TA Instructions

Hello! Welcome to Team 11's report. The checkpoints are labeled as such in the headers to make it easier for you to run, but everything has been commented out that is not necessary. The data access information is available in the "Data" section, and all dependencies / necessary downloads are show in code.

Our github repo can be accessed here: https://github.com/LoganB99/DL4H-SP24-Local-Explanations-For-Cervical-Cancer

Our video overview can be accessed here: https://drive.google.com/file/d/1VbnpcCaYxyATlkzQZPA5bLop64rc6XSg/view?usp=share_link

Mount Notebook to Google Drive

To clear up clutter, the original FAQ and Attentions are in https://colab.research.google.com/drive/1MGxB_J2TvhAANcQG8VNMvQp1QdQrcxWb?authuser=1

```
import pandas as pd
from google.colab import drive
drive.mount('/content/drive', force_remount=True)

    Mounted at /content/drive
```

```
#Testing
!pip install gspread google-auth
from google.colab import auth
auth.authenticate_user()

import gspread
from google.auth import default
creds, _ = default()

gc = gspread.authorize(creds)
```

```
Requirement already satisfied: gspread in /usr/local/lib/python3.10/dist-pack
Requirement already satisfied: google-auth in /usr/local/lib/python3.10/dist-
Requirement already satisfied: google-auth-oauthlib>=0.4.1 in /usr/local/lib/
Requirement already satisfied: StrEnum==0.4.15 in /usr/local/lib/python3.10/d
Requirement already satisfied: cachetools<6.0,>=2.0.0 in /usr/local/lib/pytho
Requirement already satisfied: pyasn1-modules>=0.2.1 in /usr/local/lib/python
Requirement already satisfied: rsa<5,>=3.1.4 in /usr/local/lib/python3.10/dis
Requirement already satisfied: requests-oauthlib>=0.7.0 in /usr/local/lib/pyt
Requirement already satisfied: pyasn1<0.7.0,>=0.4.6 in /usr/local/lib/python3
Requirement already satisfied: oauthlib>=3.0.0 in /usr/local/lib/python3.10/d
Requirement already satisfied: requests>=2.0.0 in /usr/local/lib/python3.10/d
Requirement already satisfied: charset-normalizer<4,>=2 in /usr/local/lib/pyt
Requirement already satisfied: idna<4,>=2.5 in /usr/local/lib/python3.10/dist
Requirement already satisfied: urllib3<3,>=1.21.1 in /usr/local/lib/python3.1
Requirement already satisfied: certifi>=2017.4.17 in /usr/local/lib/python3.1
```

Introduction

- Background of the problem

  Cervical Cancer prediction is a prevalent and necessary problem within today's healthcare system. Specifcally, researchers are working towards identifying risk factors and potential causes for cervical cancer. Current models, however, cannot explain why a decision is made. Local explainability techniques have been developed aiming to the causes and effects of changes within a model and explain the decision-making process at an individual prediction level, but may not be applicable in every scenario, and the explanations are not always consistent or faithful. Consequently, clinicians cannot explain why a model selected a patient as low or high risk through black-box magic models.

- Paper explanation

  The paper aims to combat the current problem of ambiguity in explainability across scenarios and analyze the existing local interpretability methods to propose methods to help clinicians determine which type of explanation models to use in a given context. Specifically, the researchers tested 5 different ML algorithms to identify the model with the highest disease predition accuracy, and then applied explainability methods to the model to identify the best practice for disease prediction. The paper then uses the predictions of the best model to generate explanations for each model across popular interpretability methods. These methods include LIME, SHAP, Diverse Counterfactual Explanations, Tree Interpreter, and Local Surrogates. Finally, each of the interpretability methods are evaluated on a set of metrics. The model found that LIME is the most robust explainability method, but no single explaination performance optimally across all metrics. Therefore, the researches suggest that clinicians should choose a method based on the setting or choose a weighted sum of metrics. This approach helps satisfy the desired explainability properties when determining patient risk in cervical cancer. As a result, the paper also recommends and influences future models to consider interpetability methods in their analysis to improve trust in the new world of generative and predictive models.

Scope of Reproducibility:

We aim to reproduce the results of the model using the UCI dataset and suggested models. We will use ADASYN to balance the dataset and remove and retrain features as one of our ablations. As another ablation, we want to test the model on the unbalanced dataset.

1. Hypothesis 1: Random Forest is the most performing model in predicting cervical cancer in terms of AUC.
2. Hypothesis 2: LIME is the most robust explainability model shown by the ROAR (remove and retrain) faithfulness metric.

Methodology

Python version in notebook: 3.10.12

Checkpoint: Dependencies

Note: because of Colab's default setup, you may have to restart the notebook and rerun after installing packages.

```
# External package installation
!pip install pandas
!pip install kaleido
!pip install gdown==4.6.0
!pip install shap
!pip install lime
!pip install interpret-community
!pip install alibi
!pip install treeinterpreter
!pip install SALib
!pip install dice-ml
!pip install pip install spectralcluster
!pip install kaleido
```

```
!pip install requests
!pip install shapash
```

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Requirement already satisfied: numpy>=1.21.0 in /usr/local/lib/python3.10/dis
Requirement already satisfied: six>=1.5 in /usr/local/lib/python3.10/dist-pac
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  Downloading kaleido-0.2.1-py2.py3-none-manylinux1_x86_64.whl (79.9 MB)
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Installing collected packages: kaleido
Successfully installed kaleido-0.2.1
Collecting gdown==4.6.0
  Downloading gdown-4.6.0-py3-none-any.whl (14 kB)
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Requirement already satisfied: six in /usr/local/lib/python3.10/dist-packages
Requirement already satisfied: tqdm in /usr/local/lib/python3.10/dist-package
Requirement already satisfied: beautifulsoup4 in /usr/local/lib/python3.10/di
Requirement already satisfied: soupsieve>1.2 in /usr/local/lib/python3.10/dis
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Requirement already satisfied: certifi>=2017.4.17 in /usr/local/lib/python3.1
Requirement already satisfied: PySocks!=1.5.7,>=1.5.6 in /usr/local/lib/pytho
Installing collected packages: gdown
  Attempting uninstall: gdown
    Found existing installation: gdown 5.1.0
    Uninstalling gdown-5.1.0:
      Successfully uninstalled gdown-5.1.0
Successfully installed gdown-4.6.0
Collecting shap
  Downloading shap-0.45.0-cp310-cp310-manylinux_2_12_x86_64.manylinux2010_x86_
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Installing collected packages: slicer, shap
Successfully installed shap-0.45.0 slicer-0.0.7
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  Preparing metadata (setup.py) ... done
Requirement already satisfied: matplotlib in /usr/local/lib/python3.10/dist-p
Requirement already satisfied: numpy in /usr/local/lib/python3.10/dist-packag
```

```
# download files and models
import gdown
import pickle
import requests

# Basic data handling and scientific computing
import numpy as np  # Numerical computing library
import pandas as pd  # Data manipulation and analysis
import random
from numpy import arange


# Visualization libraries
import seaborn as sns  # Statistical data visualization
import matplotlib.pyplot as plt  # Basic plotting library
import plotly.express as px  # Interactive plotting library
import plotly.graph_objects as go  # For creating custom plots with Plotly
from plotly.subplots import make_subplots  # For creating subplots with Plotly

# Data preprocessing and model evaluation tools
from sklearn.impute import SimpleImputer  # For handling missing data
from sklearn.model_selection import StratifiedShuffleSplit  # For creating strati
from sklearn.preprocessing import RobustScaler, StandardScaler  # Data scaling me
from sklearn.decomposition import PCA  # Principal Component Analysis
from sklearn.pipeline import Pipeline  # For creating modeling pipelines
from sklearn.metrics import accuracy_score, confusion_matrix  # Model evaluation
from sklearn.metrics import precision_recall_fscore_support  # Precision, recall,
from sklearn.metrics import roc_auc_score # AUC score

# Machine learning models
from sklearn.linear_model import LogisticRegression  # Logistic regression model
from sklearn.ensemble import RandomForestClassifier, VotingClassifier  # Ensemble
from sklearn.neighbors import KNeighborsClassifier  # k-Nearest Neighbors model
from sklearn.svm import SVC  # Support Vector Machine model
from sklearn.neural_network import MLPClassifier

# Model selection and hyperparameter tuning
from sklearn.model_selection import GridSearchCV  # For hyperparameter tuning

# Data balancing techniques
from imblearn.over_sampling import SMOTE, ADASYN  # Over-sampling techniques
from imblearn.over_sampling import RandomOverSampler  # Random over-sampling

# Additional utilities
from typing import List  # For type hints
from google.colab import drive  # Google Colab drive integration (if using Google
import warnings  # For controlling warning messages
warnings.filterwarnings('ignore')  # Suppress warning messages for cleaner output
# Plotly setup for notebooks
from plotly.offline import plot, iplot, init_notebook_mode
# init_notebook_mode(connected=True)

# Local explainability
from sklearn.inspection import permutation_importance
from sklearn.inspection import PartialDependenceDisplay, partial_dependence
from interpret_community.mimic.mimic_explainer import MimicExplainer
from interpret_community.mimic.models import LinearExplainableModel
from interpret.blackbox import MorrisSensitivity
import shap
import lime
from lime import lime_tabular
from treeinterpreter import treeinterpreter as ti
```

Checkpoint: Project Files

```
gdown.download(id='11swC5N9lqEVTp3E-K1dtBrlHQEoEkxtk', output="project_files.tgz"
!tar -xzf project_files.tgz
```

```
    Downloading...
    From: https://drive.google.com/uc?id=11swC5N9lqEVTp3E-K1dtBrlHQEoEkxtk
    To: /content/project_files.tgz
    100%|██████████| 10.5M/10.5M [00:00<00:00, 68.0MB/s]
    tar: Ignoring unknown extended header keyword 'LIBARCHIVE.xattr.com.apple.qua
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```
root = 'DL4H_Sp24_Final_Project'
```

Data

The raw dataset comes and can be downloaded from from UC Irvine Machine Learning Repository. https://archive.ics.uci.edu/dataset/383/cervical+cancer+risk+factors

Fernandes,Kelwin, Cardoso,Jaime, and Fernandes,Jessica. (2017). Cervical Cancer (Risk Factors). UCI Machine Learning Repository. https://doi.org/10.24432/C5Z310.

The dataset was collected at 'Hospital Universitario de Caracas' in Caracas, Venezuela. The dataset contains demographic information, habits, and historic medical records of 858 patients. Several patients decided not to answer some of the questions because of privacy concerns (missing values represented as '?').

The missing values certainly make some of the columns less accurate. Time since STD Diagnosis is largely unknown, followed by presence of an IUD. So there is not a perfect correlation to be determined for every feature.

We load the raw data, place it in our project directory, and display statistics, showing how many patients are without cancer and with cancer. We display the number of unknowns before we clean our data.

To clean and process the data, we convert numerical 'object' columns to integers. We replace '?'s with the median of that column. We rerun the overall statistics to confirm there are no "unknown" values and the number of cancer patients remained the same. We create a new age_category column that stratifies the ages.

We run statistics on the age category to gain context. For example, we can see things like just over 2% of the dataset is diagnosed with cancer, but 44% of those diagnosed with cancer are in their 30's, and 20% of patients who are in their 50's have cancer. (We must remember the dataset is small, which is why we sample using ADASYN). There are only 4 patients 70 or older, and they all happen to not have cancer. This does not mean age is not important.

Processing and Statistics

Checkpoint: Load Data Function

```
def load_data(data_dir):
  # implement this function to load raw data to dataframe/numpy array/tensor
    return pd.read_csv(data_dir, delimiter=',', encoding='utf-8')
```

Checkpoint: Load Raw Data

```
root = '/content/drive/My Drive/DL4H_Sp24_Final_Project/'
# dir and function to load raw data
have_access = True


try:
  data_dir = '/content/drive/My Drive/DL4H_Sp24_Final_Project/risk_factors_cervic
  raw_risk_factor_df = load_data(data_dir)
  have_access = True
except:
  have_access = False
  data_dir = 'risk_factors_cervical_cancer.csv'
  # gdown.download('https://drive.google.com/file/d/13Co6aIxBU4KXMNH56TDyQd70pkk_
  raw_risk_factor_df = load_data('DL4H_Sp24_Final_Project/risk_factors_cervical_c
  print("No access, Used Gdown!")
# https://drive.google.com/drive/folders/1AUr8BgW16UU-7XjFf8O77XAgjA27gISV?usp=sh
raw_risk_factor_df
```

```
No access, Used Gdown!
```

	Age	Number of sexual partners	First sexual intercourse	Num of pregnancies	Smokes	Smokes (years)	Smokes (packs/year)	Co
0	18	4.0	15.0	1.0	0.0	0.0	0.0	
1	15	1.0	14.0	1.0	0.0	0.0	0.0	
2	34	1.0	?	1.0	0.0	0.0	0.0	
3	52	5.0	16.0	4.0	1.0	37.0	37.0	
4	46	3.0	21.0	4.0	0.0	0.0	0.0	
...	...	...	...	...	...	...	...	
853	34	3.0	18.0	0.0	0.0	0.0	0.0	
854	32	2.0	19.0	1.0	0.0	0.0	0.0	
855	25	2.0	17.0	0.0	0.0	0.0	0.0	
856	33	2.0	24.0	2.0	0.0	0.0	0.0	
857	29	2.0	20.0	1.0	0.0	0.0	0.0	

858 rows × 36 columns

Checkpoint: Define Statistics methods

```
# calculate dataset statistics
def calculate_dataset_stats(df):
  print(len(df), " total patients")
  print(df['Dx:Cancer'].value_counts()[0], " patients without Cancer")
  print(df['Dx:Cancer'].value_counts()[1], " patients with Cancer")
  print(df.applymap(lambda x: x == "?").sum().sum(), " unknown values")
  specified_value = '?'  # Replace with the value you're interested in
  max_count = -1
  column_with_most = None

  for column in df.columns:
    if column == "STDs: Time since last diagnosis" or column == "STDs: Time since
      continue
    value_counts = df[column].value_counts()
    if specified_value in value_counts:
      if value_counts[specified_value] > max_count:
          max_count = value_counts[specified_value]
          column_with_most = column

  print(f"Column with the most '{specified_value}': {column_with_most} (Count: {m
  dataset_size = df.shape[0] * df.shape[1]
  print(100 * df.applymap(lambda x: x == "?").sum().sum()/dataset_size, " percent

  # Formatting to match the style: dtypes: float64(2), int64(2), object(1)
  formatted_summary = ", ".join([f"{k}: {v}" for k, v in df.dtypes.value_counts()
  print("dtypes:", formatted_summary)


# NOTE: this is a deviation from the source code. In the source code, category_pe
# summed up to 100 across the diagnosis, we also wanted to show the percent for e

def col_stats(df, diagnosis_column, category_column):
    """
    Calculates statistics for diagnosis distributions across categories.

    Parameters:
    - df (DataFrame): The input data frame containing the relevant data.
    - diagnosis_column (str): The name of the column containing diagnosis informa
    - category_column (str): The name of the column containing category labels (e

    Returns:
    - DataFrame: A pivot table presenting the calculated statistics.
    """
    # Calculate the overall percentage of each diagnosis-category combination.
    overall_percentages = df[[diagnosis_column, category_column]] \
        .value_counts(normalize=True) \
        .mul(100) \
        .round(decimals=4) \
        .reset_index(name='Overall_Percent')

    # Count the occurrences within each category for a diagnosis.
    diagnosis_by_category_counts = df.groupby([diagnosis_column, category_column]
        .size() \
        .reset_index(name='Count_in_Category')

    # Count the total occurrences within each category.
    total_in_category = df.groupby(category_column) \
        .size() \
        .reset_index(name='Total_in_Category')

    # Calculate the percentage of each diagnosis within specific categories.
    category_percentages = pd.merge(diagnosis_by_category_counts, total_in_catego
    category_percentages['Category_Percent'] = category_percentages['Count_in_Cat
        .div(category_percentages['Total_in_Category']) \
        .mul(100) \
        .round(decimals=4)

    # Count occurrences of each diagnosis and calculate the percentage within the
    diagnosis_counts_and_percentages = pd.merge(
        df.groupby([diagnosis_column, category_column]).size().reset_index(name='
        df.groupby(diagnosis_column).size().reset_index(name='Total_in_Diagnosis'
        on=diagnosis_column
    )
    diagnosis_counts_and_percentages['Diagnosis_Percent'] = diagnosis_counts_and_
        .div(diagnosis_counts_and_percentages['Total_in_Diagnosis']) \
        .mul(100) \
        .round(4)

    # Merge the overall percentages with category-specific percentages.
    temp_merged = pd.merge(
        overall_percentages,
        category_percentages[[diagnosis_column, category_column, 'Category_Percen
        on=[diagnosis_column, category_column]
    )

    # Merge with the diagnosis percentage data.
    final_merged = pd.merge(
        temp_merged,
        diagnosis_counts_and_percentages[[diagnosis_column, category_column, 'Dia
        on=[diagnosis_column, category_column]
    )

    # Create a pivot table for better presentation.
    final_pivot_table = final_merged.pivot(index=category_column, columns=diagnos
    final_pivot_table.fillna(0.000, inplace=True)
    return final_pivot_table

def print_unique_values_df(df: pd.DataFrame):
    for col in list(df):
        print("Number of Unique Values for "'{}'": {}".format(str(col), len(risk_
        print("dtype for {} is :{}".format(str(col), risk_factor_df[col].dtypes))
        print("-" * 150)
```

Checkpoint: Define Processing Method

