Heuristic selection for first-order theorem proving using machine learning

June 11, 2023

1 Data loading and preprocessing

Mounting drive

[ ]:
```
from google.colab import drive
drive.mount('/content/drive')
```

Importing libraries

[124]:
```
import pandas as pd
import numpy as np
from sklearn.model_selection import train_test_split
from sklearn.linear_model import Perceptron, LogisticRegression
from sklearn.naive_bayes import GaussianNB
from sklearn.tree import DecisionTreeClassifier
from sklearn.neighbors import KNeighborsClassifier
from sklearn.svm import SVC
from sklearn.metrics import accuracy_score, classification_report
from sklearn.ensemble import RandomForestClassifier, AdaBoostClassifier,␣
 ↪GradientBoostingClassifier
import xgboost as xgb
import math
from sklearn.feature_selection import SelectKBest, f_classif
import seaborn as sns
import matplotlib.pyplot as plt
from sklearn.model_selection import RandomizedSearchCV, StratifiedKFold
```

Reading files

[32]:
```
all_data_raw = pd.read_csv('/content/drive/MyDrive/Main/Ml project/
 ↪ml-prove-data/all-data-raw.csv', header = None)
test_data = pd.read_csv('/content/drive/MyDrive/Main/Ml project/ml-prove-data/
 ↪test.csv', header = None)
train_data = pd.read_csv('/content/drive/MyDrive/Main/Ml project/ml-prove-data/
 ↪train.csv', header = None)
validation_data = pd.read_csv('/content/drive/MyDrive/Main/Ml project/
 ↪ml-prove-data/validation.csv', header = None)
```

Giving column names

[33]:
```
train_data.columns = ['Stat_F1' ,'Stat_F2' ,'Stat_F3' ,'Stat_F4' ,'Stat_F5'␣
 ↪,'Stat_F6' ,'Stat_F7' ,'Stat_F8' ,'Stat_F9' ,'Stat_F10' ,
                      'Stat_F11' ,'Stat_F12' ,'Stat_F13' , 'Dynamic_F1'␣
 ↪,'Dynamic_F2' ,'Dynamic_F3' ,'Dynamic_F4' ,'Dynamic_F5' ,
                      'Dynamic_F6' ,'Dynamic_F7' ,'Dynamic_F8' ,'Dynamic_F9'␣
 ↪,'Dynamic_F10' ,'Dynamic_F11' ,'Dynamic_F12' ,'Dynamic_F13' ,
                      'Dynamic_F14' ,'Dynamic_F15' ,'Dynamic_F16'␣
 ↪,'Dynamic_F17' ,'Dynamic_F18' ,'Dynamic_F19' ,'Dynamic_F20' ,'Dynamic_F21' ,
                      'Dynamic_F22' ,'Dynamic_F23' ,'Dynamic_F24'␣
 ↪,'Dynamic_F25' ,'Dynamic_F26' ,'Dynamic_F27' ,'Dynamic_F28' ,'Dynamic_F29' ,
                      'Dynamic_F30' ,'Dynamic_F31' ,'Dynamic_F32'␣
 ↪,'Dynamic_F33' ,'Dynamic_F34' ,'Dynamic_F35' ,'Dynamic_F36' ,'Dynamic_F37' ,
                      'Dynamic_F38' ,'Heuristic1' ,'Heuristic2' ,'Heuristic3'␣
 ↪,'Heuristic4' ,'Heuristic5', 'Heuristic0' ]
```

[34]:
```
test_Data = pd.DataFrame(data=test_data.values, columns=train_data.columns)
validation_data = pd.DataFrame(data=validation_data.values, columns=train_data.
 ↪columns)
```

[35]:
```
all_data_raw.columns = ['Stat_F1' ,'Stat_F2' ,'Stat_F3' ,'Stat_F4' ,'Stat_F5'␣
 ↪,'Stat_F6' ,'Stat_F7' ,'Stat_F8' ,'Stat_F9' ,'Stat_F10' ,
                      'Stat_F11' ,'Stat_F12' ,'Stat_F13' ,'Stat_F14'␣
 ↪,'Dynamic_F1' ,'Dynamic_F2' ,'Dynamic_F3' ,'Dynamic_F4' ,'Dynamic_F5' ,
                      'Dynamic_F6' ,'Dynamic_F7' ,'Dynamic_F8' ,'Dynamic_F9'␣
 ↪,'Dynamic_F10' ,'Dynamic_F11' ,'Dynamic_F12' ,'Dynamic_F13' ,
                      'Dynamic_F14' ,'Dynamic_F15' ,'Dynamic_F16'␣
 ↪,'Dynamic_F17' ,'Dynamic_F18' ,'Dynamic_F19' ,'Dynamic_F20' ,'Dynamic_F21' ,
                      'Dynamic_F22' ,'Dynamic_F23' ,'Dynamic_F24'␣
 ↪,'Dynamic_F25' ,'Dynamic_F26' ,'Dynamic_F27' ,'Dynamic_F28' ,'Dynamic_F29' ,
                      'Dynamic_F30' ,'Dynamic_F31' ,'Dynamic_F32'␣
 ↪,'Dynamic_F33' ,'Dynamic_F34' ,'Dynamic_F35' ,'Dynamic_F36' ,'Dynamic_F37' ,
                      'Dynamic_F38' ,'Dynamic_F39' ,'Heuristic1'␣
 ↪,'Heuristic2' ,'Heuristic3' ,'Heuristic4' ,'Heuristic5']
```

