Bootstrap, Bagging, and Random Forests

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The Benefits of Averaging

A Lousy Estimator

- Let $Z, Z_1, \ldots, Z_n$ i.i.d. $\mathbb{E}Z = \mu$ and $\mathrm{Var}Z = \sigma^2$.
- We could use any single Z_i to estimate μ.
- Performance?
  - Unbiased: $\mathbb{E}Z_i = \mu$.
  - Variance of estimator would be σ^2.

Variance of a Mean

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

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

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

Averaging Independent Prediction Functions

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

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

- What's random here?

Averaging Independent Prediction Functions

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

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

- Consider $\hat{f}_{\text{avg}}(x)$ and $\hat{f}_1(x), \ldots, \hat{f}_B(x)$ as random variables. (They are.)
- $\hat{f}_1(x), \ldots, \hat{f}_B(x)$ are i.i.d.
- $\hat{f}_{\text{avg}}(x)$ and $\hat{f}_b(x)$ have the same expected value, but
- $\hat{f}_{\text{avg}}(x)$ has smaller variance:

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

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**....

Bagging

Bagging

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

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

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

Bagging for Regression

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

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

- If bootstrap samples were independent draws from P,
  - $\hat{f}_{\text{bag}}(x)$ would have the same expectation as $\hat{f}_1(x)$, but
  - $\hat{f}_{\text{bag}}(x)$ would have smaller variance.
- Empirically: Often get a similar effect for bagging.

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 ith training point, let

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

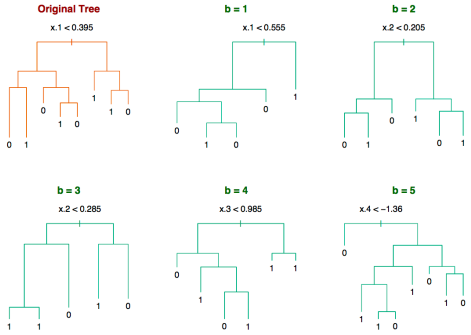
- The **OOB prediction** on x_i is

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

- The OOB error is a good estimate of the test error.
- For large enough B, OOB error is like cross validation.

Bagging Trees

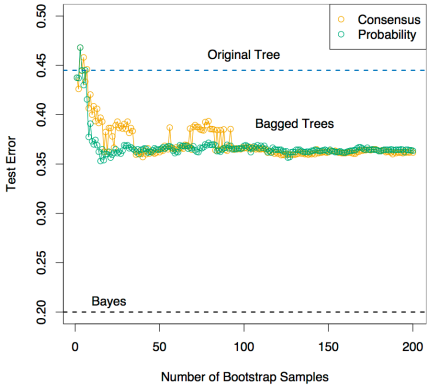
- Input space $\mathcal{X} = \mathbf{R}^5$ and output space $\mathcal{Y} = \{-1, 1\}$.
- Sample size $N = 30$ (simulated data)



From ESL Figure 8.9

Bagging Trees

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



From ESL Figure 8.10

Terms "Bias" and "Variance" in Casual Usage

- Restricting the hypothesis space $\mathcal{F}$ "**biases**" the fit
  - **towards** a simpler model and
  - **away** from the best possible fit of the training data.
- 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

- Bagging does nothing to eliminate bias.
- Hope is that bagging reduces variance.
- General sentiment is that bagging helps most when
  - Relatively unbiased base predictions
  - High variance
    - e.g. small changes in training set can cause large changes in predictions
- I'm not aware of solid theory on this...
- Empirical observation
  - Bagging trees works well.
  - Trees have high variance and low bias.
  - QED?

Random Forests

Recall the Motivating Principal of Bagging

- Averaging $\hat{f}_1, \ldots, \hat{f}_B$ reduces variance, if they're based on i.i.d. samples.
- Bootstrap samples are not indepedendent.
- This probably limits the amount of variance reduction we can get.
- Would be nice to reduce the dependence between $\hat{f}_i$'s...

Variance of a Mean of Correlated Variables

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

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

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

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

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

Random Forest

Main idea of random forests

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

Random Forest: Effect of m size