KAMRAN BALAYEV DATA MINING SEMESTER PROJECT

Climate Model Simulation Crashes

This dataset contains records of simulation crashes encountered during climate model uncertainty quantification ensembles. Ensemble members were constructed using a Latin hypercube method in LLNL's UQ Pipeline software system to sample the uncertainties of 18 model parameters within the Parallel Ocean Program (POP2) component of the Community Climate System Model (CCSM4).

Three separate Latin hypercube ensembles were conducted, each containing 180 ensemble members. 46 out of the 540 simulations failed for numerical reasons at combinations of parameter values.

The goal is to use classification to predict simulation outcomes (fail or succeed) from input parameter values, and to use sensitivity analysis and feature selection to determine the causes of simulation crashes.

Attribute Information:

The goal is to predict climate model simulation outcomes (column 21, fail or succeed) given scaled values of climate model input parameters (columns 3-20).

Column 1: Latin hypercube study ID (study 1 to study 3)

Column 2: simulation ID (run 1 to run 180)

Columns 3-20: values of 18 climate model parameters scaled in the interval [0, 1]

Column 21: simulation outcome (0 = failure, 1 = success)

Visualization of Classes via Usage of Weka

Missing Data Results

Weka tool represents that missing data rates are zero for all of the attributes

Name: Study Missing: 0 (0%)	Distinct: 3	Type: Numeric Unique: 0 (0%)
Name: Run Missing: 0 (0%)	Distinct: 180	Type: Numeric Unique: 0 (0%)
Name: vconst_corr Missing: 0 (0%)	Distinct: 540	Type: Numeric Unique: 540 (100%)
Name: vconst_2 Missing: 0 (0%)	Distinct: 540	Type: Numeric Unique: 540 (100%)
Name: vconst_3 Missing: 0 (0%)	Distinct: 540	Type: Numeric Unique: 540 (100%)
Name: vconst_4 Missing: 0 (0%)	Distinct: 540	Type: Numeric Unique: 540 (100%)
Name: vconst_5 Missing: 0 (0%)	Distinct: 540	Type: Numeric Unique: 540 (100%)
Name: vconst_7 Missing: 0 (0%)	Distinct: 540	Type: Numeric Unique: 540 (100%)
Name: ah_corr Missing: 0 (0%)	Distinct: 540	Type: Numeric Unique: 540 (100%)

Name: ah_bolus Missing: 0 (0%)	Distinct: 540	Type: Numeric Unique: 540 (100%)
Name: slm_corr Missing: 0 (0%)	Distinct: 540	Type: Numeric Unique: 540 (100%)
Name: efficiency_factor Missing: 0 (0%)	Distinct: 540	Type: Numeric Unique: 540 (100%)
Name: tidal_mix_max Missing: 0 (0%)	Distinct: 540	Type: Numeric Unique: 540 (100%)
Name: vertical_decay_scale Missing: 0 (0%)	Distinct: 540	Type: String Unique: 540 (100%)
Name: convect_corr Missing: 0 (0%)	Distinct: 540	Type: String Unique: 540 (100%)
Name: bckgrnd_vdc1 Missing: 0 (0%)	Distinct: 540	Type: Numeric Unique: 540 (100%)
Name: bckgrnd_vdc_ban Missing: 0 (0%)	Distinct: 540	Type: Numeric Unique: 540 (100%)
Name: bckgrnd_vdc_eq Missing: 0 (0%)	Distinct: 540	Type: Numeric Unique: 540 (100%)
Name: bckgrnd_vdc_psim Missing: 0 (0%)	Distinct: 540	Type: Numeric Unique: 540 (100%)
Name: Prandtl Missing: 0 (0%)	Distinct: 540	Type: Numeric Unique: 540 (100%)
Name: outcome Missing: 0 (0%)	Distinct: 2	Type: Numeric Unique: 0 (0%)

In [2]:

```
1 import numpy as np
2 import matplotlib.pyplot as plt
3 import pandas as pd
4 import seaborn as sns
5 from sklearn import preprocessing
6 from sklearn.metrics import accuracy_score
7
```

In [5]:
```
data = pd.read_csv('data/data.csv')
data.head()
```

Out[5]:

	Study	Run	vconst_corr	vconst_2	vconst_3	vconst_4	vconst_5	vconst_7	ah_corr	ah_bolu
0	1	1	0.859036	0.927825	0.252866	0.298838	0.170521	0.735936	0.428325	0.56794
1	1	2	0.606041	0.457728	0.359448	0.306957	0.843331	0.934851	0.444572	0.82801
2	1	3	0.997600	0.373238	0.517399	0.504993	0.618903	0.605571	0.746225	0.19592
3	1	4	0.783408	0.104055	0.197533	0.421837	0.742056	0.490828	0.005525	0.39212
4	1	5	0.406250	0.513199	0.061812	0.635837	0.844798	0.441502	0.191926	0.48754

5 rows × 21 columns

In [6]:
```
data.shape
```

Out[6]:
```
(540, 21)
```

In [7]:
```
data.columns
```

Out[7]:
```
Index(['Study', 'Run', 'vconst_corr', 'vconst_2', 'vconst_3', 'vconst_4',
       'vconst_5', 'vconst_7', 'ah_corr', 'ah_bolus', 'slm_corr',
       'efficiency_factor', 'tidal_mix_max',
       'vertical_decay_scale            ', 'convect_corr', 'bckgrnd_vdc1',
       'bckgrnd_vdc_ban', 'bckgrnd_vdc_eq', 'bckgrnd_vdc_psim', 'Prandtl',
       'outcome'],
      dtype='object')
```

