MODEL EVALUATION & ENSEMBLE METHODS

Model Evaluation and Selection

- Evaluation metrics: How can we measure accuracy? Other metrics to consider?
- Use **validation test set** of class-labeled tuples instead of training set when assessing accuracy
- Methods for estimating a classifier's accuracy:
  - Holdout method, random subsampling
  - Cross-validation
  - Bootstrap
- Comparing classifiers:
  - Confidence intervals
  - Cost-benefit analysis and ROC Curves

Classifier Evaluation Metrics: Confusion Matrix

Confusion Matrix:

Actual class\Predicted class	C_1	¬ C_1
C_1	**True Positives (TP)**	**False Negatives (FN)**
¬ C_1	**False Positives (FP)**	**True Negatives (TN)**

Example of Confusion Matrix:

Actual class\Predicted class	buy_computer = yes	buy_computer = no	Total
buy_computer = yes	**6954**	**46**	7000
buy_computer = no	**412**	**2588**	3000
Total	7366	2634	10000

- Given *m* classes, an entry, $\boldsymbol{CM_{i,j}}$ in a **confusion matrix** indicates # of tuples in class *i* that were labeled by the classifier as class *j*
- May have extra rows/columns to provide totals

Classifier Evaluation Metrics: Accuracy, Error Rate, Sensitivity and Specificity

A\P	C	¬C	
C	**TP**	**FN**	**P**
¬C	**FP**	**TN**	**N**
	P'	**N'**	**All**

- **Classifier Accuracy,** or recognition rate: percentage of test set tuples that are correctly classified

  Accuracy = (TP + TN)/All

- **Error rate:** *1 – accuracy*, or

  Error rate = (FP + FN)/All

- **Class Imbalance Problem**:
  - One class may be *rare*, e.g. fraud, or HIV-positive
  - Significant *majority of the negative class* and minority of the positive class
  - **Sensitivity**: True Positive recognition rate
    - **Sensitivity = TP/P**
  - **Specificity**: True Negative recognition rate
    - **Specificity = TN/N**

Classifier Evaluation Metrics: Precision and Recall, and F-measures

- **Precision**: exactness – what % of tuples that the classifier labeled as positive are actually positive

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

- **Recall:** completeness – what % of positive tuples did the classifier label as positive?
- Perfect score is 1.0

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

- Inverse relationship between precision & recall
- ***F* measure (*F_1* or *F*-score)**: harmonic mean of precision and recall,

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

- ***F_β*:** weighted measure of precision and recall
  - assigns ß times as much weight to recall as to precision

$$F_\beta = \frac{(1 + \beta^2) \times precision \times recall}{\beta^2 \times precision + recall}$$

Classifier Evaluation Metrics: Example

Actual Class\Predicted class	cancer = yes	cancer = no	Total	Recognition(%)
cancer = yes	**90**	**210**	300	30.00 (*sensitivity*
cancer = no	**140**	**9560**	9700	98.56 (*specificity)*
Total	230	9770	10000	96.40 (*accuracy*)

- *Precision* = 90/230 = 39.13% *Recall* = 90/300 = 30.00%

Evaluating Classifier Accuracy: Holdout & Cross-Validation Methods

- **Holdout method**
  - Given data is randomly partitioned into two independent sets
    - Training set (e.g., 2/3) for model construction
    - Test set (e.g., 1/3) for accuracy estimation
  - Random sampling: a variation of holdout
    - Repeat holdout k times, accuracy = avg. of the accuracies obtained
- **Cross-validation** (*k*-fold, where k = 10 is most popular)
  - Randomly partition the data into *k mutually exclusive* subsets, each approximately equal size
  - At *i*-th iteration, use D_i as test set and others as training set
  - Leave-one-out: *k* folds where *k* = # of tuples, for small sized data
  - ***Stratified cross-validation***: folds are stratified so that class dist. in each fold is approx. the same as that in the initial data

