

Assignment+1+worked+out

March 5, 2018

```
In [1]: ### RUN BEFORE ANYTHING ELSE, LOADS LIBS ###
from IPython.display import HTML
HTML(''<style>html, body{overflow-y: visible !important} .CodeMirror{min-width:105% !
%matplotlib inline
from preamble import *
plt.rcParams['savefig.dpi'] = 100 # This controls the size of your figures
# Comment out and restart notebook if you only want the last output of each cell.
InteractiveShell.ast_node_interactivity = "all"
import numpy
from sklearn.preprocessing import StandardScaler
from sklearn.pipeline import Pipeline
from sklearn.model_selection import cross_val_score
from sklearn.model_selection import train_test_split
from sklearn.linear_model import LinearRegression
from sklearn.linear_model import Ridge
from random import randint
from sklearn.model_selection import ShuffleSplit
from sklearn.neighbors import KNeighborsRegressor
from sklearn.neighbors import KNeighborsClassifier
from sklearn.linear_model import ElasticNet
from sklearn.linear_model import Lasso
from sklearn.model_selection import StratifiedShuffleSplit
from sklearn.model_selection import train_test_split
from sklearn.linear_model import LogisticRegression
from sklearn.ensemble import RandomForestClassifier
import timeit
from sklearn.model_selection import cross_val_score
from sklearn.model_selection import KFold
from sklearn.model_selection import GridSearchCV
from sklearn.model_selection import RandomizedSearchCV
from scipy.stats import expon
import pandas as pd
from sklearn.ensemble import RandomForestRegressor
from sklearn.metrics import roc_auc_score
from sklearn.ensemble import GradientBoostingClassifier
```

1 Foundations of Data Mining: Assignment 1

Please complete all assignments in this notebook. You should submit this notebook, as well as a PDF version (See File > Download as).

```
In [ ]: # Please fill in your names here
        NAME_STUDENT_1 = "Emma van Zoelen"
        NAME_STUDENT_2 = "Jules Klomp"
```

1.1 MoneyBall (5 points, 1+2+1+1)

In the early 2000s, 2 baseball scouts completely changed the game of baseball by analysing the available data about baseball players and hiring the best ones. The [MoneyBall dataset](#) contains this data (click the link for more details). The goal is to accurately predict the number of 'runs' each player can score.

```
In [179]: moneyball = oml.datasets.get_dataset(41021) # Download MoneyBall data
          # Get the predictors X and the target y
          X, y, attribute_names = moneyball.get_data(target=moneyball.default_target_attribute)
          # Describe the data with pandas, just to get an overview
          ballframe = pd.DataFrame(X, columns=attribute_names)
          ballframe.describe()
```

```
Out[179]:
```

	Team	League	Year	RA	...	RankPlayoffs	G	\
count	1232.00	1232.0	1232.00	1232.00	...	244.00	1232.00	
mean	15.67	0.5	1988.96	715.08	...	1.72	3.92	
std	9.72	0.5	14.82	93.08	...	1.10	0.62	
min	0.00	0.0	1962.00	472.00	...	0.00	0.00	
25%	7.00	0.0	1976.75	649.75	...	1.00	4.00	
50%	16.00	0.5	1989.00	709.00	...	2.00	4.00	
75%	23.00	1.0	2002.00	774.25	...	3.00	4.00	
max	38.00	1.0	2012.00	1103.00	...	4.00	7.00	

	OOPB	OSLG
count	420.00	420.00
mean	0.33	0.42
std	0.02	0.03
min	0.29	0.35
25%	0.32	0.40
50%	0.33	0.42
75%	0.34	0.44
max	0.38	0.50

[8 rows x 14 columns]

1. Visually explore the data. Plot the distribution of each feature (e.g. histograms), as well as the target. Visualize the dependency of the target on each feature (use a 2d scatter plot). Is there anything that stands out? Is there something that you think might require special treatment? - Feel free to create additional plots that help you understand the data - Only visualize the data, you don't need to change it (yet)

```

In [180]: # Import numpy
import numpy

# Print histograms attributes
Histballframe = ballframe.as_matrix(columns=None)
plt.figure(1, figsize=(5,3))
plt.subplot(1, 1, 1)
plt.hist(y)
name = "RS"
plt.title(name)

for i in range(0, 14):
    s = Histballframe[:,i]
    s = s[~numpy.isnan(s)]
    plt.figure(i+2, figsize=(5,3))
    plt.subplot(i+2, 1, 1)
    plt.hist(s)
    name = attribute_names[i]
    plt.title(name)

Out[180]: <matplotlib.figure.Figure at 0x17d06271c18>

Out[180]: <matplotlib.axes._subplots.AxesSubplot at 0x17d06271c50>

Out[180]: (array([ 16.,  48., 136., 247., 298., 236., 144.,  75.,  24.,   8.]),
          array([ 463. ,  517.6,  572.2,  626.8,  681.4,  736. ,  790.6,  845.2,
                899.8,  954.4, 1009. ])),
          <a list of 10 Patch objects>)

Out[180]: Text(0.5,1,'RS')

Out[180]: <matplotlib.figure.Figure at 0x17d0601afd0>

Out[180]: <matplotlib.axes._subplots.AxesSubplot at 0x17d05f0e6d8>

Out[180]: (array([152., 188., 152.,  98., 141., 175., 132.,  95.,  78.,  21.]),
          array([ 0. ,  3.8,  7.6, 11.4, 15.2, 19. , 22.8, 26.6, 30.4, 34.2, 38. ])),
          <a list of 10 Patch objects>)

Out[180]: Text(0.5,1,'Team')

Out[180]: <matplotlib.figure.Figure at 0x17d062ba400>

Out[180]: <matplotlib.axes._subplots.AxesSubplot at 0x17d062bfa58>

Out[180]: (array([616.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0., 616.]),
          array([0. , 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1. ])),
          <a list of 10 Patch objects>)

Out[180]: Text(0.5,1,'League')

```

```

Out[180]: <matplotlib.figure.Figure at 0x17d05f30208>
Out[180]: <matplotlib.axes._subplots.AxesSubplot at 0x17d06258208>
Out[180]: (array([100., 112., 96., 104., 130., 130., 82., 148., 150., 180.]),
          array([1962., 1967., 1972., 1977., 1982., 1987., 1992., 1997., 2002.,
                2007., 2012.]),
          <a list of 10 Patch objects>)
Out[180]: Text(0.5,1,'Year')
Out[180]: <matplotlib.figure.Figure at 0x17d0787f7f0>
Out[180]: <matplotlib.axes._subplots.AxesSubplot at 0x17d062137f0>
Out[180]: (array([ 20., 110., 239., 327., 270., 163., 77., 24., 1., 1.]),
          array([ 472. , 535.1, 598.2, 661.3, 724.4, 787.5, 850.6, 913.7,
                976.8, 1039.9, 1103. ]]),
          <a list of 10 Patch objects>)
Out[180]: Text(0.5,1,'RA')
Out[180]: <matplotlib.figure.Figure at 0x17d061df0b8>
Out[180]: <matplotlib.axes._subplots.AxesSubplot at 0x17d078a1a20>
Out[180]: (array([ 2., 17., 50., 167., 243., 291., 286., 134., 39., 3.]),
          array([ 40. , 47.6, 55.2, 62.8, 70.4, 78. , 85.6, 93.2, 100.8,
                108.4, 116. ]]),
          <a list of 10 Patch objects>)
Out[180]: Text(0.5,1,'W')
Out[180]: <matplotlib.figure.Figure at 0x17d078e3080>
Out[180]: <matplotlib.axes._subplots.AxesSubplot at 0x17d078e31d0>
Out[180]: (array([ 7., 22., 64., 193., 322., 266., 225., 81., 45., 7.]),
          array([0.277, 0.287, 0.296, 0.306, 0.315, 0.325, 0.335, 0.344, 0.354,
                0.363, 0.373])),
          <a list of 10 Patch objects>)
Out[180]: Text(0.5,1,'OBP')
Out[180]: <matplotlib.figure.Figure at 0x17d07924668>
Out[180]: <matplotlib.axes._subplots.AxesSubplot at 0x17d0793af60>
Out[180]: (array([ 13., 31., 100., 186., 276., 258., 202., 93., 57., 16.]),
          array([0.301, 0.32 , 0.339, 0.358, 0.377, 0.396, 0.415, 0.434, 0.453,
                0.472, 0.491])),
          <a list of 10 Patch objects>)

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Out[180]: Text(0.5,1,'SLG')

Out[180]: <matplotlib.figure.Figure at 0x17d0797c5c0>

Out[180]: <matplotlib.axes._subplots.AxesSubplot at 0x17d0797c518>

Out[180]: (array([ 4., 14., 41., 102., 242., 329., 229., 186., 58., 27.]),
          array([0.214, 0.222, 0.23 , 0.238, 0.246, 0.254, 0.262, 0.27 , 0.278,
                  0.286, 0.294])),
          <a list of 10 Patch objects>)

Out[180]: Text(0.5,1,'BA')

Out[180]: <matplotlib.figure.Figure at 0x17d079d34a8>

Out[180]: <matplotlib.axes._subplots.AxesSubplot at 0x17d079e7da0>

Out[180]: (array([988., 0., 0., 0., 0., 0., 0., 0., 0., 244.]),
          array([0. , 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1. ])),
          <a list of 10 Patch objects>)

Out[180]: Text(0.5,1,'Playoffs')

Out[180]: <matplotlib.figure.Figure at 0x17d07a1c7b8>

Out[180]: <matplotlib.axes._subplots.AxesSubplot at 0x17d07a1c940>

Out[180]: (array([52., 53., 44., 0., 44., 21., 0., 20., 9., 1.]),
          array([0. , 0.7, 1.4, 2.1, 2.8, 3.5, 4.2, 4.9, 5.6, 6.3, 7. ])),
          <a list of 10 Patch objects>)

Out[180]: Text(0.5,1,'RankSeason')

Out[180]: <matplotlib.figure.Figure at 0x17d07a72438>

Out[180]: <matplotlib.axes._subplots.AxesSubplot at 0x17d07a84da0>

Out[180]: (array([47., 0., 47., 0., 0., 80., 0., 68., 0., 2.]),
          array([0. , 0.4, 0.8, 1.2, 1.6, 2. , 2.4, 2.8, 3.2, 3.6, 4. ])),
          <a list of 10 Patch objects>)

Out[180]: Text(0.5,1,'RankPlayoffs')

Out[180]: <matplotlib.figure.Figure at 0x17d07abfe48>

Out[180]: <matplotlib.axes._subplots.AxesSubplot at 0x17d07adc8d0>

Out[180]: (array([ 1., 10., 23., 0., 139., 954., 0., 93., 10., 2.]),
          array([0. , 0.7, 1.4, 2.1, 2.8, 3.5, 4.2, 4.9, 5.6, 6.3, 7. ])),
          <a list of 10 Patch objects>)

```

Out[180]: Text(0.5,1,'G')

Out[180]: <matplotlib.figure.Figure at 0x17d07b0ee48>

Out[180]: <matplotlib.axes._subplots.AxesSubplot at 0x17d07b2c940>

Out[180]: (array([4., 33., 64., 89., 94., 74., 41., 15., 5., 1.]),
array([0.294, 0.303, 0.312, 0.321, 0.33 , 0.339, 0.348, 0.357, 0.366,
0.375, 0.384]),
<a list of 10 Patch objects>)

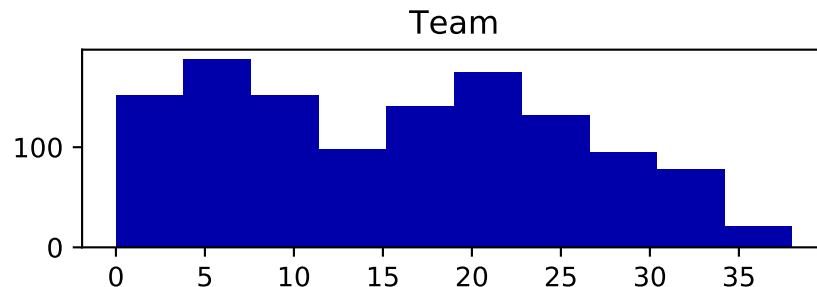
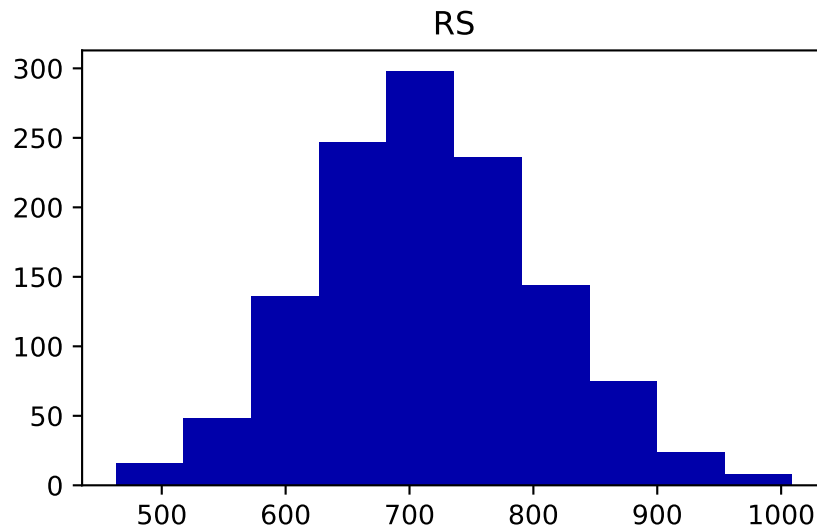
Out[180]: Text(0.5,1,'O0BP')

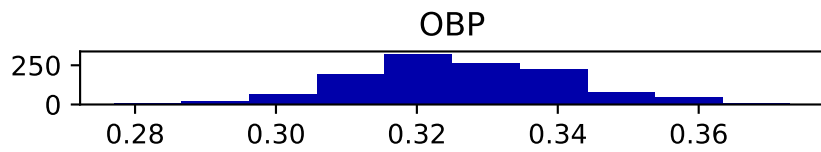
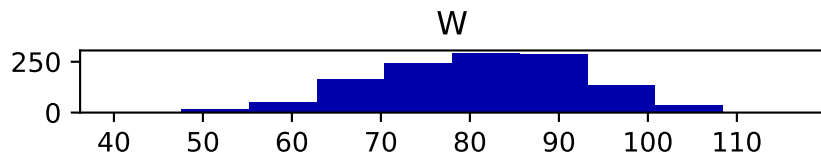
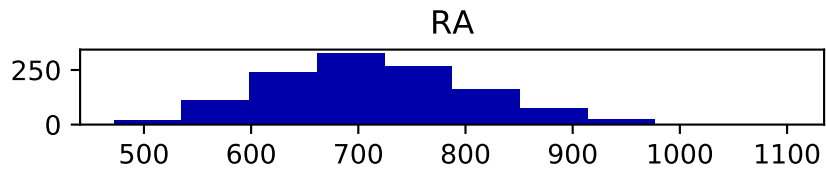
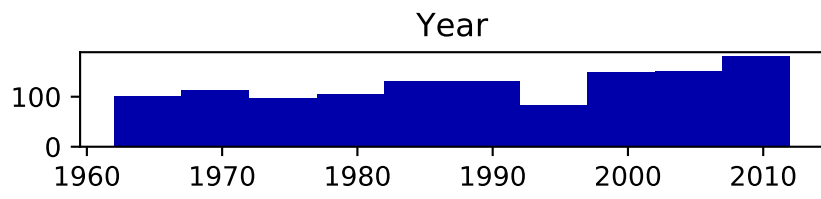
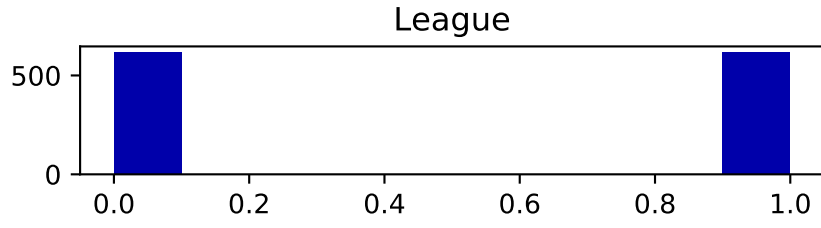
Out[180]: <matplotlib.figure.Figure at 0x17d07b67978>

