Assignment 3

Problem statement (Feature Engineering: Concrete Strength Prediction)

Goal

Using the data available in file concrete_data.xls. Apply feature engineering methods to obtain 85% to 95% accuracy (tolerance limit 95% of the time (confidence level).

Resources Available

The data for this project is available in file [https://archive.ics.uci.edu/ml/machine-learning-databases/concrete/compressive/ (https://archive.ics.uci.edu/ml/machine-learning-databases/concrete/compressive/)](https://archive.ics.uci.edu/ml/machine-learning-databases/concrete/compressive/)

Variable Information:

Given is the variable name, variable type, the measurement unit and a brief description. The concrete compressive strength is the regression problem. The order of this listing corresponds to the order of numerals along the rows of the database.

Name -- Data Type -- Measurement -- Description

- Cement (component 1) -- quantitative -- kg in a m3 mixture -- Input Variable
- Blast Furnace Slag (component 2) -- quantitative -- kg in a m3 mixture -- Input Variable
- Fly Ash (component 3) -- quantitative -- kg in a m3 mixture -- Input Variable
- Water (component 4) -- quantitative -- kg in a m3 mixture -- Input Variable
- Superplasticizer (component 5) -- quantitative -- kg in a m3 mixture -- Input Variable
- Coarse Aggregate (component 6) -- quantitative -- kg in a m3 mixture -- Input Variable
- Fine Aggregate (component 7) -- quantitative -- kg in a m3 mixture -- Input Variable
- Age -- quantitative -- Day (1~365) -- Input Variable
- **Concrete compressive strength -- quantitative -- MPa -- Output Variable**

In [25]:
```
import numpy as np
import pandas as pd

import matplotlib.pyplot as plt
import itertools
import seaborn as sns

import scipy.stats as st

from sklearn.model_selection import train_test_split


from sklearn.linear_model import LinearRegression, Ridge, Lasso
from sklearn.tree import DecisionTreeRegressor, ExtraTreeRegressor
from sklearn.ensemble import RandomForestRegressor,GradientBoostingRegressor, AdaBoostRegressor, ExtraTrees
Regressor
from sklearn.preprocessing import StandardScaler, RobustScaler, QuantileTransformer, OneHotEncoder
from sklearn.compose import ColumnTransformer
from sklearn.base import BaseEstimator
from sklearn.feature_selection import SelectKBest, f_regression
from sklearn.decomposition import PCA
from sklearn.pipeline import Pipeline
from sklearn.model_selection import GridSearchCV, cross_val_score
from sklearn.metrics import r2_score, mean_squared_error
from sklearn.utils import resample

from pprint import pprint
from time import time
import warnings
warnings.filterwarnings('ignore')

df = pd.read_csv ("concrete.csv")

print('--df.info()--')
print(df.info())
print("  ")
print('--df.columns--')
print(df.columns)
```

```
--df.info()--
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 1030 entries, 0 to 1029
Data columns (total 9 columns):
cement          1030 non-null float64
slag            1030 non-null float64
ash             1030 non-null float64
water           1030 non-null float64
superplastic    1030 non-null float64
coarseagg       1030 non-null float64
fineagg         1030 non-null float64
age             1030 non-null int64
strength        1030 non-null float64
dtypes: float64(8), int64(1)
memory usage: 72.5 KB
None

--df.columns--
Index(['cement', 'slag', 'ash', 'water', 'superplastic', 'coarseagg',
       'fineagg', 'age', 'strength'],
      dtype='object')
```

In [26]:
```
df.head()
```

Out[26]:

	cement	slag	ash	water	superplastic	coarseagg	fineagg	age	strength
0	141.3	212.0	0.0	203.5	0.0	971.8	748.5	28	29.89
1	168.9	42.2	124.3	158.3	10.8	1080.8	796.2	14	23.51
2	250.0	0.0	95.7	187.4	5.5	956.9	861.2	28	29.22
3	266.0	114.0	0.0	228.0	0.0	932.0	670.0	28	45.85
4	154.8	183.4	0.0	193.3	9.1	1047.4	696.7	28	18.29

In [27]:
```
df.describe().T
```

Out[27]:

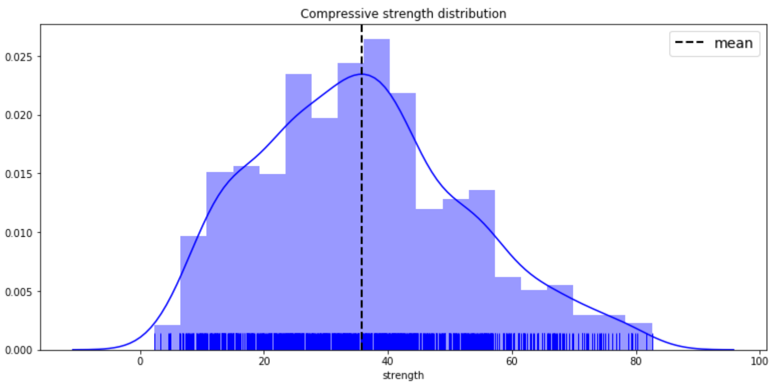
	count	mean	std	min	25%	50%	75%	max
cement	1030.0	281.167864	104.506364	102.00	192.375	272.900	350.000	540.0
slag	1030.0	73.895825	86.279342	0.00	0.000	22.000	142.950	359.4
ash	1030.0	54.188350	63.997004	0.00	0.000	0.000	118.300	200.1
water	1030.0	181.567282	21.354219	121.80	164.900	185.000	192.000	247.0
superplastic	1030.0	6.204660	5.973841	0.00	0.000	6.400	10.200	32.2
coarseagg	1030.0	972.918932	77.753954	801.00	932.000	968.000	1029.400	1145.0
fineagg	1030.0	773.580485	80.175980	594.00	730.950	779.500	824.000	992.6
age	1030.0	45.662136	63.169912	1.00	7.000	28.000	56.000	365.0
strength	1030.0	35.817961	16.705742	2.33	23.710	34.445	46.135	82.6

