Ensemble Learning

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Review

- Last week:
  - Evaluating Machine Learning Models Using Cross-Validation
  - Naïve Bayes
  - Support Vector Machines

- Assignments (Canvas):
  - Problem set 4 due tonight
  - Lab assignment 2 due next week
  - Project pre-proposal due in two weeks (finding a partner ideas)

- Questions?

Today's Topics

- One-vs-all multiclass classification
- Classifier confidence
- Evaluation: ROC and PR-curves
- Ensemble learning

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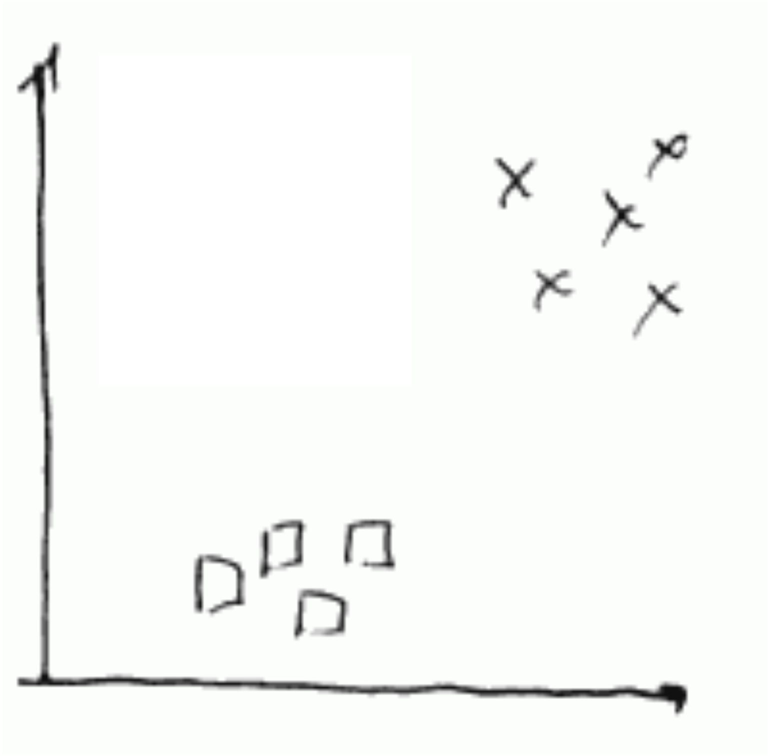
Recall: Binary vs Multiclass Classification

Binary: distinguish 2 classes



Multiclass: distinguish 3+ classes

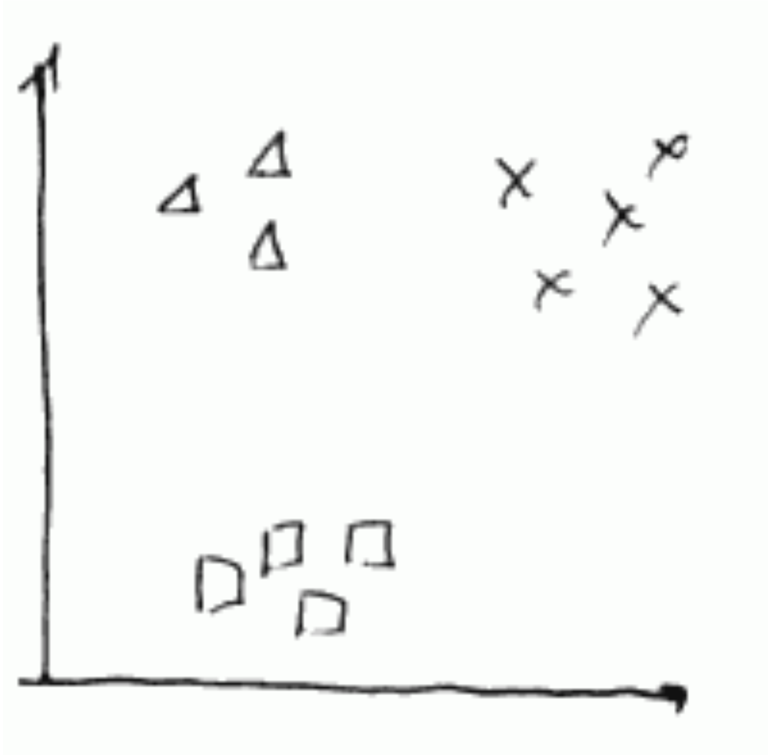


Figure Source: http://mlwiki.org/index.php/One-vs-All_Classification

Recall: Binary vs Multiclass Classification

Binary: distinguish 2 classes

Perceptron

Adaline

Support Vector Machine

Multiclass: distinguish 3+ classes

Nearest Neighbor

Decision Tree

Naïve Bayes

One-vs-All (aka, One-vs-Rest): Applying Binary Classification Methods for Multiclass Classification

- Given ‘N’ classes, train ‘N’ different classifiers: a single classifier trained per class, with the samples of that class as positive samples and all other samples as negatives; e.g.,

Figure Source: http://mlwiki.org/index.php/One-vs-All_Classification

One-vs-All (aka, One-vs-Rest): Limitation

- Often leads to unbalanced distributions during learning; i.e., when the set of negatives is much larger than the set of positives

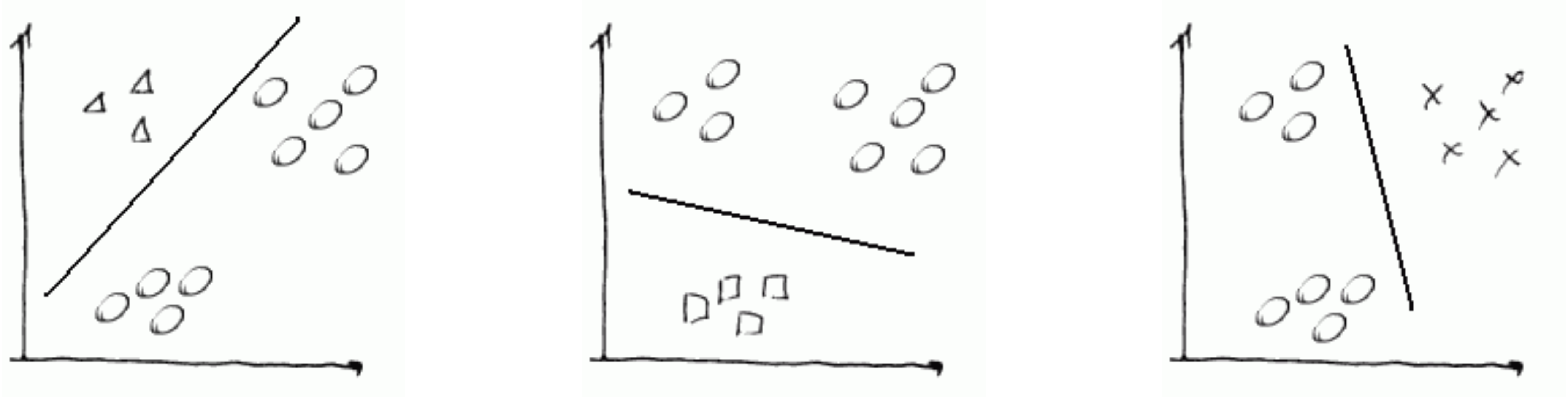
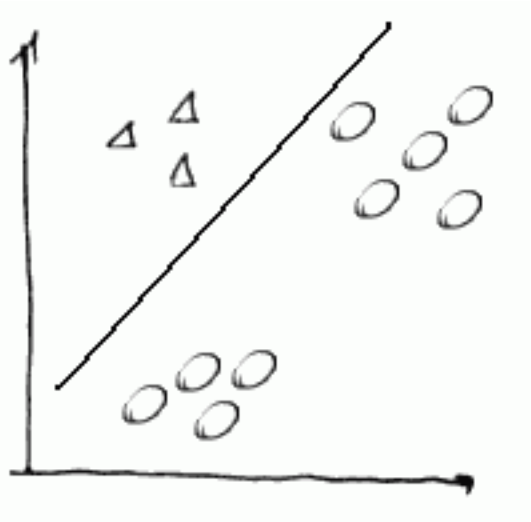
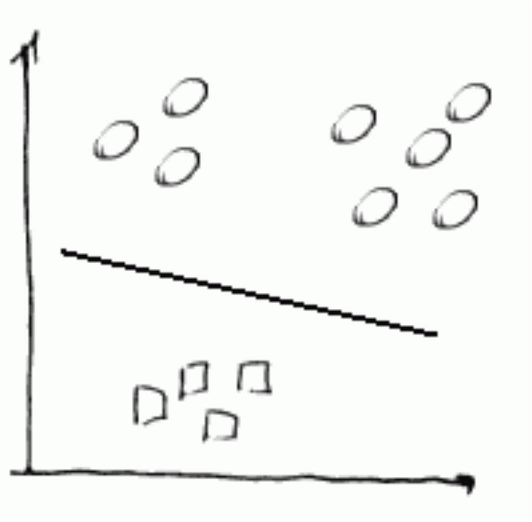


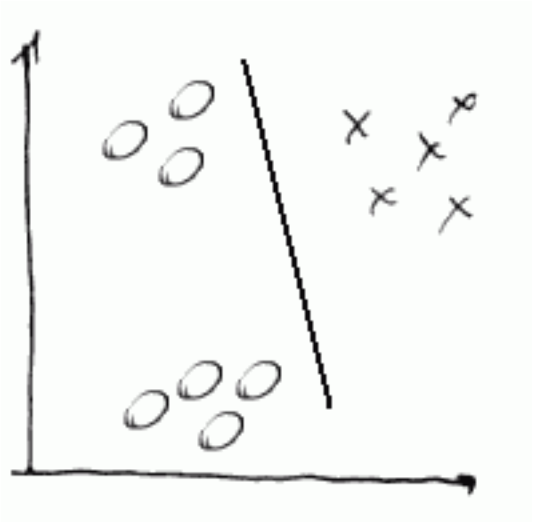
Figure Source: http://mlwiki.org/index.php/One-vs-All_Classification

One-vs-All (aka, One-vs-Rest): Class Assignment

- (Imperfect) Approach: use from N classifiers the most confident match; this requires a real-valued confidence score for its decision







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Classifier Confidence: Beyond Classification

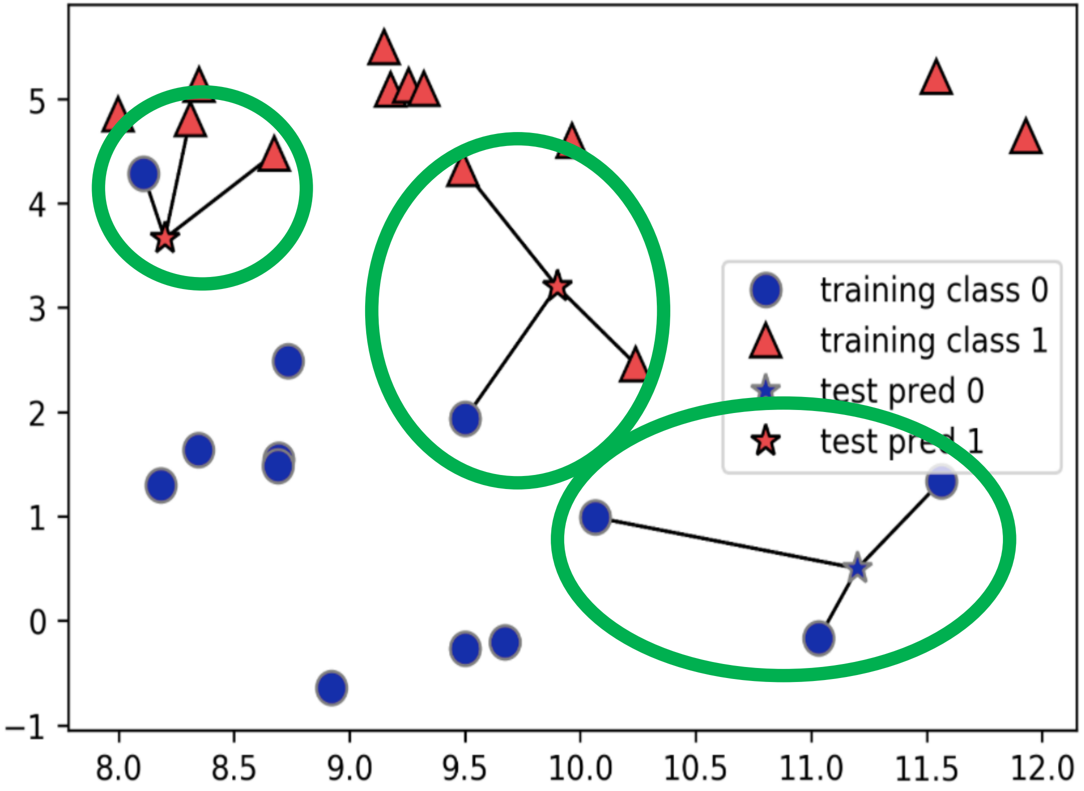
- Indicate both the predicted class and uncertainty about the choice

- When and why might you want to know about the uncertainty?
  - e.g., weather forecast: 25% chance it will rain today
  - e.g., medical treatment: when unconfident, start a patient on a drug at a lower dose and decide later whether to change the medication or dose

Classifier Confidence: How to Measure for K-Nearest Neighbors?

