# Machine Learning Engineer Nanodegree

# Capstone Project

S Iyer May 8th, 2017

## I. Definition

## **Project Overview**

Bike sharing systems are a new generation of traditional bike rentals where whole process from membership, rental and return back has become automatic. These provide an alternative means of transportation in cities by making bicycling more convenient for users, as they do not need to worry about parking or theft of their own bicycle. Cities can benefit by providing a new sustainable transportation option that can increase access to transit, but also reduce crowding on overburdened transit systems. Today, there exists great interest in these systems due to their important role in traffic, environmental and health issues.

The work presented here analyzes the effect of weather on the use of the Washington, DC, bikeshare system. Hourly weather data, including temperature, rainfall, snow, wind, fog, and humidity levels are linked to hourly usage data. This information is useful for understanding bicycling behavior and also for those planning bikeshare systems in other cities.

#### **Problem Statement**

In Washington, DC, Capital Bikeshare (CaBi) is one of the largest bikeshare system in the nation with over 1,200 bicycles at 140 stations(Alta Bicycle Share, Inc. 2012). The system grew out of an early bikesharing pilot project, SmartBike D.C., launched in 2008(Alta Bicycle Share, Inc. 2012).

A wealth of data on travel behavior is being collected by these systems and Capital Bikeshare has made the trip logs of every trip taken in the system publically available [1]. This analysis exploits the dataset of bicycle trips made using Capital Bikeshare in order to determine how bicycle usage varies under different weather conditions and other calendar factors. We predict the number of rentals every hour considering various factors like temperature (both hot and cold), humidity, windspeed, and various other weather conditions that may affect bicycle usage. We are also able to control for how patterns of daylight and darkness affect trip behavior.

These results have implications for understanding the sensitivity of bicycle usage to weather conditions and how this can affect the usefulness of bicycling as an alternative mode of travel. It is also informative for those planning or operating bikesharing systems. We'll obtain these relationships by exploring various machine learning models including linear regression, decision trees, random forest and gradient boosted trees.

#### Metrics

We'll perform the comparison of the models in terms of mean absolute error (MAE), correlation coefficient, relative absolute error (RAE), and root relative squared error (RRSE) as described by Fanaee-T et. al.[1].

$$RAE = \frac{|p_1 - a_1| + \dots + |p_n - a_n|}{|\bar{a} - a_1| + \dots + |\bar{a} - a_n|}$$

$$RRSE = \frac{(p_1 - a_1)^2 + \dots + (p_n - a_n)^2}{(\bar{a} - a_1)^2 + \dots + (\bar{a} - a_n)^2}$$

Correlation coefficient = 
$$\frac{S_{PA}}{\sqrt{S_P S_A}}$$

where,

$$S_{PA} = \frac{\sum (p_i - \bar{p})(a_i - \bar{a})}{n - 1}$$
 $S_P = \frac{\sum (p_i - \bar{p})^2}{n - 1}$ 
 $S_A = \frac{\sum (a_i - \bar{a})^2}{n - 1}$ 

In the above equations, a denotes actual target values, p denotes predicted target values,  $\bar{a}$  represents the average of actual target value,  $\bar{p}$  denotes the average of predicted target values and n denotes the sample size.

This being a regression problem (predicting count) we use squared error as the metric of choice. The relative form of these errors remove the scale of these counts (100 vs 100 million) from the comparisions.

# II. Analysis

## **Data Exploration**

The dataset "Bike-Sharing-Dataset" was obtained by the UCI Machine Learning Repository. This is a collection of databeses, domain theories and data generators which are used by the machine learning community for empirical analyses. The archive was created in 1987 by David Aha and fellow graduate students at UC Irvine. Since then it has been widely used by student, educators and researchers. The current website was designed in 2007. The UCI Machine Learning Repository is based on donations of researchers, mostly outside of UCI.