```
# process raw data
def process_data(raw_data):
    # implement this function to process the data as you need
  #these columns are not of type object, but are of type numeric
  cols_to_convert = ['Number of sexual partners', 'First sexual intercourse', 'Nu
                  'Smokes (years)', 'Smokes (packs/year)', 'Hormonal Contracept
                  'Hormonal Contraceptives (years)', 'IUD', 'IUD (years)', 'STD
                  'STDs:condylomatosis', 'STDs:cervical condylomatosis', 'STDs:
                  'STDs:vulvo-perineal condylomatosis', 'STDs:syphilis', 'STDs:
                  'STDs:genital herpes', 'STDs:molluscum contagiosum', 'STDs:AI
                  'STDs:HPV', 'STDs: Time since first diagnosis',
                  'STDs: Time since last diagnosis']

  std_cols = {'STDs:condylomatosis',
          'STDs:cervical condylomatosis',
          'STDs:vaginal condylomatosis',
          'STDs:vulvo-perineal condylomatosis',
          'STDs:syphilis',
          'STDs:pelvic inflammatory disease',
          'STDs:genital herpes',
          'STDs:molluscum contagiosum',
          'STDs:AIDS',
          'STDs:HIV',
          'STDs:Hepatitis B',
          'STDs:HPV'}
test_cols = ["Hinselmann", "Schiller", "Citology", "Biopsy"]

to_int_and_beyond = {"total_tests",
                   "total_std",
                   "Smokes",
                   "Biopsy",
                   "Dx:Cancer",
                   "Num of pregnancies",
                   "Number of sexual partners",
                   "First sexual intercourse",
                   "Hormonal Contraceptives",
                   "IUD",
                   "STDs",
                   "STDs (number)",
                   "STDs: Number of diagnosis",
                   "Dx:CIN",
                   "Dx:HPV",
                   "Dx",
                   "Hinselmann",
                   "Schiller",
                   "Biopsy",
                   "Citology"}

to_int_and_beyond = to_int_and_beyond.union(std_cols)

# convert object columns to numeric and replace with nan
raw_data[cols_to_convert] = raw_data[cols_to_convert].apply(pd.to_numeric, errc
raw_data[cols_to_convert].fillna(np.nan, inplace=True)
# replace nan values with the median of the column
imp = SimpleImputer(strategy="median")
X = imp.fit_transform(raw_data)
risk_factor_df = pd.DataFrame(X, columns=list(raw_data.columns))

# make new columns
risk_factor_df["Age"] = risk_factor_df["Age"].astype(int)
risk_factor_df["age_cat"] = risk_factor_df["Age"].apply(age_cat)
risk_factor_df["total_std"] = risk_factor_df[list(std_cols)].sum(axis=1)
risk_factor_df["total_tests"] = risk_factor_df[test_cols].sum(axis = 1)
for col in to_int_and_beyond:
  risk_factor_df[col] = risk_factor_df[col].astype(int)

# Aggregate the STD counts by age categories
std_agg = risk_factor_df.groupby("age_cat", as_index=False)[list(std_cols)].sum
return risk_factor_df, std_agg
```

```
# categorize the age ranges
def age_cat(age):
    if age < 12:
        return "Child"
    elif age < 20:
        return "Teen"
    elif age < 30:
        return "20's"
    elif age < 40:
        return "30's"
    elif age < 50:
        return "40's"
    elif age < 60:
        return "50's"
    elif age < 70:
        return "60's"
    else:
        return "70+"

def save_data(df, path):
  if have_access:
    print("Save checkpoint granted")
    df.to_csv(path, index=False)
  else:
    print("You have no access to save data, skipping save checkpoint")
```

Checkpoint: Calculate Raw Data Stats

```
print('RAW DATA STATS')
calculate_dataset_stats(raw_risk_factor_df)
```

```
RAW DATA STATS
858  total patients
840  patients without Cancer
18  patients with Cancer
3622  unknown values
Column with the most '?': IUD (Count: 117)
11.726236726236726  percent of the dataset is unknown
dtypes: object: 26, int64: 10
```

(BEFORE ADASYN) Process Data, Calculate Processed Stats, and Save Data

```
# process data set
risk_factor_df, std_agg = process_data(raw_risk_factor_df)
save_data(risk_factor_df, '/content/drive/My Drive/DL4H_Sp24_Final_Project/proces
save_data(std_agg, '/content/drive/My Drive/DL4H_Sp24_Final_Project/processed_std
```

```
Save checkpoint granted
Save checkpoint granted
```

Checkpoint: Load Processed Data

```
root
```

```
'DL4H_Sp24_Final_Project'
```

```
try:
  data_dir = '/content/drive/My Drive/DL4H_Sp24_Final_Project/processed_risk_fact
  risk_factor_df = load_data(data_dir)
  unbalanced_risk_factor_df = risk_factor_df
  data_dir = '/content/drive/My Drive/DL4H_Sp24_Final_Project/processed_std_agg.c
  std_agg = load_data(data_dir)
  have_access = True
except:
  have_access = False
  data_dir = root+'/processed_risk_factors_cervical_cancer.csv'
  # gdown.download('https://drive.google.com/file/d/1n-II-zTyOpjToeWmetQFrbZ4YKFj
  risk_factor_df = load_data(data_dir)
  unbalanced_risk_factor_df = risk_factor_df
  data_dir = root+'/processed_std_agg.csv'
  # gdown.download('https://drive.google.com/file/d/11OiEdMjfYzcMtZNh1jIWQJlIOw4i
  std_agg = load_data(data_dir)
  print("No access, Used Gdown!")
print("-" * 150)
print('PROCESSED DATA STATS')
# print overall stats, might need to edit
calculate_dataset_stats(risk_factor_df)
print("-" * 150)
# print column specific stats
print('Dx:Cancer by age category')
dxCancerByAge = col_stats(risk_factor_df, 'Dx:Cancer', 'age_cat')
print(dxCancerByAge)
```

```
No access, Used Gdown!
-----------------------------------------------------------------------------
PROCESSED DATA STATS
858  total patients
840  patients without Cancer
18  patients with Cancer
0  unknown values
Column with the most '?': None (Count: -1)
0.0  percent of the dataset is unknown
dtypes: int64: 32, float64: 6, object: 1
-----------------------------------------------------------------------------
Dx:Cancer by age category
          age_cat Overall_Percent         Category_Percent
Dx:Cancer                       0       1                0        1
0            20's         45.3380  0.5828          98.7310   1.2690  \
1            30's         24.7086  0.9324          96.3636   3.6364
2            40's          6.1772  0.3497          94.6429   5.3571
3            50's          0.4662  0.1166          80.0000  20.0000
4             70+          0.4662  0.0000         100.0000   0.0000
5            Teen         20.7459  0.1166          99.4413   0.5587

          Diagnosis_Percent
Dx:Cancer                 0        1
0                   46.3095  27.7778
1                   25.2381  44.4444
2                    6.3095  16.6667
3                    0.4762   5.5556
4                    0.4762   0.0000
5                   21.1905   5.5556
```

Checkpoint: Visualizations

Top features that correlate with cancer Dx

```
# Features that correlate with a cancer diagnosis
n = 7
target = label = "Dx:Cancer"
# correlate the numerical columns of the df
corr = risk_factor_df.select_dtypes(include=np.number).corr()
# find the top 7 correlations with Dx:Cancer
x = corr.nlargest(n,target).index
print(x)
# make a corr_df with only the top 7 columns
corr_df =  risk_factor_df[list(x)]
```

```
# recalculate the correlation
corr = corr_df.corr()
# Creating a mask for the upper triangle
mask = np.triu(np.ones_like(corr, dtype=bool), k=1)

# Use the mask to replace the upper triangle with np.nan
corr_masked = corr.where(~mask)

# Plot using Plotly Express
fig = px.imshow(corr_masked,
                color_continuous_scale="PuBu",
                labels=dict(x="Feature", y="Feature", color="Correlation"),
                x=corr.columns,  # Adding column names here
                y=corr.index)    # Adding row names here

# Update layout with title
fig.update_layout(title="Top "+str(n)+" Features Correlated With "+str(target).ca
fig.update_xaxes(showgrid=False)
fig.update_yaxes(showgrid=False)
# Show plot
fig.show()
```

```
Index(['Dx:Cancer', 'Dx:HPV', 'Dx', 'STDs:HPV', 'total_tests', 'Biopsy',
       'Schiller'],
      dtype='object')
```

Distribution of age

```
# Distribution of age
age_dist = px.histogram(risk_factor_df, x="Age", marginal="box", color_discrete_s
age_dist.update_layout(title="Age distribution")
age_dist.show()
```

Pregnancy Distribution by Age

```
#Pregancy Distribution by Age
age_preg_bar = px.box(risk_factor_df.sort_values(by="Age",ascending=True), x="age
                      color_discrete_sequence=["darkblue"], points="outliers",
                      category_orders=["Teenager", "Twenties", "Thirties", "Forti
                                       "Seventy and over"])
age_preg_bar.update_xaxes(title="Age Category")
age_preg_bar.update_yaxes(title="Number of Pregnancies")
age_preg_bar.update_layout(title="Distribution of number of pregnancies per age g
age_preg_bar.show()
```

Mayo Risk Factors (May split further)

Mayo Clinic provides many risk factors for cervical cancer, including many sexual partners, earlier sexual activity, STIs, a wekeaned immune system, smoking, and the exposure to miscarriage preventian drug DES.

We can see from the following visualizations that number of sexual partners remain fairly consistent across age ranges. We can also see a very low correlation between number of sexual partners and any relevant diagnoses.

We see a very high correlation between HPV and Cancer, but a low correlation between CIN and HPV. This could be due to the incompletenss of this dataset, that we will try to balance alter.

```
# Mayo Risk factors - sexual partners, sexual activity, STIs, immune system, smok

label = 'age_cat'
# Plotting a box plot to visualize the distribution of the number of sexual partr
# The data is sorted by age and plotted with outliers, using a blue color for the
age_num_sex_partners = px.box(risk_factor_df.sort_values(by="Age", ascending=True
                      color_discrete_sequence=["blue"], points="outliers",
                      category_orders=["Teenager", "Twenties", "Thirties", "Forti
                                       "Seventy and over"])
# Updating axis titles for better readability and clarity.
age_num_sex_partners.update_xaxes(title="Age Category")
age_num_sex_partners.update_yaxes(title="Number of Sexual Partners")
# Updating the layout to add a title to the plot.
age_num_sex_partners.update_layout(title="Distribution of number of sexual partne
# Displaying the plot.
age_num_sex_partners.show()
```

```
# Creating a scatter plot to visualize the relationship between age and number of
# The plot includes a trend line (ordinary least squares - OLS) to indicate the g
# Opacity is set to 0.4 to handle overplotting, and color represents the number c
age_num_sex_partners = px.scatter(risk_factor_df, x="Age",
                                  y="Number of sexual partners",
                                  trendline="ols",
                                  opacity=0.4,
                                  color="Num of pregnancies",
                                  color_continuous_scale="rdbu")
# Updating the layout to add a title to the plot.
age_num_sex_partners.update_layout(title="Age vs Number of Sexual Partners")
# Displaying the plot.
age_num_sex_partners.show()
```

```
# Selecting columns related to diagnoses and number of sexual partners for correl
diagnoses_num_partner_compare_cols = [label, 'Dx:HPV', "Number of sexual partners
# Calculating the correlation matrix for the selected columns.
corr_matrix = risk_factor_df[diagnoses_num_partner_compare_cols].corr(numeric_onl
# Printing the correlation matrix.
# print(corr_matrix)
# Visualizing the correlation matrix using a heatmap with text annotations for cc
diagnoses_num_partner_heatmap = px.imshow(corr_matrix,
                                          aspect="auto",
                                          color_continuous_scale="gnbu",
                                          text_auto=True)
diagnoses_num_partner_heatmap.update_layout(title='HPV vs. Sexual Partners Heatma
# Displaying the heatmap.
diagnoses_num_partner_heatmap.show()
```

```
# Selecting columns related only to diagnoses for correlation analysis.
diagnoses_cols = [label, 'Dx:CIN', 'Dx:HPV']
# Calculating the correlation matrix for the selected diagnoses columns.
diagnoses_corr_matrix = risk_factor_df[diagnoses_cols].corr(numeric_only=True)
# Visualizing the correlation matrix using a heatmap with teal-green color scale
diagnoses_heatmap = px.imshow(diagnoses_corr_matrix, aspect="auto", color_contin
# Displaying the heatmap.
diagnoses_heatmap.update_layout(title="Dx:CIN vs Dx:HPV HeatMap")
diagnoses_heatmap.show()
```

STDs

```
#data processing - to provide access of std_cols in STD graphs - do we want to ac
std_cols = {'STDs:condylomatosis',
            'STDs:cervical condylomatosis',
            'STDs:vaginal condylomatosis',
            'STDs:vulvo-perineal condylomatosis',
            'STDs:syphilis',
            'STDs:pelvic inflammatory disease',
            'STDs:genital herpes',
            'STDs:molluscum contagiosum',
            'STDs:AIDS',
            'STDs:HIV',
            'STDs:Hepatitis B',
            'STDs:HPV'}
```

```
#create historgram to understand Sum of STD occurences across age
fig = px.histogram(std_agg, x = "age_cat",
                   y = list(std_cols),
                   barmode = "group",
                   histfunc = "sum")
fig.update_layout(title = "Sum of STD occurrences across age categories")
fig.update_xaxes(title = "Age Category")
fig.update_yaxes(title = "Sum")
#show plot
fig.show()
#some discrepencies exist
```

```
#create boxplot to understand Distribution of number of sexual partners per age g
age_num_sex_partners = px.box(risk_factor_df.sort_values(by="Age",ascending=True)
                      color_discrete_sequence=["blue"], points="outliers",
                      category_orders=["Teenager", "Twenties", "Thirties", "Forti
                                       "Seventy and over"])
age_num_sex_partners.update_xaxes(title="Age Category")
age_num_sex_partners.update_yaxes(title="Number of Sexual Partners")
age_num_sex_partners.update_layout(title="Distribution of number of sexual partne
#show plot
age_num_sex_partners.show()
```

```
#create histogram to understand Count of women across age groups who have had one
fig = px.histogram(risk_factor_df.query("total_std>=0").sort_values(by=["total_st
                   x="age_cat",
                   facet_col="total_std",
                   facet_row=label,
                   color_discrete_sequence=["rebeccapurple"],
                   opacity=0.7)
fig.update_layout(title="Count of women across age groups who have had one or mor
fig.update_layout(height=1200)
#show plot
fig.show()
```

```
#create histogram to understand Count of women across age groups who have had one
fig = px.histogram(risk_factor_df.query("total_std>=0").sort_values(by=["total_st
                   x="age_cat",
                   facet_col="total_std",
                   facet_row="Dx:HPV",
                   color_discrete_sequence=["dodgerblue"],
                   opacity=0.7)
fig.update_layout(title="Count of women across age groups who have had one or mor

fig.show()
```

Tests used

Here we observe the number of tests done by patients to determine if they have Cerivcal Cancer / HPV.

