RECSM Summer School: Machine Learning for Social Sciences

Session 2.3: Bagging and Random Forests

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Bagging

Bagging

- Decision trees suffer from high variance: small changes in the training data can lead to quite different results.
- We would like to have a method with low variance: the results are similar if the method is applied repeatedly to distinct data sets (generated by the same DGP).
- Bootstrap aggregation, or bagging, is a general-purpose procedure for reducing the variance of a learning method.
- Bagging is frequently used in the context of decision trees.

Bagging

Averaging Reduces Variance

Suppose there is a set of n independent random variables $X_1, \ldots, X_n$ with variance $V(X_i) = \sigma^2,\ \forall i = 1, \ldots, n$. The variance of the mean $\bar{X}$ of these variables then is $V(\bar{X}) = \sigma^2/n$.

Bagging

- Averaging a set of variables reduces variance.
- Hence, we could reduce the variance (increase the prediction accuracy!) of a machine learning method as follows:
  - Take B training sets from the population;
  - Train the method on each training set to get predictions $\hat{f}^1(x), \hat{f}^2(x), \ldots, \hat{f}^B(x)$;
  - Average the resulting predictions

$$\hat{f}^{\mathsf{avg}}(x) = \frac{1}{B}\sum_{b=1}^{B}\hat{f}^b(x). \tag{2.3.1}$$

Bagging

- We generally do not have access to multiple training sets.
- Instead, we can bootstrap:
  - Generate B bootstrapped training sets by taking repeated samples from the (single) training set;
  - Train the method on the bth bootstrapped training set to get prediction $\hat{f}^{*b}(x)$;
  - Average all predictions to obtain

$$\hat{f}^{\text{bag}}(x) = \frac{1}{B}\sum_{b=1}^{B}\hat{f}^{*b}(x). \tag{2.3.2}$$

- This approach is called bagging!

Bagging – Applied to Regression Trees

- Construct B regression trees using B bootstrapped training sets, and average the resulting predictions.
- Each tree is grown deep and is not pruned. Hence, each tree has low bias, but high variance.
- Averaging these B trees reduces the variance.
- Bagging has been shown to give impressive improvements in accuracy by combining hundreds or thousands of trees.

Bagging – Applied to Classification Trees

- How can bagging be extended to a classification problem?
- Construct B classification trees using B bootstrapped training sets.
- For a given test observation, we record the class predicted by each of the B trees, and take a "majority vote."
- Hence, the overall prediction is the most commonly occurring class among the B predictions.

Bagging

- Increasing the number of trees B will not lead to overfitting. In practice, we want to use a value of B that is sufficiently large for the test error to have settled down.
- How do we estimate the test error of a bagged model?

Bagging

Out-of-Bag Error Estimation

Out-of-Bag Error Estimation

- With bagging, we can estimate the test error without the need to perform CV.
- Recall that the trees are repeatedly fit to bootstrapped subsets of the training set.
- It turns out that, on average, each tree is fit to around 2/3 of the training observations. The remaining 1/3 of the training observations not used to fit a given tree are called the out-of-bag (OOB) observations.

Out-of-Bag Error Estimation

- We can predict the response for observation i using all trees in which that observation was OOB. This will yield about $B/3$ predictions.
- To obtain a single prediction for observation i, we can average these predicted responses (regression) or take a majority vote (classification).
- After doing this for all n observations, we can compute the overall OOB MSE (regression) or classification error (classification).
- The resulting OOB error is a valid estimate of the test error for the bagged model.

Bagging

Measuring Variable Importance

Measuring Variable Importance

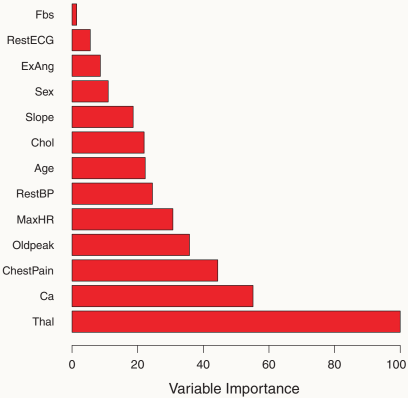
- Bagging typically has a better prediction accuracy than a single tree.
- This comes at the expense of interpretability: it is no longer possible to represent the model as a single tree and it is no longer clear which variables are most important.
- Therefore, it can be useful to compute an overall summary of the importance of each predictor using the RSS (regression) or the Gini index (classification).

Measuring Variable Importance

- For regression trees: we can record the total amount that the RSS is decreased due to splits over a given predictor, averaged over all B trees.
- For classification trees: we can record the total amount that the Gini index is decreased due to splits over a given predictor, averaged over all B trees.
- In both cases, a large value indicates an important predictor.

Measuring Variable Importance – Example

A Variable Importance Plot for the Heart Disease Data



(Source: James et al. 2013, 320)

The plot shows the mean decrease in the Gini index for each variable, relative to the largest.

Random Forests

Random Forests

- Random forests provide an improvement over bagged trees.
- They involve a small tweak that decorrelates the trees:
    - As in bagging, we build a number of decision trees on bootstrapped training samples.
    - At each split in the tree-building process, we consider a random sample of m predictors, $m < p$, as candidates for the split.
    - A new sample of m predictors is taken at each split, typically of size $m \approx \sqrt{p}$.
- Therefore, at each split in the tree, the algorithm is not even allowed to consider a majority of the available predictors.

Random Forests

- Does this sound crazy?
- Suppose that there is one very strong predictor in the training data, along with a number of moderately strong predictors.
- In bagging, most or all of the individual trees will use this strong predictor in the top split.
- Consequently, all bagged trees will look quite similar to each other, so the predictions from these trees will be highly correlated.

Random Forests

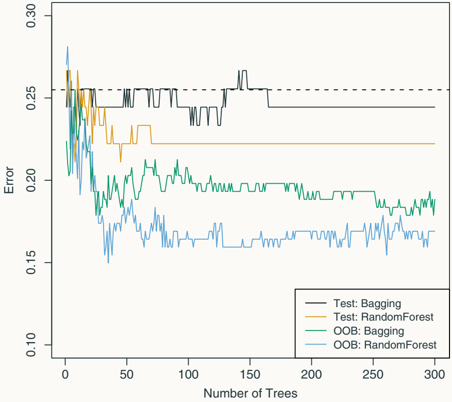
- Averaging highly correlated quantities leads to a smaller reduction in variance than averaging uncorrelated quantities.
- Therefore, bagging will not lead to a substantial reduction in variance over a single tree.
- In random forests, on average $(p - m)/p$ of the splits will not even consider the strong predictor.
- Random forests decorrelate the trees, making the average of the trees less variable and hence more reliable.

Random Forests

- The difference between bagging and random forests depends on the choice of predictor subset size m.
- If $m = p$, then the random forest is equivalent to bagging.
- As with bagging, random forests will not overfit if we increase B, so in practice we use a sufficiently large value of B (B is sufficiently large when the error rate has settled down).

Bagging and Random Forests – Example

Bagging and Random Forest Results for the Heart Disease Data



(Source: James et al. 2013, 318)

The dashed line indicates the test error resulting from a single classification tree. Random forests were applied with $m = \sqrt{p}$.