Ensemble Learning

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In Previous Lectures

- Linear Regression
- Polynomial Regression
- Training and test error
- Bias and Variance Tradeoff
- Classification
- KNN
- Logistic Regression
- SVM
- Decision trees

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In this session

- Ensemble Learning
  - Bagging (Bootstrap Aggregation)
  - Random Forests
  - Boosting

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References

For further readings, check:

Section 8.2 from the book : An Introduction to Statistical Learning. James, Gareth, Daniela Witten, Trevor Hastie, and Robert Tibshirani, 2013, ISBN: 978-1-461-47137-0

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Ensemble Learning

- Aim: take a mediocre algorithm (base model) and transform it into a super classifier without requiring any fancy new algorithm.

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How can we combine different models?

- Ensemble methods differ in training strategies and combination methods
- We will discuss two approaches
  1. Parallel training of different models using overlapping training sets (Bagging)
  2. Sequential training by iteratively re-weighting training examples such that each model focuses on a different subset of hard examples (boosting)

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Bootstrap

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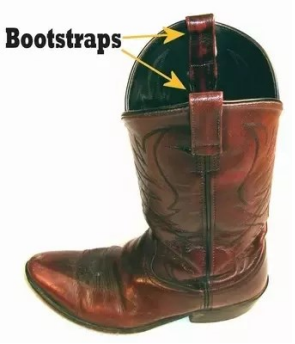
Bootstrap

- The bootstrap is a widely applicable and extremely powerful statistical tool that can be used to quantify the uncertainty associated with a given estimator or statistical learning method.
- Allows us to emulate the process of obtaining new sample sets so that we can estimate the variability in our estimate.
- Rather than repeatedly obtaining independent data sets from the population, we instead obtain distinct data sets by repeatedly sampling observations from the original data set.



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Procedure

- Suppose our original data set consists of n data points $X = \{x_1, x_2 \ldots, x_n\}$
- Multiple data sets are created as follows:
- Create a new data set X_B by drawing n points at random from X, with replacement, so that some points in X may be replicated in X_B, whereas other points in X may be absent from X_B.
- Repeat this process L times to generate L data sets each of size n and each obtained by sampling from the original data set X.

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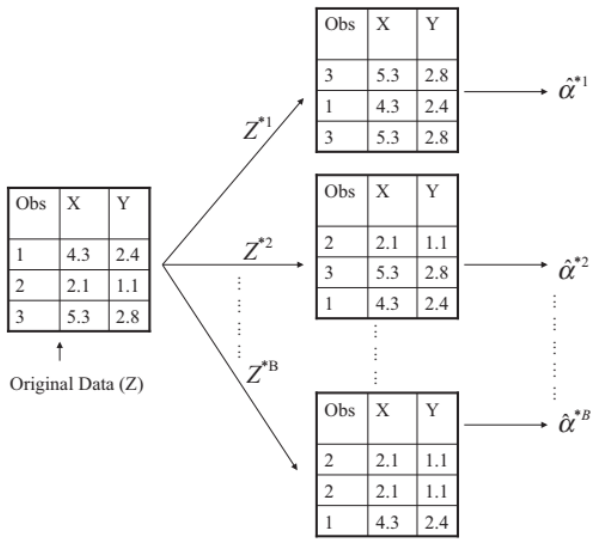
Obtain a different estimate of parameter α using a dataset Z



A graphical illustration of the bootstrap approach on a small sample containing n = 3 observations.

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Bagging

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Bagging

- Bagging: a general-purpose procedure for reducing the variance (the sensitivity of the model to the individual data points) .
- Basic idea: create different models using different bootstrapped training sets and average their prediction to produce the final output of the model
- Bagging can improve predictions for many regression and classification methods,
- It is particularly useful for decision trees (suffer from high variance).

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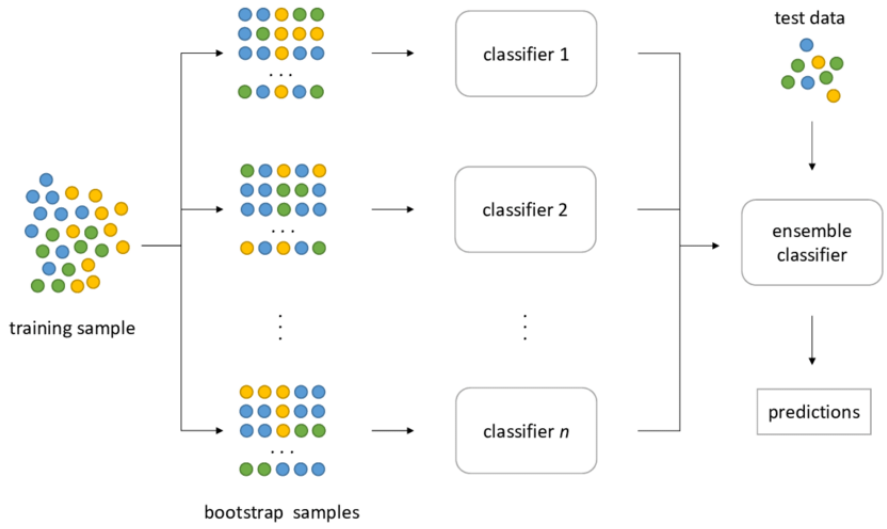
Illustration