[ ]:
```
all_data = train_data
all_data = all_data.append(validation_data)
all_data = all_data.append(test_Data)
```

2 Exploratory Data Analysis

Checking for missing values

[37]:
```
all_data.isna().sum()
```

[37]:
```
Stat_F1        0
Stat_F2        0
Stat_F3        0
Stat_F4        0
Stat_F5        0
Stat_F6        0
Stat_F7        0
Stat_F8        0
Stat_F9        0
Stat_F10       0
Stat_F11       0
Stat_F12       0
Stat_F13       0
Dynamic_F1     0
Dynamic_F2     0
Dynamic_F3     0
Dynamic_F4     0
Dynamic_F5     0
Dynamic_F6     0
Dynamic_F7     0
Dynamic_F8     0
Dynamic_F9     0
Dynamic_F10    0
Dynamic_F11    0
Dynamic_F12    0
Dynamic_F13    0
Dynamic_F14    0
Dynamic_F15    0
Dynamic_F16    0
Dynamic_F17    0
Dynamic_F18    0
Dynamic_F19    0
Dynamic_F20    0
Dynamic_F21    0
Dynamic_F22    0
Dynamic_F23    0
Dynamic_F24    0
Dynamic_F25    0
Dynamic_F26    0
Dynamic_F27    0
Dynamic_F28    0
Dynamic_F29    0
Dynamic_F30    0
Dynamic_F31    0
Dynamic_F32    0
Dynamic_F33    0
Dynamic_F34    0
```

```
Dynamic_F35    0
Dynamic_F36    0
Dynamic_F37    0
Dynamic_F38    0
Heuristic1     0
Heuristic2     0
Heuristic3     0
Heuristic4     0
Heuristic5     0
Heuristic0     0
dtype: int64
```

[38]:
```
all_data.head()
```

[38]:
```
   Stat_F1  Stat_F2  Stat_F3  Stat_F4  Stat_F5  Stat_F6  Stat_F7  Stat_F8  \
0   1.4895  0.81688   2.1168   1.7836   1.5346 -0.30543  -1.2477 -0.14537
1   1.4895  0.81688   2.1168   1.7895   1.5403 -0.31850  -1.2477 -0.14537
2   1.4895  0.81688   2.1168   1.7836   1.5346 -0.30543  -1.2477 -0.14537
3   1.4895  0.81688   2.1168   1.7836   1.5346 -0.30543  -1.2477 -0.14537
4   1.4895  0.81688   2.1168   1.7836   1.5346 -0.30543  -1.2477 -0.14537

   Stat_F9  Stat_F10  …  Dynamic_F35  Dynamic_F36  Dynamic_F37  Dynamic_F38  \
0 -0.59356  -0.23316  …     -0.48278       1.4630      0.27015      -1.5559
1 -0.59356  -0.23316  …     -0.48278       1.4801      0.21361      -1.5559
2 -0.59356  -0.23316  …     -0.48278       1.4744      0.23245      -1.5559
3 -0.59356  -0.23316  …     -0.48278       1.4401      0.34553      -1.5559
4 -0.59356  -0.23316  …     -0.48278       1.4458      0.32669      -1.5559

   Heuristic1  Heuristic2  Heuristic3  Heuristic4  Heuristic5  Heuristic0
0        -1.0        -1.0        -1.0        -1.0        -1.0         1.0
1         1.0        -1.0        -1.0        -1.0        -1.0        -1.0
2        -1.0        -1.0        -1.0        -1.0        -1.0         1.0
3        -1.0        -1.0        -1.0        -1.0        -1.0         1.0
4        -1.0        -1.0        -1.0        -1.0        -1.0         1.0

[5 rows x 57 columns]
```

