# Breast cancer prediction report

January 27, 2025

# 1 Preface

The objective of this notebook is to provide detailed visual and descriptive overiew of the dataset as well as prepare for Machine Learning modelling. Comments are added to each output in a form of explanation/key insights.

# 2 Data information and requirements

The dataset contains 166 observations of anthropometric measurements and blood analysis indicators of women being tested for detecting breast cancer. Each row represents a distinct patient observation. The data is obtained from an open access journal website for cancer research (reference:https://www.biomedcentral.com/). There is a total of 9 features and 1 target variable which are described below:

- Age age of the patient
- BMI a proportion of the weight (kg) and the squared height(m)
- Glucose- an important energy source and a component of many carbohydrates. Measure unit: mmol/L (millimoles per litre)
- Insulin- a pancreas produced hormone which regulates the amount of glucose in the blood. Measure unit : Insulin Units -100 IU - 1 ml.
- Resistin known as Adipose tissue-specific secretory factor (ADSF) specific cysteine-rich peptide hormone derived from adipose tissue.
- Adiponectin a protein hormone which regulates the glucose levels.
- MCP small cytokine that recruits monocytes, dendritic cells to the inflammation sites that are produced by tissue injury/infection.
- HOMA indicator of insulin resistance

The target variable has two values (1,2).1 indicates that the patient is diseased and 2 indicates the patient is healthy.

```
[1]: import pandas as pd
  import numpy as np
  import seaborn as sns
  import statsmodels.api as sm
  from sklearn.preprocessing import StandardScaler as sc
  from statsmodels.stats.outliers_influence import variance_inflation_factor
  from sklearn.decomposition import PCA
  import matplotlib.pyplot as plt
```

```
from sklearn.cluster import KMeans
from sklearn.linear_model import LogisticRegression
from statsmodels.discrete.discrete_model import Logit
from scipy.stats import shapiro
from sklearn.metrics import classification_report
from sklearn.metrics import accuracy_score,confusion_matrix
from matplotlib import pyplot
from sklearn.model_selection import KFold
from scipy.stats import loguniform
from sklearn.model_selection import GridSearchCV
from sklearn.svm import SVC
from sklearn.model_selection import learning_curve
from sklearn.model_selection import LeaveOneOut
from sklearn.model_selection import cross_val_score
```

# 3 Data info

```
[2]: breast_cancer=pd.read_excel('dataR2.xlsx')
[3]: breast_cancer
[3]:
          Age
                     BMI
                          Glucose
                                    Insulin
                                                 AMOH
                                                        Leptin Adiponectin \
                                             0.467409
     0
           48
               23.500000
                                70
                                      2.707
                                                        8.8071
                                                                    9.702400
     1
           83
              20.690495
                                92
                                      3.115
                                            0.706897
                                                        8.8438
                                                                    5.429285
     2
           82
               23.124670
                                91
                                      4.498
                                            1.009651 17.9393
                                                                   22.432040
                               77
     3
                                      3.226
           68
               21.367521
                                             0.612725
                                                        9.8827
                                                                    7.169560
     4
                                92
                                      3.549
                                             0.805386
                                                        6.6994
                                                                    4.819240
           86
               21.111111
     111
           45
               26.850000
                                92
                                      3.330 0.755688
                                                       54.6800
                                                                   12.100000
     112
               26.840000
                               100
                                      4.530 1.117400
                                                       12.4500
                                                                   21.420000
           62
     113
           65
               32.050000
                               97
                                      5.730
                                            1.370998
                                                       61.4800
                                                                   22.540000
     114
           72
               25.590000
                                82
                                      2.820
                                             0.570392
                                                       24.9600
                                                                   33.750000
     115
           86
              27.180000
                               138
                                     19.910 6.777364 90.2800
                                                                   14.110000
          Resistin
                      MCP.1 Classification
     0
           7.99585
                    417.114
     1
           4.06405 468.786
           9.27715
                    554.697
                                           1
     3
          12.76600
                    928.220
                                           1
          10.57635
                    773.920
                                           1
                                           2
     111 10.96000
                    268.230
                                           2
     112
          7.32000
                    330.160
                                           2
     113 10.33000
                    314.050
     114
          3.27000
                    392,460
                                           2
     115
          4.35000
                     90.090
```

## [116 rows x 10 columns]

It is worth to mention that there are no missing values.

## [4]: breast\_cancer.info()

<class 'pandas.core.frame.DataFrame'>
RangeIndex: 116 entries, 0 to 115
Data columns (total 10 columns):

#	Column	Non-Null Count	Dtype
0	Age	116 non-null	int64
1	BMI	116 non-null	float64
2	Glucose	116 non-null	int64
3	Insulin	116 non-null	float64
4	HOMA	116 non-null	float64
5	Leptin	116 non-null	float64
6	Adiponectin	116 non-null	float64
7	Resistin	116 non-null	float64
8	MCP.1	116 non-null	float64
9	Classification	116 non-null	int64

dtypes: float64(7), int64(3)

memory usage: 9.2 KB

The descriptive statistics per variable give meaningful overview of how the values are distributed. The min, max and mean values are important if we don't have specific knowledge for some variable scale.

## [5]: breast\_cancer.describe()

[5]:		Age	BMI	Glucose	Insulin	HOMA	Leptin	\
	count	116.000000	116.000000	116.000000	116.000000	116.000000	116.000000	
	mean	57.301724	27.582111	97.793103	10.012086	2.694988	26.615080	
	std	16.112766	5.020136	22.525162	10.067768	3.642043	19.183294	
	min	24.000000	18.370000	60.000000	2.432000	0.467409	4.311000	
	25%	45.000000	22.973205	85.750000	4.359250	0.917966	12.313675	
	50%	56.000000	27.662416	92.000000	5.924500	1.380939	20.271000	
	75%	71.000000	31.241442	102.000000	11.189250	2.857787	37.378300	
	max	89.000000	38.578759	201.000000	58.460000	25.050342	90.280000	
		Adiponectin	Resistin	MCP.1	Classific	ation		
	count	116.000000	116.000000	116.000000	116.0	00000		
	mean	10.180874	14.725966	534.647000	1.5	51724		
	std	6.843341	12.390646	345.912663	0.4	99475		
	min	1.656020	3.210000	45.843000	1.0	00000		
	25%	5.474283	6.881763	269.978250	1.0	00000		
	50%	8.352692	10.827740	471.322500	2.0	00000		
	75%	11.815970	17.755207	700.085000	2.0	00000		

# 4 Data exploration

# 4.0.1 Overview of target variable (# of patients per category)

The target variable which will be predicted as already mentioned can take two values.Let's see how many patients there are per category:

```
[6]: disease_group=breast_cancer.groupby('Classification').size()
      disease group=disease group.to frame()
      disease group=disease group.reset index()
 [7]: disease_group.rename(columns = {0:'count_per_category'}, inplace = True)
 [8]:
      disease_group
 [8]:
         Classification
                          count_per_category
                       1
      0
                                           52
      1
                                           64
 [9]: #window function would be useful here, but seems like they are not that powerful
      breast cancer=breast cancer.merge(disease group,on='Classification')
[10]: breast_cancer
[10]:
           Age
                       BMI
                            Glucose
                                      Insulin
                                                    AMOH
                                                           Leptin
                                                                   Adiponectin \
                                                           8.8071
                                                                       9.702400
      0
            48
                23.500000
                                 70
                                        2.707
                                               0.467409
      1
            83
                20.690495
                                 92
                                        3.115
                                               0.706897
                                                           8.8438
                                                                       5.429285
      2
            82
                23.124670
                                 91
                                        4.498
                                               1.009651
                                                          17.9393
                                                                      22.432040
      3
            68
                21.367521
                                 77
                                        3.226
                                               0.612725
                                                           9.8827
                                                                       7.169560
      4
            86
                                 92
                                                           6.6994
                21.111111
                                        3.549
                                               0.805386
                                                                       4.819240
            45
                26.850000
                                 92
                                        3.330
                                               0.755688
                                                                      12.100000
      111
                                                          54.6800
      112
            62
                26.840000
                                 100
                                        4.530
                                               1.117400
                                                          12.4500
                                                                      21.420000
      113
            65
                32.050000
                                 97
                                        5.730
                                               1.370998
                                                          61.4800
                                                                      22.540000
      114
            72
                                 82
                                               0.570392
                                                          24.9600
                25.590000
                                        2.820
                                                                      33.750000
      115
            86
                27.180000
                                 138
                                       19.910
                                               6.777364
                                                          90.2800
                                                                      14.110000
           Resistin
                        MCP.1
                               Classification
                                                count_per_category
      0
            7.99585
                      417.114
                                             1
                                                                  52
            4.06405
      1
                      468.786
                                             1
                                                                  52
                                                                  52
      2
            9.27715
                      554.697
                                             1
           12.76600
      3
                      928.220
                                             1
                                                                  52
      4
           10.57635
                      773.920
                                             1
                                                                  52
                                             2
                                                                  64
      111
           10.96000
                      268.230
```

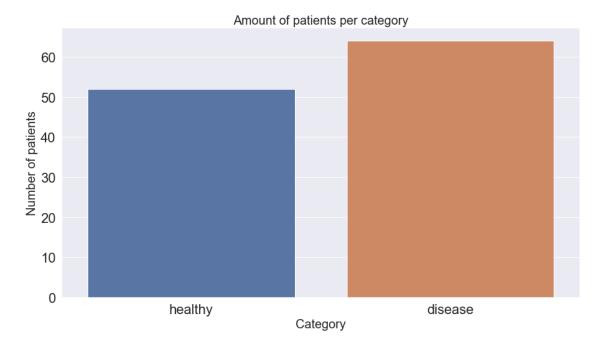
112	7.32000	330.160	2	64
113	10.33000	314.050	2	64
114	3.27000	392.460	2	64
115	4.35000	90.090	2	64

[11]: breast\_cancer['Classification\_cat']=breast\_cancer['Classification']

[116 rows x 11 columns]

Creating additional Classification categorical variable (with purpose to ease the visualization)

[13]: Text(0.5, 1.0, 'Amount of patients per category')