In [8]:
```
1 data.info
```

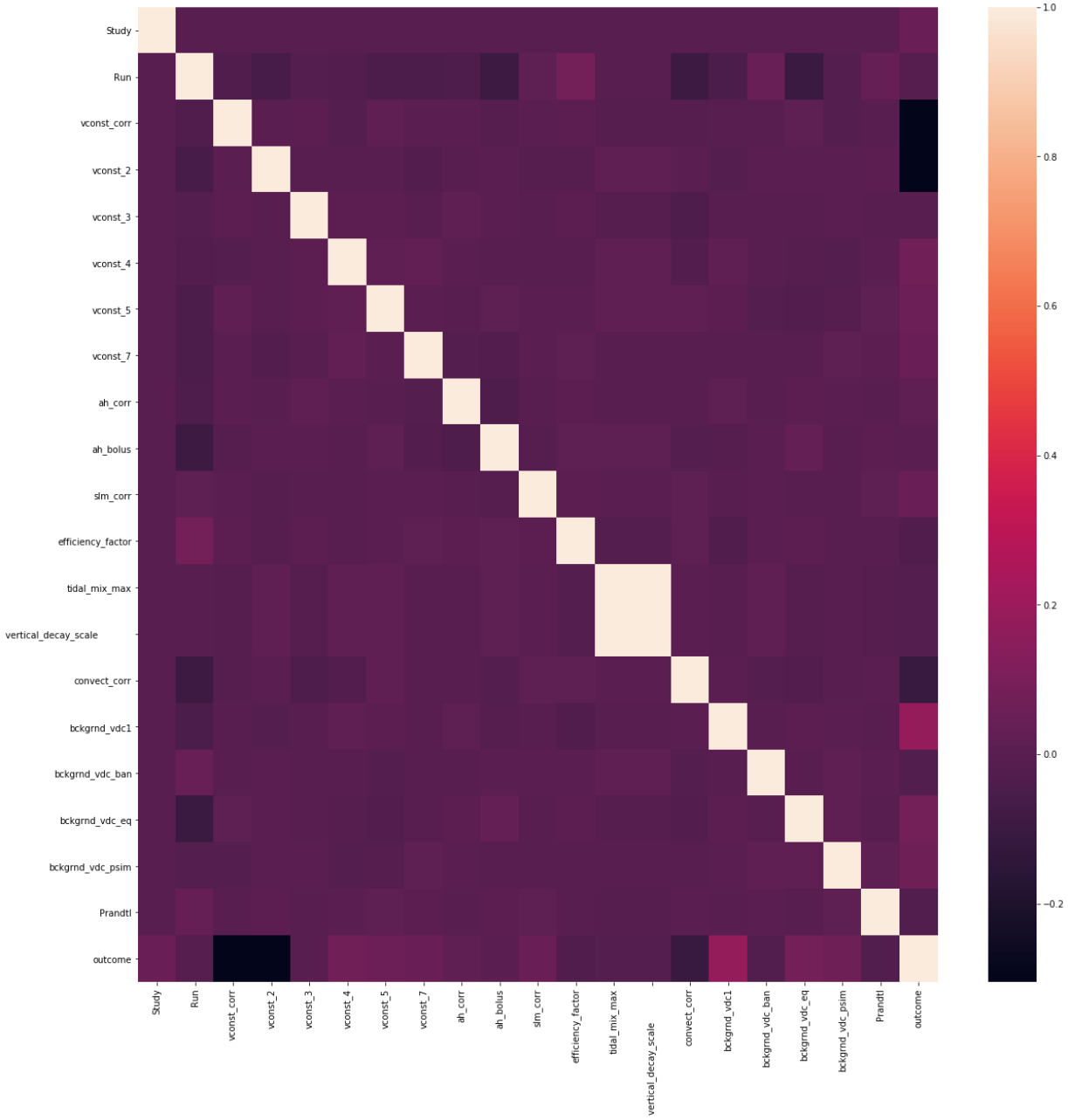
Out[8]:
```
<bound method DataFrame.info of      Study  Run  vconst_corr  vconst_2  vconst_
3  vconst_4  vconst_5  \
0         1    1     0.859036  0.927825  0.252866  0.298838  0.170521
1         1    2     0.606041  0.457728  0.359448  0.306957  0.843331
2         1    3     0.997600  0.373238  0.517399  0.504993  0.618903
3         1    4     0.783408  0.104055  0.197533  0.421837  0.742056
4         1    5     0.406250  0.513199  0.061812  0.635837  0.844798
..      ...  ...          ...       ...       ...       ...       ...
535       3  176     0.657136  0.489375  0.133713  0.411950  0.087780
536       3  177     0.915894  0.842720  0.518947  0.090622  0.336981
537       3  178     0.478600  0.941185  0.769245  0.950776  0.189406
538       3  179     0.007793  0.779287  0.867468  0.704820  0.983282
539       3  180     0.608075  0.031556  0.598264  0.794771  0.145680

     vconst_7   ah_corr  ah_bolus  ...  efficiency_factor  tidal_mix_max  \
0    0.735936  0.428325  0.567947  ...           0.245675       0.104226
1    0.934851  0.444572  0.828015  ...           0.616870       0.975786
2    0.605571  0.746225  0.195928  ...           0.679355       0.803413
3    0.490828  0.005525  0.392123  ...           0.471463       0.597879
4    0.441502  0.191926  0.487546  ...           0.551543       0.743877
..        ...       ...       ...  ...                ...            ...
535  0.356289  0.480204  0.029678  ...           0.280546       0.384117
536  0.893576  0.978703  0.674868  ...           0.798108       0.353546
537  0.112743  0.745645  0.527096  ...           0.193103       0.829563
538  0.420303  0.710612  0.174746  ...           0.761134       0.436714
539  0.378183  0.461948  0.425291  ...           0.480938       0.307816

     vertical_decay_scale             convect_corr  bckgrnd_vdc1  \
0                        0.104226      0.997518      0.448620
1                        0.975786      0.845247      0.864152
2                        0.803413      0.718441      0.924775
3                        0.597879      0.362751      0.912819
4                        0.743877      0.650223      0.522261
..                            ...           ...           ...
535                      0.384117      0.885948      0.459479
536                      0.353546      0.044796      0.347027
537                      0.829563      0.101506      0.381966
538                      0.436714      0.690132      0.981656
539                      0.307816      0.231638      0.583558

     bckgrnd_vdc_ban  bckgrnd_vdc_eq  bckgrnd_vdc_psim   Prandtl  outcome
0           0.307522        0.858310          0.796997  0.869893        0
1           0.346713        0.356573          0.438447  0.512256        1
2           0.315371        0.250642          0.285636  0.365858        1
3           0.977971        0.845921          0.699431  0.475987        1
4           0.043545        0.376660          0.280098  0.132283        1
..               ...             ...               ...       ...      ...
535         0.334482        0.573002          0.610183  0.737706        1
536         0.512499        0.810549          0.593332  0.142565        0
537         0.198811        0.867108          0.461632  0.652817        1
538         0.113193        0.364799          0.201469  0.536535        1
539         0.969365        0.464331          0.760344  0.762439        1

[540 rows x 21 columns]>
```

