HAPI_Prediction_Script

October 9, 2021

0.1 Import Libraries

[26]:
```
import pickle
import warnings
warnings.filterwarnings('ignore')
import pandas as pd
import numpy as np
from sklearn.linear_model import LogisticRegression
from sklearn.tree import DecisionTreeClassifier
from sklearn.ensemble import RandomForestClassifier
from sklearn.model_selection import GridSearchCV
import sklearn.metrics
from sklearn.model_selection import train_test_split
import matplotlib.pyplot as plt
import seaborn as sns
%matplotlib inline
from sklearn.metrics import classification_report
from sklearn.metrics import confusion_matrix
from sklearn.metrics import f1_score
from sklearn import preprocessing
from sklearn.naive_bayes import GaussianNB
import operator
from sklearn.metrics import balanced_accuracy_score
from sklearn import svm
import impyute as impy
from xgboost import XGBClassifier
from xgboost import plot_tree
import xgboost as xgb
from sklearn.experimental import enable_iterative_imputer
from sklearn.impute import IterativeImputer
import shap
from mlxtend.evaluate import bootstrap
from sklearn.metrics import roc_curve, roc_auc_score
from numpy import format_float_scientific
import inspect
from imblearn.ensemble import BalancedRandomForestClassifier
import datetime
```

