# Machine Learning in Public Health

# Lecture 8: Bagging, Random Forest, Boosting

Dr. Yang Feng

## Advantages and disadvantages of trees

- Trees are very easy to explain to people. In fact, they are even easier to explain than linear regression!
- Why? No mathematical formula needed in the communication
- Some people believe that decision trees more closely mirror human decision-making than do the regression and classification approaches seen in previous chapters.
- Trees can be displayed graphically, and are easily interpreted even by a non-expert (especially if they are small).
- Unfortunately, tress generally do not have the great predictive accuracy.
- This disadvantage motivates the ensemble methods such as bagging, random forests and boosting.

# Bagging

- The decision trees suffer from high variance.

- Bootstrap aggregation, or bagging, is a general-purpose procedure for reducing the variance of a statistical learning method; we introduce it here because it is particularly useful and frequently used in the context of decision trees.

- In this approach we generate $B$ different *bootstrapped* training data sets. We then train our method on the $b$th bootstrapped training set in order to get $\hat{f}^{*b}(x)$ (not pruned), and average all the predictions:

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

## Bagging

- Averaging these $B$ trees reduces the variance. (Why?)
- $B$ is not a critical parameter with bagging; a very large value of $B$ will not lead to overfitting.
- In practice we use $B$ sufficiently large that the error has settled down.
- For a given test observation in *classification*, we can record the class predicted by each of the $B$ trees, and take a majority vote: the overall prediction is the most commonly occurring majority class among the $B$ predictions.

## Out-of-bag Error Estimation

- For a bagged model, we can estimate the test error without doing CV or a validation set approach
- Each bagged tree makes use of a part of the original observations
- The remaining observations not used to fit a given bagged tree are referred to as the **out-of-bag** (OOB) observations
- We can predict the response for the $i$-th observation using each of the trees in which that observation was OOB

## Out-of-bag Error Estimation

- This will yield a little more than $B/3$ predictions for the $i$th observation
- To obtain a single prediction for the $i$-th observation, we can average these predicted responses (if regression is the goal) or can take a majority vote (if classification is the goal). This leads to a single OOB prediction for the $i$-th observation
- An OOB prediction can be obtained in this way for each of the $n$ observations, from which the overall OOB MSE (for a regression problem) or classification error (for a classification problem) can be computed

## Variable Importance Measures

- Although the collection of bagged trees is much more difficult to interpret than a single tree, one can obtain an overall summary of the importance of each predictor using
  - *the* `RSS` *(for bagging regression trees)*
  - *the* `Gini index` *(for bagging classification trees)*
- In the case of bagging 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. A large value indicates an important predictor
- For bagging classification trees, we can add up the total amount that the Gini index is decreased by splits over a given predictor, averaged over all $B$ trees.

# Variable Importance Measure

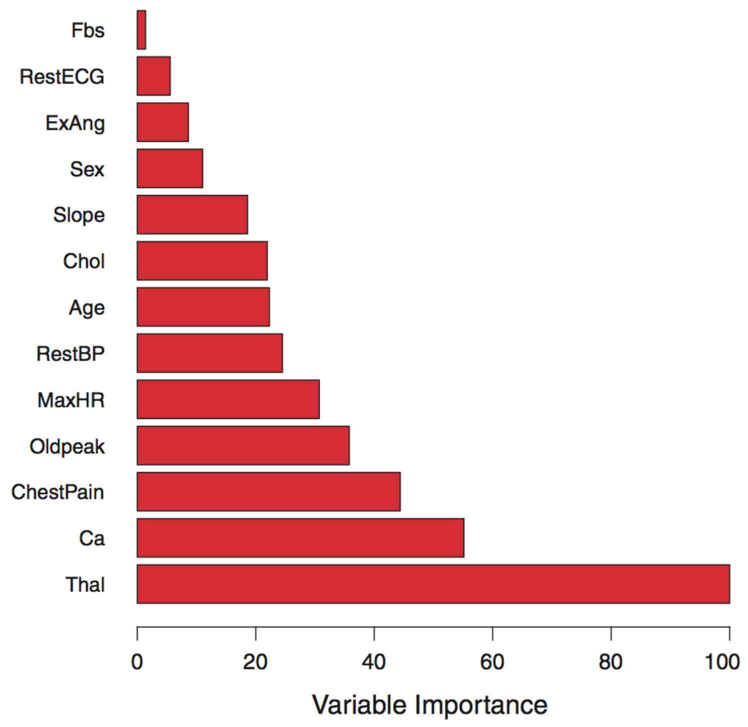


**FIGURE 8.9.** *A variable importance plot for the* Heart *data. Variable importance is computed using the mean decrease in Gini index, and expressed relative to the maximum.*