Visualization

In [9]:
```
data.hist(bins=60, figsize=(20,20))
plt.show()
```

Correlation Heatmap

In [10]:
```
plt.figure(figsize=(20,20))
sns.heatmap(data.corr())
plt.show()
```



In [11]:
```
1 data.describe()
```

Out[11]:

	Study	Run	vconst_corr	vconst_2	vconst_3	vconst_4	vconst_5	vco
count	540.000000	540.000000	540.000000	540.000000	540.000000	540.000000	540.000000	540.0
mean	2.000000	90.500000	0.500026	0.500097	0.500027	0.500119	0.500001	0.4
std	0.817254	52.008901	0.288939	0.288922	0.289067	0.288993	0.288827	0.2
min	1.000000	1.000000	0.000414	0.001922	0.001181	0.001972	0.000858	0.0
25%	1.000000	45.750000	0.249650	0.251597	0.251540	0.250158	0.250630	0.2
50%	2.000000	90.500000	0.499998	0.499595	0.500104	0.500456	0.500903	0.4
75%	3.000000	135.250000	0.750042	0.750011	0.749180	0.750348	0.748988	0.7
max	3.000000	180.000000	0.999194	0.998815	0.998263	0.997673	0.998944	0.9

8 rows × 21 columns

In [12]:
```
1 #Control if there is empty spaces or not
2 data.isnull().sum()
3
```

Out[12]:
```
Study                  0
Run                    0
vconst_corr            0
vconst_2               0
vconst_3               0
vconst_4               0
vconst_5               0
vconst_7               0
ah_corr                0
ah_bolus               0
slm_corr               0
efficiency_factor      0
tidal_mix_max          0
vertical_decay_scale   0
convect_corr           0
bckgrnd_vdc1           0
bckgrnd_vdc_ban        0
bckgrnd_vdc_eq         0
bckgrnd_vdc_psim       0
Prandtl                0
outcome                0
dtype: int64
```

Mix data set

In [13]:
```
data = data.sample(frac=1).reset_index(drop=True)
data.head()
```

Out[13]:

	Study	Run	vconst_corr	vconst_2	vconst_3	vconst_4	vconst_5	vconst_7	ah_corr	ah_bolu
0	1	142	0.649366	0.167627	0.129363	0.408177	0.066166	0.659912	0.742137	0.40681
1	3	30	0.893570	0.355212	0.066133	0.254635	0.239165	0.147224	0.255414	0.8680
2	3	149	0.379486	0.113463	0.585678	0.257807	0.920813	0.669801	0.617307	0.27416
3	3	155	0.582796	0.770086	0.333053	0.034803	0.307772	0.680384	0.174043	0.26383
4	3	105	0.763550	0.566536	0.805273	0.502555	0.078713	0.589690	0.712578	0.37926

5 rows × 21 columns

In [14]:
```
#get outcome column from dataframe
y = data['outcome']
X = data.drop('outcome',axis=1)
X.shape, y.shape
```

Out[14]: ((540, 20), (540,))

In [15]:
```
# Split data set 70 train 30 test
from sklearn.model_selection import train_test_split

X_train, X_test, y_train, y_test = train_test_split(X, y,
                                                    test_size = 0.3, random_
X_train.shape, X_test.shape
```

Out[15]: ((378, 20), (162, 20))

Classification Section

In [16]:
```
#theses lists will store the results of classification algorithms
model = []
trainAcc = []
testAcc = []

#function in order to store model and accuracy of it

def storeResults(MODEL, a,b):
    model.append(MODEL)
    trainAcc.append(round(a, 3))
    testAcc.append(round(b, 3))
```

Decision Tree Classifier

In [17]:
```
# Decision Tree model
from sklearn.tree import DecisionTreeClassifier

# instantiate the model with depth of 5
tree = DecisionTreeClassifier(max_depth = 5)
# fit the model
tree.fit(X_train, y_train)
```