0.2 Load Data

[27]:
```
df = pd.read_sas('hapi_dataset.sas7bdat')
```

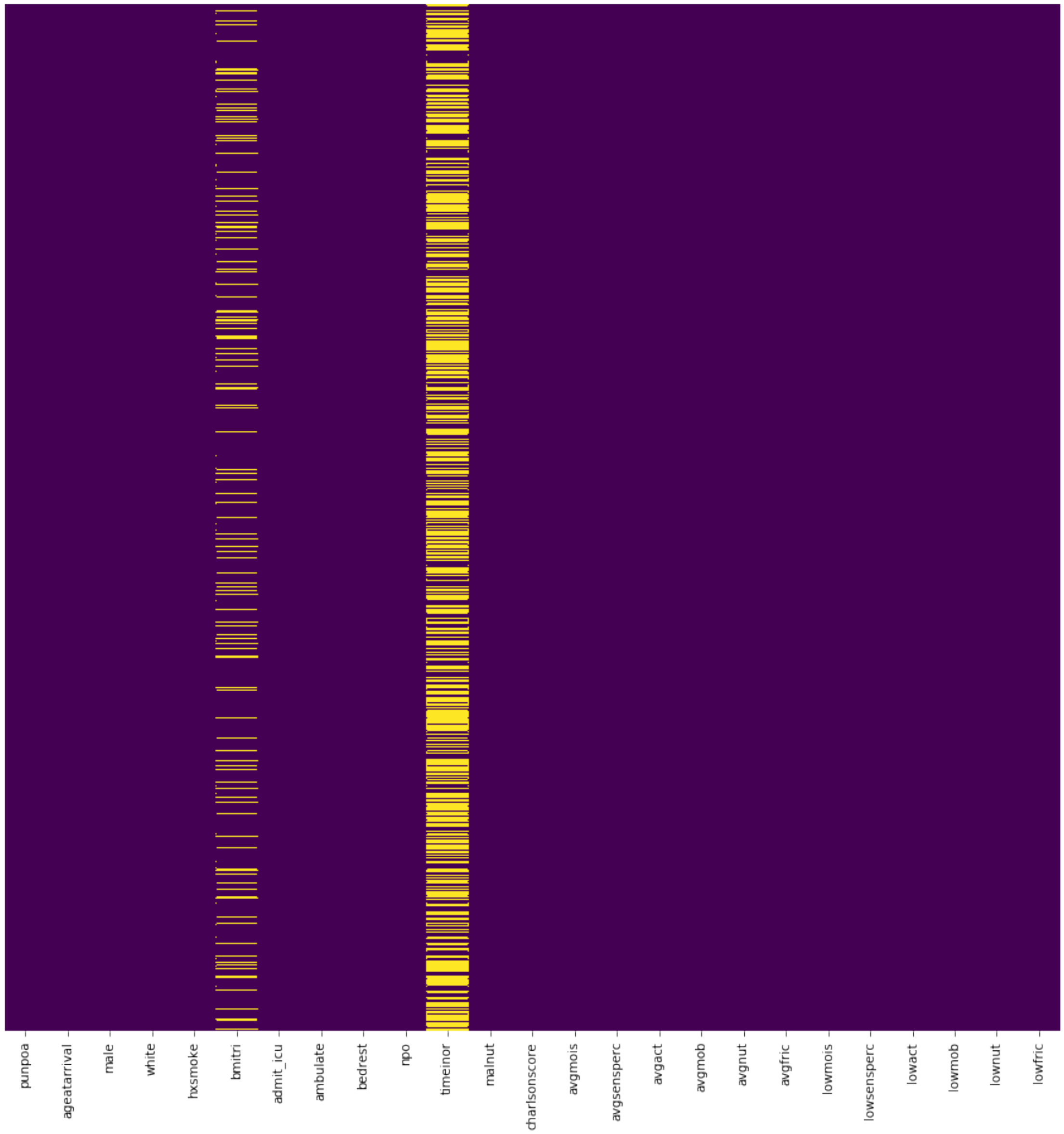
0.3 Predictor Coding and Selection

[28]:
```
# coding
df.loc[df['bmiadmission'] < 18.5, 'bmitri'] = -1
df.loc[(df['bmiadmission'] >= 18.5) & (df['bmiadmission'] < 35), 'bmitri'] = 0
df.loc[df['bmiadmission'] >= 35, 'bmitri'] = 1
df.loc[:,'wgtchgcat'] = df.loc[:,'wgtchgcat'].map({b'lost > 2 lbs':-1,b'< 2 lb␣
↪change':0,b'gained > 2 lbs':1})

# punpoa is target of interest
m3 = ['punpoa', 'ageatarrival', 'male',  'white', 'hxsmoke', 'bmitri',␣
↪'admit_icu',
      'ambulate', 'bedrest', 'npo', 'timeinor', 'malnut',␣
↪'charlsonscore','avgmois',
      'avgsensperc', 'avgact', 'avgmob', 'avgnut', 'avgfric',
      'lowmois', 'lowsensperc', 'lowact', 'lowmob', 'lownut', 'lowfric']
df = df[m3]
```

0.4 Plot Missingness

[9]:
```
fig, ax = plt.subplots(figsize=(15,15))
sns.heatmap(df.isnull(),yticklabels=False,cbar=False,cmap='viridis')
```

[9]: <matplotlib.axes._subplots.AxesSubplot at 0x1a4c7dc0b8>



0.5 Split Data into Training/Validation

[32]:
```
X,y = df.drop(columns=['punpoa']),df['punpoa']
X_train, X_test, y_train, y_test = train_test_split(X, y, train_size=0.80,␣
↪stratify=y.values, random_state=42)
```

0.6 Imputation

[34]:
```
imputer=IterativeImputer(sample_posterior=True).fit(X_train.values)
X_train.iloc[:,:] = imputer.transform(X_train.values)
X_test.iloc[:,:] = imputer.transform(X_test.values)
```

1 Main Functions

- Grid search (did bulk of search in other repositories and added ideal search parameters here)

- SHAP

- Bootstrapped AUC
- Sensitivity Analysis

- Additional plotting of ROC and SHAP per patient

[35]:
```
def perform_grid_search(estimator, options, param_grid, no_grid, X_train,␣
↪X_test, y_train, y_test, return_probs=True):
    if 'random_state' in list(inspect.getargspec(estimator))[0]:
        options['random_state']=42
    if not no_grid:
        grid_search = GridSearchCV(estimator=estimator(**options),␣
↪param_grid=param_grid, scoring='roc_auc', cv=5, verbose=False)
        grid_search.fit(X_train,y_train)
        best_params=grid_search.best_params_
    else:
        best_params=options
    options.update(best_params)
    best_estimator=estimator(**options)
    best_estimator.fit(X_train,y_train)
    y_pred=best_estimator.predict(X_test)
    if 'predict_proba' in dir(best_estimator) and return_probs:
        y_pred_probs=best_estimator.predict_proba(X_test)[:,1]
    else:
        y_pred_probs = y_pred
    fpr, tpr, thresholds = roc_curve(y_test, y_pred_probs,␣
↪drop_intermediate=False)
    roc_df = pd.DataFrame(np.vstack([fpr,tpr,thresholds]).
↪T,columns=['1-Specificity','Sensitivity','Thresholds'])
    results=pd.DataFrame(np.vstack([y_test.values,y_pred,y_pred_probs]).
↪T,columns=['y_true','y_pred','y_pred_probs'])
    return best_estimator, roc_df, results