This dataset contains the hourly and daily count of rental bikes between years 2011 and 2012 in Capital bikeshare system with the corresponding weather and seasonal information. The Laboratory of Artificial Intelligence and Decision Support (LIAAD), University of Porto, aggregated the data on two hourly and daily basis and then extracted and added the corresponding weather and seasonal information that were extracted from http://www.freemeteo.com

#### **Attribute Information:**

The dataset contains the following fields:

- instant: record index
- dteday : date
- season: season (1:springer, 2:summer, 3:fall, 4:winter)
- yr : year (0: 2011, 1:2012)
- mnth: month (1 to 12)
- hr : hour (0 to 23)
- holiday: whether day is holiday or not
- weekday: day of the week
- workingday: if day is neither weekend nor holiday is 1, otherwise is 0.
- weathersit:
  - 1: Clear, Few clouds, Partly cloudy, Partly cloudy
  - 2: Mist + Cloudy, Mist + Broken clouds, Mist + Few clouds, Mist
  - 3: Light Snow, Light Rain + Thunderstorm + Scattered clouds, Light Rain + Scattered clouds
  - 4: Heavy Rain + Ice Pallets + Thunderstorm + Mist, Snow + Fog
- temp: Normalized temperature in Celsius. The values are derived via  $(t t_m in)/(t_m ax t_m in)$ ,  $t_m in = -8$ ,  $t_m ax = +39$  (only in hourly scale)

- atemp: Normalized feeling temperature in Celsius. The values are derived via  $(t t_m in)/(t_m ax t_m in)$ ,  $t_m in = -16$ ,  $t_m ax = +50$  (only in hourly scale)
- hum: Normalized humidity. The values are divided to 100 (max)
- windspeed: Normalized wind speed. The values are divided to 67 (max)
- casual: count of casual users
- registered: count of registered users
- cnt: count of total rental bikes including both casual and registered

Given below is a random sample of 10 rows from the dataset.

instan	t dteday	seas	onyr	$\operatorname{mnt}$	h hr	holi	dayweel	kda <b>w</b> ork	ingdwagat	hersti <b>e</b> mp	at emphum	windsp	e <b>ca</b> sua	alregiste	ere <b>c</b> nt
9666	2012- 02-	1	1	2	16	0	0	0	1	0.2	0.16670.34	0.4627	16	148	164
1775	03-	1	0	3	15	0	6	0	1	0.5	0.48480.29	0.4179	170	143	313
10487	19 2012- 03-	1	1	3	1	0	0	0	1	0.46	0.45450.82	0.1343	25	88	113
17269	18 2012- 12- 27	1	1	12	9	0	4	1	1	0.26	0.21210.6	0.4925	6	127	133
13028		3	1	7	0	0	1	1	2	0.76	0.71210.58	0.2239	12	31	43
5540	2011- 08- 23	3	0	8	17	0	2	1	1	0.72	0.65150.34	0.2239	133	339	472
6754		4	0	10	23	0	4	1	2	0.58	0.54550.88	0.194	2	45	47
12572	2012- 06-	2	1	6	0	0	3	1	2	0.66	0.59090.94	0.194	7	27	34
929	13 2011- 02- 11	1	0	2	7	0	5	1	1	0.08	0.16670.73	0	1	73	74
603	2011- 01- 28	1	0	1	8	0	5	1	2	0.16	0.197 0.86	0.0896	2	155	157

The table below provides the statistical summary of each categorical column in the dataset.

	dteday	season	yr	mnth	hr	holiday	weekday	workingday	weathersit
count	17379	17379	17379	17379	17379	17379	17379	17379	17379
unique	731	4	2	12	24	2	7	2	4
top	2012-08-29 00:00:00	3	1	7	17	0	6	1	1
freq	24	4496	8734	1488	730	16879	2512	11865	11413
first	2011-01-01 00:00:00	nan	nan	nan	nan	nan	nan	nan	nan
last	2012-12-31 00:00:00	nan	nan	nan	nan	nan	nan	nan	nan

The table below provides the statistical summary of each continuous column in the dataset.

	temp	atemp	hum	windspeed	casual	registered	cnt
count	17379	17379	17379	17379	17379	17379	17379
mean	0.496987	0.475775	0.627229	0.190098	35.6762	153.787	189.463
$\operatorname{std}$	0.192556	0.17185	0.19293	0.12234	49.305	151.357	181.388
$\min$	0.02	0	0	0	0	0	1
25%	0.34	0.3333	0.48	0.1045	4	34	40
50%	0.5	0.4848	0.63	0.194	17	115	142
75%	0.66	0.6212	0.78	0.2537	48	220	281
max	1	1	1	0.8507	367	886	977

For numeric data, the table includes count, mean, std, min, max as well as the quartiles. For categorical data, the summary includes count, unique, top, and freq. The 'top' is the most common value and the 'freq' is the most common value's frequency. Timestamp column ('dteday') also include the first and last item.