```
fig = px.histogram(risk_factor_df.query("total_tests>0").sort_values(by="total_te
                   x="age_cat",
                   facet_col="total_tests",
                   facet_row=label,
                   color_discrete_sequence=["blueviolet"],
                   opacity=0.8)
fig.update_layout(title="Count of women across age groups who have had one or mor
fig.update_layout(height=1200)
fig.show()
```

```
fig = px.histogram(risk_factor_df.query("total_tests>0").sort_values(by=["total_t
                   x="age_cat",
                   facet_col="total_tests",
                   facet_row="Dx:HPV",
                   color_discrete_sequence=["coral"],
                   opacity=0.8)
fig.update_layout(title="Count of women across age groups who have had one or mor

fig.show()
```

```
fig = px.ecdf(risk_factor_df, x=["Smokes (years)",
                                 "Hormonal Contraceptives (years)",
                                 "IUD (years)"],
              color_discrete_sequence=["crimson", "deepskyblue", "chartreuse"])
fig.update_xaxes(title="Years")
fig.update_layout(title="ECDF Plot")
fig.show()
```

```
age_category_range = {
    "Age<12": "Child",
    "Age>=12 & Age<20": "Teen",
    "Age>=20 & Age<30": "20's",
    "Age>=30 & Age<40": "30's",
    "Age>=40 & Age<50": "40's",
    "Age>=50 & Age<60": "50's",
    "Age>=60 & Age<70": "60's",
    "Age>=70": "70+"}
age_prop_dict = {}
col = "Age"  # Just to get the count
for age_range, category in age_category_range.items():
    age_prop_dict[category] = risk_factor_df.query(age_range)[col].count() / len(

proportion_samples_df = pd.DataFrame.from_dict(age_prop_dict, orient="index",
                                               columns=[ "Sample Proportion"])
proportion_samples_df = proportion_samples_df.reset_index()
proportion_samples_df.columns = proportion_samples_df.columns.str.replace("index"
fig = px.pie(proportion_samples_df,
             values='Sample Proportion',
             names="Category",
             title='Age Category proportion of women sampled',color_discrete_sequ
fig.show()
proportion_samples_df
```

```
fig = make_subplots(rows=1, cols=2, specs=[[{'type': 'domain'}, {'type': 'domain'
fig = make_subplots(rows=1, cols=2, specs=[[{'type': 'domain'}, {'type': 'domain'
                    subplot_titles=["Cancer", "HPV"])
fig.add_trace(go.Pie(labels=risk_factor_df["age_cat"],
                     values=risk_factor_df[label],
                     name="Cancer", marker_colors=px.colors.sequential.RdBu),
              1, 1)
fig.add_trace(go.Pie(labels=risk_factor_df["age_cat"],
                     values=risk_factor_df["Dx:HPV"],
                     name="HPV", marker_colors=px.colors.sequential.RdBu),
              1, 2)

fig.update_traces(hole=.0, hoverinfo="label+percent+name")

fig.update_layout(
    title_text="Proportion of women across age categories with a diagnosis of Car
)
fig.show()
```

Contraceptive

```
df_hormonal_compariosn = risk_factor_df.groupby(["age_cat"], as_index=False)[["IL
fig = px.histogram(df_hormonal_compariosn, x="age_cat", y=["IUD", "Hormonal Contr
                   , color_discrete_sequence=["darkcyan", "mediumorchid"])

fig.update_xaxes(title="Age Category")
fig.update_yaxes(title="Count")
fig.update_layout(title="Age Ranges of women who use Contraceptives")

fig.show()
```

```
df_hormonal_contraceptives = risk_factor_df[
    (risk_factor_df["Hormonal Contraceptives"] == 1) & (risk_factor_df["IUD"] ==
df_hormonal_contraceptives = df_hormonal_contraceptives.sort_values(by=["Smokes",
fig = px.histogram(df_hormonal_contraceptives, x="age_cat", color="Smokes", barmo
                   color_discrete_sequence=["darkcyan", "crimson"])
fig.update_xaxes(title="Age Category")
fig.update_yaxes(title="Count")
fig.update_layout(title="Age Ranges of women who use Hormonal Contraceptives")
# fig.for_each_annotation(lambda a: a.update(text=a.text.split(":")[-1]))
fig.show()
```

```
df_IUD_contraceptives = risk_factor_df[(risk_factor_df["Hormonal Contraceptives"]
df_IUD_contraceptives = df_IUD_contraceptives.sort_values(by=["Smokes", label], a
fig = px.histogram(df_IUD_contraceptives, x="age_cat", color="Smokes", barmode="g
                   color_discrete_sequence=["darkcyan", "crimson"])
fig.update_xaxes(title="Age Category")
fig.update_yaxes(title="Sum of IUD Usage across age category")
fig.update_layout(title="Age Ranges of women who use IUD's")
fig.show()
```

```
df_both_contraceptives = risk_factor_df[(risk_factor_df["Hormonal Contraceptives"
df_both_contraceptives = df_both_contraceptives.sort_values(by="Smokes")
fig = px.histogram(df_both_contraceptives, x="age_cat", color="Smokes", barmode="
                   color_discrete_sequence=["darkcyan", "crimson"])
fig.update_xaxes(title="Age Category")
fig.update_yaxes(title="Count")
fig.update_layout(title="Age Ranges of women who use BOTH Hormonal Contracepties
fig.show()
```

ADASYN

```
test=risk_factor_df[['Number of sexual partners',   'First sexual intercourse', '

with open('summary.tex','w') as tf:
    tf.write(test.round(2).to_latex())

risk_factor_df.columns
```

```
Index(['Age', 'Number of sexual partners', 'First sexual intercourse',
       'Num of pregnancies', 'Smokes', 'Smokes (years)', 'Smokes
(packs/year)',
       'Hormonal Contraceptives', 'Hormonal Contraceptives (years)', 'IUD',
       'IUD (years)', 'STDs', 'STDs (number)', 'STDs:condylomatosis',
       'STDs:cervical condylomatosis', 'STDs:vaginal condylomatosis',
       'STDs:vulvo-perineal condylomatosis', 'STDs:syphilis',
       'STDs:pelvic inflammatory disease', 'STDs:genital herpes',
       'STDs:molluscum contagiosum', 'STDs:AIDS', 'STDs:HIV',
       'STDs:Hepatitis B', 'STDs:HPV', 'STDs: Number of diagnosis',
       'STDs: Time since first diagnosis', 'STDs: Time since last
diagnosis',
       'Dx:Cancer', 'Dx:CIN', 'Dx:HPV', 'Dx', 'Hinselmann', 'Schiller',
       'Citology', 'Biopsy', 'age_cat', 'total_std', 'total_tests'],
      dtype='object')
```

```
label="Dx:Cancer"
dx_cancer = px.histogram(risk_factor_df, y=label)
dx_cancer.update_layout(bargap=0.2)
dx_cancer.update_layout(title = "Imbalanced Classes")
dx_cancer.show()
```

Here we use ADASYN to balance the dataset

```
unbalanced_risk_factor_df = risk_factor_df
X = risk_factor_df.drop([label, "age_cat"], axis=1)
y = risk_factor_df[label].copy()
adasyn = ADASYN(random_state=42)
x_adasyn,y_adasyn = adasyn.fit_resample(X,y)
risk_factor_df = x_adasyn.join(y_adasyn)
```

Save ADASYN dataset

```
risk_factor_df["age_cat"] = risk_factor_df["Age"].apply(age_cat)
save_data(risk_factor_df, '/content/drive/My Drive/DL4H_Sp24_Final_Project/balanc
```

```
    Save checkpoint granted
```

Checkpoint: Load Balanced data

```
try:
  data_dir = '/content/drive/My Drive/DL4H_Sp24_Final_Project/balanced_risk_facto
  risk_factor_df = load_data(data_dir)
  have_access = True
except:
  have_access = False
  data_dir = root + '/balanced_risk_factors_cervical_cancer.csv'
  # gdown.download('https://drive.google.com/file/d/1-4EiqdYBbae16azaiZry7Gwhpq7X
  risk_factor_df = load_data(data_dir)
  print("No access, Used Gdown!")
risk_factor_df
label="Dx:Cancer"
```

```
    No access, Used Gdown!
```

```
dx_cancer = px.histogram(risk_factor_df, y=label)
dx_cancer.update_layout(bargap=0.2)
dx_cancer.update_layout(title = "Balanced Classes")
dx_cancer.show()
```

Checkpoint: Train Test Split

Stratifying the data on Age Category

Unbalanced

```
unbalanced_train_set = None
unbalanced_test_set = None
#Stratify the data
# 20% in test and 80% in train
unbalanced_split = StratifiedShuffleSplit(n_splits=1, test_size=0.2, random_state
for train_idx, test_idx in unbalanced_split.split(unbalanced_risk_factor_df, unba
    unbalanced_train_set = unbalanced_risk_factor_df.loc[train_idx]
    unbalanced_test_set = unbalanced_risk_factor_df.loc[test_idx]
unbalanced_cols_to_drop = ["age_cat","total_std","total_tests"]
for set_ in (unbalanced_train_set, unbalanced_test_set):
    for col in unbalanced_cols_to_drop:
        set_.drop(col, axis=1, inplace=True)


unbalanced_X_train = unbalanced_train_set.drop(label, axis=1)
unbalanced_y_train = unbalanced_train_set[label].copy()

unbalanced_X_test = unbalanced_test_set.drop(label, axis=1)
unbalanced_y_test = unbalanced_test_set[label].copy()

unbalanced_X_test.reset_index(drop=True, inplace=True)
unbalanced_y_test.reset_index(drop=True, inplace=True)
unbalanced_X_train.reset_index(drop=True, inplace=True)
unbalanced_y_train.reset_index(drop=True, inplace=True)


print("unbalanced_X_test length: ", len(unbalanced_X_test))
print("unbalanced_X_train length: ", len(unbalanced_X_train))
print("unbalanced_Y_test length: ", len(unbalanced_y_test))
print("unbalanced_Y_train length: ", len(unbalanced_y_train))
```

```
unbalanced_X_test length:  172
unbalanced_X_train length:  686
unbalanced_Y_test length:  172
unbalanced_Y_train length:  686
```

Balanced

```
train_set = None
test_set = None
#Stratify the data
# 20% in test and 80% in train
split = StratifiedShuffleSplit(n_splits=1, test_size=0.2, random_state=42)
for train_idx, test_idx in split.split(risk_factor_df, risk_factor_df["age_cat"])
    train_set = risk_factor_df.loc[train_idx]
    test_set = risk_factor_df.loc[test_idx]
cols_to_drop = ["age_cat","total_std","total_tests"]
for set_ in (train_set, test_set):
    for col in cols_to_drop:
        set_.drop(col, axis=1, inplace=True)


X_train = train_set.drop(label, axis=1)
y_train = train_set[label].copy()

X_test = test_set.drop(label, axis=1)
y_test = test_set[label].copy()

X_test.reset_index(drop=True, inplace=True)
y_test.reset_index(drop=True, inplace=True)
X_train.reset_index(drop=True, inplace=True)
y_train.reset_index(drop=True, inplace=True)


print("X_test length: ", len(X_test))
print("X_train length: ", len(X_train))
print("Y_test length: ", len(y_test))
print("Y_train length: ", len(y_train))
```

```
X_test length:  336
X_train length:  1341
Y_test length:  336
Y_train length:  1341
```

Save sets

```
#without random var
X_test.to_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/X_test.csv')
y_test.to_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/y_test.csv')
X_train.to_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/X_train.csv')
y_train.to_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/y_train.csv')
```

Checkpoint: Model Setup

We will be comparing different models: RF, SVM, LR, KNN, MLP

Model 1: Logistic Regression.

This is a simple linear model and does not have layers.

The sigmoid function is used as its activation.

lbfgs is used as the solver with L2 regularization

The default max_iter for convergence is 100.

```
param_grid = {'C': np.logspace(-5, 8, 15)}

logreg = LogisticRegression()
logreg_cv = GridSearchCV(logreg, param_grid, cv=10,refit=True)
unbalanced_logreg_cv = GridSearchCV(logreg, param_grid, cv=10,refit=True)
```

Model 2: RandomForestClassifier

Ensemble machine learning model using groups of decision trees to reduce overfitting

The default n_estimators is 100

Default criterion = gini

Convergence ends when all leaves are pure or until each leaf is equal to min_samples_leaf (by default set to 2)

```
rnd_clf = RandomForestClassifier()
unbalanced_rnd_clf = RandomForestClassifier()
```

Model 3: KNeighborsClassifier

A machine learning iterative classification method that uses a distance function to group similar data

n_neighbors (number of surrounding data points to consider) is 5 by default

```
knn_clf = KNeighborsClassifier()
knn_param_grid = {"n_neighbors": list(np.arange(1, 100, 2))}
knn_clf_cv = GridSearchCV(knn_clf, knn_param_grid, cv=10,refit=True)
unbalanced_knn_clf_cv = GridSearchCV(knn_clf, knn_param_grid, cv=10,refit=True)
```

MODEL 4: SupportVectorClassifier

Support vector models are classfication algorithm that uses hyperplances to classify data points using a maximum margin between decision boundaries and the closest data points.

The regularization parameter C is set to 1 by default.

The kernel type is set to 'rbf' (radial basis function) by default

```
svm_clf = SVC()
svc_param_grid = {'C': np.logspace(-3, 2, 6), 'gamma': np.logspace(-3, 2, 6), }
svm_clf_cv = GridSearchCV(svm_clf, svc_param_grid, cv=5, refit=True)
unbalanced_svm_clf_cv = GridSearchCV(svm_clf, svc_param_grid, cv=5, refit=True)
```

MODEL 5: MLPClassifier

MLPs are neural networks used for pattern detection.

They consist of 3 layers of nodes, an input layer, a hidden layer, and an output layer.

The default max_iter is 200.

The optimizer is 'Adam'

Each node uses a nonlinear activation function. By default this is ReLu for the hidden layer. For the output layer, softmax is used by default for multi-class classification problems and logistic for binary classification problems.

Backpropagation and gradient descent is used to to train and minimize loss.

```
nn_clf = MLPClassifier()
unbalanced_nn_clf = MLPClassifier()
```

Set up training metrics

```
# metrics to evaluate my model
# Define column names for the summary DataFrame
col_names = ["Classifier Name", "Accuracy Score", "Precision Score", "Recall Scor
# Initialize the summary DataFrame with predefined column names
unbalanced_summary_df = pd.DataFrame(columns=col_names)

# Lists to store the metrics for each estimator
unbalanced_est_name = []
unbalanced_est_acc = []
unbalanced_precision_score = []
unbalanced_recall_score = []
unbalanced_f1score = []
unbalanced_est_conf_matrix = []
unbalanced_roc=[]

# List of tuples containing the classifiers to evaluate and their respective vari
unbalanced_estimators = [
    ("UnbalancedLogisticRegression", unbalanced_logreg_cv),
    ("UnbalancedRandomForestClassifier", unbalanced_rnd_clf),
    ("UnbalancedKNeighborsClassifier", unbalanced_knn_clf_cv),
    ("UnbalancedSupportVectorClassifier", unbalanced_svm_clf_cv),
    ("UnbalancedMLPClassifier", unbalanced_nn_clf)
    ]

unbalanced_models = ['UnbalancedLogisticRegression.pkl',
                     'UnbalancedRandomForestClassifier.pkl',
                     'UnbalancedKNeighborsClassifier.pkl',
                     'UnbalancedSupportVectorClassifier.pkl',
                     'UnbalancedMLPClassifier.pkl']

summary_df = pd.DataFrame(columns=col_names)


# Lists to store the metrics for each estimator
est_name = []
est_acc = []
precision_score = []
recall_score = []
f1score = []
est_conf_matrix = []
roc=[]
```

```
# List of tuples containing the classifiers to evaluate and their respective vari
estimators = [
    ("LogisticRegression", logreg_cv),
    ("RandomForestClassifier", rnd_clf),
    ("KNeighborsClassifier", knn_clf_cv),
    ("SupportVectorClassifier", svm_clf_cv),
    ("MLPClassifier", nn_clf)
    ]
balanced_models = ['LogisticRegression.pkl',
                     'RandomForestClassifier.pkl',
                     'KNeighborsClassifier.pkl',
                     'SupportVectorClassifier.pkl',
                     'MLPClassifier.pkl']
```

Model Training

Hyperparameters: Three examples of hyperparameters we used are 'C' (regularization constant), type of kernel ('rbf'), gamma (kernel coeffient) in the Support Vector Classifier Model.

Computational Requirements: Dataset is small enough to compute on an 8 GB 2133 MHz LPDDR3 2.3 GHz Dual-Core Intel Core i5. Average run time for training is < 2 minutes. We used default epochs. For logistic regression this 100 and for MLP this is 200, unless convergence is reached earlier.

The training for the Local explainability models took hours however and we had to sample to get them done.

Unbalanced Training (Ablation)

```
# Iterate over the estimators to train
for i in range(len(unbalanced_estimators)):
    unbalanced_clf_name, unbalanced_clf = unbalanced_estimators[i]  # Unpack the
    print("Training ", unbalanced_clf_name)
    unbalanced_clf.fit(unbalanced_X_train, unbalanced_y_train)  # Train the class
    gd_model_name = root + unbalanced_clf_name + '.pkl'
    with open(gd_model_name, 'wb') as file:
      pickle.dump(unbalanced_clf, file)
unbalanced_clf_name, unbalanced_clf = '',''
```

```
Training  UnbalancedLogisticRegression
Training  UnbalancedRandomForestClassifier
Training  UnbalancedKNeighborsClassifier
Training  UnbalancedSupportVectorClassifier
Training  UnbalancedMLPClassifier
```

Balanced Training

```
for i in range(len(estimators)):
    clf_name, clf = estimators[i]  # Unpack the classifier name and the classifie
    print("Training ", clf_name)
    clf.fit(X_train, y_train)  # Train the classifier
    gd_model_name = root + clf_name + '.pkl'
    with open(gd_model_name, 'wb') as file:
      pickle.dump(clf, file)
clf_name, clf = '',''
```

```
Training  LogisticRegression
Training  RandomForestClassifier
Training  KNeighborsClassifier
Training  SupportVectorClassifier
Training  MLPClassifier
```

Double-click (or enter) to edit

Checkpoint: Result

Download pickle models with gdown

```
# LogisticRegression
unbalanced_models[0] = root +'/UnbalancedLogisticRegression.pkl'
balanced_models[0] = root +'/LogisticRegression.pkl'
# gdown.download('https://drive.google.com/file/d/1-4D7VkQ4qewUnyrzPw1izMk9WjMvQ1
# gdown.download('https://drive.google.com/file/d/1-94qCsT0VdS-CvO237Z0TeUWCouKDe
# # RandomForestClassifier
unbalanced_models[1] = root +'/UnbalancedRandomForestClassifier.pkl'
balanced_models[1] = root +'/RandomForestClassifier.pkl'
# gdown.download('https://drive.google.com/file/d/1-PBTxxalNfXQNKpX8Bg9ojFRtPGEsv
# gdown.download('https://drive.google.com/file/d/1-Qdk5tk2RCLhbfVW400S2qBI6ikStF
# # KNeighborsClassifier
unbalanced_models[2] = root +'/UnbalancedKNeighborsClassifier.pkl'
balanced_models[2] = root +'/KNeighborsClassifier.pkl'
# gdown.download('https://drive.google.com/file/d/1-Rg4cRA6NdtPeHPFnablplZ0T7e323
# gdown.download('https://drive.google.com/file/d/1-TKog0oufiDcfCJtv_gQdYTiw1rK6V
# # SupportVectorClassifier
unbalanced_models[3] = root +'/UnbalancedSupportVectorClassifier.pkl'
balanced_models[3] = root +'/SupportVectorClassifier.pkl'
# gdown.download('https://drive.google.com/file/d/1_g0BZHdpuPP9xlj0jKWJ-8fVZe4sTF
# gdown.download('https://drive.google.com/file/d/1-3sNvATHD55evt_9nSzf3nBP6XWLkr
# # MLPClassifier
unbalanced_models[4] = root +'/UnbalancedMLPClassifier.pkl'
balanced_models[4] = root +'/MLPClassifier.pkl'
# gdown.download('https://drive.google.com/file/d/1-3P6L-WKDrfMNgwp372f3vgY9Px0SE
# gdown.download('https://drive.google.com/file/d/1-DmdcIFHJFKUtAhhVW1XbVlwbfjOpW
```

Model Execution

Unbalanced evaluation (ablation)