#### 4.0.2 Exploring the anthropometric measurements (BMI)

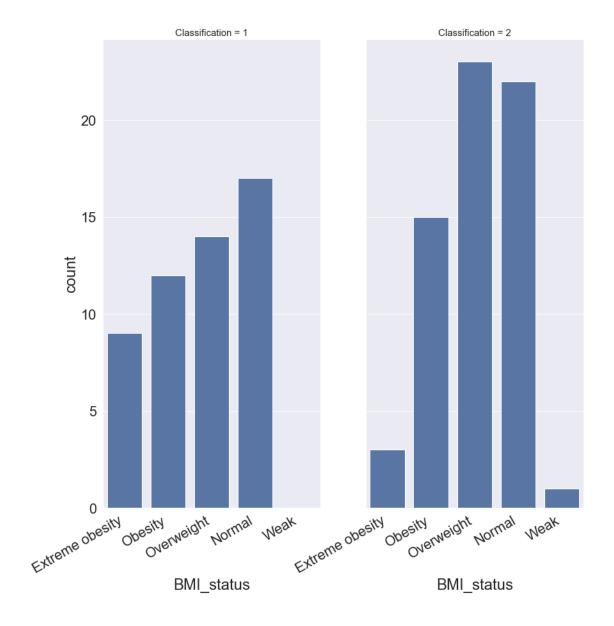
Creating variable that will categorise the patients by their BMI:

```
[14]: breast_cancer['BMI_status'] = 'zzz'
      breast_cancer.loc[(breast_cancer['BMI']>16) & (breast_cancer['BMI']<18.</pre>
       ⇔5),'BMI_status'] = 'Weak'
      breast_cancer.loc[(breast_cancer['BMI']>18.5) & (breast_cancer['BMI']<24.

¬9), 'BMI_status'] = 'Normal'

      breast_cancer.loc[(breast_cancer['BMI']>25) & (breast_cancer['BMI']<29.
       breast_cancer.loc[(breast_cancer['BMI']>30) & (breast_cancer['BMI']<34.</pre>
       ⇔9), 'BMI_status'] = 'Obesity'
      breast_cancer.loc[(breast_cancer['BMI']>34.9),'BMI_status'] = 'Extreme obesity'
[15]: count=breast_cancer.groupby(['BMI_status', 'Classification']).size()
      count=count.reset_index()
[16]: count.rename(columns = {0:'count'}, inplace = True)
[17]: count
[17]:
             BMI_status Classification count
      O Extreme obesity
                                              9
                                       1
      1 Extreme obesity
                                       2
                                              3
      2
                 Normal
                                       1
                                             17
      3
                 Normal
                                       2
                                             22
      4
                 Obesity
                                       1
                                             12
      5
                 Obesity
                                       2
                                             15
      6
             Overweight
                                       1
                                             14
      7
             Overweight
                                             23
      8
                    Weak
                                       2
                                              1
[18]: sns.set(rc = {'figure.figsize':(15,8)},font_scale=2)
      g=sns.FacetGrid(count, col='Classification', height=12, aspect=.5)
      g.map(sns.barplot, 'BMI_status', 'count', order=['Extreme_
      ⇔obesity','Obesity','Overweight','Normal','Weak'])
      g.set titles(size=15)
      g.set_xticklabels(rotation=30, horizontalalignment='right')
```

[18]: <seaborn.axisgrid.FacetGrid at 0x1bc8f561bb0>



More healthy people are categorised as 'Overweight', whereas the BMI status of diseased people (Category=1) is Normal, which means that Obesity is not an influence factor here.

# 5 Data preparation

# 5.0.1 Comparison of the univariate analysis per category. Checking for multicollinearity using Variance Inflation Factor.

The following univariate overview will provide information of how the measurements are distributed per category with the goal to see if there is significant difference between the variable values for each category. The goal of doing this: \* checking the significancy of each variable and forming hypothesis \* dropping the insignificant variables who doesn't represent the variance in the dataset or they exhibit multicollinearity with other variables is cruicalIn this case, the null hypothesis would

be: \* The variables are statistically significant and represent the variance in the data and they don't exhibit any multicollinearity. To reject the null hypothesis, the statistic tool applied is The Variance Inflation Factor (VIF) - a measure of colinearity among predictor variables within a multiple regression. It is calculated by taking the the ratio of the variance of all a given model's betas divide by the variance of a single beta if it were fit alone.

Let's first explore the univariate overview per category.

```
[19]: breast_cancer[breast_cancer['Classification']==1].describe()
      #titanic[titanic["Age"] > 35
[19]:
                                BMI
                                        Glucose
                                                    Insulin
                                                                   AMOH
                                                                            Leptin
                    Age
      count
             52.000000
                         52.000000
                                      52.000000
                                                  52.000000
                                                             52.000000
                                                                         52.000000
      mean
             58.076923
                         28.317336
                                      88.230769
                                                   6.933769
                                                               1.552398
                                                                         26.637933
                                                                         19.334699
                          5.427465
                                                   4.859793
      std
             18.957999
                                      10.191529
                                                               1.218256
      min
             24.000000
                         18.670000
                                      60.000000
                                                   2.707000
                                                               0.467409
                                                                          4.311000
      25%
             41.750000
                         23.096003
                                      82.750000
                                                   4.304000
                                                              0.879510
                                                                         11.845750
      50%
             65.000000
                         27.694389
                                      87.000000
                                                   5.483500
                                                               1.139683
                                                                         21.494850
                                                                         36.721600
      75%
             75.000000
                         32.328091
                                      93.250000
                                                   7.001000
                                                               1.774561
             89.000000
                                                  26.211000
                                                               7.111918
                                                                         83.482100
      max
                         38.578759
                                     118.000000
             Adiponectin
                            Resistin
                                                     Classification
                                                                      count_per_category
                                             MCP.1
               52.000000
                           52.000000
                                         52.000000
                                                                52.0
                                                                                     52.0
      count
      mean
                10.328205
                           11.614813
                                        499.730692
                                                                 1.0
                                                                                     52.0
                 7.631281
                           11.447053
                                        292.242157
                                                                 0.0
                                                                                      0.0
      std
      min
                 2.194280
                            3.291750
                                         45.843000
                                                                 1.0
                                                                                     52.0
      25%
                 5.454286
                            6.597523
                                        260.736500
                                                                 1.0
                                                                                     52.0
      50%
                 8.127775
                            8.929190
                                                                                     52.0
                                        471.322500
                                                                 1.0
      75%
               10.820219
                           12.808525
                                        642.933500
                                                                 1.0
                                                                                     52.0
               38.040000
                           82.100000
                                       1256.083000
                                                                                     52.0
      max
                                                                 1.0
[20]: breast cancer[breast cancer['Classification']==2].describe()
      #titanic[titanic["Age"] > 35
[20]:
                    Age
                                                                           Leptin
                                BMI
                                       Glucose
                                                   Insulin
                                                                  HOMA
                                                            64.000000
                                                                        64.000000
      count
             64.000000
                         64.000000
                                      64.00000
                                                 64.000000
             56.671875
                         26.984740
                                     105.56250
                                                 12.513219
                                                                        26.596512
      mean
                                                             3.623342
      std
             13.493155
                          4.620398
                                      26.55744
                                                 12.317738
                                                             4.588943
                                                                        19.212451
             34.000000
                         18.370000
                                      70.00000
                                                  2.432000
                                                             0.507936
                                                                         6.333900
      min
      25%
             45.000000
                         22.788722
                                      92.00000
                                                  4.406000
                                                              1.036842
                                                                        12.402925
      50%
                                      98.50000
             53.000000
                         27.408027
                                                  7.580000
                                                              2.052256
                                                                        18.877650
      75%
             68.000000
                         30.810069
                                     109.00000
                                                 16.063000
                                                              4.461312
                                                                        37.378300
      max
             86.000000
                         37.109375
                                     201.00000
                                                 58.460000
                                                            25.050342
                                                                        90.280000
             Adiponectin
                            Resistin
                                             MCP.1
                                                     Classification
                                                                      count_per_category
      count
               64.000000
                           64.000000
                                         64.000000
                                                                64.0
                                                                                     64.0
                                                                 2.0
                                                                                     64.0
               10.061167
                           17.253777
                                        563.016500
      mean
```

384.001622

0.0

0.0

12.636979

6.189466

std

min	1.656020	3.210000	90.090000	2.0	64.0
25%	5.484117	8.113675	299.188250	2.0	64.0
50%	8.446438	14.371825	465.374000	2.0	64.0
75%	12.254740	22.965170	737.762500	2.0	64.0
max	33.750000	55.215300	1698.440000	2.0	64.0

## Key insights:

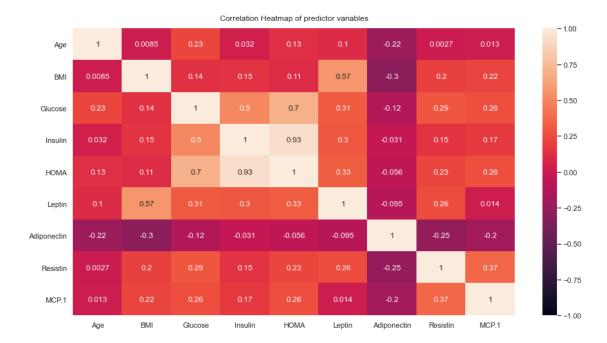
There is no significant difference between the mean Age and BMI between categories The mean glucose level for healthy people is  $\sim 20\%$  lower than the one of the diseased. A nearly 50% increase in the average Insulin levels for diseased can be noticed Mean Resistin level is also higher for diseased people \*There is no significant difference between the mean of Leptin and Adiponectin between categories

From this overview it is possible to claim that the Age and BMI are not statistically significant, but further confirmation is required.

```
Attribute
                VIF Scores
0
                  13.174889
           Age
1
           BMI
                  40.738293
2
       Glucose
                  39.585326
3
       Insulin
                  21.154744
4
          AMOH
                  22.665524
5
        Leptin
                  5.042565
6
   Adiponectin
                   3.150224
7
      Resistin
                   3.216120
8
         MCP.1
                   4.777762
```

As it is seen, the BMI and the Glucose variables have the highest VIF Scores. Let's check their correlated relationship with other variables:

```
[22]: sns.set(rc = {'figure.figsize':(15,8)})
heatmap = sns.heatmap(breast_cancer.iloc[:,:9].corr(), vmin=-1, vmax=1,
→annot=True)
heatmap.set_title('Correlation Heatmap of predictor variables',
→fontdict={'fontsize':12}, pad=12);
```



Key insights: \* Glucose has the highest correlation with Leptin. This is what I have found after doing a small reserach about their relationship:

"Circulating plasma insulin and glucose levels are thought to be major regulators of leptin secretion.Glucose metabolism rather than insulin alone is a main determinant of leptin expression." (abstract:https://academic.oup.com/jcem/article/85/3/1267/2660753)

• BMI has nearly the same VIF score as Glucose.