```

```
def run_shap(X_train, X_test, best_estimator, model_type='tree',␣
↪explainer_options={}, get_shap_values_options={}, overall=False):

    shap.initjs()

    shap_model={'tree':shap.TreeExplainer,'kernel':shap.
↪KernelExplainer,'linear':shap.LinearExplainer}[model_type]

    explainer = shap_model(best_estimator, X_train,**explainer_options)

    shap_values = explainer.shap_values(X_test,**get_shap_values_options)

    if model_type=='tree' and best_estimator.__class__.__name__!
↪='XGBClassifier':
        shap_values=np.array(shap_values)[1,...]

    shap.summary_plot(shap_values, X_test,feature_names=list(X_train),␣
↪plot_type='bar' if overall else 'dot', max_display=30)

    return explainer, shap_values

def extract_ys(Y):
    return Y[:,0], Y[:,1]

def auc(Y):
    y_true, y_pred=extract_ys(Y)
    return roc_auc_score(y_true, y_pred)

def return_bootstrap_results(results,fn,round_place=1):
    Y=results[['y_true','y_pred_probs']].values
    original, std_err, ci_bounds = bootstrap(Y, num_rounds=1000,
                                            func=fn,
                                            ci=0.95,
                                            seed=123)
    std_err=format_float_scientific(std_err,round_place)
    if float(std_err) >= 0.001:
        std_err=float(std_err)

    return "{}±{}".
↪format(float(format_float_scientific(original,round_place)),2*std_err)

def plot_roc(roc_df, results):
    plt.figure()
    ax=sns.lineplot('1-Specificity','Sensitivity',data=roc_df)
    plt.title("AUC: {}".
↪format(return_bootstrap_results(results,auc,2)))#roc_auc_score(results['y_true'],␣
↪results['y_pred_probs']))
```

```
    plt.xlabel('1-Specificity')
    plt.ylabel('Sensitivity')

def get_nearest(arr,vals=np.arange(0.1,1.,0.1)):
    idx=[]
    for val in vals:
        idx.append(np.argmin(np.abs(arr-val)))
    return np.array(idx)

def sensitivity_analysis(roc_df, intervals=0.1):
    df=roc_df.iloc[get_nearest(roc_df['Thresholds'].values,np.
 ↪arange(intervals,1.,intervals))]
    df['Specificity']=1.-df['1-Specificity']
    df=round(df[['Sensitivity','Specificity','Thresholds']].
 ↪reset_index(drop=True),2)
    return df

def shap_patient(i, explainer, shap_values, logistic=True, tree=False):
    opts={}
    expected=explainer.expected_value
    if logistic:
        opts=dict(link='logit')
    if tree:
        expected=explainer.expected_value[1]
    shap.force_plot(expected, shap_values[i, :], X_test.values[i, :],␣
 ↪feature_names=list(X_test), matplotlib=True, show=True, **opts)

def plot_rocs(roc_dict):
    for k in roc_dict:
        roc_dict[k]['Method']=k
    df=pd.concat(list(roc_dict.values()))
    plt.rcParams['figure.dpi']=300
    plt.figure(figsize=(10,10))
    plt.plot([0,1],[0,1],'--')
    sns.lineplot('1-Specificity','Sensitivity',hue='Method',data=df)
```

