A2_template_2024

July 17, 2024

1 Assignment 2: Classification

2 Using Machine Learning Tools

2.1 Overview

In this assignment, you will apply some popular machine learning techniques to the problem of classifying data from histological cell images for the diagnosis of malignant breast cancer. This will be presented as a practical scenario where you are approached by a client to solve a problem.

The main aims of this assignment are:

- to use the best practice machine learning workflow for producing a solution to a client's problem;
- to visualise and clean data;
- to train and optimise a selection of models, then choose the best;
- to obtain an unbiased measurement of the final model's performance:
- to interpret results clearly and concisely.

This assignment relates to the following ACS CBOK areas: abstraction, design, hardware and software, data and information, HCI and programming.

2.2 General instructions

This assignment is divided into several tasks. Use the spaces provided in this notebook to answer the questions posed in each task, but feel free to add additional cells to structure your notebook. Note that some questions require writing code, some require graphical results, and some require comments or analysis as text. It is your responsibility to make sure your responses are clearly labelled and your code has been fully executed (with the correct results displayed) before submission!

Do not manually edit the data set file we have provided! For marking purposes, it's important that your code can run correctly on the original data file.

This assignment uses the standard best practice machine learning workflow, building on the first assignment and course workshops, and so less detailed instructions are provided for this assignment. You should be able to implement this workflow now without low-level guidance and a substantial portion of the marks for this assignment are associated with the appropriate choices and executing this workflow correctly and efficiently. Make sure you have clean, readable code as well as producing outputs, since your coding will also count towards the marks (however, excessive commenting is

discouraged and will lose marks, so aim for a modest, well-chosen amount of comments and text in outputs).

This assignment can be solved using methods from sklearn, pandas, and matplotlib as presented in the workshops. Other libraries should not be used (even though they might have nice functionality) and occasionally certain specific functions need to be used, which will be made clear in the instruction text. You are expected to make sure that you are using functions correctly, and you should search and carefully read the documentation if unsure.

3 Scenario

A client approaches you to solve a machine learning problem for them. They run a pathology lab that processes histological images for healthcare providers and they have created a product that measures most of the same features as in the Wisconsin breast cancer data set though using different acquisitions and processing methods. Their method employs efficient stochastic sampling, making it much faster than existing methods, although slightly noisier. This method does not measure any of the 'worst' features that appear in the Wisconsin Breast Cancer Data Set. They want to be able to diagnose malignant cancer (and distinguish them from benign growths) by employing machine learning techniques, and they have asked you to implement this for them.

Their requirements are: -1) Have at least a 90% probability of detecting malignant cancer when it is present; -2) Ensure that no more than 1 in 5 healthy cases (those with benign growths) result in a false positive (labeled as malignant).

They have hand-labelled 220 samples for you, with 20 features per sample, which is all they have at the moment.

Please follow the instructions below, which will vary in level of detail.

3.1 1. Load data, visualise it and identify erroneous values [30%]

- Load the data from the csv file assignment2_data_2024.csv (found on MyUni).
- Extract the feature names and label names for use later on.
- Provide at least one text summary of the dataset. This should include key information and characteristics of the data.
- Create one graphical plot per feature. Each plot must display the feature values for the two classes (malignant and benign) separately on a single axis/panel.
- Make sure you clearly label the graphical plots with respect to feature names, axes, classes, etc.
- Identify any erroneous values in the dataset during the data visualisation or summary steps. Determine and implement, here or later, the appropriate action to handle these values (e.g., removal, correction, or none).
- Throughout this assignment, treat the *malignant* cases as the *true positive* class, following the standard convention in medicine. .

```
[1]: # This code imports some libraries that you will need.
# You should not need to modify it, though you are expected to make other

→ imports later in your code.
```

```
# Python 3.5 is required
     import sys
     assert sys.version_info >= (3, 5)
     # Common imports
     import numpy as np
     import time
     import collections
     # Pandas for overview
     import pandas as pd
     import random
     # Scikit-Learn 0.20 is required
     import sklearn
     assert sklearn._version__ >= "0.20"
     from sklearn import tree
     from sklearn import svm
     from sklearn.pipeline import Pipeline
     from sklearn.impute import SimpleImputer
     from sklearn.preprocessing import StandardScaler
     from sklearn.model_selection import GridSearchCV
     from sklearn.metrics import confusion_matrix
     from sklearn.metrics import accuracy_score, balanced_accuracy_score,_
      →recall_score, precision_score, roc_auc_score, f1_score
     from sklearn.model_selection import cross_val_score
     # Plot setup
     import matplotlib as mpl
     import matplotlib.pyplot as plt
     from matplotlib.cbook import boxplot_stats
     import seaborn as sns
     # mpl.rc('axes', labelsize=7)
     # mpl.rc('xtick', labelsize=6)
     # mpl.rc('ytick', labelsize=6)
     # mpl.rc('figure', dpi=240)
     plt.close('all')
     import seaborn as sns
[2]: # set random seed for all instances of random
     random_seed = 42
```

np.random.seed(random_seed)
random.seed(random_seed)

3.1.1 Loading in the Dataset

```
[3]: df = pd.read csv(r"./assignment2 data 2024.csv")
     df.head()
[3]:
            label
                          mean radius mean texture
                                                      mean perimeter
                                                                        mean area
        malignant 15.494653829645529
                                           15.902542
                                                           103.008265
                                                                       776.437239
        malignant 16.229870799611437
                                                                       874.712003
                                           18.785613
                                                           105.176755
     2 malignant
                   16.34567074196476
                                                           107.083804
                                                                       872.563251
                                           20.114076
        maligant 13.001009157806651
     3
                                           19.876997
                                                            85.889775
                                                                       541.281012
     4 malignant 16.416060073302194
                                           17.397533
                                                           107.857386
                                                                       891.516818
        mean smoothness mean compactness mean concavity mean concave points
     0
               0.104239
                                  0.168660
                                                  0.170572
                                                                        0.085668
     1
               0.091843
                                  0.092548
                                                  0.081681
                                                                        0.053670
     2
               0.099924
                                  0.123799
                                                  0.128788
                                                                        0.078310
     3
               0.113423
                                                  0.146214
                                                                        0.069574
                                  0.173069
               0.097321
                                  0.111530
                                                  0.125971
                                                                        0.068575
        mean symmetry
                          radius error texture error perimeter error
     0
             0.205053
                               0.653654
                                              1.096678
                                                                4.962255
     1
             0.180435
                                                                3.005373
                               0.445451
                                              1.043931
     2
             0.189756 ...
                               0.549625
                                              1.057447
                                                                3.643671
     3
             0.212078 ...
                               0.430693
                                              1.202955
                                                                3.051434
             0.179562 ...
                               0.525532
                                                                3.747194
                                              1.045900
                                                           concavity error
        area error
                    smoothness error
                                       compactness error
                                                                  0.043568
     0
         80.619370
                             0.006669
                                                0.034950
     1
         50.407958
                             0.006352
                                                0.019998
                                                                  0.025324
     2
         62.732851
                             0.006757
                                                0.031325
                                                                  0.034350
     3
         33.614356
                             0.007930
                                                0.044881
                                                                  0.042972
         59.164555
                             0.008718
                                                0.024231
                                                                  0.039763
        concave points error
                              symmetry error
                                               fractal dimension error
     0
                                                               0.004928
                    0.013765
                                     0.024093
     1
                    0.012172
                                                               0.003582
                                     0.018084
     2
                    0.015150
                                     0.021459
                                                               0.004066
     3
                                                               0.005981
                    0.014556
                                     0.035670
                    0.014202
                                     0.019236
                                                               0.004115
     [5 rows x 21 columns]
[4]: # Extract feature and labels names
     feature_names = df.columns[1:]
     target = df.columns[0]
```

3.1.2 Preliminary Visualization of the Dataset

[5]: # Provide at least one text summary of the dataset. This should include key dinformation and characteristics of the data.

df.info()

<class 'pandas.core.frame.DataFrame'>
RangeIndex: 220 entries, 0 to 219
Data columns (total 21 columns):