BMI also has high correlation with Leptin probably because Leptin is the main regulator of body weight and the main element to estimate BMI is body weight itself. Furthermore, HOMA and Insulin are also correlated with Glucose. Let's drop BMI and Glucose variables and see how the VIF scores will change.

23]:	<pre>cancer2=breast_cancer.copy()</pre>									
24]:	breast_cancer									
[24]:		Age	BMI	Glucose	Insulin	HOMA	Leptin	Adiponectin	\	
	0	48	23.500000	70	2.707	0.467409	8.8071	9.702400		
	1	83	20.690495	92	3.115	0.706897	8.8438	5.429285		
	2	82	23.124670	91	4.498	1.009651	17.9393	22.432040		
	3	68	21.367521	77	3.226	0.612725	9.8827	7.169560		
	4	86	21.111111	92	3.549	0.805386	6.6994	4.819240		
		•••	•••		•••	•••	•••			
	111	45	26.850000	92	3.330	0.755688	54.6800	12.100000		
	112	62	26.840000	100	4.530	1.117400	12.4500	21.420000		
	113	65	32.050000	97	5.730	1.370998	61.4800	22.540000		

```
114
            72
                25.590000
                                 82
                                       2.820 0.570392 24.9600
                                                                    33.750000
      115
               27.180000
            86
                                138
                                      19.910 6.777364 90.2800
                                                                    14.110000
           Resistin
                       MCP.1
                               Classification
                                               count_per_category Classification_cat \
      0
            7.99585
                     417.114
                                                                52
                                                                               healthy
                                             1
      1
            4.06405
                     468.786
                                                                52
                                                                               healthy
      2
            9.27715 554.697
                                             1
                                                                52
                                                                               healthy
      3
           12.76600
                     928.220
                                             1
                                                                52
                                                                               healthy
           10.57635
                     773.920
                                             1
                                                                52
                                                                               healthy
      . .
                                             2
                                                                               disease
      111
          10.96000
                     268.230
                                                                64
      112
           7.32000
                     330.160
                                            2
                                                                64
                                                                               disease
                                             2
      113 10.33000
                     314.050
                                                                64
                                                                               disease
                                             2
      114
            3.27000
                     392.460
                                                                64
                                                                               disease
      115
            4.35000
                      90.090
                                             2
                                                                64
                                                                               disease
           BMI_status
      0
               Normal
      1
               Normal
               Normal
      3
               Normal
      4
               Normal
      111 Overweight
      112
           Overweight
      113
              Obesity
           Overweight
      114
      115
           Overweight
      [116 rows x 13 columns]
[25]: X_vif2=X_vif.drop(['BMI', 'Glucose'], axis=1)
      vif_scores = pd.DataFrame()
      vif_scores["Attribute"] = X_vif2.columns
      # calculating VIF for each feature
      vif_scores["VIF Scores"] = [variance_inflation_factor(X_vif2.values, i) for i_
       →in range(len(X_vif2.columns))]
      display(vif_scores)
          Attribute VIF Scores
     0
                 Age
                        5.633412
     1
             Insulin
                       14.249439
     2
                AMOH
                       11.794633
     3
             Leptin
                        3.417510
     4
        Adiponectin
                        2.599688
     5
           Resistin
                        3.046963
```

#### 6 MCP.1 3.802299

The VIF scores for the remained variables decreased significantly. Insulin and HOMA still has noticeably higher scores, but not to a concerning extent. We can drop this columns from the dataset:

```
[26]:
      cancer2=cancer2.drop(['BMI','Glucose'],axis=1)
      cancer2=cancer2.drop(['BMI_status'],axis=1)
[27]:
[28]:
      breast_cancer
[28]:
            Age
                        BMI
                              Glucose
                                        Insulin
                                                      HOMA
                                                              Leptin
                                                                       Adiponectin
      0
                                   70
                                          2.707
                                                              8.8071
                                                                          9.702400
             48
                 23.500000
                                                  0.467409
      1
             83
                 20.690495
                                   92
                                                              8.8438
                                                                          5.429285
                                          3.115
                                                  0.706897
      2
             82
                 23.124670
                                                             17.9393
                                   91
                                          4.498
                                                  1.009651
                                                                         22.432040
      3
             68
                 21.367521
                                   77
                                          3.226
                                                  0.612725
                                                              9.8827
                                                                          7.169560
      4
             86
                 21.111111
                                   92
                                          3.549
                                                  0.805386
                                                              6.6994
                                                                          4.819240
      . .
      111
             45
                 26.850000
                                   92
                                          3.330
                                                  0.755688
                                                             54.6800
                                                                         12.100000
      112
                 26.840000
                                  100
                                                             12.4500
                                                                         21.420000
             62
                                          4.530
                                                  1.117400
      113
                 32.050000
                                   97
                                                  1.370998
                                                             61.4800
                                                                         22.540000
             65
                                          5.730
      114
             72
                 25.590000
                                   82
                                          2.820
                                                  0.570392
                                                             24.9600
                                                                         33.750000
      115
             86
                 27.180000
                                  138
                                         19.910
                                                  6.777364
                                                             90.2800
                                                                         14.110000
            Resistin
                         MCP.1
                                 Classification
                                                   count_per_category Classification_cat
      0
             7.99585
                       417.114
                                                1
                                                                     52
                                                                                    healthy
      1
             4.06405
                       468.786
                                                1
                                                                     52
                                                                                    healthy
      2
                                                1
                                                                     52
             9.27715
                       554.697
                                                                                    healthy
      3
            12.76600
                       928.220
                                                1
                                                                     52
                                                                                    healthy
      4
            10.57635
                       773.920
                                                1
                                                                     52
                                                                                    healthy
      . .
                 •••
                         •••
      111
            10.96000
                       268.230
                                                2
                                                                     64
                                                                                    disease
      112
                                                2
                                                                     64
             7.32000
                       330.160
                                                                                    disease
                                                2
      113
            10.33000
                       314.050
                                                                     64
                                                                                    disease
      114
             3.27000
                       392.460
                                                2
                                                                     64
                                                                                    disease
                                                2
      115
             4.35000
                        90.090
                                                                     64
                                                                                    disease
            BMI_status
      0
                Normal
                Normal
      1
      2
                Normal
      3
                Normal
      4
                Normal
            Overweight
      111
            Overweight
      112
      113
               Obesity
```

```
114 Overweight
```

115 Overweight

[116 rows x 13 columns]

Which results in a final prepared dataset:

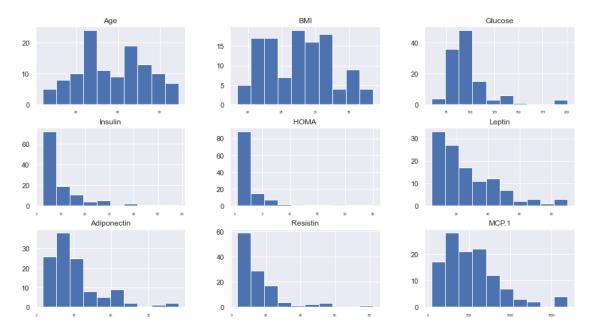
:	cano	er2							
:		Age	Insulin	HOMA	Leptin	Adiponectin	Resistin	MCP.1	\
	0	48	2.707	0.467409	8.8071	9.702400	7.99585	417.114	
	1	83	3.115	0.706897	8.8438	5.429285	4.06405	468.786	
	2	82	4.498	1.009651	17.9393	22.432040	9.27715	554.697	
	3	68	3.226	0.612725	9.8827	7.169560	12.76600	928.220	
	4	86	3.549	0.805386	6.6994	4.819240	10.57635	773.920	
		•••	•••	•••		•••	•••		
	111	45	3.330	0.755688	54.6800	12.100000	10.96000	268.230	
	112	62	4.530	1.117400	12.4500	21.420000	7.32000	330.160	
	113	65	5.730	1.370998	61.4800	22.540000	10.33000	314.050	
	114	72	2.820	0.570392	24.9600	33.750000	3.27000	392.460	
	115	86	19.910	6.777364	90.2800	14.110000	4.35000	90.090	
		<b>0</b> 3	_:¢:+:_			01 <i>:</i> f :			
	^	Clas				ry Classifica	_		
	0			1		52 52	healthy		
	1			1		52	healthy		
	2			1		52	healthy		
	3			1		52	healthy		
	4			1		52	healthy		
			•••	0	•••	0.4			
	111			2		64	disease		
	112			2		64	disease		
	113			2		64	disease		
	114			2		64	disease		
	115			2		64	disease		

[116 rows x 10 columns]

#### 5.0.2 Determine data distribution

The below histogram visualization aims to confirm the assumption that the data doesn't have Gaussian (Normal) distribution. This is nessecary to determine what kind of statistical test should be used for deriving the correlation coefficients. If a data sample is not Gaussian, then the assumptions of parametric statistical tests are violated and nonparametric statistical methods must be used, such as kendall rank correlation.

```
[30]: breast_cancer.iloc[:,:9].hist(xlabelsize=5)
```

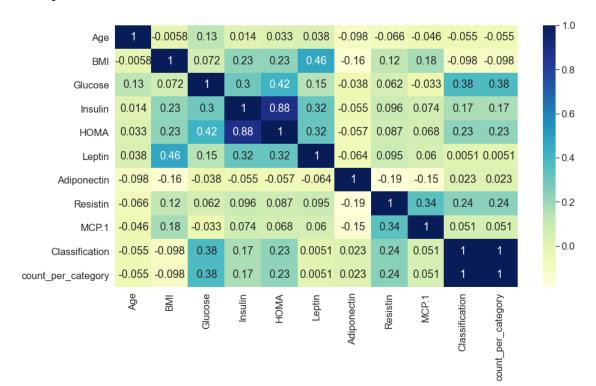


A statistical test to confirm the data sample is not drawn from Gaussian distribution using p-value: (higher the p-value, higher the chance is the data is Gaussian distributed)

Statistics=0.442, p=0.000 Sample does not look Gaussian (reject HO)

This graphical method confirms the data is not normally distributed and we can proceed to using the Kendall correlation test:

