
  - But there are different ways to average multi-class results: we will cover these shortly.
  - The support (number of instances) for each class is important to consider, e.g. in case of imbalanced classes
- Multi-label classification: each instance can have multiple labels (not covered here)

Multi-Class Confusion Matrix

True Digit	0	1	2	3	4	5	6	7	8	9
0	37	0	0	0	0	0	0	0	0	0
1	0	42	0	0	0	0	0	0	1	0
2	0	0	44	0	0	0	0	0	0	0
3	0	0	0	43	0	0	0	0	1	1
4	0	0	0	0	38	0	0	0	0	0
5	0	0	0	0	0	47	0	0	0	1
6	0	1	0	0	0	0	51	0	0	0
7	0	0	0	0	1	0	0	47	0	0
8	0	3	1	0	0	0	0	0	44	0
9	0	0	0	1	0	1	0	0	1	44

Predicted Digit

Micro vs Macro Average

Class	Predicted Class	Correct?
orange	lemon	0
orange	lemon	0
orange	apple	0
orange	orange	1
orange	apple	0
lemon	lemon	1
lemon	apple	0
apple	apple	1
apple	apple	1

Macro-average:

- Each class has equal weight.

1. Compute metric within each class
2. Average resulting metrics across classes

Class	Precision
orange	1/5 = 0.20
lemon	1/2 = 0.50
apple	2/2 = 1.00

Macro-average precision:
(0.20 + 0.50 + 1.00) / 3 = **0.57**

Micro vs Macro Average

Class	Predicted Class	Correct?
orange	lemon	0
orange	lemon	0
orange	apple	0
orange	orange	1
orange	apple	0
lemon	lemon	1
lemon	apple	0
apple	apple	1
apple	apple	1

Micro-average:

- Each instance has equal weight.
- Largest classes have most influence

1. Aggregrate outcomes across all classes
2. Compute metric with aggregate outcomes

Micro-average precision:
4 / 9 = **0.44**

Macro-Average vs Micro-Average

- If the classes have about the same number of instances, macro- and micro-average will be about the same.
- If some classes are much larger (more instances) than others, and you want to:
  - Weight your metric toward the largest ones, use micro-averaging.
  - Weight your metric toward the smallest ones, use macro-averaging.
- If the micro-average is much lower than the macro-average then examine the larger classes for poor metric performance.
- If the macro-average is much lower than the micro-average then examine the smaller classes for poor metric performance.

Multi-class Evaluation Metrics via the "Average" Parameter for a Scoring Function

- Micro: Metric on aggregated instances
- Macro: Mean per-class metric, classes have equal weight
- Weighted: Mean per-class metric, weighted by support
- Samples: for multi-label problems only

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Regression Evaluation

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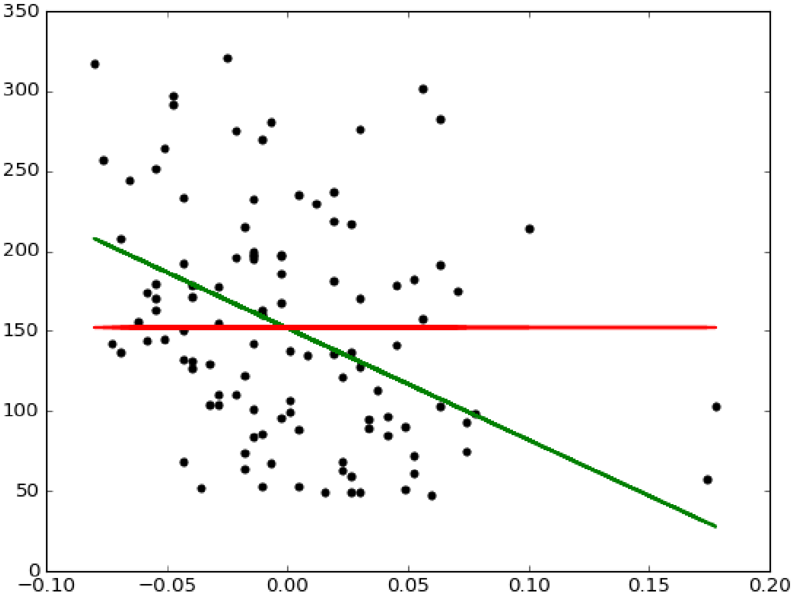
Regression metrics

- Typically r2_score is enough
  - Reminder: computes how well future instances will be predicted
  - Best possible score is 1.0
  - Constant prediction score is 0.0
- Alternative metrics include:
  - mean_absolute_error (absolute difference of target & predicted values)
  - mean_squared_error (squared difference of target & predicted values)
  - median_absolute_error (robust to outliers)

Dummy regressors

As in classification, comparison to a 'dummy' prediction model that uses a fixed rule can be useful.

For this, scikit.learn provides dummy regressors.