1.1 Return Estimators

- Logistic Regression
- Naive Bayes
- Decision Trees
- Random Forest

- XGBoost

[37]:
```
# already performed hyperparameter sweep; unpenalized model = interpretable␣
↪coefficients
best_estimator_lr, roc_df_lr, results_lr=␣
↪perform_grid_search(LogisticRegression,
                    options={'class_weight':'balanced','penalty': 'none',␣
↪'solver':'lbfgs'},
                    param_grid={'C':[np.inf]},
                    no_grid=False,
                    X_train=X_train,
                    X_test=X_test,
                    y_train=y_train,
                    y_test=y_test)
```

[38]:
```
# no hyperparameter sweep necessary
best_estimator_nb, roc_df_nb, results_nb= perform_grid_search(GaussianNB,
                    options={},
                    param_grid={},
                    no_grid=True,
                    X_train=X_train,
                    X_test=X_test,
                    y_train=y_train,
                    y_test=y_test)
```

[39]:
```
# already performed hyperparameter sweep
best_estimator_dt, roc_df_dt, results_dt=␣
↪perform_grid_search(DecisionTreeClassifier,
                    options={'class_weight':'balanced','max_features':24},
                    param_grid={'max_depth':[20],
                               'min_samples_split':[0.6],
                               'min_samples_leaf':[0.4]},
                    no_grid=False,
                    X_train=X_train,
                    X_test=X_test,
                    y_train=y_train,
                    y_test=y_test,
                    return_probs=True)
```

[18]:
```
# last stage of hyperparameter sweep
best_estimator_rf, roc_df_rf, results_rf=␣
↪perform_grid_search(BalancedRandomForestClassifier,
                    options={'n_jobs':1},
                    param_grid={'max_features':['sqrt', 'log2'],
                               'max_depth':[4,20],
                               'n_estimators':[10,20,80]},
                    no_grid=False,
```

```
                        X_train=X_train,
                        X_test=X_test,
                        y_train=y_train,
                        y_test=y_test)
```

inspect.getargspec() is deprecated since Python 3.0, use inspect.signature() or inspect.getfullargspec()

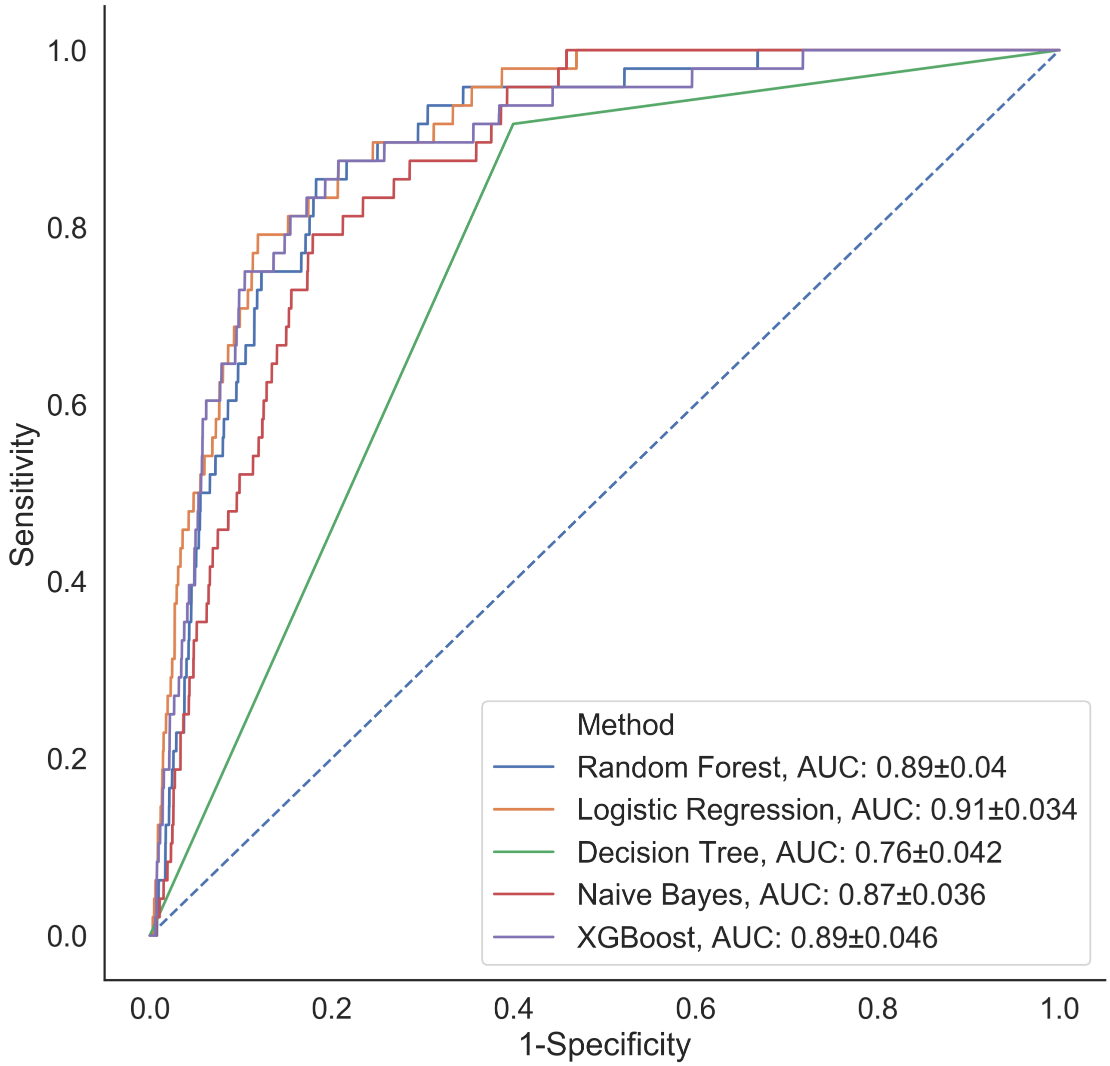
[19]:
```
# last stage of hyperparameter sweep
best_estimator_xg, roc_df_xg, results_xg= perform_grid_search(XGBClassifier,
                        options={'scale_pos_weight' : 56986/241, 'objective' :␣
 ↪'binary:logistic'},
                        param_grid={'learning_rate': [0.1],
                                      'n_estimators': [100],
                                      'max_depth': list(range(2,10,2)),
                                      'min_child_weight':list(range(1,6,2))},
                        no_grid=False,
                        X_train=X_train,
                        X_test=X_test,
                        y_train=y_train,
                        y_test=y_test)
```