#### [32]: <AxesSubplot:>



As it is visible from the above heatmap visualization, the variables that least correlate with the target variable are BMI, Age, Adiponectin, Leptin and MCP.1. Therefore, they can be dropped.

```
breast_cancer
[33]:
[33]:
                        BMI
                              Glucose
                                        Insulin
                                                              Leptin
                                                                       Adiponectin
            Age
                                                      AMOH
      0
                 23.500000
                                                              8.8071
                                                                          9.702400
             48
                                   70
                                          2.707
                                                  0.467409
      1
             83
                 20.690495
                                   92
                                          3.115
                                                  0.706897
                                                              8.8438
                                                                          5.429285
      2
             82
                 23.124670
                                   91
                                          4.498
                                                  1.009651
                                                             17.9393
                                                                         22.432040
      3
             68
                 21.367521
                                   77
                                          3.226
                                                  0.612725
                                                              9.8827
                                                                          7.169560
      4
                                   92
                                                              6.6994
             86
                 21.111111
                                          3.549
                                                  0.805386
                                                                          4.819240
      111
             45
                 26.850000
                                   92
                                          3.330
                                                 0.755688
                                                             54.6800
                                                                         12.100000
```

```
112
            62
                 26.840000
                                 100
                                        4.530 1.117400 12.4500
                                                                      21.420000
      113
                32.050000
                                  97
                                        5.730
                                               1.370998 61.4800
                                                                      22.540000
            65
      114
            72
                 25.590000
                                  82
                                        2.820
                                               0.570392
                                                          24.9600
                                                                      33.750000
      115
                 27.180000
                                       19.910
                                               6.777364 90.2800
                                                                      14.110000
            86
                                 138
           Resistin
                        MCP.1
                               {\tt Classification}
                                                count_per_category Classification_cat \
      0
            7.99585
                      417.114
                                             1
                                                                  52
                                                                                 healthy
      1
                                             1
            4.06405
                      468.786
                                                                  52
                                                                                 healthy
      2
                                             1
            9.27715
                      554.697
                                                                  52
                                                                                 healthy
      3
           12.76600
                      928.220
                                             1
                                                                  52
                                                                                 healthy
      4
           10.57635
                      773.920
                                             1
                                                                  52
                                                                                 healthy
      111
          10.96000
                      268.230
                                             2
                                                                  64
                                                                                 disease
                                             2
      112
            7.32000
                      330.160
                                                                  64
                                                                                 disease
      113
          10.33000
                      314.050
                                             2
                                                                  64
                                                                                 disease
                                             2
      114
            3.27000
                      392.460
                                                                  64
                                                                                 disease
                                             2
      115
            4.35000
                       90.090
                                                                  64
                                                                                 disease
           BMI_status
               Normal
      0
      1
               Normal
      2
               Normal
      3
               Normal
      4
               Normal
      . .
           Overweight
           Overweight
      112
      113
              Obesity
      114
           Overweight
      115
           Overweight
      [116 rows x 13 columns]
[34]: cancer=breast_cancer.copy()
      cancer=cancer.drop(['Age','BMI','Leptin','Adiponectin','MCP.
       →1','count_per_category','Classification_cat','BMI_status'],axis=1)
[36]:
     cancer
[36]:
           Glucose
                     Insulin
                                         Resistin Classification
                                   AMOH
                 70
                       2.707
                                          7.99585
      0
                              0.467409
                                                                  1
                                                                  1
      1
                 92
                       3.115
                                          4.06405
                              0.706897
      2
                       4.498
                 91
                              1.009651
                                          9.27715
      3
                       3.226
                                                                  1
                 77
                              0.612725
                                         12.76600
      4
                 92
                       3.549
                              0.805386
                                         10.57635
```

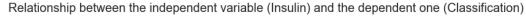
```
111
          92
                3.330 0.755688 10.96000
                                                         2
112
                                  7.32000
                                                         2
         100
                4.530 1.117400
                                                         2
113
          97
                5.730 1.370998
                                 10.33000
                                                         2
114
          82
                2.820
                       0.570392
                                  3.27000
115
         138
               19.910 6.777364
                                  4.35000
                                                         2
```

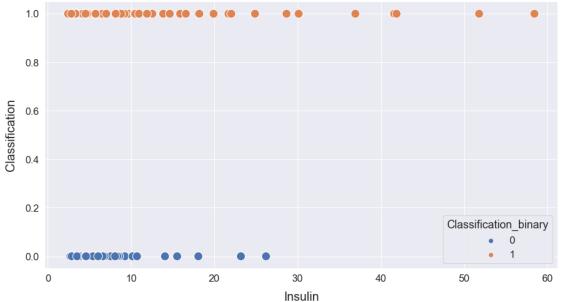
[116 rows x 5 columns]

#### 5.0.3 Exploring further the relationship between variables using Logistic Regression

There is a lot of similarities between Logistic and Linear Regression. In the case of Linear Regression, the output that has to be predicted (the y-value) can take continuous values. Although this is not the case when it comes to Logistic Regression. This type of regression aims to predict probabilities. Hence, the y-scale is 0-1 and it corresponds to the probability of a certain observation happening/not happening. The probabilities has to be transformed to log odds using the logit function. A visualization is included below to demonstrate this concept:

Transforming the Classification variable to be in a binary format:





The scatterplot shows how the Glucose variable (doesn't matter which independent variable is chosen, I chose this one) relates to the dependent variable. For example, from that visualization we can derive that patients with Glucose level of 50 are classified as 'Diseased' and the ones with 25 are classified as 'Healthy'. ALthough this scatterplot gives good sense, it is still not a Logistic Regression visualization. To make a logistic curve, a Logistic Regression() model will be fitted into the data and visualized.

```
[40]:
     model = LogisticRegression(solver='liblinear', random_state=0)
[41]:
     X_ins=cancer['Insulin'].values.reshape(-1, 1)
[42]:
     X_ins
[42]: array([[ 2.707],
             [3.115],
             [4.498],
             [ 3.226],
             [3.549],
             [ 3.226],
             [ 4.69 ],
             [6.47],
             [ 3.35 ],
             [4.952],
             [ 3.469],
             [5.663],
             [ 4.09 ],
```

- [ 6.107],
- [5.782],
- [7.553],
- [ 2.869],
- [18.077],
- [4.427],
- [14.026],
- [ 4.345],
- [ 4.53 ],
- [ 5.81 ],
- \_ \_ \_ \_
- [ 4.376],
- [5.537],
- [ 6.76 ],
- [ 6.703],
- [ 9.245],
- [ 6.817],
- [ 6.59 ],
- [15.533],
- [10.175],
- [8.576],
- [23.194],
- [ 3.855],
- [5.819],
- [4.181],
- [ 5.646],
- [5.138],
- [ 3.881],
- [ 5.376],
- [14.07],
- [5.197],
- [5.43],
- [ 8.34 ],
- [ 6.042],
- [8.079],
- [3.508],
- [10.704],
- [ 4.462],
- [26.211],
- [ 4.58 ],
- [13.852],
- [10.002],
- [ 4.56 ], [12.305],
- [21.699],
- [21.000],
- [ 2.999],
- [6.2],
- [ 4.364],
- [ 3.482],

- [5.261],
- [ 6.683],
- [ 2.64 ],
- [ 2.74 ],
- [ 6.862],
- [4.902],
- [ 3.73 ],
- [5.7],
- [ 3.42 ],
- [15.89],
- [ 3.44 ],
- [58.46], [ 6.03 ],
- [ 4.42 ],
- [36.94],
- [10.555],
- [16.635],
- [ 4.328],
- [41.611],
- [22.033],
- [3.188],
- [ 9.669],
- [28.677],
- [10.395],
- [ 4.172],
- [14.649],
- [ 2.54 ],
- [51.814],
- [12.162],
- [16.582],
- [41.894],
- [18.077],
- [30.212],
- [24.887],
- [30.13],
- [8.396],
- [ 9.208],
- [ 2.432],
- [18.2],
- [8.808],
- [ 3.012],
- [6.524],
- [10.491],
- [10.949],
- [12.548],
- [5.636],
- [ 4.713],

```
[8.15],
             [7.01],
             [11.91],
             [ 3.33 ],
             [4.53],
             [5.73],
             [ 2.82 ],
             [19.91]])
[43]: scaler=sc()
      X_transformed = scaler.fit_transform(X_ins)
[44]: y=cancer.iloc[:,5].to_numpy()
      model.fit(X_transformed,y)
[44]: LogisticRegression(random_state=0, solver='liblinear')
     Extracting the predicted probabilities from the Logistic Function:
[45]: X_probability_class_1 =model.predict_proba(X_transformed)[:, 1]
      X_probability_class_1
[45]: array([0.42899929, 0.43663294, 0.46271191, 0.43871511, 0.44478606,
             0.43871511, 0.46635192, 0.50021774, 0.44104368, 0.47132473,
             0.44328081, 0.48484552, 0.45499054, 0.49330141, 0.4871112 ,
             0.52084153, 0.43202646, 0.70796617, 0.46136685, 0.64032381,
             0.4598141 , 0.46331831, 0.48764438, 0.46040102, 0.48244724,
             0.50574325, 0.50465727, 0.55289492, 0.50682918, 0.50250424,
             0.66632932, 0.57034443, 0.54025888, 0.78168813, 0.45055275,
             0.48781577, 0.45671097, 0.4845219 , 0.47485856, 0.45104337,
             0.47938397, 0.64109581, 0.47598005, 0.48041124, 0.53578809,
             0.49206314, 0.53083702, 0.44401449, 0.5801954, 0.46202984,
             0.81839026, 0.46426603, 0.63726384, 0.46388691, 0.60959251,
             0.76162081, 0.43445937, 0.49507323, 0.46017382, 0.44352534,
             0.47719685, 0.50427622, 0.42774884, 0.42961551, 0.50768645,
             0.47037525, 0.44819538, 0.48554991, 0.44235935, 0.67235134,
             0.44273541, 0.98135608, 0.49183455, 0.46123427, 0.91078161,
             0.57742684, 0.6847356, 0.45949229, 0.93578973, 0.76621175,
             0.43800205, 0.56086923, 0.84467489, 0.57444848, 0.45654077,
             0.65118528, 0.42588423, 0.96943548, 0.60699556, 0.68386293,
             0.93707366, 0.70796617, 0.85941325, 0.80290766, 0.85865643,
             0.5368495 , 0.5521977 , 0.42387281, 0.70990061, 0.54464759,
             0.43470283, 0.50124668, 0.57623616, 0.58473669, 0.61399122,
             0.48433154, 0.46678821, 0.48650189, 0.5321845, 0.51050555,
             0.60240445, 0.44066793, 0.46331831, 0.48612108, 0.43111029,
             0.73599071])
```

