Bootstrap, Bagging, and Random Forests

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Bias and Variance

Parameters

- Suppose we have a probability distribution P.
- Often went to estimate some characteristic of P.
  - e.g. expected value, variance, kurtosis, median, etc...
- These things are called **parameters** of P.
- A **parameter** $\mu = \mu(P)$ is any function of the distribution P.
- Question: Is μ random?
- Answer: Nope. For example if P has density $f(x)$ on $\mathbf{R}$, then mean is

$$\mu = \int_{-\infty}^{\infty} x f(x)\, dx,$$

which just an integral - nothing random.

Statistics and Estimators

- Suppose $\mathcal{D}_n = (x_1, x_2, \ldots, x_n)$ is an i.i.d. sample from P.
- A **statistic** $s = s(\mathcal{D}_n)$ is any function of the data.
- A statistic $\hat{\mu} = \hat{\mu}(\mathcal{D}_n)$ is a **point estimator** of μ if $\hat{\mu} \approx \mu$.
- Question: Are statistics and/or point estimators random?
- Answer: Yes, since we're considering the data to be random.
    - The function $s(\cdot)$ isn't random, but we're plugging in random inputs.

Examples of Statistics

- Mean: $\bar{x}(\mathcal{D}_n) = \frac{1}{n}\sum_{i=1}^{n} x_i$.
- Median: $m(\mathcal{D}_n) = \text{median}(x_1, \ldots, x_n)$
- Sample variance: $\sigma^2(\mathcal{D}_n) = \frac{1}{n-1}\sum_{i=1}^{n}\left(x_i - \bar{x}(\mathcal{D}_n)\right)^2$

Fancier:

- A data histogram is a statistic.
- Empirical distribution function.
- A confidence interval.

Statistics are Random

- Statistics are random, so they have probability distributions.
- The distribution of a statistic is called a **sampling distribution**.
- We often want to know some **parameters** of the sampling distribution.
  - Most commonly the mean and the standard deviation.
- The standard deviation of the sampling distribution is called the **standard error**.
- Question: Is standard error random?
- Answer: Nope. It's a parameter of a distribution.

Bias and Variance for Real-Valued Estimators

- Let $\mu : P \mapsto \mathbf{R}$ be a real-valued parameter.
- Let $\hat{\mu} : \mathcal{D}_n \mapsto \mathbf{R}$ be an estimator of μ.

- We define the **bias** of $\hat{\mu}$ to be $\text{Bias}(\hat{\mu}) = \mathbb{E}\hat{\mu} - \mu$.
- We define the **variance** of $\hat{\mu}$ to be $\text{Var}(\hat{\mu}) = \mathbb{E}\hat{\mu}^2 - (\mathbb{E}\hat{\mu})^2$.

- An estimator is **unbiased** if $\text{Bias}(\hat{\mu}) = \mathbb{E}\hat{\mu} - \mu = 0$.

Neither bias nor variance depend on a specific sample $\mathcal{D}_n$. We are taking expectation over $\mathcal{D}_n$.

Estimating Variance of an Estimator

- To estimate $\operatorname{Var}(\hat{\mu})$ we need estimates of $\mathbb{E}\hat{\mu}$ and $\mathbb{E}\hat{\mu}^2$.
- Instead of a single sample $\mathcal{D}_n$ of size n, suppose we had
  - B independent samples of size n: $\mathcal{D}_n^1, \mathcal{D}_n^2, \ldots, \mathcal{D}_n^B$
- Can then estimate

$$
\begin{aligned}
\mathbb{E}\hat{\mu} &\approx \frac{1}{B}\sum_{i=1}^{B}\hat{\mu}\left(\mathcal{D}_n^i\right) \\
\mathbb{E}\hat{\mu}^2 &\approx \frac{1}{B}\sum_{i=1}^{B}\left[\hat{\mu}\left(\mathcal{D}_n^i\right)\right]^2
\end{aligned}
$$

and

$$
\operatorname{Var}(\hat{\mu}) \approx \frac{1}{B}\sum_{i=1}^{B}\left[\hat{\mu}\left(\mathcal{D}_n^i\right)\right]^2 - \left[\frac{1}{B}\sum_{i=1}^{B}\hat{\mu}\left(\mathcal{D}_n^i\right)\right]^2.
$$

Putting "Error Vars" on Estimator

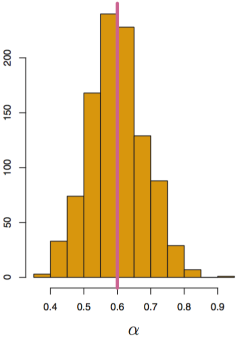
- Why do we even care about estimating variance?
- Would like to report a confidence interval for our point estimate:

$$\hat{\mu} \pm \sqrt{\widehat{\mathrm{Var}(\hat{\mu})}}$$

- (This confidence interval assumes $\hat{\mu}$ is unbiased.)
- Our **estimate of standard error** is $\sqrt{\widehat{\mathrm{Var}(\hat{\mu})}}$.