```
# Iterate over the trained models to evaluate each one
for i in range(len(unbalanced_estimators)):
    with open(unbalanced_models[i], 'rb') as file:
      downloaded_model = pickle.load(file)
    unbalanced_clf_name, _ = unbalanced_estimators[i]
    unbalanced_y_pred = downloaded_model.predict(unbalanced_X_test)  # Predict th
```

```
        # Calculate the AUROC score and append it to the roc list
        unbalanced_roc.append(roc_auc_score(unbalanced_y_test, unbalanced_y_pred, ave

        # Append classifier name to the est_name list
        unbalanced_est_name.append(unbalanced_clf_name)

        # Calculate and append accuracy to the est_acc list
        unbalanced_est_acc.append(accuracy_score(unbalanced_y_test, unbalanced_y_prec

        # Calculate precision, recall, and F1 scores and append them to their respect
        unbalanced_scores = precision_recall_fscore_support(unbalanced_y_test, unbala
        unbalanced_precision_score.append(unbalanced_scores[0])
        unbalanced_recall_score.append(unbalanced_scores[1])
        unbalanced_f1score.append(unbalanced_scores[2])

        # Append the confusion matrix for each classifier to the est_conf_matrix list
        unbalanced_est_conf_matrix.append(confusion_matrix(unbalanced_y_test, unbalar

    # Populate the summary DataFrame with the collected metrics for each classifier
    unbalanced_summary_df[col_names[0]] = unbalanced_est_name
    unbalanced_summary_df[col_names[1]] = unbalanced_est_acc
    unbalanced_summary_df[col_names[2]] = unbalanced_precision_score
    unbalanced_summary_df[col_names[3]] = unbalanced_recall_score
    unbalanced_summary_df[col_names[4]] = unbalanced_f1score
    unbalanced_summary_df[col_names[5]] = unbalanced_roc

    # plot figures to better show the results

    # it is better to save the numbers and figures for your presentation.
    unbalanced_summary_df
```

Balanced evaluation

```
# Iterate over the trained models to evaluate each one
for i in range(len(estimators)):
    with open(balanced_models[i], 'rb') as file:
      downloaded_model = pickle.load(file)
    clf_name, _ = estimators[i]
    y_pred = downloaded_model.predict(X_test)  # Predict the test set outcomes

    # Calculate the AUROC score and append it to the roc list
    roc.append(roc_auc_score(y_test, y_pred, average=None))

    # Append classifier name to the est_name list
    est_name.append(clf_name)

    # Calculate and append accuracy to the est_acc list
    est_acc.append(accuracy_score(y_test, y_pred))

    # Calculate precision, recall, and F1 scores and append them to their respect
    scores = precision_recall_fscore_support(y_test, y_pred, average="weighted")
    print(scores)
    precision_score.append(scores[0])
    recall_score.append(scores[1])
    f1score.append(scores[2])

    # Append the confusion matrix for each classifier to the est_conf_matrix list
    est_conf_matrix.append(confusion_matrix(y_test, y_pred))

# Populate the summary DataFrame with the collected metrics for each classifier
summary_df[col_names[0]] = est_name
summary_df[col_names[1]] = est_acc
summary_df[col_names[2]] = precision_score
summary_df[col_names[3]] = recall_score
summary_df[col_names[4]] = f1score
summary_df[col_names[5]] = roc

# plot figures to better show the results

# it is better to save the numbers and figures for your presentation.
summary_df
```

Model comparison

```
# compare you model with others
# you don't need to re-run all other experiments, instead, you can directly refer
```

Unbalanced comparison

```
color_scales = ["agsunset","teal","purp","viridis","viridis"]
for i in range(0,len(unbalanced_est_conf_matrix)):
    unbalanced_heatmap = px.imshow(unbalanced_est_conf_matrix[i],aspect="auto",
                        text_auto=True,
                        color_continuous_scale=color_scales[i])
    unbalanced_heatmap.update_layout(title = unbalanced_est_name[i])
    unbalanced_heatmap.update_xaxes(title="Predicted")
    unbalanced_heatmap.update_yaxes(title="Actual")
    unbalanced_heatmap.show()
```

```
#https://plotly.com/python/error-bars/
#https://problemsolvingwithpython.com/06-Plotting-with-Matplotlib/06.07-Error-Bar
unbalanced_acc_comparison = px.bar(unbalanced_summary_df, x="Classifier Name",
                        y=col_names[1:len(col_names)], labels={"value":"Test Accu
                        color_discrete_sequence=["deeppink",
                                                 "deepskyblue",
                                                 "darkviolet",
                                                 "darkorange",
                                                 "darkred"],
                        barmode="group"
                        #,error_y=[dict(type='data', array=[0.5, 1, 2],visible=Tr
                        #,error_y_minus = [dict(type='data', array=[0.5, 1, 2, 2,
                        )
unbalanced_acc_comparison.update_layout({'plot_bgcolor': 'rgba(0, 0, 0, 0)',
'paper_bgcolor': 'rgba(0, 0, 0, 0)'
})
unbalanced_acc_comparison.show()
```

Balanced comparison

Summary with heat map

```
color_scales = ["agsunset","teal","purp","viridis","viridis"]
for i in range(0,len(est_conf_matrix)):
    heatmap = px.imshow(est_conf_matrix[i],aspect="auto",
                        text_auto=True,
                        color_continuous_scale=color_scales[i])
    heatmap.update_layout(title = est_name[i])
    heatmap.update_xaxes(title="Predicted")
    heatmap.update_yaxes(title="Actual")
```

```
        heatmap.show()
```

```
#https://plotly.com/python/error-bars/
#https://problemsolvingwithpython.com/06-Plotting-with-Matplotlib/06.07-Error-Bar
acc_comparison = px.bar(summary_df, x="Classifier Name",
                        y=col_names[1:len(col_names)], labels={"value":"Test Accu
                        color_discrete_sequence=["deeppink",
                                                 "deepskyblue",
                                                 "darkviolet",
                                                 "darkorange",
                                                 "darkred"],
                        barmode="group"
                        #,error_y=[dict(type='data', array=[0.5, 1, 2],visible=Tr
                        #,error_y_minus = [dict(type='data', array=[0.5, 1, 2, 2,
                        )
acc_comparison.update_layout({'plot_bgcolor': 'rgba(0, 0, 0, 0)',
'paper_bgcolor': 'rgba(0, 0, 0, 0)'
})
acc_comparison.show()
```

** Description of Metrics**

TP: True Positive, these are the values that are positive and were predicted positive

FP: False Positive, The values which are negative but were wrongly predicted as positive

TN: True Negative, these are the values that are negative and were predicted negative

FN: False Negative, The values which are positive but were wrongly predicted as negative
Precision

Precision = TP / (TP+FP)

This metric measures the actual positive outcomes out of the total predicted positive outcomes. It attempts to identify the proportion of positive identifications that were correct. KNeighbors and SVC gave the worst precision score

In the context of diagnoising cervical cancer, this is metric would not be the most ideal to measure performance, as a negative case being labelled as a positive case is easily solved with confirmatory tests. However, one has to also consider the emotional and mental issues brought upon by being diagnosed with cervical cancer, as this can have a lingering effect even after having confirmatory tests. These tests should be done as soon as possible, as there may be another underlying illness that brought them to see a healthcare professional in the first place.

Recall

Recall = TP / (TP+FN)

This metirc measures the correctly positive predicted outocmes of the total number of positive outcomes. It answers the question of what proportions of actual positives were identified correctly. KNeighbors and SVC gave the worst precision score

In the context of diagnosing cervical cancer, we want to reduce the number of false negatives (Actual positive cases labelled as negative cases) as much possible. If an actual positive case is labelled as negative, this has serious consequecnes as the patient would go about their life without actually receiving potentially life saving treatment.

There are many reasons why a cancer can go misdiagnosed, these include:

The symptoms,especially in the early stages being mistaken for some other type of less serious illness. The actual test adminstered by a healthcare professional may give the wrong diagnosis The 5-year survival rate tells you what percent of people live at least 5 years after the cancer is found. Percent means how many out of 100. The 5-year survival rate for all people with cervical cancer is 66%. Source

Survival rates also depend on the stage of cervical cancer that is diagnosed. When detected at an early stage, the 5-year survival rate for people with invasive cervical cancer is 92%. About 44% of people with cervical cancer are diagnosed at an early stage. If cervical cancer has spread to surrounding tissues or organs and/or the regional lymph nodes, the 5-year survival rate is 58%. If the cancer has spread to a distant part of the body, the 5-year survival rate is 18%.

F1 Score

F1 Score =TP / (TP + ((FN+FP)/2))

The F1 score is defined as the harmonic mean of precision and recall. Therefore, a high F1 score means both a high precision and recall, same for low and a medium score if one score is high and the other is low.

Accuracy Accuracy = (TP + TN) / (TP + FP + TN + FN)

Data Pertubations

In this section, we take the train and test sets and add

1. random noise
2. binary variable
3. continuous variable to three separate sets

at this point, risk_factor_df is balanced data set

```
from scipy.stats import bernoulli
risk_factor_df['VAR']=bernoulli.rvs(.5, size=risk_factor_df.shape[0])
```

```
#continous
risk_factor_df['VAR']=np.random.normal(loc=0, scale=1, size=risk_factor_df.shape[
risk_factor_df.columns
```

```
Index(['Age', 'Number of sexual partners', 'First sexual intercourse',
       'Num of pregnancies', 'Smokes', 'Smokes (years)', 'Smokes
(packs/year)',
       'Hormonal Contraceptives', 'Hormonal Contraceptives (years)', 'IUD',
       'IUD (years)', 'STDs', 'STDs (number)', 'STDs:condylomatosis',
       'STDs:cervical condylomatosis', 'STDs:vaginal condylomatosis',
       'STDs:vulvo-perineal condylomatosis', 'STDs:syphilis',
       'STDs:pelvic inflammatory disease', 'STDs:genital herpes',
       'STDs:molluscum contagiosum', 'STDs:AIDS', 'STDs:HIV',
       'STDs:Hepatitis B', 'STDs:HPV', 'STDs: Number of diagnosis',
       'STDs: Time since first diagnosis', 'STDs: Time since last
diagnosis',
       'Dx:CIN', 'Dx:HPV', 'Dx', 'Hinselmann', 'Schiller', 'Citology',
       'Biopsy', 'total_std', 'total_tests', 'Dx:Cancer', 'age_cat', 'VAR'],
      dtype='object')
```

Get data and model - the source code is poorly labeled here and is not clear on the "cancer.csv" file they use

We are assuming it is the balanced dataset

```
risk_factor_df.to_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/Rcancer2.c
#modified below to replicate above filename
risk_factor_df=pd.read_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/Rcanc
```

```
risk_factor_df
```

Checkpoint: Get Original

```
# X_test=pd.read_csv(gdown.download('https://drive.google.com/file/d/1ggTvbeS9ker
X_test = pd.read_csv(root+'/X_test.csv')
X_test.drop('Unnamed: 0', inplace=True, axis=1)
# y_test=pd.read_csv(gdown.download('https://drive.google.com/file/d/1WsUWrO9Nwpc
y_test = pd.read_csv(root+'/y_test.csv')
y_test.drop('Unnamed: 0', inplace=True, axis=1)
# X_train=pd.read_csv(gdown.download('https://drive.google.com/file/d/1OnCY70gXQb
X_train = pd.read_csv(root+'/X_train.csv')
X_train.drop('Unnamed: 0', inplace=True, axis=1)
# y_train=pd.read_csv(gdown.download('https://drive.google.com/file/d/1C5euZUKZ6G
y_train = pd.read_csv(root+'/y_train.csv')
y_train.drop('Unnamed: 0', inplace=True, axis=1)
```

```
len(X_test)
```

```
    336
```

Normal

```
from scipy.stats import bernoulli

# Adding a new binary variable 'VARB' to the test dataset, with each value indepe
# from a Bernoulli distribution where the probability of a 1 is 0.5 (i.e., a fair
X_test['VARB'] = bernoulli.rvs(0.5, size=X_test.shape[0])

# Similarly, adding the 'VARB' binary variable to the training dataset.
X_train['VARB'] = bernoulli.rvs(0.5, size=X_train.shape[0])

# Adding another binary variable 'VARC' to the test dataset, with values drawn
# from the same distribution as 'VARB'.
X_test['VARC'] = bernoulli.rvs(0.5, size=X_test.shape[0])

# Adding 'VARC' to the training dataset as well.
X_train['VARC'] = bernoulli.rvs(0.5, size=X_train.shape[0])
```

```
X_test
```

```
# Loop over each column in the testing dataset
for col in X_test.columns:
    # Add Gaussian noise to each value in the current column of the testing datas
    # Noise is centered at 0 with a standard deviation of 0.1
    X_test[col] += np.random.normal(loc=0, scale=.1, size=X_test.shape[0])

    # Add Gaussian noise to each value in the current column of the training data
    # Noise is also centered at 0 with a standard deviation of 0.1
    X_train[col] += np.random.normal(loc=0, scale=.1, size=X_train.shape[0])
```

```
X_test
```

Save state from random noise

```
X_test.to_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/Noise_X_test.csv')
y_test.to_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/Noise_y_test.csv')
X_train.to_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/Noise_X_train.csv
y_train.to_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/Noise_y_train.csv
```

Checkpoint: Get Normal

```
# Noise_X_test=pd.read_csv(gdown.download('https://drive.google.com/file/d/1erD_z
Noise_X_test = pd.read_csv(root+'/Noise_X_test.csv')
Noise_X_test.drop('Unnamed: 0', inplace=True, axis=1)
# Noise_y_test=pd.read_csv(gdown.download('https://drive.google.com/file/d/1cNtkc
Noise_y_test = pd.read_csv(root+'/Noise_y_test.csv')
Noise_y_test.drop('Unnamed: 0', inplace=True, axis=1)
# Noise_X_train=pd.read_csv(gdown.download('https://drive.google.com/file/d/13SUc
Noise_X_train = pd.read_csv(root+'/Noise_X_train.csv')
Noise_X_train.drop('Unnamed: 0', inplace=True, axis=1)
Noise_y_train = pd.read_csv(root+'/Noise_y_train.csv')
# Noise_y_train=pd.read_csv(gdown.download('https://drive.google.com/file/d/1rVKc
Noise_y_train.drop('Unnamed: 0', inplace=True, axis=1)
```

```
Noise_X_test
```

Binary

```
#binary
X_test=pd.read_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/X_test.csv')
X_test.drop('Unnamed: 0', inplace=True, axis=1)
y_test=pd.read_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/y_test.csv')
y_test.drop('Unnamed: 0', inplace=True, axis=1)
X_train=pd.read_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/X_train.csv'
X_train.drop('Unnamed: 0', inplace=True, axis=1)
y_train=pd.read_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/y_train.csv'
y_train.drop('Unnamed: 0', inplace=True, axis=1)


# no random noise
from scipy.stats import bernoulli

X_test['VAR']=bernoulli.rvs(.5, size=X_test.shape[0])
X_train['VAR']=bernoulli.rvs(.5, size=X_train.shape[0])


X_test.to_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/Binary_X_test.csv'
y_test.to_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/Binary_y_test.csv'
X_train.to_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/Binary_X_train.cs
y_train.to_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/Binary_y_train.cs
```

Checkpoint: Get Binary

```
#binary
# X_test=pd.read_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/X_test.csv'
Binary_X_test = pd.read_csv(root+'/Binary_X_test.csv')
Binary_X_test.drop('Unnamed: 0', inplace=True, axis=1)
# y_test=pd.read_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/y_test.csv'
Binary_y_test = pd.read_csv(root+'/Binary_y_test.csv')
Binary_y_test.drop('Unnamed: 0', inplace=True, axis=1)
# X_train=pd.read_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/X_train.cs
Binary_X_train = pd.read_csv(root+'/Binary_X_train.csv')
Binary_X_train.drop('Unnamed: 0', inplace=True, axis=1)
Binary_y_train = pd.read_csv(root+'/Binary_y_train.csv')
# y_train=pd.read_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/y_train.cs
Binary_y_train.drop('Unnamed: 0', inplace=True, axis=1)
```

```
Binary_X_train
```

Continuous

```
#continous

# X_test=pd.read_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/X_test.csv'
X_test.drop('Unnamed: 0', inplace=True, axis=1)
# y_test=pd.read_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/y_test.csv'
y_test.drop('Unnamed: 0', inplace=True, axis=1)
# X_train=pd.read_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/X_train.cs
X_train.drop('Unnamed: 0', inplace=True, axis=1)
# y_train=pd.read_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/y_train.cs
y_train.drop('Unnamed: 0', inplace=True, axis=1)

X_test['VAR']=np.random.normal(loc=0, scale=1, size=X_test.shape[0])
X_train['VAR']=np.random.normal(loc=0, scale=1, size=X_train.shape[0])


X_test.to_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/Continuous_X_test.
y_test.to_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/Continuous_y_test.
X_train.to_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/Continuous_X_trai
y_train.to_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/Continuous_y_trai
```

Checkpoint: Get Continuous