In [28]:
```
df.apply(lambda x: sum(x.isnull()))
```

Out[28]:
```
cement          0
slag            0
ash             0
water           0
superplastic    0
coarseagg       0
fineagg         0
age             0
strength        0
dtype: int64
```

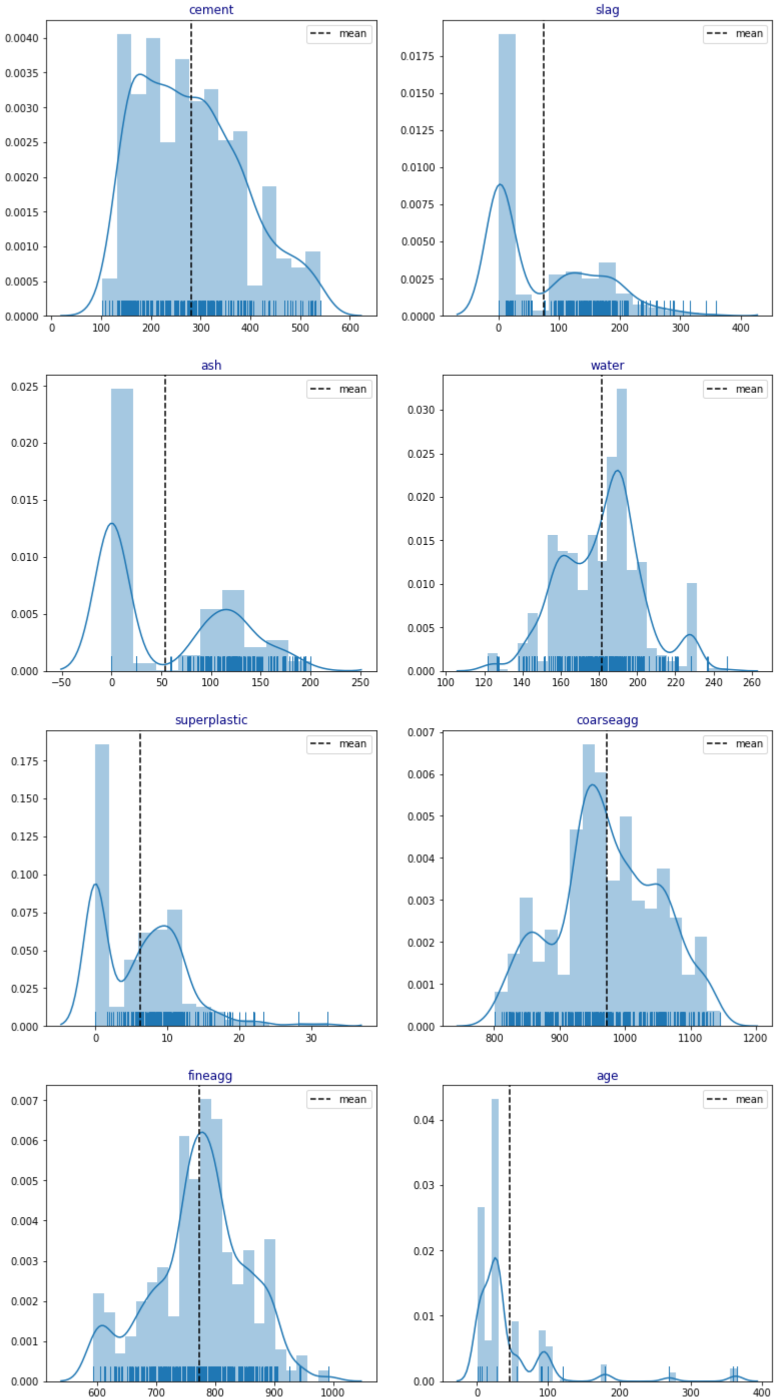
- No missing data found

In [29]:
```
plt.figure(figsize=(13,6))
sns.distplot(df["strength"],color="b",rug=True)
plt.axvline(df["strength"].mean(),
            linestyle="dashed",color="k",
            label='mean',linewidth=2)
plt.legend(loc="best",prop={"size":14})
plt.title("Compressive strength distribution")
plt.show()
```