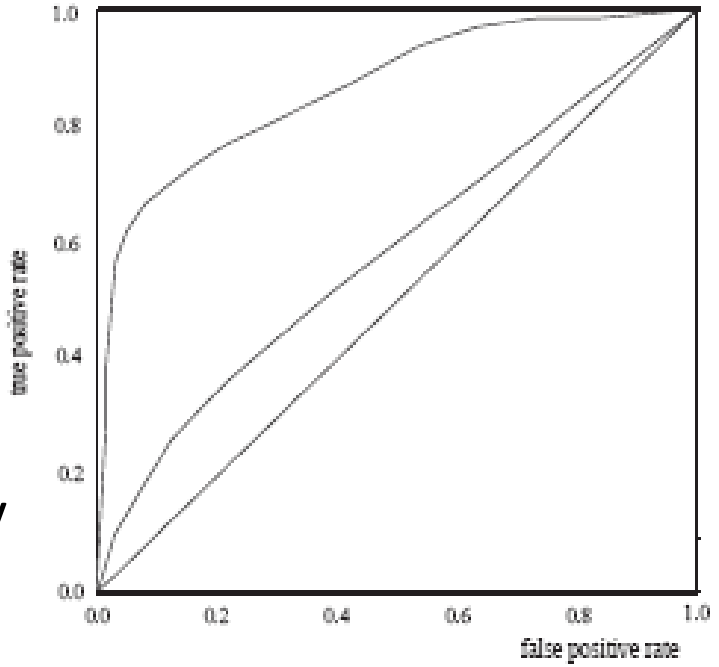
Evaluating Classifier Accuracy: Bootstrap

- **Bootstrap**
  - Works well with small data sets
  - Samples the given training tuples uniformly *with replacement*
    - i.e., each time a tuple is selected, it is equally likely to be selected again and re-added to the training set
- Several bootstrap methods, and a common one is **.632 boostrap**
  - A data set with *d* tuples is sampled *d* times, with replacement, resulting in a training set of *d* samples. The data tuples that did not make it into the training set end up forming the test set. About 63.2% of the original data end up in the bootstrap, and the remaining 36.8% form the test set (since $(1 - 1/d)^d \approx e^{-1} = 0.368$)
  - Repeat the sampling procedure *k* times, overall accuracy of the model:

$$Acc(M) = \frac{1}{k}\sum_{i=1}^{k}(0.632 \times Acc(M_i)_{test\_set} + 0.368 \times Acc(M_i)_{train\_set})$$

Model Selection: ROC Curves

- **ROC** (Receiver Operating Characteristics) curves: for visual comparison of classification models
- Originated from signal detection theory
- Shows the trade-off between the true positive rate and the false positive rate
- The area under the ROC curve is a measure of the accuracy of the model
- Rank the test tuples in decreasing order: the one that is most likely to belong to the positive class appears at the top of the list
- The closer to the diagonal line (i.e., the closer the area is to 0.5), the less accurate is the model



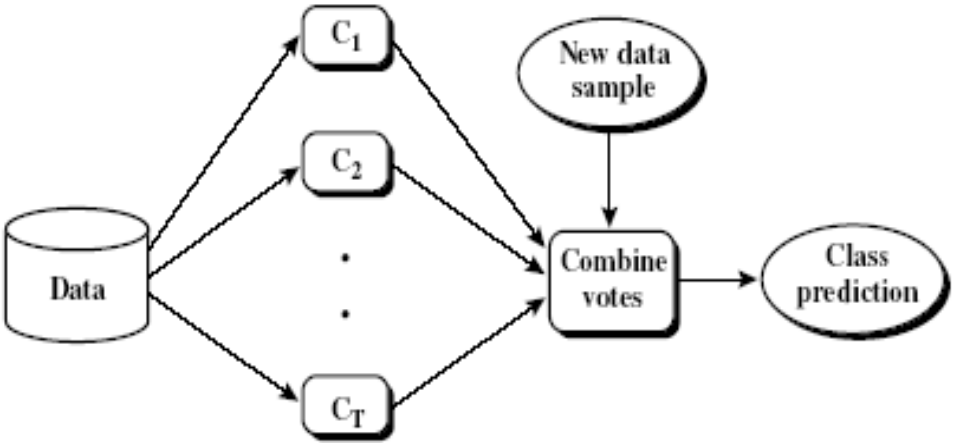
- Vertical axis represents the true positive rate
- Horizontal axis rep. the false positive rate
- The plot also shows a diagonal line
- A model with perfect accuracy will have an area of 1.0

