HAPI_Supplementary_Analyses_paper

May 21, 2022

[755]:
```
import pickle
import warnings
warnings.filterwarnings('ignore')
import pandas as pd, os
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, RandomizedSearchCV,␣
 ↪cross_val_score, StratifiedKFold
import sklearn.metrics
from sklearn.model_selection import train_test_split
import matplotlib.pyplot as plt
import seaborn as sns
from sklearn.tree import plot_tree
%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
import copy
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, glob
from mlxtend.evaluate import bootstrap
from sklearn.metrics import roc_curve, roc_auc_score
from numpy import format_float_scientific
from imblearn.ensemble import BalancedRandomForestClassifier
import inspect
```

```
import datetime
from sklearn.base import ClassifierMixin, BaseEstimator
import numpy as np
import matplotlib.pyplot as plt
from numpy.random import RandomState
from numpy.testing import assert_almost_equal
import pymc as pm
import pymc_experimental as pmx
from scipy.special import expit
import aesara
import aesara.tensor as T
from sklearn.metrics import roc_auc_score
from sklearn.neural_network import MLPClassifier
from sklearn.discriminant_analysis import LinearDiscriminantAnalysis,␣
↪QuadraticDiscriminantAnalysis
from sklearn.svm import LinearSVC
from sklearn.neighbors import KNeighborsClassifier
import dask
from dask.diagnostics import ProgressBar
import tqdm
import xarray as xr
np.random.seed(42)
```

1 Models and Convenience Functions

[188]:
```
class BART(BaseEstimator, ClassifierMixin):
    def __init__(self, m=70, alpha=0.3, train_sample=100, test_sample=1000):
        self.m=m
        self.alpha=alpha
        self.train_sample=train_sample
        self.test_sample=test_sample

    def fit(self, X, y):
        y_=y.copy()
        with pm.Model() as model:
            data=pm.Data("data",X)
            mu = pmx.BART("mu", X, y_.astype(int).values, m=self.m, alpha=self.
↪alpha)#, response="mix"
            p = pm.Deterministic("p",pm.invlogit(mu))
            y = pm.Bernoulli("y", p, observed=y_.astype(int).values)
            self.idata = pm.sample(self.train_sample,tune=self.
↪train_sample,cores=4,random_seed=12345)
        self.model=model
        return self
```

```python
    def predict(self, X):
        return self.predict_proba(X).argmax(1)

    def predict_proba(self, X):
        proba=self.predict_bart(X)
        return np.vstack([1-proba,proba]).T

    def predict_bart(self, X_new=None, rng=np.random.RandomState(42)):
        if isinstance(X_new,pd.DataFrame): X_new=X_new.values
        stacked_trees=brt.idata.sample_stats.bart_trees.stack(trees=["chain", "draw"]).to_numpy()
        preds=[dask.delayed(lambda i: np.apply_along_axis(lambda x: np.vectorize(lambda tree: tree.predict(X_new[i]))(x),1,stacked_trees))(i) for i in tqdm.trange(len(X_new))]
        with ProgressBar():
            preds=np.array(dask.compute(*preds,scheduler='threading')).sum(2)
        proba=expit(preds).mean(1)
        return proba

class BayesLogisticRegression(BaseEstimator, ClassifierMixin):
    def __init__(self, train_sample=20000, test_sample=1000, learning_rate=1e-0, batch_size=1500, intercept_prior_sigma=100, parameter_prior_sigma=10):
        self.learning_rate=learning_rate
        self.batch_size=batch_size
        self.train_sample=train_sample
        self.test_sample=test_sample
        self.intercept_prior_sigma=intercept_prior_sigma
        self.parameter_prior_sigma=parameter_prior_sigma

    def fit(self, X, y):
        coords = {
            "col": np.arange(X.shape[1]),
            "obs_id": np.arange(len(X)),
        }
        y_=y.copy()
        with pm.Model(coords=coords) as model:
            data = pm.Data("data", X)
            data_y = pm.Data("data_y", y_.astype(np.int32).values)
            a = pm.Normal("a", 0, sigma=self.intercept_prior_sigma)
            b = pm.Normal("b", 0, sigma=self.parameter_prior_sigma, shape=(1, len(coords['col'])))
            mu = pm.Deterministic("mu",a + pm.math.dot(b,data.T).flatten())
            p = pm.Deterministic("p", pm.invlogit(mu))
            y = pm.Bernoulli("y", p=p, observed=data_y)

            X_batch = pm.Minibatch(X, batch_size=self.batch_size)
```

```
            Y_batch = pm.Minibatch(y_.astype(np.int32).values, batch_size=self.
↪batch_size)

            approx = pm.fit(n=self.train_sample, obj_optimizer=pm.
↪adagrad(learning_rate=self.learning_rate),
                           more_replacements={data: X_batch, data_y:␣
↪Y_batch},random_seed=456)
        self.model=model
        self.approx=approx
        return self

    def predict(self, X):
        return self.predict_proba(X).argmax(1)

    def predict_proba(self, X):
        for i in range(2):
            trace = self.approx.sample(draws=self.test_sample)
            pm.set_data({"data": X}, model=self.model)
            ppc_test = pm.sample_posterior_predictive(trace, model=self.model,␣
↪var_names=['y','p'])
            p_test_pred = ppc_test.posterior_predictive["p"]
        proba=p_test_pred[0,...].mean(axis=0)
        return np.vstack([1-proba,proba]).T

class NaivelyCalibratedLinearSVC(LinearSVC):
    """LinearSVC with `predict_proba` method that naively scales
    `decision_function` output for binary classification. From scikit-learn␣
↪website."""

    def fit(self, X, y):
        super().fit(X, y)
        df = self.decision_function(X)
        self.df_min_ = df.min()
        self.df_max_ = df.max()
        return self

    def predict_proba(self, X):
        """Min-max scale output of `decision_function` to [0, 1]."""
        df = self.decision_function(X)
        calibrated_df = (df - self.df_min_) / (self.df_max_ - self.df_min_)
        proba_pos_class = np.clip(calibrated_df, 0, 1)
        proba_neg_class = 1 - proba_pos_class
        proba = np.c_[proba_neg_class, proba_pos_class]
        return proba
```

[522]:

```python
def perform_grid_search(estimator, options, param_grid, no_grid, X_train,␣
↪X_test, y_train, y_test, return_probs=True, add_random=True,␣
↪return_scores=False):
    if add_random: 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)
    if not return_scores:
        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
    else: return␣
↪cross_val_score(best_estimator,X_train,y_train,scoring='roc_auc', cv=5)

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.
↪reset_index(drop=True))
    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)
```

```python
    return df

def shap_patient(i, explainer, shap_values, logistic=True, tree=False, waterfall=False):
    opts={}
    expected=explainer.expected_value
    if logistic:
        opts=dict(link='logit')
    if tree:
        expected=explainer.expected_value[1]
    if not waterfall:
        shap.force_plot(expected, shap_values[i, :], X_test.values[i, :], feature_names=list(X_test), matplotlib=True, show=True, **opts)
    else:
        shap.plots.waterfall(expected, shap_values[i, :], X_test.values[i, :])

def plot_rocs(roc_dict):
    for k in roc_dict:
        roc_dict[k]['Method']=k
    df=pd.concat(list(roc_dict.values())).reset_index(drop=True)
    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)

def get_best_results(best_estimator, X_test, y_test, return_probs=True):
    if 'predict_proba' in dir(best_estimator) and return_probs:
        y_pred_probs=best_estimator.predict_proba(X_test)[:,1]
    y_pred=y_pred_probs>=0.5
    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 return_cv_results(mod,X_train,y_train, params={}):
    y_cv_res=[]
    for train_idx,val_idx in StratifiedKFold(random_state=42,shuffle=True).split(X_train,y_train):
        mod_new=(copy.deepcopy(mod) if not params else mod(**params)).fit(X_train.iloc[train_idx],y_train.iloc[train_idx])
        y_cv_res.append(dict(y_val=y_train.iloc[val_idx],y_pred=mod_new.predict_proba(X_train.iloc[val_idx])[:,1]))
    return y_cv_res
```

