Ensembles and Random Forests

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- Decision trees are easy to interpret and don't require much computation to train
 - However, capturing a complex relationship using a decision tree requires the tree be deep (lots of splits)
 - This is problematic because trees exhibit high variance and are prone to overfitting
- This presentation will focus on the random forest algorithm, a well-known ensemble model



Bagging

Random forests rely upon *bagging*, or "bootstrap aggregation", to construct a large number of decision trees:

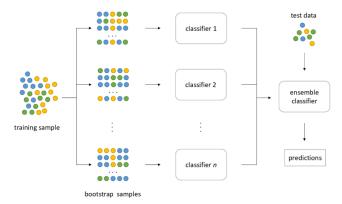


Image credit: https://hudsonthames.org/bagging-in-financial-machine-learning-sequential-bootstrapping-python/



- Bagging produces an *ensemble model* comprised of many different *base models*
 - Each base model contributes towards a final prediction, either by majority/weighted voting (classification) or simple/weighted averaging (regression)



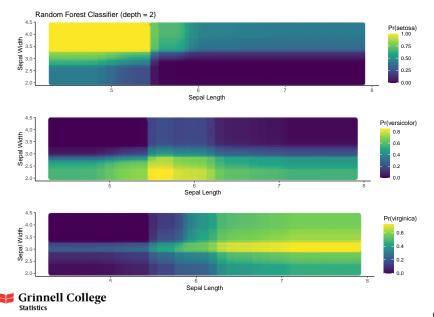
- Bagging produces an *ensemble model* comprised of many different *base models*
 - Each base model contributes towards a final prediction, either by majority/weighted voting (classification) or simple/weighted averaging (regression)
- Random forests are an ensemble model built using bagging, where each base model is a decision tree
 - What would happen if bagging were not used?



- Bagging is one strategy used by random forests to address the limitations of a single decision tree
- A second strategy is *predictor sampling*, or the random selection of limited candidate pool of predictors to be considered *at each split*
 - What might happen if predictor sampling were not used?

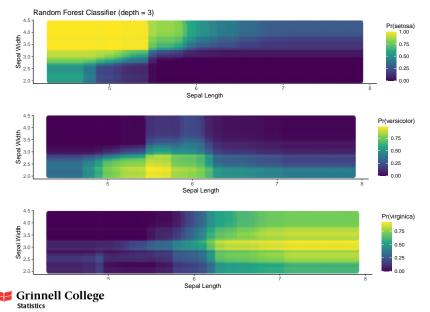


Random Forest (depth = 2)



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Random Forest (depth = 3)



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Single Decision Tree (depth = 3)

Decision Tree Classifier 4.5 -Pr(setosa) 4.0 4.0 3.5 3.5 3.0 3.0 3.0 0.75 0.50 0.25 2.0 0.00 7 5 6 å Sepal Length 4.5 Pr(versicolor) 4.0 -3.5 -3.0 -3.0 -2.5 -0.6 0.4 0.2 2.0 5 8 Sepal Length 4.5 -Pr(virginica) 4.0 4.0 Sepal Width 3.0 0.6 0.4 0.2 2.5 2.0 0.0 6 8 Sepal Length Grinnell College Statistics

- Random forests will generally offer better predictive performance than a single decision tree
 - The primary downside is that random forests are not easily interpretable
- Important tuning parameters are max_depth, min_samples_split, and max_features (the number or fraction of predictors considered at each split)
- The number of trees in the forest is also important, but including more trees past a certain point will not improve the ensemble.



Final Remarks (cont.)

max_depth and min_samples_split help prevent base models from being overfit

- By using an ensemble approach, random forests can be flexible without using deep trees
- Thus, relative to a single decision tree, you should consider using a smaller max_depth and larger min_samples_split
- max_features governs the degree of correlation between base models
 - Smaller values reduce correlations between trees (at the expense of predictive power within individual trees)
 - Default recommendations are \sqrt{p} for classification and p/3 for regression