#	Column	Non-Null Count	Dtype
0	label	220 non-null	object
1	mean radius	220 non-null	object
2	mean texture	220 non-null	float64
3	mean perimeter	220 non-null	float64
4	mean area	220 non-null	float64
5	mean smoothness	220 non-null	float64
6	mean compactness	220 non-null	float64
7	mean concavity	220 non-null	float64
8	mean concave points	220 non-null	float64
9	mean symmetry	220 non-null	float64
10	mean fractal dimension	220 non-null	float64
11	radius error	220 non-null	float64
12	texture error	220 non-null	float64
13	perimeter error	220 non-null	float64
14	area error	220 non-null	float64
15	smoothness error	220 non-null	float64
16	compactness error	220 non-null	float64
17	concavity error	220 non-null	float64
18	concave points error	220 non-null	float64
19	symmetry error	219 non-null	float64
20	fractal dimension error	220 non-null	float64
1.	67 +64(40) 1: +(0	`	

dtypes: float64(19), object(2)

memory usage: 36.2+ KB

We will first do a preliminary describe with the dirty data and after we clean these values, we can visualize the dataset again. (This will be done in step 2)

```
[6]: # Describe to show the statistics of the data df.describe()
```

```
[6]:
                          mean perimeter
                                             mean area mean smoothness
            mean texture
              220.000000
                               220.000000
                                            220.000000
                                                              220.000000
     count
               18.991963
                                89.866240
                                            620.956227
                                                                0.096480
     mean
                                 7.366180
                                                                0.004961
     std
                1.427635
                                            106.419871
    min
               15.349270
                                74.690886
                                             -2.645499
                                                                0.084651
     25%
               17.914319
                                84.911981
                                            558.731832
                                                                0.092797
     50%
               18.928256
                                88.587737
                                            603.806128
                                                                0.096457
```

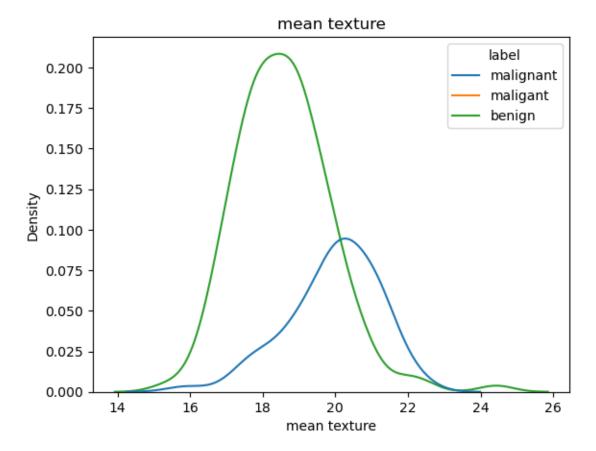
75%	19.995859	93.066393	655.690	0435	0.099817		
max	24.430831	121.247839	1103.740	0620	0.113423		
							,
	mean compactness 220.000000		-	n concave p 220.0		symmetry 20.000000	\
count	0.102879				46867	0.181850	
mean std	0.102879				4000 <i>1</i> 12548	0.101030	
min	0.075184				28701	0.157059	
25%	0.089531				38106	0.174944	
50%	0.098517				42761	0.180953	
75%	0.113276				55337	0.186354	
max	0.192880				00467	0.226448	
man	0.102000	0.201	.071	0.1	00101	0.220110	
	mean fractal dim	nension radiu	ıs error	texture er	ror perimet	er error	\
count	220.	000000 220	0.00000	220.000	000 22	20.000000	
mean	0.	103957	.393337	1.217	593	2.775090	
std	0.	606979	0.075828	0.210	182	0.579317	
min	0.	058922	.298005	0.898	026	2.059186	
25%	0.	061139	343114	1.073	344	2.394331	
50%	0.	062557	367863	1.165	727	2.610732	
75%	0.	064184	.420514	1.300	769	3.003888	
max	9.	065897	712896	2.561	348	5.903661	
		+					
count	area error smoo	220.000000	-	ness error 220.000000	concavity 6		
mean	37.781034	0.007076	4	0.025514		31901	
std	9.988655	0.001043		0.007345		4102	
min	27.693748	0.004994		0.016907		18730	
25%	31.843894	0.006372		0.020530		25373	
50%	34.007608	0.006837		0.023147		28835	
75%	39.042484	0.007675		0.027733		33620	
max	80.619370	0.011088		0.054950	0.16	3592	
	concave points e	-	ry error	fractal di	mension erro		
count	220.00		219.000000 220.000000				
mean			0.020901				
std		0.002422 0.003250 0.001259					
min			0.016181 0.002631				
25% 50%			0.018658				
50%			0.020193				
75%			0.022195		0.00404		
max	0.02	26554 (0.041861		0.01325	ΣŢ	

Visualize the distribution of each numerical feature:

Using density plots

```
[7]: for feature in feature_names[1:]:
    sns.kdeplot(data = df, x = feature, hue = "label")
    plt.title(feature)
    plt.show()
    break
```

/var/folders/gg/27ydp9614p9cpq8pg5r7rklc0000gn/T/ipykernel_90235/2683962586.py:2
: UserWarning: Dataset has 0 variance; skipping density estimate. Pass
`warn_singular=False` to disable this warning.
sns.kdeplot(data = df, x = feature, hue = "label")



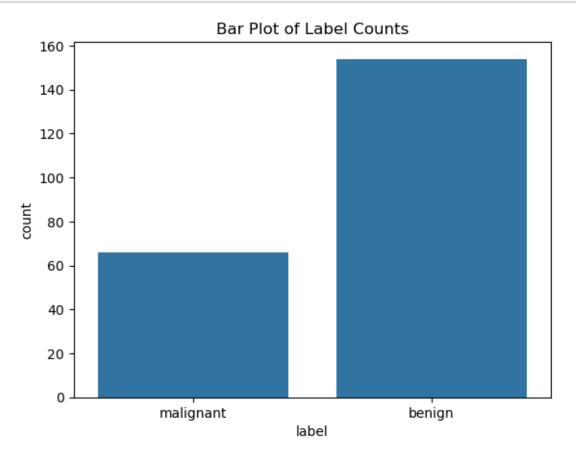
We notice that the label (target) data is dirty, we will first clean all the data, and then visualize the cleaned data.

3.1.3 Data and Error handling

From the earlier point, we will clean the label (target) data.

```
[8]: # identify which are the erroneous values df['label'].value_counts()
```

```
[8]: label
                   154
     benign
     malignant
                    65
     maligant
                     1
     Name: count, dtype: int64
 [9]: # cleaning and inspecting the new label data
      df['label'] = df["label"].str.replace("maligant", "malignant")
      df['label'].value_counts()
 [9]: label
     benign
                   154
     malignant
                    66
     Name: count, dtype: int64
[10]: # bat plot of label to show target split
      sns.countplot(data = df, x = "label")
      plt.title('Bar Plot of Label Counts')
      plt.show()
```



We notice that the column "mean radius" of not dtype float64, but an object. To know why, we

will look look for the data that's not a number.

```
[11]: # Check for non-numeric numbers in "mean radius" column
for x in df["mean radius"].value_counts().index:
    if x.replace(".", "").isdigit() == False:
        print(x)
```

-14.292182467715936 n12.254518716420597

It can be seen that there are input errors and a negative value. Since the value is mean radius (a distance), it is impossible for the values to be negative.

```
[12]: df["mean radius"] = df["mean radius"].apply(lambda x: float(x[1:]) if ('-' in_\] <math>\hookrightarrow x) or ('n' in x) else float(x)) df["mean radius"]
```

```
[12]: 0
             15.494654
      1
             16.229871
      2
             16.345671
      3
             13.001009
      4
             16.416060
      215
             13.618925
      216
             14.048464
      217
             12.879033
      218
             14.411991
      219
             12.704174
      Name: mean radius, Length: 220, dtype: float64
```