2 Load Data

[191]:
```
if not os.path.exists("data_new.pkl"):
    df = pd.read_sas('hapudataset.sas7bdat')

    # 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]

    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)
    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)
    pd.to_pickle(dict(X_train=X_train, X_test=X_test, y_train=y_train,␣
↪y_test=y_test),"data_new.pkl")
else:
    data=pd.read_pickle("data_new.pkl")
    X_train, X_test, y_train, y_test=data['X_train'], data['X_test'],␣
↪data['y_train'], data['y_test']
```

3 Fit Models

[13]:
```
results=dict()
```

[528]:
```
results["bart"]=perform_grid_search(BART,
                    options={},
                    param_grid={'alpha': [0.3,0.5,0.7],
                                'm': [10,20,30,50]},
                    no_grid=False,
```

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

```
Only 15 samples in chain.
WARNING:pymc:Only 15 samples in chain.
Multiprocess sampling (4 chains in 4 jobs)
INFO:pymc:Multiprocess sampling (4 chains in 4 jobs)
PGBART: [mu]
INFO:pymc:PGBART: [mu]

<IPython.core.display.HTML object>

<IPython.core.display.HTML object>

Sampling 4 chains for 15 tune and 15 draw iterations (60 + 60 draws total) took
60 seconds.
INFO:pymc:Sampling 4 chains for 15 tune and 15 draw iterations (60 + 60 draws
total) took 60 seconds.
100%|
            | 11446/11446 [00:00<00:00, 19436.53it/s]

[########################################] | 100% Completed |  2min  5.1s
```

[ ]:
```
results["blr"]=perform_grid_search(BayesLogisticRegression,
                    options={},
                    param_grid={'batch_size': [500,1000,1500,2500],
                                'learning_rate': [1,1e-1,1e-2]},
                    no_grid=False,
                    X_train=X_train,
                    X_test=X_test,
                    y_train=y_train,
                    y_test=y_test)
```

[224]:
```
svc=NaivelyCalibratedLinearSVC(random_state=42,penalty='l2',dual=False).
 ↪fit(X_train,y_train)
results["svc"]=get_best_results(svc, X_test, y_test)

results["svc"]=perform_grid_search(NaivelyCalibratedLinearSVC,
                    options=dict(random_state=42,dual=False),
                    param_grid=dict(penalty=['l1','l2'],
                         C=[0.01,0.1,1,10,100]),
                    no_grid=False,
                    X_train=X_train,
                    X_test=X_test,
                    y_train=y_train,
                    y_test=y_test,
                    verbose=True,
```

```
                    random=True)
```

[284]:
```
results["nn"]=perform_grid_search(MLPClassifier,
                    options=dict(random_state=42),
                    param_grid=dict(hidden_layer_sizes=[(100,),
                                                        (30,30),
                                                        (30,200,30)],
                                   alpha=[0.0001,0.001,0.01],
                                   learning_rate_init=[1e-1,1e-2,1e-3]),
                    no_grid=False,
                    X_train=X_train,
                    X_test=X_test,
                    y_train=y_train,
                    y_test=y_test,
                    verbose=True,
                    random=True)
```

[226]:
```
results["knn"]=perform_grid_search(KNeighborsClassifier,
                    options=dict(),
                    param_grid=dict(n_neighbors=[5,10,25,35,65,75,100]),
                    no_grid=False,
                    X_train=X_train,
                    X_test=X_test,
                    y_train=y_train,
                    y_test=y_test,
                    verbose=True,
                    random=False)
```

[227]:
```
results["lda"]=perform_grid_search(LinearDiscriminantAnalysis,
                    options=dict(),
                    param_grid=dict(shrinkage=[None,'auto',0.1,0.5,0.8]),
                    no_grid=False,
                    X_train=X_train,
                    X_test=X_test,
                    y_train=y_train,
                    y_test=y_test,
                    verbose=True,
                    random=False)
```

[228]:
```
results["qda"]=perform_grid_search(QuadraticDiscriminantAnalysis,
                    options=dict(),
                    param_grid=dict(reg_param=[0,0.2,0.5,0.8,1.]),
                    no_grid=False,
                    X_train=X_train,
                    X_test=X_test,
                    y_train=y_train,
                    y_test=y_test,
```

```
                    verbose=True,
                    random=False)
```

[229]:
```
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)
```

[230]:
```
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,
                                 add_random=False)
```

[231]:
```
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)
```

[232]:
```
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)
```

[233]:
```python
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)
```

4 Compile CV and Test Set Results

[530]:
```python
for k in results:
    if not isinstance(results[k],dict):
        results[k]=dict(zip(["best_estimator","roc_df","results"],results[k]))
```

[510]:
```python
cv_results={}
for k in results:
    if k not in ['bart','blr']:
        cv_results[k]=return_cv_results(results[k]['best_estimator'],X_train,y_train)
cv_results['blr']=return_cv_results(BayesLogisticRegression,X_train,y_train,results['blr']['be
get_params())
cv_results['bart']=return_cv_results(BART,X_train,y_train,results['bart']['best_estimator'].get_params())
```