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Procedure

- We generate B different bootstrapped training data sets.
- We then train our method on the b^{th} bootstrapped training set in order to get $\hat{f}^{*b}(x)$
- finally average all the predictions, to obtain

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

- For classification, you can average class probabilities (or take the majority vote)

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Out-of-Bag (OOB) Error

- There is a very straightforward way to estimate the test error of a bagged model (without the need to perform cross-validation or the validation set approach)
- Out-of-Bag (OOB) error: OOB is the mean prediction error on each training sample x_i, using only the model that did not have x_i in their bootstrapped training set.
- That is, for each observation x_i in a dataset X, calculate the average prediction error for all models that do not have x_i in their bootstrap sample.
- The resulting OOB error is a valid estimate of the test error for the bagged model, since the response for each observation is predicted using only the trees that were not fit using that observation.

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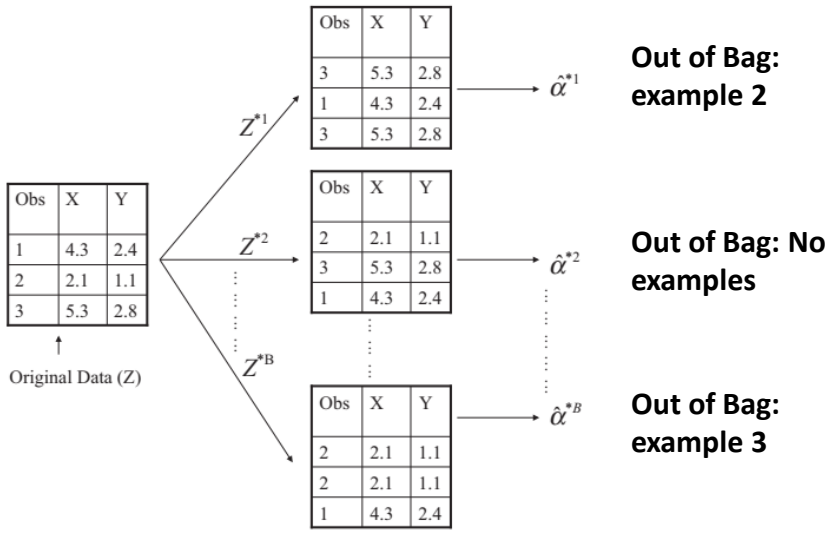

Out of Bag: example 2

Out of Bag: No examples

Out of Bag: example 3

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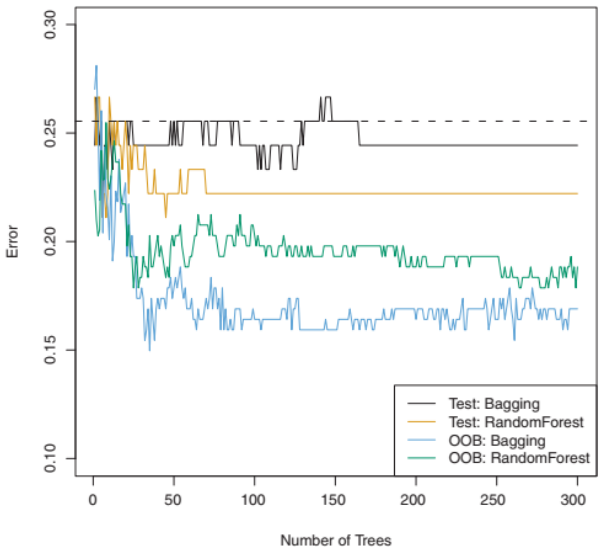
Out-of-Bag Error (Cont.)



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How can we estimate variable importance?

- Bagging typically results in improved accuracy over prediction using a single tree. Unfortunately, however, it can be difficult to interpret the resulting model.
- When we bag a large number of trees, it is no longer possible to represent the resulting statistical learning procedure using a single tree, and it is no longer clear which variables are most important to the procedure (bagging improves prediction accuracy at the expense of interpretability).

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Variable Importance Measures

- You can calculate an overall summary of the importance of each predictor using *Variable Importance Measures* such as RSS (in regression models) and Gini Index (in classification models)

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Variable Importance Measures- Regression

- For a given predictor, calculate the total amount that the RSS is decreased due to splits over a given predictor, averaged over all B trees

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Variable Importance Measures- Classification

- For a given predictor, calculate the total amount that the Gini index (measure of node *purity*—a small value indicates that a node contains predominant observations from a single class) is decreased by splits over a given predictor, averaged over all B trees.