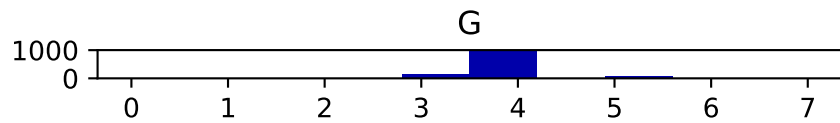
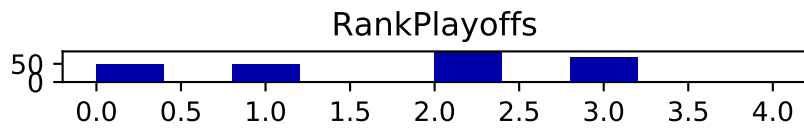
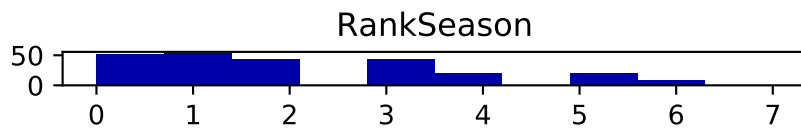
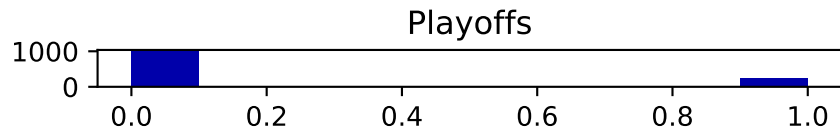
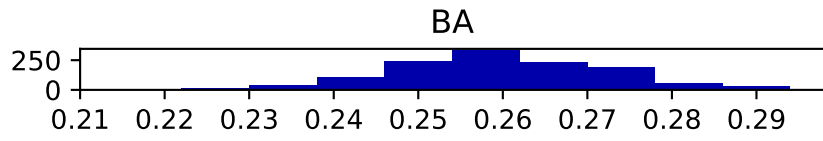
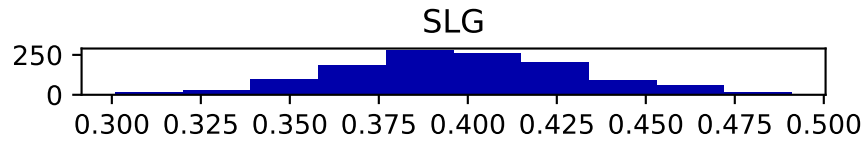
Out[180]: <matplotlib.axes._subplots.AxesSubplot at 0x17d07b679e8>

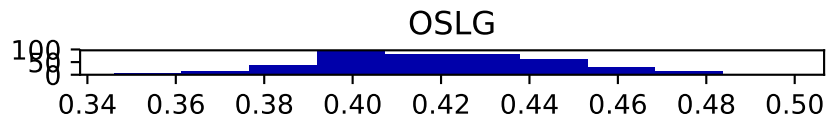
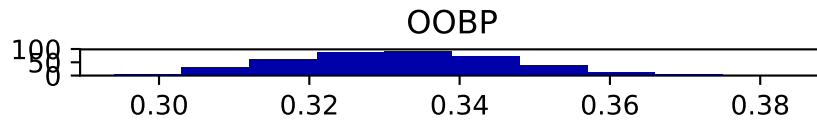
Out[180]: (array([6., 14., 36., 92., 82., 82., 61., 31., 14., 2.]),
array([0.346, 0.361, 0.377, 0.392, 0.407, 0.422, 0.438, 0.453, 0.468,
0.484, 0.499]),
<a list of 10 Patch objects>)

Out[180]: Text(0.5,1,'OSLG')









In [181]: # Print scatterplots features

```
for i in range(0, 14):
    s = Histballframe[:,i]
    plt.figure(i+2, figsize=(5,3))
    plt.subplot(i+2, 1, 1)
    plt.scatter(s,y)
    name = attribute_names[i]
    plt.title(name)
```

Out[181]: <matplotlib.figure.Figure at 0x17d05eac128>

Out[181]: <matplotlib.axes._subplots.AxesSubplot at 0x17d06027c18>

Out[181]: <matplotlib.collections.PathCollection at 0x17d08dca1d0>

Out[181]: Text(0.5,1,'Team')

Out[181]: <matplotlib.figure.Figure at 0x17d08dca5c0>

Out[181]: <matplotlib.axes._subplots.AxesSubplot at 0x17d08dcac50>

Out[181]: <matplotlib.collections.PathCollection at 0x17d08dfce48>

Out[181]: Text(0.5,1,'League')

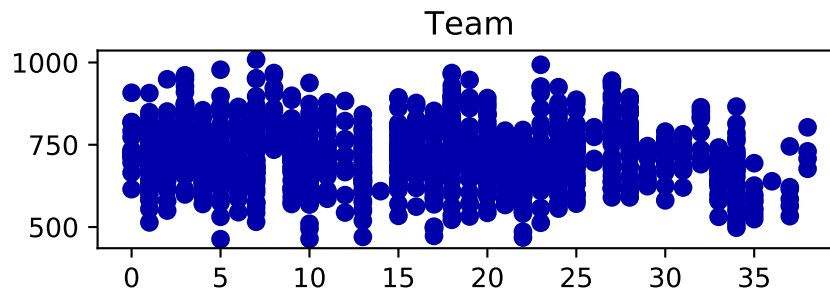
Out[181]: <matplotlib.figure.Figure at 0x17d08e07240>

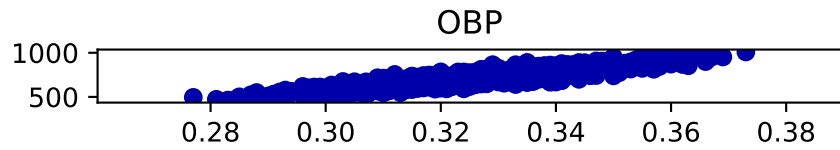
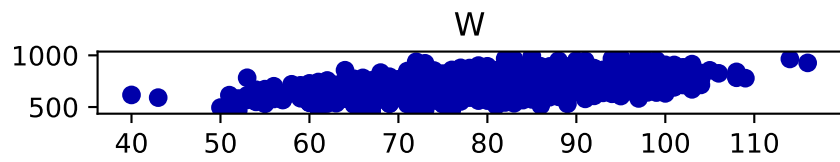
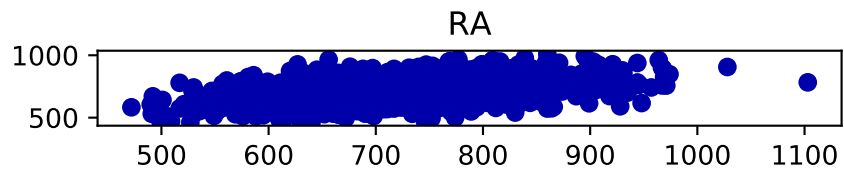
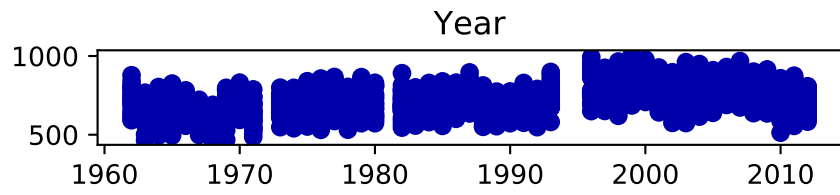
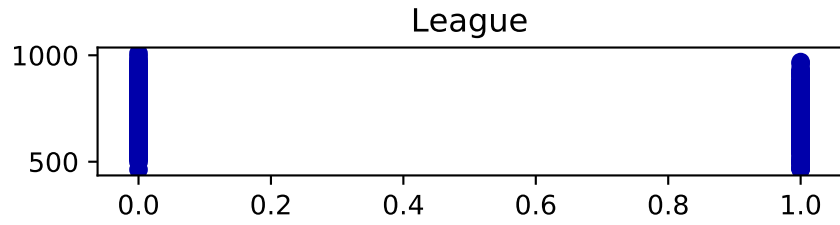
Out[181]: <matplotlib.axes._subplots.AxesSubplot at 0x17d08e078d0>

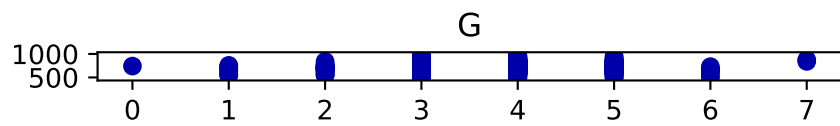
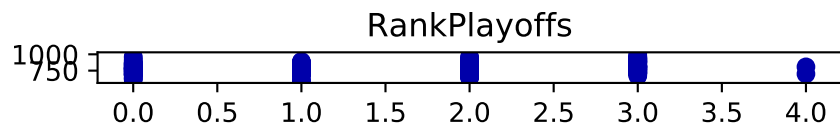
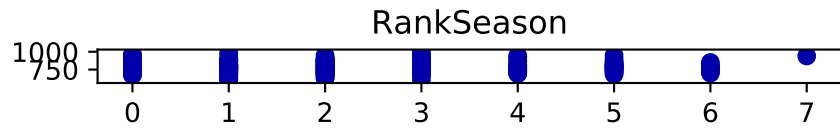
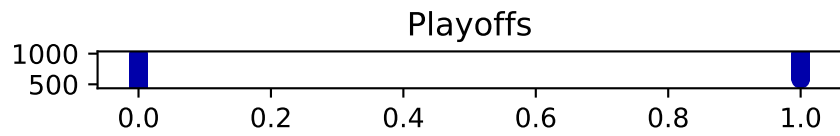
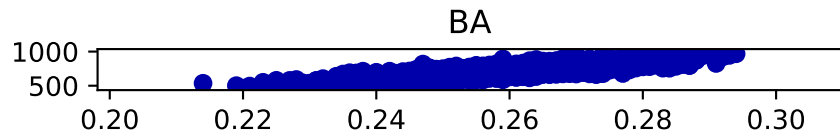
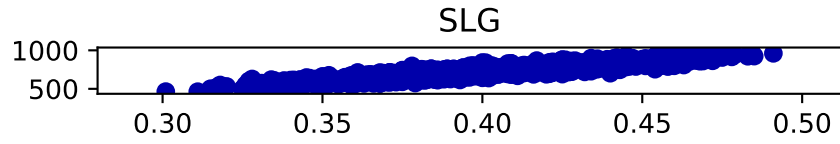
Out[181]: <matplotlib.collections.PathCollection at 0x17d08e409e8>

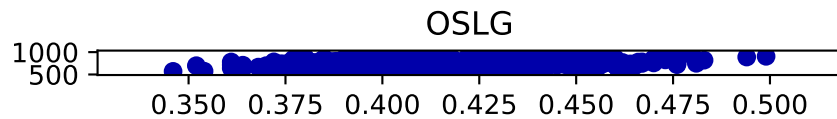
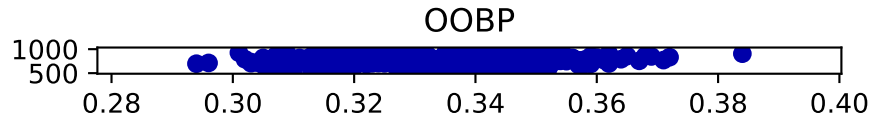
```
Out[181]: Text(0.5,1,'Year')
Out[181]: <matplotlib.figure.Figure at 0x17d08e40da0>
Out[181]: <matplotlib.axes._subplots.AxesSubplot at 0x17d08e49438>
Out[181]: <matplotlib.collections.PathCollection at 0x17d08e55860>
Out[181]: Text(0.5,1,'RA')
Out[181]: <matplotlib.figure.Figure at 0x17d08e1eac8>
Out[181]: <matplotlib.axes._subplots.AxesSubplot at 0x17d08dddeb8>
Out[181]: <matplotlib.collections.PathCollection at 0x17d08eb6a58>
Out[181]: Text(0.5,1,'W')
Out[181]: <matplotlib.figure.Figure at 0x17d08eb6e80>
Out[181]: <matplotlib.axes._subplots.AxesSubplot at 0x17d08ec1518>
Out[181]: <matplotlib.collections.PathCollection at 0x17d08efa668>
Out[181]: Text(0.5,1,'OBP')
Out[181]: <matplotlib.figure.Figure at 0x17d08efaa20>
Out[181]: <matplotlib.axes._subplots.AxesSubplot at 0x17d08f040b8>
Out[181]: <matplotlib.collections.PathCollection at 0x17d08f40198>
Out[181]: Text(0.5,1,'SLG')
Out[181]: <matplotlib.figure.Figure at 0x17d08f405c0>
Out[181]: <matplotlib.axes._subplots.AxesSubplot at 0x17d08f40c18>
Out[181]: <matplotlib.collections.PathCollection at 0x17d08f4dbe0>
Out[181]: Text(0.5,1,'BA')
Out[181]: <matplotlib.figure.Figure at 0x17d08f47cf8>
Out[181]: <matplotlib.axes._subplots.AxesSubplot at 0x17d08f21d68>
Out[181]: <matplotlib.collections.PathCollection at 0x17d08fb6240>
Out[181]: Text(0.5,1,'Playoffs')
Out[181]: <matplotlib.figure.Figure at 0x17d08fb6630>
Out[181]: <matplotlib.axes._subplots.AxesSubplot at 0x17d08fb6c88>
```

```
Out[181]: <matplotlib.collections.PathCollection at 0x17d08febd68>
Out[181]: Text(0.5,1,'RankSeason')
Out[181]: <matplotlib.figure.Figure at 0x17d08ff7160>
Out[181]: <matplotlib.axes._subplots.AxesSubplot at 0x17d08ff77b8>
Out[181]: <matplotlib.collections.PathCollection at 0x17d090318d0>
Out[181]: Text(0.5,1,'RankPlayoffs')
Out[181]: <matplotlib.figure.Figure at 0x17d09031cc0>
Out[181]: <matplotlib.axes._subplots.AxesSubplot at 0x17d0903d358>
Out[181]: <matplotlib.collections.PathCollection at 0x17d0903de80>
Out[181]: Text(0.5,1,'G')
Out[181]: <matplotlib.figure.Figure at 0x17d090471d0>
Out[181]: <matplotlib.axes._subplots.AxesSubplot at 0x17d08fccf60>
Out[181]: <matplotlib.collections.PathCollection at 0x17d090ab908>
Out[181]: Text(0.5,1,'O0BP')
Out[181]: <matplotlib.figure.Figure at 0x17d090abcc0>
Out[181]: <matplotlib.axes._subplots.AxesSubplot at 0x17d090b4358>
Out[181]: <matplotlib.collections.PathCollection at 0x17d090ec3c8>
Out[181]: Text(0.5,1,'OSLG')
```









Answer to 1 . There are clearly some features that are categorical and might be treated differently. From the histograms, we see that the features Team, League, Year, RankPlayoffs, RankSeason, Playoffs and G are such categorical features, as they do not have a normal distribution. In the scatterplots, it can also be seen that for most of those features no clear trend can be seen in relation to the result. Some of the categories seem to have better average results, but it is hard to see from the plots.

