Bagging / Random Forest

An Introduction to ensemble models

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Objectives

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- Review decision trees
- What is an ensemble model?
  - Why is it useful?
  - How does it deal with the bias-variance trade-off?
- What is bagging?
  - What are pros and cons of bagging?
- What are random forests?
  - How are they different from bagging?
  - What are the tunable hyperparameters?
- Individual Assignment
  - Implement bagging / random forests
- Pair assignment
  - Predict churn with random forests

Decision Trees

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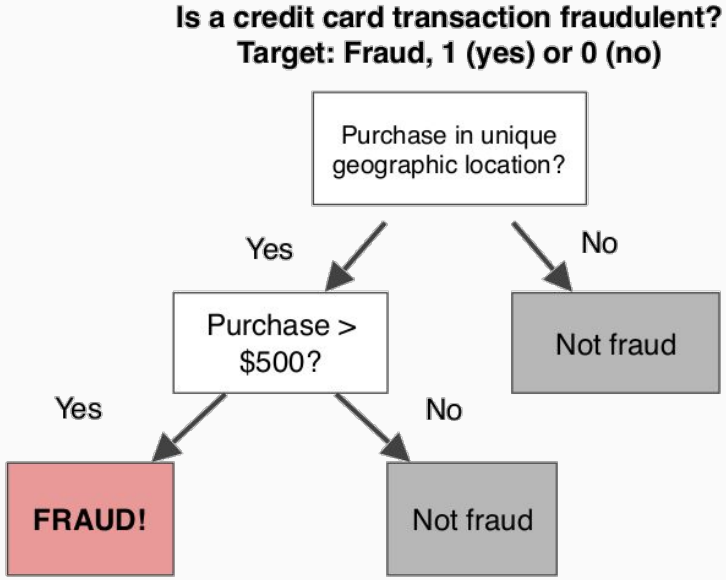
- Describe metrics used to describe the impurity in a node of categorical variables (there should be 2)
  - Shannon Entropy & Gini Index
- What about for a continuous variable?
  - RSS
- Describe how a decision tree "decides" where to make its next split.
- Are decision trees deterministic?
  - Yes
- Decision trees are non-parametric, but they have some hyper parameters that we can tune - name and describe them!
  - Max Depth, Min Samples, Max Leaf Nodes

Decision Trees Review

- Decision Trees are deterministic:
  - Once they are trained, they will arrive at the same conclusion every time given the same X values.
- Decision Trees are "nonparametric":
  - We don't make any assumptions (mean, variance, etc.) about our data when we create a tree.