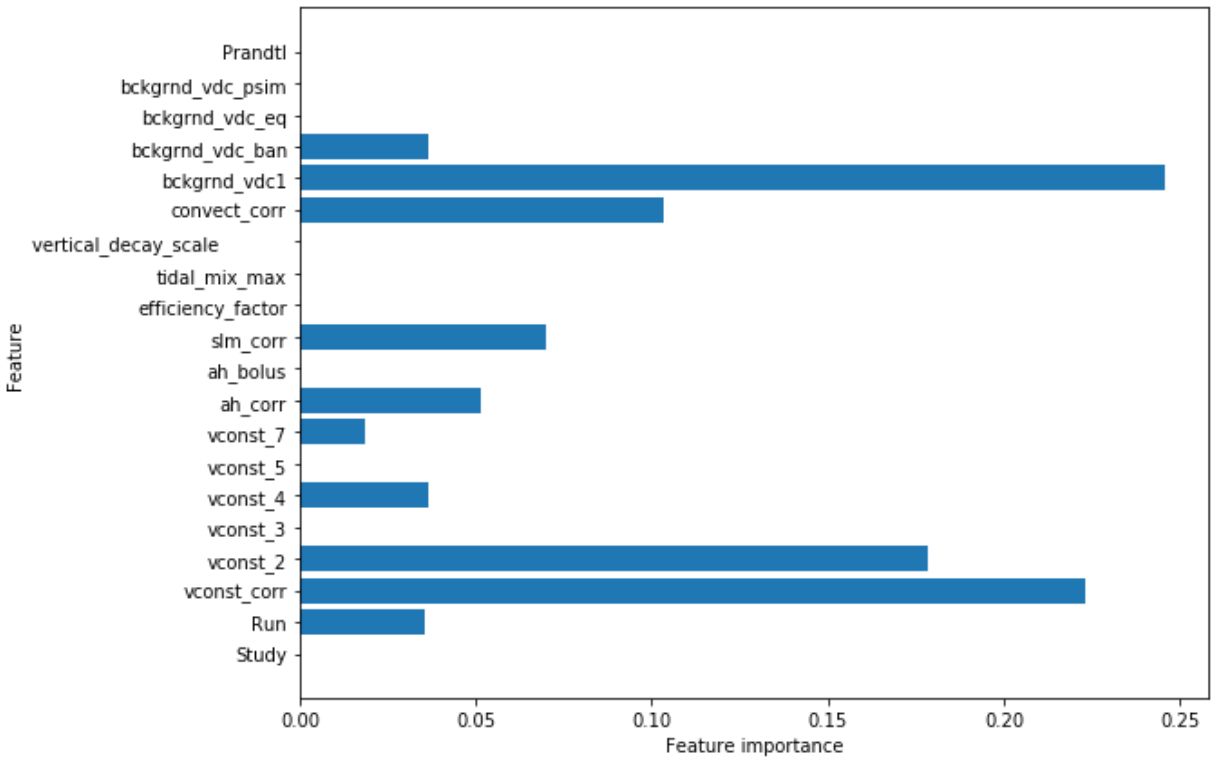
Out[17]:
```
DecisionTreeClassifier(ccp_alpha=0.0, class_weight=None, criterion='gini',
                       max_depth=5, max_features=None, max_leaf_nodes=None,
                       min_impurity_decrease=0.0, min_impurity_split=None,
                       min_samples_leaf=1, min_samples_split=2,
                       min_weight_fraction_leaf=0.0, presort='deprecated',
                       random_state=None, splitter='best')
```

In [18]:
```
##assign prediction results to the variables
yTestTree = tree.predict(X_test)
yTrainTree = tree.predict(X_train)
```

In [19]:
```
#Accuracy informations
acc_train_tree = accuracy_score(y_train,yTrainTree)
acc_test_tree = accuracy_score(y_test,yTestTree)

print("Decision Tree: Accuracy on training Data: {:.3f}".format(acc_train_tr
print("Decision Tree: Accuracy on test Data: {:.3f}".format(acc_test_tree))
```

```
Decision Tree: Accuracy on training Data: 0.981
Decision Tree: Accuracy on test Data: 0.938
```

