## **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: <a href="https://github.com/LoganB99/DL4H-SP24-Local-Explanations-For-Cervical-Cancer">https://github.com/LoganB99/DL4H-SP24-Local-Explanations-For-Cervical-Cancer</a>

Our video overview can be accessed here:

https://drive.google.com/file/d/1VbnpcCaYxyATlkzQZPA5bLop64rc6XSg/view?usp=sharing

# Mount Notebook to Google Drive

To clear up clutter, the original FAQ and Attentions are in <a href="https://colab.research.google.com/drive/1MGxB\_J2TvhAANcQG8VNMvQp1QdQrcxWb?authuser=1">https://colab.research.google.com/drive/1MGxB\_J2TvhAANcQG8VNMvQp1QdQrcxWb?authuser=1</a>

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```
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```

## 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
```

```
# 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 stratified from sklearn.preprocessing import RobustScaler, StandardScaler # Data scaling method 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 metr from sklearn.metrics import precision\_recall\_fscore\_support # Precision, recall, and 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 mod
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 Colimport warnings # For controlling warning messages

warnings.filterwarnings('ignore') # Suppress warning messages for cleaner output
# Plotly setup for notebooks

from plotly offline import plot inlot 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: <a href="https://drive.google.com/uc?id=11swC5N9lqEVTp3E-K1dtBrlHQEoEkxtk">https://drive.google.com/uc?id=11swC5N9lqEVTp3E-K1dtBrlHQEoEkxtk</a>

To: /content/project files.tgz

100% | 10.5M/10.5M [00:00<00:00, 68.0MB/s]

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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. <a href="https://archive.ics.uci.edu/dataset/383/cervical+cancer+risk+factors">https://archive.ics.uci.edu/dataset/383/cervical+cancer+risk+factors</a>

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

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_cervical_
    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_b4'
    raw_risk_factor_df = load_data('DL4H_Sp24_Final_Project/risk_factors_cervical_cancer.csv')
# https://drive.google.com/drive/folders/1AUr8BgW16UU-7XjFf8077XAgjA27gISV?usp=shar.com_risk_factor_df
```

```
# 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 for
    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: {max
  dataset size = df.shape[0] * df.shape[1]
  print(100 * df.applymap(lambda x: x == "?").sum().sum()/dataset_size, " percent o
  # 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().i"
  print("dtypes:", formatted_summary)
```

```
# NOTE: this is a deviation from the source code. In the source code, category perce
# summed up to 100 across the diagnosis, we also wanted to show the percent for each
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 information
    - category column (str): The name of the column containing category labels (e.g.
    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='0verall_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 category
    category_percentages['Category_Percent'] = category_percentages['Count_in_Category_percentages]
        .div(category_percentages['Total_in_Category']) \
        .mul(100) \
        round(decimals=4)
    # Count occurrences of each diagnosis and calculate the percentage within the di
    diagnosis counts and percentages = pd.merge(
        df.groupby([diagnosis column, category column]).size().reset index(name='Inc
        df.groupby(diagnosis_column).size().reset_index(name='Total_in_Diagnosis'),
        on=diagnosis column
    )
    diagnosis counts and percentages['Diagnosis Percent'] = diagnosis counts and pe
        .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_Percent']
                          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, 'Diagnosis_column, '
                          on=[diagnosis column, category column]
             )
             # Create a pivot table for better presentation.
             final pivot table = final merged.pivot(index=category column, columns=diagnosis
             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_fa
                          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', 'Num 
                    'Smokes (years)', 'Smokes (packs/year)', 'Hormonal Contraceptive
                    'Hormonal Contraceptives (years)', 'IUD', 'IUD (years)', 'STDs'
                    'STDs:condylomatosis', 'STDs:cervical condylomatosis', 'STDs:vag
                    'STDs:vulvo-perineal condylomatosis', 'STDs:syphilis', 'STDs:pe
                    'STDs:genital herpes', 'STDs:molluscum contagiosum', 'STDs:AIDS
                    '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, errors:
  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

```
# 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/processed
save_data(std_agg, '/content/drive/My Drive/DL4H_Sp24_Final_Project/processed_std_agg)
```