[39]:
```
all_data.info()
```

```
<class 'pandas.core.frame.DataFrame'>
Int64Index: 6118 entries, 0 to 1529
Data columns (total 57 columns):
 #   Column       Non-Null Count  Dtype
---  ------       --------------  -----
 0   Stat_F1      6118 non-null   float64
 1   Stat_F2      6118 non-null   float64
 2   Stat_F3      6118 non-null   float64
```

```
3   Stat_F4      6118 non-null   float64
4   Stat_F5      6118 non-null   float64
5   Stat_F6      6118 non-null   float64
6   Stat_F7      6118 non-null   float64
7   Stat_F8      6118 non-null   float64
8   Stat_F9      6118 non-null   float64
9   Stat_F10     6118 non-null   float64
10  Stat_F11     6118 non-null   float64
11  Stat_F12     6118 non-null   float64
12  Stat_F13     6118 non-null   float64
13  Dynamic_F1   6118 non-null   float64
14  Dynamic_F2   6118 non-null   float64
15  Dynamic_F3   6118 non-null   float64
16  Dynamic_F4   6118 non-null   float64
17  Dynamic_F5   6118 non-null   float64
18  Dynamic_F6   6118 non-null   float64
19  Dynamic_F7   6118 non-null   float64
20  Dynamic_F8   6118 non-null   float64
21  Dynamic_F9   6118 non-null   float64
22  Dynamic_F10  6118 non-null   float64
23  Dynamic_F11  6118 non-null   float64
24  Dynamic_F12  6118 non-null   float64
25  Dynamic_F13  6118 non-null   float64
26  Dynamic_F14  6118 non-null   float64
27  Dynamic_F15  6118 non-null   float64
28  Dynamic_F16  6118 non-null   float64
29  Dynamic_F17  6118 non-null   float64
30  Dynamic_F18  6118 non-null   float64
31  Dynamic_F19  6118 non-null   float64
32  Dynamic_F20  6118 non-null   float64
33  Dynamic_F21  6118 non-null   float64
34  Dynamic_F22  6118 non-null   float64
35  Dynamic_F23  6118 non-null   float64
36  Dynamic_F24  6118 non-null   float64
37  Dynamic_F25  6118 non-null   float64
38  Dynamic_F26  6118 non-null   float64
39  Dynamic_F27  6118 non-null   float64
40  Dynamic_F28  6118 non-null   float64
41  Dynamic_F29  6118 non-null   float64
42  Dynamic_F30  6118 non-null   float64
43  Dynamic_F31  6118 non-null   float64
44  Dynamic_F32  6118 non-null   float64
45  Dynamic_F33  6118 non-null   float64
46  Dynamic_F34  6118 non-null   float64
47  Dynamic_F35  6118 non-null   float64
48  Dynamic_F36  6118 non-null   float64
49  Dynamic_F37  6118 non-null   float64
50  Dynamic_F38  6118 non-null   float64
```

```
 51  Heuristic1   6118 non-null   float64
 52  Heuristic2   6118 non-null   float64
 53  Heuristic3   6118 non-null   float64
 54  Heuristic4   6118 non-null   float64
 55  Heuristic5   6118 non-null   float64
 56  Heuristic0   6118 non-null   float64
dtypes: float64(57)
memory usage: 2.7 MB
```

[40]:
```
all_data.describe()
```

[40]:

	Stat_F1	Stat_F2	Stat_F3	Stat_F4	Stat_F5	\
count	6118.000000	6118.000000	6118.000000	6118.000000	6118.000000	
mean	0.040513	0.052955	-0.000470	0.050555	0.049217	
std	0.977642	0.980589	0.998545	0.979385	0.972786	
min	-1.105200	-3.735600	-0.984110	-1.065200	-1.240100	
25%	-0.748365	-0.229907	-0.605570	-0.694180	-0.721762	
50%	-0.372350	0.425360	-0.474750	-0.323190	-0.336315	
75%	0.742862	0.831520	0.256640	0.729960	0.562390	
max	2.009400	0.831520	2.738100	2.644800	2.366200	

	Stat_F6	Stat_F7	Stat_F8	Stat_F9	Stat_F10	…	\
count	6118.000000	6118.000000	6118.000000	6118.000000	6118.000000	…	
mean	-0.007497	-0.040911	0.001915	-0.011851	0.001695	…	
std	0.980862	0.971879	0.994724	0.968021	1.006563	…	
min	-0.880580	-1.763800	-0.826370	-0.709950	-0.913580	…	
25%	-0.618170	-0.960320	-0.417770	-0.364737	-0.641410	…	
50%	-0.305430	0.310500	-0.281570	-0.201890	-0.369240	…	
75%	0.075464	0.699510	0.399430	0.156060	-0.097070	…	
max	7.194500	1.439300	32.270000	15.495000	10.654000	…	

	Dynamic_F35	Dynamic_F36	Dynamic_F37	Dynamic_F38	Heuristic1	\
count	6118.000000	6118.000000	6118.000000	6118.000000	6118.000000	
mean	-0.006171	0.038134	-0.003634	-0.037294	-0.644001	
std	0.991428	0.978672	1.004385	0.983310	0.765087	
min	-0.489900	-0.784590	-0.464860	-2.131800	-1.000000	
25%	-0.489900	-0.644062	-0.464860	-0.388068	-1.000000	
50%	-0.435790	-0.385305	-0.305720	0.330680	-1.000000	
75%	-0.235707	0.202157	0.087767	0.658180	-1.000000	
max	3.298200	2.257900	9.561500	0.932190	1.000000	

