

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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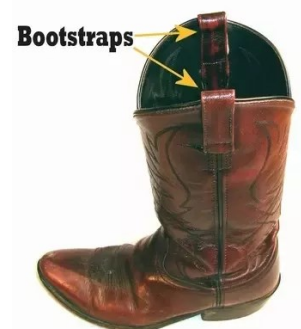
Bootstrap



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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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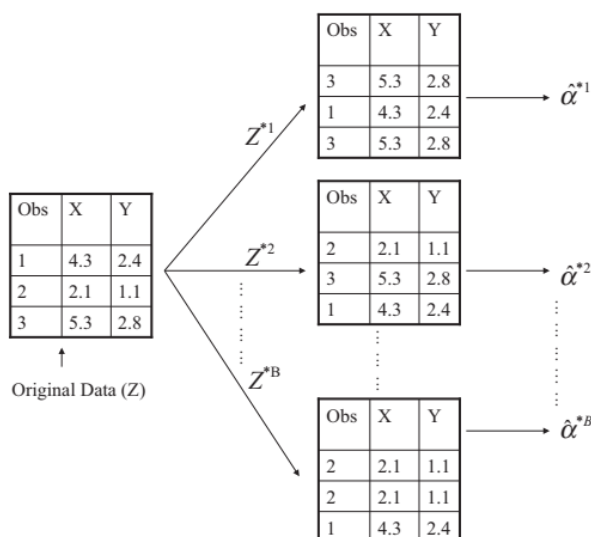
Procedure

- Suppose our original data set consists of n data points $X = \{x_1, x_2, \dots, x_n\}$
- 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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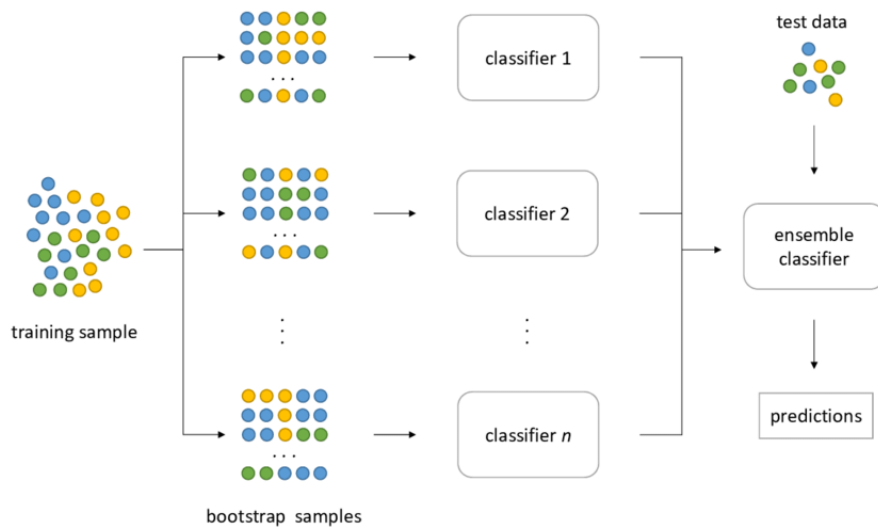
Bagging

- 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)



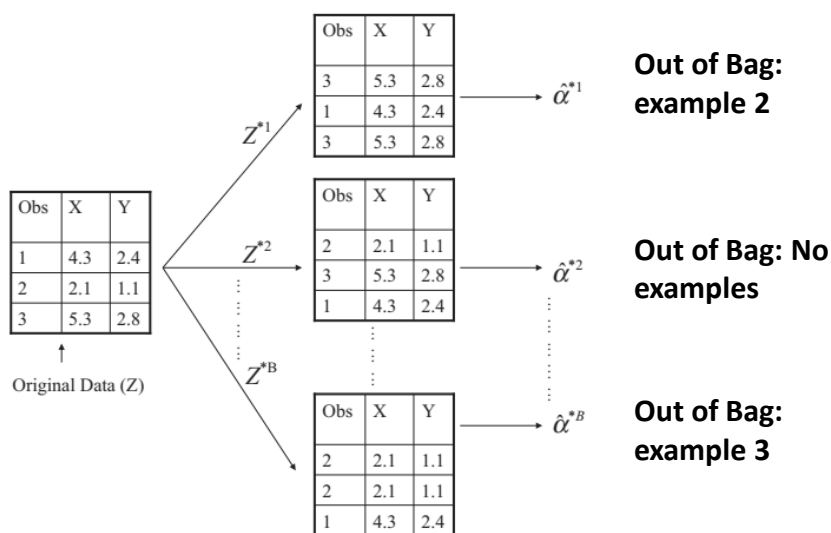
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Out-of-Bag (OOB) Error

- 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.

