rf_trials

May 26, 2020

[356]:
```
import numpy as np
import pandas as pd
from sklearn.ensemble import RandomForestClassifier
from sklearn.model_selection import train_test_split
from sklearn.feature_selection import SelectFromModel
from sklearn.metrics import accuracy_score
from sklearn import preprocessing
```

1 Transforming and Splitting Data

[357]:
```
df = pd.read_csv("data/combined_expression.csv")
```

[358]:
```
df.head()
```

[358]:
```
   CELL_LINE_NAME  classification    TSPAN6      TNMD       DPM1     SCYL3  \
0         1240121               1  6.419526  3.182094   9.320548  3.759654
1         1240122               2  7.646494  2.626819  10.153853  3.564755
2         1240123               1  8.319417  3.111183   9.643558  4.757258
3         1240124               1  9.006994  3.028173   9.686700  4.280504
4         1240127               1  7.985676  2.694729  10.676134  4.159685

   C1orf112       FGR       CFH     FUCA2  …   COL15A1   C6orf10   TMEM225  \
0  3.802619  3.215753  4.698729  7.873672  …  3.245454  2.953508  3.543429
1  3.942749  3.290760  3.551675  8.252413  …  2.786709  3.077382  3.728232
2  3.919757  3.602185  3.329644  9.076950  …  3.459089  3.085394  3.462811
3  3.147646  3.188881  3.293807  8.678790  …  2.835403  2.960303  3.415083
4  3.804637  3.481942  3.111261  7.555407  …  2.896523  2.849899  3.480114

     NOTCH4      PBX2      AGER      RNF5    AGPAT1    DFNB59     PRRT1
0  3.352022  4.672310  3.641128  3.135310  3.737072  3.450927  3.168800
1  3.208882  4.586840  3.395654  3.586800  3.519128  3.115323  3.051645
2  3.339030  4.614897  3.395845  3.419193  3.971646  3.729310  3.320022
3  3.290171  4.770123  3.400821  3.383734  3.798107  2.822404  3.297547
4  3.226128  5.832710  3.612179  3.347095  4.457963  5.198524  4.553586

[5 rows x 16383 columns]
```

[359]:
```python
X = df.drop(columns=['CELL_LINE_NAME', 'classification'])
y = df['classification']
feat_labels = list(X.columns)
```

[360]:
```python
min_max_scaler = preprocessing.MinMaxScaler()
x_scaled = min_max_scaler.fit_transform(X)
X = pd.DataFrame(x_scaled)
```

[361]:
```python
# 20% test, 80% train
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2,␣
 ↪random_state=0)
```

2 Creating the Classifier With All Features

[362]:
```python
# create and train the classifier
clf = RandomForestClassifier(n_estimators=100, random_state=0, n_jobs=-1)
clf.fit(X_train, y_train)
```

[362]:
```
RandomForestClassifier(bootstrap=True, ccp_alpha=0.0, class_weight=None,
                       criterion='gini', max_depth=None, 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=-1, oob_score=False, random_state=0, verbose=0,
                       warm_start=False)
```

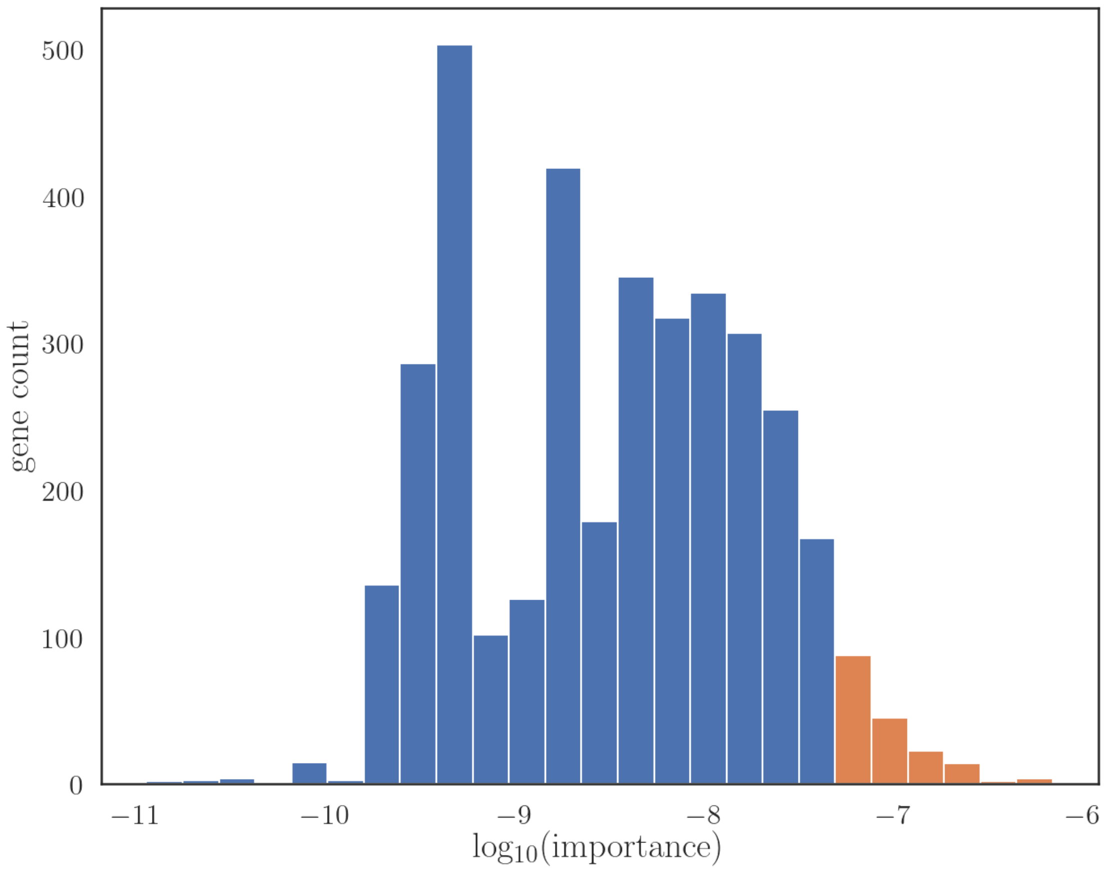
[363]:
```python
# associating each feature with its relative importance
feat_importances = list(zip(feat_labels, clf.feature_importances_))
feat_importances.sort(key = lambda x: x[1], reverse=True)
```