	Heuristic2	Heuristic3	Heuristic4	Heuristic5	Heuristic0
count	6118.000000	6118.000000	6118.000000	6118.000000	6118.000000
mean	-0.841125	-0.755476	-0.798300	-0.796012	-0.165087
std	0.540886	0.655230	0.602309	0.605331	0.986360
min	-1.000000	-1.000000	-1.000000	-1.000000	-1.000000
25%	-1.000000	-1.000000	-1.000000	-1.000000	-1.000000

```
50%      -1.000000    -1.000000    -1.000000    -1.000000    -1.000000
75%      -1.000000    -1.000000    -1.000000    -1.000000     1.000000
max       1.000000     1.000000     1.000000     1.000000     1.000000

[8 rows x 57 columns]
```

Seperating output columns

[41]:
```
test_data = all_data[['Heuristic1' ,'Heuristic2' ,'Heuristic3' ,'Heuristic4'␣
↪,'Heuristic5', 'Heuristic0']]
```

Converting multiple output columns to a single column

[42]:
```
test_data['Heuristic_no.']  = 0
for i in range(all_data.shape[0]):
  for j in range(6):
    if (test_data.iloc[i,j] == 1):
      test_data.iloc[i,6] = (j+1)%6
```

```
<ipython-input-42-e7e0f9dd4731>:1: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-
docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  test_data['Heuristic_no.']  = 0
```

[43]:
```
test_data = test_data['Heuristic_no.']
test_data = pd.DataFrame(test_data, columns =['Heuristic_no.'])
```

[44]:
```
test_data.tail()
```

[44]:

	Heuristic_no.
1525	0
1526	0
1527	5
1528	0
1529	3

Feature Selection

Determining number of features to be selected

[45]:
```
num_feature = round(math.log(all_data.shape[0],2),0)
num_feature
```

[45]: 13.0

[46]:
```
full_train_data = all_data.iloc[:,:51]
index_val = full_train_data.index
```

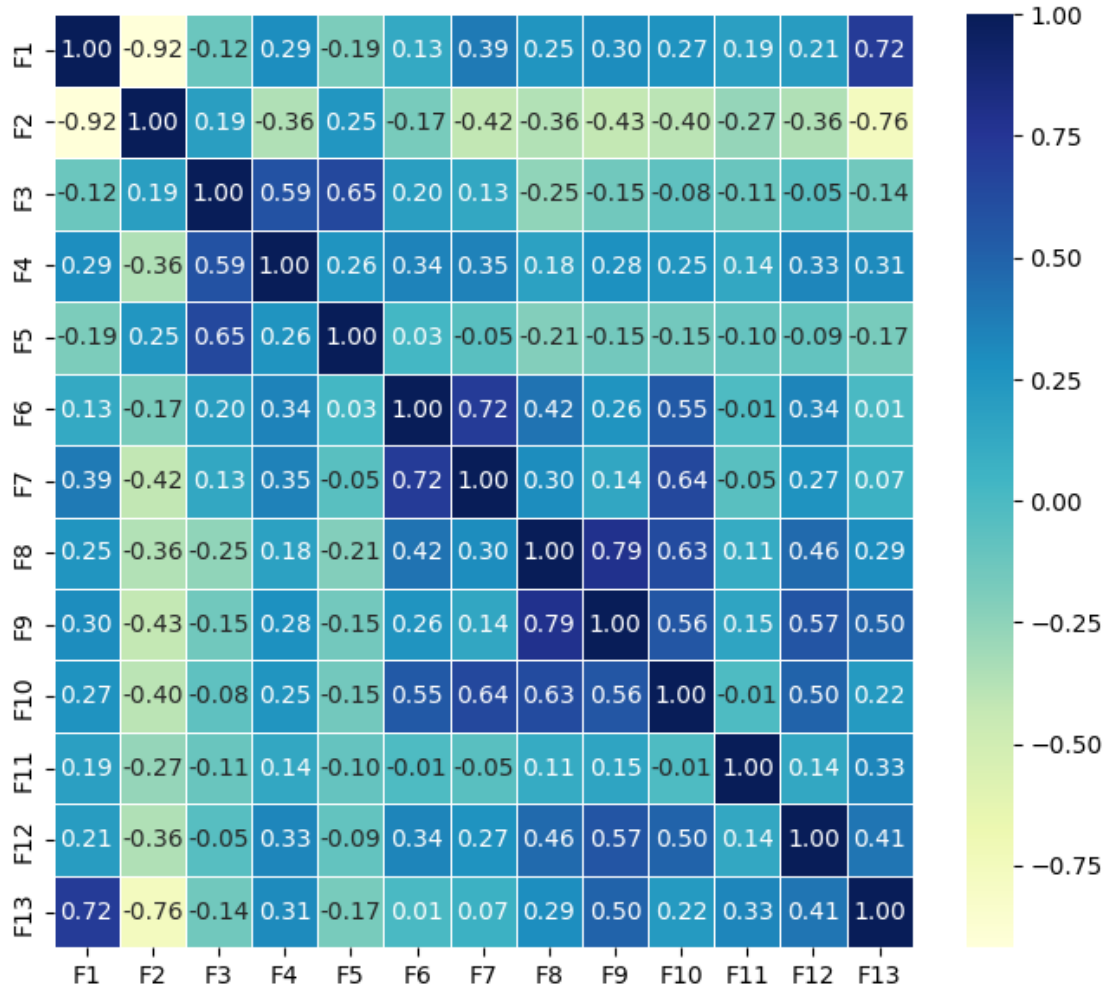
[ ]:
```
all_data = SelectKBest(f_classif, k=int(num_feature)).
 ↪fit_transform(full_train_data, test_data)
```