inspect.getargspec() is deprecated since Python 3.0, use inspect.signature() or inspect.getfullargspec()

0:03:25.294751

1.2 Plot ROCs

[46]:
```
import matplotlib
matplotlib.rcParams['figure.dpi']=400
sns.set(style='white', font_scale=1.5)
np.random.seed(123)

roc_dict={'Random Forest, AUC: {}'.
 ↪format(return_bootstrap_results(results_rf,auc,1)):roc_df_rf,
           'Logistic Regression, AUC: {}'.
 ↪format(return_bootstrap_results(results_lr,auc,1)):roc_df_lr,
           'Decision Tree, AUC: {}'.
 ↪format(return_bootstrap_results(results_dt,auc,1)):roc_df_dt,
           'Naive Bayes, AUC: {}'.
 ↪format(return_bootstrap_results(results_nb,auc,1)):roc_df_nb,
           'XGBoost, AUC: {}'.format(return_bootstrap_results(results_xg,auc,1)):
 ↪roc_df_xg}#
plot_rocs(roc_dict)
sns.despine()
```

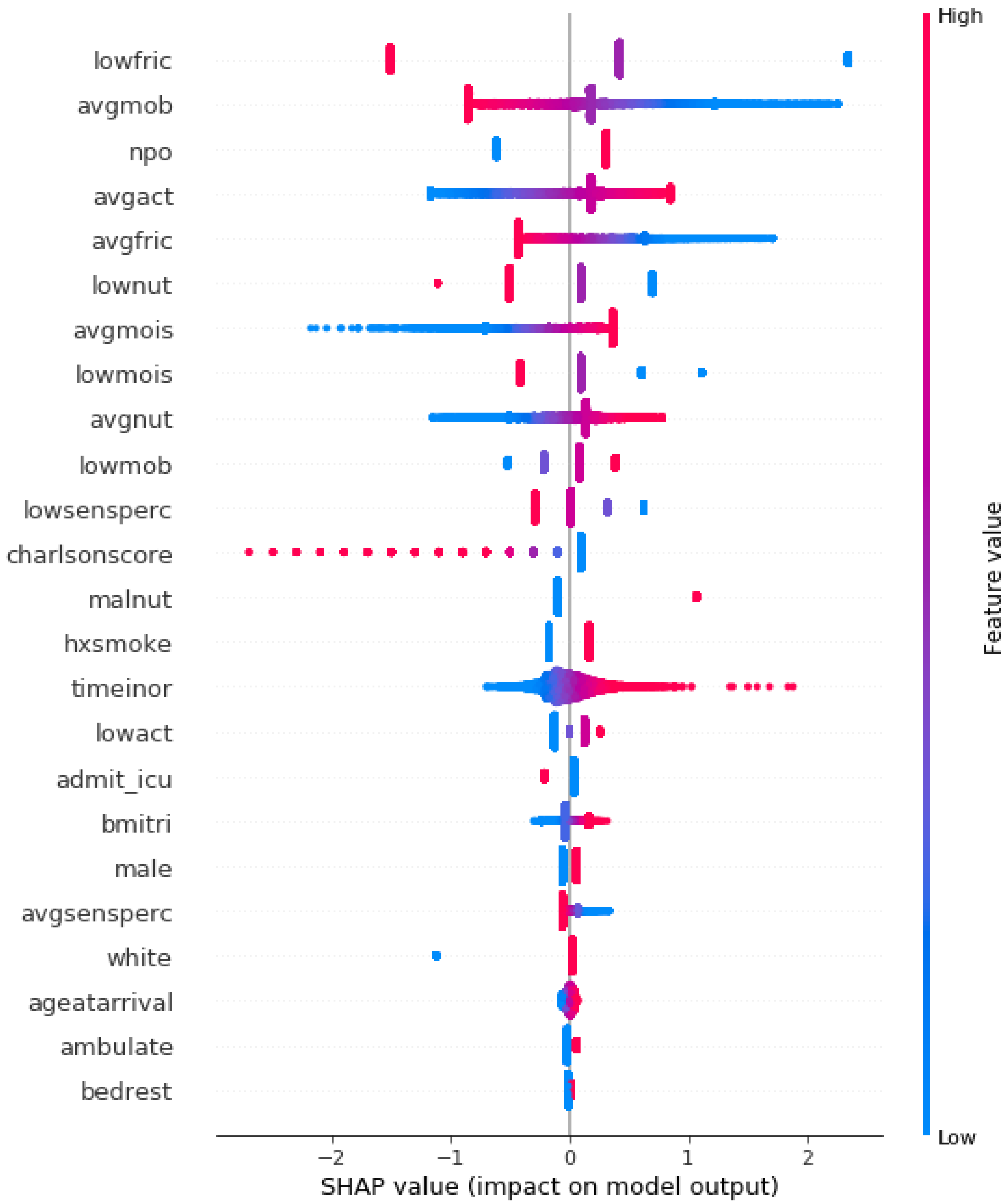


1.3 SHAP Summary and Force Plots

- Logistic Regression
- Random Forest
- XGBoost

[19]:
```
explainer_lr,shap_values_lr=run_shap(X_train, X_test, best_estimator_lr,␣
↪model_type='linear', explainer_options={}, get_shap_values_options={})
shap_importances=dict(lr=pd.DataFrame(np.abs(shap_values_lr).
↪mean(0),index=list(X_train)).sort_values([0],ascending=False))
```

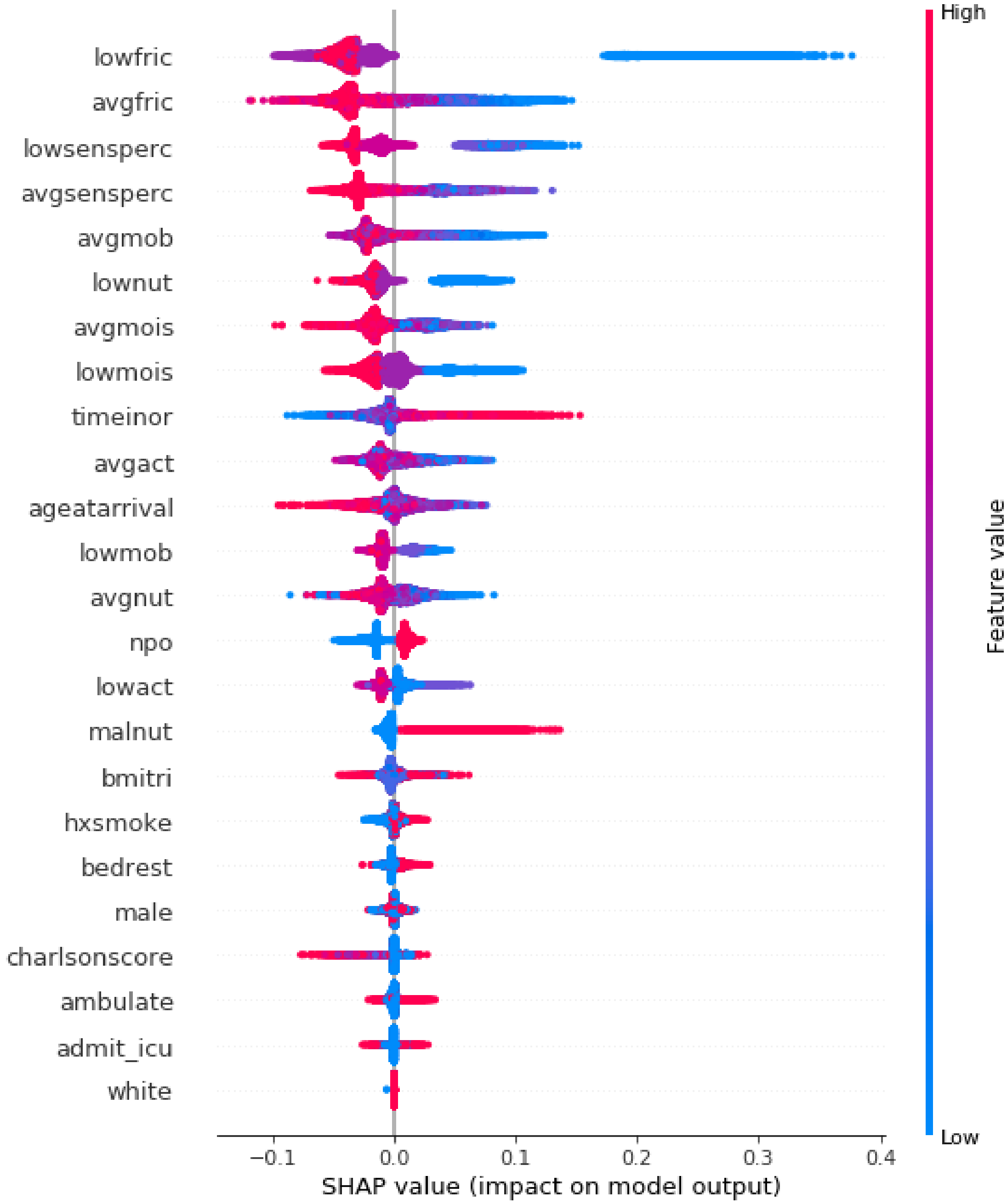
```
<IPython.core.display.HTML object>
```