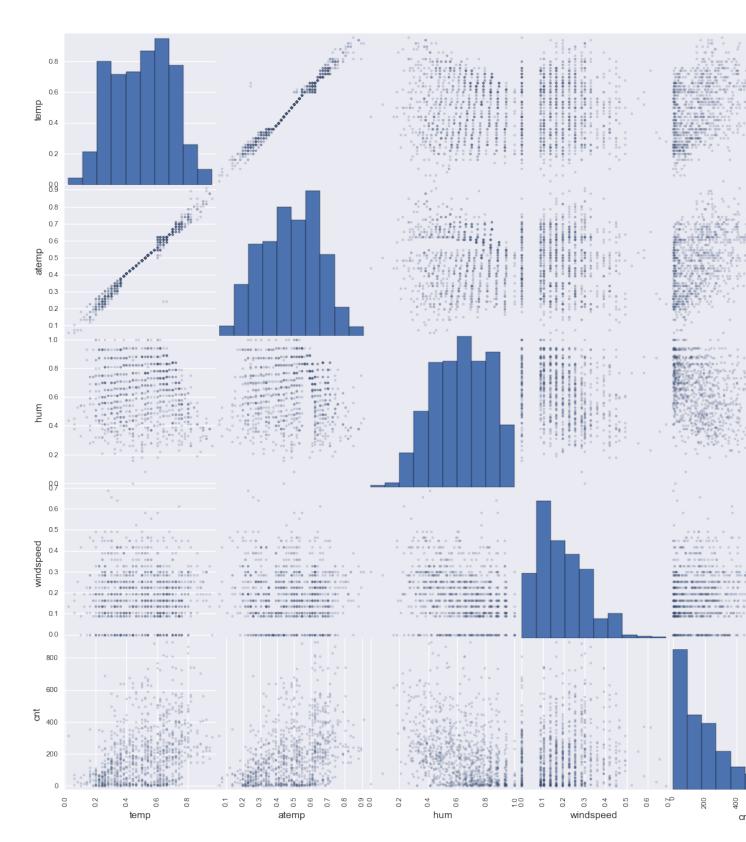
#### Observations on features:

- No data is missing from any columns.
- There are two columns 'casual' and 'registered' that add up to the output column ('cnt'). These columns should not be used in the predictive models and are removed from the data.
- There is one col 'dteday' that has the date of rental. It is redundant since year and month are already provided separately. We choose to remove this column from the data.