[366]:
```python
# plotting the feature importances
import matplotlib.pyplot as plt
plt.tight_layout()

indices = np.arange(len(feat_importances))
x, y = zip(*feat_importances)
y = [i for i in y if i > 0]
```

```
<Figure size 720x720 with 0 Axes>
```

[398]:
```python
ax1 = plt.subplot(111)
_, _, bars = plt.hist(np.log(y), bins=25, color='C0')

for bar in bars:
```

```
    if bar.get_x() >= -7.5:
        bar.set_facecolor('C1')
ax1.plot()
ax1.set_xlabel('$\mathrm{log_{10}(importance)}$', size=20)
ax1.set_ylabel('$\mathrm{gene\ count}$', size=20)
plt.tick_params(labelsize=16)
from pylab import rcParams
rcParams['figure.figsize'] = 10, 8
plt.savefig('figures/rf_importances.svg')
```



3 Testing Various Thresholds

3.1 Defining Functions for Multiple Iterations

[345]:
```
def sfm_transforms(sfm, X_train, X_test):
    X_important_train = sfm.transform(X_train)
    X_important_test = sfm.transform(X_test)
    return X_important_train, X_important_test
```

[346]:
```python
def det_accuracy(clf, X_test, y_test):
    y_pred = clf.predict(X_test)
    return accuracy_score(y_test, y_pred)
```

3.2 Testing Multiple Iterations

[381]:
```python
thresholds = np.linspace(1e-7, 1e-3, 10)
thresholds
```

[381]:
```
array([1.000e-07, 1.112e-04, 2.223e-04, 3.334e-04, 4.445e-04, 5.556e-04,
       6.667e-04, 7.778e-04, 8.889e-04, 1.000e-03])
```

[382]:
```python
thresh_accuracy = list()

j=1
for i in thresholds:
    sfm = SelectFromModel(clf, i)
    sfm.fit(X_train, y_train)
    X_important_train, X_important_test = sfm_transforms(sfm, X_train, X_test)

    clf_important = RandomForestClassifier(n_estimators=100, random_state=0,␣
 ↪n_jobs=-1)
    clf_important.fit(X_important_train, y_train)

    thresh_accuracy.append((i, det_accuracy(clf, X_test, y_test)))

    print(f'Iteration: {j}; threshold: {i}')
    j += 1
```

```
Iteration: 1; threshold: 1e-07
Iteration: 2; threshold: 0.00011119999999999999
Iteration: 3; threshold: 0.00022229999999999998
Iteration: 4; threshold: 0.00033339999999999997
Iteration: 5; threshold: 0.00044449999999999996
Iteration: 6; threshold: 0.0005556
Iteration: 7; threshold: 0.0006666999999999999
Iteration: 8; threshold: 0.0007777999999999998
Iteration: 9; threshold: 0.0008888999999999999
Iteration: 10; threshold: 0.001
```

