

Bagging and Random Forests

David S. Rosenberg

New York University

April 10, 2018

Contents

- 1 Ensemble Methods: Introduction
- 2 The Benefits of Averaging
- 3 Review: Bootstrap
- 4 Bagging
- 5 Random Forests

Ensemble Methods: Introduction

Ensembles: Parallel vs Sequential

- Ensemble methods combine multiple models
- **Parallel ensembles:** each model is built independently
 - e.g. bagging and random forests
 - Main Idea: Combine many (high complexity, low bias) models to reduce variance
- **Sequential ensembles:**
 - Models are generated sequentially
 - Try to add new models that do well where previous models lack

The Benefits of Averaging

A Poor Estimator

- Let Z, Z_1, \dots, Z_n i.i.d. $\mathbb{E}Z = \mu$ and $\text{Var}Z = \sigma^2$.
- We could use any single Z_i to estimate μ .
- Performance?
- Unbiased: $\mathbb{E}Z_i = \mu$.
- Standard error of estimator would be σ .
 - The **standard error** is the standard deviation of the sampling distribution of a statistic.
 - $\text{SD}(Z) = \sqrt{\text{Var}(Z)} = \sqrt{\sigma^2} = \sigma$.

Variance of a Mean

- Let Z, Z_1, \dots, Z_n i.i.d. $\mathbb{E}Z = \mu$ and $\text{Var}Z = \sigma^2$.
- Let's consider the average of the Z_i 's.
 - Average has the same expected value but smaller standard error:

$$\mathbb{E} \left[\frac{1}{n} \sum_{i=1}^n Z_i \right] = \mu \quad \text{Var} \left[\frac{1}{n} \sum_{i=1}^n Z_i \right] = \frac{\sigma^2}{n}.$$

- Clearly the average is preferred to a single Z_i as estimator.
- Can we apply this to reduce variance of general prediction functions?

Averaging Independent Prediction Functions

- Suppose we have B independent training sets from the same distribution.
- Learning algorithm gives B decision functions: $\hat{f}_1(x), \hat{f}_2(x), \dots, \hat{f}_B(x)$
- Define the average prediction function as:

$$\hat{f}_{\text{avg}} = \frac{1}{B} \sum_{b=1}^B \hat{f}_b$$

- What's random here?
- The B independent training sets are random, which gives rise to variation among the \hat{f}_b 's.

Averaging Independent Prediction Functions

- Fix some particular $x_0 \in \mathcal{X}$.
- Then average prediction on x_0 is

$$\hat{f}_{\text{avg}}(x_0) = \frac{1}{B} \sum_{b=1}^B \hat{f}_b(x_0).$$

- Consider $\hat{f}_{\text{avg}}(x_0)$ and $\hat{f}_1(x_0), \dots, \hat{f}_B(x_0)$ as random variables
 - Since the training sets were random
- We have no idea about the distributions of $\hat{f}_1(x_0), \dots, \hat{f}_B(x_0)$ – they could be crazy...
- But we do know that $\hat{f}_1(x_0), \dots, \hat{f}_B(x_0)$ are i.i.d. And that's all we need here...

Averaging Independent Prediction Functions

- The average prediction on x_0 is

$$\hat{f}_{\text{avg}}(x_0) = \frac{1}{B} \sum_{b=1}^B \hat{f}_b(x_0).$$

- $\hat{f}_{\text{avg}}(x_0)$ and $\hat{f}_b(x_0)$ have the same expected value, but
- $\hat{f}_{\text{avg}}(x_0)$ has smaller variance:

$$\begin{aligned} \text{Var}(\hat{f}_{\text{avg}}(x_0)) &= \frac{1}{B^2} \text{Var} \left(\sum_{b=1}^B \hat{f}_b(x_0) \right) \\ &= \frac{1}{B} \text{Var}(\hat{f}_1(x_0)) \end{aligned}$$

Averaging Independent Prediction Functions

- Using

$$\hat{f}_{\text{avg}} = \frac{1}{B} \sum_{b=1}^B \hat{f}_b$$

seems like a win.

- But in practice we don't have B independent training sets...
- Instead, we can use **the bootstrap**....

Review: Bootstrap

The Bootstrap Sample

Definition

A **bootstrap sample** from \mathcal{D}_n is a sample of size n drawn *with replacement* from \mathcal{D}_n .

