

26/04/16 DA - EXAM QUESTIONS - ENSEMBLES

2014 Q2A

→ What is an ensemble?

Ensemble (or committee) method or machine learning method that use the power of multiple models to achieve better prediction accuracy than any individual model can on its own.

An ensemble model is one that is made of two or more of less accurate models.

The output of an ensemble is due to a "voting" system. Each model in an ensemble provides an output and the most popular answer is the overall output of the ensemble.

Advantages:

- Higher accuracy
  - Many types of errors are captured
  - More output than just misclassification rate (for visualization and accuracy)
  - Can be proximal for Multi Dimensional Scaling
  - Less overfitting
  - Unlikely that all classifiers will make the same mistake
  - So long as each error is made by a minority of the classifiers, optimal classifier can be found
  - Greater predictive power compared with individual model
- EXAMPLES: RANDOM FOREST, Boosting, Bagging, RuleFit.

→ Overview of Method Used to create ensemble

Draw Diagram showing flow of data into multiple models and being merged back into a single output.

1. Multiple datasets must be made from the original training set.
2. Multiple classifiers must be constructed - each are different.
3. Combine classifiers into a single ensemble model.

Generic Formula:

$$f_{(C_m, P_n)}^m = \min_{f_{(C_m, P_n)}^m} \sum_{i=1}^N L(y_i, f_{(C_m, P_n)}^m) + \sum_{m=1}^M L(y_i, f_m)$$

- $L$  is a loss function
- Two step approach
- Choose the point  $m$ , choose a subset of  $M$  base learners out of all the space of all possible base learners
- Determine the coefficients  $c_m$
- The goal is to find "good"  $E_{m^3}^{train}$  close to target function
- Ideally we want to end up with a set of "good" classifiers with low interaction
- Change some aspect of the model as we pull the base learner
- Allow a pruning point for evaluating integrality

### Random Forests Detailed

- We assume that the user knows about the construction of single classification trees.
- Random Forest grows many classification trees
- To classify a new object from an input vector, put the input vector down the each of the trees in the forest.
- Each tree gives a classification and we say the tree "votes" for that class.
- The forest chooses the classification having the most votes (win all the trees in the forest)

Each tree is grown as follows:

1. If the number of cases in the training set is  $N$ , sample  $N$  cases at random - but with replacement, from the original dataset. This sample will be the training set for growing the tree
2. If there are  $M$  input variables, a number  $m \leq M$  is specified such that at each node,  $m$  variables are selected at random out of the  $M$  and the best split on these  $m$  is used to split the node. The value of  $m$  is held constant during the forest growing
3. Each tree is grown to the largest possible extent. There is no pruning.

Reducing  $m$  reduces both the correlation and the strength. Increase it, increase both.

Somewhere in between is an "optimal" range of  $m$ , usually quite wide.

Using the out of bag error rate a value of  $m$  in the range can quickly be found and is the only adjustable parameter to which random forest is sensitive.

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What is a Random Forest?

- RF is an ensemble method based on classification trees.
- Numerous trees are built using different training sets so as to ensure different results.
- The ensemble then predicts according to the majority.
- Classification trees are generally unstable, returning different models almost all of the time.
- For this reason, they are very suitable for ensemble methods.

Random Forests have 2 kinds of randomness built in:

1. Cases are selected at random, with replacement, and about 1/3rd of the data is not used when growing each tree. This is called 'out of bag' sample and is used to evaluate the tree. Because the out of bag sample, there is no need to split the data into test and train sets. Thus, random forests are suitable for small data sets.
2. At each split a sample  $m$  from  $M$  variables is selected. Because of this, RF are typically used when data sets have more variables than cases.

RF offer ~~higher~~ high level of predictive accuracy and an innovative set of graphical displays to reveal unexpected patterns in the data.

Two kinds of randomness built in

- Cases selected at random with replacement - training set
- At each split a random sample of  $m$  from  $M$  variables are selected
- $m$  is typically  $\sqrt{M}$
- No pruning trees placed automatically
- For each tree typically 36% of data is not used - data are called out of bag samples.
- Each tree votes for each case in the out of bag samples.
- Aggregated over all trees
- Each tree carries equal weight - each case assigned to class with the most votes.

Output: model coefficients, margin of classifier, variable importance, proximity matrix, missing value imputation, partial dependency plots.