[49]:
```
column_values =␣
 ↪['F1','F2','F3','F4','F5','F6','F7','F8','F9','F10','F11','F12','F13']
all_data = pd.DataFrame(data = all_data, index = index_val, columns =␣
 ↪column_values)
```

Heat Map

Correlation among features

[51]:
```
corr_matrix = all_data.corr()
fig, ax = plt.subplots(figsize=(8,7))
ax = sns.heatmap(corr_matrix,
 annot=True,
 linewidths=0.5,
 fmt=".2f",
 cmap="YlGnBu");
bottom, top = ax.get_ylim()
```



[52]:
```
all_data = pd.concat([all_data, test_data], axis = 1)
```

[53]:
```
all_data.head()
```

[53]:

	F1	F2	F3	F4	F5	F6	F7	F8	F9	\
0	1.5346	-1.2477	-0.23316	0.31218	-0.29103	-1.7734	-0.29911	-1.081	-0.4775	
1	1.5403	-1.2477	-0.23316	0.31218	-0.29103	-1.7734	-0.29911	-1.081	-0.4775	
2	1.5346	-1.2477	-0.23316	0.31218	-0.29103	-1.7734	-0.29911	-1.081	-0.4775	
3	1.5346	-1.2477	-0.23316	0.31218	-0.29103	-1.7734	-0.29911	-1.081	-0.4775	
4	1.5346	-1.2477	-0.23316	0.31218	-0.29103	-1.7734	-0.29911	-1.081	-0.4775	

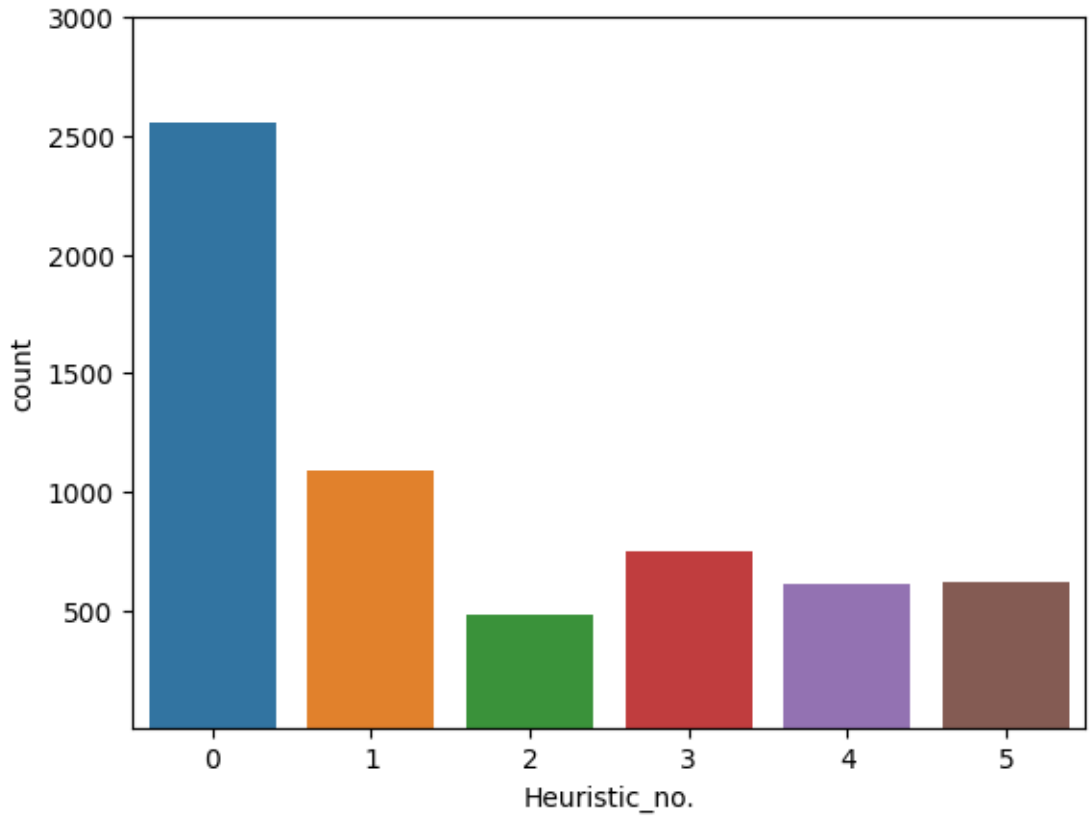
	F10	F11	F12	F13	Heuristic_no.
0	-0.51385	-0.42105	-0.65489	1.4630	0
1	-0.50588	-0.42105	-0.65489	1.4801	1
2	-0.50854	-0.42105	-0.65489	1.4744	0
3	-0.52448	-0.42105	-0.65489	1.4401	0

```
4 -0.52182 -0.42105 -0.65489  1.4458              0
```

