Bagging Trees & Random Forests

Justin Post

Recap

- MLR, Penalized MLR, & Regression Trees
  - Commonly used model with a numeric response
- Logistic Regression, Penalized Logistic Regression, & Classification Trees
  - Commonly used model with a binary response
- MLR & Logistic regression are more structured (linear)
- Trees easier to read but more variable (non-linear)

Prediction with Tree Based Methods

If we care mostly about prediction not interpretation

- Often use **bootstrapping** to get multiple samples to fit on
- Can average across many fitted trees
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Major ensemble tree methods

1. Bagging (boostrap aggregation)
2. Random Forests (extends idea of bagging - includes bagging as a special case)
3. Boosting (*slow* training of trees)

Bagging

Bagging = Bootstrap Aggregation - a general method

Bootstrapping

- resample from the data (non-parametric) or a fitted model (parameteric)
- for non-parameteric
    - treats sample as population
    - resampling done with replacement
    - can get same observation multiple times

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- for non-parameteric
    - treats sample as population
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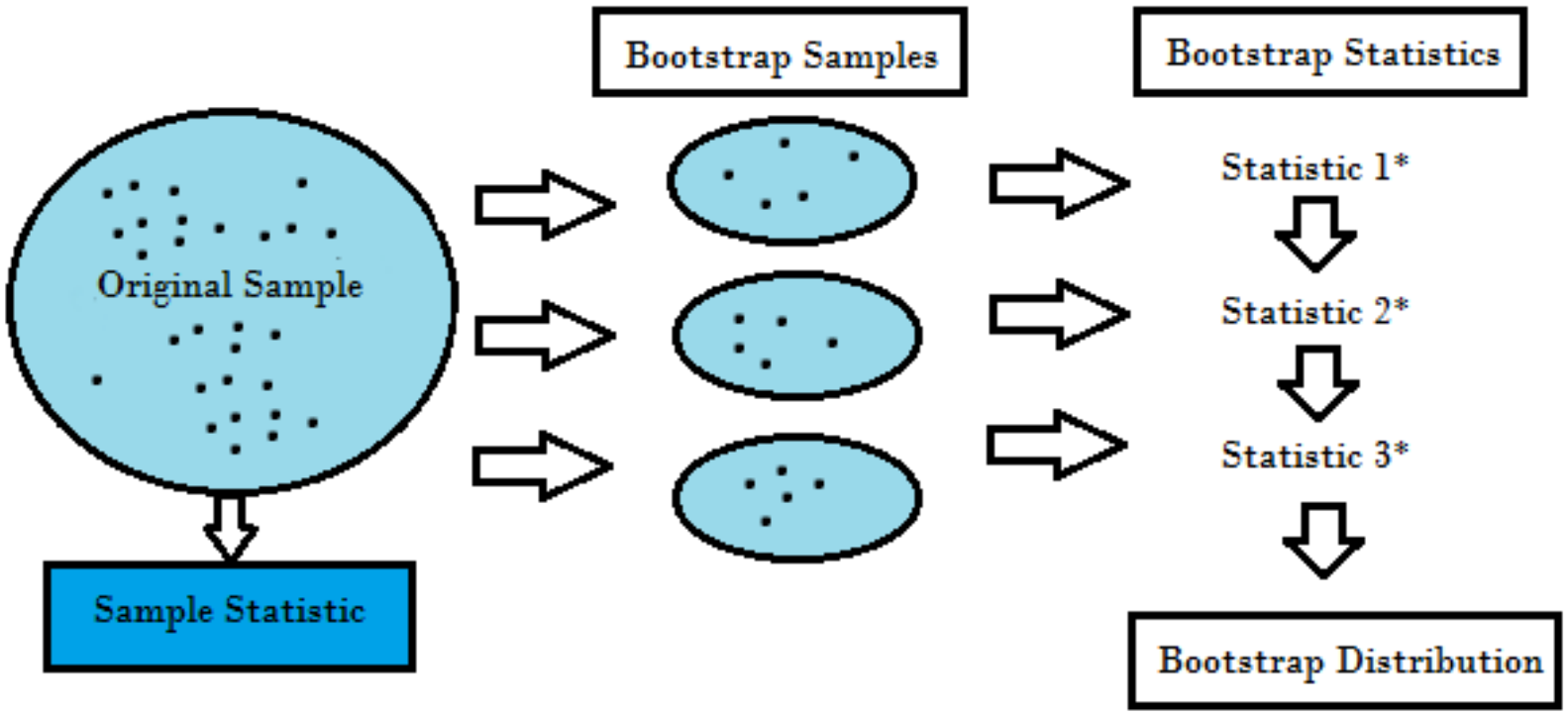
    - can get same observation multiple times
- method or estimation applied to each resample
- traditionally used to obtain standard errors (measures of variability) or construct confidence intervals