# **Exploratory Visualization**

## Correlation between continuous features

The plot below shows the pairwise correlation between the continuous features



# Observations on correlation plot:

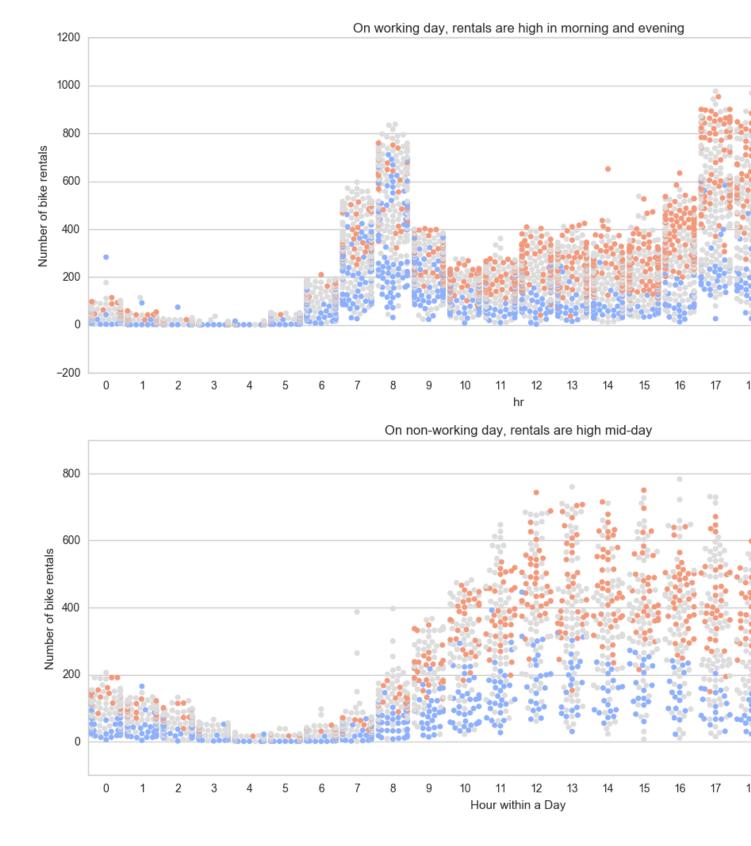
The correlation plot gives the correlation between pairwise columns in the data. The diagonals of the plot give the distribution of each column. As expected, 'temp' and 'atemp' have a strong correlation and contain

redundant information. We choose to remove 'a temp' from the Bikes dataframe. The remaining continuous features don't exhibit a correlation between themselves.

# Relationship with temperature and hour of day

Another relationship that can be visualized is between bike rentals and the temperature + hour of day. Following swarmplot provides a good visual representation of this relationship.

# Bike usage peaks with warmer temperatures



## Observations on swarm plot:

The swarm plot provides a categorical scatterplot with non-overlapping points. The swarm plot is similar to a simple scatterplot, but the points are adjusted (only along the categorical axis) so that they don't overlap. This gives a better representation of the distribution of values, although it does not scale as well to large numbers of observations (both in terms of the ability to show all the points and in terms of the computation needed to arrange them). This style of plot is often called a "beeswarm". The plot above gives the distribution of number bike rentals for each hour in the day. The colors of the data points indicate the temperature of the day.

We can observed that bike rentals are higher on working days during commute hours (morning around 8 am and evening around 5 pm). Compared to that, on a non-workingday the distribution is flat or more even during the whole day. This is expected as the major population would have a need for a bike during those hours.

Another observation from the plot is that bike rentals are higher when the temperature is moderately high (above the 3rd quartile). This is consistently seen throughout all hours for working and non-working days. This also makes sense since riding a bike would not be preferred on colder days/nights.

Thus, we can conclude that 'Temp', 'Hours', and 'workingday' are important features that we'll see during our model training.

# Algorithms and Techniques

We'll be exploring various learning techniques for this regression problem:

- Linear Regression
- Decision Tree
- Random forest (bagging)
- Gradient Boosted Regression Tree (boosting)

## III. Methodology

## **Data Preprocessing**

#### Transformation

There are some columns that require specific type casting or transformations to ensure correct usage. Furthermore, as noted earlier, some of the columns need to be excluded to avoid leakage of the response variable in the predictors. These transformations are documented in the code below.

#### Dummy encoding

Linear regression requires all columns to be of continuous types. Since we have categorical features, the best approach is to encode them to integer columns using dummy encoding using pandas.get\_dummies function:

```
# Create a new dataframe that is a copy of original
bikes_encoded = bikes.copy()

# Create dummy columns for each categorical variable and update in the new dataframe
for cat in categorical_features:
    dummy_cols = pd.get_dummies(bikes_encoded[cat], prefix=cat)

# Remove the original categorical variable from the new dataframe
bikes_encoded.drop(cat, axis=1, inplace=True)

# Add the dummy variables to the new dataframe
bikes_encoded = pd.concat([bikes_encoded, dummy_cols], axis=1)
```

#### Implementation

#### Libraries

Popular machine learning library scikit-learn was used to execute the algorithms explored in this work. Scikit-learn provides a range of supervised and unsupervised learning algorithms via a consistent interface in Python.

It is licensed under a permissive simplified BSD license and is distributed under many Linux distributions, encouraging academic and commercial use.