Checking for unbalanced classes

[54]:
```
plt.ylim(10, 3000)
sns.countplot(x = all_data['Heuristic_no.'])
```

[54]:
```
<Axes: xlabel='Heuristic_no.', ylabel='count'>
```



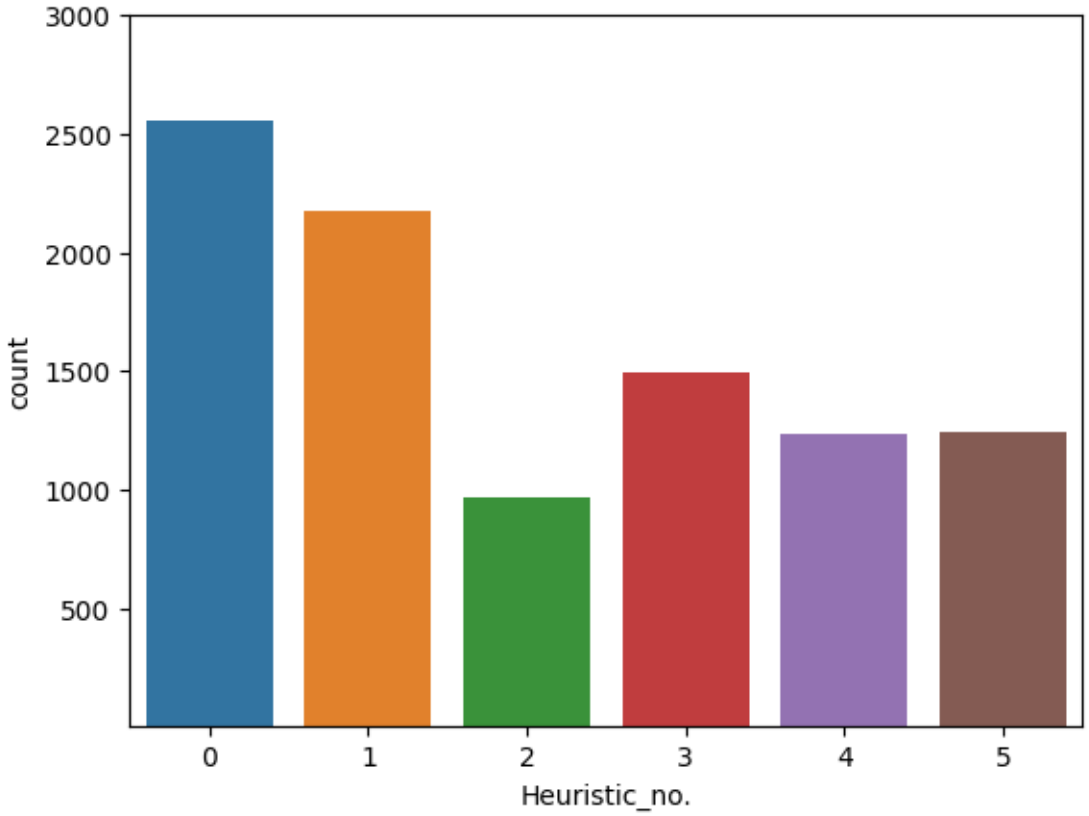
Increasing samples of minority classes to create better balance

[ ]:
```
#Seperating the 0 heuristic rows
df_filtered = all_data[all_data['Heuristic_no.'] >= 1]
df_heuristic_0  = all_data[all_data['Heuristic_no.'] == 0]

# For upscaling, replicating others
df_filtered_repl = pd.concat([df_filtered]*2)

# Combining the classes
all_data_balanced = pd.DataFrame()
all_data_balanced = all_data_balanced.append(df_filtered_repl)
```

```
all_data_balanced = all_data_balanced.append(df_heuristic_0)
all_data = all_data_balanced
```

[56]:
```
plt.ylim(10, 3000)
sns.countplot(x = all_data['Heuristic_no.'])
```

[56]: <Axes: xlabel='Heuristic_no.', ylabel='count'>



3 Modelling

Seperating and splitting train & test data

[57]:
```
num_feature = int(num_feature)
train_data = all_data.iloc[:,:num_feature]
test_data = all_data.iloc[:,num_feature]
```