- Proportion of neighbors with label *y*; e.g.,

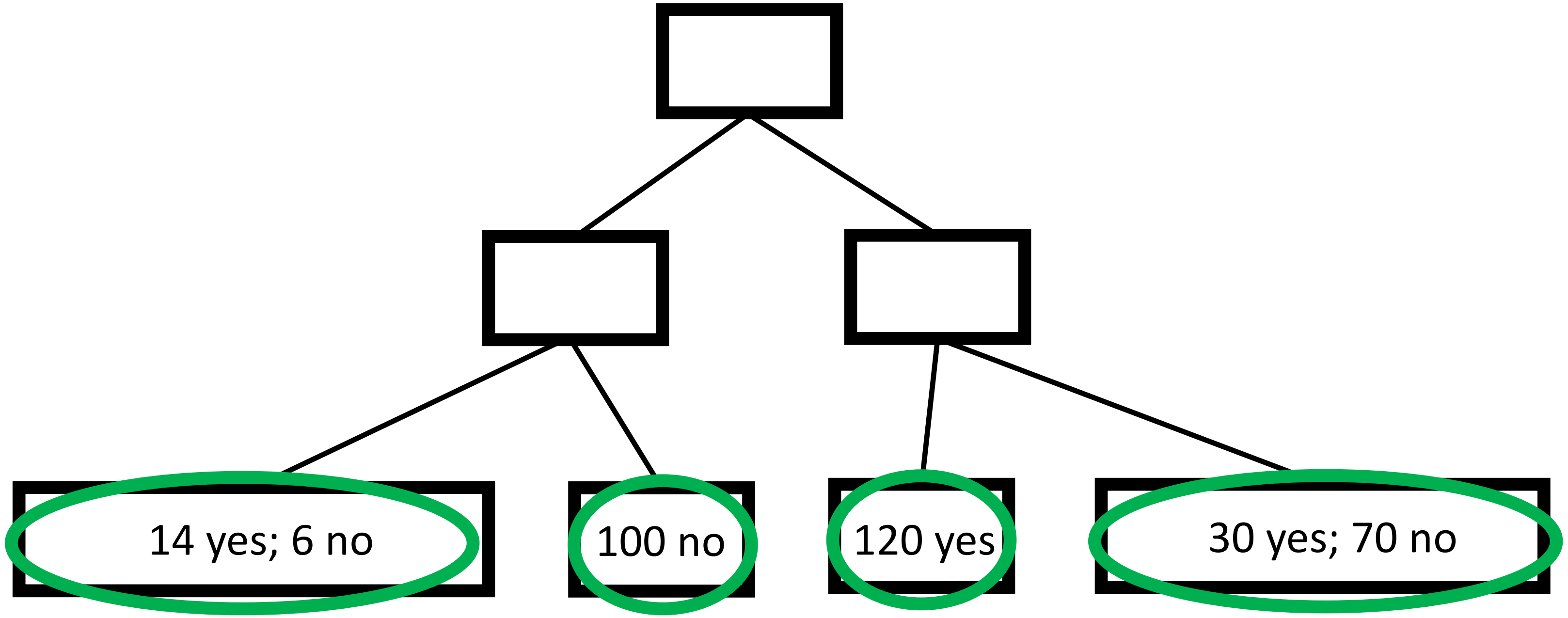
When K=3:



https://github.com/amueller/introduction_to_ml_with_python/blob/master/02-supervised-learning.ipynb

Classifier Confidence: How to Measure for Decision Trees?

- Proportion of training samples with label *y* in the leaf where for the test sample; e.g.,

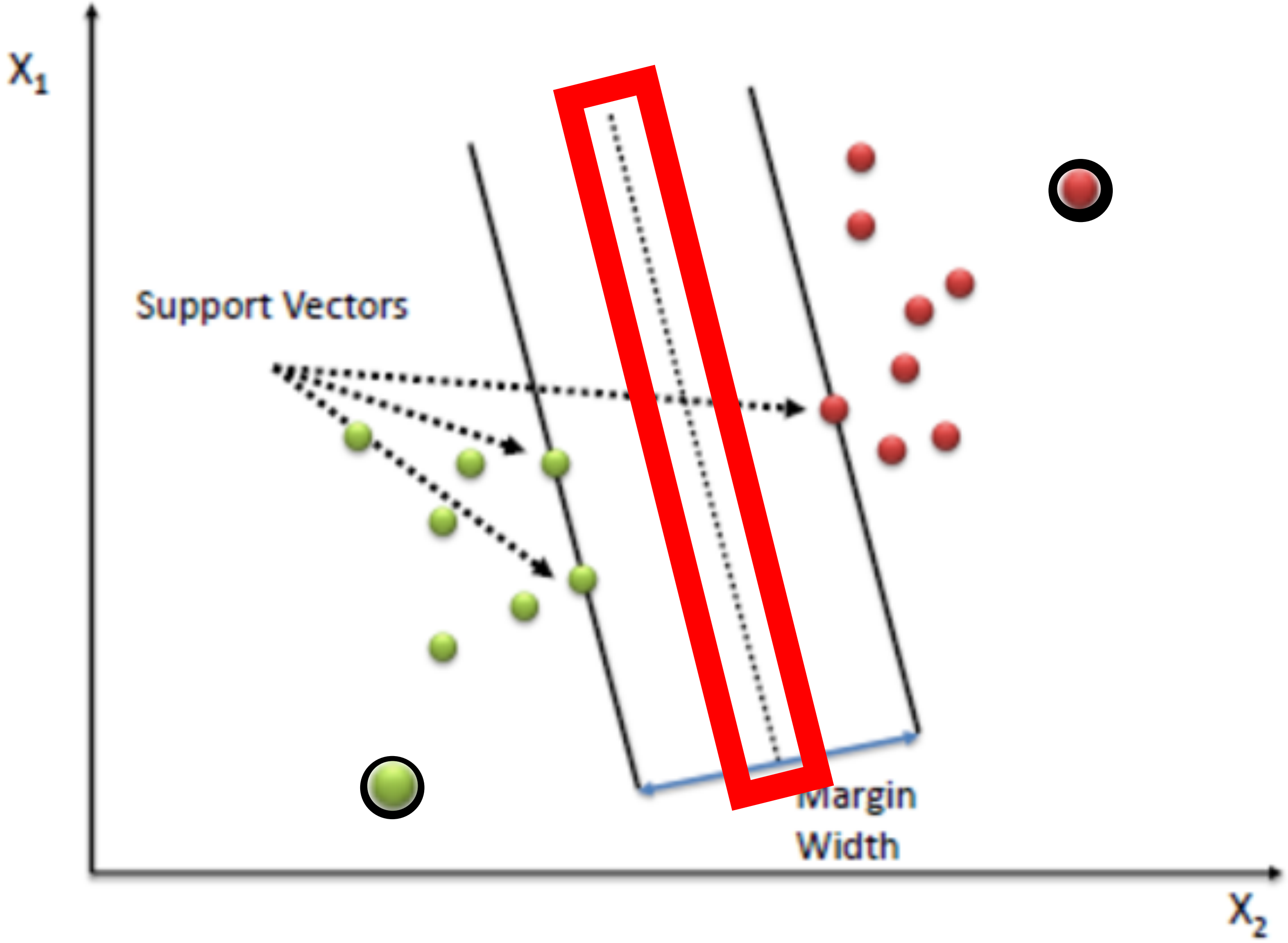


Classifier Confidence: How to Measure for Naïve Bayes?

- Conditional probability P (Y|X) for the most probable class

Classifier Confidence: How to Measure for Support Vector Machines?

- Distance to the hyperplane: e.g.,



http://chem-eng.utoronto.ca/~datamining/dmc/support_vector_machine.htm

Classifier Confidence vs Probability

- Classifiers can make mistakes in estimating their confidence level
- External calibration procedures can address this issue (e.g., using calibration curves/reliability diagrams)

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Classification from a Classifier's Confidence

- Observation: A threshold must be chosen to define the point at which the example belongs to a class or not

- Motivation: how to choose the threshold?
  - Default is 0.5
  - Yet, it can tuned to avoid different types of errors

Review: Confusion Matrix for Binary Classification

		Predicted class	
		P	N
Actual Class	P	True Positives (TP)	False Negatives (FN)
	N	False Positives (FP)	True Negatives (TN)

Python Machine Learning; Raschkka & Mirjalili

Receiver Operating Characteristic (ROC) curve

		Predicted class	
		P	*N*
Actual Class	*P*	True Positives (TP)	False Negatives (FN)
	N	False Positives (FP)	True Negatives (TN)

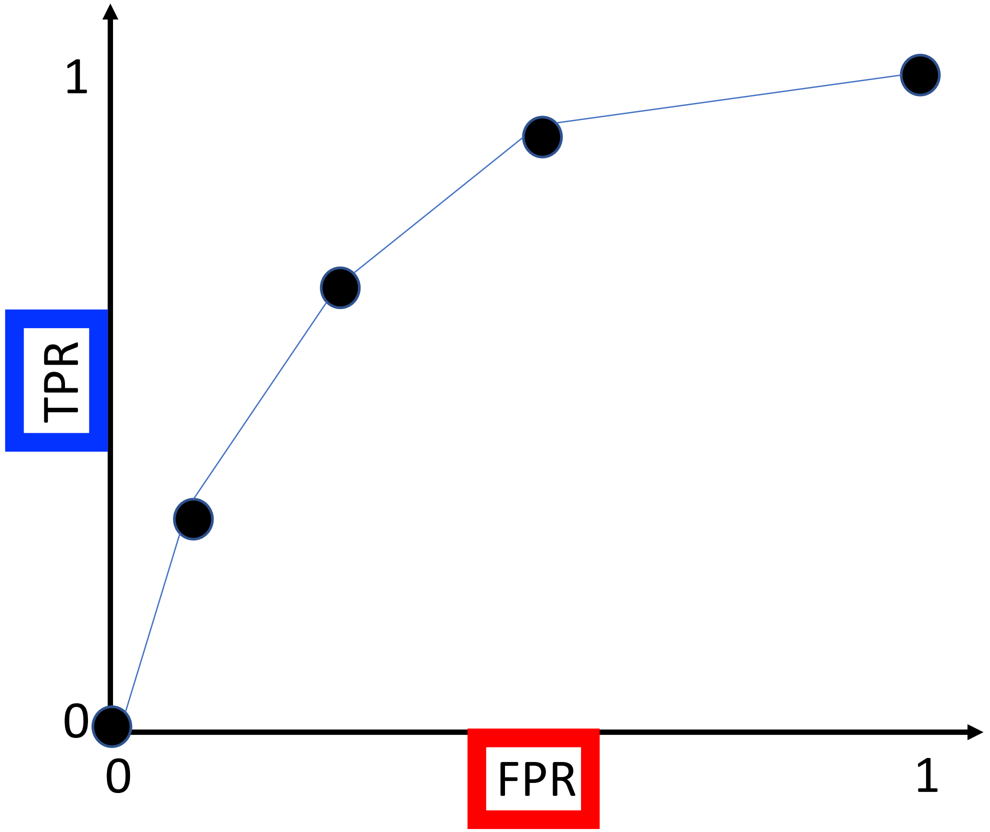
Summarizes performance based on the positive class
- A positive prediction is either correct (TP) or not (FP)

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

$$REC = TPR = \frac{TP}{P} = \frac{TP}{FN+TP}$$

Receiver Operating Characteristic (ROC) curve

To create, vary prediction threshold and compute TPR and FPR for each threshold



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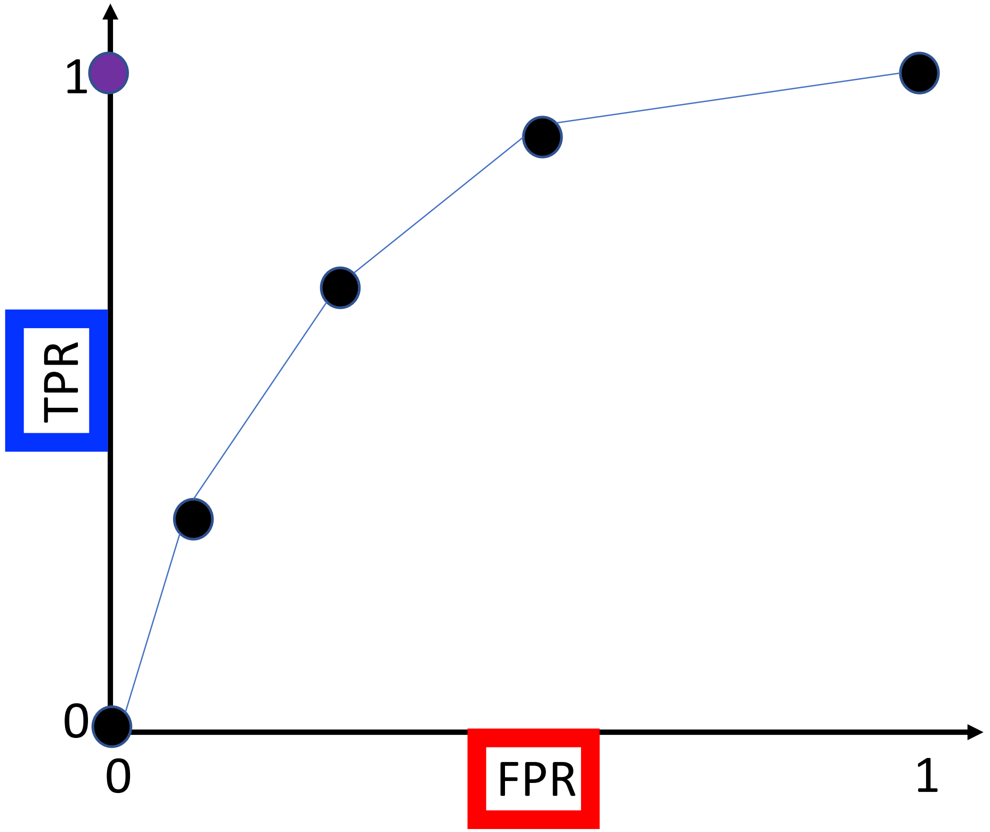
Receiver Operating Characteristic (ROC) curve

What is the coordinate for a perfect predictor?