The library is built upon the SciPy (Scientific Python) that must be installed before you can use scikit-learn. This stack that includes:

- NumPy: Base n-dimensional array package
- SciPy: Fundamental library for scientific computing
- Matplotlib: Comprehensive 2D/3D plotting
- IPython: Enhanced interactive console
- Sympy: Symbolic mathematics
- Pandas: Data structures and analysis

The vision for the library is a level of robustness and support required for use in production systems. This means a deep focus on concerns such as ease of use, code quality, collaboration, documentation and performance. Although the interface is Python, c-libraries are leverage for performance such as numpy for arrays and matrix operations, LAPACK, LibSVM and the careful use of cython.

The metric functions used in this work were implemented in Python, using the numpy library. The implementation was straightforward and documented below:

```
def rae(true_val, pred_val):
    true_mean = true_val.mean()
    diff = np.abs(true_val - pred_val)
    return diff.sum() / np.abs(true_val - true_mean).sum()

def rrse(true_val, pred_val):
    true_mean = true_val.mean()
    diff = np.square(true_val - pred_val)
    return diff.sum() / np.square(true_val - true_mean).sum()

def cc(true_val, pred_val):
```

```
true_mean, pred_mean = true_val.mean(), pred_val.mean()
spa = ((true_val - true_mean) * (pred_val - pred_mean)).sum()
sa = np.square(true_val - true_mean).sum()
sp = np.square(pred_val - pred_mean).sum()
return spa / np.sqrt(sa * sp)
```

Furthermore, various data transformations including splitting data for train and test were performed using the popular Pandas library [3]. Libraries used for plotting were seaborn[4] and matplotlib[5].

Data extraction

### Modeling methods

For each model, we employ scikit-learn functions that follow a set pattern: initialize the model and then fit using the data.

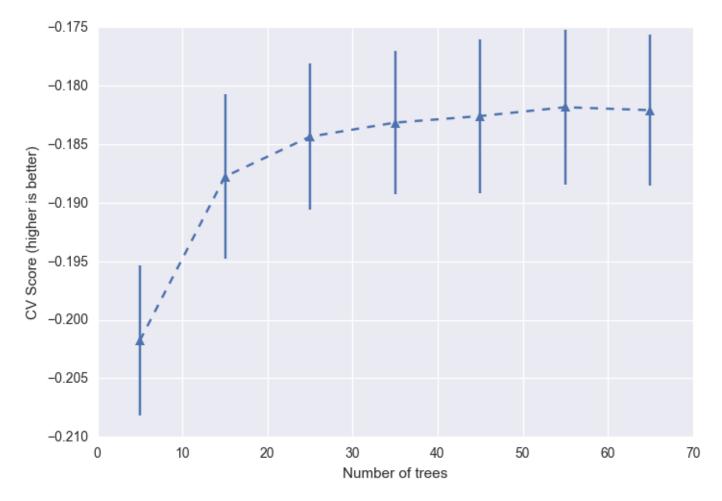
• Linear regression \_\_\_\_\_ from sklearn.linear\_model import LinearRegression # Initiate Model lin\_regr = LinearRegression(normalize=True) # Train the model lin\_regr.fit(train\_X\_encoded, train\_y\_encoded) • Decision Tree from sklearn.tree import DecisionTreeRegressor # Initiate Model dec\_tree = DecisionTreeRegressor(max\_depth=15) # Train the model dec\_tree.fit(train\_X, train\_y) \_\_\_\_\_ • Gradient Boosted Trees from sklearn.ensemble import GradientBoostingRegressor # Initiate Model gbr = GradientBoostingRegressor(n\_estimators=1000, max\_depth=3, learning\_rate=0.8) # Train the model gbr.fit(train\_X, train\_y) \_\_\_\_\_ • Random Forest from sklearn.ensemble import RandomForestRegressor # Initiate Model rand\_forest = RandomForestRegressor(n\_estimators=20, max\_depth=15)