- In a bootstrap sample, some elements of \mathcal{D}_n
 - will show up multiple times,
 - some won't show up at all.
- Each X_i has a probability $(1 - 1/n)^n$ of not being selected.
- Recall from analysis that for large n ,

$$\left(1 - \frac{1}{n}\right)^n \approx \frac{1}{e} \approx .368.$$

- So we expect $\sim 63.2\%$ of elements of \mathcal{D} will show up at least once.

The Bootstrap Method

Definition

A **bootstrap method** is when you *simulate* having B independent samples from P by taking B bootstrap samples from the sample \mathcal{D}_n .

- Given original data \mathcal{D}_n , compute B bootstrap samples D_n^1, \dots, D_n^B .
- For each bootstrap sample, compute some function

$$\phi(D_n^1), \dots, \phi(D_n^B)$$

- Work with these values as though D_n^1, \dots, D_n^B were i.i.d. P .
- **Amazing fact:** Things often come out very close to what we'd get with independent samples from P .

Bagging

Bagging

- Draw B bootstrap samples D^1, \dots, D^B from original data \mathcal{D} .
- Let $\hat{f}_1, \hat{f}_2, \dots, \hat{f}_B$ be the prediction functions for each set.
- The **bagged prediction function** is a **combination** of these:

$$\hat{f}_{\text{avg}}(x) = \text{Combine} \left(\hat{f}_1(x), \hat{f}_2(x), \dots, \hat{f}_B(x) \right)$$

- How might we combine
 - prediction functions for regression?
 - binary class predictions?
 - binary probability predictions?
 - multiclass predictions?
- Bagging proposed by Leo Breiman (1996).

Bagging for Regression

- Draw B bootstrap samples D^1, \dots, D^B from original data \mathcal{D} .
- Let $\hat{f}_1, \hat{f}_2, \dots, \hat{f}_B : \mathcal{X} \rightarrow \mathbf{R}$ be the predictions functions for each set.
- Bagged prediction function is given as

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

- Empirically, \hat{f}_{bag} often performs similarly to what we'd get from training on B independent samples:
 - $\hat{f}_{\text{bag}}(x)$ has same expectation as $\hat{f}_1(x)$, but
 - $\hat{f}_{\text{bag}}(x)$ has smaller variance than $\hat{f}_1(x)$

Out-of-Bag Error Estimation

- Each bagged predictor is trained on about 63% of the data.
- Remaining 37% are called **out-of-bag (OOB)** observations.
- For i th training point, let

$$S_i = \{b \mid D^b \text{ does not contain } i\text{th point}\}.$$

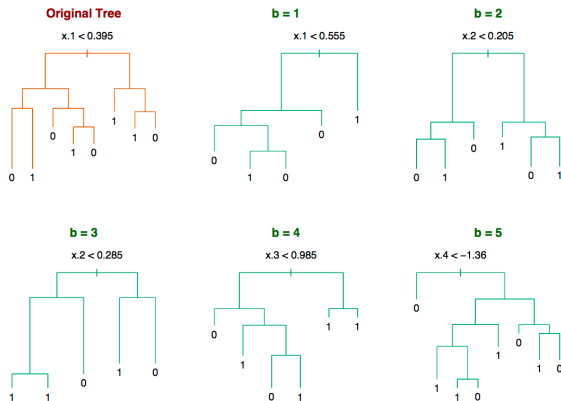
- The **OOB prediction** on x_i is

$$\hat{f}_{\text{OOB}}(x_i) = \frac{1}{|S_i|} \sum_{b \in S_i} \hat{f}_b(x_i).$$

- The OOB error is a good estimate of the test error.
- OOB error is similar to cross validation error – both are computed on training set.

Bagging Classification Trees

- Input space $\mathcal{X} = \mathbf{R}^5$ and output space $\mathcal{Y} = \{-1, 1\}$.

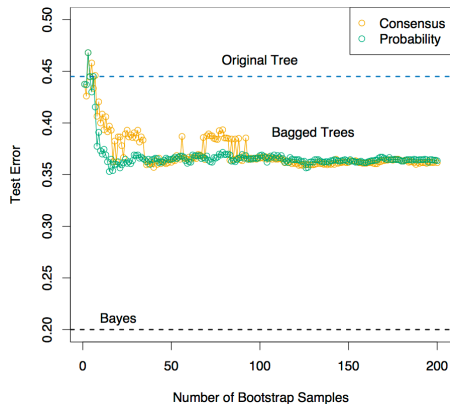


- Sample size $n = 30$
- Each bootstrap tree is quite different
- Different splitting variable at the root
- This high degree of variability from small perturbations of the training data is why tree methods are described as **high variance**.