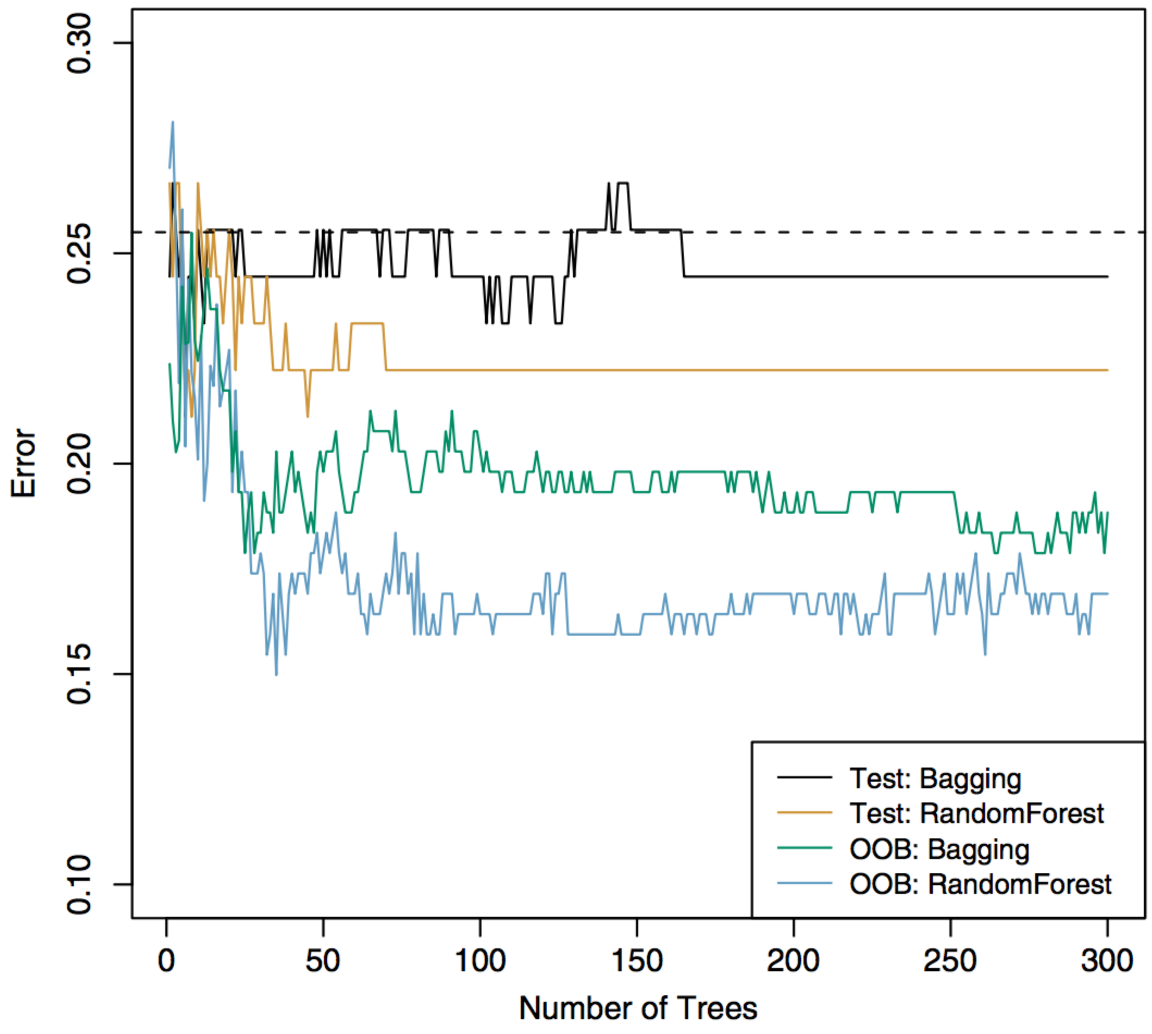
# Random Forests

- Bagging constructs trees that are too “similar” (why?), so it probably does not reduce the variance as much as we wish to.
- Random forests provide an improvement over bagged trees by way of a small tweak that *decorrelates* the trees.
- As in bagging, we build a number of decision trees on bootstrapped training samples.
- But when building these decision trees, each time a split in a tree is considered, a random sample of $m$ predictors is chosen as split candidates from the full set of $p$ predictors. The split is allowed to use **only one** of those $m$ predictors.

# Random Forests

- Bagging is a special case of random forest when $m = p$
- If you don't want to spend extra efforts on $m$, $mtry = \sqrt{p}$ is a canonical choice for classification and $mtry = p/3$ is a good choice for regression.
- As with bagging, random forests will **not overfit** if we increase $B$, so in practice we use $B$ sufficiently large for the error rate to have settled down. The default choice in the `randomForest` function is $ntree = 500$.
- Random Forest is a really good off-the-shelf algorithm!

# Test and OOB Error



## Some questions

- Q: In random forest algorithms, we restrict our attention to randomly selected m out of p features in each split. Now we change this procedure to restriction to the first $m$ features (i.e., $X_1, \cdots, X_m$) in every split. Do you expect the new procedure to work well? And why?