#### Refinement

It's not clear how many trees should be included in the Random Forest. To make a structured decision, we employ cross validation to perform a grid search across multiple number of trees.

```
Specifically we try forests with 5 trees to 65 trees, as shown below.
_____
from sklearn import model selection
from sklearn.ensemble import RandomForestRegressor
# Specify parameters for 10-fold cross validation
kfold = model_selection.KFold(n_splits=10,
                            random_state=1)
print "\n-----"
print "Average validation score:"
cv_mean_scores = []
for n_trees in range(5, 71, 10):
   # Initiate Model
   rand_forest_cv = RandomForestRegressor(n_estimators=n_trees,
                                         max_depth=20,
                                         n jobs=4)
   # Calculate and print cross-validation score
   results = model_selection.cross_val_score(rand_forest_cv, train_X, train_y, cv=kfold,
                                           scoring=metrics.make_scorer(rae, greater_is_better=False)
   print("For {0} trees is {1}".format(n_trees, results.mean()))
   cv_mean_scores.append((n_trees, results.mean(), results.std()))
Results:
Average validation score:
For 5 trees is -0.201763886736
For 15 trees is -0.18777456281
```

Average validation score:
For 5 trees is -0.201763886736
For 15 trees is -0.18777456281
For 25 trees is -0.184363069995
For 35 trees is -0.183164892377
For 45 trees is -0.182607144176
For 55 trees is -0.181847832758
For 65 trees is -0.182103770565

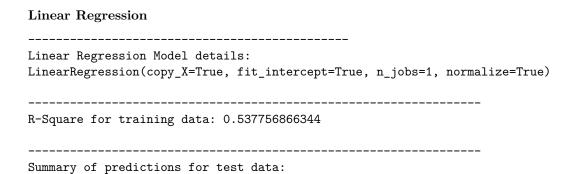


The cross validation results give the highest score for a forest with 55 trees. It is, however, important to note that the scores don't increase much after a certain point. To ensure we use a simple model (to avoid overfitting), while retaining good accuracy, we pick the simplest model that is within one standard deviation of the best model. Judging from the figure above, the forest with 25 trees fits the bill.

# IV. Results

# Model Evaluation and Validation

In this section we provide results and insights into each model.



```
Prediction
count 3476.000000
      189.386651
mean
std
      147.605852
   -194.500000
min
25%
      78.500000
     191.750000
50%
75%
      295.000000
      613.500000
max
MAE for training data: 74.9524203409
MAE for test data: 75.9496547756
RAE for training data: 0.52756830333
RAE for test data: 0.528806780634
______
RRSE for training data: 0.313859295957
RRSE for test data: 0.317508260403
CC for training data: 0.828348632183
CC for test data: 0.826556976405
```

## Analysis for Linear Regression:

1.000000 41.000000

153.000000

- Linear regression prediction includes negative output (which is not valid for cnt)
- R2 is close to 0.5, which implies that only 50% of the variance in the data is modeled by the regressor.
- Next step: Try other models to predict cnt, like Decision Tree to model greater variability in the data.

#### Decision tree:

min

25% 50%

```
_____
Decision Tree Model details:
DecisionTreeRegressor(criterion='mse', max_depth=15, max_features=None,
         max_leaf_nodes=None, min_impurity_split=1e-07,
         min_samples_leaf=1, min_samples_split=2,
         min_weight_fraction_leaf=0.0, presort=False, random_state=None,
         splitter='best')
Summary of predictions for test data:
      Prediction
count 3476.000000
mean 193.543441
std 179.346887
```

75% 290.000000 max 919.000000

-----

MAE for training data: 9.54837085521 MAE for test data: 33.8699654776

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RAE for training data: 0.0672082074032 RAE for test data: 0.235822894222

\_\_\_\_\_

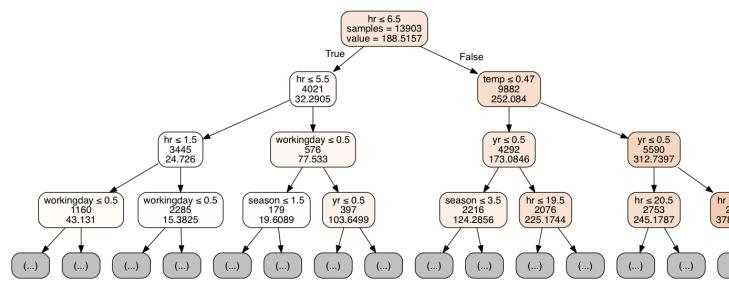
RRSE for training data: 0.0132821892645 RRSE for test data: 0.103842051796