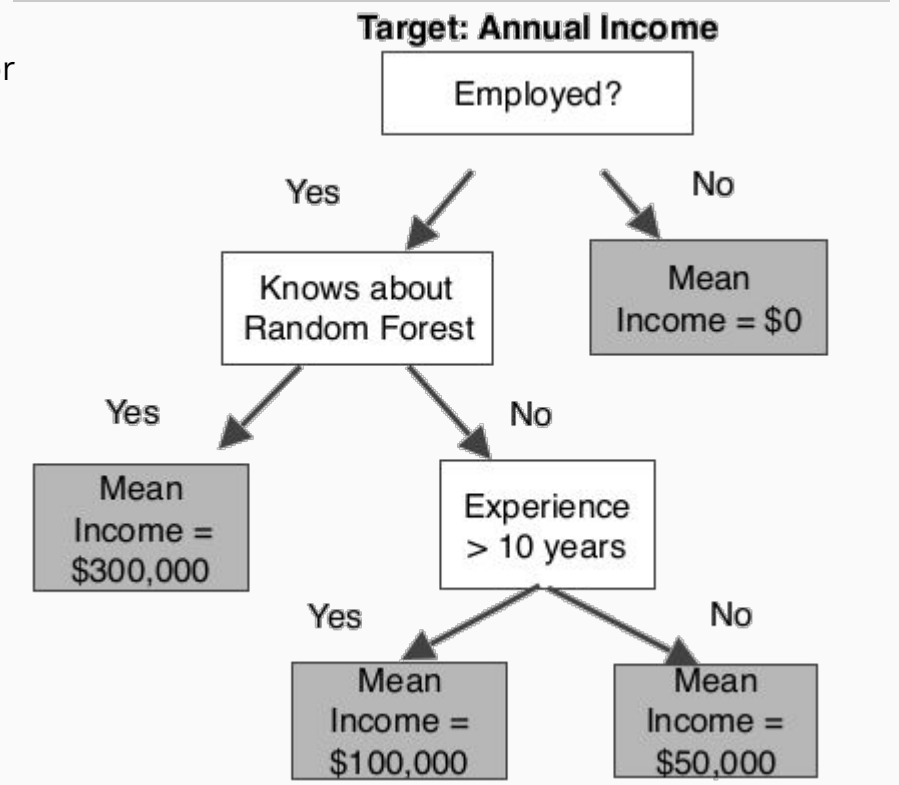
Decision Trees: Regression

Each split tries to minimize the Total Squared Error

$$\sum_{j=1}^{J} \sum_{i \in R_j} (y_i - \hat{y}_{R_J})^2$$

Where J is the number of child nodes and R is each child node

The model output is typically the mean within each leaf node



Pros and Cons of Decision Trees

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Pros

- Handle non-linear relationships well
- Highly interpretable (unless we have a ton of features)
- Useful for classification & regression
- No feature scaling required

Cons

- Expensive to train
- **Often poor predictors (high variance)**

Ensemble Models: Wisdom of the Crowd

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Suppose you are trying to guess how many Skittles are in a jar.

- Looks like I have a water bottle here!
  - Guess how many are in the jar and submit your answer:
  - https://goo.gl/forms/7Q1fw2tPB4ZYRkWF3
- Do you think your guess was better than average?
- Let's see: Results

Ensemble Model

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Combines multiple weak learners to form a strong learner

- Basic Idea: Wisdom of the Crowd
  - Run multiple models on the data and aggregate the predictive results to produce an overall prediction that is better than any of the individual models could do on their own
  - The overall prediction is the **average prediction** for a regressor or
  - **Plurality choice** for a classifier (or the average of the percentages of each class)

Ensemble for decision trees?

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- What is a common pitfall of decision trees?
  - Overfitting to the data
  - Let's try using a large number of trees to reduce variance
- What if we just build a bunch of decision trees and average the results?
  - Do you foresee any issues?

Ensemble for decision trees?

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- Decision trees are deterministic (given the same data, they will return the same splits)
  - An ensemble model won't work here!
- How can we solve this?
  - Train each learner on a different subset of the data
  - But how do we do this when we only have one set of data to work with?
    - Bootstrapping!

Bootstrapping Review

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- What is a bootstrap sample?
  - Given n data points we select a sample of n points with replacement
- What have we used it for?
  - Return better estimates of sample statistics (95% confidence interval for example)

How to bootstrap

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- Method
  - Start with your dataset of size n
  - Sample from your dataset with replacement to create one bootstrap sample of size n
  - Repeat B times
  - Each bootstrap sample can then be used as a separate dataset for estimation or model fitting
- Advantages
  - Requires no theoretical calculations
  - Available regardless of how complicated the estimator might be

Bias and Variance Review

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- Bias:
  - Error from failure to match the training set
  - Caused by choosing a model that is too simple

- Variance:
  - Error due to random noise specific to our training set
  - Decreases as we get more data

Bias Variance Trade-off for Bushy Trees

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- What's great about bushy decision trees?
  - Low bias
- What's not so great about them?
  - High variance
- Bias
  - Trees can be low bias by being highly complex
- Variance
  - "Given a set of n independent observations Z_1 ,...,Z_n , each with variance σ^2 , the variance of the mean Z-bar of the observations is given by σ^2 / n. In other words, averaging a set of observations reduces variance."
    -- Introduction to Statistical Learning

$$\text{Variance} = \frac{\sigma^2}{B}$$

Where B is the number of independent estimators

Bagging

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Bagging* , or **B**ootstrap **ag**gregation, is a general-purpose procedure **for reducing the variance** of a statistical learning method

- Bootstrapped trees provide low-bias, high variance predictors
- Trees are generally grown deep and are not pruned, hence each individual tree has high variance, but low bias
- Averaged predictors are still low-bias
- Averaged estimators are lower variance than single predictors
- The number of trees B is not a critical parameter with bagging; using a very large B won't lead to overfitting
- In practice we want to use a large enough B such that our test error has settled down

*Bagging is a general ensemble procedure often used with trees

Bagging

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- This seems a little like cheating right?
- What did we assume about our estimators?
  - Independence
  - Bootstrapped samples are not independent

$$Var\left(\hat{f}_{bag}(x_0)\right) = \rho\sigma^2 + \frac{(1-\rho)\sigma^2}{B}$$

- ρ = rho, the correlation coefficient for the different samples
- As rho goes towards one, the effect of multiple estimators on decreasing variance weakens
- Only the uncorrelated parts of the sample decrease variance

Bagging Review

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- What is an ensemble method?
- Why do we need to bootstrap?
- The general idea of bagging is to start with ___ bias, ___ variance trees and aggregate across multiple models to decrease _____
- Why are bootstrapped samples correlated?