2 . Compare all linear regression algorithms that we covered in class (Linear Regression, Ridge, Lasso and ElasticNet), as well as kNN. Evaluate using cross-validation and the R^2 score, with the default parameters. Does scaling the data with StandardScaler help? Provide a concise but meaningful interpretation of the results. - Preprocess the data as needed (e.g. are there nominal features that are not ordinal?). If you don't know how to proceed, remove the feature and continue.

```
In [182]: # Preprocessing the data: get dummies
```

```
# Delete features OOBP and OSLG, because they have a lot of missing values but are f
del ballframe['OOBP']
del ballframe['OSLG']
```

```
# Get dummies for categorical features
ballframe_dummies = pd.get_dummies(ballframe, columns=['Team', 'League', 'Year', 'Ra
```

```
In [183]: # Preprocessing the data: convert into NumPy Array
```

```
# extract NumPy arrays
X = ballframe_dummies.values

print("X.shape: {} y.shape: {}".format(X.shape, y.shape))
```

```
X.shape: (1232, 116) y.shape: (1232,)
```

```
In [184]: # StandardScaler
```

```
from sklearn.preprocessing import StandardScaler
```

```
from sklearn.pipeline import Pipeline
```

```
scaler = StandardScaler()
```

```
In [185]: # Linear Regression Model
```

```
from sklearn.model_selection import cross_val_score
from sklearn.model_selection import train_test_split
from sklearn.linear_model import LinearRegression
```

```
lr = LinearRegression()
```

```
pipeline_lr = Pipeline([('transformer', scaler), ('estimator', lr)])
```

```
lr_scores = cross_val_score(lr, X, y, cv=10)
```

```
lr_scores_scaled = cross_val_score(pipeline_lr, X, y, cv=10)
```

```
print("Cross-validation scores (R2): {}".format(lr_scores))
```

```
print(numpy.mean(lr_scores))
```

```
print("Cross-validation scores scaled (R2): {}".format(lr_scores_scaled))
```

```
print(numpy.mean(lr_scores_scaled))
```

```
Cross-validation scores (R2): [0.914 0.886 0.919 0.939 0.913 0.863 0.912 0.923 0.944 0.923]
0.9136845732764334
```

```
Cross-validation scores scaled (R2): [-2.880e+06 -2.811e+06 -1.344e+07 -5.772e+06 -5.210e+08
-5.392e+06 -5.092e+07 -5.824e+07 -4.840e+06]
-68119723.7684226
```

```
In [186]: # Ridge
```

```
from sklearn.linear_model import Ridge
```

```
ridge = Ridge()
```

```
pipeline_ridge = Pipeline([('transformer', scaler), ('estimator', ridge)])
```

```
ridge_scores = cross_val_score(ridge, X, y, cv=10)
```

```
ridge_scores_scaled = cross_val_score(pipeline_ridge, X, y, cv=10)
```

```
print("Cross-validation scores (R2): {}".format(ridge_scores))
```

```
print(numpy.mean(ridge_scores))
```

```
print("Cross-validation scores (R2): {}".format(ridge_scores_scaled))
```

```
print(numpy.mean(ridge_scores_scaled))
```

```
Cross-validation scores (R2): [0.818 0.743 0.835 0.81 0.841 0.858 0.815 0.816 0.854 0.828]
0.8218003937786371
```

Cross-validation scores (R^2): [0.916 0.888 0.92 0.94 0.912 0.862 0.912 0.923 0.944 0.923]
0.91399626474137

In [187]: # *Lasso*

```
from sklearn.linear_model import Lasso

lasso = Lasso()

pipeline_lasso = Pipeline([('transformer', scaler), ('estimator', lasso)])

lasso_scores = cross_val_score(lasso, X, y, cv=10)
lasso_scores_scaled = cross_val_score(pipeline_lasso, X, y, cv=10)

print("Cross-validation scores ( $R^2$ ): {}".format(lasso_scores))
print(numpy.mean(lasso_scores))

print("Cross-validation scores ( $R^2$ ): {}".format(lasso_scores_scaled))
print(numpy.mean(lasso_scores_scaled))
```

Cross-validation scores (R^2): [0.791 0.679 0.818 0.804 0.824 0.821 0.79 0.774 0.831 0.829]
0.796011952506216

Cross-validation scores (R^2): [0.918 0.888 0.923 0.934 0.907 0.912 0.913 0.924 0.946 0.93]
0.9196118331978367

In [188]: # *ElasticNet*

```
from sklearn.linear_model import ElasticNet

elasticn = ElasticNet()

pipeline_elasticn = Pipeline([('transformer', scaler), ('estimator', elasticn)])

elasticn_scores = cross_val_score(elasticn, X, y, cv=10)
elasticn_scores_scaled = cross_val_score(pipeline_elasticn, X, y, cv=10)

print("Cross-validation scores ( $R^2$ ): {}".format(elasticn_scores))
print(numpy.mean(elasticn_scores))

print("Cross-validation scores ( $R^2$ ): {}".format(elasticn_scores_scaled))
print(numpy.mean(elasticn_scores_scaled))
```

Cross-validation scores (R^2): [0.791 0.68 0.817 0.802 0.825 0.822 0.792 0.774 0.831 0.829]
0.7962006465612156

Cross-validation scores (R^2): [0.884 0.827 0.859 0.819 0.84 0.854 0.85 0.846 0.87 0.886]
0.8534467360388138


```

In [189]: # kNN

from sklearn.neighbors import KNeighborsRegressor

knn = KNeighborsRegressor(n_neighbors=6)

pipeline_knn = Pipeline([('transformer', scaler), ('estimator', knn)])

knn_scores = cross_val_score(knn, X, y, cv=10)
knn_scores_scaled = cross_val_score(pipeline_knn, X, y, cv=10)

print("Cross-validation scores (R^2): {}".format(knn_scores))
print(numpy.mean(knn_scores))

print("Cross-validation scores (R^2): {}".format(knn_scores_scaled))
print(numpy.mean(knn_scores_scaled))

Cross-validation scores (R^2): [0.775 0.55 0.685 0.571 0.811 0.792 0.791 0.689 0.656 0.733]
0.705246606343064
Cross-validation scores (R^2): [0.499 0.478 0.467 0.276 0.522 0.629 0.385 0.424 0.404 0.426]
0.45107928209098036

```

Answer to 2 . There are clear differences in the results of the different algorithms without scaling. Without scaling, Linear Regression performs quite a lot better than all the other algorithms. After scaling, however, Linear Regression basically doesn't get any result at all. The scaling makes all features evenly important, but it might distort the effect of the categorical features. There is probably some extreme overfitting on these features going on. Both Ridge and Lasso reach the same performance of Linear Regression after scaling, showing that they are better able to deal with the data when it is scaled. ElasticNet improves as well, though not to the same level. Performance of kNN decreases after scaling, which is logical, as the target variable hasn't been scaled. Since kNN works on absolute distance between points, the scaling distorts the result. To get a valuable result, the target variable should be scaled within the same range.

3 . Do a default, shuffled train-test split and optimize the linear models for the degree of regularization (α) and choice of penalty (L1/L2). For Ridge and Lasso, plot a curve showing the effect of the training and test set performance (R^2) while increasing the degree of regularization for different penalties. For ElasticNet, plot a heatmap $\alpha \times l1_ratio \rightarrow R^2$ using test set performance. Report the optimal performance. Again, provide a concise but meaningful interpretation. What does the regularization do? Can you get better results? - Think about how you get the L1/L2 loss. This is not a hyperparameter in regression. - We've seen how to generate such heatmaps in Lecture 3.

```

In [190]: # Create default shuffled train-test split
from sklearn.model_selection import train_test_split

X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=0, shuffle=True)

In [191]: # Optimize alpha, L1 and L2
import numpy

```

```

ridge_curve_train, ridge_curve_test = [], []

lasso_curve_train, lasso_curve_test = [], []

elastictn_heatmap = []

alpha_val = [0.0001, 0.0005, 0.001, 0.005, 0.01, 0.05, 0.1, 0.5, 1, 5, 10]

for i in [0.0001, 0.0005, 0.001, 0.005, 0.01, 0.05, 0.1, 0.5, 1, 5, 10]:
    ridge_optimize = Ridge(alpha = i).fit(X_train, y_train)
    ridge_curve_train.append(ridge_optimize.score(X_train, y_train))
    ridge_curve_test.append(ridge_optimize.score(X_test, y_test))

for i in [0.0001, 0.0005, 0.001, 0.005, 0.01, 0.05, 0.1, 0.5, 1, 5, 10]:
    lasso_optimize = Lasso(alpha = i).fit(X_train, y_train)
    lasso_curve_train.append(lasso_optimize.score(X_train, y_train))
    lasso_curve_test.append(lasso_optimize.score(X_test, y_test))

for i in range (0, 11):
    elastictn_heatmap.append([])
    for k in [0.0001, 0.0005, 0.001, 0.005, 0.01, 0.05, 0.1, 0.5, 1]:
        elastictn_optimize = ElasticNet(alpha = alpha_val[i], l1_ratio = k).fit(X_train, y_train)
        elastictn_heatmap[i].append(elastictn_optimize.score(X_test, y_test))

```

```

In [192]: print(ridge_curve_train)
print(ridge_curve_test)
plt.plot(ridge_curve_train)
plt.plot(ridge_curve_test)
plt.xticks([0,1,2,3,4,5,6,7,8,9,10], [0.0001, 0.0005, 0.001, 0.005, 0.01, 0.05, 0.1, 0.5, 1, 5, 10])
plt.xlabel("Alpha value")
plt.ylabel("R^2 score")

```

```

[0.9553079170821583, 0.95530212490783, 0.9552852280041161, 0.954903258526907, 0.95415197886097,
0.9446323593615862, 0.9449377495664446, 0.9450109463229461, 0.9450889139760436, 0.94461328632,

```

```

Out[192]: [<matplotlib.lines.Line2D at 0x17d07a99cf8>]

```

```

Out[192]: [<matplotlib.lines.Line2D at 0x17d07a99748>]

```

```

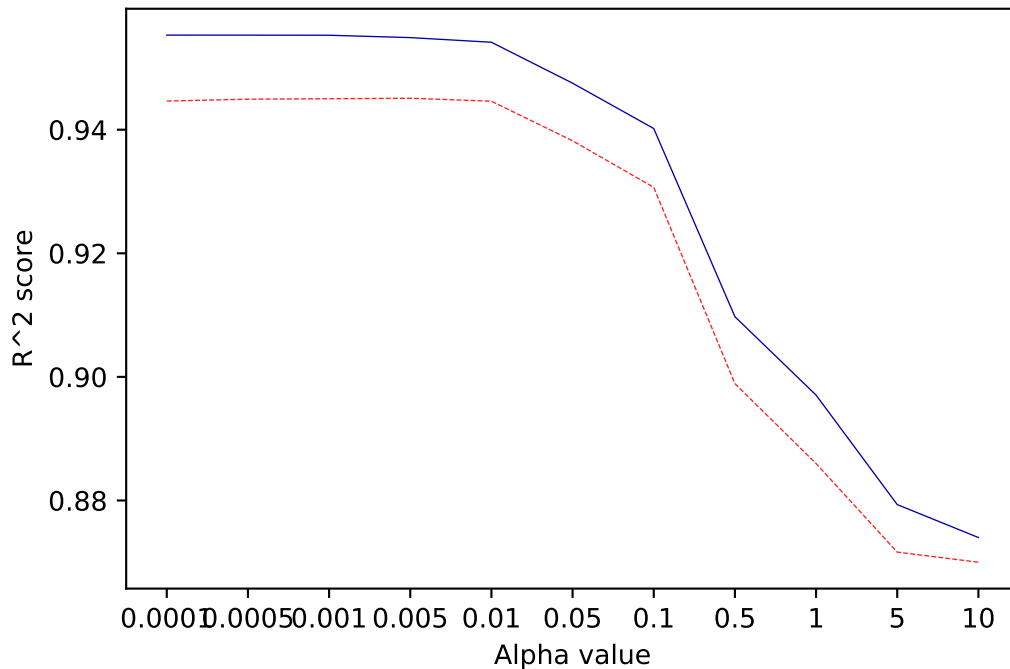
Out[192]: ([<matplotlib.axis.XTick at 0x17d0918fcf8>,
<matplotlib.axis.XTick at 0x17d090187b8>,
<matplotlib.axis.XTick at 0x17d0910d588>,
<matplotlib.axis.XTick at 0x17d07ab4be0>,
<matplotlib.axis.XTick at 0x17d07b1d128>,
<matplotlib.axis.XTick at 0x17d07b1d860>,
<matplotlib.axis.XTick at 0x17d07b22208>,
<matplotlib.axis.XTick at 0x17d07b226a0>,

```

```
<matplotlib.axis.XTick at 0x17d07b22e48>,  
<matplotlib.axis.XTick at 0x17d07b2ce48>,  
<matplotlib.axis.XTick at 0x17d07b2c390>],  
<a list of 11 Text xticklabel objects>
```

Out[192]: Text(0.5,0,'Alpha value')

Out[192]: Text(0,0.5,'R^2 score')



```
In [193]: print(lasso_curve_train)  
          print(lasso_curve_test)  
          plt.plot(lasso_curve_train)  
          plt.plot(lasso_curve_test)  
          plt.xticks([0,1,2,3,4,5,6,7,8,9,10], [0.0001, 0.0005, 0.001, 0.005, 0.01, 0.05, 0.1,  
          plt.xlabel("Alpha value")  
          plt.ylabel("R^2 score")
```

```
[0.9553079224300998, 0.9553019511773134, 0.955283541435668, 0.9549727806010627, 0.954600733329,  
[0.9448996314791974, 0.9449744867278487, 0.9451204905307454, 0.945636691510753, 0.945701681282
```

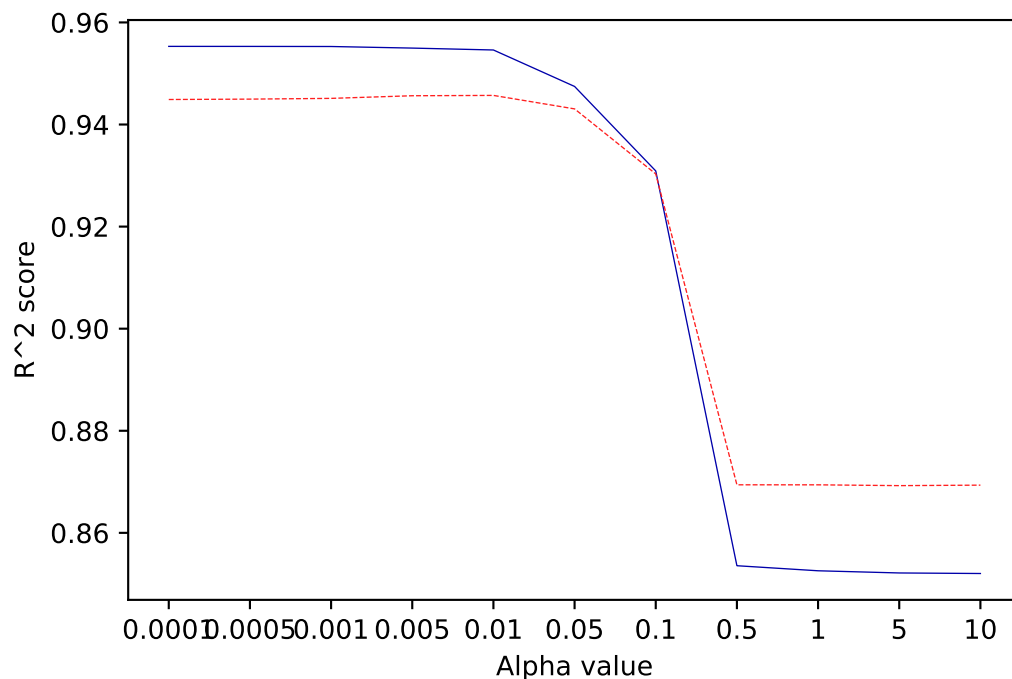
Out[193]: [<matplotlib.lines.Line2D at 0x17d07caa898>]

Out[193]: [<matplotlib.lines.Line2D at 0x17d07caa0f0>]

```
Out[193]: ([<matplotlib.axis.XTick at 0x17d07b4b390>,
<matplotlib.axis.XTick at 0x17d07a3c080>,
<matplotlib.axis.XTick at 0x17d07a3c240>,
<matplotlib.axis.XTick at 0x17d07c81c50>,
<matplotlib.axis.XTick at 0x17d07c81908>,
<matplotlib.axis.XTick at 0x17d07cc35c0>,
<matplotlib.axis.XTick at 0x17d07cc3668>,
<matplotlib.axis.XTick at 0x17d07cc3b00>,
<matplotlib.axis.XTick at 0x17d07961908>,
<matplotlib.axis.XTick at 0x17d079610b8>,
<matplotlib.axis.XTick at 0x17d07cbdef0>],
<a list of 11 Text xticklabel objects>)
```

```
Out[193]: Text(0.5,0,'Alpha value')
```

```
Out[193]: Text(0,0.5,'R^2 score')
```



```
In [194]: elasticn_heatmap = np.array(elasticn_heatmap)
print(elasticn_heatmap)
```

```
plt.imshow(elasticn_heatmap, cmap='hot')
```

```
plt.xticks([0,1,2,3,4,5,6,7,8], [0.0001, 0.0005, 0.001, 0.005, 0.01, 0.05, 0.1, 0.5,
plt.yticks([0,1,2,3,4,5,6,7,8,9,10], [0.0001, 0.0005, 0.001, 0.005, 0.01, 0.05, 0.1,
plt.xlabel("L1 Ratio")
plt.ylabel("Alpha value")
```

```
[0.932 0.932 0.932 0.932 0.932 0.932 0.933 0.939 0.945]
[0.901 0.901 0.901 0.901 0.901 0.902 0.903 0.916 0.945]
[0.887 0.887 0.887 0.887 0.887 0.888 0.889 0.901 0.945]
[0.872 0.872 0.872 0.872 0.872 0.872 0.872 0.876 0.946]
[0.87 0.87 0.87 0.87 0.87 0.87 0.87 0.872 0.946]
[0.87 0.87 0.87 0.87 0.87 0.87 0.87 0.87 0.943]
[0.87 0.87 0.87 0.87 0.87 0.87 0.87 0.87 0.93 ]
[0.87 0.87 0.87 0.87 0.87 0.87 0.87 0.87 0.869]
[0.87 0.87 0.87 0.87 0.87 0.87 0.87 0.87 0.869]
[0.869 0.869 0.869 0.869 0.869 0.869 0.869 0.869 0.869]
[0.865 0.865 0.865 0.865 0.865 0.865 0.866 0.868 0.869]]
```