\_\_\_\_\_

CC for training data: 0.993336714217 CC for test data: 0.947327629461

-----

Let's visualize the decision tree to get an idea of how it splits on features:



Analysis for Decision Tree:

- Performance for decision tree is much better than linear regression (higher CC and lower error)
- The top of the tree contains nodes that primarily use hr, temp, workingday as the split features. This indicates the importance of these particular features.
- There are signs of overfitting since the training error is low but the test error is still reasonably high. We can use ensemble techniques to overcome the overfitting effects.

## **Gradient Boosted Trees**

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Gradient Boosted Regression Trees:

```
max_leaf_nodes=None, min_impurity_split=1e-07,
min_samples_leaf=1, min_samples_split=2,
min_weight_fraction_leaf=0.0, n_estimators=1000,
presort='auto', random_state=None, subsample=1.0, verbose=0,
warm_start=False)
```

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#### Summary of predictions for test data:

	Prediction
count	3476.000000
mean	193.249137
std	179.457494
min	-165.000000
25%	43.000000
50%	156.000000
75%	293.250000
max	909.000000

MAE for training data: 20.8884413436 MAE for test data: 29.9496547756

\_\_\_\_\_\_

RAE for training data: 0.147027667802 RAE for test data: 0.208527353676

\_\_\_\_\_

RRSE for training data: 0.029217618587 RRSE for test data: 0.0605477754712

-----

CC for training data: 0.98529362356 CC for test data: 0.96935713163

\_\_\_\_\_\_

# Analysis for Gradient Boosted Trees:

• The test error has decreased, with the training and test error closer to each other. That indicates a drop in variance (overfitting).

## **Random Forest**

```
Random Forest Model with Cross-Validation details:
```

-----

Summary of predictions for test data:

Prediction
3476.000000
193.671461
175.455396
1.000000
47.000000
156.500000
287.000000
918.000000

\_\_\_\_\_

MAE for training data: 10.3020930734 MAE for test data: 26.5261795167

\_\_\_\_\_

RAE for training data: 0.0725134390427 RAE for test data: 0.184691077717

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RRSE for training data: 0.00912075968267

RRSE for test data: 0.058918498909

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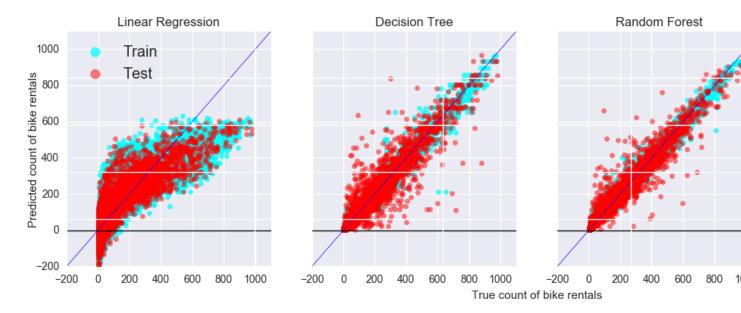
CC for training data: 0.995516131278 CC for test data: 0.970138513161

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## Justification

Given below is a comparison of the performance of four models on the test data set.

Modeling technique	mae	rae	rrse	cc
Linear regression	76.726	0.5403	0.3248	0.8217
Decision Tree	35.177	0.2477	0.1177	0.9410
Gradient Boosted Tree	29.9496	0.2085	0.06054	0.9693
Random Forest	26.63	0.1876	0.06549	0.9667



The figure above compares the performance of the four models on the training (cyan) and testing (red) datasets. The x-axis represents the true count of each data point and the y-axis represents the prediction for that point. The ideal model would have all points on the diagonal (blue line). Further, since this is a count, all points should be positive, implying that the ideal model should have all prediction points above the x-axis (black line).