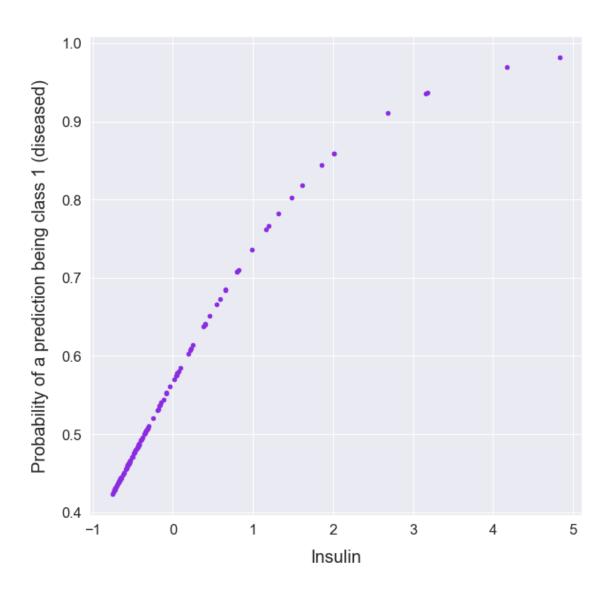
[5.75],

```
[46]:
            Insulin probability_class1
                                0.428999
          -0.728739
          -0.688038
      1
                                0.436633
      2
          -0.550073
                                0.462712
          -0.676965
                                0.438715
          -0.644743
                                0.444786
      4
      111 -0.666590
                                0.440668
      112 -0.546881
                                0.463318
      113 -0.427172
                                0.486121
      114 -0.717467
                                0.431110
      115 0.987394
                                0.735991
```

[116 rows x 2 columns]

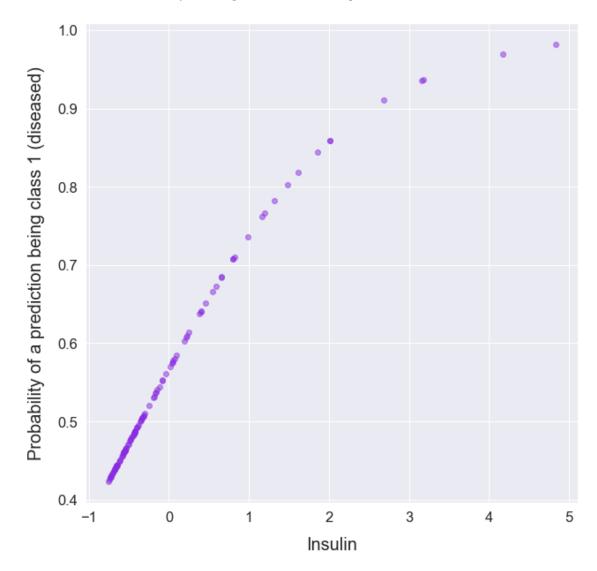
The final visualization has a logistic curve fitted to the observations. The log odds is calculated using the logit function on the y-axis for each observation.

<Figure size 1080x576 with 0 Axes>



```
plt.ylabel("Probability of a prediction being class 1 (diseased)", u collabelpad=14, fontsize = 20)
```

[50]: Text(0, 0.5, 'Probability of a prediction being class 1 (diseased)')



# 5.0.4 Clustering analysis using K-Means clustering - are there clusters in the data?

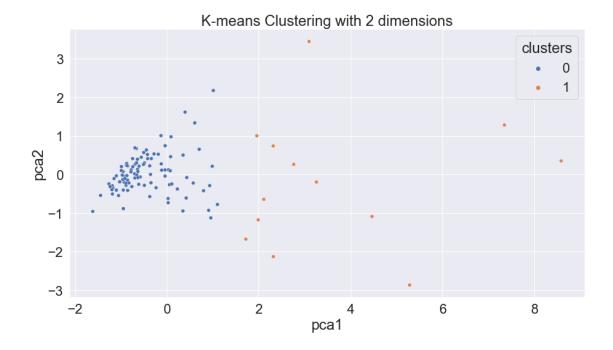
The goal of this section is to perform clustering analysis on the features so that additional insights of the feature space is provided. Typically, clustering algorithms are applied in a context of unsupervised learning task, but they can also be applicable to explore any clusters in the datasets if with the help of visualization. An additional technique, dimensionality reduction, will be used for creating 2-dimensional feature dataset. Dimensionality reduction refers to techniques of decreasing the number of variables in the dataset. Mainly, it is applicable to ease the ML execution. In this case, it will be used to decrease the volume of the data that will be clustered. The method of applying this technique is

PCA (Principal Component Analysis). Principal component analysis (PCA) involves a mathematical procedure that transforms a number of (possibly) correlated variables into a (smaller) number of uncorrelated variables called principal components. Before starting with any execution, the data should be pre-processed. Scaling will be used to achieve this goal. The reason for performing pre-processing is related to how the PCA function will analyse the values of the variables. Since the variables are not sharing the same scale, some of them might have larger variation and since the goal of the PCA is to maximize the variance per variable, the result will be that some of the variables will be assigned with more importance than others, which is not the end goal and will lead to misleading results.

Standardizing data:

```
[51]: Y =cancer['Classification']
      X =cancer.iloc[:,:-2]
      columns = X.columns
      scaler = sc()
      X_std = scaler.fit_transform(X)
      X_std = pd.DataFrame(X_std, columns = columns)
      X_std.head()
[51]:
          Glucose
                    Insulin
                                 HOMA Resistin
      0 -1.239222 -0.728739 -0.614282 -0.545517
      1 -0.258299 -0.688038 -0.548240 -0.864214
      2 -0.302887 -0.550073 -0.464752 -0.441660
      3 -0.927110 -0.676965 -0.574210 -0.158867
      4 -0.258299 -0.644743 -0.521081 -0.336352
[52]: #extracting the features from the standardised dataset
      features = list(X_std.columns)[:-1]
      ###creating feature dataset (with the purpose of not working directly on the
       ⇔original standardised one)
      data = X_std[features]
[53]: #creating 2 clusters (the number of clusters is randomly chosen)
      clustering_kmeans = KMeans(n_clusters=2)
      data['clusters'] = clustering_kmeans.fit_predict(data)
     The data is already clustered. Time for PCA:
[54]: reduced data = PCA(n components=2).fit transform(data)
      results = pd.DataFrame(reduced_data,columns=['pca1','pca2'])
[55]: pca1=results[['pca1']]
      pca2=results[['pca2']]
     This is the resulting dataset.
[56]: results
```

```
[56]:
               pca1
                         pca2
          -1.444573 -0.539831
      0
      1
          -0.887192 0.244921
      2
          -0.777763 0.121084
      3
          -1.232876 -0.313752
          -0.845227 0.217554
      111 -0.866403 0.231364
      112 -0.555884 0.448676
      113 -0.510255 0.262423
      114 -1.151616 -0.104742
      115 2.316055 0.742823
      [116 rows x 2 columns]
     Here we create a variable that has a copy of the Classification variable (the target output) with the
     purpose of appending it to the newly created dimensionality reducted dataset:
[57]: x1=cancer[['Classification']]
      joined=X_std.join(x1)
[58]: joined=joined[['Classification']]
[59]: joined=results.join(joined)
[60]: joined
[60]:
               pca1
                          pca2
                                Classification
      0
          -1.444573 -0.539831
      1
          -0.887192 0.244921
                                              1
      2
          -0.777763 0.121084
                                              1
      3
          -1.232876 -0.313752
                                              1
      4
          -0.845227
                     0.217554
                                              1
      111 -0.866403 0.231364
                                             2
                                             2
      112 -0.555884 0.448676
                                             2
      113 -0.510255 0.262423
                                              2
      114 -1.151616 -0.104742
      115 2.316055 0.742823
                                             2
      [116 rows x 3 columns]
[61]: sns.set(rc = {'figure.figsize': (15,8)},font_scale=2)
      sns.scatterplot(x="pca1", y="pca2", hue=data['clusters'], data=results)
      plt.title('K-means Clustering with 2 dimensions')
      plt.show()
```



There are no distinguishable clusters.

## 6 Conclusion

Several techniques were applied to perform initial exploration on the data including correlation heatmap, basic barplots for quantitive analysis as well as a more advanced data mining technique - clustering. A null hypothesis was formed for checking the significancy of the variables which was rejected by a VIF score method applied on the features. This was important step towards the next phase-Data provisioning which resulted in creating two datasets - 'cancer2' derived from rejecting the null hypothesis by the VIF analysis and the 'joined' dataset, derived from the clustering analysis.

# 7 Modelling

So far, the dataset has been analyzed and prepared for the current phase-Modelling. To choose what kind of model should be fitted, several aspects are taken into account. From analyzing the data in previous phases, it is clear this is a supervised problem since each instance is labelled. The target variable is in binary format representing 2 classes - 1 (class='diseased') and 0 (class='healthy'). So therefore, algorithms which classifies the instances into those 2 classes should be fitted into the data. SVM classifier would be applicable.

#### 7.0.1 Pre-processing data and splitting it into train and test sets

The first step that should be performed is is to scale the data so that each feature lies within the same range. This is already done from the previous section for the CLuster Analysis. In case of SVM, the distance between the points is measured and it is essential the data is scaled for accurate interpretation of the classifier.

```
[62]: y =cancer[['Classification_binary']]
    print(y)
    print(X_std)
```

```
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115
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```

```
[116 rows x 1 columns]
```

```
Glucose
                Insulin
                             HOMA Resistin
   -1.239222 -0.728739 -0.614282 -0.545517
0
   -0.258299 -0.688038 -0.548240 -0.864214
   -0.302887 -0.550073 -0.464752 -0.441660
3
   -0.927110 -0.676965 -0.574210 -0.158867
4
   -0.258299 -0.644743 -0.521081 -0.336352
111 -0.258299 -0.666590 -0.534786 -0.305255
    0.098400 -0.546881 -0.435039 -0.600299
113 -0.035362 -0.427172 -0.365106 -0.356320
114 -0.704173 -0.717467 -0.585883 -0.928577
115 1.792721 0.987394 1.125766 -0.841036
```

#### [116 rows x 4 columns]

The train\_test\_split method is the most common way to split the data into two sets. The data is split into a training set which the model is fit into and a test set used for evaluating the model performance on an unseen data.