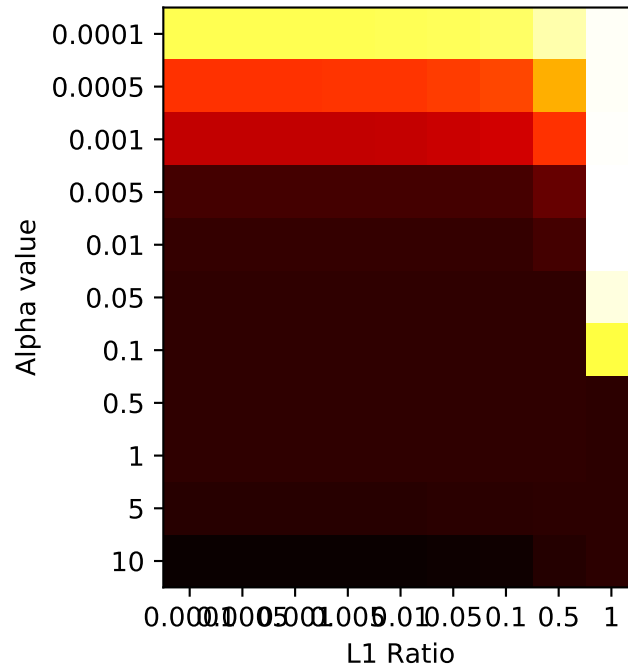
Out[194]: <matplotlib.image.AxesImage at 0x17d07c486d8>

Out[194]: ([<matplotlib.axis.XTick at 0x17d07a61d30>, <matplotlib.axis.XTick at 0x17d07accb00>, <matplotlib.axis.XTick at 0x17d08d72160>, <matplotlib.axis.XTick at 0x17d07c48e80>, <matplotlib.axis.XTick at 0x17d07c5b0b8>, <matplotlib.axis.XTick at 0x17d07c5b2e8>, <matplotlib.axis.XTick at 0x17d08d47f60>, <matplotlib.axis.XTick at 0x17d08d47940>, <matplotlib.axis.XTick at 0x17d08d475f8>], <a list of 9 Text xticklabel objects>)

Out[194]: ([<matplotlib.axis.YTick at 0x17d07cc3898>, <matplotlib.axis.YTick at 0x17d08d72710>, <matplotlib.axis.YTick at 0x17d08d47710>, <matplotlib.axis.YTick at 0x17d07c5bef0>, <matplotlib.axis.YTick at 0x17d04b2b320>, <matplotlib.axis.YTick at 0x17d0793ad30>, <matplotlib.axis.YTick at 0x17d0793a550>, <matplotlib.axis.YTick at 0x17d061f8a90>, <matplotlib.axis.YTick at 0x17d061f8160>, <matplotlib.axis.YTick at 0x17d078e9b00>, <matplotlib.axis.YTick at 0x17d078e95f8>], <a list of 11 Text yticklabel objects>)

Out[194]: Text(0.5,0,'L1 Ratio')

Out[194]: Text(0,0.5,'Alpha value')



Answer to 3 . Optimal performance for both Ridge and Lasso is for very small values of alpha: 0.01 or smaller. ElasticNet performs best at an L1 ratio of 1, with an alpha of 0.05 or smaller. This means that it only uses L1 regularization, just like Lasso, with a similar optimal alpha as well. Apparently, the model is not very likely to overfit, as higher regularization doesn't improve performance. ElasticNet does show that L1 regularization here works better.

4 . Visualize the coefficients of the optimized models. Do they agree on which features are important? Compare the results with the feature importances returned by a RandomForest. Does it agree with the linear models? What would look for when scouting for a baseball player?

```
In [195]: ridge_optimal = Ridge(alpha = 0.01).fit(X_train, y_train)
lasso_optimal = Lasso(alpha = 0.01).fit(X_train, y_train)
elasticn_optimal = ElasticNet(alpha = 0.01, l1_ratio = 1).fit(X_train, y_train)

plt.plot(ridge_optimal.coef_, 's', label="Ridge")
plt.plot(lasso_optimal.coef_, '^', label="Lasso")
plt.plot(elasticn_optimal.coef_, 'v', label="ElasticNet")
plt.xlabel("Coefficient index")
plt.ylabel("Coefficient magnitude")
plt.ylim(-25, 25)
plt.legend()
```

Out[195]: [<matplotlib.lines.Line2D at 0x17d05fb6cf8>]

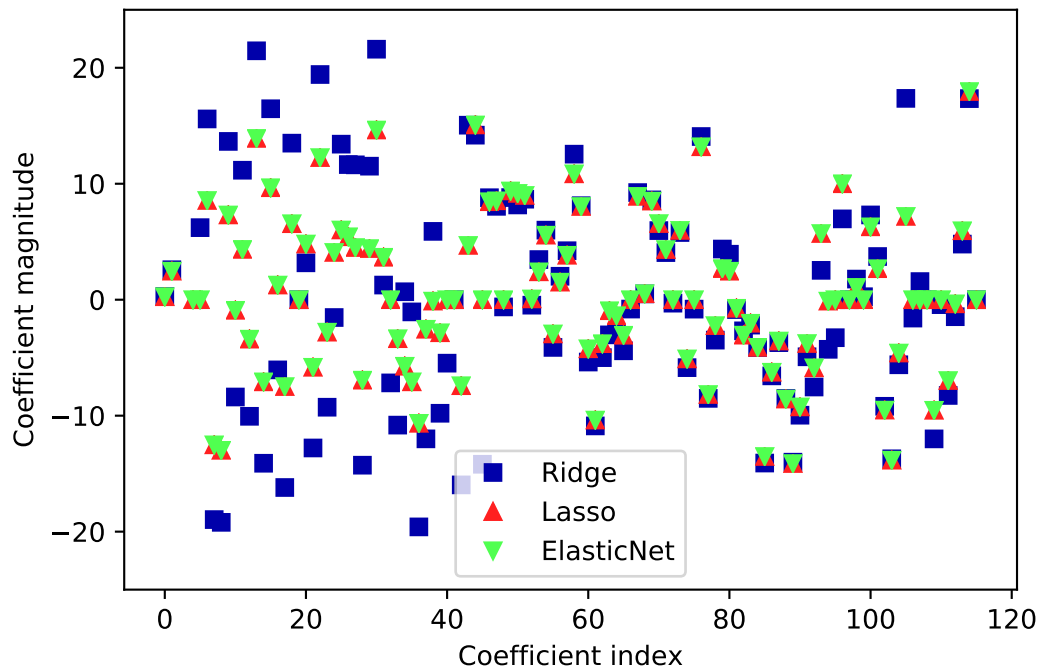
Out[195]: [<matplotlib.lines.Line2D at 0x17d029913c8>]

Out[195]: [<matplotlib.lines.Line2D at 0x17d07d05860>]

```

Out[195]: Text(0.5,0,'Coefficient index')
Out[195]: Text(0,0.5,'Coefficient magnitude')
Out[195]: (-25, 25)
Out[195]: <matplotlib.legend.Legend at 0x17d07d05c18>

```



```

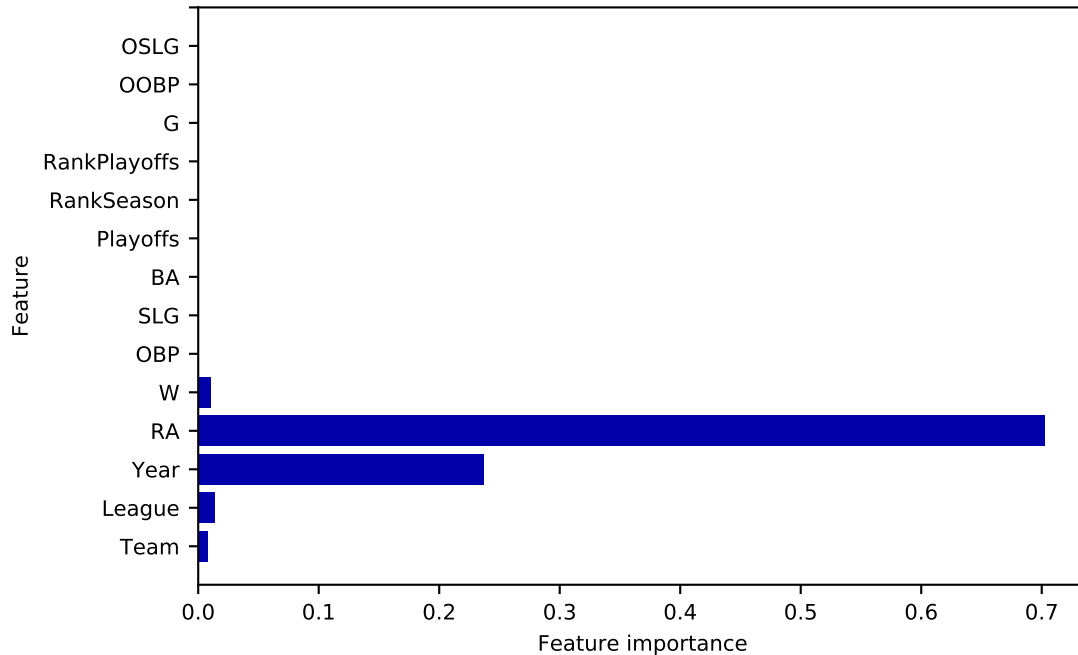
In [126]: # Feature importances RandomForest
from sklearn.ensemble import RandomForestRegressor

randomforest = RandomForestRegressor().fit(X_train, y_train)

def plot_feature_importances_moneyball(model):
    n_features = X.shape[1]
    plt.barh(range(n_features), model.feature_importances_, align='center')
    plt.yticks(np.arange(n_features), attribute_names)
    plt.xlabel("Feature importance")
    plt.ylabel("Feature")
    plt.ylim(-1, 14)

plt.rcParams.update({'font.size':8})
plot_feature_importances_moneyball(randomforest)

```



Answer to 4 . Lasso and ElasticNet clearly agree fully on which features are important. This makes sense, as they make use of the same regularization parameter. Ridge uses different features. It generally agrees on the importance of the features that were made into dummies, but is a bit more extreme on the importance of the original features. The feature importances returned by a RandomForest are much more specific and condensed, it mostly only uses RA and Year as a predictor of the result. It feels logical that the the Run Average is considered so important, as it is one of the features that objectively looks at the performance of a player. According to the model it matters a lot whether a player has a 'good year', that is something I would probably not look at when scouting for a baseball player. Features like the On-base percentage and the slugging percentage seem like good objective predictors of performance. However, in real life I would maybe also look at current fitness of the player and sensibility to strategy, something which is not present in this dataset.

1.2 Nepalese character recognition (5 points, 1+2+2)

The [Devnagari-Script dataset](#) contains 92,000 images (32x32 pixels) of 46 characters from Devanagari script. Your goal is to learn to recognize the right letter given the image.

```
In [17]: devnagari = oml.datasets.get_dataset(40923) # Download Devnagari data
# Get the predictors X and the labels y
X, y = devnagari.get_data(target=devnagari.default_target_attribute);
#classes = devnagari.retrieve_class_labels(target_name='character') # This one takes
```

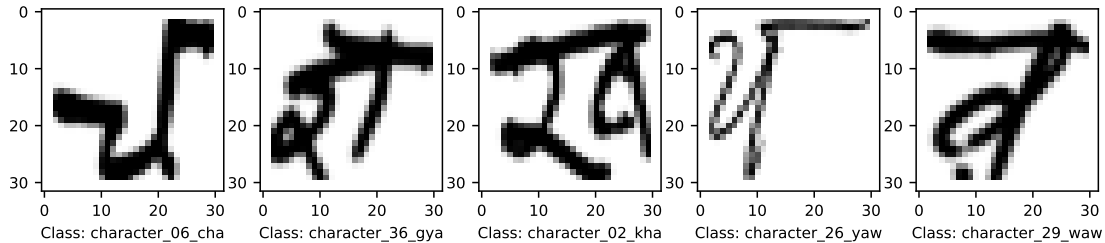
```
In [35]: # Take some random examples, reshape to a 32x32 image and plot
fig, axes = plt.subplots(1, 5, figsize=(10, 5))
for i in range(5):
```



```

n = randint(0,90000)
axes[i].imshow(X[n].reshape(32, 32), cmap=plt.cm.gray_r)
axes[i].set_xlabel("Class: %s" % (classes[y[n]]))
plt.show();

```



1. Evaluate k-Nearest Neighbors, Logistic Regression and RandomForests with their default settings.

- Take a stratified 10% subsample of the data.
- Use the default train-test split and predictive accuracy. Is predictive accuracy a good scoring measure for this problem?
- Try to build the same models on increasingly large samples of the dataset (e.g. 10%, 20%,...). Plot the training time and the predictive performance for each. Stop when the training time becomes prohibitively large (this will be different for different models).

```

In [ ]: #Running K-Nearest Neighbors Classifier, first on 10% subsample, then on gradually big
#compute times

```

```

a = [0.1, 0.2, 0.3]
ComputeTimeKNN = []
PerformanceKNN = []
#Taking a xx% stratified subsample of the data. As can be seen from the plotted comput
#of the data, 30% is the biggest subsample with a reasonable compute time.
for i in a:
    sss = StratifiedShuffleSplit(n_splits=3, train_size=i, random_state=0)

    for train_index, test_index in sss.split(X, y):
        X_new, X_excluded = X[train_index], X[test_index]
        y_new, y_excluded = y[train_index], y[test_index]
        X_train, X_test, y_train, y_test = train_test_split(X_new, y_new, random_state=0)
        print("%s %f:" % ("subsample fraction", i))
        start_time = timeit.default_timer()
        knn = KNeighborsClassifier().fit(X_train, y_train)
        print("Test set score KNN: {:.2f}".format(knn.score(X_test, y_test)))
        compute_time = timeit.default_timer() - start_time
        PerformanceKNN.append(knn.score(X_test, y_test))

```

```
ComputeTimeKNN.append(compute_time)

plt.plot(a, ComputeTimeKNN)
plt.xlabel('Subsample of data in %')
plt.ylabel('Compute time of KNN model')

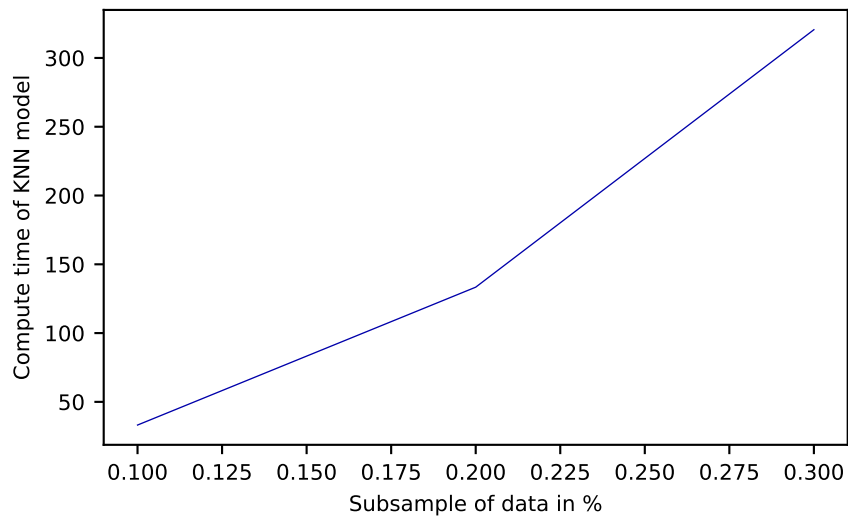
plt.show()
plt.plot(a, PerformanceKNN)
plt.xlabel('Subsample used in training')
plt.ylabel('Predictive Performance KNN')
```

```
subsample fraction 0.100000:
Test set score KNN: 0.73
subsample fraction 0.200000:
Test set score KNN: 0.80
subsample fraction 0.300000:
Test set score KNN: 0.84
```

```
Out[ ]: [<matplotlib.lines.Line2D at 0x106c359e8>]
```

```
Out[ ]: Text(0.5,0,'Subsample of data in %')
```