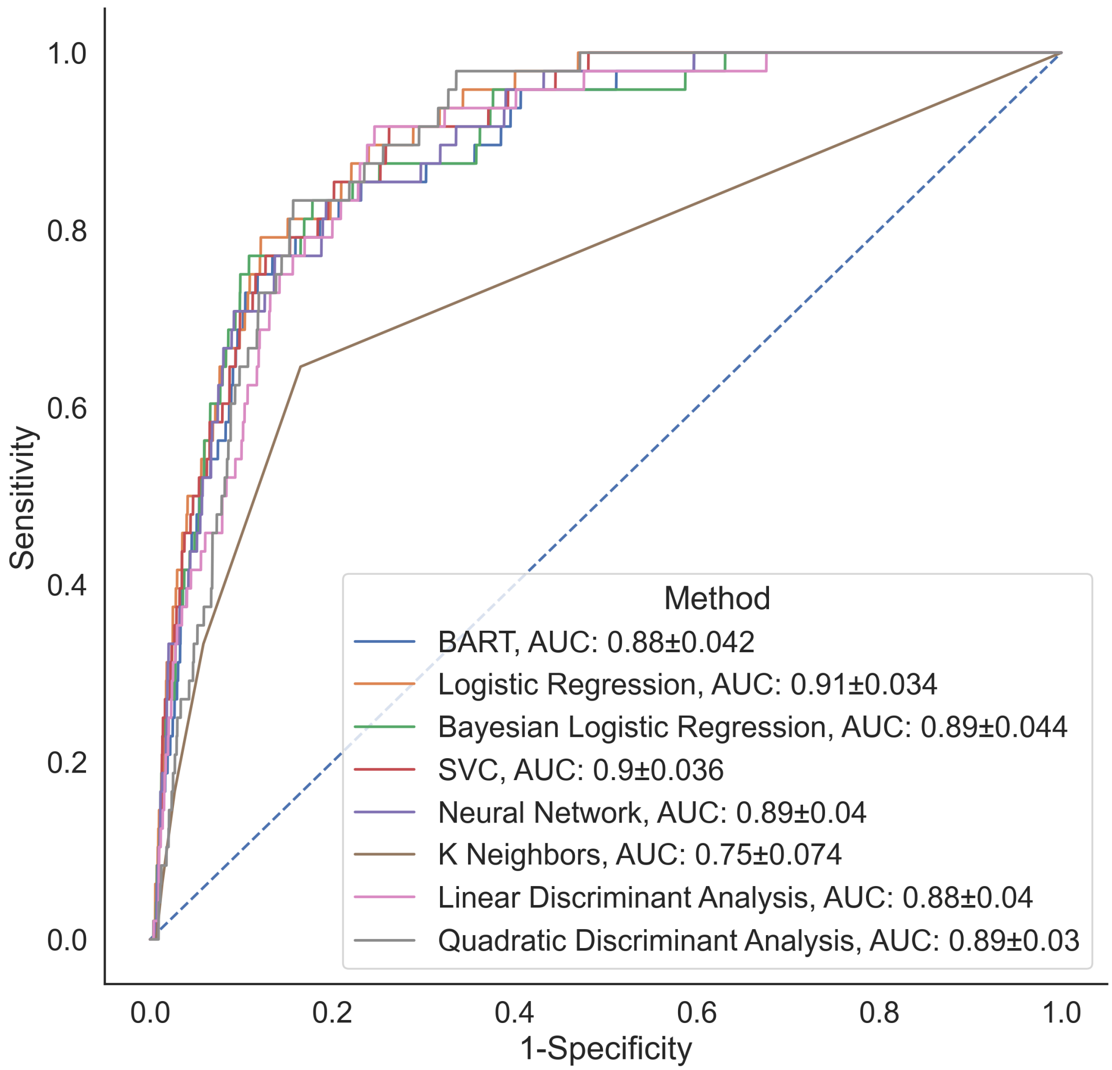
[526]:
```python
pd.to_pickle(cv_results,"cv_results.pkl")
```

[238]:
```python
for k in results:
    try:
        pd.to_pickle(results[k],f"model_results/{k}.pkl")
    except:
        pass
```

[846]:
```python
if False: results={os.path.basename(f).replace(".pkl",""):pd.read_pickle(f) for f in glob.glob("model_results/*")}
```

5 Visualize Comparison Methods

[287]:
```
import matplotlib
matplotlib.rcParams['figure.dpi']=400
sns.set(style='white', font_scale=1.5)
np.random.seed(123)

roc_dict={
          'BART, AUC: {}'.
 ↪format(return_bootstrap_results(results['bart']['results'],auc,1)):
 ↪results['bart']['roc_df'],
          'Logistic Regression, AUC: {}'.
 ↪format(return_bootstrap_results(results['lr']['results'],auc,1)):
 ↪results['lr']['roc_df'],
          'Bayesian Logistic Regression, AUC: {}'.
 ↪format(return_bootstrap_results(results['blr']['results'],auc,1)):
 ↪results['blr']['roc_df'],
          'SVC, AUC: {}'.
 ↪format(return_bootstrap_results(results['svc']['results'],auc,1)):
 ↪results['svc']['roc_df'],
          'Neural Network, AUC: {}'.
 ↪format(return_bootstrap_results(results['nn']['results'],auc,1)):
 ↪results['nn']['roc_df'],
          'K Neighbors, AUC: {}'.
 ↪format(return_bootstrap_results(results['knn']['results'],auc,1)):
 ↪results['knn']['roc_df'],
          'Linear Discriminant Analysis, AUC: {}'.
 ↪format(return_bootstrap_results(results['lda']['results'],auc,1)):
 ↪results['lda']['roc_df'],
          'Quadratic Discriminant Analysis, AUC: {}'.
 ↪format(return_bootstrap_results(results['qda']['results'],auc,1)):
 ↪results['qda']['roc_df'],
}
plot_rocs(roc_dict)
sns.despine()
```



6 Nonparametric Bootstrapping of Test Set and CV AUCs

[305]:
```
import tqdm

bootstrapped_aucs={}
for k in results:
    np.random.seed(42)
    idx=np.arange(len(results['xg']['results'])).astype(int)
    pred=results[k]['results'].iloc[:,[0,-1]]
    aucs=[]
    for i in tqdm.trange(1000):
        idx_new=np.random.choice(idx,len(idx),replace=True)
```

```
        pred_new=pred.iloc[idx_new]
        aucs.append(roc_auc_score(*pred_new.values.T.tolist()))
    bootstrapped_aucs[k]=np.array(aucs)
```

```
100%|
               | 1000/1000 [00:07<00:00, 135.99it/s]
100%|
               | 1000/1000 [00:07<00:00, 135.89it/s]
100%|
               | 1000/1000 [00:07<00:00, 136.30it/s]
100%|
               | 1000/1000 [00:07<00:00, 130.82it/s]
100%|
               | 1000/1000 [00:07<00:00, 128.72it/s]
100%|
               | 1000/1000 [00:07<00:00, 134.49it/s]
100%|
               | 1000/1000 [00:07<00:00, 132.82it/s]
100%|
               | 1000/1000 [00:06<00:00, 149.43it/s]
100%|
               | 1000/1000 [00:07<00:00, 138.11it/s]
100%|
               | 1000/1000 [00:08<00:00, 115.00it/s]
100%|
               | 1000/1000 [00:08<00:00, 124.89it/s]
100%|
               | 1000/1000 [00:07<00:00, 127.86it/s]
```

[548]:
```
cv_auc_dict={}
for k in cv_results:
    cv_auc_dict[k]=[]
    np.random.seed(42)
    for fold in range(5):
        cv_auc_dict[k].
 ↪append(roc_auc_score(cv_results[k][fold]['y_val'],cv_results[k][fold]['y_pred']))
```

[541]:
```
cv_auc_bootstrap_dict={}
for k in cv_results:
    cv_auc_bootstrap=[]
    np.random.seed(42)
    idxs=[np.arange(len(cv_results[k][i]['y_val'])).astype(int) for i in␣
 ↪range(5)]
    for i in tqdm.trange(1000):
        idxs_new=[np.random.choice(idxs[fold],len(idxs[fold]),replace=True) for␣
 ↪fold in range(5)]
        aucs_tmp=[]
```

```
        for fold in range(5):
            aucs_tmp.append(roc_auc_score(cv_results[k][fold]['y_val'].
↪iloc[idxs_new[fold]],cv_results[k][fold]['y_pred'][idxs_new[fold]]))
        cv_auc_bootstrap.append(np.mean(aucs_tmp))
    cv_auc_bootstrap_dict[k]=np.array(cv_auc_bootstrap)
```

```
100%|
               | 1000/1000 [00:15<00:00, 62.75it/s]
100%|
               | 1000/1000 [00:16<00:00, 62.46it/s]
100%|
               | 1000/1000 [00:12<00:00, 80.23it/s]
100%|
               | 1000/1000 [00:15<00:00, 62.78it/s]
100%|
               | 1000/1000 [00:18<00:00, 54.56it/s]
100%|
               | 1000/1000 [00:15<00:00, 63.13it/s]
100%|
               | 1000/1000 [00:16<00:00, 60.14it/s]
100%|
               | 1000/1000 [00:12<00:00, 79.61it/s]
100%|
               | 1000/1000 [00:14<00:00, 67.88it/s]
100%|
               | 1000/1000 [00:17<00:00, 58.14it/s]
100%|
               | 1000/1000 [00:16<00:00, 61.37it/s]
100%|
               | 1000/1000 [00:15<00:00, 66.51it/s]
```