Decorrelating Trees

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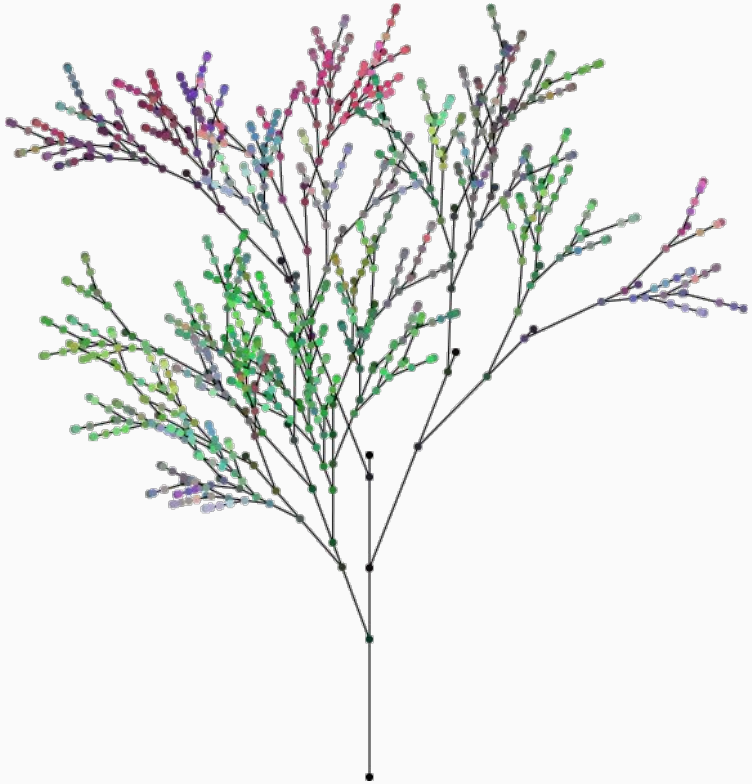
- Bagged trees are correlated because:
  - Bootstrap samples are about the same (approximately ⅔)
    - Can't do much about this
  - Influential features tend to be the same
    - We **can** fix this

Random Forests

Everyone's Favorite ML algorithm



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http://luc.devroye.org/lucsforest2008/

Random Forests

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- Ensemble method similar to bagging
- Trees are trained on bootstrapped samples
- But, at each split we only use a random subset of features (subset sampling)
  - Only use some features to make splits
  - This prevents trees from always making the same splits
  - Subset of features is resampled at every split
  - Smaller subset of features = less correlation between trees

Tuning Random Forests

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- Tuning
  - m = number of features included at each split
  - p = total number of features
  - m = $\sqrt{p}$ (sklearn default) or m = p/3 features
- Performance
  - Random forests are robust to overfitting and other issues associated with decision trees
  - Generally use a large number of bushy trees
  - Often has state-of-the-art performance without much tuning

Random Forest Parameters

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- Total number of trees (n_estimators)
- Number of features to consider at each split (max_features)
- Individual decision tree parameters
  - E.g., tree depth (max_depth), pruning (min_samples_split, min_samples_leaf)

How many trees should we use?

- Variance decreases with more trees
  - But with diminishing returns
- Runtime scales linearly with the number of trees
- More is still better, but start small first to reduce computation time

Random Forest Pros and Cons

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- Pros
  - Often give near state-of-the-art performance
  - Good out-of-the-box performance
  - No feature scaling needed
  - Models nonlinear relationships
- Cons
  - Can be expensive to train (though can be done in parallel)
  - Models can be quite large (the pickled version of a several hundred tree model can easily be several GBs)
  - Not interpretable (although techniques such as predicted value plots can help)

Random Forests Review

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- How is random forest an improvement over bagging?
- As the subset of features (m) available at each split increases, tree correlation _____
- What are two pros of Random Forests?
- Two cons?

Afternoon

Random Forest in Sklearn

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class sklearn.ensemble.**RandomForestClassifier**(*n_estimators='warn'*, *criterion='gini'*, *max_depth=None*, *min_samples_split=2*, *min_samples_leaf=1*, *min_weight_fraction_leaf=0.0*, *max_features='auto'*, *max_leaf_nodes=None*, *min_impurity_decrease=0.0*, *min_impurity_split=None*, *bootstrap=True*, *oob_score=False*, *n_jobs=None*, *random_state=None*, *verbose=0*, *warm_start=False*, *class_weight=None*)[source]

```
from sklearn.ensemble import RandomForestClassifier # or RandomForestRegressor

rfc = RandomForestClassifier(n_estimators = 100, n_jobs = -1)
rfc.fit(X_train)

y_pred = rfc.predict(X_test)
```

Out of Bag Score (OOB Score)

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OOB Score is a quick and dirty "replacement" for cross validation

- We already have data that each tree has not seen yet -- each bootstrapped sample only includes about ⅔ of the data.
- We can feed the data that wasn't used in a tree as a **test set** for that tree.
- We can then aggregate the *accuracy score** for each of our points (each test data point tested on ~⅓ of our trees)

*The downside is that oob_score in sklearn only computes accuracy or R^2, so if we want precision, recall, or other metrics we will still need to cross validate

```
rf = RandomForestClassifier(n_estimators=100, oob_score=True)
rf.fit(X_train, y_train)
print(rf.oob_score_)
```

Interpreting Tree Models

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Recall, one of the main strengths of Decision Trees is interpretability.

