data1030-final

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1 DATA1030 Final

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INSTRUCTIONS **EdStem:**

- Come up with a classification or regression problem!
- The goal of the final project is to develop a supervised ML pipeline from scratch by following the eight steps outlined in the lecture notes.
- There are three main reasons why a ML problem is difficult:
  1) missing data
  2) dataset is not IID (e.q., time series data, or one object is described by multiple data points - group structure)
  3) dataset is large (more than 100k points) so it is difficult to manage it on your laptop
- Choose a dataset with at least one of these difficulties!

Rubric: - Select a dataset and have an interesting/valuable/relevant classification or regression problem in mind to solve - The purpose of the semester-long project is to give you hands-on experience working with a machine learning pipeline. For the final presentation, the focus is on cross validation, the algorithms and parameters you tried, scores and uncertainties, and model explanations. The presentation is intended as a summary of your final project report.

1) EDA
2) splitting
3) preprocessing
4) evaluation metric
5) ML models
6) hyperparamter tuning
7) interpretability

PROJECT **Topic:** - predicting survival outcome of heart failure patients

Data: - PhysioNet - Hospitalized patients with heart failure: integrating electronic healthcare records and external outcome data - Zhang, Z., Cao, L., Zhao, Y., Xu, Z., Chen, R., Lv, L., & Xu, P. (2022). Hospitalized patients with heart failure: integrating electronic healthcare records and external outcome data (version 1.3). *PhysioNet*. RRID:SCR_007345. https://doi.org/10.13026/5m60-vs44 - original publication: Zhang Z, Cao L, Chen R, Zhao Y, Lv L, Xu Z, Xu P. Electronic healthcare records and external outcome data for hospitalized patients with heart failure. Sci Data. 2021 Feb 5;8(1):46. doi: 10.1038/s41597-021-00835-9. PMID: 33547290; PMCID: PMC7865067 - patients who were admitted to a hospital in Sichuan, China between 2016 and 2019 - 168 variables for

2,008 patients with heart failure - Medications administered during the hospitalization are recorded in dat_md.csv. - Subsequent admission & mortality = follow-up at 28 days, 3 months, 6 months -> classification problem (discrete ordinal)

[ ]:
```
# IMPORT PACKAGES
import pandas as pd
import numpy as np

# EDA
import seaborn as sns
import matplotlib.pyplot as plt

# splitting
from sklearn.model_selection import train_test_split
from sklearn.model_selection import StratifiedKFold

# preprocessing
from sklearn.preprocessing import StandardScaler, OneHotEncoder, OrdinalEncoder
from sklearn.compose import ColumnTransformer
from sklearn.pipeline import Pipeline
from sklearn.impute import SimpleImputer
from sklearn.preprocessing import LabelEncoder
from sklearn.utils.class_weight import compute_sample_weight
from sklearn.experimental import enable_iterative_imputer
from sklearn.impute import IterativeImputer
# from sklearn.ensemble import RandomForestRegressor
# from sklearn.ensemble import ExtraTreesRegressor
from sklearn.impute import KNNImputer

# models
from sklearn.pipeline import Pipeline
from imblearn.pipeline import Pipeline as ImbPipeline
from sklearn.model_selection import ParameterGrid
from sklearn.model_selection import GridSearchCV
from sklearn.linear_model import LogisticRegression
from sklearn.svm import SVC
from sklearn.ensemble import RandomForestClassifier
import xgboost

# metrics
from sklearn.metrics import f1_score

# interpretability
from sklearn.metrics import confusion_matrix
from sklearn.metrics import ConfusionMatrixDisplay
import shap
```

[19]:
```python
# IMPORT DATA

# csv to df
df_og = pd.read_csv('heartfailure-ehr-data/dat.csv')

# display all
pd.set_option('display.max_columns', None)
pd.set_option('display.max_rows', None)

# print(df_og.head())
# print(df_og.describe())
# print(df_og.shape) # (2008, 167)
```

[20]:
```python
# FINAL DF
df = df_og.copy()

# print(df.columns)

# create 1 y var:
# initial y options based on project goal of predicting survival outcome
drop_cols = ["Unnamed: 0", "inpatient.number", "outcome.during.
 ↪hospitalization", "death.within.28.days", "re.admission.within.28.days",␣
 ↪"death.within.3.months", "re.admission.within.3.months",
             "death.within.6.months", "re.admission.within.6.months", "time.of.
 ↪death..days.from.admission.", "re.admission.time..days.from.admission.",
             "return.to.emergency.department.within.6.months", "time.to.
 ↪emergency.department.within.6.months"]

# make y categorical -> death @ hosp, 28d, 3mo, 6mo, alive 6mo
y_series = pd.Series(name = 'survival.outcome')
for row in range(len(df)):
    if df.loc[row, "outcome.during.hospitalization"] == 'Dead':
        outcome = 'death.at.hospital'
    elif df.loc[row, "death.within.28.days"] == 1:
        outcome = 'death.within.28d'
    elif df.loc[row, "death.within.3.months"] == 1:
        outcome = 'death.within.3m'
    elif df.loc[row, "death.within.6.months"] == 1:
        outcome = 'death.within.6m'
    else:
        outcome = 'alive.after.6m'
    y_series[row] = outcome

# drop original y cols
df = df.drop(columns=drop_cols)

# drop column with all missing values:
```

```
# which columns completely missing:
# for col in df.columns:
#     if df[col].isnull().sum() == len(df):
#         print(col)
# cholinesterase

df = df.drop(columns=['cholinesterase'])

df['survival.outcome'] = y_series
```

[4]:
```
# EDA
# final dataset
X = df.loc[:, df.columns != 'survival.outcome']
y = df['survival.outcome']

# print(y.head())
print(y.shape) # (2008,)
# # print(X.head())
print(X.shape) # (2008, 154)
```

```
(2008,)
(2008, 153)
```

[21]:
```
# EDA
# check class balance:
print(y.value_counts(normalize=False))
print(y.value_counts(normalize=True))

# iid & imbalanced
# -> kfold shuffle, class_weight, f-score
```

```
survival.outcome
alive.after.6m       1951
death.within.28d       28
death.within.6m        15
death.at.hospital      11
death.within.3m         3
Name: count, dtype: int64
survival.outcome
alive.after.6m       0.971614
death.within.28d     0.013944
death.within.6m      0.007470
death.at.hospital    0.005478
death.within.3m      0.001494
Name: proportion, dtype: float64
```