7 CV Results Across Folds and Final Averages with 95% CI

[558]:
```
pd.concat([pd.DataFrame(cv_auc_dict).T,pd.DataFrame({k:np.quantile(v,[0.025,0.
↪5,0.975]) for k,v in cv_auc_bootstrap_dict.items()}).T],axis=1)
```

[558]:
```
            0         1         2         3         4         0         1  \
svc  0.921016  0.927512  0.891727  0.857496  0.938346  0.886922  0.907681
nn   0.916311  0.933244  0.894160  0.855528  0.938827  0.889730  0.908005
knn  0.771517  0.786700  0.773297  0.702108  0.851724  0.743994  0.777946
lda  0.894562  0.920447  0.885559  0.845985  0.928837  0.874135  0.895818
qda  0.865296  0.874820  0.862614  0.875682  0.912151  0.851973  0.878705
```

lr	0.907953	0.917067	0.892731	0.858048	0.935814	0.881971	0.902915
nb	0.860681	0.917132	0.880196	0.849523	0.921256	0.864556	0.886324
dt	0.737115	0.783344	0.767718	0.712494	0.777913	0.736596	0.756542
rf	0.896381	0.936123	0.895808	0.841807	0.926263	0.878593	0.899922
xg	0.898649	0.926911	0.886345	0.849638	0.933460	0.880296	0.899127
blr	0.907492	0.928557	0.896443	0.869342	0.936045	0.889997	0.907853
brt	0.912484	0.931174	0.913993	0.879183	0.945253	0.899406	0.916642

	2
svc	0.924806
nn	0.925033
knn	0.810999
lda	0.913166
qda	0.900174
lr	0.919607
nb	0.905758
dt	0.774078
rf	0.918944
xg	0.917566
blr	0.925174
brt	0.932322

8 Test Set 95% CI

[835]:
```python
pd.concat([pd.DataFrame({k:np.quantile(v,[0.5,0.025,0.975]) for k,v in bootstrapped_aucs.items()}).T],axis=1)
```

[835]:

	0	1	2
svc	0.899452	0.860265	0.929901
nn	0.890105	0.848793	0.924575
knn	0.750720	0.676019	0.816482
lda	0.884372	0.839300	0.917000
qda	0.891296	0.857343	0.916772
lr	0.907055	0.869431	0.934614
nb	0.865701	0.828666	0.897776
dt	0.758902	0.716284	0.792318
rf	0.896915	0.857940	0.926435
xg	0.887943	0.845535	0.924111
blr	0.890151	0.843100	0.925787
bart	0.884963	0.840583	0.920440

9 Pairwise AUC differences between models for CV and Test Set

[833]:
```
df_res=pd.DataFrame([np.hstack([(k1,k2),np.
↪quantile(bootstrapped_aucs[k1]-bootstrapped_aucs[k2],[0.5,0.025,0.975])])␣
↪for k1,k2 in [x.split("-") for x in set(["-".join(sorted([k1,k2])) for k1 in␣
↪results for k2 in results if k1!
↪=k2])]],columns=['algo1','algo2','Estimate','2.5%CI','97.5%CI'])
df_res.iloc[:,-3:]=df_res.iloc[:,-3:].astype(float)
df_res['Reject H0']=df_res.iloc[:,-2:].apply(lambda x: len(np.where(np.
↪logical_and(0<=x.values[1], 0>=x.values[0]))[0])==0,axis=1)
df_res.to_csv("test_auc_res.csv")
```

[832]:
```
df_res_cv=pd.DataFrame([np.hstack([(k1,k2),np.
↪quantile(cv_auc_bootstrap_dict[k1]-cv_auc_bootstrap_dict[k2],[0.5,0.025,0.
↪975])]) for k1,k2 in [x.split("-") for x in set(["-".join(sorted([k1,k2]))␣
↪for k1 in cv_results for k2 in cv_results if k1!
↪=k2])]],columns=['algo1','algo2','Estimate','2.5%CI','97.5%CI'])
df_res_cv.iloc[:,-3:]=df_res_cv.iloc[:,-3:].astype(float)
df_res_cv['Reject H0']=df_res_cv.iloc[:,-2:].apply(lambda x: len(np.where(np.
↪logical_and(0<=x.values[1], 0>=x.values[0]))[0])==0,axis=1)
df_res_cv.to_csv("cv_auc_res.csv")
```

10 Bootstrapping SHAP interpretation methods

[827]:
```
explainer_rf,shap_values_rf=run_shap(X_train, X_test,␣
↪results['rf']['best_estimator'], model_type='tree', explainer_options={},␣
↪get_shap_values_options=dict(approximate=True))
explainer_xg,shap_values_xg=run_shap(X_train, X_test,␣
↪results['xg']['best_estimator'], model_type='tree',␣
↪get_shap_values_options=dict(approximate=True))
explainer_lr,shap_values_lr=run_shap(X_train, X_test,␣
↪results['lr']['best_estimator'], model_type='linear', explainer_options={},␣
↪get_shap_values_options=dict())
```

[562]:
```
shap_values=dict(lr=shap_values_lr,
                 rf=shap_values_rf,
                 xg=shap_values_xg)
```

[610]:
```
def calc_global_importance(shap_values):
    return np.abs(shap_values).sum(0)#(-np.abs(shap_values).sum(0)).argsort()

bootstrapped_importances={}
idx=np.arange(len(shap_values['lr'])).astype(int)
for k in shap_values:
```

```
    np.random.seed(42)
    bootstrapped_importances[k]=[]
    for i in tqdm.trange(1000):
        bootstrapped_importances[k].
↪append(calc_global_importance(shap_values[k][np.random.
↪choice(idx,len(idx),replace=True)]))
bootstrapped_importances=pd.DataFrame(bootstrapped_importances)
```

```
100%|
              | 1000/1000 [00:01<00:00, 812.30it/s]
100%|
              | 1000/1000 [00:01<00:00, 996.64it/s]
100%|
              | 1000/1000 [00:01<00:00, 942.14it/s]
```

11 Comparing SHAP global importances with spearman and RBO

[750]:
```
import rbo
test_features=np.arange(len(X_test.columns)).astype(int)

rbo_lr_rf=pd.DataFrame(bootstrapped_importances[['lr','rf']].applymap(lambda x:␣
↪test_features[(-x).argsort()]).apply(lambda x: rbo.RankingSimilarity(*x.
↪tolist()).rbo_ext(p=0.9),axis=1),columns=['r'])
rbo_lr_xg=pd.DataFrame(bootstrapped_importances[['lr','xg']].applymap(lambda x:␣
↪test_features[(-x).argsort()]).apply(lambda x: rbo.RankingSimilarity(*x.
↪tolist()).rbo_ext(p=0.9),axis=1),columns=['r'])
rbo_rf_xg=pd.DataFrame(bootstrapped_importances[['rf','xg']].applymap(lambda x:␣
↪test_features[(-x).argsort()]).apply(lambda x: rbo.RankingSimilarity(*x.
↪tolist()).rbo_ext(p=0.9),axis=1),columns=['r'])
```