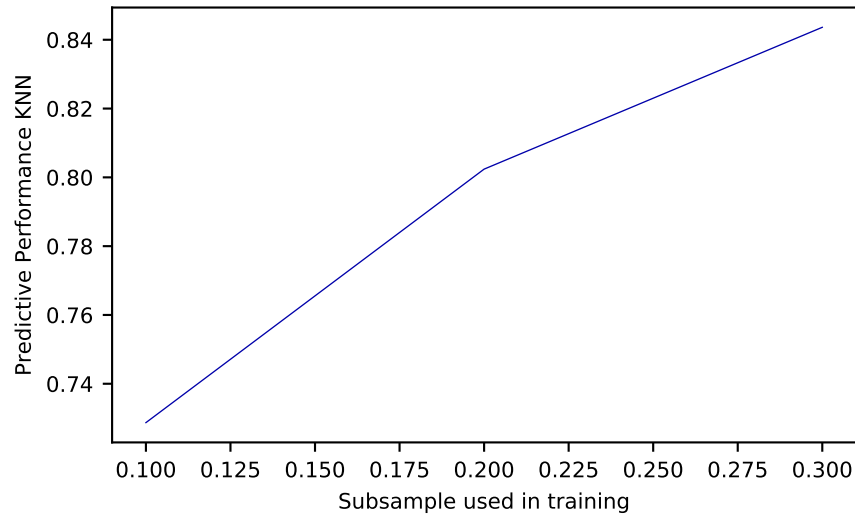
```
Out[ ]: Text(0,0.5,'Compute time of KNN model')
```



```
Out[ ]: [<matplotlib.lines.Line2D at 0x106cd6908>]
```

```
Out[ ]: Text(0.5,0,'Subsample used in training')
```

```
Out[ ]: Text(0,0.5,'Predictive Performance KNN')
```



In [18]: *#Running Logistic Regression, first on 10% subsample, then on gradually bigger sample
#times*

*#Logistic Regression seems to be quite a bit more computationally intensive. 10% seem
#size for which the computation time is still reasonable. After that, the computation*

```

ComputeTimeLR = []
PerformanceLR = []
a = [0.1]
for i in a:
    sss = StratifiedShuffleSplit(n_splits=3, train_size=i, random_state=0)

    for train_index, test_index in sss.split(X, y):
        X_new, X_excluded = X[train_index], X[test_index]
        y_new, y_excluded = y[train_index], y[test_index]
    X_train, X_test, y_train, y_test = train_test_split(X_new, y_new, random_state=0)
    print("%s %f:" %("subsample fraction", i))
    start_time = timeit.default_timer()
    lr = LogisticRegression().fit(X_train, y_train)
    print("Test set score LR: {:.2f}".format(lr.score(X_test, y_test)))
    compute_time = timeit.default_timer() - start_time
    PerformanceLR.append(lr.score(X_test, y_test))
    ComputeTimeLR.append(compute_time)

plt.scatter(a, ComputeTimeLR)
plt.xlabel('Subsample of data ')
plt.ylabel('Compute time of LR model')

plt.show()

```

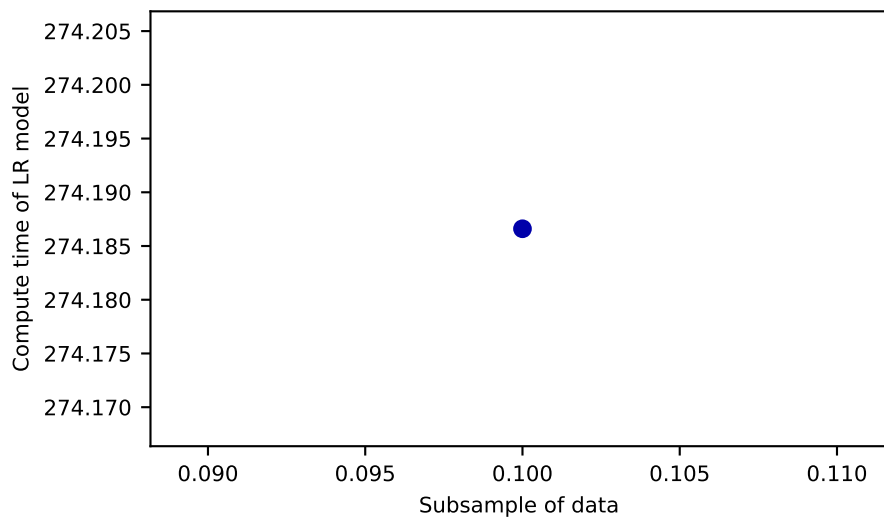
```
plt.scatter(a, PerformanceLR)
plt.xlabel('Subsample used in training')
plt.ylabel('Predictive Performance LR')
```

```
subsample fraction 0.100000:
Test set score LR: 0.49
```

```
Out[18]: <matplotlib.collections.PathCollection at 0x1c12b1b198>
```

```
Out[18]: Text(0.5,0,'Subsample of data ')
```

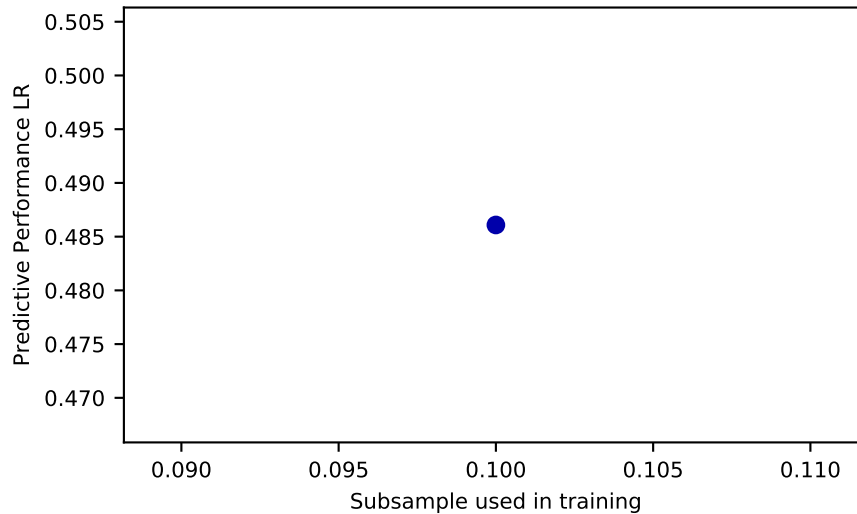
```
Out[18]: Text(0,0.5,'Compute time of LR model')
```



```
Out[18]: <matplotlib.collections.PathCollection at 0x109aa0518>
```

```
Out[18]: Text(0.5,0,'Subsample used in training')
```

```
Out[18]: Text(0,0.5,'Predictive Performance LR')
```



In [5]: *#Running Random Forest Classifier, first on 10% subsample, then on gradually bigger sa
#times. The compute time doesn't skyrocket like with the other classification methods.*

```

ComputeTimeRF = []
PerformanceRF = []
a = [0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9]
for i in a:
    sss = StratifiedShuffleSplit(n_splits=3, train_size=i, random_state=0)

    for train_index, test_index in sss.split(X, y):
        X_new, X_excluded = X[train_index], X[test_index]
        y_new, y_excluded = y[train_index], y[test_index]
        X_train, X_test, y_train, y_test = train_test_split(X_new, y_new, random_state=0)
        print("%s %f:" %("subsample fraction", i))
        start_time = timeit.default_timer()
        rf = RandomForestClassifier().fit(X_train, y_train)
        print("Test set score RF: {:.2F}".format(rf.score(X_test, y_test)))
        compute_time = timeit.default_timer() - start_time
        PerformanceRF.append(rf.score(X_test, y_test))
        ComputeTimeRF.append(compute_time)

plt.plot(a, ComputeTimeRF)
plt.xlabel('Subsample of data')
plt.ylabel('Compute time of RF model')

plt.show()
plt.plot(a, PerformanceRF)
plt.xlabel('Subsample used in training')
plt.ylabel('Predictive Performance RF')

```

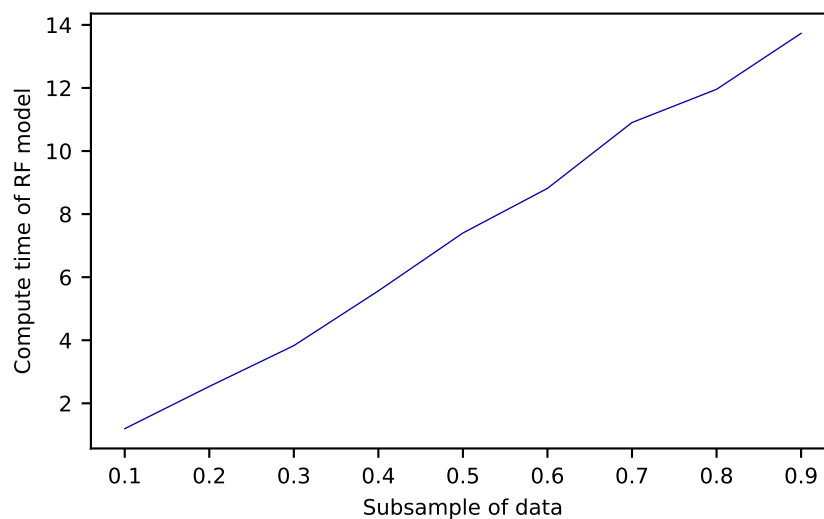
```
plt.show()
```

```
subsample fraction 0.100000:  
Test set score RF: 0.57  
subsample fraction 0.200000:  
Test set score RF: 0.64  
subsample fraction 0.300000:  
Test set score RF: 0.69  
subsample fraction 0.400000:  
Test set score RF: 0.70  
subsample fraction 0.500000:  
Test set score RF: 0.73  
subsample fraction 0.600000:  
Test set score RF: 0.75  
subsample fraction 0.700000:  
Test set score RF: 0.75  
subsample fraction 0.800000:  
Test set score RF: 0.76  
subsample fraction 0.900000:  
Test set score RF: 0.77
```

```
Out [5]: [<matplotlib.lines.Line2D at 0x10b4185f8>]
```

```
Out [5]: Text(0.5,0,'Subsample of data')
```

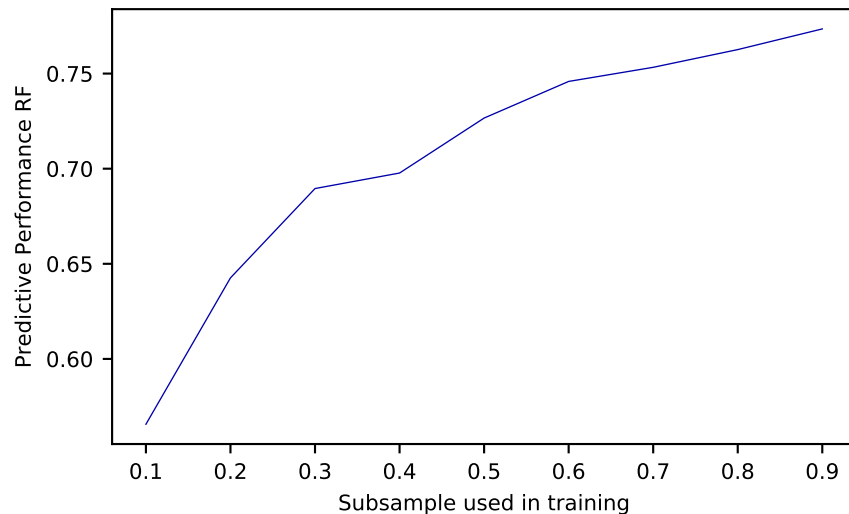
```
Out [5]: Text(0,0.5,'Compute time of RF model')
```



```
Out [5]: [<matplotlib.lines.Line2D at 0x10b45b320>]
```

```
Out [5]: Text(0.5,0,'Subsample used in training')
```

```
Out [5]: Text(0,0.5,'Predictive Performance RF')
```



Answer to 1. The simple predictive accuracy metric (percentage of accurate predictions against total predictions) was used to assess the performance of the models created. While this predictive accuracy somewhat helps in assessing the performance of the models, it doesn't tell the whole story. It is important to note that the classification problem at hand consists of 46 classes (the number of Nepalese Characters). A random model would give 2,17% accuracy. This opposed to a simple 2 classes problem, where a random model would give 50% accuracy. an accuracy in the range of 70-80% is fairly good, while for a 2-class problem the performance would be abysmal. To more fully understand the performance of the models, a confusion matrix could be created. Weights can be attributed to certain wrong predictions to train them out of the models. Although there are many examples where this would be of importance (e.g. disease prediction), in this particular case there seems no need to give certain wrong predictions more weight than others. So even though predictive accuracy doesn't tell the whole story, in this specific classification problem it is a fine metric.

2 . Optimize the value for the number of neighbors k (keep $k < 50$) and the number of trees (keep $n_estimators < 100$) on the stratified 10% subsample. - Use 10-fold crossvalidation and plot k and $n_estimators$ against the predictive accuracy. Which value of k , $n_estimators$ should you pick?

```
In [8]: X, y = devnagari.get_data(target=devnagari.default_target_attribute);

#Create 10% stratified subsample
sss = StratifiedShuffleSplit(n_splits=5, train_size=0.1, random_state=0)

for train_index, test_index in sss.split(X, y):
    X_new, X_val = X[train_index], X[test_index]
    y_new, y_val = y[train_index], y[test_index]
#Vary number of neighbors from 1 to 41 in steps of 10
```

```

a = numpy.arange(1,42,10)

PerformanceKNNk = []
for i in a:
    knn = KNeighborsRegressor(n_neighbors=i)
    kfold = KFold(n_splits=10)
    PerformanceKNNk.append(np.mean(cross_val_score(knn, X_new, y_new, cv=kfold)))

plt.scatter(a, PerformanceKNNk)
plt.xlabel("Number of neighbors")
plt.ylabel("Mean cv score")
plt.show()
#from the scatterplot it seems the optimal k value is between 1 and 11, therefore try
a = numpy.arange(1,11,1)
PerformanceKNNk = []
for i in a:
    knn = KNeighborsRegressor(n_neighbors=i)
    kfold = KFold(n_splits=10)
    PerformanceKNNk.append(np.mean(cross_val_score(knn, X_new, y_new, cv=kfold)))

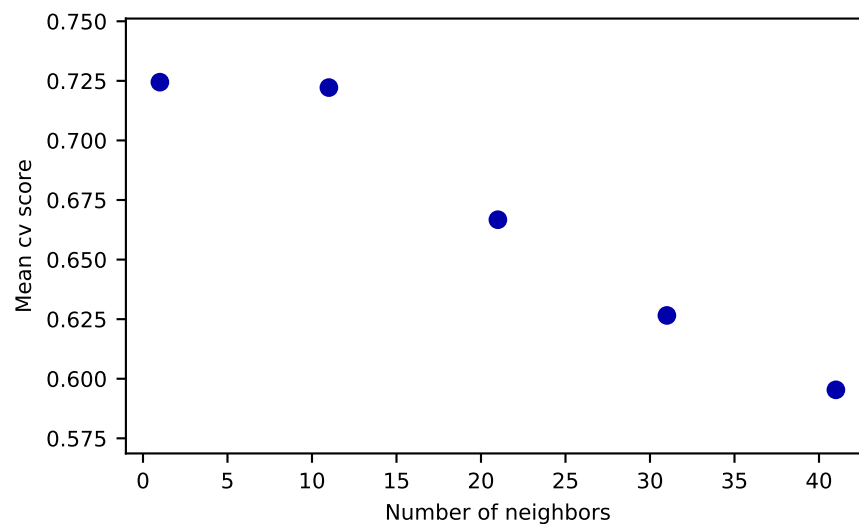
plt.scatter(a, PerformanceKNNk)
plt.xlabel("Number of neighbors")
plt.ylabel("Mean cv score")
plt.show()

```

Out[8]: <matplotlib.collections.PathCollection at 0x1c0c062048>

Out[8]: Text(0.5,0,'Number of neighbors')

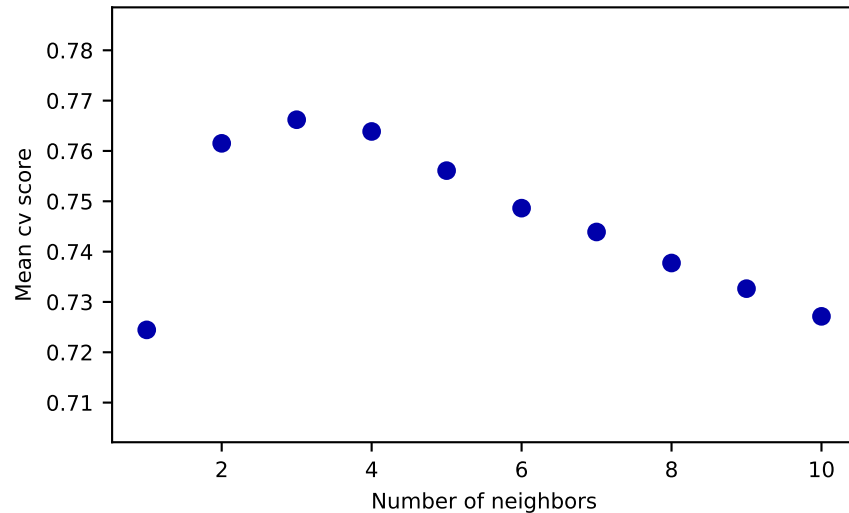
Out[8]: Text(0,0.5,'Mean cv score')