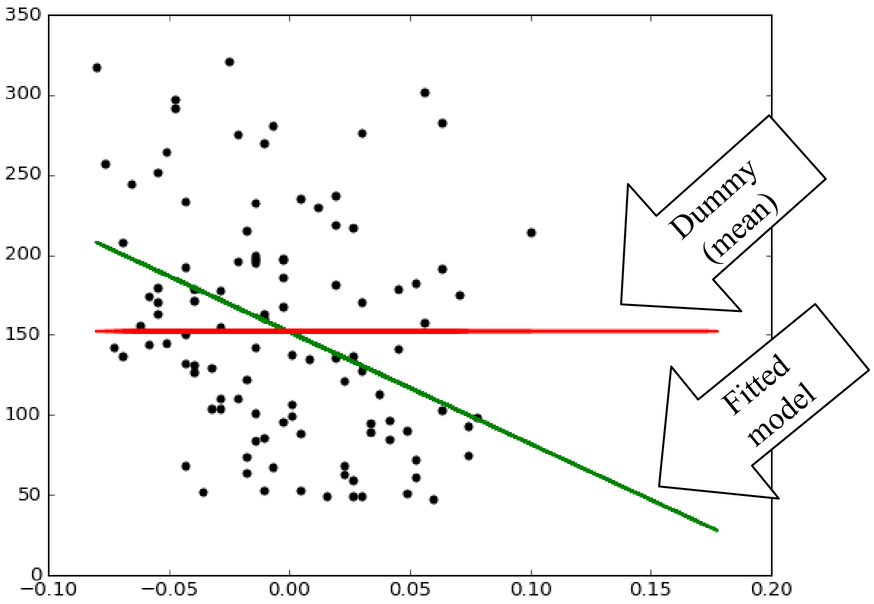


Dummy regressors

As in classification, comparison to a 'dummy' prediction model that uses a fixed rule can be useful.

For this, scikit.learn provides dummy regressors.

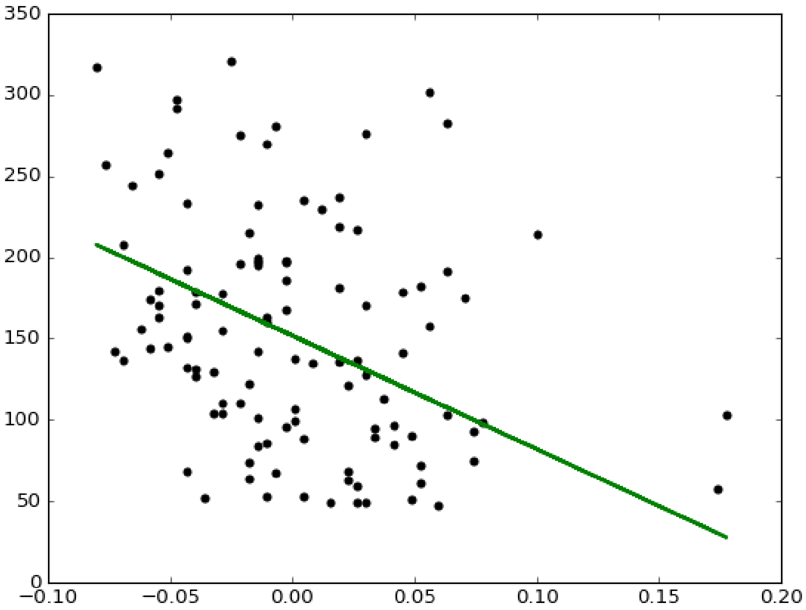
```
Linear model, coefficients: [-698.80206267]
Mean squared error (dummy): 4965.13
Mean squared error (linear model): 4646.74
r2_score (dummy): -0.00
r2_score (linear model): 0.06
```



Dummy regressors

The DummyRegressor class implements four simple baseline rules for regression, using the `strategy` parameter:

- `mean` predicts the mean of the training target values.
- `median` predicts the median of the training target values.
- `quantile` predicts a user-provided quantile of the training target values (e.g. value at the 75th percentile)
- `constant` predicts a custom constant value provided by the user.



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Optimizing Classifiers for Different Evaluation Metrics