Issues Affecting Model Selection

- **Accuracy**
  - classifier accuracy: predicting class label
- **Speed**
  - time to construct the model (training time)
  - time to use the model (classification/prediction time)
- **Robustness**: handling noise and missing values
- **Scalability**: efficiency in disk-resident databases
- **Interpretability**
  - understanding and insight provided by the model
- Other measures, e.g., goodness of rules, such as decision tree size or compactness of classification rules

Ensemble Methods: Techniques to Improve Classification Accuracy

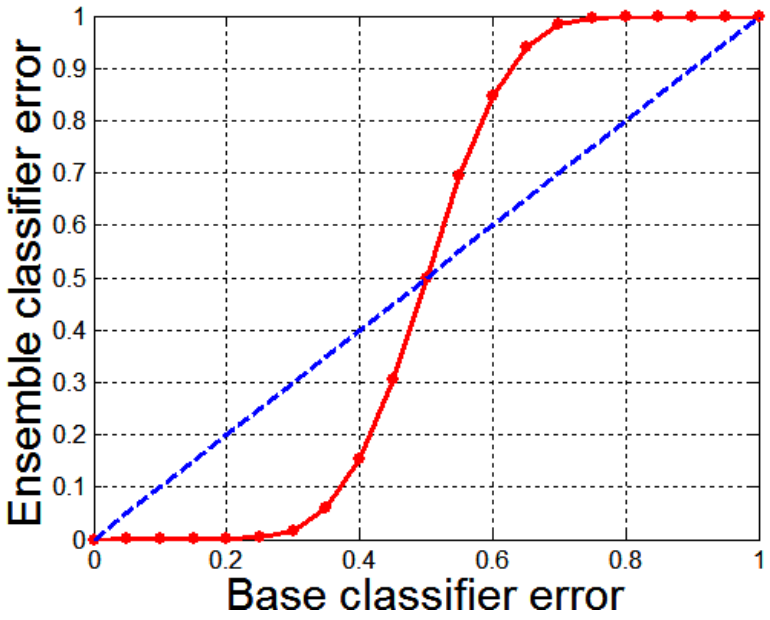
Ensemble Methods: Increasing the Accuracy



- Ensemble methods
  - Use a combination of models to increase accuracy
  - Combine a series of k learned models, M_1, M_2, …, M_k, with the aim of creating an improved model M*
- Popular ensemble methods
  - Bagging: averaging the prediction over a collection of classifiers
  - Boosting: weighted vote with a collection of classifiers
  - Ensemble: combining a set of heterogeneous classifiers

Why Ensemble Methods work?

- Suppose there are 25 base classifiers
  - Each classifier has error rate, $\varepsilon = 0.35$
  - Assume errors made by classifiers are uncorrelated
  - Probability that the ensemble classifier makes a wrong prediction:



$$P(X \geq 13) = \sum_{i=13}^{25} \binom{25}{i} \varepsilon^i (1-\varepsilon)^{25-i} = 0.06$$

Types of Ensemble Methods

- Manipulate data distribution
  - Example: bagging, boosting
- Manipulate input features
  - Example: random forests
- Manipulate class labels
  - Example: error-correcting output coding

Bagging: Boostrap Aggregation

- Analogy: Diagnosis based on multiple doctors' majority vote
- Training
  - Given a set D of *d* tuples, at each iteration *i*, a training set D_i of *d* tuples is sampled with replacement from D (i.e., bootstrap)
  - A classifier model M_i is learned for each training set D_i
- Classification: classify an unknown sample **X**
  - Each classifier M_i returns its class prediction
  - The bagged classifier M* counts the votes and assigns the class with the most votes to **X**
- Prediction: can be applied to the prediction of continuous values by taking the average value of each prediction for a given test tuple
- Accuracy
  - Often significantly better than a single classifier derived from D
  - For noise data: not considerably worse, more robust
  - Proved improved accuracy in prediction

Bagging Algorithm

Algorithm 5.6 Bagging Algorithm

1: Let k be the number of bootstrap samples.
2: **for** $i = 1$ to k **do**
3: Create a bootstrap sample of size n, D_i.
4: Train a base classifier C_i on the bootstrap sample D_i.
5: **end for**
6: $C^*(x) = \arg\max_y \sum_i \delta\big(C_i(x) = y\big)$, $\{\delta(\cdot) = 1$ if its argument is true, and 0 otherwise.$\}$