[22]:
```
# data types
# continuous:
continuous_ftrs = X.select_dtypes(include=['int64', 'float64']).columns.tolist()

# categorical:
all_cat_ftrs = X.select_dtypes(include=['object', 'category', 'bool']).columns
# ordinal vs. nominal:
# for col in all_cat_ftrs:
#     print(f"\n{col}: {X[col].unique()}")
# ordinal:
    # NYHA.cardiac.function.classification: ['III' 'II' 'IV']
    # Killip.grade: ['III' 'I' 'II' 'IV']
    # consciousness: ['Clear' 'ResponsiveToPain' 'ResponsiveToSound'␣
 ↪'Nonresponsive']
    # respiratory.support.: [nan 'NIMV' 'IMV']
    # ageCat: ['(69,79]' '(59,69]' '(79,89]' '(49,59]' '(89,110]' '(29,39]'␣
 ↪'(39,49]' '(21,29]']
# binary (but want to assign 0/1):
    # admission.way: ['NonEmergency' 'Emergency']
    # type.II.respiratory.failure: ['NonTypeII' 'TypeII']
    # oxygen.inhalation: ['OxygenTherapy' 'AmbientAir']
ordinal_ftrs = ['NYHA.cardiac.function.classification', 'Killip.grade',␣
 ↪'consciousness', 'respiratory.support.', 'ageCat',
                'admission.way', 'type.II.respiratory.failure', 'oxygen.
 ↪inhalation']
ordinal_cats = [['II', 'III', 'IV'],  # NYHA.cardiac.function.classification
                ['I', 'II', 'III', 'IV'],  # Killip.grade
                ['Clear', 'ResponsiveToSound', 'ResponsiveToPain',␣
 ↪'Nonresponsive'],  # consciousness
                ['NA', 'NIMV', 'IMV'],  # respiratory.support.
                ['(21,29]', '(29,39]', '(39,49]', '(49,59]', '(59,69]',␣
 ↪'(69,79]', '(79,89]', '(89,110]'],  # ageCat
                ['NonEmergency', 'Emergency'],  # admission.way
                ['NonTypeII', 'TypeII'],  # type.II.respiratory.failure
                ['AmbientAir', 'OxygenTherapy']  # oxygen.inhalation
                ]
# nominal:
nominal_ftrs = list(set(all_cat_ftrs) - set(ordinal_ftrs))
```

[7]:
```
# EDA

# continuous = histogram
# ordinal = barplot (correct order)
# categorical = barplot
# continuous v. continuous = scatterplot, heatmap
# continuous v. categorical = category-specific histogram, boxplot, violin plot␣
 ↪(>3-4)
```

```
# categorical v. categorical = stacked barplot
```

[8]:
```
# EDA
# visualize individual variables:

# continuous = histogram
# for col in continuous_ftrs:
#     plt.figure(figsize=(4, 3)) # size to manage cell output
#     plt.hist(X[col])#, kde=True)
#     plt.title(f'Distribution of {col}')
#     plt.xlabel(col)
#     plt.ylabel('Frequency')
#     plt.show()
```

[9]:
```
# EDA
# visualize individual variables:

# nominal = barplot
# for col in nominal_ftrs:
#     plt.figure(figsize=(4, 3)) # size to manage cell output
#     sns.countplot(data=X, x=col)
#     plt.title(f'Distribution of {col}')
#     plt.xlabel(col)
#     plt.ylabel('Count')
#     plt.show()
```

[10]:
```
# EDA
# visualize individual variables:

# ordinal = barplot (in given order)
# for col in  ordinal_ftrs:
#     plt.figure(figsize=(4, 3)) # size to manage cell output
#     order = ordinal_cats[ordinal_ftrs.index(col)]
#     sns.countplot(data=X, x=col, order=order)
#     plt.title(f'Distribution of {col}')
#     plt.xlabel(col)
#     plt.ylabel('Count')
#     plt.show()
```

[11]:
```
# EDA
# visualize outcome vs. features:

# categorical v. categorical = stacked bar plot
# for col in nominal_ftrs:
#     count_matrix = df.groupby([col, 'survival.outcome']).size().unstack()
#     count_matrix_norm = count_matrix.div(count_matrix.sum(axis=1),axis=0)
#     count_matrix_norm.plot(kind='bar', stacked=True, cmap='Paired',␣
↪figsize=(4, 3)) # size to manage cell output
#     plt.title(f'{col} vs. Survival Outcome')
#     plt.xlabel(col)
#     plt.ylabel('Count')
#     plt.legend(title='Survival Outcome', fontsize='small')
#     # plt.tight_layout()
#     plt.show()

# for col in ordinal_ftrs:
#     count_matrix = df.groupby([col, 'survival.outcome']).size().unstack()
#     count_matrix_norm = count_matrix.div(count_matrix.sum(axis=1),axis=0)

#     count_matrix_norm.plot(kind='bar', stacked=True, cmap='Paired',␣
↪figsize=(4, 3)) # size to manage cell output
#     plt.title(f'{col} vs. Survival Outcome')
#     plt.xlabel(col)
#     plt.ylabel('Count')
#     plt.legend(title='Survival Outcome', fontsize='small')
#     # plt.tight_layout()
#     plt.show()
```

[12]:
```
# EDA
# continuous x v. outcome:

# categorical x continuous = category-specific histograms, box plot, violin plot
# for col in continuous_ftrs:
#     df[[col,'survival.outcome']].boxplot(by='survival.outcome',␣
↪figsize=(4,3)) # size to manage cell output
#     # plt.title(f'survival outcome by {col}')
#     plt.xlabel('survival outcome')
#     plt.ylabel(col)
#     plt.tight_layout()
#     plt.xticks(rotation=45)
#     plt.show()
```

[23]:
```
# EDA
# missing values
# how many missing values per column
missing_vals = df.isnull().sum()
missing_perc = (missing_vals / len(df)) * 100

# print(missing_vals)
# print(missing_perc)
# for col in df.columns:
#     miss = missing_vals[col]
#     perc = missing_perc[col]
#     if miss > 0:
#         print(f"{col}: {perc:.2f}%")

# cols with missing values 100-90, 80-90, 70-79, 60-69, 50-59, 40-49, 30-39,␣
↪20-29, 10-19, 1-9%
bins = [0, 10, 20, 30, 40, 50, 60, 70, 80, 90, 100]
labels = ['0-9%', '10-19%', '20-29%', '30-39%', '40-49%', '50-59%', '60-69%',␣
↪'70-79%', '80-89%', '90-100%']
df_missing = pd.DataFrame({'column': missing_vals.index, 'missing_count':␣
↪missing_vals.values})
df_missing['missing_perc'] = (df_missing['missing_count'] / len(df_og)) * 100
df_missing['missing_bin'] = pd.cut(df_missing['missing_perc'], bins=bins,␣
↪labels=labels, right=False)
missing_bin_counts = df_missing['missing_bin'].value_counts().sort_index()
print(missing_bin_counts)

# total missing values in dataset:
total_missing = missing_vals.sum()
total_values = df_og.size
overall_missing_perc = (total_missing / total_values) * 100
print(f"total missing values: {total_missing}")
print(f"overall missing percentage: {overall_missing_perc:.2f}%")

cont_missing = df[continuous_ftrs].isnull().sum().sum()
cont_missing_perc = (cont_missing / (len(continuous_ftrs) * len(df))) * 100
print(f"total missing values in continuous features: {cont_missing}")
print(f"total missing percentage in continuous features: {cont_missing_perc:.
↪2f}%")
nom_missing = df[nominal_ftrs].isnull().sum().sum()
nom_missing_perc = (nom_missing / (len(nominal_ftrs) * len(df))) * 100
print(f"total missing values in nominal features: {nom_missing}")
print(f"total missing percentage in nominal features: {nom_missing_perc:.2f}%")
ord_missing = df[ordinal_ftrs].isnull().sum().sum()
ord_missing_perc = (ord_missing / (len(ordinal_ftrs) * len(df))) * 100
print(f"total missing values in ordinal features: {ord_missing}")
print(f"total missing percentage in ordinal features: {ord_missing_perc:.2f}%")
```

```
missing_bin
0-9%       103
10-19%       7
20-29%       3
30-39%       1
40-49%       0
50-59%      25
60-69%       2
70-79%       4
80-89%       3
```

```
90-100%      6
Name: count, dtype: int64
total missing values: 57562
overall missing percentage: 17.17%
total missing values in continuous features: 55569
total missing percentage in continuous features: 19.91%
total missing values in nominal features: 27
total missing percentage in nominal features: 0.22%
total missing values in ordinal features: 1966
total missing percentage in ordinal features: 12.24%
```