[751]:
```
from scipy.stats import pearsonr, spearmanr, kendalltau

spearmanr_lr_rf=pd.DataFrame(bootstrapped_importances[['lr','rf']].apply(lambda␣
↪x: spearmanr(*x.tolist()),axis=1).tolist(),columns=['r','p'])
spearmanr_lr_xg=pd.DataFrame(bootstrapped_importances[['lr','xg']].apply(lambda␣
↪x: spearmanr(*x.tolist()),axis=1).tolist(),columns=['r','p'])
spearmanr_rf_xg=pd.DataFrame(bootstrapped_importances[['rf','xg']].apply(lambda␣
↪x: spearmanr(*x.tolist()),axis=1).tolist(),columns=['r','p'])
```

[752]:
```
pd.concat([
           spearmanr_lr_rf['r'],
           spearmanr_lr_xg['r'],
           spearmanr_rf_xg['r'],
           spearmanr_rf_xg['r']-spearmanr_lr_rf['r'],
           spearmanr_rf_xg['r']-spearmanr_lr_xg['r'],
```

```
            spearmanr_lr_xg['r']-spearmanr_lr_rf['r'],
            rbo_lr_rf['r'],
            rbo_lr_xg['r'],
            rbo_rf_xg['r'],
            rbo_rf_xg['r']-rbo_lr_rf['r'],
            rbo_rf_xg['r']-rbo_lr_xg['r'],
            rbo_lr_xg['r']-rbo_lr_rf['r']],axis=1).apply(lambda x:np.
 ↪quantile(x,[0.5,0.025,0.975]).tolist(),axis=0).T
```

[752]:

```
          0         1         2
r  0.706087  0.690435  0.713043
r  0.731592  0.724163  0.747278
r  0.759915  0.747714  0.772115
r  0.054688  0.039867  0.069507
r  0.023965  0.011765  0.037473
r  0.028114  0.015921  0.050743
r  0.682958  0.679083  0.682958
r  0.637664  0.636738  0.644651
r  0.669883  0.666009  0.672498
r -0.013074 -0.016949 -0.009200
r  0.029604  0.025730  0.033146
r -0.045293 -0.049168 -0.034433
```

12 Comparing SHAP with LIME

[828]:

```
class helper_object():
    """
    This wraps the shap object.
    It takes as input i, which indicates the index of the observation to be␣
 ↪explained.
    """
    def __init__(self, i, X, shap_values, explainer):
        self.base_values = explainer.expected_value[1]
        self.data = X.iloc[i]
        self.feature_names = X.columns.to_list()
        self.values = shap_values[i]

class helper_object_xg():
    """
    This wraps the shap object.
    It takes as input i, which indicates the index of the observation to be␣
 ↪explained.
    """
    def __init__(self, i, X, shap_values, explainer):
```

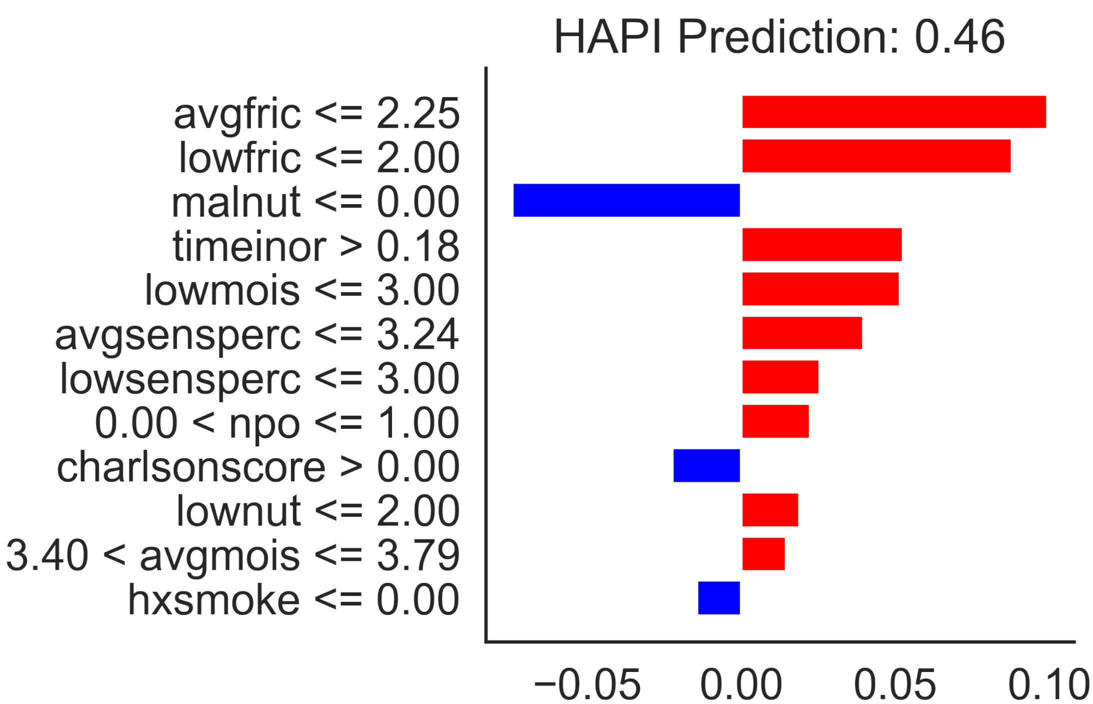
```
        self.base_values = (explainer.expected_value)#(lambda x: 1/(1+np.
↪exp(-x)))
        self.data = X.iloc[i]
        self.feature_names = X.columns.to_list()
        self.values = (shap_values[i])#(lambda x: 1/(1+np.exp(-x)))
```

[785]:
```
import lime
import lime.lime_tabular
from lime.explanation import Explanation

class Explanation2(object):

    def __init__(self,explainer,*args,**kwargs):
        self.explainer=explainer
        self.mode=self.explainer.mode
        self.class_names=self.explainer.class_names

    def as_pyplot_figure(self, label=1, figsize=(4,4), **kwargs):
        """Returns the explanation as a pyplot figure.
        Will throw an error if you don't have matplotlib installed
        Args:
            label: desired label. If you ask for a label for which an
                   explanation wasn't computed, will throw an exception.
                   Will be ignored for regression explanations.
            figsize: desired size of pyplot in tuple format, defaults to (4,4).
            kwargs: keyword arguments, passed to domain_mapper
        Returns:
            pyplot figure (barchart).
        """
        import matplotlib.pyplot as plt
        exp = self.explainer.as_list(label=label, **kwargs)
        fig = plt.figure(figsize=figsize)
        vals = [x[1] for x in exp]
        names = [x[0] for x in exp]
        vals.reverse()
        names.reverse()
        colors = ['red' if x > 0 else 'blue' for x in vals]
        pos = np.arange(len(exp)) + .5
        plt.barh(pos, vals, align='center', color=colors)
        plt.yticks(pos, names)
        if self.mode == "classification":
            title = 'Local explanation for class %s' % self.class_names[label]
        else:
            title = 'Local explanation'
        plt.title(title)
        return fig
```