[33]:
```
explainer_rf,shap_values_rf=run_shap(X_train, X_test, best_estimator_rf,␣
↪model_type='tree', explainer_options={},␣
↪get_shap_values_options=dict(approximate=True))
shap_importances.update(dict(rf=pd.DataFrame(np.abs(shap_values_rf).
↪mean(0),index=list(X_train)).sort_values([0],ascending=False)))
```

```
<IPython.core.display.HTML object>
```

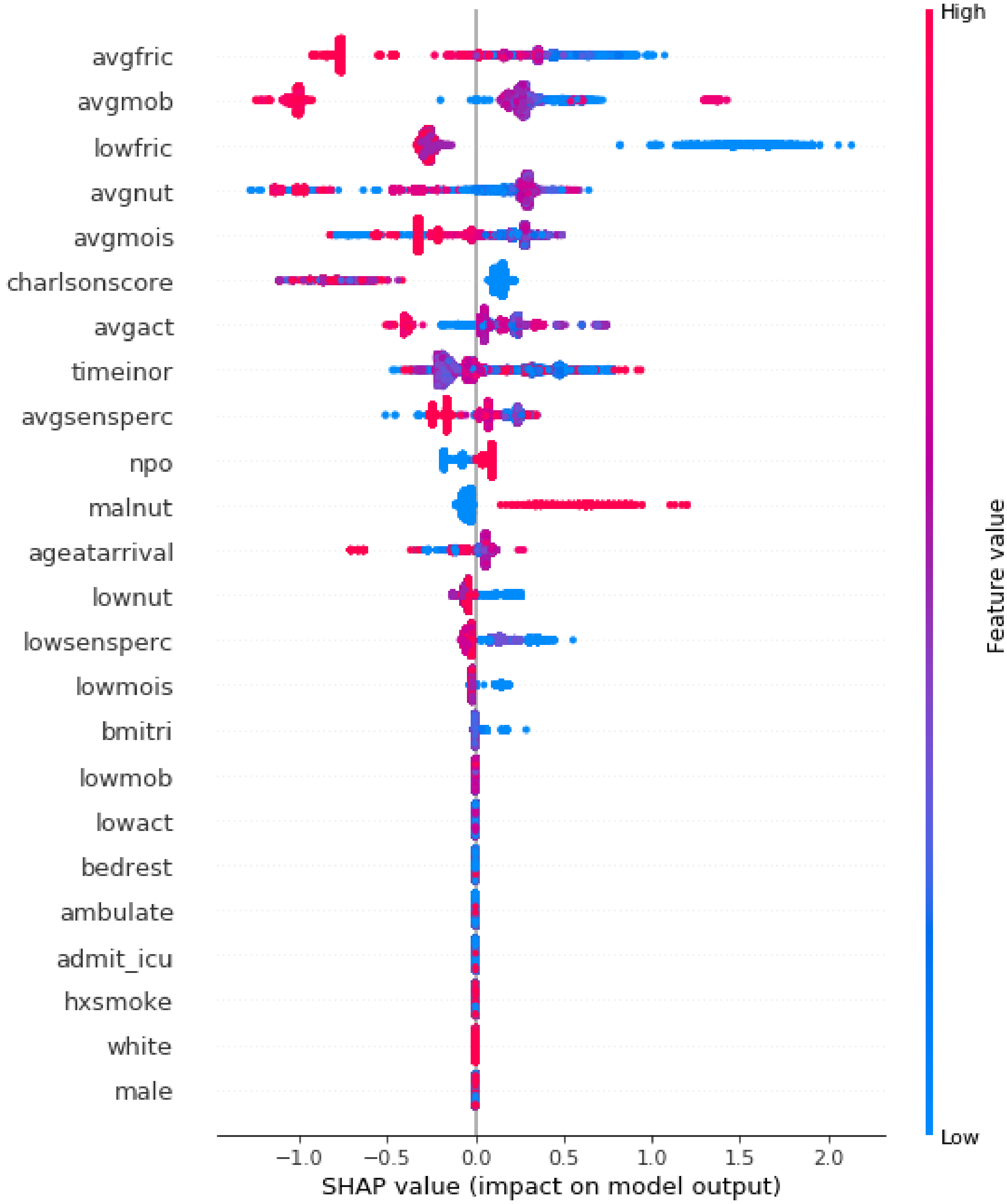
```
Passing 45781 background samples may lead to slow runtimes. Consider using
shap.sample(data, 100) to create a smaller background data set.
```



[30]:
```
explainer_xg,shap_values_xg=run_shap(X_train, X_test, best_estimator_xg,␣
↪model_type='tree', explainer_options={}, get_shap_values_options={})
```

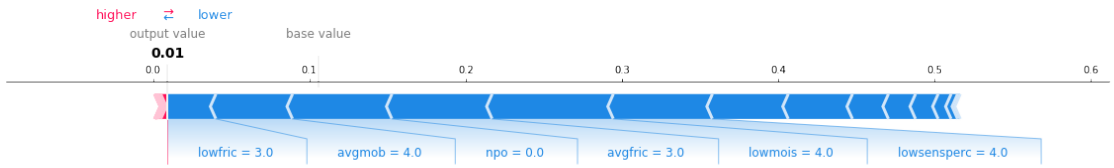
```
shap_importances.update(dict(xg=pd.DataFrame(np.abs(shap_values_xg).
↪mean(0),index=list(X_train)).sort_values([0],ascending=False)))
```