[24]:
```
# SPLITTING

# split during model iteration over multiple random states
random_states = [42, 52, 62, 72, 82]
```

[15]:
```
# PREPROCESSING

# preprocess during model iteration over multiple random states
# random_states = [42, 52, 62, 72, 82]

# encode & impute
# continuous -> StandardScaler
# nominal -> OneHotEncoder
# ordinal -> OrdinalEncoder

# IterativeImputer not reasonable with iteration through such high # features
# -> use KNN Imputer
```

[28]:
```
# MODELS
# logistic regression (classification)

# nominal transformer:
nominal_transformer = Pipeline(steps=[('imputer',␣
 ↪SimpleImputer(strategy='constant', fill_value='missing')),
                                      ('onehot',␣
 ↪OneHotEncoder(sparse_output=False, handle_unknown='ignore'))])
# ordinal transformer:
# We need to replace the NaN with a string first!
ordinal_transformer = Pipeline(steps=[('imputer',␣
 ↪SimpleImputer(strategy='constant', fill_value='NA')),
                                      ('ordinal', OrdinalEncoder(categories =␣
 ↪ordinal_cats))])
# continuous transformer:
# KNN Imputer
numeric_transformer = Pipeline(steps=[('imputer', KNNImputer(n_neighbors=10)),
                                      ('scaler', StandardScaler())])
```

```
# preprocessor:
preprocessor = ColumnTransformer(transformers=[('num', numeric_transformer,␣
 ↪continuous_ftrs),
                                                ('cat', nominal_transformer,␣
 ↪nominal_ftrs),
                                                ('ord', ordinal_transformer,␣
 ↪ordinal_ftrs)])

# hyperparameter tuning:
lr_param_grid = {'logreg__penalty': ['l2'],
                 'logreg__C': np.logspace(-3,0,10),
                 'logreg__max_iter': [1000]}

# initialize result collection:
lr_test_scores = []
lr_models = []

# model:
for rs in random_states:
        # splitting: stratified kfold
        kf1 = StratifiedKFold(n_splits=3, shuffle=True, random_state=rs) #n 3␣
 ↪bc smallest class size = 3
        for other_idx, test_idx in kf1.split(X, y):
          X_other = X.iloc[other_idx]
          X_test = X.iloc[test_idx]
          y_other = y.iloc[other_idx] # y transformed
          y_test = y.iloc[test_idx]

        # pipeline:
        model = LogisticRegression(random_state = rs, class_weight='balanced')

        pipeline = Pipeline(steps=[('preprocessor', preprocessor),
                                   ('logreg', model)])

        # cross validation:
        kf2 = StratifiedKFold(n_splits=2, shuffle=True, random_state=rs) #n 2␣
 ↪bc smallest class size = 2
        grid = GridSearchCV(pipeline, param_grid=lr_param_grid, scoring =␣
 ↪'f1_weighted', cv=kf2, return_train_score = True, verbose=True)

        # model fitting:
        grid.fit(X_other, y_other)

        # results:
        lr_models.append(grid)
        y_test_pred = lr_models[-1].predict(X_test)
        # test-score = f1_weighted
        test_score = f1_score(y_test, y_test_pred, average='weighted')
        lr_test_scores.append(test_score)

# best model:
lr_best_model_idx = np.argmax(lr_test_scores)
lr_best_model = lr_models[lr_best_model_idx]
lr_best_hyperparams = lr_best_model.best_params_
lr_best_test_score = lr_test_scores[lr_best_model_idx]

print("best model hyperparameters: ", lr_best_hyperparams)
print("best model test f1: ", lr_best_test_score)

# results (plot later)
lr_mean = np.mean(lr_test_scores)
lr_std = np.std(lr_test_scores)
```

```
Fitting 2 folds for each of 10 candidates, totalling 20 fits
Fitting 2 folds for each of 10 candidates, totalling 20 fits
Fitting 2 folds for each of 10 candidates, totalling 20 fits
Fitting 2 folds for each of 10 candidates, totalling 20 fits
Fitting 2 folds for each of 10 candidates, totalling 20 fits
best model hyperparameters:  {'logreg__C': np.float64(1.0), 'logreg__max_iter':
1000, 'logreg__penalty': 'l2'}
best model test f1:  0.9447422523313181
```