```
#Continuous
# X_test=pd.read_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/X_test.csv'
Continuous_X_test = pd.read_csv(root+'/Continuous_X_test.csv')
Continuous_X_test.drop('Unnamed: 0', inplace=True, axis=1)
# y_test=pd.read_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/y_test.csv'
Continuous_y_test = pd.read_csv(root+'/Continuous_y_test.csv')
Continuous_y_test.drop('Unnamed: 0', inplace=True, axis=1)
# X_train=pd.read_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/X_train.cs
Continuous_X_train = pd.read_csv(root+'/Continuous_X_train.csv')
Continuous_X_train.drop('Unnamed: 0', inplace=True, axis=1)
Continuous_y_train = pd.read_csv(root+'/Continuous_y_train.csv')
# y_train=pd.read_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/y_train.cs
Continuous_y_train.drop('Unnamed: 0', inplace=True, axis=1)
```

```
Continuous_X_test
```

Checkpoint: Set rnd_clf Models

Fit on the continuous pertubation from the previous section

```
rnd_clf = RandomForestClassifier()
rnd_clf.fit(X_train, y_train)
noise_rnd_clf = RandomForestClassifier()
noise_rnd_clf.fit(Noise_X_train, Noise_y_train)
binary_rnd_clf = RandomForestClassifier()
binary_rnd_clf.fit(Binary_X_train, Binary_y_train)
continuous_rnd_clf = RandomForestClassifier()
continuous_rnd_clf.fit(Continuous_X_train, Continuous_y_train)
```

```
model=rnd_clf
noise_model = noise_rnd_clf
binary_model = binary_rnd_clf
continuous_model = continuous_rnd_clf
```

Local Methods

SAVE THE DATA SO THIS IS NOT A CHECKPOINT

We generated feature importance explanations using LIME, three variants of SHAP (Tree-SHAP (TSHAP), Kernel-SHAP (KSHAP) and Sampling-SHAP (SSHAP)), Tree Interpreter, DICE and Local Surrogates.

LIME is a model-agnostic technique for explaining the predictions of machine learning models on a local, instance-specific basis. LIME approximates the predictions of f(x) by with a simpler g(x) for an instance of interest x.

SHAP values explain the output of any machine learning model by attributing a value to each feature for a prediction based on their contributions towards that prediction. This is done by considering all possible feature combinations. There are many variants of KSHAP.

DICE is a model-agnostic method for generating diverse and interpretable counterfactual explanations for individual predictions. DICE finds instances similar to original instance x, but with different predicted outcomes. Optimization requires minimizing a distance metric between the counterfactuals and x, subject to constraints that ensure dissimilarity among generated counterfactuals. Counterfactuals are generated by perturbing the features of x while staying within the feasible range of feature values.

Tree Interpreter is a model-specific method for interpreting predictions of tree-based models, such as random forests. It provides a way to attribute feature importance values for predictions made by tree-based models, by tracing the decision path of an instance through the tree and measuring the contribution of each feature towards the prediction. This is done by summing the changes in prediction associated with each decision node along the path, weighted by the proportion of instances that pass through each decision node.

Local Surrogates (Molnar, 2022) are model-specific methods for interpreting predictions of machine learning models that aim to provide insights into the decision-making process of the black-box model for a specific prediction, by fitting a simpler model, such as linear regression or decision tree, using the training data in the local neighborhood of the instance of interest. Local surrogates generate explanations in the form of interpretable models or feature importance values, depending on the specific method used.

Source: [1] Ayad, W., Bonnier, T., Bosch, B., Read, J., & Parbhoo, S. (2023). Which Explanation Makes Sense? A Critical Evaluation of Local Explanations for Assessing Cervical Cancer Risk Factors. Ecole polytechnique, 1-50.

Initialize function

```
def run_explainers(mode, model, X_train, X_test, y_train, y_test):
  # Initialize various SHAP explainers and a DataFrame to hold zero-initialized c
  # This DataFrame uses the same structure and column names as X_test.
  GloSur = kernelSHAP = treeSHAP = samplingSHAP = limecontrib = ticontrib = dicec
      pd.DataFrame([[0.0] * X_test.shape[1]] * X_test.shape[0], columns=X_test.cc

  # Initialize dictionaries to store feature importances from different explainer
  fi_1 = fi_2 = fi_3 = fi_4 = fi_5 = fi_6 = fi_7 = {f'{x}': 0.0 for x in X_test.c

  # Initialize a dictionary to store results temporarily.
  res = dict()

  # Retrieve the list of feature names from the test dataset.
```

```
features = X_test.columns

## GloSur

# Print a header for the GloSur results section.
print("-GLOSUR-")

# Set up the GloSur explainer using a linear model as the surrogate to approxim
explainer = MimicExplainer(model,
                          X_train,
                          LinearExplainableModel,
                          augment_data=False,  # Do not augment data; use the c
                          features=features,  # List of features to explain.
                          model_task="classification")  # Task type (classifica

# Generate global explanations based on the entire test dataset.
global_explanation = explainer.explain_global(X_test)

# Extract local importance values for each instance and convert them into a Dat
temp = pd.DataFrame(global_explanation.local_importance_values[1], columns=feat

# Update the GloSur DataFrame with new importance values, adding to existing va
GloSur = GloSur.add(temp, fill_value=0)

# Reset the results dictionary and retrieve feature importance as a dictionary
res = dict()
res = global_explanation.get_feature_importance_dict()

# Update fi_1 dictionary with aggregated feature importances, combining existin
fi_1 = {k: fi_1.get(k, 0) + res.get(k, 0) for k in set(fi_1)}
fi_1
## KSHAP

# We had to use kmeans to summarize. the full data would have taken hours
# Setting a smaller K to be able to train


print("-KSHAP-")
# KSHAP
K = 10  # Adjust. 1341 is too big

# Step 1: Summarize the background data
X_train_summary = shap.kmeans(X_train, K)

# Step 2: Create the explainer
```

```
explainer = shap.KernelExplainer(model.predict_proba, X_train_summary, feature_

# Step 3: Calculate SHAP values
shap_values = explainer.shap_values(X_test)

# Convert SHAP values to DataFrame for easier manipulation (assuming binary cla
temp = pd.DataFrame(shap_values[1], columns=features)

kernelSHAP = kernelSHAP.add(temp, fill_value=0)

# Step 5: Compute Feature Importance
res = {feature: np.mean(np.abs(kernelSHAP[feature])) for feature in kernelSHAP.

# Update or initialize feature importances
fi_2 = {k: fi_2.get(k, 0) + res.get(k, 0) for k in set(fi_2)}
fi_2
## TShap



print("-TSHAP-")
# TSHAP TODO acction check_additivity=False
explainer = shap.TreeExplainer(model,X_train, check_additivity=False)
shap_values = explainer.shap_values(X_test)

temp=pd.DataFrame(shap_values[1], columns=features)
treeSHAP=treeSHAP.add(temp, fill_value=0)

res = dict()
for i in list(treeSHAP.columns):
  res[i]=np.mean(np.abs(treeSHAP[i]))
fi_3={k: fi_3.get(k, 0) + res.get(k, 0) for k in set(fi_3)}
fi_3
## SSHAP
print("-SSHAP-")
# Reduce the number of samples used for explanations
X_train_sampled = shap.sample(X_train, 20)  # for example, sample 20 instances

# Create the SamplingExplainer using the sampled training data
explainer = shap.explainers.Sampling(model.predict_proba, X_train_sampled)
shap_values = explainer.shap_values(X_test)
temp = pd.DataFrame(shap_values[1], columns=features)
samplingSHAP = samplingSHAP.add(temp, fill_value=0)

# Aggregate and compute feature importance
res = {feature: np.mean(np.abs(samplingSHAP[feature])) for feature in samplingS
```

```
fi_4 = {k: fi_4.get(k, 0) + res.get(k, 0) for k in set(fi_4)}
fi_4
## LIME
print("-LIME-")

# LIME
explainer = lime.lime_tabular.LimeTabularExplainer(X_train.values,mode='classif

all=[]
for i in range (len(X_test)):
  exp = explainer.explain_instance(X_test.iloc[i], model.predict_proba, num_fea
  all.append(sorted(exp.as_map()[1]))


all_res=[]
for i in range(len(all)):
  res = dict()
  for j in range(len(all[0])):
    res[features[j]] = all[i][j][1]
  all_res.append(res)

temp=pd.DataFrame(all_res, columns=features)
limecontrib=limecontrib.add(temp, fill_value=0)

res = dict()
for j in list(limecontrib.columns):
  res[j]=np.mean(np.abs(limecontrib[j]))
fi_5={k: fi_5.get(k, 0) + res.get(k, 0) for k in set(fi_5)}
fi_5
## Tree Interpreter
# Random forest classifier is not correct model type.
# Base learner needs to be a DecisionTreeClassifier or DecisionTreeRegressor.
# Average out the trees in the estimators
# Prepare containers for the individual tree results
all_contributions = []
all_biases = []

# Iterate over each tree in the RandomForest
for tree in model.estimators_:
    prediction, bias, contributions = ti.predict(tree, X_test)
    all_biases.append(bias)
    all_contributions.append(contributions)

# Convert the lists into numpy arrays for easier mean calculation
all_contributions = np.array(all_contributions)
```

```
all_biases = np.array(all_biases)

# Calculate the mean contributions and biases across all trees
mean_contributions = np.mean(all_contributions, axis=0)
mean_biases = np.mean(all_biases, axis=0)

# Organize contributions into a DataFrame
all_res = []
for i in range(len(mean_contributions)):
    res = dict()
    for j in range(len(features)):
        res[features[j]] = mean_contributions[i, j, 1]  # Index 1 for contribut
    all_res.append(res)

temp = pd.DataFrame(all_res, columns=features)
ticontrib = temp.sum()

# Calculate the mean of absolute values of contributions for each feature
res = {feature: np.mean(np.abs(ticontrib[feature])) for feature in ticontrib.ir
fi_6 = {k: fi_6.get(k, 0) + res.get(k, 0) for k in set(fi_6)}
fi_6
## DICE
# df.select_dtypes(exclude=int)
label = "Dx:Cancer"
temp1=X_train
temp1['Dx:Cancer']=y_train
temp2=X_test
temp2['Dx:Cancer']=y_test

temp3=pd.concat([temp1,temp2])

risk_factor_df=temp3
#debugging
# print(risk_factor_df.columns==X_test.columns)
# print(risk_factor_df.columns)
# X_test.columns
# print('df dtypes:', risk_factor_df.dtypes)
# print('X_test dtypes: ', X_test.dtypes)

print("-DICE-")
import dice_ml
df=risk_factor_df

# print("Label (outcome name):", label)
# print("Is label in DataFrame columns?", label in df.columns)
```

```
    # print(df.columns == X_test.columns)
    cont_features = list(df.columns)
    cont_features.remove(label)

    # Sample a fraction of the data
    # Gaussian Noise took way too long
    frac = .1
    total_CFS=10
    if mode == 'Noise':
      frac = .02
      total_CFS=5
    sampled_df = df.sample(frac=frac, random_state=42)  # Ensure reproducibility

    # Continue with the sampled DataFrame
    d = dice_ml.Data(dataframe=sampled_df, continuous_features=cont_features, outco
    m = dice_ml.Model(model=model, backend="sklearn")
    exp = dice_ml.Dice(d, m, method="random")

    #modification to remove label
    # query_instance = X_test
    query_instance = X_test.drop(columns=[label])
    e1 = exp.generate_counterfactuals(query_instance, total_CFs=total_CFS, desired_
                                      desired_class="opposite",
                                      permitted_range=None, features_to_vary="all")

    imp = exp.local_feature_importance(query_instance, posthoc_sparsity_param=None)
    dicecontrib=pd.DataFrame.from_dict(imp.local_importance)

    res = dict()
    for j in list(dicecontrib.columns):
      res[j]=np.mean(np.abs(dicecontrib[j]))
    fi_7={k: fi_7.get(k, 0) + res.get(k, 0) for k in set(fi_7)}
    fi_7

    GloSur.to_csv(f"/content/drive/My Drive/DL4H_Sp24_Final_Project/{mode}_glosur.c
    kernelSHAP.to_csv(f"/content/drive/My Drive/DL4H_Sp24_Final_Project/{mode}_Ksha
    treeSHAP.to_csv(f"/content/drive/My Drive/DL4H_Sp24_Final_Project/{mode}_Tshap.
    samplingSHAP.to_csv(f"/content/drive/My Drive/DL4H_Sp24_Final_Project/{mode}_Ss
    limecontrib.to_csv(f"/content/drive/My Drive/DL4H_Sp24_Final_Project/{mode}_lim
    ticontrib.to_csv(f"/content/drive/My Drive/DL4H_Sp24_Final_Project/{mode}_ti.cs
    dicecontrib.to_csv(f"/content/drive/My Drive/DL4H_Sp24_Final_Project/{mode}_dic

    dics = []
```

```
fi_1['Method'] = 'Surrogates'
dics.append(fi_1)
fi_2['Method'] = 'KSHAP'
dics.append(fi_2)
fi_3['Method'] = 'TSHAP'
dics.append(fi_3)
fi_4['Method'] = 'SSHAP'
dics.append(fi_4)
fi_5['Method'] = 'LIME'
dics.append(fi_5)
fi_6['Method'] = 'TI'
dics.append(fi_6)
fi_7['Method'] = 'DICE'
dics.append(fi_7)


dics = pd.DataFrame(dics)
methods=dics['Method']
dics['Method']=methods
dics.to_csv(f"/content/drive/My Drive/DL4H_Sp24_Final_Project/{mode}_localExpla
print(mode, " is complete!")
```

```
def run_explainers_ti(mode, model, X_train, X_test, y_train, y_test):
  # Initialize a dictionary to store results temporarily.
  print(f'starting {mode}')
  res = dict()

  # Retrieve the list of feature names from the test dataset.
  features = X_test.columns
  # Initialize an empty DataFrame to store contributions from all trees
  all_contributions = pd.DataFrame(columns=features, index=X_test.index)
  all_contributions.fillna(0, inplace=True)
  # print(len(model.estimators_))
  # Iterate over each estimator (tree) in the random forest
  for tree in model.estimators_:
      prediction, bias, contributions = ti.predict(tree, X_test)

      # Sum up the contributions for each feature from this tree
      for i in range(len(X_test)):
          all_contributions.iloc[i] += contributions[i][:,1]  # assuming contribu

  # Now average the contributions across all trees
  average_contributions = all_contributions / len(model.estimators_)
  # Compute the mean of absolute contributions for each feature
  feature_importance = average_contributions.abs().mean()
  fi_dict = feature_importance.to_dict()
  average_contributions.to_csv(f"/content/drive/My Drive/DL4H_Sp24_Final_Project/
  file_path = f"/content/drive/My Drive/DL4H_Sp24_Final_Project/{mode}_localExpla

  # Load the existing data from CSV
  dics = pd.read_csv(file_path)

  # Find the index of the row where the Method is 'TI'
  ti_index = dics[dics['Method'] == 'TI'].index

  # Update the 'TI' row with the correct dictionary values
  for key in fi_dict:
      if key in dics.columns:
          dics.loc[ti_index, key] = fi_dict[key]

  # Save the updated DataFrame back to CSV
  dics.to_csv(file_path, index=False)

  print(f"Updated the TI method in {file_path}")
```

Continuous (Done)

```
# run_explainers('Continuous', continuous_rnd_clf, Continuous_X_train, Continuous
```

Original (Done)

```
#run_explainers('Original', rnd_clf, X_train, X_test, y_train, y_test)
```

Binary (Done)

```
#run_explainers('Binary', binary_rnd_clf, Binary_X_train, Binary_X_test, Binary_y
```

Gaussian Noise (Done)

We had to further decrease the dice sampling for this, otherwise the training was taking too long

```
#run_explainers('Noise', noise_rnd_clf, Noise_X_train, Noise_X_test, Noise_y_trai
```

Rerun TI

```
# run_explainers_ti('Original', rnd_clf, X_train, X_test, y_train, y_test)
# run_explainers_ti('Continuous', continuous_rnd_clf, Continuous_X_train, Continu
# run_explainers_ti('Binary', binary_rnd_clf, Binary_X_train, Binary_X_test, Bina
# run_explainers_ti('Noise', noise_rnd_clf, Noise_X_train, Noise_X_test, Noise_y_
```

```
    starting Original
    Updated the TI method in /content/drive/My Drive/DL4H_Sp24_Final_Project/Orig
    starting Continuous
    Updated the TI method in /content/drive/My Drive/DL4H_Sp24_Final_Project/Cont
    starting Binary
    Updated the TI method in /content/drive/My Drive/DL4H_Sp24_Final_Project/Bina
    starting Noise
    Updated the TI method in /content/drive/My Drive/DL4H_Sp24_Final_Project/Nois
```

Evaluation

```
#get explanations

instance=291
```

Checkpoint: Get original contributions

```
#DL
gscontrib = pd.read_csv(root+'/Original_glosur.csv')
kercontrib = pd.read_csv(root+'/Original_Kshap.csv')
samcontrib = pd.read_csv(root+'/Original_Sshap.csv')
trecontrib = pd.read_csv(root+'/Original_Tshap.csv')
limecontrib = pd.read_csv(root+'/Original_lime.csv')
ticontrib = pd.read_csv(root+'/Original_ti.csv')
dicecontrib = pd.read_csv(root+'/Original_dice.csv')
all_fi = pd.read_csv(root+'/Original_localExplainMethods.csv')
```

Noise Contributions