Save checkpoint granted Save checkpoint granted

Checkpoint: Load Processed Data

root

```
try:
  data_dir = '/content/drive/My Drive/DL4H_Sp24_Final_Project/processed_risk_factors
  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.csv
  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-zTy0pjToeWmetQFrbZ4YKFjfZ0
  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/110iEdMjfYzcMtZNh1jIWQJlIOw4iEbl
  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
                                            1
                                                                       1
                 20's
                              45.3380 0.5828
                                                       98.7310
                                                                  1.2690 \
                              24.7086 0.9324
                                                                  3.6364
    1
                 30's
                                                       96.3636
    2
                 40's
                               6.1772 0.3497
                                                       94.6429
                                                                5.3571
    3
                                                       80.0000 20.0000
                 50's
                               0.4662 0.1166
    4
                 70+
                               0.4662 0.0000
                                                      100.0000
                                                                  0.0000
    5
                 Teen
                              20.7459 0.1166
                                                       99.4413
                                                                  0.5587
              Diagnosis_Percent
    Dx:Cancer
                        46.3095 27.7778
    0
    1
                        25.2381
                                 44.4444
    2
                         6.3095
                                 16.6667
```

5.5556

0.4762

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
                                 # Adding row names here
                y=corr.index)
# Update layout with title
fig.update_layout(title="Top "+str(n)+" Features Correlated With "+str(target).capi
fig.update xaxes(showgrid=False)
fig.update_yaxes(showgrid=False)
# Show plot
fig.show()
```

## → Distribution of age

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

## Pregnancy Distribution by Age

## ✓ 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.

```
# 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 and diagnoses_heatmap = px.imshow(diagnoses_corr_matrix, aspect="auto", color_continuous # 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 add .
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 ground 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", "Forties' "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 partners #show plot
age_num_sex_partners.show()
```

#### ✓ Tests used

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

```
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(ris
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_sequence
fig.show()
proportion_samples_df
```

Contraceptive

```
df_IUD_contraceptives = risk_factor_df[(risk_factor_df["Hormonal Contraceptives"] =:
df_IUD_contraceptives = df_IUD_contraceptives.sort_values(by=["Smokes", label], asce
fig = px.histogram(df_IUD_contraceptives, x="age_cat", color="Smokes", barmode="ground 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="grocolor_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 and fig.show()
```

#### ✓ ADASYN

with open('summary.tex','w') as tf:

test=risk\_factor\_df[['Number of sexual partners', 'First sexual intercourse', 'Nur

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/balanced_
Save checkpoint granted
```

#### Checkpoint: Load Balanced data

```
try:
  data dir = '/content/drive/My Drive/DL4H Sp24 Final Project/balanced risk factors
  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/1-4EiqdYBbae16azaiZry7Gwhpq7Xhwl
  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=4%)
for train idx, test idx in unbalanced split.split(unbalanced risk factor df, unbalanced risk factor df, unbalanced split.split(unbalanced risk factor df, unbalanced risk factor df, un
         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("Y_test 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 Score"
# 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 variab
unbalanced estimators = [
    ("UnbalancedLogisticRegression", unbalanced_logreg_cv),
    ("UnbalancedRandomForestClassifier", unbalanced_rnd_clf),
    ("UnbalancedKNeighborsClassifier", unbalanced_knn_clf_cv),
    ("UnbalancedSupportVectorClassifier", unbalanced_svm_clf_cv),
    ("UnbalancedMLPClassifier", unbalanced_nn_clf)
    1
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 variab
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 coefficient) 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 cla
    print("Training ", unbalanced_clf_name)
    unbalanced_clf.fit(unbalanced_X_train, unbalanced_y_train) # Train the classif:
    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
    Training UnbalancedMLPClassifier
```

## Balanced Training

```
for i in range(len(estimators)):
    clf_name, clf = estimators[i] # Unpack the classifier name and the classifier operint("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/1-4D7VkQ4qewUnyrzPw1izMk9WjMvQ13D,
# gdown.download('https://drive.google.com/file/d/1-94qCsT0VdS-Cv0237Z0TeUWCouKDeyl,
# # RandomForestClassifier
unbalanced_models[1] = root +'/UnbalancedRandomForestClassifier.pkl'
balanced_models[1] = root +'/RandomForestClassifier.pkl'
# gdown.download('https://drive.google.com/file/d/1-PBTxxalNfXQNKpX8Bg9ojFRtPGEsvbw,
# gdown.download('https://drive.google.com/file/d/1-Qdk5tk2RCLhbfVW400S2qBI6ikStRBh,
# # KNeighborsClassifier
unbalanced_models[2] = root +'/UnbalancedKNeighborsClassifier.pkl'
balanced_models[2] = root +'/KNeighborsClassifier.pkl'
# gdown.download('https://drive.google.com/file/d/1-Rg4cRA6NdtPeHPFnablplZ0T7e323Qg,
# gdown.download('https://drive.google.com/file/d/1-TKog0oufiDcfCJtv_gQdYTiw1rK6VkN,
# # SupportVectorClassifier
unbalanced_models[3] = root +'/UnbalancedSupportVectorClassifier.pkl'
balanced_models[3] = root +'/SupportVectorClassifier.pkl'
# gdown.download('https://drive.google.com/file/d/1_g0BZHdpuPP9xlj0jKWJ-8fVZe4sTPkA,
# gdown.download('https://drive.google.com/file/d/1-3sNvATHD55evt_9nSzf3nBP6XWLknjL,
# # MLPClassifier
unbalanced_models[4] = root +'/UnbalancedMLPClassifier.pkl'
balanced_models[4] = root +'/MLPClassifier.pkl'
# gdown.download('https://drive.google.com/file/d/1-3P6L-WKDrfMNgwp372f3vgY9Px0SEIm,
# gdown.download('https://drive.google.com/file/d/1-DmdcIFHJFKUtAhhVW1XbVlwbfj0pWS2,
```