Histogram of Estimator

- Want to estimate $\alpha = \alpha(P)$ for some known P, and some complicated α.
- Point estimator $\hat{\alpha} = \hat{\alpha}(\mathcal{D}_{100})$ for samples of size 100.
- Histogram of $\hat{\alpha}$ for 1000 random datasets of size 100:



Pink line indicates true value of α. This is Figure 5.10 from *An Introduction to Statistical Learning, with applications in R* (Springer, 2013).

Practical Issue

- We typically get only one sample $\mathcal{D}_n$.
- We could divide it into B groups.
- Our estimator would be $\hat{\mu} = \hat{\mu}\left(\mathcal{D}_{n/B}\right)$.
- And we could get a variance estimate for $\hat{\mu}$.
- But the estimator itself would not be as good as if we used all data:

$$\hat{\mu} = \hat{\mu}(\mathcal{D}_n).$$

- Can we get the best of both worlds?
  - A good point estimate AND a variance estimate?

The Bootstrap

The Bootstrap Sample

Definition

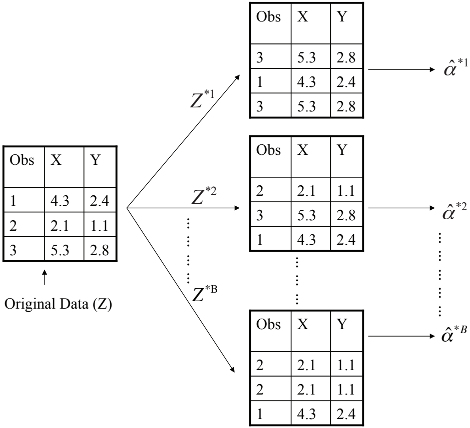
A **bootstrap sample** from $\mathcal{D}_n = \{x_1, \ldots, x_n\}$ is a sample of size n drawn *with replacement* from $\mathcal{D}_n$.

- 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 ~63.2% of elements of $\mathcal{D}$ will show up at least once.

The Bootstrap Sample



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.

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.

Independent vs Bootstrap Samples

- Want to estimate $\alpha = \alpha(P)$ for some known P and some complicated α.
- Point estimator $\hat{\alpha} = \hat{\alpha}(\mathcal{D}_{100})$ for samples of size 100.
- Histogram of $\hat{\alpha}$ based on
  - 1000 independent samples of size 100, vs
  - 1000 bootstrap samples of size 100

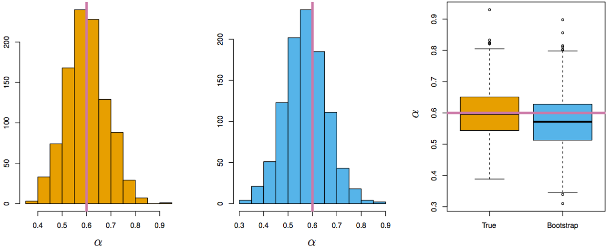


Figure 5.10 from *ISLR* (Springer, 2013) with permission from the authors: G. James, D. Witten, T. Hastie and R. Tibshirani.

The Bootstrap in Practice

- Suppose we have an estimator $\hat{\mu} = \hat{\mu}(\mathcal{D}_n)$.
- To get error bars, we can compute the "bootstrap variance".
  - Draw B bootstrap samples.
  - Compute empirical variance of $\hat{\mu}(\mathcal{D}_n^1), \ldots, \hat{\mu}(\mathcal{D}_n^B)$..
- Could report

$$\hat{\mu}(\mathcal{D}_n) \pm \sqrt{\text{Bootstrap Variance}}$$

The Benefits of Averaging

A Lousy Estimator

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

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

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

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

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

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

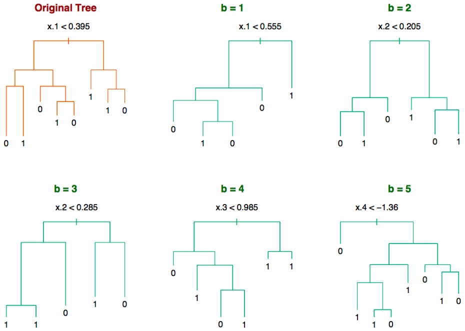
- The **OOB prediction** on x_i is

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

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

Bagging Trees

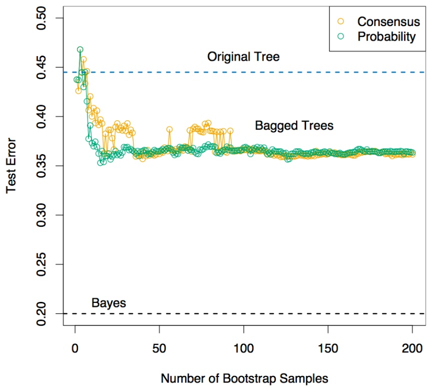
- Input space $\mathcal{X} = \mathbf{R}^5$ and output space $\mathcal{Y} = \{-1, 1\}$.
- Sample size $N = 30$ (simulated data)



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 $\operatorname{Var} Z = \sigma^2$,

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

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

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

- 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