```
[63]: from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X_std,np.ravel(y),_u

-test_size = 0.25,random_state=4)
```

It would be helpful to check the class distributions, because if there are more observations of class 0 than there is of class 1 or vice versa the data will be considered as biased and therefore the classifier interpretation will not be reliable. The np. bincount() function will count the occurrences of each value in the array (how many 0s and 1s are present in it.)

```
[64]: np.bincount(y_train)
```

```
[64]: array([37, 50], dtype=int64)
```

There is relatively good class balance in the training set.

#### 7.0.2 Support vector machine implementation

In this section, the choen model will be fitted into the data with default parameters. The model learns from the training data and makes predictions on the test data with the goal to estimate how well the model generalises on unseen data.

```
[65]: classifier = SVC() classifier.fit(X_train, y_train)
```

[65]: SVC()

Retrieve predictions:

#### 7.0.3 Model performance

An accuracy score will be used to check the overall score of the model by comparing the correctly predicted labels out of the total in the test set.

```
[67]: accuracy_score(y_pred,y_test)
```

#### [67]: 0.8275862068965517

82% is almost completely aligned with the pre-defined goal of ~85 %. Although this is an acceptable result, there is still no clarity how the model is performing per class. This insight is essential since it might be possible that certain class has more weight than other/s.

```
[68]: print(classification_report(y_test,y_pred))
```

	precision	recall	f1-score	support
0	0.81	0.87	0.84	15
1	0.85	0.79	0.81	14
accuracy			0.83	29
macro avg	0.83	0.83	0.83	29
weighted avg	0.83	0.83	0.83	29

```
[69]: cm4 = confusion_matrix(y_pred, y_test)
print(cm4)
```

```
[[13 3]
[ 2 11]]
```

The classification report goes along with the confusion matrix. The retrieved confusion matrix can be interpreted as follows:

As mentioned, there are 2 possible classes 0 (healthy) and 0 (diseased). The sum of all numbers is 29, that means that the classifier made 29 predictions in total. The numbers 13 and 11 are the correctly predicted labels for each class whereas 2 and 3 are the incorrectly predicted labels. If the array is interpreted column-wise, each column corresponds to a certain class. With that being mentioned, 13 out of 15 patients were actually healthy and they were predicted as healthy and 2 were healthy, but classified as 'diseased'. Identical interpretation applies to class 1: Out of 14 diseased patients, 11 were correctly classified as diseased and 3 were diseased, but classified as 'healthy'. The basic terms behind this explanation are the following: \* true positives (TP): These are cases in which it is predicted 1 and the observations do belong to class 1. \* true negatives (TN): Predicted 0, and the observations do belong to class 0. \* false positives (FP): Predicted 1, but they belong to class 0. but they don't actually have the disease. (Also known as a "Type I error.") \* false negatives (FN): Predicted 0, but they belong to class 1.

There are certain calculations that can be made using each of these terms retrieved from the confusion matrix for binary classifier and some of them are also represented in the classification report: \* Accuracy: Overall, how often is the classifier correct? : (TP+TN)/total = (13+11)/29 = 0.83 \* Misclassification Rate: Overall, how often is it wrong? : (FP+FN)/total = (3+2)/29 = 0.17; equivalent to 1 minus Accuracy and it is also known as "Error Rate" \* True Positive Rate: When it's actually yes, how often does it predict yes? : TP/actual yes = 11/13 = 0.85 also known as "Sensitivity" or "Recall" \* False Positive Rate: When it's actually no, how often does it predict yes? : FP/actual no = 3/16 = 0.19 \* True Negative Rate: When it's actually no, how often does it predict no? : TN/actual no = 11/16 = 0.68; equivalent to 1 minus False Positive Rate and also known as "Specificity" \* Precision: When it predicts yes, how often is it correct? : TP/predicted yes = 11/14 = 0.79

For this model, it is desired that the model has low false positive rate (it won't be nice to be told you don't have cancer but in fact you do have). A FP rate of 0.19 is acceptable.

# 7.0.4 Estimating model performance using k-fold cross validation

In the current case, the data size is not big enough which can result in producing a model that overfits the data (learning too much from the training data). To check for overfitting, cross-validation should be performed. There are many cross-validation techniques, but the one which I will focus on in this notebook is called k-fold cross validation. The parameter that the KFold () function takes is n\_splits which has to be carefully selected - it determines the number of folds the data will be split into. What happens after splitting the data into these folds is, part of the observations within each fold are used for testing the model, and the rest for training. The beneficial thing about this method is that each observation is included in a test set only once. The next question is - how to determine the k value for the n\_splits parameter?

#### 7.0.5 Sensitivity analysis of K

To choose the optimal k number, we need to test different k-values on the dataset. This can be achieved by using a leave-one-out cross-validation (LOOCV), a computationally expensive version of cross-validation where k=N, and N is the total number of examples in the training dataset. That is, each sample in the training set is given an example to be used alone as the test evaluation dataset and it can provide a good estimate of model performance given the available data. We

can then compare the mean classification accuracy for different k values to the mean classification accuracy from LOOCV on the same dataset. The difference between the scores provides a rough proxy for how well a k value approximates the ideal model evaluation test condition.

```
[70]: # evaluate the model using a given test condition

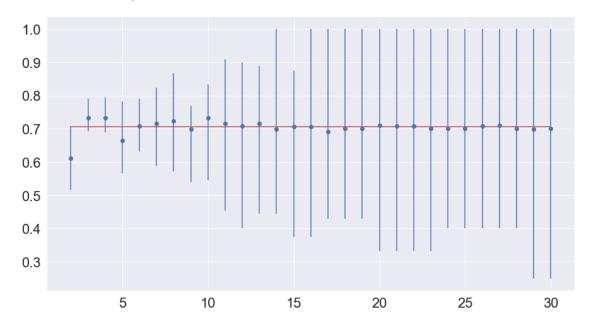
def evaluate_model(cv):
    scores = cross_val_score(classifier, X, y, scoring='accuracy', cv=cv,u
n_jobs=-1)

return scores.mean(), scores.min(), scores.max()
```

```
[71]: # define folds to test
      folds = range(2,31)
      # record mean and min/max of each set of results
      means, mins, maxs = list(),list(),list()
      ideal, _, _ = evaluate_model(LeaveOneOut())
      print('Ideal: %.3f' % ideal)
      # evaluate each k value
      for k in folds:
      # define the test condition
       cv = KFold(n_splits=k, shuffle=True, random_state=1)
       # evaluate k value
      k_mean, k_min, k_max = evaluate_model(cv)
       # report performance
       print('> folds=%d, accuracy=%.3f (%.3f,%.3f)' % (k, k_mean, k_min, k_max))
       # store mean accuracy
       means.append(k_mean)
      # store min and max relative to the mean
      mins.append(k_mean - k_min)
      maxs.append(k_max - k_mean)
      # line plot of k mean values with min/max error bars
      pyplot.errorbar(folds, means, yerr=[mins, maxs], fmt='o')
      # plot the ideal case in a separate color
      pyplot.plot(folds, [ideal for _ in range(len(folds))], color='r')
      # show the plot
      pyplot.show()
```

```
Ideal: 0.707
> folds=2, accuracy=0.612 (0.517,0.707)
> folds=3, accuracy=0.733 (0.692,0.789)
> folds=4, accuracy=0.733 (0.690,0.793)
> folds=5, accuracy=0.664 (0.565,0.783)
> folds=6, accuracy=0.707 (0.632,0.789)
> folds=7, accuracy=0.716 (0.588,0.824)
> folds=8, accuracy=0.724 (0.571,0.867)
> folds=9, accuracy=0.699 (0.538,0.769)
> folds=10, accuracy=0.733 (0.545,0.833)
> folds=11, accuracy=0.717 (0.455,0.909)
```

```
> folds=12, accuracy=0.707 (0.400,0.900)
> folds=13, accuracy=0.716 (0.444,0.889)
> folds=14, accuracy=0.699 (0.444,1.000)
> folds=15, accuracy=0.707 (0.375,0.875)
> folds=16, accuracy=0.706 (0.375,1.000)
> folds=17, accuracy=0.692 (0.429,1.000)
> folds=18, accuracy=0.700 (0.429,1.000)
> folds=19, accuracy=0.701 (0.429,1.000)
> folds=20, accuracy=0.710 (0.333,1.000)
> folds=21, accuracy=0.708 (0.333,1.000)
> folds=22, accuracy=0.708 (0.333,1.000)
> folds=23, accuracy=0.701 (0.333,1.000)
> folds=24, accuracy=0.700 (0.400,1.000)
> folds=25, accuracy=0.700 (0.400,1.000)
> folds=26, accuracy=0.708 (0.400,1.000)
> folds=27, accuracy=0.709 (0.400,1.000)
> folds=28, accuracy=0.700 (0.400,1.000)
> folds=29, accuracy=0.698 (0.250,1.000)
> folds=30, accuracy=0.700 (0.250,1.000)
```



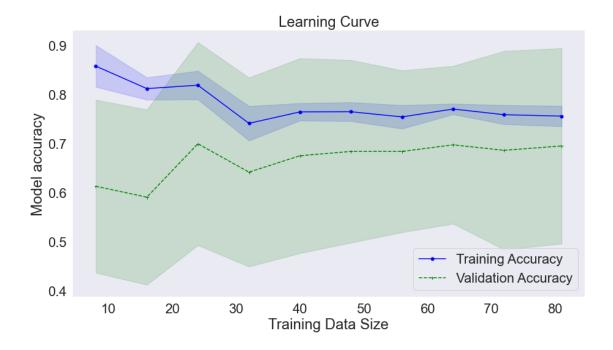
0.707 -> k=15.

```
print('Accuracy -val set: %.2f% (%.2f)' % (results.mean()*100, results.std()))
```

Accuracy -val set: 63.81% (0.22)

It is noticeable that the accuracy score is significantly lower than the one retrieved earlier from splitting the data using simple train\_test\_split. That's why it is important that the dataset is large enough. When a data is large enough it will be representative and a good balance between bias and variance will be achieved. The below visualization will illustrate the training vs validation accuracy for different training sizes which will further prove the point that the data size is essential. The learning curve () function will be used to plot the training vs the validation accuracy using the kfold variable defined earlier as the cross-validation method passed to the cv parameter.