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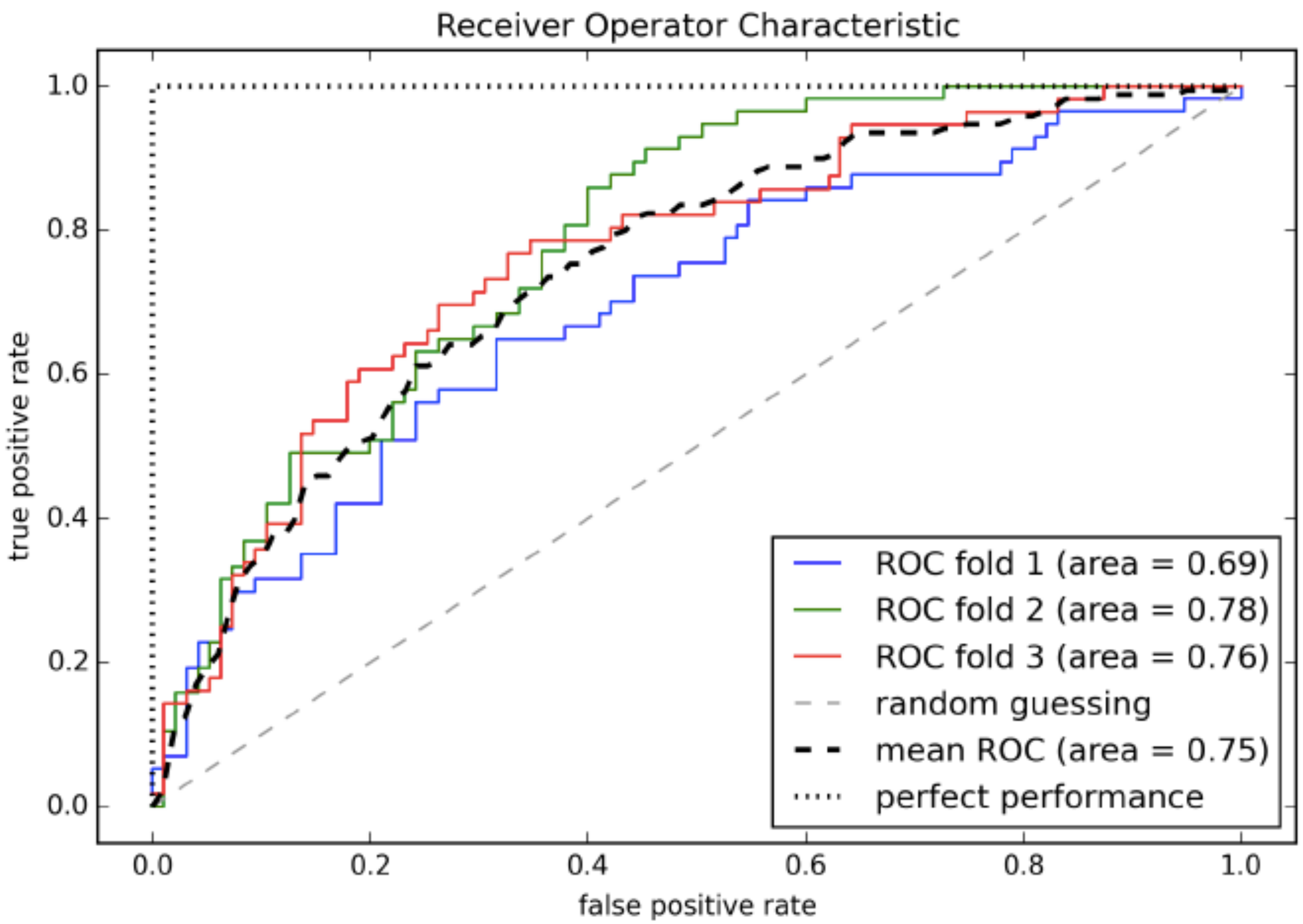
ROC Curve: Area Under Curve (AUC)

Which of the first three methods performs best overall?



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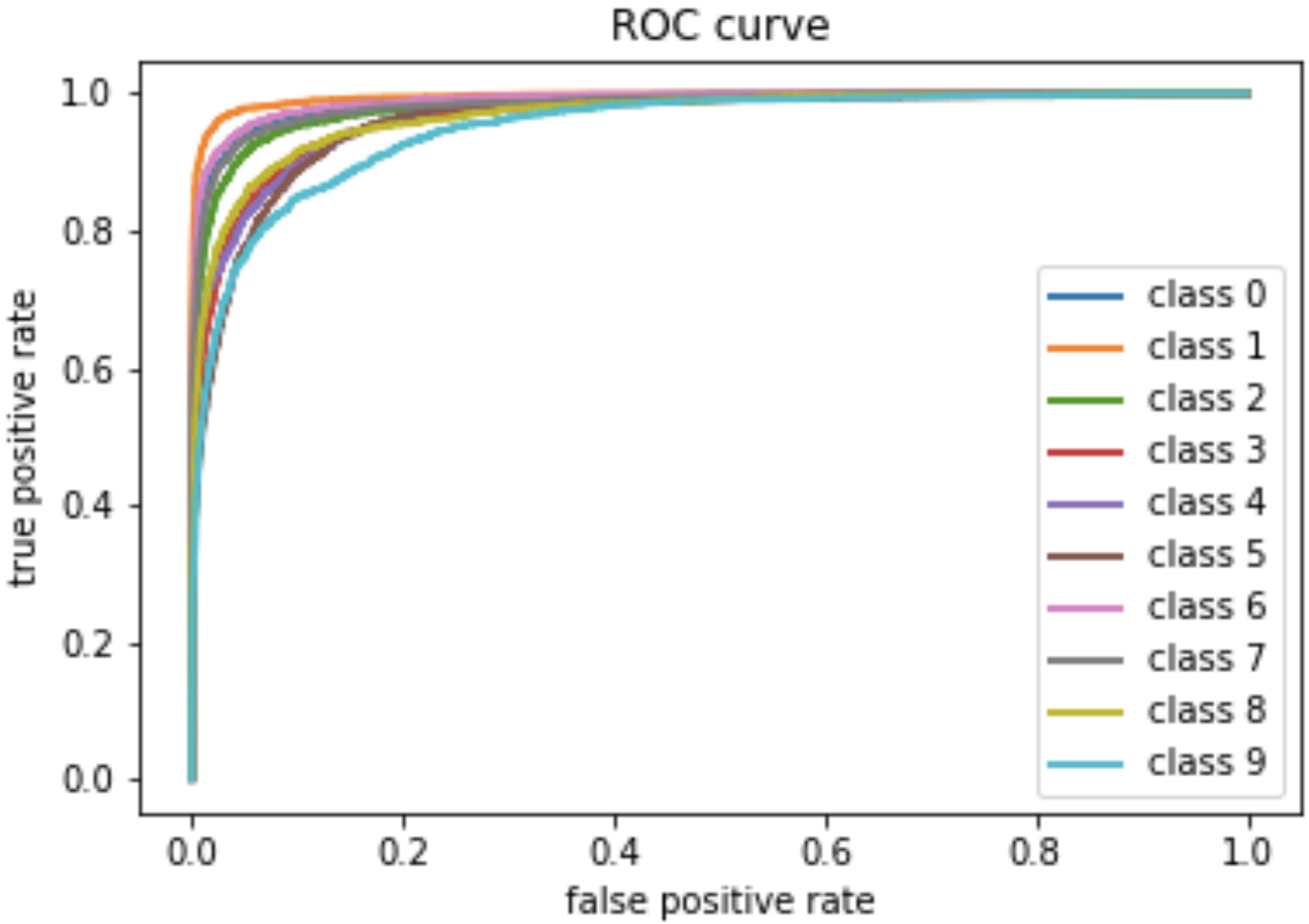
Python Machine Learning; Raschkka & Mirjalili

ROC Curve: Multiclass Classification

- Plot curve per class:



https://stackoverflow.com/questions/56090541/how-to-plot-precision-and-recall-of-multiclass-classifier

Precision-Recall (PR) Curve

		Predicted class	
		P	N
Actual Class	P	True Positives (TP)	False Negatives (FN)
	N	False Positives (FP)	True Negatives (TN)

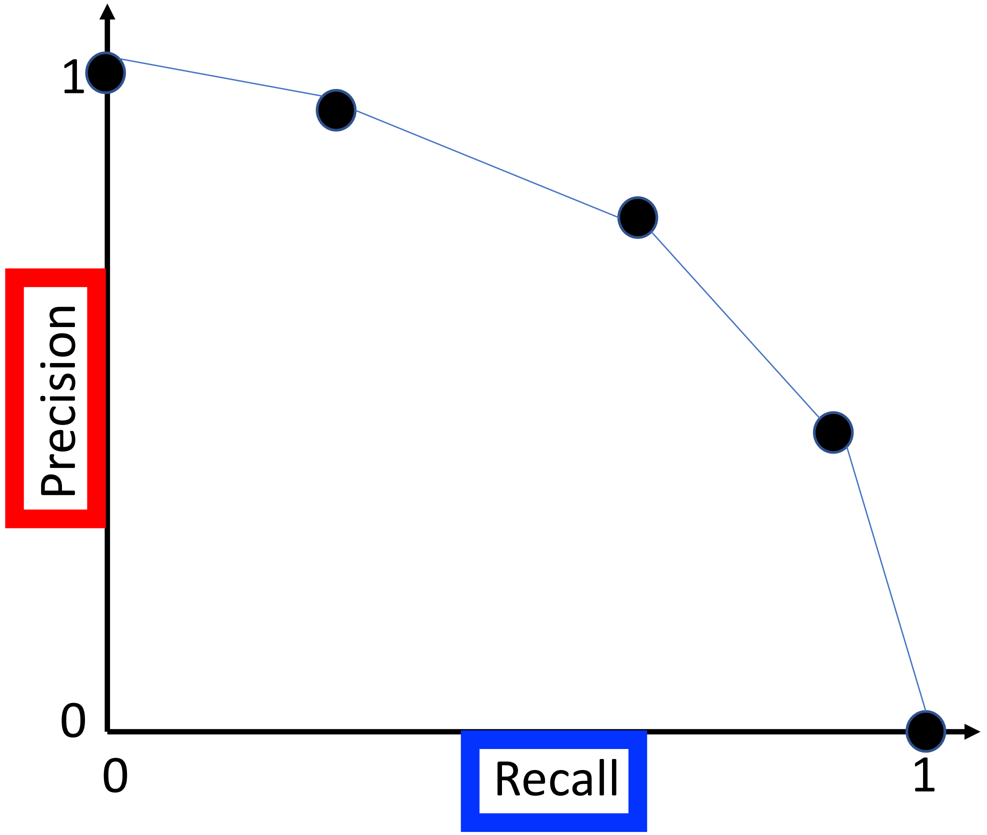
Summarizes performance based only on the positive class (ignores true negatives):

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

$$REC = TPR = \frac{TP}{P} = \frac{TP}{FN + TP}$$

Precision-Recall (PR) Curve

To create, vary prediction threshold and compute precision and recall for each threshold