Non-Parametric Bootstrapping



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1. Create a bootstrap sample (same size as actual sample)
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4. Final prediction is average of these predictions
    - $\hat{y}(x) = \frac{1}{B}\sum_{j=1}^{B}\hat{y}^{*j}(x)$

Bagging

For Classification Trees:

1. Create a bootstrap sample (same size as actual sample)
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4. (One option) Use **majority vote** as final classification prediction (i.e. use most common prediction made by all bootstrap trees)

Bagging Example

```
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
bike_data = pd.read_csv("data/bikeDetails.csv")
#create response and new predictor
bike_data['log_selling_price'] = np.log(bike_data['selling_price'])
bike_data['log_km_driven'] = np.log(bike_data['km_driven'])
#Add a Categorical Predictor via a Dummy Variable
bike_data["one_owner"] = pd.get_dummies(bike_data["owner"]).iloc[:,0]
pd.get_dummies(bike_data["owner"])
```

```
##       1st owner  2nd owner  3rd owner  4th owner
## 0             1          0          0          0
## 1             1          0          0          0
## 2             1          0          0          0
## 3             1          0          0          0
## 4             0          1          0          0
## ...         ...        ...        ...        ...
## 1056          1          0          0          0
## 1057          1          0          0          0
## 1058          0          1          0          0
## 1059          1          0          0          0
## 1060          1          0          0          0
##
## [1061 rows x 4 columns]
```

Bagging Example

- We can use the `RandomForestRegressor` function with `max_features` set to `None`
- No tuning parameters really needed. Can set `max_depth` or `min_samples_leaf` as before
- Default says to train on 100 trees (bootstrap samples)

```
from sklearn.ensemble import RandomForestRegressor
bag_tree = RandomForestRegressor(max_features = None, n_estimators = 500)
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from sklearn.ensemble import RandomForestRegressor
bag_tree = RandomForestRegressor(max_features = None, n_estimators = 500)
bag_tree.fit(bike_data[['log_km_driven', 'year']],
             bike_data['log_selling_price'])
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```

- Still predict with `.predict()`

```
print(bag_tree.predict(np.array([[9.5, 1990], [9.5, 2015], [10.6, 1990], [10.6, 2015]])))
```

```
## [10.79793114 10.78809644  9.77939894 10.4513258 ]
##
## C:\python\lib\site-packages\sklearn\base.py:450: UserWarning: X does not have valid feature names, but RandomForestRegres
##   warnings.warn(
```

```
print(np.exp(bag_tree.predict(np.array([[9.5, 1990], [9.5, 2015], [10.6, 1990], [10.6, 2015]]))))
```

```
## [48919.48868338 48440.73851228 17666.03126062 34590.20418069]
##
## C:\python\lib\site-packages\sklearn\base.py:450: UserWarning: X does not have valid feature names, but RandomForestRegres
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```