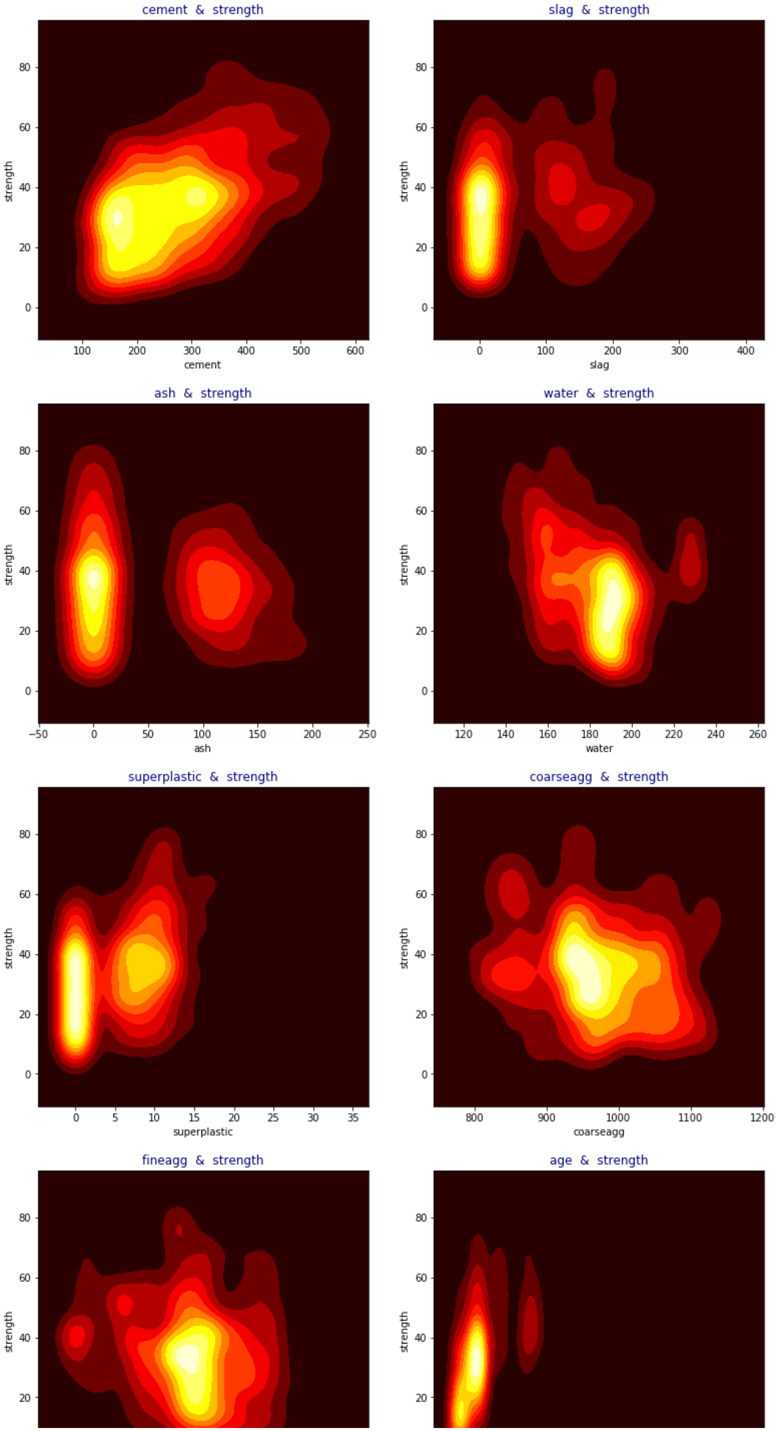
- The Compressive Streng is normal distributed

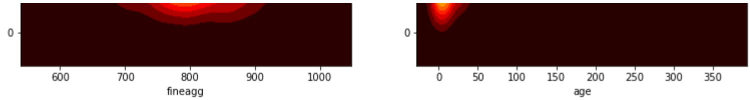
In [30]:
```
cols = [i for i in df.columns if i not in 'strength']
length = len(cols)
cs = ["b","r","g","c","m","k","lime","c"]
fig = plt.figure(figsize=(13,25))

for i,j,k in itertools.zip_longest(cols,range(length),cs):
    plt.subplot(4,2,j+1)
    ax = sns.distplot(df[i],rug=True)
    ax.set_facecolor("w")
    plt.axvline(df[i].mean(),linestyle="dashed",label="mean",color="k")
    plt.legend(loc="best")
    plt.title(i,color="navy")
    plt.xlabel("")
```


cement
mean
slag
mean
ash
mean
water
mean
superplastic
mean
coarseagg
mean
fineagg
mean
age
mean

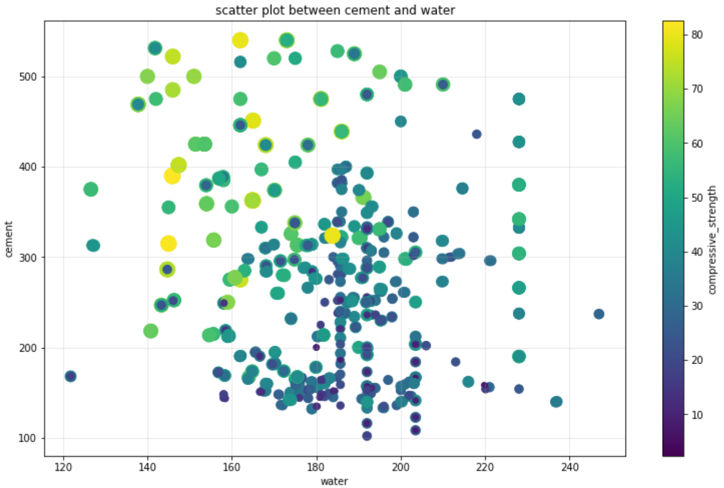
- Several features are skew to the left of the distribution (slag, ash, superplastic and age)

In [31]:
```
cols = [i for i in df.columns if i not in 'strength']
length = len(cols)

plt.figure(figsize=(13,27))
for i,j in itertools.zip_longest(cols,range(length)):
    plt.subplot(4,2,j+1)
    sns.kdeplot(df[i],
                df["strength"],
                cmap="hot",
                shade=True)
    plt.title(i+"  &  strength",color="navy")
```