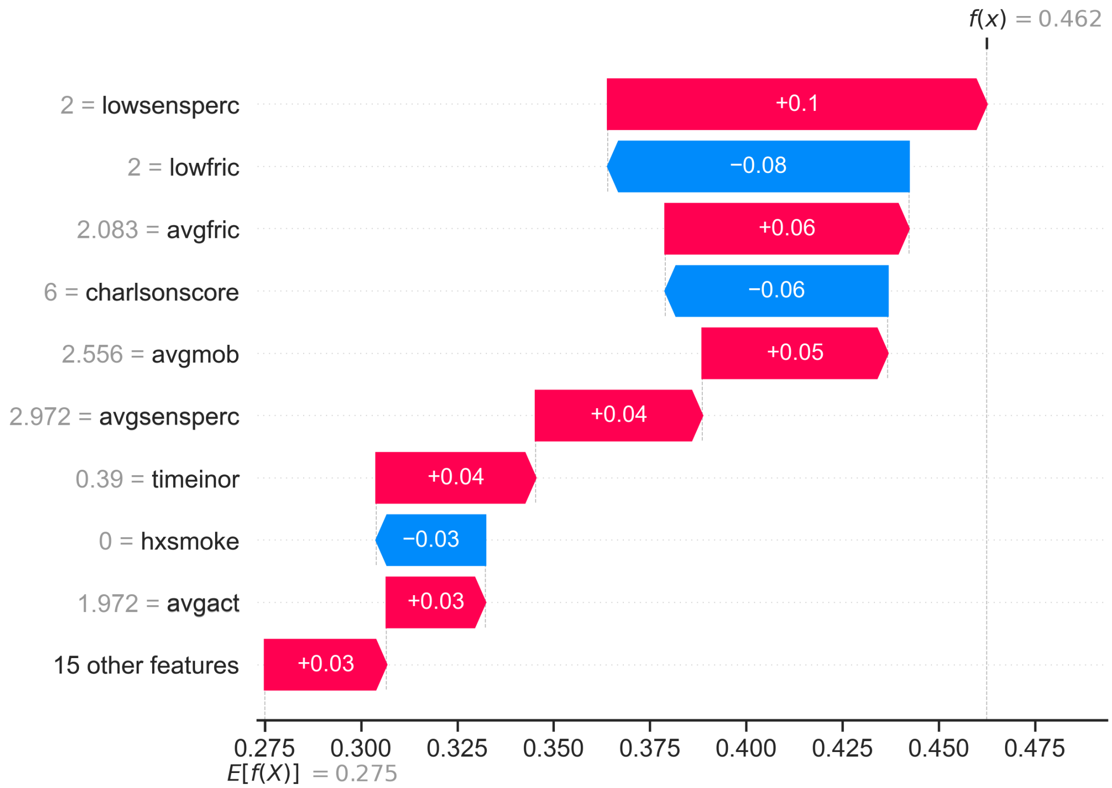
```
explainer = lime.lime_tabular.LimeTabularExplainer(X_train.values,␣
↪mode="classification",feature_names=X_train.columns)
```

[830]:
```
explanation=Explanation2(explainer.explain_instance(X_test[y_test==1].
↪values[0], results['rf']['best_estimator'].predict_proba, labels=[1],␣
↪num_features=X_test.shape[1]//2))
explanation.as_pyplot_figure()
sns.despine()
plt.title(f"HAPI Prediction: {round(results['rf']['results'].
↪values[y_test==1][0,-1],2)}")
```

[830]:
```
Text(0.5, 1.0, 'HAPI Prediction: 0.46')
```

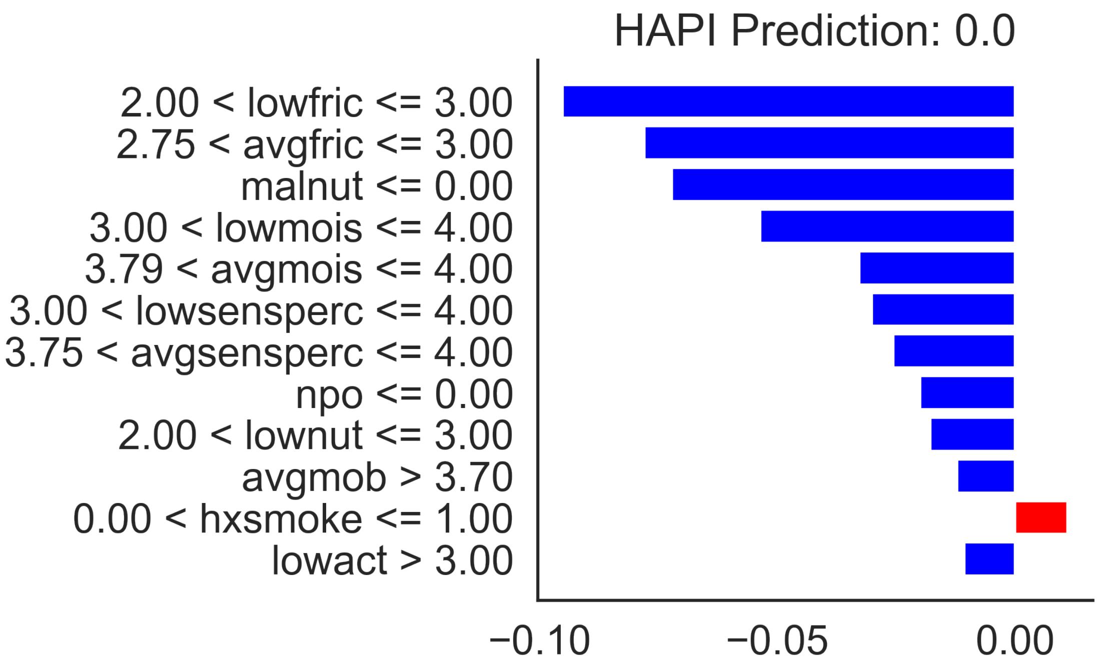


[374]:
```
shap.plots.waterfall(helper_object(np.
↪where(y_test==1)[0][0],X_test,shap_values_rf,explainer_rf))#expected,␣
↪shap_values[i, :], X_test.values[i, :])
```