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Random Forest

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Random Forests

- Random forests provide an improvement over bagged trees by way of a random small tweak that *decorrelates* the trees.
- You may consider Random forest as many, relatively uncorrelated, models that operate as a committee to make decisions

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Random Forests - Random Variable Selection

- As in bagging, we build a number forest of decision trees on bootstrapped training samples.
- However, when building these decision trees, each time a split in a tree is considered, we select a random sample of m predictors (out of the available p predictors).
- The split is allowed to use only one of those m predictors and a fresh sample of m predictors is taken at each split.
- Typically we choose $m \approx \sqrt{p}$—that is, the number of predictors considered at each split is approximately equal to the square root of the total number of predictors.
- Why do we make random variable selection?

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Random Forests - Random Variable Selection (Cont.)

- Why do we need random variable selection in random forests? the algorithm is not even allowed to consider a majority of the available predictors when preforming the splitting.
- The answer is: to build a set of relatively *uncorrelated models.*
- Averaging many highly correlated quantities does not lead to as large of a reduction in variance as averaging many uncorrelated quantities.

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Uncorrelated trees

- Suppose that there is one very strong predictor in the data set, along with a number of other moderately strong predictors.
- Then in the collection of bagged trees, most or all of the trees will use this strong predictor in the top split (will look quite similar to each other).
- Hence the predictions from the bagged trees will be highly correlated (does not lead to a sufficient reduction in variance).
- Random forests overcome this problem by forcing each split to consider only a subset of the predictors.

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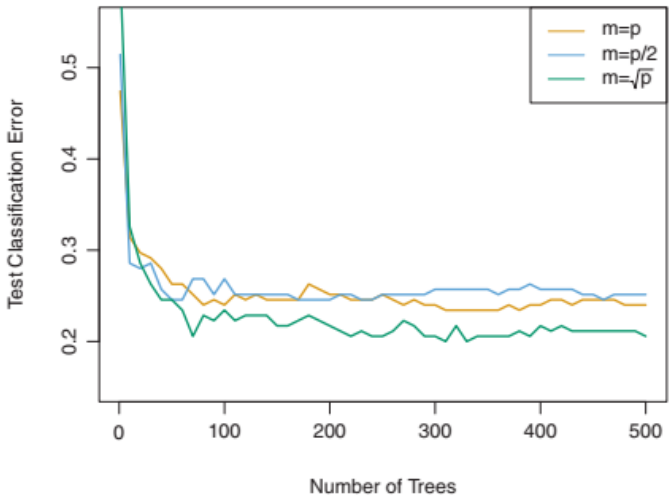
Impact of choosing different m values



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Boosting

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Boosting – Basic idea

- The principal difference between boosting and the bagging algorithm is is that the base models are trained in sequence.
- Each model is trained using information from previously trained models.
- Boosting does not involve bootstrap sampling; instead each tree is fit on a *modified version of the original data set.*

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Boosting for Regression Trees - Algorithm

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:
   $$\hat{f}(x) \leftarrow \hat{f}(x) + \lambda \hat{f}^b(x).$$
   (c) Update the residuals,
   $$r_i \leftarrow r_i - \lambda \hat{f}^b(x_i).$$
3. Output the boosted model,
   $$\hat{f}(x) = \sum_{b=1}^{B} \lambda \hat{f}^b(x).$$

Tuning Parameters:

- B, number of models
- d, depth of each model
- λ: shrinkage parameter

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Basic idea

- Fit a decision tree to the residuals from the model (mistakes of this model), rather than the outcome Y , as the response.
- By fitting small trees to the residuals, we slowly improve $\hat{f}$ in areas where it does not perform well.
- The shrinkage parameter λ slows the process down even further, allowing more and different shaped trees to attack the residuals

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- Suppose the value you are predicting is 12 and $\lambda = 0.1$
- First model: predicts 6 (i.e. residue: 6)
- Second model tries to predict 6, let's say it predicts 4.5
- Total prediction (6+0.1*4.5=6.45) – residue:5.55

…….

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Tuning Parameters

1. The number of trees B. Unlike bagging and random forests, boosting can overfit if B is too large, although this overfitting tends to occur slowly if at all. (We use cross-validation to select B).
2. The shrinkage parameter λ, a small positive number. This controls the rate at which boosting learns. Typical values are 0.01 or 0.001, and the right choice can depend on the problem. Very small λ can require using a very large value of B in order to achieve good performance.
3. 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. In this case, the boosted ensemble is fitting an additive model, since each term involves only a single variable.

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