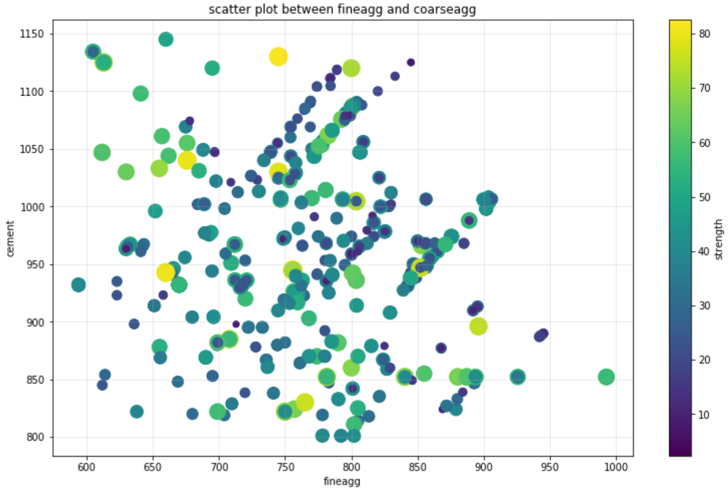

cement & strength
strength
cement
slag & strength
strength
slag
ash & strength
strength
ash
water & strength
strength
water
superplastic & strength
strength
superplastic
coarseagg & strength
strength
coarseagg
fineagg & strength
strength
age & strength
strength



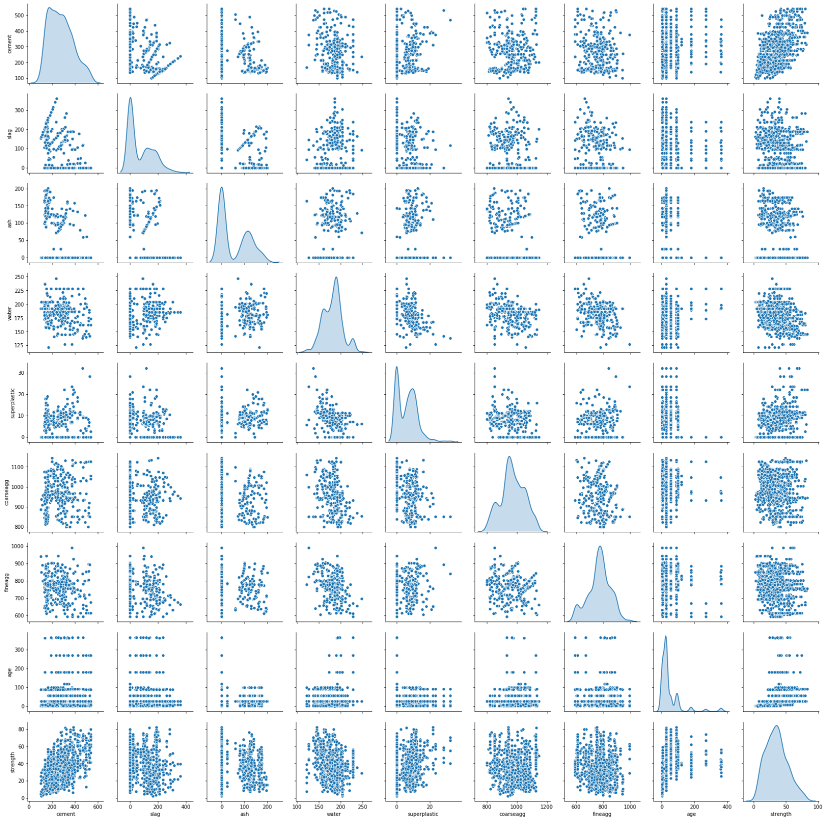
In [32]:
```python
fig = plt.figure(figsize=(13,8))
ax = fig.add_subplot(111)
plt.scatter(df["water"],df["cement"],
            c=df["strength"],s=df["strength"]*3,
            linewidth=1)
ax.set_facecolor("w")
ax.set_xlabel("water")
ax.set_ylabel("cement")
lab = plt.colorbar()
lab.set_label("compressive_strength")
plt.title("scatter plot between cement and water")
plt.grid(True,alpha=.3)
plt.show()
```



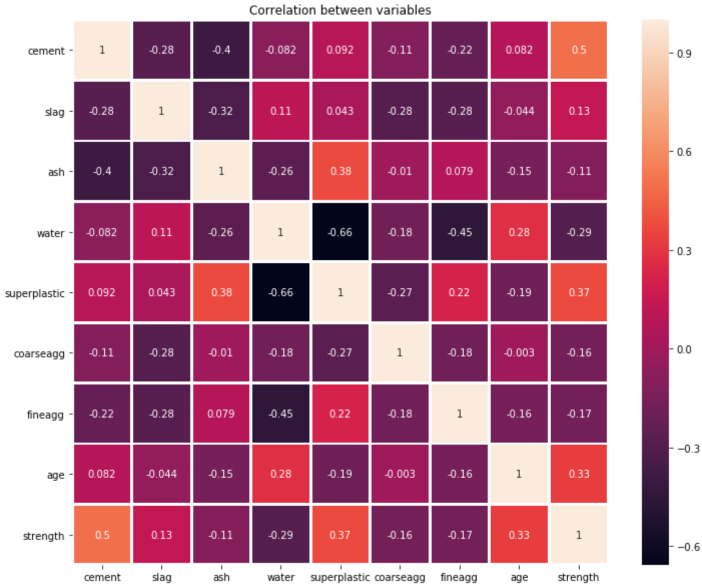
In [33]:
```
fig = plt.figure(figsize=(13,8))
ax = fig.add_subplot(111)
plt.scatter(df["fineagg"],df["coarseagg"],
            c=df["strength"],s=df["strength"]*4,
            linewidth=1)
ax.set_facecolor("w")
ax.set_xlabel("fineagg")
ax.set_ylabel("cement")
lab = plt.colorbar()
lab.set_label("strength")
plt.title("scatter plot between fineagg and coarseagg")
plt.grid(True,alpha=.3)
plt.show()
```



In [36]:
```
sns.pairplot(df, diag_kind="kde")
plt.show()
```



In [37]:
```
cor = df.corr()

plt.figure(figsize=(12,10))

sns.heatmap(cor,annot=True,linewidth=2)
plt.title("Correlation between variables")
plt.show()
```



- **cement, water, age and superplastic** are highly correlated to **strength**
- **superplastic and ash** are highly correlated
- **age and water** both are highly correlated

Data Cleaning

Identify the outlier

By using inter quarter range (IQR) method to detect and remove the outlier

Using IQR method is better than z-score approach, because most of the concrete data is skewed to left as show in the plots.