[29]:
```
# MODELS
# SVC

# same trasforners as log reg

# hyperparameter tuning:
svc_param_grid = {'svc__C': np.logspace(-3,0,10),
                  'svc__gamma': np.logspace(-3,0,10)}

# initialize result collection:
svc_test_scores = []
svc_models = []

# model:
for rs in random_states:
        # splitting: stratified kfold
        kf1 = StratifiedKFold(n_splits=3, shuffle=True, random_state=rs) #n 3␣
 ↪bc smallest class size = 3
        for other_idx, test_idx in kf.split(X, y):
          X_other = X.iloc[other_idx]
          X_test = X.iloc[test_idx]
          y_other = y.iloc[other_idx] # y transformed
          y_test = y.iloc[test_idx]

        # pipeline:
        model = SVC(random_state = rs, class_weight='balanced')
        pipeline = Pipeline(steps=[('preprocessor', preprocessor),
                                   ('svc', model)])

        # cross validation:
        kf2 = StratifiedKFold(n_splits=2, shuffle=True, random_state=rs) #n 2␣
↪bc smallest class size = 2
        grid = GridSearchCV(pipeline, param_grid=svc_param_grid, scoring =␣
↪'f1_weighted',
                            cv=kf2, return_train_score = True, verbose=True)

        # model fitting:
        grid.fit(X_other, y_other)

        # results:
        svc_models.append(grid)
        y_test_pred = svc_models[-1].predict(X_test)
        # test-score = f1_weighted
        test_score = f1_score(y_test, y_test_pred, average='weighted')
        svc_test_scores.append(test_score)


# best model:
svc_best_model_idx = np.argmax(svc_test_scores)
svc_best_model = svc_models[svc_best_model_idx]
svc_best_hyperparams = svc_best_model.best_params_
svc_best_test_score = svc_test_scores[svc_best_model_idx]

print("best model hyperparameters: ", svc_best_hyperparams)
print("best model test f1: ", svc_best_test_score)

# results (plot later)
svc_mean = np.mean(svc_test_scores)
svc_std = np.std(svc_test_scores)
```

```
Fitting 2 folds for each of 100 candidates, totalling 200 fits
Fitting 2 folds for each of 100 candidates, totalling 200 fits
Fitting 2 folds for each of 100 candidates, totalling 200 fits
Fitting 2 folds for each of 100 candidates, totalling 200 fits
Fitting 2 folds for each of 100 candidates, totalling 200 fits
best model hyperparameters:  {'svc__C': np.float64(0.46415888336127775),
'svc__gamma': np.float64(0.004641588833612777)}
```

```
best model test f1:  0.957290794077231
```

[30]:
```
# MODELS
# RFC

# preprocessing: don't impute tree models -> trees only need preprocessing to␣
↪numeric
# same categorical encoders as logreg & SVC
# # nominal encoder:
# nominal_transformer = Pipeline(steps=[('imputer',␣
↪SimpleImputer(strategy='constant', fill_value='missing')),
#                                    ('onehot', OneHotEncoder(sparse_output=False,␣
↪handle_unknown='ignore'))])
# # ordinal encoder:
# ordinal_transformer = Pipeline(steps=[('imputer',␣
↪SimpleImputer(strategy='constant', fill_value='NA')),
#                                    ('ordinal', OrdinalEncoder(categories =␣
↪ordinal_cats))])
# continuous encoder: no imputation for tree models

# preprocessor:
preprocessor = ColumnTransformer(transformers=[('cat', nominal_transformer,␣
↪nominal_ftrs),
                                                ('ord', ordinal_transformer,␣
↪ordinal_ftrs)])

# hyperparameter tuning:
rfc_param_grid = {'rfc__n_estimators': [10,50,100,500],
                  'rfc__max_features': np.linspace(0.1,0.9,5),
                  'rfc__max_depth': [1,10,30]}

# initialize result collection:
rfc_test_scores = []
rfc_models = []

# model:
for rs in random_states:
        # splitting: kfold on other
        kf1 = StratifiedKFold(n_splits=3, shuffle=True, random_state=rs) #n 3␣
↪bc smallest class size = 3
        for other_idx, test_idx in kf1.split(X, y):
          X_other = X.iloc[other_idx]
          X_test = X.iloc[test_idx]
          y_other = y.iloc[other_idx] # y transformed
          y_test = y.iloc[test_idx]

        # pipeline:
```

```
        model = RandomForestClassifier(random_state=rs,␣
↪class_weight='balanced_subsample') # balanced_subsample for imbalanced
        pipeline = Pipeline(steps=[('preprocessor', preprocessor),
                                   ('rfc', model)])

        # cross validation:
        kf2 = StratifiedKFold(n_splits=2, shuffle=True, random_state=rs) #n 2␣
↪bc smallest class size = 2
        grid = GridSearchCV(pipeline, param_grid=rfc_param_grid, scoring =␣
↪'f1_weighted',
                            cv=kf2, return_train_score = True, verbose=True)

        # model fitting:
        grid.fit(X_other, y_other)

        # results
        rfc_models.append(grid)
        y_test_pred = rfc_models[-1].predict(X_test)
        # test-score = f1_weighted
        test_score = f1_score(y_test, y_test_pred, average='weighted')
        rfc_test_scores.append(test_score)

# best model:
rfc_best_model_idx = np.argmax(rfc_test_scores)
rfc_best_model = rfc_models[rfc_best_model_idx]
rfc_best_hyperparams = rfc_best_model.best_params_
rfc_best_test_score = rfc_test_scores[rfc_best_model_idx]

print("best model hyperparameters: ", rfc_best_hyperparams)
print("best model test f1: ", rfc_best_test_score)

# results (plot later)
rfc_mean = np.mean(rfc_test_scores)
rfc_std = np.std(rfc_test_scores)
```

```
Fitting 2 folds for each of 60 candidates, totalling 120 fits
Fitting 2 folds for each of 60 candidates, totalling 120 fits
Fitting 2 folds for each of 60 candidates, totalling 120 fits
Fitting 2 folds for each of 60 candidates, totalling 120 fits
Fitting 2 folds for each of 60 candidates, totalling 120 fits
best model hyperparameters:  {'rfc__max_depth': 30, 'rfc__max_features':
np.float64(0.9), 'rfc__n_estimators': 10}
best model test f1:  0.9580779018335805
```