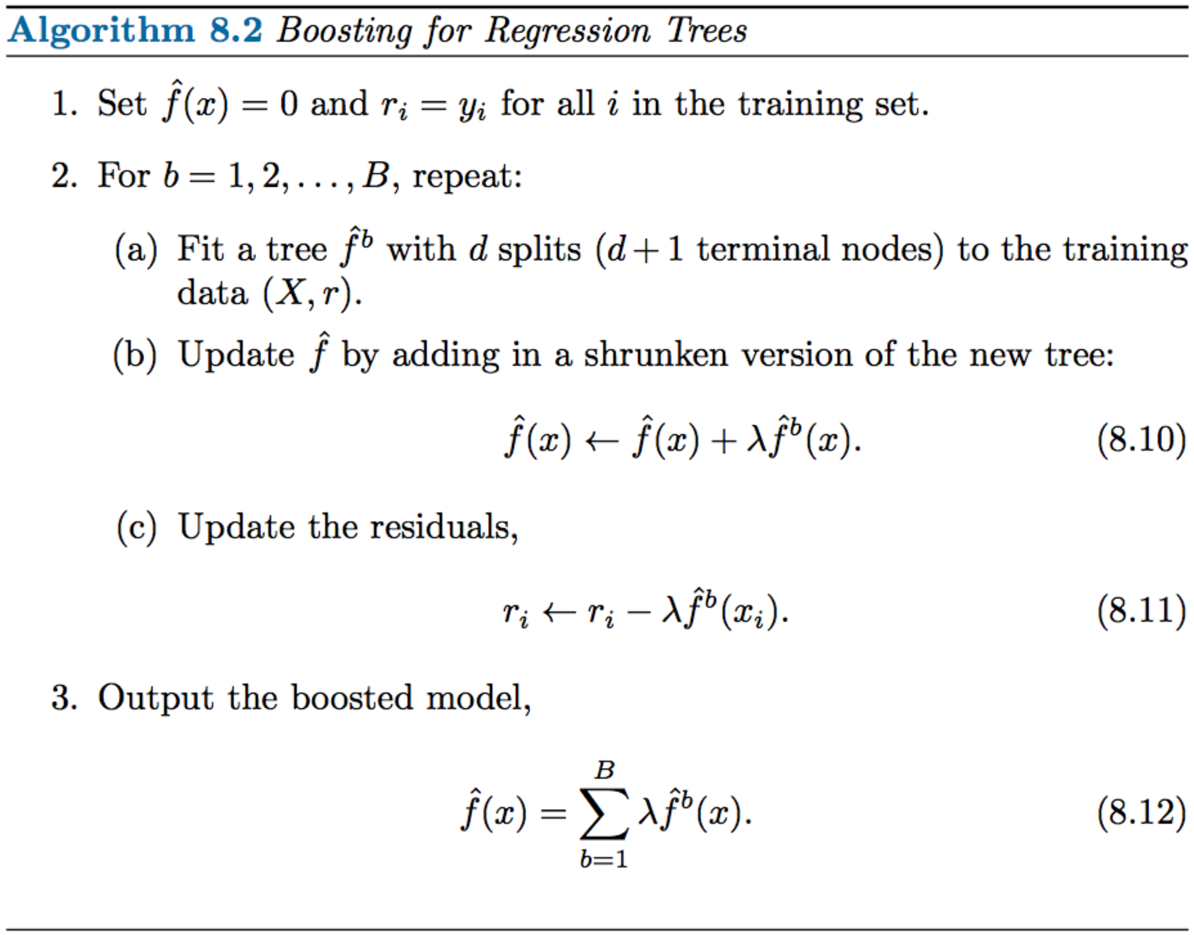
- Q: Is random forest always a better algorithm compared to decision trees?

- Q: What are the sources of randomness random forests have? Hint: 2.

- Q: (brainstorm, no clear answer): Can you think of some ways to combine linear regression and decision trees / random forest?

## Boosting

- Like bagging, boosting is a general approach that can be applied to many statistical learning methods for regression or classification.



**Algorithm 8.2** *Boosting for Regression Trees*

```
1. Set $\hat{f}(x) = 0$ and $r_i = y_i$ for all $i$ in the training set.
2. For $b = 1, 2, \ldots, B$, repeat:
    (a) Fit a tree $\hat{f}^b$ with $d$ splits ($d+1$ terminal nodes) to the training data $(X, r)$.
    (b) Update $\hat{f}$ by adding in a shrunken version of the new tree:
        $\hat{f}(x) \leftarrow \hat{f}(x) + \lambda \hat{f}^b(x).$   (8.10)
    (c) Update the residuals,
        $r_i \leftarrow r_i - \lambda \hat{f}^b(x_i).$   (8.11)
3. Output the boosted model,
    $\hat{f}(x) = \sum_{b=1}^{B} \lambda \hat{f}^b(x).$   (8.12)
```

## In the boosting tree algorithm

- We use cross-validation to select $B$.
- The shrinkage parameter $\lambda$, a small positive number. This controls the rate at which boosting learns. Typical values are $0.01$ or $0.001$.
- The number $d$ of splits in each tree, which controls the complexity of the boosted ensemble. Often $d = 1$ works well, in which case each tree is a *stump*, consisting of a single split. More generally $d$ is the interaction depth.
- Boosting is a *slow* learner.