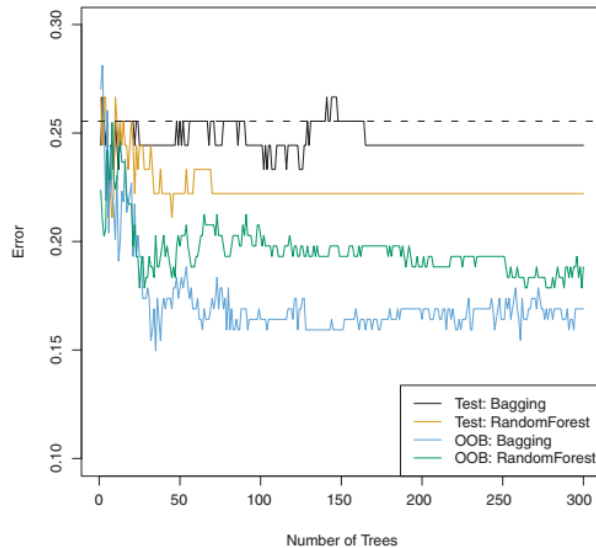


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Out-of-Bag Error (Cont.)



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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 performing 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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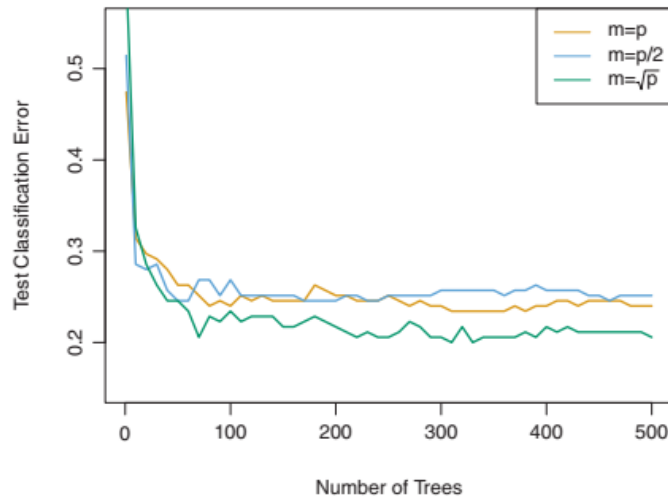
Uncorrelated trees

- 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 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 $b = 1, 2, \dots, B$, 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 shrunk 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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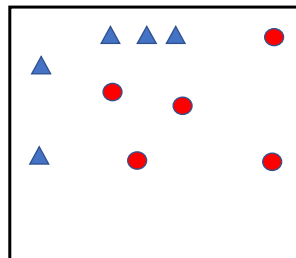
Tuning Parameters

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.



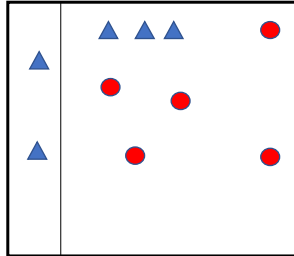
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Adaboost



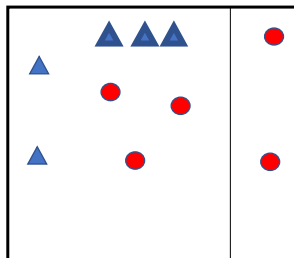
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Model 1



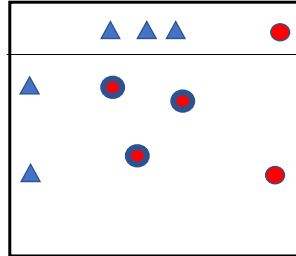
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Model 2



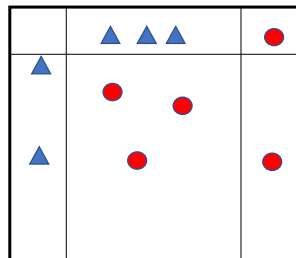
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Model 3



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Cobine



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