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Precision-Recall (PR) Curve

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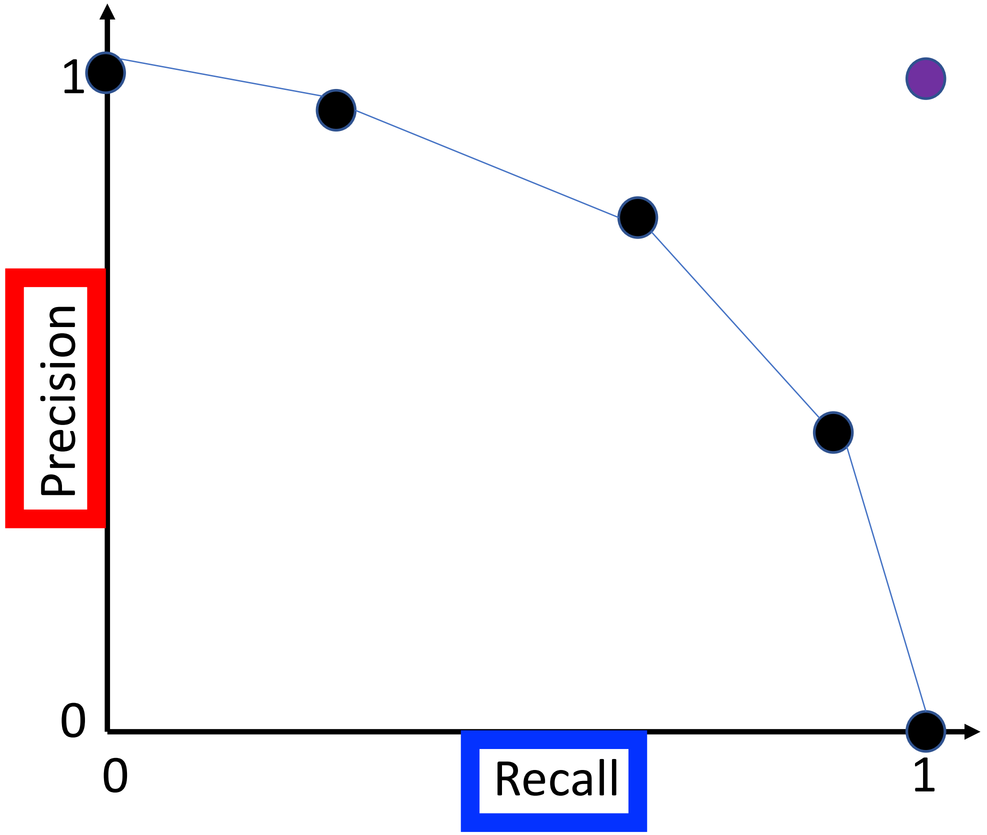

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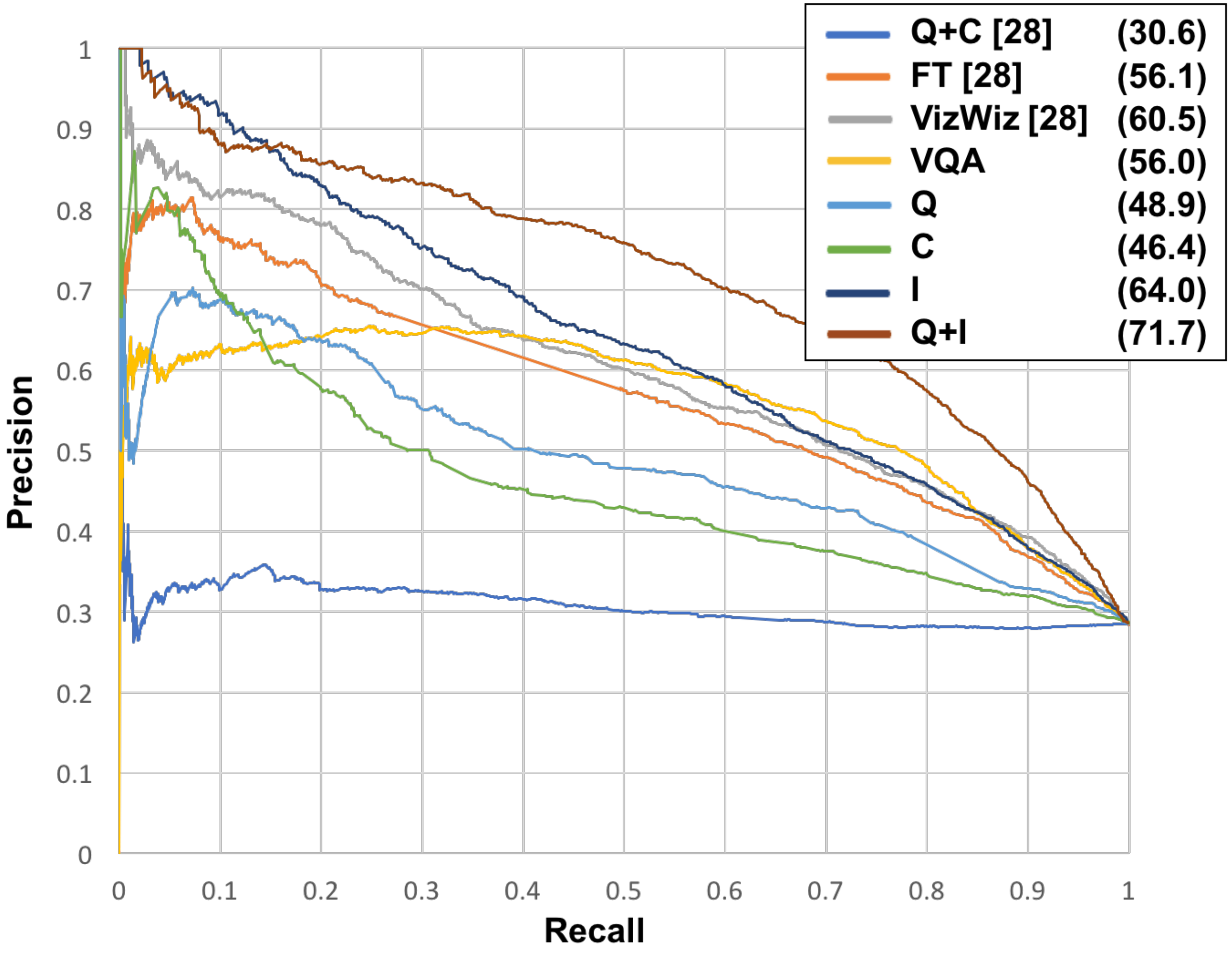
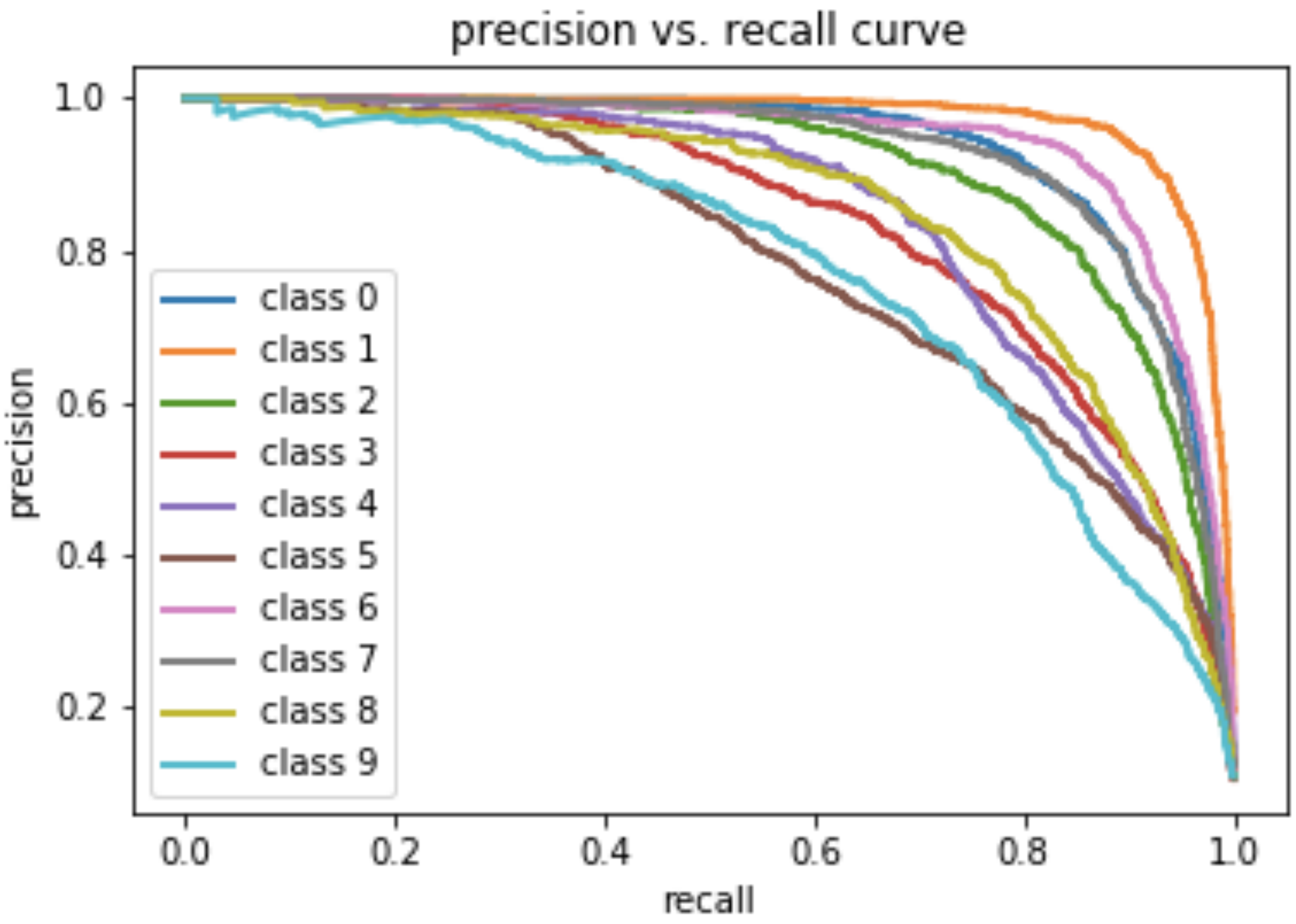
PR Curve: Area Under Curve (AUC)



- Which classifier is the best?

PR Curve: Multiclass Classification

- Plot curve per class:



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Group Discussion: Evaluation Curves

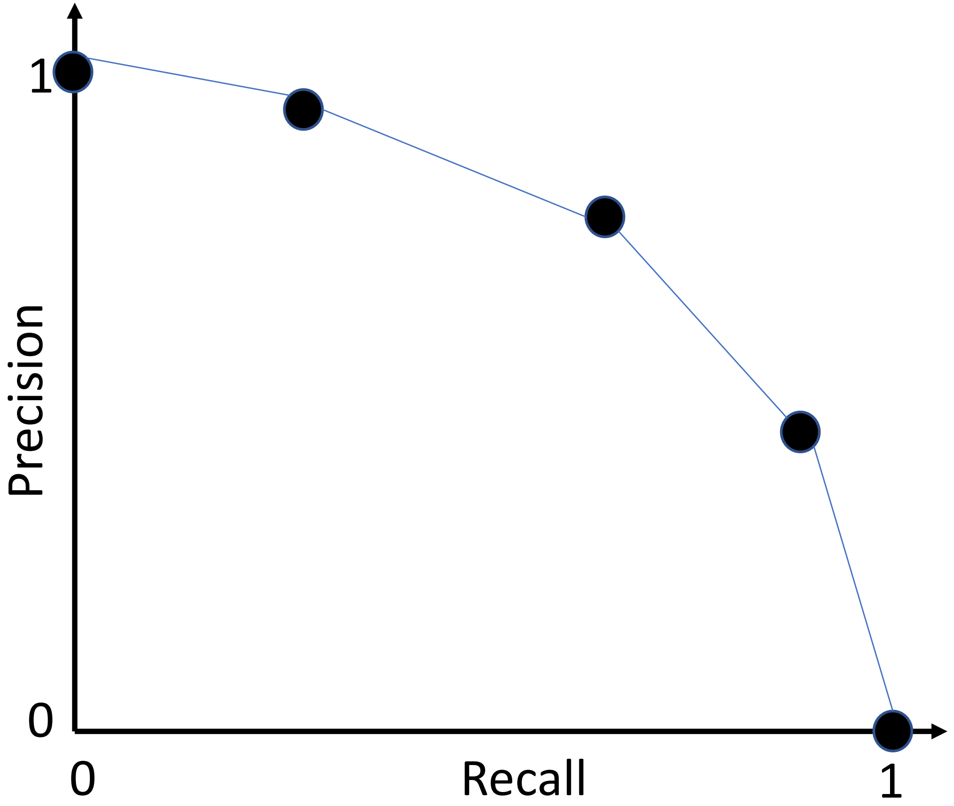
1. Assume you are building a classifier for these applications:
    - Detecting offensive content online
    - Medical diagnoses
    - Detecting shoplifters
    - Deciding whether a person is guilty of a crime

What classifier threshold would you choose for each application and why?

2. When would you choose to evaluate with a PR curve versus a ROC curve?

3. What is the area under the ROC and PR curves for a perfect classifier?

Assume the following thresholds were used to create the curve: 0, 0.25, 0.5, 0.75, 1.



Today’s Topics

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Idea: How Many Predictors to Use?

More than 1: Ensemble

Why Choose Ensemble Instead of an Algorithm?