[58]:
```
x_train, x_test, y_train, y_test = train_test_split(train_data, test_data ,␣
↪test_size = 0.1, random_state = 0)
```

Applying Classifier models:

[59]:
```
clf1 = Perceptron()
clf2 = LogisticRegression(max_iter = 200)
clf3 = SVC()
clf4 = DecisionTreeClassifier()
clf5 = KNeighborsClassifier()
clf6 = GaussianNB()
```

Hyper parameter tuning for XGBClassifier

[60]:
```
parameters = {'n_estimators':[25,50,100,150,200],
              'max_depth':[1,3,5,7,9,None],
              'gamma':[0.5, 1, 2, 5]}

folds = 3
param_comb = 5
XGB = xgb.XGBClassifier(objective="multi:softprob", random_state=42)
skf = StratifiedKFold(n_splits=folds)
grid = RandomizedSearchCV(estimator = XGB, param_distributions=parameters)
grid.fit(x_train, y_train)
print('\n Best hyperparameters:')
print(grid.best_params_)
```

```
 Best hyperparameters:
{'n_estimators': 50, 'max_depth': 9, 'gamma': 1}
```

[61]:
```
clf7 = AdaBoostClassifier(n_estimators = 50, learning_rate = 1.0)
clf8 = GradientBoostingClassifier(n_estimators = 50, learning_rate= 0.5,␣
 ↪max_depth = None, )
clf9 = RandomForestClassifier(max_depth = 3, n_estimators =50, criterion =␣
 ↪'entropy')
clf10 = xgb.XGBClassifier(objective="multi:softprob", random_state=42,␣
 ↪n_estimators= 50, gamma = 1, max_depth= 9)
```

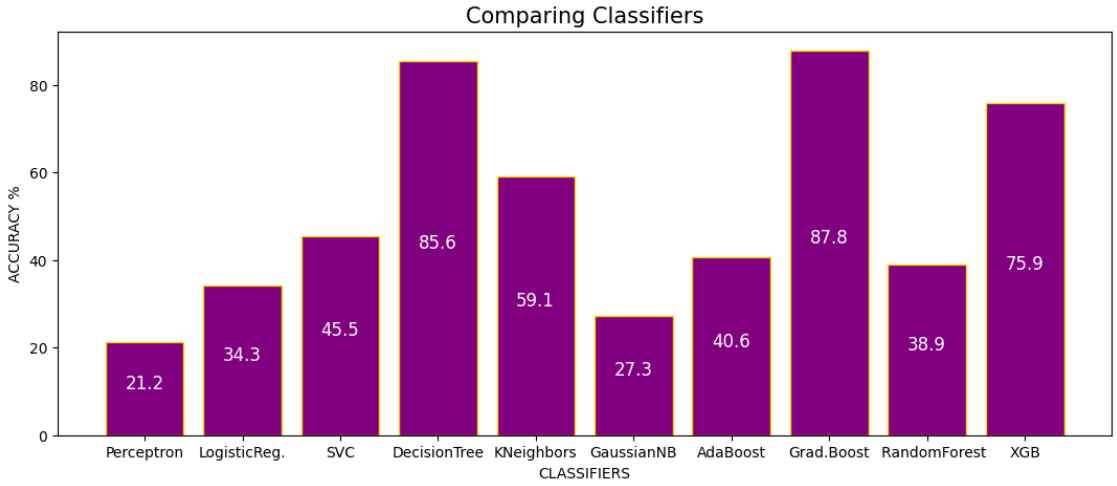
Predicting output and calculating accuracy score

[67]:
```
result = [0,0,0,0,0,0,0,0,0,0]
clf1.fit(x_train, y_train)
pred1 = clf1.predict(x_test)
acc1 = accuracy_score(y_test, pred1)
result[0] = (acc1)

clf2.fit(x_train, y_train)
pred2 = clf2.predict(x_test)
acc2 = accuracy_score(y_test, pred2)
result[1] = (acc2)

clf3.fit(x_train, y_train)
```

```
pred3 = clf3.predict(x_test)
acc3 = accuracy_score(y_test, pred3)
result[2] = (acc3)

clf4.fit(x_train, y_train)
pred4 = clf4.predict(x_test)
acc4 = accuracy_score(y_test, pred4)
result[3] = (acc4)

clf5.fit(x_train, y_train)
pred5 = clf5.predict(x_test)
acc5 = accuracy_score(y_test, pred5)
result[4] = (acc5)

clf6.fit(x_train, y_train)
pred6 = clf6.predict(x_test)
acc6 = accuracy_score(y_test, pred6)
result[5] = (acc6)

clf7.fit(x_train, y_train)
pred7 = clf7.predict(x_test)
acc7 = accuracy_score(y_test, pred7)
result[6] = (acc7)

clf8.fit(x_train, y_train)
pred8 = clf8.predict(x_test)
acc8 = accuracy_score(y_test, pred8)
result[7] = (acc8)

clf9.fit(x_train, y_train)
pred9 = clf9.predict(x_test)
acc9 = accuracy_score(y_test, pred9)
result[8] = (acc9)

clf10.fit(x_train, y_train)
pred10 = clf10.predict(x_test)
acc10 = accuracy_score(y_test, pred10)
result[9] = acc10
result = [i*100 for i in result]
```