```
#RF
gscontrib_noise = pd.read_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/No
kercontrib_noise = pd.read_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/N
samcontrib_noise = pd.read_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/N
trecontrib_noise = pd.read_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/N
limecontrib_noise = pd.read_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/
ticontrib_noise = pd.read_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/No
dicecontrib_noise = pd.read_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/
all_fi_noise = pd.read_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/Noise
```

Continuous contributions

```
#VAR continue
gscontrib_continuous = pd.read_csv('/content/drive/My Drive/DL4H_Sp24_Final_Proje
kercontrib_continuous = pd.read_csv('/content/drive/My Drive/DL4H_Sp24_Final_Proj
samcontrib_continuous = pd.read_csv('/content/drive/My Drive/DL4H_Sp24_Final_Proj
trecontrib_continuous = pd.read_csv('/content/drive/My Drive/DL4H_Sp24_Final_Proj
limecontrib_continuous = pd.read_csv('/content/drive/My Drive/DL4H_Sp24_Final_Pro
ticontrib_continuous = pd.read_csv('/content/drive/My Drive/DL4H_Sp24_Final_Proje
dicecontrib_continuous = pd.read_csv('/content/drive/My Drive/DL4H_Sp24_Final_Pro
all_fi_continuous = pd.read_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/
```

Binary Contributions

```
#VAR binary
gscontrib_binary = pd.read_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/B
kercontrib_binary = pd.read_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/
samcontrib_binary = pd.read_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/
trecontrib_binary = pd.read_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/
limecontrib_binary = pd.read_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project
ticontrib_binary = pd.read_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/B
dicecontrib_binary = pd.read_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project
all_fi_binary = pd.read_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/Bina
```

Checkpoint: explain

```
#TOOLS
all_fi.fillna(0, inplace=True)
all_fi.iloc[:,:-1]=np.abs(all_fi.iloc[:,:-1])
all_fi.reset_index(drop=True, inplace=True)
label="Dx:Cancer"
methods=all_fi['Method'].to_list()
weights=[gscontrib, kercontrib, trecontrib, samcontrib, limecontrib, ticontrib, c


#Normalize
gscontrib_norm=gscontrib.div(gscontrib.sum(axis=1), axis=0)
kercontrib_norm=kercontrib.div(kercontrib.sum(axis=1), axis=0)
samcontrib_norm=samcontrib.div(samcontrib.sum(axis=1), axis=0)
trecontrib_norm=trecontrib.div(trecontrib.sum(axis=1), axis=0)
limecontrib_norm=limecontrib.div(limecontrib.sum(axis=1), axis=0)
ticontrib_norm=ticontrib.div(ticontrib.sum(axis=1), axis=0)
dicecontrib_norm=dicecontrib.div(dicecontrib.sum(axis=1), axis=0)
```

```
#One Instance
risk_factor_df.describe().iloc[1]
```

```
Age                                   29.375075
Number of sexual partners              2.555158
First sexual intercourse              17.480024
Num of pregnancies                     2.267740
Smokes                                 0.077519
Smokes (years)                         1.362854
Smokes (packs/year)                    0.796284
Hormonal Contraceptives                0.586166
Hormonal Contraceptives (years)        2.368868
IUD                                    0.129398
IUD (years)                            1.147927
STDs                                   0.047108
STDs (number)                          0.079308
STDs:condylomatosis                    0.026237
STDs:cervical condylomatosis           0.000000
STDs:vaginal condylomatosis            0.002385
STDs:vulvo-perineal condylomatosis     0.025641
STDs:syphilis                          0.010733
STDs:pelvic inflammatory disease       0.000596
STDs:genital herpes                    0.000596
STDs:molluscum contagiosum             0.000596
STDs:AIDS                              0.000000
STDs:HIV                               0.010733
STDs:Hepatitis B                       0.000596
STDs:HPV                               0.001193
STDs: Number of diagnosis              0.044723
STDs: Time since first diagnosis       4.245497
STDs: Time since last diagnosis        3.287024
Dx:CIN                                 0.005367
Dx:HPV                                 0.412045
Dx                                     0.388790
Hinselmann                             0.030411
Schiller                               0.115683
Citology                               0.067382
Biopsy                                 0.085868
total_std                              0.079308
total_tests                            0.536076
Dx:Cancer                              0.499106
Name: mean, dtype: float64
```

```
xx=risk_factor_df.describe().iloc[1]
```

```
instance=3
```

```
xx=X_test.iloc[instance]
idx=list(xx.to_numpy().nonzero()[0])
xx=xx.to_frame()
xxx=xx.T.columns
new=pd.DataFrame()
for i in range(len(xxx)):
  if i in idx:
     new[xxx[i]]=xx.T[xxx[i]]

new.T.round(2)
```

```
with open('instance.tex','w') as tf:
    tf.write(new.T.round(2).to_latex())
```

```
#Instance dataframe
one_instance=[]

for i in range(len(methods)):
  one_instance.append(weights[i].iloc[instance])

one_instance=pd.DataFrame(one_instance, columns=X_test.columns)
one_instance['methods']=methods
one_instance.set_index('methods', inplace=True)

# one_instance.to_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/one_instar
```

```
one_instance
```

```
instance=291
var='W'
maxx=10
f=''
vale=0


# Initialize a LIME Explainer for tabular data, specifying the training dataset,
explainer = lime.lime_tabular.LimeTabularExplainer(X_train.values, mode='classifi

# Explain the prediction of a specific instance from the test dataset using the t
exp = explainer.explain_instance(X_test.iloc[instance], model.predict_proba, num_
```

The model is confident this instance is of class 1.

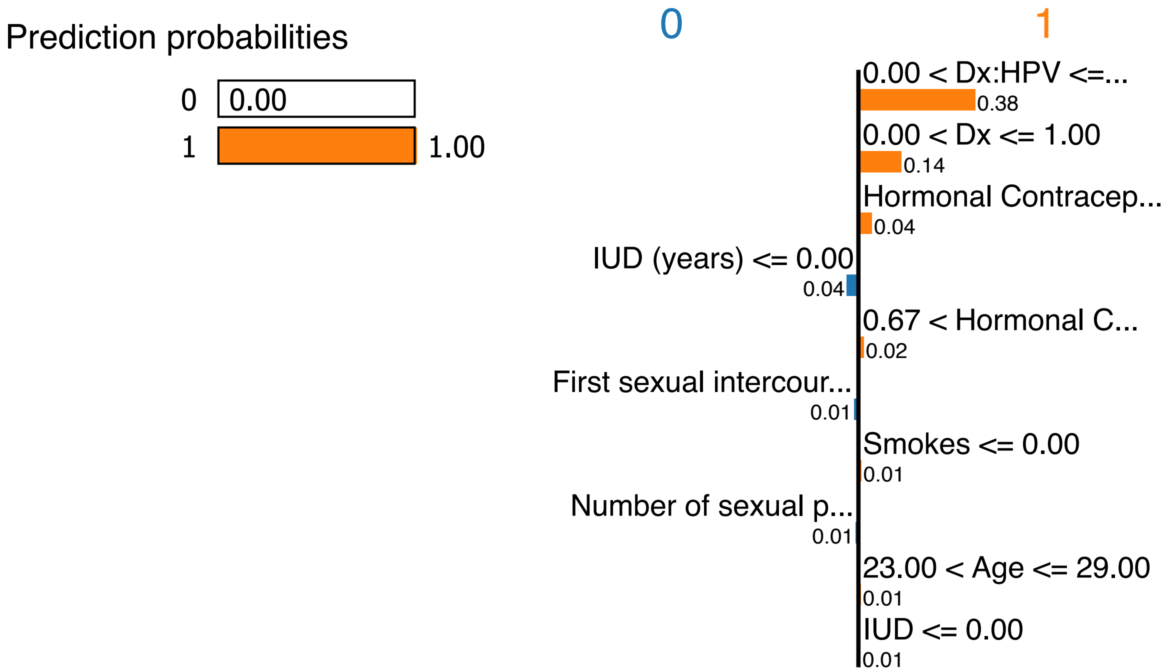
```
# glosar contribution
items = gscontrib.iloc[instance].to_dict()
t = []
count=0
for i, item in enumerate(items):
  if abs(items[item]) > 0.0 :
    t.append((i, items[item]))

t = sorted(t, key=lambda tup: abs(tup[1]),  reverse=True)

exp_test = {1: t[0:maxx]}


exp.local_exp = exp_test
exp.show_in_notebook(show_table=False,show_predicted_value=False)
```

```
%matplotlib inline
fig = exp.as_pyplot_figure()
plt.xlabel("Local Surrogates")
```

```
# fig.savefig('/content/drive/My Drive/DL4H_Sp24_Final_Project/'+str(var)+'surrog
items = kercontrib.iloc[instance].to_dict()
t = []
count=0
for i, item in enumerate(items):
  if abs(items[item]) > 0.0 :
    t.append((i, items[item]))

t = sorted(t, key=lambda tup: abs(tup[1]),  reverse=True)

exp_test = {1: t[0:maxx]}


exp.local_exp = exp_test
exp.show_in_notebook(show_table=False,show_predicted_value=False)
```

```
%matplotlib inline
fig = exp.as_pyplot_figure()
plt.xlabel("kernel SHAP")
# fig.savefig('/content/drive/My Drive/DL4H_Sp24_Final_Project/'+str(var)+'kernel
items = trecontrib.iloc[instance].to_dict()
t = []
count=0
for i, item in enumerate(items):
  if abs(items[item]) > 0.0 :
    t.append((i, items[item]))

t = sorted(t, key=lambda tup: abs(tup[1]),  reverse=True)

exp_test = {1: t[0:maxx]}


exp.local_exp = exp_test
exp.show_in_notebook(show_table=True,show_predicted_value=False)
```

```
%matplotlib inline
fig = exp.as_pyplot_figure()
plt.xlabel("Tree SHAP")
# fig.savefig('/content/drive/My Drive/DL4H_Sp24_Final_Project/'+str(var)+'treeSH
items = samcontrib.iloc[instance].to_dict()
t = []
count=0
for i, item in enumerate(items):
  if abs(items[item]) > 0.0 :
    t.append((i, items[item]))

t = sorted(t, key=lambda tup: abs(tup[1]),  reverse=True)

exp_test = {1: t[0:maxx]}


exp.local_exp = exp_test
exp.show_in_notebook(show_table=True,show_predicted_value=False)
```



Feature	Value
Dx:HPV	1.00
Dx	1.00
Hormonal Contraceptives	0.00
IUD (years)	0.00
Hormonal Contraceptives (years)	0.86
First sexual intercourse	14.00
Smokes	0.00
Number of sexual partners	2.00
Age	27.00
IUD	0.00

```
%matplotlib inline
fig = exp.as_pyplot_figure()
plt.xlabel("Sampling SHAP")
# fig.savefig('/content/drive/My Drive/DL4H_Sp24_Final_Project/'+str(var)+'sampli
items = limecontrib.iloc[instance].to_dict()
t = []
count=0
for i, item in enumerate(items):
  if abs(items[item]) > 0.0 :
    t.append((i, items[item]))

t = sorted(t, key=lambda tup: abs(tup[1]),  reverse=True)

exp_test = {1: t[0:maxx]}


exp.local_exp = exp_test
exp.show_in_notebook(show_table=True,show_predicted_value=False)
```

```
%matplotlib inline
fig = exp.as_pyplot_figure()
plt.xlabel("LIME")
# fig.savefig('/content/drive/My Drive/DL4H_Sp24_Final_Project/'+str(var)+'lime'+
items = ticontrib.iloc[instance].to_dict()
t = []
count=0
for i, item in enumerate(items):
  if abs(items[item]) > 0.0 :
    t.append((i, items[item]))

t = sorted(t, key=lambda tup: abs(tup[1]),  reverse=True)

exp_test = {1: t[0:maxx]}


exp.local_exp = exp_test
exp.show_in_notebook(show_table=False,show_predicted_value=False)
```

```
%matplotlib inline
fig = exp.as_pyplot_figure()
plt.xlabel("Tree Interpreter")
# fig.savefig('/content/drive/My Drive/DL4H_Sp24_Final_Project/'+str(var)+'ti'+st
items = dicecontrib.iloc[instance].to_dict()
t = []
count=0
for i, item in enumerate(items):
  if abs(items[item]) > 0.0 :
    t.append((i, items[item]))

t = sorted(t, key=lambda tup: abs(tup[1]),  reverse=True)

exp_test = {1: t[0:maxx]}

exp.local_exp = exp_test
exp.show_in_notebook(show_table=False,show_predicted_value=False)
```

```
%matplotlib inline
fig = exp.as_pyplot_figure()
plt.xlabel("DiCE")
# fig.savefig('/content/drive/My Drive/DL4H_Sp24_Final_Project/'+str(var)+'dice'+
```

Checkpoint ROAR

The Faithfulness Metric: RemOve And Retrain (ROAR) (Hooker et al., 2018) is a machine learning interpretability metric that involves iteratively removing a subset of features from a dataset, retraining the model on the reduced dataset, and then evaluating the changes in model accuracy or feature importance.

```
from sklearn.model_selection import cross_val_score

def roar(featImp, feature_to_predict, datapath, savepath, dataname):
    # Define line styles for plotting
    a = ['ro--', 'go--', 'mo--', 'yo--', 'co--', 'ko--', 'bo--']
    # Define percentages of features to remove in each iteration
    pourc = [0, 10, 20, 30, 40, 60, 70, 90]
    # Set font size for plots
    font = {'size': 14}
    plt.rc('font', **font)

    # Iterate over each row of feature importances (each method's importance)
    for k in range(featImp.shape[0]):
        accuracies = []
        # Iterate over defined percentages to remove features incrementally
        for i in pourc:
            # Extract feature importances, assuming 'Method' column exists and ne
            fi = featImp.iloc[k, :].drop('Method')
            # Sort features by importance
            fi = fi.to_dict()
            fi = dict(sorted(fi.items(), key=lambda x: x[1], reverse=True))
            fii = list(fi.keys())

            # Load the dataset
            df = pd.read_csv(datapath)
            # Calculate the number of top features to remove based on percentage
            top = int((len(fii) * i) / 100)
            if top >= len(fii):
                print(f"Skipping removal of top {top} features as it exceeds avai
                accuracies.append(None)
                continue
            remaining_features = fii[top:] + [feature_to_predict]

            print(f"Removing top {top} features, which are: {fii[:top]}")

            # Select the remaining features in the dataset
            df = df[remaining_features]
            X = df.drop(feature_to_predict, axis=1).values
            y = df[feature_to_predict].values

            # Check if there are any features left to train the model
            if X.shape[1] == 0:
                print("No features left to train the model.")
                accuracies.append(None)
                continue

            # Initialize the classifier and perform cross-validation
            model = RandomForestClassifier(random_state=42)
            try:
                scores = cross_val_score(model, X, y, cv=10)
                accuracies.append(np.mean(scores))
            except Exception as e:
                print(f"Error while fitting the model: {e}")
                accuracies.append(None)

        # Plot the results for the current feature importance row
        plt.plot(pourc, accuracies, a[k], label=f"{featImp.iloc[k, :]['Method']}

    # Configure and display the plot
    plt.xlabel('% removed features for ' + dataname)
    plt.ylabel('Accuracy')
    plt.legend(loc='upper right')
    # plt.savefig(savepath + 'roar.png', bbox_inches='tight', dpi=300)
    plt.show()



datapath=root + '/Rcancer2.csv'
savepath= '/content/drive/My Drive/DL4H_Sp24_Final_Project/'
dataname='Cervical cancer'
# print(all_fi.columns)
# roar(all_fi, label, datapath, savepath, dataname)
```

```
from PIL import Image
im = Image.open(root+"/roar.png")
im
```

SHAPASH Contribution Plots (Age)

```
from shapash.explainer.consistency import Consistency
from shapash import SmartExplainer

print("Training Data Shape:", X_train.shape)
print("Testing Data Shape:", X_test.shape)
print("Training Features:", X_train.columns.tolist())
print("Testing Features:", X_test.columns.tolist())

cns=Consistency()
xpl = SmartExplainer(model=model)
xpl.compile(x=X_test)

from sklearn.ensemble import RandomForestClassifier
xpl = SmartExplainer(model=model)
xpl.compile(
    x=X_test,
)
```

```
Training Data Shape: (1341, 35)
Testing Data Shape: (336, 35)
Training Features: ['Age', 'Number of sexual partners', 'First sexual interco
Testing Features: ['Age', 'Number of sexual partners', 'First sexual intercou
INFO: Shap explainer type - <shap.explainers._tree.TreeExplainer object at 0x
INFO: Shap explainer type - <shap.explainers._tree.TreeExplainer object at 0x
```

```
img=xpl.plot.contribution_plot(0)
img.show()
```

```
# img.write_image('/content/drive/My Drive/DL4H_Sp24_Final_Project/contribage.png
xpl = SmartExplainer(model=model)
xpl.compile(x=X_test,contributions=kercontrib)
```

```
img=xpl.plot.contribution_plot(0)
img.show()
```

```
# img.write_image('/content/drive/My Drive/DL4H_Sp24_Final_Project/contribagekerr
xpl = SmartExplainer(model=model)
xpl.compile(x=X_test,contributions=samcontrib)
img=xpl.plot.contribution_plot(0)
img.show()
```

```
# img.write_image('/content/drive/My Drive/DL4H_Sp24_Final_Project/contribagesamp
xpl = SmartExplainer(model=model)
xpl.compile(x=X_test,contributions=trecontrib)
img=xpl.plot.contribution_plot(0)
img.show()
```