#### 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 the '
    # Calculate the AUROC score and append it to the roc list
    unbalanced_roc.append(roc_auc_score(unbalanced_y_test, unbalanced_y_pred, average
    # 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_pred))
    # Calculate precision, recall, and F1 scores and append them to their respective
    unbalanced scores = precision recall fscore support(unbalanced y test, unbalance
    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, unbalanced
# 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 respective
    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 tl
```

#### Unbalanced comparison

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

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

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 outcomes 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 consequences 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[0]
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.csv
#modified below to replicate above filename
risk\_factor\_df=pd.read\_csv('/content/drive/My Drive/DL4H\_Sp24\_Final\_Project/Rcancer2.

risk\_factor\_df

Checkpoint: Get Original

```
# X_test=pd.read_csv(gdown.download('https://drive.google.com/file/d/1ggTvbeS9kerpV'
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/1WsUWr09Nwpd6K,
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/1OnCY70gXQbT3:
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/1C5euZUKZ6GLel
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 independed # from a Bernoulli distribution where the probability of a 1 is 0.5 (i.e., a fair condition to the same distribution where the probability of a 1 is 0.5 (i.e., a fair condition to the training dataset)

# 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 dataset
    # 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 datase:
# 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_zgc'
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/1cNtkdYal
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/13SUdzZonaise_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/1rVKdQal
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.csv'
y_train.to_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/Binary_y_train.csv'
```

## 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.csv')
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.csv')
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.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)

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.cs' y\_test.to\_csv('/content/drive/My Drive/DL4H\_Sp24\_Final\_Project/Continuous\_y\_test.cs' X\_train.to\_csv('/content/drive/My Drive/DL4H\_Sp24\_Final\_Project/Continuous\_X\_train.csv('/content/drive/My Drive/DL4H\_Sp24\_Final\_Project/Continuous\_y\_train.csv('/content/drive/My Drive/DL4H\_Sp24\_Final\_Project/Content/drive/My Drive/DL4H\_Sp24\_Final\_Project/Content/drive/My Drive/DL4H\_Sp24\_Final\_Project/Content/drive/My Drive/DL4H\_Sp24\_Final\_Project/Content/drive/My Drive/DL4H\_Sp24\_Final\_Project/Content/drive/My Drive/DL4H\_Sp24\_Final\_Project/Content/drive/My Drive/DL4H\_Sp24\_Final\_Project/Content/drive/My Drive/DL4H\_Sp24\_Final\_Project/Content/drive/My Drive/DL4H\_Sp24\_Final\_Project/Content/drive/My Drive/DL4H\_Sp24\_Final\_Project/Content/drive/DL4H\_Sp

#### 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.csv'
Continuous_X_train = pd.read_csv(root+'/Continuous_X_train.csv')
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.csv'
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 con
  # This DataFrame uses the same structure and column names as X test.
  GloSur = kernelSHAP = treeSHAP = samplingSHAP = limecontrib = ticontrib = dicecon
      pd.DataFrame([[0.0] * X test.shape[1]] * X test.shape[0], columns=X test.columnum.
  # Initialize dictionaries to store feature importances from different explainers.
  fi 1 = fi 2 = fi 3 = fi 4 = fi 5 = fi 6 = fi 7 = \{f'\{x\}': 0.0 \text{ for } x \text{ in } X \text{ test.col}\}
  # 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 approximate
  explainer = MimicExplainer(model,
                            X train.
                            LinearExplainableModel,