In [38]:
```
Q1 = df.quantile(0.25)
Q3 = df.quantile(0.75)
IQR = Q3 - Q1

df_out = df[~((df < (Q1 - 1.5 * IQR)) |(df > (Q3 + 1.5 * IQR))).any(axis=1)]
df_out.shape
```

Out[38]: (941, 9)

Spliting Data

Split By ratio of 70:30

In [39]:
```
X_train, X_test, y_train, y_test = train_test_split( df_out.loc[:, df_out.columns != 'strength'], df_out["s
trength"], test_size=0.3, random_state = 0)
```

Modelling

Modelling with Pipeline and GridSearchCV

Preprocessing Pipeline

ColumnTransformer for Numeric Transformer and Categorical Transformer

- In this case study, no categorical features
- All the numeric features will be transformed by the scaler of QuantileTransformer().

In [40]:
```
numeric_features = [i for i in df_out.columns if i not in 'strength']
numeric_transformer = Pipeline(steps=[
    ('scaler',  QuantileTransformer())])

categorical_features = []
categorical_transformer = Pipeline(steps=[
    ('onehot', OneHotEncoder(handle_unknown='ignore'))])

preprocessor = ColumnTransformer(
    transformers=[
        ('num', numeric_transformer, numeric_features),
        ('cat', categorical_transformer, categorical_features)])
```

Modelling

Preparing the pipeline that streamline the whole process from preprocessing to testing the model

1. Preprocessor is pre-defined as aboved, which is **QuantileTransformer()**
2. To improve the model by reducing the dimension, two strategy, **PCA() and SelectKBest(f_regression)** will be decided
3. Regressor will also be decided from **Ridge(), Lasso(), RandomForestRegressor(), GradientBoostingRegressor(), ExtraTreesRegressor(), and DecisionTreeRegressor()**.
4. All the **hyperparameter ranges** also is defined.
5. All the above step will be streamlined by **pipeline**.
6. **GridSearchCV** is used to choose the best estimator amongst all the combination.

Evaluation for the scoring

1. **"neg_means_square_error"** is chosen for this case. Higher number of "neg_means_square_error" is better, or can be interpreted as value nearer to 0 is better.