Out [8]: <matplotlib.collections.PathCollection at 0x1c0c62a2b0>

Out [8]: Text(0.5,0,'Number of neighbors')

Out [8]: Text(0,0.5,'Mean cv score')



```
In [15]: X, y = devnagari.get_data(target=devnagari.default_target_attribute);
```

```
PerformanceRFn = []
```

```
sss = StratifiedShuffleSplit(n_splits=5, train_size=0.1, random_state=0)
```

```
for train_index, test_index in sss.split(X,y):
```

```
    X_new, X_out = X[train_index], X[test_index]
```

```
    y_new, y_val = y[train_index], y[test_index]
```

```
a = numpy.arange(10,101,10)
```

```
for i in a:
```

```
    rf = RandomForestClassifier(n_estimators=i)
```

```
    kfold = KFold(n_splits=10)
```

```
    PerformanceRFn.append(np.mean(cross_val_score(rf, X_new, y_new, cv=kfold)))
```

```
plt.scatter(a, PerformanceRFn)
```

```
plt.xlabel("Number of trees")
```

```
plt.ylabel("Mean cv score")
```

```
plt.show()
```

```
a = numpy.arange(90,100,1)
```

```
PerformanceRFn = []
```

```
for i in a:
```

```
    rf = RandomForestClassifier(n_estimators=i)
```

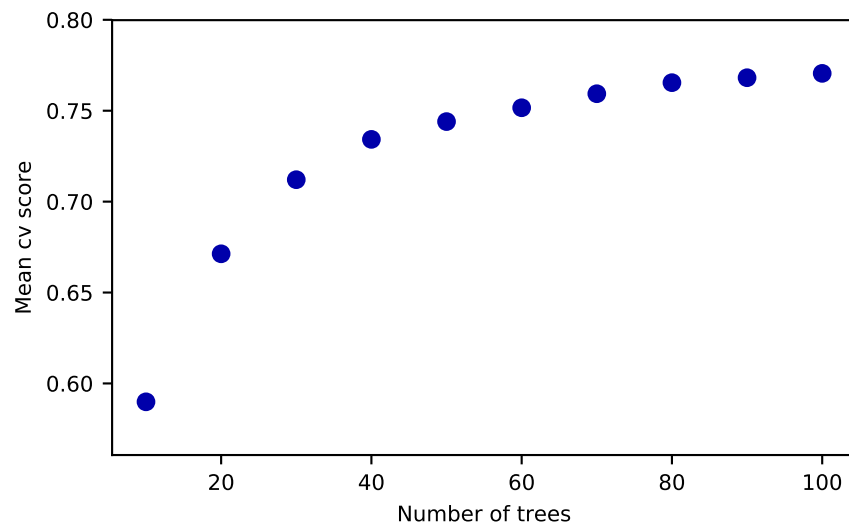
```
kfold = KFold(n_splits=10)
PerformanceRfn.append(np.mean(cross_val_score(rf, X_new, y_new, cv=kfold)))

plt.scatter(a, PerformanceRfn)
plt.xlabel("Number of trees")
plt.ylabel("Mean cv score")
plt.show()
```

Out[15]: <matplotlib.collections.PathCollection at 0x1c0c61b860>

Out[15]: Text(0.5,0,'Number of trees')

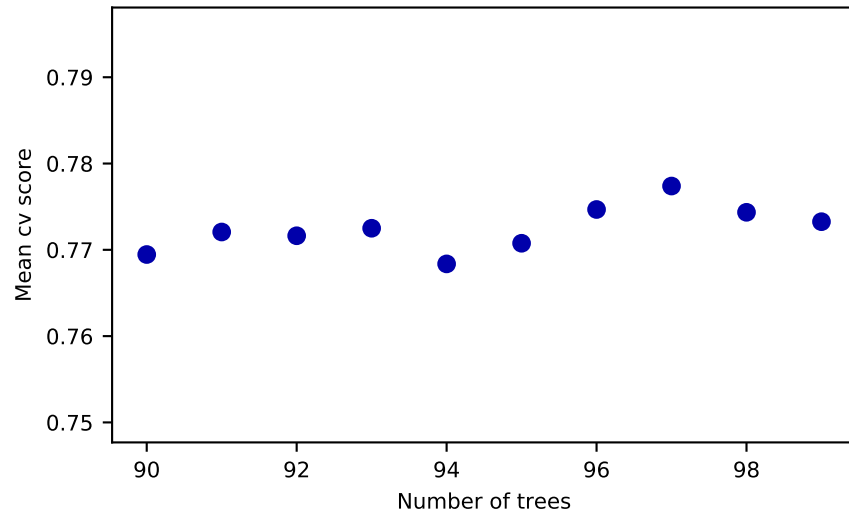
Out[15]: Text(0,0.5,'Mean cv score')



Out[15]: <matplotlib.collections.PathCollection at 0x1c0c5c2908>

Out[15]: Text(0.5,0,'Number of trees')

Out[15]: Text(0,0.5,'Mean cv score')



Answer to 2. From the plots, it can be gathered that the optimal value for `k_neighbors` is 3 And for `n_estimators` this value is 97 (keeping below 100)

3. For the RandomForest, optimize both `n_estimators` and `max_features` at the same time on the entire dataset. - Use a nested cross-validation and a random search over the possible values, and measure the accuracy. Explore how fine-grained this grid/random search can be, given your computational resources. What is the optimal performance you find? - Hint: choose a nested cross-validation that is feasible. Don't use too many folds in the outer loop. - Repeat the grid search and visualize the results as a plot (heatmap) `n_estimators` \times `max_features` \rightarrow ACC with ACC visualized as the color of the data point. Try to make the grid as fine as possible. Interpret the results. Can you explain your observations? What did you learn about tuning RandomForests?

```
In [22]: X, y = devnagari.get_data(target=devnagari.default_target_attribute);
        sss = StratifiedShuffleSplit(n_splits=5, train_size=0.2, random_state=0)
```

```
for train_index, test_index in sss.split(X,y):
    X_new, X_out = X[train_index], X[test_index]
    y_new, y_val = y[train_index], y[test_index]
n_estimators = [25, 50, 100, 200, 400, 800]
max_features = [1, 2, 4, 8, 16, 32, 64, 128]
rfc = RandomForestClassifier(n_estimators = n_estimators, max_features = max_features)
inner_cv = KFold(n_splits=3, shuffle=True, random_state=1)
outer_cv = KFold(n_splits=3, shuffle=True, random_state=1)
param_grid = {'n_estimators': n_estimators, 'max_features': max_features}
rscv = RandomizedSearchCV(RandomForestClassifier(n_estimators = n_estimators,
                                                max_features = max_features),
                        param_distributions=param_grid, n_iter=10, cv=inner_cv, n_j
scores = cross_val_score(rscv, X_new, y_new, cv=outer_cv)
print(scores)
rscv.fit(X_new, y_new)
rscv.best_params_
```

```
[0.834 0.841 0.83 ]
```

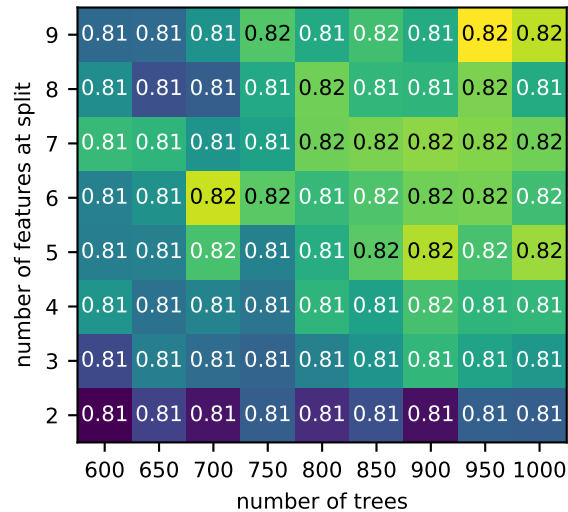
```
Out [22]: RandomizedSearchCV(cv=KFold(n_splits=3, random_state=1, shuffle=True),
                             error_score='raise',
                             estimator=RandomForestClassifier(bootstrap=True, class_weight=None, criterion=
                             max_depth=None, max_features=[1, 2, 4, 8, 16, 32, 64, 128],
                             max_leaf_nodes=None, min_impurity_decrease=0.0,
                             min_impurity_split=None, min_samples_leaf=1,
                             min_samples_split=2, min_weight_fraction_leaf=0.0,
                             n_estimators=[25, 50, 100, 200, 400, 800], n_jobs=1,
                             oob_score=False, random_state=None, verbose=0,
                             warm_start=False),
                             fit_params=None, iid=True, n_iter=10, n_jobs=2,
                             param_distributions={'n_estimators': [25, 50, 100, 200, 400, 800]}, 'max_fea
                             pre_dispatch='2*n_jobs', random_state=None, refit=True,
                             return_train_score='warn', scoring=None, verbose=0)
```

```
Out [22]: {'max_features': 2, 'n_estimators': 800}
```

```
In [23]: #set new parameter grid
n_estimators = [600, 650, 700, 750, 800, 850, 900, 950, 1000]
max_features = [2, 3, 4, 5, 6, 7, 8, 9]
param_grid = {'n_estimators': n_estimators, 'max_features': max_features}
grid_search = GridSearchCV(rfc, param_grid, cv=3, n_jobs=2)
X_train, X_test, y_train, y_test = train_test_split(X_new, y_new, random_state=0)
grid_search.fit(X_train, y_train)
```

```
Out [23]: GridSearchCV(cv=3, error_score='raise',
                       estimator=RandomForestClassifier(bootstrap=True, class_weight=None, criterion=
                       max_depth=None, max_features=[1, 2, 4, 8, 16, 32, 64, 128],
                       max_leaf_nodes=None, min_impurity_decrease=0.0,
                       min_impurity_split=None, min_samples_leaf=1,
                       min_samples_split=2, min_weight_fraction_leaf=0.0,
                       n_estimators=[25, 50, 100, 200, 400, 800], n_jobs=1,
                       oob_score=False, random_state=None, verbose=0,
                       warm_start=False),
                       fit_params=None, iid=True, n_jobs=2,
                       param_grid={'n_estimators': [600, 650, 700, 750, 800, 850, 900, 950, 1000]}, 'ma
                       pre_dispatch='2*n_jobs', refit=True, return_train_score='warn',
                       scoring=None, verbose=0)
```

```
In [27]: #display results in heatmap
results = pd.DataFrame(grid_search.cv_results_)
scores = np.array(results.mean_test_score).reshape(8, 9)
mglearn.tools.heatmap(scores, xlabel='number of trees', xticklabels=param_grid['n_est
                        ylabel='number of features at split', yticklabels=param_grid['ma
```



Answer to 3.

For the random grid search, a relative small number of possibilities (10) were explored, using 20% of the data. This was a necessary consideration, as many runs on either the full data set or larger number of possibilities resulted in system crashes due to running out of memory (on an 8GB machine). It is therefore very likely that the optimal solution found is not close to the true optimal solution, but it will have to make do. The optimal values for `N_estimators` is 800, combined with `max_features` 2. `N_jobs=2` was taken as a precaution as to not overload the system. with these values, a more focussed full grid search is performed, with 9 and 8 values respectively for the hyperparameters. The heatmap shows a higher concentration of high scores (0.82) generally towards a larger number of features at split, the same seems true for larger number of trees. The optimal values seem to be `Max_feature` = 9 and `N_estimators` is 950, which is interesting, considering the random search gave `Max_features` = 2 as being optimal. But as said before, it is difficult to draw strong conclusions from this run, as the initial random grid search was limited, it could be that this optimum is merely a local optimum. The main takeaway is that (random) grid search is hugely computationally expensive, especially on a mobile machine with less power. A more extensive initial random grid search would have been much preferred and would have allowed to draw stronger conclusions from the finer grid search. Going straight for a grid search would be almost impossible to get optimal values near their true optimals, but by doing a random search first, an estimation of the optimals can be made and the search can be narrowed down significantly.

1.3 3. Understanding Ensembles (5 points (3+2))

Do a deeper analysis of how RandomForests and Gradient Boosting reduce their prediction error. We'll use the MAGIC telescope dataset (<http://www.openml.org/d/1120>). When high-energy particles hit the atmosphere, they produce chain reactions of other particles called 'showers', and you need to detect whether these are caused by gamma rays or cosmic rays.

```
In [ ]: # Get the data
        magic_data = oml.datasets.get_dataset(1120) # Download MAGIC Telescope data
        X, y = magic_data.get_data(target=magic_data.default_target_attribute);
```

```
In [ ]: # Quick visualization
X, y, attribute_names = magic_data.get_data(target=magic_data.default_target_attribute)
magic = pd.DataFrame(X, columns=attribute_names)
magic.plot(figsize=(20,10))
# Also plot the target: 1 = gamma, 0 = background
pd.DataFrame(y).plot(figsize=(20,1));
```

1. Do a bias-variance analysis of both algorithms. For each, vary the number of trees on a log scale from 1 to 1024, and plot the bias error (squared), variance, and total error (in one plot per algorithm). Interpret the results. Which error is highest for small ensembles, and which reduced most by each algorithm as you use a larger ensemble? When are both algorithms under- or over-fitting? Provide a detailed explanation of why random forests and gradient boosting behave this way. - See lecture 3 for an example on how to do the bias-variance decomposition - To save time, you can use a 10% stratified subsample in your initial experiments, but show the plots for the full dataset in your report.

```
In [9]: from sklearn.model_selection import ShuffleSplit
from sklearn.model_selection import StratifiedShuffleSplit
import numpy
treensrs = numpy.logspace(0, 10, base=2, num=11)

bias_forest, variance_forest, error_forest = [], [], []

# RandomForest
from sklearn.ensemble import RandomForestClassifier

# Take 10% stratified subsample
#sss = StratifiedShuffleSplit(n_splits=3, test_size=(0.9), random_state=0)

#for train_index, test_index in sss.split(X, y):
#    X_new, X_excluded = X[train_index], X[test_index]
#    y_new, y_excluded = y[train_index], y[test_index]

X_new = X
y_new = y

# Bootstraps
n_repeat = 100
shuffle_split = ShuffleSplit(test_size=0.33, n_splits=n_repeat)

for i in treensrs:
    forest = RandomForestClassifier(n_estimators=int(i), random_state=2) # vary n_estimators
    # Store sample predictions
    y_all_pred = [[] for _ in range(len(y_new))]

    # Train classifier on each bootstrap and score predictions
    for i, (train_index, test_index) in enumerate(shuffle_split.split(X_new)):
```

```

# Train and predict
forest.fit(X_new[train_index], y_new[train_index])
y_pred = forest.predict(X_new[test_index])

# Store predictions
for i,index in enumerate(test_index):
    y_all_pred[index].append(y_pred[i])

# Compute bias, variance, error
bias_sq = sum([(1 - x_new.count(y[i])/len(x_new))**2 * len(x_new)/n_repeat
               for i,x_new in enumerate(y_all_pred)])
var = sum([(1 - ((x_new.count(0)/len(x_new))**2 + (x_new.count(1)/len(x_new))**2)
           for i,x_new in enumerate(y_all_pred)])
error = sum([(1 - x_new.count(y[i])/len(x_new)) * len(x_new)/n_repeat
             for i,x_new in enumerate(y_all_pred)])

bias_forest.append(bias_sq)
variance_forest.append(var)
error_forest.append(error)

print("Bias squared: %.2f, Variance: %.2f, Total error: %.2f" % (bias_sq, var, error))

```

```

Out [9]: RandomForestClassifier(bootstrap=True, class_weight=None, criterion='gini',
                                max_depth=None, max_features='auto', max_leaf_nodes=None,
                                min_impurity_decrease=0.0, min_impurity_split=None,
                                min_samples_leaf=1, min_samples_split=2,
                                min_weight_fraction_leaf=0.0, n_estimators=1, n_jobs=1,
                                oob_score=False, random_state=2, verbose=0, warm_start=False)

```

```

Out [9]: RandomForestClassifier(bootstrap=True, class_weight=None, criterion='gini',
                                max_depth=None, max_features='auto', max_leaf_nodes=None,
                                min_impurity_decrease=0.0, min_impurity_split=None,
                                min_samples_leaf=1, min_samples_split=2,
                                min_weight_fraction_leaf=0.0, n_estimators=1, n_jobs=1,
                                oob_score=False, random_state=2, verbose=0, warm_start=False)

