Project 2 - 605840292

May 16, 2023

1 Project 2 - Binary Classification Comparative Methods

For this project we're going to attempt a binary classification of a dataset using multiple methods and compare results.

Our goals for this project will be to introduce you to several of the most common classification techniques, how to perform them and tweek parameters to optimize outcomes, how to produce and interpret results, and compare performance. You will be asked to analyze your findings and provide explanations for observed performance.

DEFINITIONS

Binary Classification: In this case a complex dataset has an added 'target' label with one of two options. Your learning algorithm will try to assign one of these labels to the data.

Supervised Learning: This data is fully supervised, which means it's been fully labeled and we can trust the veracity of the labeling.

1.1 Submission Details

Project is due May 17th at 12:00 pm (Wednesday Noon). To submit the project, please save the notebook as a pdf file and submit the assignment via Gradescope. In addition, make sure that all figures are legible and sufficiently large. For best pdf results, we recommend downloading Latex and print the notebook using Latex.

1.2 Loading Essentials and Helper Functions

```
[1]: #Here are a set of libraries we imported to complete this assignment.

#Feel free to use these or equivalent libraries for your implementation import numpy as np # linear algebra import pandas as pd # data processing, CSV file I/O (e.g. pd.read_csv) import matplotlib.pyplot as plt # this is used for the plot the graph import os import time

#Sklearn classes

from sklearn.model_selection import train_test_split, cross_val_score,u

GridSearchCV, KFold

from sklearn import metrics

from sklearn.svm import SVC #SVM classifier
```

```
from sklearn.linear_model import LogisticRegression
     from sklearn.neighbors import KNeighborsClassifier
     from sklearn.metrics import confusion_matrix
     import sklearn.metrics.cluster as smc
     from sklearn.pipeline import Pipeline
     from sklearn.preprocessing import StandardScaler, OneHotEncoder, Normalizer, U
      →MinMaxScaler
     from sklearn.compose import ColumnTransformer, make_column_transformer
     from matplotlib import pyplot
     import itertools
     %matplotlib inline
     #Sets random seed
     import random
     random.seed(42)
[2]: # Helper function allowing you to export a graph
     def save fig(fig_id, tight_layout=True, fig_extension="png", resolution=300):
         path = os.path.join(fig_id + "." + fig_extension)
         print("Saving figure", fig_id)
         if tight_layout:
             plt.tight_layout()
         plt.savefig(path, format=fig_extension, dpi=resolution)
[3]: # Helper function that allows you to draw nicely formatted confusion matrices
     def draw_confusion_matrix(y, yhat, classes):
         111
             Draws a confusion matrix for the given target and predictions
             Adapted from scikit-learn and discussion example.
         111
         plt.cla()
         plt.clf()
         matrix = confusion_matrix(y, yhat)
         plt.imshow(matrix, interpolation='nearest', cmap=plt.cm.YlOrBr)
         plt.title("Confusion Matrix")
         plt.colorbar()
         num_classes = len(classes)
         plt.xticks(np.arange(num_classes), classes, rotation=90)
         plt.yticks(np.arange(num_classes), classes)
         fmt = 'd'
```

```
thresh = matrix.max() / 2.
         for i, j in itertools.product(range(matrix.shape[0]), range(matrix.
      ⇔shape[1])):
             plt.text(j, i, format(matrix[i, j], fmt),
                      horizontalalignment="center",
                      color="white" if matrix[i, j] > thresh else "black")
         plt.ylabel('True label')
         plt.xlabel('Predicted label')
         plt.tight_layout()
         plt.show()
[4]: def heatmap(data, row_labels, col_labels, figsize = (20,12), cmap = "YlGn",
                 cbar_kw={}, cbarlabel="", valfmt="{x:.2f}",
                 textcolors=("black", "white"), threshold=None):
         HHHH
         Create a heatmap from a numpy array and two lists of labels.
         Taken from matplotlib example.
         Parameters
         data
             A 2D numpy array of shape (M, N).
         row_labels
             A list or array of length M with the labels for the rows.
         col_labels
             A list or array of length N with the labels for the columns.
             A `matplotlib.axes.Axes` instance to which the heatmap is plotted. If
             not provided, use current axes or create a new one. Optional.
             A string that specifies the colormap to use. Look at matplotlib docs\sqcup
      \hookrightarrow for information.
             Optional.
         cbar_kw
             A dictionary with arguments to `matplotlib.Figure.colorbar`. Optional.
         cbarlabel
             The label for the colorbar. Optional.
         valfmt
             The format of the annotations inside the heatmap. This should either
             use the string format method, e.g. "x \in \{x: 2f\}", or be a
             `matplotlib.ticker.Formatter`. Optional.
         textcolors
             A pair of colors. The first is used for values below a threshold,
             the second for those above. Optional.
         threshold
```

```
Value in data units according to which the colors from textcolors are
    applied. If None (the default) uses the middle of the colormap as
11 11 11
plt.figure(figsize = figsize)
ax = plt.gca()
# Plot the heatmap
im = ax.imshow(data,cmap=cmap)
# Create colorbar
cbar = ax.figure.colorbar(im, ax=ax, **cbar_kw)
cbar.ax.set_ylabel(cbarlabel, rotation=-90, va="bottom")
# Show all ticks and label them with the respective list entries.
ax.set_xticks(np.arange(data.shape[1]), labels=col_labels)
ax.set_yticks(np.arange(data.shape[0]), labels=row_labels)
# Let the horizontal axes labeling appear on top.
ax.tick_params(top=True, bottom=False,
               labeltop=True, labelbottom=False)
# Rotate the tick labels and set their alignment.
plt.setp(ax.get_xticklabels(), rotation=-30, ha="right",
         rotation_mode="anchor")
# Turn spines off and create white grid.
ax.spines[:].set_visible(False)
ax.set_xticks(np.arange(data.shape[1]+1)-.5, minor=True)
ax.set_yticks(np.arange(data.shape[0]+1)-.5, minor=True)
ax.grid(which="minor", color="w", linestyle='-', linewidth=3)
ax.tick_params(which="minor", bottom=False, left=False)
# Normalize the threshold to the images color range.
if threshold is not None:
    threshold = im.norm(threshold)
else:
    threshold = im.norm(data.max())/2.
# Set default alignment to center, but allow it to be
# overwritten by textkw.
kw = dict(horizontalalignment="center",
          verticalalignment="center")
# Get the formatter in case a string is supplied
```

```
if isinstance(valfmt, str):
             valfmt = matplotlib.ticker.StrMethodFormatter(valfmt)
         # Loop over the data and create a `Text` for each "pixel".
         # Change the text's color depending on the data.
         texts = []
         for i in range(data.shape[0]):
             for j in range(data.shape[1]):
                 kw.update(color=textcolors[int(im.norm(data[i, j]) > threshold)])
                 text = im.axes.text(j, i, valfmt(data[i, j], None), **kw)
                 texts.append(text)
[5]: def make_meshgrid(x, y, h=0.02):
         """Create a mesh of points to plot in
         Parameters
         x: data to base x-axis meshgrid on
         y: data to base y-axis meshgrid on
         h: stepsize for meshgrid, optional
         Returns
```

```
xx, yy: ndarray
    11 11 11
    x \min, x \max = x.\min() - 1, x.\max() + 1
    y_{min}, y_{max} = y.min() - 1, y.max() + 1
    xx, yy = np.meshgrid(np.arange(x_min, x_max, h), np.arange(y_min, y_max, h))
    return xx, yy
def plot_contours(clf, xx, yy, **params):
    """Plot the decision boundaries for a classifier.
    Parameters
    _____
    ax: matplotlib axes object
    clf: a classifier
    xx: meshgrid ndarray
    yy: meshqrid ndarray
    params: dictionary of params to pass to contourf, optional
    Z = clf.predict(np.c_[xx.ravel(), yy.ravel()])
    Z = Z.reshape(xx.shape)
    out = plt.contourf(xx, yy, Z, **params)
    return out
```

```
def draw_contour(x,y,clf, class_labels = ["Negative", "Positive"]):
    """
    Draws a contour line for the predictor

    Assumption that x has only two features. This functions only plots the
    ifirst two columns of x.

    """

    X0, X1 = x[:, 0], x[:, 1]
    xx0, xx1 = make_meshgrid(X0,X1)

plt.figure(figsize = (10,6))
    plot_contours(clf, xx0, xx1, cmap="PiYG", alpha=0.8)
    scatter=plt.scatter(X0, X1, c=y, cmap="PiYG", s=30, edgecolors="k")
    plt.legend(handles=scatter.legend_elements()[0], labels=class_labels)

plt.xlim(xx0.min(), xx0.max())
    plt.ylim(xx1.min(), xx1.max())
```

2 Example Project

In this part, we will go over how to perform a Binary classification task using a variety of models. We will provide examples of how to train and evaluate these models.

2.1 Dataset Description

Healthcare is an important industry that uses machine learning to aid doctors in diagnosing many different kinds of illnesses and diseases. For this example project, we will be using the Breast Cancer Wisconsin Dataset to determine whether a mass found in a body is benign or malignant.

Features are computed from a digitized image of a fine needle aspirate (FNA) of a breast mass. They describe characteristics of the cell nuclei present in the image.

Feature Information:

```
Column 1: ID number
```

```
Column 2: Diagnosis (M = malignant, B = benign)
```

Ten real-valued features are computed for each cell nucleus:

- 1. radius (mean of distances from center to points on the perimeter)
- 2. texture (standard deviation of gray-scale values)
- 3. perimeter
- 4. area
- 5. smoothness (local variation in radius lengths)
- 6. compactness (perimeter^2 / area 1.0)
- 7. concavity (severity of concave portions of the contour)
- 8. concave points (number of concave portions of the contour)

9. symmetry

```
10. fractal dimension ("coastline approximation" - 1)
```

Due to the statistical nature of the test, we are not able to get exact measurements of the previous values. Instead, the dataset contains the mean and standard error of the real-valued features.

Columns 3-12 present the mean of the measured values

Columns 13-22 present the standard error of the measured values

2.2 Load and Analyze the dataset

```
[6]: #Load Data
data = pd.read_csv('datasets/breast_cancer_data.csv')
```

Always look at your dataset after loading it. Use information from .describe and .info to learn more about the dataset.

```
data.head(5)
[7]:
[7]:
               id diagnosis
                              radius_mean
                                            texture_mean
                                                           perimeter_mean
                                                                             area_mean
     0
          842302
                           М
                                     17.99
                                                    10.38
                                                                    122.80
                                                                                1001.0
     1
          842517
                           М
                                     20.57
                                                    17.77
                                                                    132.90
                                                                                1326.0
                           М
     2
        84300903
                                     19.69
                                                    21.25
                                                                    130.00
                                                                                1203.0
                           М
                                     11.42
                                                    20.38
                                                                     77.58
     3
        84348301
                                                                                 386.1
        84358402
                           Μ
                                     20.29
                                                    14.34
                                                                    135.10
                                                                                1297.0
        smoothness mean
                           compactness_mean
                                               concavity_mean
                                                                concave points_mean \
     0
                 0.11840
                                     0.27760
                                                       0.3001
                                                                             0.14710
                 0.08474
     1
                                     0.07864
                                                       0.0869
                                                                             0.07017
     2
                 0.10960
                                     0.15990
                                                       0.1974
                                                                             0.12790
     3
                 0.14250
                                     0.28390
                                                       0.2414
                                                                             0.10520
     4
                 0.10030
                                     0.13280
                                                       0.1980
                                                                             0.10430
           radius_se
                        texture_se
                                    perimeter_se
                                                    area_se
                                                              smoothness_se
     0
               1.0950
                            0.9053
                                            8.589
                                                     153.40
                                                                   0.006399
               0.5435
                                            3.398
                                                      74.08
     1
                            0.7339
                                                                   0.005225
     2
               0.7456
                            0.7869
                                            4.585
                                                      94.03
                                                                   0.006150
     3
                                                      27.23
               0.4956
                                            3.445
                                                                   0.009110
                            1.1560
     4
               0.7572
                            0.7813
                                            5.438
                                                      94.44
                                                                   0.011490
                          concavity_se
        compactness_se
                                         concave points_se
                                                              symmetry_se
     0
                0.04904
                               0.05373
                                                    0.01587
                                                                  0.03003
     1
                0.01308
                               0.01860
                                                    0.01340
                                                                  0.01389
     2
                0.04006
                               0.03832
                                                    0.02058
                                                                  0.02250
     3
                0.07458
                               0.05661
                                                    0.01867
                                                                  0.05963
     4
                0.02461
                               0.05688
                                                    0.01885
                                                                  0.01756
```

fractal_dimension_se

0	0.006193
1	0.003532
2	0.004571
3	0.009208
4	0.005115

[5 rows x 22 columns]

[8]: data.describe()

[8]:		id	rad	lius_mean	text	cure_mean	per	rimeter_mean	area	a_mean	\
	count	5.690000e+02	56	9.000000	56	39.000000		569.000000	569.0	000000	
	mean	3.037183e+07	1	4.127292	1	19.289649		91.969033	654.8	389104	
	std	1.250206e+08		3.524049		4.301036		24.298981	351.9	914129	
	min	8.670000e+03		6.981000		9.710000		43.790000	143.	500000	
	25%	8.692180e+05	1	1.700000	-	16.170000		75.170000	420.3	300000	
	50%	9.060240e+05	1	3.370000	-	18.840000		86.240000	551.	100000	
	75%	8.813129e+06	1	5.780000	2	21.800000		104.100000	782.	700000	
	max	9.113205e+08	2	8.110000	3	39.280000		188.500000	2501.0	000000	
		smoothness_mea	a n	compactne	ac ma	an conca	,,i+,	y_mean conc	ave poi	nta maa	n \
	count	569.0000		-	.0000			y_mean conc 000000	-	9.00000	
	mean	0.0963			0.1043			088799		0.04891	
	std	0.0140			0.0528			079720		0.038803	
	min	0.0526			0.0320			000000		0.00000	
	25%	0.0863			0.0649			029560		0.02031	
	50%	0.0958			0.092630 0.061540		0.033500				
			. 1304			0.074000					
	max				.3454			0.201200			
	man	0.1001		0.010			٠.	120000			Ü
		symmetry_mean		radius_	se t	exture_se	ре	erimeter_se	area	a_se \	
	count	569.000000	•••	569.0000	-	- 569.000000	1	569.000000	569.000	_	
	mean	0.181162	•••	0.4051	.72	1.216853		2.866059	40.33	7079	
	std	0.027414	•••	0.2773	313	0.551648		2.021855	45.49	1006	
	min	0.106000	•••	0.1115	00	0.360200		0.757000	6.80	2000	
	25%	0.161900	•••	0.2324	00	0.833900		1.606000	17.85	0000	
	50%	0.179200	•••	0.3242	200	1.108000		2.287000	24.53	0000	
	75%	0.195700	•••	0.4789	000	1.474000		3.357000	45.19	0000	
	max	0.304000	•••	2.8730	000	4.885000		21.980000	542.20	0000	
										,	
		smoothness_se	co	mpactness	_	concavity	_	concave po	_	\	
	count	569.000000		569.000		569.000			.000000		
	mean	0.007041		0.025		0.031			0.011796		
	std	0.003003		0.017		0.030			.006170		
	min	0.001713		0.002		0.000			0.000000		
	25%	0.005169		0.013		0.015			.007638		
	50%	0.006380		0.020	450	0.025	890	C	.010930		

75% max	0.00814 0.03113		0.042050 0.396000	0.014710 0.052790
count mean	symmetry_se 569.000000 0.020542	fractal_dimension_se 569.000000 0.003795		
std	0.008266	0.002646		
min	0.007882	0.000895		
25%	0.015160	0.002248		
50%	0.018730	0.003187		
75%	0.023480	0.004558		
max	0.078950	0.029840		

[8 rows x 21 columns]

[9]: data.info()

<class 'pandas.core.frame.DataFrame'>
RangeIndex: 569 entries, 0 to 568
Data columns (total 22 columns):

#	Column	Non-Null Count	Dtype
0	id	569 non-null	 int64
1	diagnosis	569 non-null	object
2	radius_mean	569 non-null	float64
3	texture_mean	569 non-null	float64
4	perimeter_mean	569 non-null	float64
5	area_mean	569 non-null	float64
6	smoothness_mean	569 non-null	float64
7	compactness_mean	569 non-null	float64
8	concavity_mean	569 non-null	float64
9	concave points_mean	569 non-null	float64
10	symmetry_mean	569 non-null	float64
11	fractal_dimension_mean	569 non-null	float64
12	radius_se	569 non-null	float64
13	texture_se	569 non-null	float64
14	perimeter_se	569 non-null	float64
15	area_se	569 non-null	float64
16	smoothness_se	569 non-null	float64
17	compactness_se	569 non-null	float64
18	concavity_se	569 non-null	float64
19	concave points_se	569 non-null	float64
20	symmetry_se	569 non-null	float64
21	fractal_dimension_se	569 non-null	float64
٠.	67 .04(00)04(4)	1 1 1 (4)	

dtypes: float64(20), int64(1), object(1)

memory usage: 97.9+ KB

While .info shows that every entry has 569 non-null and there are 569 entries, it is good to explicitly

check for nulls.

[10]:	data.isnull().sum()	
[10]:	id	0
	diagnosis	0
	radius_mean	0
	texture_mean	0
	perimeter_mean	0
	area_mean	0
	smoothness_mean	0
	compactness_mean	0
	concavity_mean	0
	concave points_mean	0
	symmetry_mean	0
	fractal_dimension_mean	0
	radius_se	0
	texture_se	0
	perimeter_se	0
	area_se	0
	smoothness_se	0
	compactness_se	0
	concavity_se	0
	concave points_se	0
	symmetry_se	0
	<pre>fractal_dimension_se dtype: int64</pre>	0

Awesome! No need for imputation!

While we are looking at the dataset, we shall remove the "id" column.

```
[11]: data = data.drop(["id"],axis= 1)
```

2.2.1 Looking at the target labels

For this project, we wish to classify the diagnosis column.

```
[12]: data["diagnosis"]
[12]: 0
              М
      1
              Μ
      2
              М
      3
              М
      4
              М
      564
              Μ
      565
              Μ
      566
              Μ
```

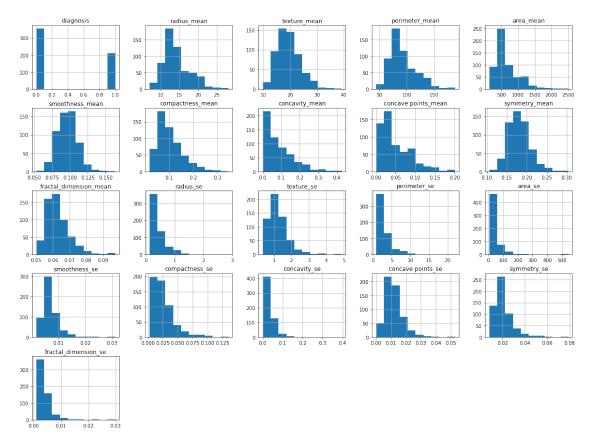
```
567 M
568 B
Name: diagnosis, Length: 569, dtype: object
```

We need to transform this column into numerical column so that we may use them in our models. To do this, we will employ the LabelEncoder to automatically transform all the target label.

```
[13]: from sklearn.preprocessing import LabelEncoder
      le = LabelEncoder()
      data['diagnosis'] = le.fit_transform(data['diagnosis'])
      print(le.classes_)
      ['B' 'M']
[14]: data['diagnosis']
[14]: 0
             1
      1
             1
      2
      3
      4
      564
             1
      565
             1
      566
             1
      567
      568
      Name: diagnosis, Length: 569, dtype: int64
```

2.2.2 Let's look at a histogram of the full dataset.

Its always good to get a global view of your datasets by looking at their histograms. You might see some interesting trends.

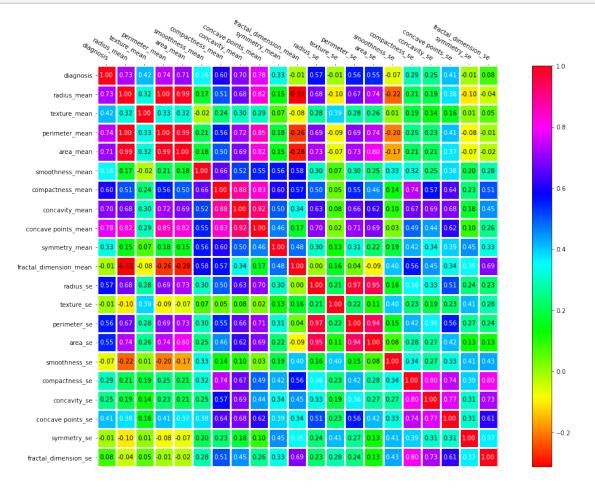


From the histograms, we can see some interesting trends. Possible observations:

- Many of the _se columns indicate a heavy skewness towards low values and have large tails
- Many of the _mean columns look more Gaussian in shape
- There is a large disparity between the ranges of certain features. For example, radius mean can go from 0 to 25 while smoothness_mean is in the range [0.050,0.150]. This indicates we will have to normalize or standardize the features if the models are sensitive to such measures.

2.2.3 Looking at the correlation matrix to get an idea about which features are important

```
[16]: correlations = data.corr()
    columns = list(data)
    #Creates the heatmap
    heatmap(correlations.values,columns,figsize = (20,12),cmap="hsv")
```



```
[17]: #Let's specifically look at the correlations of our target feature correlations["diagnosis"].sort_values(ascending=False)
```

```
[17]: diagnosis
                                 1.000000
      concave points_mean
                                 0.776614
      perimeter_mean
                                 0.742636
      radius_mean
                                 0.730029
      area_mean
                                 0.708984
      concavity_mean
                                 0.696360
      compactness_mean
                                 0.596534
      radius_se
                                 0.567134
```

```
perimeter_se
                           0.556141
                           0.548236
area_se
texture_mean
                           0.415185
concave points_se
                           0.408042
smoothness_mean
                           0.358560
symmetry_mean
                           0.330499
compactness_se
                           0.292999
concavity_se
                           0.253730
fractal_dimension_se
                           0.077972
symmetry_se
                          -0.006522
texture_se
                          -0.008303
fractal_dimension_mean
                          -0.012838
smoothness se
                          -0.067016
Name: diagnosis, dtype: float64
```

We can see that there is a lot of correlation between the features and the target label. Thus, we can expect to learn something from the data

2.2.4 When doing classification, check if classes are heavily imbalanced.

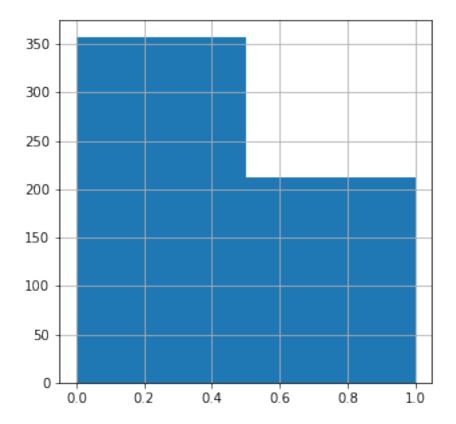
It is important that the dataset does not prefer one class over any others. Otherwise, it may bias the model to not learn the minority classes well.

Lets use a histogram and count the number of elements in each class.

```
[19]: data['diagnosis'].hist(bins=2, figsize=(5,5))
data['diagnosis'].value_counts()
```

[19]: 0 357 1 212

Name: diagnosis, dtype: int64



There is a bit of an imbalance which is something to keep in mind if we find that our models do not perform well on the minority classes. For our purposes, this imbalance is not big enough to be an issue so we will not perform balancing techniques for this dataset.

Since the dataset is small though, we want to be careful when making training and testing splits to ensure that there is enough of each class for both splits. We will show how to perform this shortly.

2.2.5 Setting up the data

Before starting any model training, we have to split up the target labels from our features.

```
[20]: y = data["diagnosis"]
x = data.drop(["diagnosis"],axis = 1)
```

Now, we also split the data into training and testing data. To ensure that there is not an imbalance of classes in the training and testing set, we will use the stratify parameter in train_test_split to perform stratified sampling on the data (Recall from lecture how stratified sampling is performed).

```
[22]: train_raw, test_raw, target, target_test = train_test_split(x,y, test_size=0.2, stratify= y, random_state=0)
```

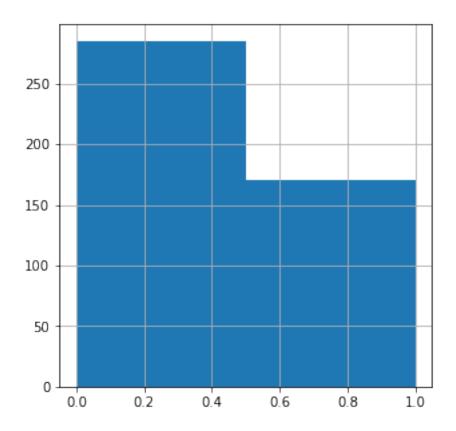
Note that we named the input feature data as raw to indicate that there has been no pre-processing on them such as standardization. Shortly, we will show the affect that pre-processing has on the performance of the model.

Let us quickly test that the splits are somewhat balanced.

[23]: #Training classes
 target.hist(bins=2, figsize=(5,5))
 target.value_counts()

[23]: 0 285 1 170

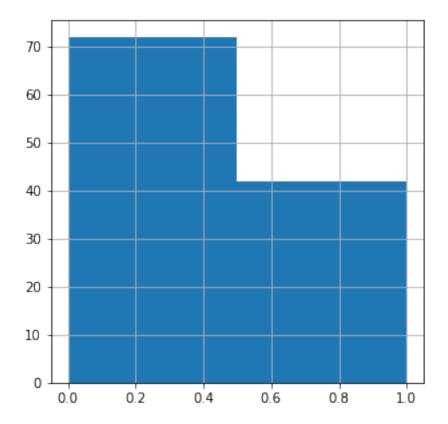
Name: diagnosis, dtype: int64



[24]: #Testing classes
target_test.hist(bins=2, figsize=(5,5))
target_test.value_counts()

[24]: 0 72 1 42

Name: diagnosis, dtype: int64



We can see that the class balance is about the same as before the split. In fact, we can see that if a classifier just guessed class 0, it would have an accuracy of $100 * \frac{72}{72+42} = 63.15\%$. We can consider this the baseline accuracy to compare against.

2.3 Models for Classification: KNN

For our first model, we will use KNN classification. This is a model we have seen many times throughout the course and it would be interesting to see how well it performs.

2.3.1 Simple KNN classification with K=3

Let us try KNN on the raw data with simply 3 nearest neighbors. We use the sklearn metric library to calculate the measures of interest. In this case, we focus on accuracy.

```
[25]: # k-Nearest Neighbors algorithm
knn = KNeighborsClassifier(n_neighbors=3)
knn.fit(train_raw, target)
predicted = knn.predict(test_raw)
[26]: print("%-12s %f" % ('Accuracy:', metrics.accuracy_score(target_test,predicted)))
```

Accuracy: 0.877193

We can see that there is already a huge improvement in accuracy on comparison to the baseline of 63.15%. Let's see the effect that standardizing the input features would have on the KNN performance.

2.3.2 Affect of pre-processing on KNN

```
[31]: # k-Nearest Neighbors algorithm
knn = KNeighborsClassifier(n_neighbors=3)
knn.fit(train, target)
testing_result = knn.predict(test)
predicted = knn.predict(test)
```

```
[32]: print("%-12s %f" % ('Accuracy:', metrics.accuracy_score(target_test,predicted)))
```

Accuracy: 0.921053

We can see that with pre-processing we were able to get a much better classification accuracy.

Here we only used StandardScaler. Lets see if other pre-processing techniques could have also worked. As such, lets look at MinMaxScaler and Normalizer:

```
print("%-12s %f" % ('Accuracy:', metrics.

accuracy_score(target_test,predicted)))
```

StandardScaler()

Accuracy: 0.903509

MinMaxScaler()

Accuracy: 0.912281

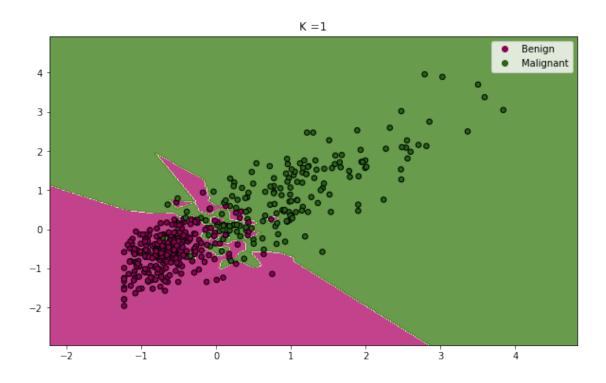
Normalizer()

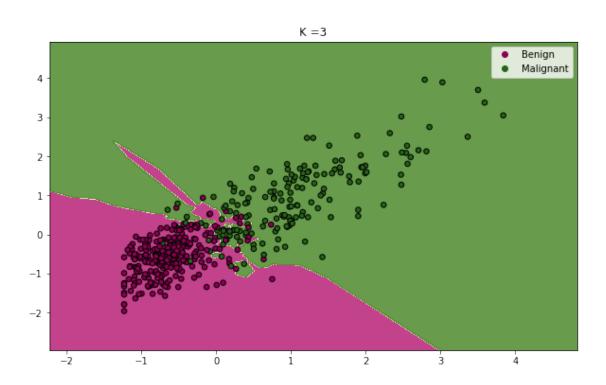
Accuracy: 0.885965

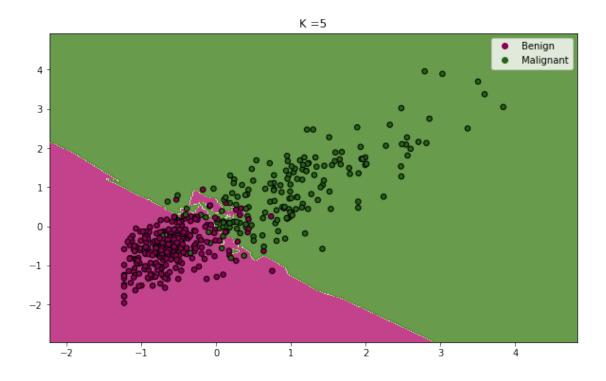
We can see that MinMaxScaler had the same performance as StandardScaler. Yet, Normalizer did not improve the model.

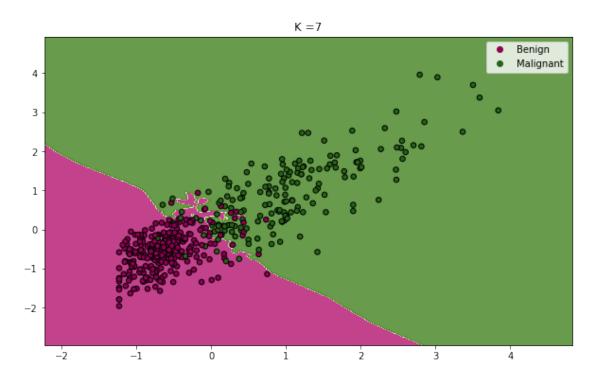
2.3.3 Visualizing decision boundaries for KNN

Its always nice to see the decision boundaries a model decides upon. Let's see how the decision boundary changes as function of k when only using the two most correlated features to the target labels: concave_points_mean and perimeter_mean.









We can see that as k gets larger, the decision boundary gets smoother.

2.4 Models for Classification: Logistic Regression

While KNN is a very powerful model, it does come with a few issues such as

- Require storing the full training dataset
- Prediction is done by comparing new sample will all samples in training set which is timeconsuming

These issues arise because KNN is a non-parametric model which means that it does not summarize the data into a finite set of parameters.

Let us now look at Logistic Regression which is an example of a **parametric** model.

2.4.1 Simple Logistic Regression

First, let us see how logistic regression performs without any regularization.

```
[35]: log_reg = LogisticRegression(penalty = "12", max_iter = 1000, solver = "lbfgs", L
       C=(10**30)/1)
      #C is choosen to be high to remove regularization
      #We could have chosen penalty = "none" since lbfgs supports it but this option_
       ⇔is not possible for all solvers.
      log_reg.fit(train_raw, target)
      testing_result = log_reg.predict(test_raw)
      predicted = log_reg.predict(test_raw)
      print("%-12s %f" % ('Accuracy:', metrics.accuracy_score(target_test,predicted)))
     Accuracy:
                  0.947368
     /Users/mac/opt/anaconda3/lib/python3.9/site-
     packages/sklearn/linear_model/_logistic.py:814: ConvergenceWarning: lbfgs failed
```

to converge (status=1):

STOP: TOTAL NO. of ITERATIONS REACHED LIMIT.

Increase the number of iterations (max_iter) or scale the data as shown in: https://scikit-learn.org/stable/modules/preprocessing.html Please also refer to the documentation for alternative solver options: https://scikit-learn.org/stable/modules/linear_model.html#logisticregression n_iter_i = _check_optimize_result(

We can see that Logistic Regression is actually performing much better than any of the KNN models we tried. We can also see the parameters that the model learned.

```
[36]: #Parameters for each feature
      log_reg.coef_
```

```
[36]: array([[ 9.75423152e+00, 5.06832782e-01, -1.63991042e+00,
              1.01663531e-02, 4.16595527e+01, 2.35566119e+01,
```

```
7.32616576e+01, 6.70896388e+01, 2.46406166e+01,
-4.92793866e-01, -3.36139407e+01, -2.64891845e+00,
1.22770175e+00, 4.02112983e-01, -2.27236940e+00,
-5.13525815e+01, -7.17092758e+01, -8.21666313e+00,
-1.80542274e+01, -1.15006379e+01]])

[37]: #Intercept term
log reg.intercept
```

```
log_reg.intercept_
```

```
[37]: array([-20.4799503])
```

```
[38]: print("Number of Features in data:", train_raw.shape[1])
print("Number of Parameters:", len(log_reg.coef_[0]))
```

```
Number of Features in data: 20
Number of Parameters: 20
```

Since we are using Logistic Regression where we model the log odds with a linear function, it makes sense that we have a parameter/coefficient for each input feature.

2.4.2 Parameters for Logistic Regression

In Sci-kit Learn, the following are just some of the parameters we can pass into Logistic Regression:

- penalty: {'l1', 'l2', 'elasticnet', 'none'} default="l2"
 - Specifies the type of regularization to use. Not all penalties work for each solver.
- C: positive float, default=1
 - Inverse of the regularization strength. You can treat C as $\frac{1}{\lambda}$ as shown in lecture. Thus, as C gets smaller, the regularization strength increases.
- solver: {'newton-cg', 'lbfgs', 'liblinear', 'sag', 'saga'}, default='lbfgs'
 - Algorithm to use in the optimization problem. Each algorithms solves logistic regression using different iterative methods that are based on the gradient. Read the sci-kit learn documentation for more information.
- max iter: int, default=100
 - Maximum number of iterations taken for the solvers to converge.

Each parameter has a different effect on the model. Let's look at how the choose of max_iter affects the model performance on the raw data and the standardized dataset.

Raw Data Accuracy: 0.938596 Preprocessed Data Accuracy: 0.947368

We see that the accuraccies are pretty close to each other. Lets see what happens when we decrease the max iter.

```
[41]: log_reg = LogisticRegression(penalty = "12",max_iter = 70, solver = "lbfgs", C=⊔
→0.01)

#Train raw is the data before preprocessing
log_reg.fit(train_raw, target)
predicted = log_reg.predict(test_raw)
print("%-12s %f" % ('Raw Data Accuracy:', metrics.
→accuracy_score(target_test,predicted)))
```

Raw Data Accuracy: 0.921053

/Users/mac/opt/anaconda3/lib/python3.9/sitepackages/sklearn/linear_model/_logistic.py:814: ConvergenceWarning: lbfgs failed to converge (status=1): STOP: TOTAL NO. of ITERATIONS REACHED LIMIT.

Increase the number of iterations (max_iter) or scale the data as shown in: https://scikit-learn.org/stable/modules/preprocessing.html

Please also refer to the documentation for alternative solver options:

 $\verb|https://scikit-learn.org/stable/modules/linear_model.html#logistic-regression| \\$

n_iter_i = _check_optimize_result(

Ooops! The model did not seem to converge. Its seem that the scale of the features strongly affects the convergence speed of the iterative algorithm. As suggested, we can fix this issue by increaing the max_iter, re-scaling the data, or using a different solver.

```
[42]: #Train is the data after preprocessing (using Standard scalar)
log_reg.fit(train, target)
predicted = log_reg.predict(test)

print("%-12s %f" % ('Preprocessed Data Accuracy:', metrics.

→accuracy_score(target_test,predicted)))
```

Preprocessed Data Accuracy: 0.947368

2.4.3 Cross Validation for Logistic Regression

Let us do a little experiment using cross validation to see how each term affects the logistic regression. We will perform this example on the standardized data.

```
[43]: #You may even do Cross validation for classification
      from sklearn.model_selection import GridSearchCV
      #Note that this a list of dict
      #Each dict describes the combination of parameters to check
      parameters = [
          {"penalty": ["12"],
          "C": [0.01,1,100],
          "solver": ["lbfgs","liblinear"]},#These solvers support penalty = "l2"
          {"penalty": ["none"],
          "C": [1], #Specified to prevent error message
          "solver": ["lbfgs", "newton-cg"]}, #These solvers support penalty = "none"
      ]
      #instantiate model
      #Implementing cross validation
      k = 3
      kf = KFold(n_splits=k, random_state=None)
      log_reg = LogisticRegression(penalty = "none", max_iter = 1000, solver = ___
      →"lbfgs") #will change parameters during CV
      grid = GridSearchCV(log_reg , parameters, cv = kf, scoring = "accuracy")
      grid.fit(train,target)
```

scoring='accuracy')

```
[44]: #Put results into Dataframe
      res= pd.DataFrame(grid.cv_results_)
[44]:
         mean_fit_time
                         std_fit_time
                                        mean_score_time
                                                          std_score_time param_C
      0
                                                0.001001
                                                                 0.000107
                                                                             0.01
              0.009472
                             0.001411
      1
              0.012911
                             0.015354
                                                0.000847
                                                                 0.000324
                                                                              0.01
      2
                                                0.001141
              0.028138
                             0.014131
                                                                 0.000399
      3
              0.004245
                             0.000911
                                                0.002702
                                                                 0.000691
                                                                                 1
      4
              0.040667
                             0.005057
                                                0.000490
                                                                 0.000014
                                                                               100
      5
              0.002956
                             0.000118
                                                0.000463
                                                                 0.000013
                                                                               100
      6
              0.087847
                             0.049634
                                                0.000490
                                                                 0.000010
                                                                                 1
      7
                                                0.000517
                                                                                 1
              0.074966
                             0.057169
                                                                 0.000014
        param_penalty param_solver
                    12
      0
                              lbfgs
                    12
                          liblinear
      1
      2
                    12
                              lbfgs
      3
                    12
                          liblinear
      4
                    12
                              lbfgs
      5
                    12
                          liblinear
      6
                              lbfgs
                  none
      7
                  none
                          newton-cg
                                                       params split0_test_score
      0
           {'C': 0.01, 'penalty': '12', 'solver': 'lbfgs'}
                                                                         0.914474
      1
         {'C': 0.01, 'penalty': '12', 'solver': 'liblin...
                                                                       0.921053
      2
              {'C': 1, 'penalty': '12', 'solver': 'lbfgs'}
                                                                         0.960526
          {'C': 1, 'penalty': '12', 'solver': 'liblinear'}
      3
                                                                         0.960526
            {'C': 100, 'penalty': '12', 'solver': 'lbfgs'}
      4
                                                                         0.947368
         {'C': 100, 'penalty': '12', 'solver': 'libline...
                                                                       0.947368
            {'C': 1, 'penalty': 'none', 'solver': 'lbfgs'}
                                                                         0.934211
         {'C': 1, 'penalty': 'none', 'solver': 'newton-...
                                                                       0.940789
         split1_test_score
                             split2_test_score
                                                  mean_test_score
                                                                    std_test_score
      0
                   0.927632
                                                                          0.008425
                                       0.907285
                                                         0.916463
                   0.953947
                                                                          0.014288
      1
                                       0.927152
                                                         0.934051
      2
                   0.960526
                                       0.947020
                                                         0.956024
                                                                          0.006367
      3
                   0.960526
                                       0.953642
                                                         0.958232
                                                                          0.003245
      4
                   0.947368
                                       0.907285
                                                         0.934007
                                                                          0.018896
      5
                   0.953947
                                       0.907285
                                                         0.936200
                                                                          0.020622
      6
                   0.953947
                                       0.907285
                                                         0.931814
                                                                          0.019125
      7
                   0.953947
                                       0.920530
                                                         0.938422
                                                                          0.013745
```

rank test score

```
0
                       8
                       5
1
2
                       2
3
                       1
4
                       6
5
                       4
6
                       7
7
                       3
```

```
[45]: #Extract the columns that specify the score and the parameters for each row res[["rank_test_score","param_C","param_penalty","param_solver","mean_test_score"]]
```

[45]:	rank_test_score	param_C	param_penalty	param_solver	mean_test_score
0	8	0.01	12	lbfgs	0.916463
1	5	0.01	12	liblinear	0.934051
2	2	1	12	lbfgs	0.956024
3	1	1	12	liblinear	0.958232
4	6	100	12	lbfgs	0.934007
5	4	100	12	liblinear	0.936200
6	7	1	none	lbfgs	0.931814
7	3	1	none	newton-cg	0.938422

We can see that the choice of these parameters can strongly affect performance of the classifier. Lets check the performance of the best parameters on the test set.

```
[46]: #Train raw is the data before preprocessing
predicted = grid.predict(test)
print("%-12s %f" % ('Accuracy:', metrics.accuracy_score(target_test,predicted)))
```

Accuracy: 0.938596

Note that this test accuracy is not as good as some of the other logistic regression examples we've shown.

2.4.4 Speedtest between KNN and Logistic Regression

Lets see how long KNN and Logistic Regression take to perform training and testing.

```
[47]: scaler = StandardScaler()
    train = scaler.fit_transform(train_raw)
    test = scaler.fit_transform(test_raw)

log_reg = LogisticRegression(penalty = "none",max_iter = 1000)
    knn = KNeighborsClassifier(n_neighbors=3)

t0 = time.time()
    knn.fit(train, target)
    t1 = time.time()
```

```
print("KNN Training Time : ", t1-t0)

t0 = time.time()
log_reg.fit(train, target)
t1 = time.time()
print("Logistic Regression Training Time : ", t1-t0)
```

KNN Training Time : 0.0008308887481689453 Logistic Regression Training Time : 0.19958877563476562

```
[48]: t0 = time.time()
knn.predict(test)
t1 = time.time()
print("KNN Testing Time : ", t1-t0)

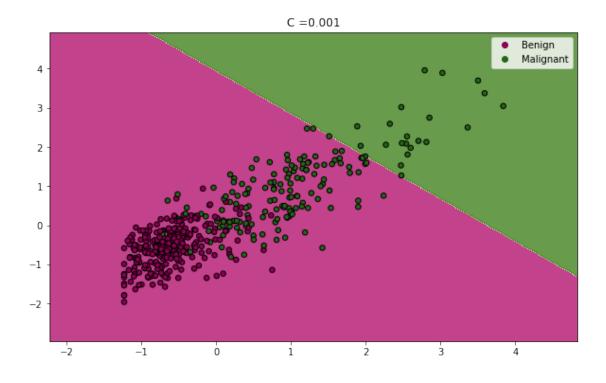
t0 = time.time()
log_reg.predict(test)
t1 = time.time()
print("Logistic Regression Testing Time : ", t1-t0)
```

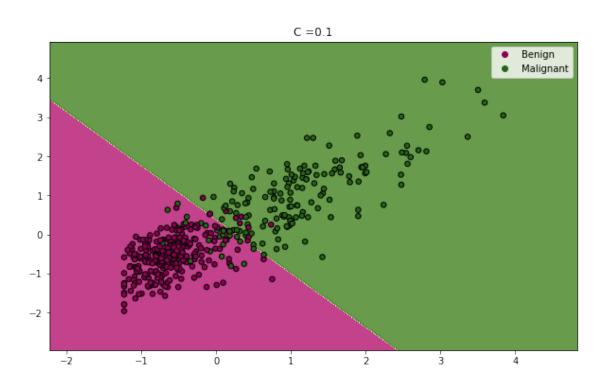
KNN Testing Time : 0.022438764572143555
Logistic Regression Testing Time : 0.0005810260772705078

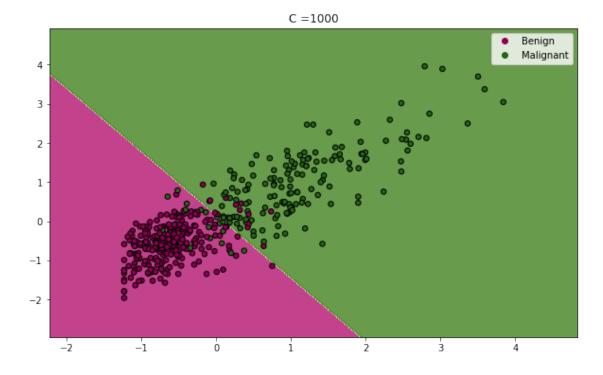
This simple test shows that Logistic Regression is slower than KNN during Training time but is much faster during testing time.

2.4.5 Visualizing decision boundaries for Logistic Regression

Now, lets look at the decision boundary caused by Logistic Regression. Same as for KNN, we use the two most correlated features to the target labels: concave_points_mean and perimeter_mean. This way, we can visualize the 2D decision boundary.





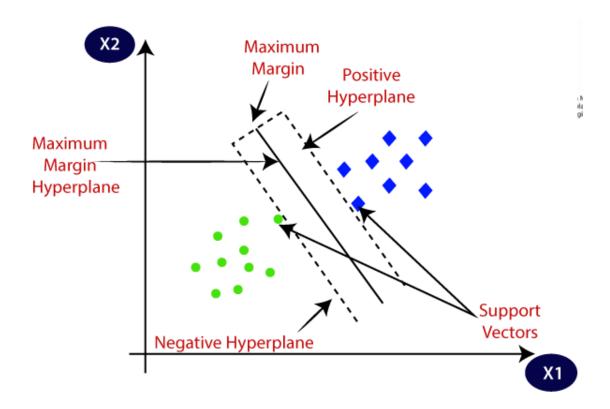


We can see as the regularization strength changes, the decision boundary moves as well. Additionally, we can clearly see that the decision boundary is a line since this is a linear model.

2.5 Models for Classification: SVM

We now discuss another type of linear classification model known as Support Vector Machines (SVM). Where Logistic Regression was motivated probability theory, SVM is motivated by geometeric arguments. Specifically, SVM finds a separating hyperline that maximizes the margin (i.e. distance from each class). The hyperplane is used to classify the points by designating every sample on of side of the hyperplane as the positive class and the other side as the negative class.

The hyperplane is determine by a few sample points known as support vectors that uniquely characterize the hyperplane.



Note that it may not always be possible to find a hyperplane that completely separates the classes. Thus, we use what is known as Soft-Margin SVM which aims to maximize the margin while minizming the distance on the classes that are on the wrong side.

All Sci-kit learn implementations of SVM that we use are soft-margin SVM.

2.5.1 Simple SVM classification

```
[50]: svm = SVC()
svm.fit(train, target)
predicted = svm.predict(test)
print("%-12s %f" % ('Accuracy:', metrics.accuracy_score(target_test,predicted)))
```

Accuracy: 0.921053

2.5.2 Parameters for SVM

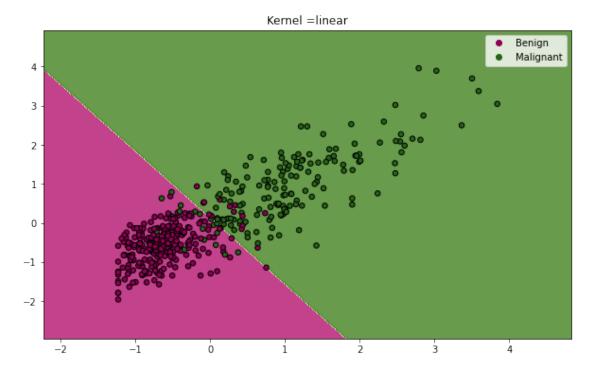
In Sci-kit Learn, the following are just some of the parameters we can pass into Logistic Regression:

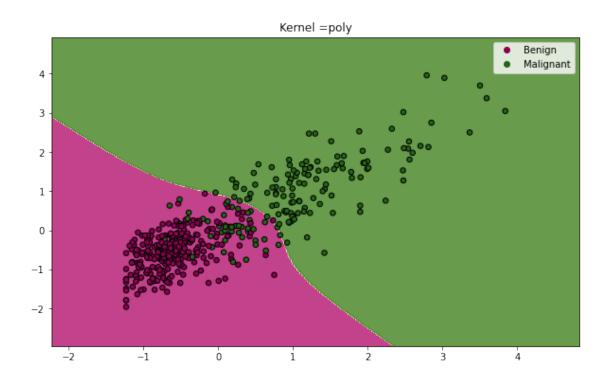
- C: positive float, default=1
 - Inverse of the regularization strength. You can treat C as $\frac{1}{\lambda}$ as shown in lecture. Thus, as C gets smaller, the regularization strength increases. SVM only uses the L2 regularization.
- kernel: {'linear', 'poly', 'rbf', 'sigmoid'}, default='rbf'
 - Specifies the kernel type to be used in the algorithm. A kernel specifies a mapping into a higher dimension space to allow for non-linear decision boundaries.
- degree: int, default=3

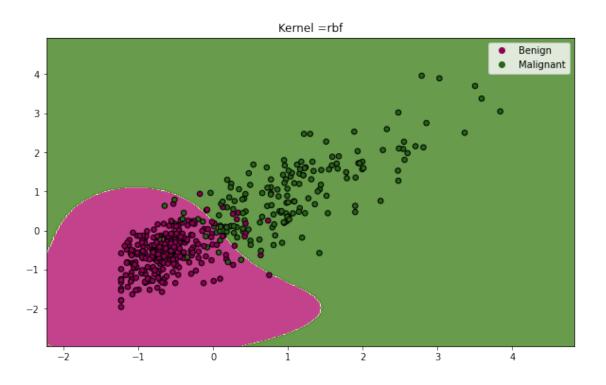
- Degree of the polynomial kernel function ('poly'). Ignored by all other kernels.

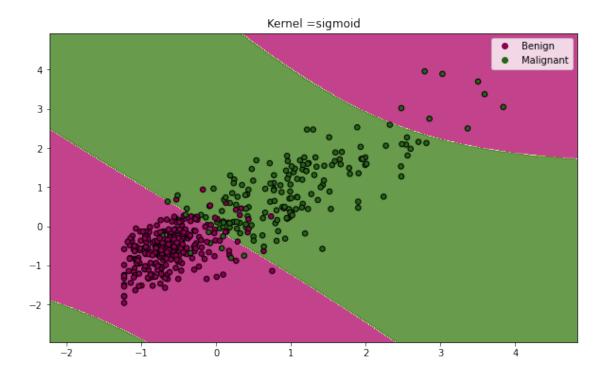
2.5.3 Visualizing decision boundaries for SVM

Now, lets look at the decision boundary caused by SVM with different kernels. Same as for KNN and Logistic Regression, we use the two most correlated features to the target labels: concave_points_mean and perimeter_mean. This way, we can visualize the 2D decision boundary.









We can see that the decision boundary is not always linear because we are using non-linear kernels.

2.6 Important Measures for Classifications

Now that we have gone over a few models for binary classification, let's explore the different ways we can measure the performance of these models.

```
[52]: #Example classifier
log_reg = LogisticRegression(max_iter = 1000)
log_reg.fit(train_raw, target)
predicted = log_reg.predict(test_raw)
```

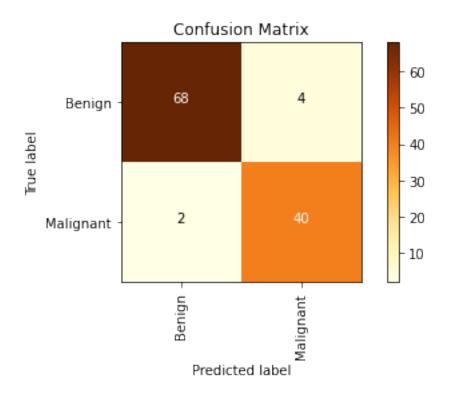
Here are just some of the most important measures of interest. We use the convention to refer to the class labeled as 1 as the positive class.

- Accuracy: The percentage of predictions that are correct. Use metrics.accuracy_score
- Precision: Number of labels correctly classified as positive positive among all the predictions that were classified as positive. Use metrics.precision_score
- Recall: Number of labels correctly classified as positive. Percentage of predictions that are correctly positive among all the labels where the true class is positive. Also known as the probability of detecting when a class is positive. Use metrics.recall_score
- **F1 Score:** Harmonic mean of the precision and recall. Highest value is 1 when both precision and recall are 1, i.e. perfect. Lowest value is 0 when either precision or recall is zero. Provides an aggregate score to analyze both precision and recall. Use metrics.f1_score

We can calculate these measures by using a confusion matrix as well.

Accuracy: 0.947368
Precision: 0.909091
Recall: 0.952381
F1 Score: 0.930233
Confusion Matrix:

[[68 4] [2 40]]



3 TODO: Using classification methods to classify heart disease

Now that you have some examples of the classifiers that Sci-kit learn has to offers, let try to apply them to a new dataset.

3.1 Background: The Dataset

For this exercise we will be using a subset of the UCI Heart Disease dataset, leveraging the fourteen most commonly used attributes. All identifying information about the patient has been scrubbed. You will be asked to classify whether a patient is suffering from heart disease based on a host of potential medical factors.

The dataset includes 14 columns. The information provided by each column is as follows:

```
age: Age in years
sex: (1 = \text{male}; 0 = \text{female})
cp: Chest pain type (0 = asymptomatic; 1 = atypical angina; 2 = non-anginal pain; 3 = typical
angina)
trestbps: Resting blood pressure (in mm Hg on admission to the hospital)
chol: cholesterol in mg/dl
fbs Fasting blood sugar > 120 \text{ mg/dl} (1 = \text{true}; 0 = \text{false})
restecg: Resting electrocardiographic results (0= showing probable or definite left ventricular hy-
pertrophy by Estes' criteria; 1 = normal; 2 = having ST-T wave abnormality (T wave inversions
and/or ST elevation or depression of > 0.05 \text{ mV})
thalach: Maximum heart rate achieved
exang: Exercise induced angina (1 = \text{ves}; 0 = \text{no})
oldpeak: Depression induced by exercise relative to rest
slope: The slope of the peak exercise ST segment (0 = \text{downsloping}; 1 = \text{flat}; 2 = \text{upsloping})
ca: Number of major vessels (0-3) colored by flourosopy
thal: 1 = \text{normal}; 2 = \text{fixed defect}; 7 = \text{reversable defect}
sick: Indicates the presence of Heart disease (True = Disease; False = No disease)
```

3.2 [25 pts] Part 1. Load the Data and Analyze

Let's first load our dataset so we'll be able to work with it. (correct the relative path if your notebook is in a different directory than the csv file.)

```
[97]: data = pd.read_csv('datasets/heartdisease.csv')
```

3.2.1 [5 pts] Looking at the data

std

0.612277

Now that our data is loaded, let's take a closer look at the dataset we're working with. Use the head method, the describe method, and the info method to display some of the rows so we can visualize the types of data fields we'll be working with.

```
[98]:
      data.head(5)
                                                 restecg
[98]:
                         trestbps
                                     chol
                                           fbs
                                                           thalach
                                                                     exang
                                                                             oldpeak
                                                                                       slope
          age
               sex
                     ср
      0
                      3
                                                        0
                                                                          0
                                                                                  2.3
                                                                                            0
           63
                               145
                                      233
                                              1
                                                                150
                  1
      1
           37
                      2
                                              0
                                                        1
                                                                          0
                                                                                  3.5
                                                                                            0
                  1
                               130
                                      250
                                                                187
      2
                                      204
           41
                 0
                      1
                               130
                                              0
                                                        0
                                                                172
                                                                          0
                                                                                  1.4
                                                                                            2
      3
                      1
                                              0
                                                                          0
                                                                                            2
           56
                  1
                               120
                                      236
                                                        1
                                                                178
                                                                                  0.8
      4
           57
                  0
                      0
                               120
                                      354
                                              0
                                                        1
                                                                163
                                                                          1
                                                                                  0.6
                                                                                            2
              thal
                      sick
          ca
      0
           0
                  1
                     False
                  2
      1
           0
                     False
      2
           0
                  2
                     False
      3
           0
                  2
                     False
      4
           0
                  2
                     False
[99]:
      data.describe()
[99]:
                                                         trestbps
                                                                           chol
                                                                                          fbs
                      age
                                    sex
                                                  ср
                                                                                  303.000000
      count
              303.000000
                            303.000000
                                         303.000000
                                                       303.000000
                                                                    303.000000
               54.366337
                              0.683168
                                            0.966997
                                                       131.623762
                                                                    246.264026
                                                                                    0.148515
      mean
      std
                9.082101
                              0.466011
                                            1.032052
                                                        17.538143
                                                                     51.830751
                                                                                    0.356198
      min
               29.000000
                              0.00000
                                           0.00000
                                                        94.000000
                                                                    126.000000
                                                                                    0.000000
      25%
                                           0.00000
                                                       120.000000
                                                                    211.000000
                                                                                    0.00000
               47.500000
                              0.000000
      50%
               55.000000
                              1.000000
                                            1.000000
                                                       130.000000
                                                                    240.000000
                                                                                    0.000000
      75%
               61.000000
                              1.000000
                                           2.000000
                                                       140.000000
                                                                    274.500000
                                                                                    0.000000
               77.000000
                              1.000000
                                           3.000000
                                                       200.000000
      max
                                                                    564.000000
                                                                                    1.000000
                  restecg
                               thalach
                                               exang
                                                          oldpeak
                                                                          slope
                                                                                           ca
                                                       303.000000
                                                                    303.000000
      count
              303.000000
                            303.000000
                                         303.000000
                                                                                  303.000000
                            149.646865
                                           0.326733
                                                         1.039604
                                                                      1.399340
                                                                                    0.729373
      mean
                0.528053
      std
                0.525860
                             22.905161
                                           0.469794
                                                         1.161075
                                                                      0.616226
                                                                                    1.022606
      min
                0.000000
                             71.000000
                                           0.000000
                                                         0.00000
                                                                      0.000000
                                                                                    0.000000
      25%
                            133.500000
                                           0.00000
                                                                                    0.00000
                0.000000
                                                         0.00000
                                                                      1.000000
      50%
                1.000000
                            153.000000
                                           0.000000
                                                         0.800000
                                                                      1.000000
                                                                                    0.000000
      75%
                1.000000
                            166.000000
                                            1.000000
                                                         1.600000
                                                                      2.000000
                                                                                    1.000000
                            202.000000
                                                                      2.000000
      max
                2.000000
                                            1.000000
                                                         6.200000
                                                                                    4.000000
                     thal
              303.000000
      count
      mean
                2.313531
```

```
min
          0.000000
25%
          2.000000
50%
          2.000000
75%
          3.000000
          3.000000
max
```

[100]: data.info()

<class 'pandas.core.frame.DataFrame'> RangeIndex: 303 entries, 0 to 302 Data columns (total 14 columns):

#	Column	Non-Null Count	Dtype
0	age	303 non-null	int64
1	sex	303 non-null	int64
2	ср	303 non-null	int64
3	trestbps	303 non-null	int64
4	chol	303 non-null	int64
5	fbs	303 non-null	int64
6	restecg	303 non-null	int64
7	thalach	303 non-null	int64
8	exang	303 non-null	int64
9	oldpeak	303 non-null	float64
10	slope	303 non-null	int64
11	ca	303 non-null	int64
12	thal	303 non-null	int64
13	sick	303 non-null	bool
dtype	es: bool(1), float64(1),	int64(12)

memory usage: 31.2 KB

Sometimes data will be stored in different formats (e.g., string, date, boolean), but many learning methods work strictly on numeric inputs. Additionally, some numerical features can represent categorical features which need to be pre-processed. Are there any columns that need to be transformed and why?

I think "sick" variabel need to encode to numerical labels. And not sure whether oldpeak need to transform.

Determine if we're dealing with any null values. If so, report on which columns?

[101]: data.isnull().sum() [101]: age 0 0 sex 0 ср trestbps 0 chol 0 fbs 0 restecg 0

```
thalach 0
exang 0
oldpeak 0
slope 0
ca 0
thal 0
sick 0
dtype: int64
```

There's no missing value and do not need to remove any column. It's ready to imputate data.

3.2.2 [5 pts] Transform target label into numerical value

Before we begin our analysis, we need to fix the field(s) that will be problematic. Specifically, convert our boolean "sick" variable into a binary numeric target variable (values of either '0' or '1') using the label encoder from scikit-learn, place this new array into a new column of the DataFrame named "target", and then drop the original "sick" column from the dataframe. Afterward, use head to print the first 5 rows

```
[102]: le = LabelEncoder()
        data['target'] = le.fit transform(data['sick'])
[103]: data = data.drop(["sick"],axis = 1)
        data.head(5)
[103]:
           age
                 sex
                       ср
                           trestbps
                                       chol
                                              fbs
                                                    restecg
                                                              thalach
                                                                         exang
                                                                                 oldpeak
                                                                                           slope
                                                           0
                                                                                     2.3
                                                                                                0
        0
            63
                        3
                                 145
                                        233
                                                                   150
                                                                             0
                   1
                                                1
                        2
                                                                                                0
        1
            37
                   1
                                 130
                                        250
                                                0
                                                           1
                                                                   187
                                                                             0
                                                                                     3.5
        2
                                                                                                2
                                                           0
                                                                             0
                                                                                     1.4
            41
                   0
                        1
                                 130
                                        204
                                                0
                                                                   172
        3
            56
                        1
                                 120
                                        236
                                                0
                                                           1
                                                                   178
                                                                             0
                                                                                     0.8
                                                                                                2
                   1
                                 120
                                                                                                2
            57
                   0
                                        354
                                                0
                                                           1
                                                                   163
                                                                             1
                                                                                     0.6
                      target
               thal
           ca
        0
            0
                   1
                            0
                   2
                            0
        1
            0
                   2
        2
            0
                            0
                            0
        3
            0
                   2
                   2
                            0
```

3.2.3 [5 pts] Plotting histogram of data

Now that we have a feel for the data-types for each of the variables, plot histograms of each field.

```
<AxesSubplot:title={'center':'trestbps'}>],
   [<AxesSubplot:title={'center':'chol'}>,
    <AxesSubplot:title={'center':'fbs'}>,
    <AxesSubplot:title={'center':'restecg'}>,
    <AxesSubplot:title={'center':'thalach'}>],
    [<AxesSubplot:title={'center':'exang'}>,
     <AxesSubplot:title={'center':'oldpeak'}>,
    <AxesSubplot:title={'center':'slope'}>,
    <AxesSubplot:title={'center':'ca'}>],
    [<AxesSubplot:title={'center':'thal'}>,
     <AxesSubplot:title={'center':'target'}>, <AxesSubplot:>,
    <AxesSubplot:>]], dtype=object)
                                                                     60
                      150
                                              100
                                                                     50
40
                                                                     40
                       100
                                                                     30
20
                                                                     20
10
                                                                     10
                                                                                160
                                                                                    180
                                             120
                       200
80
                                             100
                      150
60
                       100
                                              60
                                              40
                                                                    175
200
                                             140
                      140
                                             120
                                                                    150
                      120
                                                                    125
                                             100
                      100
                       80
                                                                    100
100
                                                                     75
                       60
                       40
                                                                     50
50
                      150
125
                      125
100
                       100
                       75
```

From the histograms, we can see some interesting trends. Possible observations:

- Many of the oldpeak, ca indicate a heavy skewness towards low values and have large tails
- Many of the age, trestbps, thalach, chol columns look more Gaussian in shape
- There is a large disparity between the ranges of certain features. For example, **chol can go** from 0 to 500 while **age is in the range** [30,70]. This indicates we will have to normalize or standardize the features if the models are sensitive to such measures.

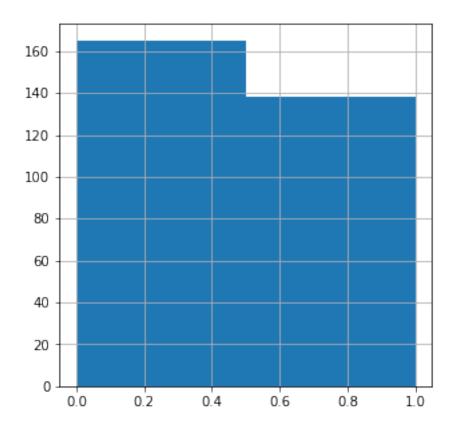
3.2.4 [5 pts] Looking at class balance

We also want to make sure we are dealing with a balanced dataset. In this case, we want to confirm whether or not we have an equitable number of sick and healthy individuals to ensure that our classifier will have a sufficiently balanced dataset to adequately classify the two. Plot a histogram specifically of the sick target, and conduct a count of the number of sick and healthy individuals and report on the results:

```
[105]: data['target'].hist(bins=2, figsize=(5,5))
data['target'].value_counts()
```

[105]: 0 165 1 138

Name: target, dtype: int64



There is a little bit of an imbalance. For our purposes, this imbalance is not big enough to be an issue so we will not perform balancing techniques for this dataset. Since the dataset is small though, so we just making training and testing splits carefully to ensure that there is enough of each class for both splits.

Balanced datasets are important to ensure that classifiers train adequately and don't overfit, however arbitrary balancing of a dataset might introduce its own issues.

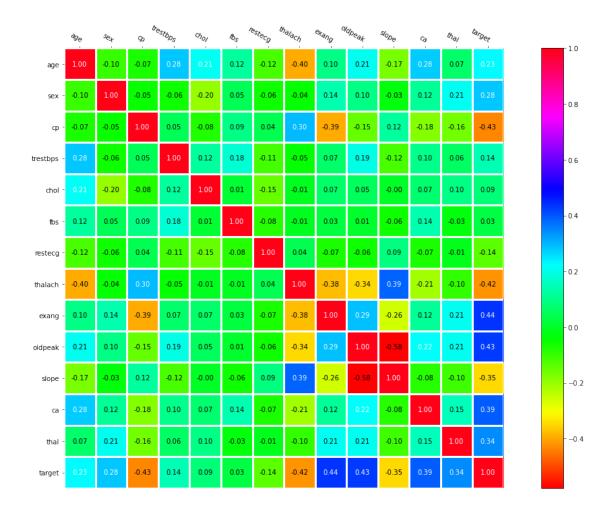
Discuss some of the problems that might arise by artificially balancing a dataset.

- Loss of Information: lead to a loss of valuable information and reduce the diversity of the dataset.
- Bias in Training: in oversampling the minority class, the model might be exposed to redundant or synthetic instances, which can lead to overfitting.
- Increased Model Complexity: Balancing a dataset often involves generating synthetic samples or replicating existing ones which can increase the complexity of the model training process.
- Imbalance in Evaluation: If the test set or validation set is not balanced in the same way as the training set, the model's performance metrics can be misleading.
- Addressing the Wrong Issue: might overlook the underlying reasons for the class imbalance, such as data collection biases or naturally imbalanced distributions, and fail to address the root cause.

3.2.5 [5 pts] Looking at Data Correlation

Now that we have our dataframe prepared let's start analyzing our data. For this next question let's look at the correlations of our variables to our target value. First, use the heatmap function to plot the correlations of the data.

```
[106]: correlations = data.corr()
columns = list(data)
#Creates the heatmap
heatmap(correlations.values,columns,figsize = (20,12),cmap="hsv")
```



Next, show the correlation to the "target" feature only and sorr them in descending order.

[107]: correlations["target"].sort_values(ascending=False)

```
[107]: target
                    1.000000
       exang
                    0.436757
       oldpeak
                    0.430696
       ca
                    0.391724
                    0.344029
       thal
                    0.280937
       sex
       age
                    0.225439
       trestbps
                    0.144931
       chol
                    0.085239
       fbs
                    0.028046
                   -0.137230
       restecg
                   -0.345877
       slope
       thalach
                   -0.421741
                   -0.433798
       ср
```

Name: target, dtype: float64

From the heatmap values and the description of the features, why do you think some variables correlate more highly than others? (This question is just to get you thinking and there is no perfect answer since we have no medical background)

exang has **highest correlation**: It indicates that individuals experiencing angina during exercise may have compromised blood flow to the heart due to narrowed or blocked arteries.

oldpeak: Heart disease can contribute to depression, and depression can affect cardiovascular health by influencing behaviors, such as decreased physical activity or adherence to treatment plans.

3.3 [25 pts] Part 2. Prepare the Data and run a KNN Model

Before running our various learning methods, we need to do some additional prep to finalize our data. Specifically you'll have to cut the classification target from the data that will be used to classify, and then you'll have to divide the dataset into training and testing cohorts.

Specifically, we're going to ask you to prepare 2 batches of data. The first batch will simply be the raw numeric data that hasn't gone through any additional pre-processing. The second batch will be data that you will pipeline using pre-processing methods. We will then feed both of these datasets into a classifier to showcase just how important this step can be!

3.3.1 [2 pts] Separate target labels from data

Save the label column as a separate array and then make a new dataframe without the target.

```
[122]: y = data["target"]
x = data.drop(["target"],axis = 1)
```

3.3.2 [5 pts] Balanced Train Test Split

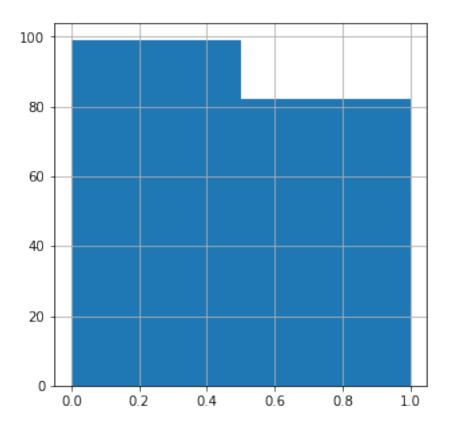
82

1

Now, create your 'Raw' unprocessed training data by dividing your dataframe into training and testing cohorts, with your training cohort consisting of 60% of your total dataframe. To ensure that the train and test sets have balanced classes, use the stratify command of train_test_split. Output the resulting shapes of your training and testing samples to confirm that your split was successful. Additionally, output the class counts for the training and testing cohorts to confirm that there is no artifical class imbalance.

Note: Use randomstate = 0 to ensure that the same train/test split happens everytime for ease of grading.

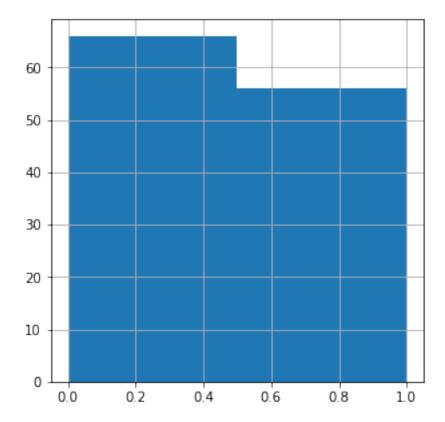
Name: target, dtype: int64



[125]: #Testing classes
 target_test.hist(bins=2, figsize=(5,5))
 target_test.value_counts()

[125]: 0 66 1 56

Name: target, dtype: int64



We can see that the class balance is about the same as before the split. In fact, we can see that if a classifier just guessed class 0, it would have an accuracy of $100 * \frac{66}{66+56} = 54.10\%$. We can consider this the baseline accuracy to compare against.

3.3.3 [5 pts] KNN on raw data

Now, let's try a classification model on this data. We'll first use KNN since it is the one we are most familiar with.

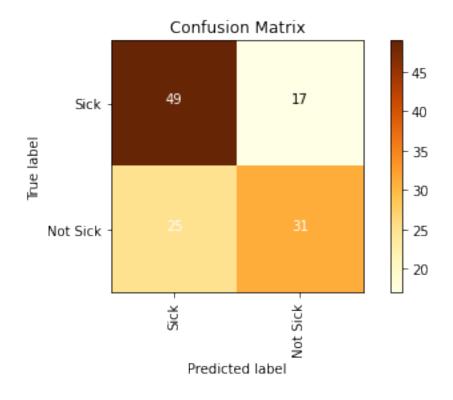
One thing we noted in class was that because KNN relies on Euclidean distance, it is highly sensitive to the relative magnitude of different features. Let's see that in action! Implement a K-Nearest Neighbor algorithm on our data and report the results. For this initial implementation, simply use the default settings. Refer to the KNN Documentation for details on implementation. Report on the test accuracy of the resulting model and print out the confusion matrix.

Recall that accurracy can be calculated easily using metrics.accuracy_score and that we have a helper function to draw the confusion matrix.

```
[126]: # k-Nearest Neighbors algorithm
knn = KNeighborsClassifier()
knn.fit(train_raw, target)
predicted = knn.predict(test_raw)
```

Accuracy: 0.655738
Precision: 0.645833
Recall: 0.553571
F1 Score: 0.596154
Confusion Matrix:

[[49 17] [25 31]]



3.3.4 [5 pts] KNN on preprocessed data

Now lets implement a pipeline to preprocess the data. For the pipeline, use StandardScaler on the numerical features and one-hot encoding on the categorical features. For reference on how to make a pipeline, please look at project 1.

For reference, the categorical features are ['sex', 'cp', 'fbs', 'restecg', 'exang', 'slope', 'ca', 'thal'].

Now use the pipeline to transform the data and then apply the same KNN classifier with this new training/testing data. Report the test accuraccy. Discuss the implications of the different results you are obtaining.

Note: Remember to use fit transform on the training data and transform on the testing data.

```
[136]: #Transform raw data
train = pipeline.fit_transform(train_raw)
test = pipeline.transform(test_raw) #Note that there is no fit calls
```

```
[137]: # k-Nearest Neighbors algorithm
knn = KNeighborsClassifier()
knn.fit(train, target)
testing_result = knn.predict(test)
predicted = knn.predict(test)
```

```
[138]: print("%-12s %f" % ('Accuracy:', metrics.accuracy_score(target_test,predicted)))
```

Accuracy: 0.754098

Accuracy of processed data is better than the raw data with 10%

3.3.5 [8 pts] KNN Parameter optimization for n neighbors

The KNN Algorithm includes an n_neighbors attribute that specifies how many neighbors to use when developing the cluster. (The default value is 5, which is what your previous model used.) Lets now try n values of: 1, 2, 3, 5, 7, 9, 10, 20, and 50. Run your model for each value and report the test accuracy for each. (HINT leverage python's ability to loop to run through the array and generate results without needing to manually code each iteration).

```
[149]: #k_r = [1, 2, 3, 5, 7, 9, 10, 20, 50]
for k in [1, 2, 3, 5, 7, 9, 10, 20, 50]:
    knn = KNeighborsClassifier(n_neighbors=k)
    knn.fit(train, target)
```

```
Accuracy for k = 1 is 0.770492
Accuracy for k = 2 is 0.745902
Accuracy for k = 3 is 0.754098
Accuracy for k = 5 is 0.754098
Accuracy for k = 7 is 0.762295
Accuracy for k = 9 is 0.778689
Accuracy for k = 10 is 0.778689
Accuracy for k = 20 is 0.778689
Accuracy for k = 50 is 0.778689
```

Comment for which value of n did the KNN model perform the best. Did the model perform strictly better or strictly worse as the value of n increased?

K=9 should be the best KNN model because it has relatively high accuracy and low complexity.

So we have a model that seems to work well. But let's see if we can do better! To do so we'll employ Logistic Regression and SVM to improve upon the model and compare the results.

For the rest of the project, you will only be using the transformed data and not the raw data. DO NOT USE THE RAW DATA ANYMORE.

3.4 [20 pts] Part 3. Additional Learning Methods: Logistic Regression

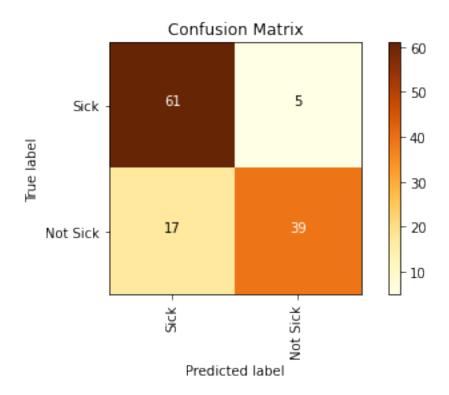
Let's now try Logistic Regression. Recall that Logistic regression is a statistical model that in its basic form uses a logistic function to model a binary dependent variable.

3.4.1 [5 pts] Run the default Logistic Regression

Implement a Logistical Regression Classifier. Review the Logistical Regression Documentation for how to implement the model. Use the default settings. Report on the test accuracy and print out the confusion matrix.

```
[150]: log_reg = LogisticRegression()
    log_reg.fit(train, target)
    testing_result = log_reg.predict(test)
    predicted = log_reg.predict(test)

print("%-12s %f" % ('Accuracy:', metrics.accuracy_score(target_test,predicted)))
    draw_confusion_matrix(target_test, predicted, ['Sick', 'Not Sick'])
```



3.4.2 [5 pts] Compare Logistic Regression and KNN

In your own words, describe the key differences between Logistic Regression and KNN? When would you use one over the other?

Difference:

- Algorithm Type: Logistic Regression: binary or multi-class classification; It models the relationship between the independent variables and the **probability** using a logistic function. KNN: k nearest neighbors based on a distance metric.
- Decision Boundary: Logistic Regression: linear decision boundary KNN: non-linear decision boundary.
- Model Interpretability: Logistic Regression: interpretable results by estimating coefficients that indicate the influence of each feature on the outcome. KNN: It doesn't provide direct interpretability as it relies on distance-based calculations.
- Training and Prediction Time: Logistic Regression: faster KNN: slower
- Parametric: Logistic Regression: parametric KNN: non-parametric

When to use:

Logistic Regression: - interpretability and understanding the impact of features on the outcome - The relationship between features and the log-odds of the target variable is believed to be linear or can be linearized. - The dataset has a large number of features or a large number of training examples, as logistic regression can handle these scenarios efficiently.

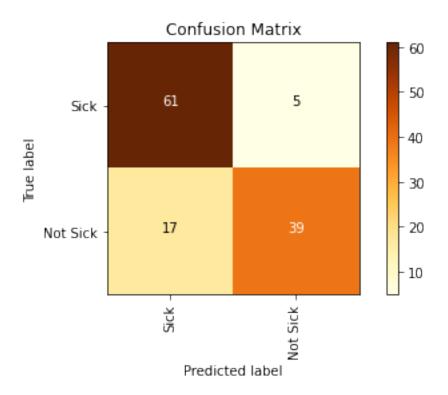
KNN: - The decision boundary is complex and likely to be non-linear. - The dataset is relatively small or moderate in size, as KNN does not scale well with large datasets. - There is no clear functional relationship between the features and the target variable.

3.4.3 [5 pts] Tweaking the Logistic Regression

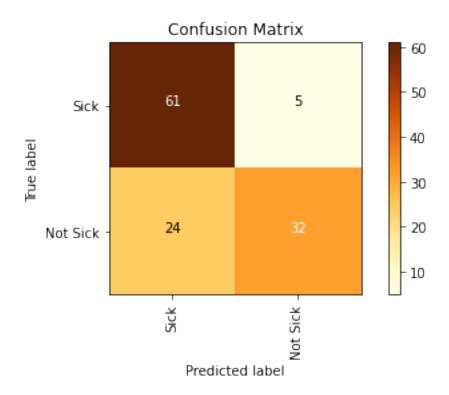
What are some parameters we can change that will affect the performance of Logistic Regression?

- penalty
- max iter
- solver
- C (mainly)

Implement Logistic Regression with solver= 'liblinear', max_iter= 1000, penalty = 'l2', and C=1. Report on the test accuracy and print out the confusion matrix.



Now, Implement Logistic Regression with solver= 'liblinear', max_iter= 1000, penalty = 'l2', and C=0.0001. Report on the test accuracy and print out the confusion matrix.

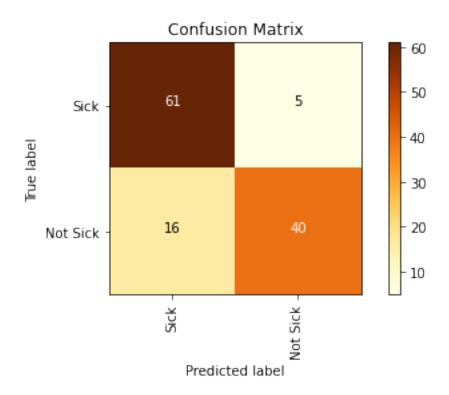


Did the accuraccy drop or improve? Why?

Does not improve because we make C smaller. As C gets smaller, the regularization strength increases. It makes penalty increase and leads to lower accuracy.

3.4.4 [5 pts] Trying out different penalties

Now, Implement Logistic Regression with solver= 'liblinear', max_iter= 1000, penalty = 'l1', and C=1. Report on the test accuracy and print out the confusion matrix.



Describe what the purpose of a penalty term is and how the change from L2 to L1 affected the model.

purpose:

• helps prevent overfitting and improve the model's generalization ability. The penalty term is added to the loss function during training, influencing the model's parameter estimation process.

change:

- Sparsity of Features: L1 regularization tends to drive some of the coefficients to exactly zero. L2 will make coefficient close to 0 but not equal 0.
- Model Complexity: L1 regularization generally produces models with lower complexity compared to L2 regularization.
- Robustness to Outliers: L1 regularization is generally more robust to outliers compared to L2 regularization because L2 regularization penalizes the squared magnitude of coefficients, which can be greatly affected by outliers.

3.5 [20 pts] Part 4. Additional Learning Methods: SVM (Support Vector Machine)

A Support Vector Machine (SVM) is a discriminative classifier formally defined by a separating hyperplane. In other words, given labeled training data (supervised learning), the algorithm outputs

an optimal hyperplane which categorizes new examples. In two dimensional space this hyperplane is a line dividing a plane in two parts each corresponding to one of the two classes.

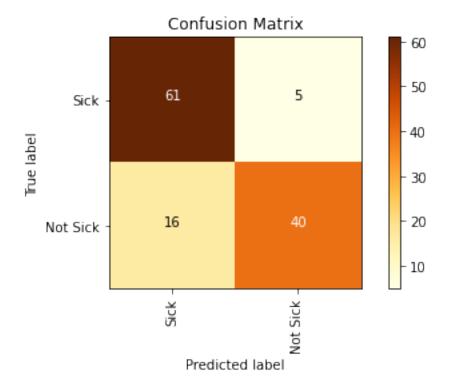
Recall that Sci-kit learn uses soft-margin SVM to account for datasets that are not separable.

3.5.1 [5 pts] Run default SVM classifier

Implement a Support Vector Machine classifier on your pipelined data. Review the SVM Documentation for how to implement a model. For this implementation you can simply use the default settings. Report on the test accuracy and print out the confusion matrix.

```
[154]: svm = SVC()
    svm.fit(train, target)
    predicted = svm.predict(test)
    print("%-12s %f" % ('Accuracy:', metrics.accuracy_score(target_test,predicted)))
    draw_confusion_matrix(target_test, predicted4, ['Sick', 'Not Sick'])
```

Accuracy: 0.803279



Print out the number of support vectors that SVC has determined. Look at the documentation for how to get this.

```
[155]: print("number of Support vectors:", svm.n_support_)
print("Total number of Support vectors:", sum(svm.n_support_))
```

```
number of Support vectors: [54 52]
Total number of Support vectors: 106
```

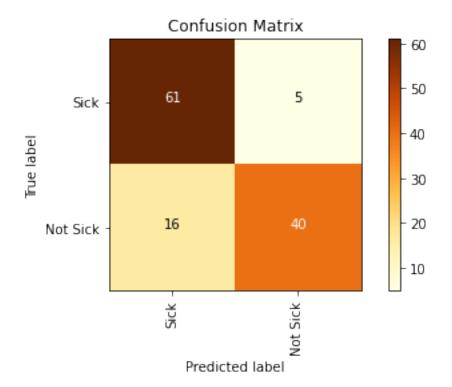
You may find that there are quite a few support vectors. This is due in part to the small number of samples in the training set and the choice of kernel.

3.5.2 [5 pts] Use a Linear SVM

Rerun your SVM, but now modify your model parameter kernel to equal 'linear'. Report on the test accuracy and print out the confusion matrix. Also, print out the number of support vectors.

```
[156]: svm = SVC(kernel='linear')
svm.fit(train, target)
predicted = svm.predict(test)
print("%-12s %f" % ('Accuracy:', metrics.accuracy_score(target_test,predicted)))
draw_confusion_matrix(target_test, predicted4, ['Sick', 'Not Sick'])
```

Accuracy: 0.844262



```
[157]: print("number of Support vectors:", svm.n_support_)
    print("Total number of Support vectors:", sum(svm.n_support_))
```

number of Support vectors: [34 31]
Total number of Support vectors: 65

You will notice that number of support vectors has decreased significantly.

3.5.3 [5 pts] Compare default SVM and Linear SVM

Explain the what the new results you've achieved mean. Read the documentation to understand what you've changed about your model and explain why changing that input parameter might impact the results in the manner you've observed.

linear SVM has higher accuracy and less number of support vector

linear SVM operates directly in the original feature space and focuses on capturing linear relationships, making it suitable for linearly separable data or cases where non-linear relationships are not significant. However, default SVM with non-linear kernels can provide better accuracy when dealing with complex, non-linear relationships. The choice between linear SVM and default SVM depends on the characteristics of the data, the complexity of the problem, and the trade-offs between accuracy and model simplicity.

Number of Support Vectors:

- Linear SVM: with simpler linear decision boundary, requires fewer support vectors to accurately separate the classes
- Default SVM: its ability to capture complex relationships, may require more support vectors to model intricate decision boundaries accurately

3.5.4 [5 pts] Compare SVM and Logistic Regression

Both logistic regression and linear SVM are trying to classify data points using a linear decision boundary but achieve it in different ways. In your own words, explain the difference between the ways that Logistic Regression and Linear SVM find the boundary?

- logistic regression estimates the probability of class membership using a sigmoid function and fits the best-fitting line based on the likelihood of observed class labels.
- Linear SVM finds the optimal hyperplane that maximizes the margin between classes and determines the decision boundary based on this hyperplane.

3.6 [10 pts] Part 5: Cross Validation and Model Selection

You've sampled a number of different classification techniques and have seen their performance on the dataset. Before we draw any conclusions on which model is best, we want to ensure that our results are not the result of the random sampling of our data we did with the Train-Test-Split. To ensure otherwise, we will conduct a K-Fold Cross-Validation with GridSearch to determine which model perform best and assess its performance on the test set.

3.6.1 [10 pts] Model Selection

Run a GridSearchCV with 3-Fold Cross Validation. You will be running each classification model with different parameters.

```
KNN: - n_neighbors = [1,3,5,7] - metric = ["euclidean", "manhattan"] #Different Distance functions
Logistic Regression: - penalty = ["l1", "l2"] - solver = ["liblinear"] - C = [0.0001,0.1,10]
SVM: - kernel = ["linear", "rbf"] - C = [0.0001,0.1,10]
```

Make sure to train and test your model on the transformed data and not on the raw data.

After using GridSearchCV, put the results into a pandas Dataframe and print out the whole table.

```
[158]: clf1 = KNeighborsClassifier()
      clf2 = LogisticRegression()
      clf3 = SVC()
      parameters = [
          {'classifier__n_neighbors':[1,3,5,7], 'classifier__metric':
       {'classifier_penalty':["11","12"], 'classifier_solver':["liblinear"],
       {'classifier_kernel':["linear", "rbf"], 'classifier_C':[0.0001,0.1,10],
       [161]: #Implementing cross validation
      k = 3
      kf = KFold(n_splits=k, random_state=None)
      pipeline = Pipeline([('classifier', clf1)])
      grid = GridSearchCV(pipeline,parameters,cv=kf, scoring ="accuracy")
      grid.fit(train,target)
      res = pd.DataFrame(grid.cv_results_)
      res
     /Users/mac/opt/anaconda3/lib/python3.9/site-
     packages/sklearn/model_selection/_validation.py:372: FitFailedWarning:
     6 fits failed out of a total of 48.
     The score on these train-test partitions for these parameters will be set to
     If these failures are not expected, you can try to debug them by setting
     error_score='raise'.
     Below are more details about the failures:
     6 fits failed with the following error:
     Traceback (most recent call last):
       File "/Users/mac/opt/anaconda3/lib/python3.9/site-
     packages/sklearn/model_selection/_validation.py", line 680, in _fit_and_score
         estimator.fit(X_train, y_train, **fit_params)
       File "/Users/mac/opt/anaconda3/lib/python3.9/site-
     packages/sklearn/pipeline.py", line 394, in fit
         self._final_estimator.fit(Xt, y, **fit_params_last_step)
       File "/Users/mac/opt/anaconda3/lib/python3.9/site-
     packages/sklearn/linear_model/_logistic.py", line 1464, in fit
```

```
raise ValueError("Penalty term must be positive; got (C=%r)" % self.C)
      ValueError: Penalty term must be positive; got (C='0.0001,0.1,10')
        warnings.warn(some_fits_failed_message, FitFailedWarning)
      /Users/mac/opt/anaconda3/lib/python3.9/site-
      packages/sklearn/model_selection/_search.py:969: UserWarning: One or more of the
      test scores are non-finite: [0.76812386 0.82887067 0.82905282 0.81247723
      0.76256831 0.82887067
       0.82896175 0.82349727
                                                 nan 0.54744991 0.54744991
       0.86202186 0.73570128 0.83460838 0.78469945]
        warnings.warn(
[161]:
           mean_fit_time
                           std_fit_time
                                          mean_score_time
                                                            std_score_time
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                                                 0.007533
       0
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                0.002447
                               0.001177
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                                                                  0.001910
       2
                0.001554
                               0.000683
                                                 0.004909
                                                                  0.000894
       3
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       4
                0.000939
                               0.000079
                                                 0.004545
                                                                  0.001974
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                0.000931
                               0.000061
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       6
                KNeighborsClassifier()
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       7
                KNeighborsClassifier()
                                                        manhattan
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                  LogisticRegression()
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                  LogisticRegression()
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           SVC(C=0.1, kernel='linear')
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           SVC(C=0.1, kernel='linear')
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           SVC(C=0.1, kernel='linear')
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           SVC(C=0.1, kernel='linear')
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       15
           SVC(C=0.1, kernel='linear')
                                                               NaN
```

```
\verb|param_classifier_n_neighbors param_classifier_C \setminus
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```
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    {'classifier': KNeighborsClassifier(), 'classi...
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    {'classifier': KNeighborsClassifier(), 'classi...
6
                                                                  0.786885
7
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    {'classifier': LogisticRegression(), 'classifi...
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   {'classifier': SVC(C=0.1, kernel='linear'), 'c...
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                                                                  0.459016
    {'classifier': SVC(C=0.1, kernel='linear'), 'c...
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                                                                  0.573770
   {'classifier': SVC(C=0.1, kernel='linear'), 'c...
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   {'classifier': SVC(C=0.1, kernel='linear'), 'c...
                                                                  0.754098
                        split2_test_score
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0
             0.783333
                                                                     0.021509
                                  0.783333
                                                    0.768124
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                                                                     0.046167
3
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                                                    0.812477
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                                                                     0.032717
7
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                                                    0.862022
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                                                                     0.046205
    rank_test_score
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```

```
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10
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11
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12
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13
                    12
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                     9
```

What was the best model and what was it's score?

```
[162]: print(grid.best_score_)
print(grid.best_estimator_)
```

0.8620218579234972
Pipeline(steps=[('classifier', SVC(C=0.1, kernel='linear'))])

Using the best model you have, report the test accuracy and print out the confusion matrix

```
[164]: svmbest = SVC(kernel='linear', C=0.1)
    svmbest.fit(train, target)
    predicted = svmbest.predict(test)
    print("%-12s %f" % ('Accuracy:', metrics.accuracy_score(target_test,predicted)))
    draw_confusion_matrix(target_test, predicted4, ['Sick', 'Not Sick'])
```