- Reduces probability for making a wrong prediction, assuming:
  - Classifiers are independent (not true in practice!)
- Suppose:
  - n classifiers for binary classification task
  - Each classifier has same error rate ε
  - Probability mass function indicates the probability of error from an ensemble:

Number of classifiers

Classifier error rate

$$P(y \geq k) = \sum_{k}^{\boxed{n}} \boxed{\binom{n}{k}} \varepsilon^{k} (1 - \boxed{\varepsilon})^{n-k} = \boxed{\varepsilon_{ensemble}}$$

Error probability

ways to choose *k* subsets from set of size *n*

  - e.g., n = 11, ε = 0.25; k = 6: probability of error is ~0.034 which is much lower than probability of error from a single algorithm (0.25)

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How to Get Diverse Classifiers?

$$P(y \geq k) = \sum_{k}^{n} \binom{n}{k} \varepsilon^{k} (1-\varepsilon)^{n-k} = \varepsilon_{ensemble}$$

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- Suppose:
  - n classifiers for binary classification task
  - Probability mass function indicates the probability of error from an ensemble:

than probability of error from a single algorithm (0.25)

1. Use different algorithms

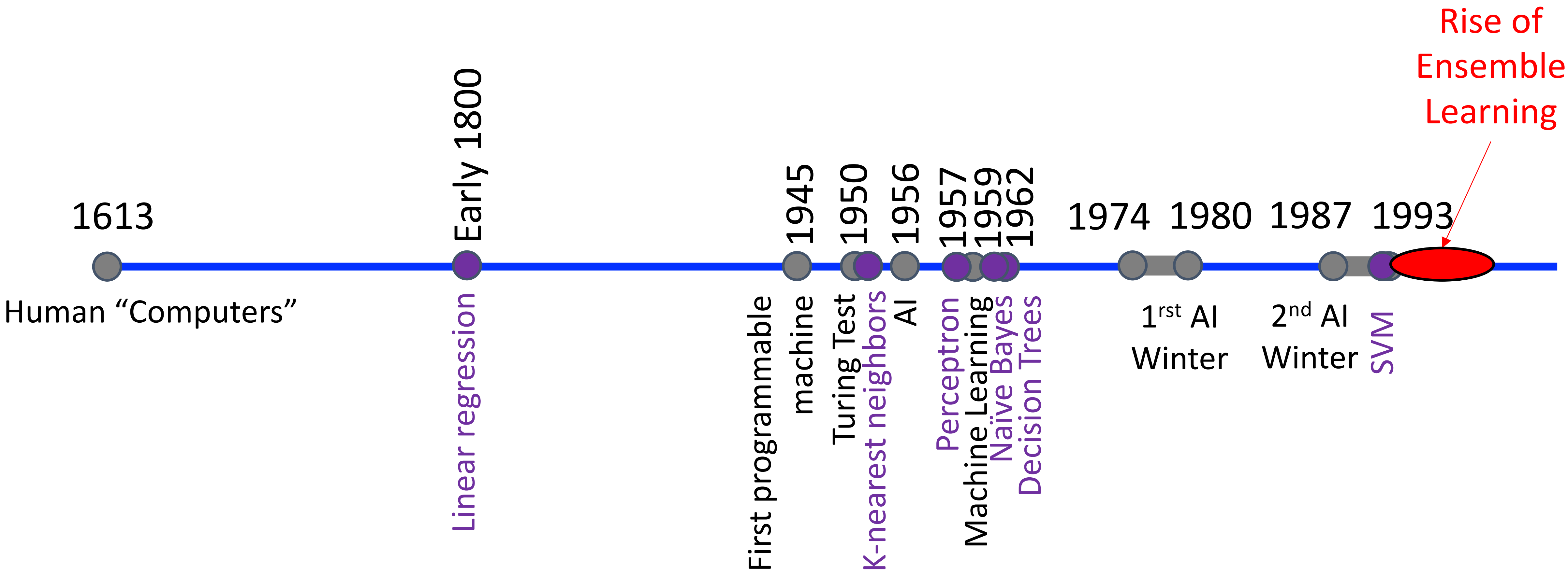
2. Use different features

2. Use different training data

How to Predict with an Ensemble?

- Majority Voting
  - Return most popular prediction from multiple prediction algorithms
- Bootstrap Aggregation, aka Bagging
  - Resample data to train algorithm on different random subsets
- Boosting
  - Reweight data to train algorithms to specialize on different “hard” examples
- Stacking
  - Train a model that learns how to aggregate classifiers’ predictions

Historical Context of ML Models



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Majority Voting

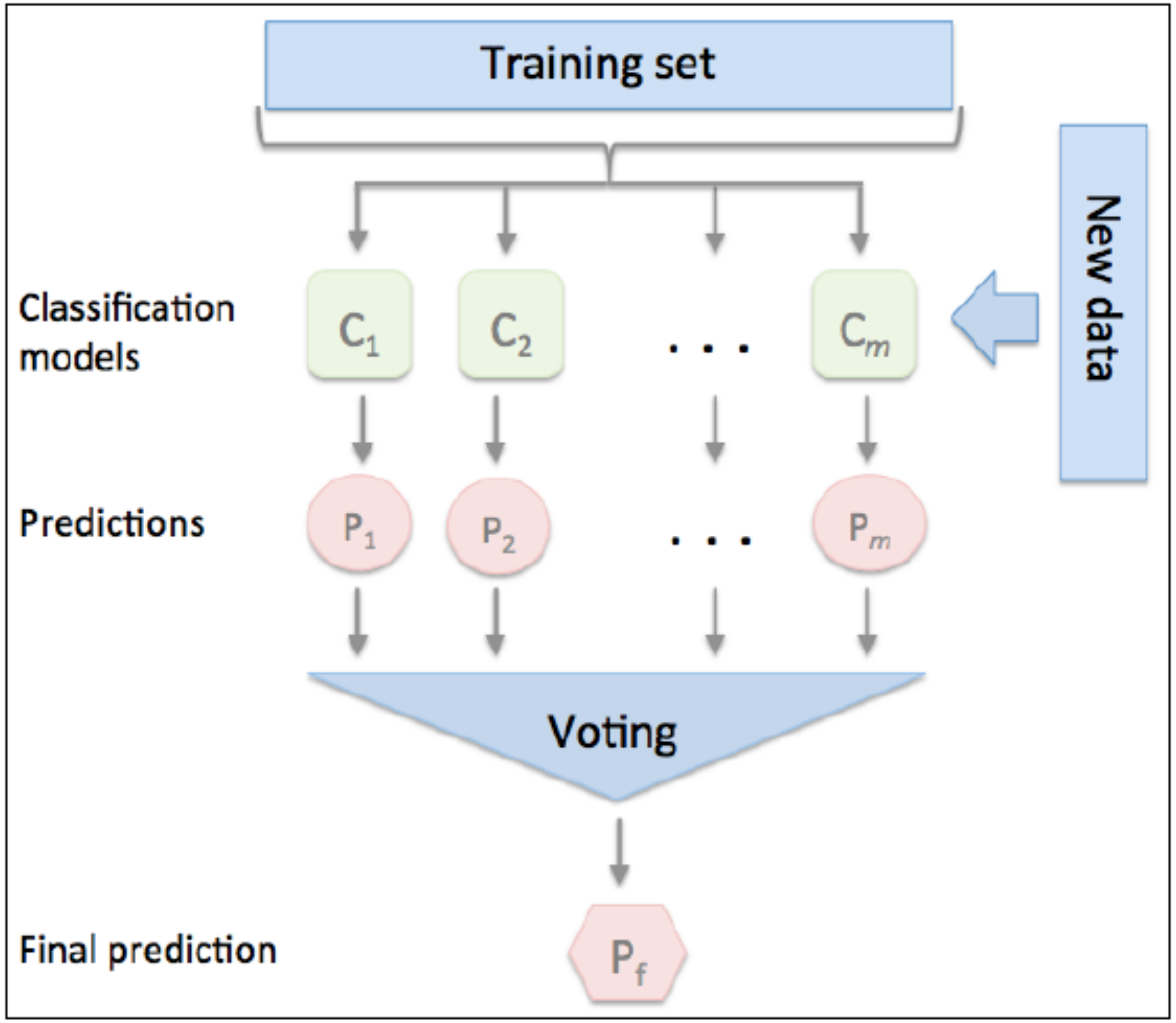
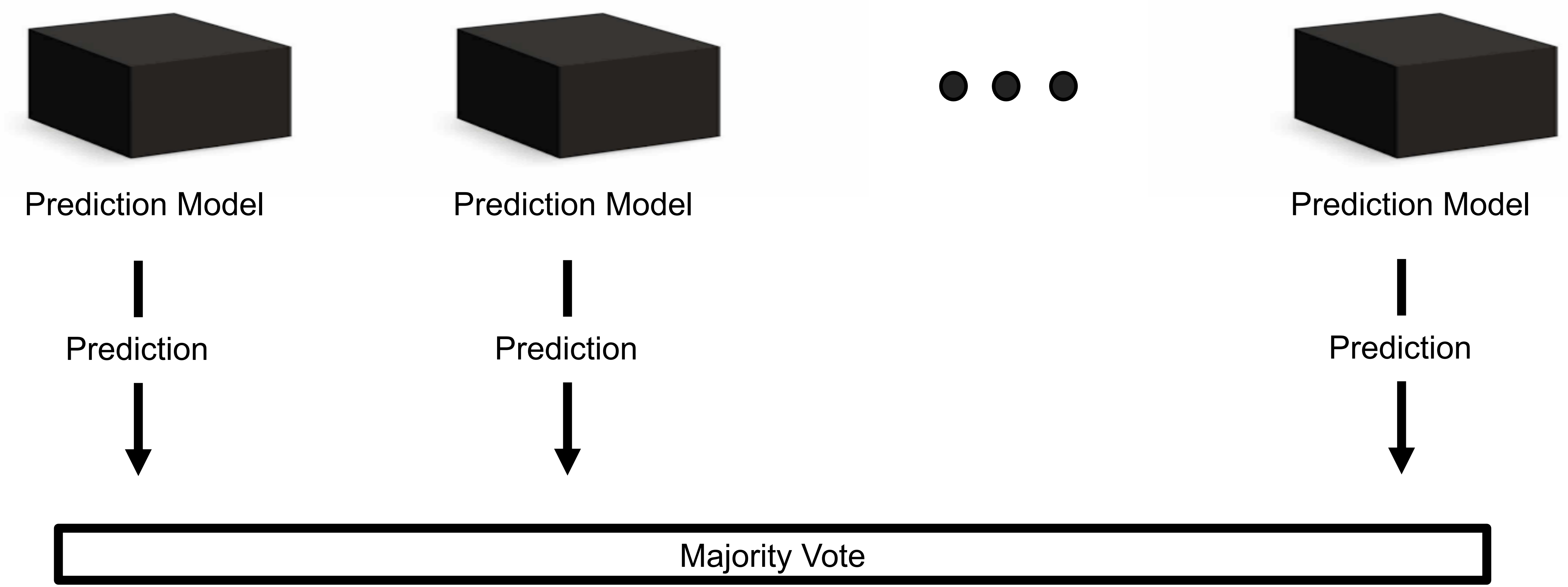


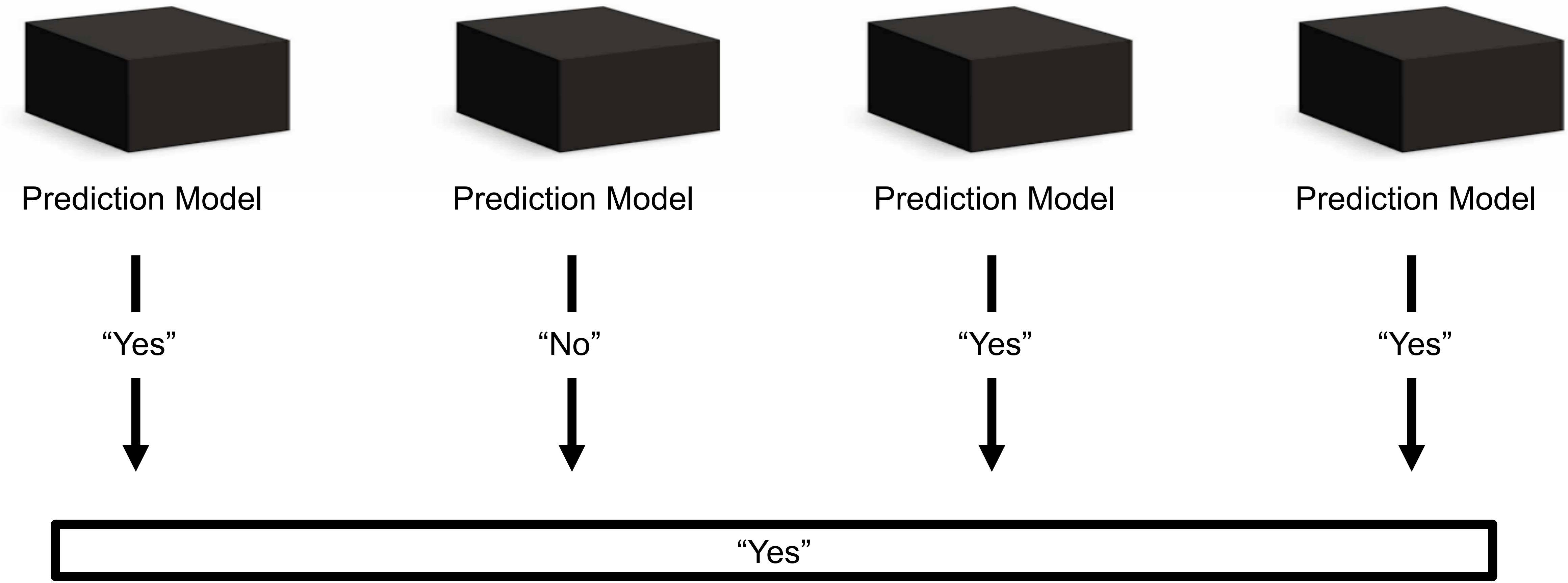
Figure Credit: Raschka & Mirjalili, Python Machine Learning.