```

```

Out [9]: RandomForestClassifier(bootstrap=True, class_weight=None, criterion='gini',
                                max_depth=None, max_features='auto', max_leaf_nodes=None,
                                min_impurity_decrease=0.0, min_impurity_split=None,
                                min_samples_leaf=1, min_samples_split=2,
                                min_weight_fraction_leaf=0.0, n_estimators=1, n_jobs=1,
                                oob_score=False, random_state=2, verbose=0, warm_start=False)

```

```

Out [9]: RandomForestClassifier(bootstrap=True, class_weight=None, criterion='gini',
                                max_depth=None, max_features='auto', max_leaf_nodes=None,
                                min_impurity_decrease=0.0, min_impurity_split=None,
                                min_samples_leaf=1, min_samples_split=2,

```

```
min_weight_fraction_leaf=0.0, n_estimators=1, n_jobs=1,  
oob_score=False, random_state=2, verbose=0, warm_start=False)
```

```
Out [9]: RandomForestClassifier(bootstrap=True, class_weight=None, criterion='gini',  
max_depth=None, max_features='auto', max_leaf_nodes=None,  
min_impurity_decrease=0.0, min_impurity_split=None,  
min_samples_leaf=1, min_samples_split=2,  
min_weight_fraction_leaf=0.0, n_estimators=1, n_jobs=1,  
oob_score=False, random_state=2, verbose=0, warm_start=False)
```

```
Out [9]: RandomForestClassifier(bootstrap=True, class_weight=None, criterion='gini',  
max_depth=None, max_features='auto', max_leaf_nodes=None,  
min_impurity_decrease=0.0, min_impurity_split=None,  
min_samples_leaf=1, min_samples_split=2,  
min_weight_fraction_leaf=0.0, n_estimators=1, n_jobs=1,  
oob_score=False, random_state=2, verbose=0, warm_start=False)
```

```
Out [9]: RandomForestClassifier(bootstrap=True, class_weight=None, criterion='gini',  
max_depth=None, max_features='auto', max_leaf_nodes=None,  
min_impurity_decrease=0.0, min_impurity_split=None,  
min_samples_leaf=1, min_samples_split=2,  
min_weight_fraction_leaf=0.0, n_estimators=1, n_jobs=1,  
oob_score=False, random_state=2, verbose=0, warm_start=False)
```

```
Out [9]: RandomForestClassifier(bootstrap=True, class_weight=None, criterion='gini',  
max_depth=None, max_features='auto', max_leaf_nodes=None,  
min_impurity_decrease=0.0, min_impurity_split=None,  
min_samples_leaf=1, min_samples_split=2,  
min_weight_fraction_leaf=0.0, n_estimators=1, n_jobs=1,  
oob_score=False, random_state=2, verbose=0, warm_start=False)
```

```
Out [9]: RandomForestClassifier(bootstrap=True, class_weight=None, criterion='gini',  
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Bias squared: 577.38, Variance: 668.21, Total error: 1245.59

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```

Bias squared: 684.77, Variance: 422.62, Total error: 1107.39

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```

Bias squared: 618.35, Variance: 329.28, Total error: 947.63

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```

Bias squared: 607.83, Variance: 245.20, Total error: 853.03

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Bias squared: 620.29, Variance: 188.43, Total error: 808.72

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    min_samples_leaf=1, min_samples_split=2,
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```

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```

Bias squared: 634.32, Variance: 145.04, Total error: 779.36

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Bias squared: 651.62, Variance: 117.86, Total error: 769.48

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    min_impurity_decrease=0.0, min_impurity_split=None,
    min_samples_leaf=1, min_samples_split=2,
    min_weight_fraction_leaf=0.0, n_estimators=128, n_jobs=1,
    oob_score=False, random_state=2, verbose=0, warm_start=False)
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```

Bias squared: 658.30, Variance: 101.39, Total error: 759.69

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Out [9]: RandomForestClassifier(bootstrap=True, class_weight=None, criterion='gini',
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```


Bias squared: 667.32, Variance: 92.63, Total error: 759.95

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Bias squared: 669.96, Variance: 85.23, Total error: 755.19

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    oob_score=False, random_state=2, verbose=0, warm_start=False)
```

```
Out [9]: RandomForestClassifier(bootstrap=True, class_weight=None, criterion='gini',
    max_depth=None, max_features='auto', max_leaf_nodes=None,
    min_impurity_decrease=0.0, min_impurity_split=None,
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Out [9]: RandomForestClassifier(bootstrap=True, class_weight=None, criterion='gini',
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    oob_score=False, random_state=2, verbose=0, warm_start=False)
```

Bias squared: 668.26, Variance: 84.75, Total error: 753.01

```
In [10]: print(bias_forest)
print(variance_forest)
print(error_forest)
```

```
plt.plot(bias_forest, label = "Bias Squared")
plt.plot(variance_forest, label = "Variance", linestyle='-')
plt.plot(error_forest, color='g', label="Total Error", linestyle='-')
plt.xticks([0,1,2,3,4,5,6,7,8,9,10], treenrs)
plt.xlabel("Number of Trees")
```

```
plt.legend(bbox_to_anchor=(0., 1.02, 1., .102), loc=3, ncol=2, mode="expand", borderaxes
```

```
[577.3771775231379, 684.7718043551013, 618.3464755284955, 607.829488189841, 620.290278444065, 6
[668.212822476837, 422.61819564489, 329.2835244715022, 245.20051181016072, 188.42972155593546,
[1245.5899999998956, 1107.389999999967, 947.6299999999704, 853.0299999999836, 808.7199999999899
```

```
Out [10]: [<matplotlib.lines.Line2D at 0x24358c663c8>]
```

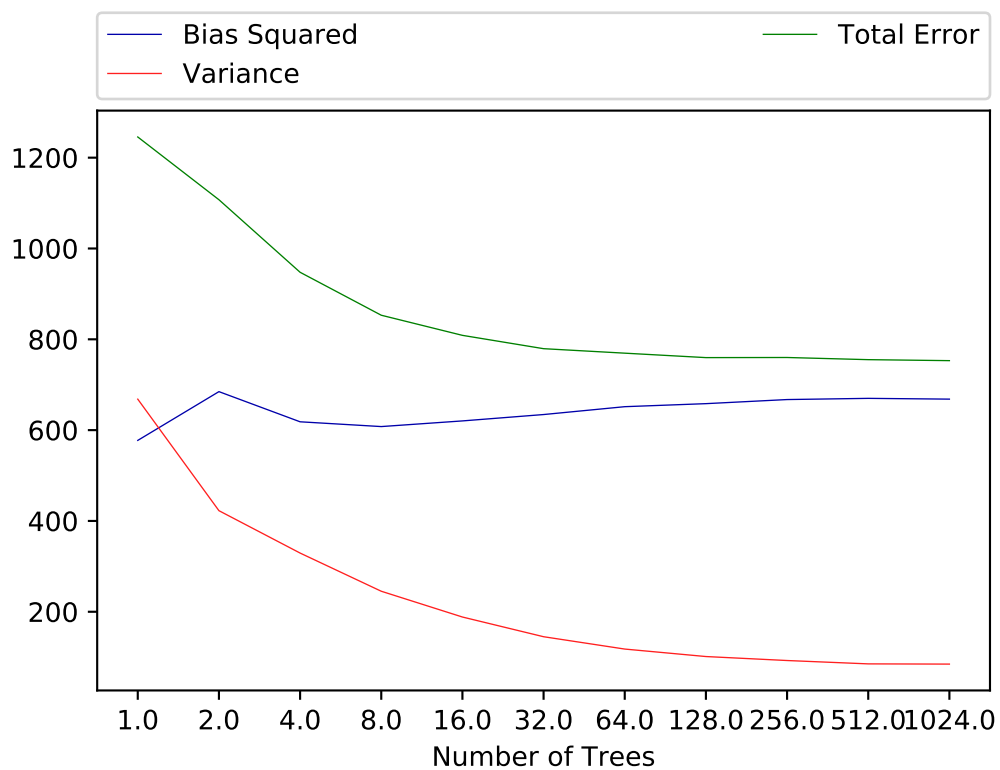
Out[10]: [<matplotlib.lines.Line2D at 0x24355ab5518>]

Out[10]: [<matplotlib.lines.Line2D at 0x24358c66898>]

Out[10]: ([<matplotlib.axis.XTick at 0x24355a6b0f0>,
<matplotlib.axis.XTick at 0x24351956fd0>,
<matplotlib.axis.XTick at 0x243559657f0>,
<matplotlib.axis.XTick at 0x24358c6c828>,
<matplotlib.axis.XTick at 0x24358c6ce48>,
<matplotlib.axis.XTick at 0x24358c6d4a8>,
<matplotlib.axis.XTick at 0x24358c6db00>,
<matplotlib.axis.XTick at 0x24358c71198>,
<matplotlib.axis.XTick at 0x24358c717f0>,
<matplotlib.axis.XTick at 0x24358c71e48>,
<matplotlib.axis.XTick at 0x24358c754e0>],
<a list of 11 Text xticklabel objects>)

Out[10]: Text(0.5,0,'Number of Trees')

Out[10]: <matplotlib.legend.Legend at 0x24358c6de48>



```
In [11]: # Gradient Boosting
         from sklearn.ensemble import GradientBoostingClassifier
```

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bias_gbrt, variance_gbrt, error_gbrt = [], [], []

for i in treenrs:
    gbrt = GradientBoostingClassifier(n_estimators=int(i), random_state=0) # vary n_e
    # Store sample predictions
    y_all_pred = [[] for _ in range(len(y_new))]

    # Train classifier on each bootstrap and score predictions
    for i, (train_index, test_index) in enumerate(shuffle_split.split(X_new)):
        # Train and predict
        gbrt.fit(X_new[train_index], y_new[train_index])
        y_pred = gbrt.predict(X_new[test_index])

        # Store predictions
        for i, index in enumerate(test_index):
            y_all_pred[index].append(y_pred[i])

    # Compute bias, variance, error
    bias_sq = sum([(1 - x_new.count(y[i])/len(x_new))**2 * len(x_new)/n_repeat
                  for i, x_new in enumerate(y_all_pred)])
    var = sum([(1 - ((x_new.count(0)/len(x_new))**2 + (x_new.count(1)/len(x_new))**2)
              for i, x_new in enumerate(y_all_pred)])
    error = sum([(1 - x_new.count(y[i])/len(x_new)) * len(x_new)/n_repeat
                for i, x_new in enumerate(y_all_pred)])

    bias_gbrt.append(bias_sq)
    variance_gbrt.append(var)
    error_gbrt.append(error)

print("Bias squared: %.2f, Variance: %.2f, Total error: %.2f" % (bias_sq, var, error))

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min_impurity_decrease=0.0, min_impurity_split=None,
min_samples_leaf=1, min_samples_split=2,
min_weight_fraction_leaf=0.0, n_estimators=1, presort='auto',
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min_impurity_decrease=0.0, min_impurity_split=None,
min_samples_leaf=1, min_samples_split=2,
min_weight_fraction_leaf=0.0, n_estimators=1, presort='auto',
random_state=0, subsample=1.0, verbose=0, warm_start=False)
```

```
Out[11]: GradientBoostingClassifier(criterion='friedman_mse', init=None,
learning_rate=0.1, loss='deviance', max_depth=3,
max_features=None, max_leaf_nodes=None,
min_impurity_decrease=0.0, min_impurity_split=None,
min_samples_leaf=1, min_samples_split=2,
min_weight_fraction_leaf=0.0, n_estimators=1, presort='auto',
random_state=0, subsample=1.0, verbose=0, warm_start=False)
```

```
Out[11]: GradientBoostingClassifier(criterion='friedman_mse', init=None,
    learning_rate=0.1, loss='deviance', max_depth=3,
    max_features=None, max_leaf_nodes=None,
    min_impurity_decrease=0.0, min_impurity_split=None,
    min_samples_leaf=1, min_samples_split=2,
    min_weight_fraction_leaf=0.0, n_estimators=1, presort='auto',
    random_state=0, subsample=1.0, verbose=0, warm_start=False)
```

```
Out[11]: GradientBoostingClassifier(criterion='friedman_mse', init=None,
    learning_rate=0.1, loss='deviance', max_depth=3,
    max_features=None, max_leaf_nodes=None,
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Out[11]: GradientBoostingClassifier(criterion='friedman_mse', init=None,
    learning_rate=0.1, loss='deviance', max_depth=3,
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Out[11]: GradientBoostingClassifier(criterion='friedman_mse', init=None,
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Out[11]: GradientBoostingClassifier(criterion='friedman_mse', init=None,
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    min_weight_fraction_leaf=0.0, n_estimators=1, presort='auto',
    random_state=0, subsample=1.0, verbose=0, warm_start=False)
```

Bias squared: 2206.91, Variance: 0.00, Total error: 2206.91

```
Out[11]: GradientBoostingClassifier(criterion='friedman_mse', init=None,
    learning_rate=0.1, loss='deviance', max_depth=3,
    max_features=None, max_leaf_nodes=None,
    min_impurity_decrease=0.0, min_impurity_split=None,
    min_samples_leaf=1, min_samples_split=2,
    min_weight_fraction_leaf=0.0, n_estimators=2, presort='auto',
    random_state=0, subsample=1.0, verbose=0, warm_start=False)
```

```
Out[11]: GradientBoostingClassifier(criterion='friedman_mse', init=None,
    learning_rate=0.1, loss='deviance', max_depth=3,
    max_features=None, max_leaf_nodes=None,
    min_impurity_decrease=0.0, min_impurity_split=None,
    min_samples_leaf=1, min_samples_split=2,
    min_weight_fraction_leaf=0.0, n_estimators=2, presort='auto',
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Out[11]: GradientBoostingClassifier(criterion='friedman_mse', init=None,
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    min_weight_fraction_leaf=0.0, n_estimators=2, presort='auto',
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    min_samples_leaf=1, min_samples_split=2,
    min_weight_fraction_leaf=0.0, n_estimators=2, presort='auto',
    random_state=0, subsample=1.0, verbose=0, warm_start=False)

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    min_weight_fraction_leaf=0.0, n_estimators=2, presort='auto',
    random_state=0, subsample=1.0, verbose=0, warm_start=False)

Out[11]: GradientBoostingClassifier(criterion='friedman_mse', init=None,
    learning_rate=0.1, loss='deviance', max_depth=3,
```

```
max_features=None, max_leaf_nodes=None,
min_impurity_decrease=0.0, min_impurity_split=None,
min_samples_leaf=1, min_samples_split=2,
min_weight_fraction_leaf=0.0, n_estimators=2, presort='auto',
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min_impurity_decrease=0.0, min_impurity_split=None,
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```

```
min_samples_leaf=1, min_samples_split=2,  
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min_samples_leaf=1, min_samples_split=2,
```

```
min_weight_fraction_leaf=0.0, n_estimators=2, presort='auto',
random_state=0, subsample=1.0, verbose=0, warm_start=False)
```

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Out[11]: GradientBoostingClassifier(criterion='friedman_mse', init=None,
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Out[11]: GradientBoostingClassifier(criterion='friedman_mse', init=None,
    learning_rate=0.1, loss='deviance', max_depth=3,
```

```
max_features=None, max_leaf_nodes=None,
min_impurity_decrease=0.0, min_impurity_split=None,
min_samples_leaf=1, min_samples_split=2,
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Out[11]: GradientBoostingClassifier(criterion='friedman_mse', init=None,
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min_samples_leaf=1, min_samples_split=2,
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random_state=0, subsample=1.0, verbose=0, warm_start=False)
```

```
Out[11]: GradientBoostingClassifier(criterion='friedman_mse', init=None,
learning_rate=0.1, loss='deviance', max_depth=3,
max_features=None, max_leaf_nodes=None,
min_impurity_decrease=0.0, min_impurity_split=None,
min_samples_leaf=1, min_samples_split=2,
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```

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```

Bias squared: 2206.70, Variance: 0.00, Total error: 2206.70

```
Out[11]: GradientBoostingClassifier(criterion='friedman_mse', init=None,
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    random_state=0, subsample=1.0, verbose=0, warm_start=False)

Out[11]: GradientBoostingClassifier(criterion='friedman_mse', init=None,
    learning_rate=0.1, loss='deviance', max_depth=3,
```



```
max_features=None, max_leaf_nodes=None,
min_impurity_decrease=0.0, min_impurity_split=None,
min_samples_leaf=1, min_samples_split=2,
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min_weight_fraction_leaf=0.0, n_estimators=4, presort='auto',
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    random_state=0, subsample=1.0, verbose=0, warm_start=False)

Out[11]: GradientBoostingClassifier(criterion='friedman_mse', init=None,
    learning_rate=0.1, loss='deviance', max_depth=3,
```

```
max_features=None, max_leaf_nodes=None,
min_impurity_decrease=0.0, min_impurity_split=None,
min_samples_leaf=1, min_samples_split=2,
min_weight_fraction_leaf=0.0, n_estimators=4, presort='auto',
random_state=0, subsample=1.0, verbose=0, warm_start=False)
```