                             augment data=False, # Do not augment data; use the orio
                             features=features, # List of features to explain.
                            model_task="classification") # Task type (classification)
  # 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 DataF
  temp = pd.DataFrame(global explanation.local importance values[1], columns=feature
  # Update the GloSur DataFrame with new importance values, adding to existing value
  GloSur = GloSur.add(temp, fill value=0)
  # Reset the results dictionary and retrieve feature importance as a dictionary from
  res = dict()
  res = global explanation.get feature importance dict()
  # Update fi_1 dictionary with aggregated feature importances, combining existing \
  fi 1 = \{k: fi 1.qet(k, 0) + res.qet(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 pe
# Step 3: Calculate SHAP values
shap values = explainer.shap values(X test)
# Convert SHAP values to DataFrame for easier manipulation (assuming binary class:
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.co
# Update or initialize feature importances
fi_2 = \{k: fi_2.get(k, 0) + res.get(k, 0) \text{ for } k \text{ 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 samplingSHAI
fi_4 = \{k: fi_4.get(k, 0) + res.get(k, 0) \text{ for } k \text{ in } set(fi_4)\}
fi 4
## LIME
print("-LIME-")
# LIME
explainer = lime.lime tabular.LimeTabularExplainer(X train.values,mode='classific
all=[]
for i in range (len(X test)):
  exp = explainer.explain_instance(X_test.iloc[i], model.predict_proba, num_featu
  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) \text{ for } k \text{ 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 contribution
    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.index
fi 6 = \{k: fi 6.qet(k, 0) + res.qet(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':
```

```
DL4H_Team_11 - Colab
  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, outcome_
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_rail
                                   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) \text{ for } k \text{ in } set(fi_7)\}
fi_7
GloSur.to_csv(f"/content/drive/My Drive/DL4H_Sp24_Final_Project/{mode}_glosur.csv'
kernelSHAP.to_csv(f"/content/drive/My Drive/DL4H_Sp24_Final_Project/{mode}_Kshap.u
treeSHAP.to csv(f"/content/drive/My Drive/DL4H Sp24 Final Project/{mode} Tshap.cs<sup>1</sup>
samplingSHAP.to_csv(f"/content/drive/My Drive/DL4H_Sp24_Final_Project/{mode}_Sshap
limecontrib.to csv(f"/content/drive/My Drive/DL4H Sp24 Final Project/{mode} lime...
ticontrib.to_csv(f"/content/drive/My Drive/DL4H_Sp24_Final_Project/{mode}_ti.csv"
dicecontrib.to_csv(f"/content/drive/My Drive/DL4H_Sp24_Final_Project/{mode}_dice.
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)

dics.append(fi\_7)

fi\_7['Method'] = 'DICE'

dics = pd.DataFrame(dics)
methods=dics['Method']
dics['Method']=methods

```
dics.to_csv(f"/content/drive/My Drive/DL4H_Sp24_Final_Project/{mode}_localExplain/
  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 contribution
  # 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/{mod
  file path = f"/content/drive/My Drive/DL4H Sp24 Final Project/{mode} localExplainMe
  # 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}")

Explainers commented outed for time

# Continuous (Done)

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

## 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_t
```

# 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_train,
```

# run\_explainers\_ti('Original', rnd\_clf, X\_train, X\_test, y\_train, y\_test)

### Rerun TI

```
# run_explainers_ti('Continuous', continuous_rnd_clf, Continuous_X_train, Continuous
# run_explainers_ti('Binary', binary_rnd_clf, Binary_X_train, Binary_X_test, Binary_
# run_explainers_ti('Noise', noise_rnd_clf, Noise_X_train, Noise_X_test, Noise_y_tra

    starting Original
    Updated the TI method in /content/drive/My Drive/DL4H_Sp24_Final_Project/Original
    starting Continuous
    Updated the TI method in /content/drive/My Drive/DL4H_Sp24_Final_Project/Continustanting Binary
    Updated the TI method in /content/drive/My Drive/DL4H_Sp24_Final_Project/Binary
    starting Noise
    Updated the TI method in /content/drive/My Drive/DL4H_Sp24_Final_Project/Noise_1
```