In [41]:
```
class DummyEstimator(BaseEstimator):
    def fit(self): pass
    def score(self): pass

# Create a pipeline
pipe = Pipeline([('preprocessor', preprocessor),
                 ('reduce_dim', PCA()),
                 ('regressor', DummyEstimator())]) # Placeholder Estimator

#prepareing for the hyperparemeter to be tuned
n_features_to_test = np.arange(1, 9)
alpha_to_test = 2.0**np.arange(-6, +6)
linear_regressor = [Ridge(),
                    Lasso()]

ensemble_regressor = [RandomForestRegressor(bootstrap=True, oob_score=True, n_jobs=-1),
                      GradientBoostingRegressor(),
                      ExtraTreesRegressor(bootstrap=True, oob_score =True, n_jobs=-1)]

tree_regressor = [DecisionTreeRegressor(),
                  ExtraTreeRegressor() ]

params = [
        {'reduce_dim': [PCA()],
         'reduce_dim__n_components': n_features_to_test,
         'regressor': linear_regressor,
         'regressor__alpha': alpha_to_test,
         "regressor__random_state" : [1]},

        {'reduce_dim': [PCA()],
         'reduce_dim__n_components': n_features_to_test,
         "regressor": ensemble_regressor,
         "regressor__random_state" : [1],
         "regressor__n_estimators" : [10,50,100],
         "regressor__max_depth": [3, 5, 10, None],
         "regressor__min_samples_split": [2, 5, 10, 15]},

        {'reduce_dim': [PCA()],
         'reduce_dim__n_components': n_features_to_test,
         "regressor": tree_regressor,
         "regressor__random_state" : [1],
         "regressor__max_depth": [3, 5, 10, None],
         "regressor__min_samples_split": [2, 5, 10, 15]},

        {'reduce_dim': [SelectKBest(f_regression)],
         'reduce_dim__k': n_features_to_test,
         'regressor': linear_regressor,
         'regressor__alpha': alpha_to_test,
         "regressor__random_state" : [1]},

        {'reduce_dim': [SelectKBest(f_regression)],
         'reduce_dim__k': n_features_to_test,
         "regressor": ensemble_regressor,
         "regressor__random_state" : [1],
         "regressor__n_estimators" : [10,50,100],
         "regressor__max_depth": [3, 5, 10, None],
         "regressor__min_samples_split": [2, 5, 10, 15]},

        {'reduce_dim': [SelectKBest(f_regression)],
         'reduce_dim__k': n_features_to_test,
         "regressor": tree_regressor,
         "regressor__random_state" : [1],
         "regressor__max_depth": [3, 5, 10, None],
         "regressor__min_samples_split": [2, 5, 10, 15]}

        ]


gridsearch = GridSearchCV(pipe, params, scoring='neg_mean_squared_error', cv=5, n_jobs=-1, verbose=2)

print("pipeline:", [name for name, _ in pipe.steps])
print("parameters:")
pprint(params)
t0 = time()
gridsearch.fit(X_train, y_train)
print("done in %0.3fs" % (time() - t0))
print()
print('Negative MSE score is: ', gridsearch.score(X_test, y_test))
```

```
pipeline: ['preprocessor', 'reduce_dim', 'regressor']
parameters:
[{'reduce_dim': [PCA(copy=True, iterated_power='auto', n_components=None, random_state=None,
  svd_solver='auto', tol=0.0, whiten=False)],
  'reduce_dim__n_components': array([1, 2, 3, 4, 5, 6, 7, 8]),
  'regressor': [Ridge(alpha=1.0, copy_X=True, fit_intercept=True, max_iter=None,
   normalize=False, random_state=None, solver='auto', tol=0.001),
                Lasso(alpha=1.0, copy_X=True, fit_intercept=True, max_iter=1000,
   normalize=False, positive=False, precompute=False, random_state=None,
   selection='cyclic', tol=0.0001, warm_start=False)],
  'regressor__alpha': array([1.5625e-02, 3.1250e-02, 6.2500e-02, 1.2500e-01, 2.5000e-01,
       5.0000e-01, 1.0000e+00, 2.0000e+00, 4.0000e+00, 8.0000e+00,
       1.6000e+01, 3.2000e+01]),
  'regressor__random_state': [1]},
 {'reduce_dim': [PCA(copy=True, iterated_power='auto', n_components=None, random_state=None,
  svd_solver='auto', tol=0.0, whiten=False)],
  'reduce_dim__n_components': array([1, 2, 3, 4, 5, 6, 7, 8]),
  'regressor': [RandomForestRegressor(bootstrap=True, criterion='mse', 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='warn', n_jobs=-1,
           oob_score=True, random_state=None, verbose=0, warm_start=False),
                GradientBoostingRegressor(alpha=0.9, criterion='friedman_mse', init=None,
             learning_rate=0.1, loss='ls', 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=100, n_iter_no_change=None, presort='auto',
             random_state=None, subsample=1.0, tol=0.0001,
             validation_fraction=0.1, verbose=0, warm_start=False),
                ExtraTreesRegressor(bootstrap=True, criterion='mse', 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='warn', n_jobs=-1,
          oob_score=True, random_state=None, verbose=0, warm_start=False)],
  'regressor__max_depth': [3, 5, 10, None],
  'regressor__min_samples_split': [2, 5, 10, 15],
  'regressor__n_estimators': [10, 50, 100],
  'regressor__random_state': [1]},
 {'reduce_dim': [PCA(copy=True, iterated_power='auto', n_components=None, random_state=None,
  svd_solver='auto', tol=0.0, whiten=False)],
  'reduce_dim__n_components': array([1, 2, 3, 4, 5, 6, 7, 8]),
  'regressor': [DecisionTreeRegressor(criterion='mse', max_depth=None, 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=False, random_state=None, splitter='best'),
                ExtraTreeRegressor(criterion='mse', 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, random_state=None,
          splitter='random')],
  'regressor__max_depth': [3, 5, 10, None],
  'regressor__min_samples_split': [2, 5, 10, 15],
  'regressor__random_state': [1]},
 {'reduce_dim': [SelectKBest(k=10, score_func=<function f_regression at 0x00000220832B07B8>)],
  'reduce_dim__k': array([1, 2, 3, 4, 5, 6, 7, 8]),
  'regressor': [Ridge(alpha=1.0, copy_X=True, fit_intercept=True, max_iter=None,
   normalize=False, random_state=None, solver='auto', tol=0.001),
                Lasso(alpha=1.0, copy_X=True, fit_intercept=True, max_iter=1000,
   normalize=False, positive=False, precompute=False, random_state=None,
   selection='cyclic', tol=0.0001, warm_start=False)],
  'regressor__alpha': array([1.5625e-02, 3.1250e-02, 6.2500e-02, 1.2500e-01, 2.5000e-01,
       5.0000e-01, 1.0000e+00, 2.0000e+00, 4.0000e+00, 8.0000e+00,
       1.6000e+01, 3.2000e+01]),
  'regressor__random_state': [1]},
 {'reduce_dim': [SelectKBest(k=10, score_func=<function f_regression at 0x00000220832B07B8>)],
  'reduce_dim__k': array([1, 2, 3, 4, 5, 6, 7, 8]),
  'regressor': [RandomForestRegressor(bootstrap=True, criterion='mse', 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='warn', n_jobs=-1,
           oob_score=True, random_state=None, verbose=0, warm_start=False),
                GradientBoostingRegressor(alpha=0.9, criterion='friedman_mse', init=None,
             learning_rate=0.1, loss='ls', 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=100, n_iter_no_change=None, presort='auto',
             random_state=None, subsample=1.0, tol=0.0001,
             validation_fraction=0.1, verbose=0, warm_start=False),
```

```
                ExtraTreesRegressor(bootstrap=True, criterion='mse', 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='warn', n_jobs=-1,
          oob_score=True, random_state=None, verbose=0, warm_start=False)],
  'regressor__max_depth': [3, 5, 10, None],
  'regressor__min_samples_split': [2, 5, 10, 15],
  'regressor__n_estimators': [10, 50, 100],
  'regressor__random_state': [1]},
 {'reduce_dim': [SelectKBest(k=10, score_func=<function f_regression at 0x00000220832B07B8>)],
  'reduce_dim__k': array([1, 2, 3, 4, 5, 6, 7, 8]),
  'regressor': [DecisionTreeRegressor(criterion='mse', max_depth=None, 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=False, random_state=None, splitter='best'),
                ExtraTreeRegressor(criterion='mse', 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, random_state=None,
          splitter='random')],
  'regressor__max_depth': [3, 5, 10, None],
  'regressor__min_samples_split': [2, 5, 10, 15],
  'regressor__random_state': [1]}]
Fitting 5 folds for each of 3200 candidates, totalling 16000 fits

[Parallel(n_jobs=-1)]: Using backend LokyBackend with 8 concurrent workers.
[Parallel(n_jobs=-1)]: Done  25 tasks      | elapsed:   22.9s
[Parallel(n_jobs=-1)]: Done 146 tasks      | elapsed:   24.8s
[Parallel(n_jobs=-1)]: Done 349 tasks      | elapsed:   28.0s
[Parallel(n_jobs=-1)]: Done 835 tasks      | elapsed:   34.5s
[Parallel(n_jobs=-1)]: Done 1325 tasks      | elapsed:   53.5s
[Parallel(n_jobs=-1)]: Done 1770 tasks      | elapsed:  1.3min
[Parallel(n_jobs=-1)]: Done 2297 tasks      | elapsed:  1.7min
[Parallel(n_jobs=-1)]: Done 2904 tasks      | elapsed:  2.3min
[Parallel(n_jobs=-1)]: Done 3593 tasks      | elapsed:  3.0min
[Parallel(n_jobs=-1)]: Done 4362 tasks      | elapsed:  3.7min
[Parallel(n_jobs=-1)]: Done 5213 tasks      | elapsed:  4.5min
[Parallel(n_jobs=-1)]: Done 6144 tasks      | elapsed:  5.5min
[Parallel(n_jobs=-1)]: Done 7487 tasks      | elapsed:  6.3min
[Parallel(n_jobs=-1)]: Done 9418 tasks      | elapsed:  7.0min
[Parallel(n_jobs=-1)]: Done 10593 tasks      | elapsed:  8.1min
[Parallel(n_jobs=-1)]: Done 11848 tasks      | elapsed:  9.2min
[Parallel(n_jobs=-1)]: Done 13185 tasks      | elapsed: 10.6min
[Parallel(n_jobs=-1)]: Done 14602 tasks      | elapsed: 12.2min
[Parallel(n_jobs=-1)]: Done 16000 out of 16000 | elapsed: 12.6min finished

done in 759.002s

Negative MSE score is:  -24.77230601825275
```