[31]:
```
# MODELS
# XGB
# preprocessing: don't impute tree models -> trees only need preprocessing to␣
↪numeric
# same preprocessor as RFC
# # nominal encoder:
# nominal_transformer = Pipeline(steps=[('imputer',␣
↪SimpleImputer(strategy='constant', fill_value='missing')),
#                                  ('onehot', OneHotEncoder(sparse_output=False,␣
↪handle_unknown='ignore'))])
# # ordinal encoder:
# ordinal_transformer = Pipeline(steps=[('imputer',␣
↪SimpleImputer(strategy='constant', fill_value='NA')),
#                                  ('ordinal', OrdinalEncoder(categories =␣
↪ordinal_cats))])
# continuous encoder: no imputation for tree models

# # preprocessor:
# preprocessor = ColumnTransformer(transformers=[('cat', nominal_transformer,␣
↪nominal_ftrs),
#                                                 ('ord', ordinal_transformer,␣
↪ordinal_ftrs)])

# hyperparameter tuning:
xgb_param_grid = {'xgb__n_estimators': [10,50,100],
              'xgb__max_depth': [5,30,50],
              'xgb__learning_rate': [0.01, 0.05, 0.1],
              'xgb__reg_lambda': np.logspace(-2,2,5),
              'xgb__subsample': [0.3, 0.5, 0.7]}

# initialize result collection:
xgb_test_scores = []
xgb_models = []
xgb_test_sets = [] # best model -> save test set for cm

# y label encoder: (not in preprocessor)
# fit on the full set (y) to create a stable mapping label -> no leakage bc␣
↪only records which string label maps to which integer, doesn't learn␣
↪relationship between X & y
y_labenc = LabelEncoder()
y_labenc.fit(y)

# model:
for rs in random_states:
        # splitting: stratified kfold
        kf1 = StratifiedKFold(n_splits=3, shuffle=True, random_state=rs) #n 3␣
↪bc smallest class size = 3
        for other_idx, test_idx in kf1.split(X, y):
          X_other = X.iloc[other_idx]
          X_test = X.iloc[test_idx]
          y_other = y.iloc[other_idx] # y transformed
          y_test = y.iloc[test_idx]

        # transform y other & test using label encoder fitted on full y
        y_other_enc = y_labenc.transform(y_other)
        y_test_enc = y_labenc.transform(y_test)

        # pipeline:
        # model = xgboost.XGBClassifier(early_stopping_rounds=40,␣
↪enable_categorical=True) # true/false
        model = xgboost.XGBClassifier(enable_categorical=True)
        pipeline = Pipeline(steps=[('preprocessor', preprocessor),
                                   ('xgb', model)])

        # cross validation:
        kf2 = StratifiedKFold(n_splits=2, shuffle=True, random_state=rs) #n 2␣
↪bc smallest class size = 2
        grid = GridSearchCV(pipeline, param_grid=xgb_param_grid, scoring =␣
↪'f1_weighted',
                            cv=kf2, return_train_score=True, verbose=True,␣
↪error_score='raise')

        # model fitting:
        # no early stopping with GridSearchCV
        class_weights = compute_sample_weight(class_weight='balanced',␣
↪y=y_other_enc)
        grid.fit(X_other, y_other_enc, xgb__sample_weight=class_weights,␣
↪xgb__verbose=False) # verbose = validation_0-mlogloss output

        # results
        xgb_models.append(grid)
        y_test_pred = xgb_models[-1].predict(X_test)

        # test-score = f1_weighted
        test_score = f1_score(y_test_enc, y_test_pred, average='weighted')
        xgb_test_scores.append(test_score)
        xgb_test_sets.append((X_test, y_test_enc))

        # sanity check
        # print(test_score)

# best model:
xgb_best_model_idx = np.argmax(xgb_test_scores)
xgb_best_model = xgb_models[xgb_best_model_idx]
```

```
xgb_best_hyperparams = xgb_best_model.best_params_
xgb_best_test_score = xgb_test_scores[xgb_best_model_idx]

print("best model hyperparameters: ", xgb_best_hyperparams)
print("best model test f1: ", xgb_best_test_score)

# results (plot later)
xgb_mean = np.mean(xgb_test_scores)
xgb_std = np.std(xgb_test_scores)
```

```
Fitting 2 folds for each of 405 candidates, totalling 810 fits
Fitting 2 folds for each of 405 candidates, totalling 810 fits
Fitting 2 folds for each of 405 candidates, totalling 810 fits
Fitting 2 folds for each of 405 candidates, totalling 810 fits
Fitting 2 folds for each of 405 candidates, totalling 810 fits
best model hyperparameters:  {'xgb__learning_rate': 0.05, 'xgb__max_depth': 30,
'xgb__n_estimators': 50, 'xgb__reg_lambda': np.float64(1.0), 'xgb__subsample':
0.3}
best model test f1:  0.9699978646166987
```

[47]:
```
# BEST MODEL

# all 'best' models:
print("lr: ", lr_mean, ", ", lr_std)
print("svc: ", svc_mean, ", ", svc_std)
print("rfc: ", rfc_mean, ", ", rfc_std)
print("xgb: ", xgb_mean, ", ", xgb_std)

# xgb:
# best model hyperparameters:  {'xgb__learning_rate': 0.05, 'xgb__max_depth':␣
 ↪30, 'xgb__n_estimators': 50, 'xgb__reg_lambda': np.float64(0.01),␣
 ↪'xgb__subsample': 0.5}
# best model test f1:  0.9600153034352713

best_model = xgb_best_model
best_X_test, best_y_test = xgb_test_sets[xgb_best_model_idx]
```

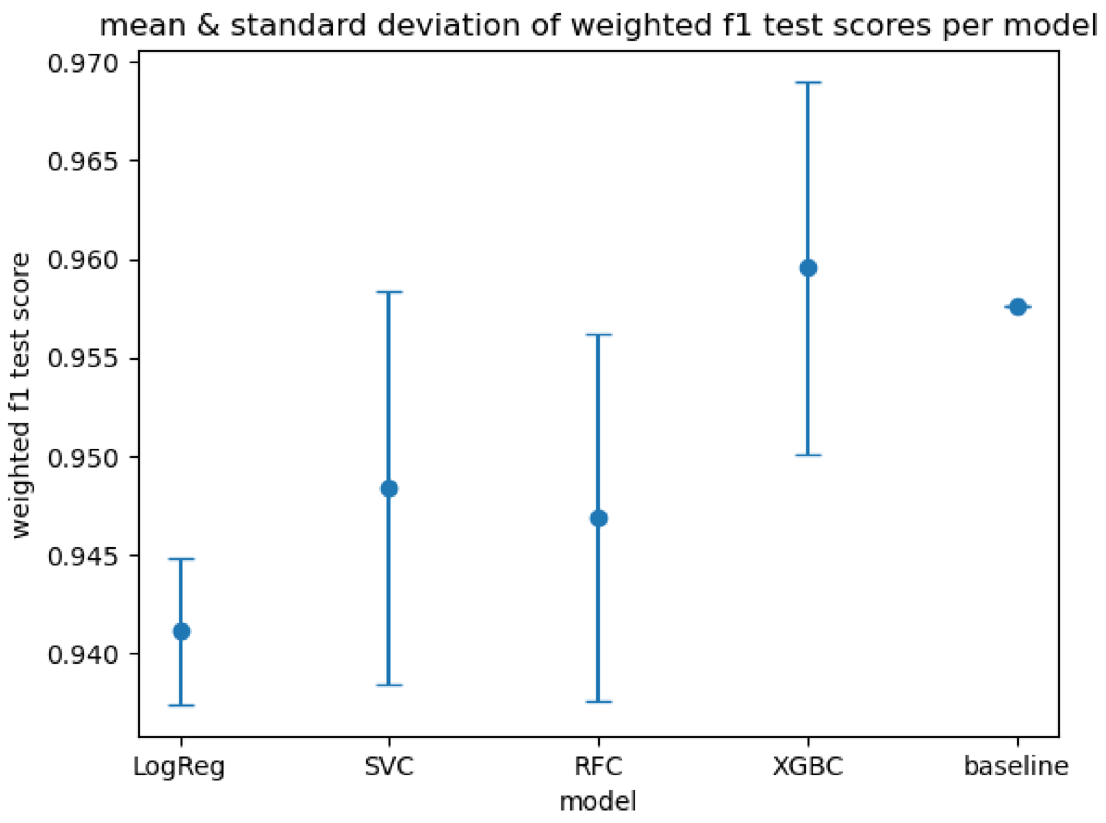
```
lr:  0.9411238583535871 ,  0.003720000194119701
svc:  0.9483896831638686 ,  0.009935752032979972
rfc:  0.9468757082403811 ,  0.00931753233832749
xgb:  0.9595519771332045 ,  0.009438372944090704
```