We then check for null values in the data.

```
[13]: # Check for null values in the dataset df.isnull().sum()
```

```
[13]: label
                                  0
      mean radius
                                  0
      mean texture
                                  0
      mean perimeter
                                  0
      mean area
                                  0
      mean smoothness
                                  0
      mean compactness
                                  0
      mean concavity
      mean concave points
                                  0
      mean symmetry
                                  0
      mean fractal dimension
                                  0
      radius error
                                  0
      texture error
                                  0
      perimeter error
                                  0
```

```
0
      area error
      smoothness error
                                 0
      compactness error
      concavity error
      concave points error
                                 0
      symmetry error
                                 1
      fractal dimension error
                                0
      dtype: int64
[14]: df[df["symmetry error"].isna()]
           label mean radius mean texture mean perimeter
Γ14]:
                                                              mean area \
      218 benign
                     14.411991
                                   18.970674
                                                   93.423809 671.128126
           mean smoothness mean compactness mean concavity mean concave points \
                  0.086304
                                    0.090118
                                                    0.070882
                                                                         0.039482
      218
           mean symmetry ... radius error texture error perimeter error \
      218
                0.175789 ...
                                0.356964
                                                1.030049
                                                                  2.56017
           area error smoothness error compactness error concavity error \
      218
          35.435273
                               0.005784
                                                  0.022279
                                                                   0.025244
           concave points error symmetry error fractal dimension error
                        0.00999
      218
                                            NaN
                                                                0.003255
      [1 rows x 21 columns]
```

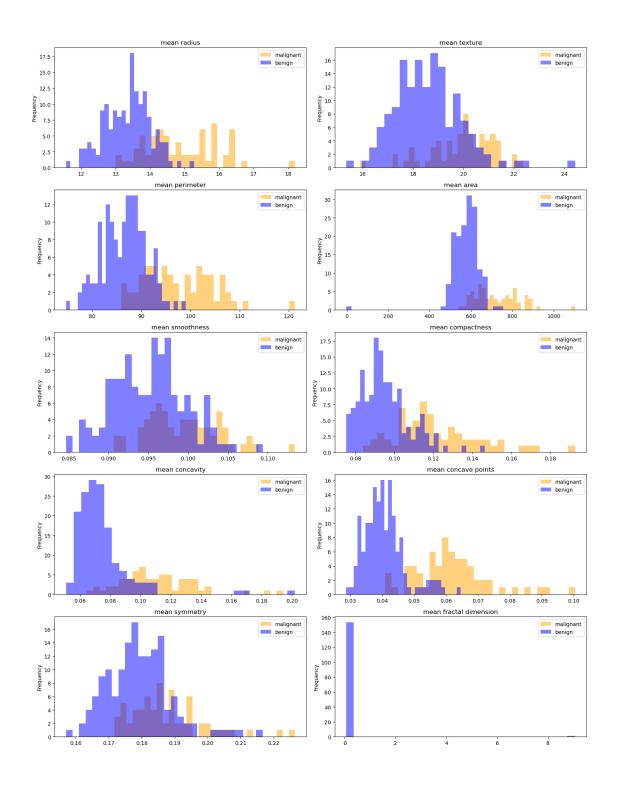
Note: Imputation will be part of the preprocessing pipeline to account for data leakage.

3.1.4 Visualization and Outlier Analysis

Visualization of data distirbutions Using histograms

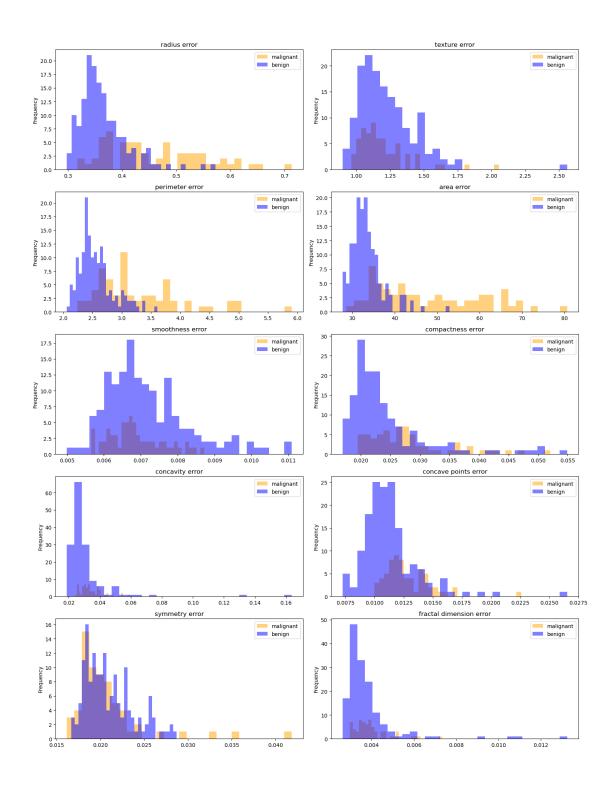
```
ax.set_title(v)
ax.set_ylabel('Frequency')
ax.legend()

# Adjust layout
plt.tight_layout(rect=[0, 0, 1, 0.95]) # Leave space at the top for the legend
plt.show()
```



[16]: # Create subplots of mean features
fig, axs = plt.subplots(5, 2, figsize=(15, 20)) # Adjust the figure size as

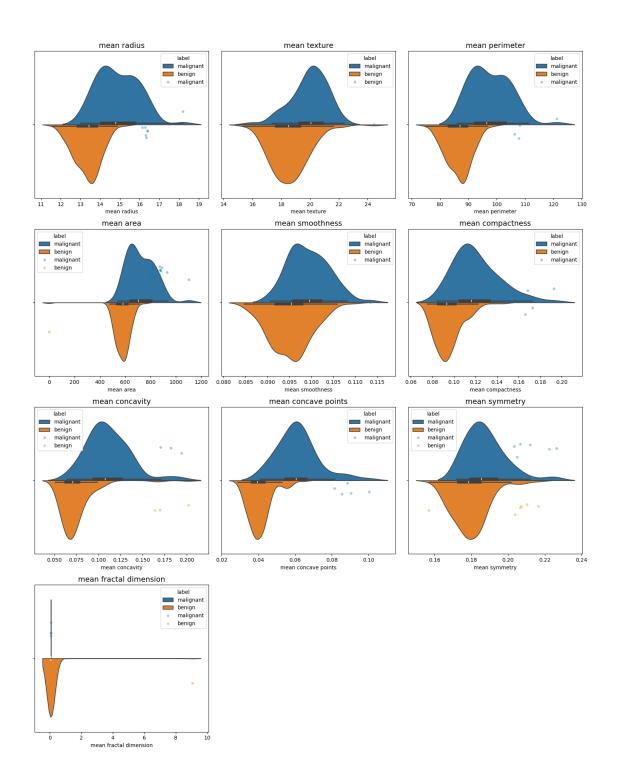
→needed



Outlier analysis with violinplots Using violinplots and stripplots complementing distribution analysis (Added outside matplotlib)

NOTE: Dots refer to the defintion of a statistical outlier where $\hat{x} \pm 1.5*IQR$

```
[17]: fig, axs = plt.subplots(4, 3, figsize=(15, 20)) # Adjust the figure size as
       \rightarrowneeded
      for i, v in enumerate([feature for feature in feature_names if 'mean' in_
       →feature]):
          row, col = divmod(i, 3) # Calculate row and column index for the subplot
          ax = axs[row, col] # Select the appropriate axes for the current plot
          sns.violinplot(data=df, x=v, hue="label", ax=ax, split=True)
          # Identify outliers with IQR
          stats = boxplot_stats(df[v])
          outliers = [item for stat in stats for item in stat['fliers']]
          # Filter df for outliers in the current feature and plot
          sns.stripplot(data=df[df[v].isin(outliers)], x=v, hue="label", ax=ax,_u
       ⇒alpha=0.4, dodge=True)
          ax.set_title(v, fontsize=14) # Adjust title font size as needed
      total_plots = len([feature for feature in feature_names if 'mean' in feature])
      for j in range(total_plots, 4*3):
          row, col = divmod(j, 3)
          axs[row, col].axis('off')
      # Adjust layout
      plt.tight_layout(rect=[0, 0, 1, 0.95])
     plt.show()
```