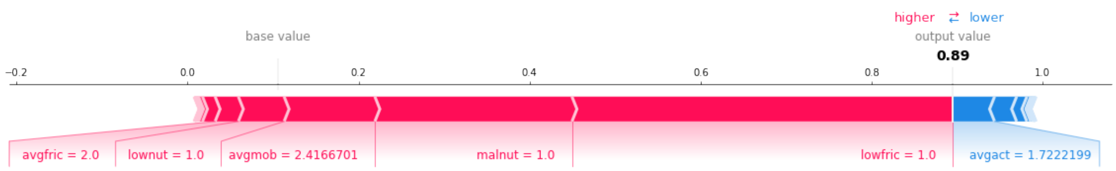
```
<IPython.core.display.HTML object>
```



[21]:

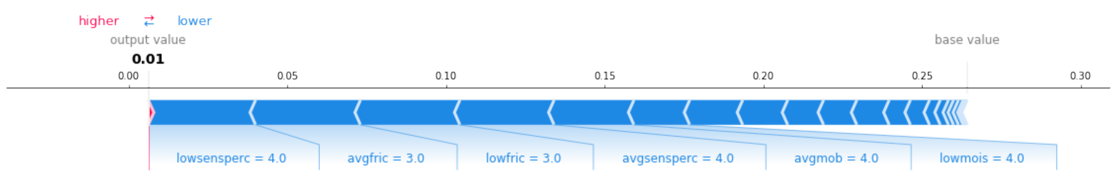
```
i=7
shap_patient(i, explainer_lr, shap_values_lr, logistic=True)
i=300
shap_patient(i, explainer_lr, shap_values_lr, logistic=True)
```

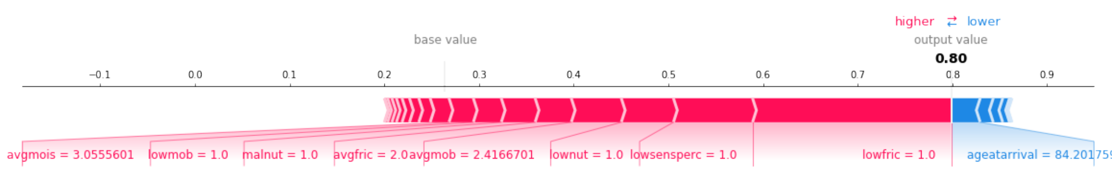




[38]:

```
i=7
shap_patient(i, explainer_rf, shap_values_rf, logistic=False,tree=True)
i=300
shap_patient(i, explainer_rf, shap_values_rf, logistic=False,tree=True)
```





[ ]:
```
i=7
shap_patient(i, explainer_xg, shap_values_xg, logistic=False,tree=False)
i=300
shap_patient(i, explainer_xg, shap_values_xg, logistic=False,tree=False)
```

1.4 SHAP Force Plots Across Cohort

- Logistic Regression
- Random Forest
- XGBoost

[ ]:
```
shap.initjs()
shap.force_plot(explainer_lr.expected_value, shap_values_lr[:300],link='logit')
```

[ ]:
```
shap.initjs()
shap.force_plot(explainer_rf.expected_value[0], shap_values_rf[:300])
```

[ ]:
```
shap.initjs()
shap.force_plot(explainer_xg.expected_value, shap_values_xg[:300])
```

1.5 Compare LR, RF, XGBoost SHAP Importances

[32]:
```
for k in shap_importances:
    shap_importances[k]=shap_importances[k].loc[list(X_train)]
```

[33]:
```
from scipy.stats import spearmanr
df_rank=pd.DataFrame(columns=list(shap_importances.
 ↪keys()),index=list(shap_importances.keys()))
for k in shap_importances:
    for k2 in shap_importances:
        df_rank.loc[k,k2]=','.join([str(round(x,4)) for x in␣
 ↪spearmanr(shap_importances[k], shap_importances[k2])])
```

[34]:
```
# rank ordered
df_importance=pd.concat(shap_importances.values(),axis=1)
df_importance.columns=['lr','rf','xg']
df_importance=df_importance.iloc[np.argsort(-df_importance['lr'])].apply(lambda␣
 ↪x: np.argsort(-x),axis=0)
df_importance+1
```

[34]:

	lr	rf	xg
lowfric	1	1	5
avgmob	2	5	2
lownut	3	11	1
npo	4	3	8
avgfric	5	19	6
avgmois	6	6	12
avgact	7	16	7
avgnut	8	2	16
lowmois	9	9	19
lowmob	10	4	4
lowsensperc	11	7	14
charlsonscore	12	15	24
hxsmoke	13	14	3
malnut	14	8	11
lowact	15	24	9
timeinor	16	10	22
admit_icu	17	13	13
white	18	20	10
avgsensperc	19	22	17
ambulate	20	12	18
male	21	23	20
bmitri	22	21	21
bedrest	23	17	23
ageatarrival	24	18	15

[35]:

```
# raw values
df_importance=pd.concat(shap_importances.values(),axis=1)
df_importance.columns=['lr','rf','xg']
df_importance=df_importance.iloc[np.argsort(-df_importance['lr'])]
df_importance
```