In [20]:
```
#Feature Importance
plt.figure(figsize=(9,7))
n_features = X_train.shape[1]
plt.barh(range(n_features), tree.feature_importances_, align='center')
plt.yticks(np.arange(n_features), X_train.columns)
plt.xlabel("Feature importance")
plt.ylabel("Feature")
plt.show()
```



In [21]:
```
#Store the accuracy result
storeResults('Decision Tree', acc_train_tree, acc_test_tree)
```

Random Forest Classifier

In [22]:
```
# Random Forest model
from sklearn.ensemble import RandomForestClassifier

# instantiate the model
forest = RandomForestClassifier(max_depth=5)

# fit the model
forest.fit(X_train, y_train)
```

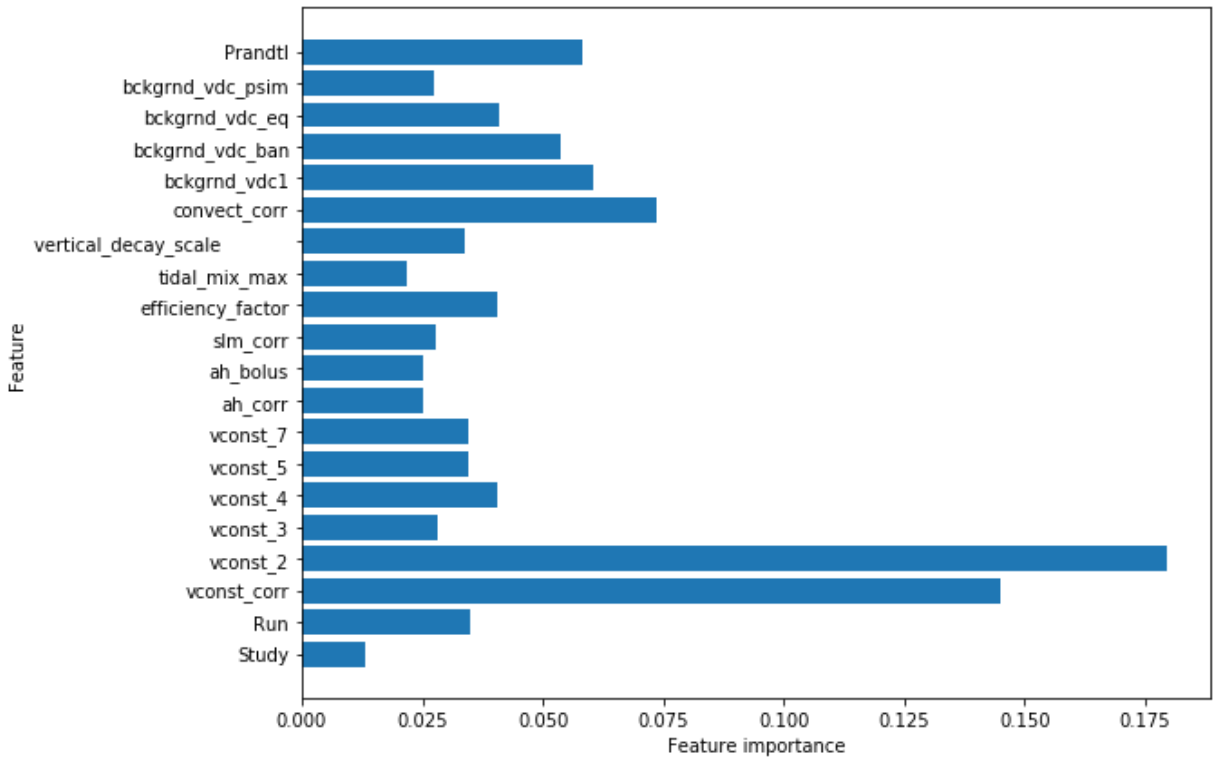
Out[22]:
```
RandomForestClassifier(bootstrap=True, ccp_alpha=0.0, class_weight=None,
                       criterion='gini', max_depth=5, max_features='auto',
                       max_leaf_nodes=None, max_samples=None,
                       min_impurity_decrease=0.0, min_impurity_split=None,
                       min_samples_leaf=1, min_samples_split=2,
                       min_weight_fraction_leaf=0.0, n_estimators=100,
                       n_jobs=None, oob_score=False, random_state=None,
                       verbose=0, warm_start=False)
```