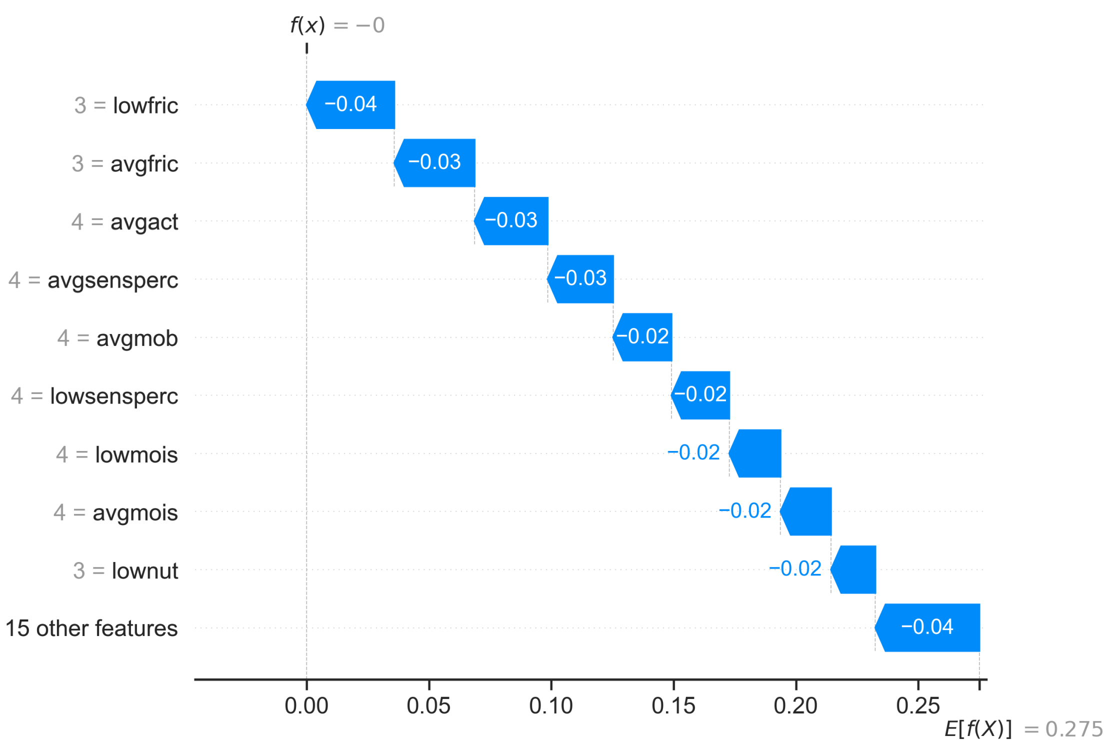


[807]:
```python
explanation=Explanation2(explainer.explain_instance(X_test[y_test==0].
    values[0], results['rf']['best_estimator'].predict_proba, labels=[1],
    num_features=X_test.shape[1]//2))
# explanation.show_in_notebook(show_table=True, show_all=False)
explanation.as_pyplot_figure()
sns.despine()
plt.title(f"HAPI Prediction: {round(results['rf']['results'].
    values[y_test==0][0,-1],2)}")
```

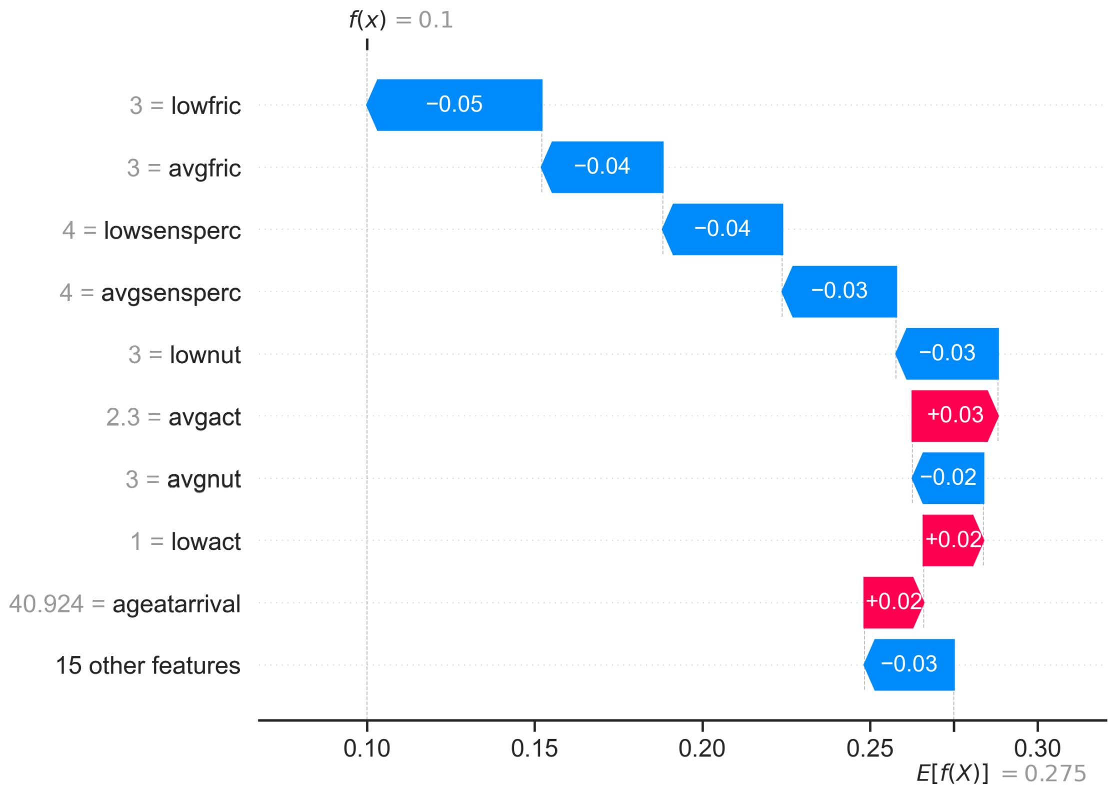
[807]:
```
Text(0.5, 1.0, 'HAPI Prediction: 0.0')
```



[480]:
```
shap.plots.waterfall(helper_object(np.
↪where(y_test==0)[0][0],X_test,shap_values_rf,explainer_rf))#expected,␣
↪shap_values[i, :], X_test.values[i, :])
```

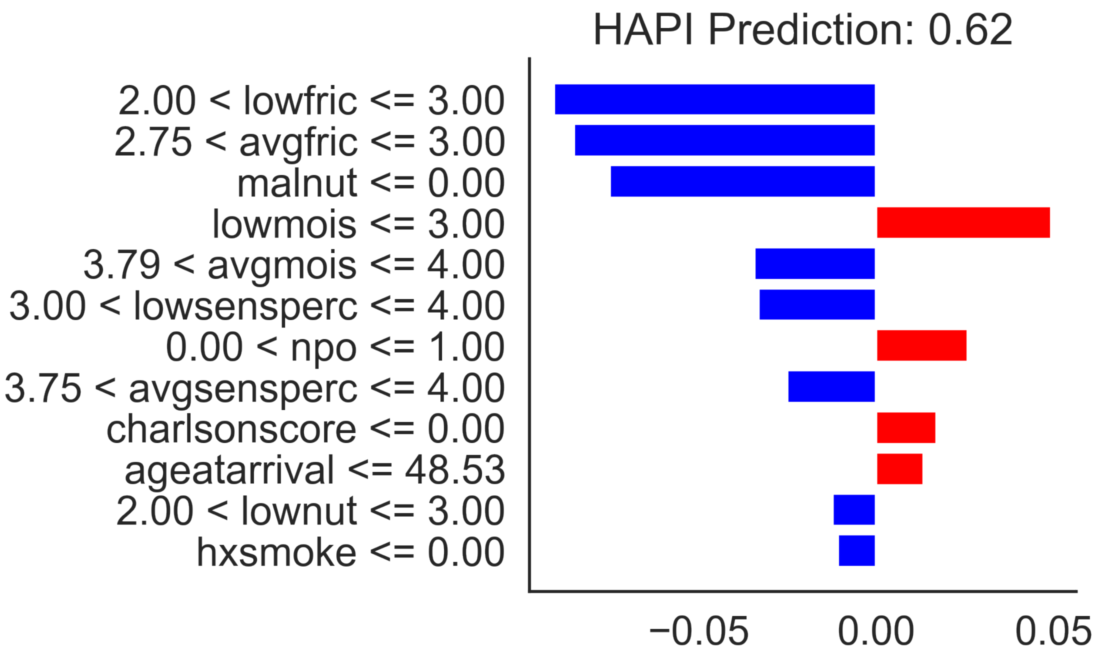


[481]:
```
shap.plots.waterfall(helper_object(np.
 ↪where(y_test==0)[0][15],X_test,shap_values_rf,explainer_rf))#expected,␣
 ↪shap_values[i, :], X_test.values[i, :])
```