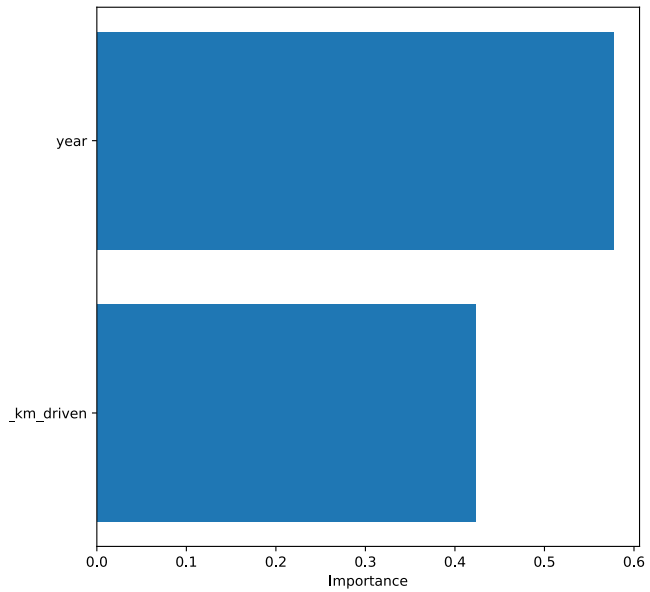
Bagging Example

- Can look at variable importance measure

```
bag_tree.feature_importances_
```

```
## array([0.42265995, 0.57734005])
```

```
plt.barh(bike_data.columns[[8,2]], bag_tree.feature_importances_); plt.xlabel("Importance");plt.show()
```



Bagging Example

- Fit the bagged tree model

```
bag_tree2 = RandomForestRegressor(max_features = None, n_estimators = 500)
bag_tree2.fit(bike_data[['log_km_driven', 'year', 'one_owner']],
              bike_data['log_selling_price'])
```

- Compare predictions between models

```
to_predict = np.array([[9.5, 1990, 1], [9.5, 1990, 0], [9.5, 2000, 1], [9.5, 2000, 0]])
pred_compare = pd.DataFrame(zip(bag_tree.predict(to_predict[:,0:2]), bag_tree2.predict(to_predict)),
                            columns = ["No Cat", "Cat"])
```

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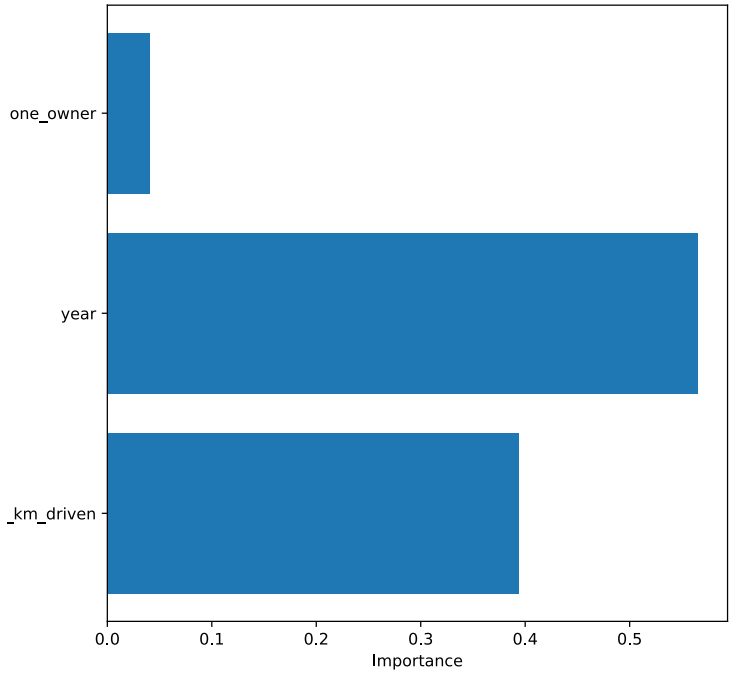
```

```
pd.concat([pred_compare, np.exp(pred_compare)], axis = 1)
```

```
##       No Cat        Cat        No Cat           Cat
## 0  10.797931  10.323810  48919.488683  30449.054146
## 1  10.797931  11.029802  48919.488683  61685.369810
## 2   9.828104   9.686956  18547.750316  16106.135206
## 3   9.828104  10.014984  18547.750316  22358.996299
```

Variable Importance

```
plt.barh(bike_data.columns[[8,2, 9]], bag_tree2.feature_importances_); plt.xlabel("Importance");plt.show()
```



Compare CV Error of Bagged Tree to Other Models