```
[73]: # Use learning curve to get training and test scores along with train sizes
      train_sizes, train_scores, test_scores = learning_curve(estimator=SVC(),_
       →X=X_train, y=y_train,
                                                              cv=kfold, train_sizes=np.
       \hookrightarrowlinspace(0.1, 1.0, 10),
                                                            n_{jobs=1}
      # Calculate training and test mean and std
      train_mean = np.mean(train_scores, axis=1)
      train_std = np.std(train_scores, axis=1)
      test_mean = np.mean(test_scores, axis=1)
      test_std = np.std(test_scores, axis=1)
      # Plot the learning curve
      plt.plot(train_sizes, train_mean, color='blue', marker='o', markersize=5,u
       ⇔label='Training Accuracy')
      plt.fill_between(train_sizes, train_mean + train_std, train_mean - train_std,__
       ⇔alpha=0.15, color='blue')
      plt.plot(train_sizes, test_mean, color='green', marker='+', markersize=5,u
       ⇔linestyle='--', label='Validation Accuracy')
      plt.fill_between(train_sizes, test_mean + test_std, test_mean - test_std,__
       ⇒alpha=0.15, color='green')
      plt.title('Learning Curve')
      plt.xlabel('Training Data Size')
      plt.ylabel('Model accuracy')
      plt.grid()
      plt.legend(loc='lower right')
      plt.show()
```



From this visualization it can be noted that the for training sample size less than 25, the difference between training and validation accuracy is much larger. This is the case of overfitting. For training size greater than 30, the model is better. It is a sign of good bias-variance trade-off.

#### 7.0.6 Conclusion from cross-validation

It can be seen that the model is overfitting which is confirmed from comparing the cross-validation. The goal is to achieve a good bias-variance trade off after all. It can be seen from the above visualization that for larger training samples, the training and the validation accuracy are balanced which is the goal. The bottleneck here as already mentioned is that there is not enough data to use for training and thus improving the model performance is not currently possible from this aspect. And if the n\_splits of the cross-validation method increases, the error will increase as well. And we don't want to have any overlap in the training and testing folds that are retrieved from the KFold method. What can be done in this case is, tuning the parameters of the model so that is learns appropriately from the available data.

#### 7.0.7 Cross-validation further evaluation

Confusion matrix will still be used to evaluate the model from the cross validation. In this case, we need to retrieve the predictions made in each fold and compare them with the test labels also retrieved from every fold (of course there might be other ways to achieve the same)

The itterator below goes through each of the folds and appends the test and predicted values. This is possible since the kfold.split provides the test and train indexes.

```
[74]: X2=X_std.to_numpy()
```

[75]: y2=cancer['Classification\_binary'].to\_numpy()

```
[76]: for train_index, test_index in kfold.split(X2):
            print(train_index, test_index)
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[77]: def evaluate_model(X2,y2):
          kfold =KFold(n_splits=15)
          predicted_targets = np.array([])
          actual_targets = np.array([])
          for train_index, test_index in kfold.split(X2):
              X_train2, X_test2, y_train2, y_test2 = __

¬X2[train_index],X2[test_index],y2[train_index],y2[test_index]

              # Fit the classifier
              classifier2 =SVC().fit(X_train2,y_train2)
              # Predict the labels of the test set samples
              predicted_labels = classifier2.predict(X_test2)
              predicted_targets = np.append(predicted_targets, predicted_labels)
              actual_targets = np.append(actual_targets,y_test2)
          return predicted_targets, actual_targets
[78]: predicted_target, actual_target = evaluate_model(X2,y2)
      confusion_matrix(actual_target,predicted_target)
[78]: array([[31, 21],
             [21, 43]], dtype=int64)
[79]: print(classification_report(actual_target,predicted_target))
                                 recall f1-score
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                                                         116
         accuracy
```

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macro avg 0.63 0.63 0.63 116
weighted avg 0.64 0.64 0.64 116
```

Since we are interested in observing the False Positive rate, in this case it is 21/52 = 0.4 but this is more realistic and reliable score of the model skill.

## 7.0.8 Hyperparameter tuning using Grid Search

Besides that cross-validation is extremely powerful in estimating the model skill, this method can be used as a parameter to the Grid Search. Grid search is a method that scans the data and search for optimal parameters for a given model.

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Fitting 15 folds for each of 75 candidates, totalling 1125 fits
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[CV 15/15] END .C=0.1, gamma=0.1, kernel=linear;, score=1.000 total time=
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[CV 1/15] END .C=0.1, gamma=0.1, kernel=sigmoid;, score=0.667 total time=
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[CV 2/15] END .C=0.1, gamma=0.1, kernel=sigmoid;, score=0.667 total time=
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[CV 3/15] END .C=0.1, gamma=0.1, kernel=sigmoid;, score=0.500 total time=
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[CV 4/15] END .C=0.1, gamma=0.1, kernel=sigmoid;, score=0.667 total time=
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[CV 5/15] END .C=0.1, gamma=0.1, kernel=sigmoid;, score=0.500 total time=
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[CV 6/15] END .C=0.1, gamma=0.1, kernel=sigmoid;, score=0.667 total time=
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[CV 9/15] END .C=0.1, gamma=0.1, kernel=sigmoid;, score=0.333 total time=
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[CV 10/15] END C=0.1, gamma=0.1, kernel=sigmoid;, score=0.500 total time=
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[CV 2/15] END C=0.1, gamma=0.01, kernel=sigmoid;, score=0.667 total time=
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[CV 3/15] END C=0.1, gamma=0.01, kernel=sigmoid;, score=0.500 total time=
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[CV 7/15] END C=0.1, gamma=0.01, kernel=sigmoid;, score=0.333 total time=
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[CV 12/15] END C=0.1, gamma=0.001, kernel=linear;, score=0.667 total time=
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[CV 9/15] END ..C=0.1, gamma=0.0001, kernel=rbf;, score=0.333 total time=
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[CV 12/15] END .C=0.1, gamma=0.0001, kernel=rbf;, score=0.333 total time=
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[CV 15/15] END .C=0.1, gamma=0.0001, kernel=rbf;, score=0.600 total time=
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[CV 9/15] END C=0.1, gamma=0.0001, kernel=linear;, score=0.833 total time=
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- [CV 10/15] END C=0.1, gamma=0.0001, kernel=linear;, score=0.667 total time= 0.0s
- [CV 11/15] END C=0.1, gamma=0.0001, kernel=linear;, score=0.833 total time= 0.0s
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- [CV 6/15] END C=0.1, gamma=0.0001, kernel=sigmoid;, score=0.667 total time=0.0s
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0.0s
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- [CV 15/15] END .C=100, gamma=0.0001, kernel=rbf;, score=0.600 total time= 0.0s [CV 1/15] END C=100, gamma=0.0001, kernel=linear;, score=0.833 total time= 0.0s [CV 2/15] END C=100, gamma=0.0001, kernel=linear;, score=0.833 total time= 0.00
- [CV 3/15] END C=100, gamma=0.0001, kernel=linear;, score=0.500 total time= 0.0s
- [CV 4/15] END C=100, gamma=0.0001, kernel=linear;, score=0.500 total time= 0.0s
- [CV 5/15] END C=100, gamma=0.0001, kernel=linear;, score=0.667 total time= 0.0s
- [CV 6/15] END C=100, gamma=0.0001, kernel=linear;, score=1.000 total time= 0.0s
- [CV 7/15] END C=100, gamma=0.0001, kernel=linear;, score=0.500 total time= 0.0s
- [CV 8/15] END C=100, gamma=0.0001, kernel=linear;, score=0.333 total time= 0.0s
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- [CV 9/15] END C=100, gamma=0.0001, kernel=sigmoid;, score=0.333 total time=

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[CV 5/15] END .C=1000, gamma=0.1, kernel=linear;, score=0.667 total time=
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[CV 1/15] END C=1000, gamma=0.001, kernel=linear;, score=0.833 total time=
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- [CV 2/15] END C=1000, gamma=0.001, kernel=linear;, score=0.833 total time= 0.0s
- [CV 3/15] END C=1000, gamma=0.001, kernel=linear;, score=0.500 total time= 0.0s
- [CV 4/15] END C=1000, gamma=0.001, kernel=linear;, score=0.667 total time= 0.0s
- [CV 5/15] END C=1000, gamma=0.001, kernel=linear;, score=0.667 total time= 0.0s
- [CV 6/15] END C=1000, gamma=0.001, kernel=linear;, score=1.000 total time= 0.0s
- [CV 7/15] END C=1000, gamma=0.001, kernel=linear;, score=0.500 total time=0.0s
- [CV 8/15] END C=1000, gamma=0.001, kernel=linear;, score=0.333 total time= 0.0s
- [CV 9/15] END C=1000, gamma=0.001, kernel=linear;, score=0.667 total time= 0.0s  $\,$
- [CV 10/15] END C=1000, gamma=0.001, kernel=linear;, score=0.500 total time= 0.0s
- [CV 11/15] END C=1000, gamma=0.001, kernel=linear;, score=0.833 total time= 0.0s
- [CV 12/15] END C=1000, gamma=0.001, kernel=linear;, score=0.667 total time= 0.0s
- [CV 13/15] END C=1000, gamma=0.001, kernel=linear;, score=0.600 total time= 0.0s
- [CV 14/15] END C=1000, gamma=0.001, kernel=linear;, score=0.400 total time= 0.0s
- [CV 15/15] END C=1000, gamma=0.001, kernel=linear;, score=1.000 total time= 0.0s  $\,$
- [CV 1/15] END C=1000, gamma=0.001, kernel=sigmoid;, score=0.833 total time= 0.0s
- [CV 2/15] END C=1000, gamma=0.001, kernel=sigmoid;, score=0.833 total time= 0.0s
- [CV 3/15] END C=1000, gamma=0.001, kernel=sigmoid;, score=0.500 total time= 0.0s
- [CV 4/15] END C=1000, gamma=0.001, kernel=sigmoid;, score=0.500 total time= 0.0s
- [CV 5/15] END C=1000, gamma=0.001, kernel=sigmoid;, score=0.667 total time= 0.0s
- [CV 6/15] END C=1000, gamma=0.001, kernel=sigmoid;, score=1.000 total time= 0.0s
- [CV 7/15] END C=1000, gamma=0.001, kernel=sigmoid;, score=0.500 total time= 0.0s
- [CV 8/15] END C=1000, gamma=0.001, kernel=sigmoid;, score=0.167 total time= 0.0s  $\,$
- [CV 9/15] END C=1000, gamma=0.001, kernel=sigmoid;, score=0.667 total time= 0.0s
- [CV 10/15] END C=1000, gamma=0.001, kernel=sigmoid;, score=0.667 total time= 0.0s