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Out[11]: GradientBoostingClassifier(criterion='friedman_mse', init=None,
learning_rate=0.1, loss='deviance', max_depth=3,
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min_impurity_decrease=0.0, min_impurity_split=None,  
min_samples_leaf=1, min_samples_split=2,  
min_weight_fraction_leaf=0.0, n_estimators=4, presort='auto',  
random_state=0, subsample=1.0, verbose=0, warm_start=False)
```

```
Out[11]: GradientBoostingClassifier(criterion='friedman_mse', init=None,  
learning_rate=0.1, loss='deviance', max_depth=3,  
max_features=None, max_leaf_nodes=None,  
min_impurity_decrease=0.0, min_impurity_split=None,  
min_samples_leaf=1, min_samples_split=2,
```

```
min_weight_fraction_leaf=0.0, n_estimators=4, presort='auto',
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    learning_rate=0.1, loss='deviance', max_depth=3,
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max_features=None, max_leaf_nodes=None,  
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```

Bias squared: 1341.48, Variance: 65.76, Total error: 1407.24

```
Out[11]: GradientBoostingClassifier(criterion='friedman_mse', init=None,  
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min_samples_leaf=1, min_samples_split=2,  
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```

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Out[11]: GradientBoostingClassifier(criterion='friedman_mse', init=None,  
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    learning_rate=0.1, loss='deviance', max_depth=3,
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max_features=None, max_leaf_nodes=None,
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min_samples_leaf=1, min_samples_split=2,
min_weight_fraction_leaf=0.0, n_estimators=8, presort='auto',
random_state=0, subsample=1.0, verbose=0, warm_start=False)
```

```
Out[11]: GradientBoostingClassifier(criterion='friedman_mse', init=None,
learning_rate=0.1, loss='deviance', max_depth=3,
max_features=None, max_leaf_nodes=None,
min_impurity_decrease=0.0, min_impurity_split=None,
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```

Bias squared: 1187.55, Variance: 61.29, Total error: 1248.84

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Bias squared: 968.76, Variance: 75.58, Total error: 1044.34

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presort='auto', random_state=0, subsample=1.0, verbose=0,
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Out[11]: GradientBoostingClassifier(criterion='friedman_mse', init=None,
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```

Bias squared: 855.65, Variance: 74.04, Total error: 929.69

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    min_impurity_decrease=0.0, min_impurity_split=None,
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Out[11]: GradientBoostingClassifier(criterion='friedman_mse', init=None,
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```

Bias squared: 770.23, Variance: 70.82, Total error: 841.05

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min_impurity_decrease=0.0, min_impurity_split=None,
min_samples_leaf=1, min_samples_split=2,
min_weight_fraction_leaf=0.0, n_estimators=128,
```

```
presort='auto', random_state=0, subsample=1.0, verbose=0,
warm_start=False)
```

```
Out[11]: GradientBoostingClassifier(criterion='friedman_mse', init=None,
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```

Bias squared: 715.12, Variance: 77.95, Total error: 793.07

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min_samples_leaf=1, min_samples_split=2,
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Bias squared: 675.61, Variance: 91.53, Total error: 767.14

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    min_weight_fraction_leaf=0.0, n_estimators=512,
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Out[11]: GradientBoostingClassifier(criterion='friedman_mse', init=None,
    learning_rate=0.1, loss='deviance', max_depth=3,
    max_features=None, max_leaf_nodes=None,
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    presort='auto', random_state=0, subsample=1.0, verbose=0,
    warm_start=False)
```

Bias squared: 636.53, Variance: 112.22, Total error: 748.75

```
Out[11]: GradientBoostingClassifier(criterion='friedman_mse', init=None,
    learning_rate=0.1, loss='deviance', max_depth=3,
    max_features=None, max_leaf_nodes=None,
    min_impurity_decrease=0.0, min_impurity_split=None,
    min_samples_leaf=1, min_samples_split=2,
    min_weight_fraction_leaf=0.0, n_estimators=1024,
    presort='auto', random_state=0, subsample=1.0, verbose=0,
    warm_start=False)
```

```
Out[11]: GradientBoostingClassifier(criterion='friedman_mse', init=None,
    learning_rate=0.1, loss='deviance', max_depth=3,
```

```
max_features=None, max_leaf_nodes=None,
min_impurity_decrease=0.0, min_impurity_split=None,
min_samples_leaf=1, min_samples_split=2,
min_weight_fraction_leaf=0.0, n_estimators=1024,
presort='auto', random_state=0, subsample=1.0, verbose=0,
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```

Bias squared: 611.76, Variance: 135.73, Total error: 747.49

```

In [12]: print(bias_gbrt)
         print(variance_gbrt)
         print(error_gbrt)

plt.plot(bias_gbrt, label = "Bias Squared")
plt.plot(variance_gbrt, label = "Variance", linestyle='-')
plt.plot(error_gbrt, color='g', label="Total Error", linestyle='-')
plt.xticks([0,1,2,3,4,5,6,7,8,9,10], treesrs)
plt.xlabel("Number of Trees")

plt.legend(bbox_to_anchor=(0., 1.02, 1., .102), loc=3, ncol=2, mode="expand", borderaxes=1)

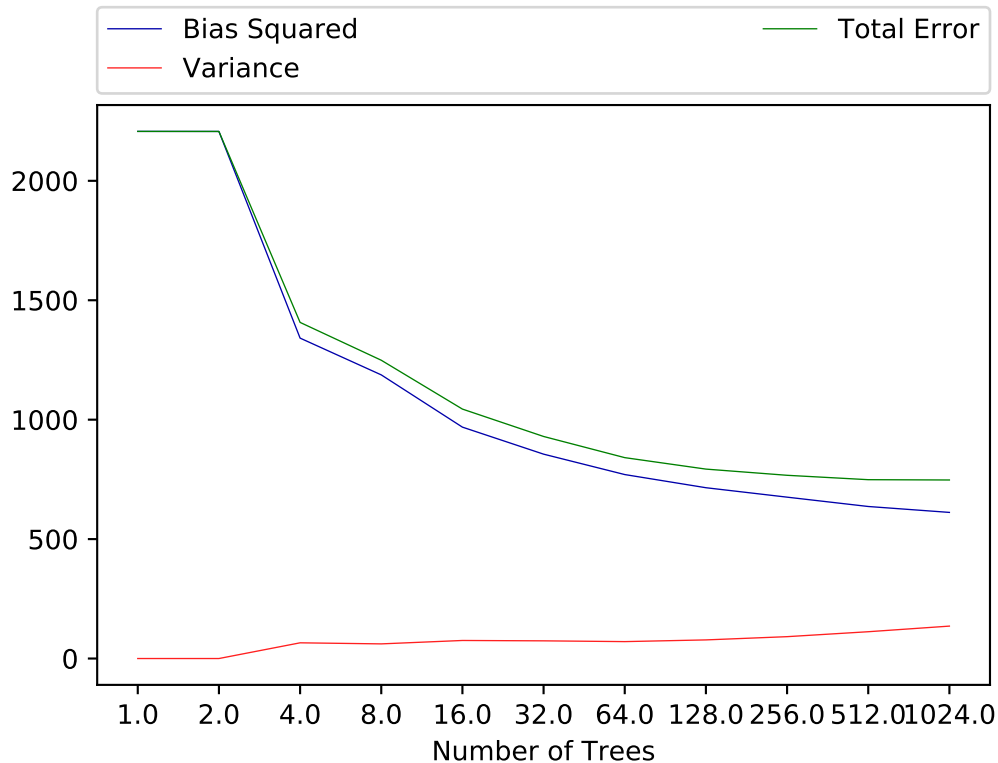
[2206.9099999999094, 2206.699999999907, 1341.4757829835203, 1187.5455013354745, 968.7640916177007,
0.0, 0.0, 65.7642170164546, 61.29449866450801, 75.5759083822976, 74.04283899431623, 70.82239100000001,
[2206.9099999999094, 2206.699999999907, 1407.2399999999625, 1248.83999999997, 1044.3399999999999]

Out[12]: [<matplotlib.lines.Line2D at 0x24358411c18>]
Out[12]: [<matplotlib.lines.Line2D at 0x24358c75198>]
Out[12]: [<matplotlib.lines.Line2D at 0x24356be8198>]
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<matplotlib.axis.XTick at 0x24356bfb710>,
<matplotlib.axis.XTick at 0x24356bfbd68>],
<a list of 11 Text xticklabel objects>)

Out[12]: Text(0.5,0,'Number of Trees')

Out[12]: <matplotlib.legend.Legend at 0x24356bfbc88>

```



Answer to 1. As can be gathered from the plot, the total error for the random forest ensemble model keeps decreasing with the number of tree increasing. The start of the curves are interesting, with bias starting off low, rising, then decreasing and then rising again above 8 trees. This likely is a sign of underfitting with the number of trees anywhere below 16. The theory behind random forest ensemble is taking a vast amount of weak models that together make a strong model. This, however, needs scale and an ensemble of 16 or under trees will not cumulate in a strong model. Although it is a bit tricky to assess the slopes of the curves near the end, it seems the decrease in variance with 512 or above number of trees is offset fully by an increase in bias. This is a sign of overfitting. Gradient boosting works differently from random forest. Whereas RF decreases the total error by decreasing variance, GB starts off with low variance and decreases the total error by bringing down bias. Because after each iteration, the newly created tree focusses on getting the predictions right that the previous one got wrong. This also means that the first few iterations aren't very accurate as it hasn't had the time to learn from the previous mistakes, leading to underfitting. This seems very evident with number of trees at 16 and below. This method of learning also means that when the focus stays on the mistakes of the trees, the model will eventually overfit as it gives excessive weight to datapoints that are difficult to predict, and that might be outliers that preferably are ignored. Even though it is again somewhat difficult to assess, the curve of the variance seems to significantly increase from number of trees at 256 and onwards.

2 . A *validation curve* can help you understand when a model starts under- or overfitting. It plots both training and test set error as you change certain characteristics of your model, e.g. one or more hyperparameters. Build validation curves for gradient boosting, evaluated using AUROC, by varying the number of iterations between 1 and 500. In addition, use at least two values for the learning rate (e.g. 0.1 and 1), and tree depth (e.g. 1 and 4). This will yield at least

4 curves. Interpret the results and provide a clear explanation for the results. When is the model over- or underfitting? Discuss the effect of the different combinations learning rate and tree depth and provide a clear explanation. - While scikit-learn has a `validation_curve` function, we'll use a modified version (below) that provides a lot more detail and can be used to study more than one hyperparameter. You can use a default train-test split.

```
In [13]: # Plots validation curves for every classifier in clfs.
# Also indicates the optimal result by a vertical line
# Uses 1-AUROC, so lower is better
from sklearn.metrics import roc_auc_score
from sklearn.ensemble import GradientBoostingClassifier
from sklearn.model_selection import train_test_split

gbrt1 = GradientBoostingClassifier(n_estimators=500, random_state=0, learning_rate=0.1)
gbrt2 = GradientBoostingClassifier(n_estimators=500, random_state=0, learning_rate=1,
gbrt3 = GradientBoostingClassifier(n_estimators=500, random_state=0, learning_rate=0.01)
gbrt4 = GradientBoostingClassifier(n_estimators=500, random_state=0, learning_rate=1,

clfs = [gbrt1, gbrt2, gbrt3, gbrt4]

X_train, X_test, y_train, y_test = train_test_split(X_new, y_new, random_state=0)

gbrt1_fit = gbrt1.fit(X_train, y_train)
gbrt2_fit = gbrt2.fit(X_train, y_train)
gbrt3_fit = gbrt3.fit(X_train, y_train)
gbrt4_fit = gbrt4.fit(X_train, y_train)

def validation_curve(clfs, X_test, y_test, X_train, y_train):
    for n,clf in enumerate(clfs):
        test_score = np.empty(len(clf.estimators_))
        train_score = np.empty(len(clf.estimators_))

        print(clf.estimators_)

        for i, pred in enumerate(clf.staged_decision_function(X_test)):
            test_score[i] = 1-roc_auc_score(y_test, pred)

        for i, pred in enumerate(clf.staged_decision_function(X_train)):
            train_score[i] = 1-roc_auc_score(y_train, pred)

        best_iter = np.argmin(test_score)
        learn = clf.get_params()['learning_rate']
        depth = clf.get_params()['max_depth']
        test_line = plt.plot(test_score,
                             label='learn=%.1f depth=%i (%.2f)%(learn,depth,
                             test_score[best_iter])

        colour = test_line[-1].get_color()
        plt.plot(train_score, '--', color=colour)
```

```
plt.xlabel("Number of boosting iterations")
plt.ylabel("1 - area under ROC")
plt.axvline(x=best_iter, color=colour)
```

```
plt.legend(loc='best')
```

```
validation_curve(clfs, X_test, y_test, X_train, y_train)
```

```
[[DecisionTreeRegressor(criterion='friedman_mse', max_depth=1,
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```

```

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```

```

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```
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```

min_weight_fraction_leaf=0.0, presort='auto',
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max_features=None, max_leaf_nodes=None,
min_impurity_decrease=0.0, min_impurity_split=None,
min_samples_leaf=1, min_samples_split=2,
min_weight_fraction_leaf=0.0, presort='auto',
random_state=<mtrand.RandomState object at 0x0000024356BF98B8>,
splitter='best')]
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splitter='best')]
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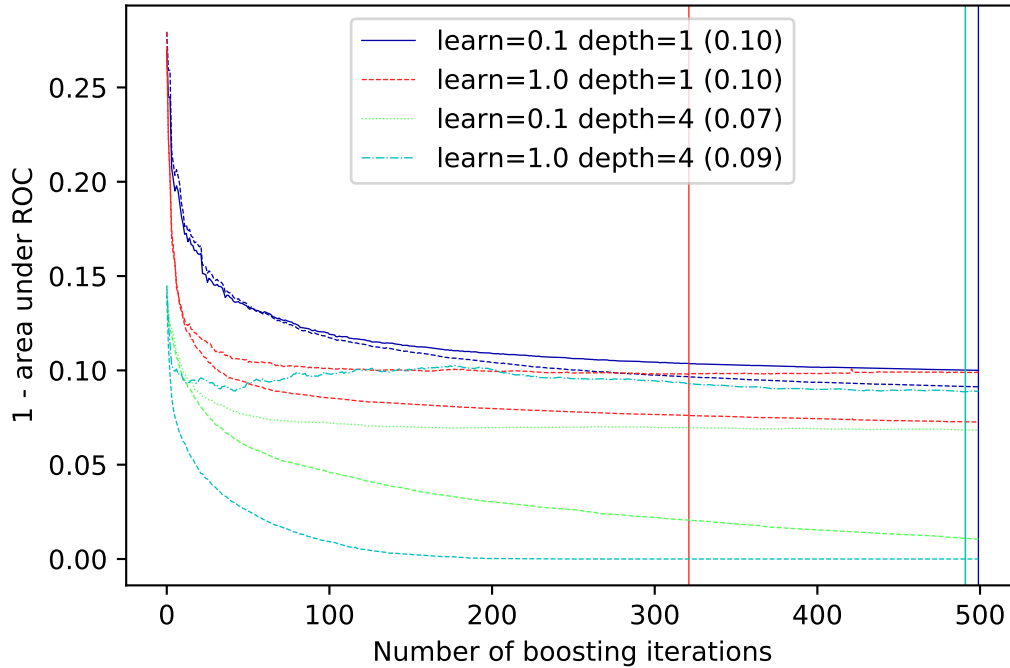
```

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max_features=None, max_leaf_nodes=None,
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random_state=<trand.RandomState object at 0x0000024356E86900>,
splitter='best')]
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random_state=<trand.RandomState object at 0x0000024356E86900>,
splitter='best')]

```

```
[DecisionTreeRegressor(criterion='friedman_mse', max_depth=4,
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```



Answer to 2 . As can be seen in the figure, while a model with a learning rate of 1 and a depth of 4 gets the smallest error in total, there is a very large difference between training and test set performance. The performance on the training set is very good, while the performance on the test set is very close to the performance of other models, which indicates overfitting on the training set. A model with a learning rate of 0.1 and a depth of shows the exact opposite, as it generally has the largest error of all four models, but has almost equal performance on train and test set. In this case, the model might be slightly underfitting. Looking at the results, they are quite logical considering the model parameters. Both a higher learning rate and a greater depth provide smaller errors, which makes sense as the model will try to fit the data more strongly and has more depth to try to do so. Also, the higher both values, the larger the difference between train and test set will be, as the model starts overfitting. To create a good model, a trade-off between learning rate and depth must be made to achieve good results without overfitting too much.