However, when we aggregate our trees with simple Bagging or Random Forests, it's not so easy…

- We can no longer simply rank our features in the order in which they were split on
- We can look at ***Feature Importances*** *(Note: not as interpretable as coefficients for a linear regression)*

Feature Importances

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- Measure the total amount the information gain increases due to splits over a given feature

  rf.feature_importances_ (where rf is your fit RandomForestClassifier / RandomForestRegressor) does this

Measuring Feature importance

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Let's get some intuition for how we calculate feature importances…

1. For each feature m_j, we calculate the decrease in our impurity criterion (MSE, Gini, etc.) for the node(s) that split on m_j
2. We then weight it by how many points passed through the nodes that split on m_j
3. And finally, we average the calculations for steps 1 and 2 across our entire forest

Leave One Out Feature Importance

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Two more methods...

- When tree B_i is grown, score it with OOB, then remove that feature and score it again to measure the change in your validation metric(s)
  - This is called **Leave One Out Feature Importances**

- Iterate through features dropping m_j out and plotting feature importances -- help with "multicollinearity"

What does feature importance not tell us?

- It is difficult to learn the effect size and direction of a feature
- For most real world problems, features don't have a constant effect size across all X-values
    - Effect direction can even reverse at different levels of X.

Partial Dependence Plots

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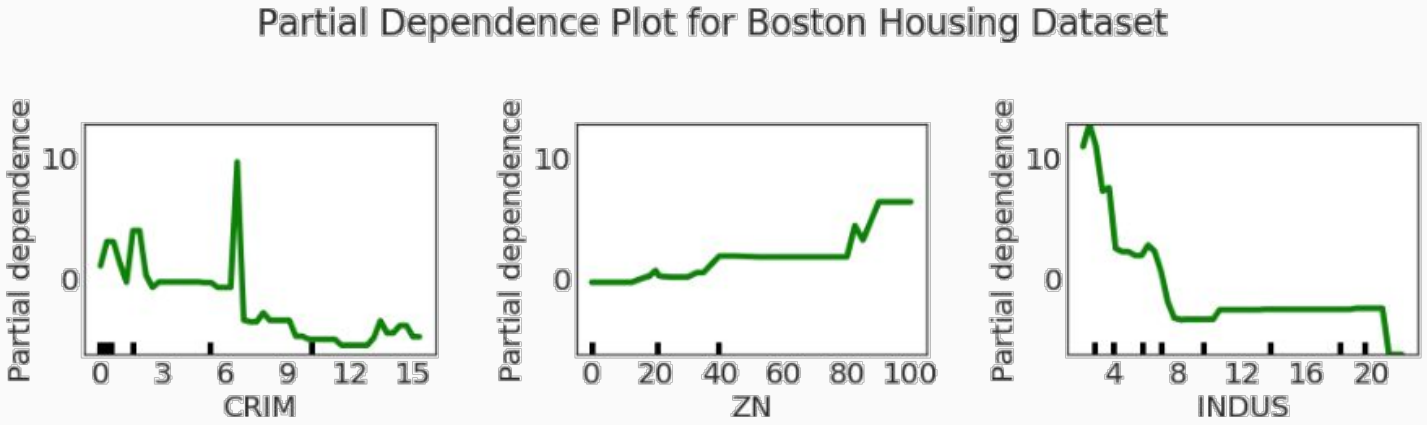
How can we view how a single variable affects the prediction?

- Permute values for each feature column and compare predictive "success" of the feature at each value
- Compare one (or two, if you use a 3D plot) features and how predictive they are at different values
- How to interpret y - axis:
  - "The partial dependence curve at a certain feature value represents the average prediction when we force all data points to take on that feature value."[1]

1. https://christophm.github.io/interpretable-ml-book/pdp.html

Partial Dependence Plots



Partial Dependence Plots

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They can be used for all kinds of models, not just trees!

To the notebook!

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- Jupyter-notebook comparing decision trees with random forests
- Examples of feature importances and partial dependence plots
- Example usage of sklearn implementations

Predicting churn with sklearn

Random Forests

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