Introduction to Machine Learning

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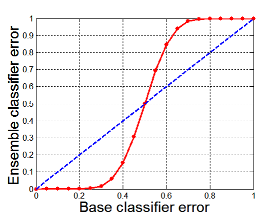
Ensemble Methods

- Construct a set of classifiers from the training data
- Predict class label of test records by combining the predictions made by multiple classifiers

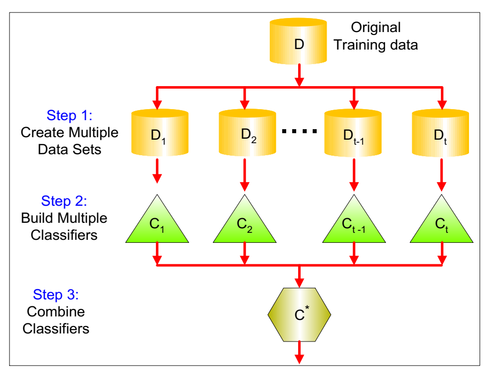
Why Ensemble Methods work?

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



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

General Approach



Types of Ensemble Methods

- Bayesian ensemble
  - Example: Mixture of Gaussian
- Manipulate data distribution
  - Example: Resampling method
- Manipulate input features
  - Example: Feature subset selection
- Manipulate class labels
  - Example: error-correcting output coding
- Introduce randomness into learning algorithm
  - Example: Random forests

Bagging

- Sampling with replacement

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

- Build classifier on each bootstrap sample
- Each sample has probability $1 - (1 – 1/n)^n$ of being selected
- On average, each bootstrap data contains ~63% of original data

Bagging Algorithm

Algorithm 5.6 Bagging Algorithm

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

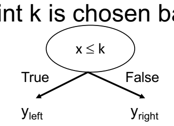
Bagging Example

- 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 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

- 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

Random Forests

- Class of ensemble methods specifically designed for decision tree classifiers
- Bagging using decision trees is a special case of random forests
- RF method combines Breiman's "bagging" idea with the random feature selection.

Random Forests

Each tree is constructed using the following algorithm:

Given
- Let the number of training cases be *N*, and the number of variables in the classifier be *M*.
- *m* be the number of input variables used to determine the decision at a node of the tree; *m* should be much less than *M*.

Generate training data (bootstrap)
- Choose a training set for each tree by choosing *n* times with replacement from all *N* available training cases (i.e. take a bootstrap sample). Use the rest of the cases to estimate the error of the tree, by predicting their classes.
- For each node of the tree, randomly choose *m* variables on which to base the decision at that node. Calculate the best split based on these *m* variables in the training set.
- Each tree is fully grown and not pruned

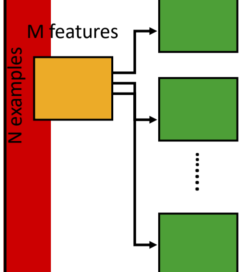
Prediction
- Each tree is used to predict the label. Voting scheme is used to determine the final class label.

Random Forests

- Class of ensemble methods specifically designed for decision tree classifiers
- Bagging using decision trees is a special case of random forests
- RF method combines Breiman's "bagging" idea with the random feature selection.

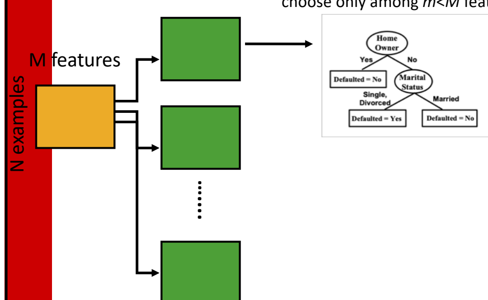
Random Forest Construction

Create bootstrap samples from the training data

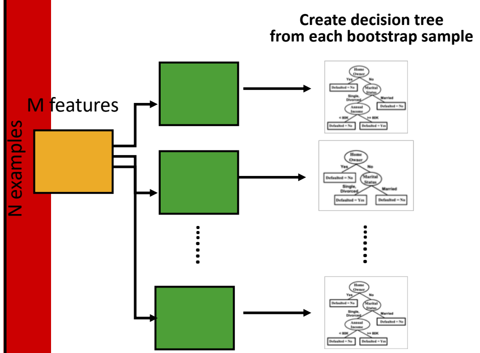


Random Forest Construction

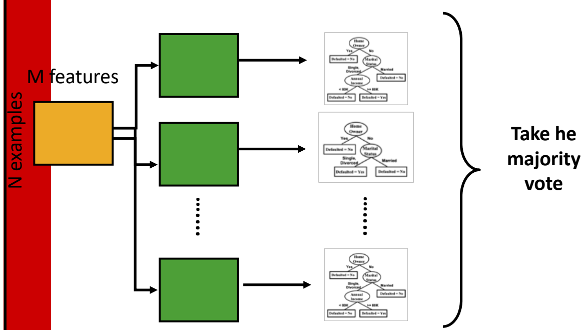
At each node in choosing the split feature choose only among *m*<*M* features



Random Forest Construction



Random Forest Prediction



Random Forests

- Advantages
  - One accurate and widely used algorithm
  - Can handle large number of features without need for feature selection first
  - Provides estimates of which variables are important
  - Handles missing data well
- Disadvantages
  - May lead to overfitting on some datasets
  - May be biased towards attributes that result in large number splits

Practice

- On one or more of UCI ML Repository (http://archive.ics.uci.edu/ml/)
  - Construct decision tree
  - Construct random forest
  - Compare and contrast both
- Acknowledgements
  - Slides adopted from UMN and CMU classes