```
# img.write_image('/content/drive/My Drive/DL4H_Sp24_Final_Project/contribagetree
xpl = SmartExplainer(model=model)
xpl.compile(x=X_test,contributions=limecontrib)
img=xpl.plot.contribution_plot(0)
img.show()
```

```
# img.write_image('/content/drive/My Drive/DL4H_Sp24_Final_Project/contribagelime
xpl = SmartExplainer(model=model)
xpl.compile(x=X_test,contributions=ticontrib)
img=xpl.plot.contribution_plot(0)
img.show()
```

```
# img.write_image('/content/drive/My Drive/DL4H_Sp24_Final_Project/contribageti.p
xpl = SmartExplainer(model=model)
xpl.compile(x=X_test,contributions=gscontrib)
img=xpl.plot.contribution_plot(0)
img.show()
```

```
# img.write_image('/content/drive/My Drive/DL4H_Sp24_Final_Project/contribageGlos
xpl = SmartExplainer(model=model)
dicecontrib = dicecontrib[X_test.columns]
xpl.compile(x=X_test,contributions=dicecontrib)
img=xpl.plot.contribution_plot(0)
img.show()
```

```
# img.write_image('/content/drive/My Drive/DL4H_Sp24_Final_Project/contribageDice
fig_image=xpl.plot.contribution_plot(29)
fig_image.show()
# plt.savefig('/content/drive/My Drive/DL4H_Sp24_Final_Project/contdxhpv.png')
```

Consistency Plots

```
pairwise_consistency=cns.calculate_all_distances(methods, weights)
```

```
test=pairwise_consistency[1].round(2)
```

```
test.style.background_gradient(cmap='Paired_r')
```

```
root = 'DL4H_Sp24_Final_Project'
```

```
with open(root + '/consistency.tex','w') as tf:
    tf.write(test.to_latex())
```

```
corr = pairwise_consistency[1]
mask = np.zeros_like(corr)
mask[np.triu_indices_from(mask)] = True
fig = plt.figure(figsize=(9, 11))
with sns.axes_style("white"):

    ax = sns.heatmap(corr, mask=mask, square=True,annot=True, annot_kws={'fontsiz
                xticklabels=methods, yticklabels=methods, cmap="Reds", cbar=True)
    ax.set_title("Cervical cancer risk factors", color='xkcd:medium blue', fontsi
    ax.set_ylabel('Top Feature\nAgreement (N=10)', color='xkcd:medium blue', font



    plt.show()
```

```
# fig.savefig(root+'/consistency_png', bbox_inches='tight', dpi=300)
```

```
for i in pairwise_consistency[1].columns:
  print(i, round(np.mean(pairwise_consistency[1][i]),2))
```

```
Surrogates 0.56
KSHAP 0.45
TSHAP 0.42
SSHAP 0.45
LIME 0.5
TI 0.49
DICE 1.1
```

Compactness

```
def get_distance(selection, contributions, mode, nb_features):

    if mode == "classification" and len(contributions) == 2:
        contributions = contributions[1]
    assert nb_features <= contributions.shape[1]

    contributions = contributions.loc[selection].values
    top_features = np.array([sorted(row, key=abs, reverse=True) for row in contri
    output_top_features = np.sum(top_features[:, :], axis=1)
    output_all_features = np.sum(contributions[:, :], axis=1)

    if mode == "regression":
        distance = abs(output_top_features - output_all_features) / abs(output_al
    elif mode == "classification":
        distance = abs(output_top_features - output_all_features)
    return distance


def get_min_nb_features(selection, contributions, mode, distance):

    assert 0 <= distance <= 1

    if mode == "classification" and len(contributions) == 2:
        contributions = contributions[1]
    contributions = contributions.loc[selection].values
    features_needed = []
    # For each instance, add features one by one (ordered by SHAP) until we get c
    for i in range(contributions.shape[0]):
        ids = np.flip(np.argsort(np.abs(contributions[i, :])))
        output_value = np.sum(contributions[i, :])

        score = 0
        for j, idx in enumerate(ids):
            # j : number of features needed
            # idx : positions of the j top shap values
            score += contributions[i, idx]
            # CLOSE_ENOUGH
            if mode == "regression":
                if abs(score - output_value) < distance * abs(output_value):
                    break
            elif mode == "classification":
                if abs(score - output_value) < distance:
                    break
        features_needed.append(j + 1)
    return features_needed



def compute_features_compacity(case, contributions, selection, distance, nb_featu
        #if (case == "classification") and (len(classes) > 2):
        #    raise AssertionError("Multi-class classification is not supported")

        features_needed = get_min_nb_features(selection, contributions, case, dis
        distance_reached = get_distance(selection, contributions, case, nb_featur
        # We clip large approximations to 100%
        distance_reached = np.clip(distance_reached, 0, 1)

        return {"features_needed": features_needed, "distance_reached": distance_


compacities=[]

for weight in weights:
  rr=compute_features_compacity(case="classification", contributions=weight, sele
  #rr=compute_features_compacity(case="classification", contributions=weight, sel
  compacities.append(pd.DataFrame.from_dict(rr))
```

```
maxx=[]
for c in compacities:
  maxx.append(c.iloc[c.distance_reached.idxmax()].tolist())
compacity=pd.DataFrame(data=maxx, columns=['features_needed', 'distance_reached']
compacity['Method']=methods
compacity.set_index('Method', drop=True).round(2)
```

```
with open(root+'/compactness'+str(instance)+'.tex','w') as tf:
    tf.write(compacity.to_latex())
```

```
xpl = SmartExplainer(model=model)
xpl.compile(x=X_test,contributions=gscontrib)
img=xpl.plot.compacity_plot()
img.show()
```

```
# img.write_image('/content/drive/My Drive/DL4H_Sp24_Final_Project/compactGlosur.
xpl = SmartExplainer(model=model)
xpl.compile(x=X_test,contributions=kercontrib)
img=xpl.plot.compacity_plot()
img.show()
```

```
# img.write_image('/content/drive/My Drive/DL4H_Sp24_Final_Project/compactker.png
xpl = SmartExplainer(model=model)
xpl.compile(x=X_test,contributions=trecontrib)
img=xpl.plot.compacity_plot()
img.show()
```

```
# img.write_image('/content/drive/My Drive/DL4H_Sp24_Final_Project/compacttree.pr
xpl = SmartExplainer(model=model)
xpl.compile(x=X_test,contributions=limecontrib)
img=xpl.plot.compacity_plot()
img.show()
```

```
# img.write_image('/content/drive/My Drive/DL4H_Sp24_Final_Project/compactlime.pr
xpl = SmartExplainer(model=model)
xpl.compile(x=X_test,contributions=samcontrib)
img=xpl.plot.compacity_plot()
img.show()
```

```
# img.write_image('/content/drive/My Drive/DL4H_Sp24_Final_Project/compactsamplir
xpl = SmartExplainer(model=model)
xpl.compile(x=X_test,contributions=ticontrib)
img=xpl.plot.compacity_plot()
img.show()
```

```
# img.write_image('/content/drive/My Drive/DL4H_Sp24_Final_Project/compactti.png'
xpl = SmartExplainer(model=model)
xpl.compile(x=X_test,contributions=dicecontrib)
img=xpl.plot.compacity_plot()
img.show()
```

```
# img.write_image('/content/drive/My Drive/DL4H_Sp24_Final_Project/compactdice.pr
```

Stability

```
from sklearn.preprocessing import normalize
```

```
def _compute_distance(x1, x2, mean_vector, epsilon=0.0000001):
    """
    Compute distances between data points by using L1 on normalized data : sum(ab
    Parameters
    ----------
    x1 : array
        First vector
    x2 : array
        Second vector
    mean_vector : array
        Each value of this vector is the std.dev for each feature in dataset
    Returns
    -------
    diff : float
        Returns :math:`\\sum(\\frac{|x1-x2|}{mean\_vector+epsilon})`
    """
    diff = np.sum(np.abs(x1 - x2) / (mean_vector + epsilon))
    return diff


def _compute_similarities(instance, dataset):
    """
    Compute pairwise distances between an instance and all other data points
    Parameters
    ----------
    instance : 1D array
        Reference data point
    dataset : 2D array
        Entire dataset used to identify neighbors
    Returns
    -------
    similarity_distance : array
        V[j] == distance between actual instance and instance j
    """
    mean_vector = np.array(dataset, dtype=np.float32).std(axis=0)
    similarity_distance = np.zeros(dataset.shape[0])

    for j in range(0, dataset.shape[0]):
        # Calculate distance between point and instance j
        dist = _compute_distance(instance, dataset[j], mean_vector)
        similarity_distance[j] = dist

    return similarity_distance
```

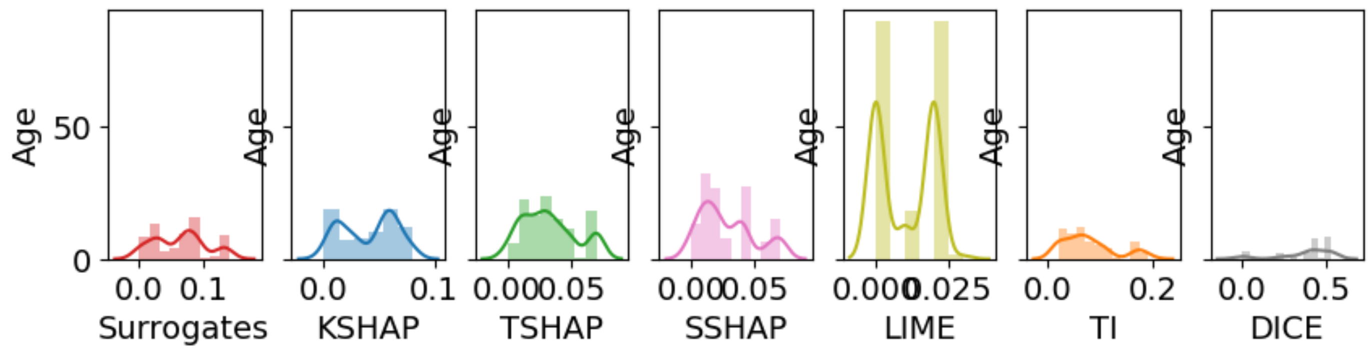
```
def _get_radius(dataset, n_neighbors, sample_size=50, percentile=95):
    """
    Calculate the maximum allowed distance between points to be considered as nei
    Parameters
    ----------
    dataset : DataFrame
        Pool to sample from and calculate a radius
    n_neighbors : int
        Maximum number of neighbors considered per instance
    sample_size : int, optional
        Number of data points to sample from dataset, by default 500
    percentile : int, optional
        Percentile used to calculate the distance threshold, by default 95
    Returns
    -------
    radius : float
        Distance threshold
    """
    # Select 500 points max to sample
    size = min([dataset.shape[0], sample_size])
    # Randomly sample points from dataset
    sampled_instances = dataset[np.random.randint(0, dataset.shape[0], size), :]
    # Define normalization vector
    mean_vector = np.array(dataset, dtype=np.float32).std(axis=0)
    # Initialize the similarity matrix
    similarity_distance = np.zeros((size, size))
    # Calculate pairwise distance between instances
    for i in range(size):
        for j in range(i, size):
            dist = _compute_distance(sampled_instances[i], sampled_instances[j],
            similarity_distance[i, j] = dist
            similarity_distance[j, i] = dist
    # Select top n_neighbors
    ordered_X = np.sort(similarity_distance)[:, 1: n_neighbors + 1]
    # Select the value of the distance that captures XX% of all distances (percer
    return np.percentile(ordered_X.flatten(), percentile)


def find_neighbors(selection, dataset, model, mode, n_neighbors=30):
    """
    For each instance, select neighbors based on 3 criteria:
    1. First pick top N closest neighbors (L1 Norm + st. dev normalization)
    2. Filter neighbors whose model output is too different from instance (see cc
    3. Filter neighbors whose distance is too big compared to a certain thresholc
    Parameters
    ----------
    selection : list
        Indices of rows to be displayed on the stability plot
    dataset : DataFrame
        Entire dataset used to identify neighbors
    model : model object
        ML model
    mode : str
        "classification" or "regression"
    n_neighbors : int, optional
        Top N neighbors initially allowed, by default 10
    Returns
    -------
    all_neighbors : list of 2D arrays
        Wrap all instances with corresponding neighbors in a list with length (#i
        Each array has shape (#neighbors, #features) where #neighbors includes th
    """
    instances = dataset.loc[selection].values

    all_neighbors = np.empty((0, instances.shape[1] + 1), float)
    """Filter 1 : Pick top N closest neighbors"""
    for instance in instances:
        c = _compute_similarities(instance, dataset.values)
        # Pick indices of the closest neighbors (and include instance itself)
        neighbors_indices = np.argsort(c)[: n_neighbors + 1]
        # Return instance with its neighbors
        neighbors = dataset.values[neighbors_indices]
        # Add distance column
        neighbors = np.append(neighbors, c[neighbors_indices].reshape(n_neighbors
        all_neighbors = np.append(all_neighbors, neighbors, axis=0)

    # Calculate predictions for all instances and corresponding neighbors
    if mode == "regression":
        # For XGB it is necessary to add columns in df, otherwise columns mismatc
        predictions = model.predict(pd.DataFrame(all_neighbors[:, :-1], columns=c
    elif mode == "classification":
        predictions = model.predict_proba(pd.DataFrame(all_neighbors[:, :-1], col

    # Add prediction column
    all_neighbors = np.append(all_neighbors, predictions.reshape(all_neighbors.sh
    # Split back into original chunks (1 chunck = instance + neighbors)
    all_neighbors = np.split(all_neighbors, instances.shape[0])

    """Filter 2 : neighbors with similar blackbox output"""
    # Remove points if prediction is far away from instance prediction
    if mode == "regression":
        # Trick : use enumerate to allow the modifcation directly on the iterator
        for i, neighbors in enumerate(all_neighbors):
            all_neighbors[i] = neighbors[abs(neighbors[:, -1] - neighbors[0, -1])
    elif mode == "classification":
        for i, neighbors in enumerate(all_neighbors):
            all_neighbors[i] = neighbors[abs(neighbors[:, -1] - neighbors[0, -1])

    """Filter 3 : neighbors below a distance threshold"""
    # Remove points if distance is bigger than radius
    radius = _get_radius(dataset.values, n_neighbors)

    for i, neighbors in enumerate(all_neighbors):
        # -2 indicates the distance column
        all_neighbors[i] = neighbors[neighbors[:, -2] < radius]
    return all_neighbors

def shap_neighbors(instance, x_encoded, contributions, mode):
    """
    For an instance and corresponding neighbors, calculate various
    metrics (described below) that are useful to evaluate local stability
    Parameters
    ----------
    instance : 2D array
        Instance + neighbours with corresponding features
    x_encoded : DataFrame
        Entire dataset used to identify neighbors
    contributions : DataFrame
        Calculated contribution values for the dataset
    Returns
    -------
    norm_shap_values : array
        Normalized SHAP values (with corresponding sign) of instance and its neig
    average_diff : array
        Variability (stddev / mean) of normalized SHAP values (using L1) across n
    norm_abs_shap_values[0, :] : array
        Normalized absolute SHAP value of the instance
    """
    # Extract SHAP values for instance and neighbors
    # :-2 indicates that two columns are disregarded : distance to instance and m
    ind = pd.merge(x_encoded.reset_index(), pd.DataFrame(instance[:, :-2], column
        .set_index(x_encoded.index.name if x_encoded.index.name is not None else
    # If classification, select contrbutions of one class only
    if mode == "classification" and len(contributions) == 2:
        contributions = contributions[1]
    shap_values = contributions.loc[ind]
    # For neighbors comparison, the sign of SHAP values is taken into account
    norm_shap_values = normalize(shap_values, axis=1, norm="l1")
    # But not for the average impact of the features across the dataset
    norm_abs_shap_values = normalize(np.abs(shap_values), axis=1, norm="l1")
    # Compute the average difference between the instance and its neighbors
    # And replace NaN with 0
    average_diff = np.divide(norm_shap_values.std(axis=0), norm_abs_shap_values.m
                             out=np.zeros(norm_abs_shap_values.shape[1]),
                             where=norm_abs_shap_values.mean(axis=0) != 0)

    return norm_shap_values, average_diff, norm_abs_shap_values[0, :]


def get_distance(selection, contributions, mode, nb_features):
    """
    Determine how close we get to the output with all features by using only a su
    Parameters
    ----------
    selection : list
        Indices of rows to be displayed on the stability plot
    contributions : DataFrame
        Calculated contribution values for the dataset
    mode : str
        "classification" or "regression"
    nb_features : int, optional
        Number of features used, by default 5
    Returns
    -------
    distance : array
        List of distances for each instance by using top selected features (ex: r

        * For regression:

            * normalized distance between the output of current model and output
        * For classifciation:
            * distance between probability outputs (absolute value)
    """
    if mode == "classification" and len(contributions) == 2:
        contributions = contributions[1]
    assert nb_features <= contributions.shape[1]

    contributions = contributions.loc[selection].values
    top_features = np.array([sorted(row, key=abs, reverse=True) for row in contri
    output_top_features = np.sum(top_features[:, :], axis=1)
    output_all_features = np.sum(contributions[:, :], axis=1)

    if mode == "regression":
        distance = abs(output_top_features - output_all_features) / abs(output_al
    elif mode == "classification":
        distance = abs(output_top_features - output_all_features)
    return distance




def compute_features_stability (case, x, selection, contributions):
        """
        For a selection of instances, compute features stability metrics used in
        methods `local_neighbors_plot` and `local_stability_plot`.
        - If selection is a single instance, the method returns the (normalized)
        of instance and corresponding neighbors.
        - If selection represents multiple instances, the method returns the aver
        of instances and neighbors (=amplitude), as well as the variability of th
        Parameters
        ----------
        selection: list
            Indices of rows to be displayed on the stability plot
        Returns
        -------
        Dictionary
            Values that will be displayed on the graph. Keys are "amplitude", "va
        """
        #if (case == "classification") and (len(self._classes) > 2):
        #    raise AssertionError("Multi-class classification is not supported")
        x_encoded=x
        x_init=x
        all_neighbors = find_neighbors(selection, x_encoded, model, case)