[35]:

	lr	rf	xg
lowfric	1.077155	0.063974	0.445495
avgmob	0.444859	0.014991	0.496902
lownut	0.426227	0.026242	0.081018
npo	0.399199	0.012205	0.091580
avgfric	0.372795	0.039484	0.498970
avgmois	0.338860	0.023171	0.237259
avgact	0.322387	0.010141	0.195262
avgnut	0.288830	0.009063	0.380236
lowmois	0.251743	0.012955	0.031901
lowmob	0.224512	0.007830	0.000000
lowsensperc	0.200263	0.030168	0.076142
charlsonscore	0.177295	0.002507	0.234391
hxsmoke	0.175196	0.003645	0.000000
malnut	0.169195	0.009453	0.090302

lowact	0.111169	0.009586	0.000000
timeinor	0.084059	0.018423	0.193365
admit_icu	0.056460	0.001027	0.000000
white	0.051750	0.000003	0.000000
avgsensperc	0.049866	0.026165	0.168168
ambulate	0.048464	0.003567	0.000000
male	0.045987	0.001865	0.000000
bmitri	0.033076	0.003149	0.007451
bedrest	0.014670	0.002198	0.000000
ageatarrival	0.010834	0.009001	0.081082

1.6 Compare Logistic Regression SHAP with Normalized Regression Coefficients

[350]:

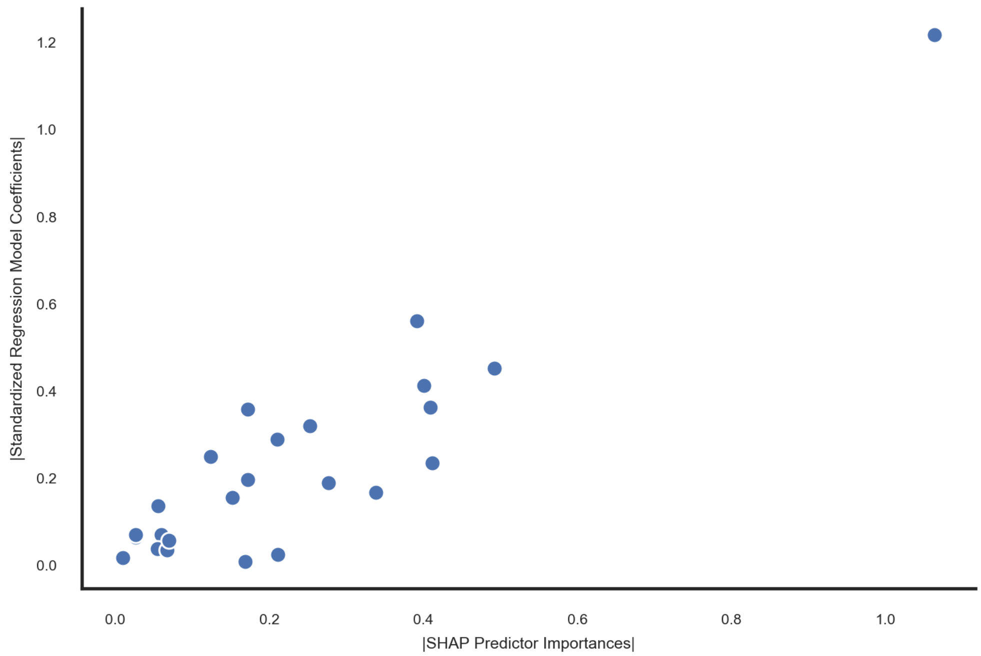
```
import statsmodels.api as sm
import numpy as np
import statsmodels
from sklearn.preprocessing import StandardScaler
np.random.seed(42)

class SMWrapper(BaseEstimator, RegressorMixin):
    """ A universal sklearn-style wrapper for statsmodels regressors https://
↪stackoverflow.com/questions/41045752/
↪using-statsmodel-estimations-with-scikit-learn-cross-validation-is-it-possible"""
    def __init__(self, model_class, fit_intercept=True, kwargs=dict()):
        self.model_class = model_class
        self.fit_intercept = fit_intercept
        self.kwargs=kwargs
    def fit(self, X, y):
        if self.fit_intercept:
            X = sm.add_constant(X)
        self.model_ = self.model_class(y, X, **self.kwargs)
        self.results_ = self.model_.fit()
    def predict(self, X):
        if self.fit_intercept:
            X = sm.add_constant(X)
        return self.results_.predict(X)
LogReg=SMWrapper(sm.GLM,kwargs=dict(family=sm.families.Binomial()))
LogReg.fit(X_train,y_train)

X_train2 = sm.add_constant(StandardScaler().fit_transform(X_train))
y_train2 = y_train
LogReg.fit(X_train2,y_train2)
res=pd.read_html(LogReg.results_.summary().tables[1].as_html(),header=0,␣
↪index_col=0)[0]
res.index=['const']+list(X_train)
```

[353]:

```
sns.set(font_scale=0.5,style='white')
sns.scatterplot(np.abs(shap_values_lr).mean(0),res['coef'].iloc[1:].abs())
sns.despine()
plt.xlabel('|SHAP Predictor Importances|')
plt.ylabel('|Standardized Regression Model Coefficients|')
```

[353]:

```
Text(0, 0.5, '|Standardized Regression Model Coefficients|')
```



[336]:
```
from scipy.stats import pearsonr
pearsonr(np.abs(shap_values_lr).mean(0),res['coef'].iloc[1:].abs())
```

[336]: (0.9137826728973484, 4.5060919640262534e-10)