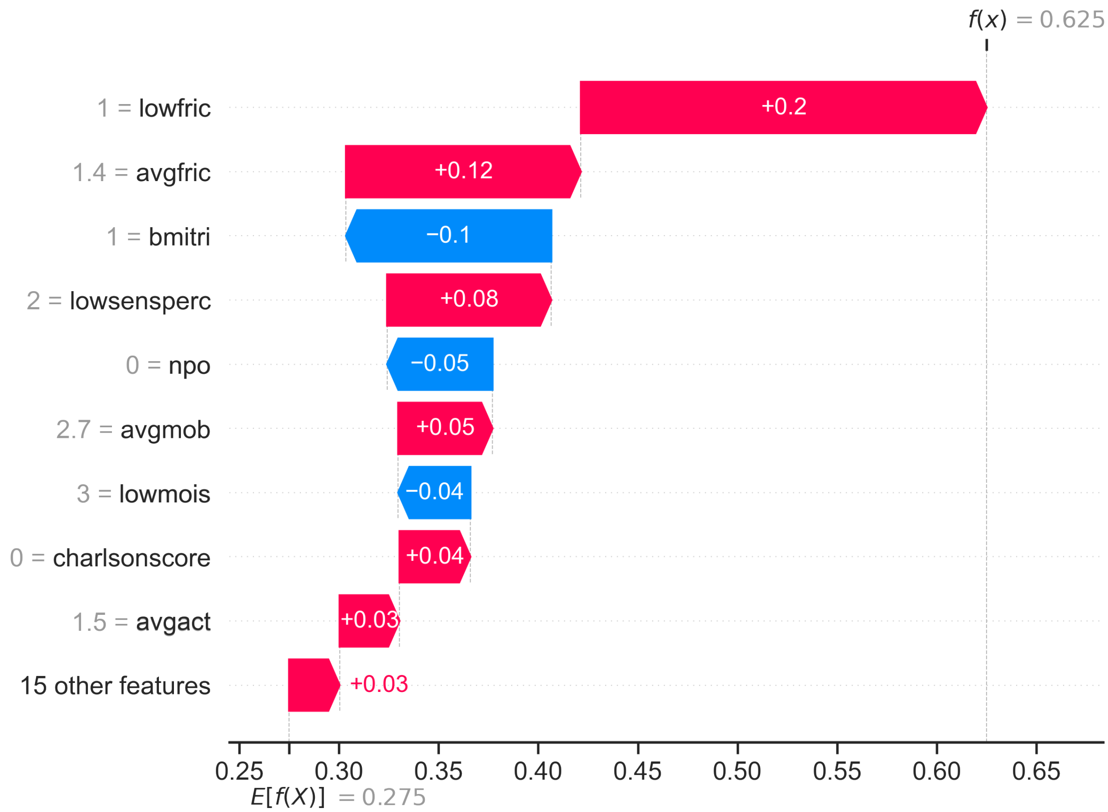
[806]:
```
explanation=Explanation2(explainer.explain_instance(X_test[y_test==0].
 ↪values[15], results['rf']['best_estimator'].predict_proba, labels=[1],␣
 ↪num_features=X_test.shape[1]//2))
explanation.as_pyplot_figure()
sns.despine()
plt.title(f"HAPI Prediction: {round(results['rf']['results'].
 ↪values[y_test==1][15,-1],2)}")
```

[806]:
```
Text(0.5, 1.0, 'HAPI Prediction: 0.62')
```



[770]:

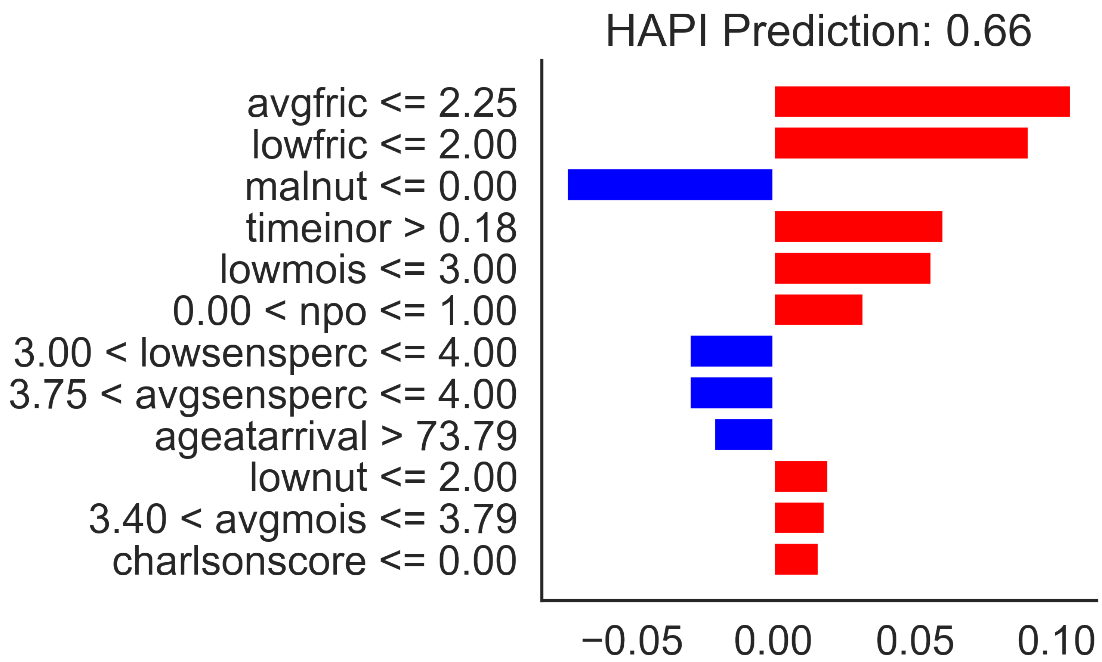
```
matplotlib.rcParams['figure.dpi']=300
shap.plots.waterfall(helper_object(np.
  ↪where(y_test==1)[0][15],X_test,shap_values_rf,explainer_rf))#expected,␣
  ↪shap_values[i, :], X_test.values[i, :])
```



[805]:

```
explanation=Explanation2(explainer.explain_instance(X_test[y_test==1].
 ↪values[25], results['rf']['best_estimator'].predict_proba, labels=[1],␣
 ↪num_features=X_test.shape[1]//2))
explanation.as_pyplot_figure()
sns.despine()
plt.title(f"HAPI Prediction: {round(results['rf']['results'].
 ↪values[y_test==1][25,-1],2)}")
```

[805]: Text(0.5, 1.0, 'HAPI Prediction: 0.66')



HAPI Prediction: 0.66
avgfric <= 2.25
lowfric <= 2.00
malnut <= 0.00
timeinor > 0.18
lowmois <= 3.00
0.00 < npo <= 1.00
3.00 < lowsensperc <= 4.00
3.75 < avgsensperc <= 4.00
ageatarrival > 73.79
lownut <= 2.00
3.40 < avgmois <= 3.79
charlsonscore <= 0.00
−0.05
0.00
0.05
0.10


```
[ ]:
```