[33]:
```
# BASELINE

# multiclass classification: baseline = predict majority class for all points
# majority class = alive.after.6m = 0
majority_class = 0
y_baseline_pred = [majority_class] * len(best_y_test)
```

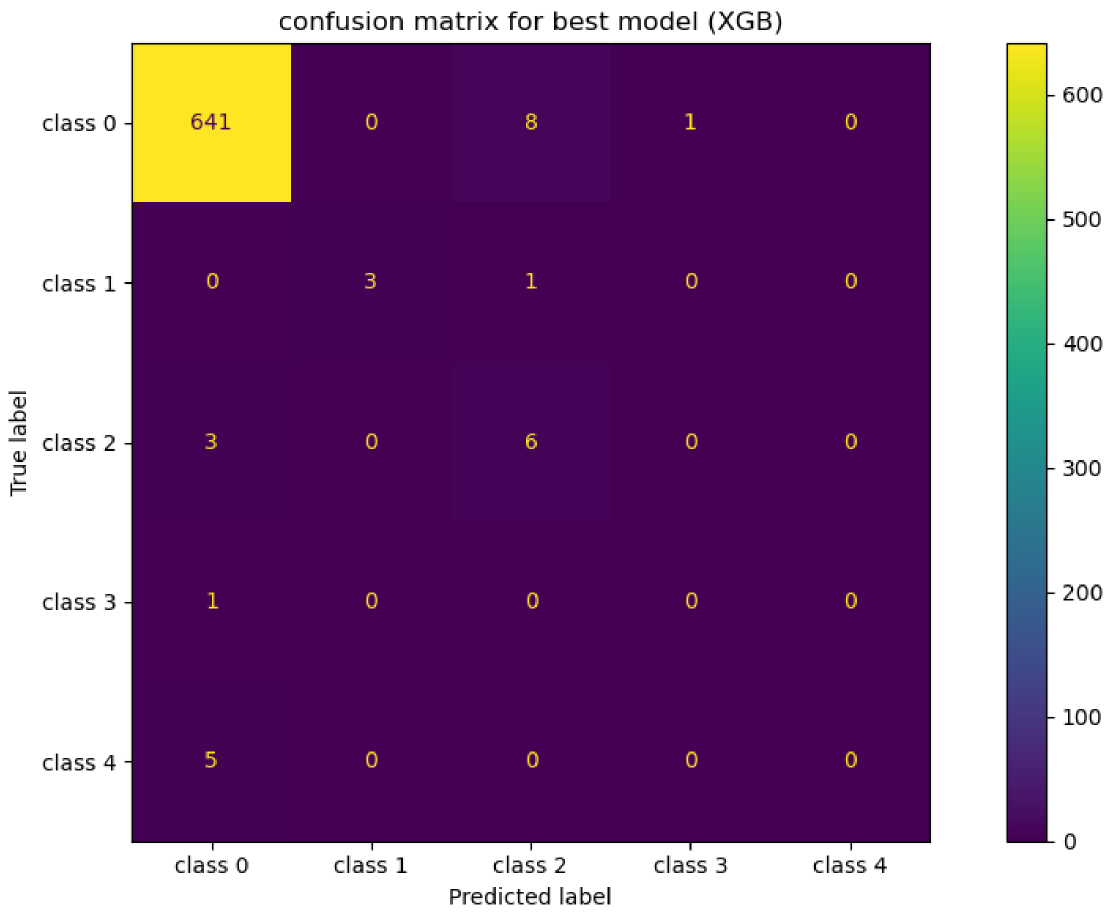
```
baseline_test_score = f1_score(best_y_test, y_baseline_pred, average='weighted')
print("baseline test f1: ", baseline_test_score)
```

```
baseline test f1:  0.9576036563460791
```

[41]:
```
# RESULTS
# plot means and standard deviations

labels = ['LogReg', 'SVC', 'RFC', 'XGBC', 'baseline']
means = [lr_mean, svc_mean, rfc_mean, xgb_mean, baseline_test_score]
stds = [lr_std, svc_std, rfc_std, xgb_std, 0] # assume baseline std=0

fig = plt.figure()
plt.errorbar(labels, means, yerr=stds, fmt='o', capsize=5, label='mean with␣
 ↪std')
plt.xlabel('model')
plt.ylabel('weighted f1 test score')
plt.title('mean & standard deviation of weighted f1 test scores per model')
plt.show()

fig.savefig("mean_sd.png", dpi=300)
```



[39]:
```
# INTERPRETABILITY
# confusion matrix
# best model:

# predict:
y_true = best_y_test
y_pred = best_model.predict(best_X_test)

# overall confusion matrix
cm = confusion_matrix(y_true, y_pred)
disp = ConfusionMatrixDisplay(cm,display_labels=['class 0', 'class 1', 'class␣
 ↪2', 'class 3', 'class 4'])
fig, ax = plt.subplots(figsize=(10,6))
disp.plot(ax=ax)
plt.title('confusion matrix for best model (XGB)')
plt.tight_layout()
plt.show()

fig.savefig("conf_matx.png", dpi=300)
```