In [42]:

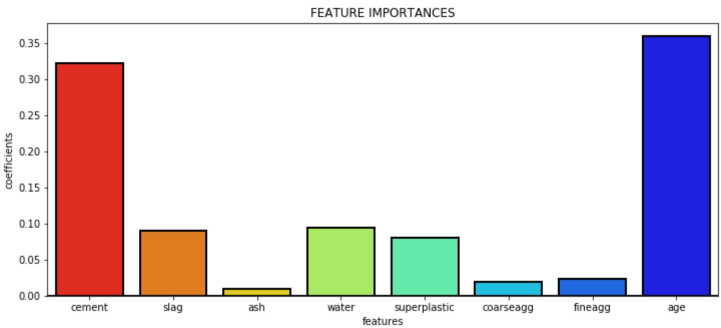
```
gridsearch.best_params_
```

Out[42]:

```
{'reduce_dim': SelectKBest(k=8, score_func=<function f_regression at 0x00000220832B07B8>),
 'reduce_dim__k': 8,
 'regressor': GradientBoostingRegressor(alpha=0.9, criterion='friedman_mse', init=None,
              learning_rate=0.1, loss='ls', max_depth=5, max_features=None,
              max_leaf_nodes=None, min_impurity_decrease=0.0,
              min_impurity_split=None, min_samples_leaf=1,
              min_samples_split=10, min_weight_fraction_leaf=0.0,
              n_estimators=100, n_iter_no_change=None, presort='auto',
              random_state=1, subsample=1.0, tol=0.0001,
              validation_fraction=0.1, verbose=0, warm_start=False),
 'regressor__max_depth': 5,
 'regressor__min_samples_split': 10,
 'regressor__n_estimators': 100,
 'regressor__random_state': 1}
```

In [43]:
```
plt.figure(figsize=(12,5))
coef = pd.DataFrame(gridsearch.best_estimator_.named_steps['regressor'].feature_importances_)
coef["feat"] = X_train.columns
ax2 = sns.barplot(coef["feat"],coef[0],palette="jet_r",
                  linewidth=2,edgecolor="k"*coef["feat"].nunique())

ax2.axhline(0,color="k",linewidth=2)
plt.ylabel("coefficients")
plt.xlabel("features")
plt.title('FEATURE IMPORTANCES')
```

Out[43]: Text(0.5, 1.0, 'FEATURE IMPORTANCES')



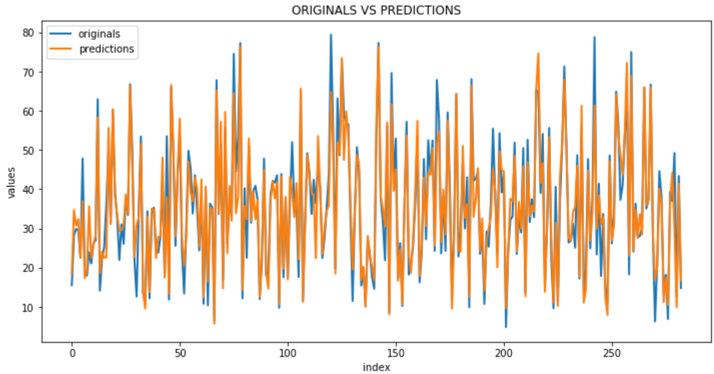
- The features importance show similarity to the correlation chart