In [23]:
```
##assign prediction results to the variables
y_test_forest = forest.predict(X_test)
y_train_forest = forest.predict(X_train)
```

In [24]:
```
#Accuracy informations
acc_train_forest = accuracy_score(y_train,y_train_forest)
acc_test_forest = accuracy_score(y_test,y_test_forest)

print("Random forest: Accuracy on training Data: {:.3f}".format(acc_train_fo
print("Random forest: Accuracy on test Data: {:.3f}".format(acc_test_forest)
```

```
Random forest: Accuracy on training Data: 0.955
Random forest: Accuracy on test Data: 0.932
```

In [25]:
```
#Feature Importance
plt.figure(figsize=(9,7))
n_features = X_train.shape[1]
plt.barh(range(n_features), forest.feature_importances_, align='center')
plt.yticks(np.arange(n_features), X_train.columns)
plt.xlabel("Feature importance")
plt.ylabel("Feature")
plt.show()
```



In [26]:
```
#Sonucu tut
storeResults('Random Forest', acc_train_forest, acc_test_forest)
```

Support Vector Machines

In [27]:
```
#Support vector machine model
from sklearn.svm import SVC

# instantiate the model
svm = SVC(kernel='linear', C=1.0, random_state=12)
#fit the model
svm.fit(X_train, y_train)
```

Out[27]:
```
SVC(C=1.0, break_ties=False, cache_size=200, class_weight=None, coef0=0.0,
    decision_function_shape='ovr', degree=3, gamma='scale', kernel='linear',
    max_iter=-1, probability=False, random_state=12, shrinking=True, tol=0.001,
    verbose=False)
```

In [28]:
```
####assign prediction results to the variables
y_test_svm = svm.predict(X_test)
y_train_svm = svm.predict(X_train)
```

In [29]:
```
#Accuracy informations
acc_train_svm = accuracy_score(y_train,y_train_svm)
acc_test_svm = accuracy_score(y_test,y_test_svm)

print("SVM: Accuracy on training Data: {:.3f}".format(acc_train_svm))
print("SVM : Accuracy on test Data: {:.3f}".format(acc_test_svm))
```

```
SVM: Accuracy on training Data: 0.950
SVM : Accuracy on test Data: 0.963
```

In [30]:
```
#Store results
storeResults('SVM', acc_train_svm, acc_test_svm)
```

KNN

In [31]:
```
from sklearn.neighbors import KNeighborsClassifier
neigh = KNeighborsClassifier(n_neighbors=3)
neigh.fit(X_train,y_train)
y_pred = neigh.predict(X_test)
accuracy_score(y_test, y_pred)
from sklearn import metrics
metrics.accuracy_score(y_test, y_pred)*100
```

Out[31]:
```
91.9753086419753
```

In [32]:
```
##assign prediction results to the variables
y_test_knn=neigh.predict(X_test)
y_train_knn = neigh.predict(X_train)
```

In [33]:
```
#Accuracy information
trainAccKnn = accuracy_score(y_train,y_train_knn)
testAccKnn = accuracy_score(y_test,y_test_knn)

print("Random forest: Accuracy on training Data: {:.3f}".format(trainAccKnn))
print("Random forest: Accuracy on test Data: {:.3f}".format(testAccKnn))
```

```
Random forest: Accuracy on training Data: 0.913
Random forest: Accuracy on test Data: 0.920
```

In [34]:
```
#Store result
storeResults('KNN', trainAccKnn, testAccKnn)
```

In [41]:
```
#Create dataframe in order to store all algorithms and their performances.
results = pd.DataFrame({ 'model': model,
    'Train Accuracy': trainAcc,
    'Test Accuracy': testAcc})
results
```

Out[41]:

	model	Train Accuracy	Test Accuracy
0	Decision Tree	0.981	0.938
1	Random Forest	0.955	0.932
2	SVM	0.950	0.963
3	KNN	0.913	0.920

In [42]:
```
#Sort in  descending order
results.sort_values(by=['Test Accuracy', 'Train Accuracy'], ascending=False)
```

Out[42]:

	model	Train Accuracy	Test Accuracy
2	SVM	0.950	0.963
0	Decision Tree	0.981	0.938
1	Random Forest	0.955	0.932
3	KNN	0.913	0.920