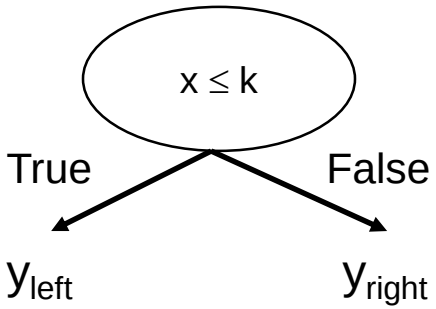
Bagging Example

- Consider 1-dimensional data set:

Original Data:

x	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1
y	1	1	1	-1	-1	-1	-1	1	1	1

- Classifier is a decision stump
  - Decision rule: $x \leq k$ versus $x > k$
  - Split point k is chosen based on entropy



Bagging Example

Bagging Round 1:

x	0.1	0.2	0.2	0.3	0.4	0.4	0.5	0.6	0.9	0.9
y	1	1	1	1	-1	-1	-1	-1	1	1

x <= 0.35 ➔ y = 1
x > 0.35 ➔ y = -1

Bagging Round 2:

x	0.1	0.2	0.3	0.4	0.5	0.5	0.9	1	1	1
y	1	1	1	-1	-1	-1	1	1	1	1

x <= 0.7 ➔ y = 1
x > 0.7 ➔ y = 1

Bagging Round 3:

x	0.1	0.2	0.3	0.4	0.4	0.5	0.7	0.7	0.8	0.9
y	1	1	1	-1	-1	-1	-1	-1	1	1

x <= 0.35 ➔ y = 1
x > 0.35 ➔ y = -1

Bagging Round 4:

x	0.1	0.1	0.2	0.4	0.4	0.5	0.5	0.7	0.8	0.9
y	1	1	1	-1	-1	-1	-1	-1	1	1

x <= 0.3 ➔ y = 1
x > 0.3 ➔ y = -1

Bagging Round 5:

x	0.1	0.1	0.2	0.5	0.6	0.6	0.6	1	1	1
y	1	1	1	-1	-1	-1	-1	1	1	1

x <= 0.35 ➔ y = 1
x > 0.35 ➔ y = -1

Bagging Example

Bagging Round 6:

x	0.2	0.4	0.5	0.6	0.7	0.7	0.7	0.8	0.9	1
y	1	-1	-1	-1	-1	-1	-1	1	1	1

x <= 0.75 ➔ y = -1
x > 0.75 ➔ y = 1

Bagging Round 7:

x	0.1	0.4	0.4	0.6	0.7	0.8	0.9	0.9	0.9	1
y	1	-1	-1	-1	-1	1	1	1	1	1

x <= 0.75 ➔ y = -1
x > 0.75 ➔ y = 1

Bagging Round 8:

x	0.1	0.2	0.5	0.5	0.5	0.7	0.7	0.8	0.9	1
y	1	1	-1	-1	-1	-1	-1	1	1	1

x <= 0.75 ➔ y = -1
x > 0.75 ➔ y = 1

Bagging Round 9:

x	0.1	0.3	0.4	0.4	0.6	0.7	0.7	0.8	1	1
y	1	1	-1	-1	-1	-1	-1	1	1	1

x <= 0.75 ➔ y = -1
x > 0.75 ➔ y = 1

Bagging Round 10:

x	0.1	0.1	0.1	0.1	0.3	0.3	0.8	0.8	0.9	0.9
y	1	1	1	1	1	1	1	1	1	1

x <= 0.05 ➔ y = 1
x > 0.05 ➔ y = 1

Bagging Example

- Summary of Training sets:

Round	Split Point	Left Class	Right Class
1	0.35	1	-1
2	0.7	1	1
3	0.35	1	-1
4	0.3	1	-1
5	0.35	1	-1
6	0.75	-1	1
7	0.75	-1	1
8	0.75	-1	1
9	0.75	-1	1
10	0.05	1	1

Bagging Example

- Assume test set is the same as the original data
- Use majority vote to determine class of ensemble classifier