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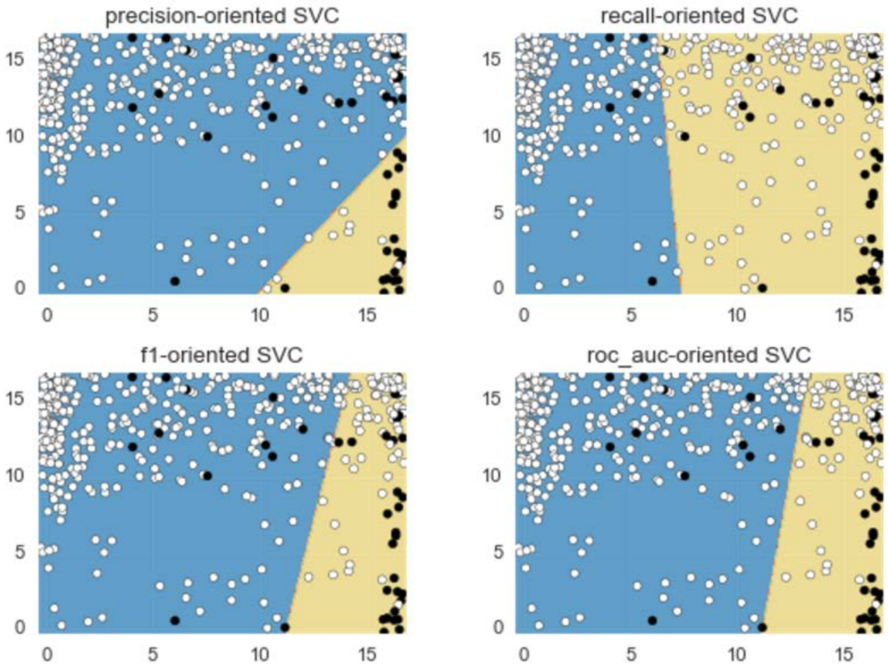
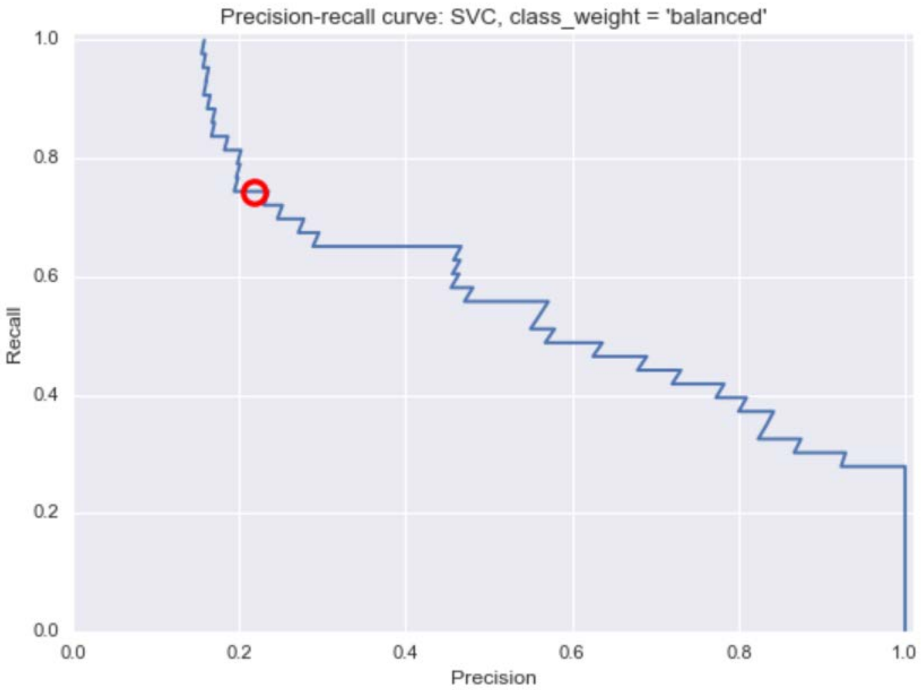
Model Selection Using Evaluation Metrics

- Train/test on same data
  - Single metric.
  - Typically overfits and likely won't generalize well to new data.
  - But can serve as a sanity check: low accuracy on the training set may indicate an implementation problem.
- Single train/test split
  - Single metric.
  - Speed and simplicity.
  - Lack of variance information
- K-fold cross-validation
  - K train-test splits.
  - Average metric over all splits.
  - Can be combined with parameter grid search: GridSearchCV (def. cv = 3)

Example: Optimizing a Classifier Using Different Evaluation Metrics



Example: Precision-Recall Curve of Default Support Vector Classifier



Training, Validation, and Test Framework for Model Selection and Evaluation

- Using only cross-validation or a test set to do model selection may lead to more subtle overfitting / optimistic generalization estimates
- Instead, use three data splits:
  1. Training set (model building)
  2. Validation set (model selection)
  3. Test set (final evaluation)
- In practice:
  - Create an initial training/test split
  - Do cross-validation on the training data for model/parameter selection
  - Save the held-out test set for final model evaluation

Concluding Notes

- Accuracy is often not the right evaluation metric for many real-world machine learning tasks
  - False positives and false negatives may need to be treated very differently
  - Make sure you understand the needs of your application and choose an evaluation metric that matches your application, user, or business goals.
- Examples of additional evaluation methods include:
  - Learning curve: How much does accuracy (or other metric) change as a function of the amount of training data?
  - Sensitivity analysis: How much does accuracy (or other metric) change as a function of key learning parameter values?