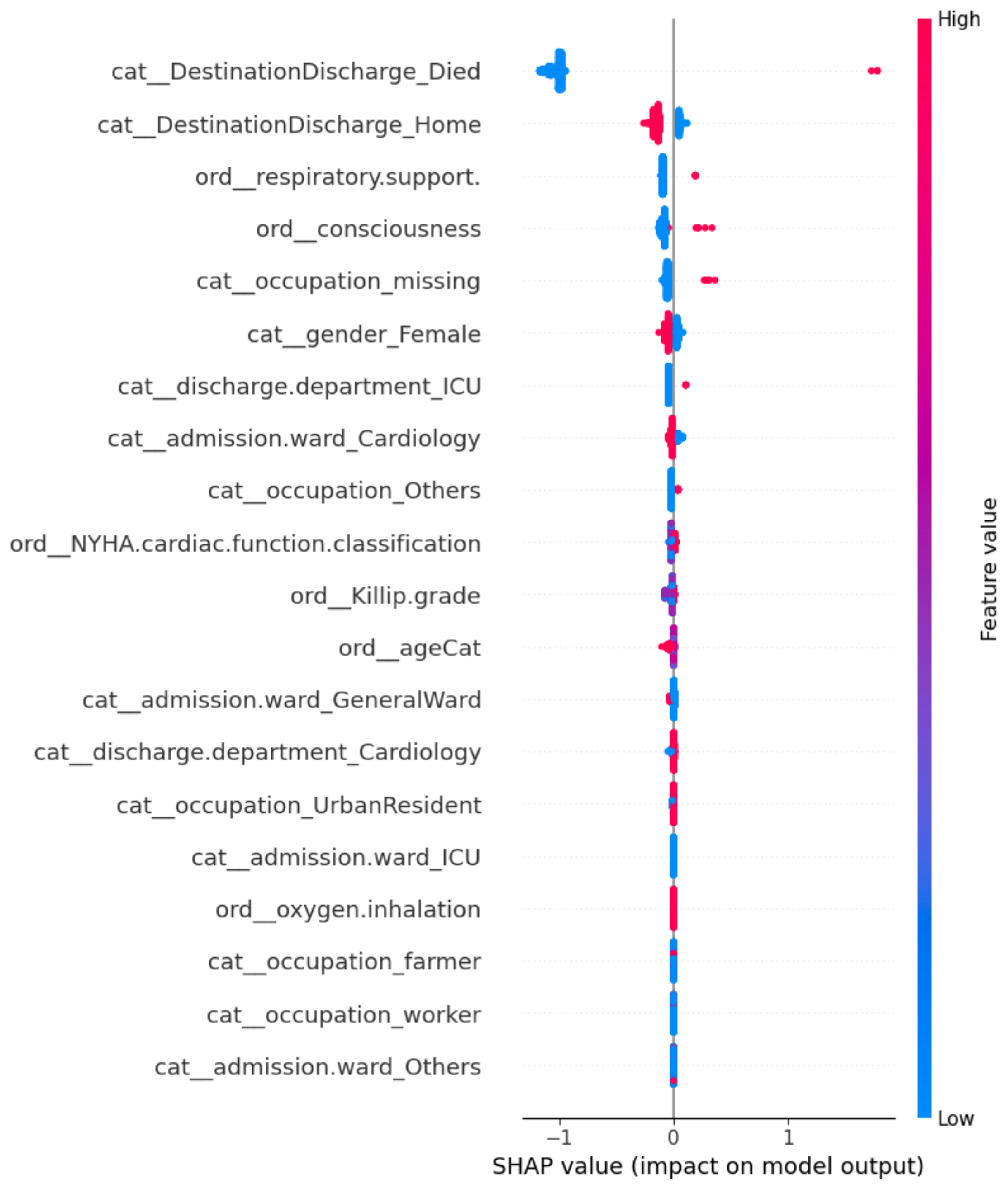


```
[ ]: # INTERPRETABILITY
     # global feature importances - xgb feature_importances_
     best_model_step = best_model.best_estimator_.named_steps['xgb']
     importances = best_model_step.feature_importances_
     ftr_names = best_model.best_estimator_.named_steps['preprocessor'].
      ↪get_feature_names_out()
     ftr_importance_df = pd.DataFrame({'feature': ftr_names,
                                       'importance': importances})
     ftr_importance_df = ftr_importance_df.sort_values(by='importance',␣
      ↪ascending=False) # sort descending

     ftr_importance_df
```

```
[ ]:                                       feature  importance
     10               cat__DestinationDischarge_Died    0.108454
     26                   ord__respiratory.support.    0.084143
     19        cat__discharge.department_Cardiology    0.066198
     4                      cat__occupation_missing    0.065827
     12               cat__DestinationDischarge_Home    0.054816
     6              cat__admission.ward_Cardiology    0.053379
     1                       cat__occupation_Others    0.050983
     13            cat__DestinationDischarge_Unknown    0.046431
     27                                 ord__ageCat    0.041249
     28                          ord__admission.way    0.039064
     24                           ord__Killip.grade    0.038888
     14                          cat__gender_Female    0.035087
     7             cat__admission.ward_GeneralWard    0.032934
     23    ord__NYHA.cardiac.function.classification    0.030319
     3                       cat__occupation_farmer    0.029714
     20       cat__discharge.department_GeneralWard    0.027263
     17             cat__type.of.heart.failure_Left    0.026680
     29             ord__type.II.respiratory.failure    0.025906
     11  cat__DestinationDischarge_HealthcareFacility    0.024827
     21               cat__discharge.department_ICU    0.021101
     25                          ord__consciousness    0.020541
     16             cat__type.of.heart.failure_Both    0.018168
     2                cat__occupation_UrbanResident    0.017123
     22            cat__discharge.department_Others    0.016507
     8                      cat__admission.ward_ICU    0.010975
     9                   cat__admission.ward_Others    0.007984
     30                       ord__oxygen.inhalation    0.005441
     0                      cat__occupation_Officer    0.000000
     18            cat__type.of.heart.failure_Right    0.000000
     5                       cat__occupation_worker    0.000000
     15                            cat__gender_Male    0.000000
```

```
[120]: # INTERPRETABILITY
       # local feature importances - SHAP
       best_pipe = grid.best_estimator_

       shap.initjs()
       explainer = shap.TreeExplainer(best_pipe[1])
       X_test_transformed = best_pipe[0].transform(best_X_test)
       # shap_values = explainer.shap_values(X_test_transformed)

       # print(np.shape(X_test_transformed)) # (669, 31)
       # print(np.shape(shap_values)) # (669, 31, 5)

       # index = 0 # the index of the point to explain
       # print(explainer.expected_value[0]) # we explain class 0 predictions

       feature_names = best_pipe[0].get_feature_names_out()
       # shap.force_plot(explainer.expected_value[0], shap_values[index,:,0], features␣
        ↪= X_test_transformed[index,:],feature_names = feature_names,
       #                        matplotlib=True, show=False)
       # # fig.title('SHAP force plot for class 0')
       # # plt.show()
       # # fig.savefig("shap.png", dpi=300)
       # # Get the current figure and axes

       # fig, ax = plt.gcf(), plt.gca()
       # # fig.set_size_inches(12, 4)    # taller canvas


       # for text in ax.texts:
       #     # text.set_rotation(15) # Rotate by 45 degrees
       #     # x, y = text.get_position()
       #     # text.set_position((x, y - 0.5))   # push
       #     if text.get_color() in ('#ff0052', '#008bff'):   # feature labels
       #         text.set_rotation(45)
       #         x, y = text.get_position()
       #         text.set_position((x, y - 0.5))

       # # plt.tight_layout()
       # plt.show()

       shap.summary_plot(shap_values[:,:,1], X_test_transformed,feature_names =␣
        ↪feature_names)
```

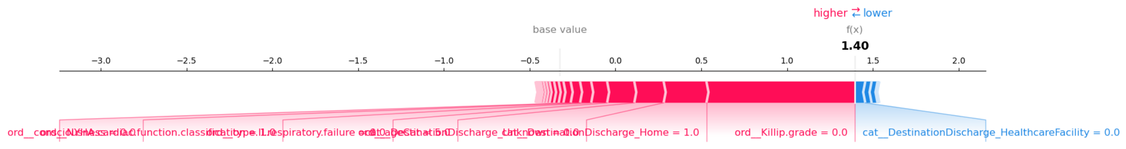
```
<IPython.core.display.HTML object>
```