Round	x=0.1	x=0.2	x=0.3	x=0.4	x=0.5	x=0.6	x=0.7	x=0.8	x=0.9	x=1.0
1	1	1	1	-1	-1	-1	-1	-1	-1	-1
2	1	1	1	1	1	1	1	1	1	1
3	1	1	1	-1	-1	-1	-1	-1	-1	-1
4	1	1	1	-1	-1	-1	-1	-1	-1	-1
5	1	1	1	-1	-1	-1	-1	-1	-1	-1
6	-1	-1	-1	-1	-1	-1	-1	1	1	1
7	-1	-1	-1	-1	-1	-1	-1	1	1	1
8	-1	-1	-1	-1	-1	-1	-1	1	1	1
9	-1	-1	-1	-1	-1	-1	-1	1	1	1
10	1	1	1	1	1	1	1	1	1	1
Sum	2	2	2	-6	-6	-6	-6	2	2	2
Sign	1	1	1	-1	-1	-1	-1	1	1	1

Predicted Class

Boosting

- Analogy: Consult several doctors, based on a combination of weighted diagnoses—weight assigned based on the previous diagnosis accuracy
- How boosting works?
  - **Weights** are assigned to each training tuple
  - A series of k classifiers is iteratively learned
  - After a classifier M_i is learned, the weights are updated to allow the subsequent classifier, M_{i+1}, to **pay more attention to the training tuples that were misclassified** by M_i
  - The final **M* combines the votes** of each individual classifier, where the weight of each classifier's vote is a function of its accuracy
- Boosting algorithm can be extended for numeric prediction
- Comparing with bagging: Boosting tends to have greater accuracy, but it also risks overfitting the model to misclassified data

Boosting

- An iterative procedure to adaptively change distribution of training data by focusing more on previously misclassified records
  - Initially, all N records are assigned equal weights
  - Unlike bagging, weights may change at the end of each boosting round

Boosting

- Records that are wrongly classified will have their weights increased
- Records that are classified correctly will have their weights decreased

Original Data	1	2	3	4	5	6	7	8	9	10
Boosting (Round 1)	7	3	2	8	7	9	4	10	6	3
Boosting (Round 2)	5	4	9	4	2	5	1	7	4	2
Boosting (Round 3)	4	4	8	10	4	5	4	6	3	4

- Example 4 is hard to classify
- Its weight is increased, therefore it is more likely to be chosen again in subsequent rounds

Adaboost (Freund and Schapire, 1997)

- Given a set of *d* class-labeled tuples, ($\mathbf{X_1}$, y_1), …, ($\mathbf{X_d}$, y_d)
- Initially, all the weights of tuples are set the same (1/d)
- Generate k classifiers in k rounds. At round i,
  - Tuples from D are sampled (with replacement) to form a training set D_i of the same size
  - Each tuple's chance of being selected is based on its weight
  - A classification model M_i is derived from D_i
  - Its error rate is calculated using D_i as a test set
  - If a tuple is misclassified, its weight is increased, o.w. it is decreased
- Error rate: err($\mathbf{X_j}$) is the misclassification error of tuple $\mathbf{X_j}$. Classifier M_i error rate is the sum of the weights of the misclassified tuples:

$$error(M_i) = \sum_{j}^{d} w_j \times err(\mathbf{X_j})$$

- The weight of classifier M_i's vote is

$$\log \frac{1 - error(M_i)}{error(M_i)}$$

AdaBoost Algorithm

Algorithm 5.7 AdaBoost Algorithm

1: $\mathbf{w} = \{w_j = 1/n \mid j = 1, 2, \cdots, n\}$. {Initialize the weights for all n instances.}
2: Let k be the number of boosting rounds.
3: **for** $i = 1$ to k **do**
4: Create training set D_i by sampling (with replacement) from D according to w.
5: Train a base classifier C_i on D_i.
6: Apply C_i to all instances in the original training set, D.
7: $\epsilon_i = \frac{1}{n}\left[\sum_j w_j \, \delta\left(C_i(x_j) \neq y_j\right)\right]$ {Calculate the weighted error}
8: **if** $\epsilon_i > 0.5$ **then**
9: $\mathbf{w} = \{w_j = 1/n \mid j = 1, 2, \cdots, n\}$. {Reset the weights for all n instances.}
10: Go back to Step 4.
11: **end if**
12: $\alpha_i = \frac{1}{2} \ln \frac{1-\epsilon_i}{\epsilon_i}$.
13: Update the weight of each instance according to equation (5.88).
14: **end for**
15: $C^*(\mathbf{x}) = \arg\max_y \sum_{j=1}^{T} \alpha_j \delta(C_j(\mathbf{x}) = y)\big)$.