Majority Voting

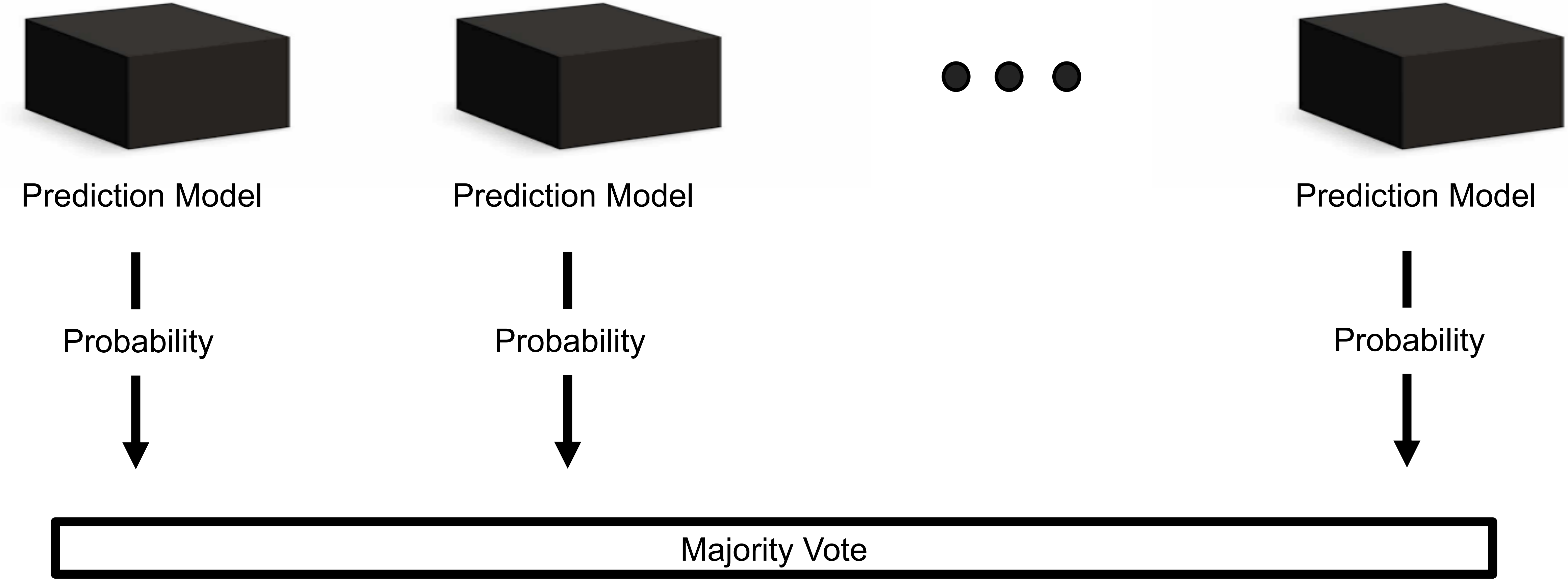


Majority Voting: Binary Task

e.g., “Is it sunny today?”

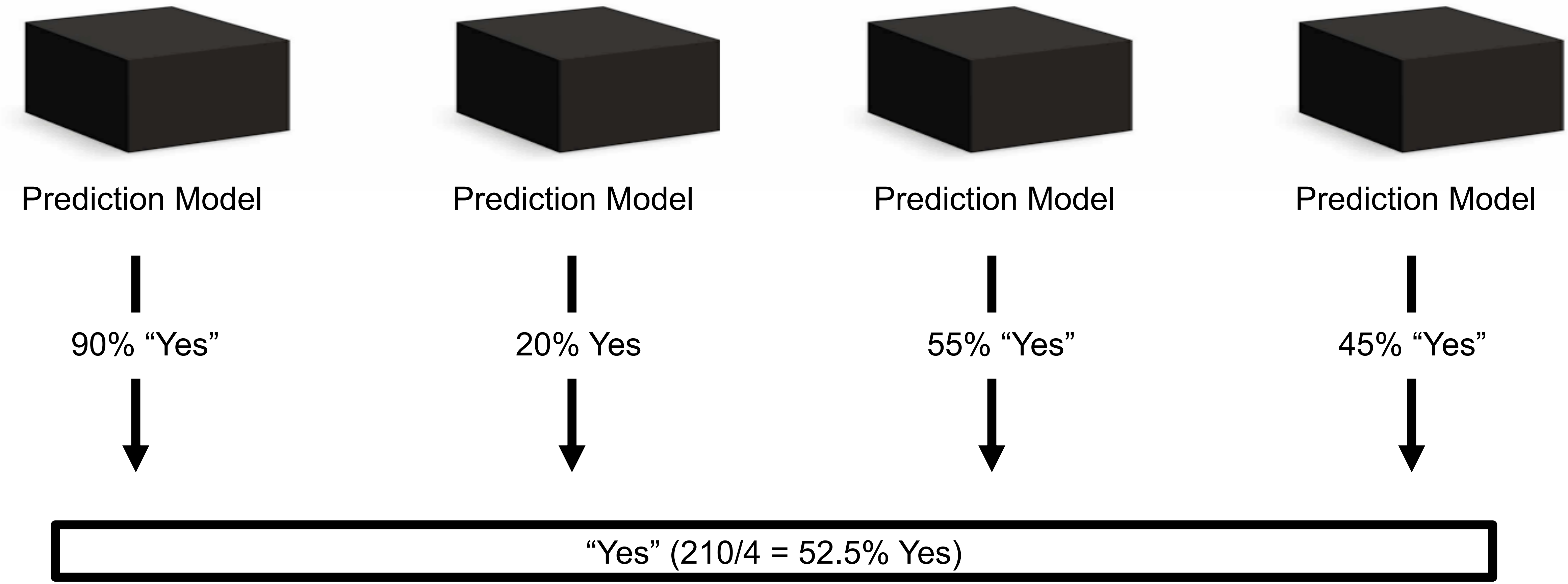


Majority Voting: “Soft” (not “Hard”)



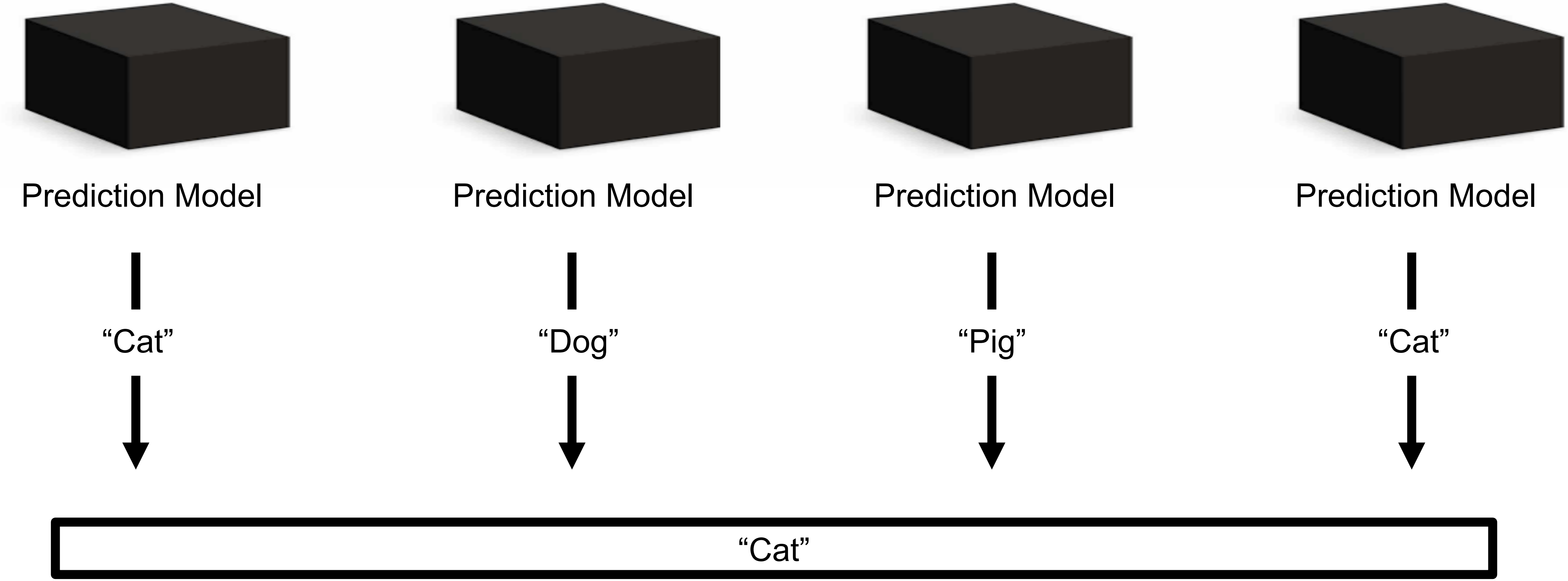
Majority Voting: Soft Voting on Binary Task

e.g., “Is it sunny today?”



Plurality Voting: Non-Binary Task

e.g., “What object is in the image?”



Majority Voting: Regression

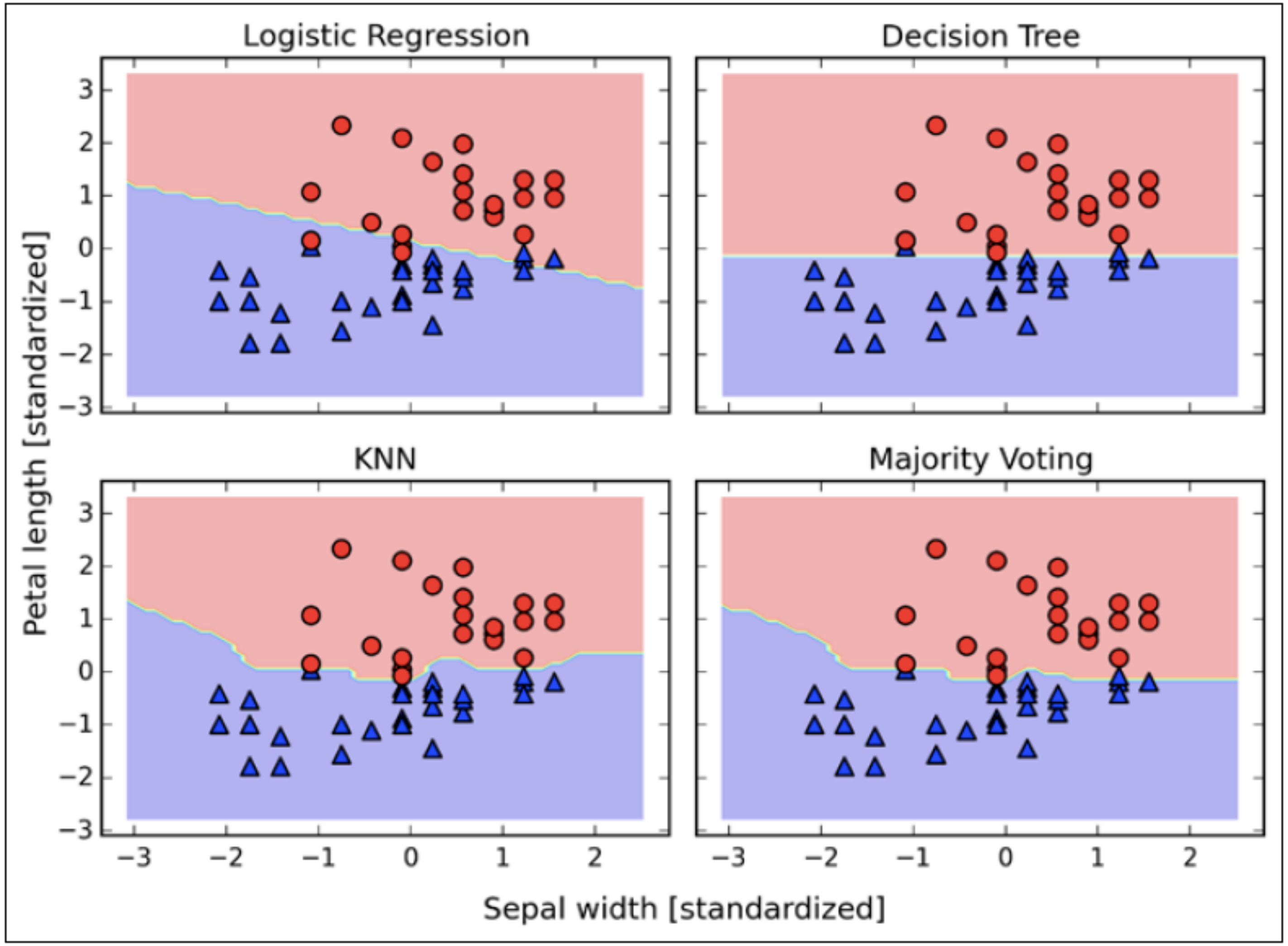
e.g., “Is it sunny today?”