## 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/Noise kercontrib_noise = pd.read_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/Noise samcontrib_noise = pd.read_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/Noise trecontrib_noise = pd.read_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/Noise limecontrib_noise = pd.read_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/Noise ticontrib_noise = pd.read_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/Noise dicecontrib_noise = pd.read_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/Noise all_fi_noise = pd.read_csv('/content/drive/My Drive/DL4H_Sp24_Final_Project/Noise_left)
```

## Continuous contributions

#### **#VAR** continue

gscontrib\_continuous = pd.read\_csv('/content/drive/My Drive/DL4H\_Sp24\_Final\_Project, kercontrib\_continuous = pd.read\_csv('/content/drive/My Drive/DL4H\_Sp24\_Final\_Project samcontrib\_continuous = pd.read\_csv('/content/drive/My Drive/DL4H\_Sp24\_Final\_Project trecontrib\_continuous = pd.read\_csv('/content/drive/My Drive/DL4H\_Sp24\_Final\_Project limecontrib\_continuous = pd.read\_csv('/content/drive/My Drive/DL4H\_Sp24\_Final\_Project ticontrib\_continuous = pd.read\_csv('/content/drive/My Drive/DL4H\_Sp24\_Final\_Project, dicecontrib\_continuous = pd.read\_csv('/content/drive/My Drive/DL4H\_Sp24\_Final\_Project all\_fi\_continuous = pd.read\_csv('/content/drive/My Drive/DL4H\_Sp24\_Final\_Project/Content/drive/My Drive/DL4H\_Sp24\_Final\_Project/Content/Drive/DL4H\_Sp24\_Final\_Project/Content/Drive/DL4H\_Sp24\_Final\_Project/Content/Drive/DL4H\_Sp24\_Final\_Project/Content/Drive/DL4H\_Sp24\_Final\_Project/Content/Drive/DL4H\_Sp24\_Final\_Project/Content/Drive/DL4H\_Sp24\_Final\_Project/Content/Drive/DL4H\_Sp24\_Final\_Project/Content/Drive/DL4H\_Sp24\_Final\_Project/Content/Drive/DL4H\_Sp24\_Final\_Project/Content/Drive/DL4H\_Sp24\_Final\_Project/C

## Binary Contributions

#### **#VAR** binary

gscontrib\_binary = pd.read\_csv('/content/drive/My Drive/DL4H\_Sp24\_Final\_Project/Binkercontrib\_binary = pd.read\_csv

# 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, dicc
#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)
dicecontrib_norm=dicecontrib.div(dicecontrib.sum(axis=1), axis=0)
```

# #One Instance risk\_factor\_df.describe().iloc[1]

A	20 275075
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_instance
one_instance
```

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

# Initialize a LIME Explainer for tabular data, specifying the training dataset, the explainer = lime.lime\_tabular.LimeTabularExplainer(X\_train.values, mode='classifica'

# Explain the prediction of a specific instance from the test dataset using the transexp = explainer.explain\_instance(X\_test.iloc[instance], model.predict\_proba, num\_feature.explain\_instance(X\_test.iloc[instance], model.predict\_proba, num\_feature.explain\_instance(X\_test.iloc(instance), num\_feature.explain\_instance(X\_test.iloc(instance), num\_feature.explain\_instance

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)+'surrogate
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)+'kernelSH/
```

```
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)+'treeSHAP
```

```
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)
```

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

```
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'+st
```

```
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'+str()
```

```
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'+st
```

# 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 need:
            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 availal
                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']} fo
    # 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 intercours' Testing Features: ['Age', 'Number of sexual partners', 'First sexual intercours' INFO: Shap explainer type — <shap.explainers.\_tree.TreeExplainer object at 0x7f(INFO: Shap explainer type — <shap.explainer object at 0x7f(INFO: Shap explainer object at 0x7f(INFO: Sh

img=xpl.plot.contribution\_plot(0)
img.show()

# img.write\_image('/content/drive/My Drive/DL4H\_Sp24\_Final\_Project/contribage.png')

img.show()

```
5/5/24, 10:38 PM
                                               DL4H_Team_11 - Colab
    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/contribagekernel
    xpl = SmartExplainer(model=model)
    xpl.compile(x=X_test,contributions=samcontrib)
    img=xpl.plot.contribution_plot(0)
```

# img.write\_image('/content/drive/My Drive/DL4H\_Sp24\_Final\_Project/contribagesampli)

```
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.pu

```
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.pu

```
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.png

```
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/contribageGlosur

```
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.pu
```

```
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')
```

```
# 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]</pre>
    contributions = contributions.loc[selection].values
    top features = np.array([sorted(row, key=abs, reverse=True) for row in contribu-
    output ton features - nn sum(ton features[: :1 avis-1)
compacities=[]
for weight in weights:
  rr=compute_features_compacity(case="classification", contributions=weight, select:
  #rr=compute features compacity(case="classification", contributions=weight, selec
  compacities.append(pd.DataFrame.from_dict(rr))
    ICCUITE GESCUICC
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)
```

l- -- - I -