        # Check if entry is a single instance or not
        if len(selection) == 1:
            # Compute explanations for instance and neighbors
            norm_shap, _, _ = shap_neighbors(all_neighbors[0], x_encoded, contrib
            local_neighbors = {"norm_shap": norm_shap}
            return local_neighbors
        else:
            numb_expl = len(selection)
            amplitude = np.zeros((numb_expl, x_init.shape[1]))
            variability = np.zeros((numb_expl, x_init.shape[1]))
            # For each instance (+ neighbors), compute explanation
            for i in range(numb_expl):
                (_, variability[i, :], amplitude[i, :],) = shap_neighbors(all_nei
            features_stability = {"variability": variability, "amplitude": amplit
            return features_stability


features=list(X_test.columns)


frames=[]
for weight in weights:
  #fs= compute_features_stability (case="classification", x=X_test, selection=lis
  fs= compute_features_stability (case="classification", x=X_test, selection=[ins
  frames.append(fs)
```

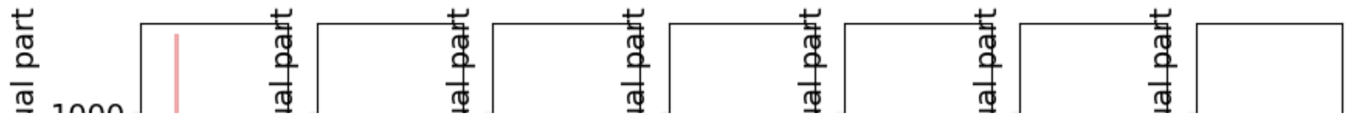
One Instance

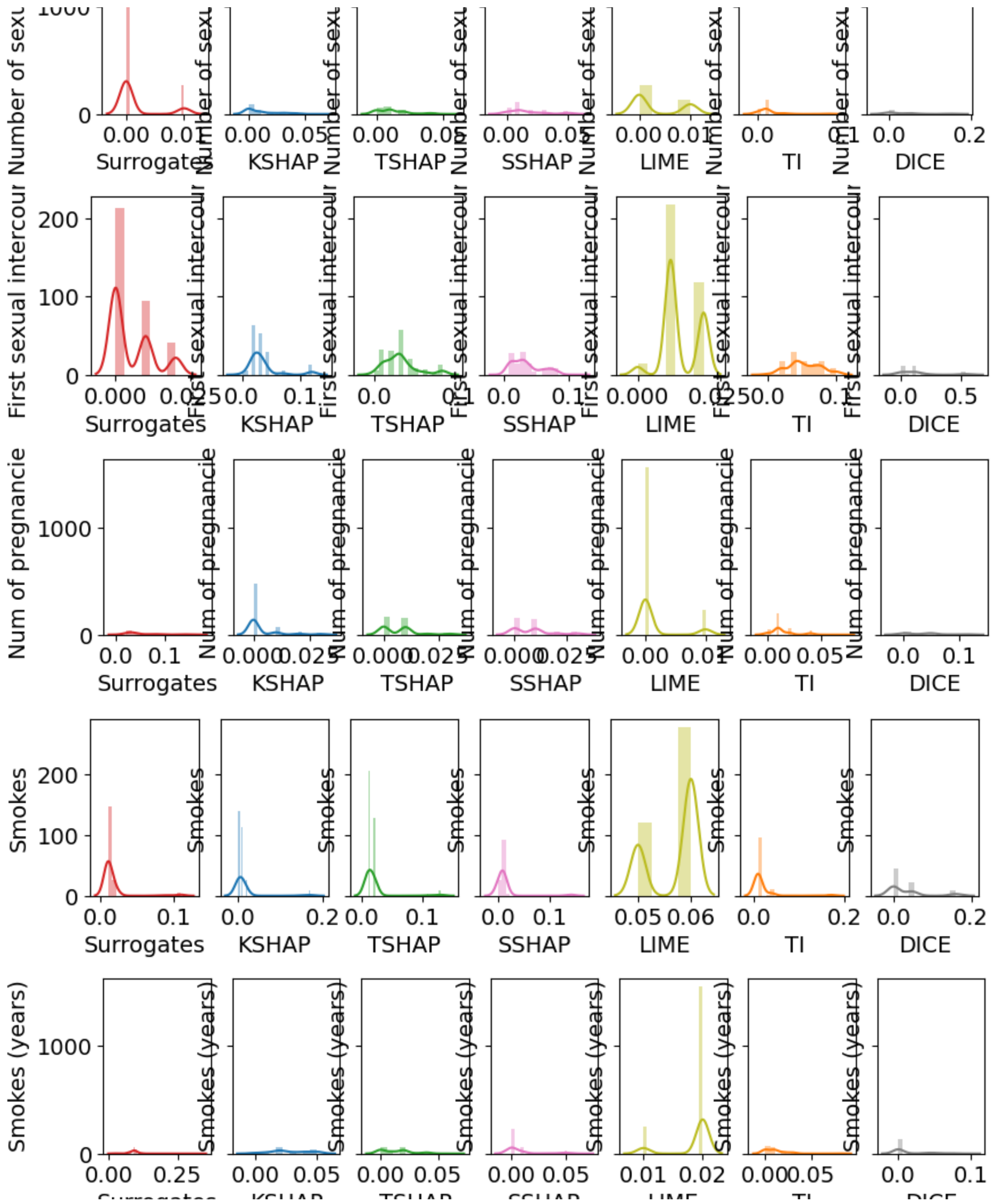
```
colors = ['tab:red', 'tab:blue', 'tab:green', 'tab:pink', 'tab:olive',  'tab:oran

for j in range(len(features)):
  fig, axes = plt.subplots(1, 7, figsize=(12, 2), sharey=True, dpi=100)
  t=0

  for fg, fs in enumerate(frames):
    am=[]

    for i in range(len(fs['norm_shap'])):
      am.append(round(fs['norm_shap'][i][j], 2)) # i INSCTANCE j Feature
    sns.distplot(am, ax=axes[fg], color=colors[t], axlabel=methods[t])
    t=t+1
    axes[fg].set_ylabel(features[j])
  # plt.savefig(root+'/'+str(var)+str(instance)+str(features[j])[:10]+'.png', bbc
  plt.show()
```

Multiple Instances

```
features=X_test.columns


#compute_features_compacity(case="classification", contributions=weight, selectic
frames=[]
for weight in weights:
  fs= compute_features_stability (case="classification", x=X_test, selection=list
  #fs= compute_features_stability (case="classification", x=X_test, selection=[1,
  frames.append(fs)


colors = ['tab:red', 'tab:blue', 'tab:green', 'tab:pink', 'tab:olive',  'tab:orar

for j in range(len(features)):
  fig, axes = plt.subplots(1, 7, figsize=(10, 2), sharey=True, dpi=100)
  t=0
  for fg, fs in enumerate(frames):
    vr=[]
    am=[]
    for i in range(len(fs['variability'])):
      vr.append(round(fs['variability'][i][j], 2)) # i INSCTANCE j Feature
      am.append(round(fs['amplitude'][i][j], 2))
    axes[fg].set_ylabel(features[j])
    sns.distplot(am, ax=axes[fg], color=colors[t], axlabel=methods[t])
    t=t+1
    #print('VR', vr)

  # plt.savefig(root+'/'+str(var)+str(features[j])[:10]+'.png')
  plt.show()
```






Number of sext
1000
0
0.00
0.01
Surrogates
KSHAP
TSHAP
SSHAP
LIME
TI
DICE
First sexual intercour
200
100
Num of pregnancie
Smokes
Smokes (years)
0.05
0.06
0.1
0.2
0.25
0.025
0.5

```
t=0
for fg, fs in enumerate(frames):
  vr=[]
  am=[]
  for j in range(len(features)):
    vr.append(np.mean(fs['variability'][j])) # i INSCTANCE j Feature
    am.append(np.std(fs['variability'][j]))
  print(methods[t], round(np.mean(vr),2))
  print(methods[t], round(np.std(am),2))
  t+=1
```

```
Surrogates 0.22
Surrogates 0.22
KSHAP 0.31
KSHAP 0.25
TSHAP 0.41
TSHAP 0.11
SSHAP 0.37
SSHAP 0.14
LIME 0.66
LIME 0.02
TI 0.48
TI 0.1
DICE 1.28
DICE 0.1
```

```
xpl.plot.stability_plot(selection=[0, 1, 3])
```

```
fig_image=xpl.plot.stability_plot()
#plt.xlabel("Local Surrogates")
# plt.savefig(root + '/stabplot.png')
```

```
for w in weights:
  xpl = SmartExplainer(model=model)
  w = w[X_test.columns]
  xpl.compile(x=X_test,contributions=w)
  xpl.plot.stability_plot()
```

Feature and Rank Disagreement

```
from scipy.stats import spearmanr
import numpy as np
import itertools

def intersection(r1, r2):
    return list(set(r1) & set(r2))

def check_size(r1, r2):
    assert len(r1) == len(r2), 'Both rankings should be the same size'

def feature_agreement(r1, r2):
    """
    Measures the fraction of common features between the
    sets of top-k features of the two rankings.

    From Krishna et al. (2022), The Disagreement Problem in
    Explainable Machine Learning: A Practitioner's Perspective

    Parameters
    ---------------
    r1, r2 : list
        Two feature rankings of identical shape
    """
    check_size(r1, r2)
    k = len(r1)

    return len(intersection(r1, r2)) / k

def rank_agreement(r1, r2):
    """
    Stricter than feature agreement, rank agreement checks
    that the feature order is comparable between the two rankings.

    From Krishna et al. (2022), The Disagreement Problem in
    Explainable Machine Learning: A Practitioner's Perspective

    Parameters
    ---------------
    r1, r2 : list
        Two feature rankings of identical shape
    """
    check_size(r1, r2)
    k = len(r1)

    return np.sum([True if x==y else False for x,y in zip(r1,r2)]) / k

def weak_rank_agreement(r1, r2):
    """
    Check if the rank is approximately close (within one rank).
    """
    check_size(r1, r2)
    k = len(r1)
    window_size=1

    rank_agree=[]
    for i, v in enumerate(r1):
        if i == 0:
            if v in r2[i:i+window_size+1]:
                rank_agree.append(True)
            else:
                rank_agree.append(False)
        else:
            if v in r2[i-window_size:i+window_size+1]:
                rank_agree.append(True)
            else:
                rank_agree.append(False)

    return np.sum(rank_agree)/k


def rank_correlation(r1, r2):
    return spearmanr(r1, r2)


def to_rankings(df, instance):
    """
    Convert feature attributions to a list of top features.
    """
    contrib_features = df.columns


    vals = df[contrib_features].values[instance,:]
    rankings = np.argsort(np.absolute(vals))[::-1]
    features = vals[rankings]
    return rankings


def compute_matrices(weights, instance):
    n_rankings = len(methods)

    feature_agree = np.zeros((n_rankings, n_rankings))
    rank_agree = np.zeros((n_rankings, n_rankings))
    corr = np.zeros((n_rankings, n_rankings))


    for i, j in itertools.product(range(n_rankings), range(n_rankings)):
        r1 = to_rankings(weights[i], instance)[:10]
        r2 = to_rankings(weights[j], instance)[:10]
        feature_agree[i,j] = feature_agreement(r1, r2)
        rank_agree[i,j] = rank_agreement(r1, r2)

    return feature_agree, rank_agree


feature_agree, rank_agree = compute_matrices(weights, instance)


corr = feature_agree
mask = np.zeros_like(corr)
mask[np.triu_indices_from(mask)] = True
fig = plt.figure(figsize=(9, 11))
with sns.axes_style("white"):

    ax = sns.heatmap(corr, mask=mask, square=True,annot=True, annot_kws={'fontsiz
                xticklabels=methods, yticklabels=methods, cmap="Reds", cbar=True)
    ax.set_title("Cervical cancer risk factors", color='xkcd:medium blue', fontsi
    ax.set_ylabel('Top Feature\nAgreement (N=10)', color='xkcd:medium blue', font
    ax.text(0.95,
                0.95,
                f"(a)",
                fontsize=14,
                alpha=0.8,
                ha="center",
                va="center",
                transform=ax.transAxes,
            )
    data=corr
    avg = np.mean(data[mask==0])
    text = f'Avg. Agrmnt : {avg:.2f}'
    ax.annotate(text, (1.0, 0.84), xycoords='axes fraction', fontsize=14, ha='rig

    avg = np.mean(data[4:, :4])
    text = f'Avg. Agrmnt b/t FI & FR: {avg:.2f}'
    ax.annotate(text, (1.0, 0.79), xycoords='axes fraction', fontsize=14, ha='rig




    plt.show()
```

```
# fig.savefig(root + '/featagrem'+str(instance)+'.png', bbox_inches='tight', dpi=


corr = rank_agree
mask = np.zeros_like(corr)
mask[np.triu_indices_from(mask)] = True
fig = plt.figure(figsize=(9, 11))
with sns.axes_style("white"):
```

```
ax = sns.heatmap(corr, mask=mask, square=True,annot=True, annot_kws={'fontsiz
            xticklabels=methods, yticklabels=methods, cmap="Reds")
ax.set_title("Cervical cancer risk factors", color='xkcd:medium blue', fontsi
ax.set_ylabel('Feature Rank\nAgreement (N=10)', color='xkcd:medium blue',font

ax.text(0.95,
            0.95,
            f"(b)",
            fontsize=14,
            alpha=0.8,
            ha="center",
            va="center",
            transform=ax.transAxes,
        )
data=corr
avg = np.mean(data[mask==0])
text = f'Avg. Agrmnt : {avg:.2f}'
ax.annotate(text, (1.0, 0.84), xycoords='axes fraction', fontsize=14, ha='rig

avg = np.mean(data[4:, :4])
text = f'Avg. Agrmnt b/t FI & FR: {avg:.2f}'
ax.annotate(text, (1.0, 0.79), xycoords='axes fraction', fontsize=14, ha='rig



plt.show()
```

```
# fig.savefig(root + '/rankagrem'+str(instance)+'.png', bbox_inches='tight', dpi=
```

Discussion & Results

Results

In our reproduction of the hypothesis that the Random Forest Classifier is the best model with the highest ROC, we were able to reproduct the results almost exaclty (as seen in section Model Execution - Balanced Evalutation). The results varied at bit from the original results (reasonings as to why in the discussion section below), but the Random Forest Classifier model was tied for the second best AUC score, just behind the Logistic Regression. We determined would be most RandomForestClassifier would still be the most reliable model to continue the reproduction with because of its high accuracy as well it's compatibility with later models used in the explainability study (some of which are only compatibile with tree models).

In our ablation using an unbalanced dataset, we produced vary similar results to the original study. We found that the all of the models resulted in the same AUC score (1.0), except for the KNNClassifier. Using these results, we could determine that the RandomForestClassifier is a strong model to continue testing with (as seen in section "Model Execution"), agreeing with the original paper's detrimation.

Secondly, in our testing of the hypothesis of LIME being the most faithful explanation, we did find that this was the correct result as the LIME had the highest accuracy with the removal of features, while the other interpretability methods decreased in accuracy with the remove of features (as seen in section Checkpoint ROAR). In our ROAR testing, there was a larger dip in accuracy at 70% removed features, showing marginally less robustness that the original claim. but still verifying that LIME is the most faithful model. LIME helps use other variable to explain a cancer diagnosis.

Overall, we were able to reproduce and verify the claims made by the orgiinal paper, even with the inclusion of our ablations. With more time, we would like to run the tests on that entire dataset, in order to verify the claims.

Discussion

Reproducabilty and Results Deviations:

We were able to acquire, process, and visual the data, and run the 5 models and ablations against the data with common Python libraries and minimal confusion. The paper we chose has shown to be reproducible to an extent. We were able to replicate the experiments proposed in the paper as well as our ablations, but our results varied. One major reason for this was likely due to the sampling methods we introduced, as we reduced the size of our training data sets in order to be able to train our models in a suitable amount of time for this project. Our dataset was not as diverse, as it was almost 1:1 HPV to Cancer. Other discepencies were likely because in the original author's Github model, they chose to continue their local explainability experiments with the Neural Network model, even though the Random Forest Classifier performed better. We corrected this in our reproduction. Additionally, we we were able to display the TI contribution, which was unsuccessful in the source code. We ran only a set of the results against a subset of the source data variations, as we believe this is suitable to compare.

During the reproduction, moving the data to adapt to our local enviroments in a shareable format was initially difficult, but ultimateley possible. Processsing data was also hard, as the data set needed reformatting to work correctly with some models. Transferring the code and adding ablations was successful because of the heavily commented and organized code that could be split into many sections. Descriptions for the 4 types of train/test data sets would have been helpful in understanding the training function and levels. In addition, in order to make this paper more easy to reproduce, we would suggest adding checkpoints to the program as well as providing more documentation regarding data cleaning.

References

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