From HTF Figure 8.9

Comparing Classification Combination Methods

- Two ways to combine classifications: consensus class or average probabilities.



From HTF Figure 8.10

Terms “Bias” and “Variance” in Casual Usage (Warning! Confusion Zone!)

- Restricting the hypothesis space \mathcal{F} “**biases**” the fit
 - **away** from the best possible fit of the training data, and
 - **towards** a [usually] simpler model.
- Full, unpruned decision trees have very little bias.
- Pruning decision trees introduces a bias.
- **Variance** describes how much the fit changes across different random training sets.
- If different random training sets give very similar fits, then algorithm has high **stability**.
- Decision trees are found to be high variance (i.e. not very stable).

Conventional Wisdom on When Bagging Helps

- Hope is that bagging reduces variance without making bias worse.
- General sentiment is that bagging helps most when
 - Relatively unbiased base prediction functions
 - High variance / low stability
 - i.e. small changes in training set can cause large changes in predictions
- Hard to find clear and convincing theoretical results on this
- But following this intuition leads to improved ML methods, e.g. Random Forests

Random Forests

Recall the Motivating Principal of Bagging

- Averaging $\hat{f}_1, \dots, \hat{f}_B$ reduces variance, if they're based on i.i.d. samples from $P_{\mathcal{X} \times \mathcal{Y}}$
- Bootstrap samples are
 - independent samples from the training set, but
 - are **not** independent samples from $P_{\mathcal{X} \times \mathcal{Y}}$.
- This dependence limits the amount of variance reduction we can get.
- Would be nice to reduce the dependence between \hat{f}_i 's...

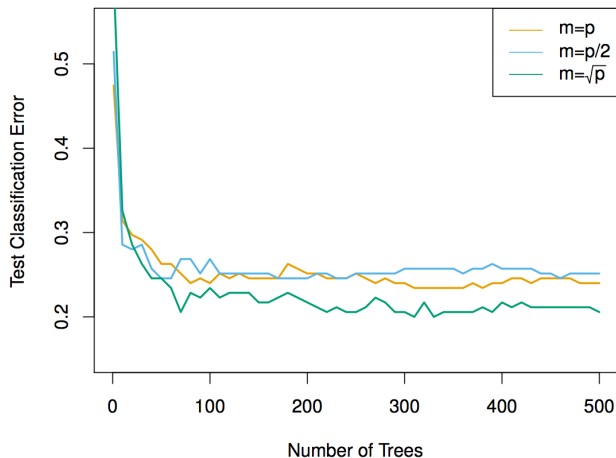
Main idea of random forests

Use **bagged decision trees**, but modify the tree-growing procedure to reduce the dependence between trees.

- **Key step** in random forests:
 - When constructing **each tree node**, restrict choice of splitting variable to a randomly chosen subset of features of size m .
- Typically choose $m \approx \sqrt{p}$, where p is the number of features.
- Can choose m using cross validation.

- Usual approach is to build very deep trees (low bias)
- Diversity in individual tree prediction functions from
 - bootstrap samples (somewhat different training data) and
 - randomized tree building
- Bagging seems to work better when we are combining a diverse set of prediction functions.

Random Forest: Effect of m size



From *An Introduction to Statistical Learning, with applications in R* (Springer, 2013) with permission from the authors: G. James, D. Witten, T. Hastie and R. Tibshirani.

Appendix

Variance of a Mean of Correlated Variables

- For Z, Z_1, \dots, Z_n i.i.d. with $\mathbb{E}Z = \mu$ and $\text{Var}Z = \sigma^2$,

$$\mathbb{E} \left[\frac{1}{n} \sum_{i=1}^n Z_i \right] = \mu \quad \text{Var} \left[\frac{1}{n} \sum_{i=1}^n Z_i \right] = \frac{\sigma^2}{n}.$$

- What if Z 's are correlated?
- Suppose $\forall i \neq j, \text{Corr}(Z_i, Z_j) = \rho$. Then

$$\text{Var} \left[\frac{1}{n} \sum_{i=1}^n Z_i \right] = \rho \sigma^2 + \frac{1-\rho}{n} \sigma^2.$$

- For large n , the $\rho \sigma^2$ term dominates – limits benefit of averaging.