Prediction Model | Prediction Model | Prediction Model | Prediction Model

90% “Yes” | 20% Yes | 55% “Yes” | 45% “Yes”

52.5% (average prediction)

Majority Voting: Example of Decision Boundary



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Bagging

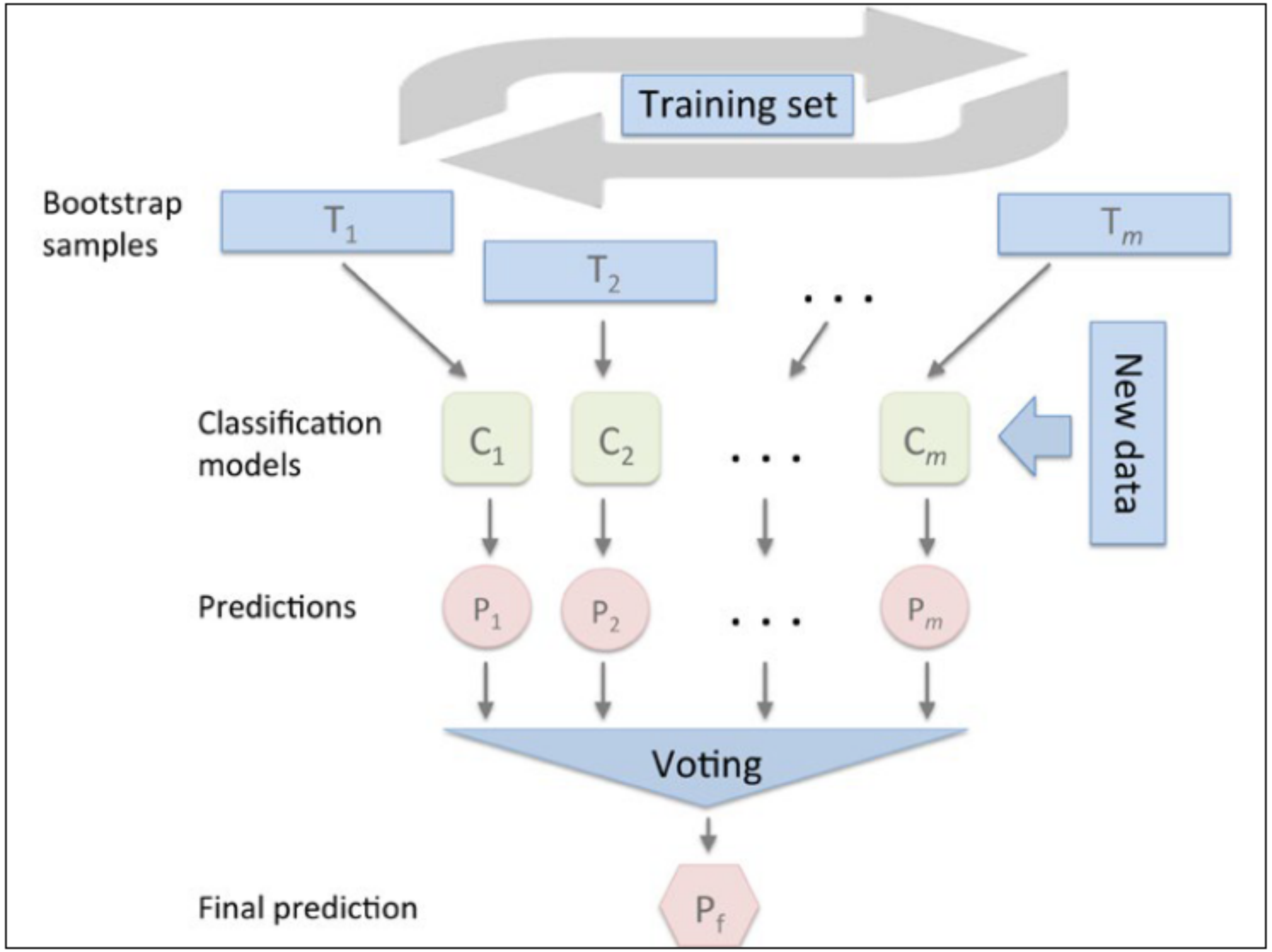


Figure Credit: Raschka & Mirjalili, Python Machine Learning.

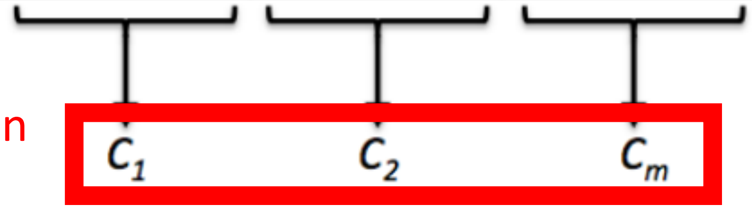
Bagging: Training

- Build ensemble from “bootstrap samples” drawn with replacement
- e.g.,

Duplicate data can occur for training

Some examples missing from training data; e.g., round 1

Sample indices	Bagging round 1	Bagging round 2	...
1	2	7	...
2	2	3	...
3	1	2	...
4	3	1	...
5	7	1	...
6	2	7	...
7	4	7	...



Each classifier trained on different subset of data

Breiman, Bagging Predictors, 1994.

Ho, Random Decision Forests, 1995.

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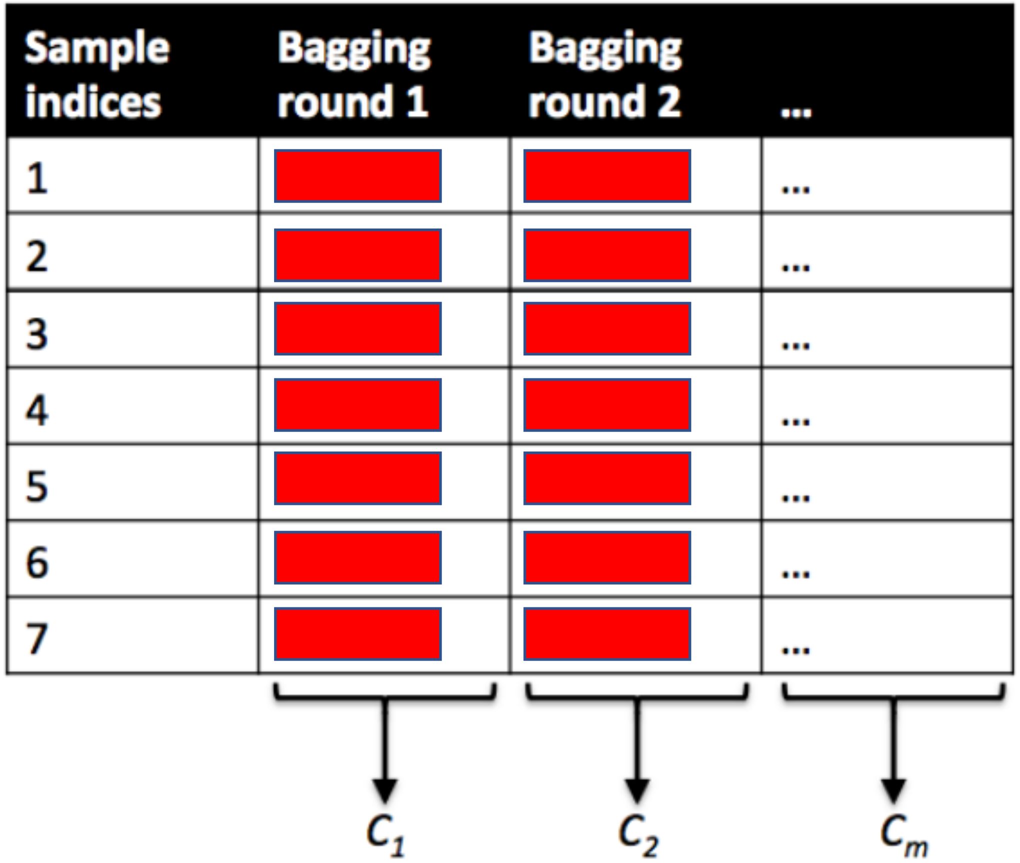
- e.g.,



Class Demo:
- Pick a number from the bag

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Bagging: Predicting

Prediction Model Prediction Model Prediction Model Prediction Model

- Predict as done for “majority voting”
  - e.g., “hard” voting
  - e.g., “soft” voting
  - e.g., averaging values for regression

Bagging: Random Forest

- Build ensemble from "bootstrap samples" drawn with replacement
- e.g.,

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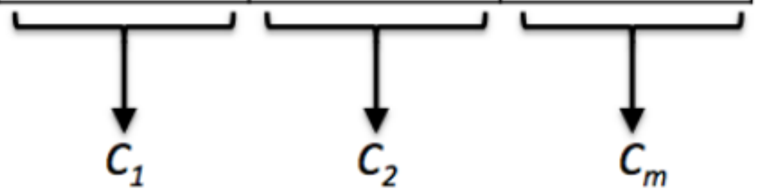

Fit decision trees by also selecting random feature subsets

Breiman, Bagging Predictors, 1994.
Ho, Random Decision Forests, 1995.
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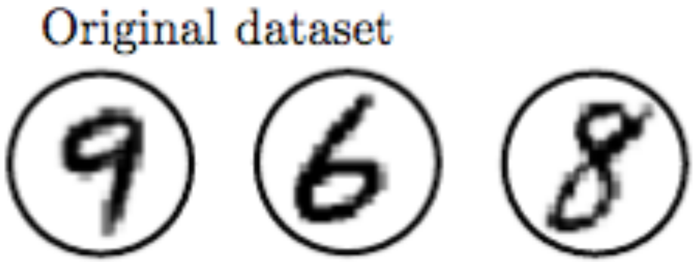
Bagging: Intuition (Train an 8 detector)



Fellow et al., Deep Learning (chapter 7), 2016.

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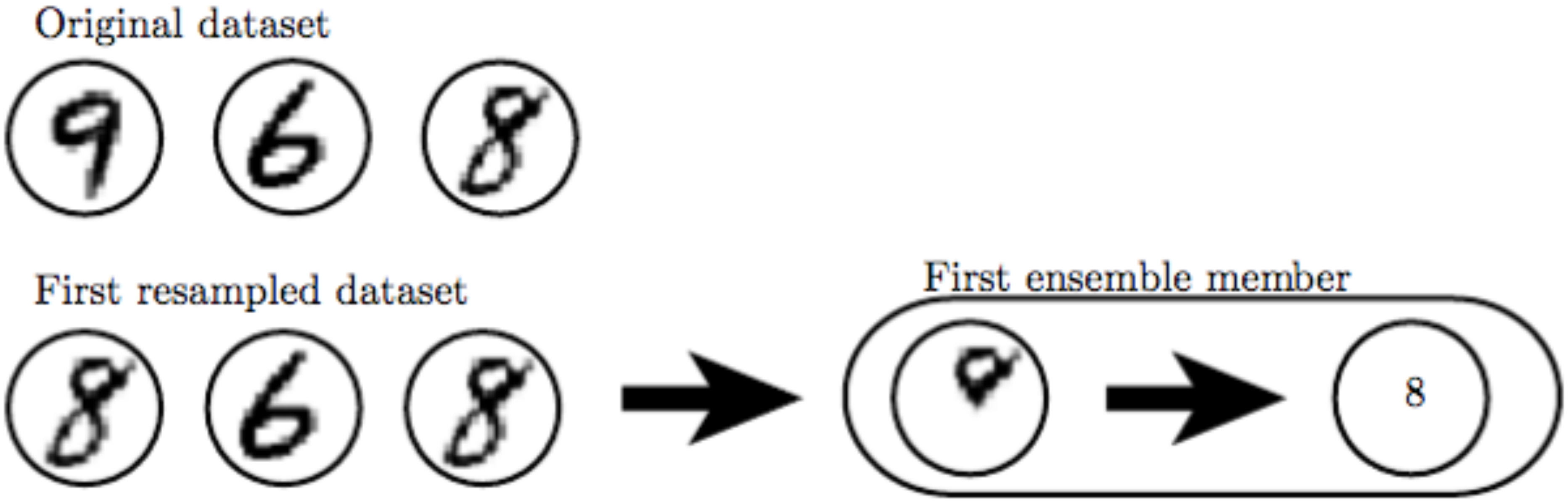