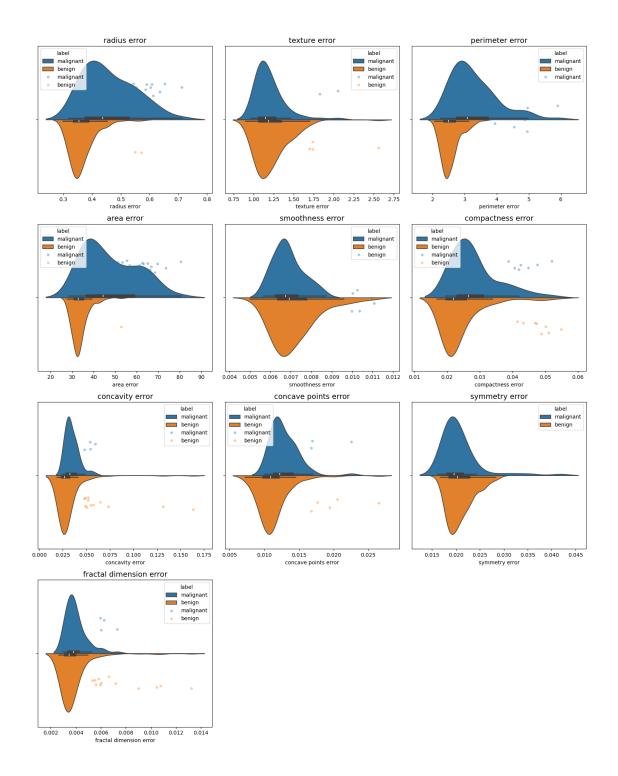


This plots the violinplots of both malignant and bening values w.r.t each outlier values for the mean measurement features. We will use the distributions to serve as guidance with the outliers to "eyeball" *unreasonable values*. This process will be repeated as well for the error measurement features.

```
[18]: # Removing outliers of the "mean" feautures by setting these as np.nan
      # We will manually remove problematic outliers and replace these to be with np.
       ⇔nan to be imputed in step 2
      df.loc[((df["mean radius"] > 18) & (df["label"] == 'malignant')), "mean,
       ⇔radius"] = np.nan
      df["mean perimeter"] = df["mean perimeter"].apply(lambda x: np.nan if x > 120__
       ⇔else x)
      df["mean compactness"] = df["mean compactness"].apply(lambda x: np.nan if x > 0.
       \rightarrow16 else x)
      df.loc[(df["mean area"] < 200) & (df["label"] == 'benign'), "mean area"] = np.
       ⊶nan
      df.loc[(df["mean area"] > 850) & (df["label"] == 'malignant'), "mean area"] =
       ⇔np.nan
      df.loc[(df["mean texture"] > 24) & (df["label"] == 'benign'), "mean texture"] =
       ⇔np.nan
      df["mean symmetry"] = df["mean symmetry"].apply(lambda x: np.nan if x >= 0.20_{\square})
       ⇔else x)
      df["mean concavity"] = df["mean concavity"].apply(lambda x: np.nan if x > 0.170_{LI})
       ⇔else x)
      df["mean fractal dimension"] = df["mean fractal dimension"].apply(lambda x: np.
       \rightarrownan if x > 1 else x)
[19]: fig, axs = plt.subplots(4, 3, figsize=(15, 20)) # Adjust the figure size as_
       \neg needed
      for i, v in enumerate([feature for feature in feature_names if 'error' in__
       →featurel):
          row, col = divmod(i, 3) # Calculate row and column index for the subplot
          ax = axs[row, col] # Select the appropriate axes for the current plot
          sns.violinplot(data=df, x=v, hue="label", ax=ax, split=True)
          # Identify outliers with IQR
          stats = boxplot_stats(df[v])
          outliers = [item for stat in stats for item in stat['fliers']]
          # Filter df for outliers in the current feature and plot
          sns.stripplot(data=df[df[v].isin(outliers)], x=v, hue="label", ax=ax,_u
       ⇒alpha=0.4, dodge=True)
          ax.set_title(v, fontsize=14) # Adjust title font size as needed
```

```
total_plots = len([feature for feature in feature_names if 'mean' in feature])
for j in range(total_plots, 4*3):
    row, col = divmod(j, 3)
    axs[row, col].axis('off')

# Adjust layout
plt.tight_layout(rect=[0, 0, 1, 0.95]) # Leave space at the top for the legend
plt.show()
```



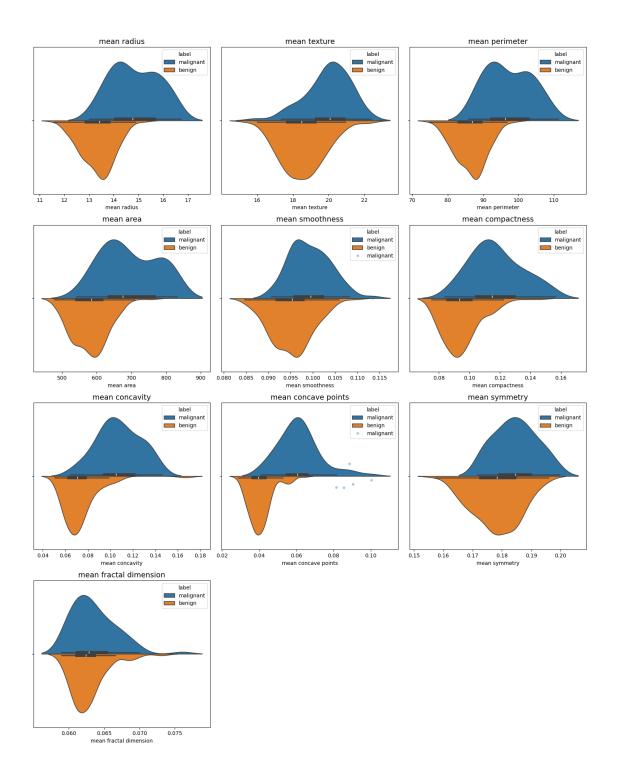
[20]: # Removing outliers of the "error" features

We will manually remove problematic outliers and replace these to be with np.

onan to be imputed in step 2

Visualization after Data Cleaning and Outlier Analysis

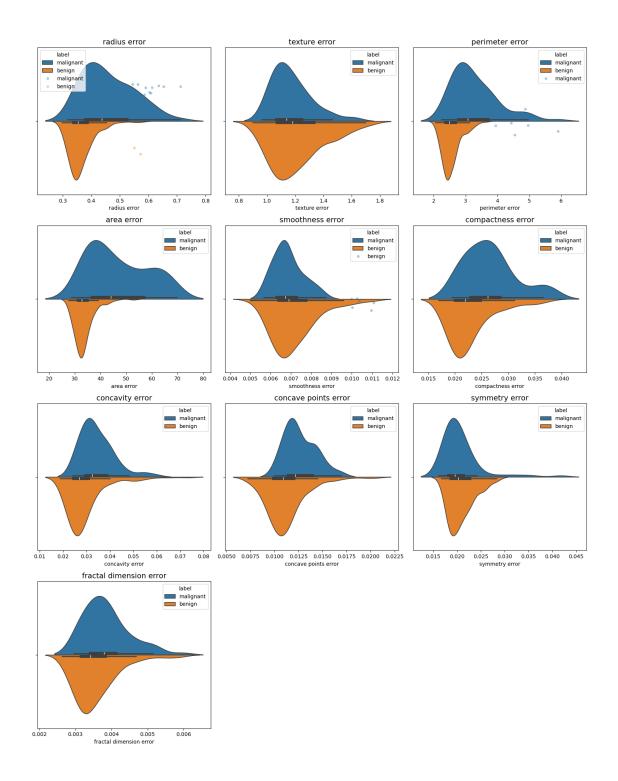
```
[21]: fig, axs = plt.subplots(4, 3, figsize=(15, 20)) # Adjust the figure size as
       \rightarrowneeded
      for i, v in enumerate([feature for feature in feature_names if 'mean' in_
       ofeaturel):
          row, col = divmod(i, 3) # Calculate row and column index for the subplot
          ax = axs[row, col] # Select the appropriate axes for the current plot
          sns.violinplot(data=df, x=v, hue="label", ax=ax, split=True)
          # Identify outliers with IQR
          stats = boxplot_stats(df[v])
          outliers = [item for stat in stats for item in stat['fliers']]
          # Filter df for outliers in the current feature and plot
          sns.stripplot(data=df[df[v].isin(outliers)], x=v, hue="label", ax=ax,_u
       →alpha=0.4, dodge=True)
          ax.set_title(v, fontsize=14) # Adjust title font size as needed
      total_plots = len([feature for feature in feature_names if 'mean' in feature])
      for j in range(total_plots, 4*3):
          row, col = divmod(j, 3)
          axs[row, col].axis('off')
      # Adjust layout
      plt.tight_layout(rect=[0, 0, 1, 0.95]) # Leave space at the top for the legend
      plt.show()
```