Margins of classifier - Proportion of votes for each class

Assign vote to class with highest proportion of votes

Margin of a vote = proportion of votes for correct class - max proportion assigned other class

Should be large

Under majority vote, positive margin need correct classification

### Vote Importance

- Two approaches: - Contribution to fit

• Residual in fitting model e.g. GLM

- Contribution to prediction method

Can calculate for each class

Can calculate overall result

### Prediction method:

- For each tree ~~calculate~~ calculate % misclassified ( $v_i$ ) for each class and overall using 008 codes
- For each predictor randomly sort the code and put code from the tree again
- Calculate % misclassified again ( $v_{s,i}$ ) for each class and overall
- Calculate difference  $v_i - v_{s,i}$
- Average results over all trees

### Proximity of code

- Calculate  $N \times N$  proximity matrix  $p(i,j)$
- Every element initially set to 0
- If code  $i$  and code  $j$  end up in the same node  
 $p(i,j) = p(i,j) + 1$
- Accumulate over all trees and summate
- Can use this proximity matrix as input into MDS
- Degree to which individual observations are classified alike
- Grow tree as usual - Drop all branching data down tree

### Partial Dependency Plot

- Shows how each predictor is related to response holding other variables constant.
- Let  $x$  be the initial predictor of interest with  $V$  distinct values.
- Construct  $V$  data sets for each of the  $V$  values of  $x$  leaving all other variables unchanged.
- For the  $V$  datasets, predict the response using random forest.
- Calculate a single value averaged over all observations for each dataset.
- Average these predictions over lines.
- It is common in output still that  $n=2$ .

### Advantages

- Simple to implement
- Good classifier
- Lots of other information
- Works with large number of variables
- Different types of variable
- Can use proximity matrix as input into MDS
- It's accuracy is as good as individual and sometimes better
- Relatively robust to outliers and noise
- Faster than bagging or boosting
- It gives useful internal estimates of error, strength, correlation and variable importance
- It's simple and easily parallelised

- $\rho$  correlation between the trees depends on  $m$
- Increasing  $\rho$  increases the forest error rate
- Increasing strength of individual trees decreases forest error rate
- The larger  $m$  is the "better" the tree
- Reducing  $m$  reduces both the correlation and the strength
- Increasing  $m$  increases both correlation and strength
- Find optimum  $m$  suggested  $m = \sqrt{M}$

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### Partial Dependency Plot

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- Construct  $v$  data sets for each of the  $v$  values of  $x$  leaving all other variables unchanged
- For the  $v$  datasets, predict the response using random forest
- Calculate a single value averaged over all observations for each dataset
- Average these predictions over trees
- $k$  calculated in output cell  $k=1, 2$

### (A) Advantages

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Tuning Parameters - Node Size for growing tree!

- Number of trees
- Number of predicted samples

- Cannot include cuts like a single tree
- Can alter priors

From the random forest

Margin is the difference between the maximum class and the next largest class  
i.e. predicted hair colour is brown, black, blonde

For pupil, say 80% say black, 10% blonde & 10% brown. the margin is 80 to 10 = 70.

Margin is used by the forest

Missing data can be dealt with in 2 ways:

- simplest method is to replace any missing data with the median
- More complete method involves beginning with a rough guess of the value of missing data  
→ full size random forest is grown  
→ For variable M with a missing value, an average of over all missing non-missing cases is taken and weighted by proximity
- Above process is repeated until the best average

ADA Boost:

- Variation of an ensemble method
- (Composite) of a # of weak learners - individual trees which are only slightly more accurate than random guessing - and weights for each of these learners, depending on which local area of the graph it is operating on
- Adapts in the sense that subsequent weak learners are trained in favour of those instances misclassified by previous classifier
- Suitable to noisy data and outliers
- Individual learners can be weak but adding a learner as learner or better than random guessing the final model can be proven to converge to a strong learner.

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- Heart of algorithm is how it examines each weak learner and assigns an alpha weight
- You go through the pool of classifiers and find the one which does the best job  
Minimizing classification error. You then increase the weights of the samples which are wrongly classified so the next classifier has to work better on these samples.  
Then you go through the pool again
- Emphasis increases data to focus on vulnerable info

### Adv Disadv

- Powerful classification algorithm
- Can achieve similar classification result with much less tweaking of parameters or settings
- Can be sensitive to noisy data and outliers
- Can be less susceptible to overfitting problem
- Simple to implement
- Does feature selection resulting in relatively simple classifiers
- Instead of re-sampling, use training set re-weighting
- Possibly suboptimal solution
- Lose the simple interpretability of classification trees
- Computation is more difficult
- No prior knowledge needed about weak learners
- No parameter to tune except (T)
- From empirical evidence, AdaBoost is particularly vulnerable to uniform noise
- Boosting performs an exhaustive search for best predictor to split on, whereas random forest model only searches a small subset of data
- Boosting grows trees in series, with later trees dependent on the result of previous trees, RF grows in parallel, independent of one another
- On a large training set, boosting can be slow with many predictors, while RF model selects only a subset of predictors for each split, which can handle significantly larger problems before dying