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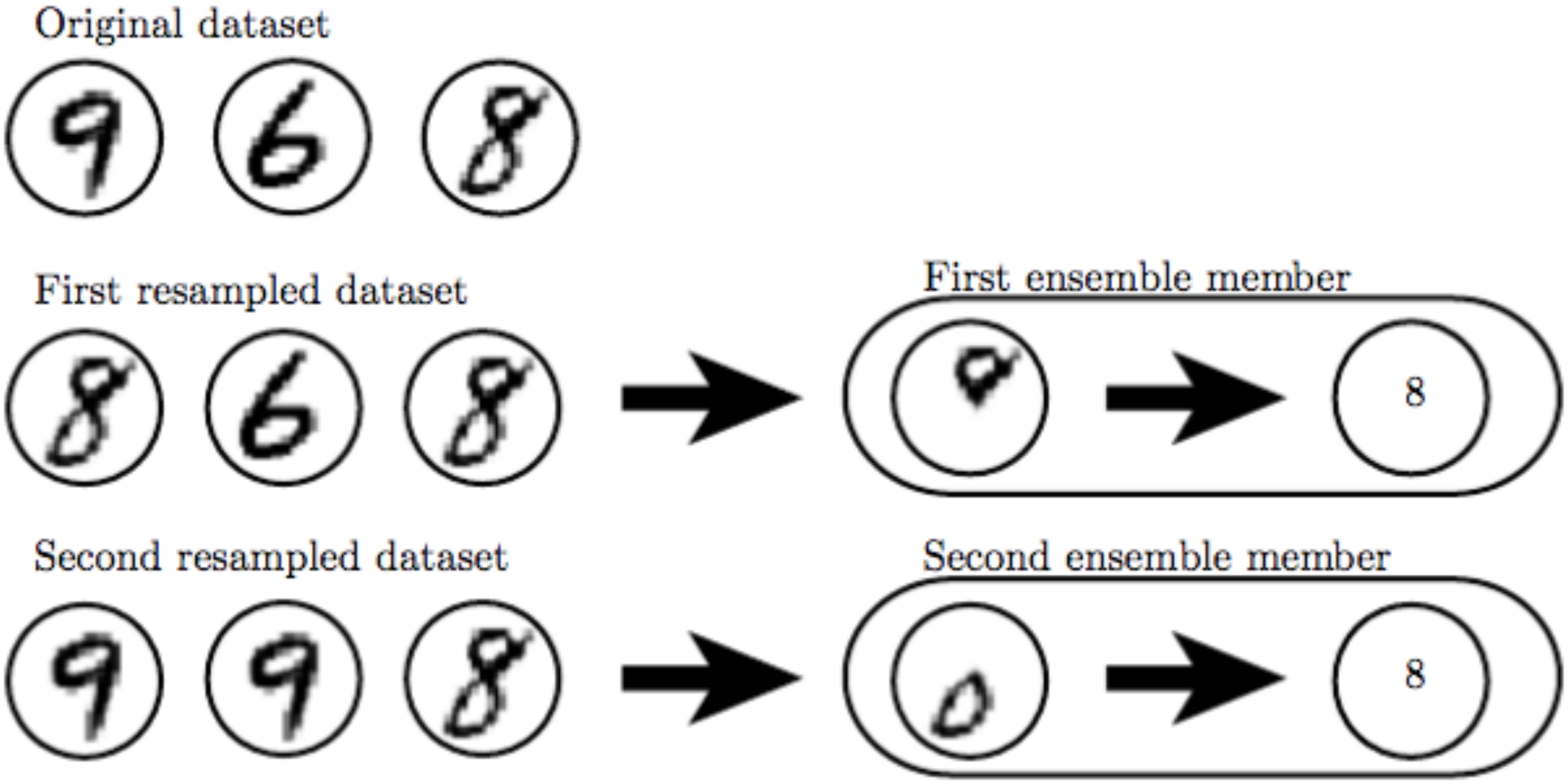

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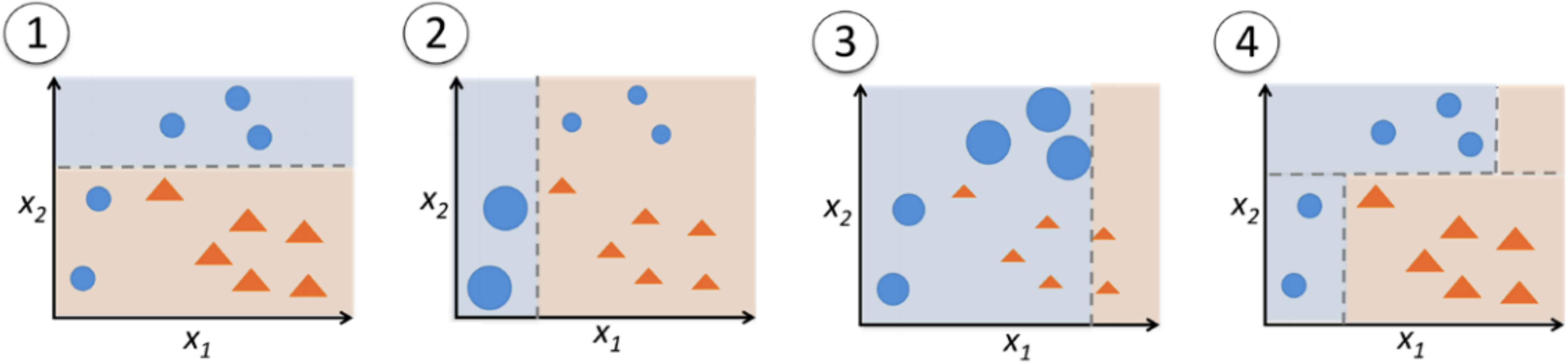
Boosting

- Key idea: sequentially train predictors that each try to correctly predict examples that were hard for previous predictors

- Original Algorithm:
  - Train classifier 1: use random subset of examples without replacement
  - Train classifier 2: use a second random subset of examples without replacement and add 50% of examples misclassified by classifier 1
  - Train classifier 3: use examples that classifiers 1 and 2 disagree on
  - Predict using majority vote from 3 classifiers

Boosting – Adaboost (**Ada**ptive **Boost**ing)



Assign equal weights to all examples

- Assign larger weights to previous misclassifications
- Assign smaller weights to previous correct classifications

- Assign larger weights to training samples C_1 and C_2 disagree on
- Assign smaller weights to previous correct classifications

Predict with weighted majority vote

Freund and Schapire, Experiments with a New Boosting Algorithm, 1996.

Raschka and Mirjalili; Python Machine Learning

Boosting – Adaboost (**Ada**ptive **Boost**ing)

e.g., 1d dataset

Sample indices	x	y	Weights	$\hat{y}(x <= 3.0)$?	Correct?	Updated weights
1	1.0	1	0.1	1	Yes	0.072
2	2.0	1	0.1	1	Yes	0.072
3	3.0	1	0.1	1	Yes	0.072
4	4.0	-1	0.1	-1	Yes	0.072
5	5.0	-1	0.1	-1	Yes	0.072
6	6.0	-1	0.1	-1	Yes	0.072
7	7.0	1	0.1	-1	No	0.167
8	8.0	1	0.1	-1	No	0.167
9	9.0	1	0.1	-1	No	0.167
10	10.0	-1	0.1	-1	Yes	0.072

Round 2: update weights

Round 1: training data, weights, predictions

Raschka and Mirjalili; Python Machine Learning

Boosting – Adaboost (**Ada**ptive **Boost**ing)

e.g., 1d dataset

1. Compute error rate (sum misclassified examples' weights):

$$\varepsilon = 0.1\times 0 + 0.1\times 0 + 0.1\times 0 + 0.1\times 0 + 0.1\times 0 + 0.1\times 0 + 0.1\times 1 + 0.1\times 1 + 0.1\times 1 + 0.1\times 0 = \frac{3}{10} = 0.3$$

2. Compute coefficient used to update weights and make majority vote prediction:

$$\alpha_j = 0.5\log\left(\frac{1-\varepsilon}{\varepsilon}\right) \approx 0.424$$

3. Update weight vector:

$$\boldsymbol{w} := \boldsymbol{w} \times \exp\left(-\alpha_j \times \hat{\boldsymbol{y}} \times \boldsymbol{y}\right)$$

- Correct predictions will decrease weight and vice versa

$$0.1\times\exp\left(-0.424\times 1\times 1\right) \approx 0.065 \quad 0.1\times\exp\left(-0.424\times(-1)\times(1)\right) \approx 0.153$$

4. Normalize weights to sum to 1:

$$\boldsymbol{w} := \frac{\boldsymbol{w}}{\sum_i w_i}$$

$$\sum_i w_i = 7\times 0.065 + 3\times 0.153 = 0.914$$

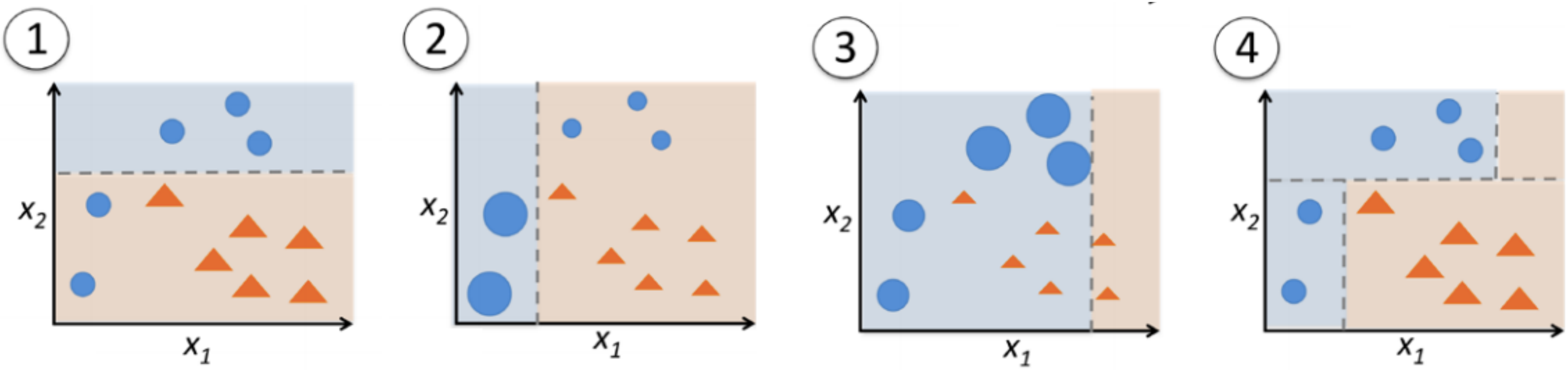
Correct?	Updated weights
Yes	0.072
Yes	0.072
Yes	0.072
Yes	0.072
Yes	0.072
Yes	0.072
No	0.167
No	0.167
No	0.167
Yes	0.072

$0.065 / 0.914$

$0.153 / 0.914$

Raschka and Mirjalili; Python Machine Learning

Boosting – Adaboost (**Ada**ptive **Boost**ing)



To predict, use α calculated for each classifier as its weight when voting with all trained classifiers.

Idea: value the prediction of each classifier based on the accuracies they had on the training dataset.

Raschka and Mirjalili; Python Machine Learning

How to Predict with an Ensemble of Algorithms?

- Majority Voting
  - Return most popular prediction from multiple prediction algorithms
- Bootstrap Aggregation, aka Bagging
  - Train algorithm repeatedly on different random subsets of the training set
- Boosting
  - Train algorithms that each specialize on different “hard” training examples
- Stacking
  - Train a model that learns how to aggregate classifiers’ predictions

Stacked Generalization, aka Stacking

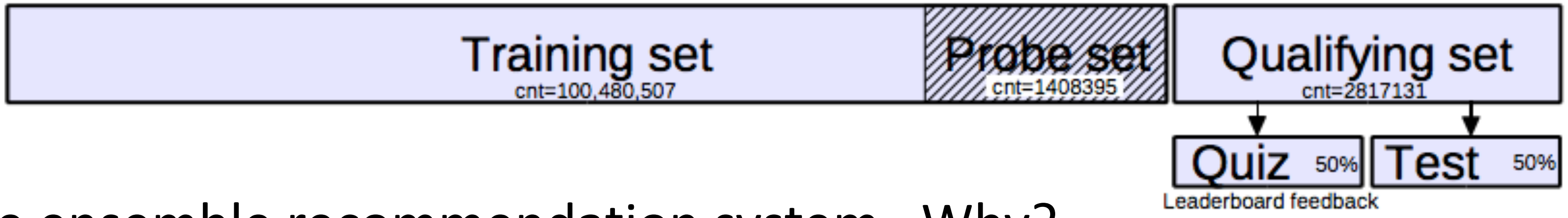
- Train meta-learner to learn the optimal weighting of each classifiers' predictions for making the final prediction
- Algorithm:
  1. Split dataset into three disjoint sets.
  2. Train several base learners on the first partition.
  3. Test the base learners on the second partition and third partition.
  4. Train meta-learner on second partition using classifiers' predictions as features
  5. Evaluate meta-learner on third prediction using classifiers' predictions as features

David, H. Wolpert, Stacked Generalization, 1992.

Tutorial: http://blog.kaggle.com/2017/06/15/stacking-made-easy-an-introduction-to-stacknet-by-competitions-grandmaster-marios-michailidis-kazanova/

Ensemble Learner Won Netflix Prize "Challenge"

- In 2009 challenge, winning team won $1 million using ensemble approach:
  - https://www.netflixprize.com/assets/GrandPrize2009_BPC_BigChaos.pdf
  - Dataset: 5-star ratings on 17770 movies from 480189 "anonymous" users collected by Netflix over ~7 years. In total, the number of ratings is 100,480,507.



- Netflix did not use ensemble recommendation system. Why?
  - "We evaluated some of the new methods offline but the additional accuracy gains that we measured did not seem to justify the engineering effort needed to bring them into a production environment" - https://medium.com/netflix-techblog/netflix-recommendations-beyond-the-5-stars-part-1-55838468f429
  - Computationally slow and complex from using "sequential" training of learners

Yehuda Koren, The BellKor Solution to the Netflix Grand Prize, 2009.

Today's Topics

- One-vs-all multiclass classification
- Classifier confidence
- Evaluation: ROC and PR-curves
- Ensemble learning