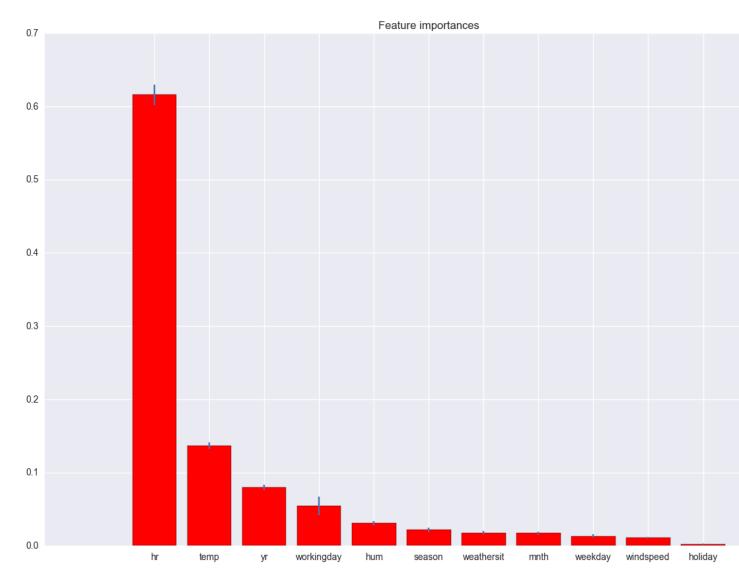
We can see from the comparison figure that linear regression performs poorly when compared to our ideal model. The points have high variability along the x-axis, with no prediction going over about 600. The linear model also makes the egregious mistake of predicting negative counts (min value of about -200).

Compared to the linear model, decision tree makes good predictions. Most of the points lie along the diagonal, but have considerable variability around that line. The test data points have higher variance than train, again an indicative of overfitting.

Random forest and Gradient Boosted Trees show better performance than Decision Tree with lower variability around the diagonal line. The train and test performance is comparable in either case. The boosting method, however, also falls prey to predicting negative counts for low cardinality rentals. Considering this conspicuous inaccuracy, we can conclude that random forest is the best model for this problem among the four tried in this work.

# V. Conclusion

#### Free-Form Visualization



The figure above gives the importance of each feature used in the final Random Forest model. The top five important features in descending order are hr (which hour was the bike rented), temp (temperature at the time), year (rental year), workingday (whether the day was a working day or not) and hum (humidity). The fact that hr and temp played the most important part was also apparent from the swarm plot in the 'Exploratory Visualization' section.

#### Reflection

In the world of bicycle research, data collection is often both challenging and expensive. Additionally, research regarding the relationship between weather and cycling is typically conducted based on daily averages and not necessarily at the precise time that the trip was taken. The latter is more meaningful as weather can vary throughout the day. Through data collection technology embedded within bikeshare systems, the ability to understand different impacts on at least bikeshare trips is possible. The weather of Washington, DC contains almost all variations. It rains and snows, has cold days and hot days and can be excessively humid at times.

This analysis helps to better document the relative impact of various weather conditions on bikesharing trips in Washington, DC, considering the precise weather observation at the time the trip was taken. The results of this analysis show that fewer trips are made in rain, high humidity, high wind speeds, and low temperatures, while trips increase with higher temperatures especially in the evenings.

#### Improvement

From our analysis, we concluded that Random Forest model worked better than Gradient Boosted Trees. In practice, Gradient Boosted Trees provide good results, but require fine tuning of several hyperparameters including the number of trees, the depth (or number of leaves), and the shrinkage (or learning rate). The model in this analysis was tuned significantly which could explain some of the negative predictions. The author believes boosted trees would yield best results if tuned correctly.

The year feature being important is surprising, but understandable since this is data for limited years - there could be year-specific trends, which might get washed out if the analysis is run on multiple years. Re-running this analysis on a bigger dataset would be an interesting exercise.

An additional analysis that was outside the scope of this study is to embed the data, with metro and other transportation information. Bike rentals are expected to have a strong correlation with the availability of public transportation systems. (Example: do bike rentals increase in evening if public transportation becomes less frequent?).

#### References

[1] Fanaee-T, H. & Gama, J. Prog Artif Intell (2014) 2: 113. doi:10.1007/s13748-013-0040-3 [2] Scikit-learn: Machine Learning in Python, Pedregosa et al., JMLR 12, pp. 2825-2830, 2011.