[22]: fig, axs = plt.subplots(4, 3, figsize=(15, 20)) # Adjust the figure size as⊔

→needed

```
for i, v in enumerate([feature for feature in feature_names if 'error' in_
 →feature]):
    row, col = divmod(i, 3) # Calculate row and column index for the subplot
    ax = axs[row, col] # Select the appropriate axes for the current plot
    sns.violinplot(data=df, x=v, hue="label", ax=ax, split=True)
    # Identify outliers with IQR
    stats = boxplot_stats(df[v])
    outliers = [item for stat in stats for item in stat['fliers']]
    # Filter df for outliers in the current feature and plot
    sns.stripplot(data=df[df[v].isin(outliers)], x=v, hue="label", ax=ax, u
 →alpha=0.4, dodge=True)
    ax.set_title(v, fontsize=14) # Adjust title font size as needed
total_plots = len([feature for feature in feature_names if 'mean' in feature])
for j in range(total_plots, 4*3):
   row, col = divmod(j, 3)
    axs[row, col].axis('off')
# Adjust layout
plt.tight_layout(rect=[0, 0, 1, 0.95]) # Leave space at the top for the legend
plt.show()
```



```
[23]: ### Final step -> transform target into proper binary values
    df['label'] = df['label'].apply(lambda x: 1 if x == 'malignant' else 0)

[24]: df.info()
```

<class 'pandas.core.frame.DataFrame'>
RangeIndex: 220 entries, 0 to 219
Data columns (total 21 columns):

#	Column	Non-Null Count	Dtype
0	label	220 non-null	int64
1	mean radius	219 non-null	float64
2	mean texture	219 non-null	float64
3	mean perimeter	219 non-null	float64
4	mean area	210 non-null	float64
5	mean smoothness	220 non-null	float64
6	mean compactness	216 non-null	float64
7	mean concavity	216 non-null	float64
8	mean concave points	220 non-null	float64
9	mean symmetry	206 non-null	float64
10	mean fractal dimension	219 non-null	float64
11	radius error	220 non-null	float64
12	texture error	217 non-null	float64
13	perimeter error	220 non-null	float64
14	area error	218 non-null	float64
15	smoothness error	220 non-null	float64
16	compactness error	206 non-null	float64
17	concavity error	218 non-null	float64
18	concave points error	218 non-null	float64
19	symmetry error	219 non-null	float64
20	fractal dimension error	210 non-null	float64
1.	67 (64(60) : (64(4)		

dtypes: float64(20), int64(1)

memory usage: 36.2 KB

3.2 2. Prepare data and models, and make baseline measurements [20%]

- Split data into appropriate sets using the **stratify** option to obtain consistent proportions of classes in each set.
- Decide on appropriate pre-processing steps for the data.
- Implement a very simple baseline model that makes purely random predictions of the class.
- Measure the baseline performance with the following metrics:
 - accuracy
 - balanced accuracy: accounts for imblanaced datasets, defined as (sensitivity + specificity)/2
 - recall
 - precision
 - auc
 - f1score
 - fbeta scores with beta=0.1
 - fbeta score with beta=10
- Also display a confusion matrix for the baseline predictions.
- As a second baseline, implement an SGD classifier and fit it once (without hyper-parameter optimisation) and then display the same performance metrics and a confusion matrix for its

results.

3.2.1 Data Preprocessing Definition

```
[27]: # Some helpful code that you can use if you wish (or not)

from sklearn.metrics import fbeta_score, make_scorer

def f10_score(yt,yp):
    return fbeta_score(yt, yp, beta=10)

def f01_score(yt,yp):
    return fbeta_score(yt, yp, beta=0.1)

f10_scorer = make_scorer(fbeta_score, beta=10)
  f01_scorer = make_scorer(fbeta_score, beta=0.1)
```

```
def print_baseline_metrics(y_true, y_pred):
    print(f"Accuracy: {accuracy_score(y_true, y_pred)}")
    print(f"Balanced Accuracy: {balanced_accuracy_score(y_true, y_pred)}")
    print(f"Recall: {recall_score(y_true, y_pred)}")
    print(f"Precision: {precision_score(y_true, y_pred)}")
    print(f"ROC AUC: {roc_auc_score(y_true, y_pred)}")
    print(f"F1 Score: {f1_score(y_true, y_pred)}")
    print(f"fbeta_scores with beta=0.1: {f01_score(y_true, y_pred)}")
    print(f"fbeta_scores with beta=10: {f10_score(y_true, y_pred)}")
```

3.2.2 Simple Baseline of Random Predictions

```
[29]: baseline_predictions = np.random.choice([0, 1], size=len(y_train))
print_baseline_metrics(y_train, baseline_predictions)
```

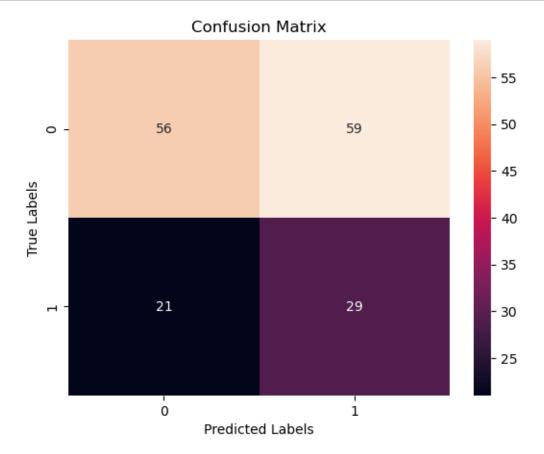
Accuracy: 0.5151515151515151

Balanced Accuracy: 0.5334782608695652

Recall: 0.58

Precision: 0.32954545454545453 ROC AUC: 0.5334782608695652 F1 Score: 0.42028985507246375

fbeta_scores with beta=0.1: 0.3309604519774011 fbeta_scores with beta=10: 0.5756682389937107



3.2.3 Baseline SGD Classifier

[32]: base_sgd_pred = SGD_pipeline.fit(X_train, y_train).predict(X_train)
 train_baseline_predictions = SGD_pipeline.predict(X_train)
print(f"F1 on train set: {f1_score(y_train, train_baseline_predictions)}")
 print_baseline_metrics(y_train, base_sgd_pred)
 plot_confusion_matrix(y_train, base_sgd_pred)

Accuracy: 0.98787878787879

Balanced Accuracy: 0.991304347826087

Recall: 1.0

Precision: 0.9615384615384616 ROC AUC: 0.9913043478260869 F1 Score: 0.9803921568627451

fbeta_scores with beta=0.1: 0.9619047619047619 fbeta_scores with beta=10: 0.9996041171813144

Confusion Matrix - 100 - 80 - 60 - 40 - 20 - Predicted Labels

```
[33]: # Getting Comparable CV Score

cv_score = cross_val_score(SGD_pipeline, X_train, y_train, cv=4, scoring='f1')

print(f"Mean F1 score on CV: {cv_score.mean()}")
```

Mean F1 score on CV: 0.9080964325529542

3.3 3. Model Optimisation [40%]

3.3.1 3.1 Performance metric

Choose one performance metric from the above set. State your choice and explain why you chose it. [50 words maximum]

The aim of the requirements are at least 90% of detecting malignant cancer when it is present - maximizing Precision, and ensure that no more than 1 in 5 healthy cases result in a false postive - minimizing False Positive Rate. To optimize for a combination of these: use F1-score.

$$F1 = 2 \times \frac{\text{precision} \times \text{recall}}{\text{precision} + \text{recall}}$$

3.3.2 3.2 Hyper-parameter optimisation

- Perform a hyper-parameter optimisation (using appropriate methods) on three models:
 - SGD Classifer
 - SVM
 - One other model of your choice
- Display the results of each model (including confusion matrices) and choose the best model.
- Choose the best model and display the final results of this model.

SGD Classifier

```
[34]: SGD_param_grid = {
    'SGD_loss': ['hinge', 'modified_huber', 'squared_hinge', 'perceptron'],
    'SGD_penalty': ['12', '11', 'elasticnet'],
    'SGD_alpha': [0.001, 0.01, 0.1],
}
SGD_grid_search = GridSearchCV(SGD_pipeline, SGD_param_grid, cv=4, scoring='f1')
```

```
[35]: SGD_grid_search.fit(X_train, y_train)
```

```
/Users/nic/Uni/CS7317/.venv/lib/python3.12/site-
packages/sklearn/linear_model/_stochastic_gradient.py:744: ConvergenceWarning:
Maximum number of iteration reached before convergence. Consider increasing
max_iter to improve the fit.
   warnings.warn(
/Users/nic/Uni/CS7317/.venv/lib/python3.12/site-
packages/sklearn/linear_model/_stochastic_gradient.py:744: ConvergenceWarning:
```

```
Maximum number of iteration reached before convergence. Consider increasing
max_iter to improve the fit.
  warnings.warn(
/Users/nic/Uni/CS7317/.venv/lib/python3.12/site-
packages/sklearn/linear model/ stochastic gradient.py:744: ConvergenceWarning:
Maximum number of iteration reached before convergence. Consider increasing
max iter to improve the fit.
  warnings.warn(
/Users/nic/Uni/CS7317/.venv/lib/python3.12/site-
packages/sklearn/linear_model/_stochastic_gradient.py:744: ConvergenceWarning:
Maximum number of iteration reached before convergence. Consider increasing
max_iter to improve the fit.
  warnings.warn(
/Users/nic/Uni/CS7317/.venv/lib/python3.12/site-
packages/sklearn/linear_model/_stochastic_gradient.py:744: ConvergenceWarning:
Maximum number of iteration reached before convergence. Consider increasing
max_iter to improve the fit.
 warnings.warn(
/Users/nic/Uni/CS7317/.venv/lib/python3.12/site-
packages/sklearn/linear_model/_stochastic_gradient.py:744: ConvergenceWarning:
Maximum number of iteration reached before convergence. Consider increasing
max iter to improve the fit.
  warnings.warn(
/Users/nic/Uni/CS7317/.venv/lib/python3.12/site-
packages/sklearn/linear_model/_stochastic_gradient.py:744: ConvergenceWarning:
Maximum number of iteration reached before convergence. Consider increasing
max_iter to improve the fit.
  warnings.warn(
/Users/nic/Uni/CS7317/.venv/lib/python3.12/site-
packages/sklearn/linear_model/_stochastic_gradient.py:744: ConvergenceWarning:
Maximum number of iteration reached before convergence. Consider increasing
max_iter to improve the fit.
  warnings.warn(
/Users/nic/Uni/CS7317/.venv/lib/python3.12/site-
packages/sklearn/linear model/ stochastic gradient.py:744: ConvergenceWarning:
Maximum number of iteration reached before convergence. Consider increasing
max_iter to improve the fit.
  warnings.warn(
/Users/nic/Uni/CS7317/.venv/lib/python3.12/site-
packages/sklearn/linear_model/_stochastic_gradient.py:744: ConvergenceWarning:
Maximum number of iteration reached before convergence. Consider increasing
max_iter to improve the fit.
  warnings.warn(
/Users/nic/Uni/CS7317/.venv/lib/python3.12/site-
packages/sklearn/linear_model/_stochastic_gradient.py:744: ConvergenceWarning:
```

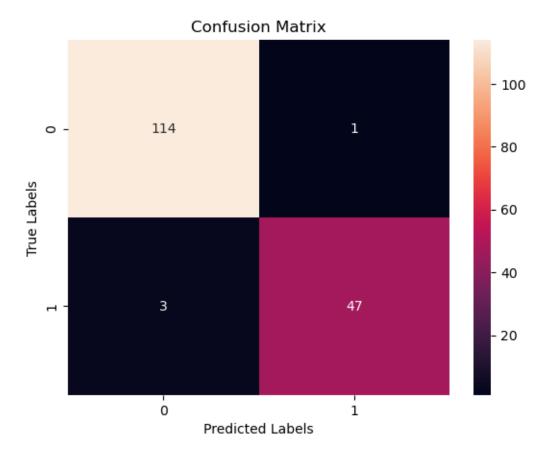
Maximum number of iteration reached before convergence. Consider increasing

max_iter to improve the fit.

warnings.warn(

```
/Users/nic/Uni/CS7317/.venv/lib/python3.12/site-
     packages/sklearn/linear_model/_stochastic_gradient.py:744: ConvergenceWarning:
     Maximum number of iteration reached before convergence. Consider increasing
     max_iter to improve the fit.
       warnings.warn(
     /Users/nic/Uni/CS7317/.venv/lib/python3.12/site-
     packages/sklearn/linear_model/_stochastic_gradient.py:744: ConvergenceWarning:
     Maximum number of iteration reached before convergence. Consider increasing
     max_iter to improve the fit.
       warnings.warn(
     /Users/nic/Uni/CS7317/.venv/lib/python3.12/site-
     packages/sklearn/linear_model/_stochastic_gradient.py:744: ConvergenceWarning:
     Maximum number of iteration reached before convergence. Consider increasing
     max_iter to improve the fit.
       warnings.warn(
[35]: GridSearchCV(cv=4,
                  estimator=Pipeline(steps=[('preprocessing',
                                             Pipeline(steps=[('imputer',
                                                             SimpleImputer()),
                                                             ('scaler',
                                                             StandardScaler())])),
                                            ('SGD',
                                             SGDClassifier(random_state=42))]),
                  param_grid={'SGD_alpha': [0.001, 0.01, 0.1],
                              'SGD__loss': ['hinge', 'modified_huber',
                                            'squared_hinge', 'perceptron'],
                              'SGD_penalty': ['12', '11', 'elasticnet']},
                  scoring='f1')
[36]: SGD_best_estimator = SGD_grid_search.best_estimator_
     print(SGD_best_estimator)
     print(f"mean F1 score of the best estimator in Grid Search: {SGD grid search.
       ⇔best_score_}")
     print(f"Std. Dev of f1 of estimator: {SGD_grid_search.
       Pipeline(steps=[('preprocessing',
                     Pipeline(steps=[('imputer', SimpleImputer()),
                                     ('scaler', StandardScaler())])),
                     ('SGD',
                     SGDClassifier(alpha=0.01, penalty='elasticnet',
                                   random_state=42))])
     mean F1 score of the best estimator in Grid Search: 0.91916666666666667
     Std. Dev of f1 of estimator: 0.07484706629743967
[37]: SGD_y_pred = SGD_best_estimator.predict(X_train)
```

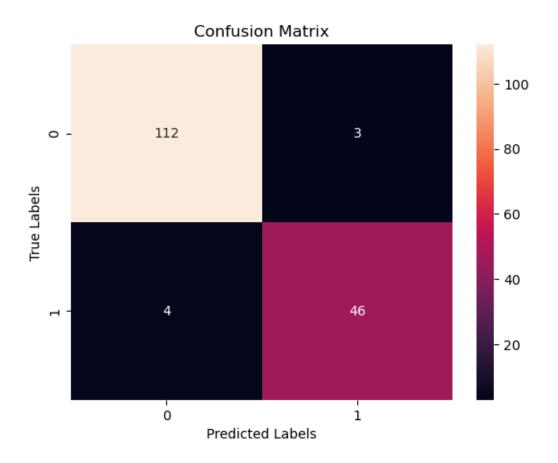
F1 score of the best estimator on entire trainset: 0.9591836734693877



```
SVM_grid_search = GridSearchCV(SVM_pipeline, SVM_param_grid, cv=4, scoring='f1')
[40]: SVM_grid_search.fit(X_train, y_train)
[40]: GridSearchCV(cv=4,
                   estimator=Pipeline(steps=[('preprocessing',
                                              Pipeline(steps=[('imputer',
                                                                SimpleImputer()),
                                                               ('scaler',
                                                                StandardScaler())])),
                                              ('SVM', SVC(random_state=42))]),
                   param_grid={'SVM__C': [0.1, 1, 5, 10, 20],
                               'SVM__degree': [1, 2, 3, 4],
                               'SVM__gamma': [0.1, 1, 10, 100],
                               'SVM_kernel': ['linear', 'poly', 'rbf', 'sigmoid']},
                   scoring='f1')
[41]: SVM_best_estimator = SVM_grid_search.best_estimator_
      print(SVM_best_estimator)
      print(f"Mean F1 score of the best estimator in Grid Search: {SVM_grid_search.
       ⇔best_score_}")
      print(f"Std. Dev of f1 of estimator: {SVM grid search.
       ocv_results_['std_test_score'][SVM_grid_search.best_index_]}")
     Pipeline(steps=[('preprocessing',
                      Pipeline(steps=[('imputer', SimpleImputer()),
                                       ('scaler', StandardScaler())])),
                      ('SVM',
                      SVC(C=0.1, degree=1, gamma=0.1, kernel='linear',
                          random state=42))])
     Mean F1 score of the best estimator in Grid Search: 0.9323076923076923
     Std. Dev of f1 of estimator: 0.05669392545442547
[42]: SVM_y_pred = SVM_best_estimator.predict(X_train)
      print(f"F1 score of the best estimator on entire trainset: {f1 score(y train, |

SVM_y_pred)}")
      plot_confusion_matrix(y_train, SVM_y_pred)
```

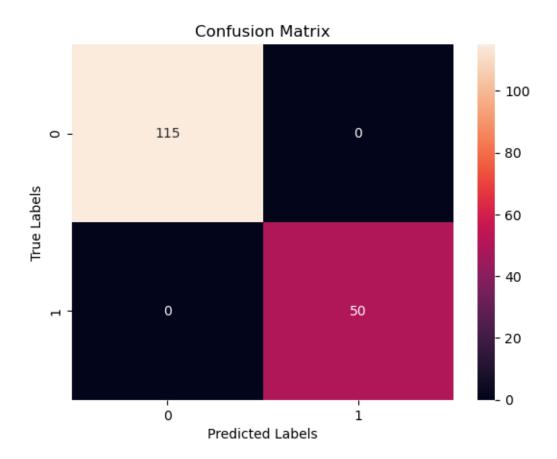
F1 score of the best estimator on entire trainset: 0.9292929292929293



```
Random Forest
[43]: from sklearn.ensemble import RandomForestClassifier
      RF_pipeline = Pipeline(steps = [
          ('preprocessing', preprocessing_pipeline),
          ('RF', RandomForestClassifier(random_state=random_seed, n_jobs = -1))
      ])
[44]: RF_param_grid = {
          'RF_n_estimators': [50, 100, 200, 400],
          'RF_max_depth': [None, 5, 10, 20],
          'RF__criterion': ["gini", "entropy", "log_loss"],
          'RF__max_features': [None, 'sqrt', 'log2'],
          'RF__class_weight': ['balanced', 'balanced_subsample', None]
      }
      RF_grid_search = GridSearchCV(RF_pipeline, RF_param_grid, cv=4, scoring='f1',_
       \rightarrown_jobs=-1)
[45]: RF_grid_search.fit(X_train, y_train)
```

```
[45]: GridSearchCV(cv=4,
                  estimator=Pipeline(steps=[('preprocessing',
                                            Pipeline(steps=[('imputer',
                                                             SimpleImputer()),
                                                            ('scaler',
                                                             StandardScaler())])),
                                            ('RF',
                                            RandomForestClassifier(n_jobs=-1,
     random_state=42))]),
                  n_{jobs}=-1,
                  param_grid={'RF__class_weight': ['balanced', 'balanced_subsample',
                                                  None],
                              'RF__criterion': ['gini', 'entropy', 'log_loss'],
                              'RF__max_depth': [None, 5, 10, 20],
                              'RF_max_features': [None, 'sqrt', 'log2'],
                              'RF_n_estimators': [50, 100, 200, 400]},
                  scoring='f1')
[46]: RF_best_estimator = RF_grid_search.best_estimator_
     print(RF_best_estimator)
     print(f"Mean F1 score of the best estimator on gridsearch: {RF_grid_search.
       ⇔best_score_}")
     print(f"Std. Dev of f1 of estimator: {RF_grid_search.
       Pipeline(steps=[('preprocessing',
                     Pipeline(steps=[('imputer', SimpleImputer()),
                                     ('scaler', StandardScaler())])),
                     ('RF',
                     RandomForestClassifier(class_weight='balanced',
                                            criterion='entropy', max_features=None,
                                           n_jobs=-1, random_state=42))])
     Mean F1 score of the best estimator on gridsearch: 0.9065663322185062
     Std. Dev of f1 of estimator: 0.03558755263053043
[47]: RF_y_pred = RF_best_estimator.predict(X_train)
     print(f"F1 score of the best estimator on validation: {f1_score(y_train,_
       →RF_y_pred)}")
     plot_confusion_matrix(y_train, RF_y_pred)
```

F1 score of the best estimator on validation: 1.0

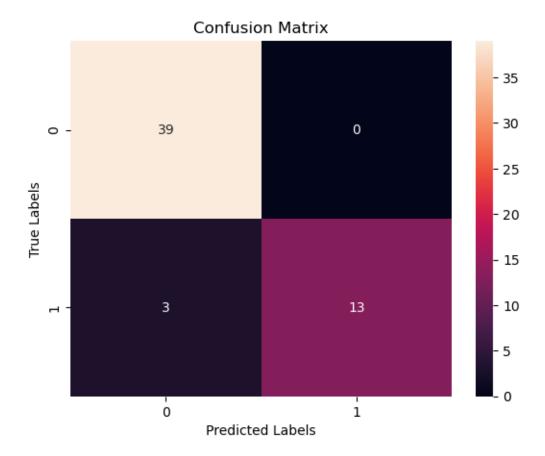


From the experimentation above, we see that SVM classifier performed the best out of all the other models. We then train it with the full X_train and y_train dataset.

Model	Mean F1 from GridSearchCV
Baseline SGD	0.9098
SGD	0.9192
SVM	0.9323
Random Forest	0.9065

```
[59]: best_model_test_pred = best_model.predict(X_test)
    print(f"F1 score of the best estimator on test: {f1_score(y_test, u best_model_test_pred)}")
    plot_confusion_matrix(y_test, best_model_test_pred)
```

F1 score of the best estimator on test: 0.896551724137931



3.3.3 3.3 Final results

From the final results calculate the *probability* that a sample from a person with a malignant tumour is given a result that they do not have cancer.

39 0 3 13

```
[61]: # We look for getting a predicted of 0, given a true lable of 1 print(f'{fn/(fn+tp)*100}%')
```

3.4 4. Decision Boundaries [10%]

- To finish up, the client wants a visualisation of how the final model is working and your line manager has asked you to show some of the decision boundaries.
- The client also wants to know if your method has met their performance specifications.
- Follow the next three steps (4.1, 4.2 and 4.3) to do these things.

3.4.1 4.1 Discriminative features

Although it is only possible to know the true usefulness of a feature when you've combined it with others in a machine learning method, it is still helpful to have some measure for how discriminative each feature is on its own. One common method for doing this is to calculate a T-score (often used in statistics, and in the LDA machine learning method) for each feature.

The formula for the T-score is:

```
(\text{mean}(x2) - \text{mean}(x1))/(0.5*(\text{stddev}(x2) + \text{stddev}(x1)))
```

where x1 and x2 are the feature values corresponding to the two classes. Large values for the T-score (either positive or negative) indicate discriminative ability.

Calculate the T-score for each feature and print out the best 4 features according to this score.

```
[63]: sorted_t_scores = sorted(t_scores.items(), key=lambda x: x[1], reverse=True) print(sorted_t_scores[:4])
```

```
[('mean concave points', np.float64(2.338207079841026)), ('mean perimeter', np.float64(1.9656491051417186)), ('mean concavity', np.float64(1.932435828786661)), ('mean radius', np.float64(1.8482466099087533))]
```

3.4.2 Visualise decision boundaries

Display the decision boundaries for each pair of features from the best 4 chosen above. You can use the functions below to help if you like.

Instead of using the simple mean as the input for xmean in plot_contours, use the following:

```
_0.5*(mean(x1) + mean(x2))_
```

where x1 and x2 are the data associated with the two classes. This way of calculating a "mean" point takes into account any imbalance between the classes.

```
[54]: def make_meshgrid(x, y, ns=100):
          """Create a mesh of points to plot in
          Parameters
          x: data to base x-axis meshgrid on (only min and max used)
          y: data to base y-axis meshgrid on (only min and max used)
          ns: number of steps in grid, optional
          Returns
          _____
          xx, yy: ndarray
          11 11 11
          x_{min}, x_{max} = x.min(), x.max()
          y_{min}, y_{max} = y_{min}(), y_{max}()
          hx = (x_max - x_min)/ns
          hy = (y_max - y_min)/ns
          xx, yy = np.meshgrid(np.arange(x_min, x_max + hx, hx), np.arange(y_min,_
       \rightarrowy_max + hy, hy))
          return xx, yy
```

```
[77]: def plot_contours(clf, xx, yy, xmean, n1, n2, ax, **params):
          """Plot the decision boundaries for a classifier.
          Parameters
          _____
          clf: a classifier
          xx: meshgrid ndarray
          yy: meshgrid ndarray
          xmean: 1d array of N mean values (used to populate constant features with)
          n1, n2: index numbers of features that change
                     that is, which features xx and yy represent, from the set of N_{\sqcup}
       \hookrightarrow features
          params: dictionary of params to pass to contourf, optional
          11 11 11
          # The following lines makes an MxN matrix to pass to the classifier (\#_{\sqcup}
       \hookrightarrow samples x \# features)
          # It does this by multiplying Mx1 and 1xN matrices, where the former is
       ⇔filled with 1's
          # where M is the number of grid points in xx and N is the number of
       ⇔features in xmean
          # It is done in such a way that the xmean vector is replaced in each row
          fullx = np.ones((xx.ravel().shape[0],1)) * np.reshape(xmean,(1,-1))
```

```
fullx[:,n1] = xx.ravel()
fullx[:,n2] = yy.ravel()
Z = clf.predict(fullx)
Z = Z.reshape(xx.shape)
out = ax.contourf(xx, yy, Z, **params)
return out
```

```
[56]: from itertools import combinations
best_features = [f[0] for f in sorted_t_scores[:4]]

feature_pairs = list(combinations(best_features, 2))
print(feature_pairs)
```

[('mean concave points', 'mean perimeter'), ('mean concave points', 'mean concavity'), ('mean concave points', 'mean radius'), ('mean perimeter', 'mean concavity'), ('mean perimeter', 'mean radius'), ('mean concavity', 'mean radius')]

```
[82]: import matplotlib.patches as mpatches
      class_means = 0.5 * (benign.iloc[:,1:].mean() + malignant.iloc[:,1:].mean())
      fig, axs = plt.subplots(3, 2, figsize=(15, 20))
      for i, (x, y) in enumerate(feature_pairs):
          ax = axs[i // 2, i % 2]
          # title for the plots
          title = f''\{x\} vs \{y\}''
          # Set-up grid for plotting.
          X0, X1 = X_train[x], X_train[y]
          xx, yy = make_meshgrid(X0, X1)
          plot_contours(best_model, xx, yy, class_means, X_train.columns.get_loc(x),__
       →X_train.columns.get_loc(y), ax, cmap=plt.cm.coolwarm, alpha=0.8)
          ax.scatter(X0, X1, c=y train, cmap=plt.cm.coolwarm, s=20, edgecolors='k')
          ax.set_xlim(xx.min(), xx.max())
          ax.set_ylim(yy.min(), yy.max())
          ax.set_xlabel(x)
          ax.set ylabel(y)
          ax.legend(handles=[mpatches.Patch(color='Blue', label='Benign'), mpatches.
       →Patch(color='red', label='Malignant')])
          ax.set_xticks(())
          ax.set_yticks(())
          ax.set_title(title)
      plt.show()
```

/Users/nic/Uni/CS7317/.venv/lib/python3.12/site-packages/sklearn/base.py:493: UserWarning: X does not have valid feature names, but SimpleImputer was fitted with feature names

```
warnings.warn(
```

No artists with labels found to put in legend. Note that artists whose label start with an underscore are ignored when legend() is called with no argument.

/Users/nic/Uni/CS7317/.venv/lib/python3.12/site-packages/sklearn/base.py:493: UserWarning: X does not have valid feature names, but SimpleImputer was fitted with feature names

warnings.warn(

No artists with labels found to put in legend. Note that artists whose label start with an underscore are ignored when legend() is called with no argument. /Users/nic/Uni/CS7317/.venv/lib/python3.12/site-packages/sklearn/base.py:493: UserWarning: X does not have valid feature names, but SimpleImputer was fitted with feature names

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warnings.warn(

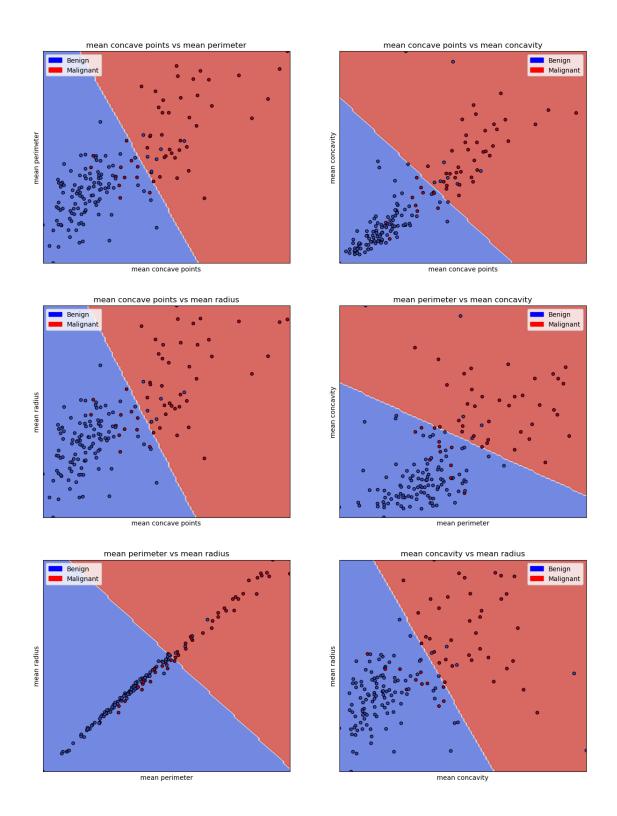
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warnings.warn(

No artists with labels found to put in legend. Note that artists whose label start with an underscore are ignored when legend() is called with no argument.



3.4.3 4.3 Performance specification

Does the final model meet the client's criteria? Explain why or why not. [100 words maximum]

The two requirements that the client is looking for is for a Recall of 90% and a False Positive Rate below 20%. The final model does not fulfill the client's criteria because the mean F1 metric of the best model is at 0.9323 with a standard deviation of 0.0567 after cross-fold validation but when generalizing this to the outsample data, we see that the F1 score is at 0.89, but the Recall of the model is at 81.25% with a False Positive Rate of 0%. The performance of the model only hits one of the two requirements.