[123]:
```
classifier_list = ['Perceptron','LogisticReg.','SVC','DecisionTree',
                   'KNeighbors','GaussianNB','AdaBoost',
                   'Grad.Boost','   RandomForest','XGB']
plt.figure(figsize=(13, 5))
plt.bar(classifier_list, result, color = 'purple', edgecolor = 'gold')
for index, val in enumerate(result):
```

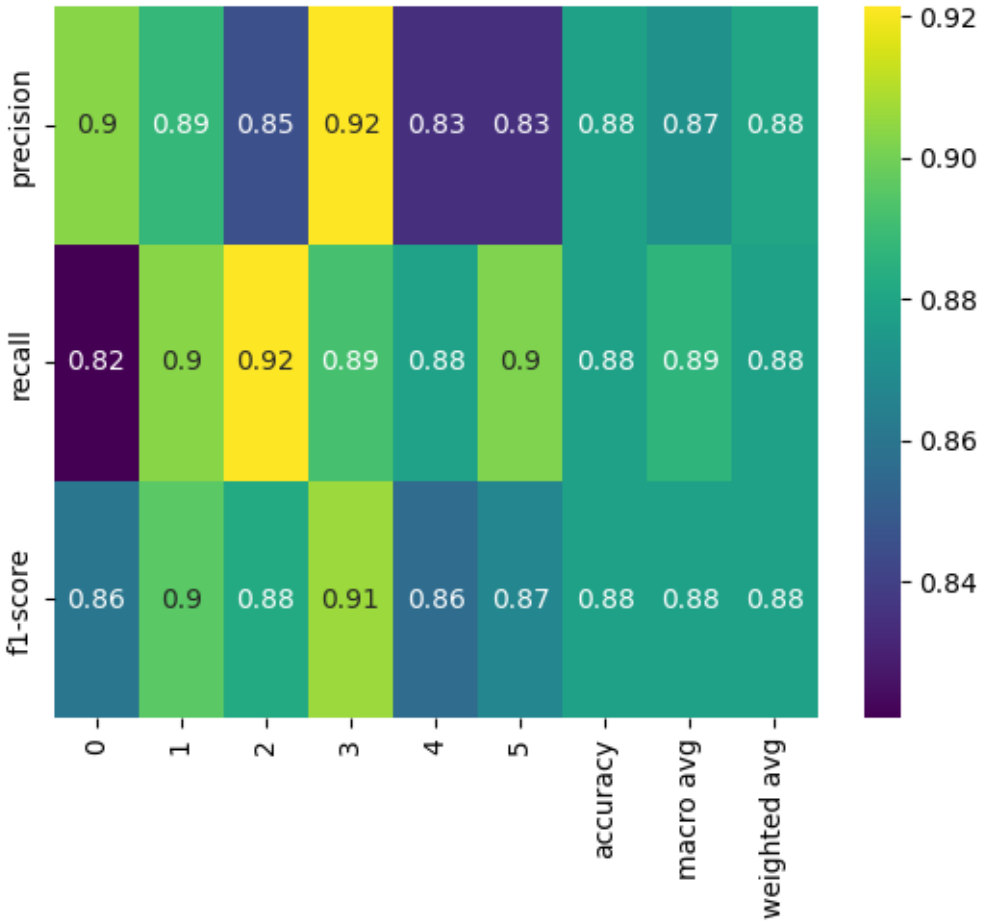
```
  plt.text(index-0.2, val/2 , str(round(val, 1)), color = 'white', size =␣
 ↪'large')
plt.xlabel("CLASSIFIERS")
plt.ylabel("ACCURACY %")
plt.title("Comparing Classifiers", fontsize = 15)
plt.show()
```



3.1 Classification report of best classifier:

GradientBoosting

[121]:
```
cr = classification_report(y_test, pred8,output_dict=True)
map = sns.heatmap(pd.DataFrame(cr).iloc[:-1, :], annot=True, cmap="viridis")
plt.show()
```


precision
recall
f1-score
0.9
0.89
0.85
0.92
0.83
0.83
0.88
0.87
0.88
0.82
0.9
0.92
0.89
0.88
0.9
0.88
0.89
0.88
0.86
0.9
0.88
0.91
0.86
0.87
0.88
0.88
0.88
0
1
2
3
4
5
accuracy
macro avg
weighted avg
0.92
0.90
0.88
0.86
0.84

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