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[CV 11/15] END C=1000, gamma=0.001, kernel=sigmoid;, score=1.000 total time=
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[CV 12/15] END C=1000, gamma=0.001, kernel=sigmoid;, score=0.667 total time=
[CV 13/15] END C=1000, gamma=0.001, kernel=sigmoid;, score=0.600 total time=
[CV 14/15] END C=1000, gamma=0.001, kernel=sigmoid;, score=0.400 total time=
0.0s
[CV 15/15] END C=1000, gamma=0.001, kernel=sigmoid;, score=1.000 total time=
0.0s
[CV 1/15] END .C=1000, gamma=0.0001, kernel=rbf;, score=0.833 total time=
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[CV 2/15] END .C=1000, gamma=0.0001, kernel=rbf;, score=0.833 total time=
                                                                             0.0s
[CV 3/15] END .C=1000, gamma=0.0001, kernel=rbf;, score=0.667 total time=
                                                                             0.0s
[CV 4/15] END .C=1000, gamma=0.0001, kernel=rbf;, score=0.500 total time=
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[CV 5/15] END .C=1000, gamma=0.0001, kernel=rbf;, score=0.667 total time=
                                                                             0.0s
[CV 6/15] END .C=1000, gamma=0.0001, kernel=rbf;, score=1.000 total time=
                                                                             0.0s
[CV 7/15] END .C=1000, gamma=0.0001, kernel=rbf;, score=0.333 total time=
                                                                             0.0s
[CV 8/15] END .C=1000, gamma=0.0001, kernel=rbf;, score=0.167 total time=
                                                                             0.0s
[CV 9/15] END .C=1000, gamma=0.0001, kernel=rbf;, score=0.667 total time=
                                                                             0.0s
[CV 10/15] END C=1000, gamma=0.0001, kernel=rbf;, score=0.500 total time=
                                                                             0.0s
[CV 11/15] END C=1000, gamma=0.0001, kernel=rbf;, score=1.000 total time=
                                                                             0.0s
[CV 12/15] END C=1000, gamma=0.0001, kernel=rbf;, score=0.667 total time=
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[CV 13/15] END C=1000, gamma=0.0001, kernel=rbf;, score=0.600 total time=
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[CV 14/15] END C=1000, gamma=0.0001, kernel=rbf;, score=0.600 total time=
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[CV 15/15] END C=1000, gamma=0.0001, kernel=rbf;, score=1.000 total time=
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[CV 3/15] END C=1000, gamma=0.0001, kernel=linear;, score=0.500 total time=
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[CV 6/15] END C=1000, gamma=0.0001, kernel=linear;, score=1.000 total time=
[CV 7/15] END C=1000, gamma=0.0001, kernel=linear;, score=0.500 total time=
[CV 8/15] END C=1000, gamma=0.0001, kernel=linear;, score=0.333 total time=
[CV 9/15] END C=1000, gamma=0.0001, kernel=linear;, score=0.667 total time=
[CV 10/15] END C=1000, gamma=0.0001, kernel=linear;, score=0.500 total time=
[CV 11/15] END C=1000, gamma=0.0001, kernel=linear;, score=0.833 total time=
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[CV 12/15] END C=1000, gamma=0.0001, kernel=linear;, score=0.667 total time=
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[CV 13/15] END C=1000, gamma=0.0001, kernel=linear;, score=0.600 total time=
     0.0s
     [CV 14/15] END C=1000, gamma=0.0001, kernel=linear;, score=0.400 total time=
     0.0s
     [CV 15/15] END C=1000, gamma=0.0001, kernel=linear;, score=1.000 total time=
     [CV 1/15] END C=1000, gamma=0.0001, kernel=sigmoid;, score=0.833 total time=
     [CV 2/15] END C=1000, gamma=0.0001, kernel=sigmoid;, score=0.833 total time=
     0.0s
     [CV 3/15] END C=1000, gamma=0.0001, kernel=sigmoid;, score=0.500 total time=
     0.0s
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     [CV 5/15] END C=1000, gamma=0.0001, kernel=sigmoid;, score=0.667 total time=
     0.0s
     [CV 6/15] END C=1000, gamma=0.0001, kernel=sigmoid;, score=1.000 total time=
     0.0s
     [CV 7/15] END C=1000, gamma=0.0001, kernel=sigmoid;, score=0.333 total time=
     [CV 8/15] END C=1000, gamma=0.0001, kernel=sigmoid;, score=0.167 total time=
     [CV 9/15] END C=1000, gamma=0.0001, kernel=sigmoid;, score=0.833 total time=
     0.0s
     [CV 10/15] END C=1000, gamma=0.0001, kernel=sigmoid;, score=0.667 total time=
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     [CV 11/15] END C=1000, gamma=0.0001, kernel=sigmoid;, score=0.833 total time=
     0.0s
     [CV 12/15] END C=1000, gamma=0.0001, kernel=sigmoid;, score=0.667 total time=
     0.0s
     [CV 13/15] END C=1000, gamma=0.0001, kernel=sigmoid;, score=0.600 total time=
     0.0s
     [CV 14/15] END C=1000, gamma=0.0001, kernel=sigmoid;, score=0.400 total time=
     [CV 15/15] END C=1000, gamma=0.0001, kernel=sigmoid;, score=1.000 total time=
     0.0s
[80]: GridSearchCV(cv=KFold(n_splits=15, random_state=None, shuffle=False),
                   estimator=SVC(),
                   param_grid={'C': [0.1, 1, 10, 100, 1000],
                               'gamma': [1, 0.1, 0.01, 0.001, 0.0001],
                               'kernel': ['rbf', 'linear', 'sigmoid']},
                   verbose=3)
[81]: # print best parameter after tuning
      print(grid.best_params_)
```

0.0s

```
# print how our model looks after hyper-parameter tuning
      print(grid.best_estimator_)
     {'C': 1, 'gamma': 1, 'kernel': 'sigmoid'}
     SVC(C=1, gamma=1, kernel='sigmoid')
     Fitting the best estimated model from the Grid Search:
[82]: classifier0 = SVC(C=1, gamma=1,kernel='sigmoid')
      classifier0.fit(X_train, y_train)
[82]: SVC(C=1, gamma=1, kernel='sigmoid')
[83]: y_grid_pred = classifier0.predict(X_test)
      # print classification report
      print(classification_report(y_test,y_grid_pred))
                   precision
                                 recall f1-score
                                                     support
                0
                         0.78
                                   0.93
                                              0.85
                                                          15
                         0.91
                                   0.71
                                             0.80
                                                          14
                                             0.83
                                                          29
         accuracy
                                             0.82
                                                          29
        macro avg
                         0.84
                                   0.82
     weighted avg
                         0.84
                                   0.83
                                             0.83
                                                          29
[84]: accuracy_score(y_test,y_grid_pred)
[84]: 0.8275862068965517
[85]: cm5 = confusion matrix(y grid pred, y test)
      print(cm5)
     [[14 4]
      [ 1 10]]
     Still acceptable False Positive rate from the tuned model.
     7.0.9 Re-comparing the tuned model training and validation accuracy
[86]: # Use learning curve to get training and test scores along with train sizes
      train_sizes, train_scores, test_scores = learning_curve(estimator=SVC(C=1,__

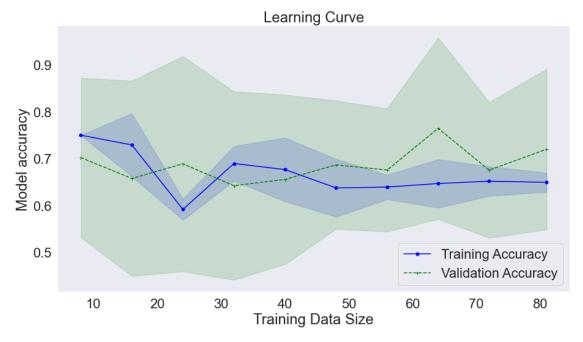
→gamma=1,kernel='sigmoid'), X=X_train, y=y_train,
```

 $\rightarrow$ linspace(0.1, 1.0, 10),

cv=kfold, train\_sizes=np.

 $n_jobs=1)$ 

```
# Calculate training and test mean and std
train_mean = np.mean(train_scores, axis=1)
train_std = np.std(train_scores, axis=1)
test_mean = np.mean(test_scores, axis=1)
test_std = np.std(test_scores, axis=1)
# Plot the learning curve
plt.plot(train_sizes, train_mean, color='blue', marker='o', markersize=5,u
 ⇔label='Training Accuracy')
plt.fill_between(train_sizes, train_mean + train_std, train_mean - train_std,__
 ⇔alpha=0.15, color='blue')
plt.plot(train_sizes, test_mean, color='green', marker='+', markersize=5,_
 ⇔linestyle='--', label='Validation Accuracy')
plt.fill_between(train_sizes, test_mean + test_std, test_mean - test_std,_u
 ⇒alpha=0.15, color='green')
plt.title('Learning Curve')
plt.xlabel('Training Data Size')
plt.ylabel('Model accuracy')
plt.grid()
plt.legend(loc='lower right')
plt.show()
```



Comparing individual accuracy scores of the validation and training sets is not always enough. By

re-computing the learning curve for this graph we can observe if after tuning the hyper-parameters of the model, the overfitting is minimized. Looking at the lines of the graph, I would say this is the perfect scenario - it is obvious that with these set of hyper-parameters, the model doesn't overfit the data that much.

## 8 Conclusion

In the phase 'Modelling', first we started with building a simple SVM classifier and test its accuracy. Although the model gave high accuracy and acceptable confusion matrix, this is still not enough to draw the final conclusion that this model has to be selected. Therefore, a cross-validation was executed with pre-defined value of k. Via this method, the model was run on each fold and its performance across each of those folds was computed and evaluated via confusion matrix. It showed that the False Positive Rate in fact is much higher. Afterwards, the resulted cross-validation was passed as parameter to the GridSearch to obtain the best estimated model with the goal to see if the overfitting is reduced. Overall, further training was needed to fit a model on such limited data sample but at the end, the overfitting was reduced and the False Positive rate is acceptable.