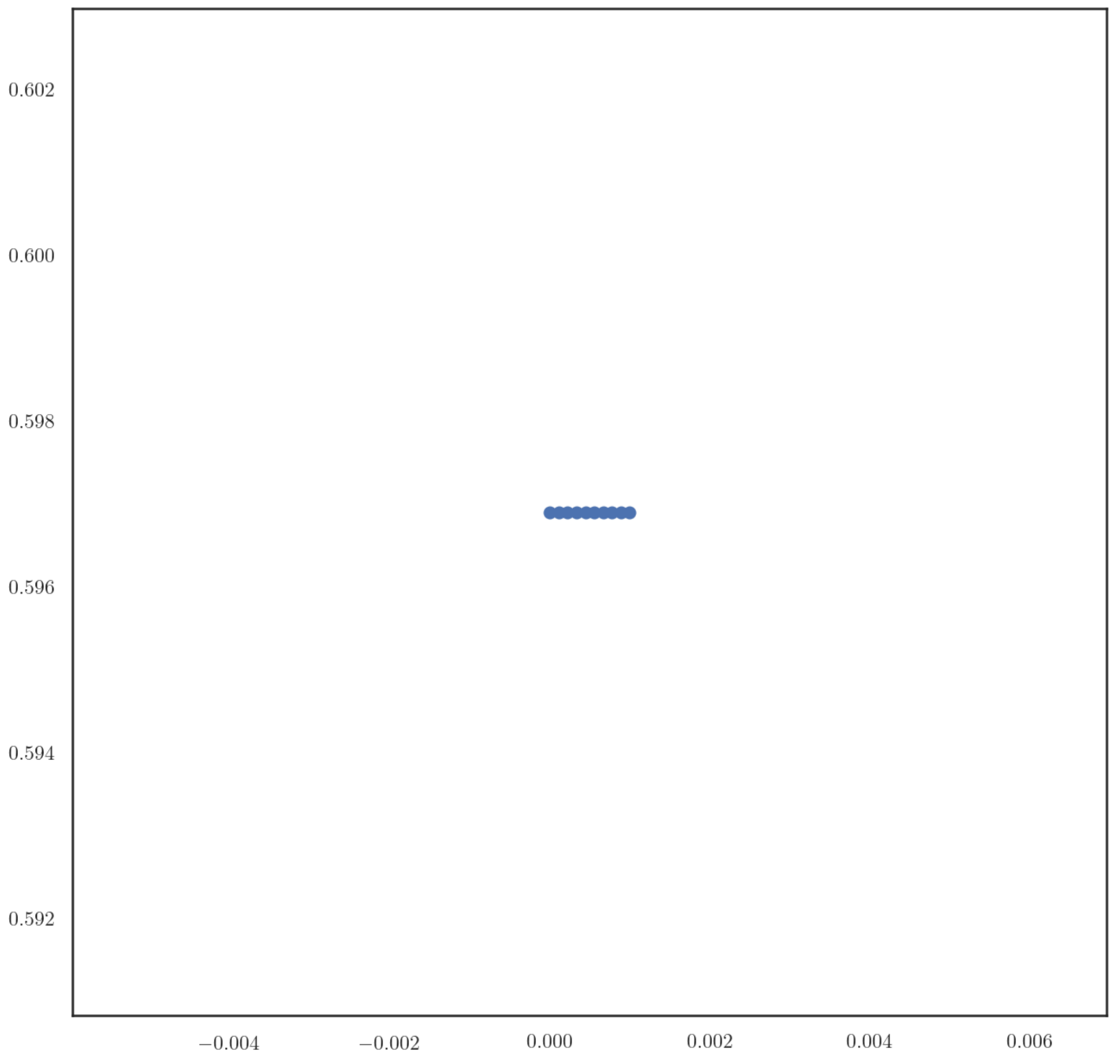
[383]:
```python
thresh_accuracy
```

[383]:
```
[(1e-07, 0.5968992248062015),
 (0.00011119999999999999, 0.5968992248062015),
 (0.00022229999999999998, 0.5968992248062015),
 (0.00033339999999999997, 0.5968992248062015),
 (0.00044449999999999996, 0.5968992248062015),
```

```
 (0.0005556, 0.5968992248062015),
 (0.0006666999999999999, 0.5968992248062015),
 (0.0007777999999999998, 0.5968992248062015),
 (0.0008888999999999999, 0.5968992248062015),
 (0.001, 0.5968992248062015)]
```

[384]:
```
# testList2 = [(np.log(elem1), elem2) for elem1, elem2 in thresh_accuracy]
plt.scatter(*zip(*thresh_accuracy))
```

[384]: <matplotlib.collections.PathCollection at 0x1a2c3065f8>



[385]:
```
len(thresh_accuracy)
thresh_accuracy
```

```
[385]: [(1e-07, 0.5968992248062015),
 (0.00011119999999999999, 0.5968992248062015),
 (0.00022229999999999998, 0.5968992248062015),
 (0.00033339999999999997, 0.5968992248062015),
 (0.00044449999999999996, 0.5968992248062015),
 (0.0005556, 0.5968992248062015),
 (0.0006666999999999999, 0.5968992248062015),
 (0.0007777999999999998, 0.5968992248062015),
 (0.0008888999999999999, 0.5968992248062015),
 (0.001, 0.5968992248062015)]
```

4 Threshold to Choose

The accuracy does not significantly differ across the thresholds chosen. Therefore, a threshold of 1e-3 of importance will be used as the cutoff as it provides a relatively small subset of the 16833 genes. This gives 40 genes as the subset to analyze.