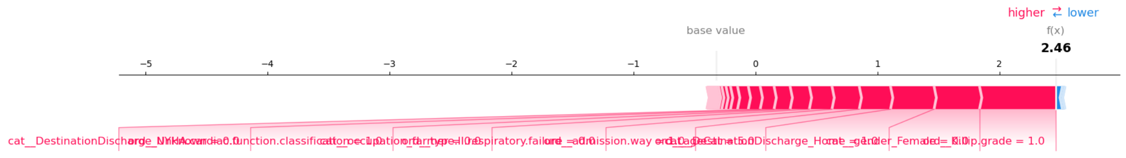


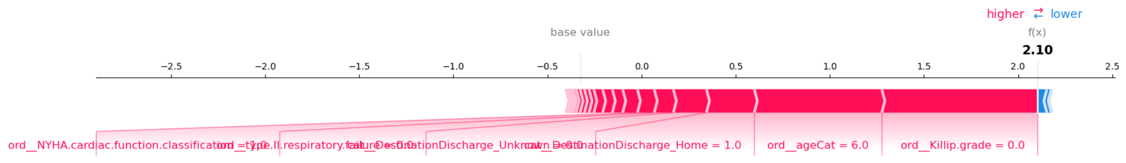
[ ]:
```
# local feature importances - SHAP
best_pipe = grid.best_estimator_

shap.initjs()
explainer = shap.TreeExplainer(best_pipe[1])
X_test_transformed = best_pipe[0].transform(best_X_test)
shap_values = explainer.shap_values(X_test_transformed)
```

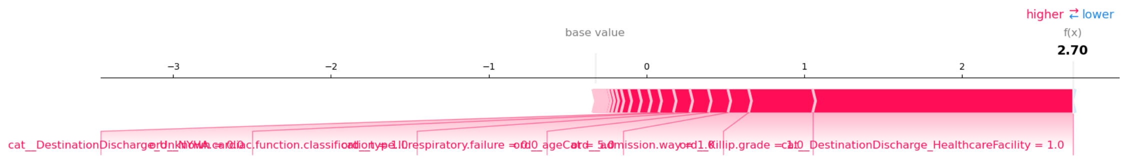
```
# print(np.shape(X_test_transformed)) # (669, 31)
# print(np.shape(shap_values)) # (669, 31, 5)

print("expected value: ", explainer.expected_value[0])


for i in range(5):
    index = i # the index of the point to explain

    feature_names = best_pipe[0].get_feature_names_out()
    shap.force_plot(explainer.expected_value[0], shap_values[index,:,0],␣
 ↪features = X_test_transformed[index,:],feature_names = feature_names,
                        matplotlib=True)
    # fig.savefig(f"shap_{i}.png", dpi=300)
```

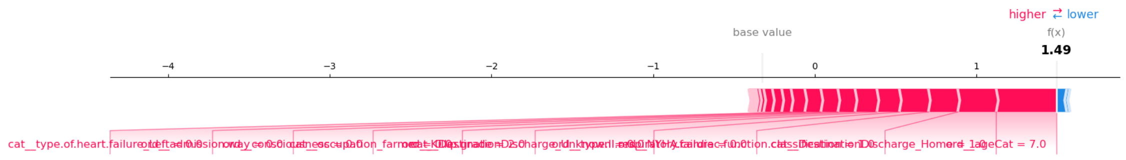
```
<IPython.core.display.HTML object>

expected value:  -0.3249051
```











[140]:
```python
# pipeline: best_pipe[0] = preprocessor, best_pipe[1] = xgb estimator
best_est = best_pipe[1]
preproc = best_pipe[0]

# transform test set once
X_test_transformed = preproc.transform(best_X_test)   # numpy array
feature_names = preproc.get_feature_names_out()

# class names (if you used a LabelEncoder)

class_names = list(y_labenc.classes_)

# create explainer (TreeExplainer for tree models)
explainer = shap.TreeExplainer(best_est)
shap_values = explainer.shap_values(X_test_transformed)  # could be list or ndarray

# print(shap_values.shape)

# shap_values can be either:
# # - a list of arrays: shap_values[c] shape (n_samples, n_features)
# # - or an ndarray shape (n_samples, n_features, n_classes)
# if isinstance(shap_values, list):
# n_classes = len(shap_values)
    # ensure each element is (n_samples, n_features)
# else:
#     # convert to list of per-class arrays for simpler indexing below
```

```
n_classes = shap_values.shape[2]
shap_values = [shap_values[:, :, c] for c in range(n_classes)]

sample_idx = 5   # the sample you want to explain

shap.initjs()
for c in range(n_classes):
    print(f"SHAP force plot for class {class_names[c]}:")
    base = explainer.expected_value[c]      # baseline for class c
    sv = shap_values[c][sample_idx]         # shape (n_features,)
    display(shap.force_plot(base, sv, X_test_transformed[sample_idx],
                            feature_names=feature_names))

# shap.initjs()
# for c in range(n_classes):
#     print(f"SHAP force plot for class {class_names[c]}:")
#     base = explainer.expected_value[c]      # baseline for class c
#     sv = shap_values[c][sample_idx]         # shape (n_features,)
#     display(shap.force_plot(base, sv, X_test_transformed[sample_idx],
#                             feature_names=feature_names, matplotlib=True,␣
 ↪show=False))
#     # plt.xticks(rotation=45)
# plt.tight_layout()
# plt.show()

# for c in range(n_classes):
#     base = explainer.expected_value[c]
#     sv = shap_values[c][sample_idx]

#     # create the matplotlib force plot (returns a Matplotlib Figure)
#     fig = shap.force_plot(base, sv, X_test_transformed[sample_idx],
#                           feature_names=feature_names, matplotlib=True,␣
 ↪show=False)

#     # rotate x tick labels on all axes in the figure
#     for ax in fig.axes:
#         for lbl in ax.get_xticklabels():
#             lbl.set_rotation(45)
#             lbl.set_ha('right')

#     plt.tight_layout()
#     display(fig)
#     plt.close(fig)
```

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

```
SHAP force plot for class alive.after.6m:
```

```
<shap.plots._force.AdditiveForceVisualizer at 0x1386ab8f0>

SHAP force plot for class death.at.hospital:

<shap.plots._force.AdditiveForceVisualizer at 0x13a09d400>

SHAP force plot for class death.within.28d:

<shap.plots._force.AdditiveForceVisualizer at 0x13a09d400>

SHAP force plot for class death.within.3m:

<shap.plots._force.AdditiveForceVisualizer at 0x1383f5be0>

SHAP force plot for class death.within.6m:

<shap.plots._force.AdditiveForceVisualizer at 0x1384b6cc0>
```