```
from sklearn.model_selection import GridSearchCV, cross_validate
from sklearn.linear_model import LinearRegression
from sklearn.tree import DecisionTreeRegressor
bag_cv = cross_validate(RandomForestRegressor(n_estimators = 500, max_depth = 4, min_samples_leaf = 10),
                        bike_data[['log_km_driven', 'year', 'one_owner']],
                        bike_data['log_selling_price'], cv = 5, scoring = "neg_mean_squared_error")
```

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```
rtree_tune = GridSearchCV(DecisionTreeRegressor(),
                          {'max_depth': range(2,15),'min_samples_leaf':[3, 10, 50, 100]}, cv = 5,
                          scoring = "neg_mean_squared_error") \
                          .fit(bike_data[['log_km_driven', 'year', 'one_owner']],
                                         bike_data['log_selling_price'])
rtree_cv = cross_validate(rtree_tune.best_estimator_,
                        bike_data[['log_km_driven', 'year', 'one_owner']],
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                        bike_data['log_selling_price'], cv = 5, scoring = "neg_mean_squared_error")
```

```
mlr_cv = cross_validate(LinearRegression(),
                        bike_data[['log_km_driven', 'year', 'one_owner']],
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from sklearn.linear_model import LinearRegression
from sklearn.tree import DecisionTreeRegressor
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                        bike_data['log_selling_price'], cv = 5, scoring = "neg_mean_squared_error")
```

```
print(np.sqrt([-sum(bag_cv['test_score'])/5, -sum(rtree_cv['test_score'])/5, -sum(mlr_cv['test_score'])/5]))
```

```
## [0.50498791 0.51469632 0.51735197]
```

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- Often use **bootstrapping** to get multiple samples to fit on
- Can average across many fitted trees
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1. Bagging (boostrap aggregation)
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But why?

- If a really strong predictor exists, every bootstrap tree will probably use it for the first split (2nd split, etc.)
- Makes bagged trees predictions more correlated
- Correlation --> smaller reduction in variance from aggregation

Random Forests

By randomly selecting a subset of predictors, a good predictor or two won't dominate the tree fits

- Rules of thumb say use `num_features` = $\sqrt{\#\text{ predictors}}$ (classification) or `num_features` = $\#\text{ predictors}/3$ (regression) (randomly selected) predictors
- If `num_features` = number of predictors then you have bagging!
  - Default for `RandomForestRegressor()`
- Better to determine `num_features` via CV (or other measure)

Random Forests

- Select best random forest model using `GridSearchCV()`

```
parameters = {"max_features": range(1,4), "max_depth": [3, 4, 5, 10, 15],'min_samples_leaf':[3, 10, 50, 100]}
rf_tune = GridSearchCV(RandomForestRegressor(n_estimators = 500),
                       parameters, cv = 5, scoring = "neg_mean_squared_error")
rf_tune.fit(bike_data[['log_km_driven', 'year', 'one_owner']],
            bike_data['log_selling_price'])
```

```
print(rf_tune.best_estimator_)
```

```
## RandomForestRegressor(max_depth=5, max_features=2, min_samples_leaf=3,
##                       n_estimators=500)
```

Random Forests

Compare all model CV errors

```
rf_cv = cross_validate(rf_tune.best_estimator_,
                       bike_data[['log_km_driven', 'year', 'one_owner']],
                       bike_data['log_selling_price'], cv = 5,
                       scoring = "neg_mean_squared_error")

print(np.sqrt([-sum(bag_cv['test_score'])/5, -sum(rtree_cv['test_score'])/5,
               -sum(mlr_cv['test_score'])/5, -sum(rf_cv['test_score'])/5]))
```

```
## [0.50498791 0.51469632 0.51735197 0.50318953]
```

Recap

Averaging many trees can greatly improve prediction

- Comes at a loss of interpretability
- Variable importance measures can be used

Bagging

- Fit many trees on bootstrap samples and combine predictions in some way

Random Forest

- Do bagging but randomly select the predictors to use for each split