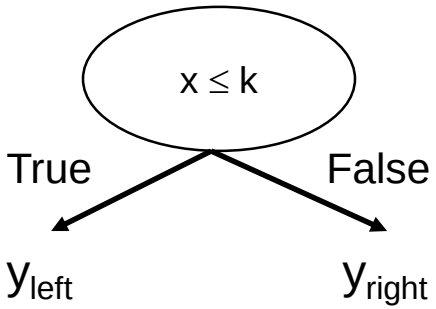
AdaBoost Example

- Consider 1-dimensional data set:

Original Data:

x	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1
y	1	1	1	-1	-1	-1	-1	1	1	1

- Classifier is a decision stump
  - Decision rule: $x \leq k$ versus $x > k$
  - Split point k is chosen based on entropy



AdaBoost Example

- Training sets for the first 3 boosting rounds:

Boosting Round 1:

x	0.1	0.4	0.5	0.6	0.6	0.7	0.7	0.7	0.8	1
y	1	-1	-1	-1	-1	-1	-1	-1	1	1

Boosting Round 2:

x	0.1	0.1	0.2	0.2	0.2	0.2	0.3	0.3	0.3	0.3
y	1	1	1	1	1	1	1	1	1	1

Boosting Round 3:

x	0.2	0.2	0.4	0.4	0.4	0.4	0.5	0.6	0.6	0.7
y	1	1	-1	-1	-1	-1	-1	-1	-1	-1

- Summary:

Round	Split Point	Left Class	Right Class	alpha
1	0.75	-1	1	1.738
2	0.05	1	1	2.7784
3	0.3	1	-1	4.1195

AdaBoost Example

- Weights

Round	x=0.1	x=0.2	x=0.3	x=0.4	x=0.5	x=0.6	x=0.7	x=0.8	x=0.9	x=1.0
1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
2	0.311	0.311	0.311	0.01	0.01	0.01	0.01	0.01	0.01	0.01
3	0.029	0.029	0.029	0.228	0.228	0.228	0.228	0.009	0.009	0.009

- Classification

Round	x=0.1	x=0.2	x=0.3	x=0.4	x=0.5	x=0.6	x=0.7	x=0.8	x=0.9	x=1.0
1	-1	-1	-1	-1	-1	-1	-1	1	1	1
2	1	1	1	1	1	1	1	1	1	1
3	1	1	1	-1	-1	-1	-1	-1	-1	-1
Sum	5.16	5.16	5.16	-3.08	-3.08	-3.08	-3.08	0.397	0.397	0.397
Sign	1	1	1	-1	-1	-1	-1	1	1	1

Predicted Class

Random Forest (Breiman 2001)

- Random Forest:
  - Each classifier in the ensemble is a *decision tree* classifier and is generated using a random selection of attributes at each node to determine the split
  - During classification, each tree votes and the most popular class is returned
- Two Methods to construct Random Forest:
  - Forest-RI (*random input selection*): Randomly select, at each node, F attributes as candidates for the split at the node. The CART methodology is used to grow the trees to maximum size
  - Forest-RC (*random linear combinations*): Creates new attributes (or features) that are a linear combination of the existing attributes (reduces the correlation between individual classifiers)
- Comparable in accuracy to Adaboost, but more robust to errors and outliers
- Insensitive to the number of attributes selected for consideration at each split, and faster than bagging or boosting

Classification of Class-Imbalanced Data Sets

- Class-imbalance problem: Rare positive example but numerous negative ones, e.g., medical diagnosis, fraud, oil-spill, fault, etc.
- Traditional methods assume a balanced distribution of classes and equal error costs: not suitable for class-imbalanced data
- Typical methods for imbalance data in 2-class classification:
  - **Oversampling**: re-sampling of data from positive class
  - **Under-sampling**: randomly eliminate tuples from negative class
  - **Threshold-moving**: moves the decision threshold, t, so that the rare class tuples are easier to classify, and hence, less chance of costly false negative errors
  - Ensemble techniques: Ensemble multiple classifiers introduced above
- Still difficult for class imbalance problem on multiclass tasks