In [44]:
```
predict = gridsearch.best_estimator_.predict(X_test)

print ("RMSE:", np.sqrt(mean_squared_error(y_test,predict)) )
print ("R2 Score",r2_score(y_test,predict))
prediction = pd.DataFrame(predict)
cross_val = cross_val_score(gridsearch.best_estimator_ ,X_train,y_train,cv=5,scoring="neg_mean_squared_erro
r")
cross_val = cross_val.ravel()

cv_mean = cross_val.mean()
cv_std = cross_val.std()

cv_rmse_mean = cv_mean
cv_rmse_std = cv_std
print ("cv-mean :", cv_rmse_mean)
print ("cv-std  :", cv_rmse_std)
```

```
RMSE: 4.97717851982955 75
R2 Score 0.9114174585277182
cv-mean : -24.80080040602669
cv-std  : 6.109235990863117
```

In [45]:
```
plt.figure(figsize=(13,28))
plt.subplot(211)

testy = y_test.reset_index()["strength"]

ax = testy.plot(label="originals",figsize=(12,13),linewidth=2)
ax = prediction[0].plot(label = "predictions",figsize=(12,13),linewidth=2)
plt.legend(loc="best")
plt.title("ORIGINALS VS PREDICTIONS")
plt.xlabel("index")
plt.ylabel("values")
```

Out[45]:
```
Text(0, 0.5, 'values')
```



- The predicted value is following the original value

In [46]:
```
gridsearch.best_estimator_.named_steps['regressor']
```

Out[46]:
```
GradientBoostingRegressor(alpha=0.9, criterion='friedman_mse', init=None,
                    learning_rate=0.1, loss='ls', max_depth=5, max_features=None,
                    max_leaf_nodes=None, min_impurity_decrease=0.0,
                    min_impurity_split=None, min_samples_leaf=1,
                    min_samples_split=10, min_weight_fraction_leaf=0.0,
                    n_estimators=100, n_iter_no_change=None, presort='auto',
                    random_state=1, subsample=1.0, tol=0.0001,
                    validation_fraction=0.1, verbose=0, warm_start=False)
```

Confidance Interval for the Model

By using bootstrap and resample method to test the model

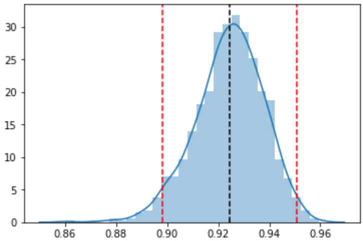
In [47]:
```
# configure bootstrap
n_iterations = 1000              # Number of bootstrap samples to create

# run bootstrap
RMSEstats = list()
R2stats = list()
for i in range(n_iterations):
    # prepare train and test sets
    df_resample = resample(df_out)  # Sampling with replacement
    X_train, X_test, y_train, y_test = train_test_split( df_resample.loc[:, df_resample.columns != 'strengt
h'],
                                                         df_resample["strength"],
                                                         test_size=0.5,
                                                         random_state = 0)
    # fit model
    model = gridsearch.best_estimator_.named_steps['regressor']
    model.fit(X_train, y_train)
    # evaluate model
    predictions = model.predict(X_test)
    RMSE_score = np.sqrt(mean_squared_error(y_test, predictions))
    R2_score = r2_score(y_test, predictions)
    RMSEstats.append(RMSE_score)
    R2stats.append(R2_score)
```

The distribution of the R^2 score of the model

In [48]:
```
upper = np.mean(R2stats)+1.96*np.std(R2stats)
lower = np.mean(R2stats)-1.96*np.std(R2stats)
print('R2 score mean is %.2f (+/- %.3f) with 95%% confidence interval' % (np.mean(R2stats),1.96*np.std(R2st
ats)))

sns.distplot(R2stats)
plt.axvline(np.mean(R2stats),linestyle="dashed",color="k")
plt.axvline(lower,linestyle="dashed",color="r")
plt.axvline(upper,linestyle="dashed",color="r")
```

```
R2 score mean is 0.92 (+/- 0.026) with 95% confidence interval
```

Out[48]: <matplotlib.lines.Line2D at 0x22084360780>

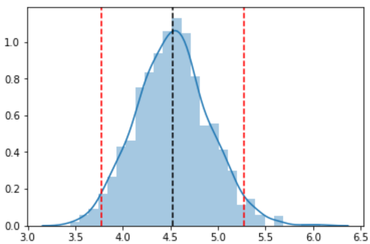


The distribution of the RMSE of the model

In [49]:
```
upper = np.mean(RMSEstats)+1.96*np.std(RMSEstats)
lower = np.mean(RMSEstats)-1.96*np.std(RMSEstats)
print('RMSE score mean is %.2f (+/- %.3f) with 95%% confidence interval' % (np.mean(RMSEstats),1.96*np.std(
RMSEstats)))

sns.distplot(RMSEstats)
plt.axvline(np.mean(RMSEstats),linestyle="dashed",color="k")
plt.axvline(lower,linestyle="dashed",color="r")
plt.axvline(upper,linestyle="dashed",color="r")
```

```
RMSE score mean is 4.52 (+/- 0.752) with 95% confidence interval
```

Out[49]: <matplotlib.lines.Line2D at 0x22086e7bcf8>



Conclusion

- **GradientBoostingRegressor** has been **selected** with **tuned hyperparameter** from GridSearchCV
- By **bootstraping and resample**, the performance of the model is measured.
- It has **lowest** the **Root Means Square Error**, where
  - **RMSE = 4.52 (+/- 0.752)**
  - **R2_score = 0.92 (+/- 0.026)**

GradientBoostingRegressor performed better. It is a type of inductively generated tree ensemble model. **At each step, a new tree is trained against the negative gradient of the loss function**, which is analogous to (or identical to, in the case of least-squares error) the residual error.

RMSE is the **square root of the variance of the residuals** and it is a better measure of how accurately the model predicts the response compare to R2 score. This is because **RMSE is an absolute measure of fit** whereas **R2 is a relative measure of fit**.

In [ ]: