Understanding KNN w.r.t different Distance metrics

Before I jump on to KNN or other similar distance dependent algorithms lets first take a moment to understand the various distance metrics.

My objective for creating this notebook is understanding the various distances which we can leverage while working on a usecase because there is no single distance metric that can be applied in every problem.

Notebook Contents

Packages_Import

In [127…

```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns
import scipy
```

```
import statsmodels as stm

from sklearn.datasets import load_breast_cancer
from sklearn.neighbors import KNeighborsClassifier, DistanceMetric, RadiusNeighborsC

%matplotlib inline
```

Distance_Calculations

CASE-I

Entire variable as an one row vector

In [2]:
```
X = np.array([[1,2,3]])
Y = np.array([[3,4,5]])
X,Y
```

Out[2]:
```
(array([[1, 2, 3]]), array([[3, 4, 5]]))
```

In [3]:
```
X.shape, Y.shape, X.ndim, Y.ndim
```

Out[3]:
```
((1, 3), (1, 3), 2, 2)
```

1.1.Euclidean_Distance

In [4]:
```
eu_dist = DistanceMetric.get_metric('euclidean')
```

In [5]:
```
#Pair-wise distance
eu_dist.pairwise(X,Y)
```

Out[5]:
```
array([[3.46410162]])
```

In [6]:
```
#Reduced distance is squared values in case of Euclidean
eu_dist.dist_to_rdist(X), eu_dist.dist_to_rdist(Y)
```

Out[6]:
```
(array([[1, 4, 9]], dtype=int32), array([[ 9, 16, 25]], dtype=int32))
```

In [7]:
```
#Reduced distance is squared root of values in case of Euclidean
eu_dist.rdist_to_dist(X), eu_dist.rdist_to_dist(Y)
```

Out[7]:
```
(array([[1.        , 1.41421356, 1.73205081]]),
 array([[1.73205081, 2.        , 2.23606798]]))
```

1.2.Manhattan_Distance

In [8]:
```
man_hat_dist = DistanceMetric.get_metric('manhattan')
```

In [9]:
```
man_hat_dist.pairwise(X,Y)
```

Out[9]:
```
array([[6.]])
```

In [10]:
```
#Reduced distance is same values in case of Manhattan
man_hat_dist.dist_to_rdist(X), man_hat_dist.dist_to_rdist(Y)
```

Out[10]:
```
(array([[1, 2, 3]]), array([[3, 4, 5]]))
```

In [11]:
```
#Reduced distance is same values in case of Manhattan
man_hat_dist.rdist_to_dist(X), man_hat_dist.rdist_to_dist(Y)
```

Out[11]:
```
(array([[1, 2, 3]]), array([[3, 4, 5]]))
```

CASE-II

Entire variable as an one column vector

In [12]:
```
XX = X.copy().reshape(3,1)
YY = Y.copy().reshape(3,1)
```

In [13]:
```
XX,YY
```

Out[13]:
```
(array([[1],
        [2],
        [3]]),
 array([[3],
        [4],
        [5]]))
```

2.1.Euclidean_Distance

In [14]:
```
eu_dist.pairwise(XX,YY)
```

Out[14]:
```
array([[2., 3., 4.],
       [1., 2., 3.],
       [0., 1., 2.]])
```

In [15]:
```
eu_dist.dist_to_rdist(XX), eu_dist.dist_to_rdist(YY)
```

Out[15]:
```
(array([[1],
        [4],
        [9]], dtype=int32),
 array([[ 9],
        [16],
        [25]], dtype=int32))
```

2.2.Manhattan_Distance

In [16]:
```
man_hat_dist.pairwise(XX,YY)
```

Out[16]:
```
array([[2., 3., 4.],
       [1., 2., 3.],
       [0., 1., 2.]])
```

In [17]:
```
man_hat_dist.dist_to_rdist(XX), man_hat_dist.dist_to_rdist(YY)
```

Out[17]:
```
(array([[1],
        [2],
        [3]]),
 array([[3],
        [4],
        [5]]))
```

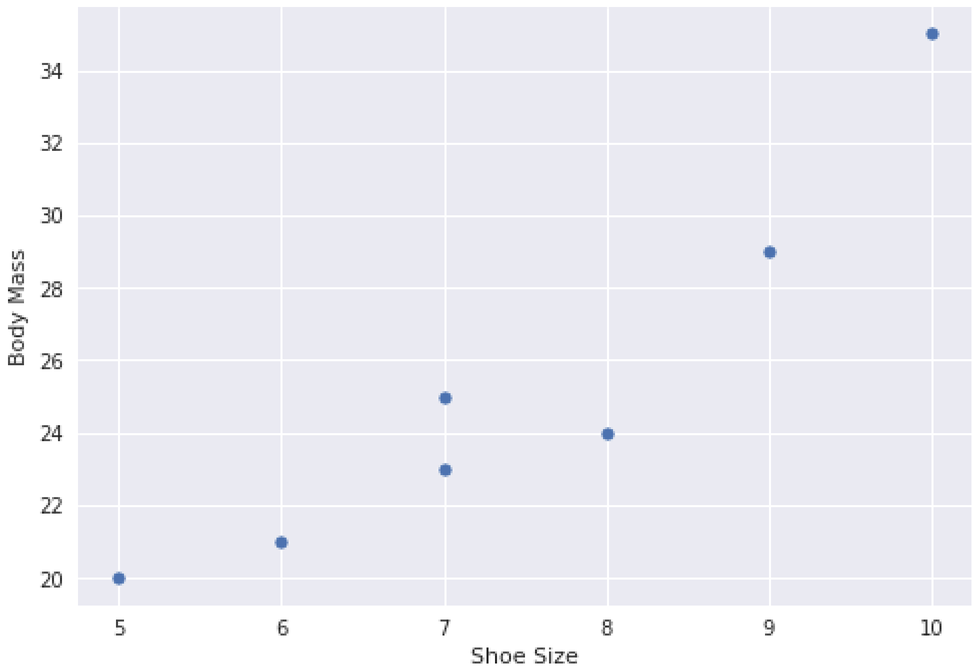
CASE-III

Working with real-valued integer variables

In [18]:
```
shoe_size = np.array([7,8,9,10,6,5,7])
body_mass = np.array([23,24,29,35,21,20,25])
shoe_size, body_mass, shoe_size.shape, shoe_size.ndim, body_mass.shape, body_mass.nd
```

Out[18]:
```
(array([ 7,  8,  9, 10,  6,  5,  7]),
 array([23, 24, 29, 35, 21, 20, 25]),
 (7,),
 1,
 (7,),
 1)
```

In [19]:
```
with plt.style.context('seaborn'):
    sns.scatterplot(x=shoe_size,y=body_mass,palette='inferno')
    plt.xlabel('Shoe Size')
    plt.ylabel('Body Mass')
```



In [20]:
```
[shoe_size[5],body_mass[5]], [shoe_size[4],body_mass[4]]
```

Out[20]:
```
([5, 20], [6, 21])
```

3.1.Euclidean_Distance

In [21]:
```
eu_dist.pairwise([[shoe_size[5],body_mass[5]]], [[shoe_size[4],body_mass[4]]])
```

Out[21]:
```
array([[1.41421356]])
```

3.2.Manhattan_Distance

In [22]:
```
man_hat_dist.pairwise([[shoe_size[5],body_mass[5]]], [[shoe_size[4],body_mass[4]]])
```

Out[22]:
```
array([[2.]])
```

3.3.Chebyshev_Distance

In [23]:
```
chby_dist = DistanceMetric.get_metric('chebyshev')
```

In [24]:
```
chby_dist.pairwise([[shoe_size[5],body_mass[5]]], [[shoe_size[4],body_mass[4]]])
```

Out[24]:
```
array([[1.]])
```

In [25]:
```
shoe_size.reshape((1,7)),body_mass.reshape((1,7))
```

Out[25]:
```
(array([[ 7,  8,  9, 10,  6,  5,  7]]), array([[23, 24, 29, 35, 21, 20, 25]]))
```

In [26]:
```
chby_dist.pairwise(shoe_size.reshape((1,7)),body_mass.reshape((1,7))) ## 35 - 10 = 2
```

Out[26]:
```
array([[25.]])
```

3.4.Mahalanobis_Distance

In [27]:
```
body_data_df = pd.DataFrame({'shoe_size':shoe_size, 'body_mass':body_mass})
```

In [28]:
```
np.square(body_data_df.corr())
```

Out[28]:

	shoe_size	body_mass
shoe_size	1.000000	0.879253
body_mass	0.879253	1.000000

In [29]:
```
np.square(np.corrcoef(shoe_size,body_mass))
```

Out[29]:
```
array([[1.       , 0.8792535],
       [0.8792535, 1.       ]])
```

In [30]:
```
## Calculating Mahalanobis Distance ::: (X - mu) * inv(cov(X)) * (X - mu).T
x_min_mu = body_data_df - np.mean(body_data_df)
inv_cov_x = pd.DataFrame(scipy.linalg.inv(body_data_df.cov()))
x_min_mu_T = x_min_mu.T
```

In [31]:
```
x_min_mu.shape, inv_cov_x.shape, x_min_mu_T.shape
```

Out[31]:
```
((7, 2), (2, 2), (2, 7))
```

In [32]:
```
mahanalobis_dists_matrix = pd.DataFrame(np.dot(np.dot(x_min_mu,inv_cov_x),x_min_mu_T
mahanalobis_dists_matrix
```

Out[32]:

	0	1	2	3	4	5	6
0	0.416337	0.875584	0.014185	-1.177375	0.287251	-0.171996	-0.243986
1	0.875584	2.705124	0.959986	-1.678823	-0.060287	-1.889828	-0.911756
2	0.014185	0.959986	1.002187	0.818488	-0.705715	-1.651516	-0.437615
3	-1.177375	-1.678823	0.818488	4.065489	-1.425616	-0.924168	0.322005
4	0.287251	-0.060287	-0.705715	-1.425616	0.709262	1.056800	0.138306
5	-0.171996	-1.889828	-1.651516	-0.924168	1.056800	2.774632	0.806076
6	-0.243986	-0.911756	-0.437615	0.322005	0.138306	0.806076	0.326970

In [33]:
```
np.diagonal(mahanalobis_dists_matrix)
```

Out[33]:
```
array([0.41633666, 2.70512442, 1.00218689, 4.0654885 , 0.70926178,
       2.77463207, 0.32696968])
```

CASE-IV

Working with DataFrame object

Understood `Mahalanobis Distance` via link :: https://www.machinelearningplus.com/statistics/mahalanobis-distance/

In [34]:
```
filepath = 'https://raw.githubusercontent.com/selva86/datasets/master/diamonds.csv'
df = pd.read_csv(filepath).iloc[0:500, [0,4,6]]
df.shape, df.ndim, df.head()
```

Out[34]:
```
((500, 3),
 2,
    carat  depth  price
 0   0.23   61.5    326
 1   0.21   59.8    326
```

```
2    0.23    56.9    327
3    0.29    62.4    334
4    0.31    63.3    335)
```

In [36]:

```
def mahalanobis(x=None, data=None):
    """This function generates the Mahalanobis Distance"""
    x_min_mu = x - np.mean(data)
    cov = np.cov(data.values.T)
    inv_cov_x = scipy.linalg.inv(cov)
    first_term = np.dot(x_min_mu, inv_cov_x)
    mahal_dist = np.dot(first_term, x_min_mu.T)
    return mahal_dist.diagonal(), inv_cov_x

df_x = df[['carat', 'depth', 'price']].head(500)
df_x['mahala'],VI = mahalanobis(x=df_x, data=df[['carat', 'depth', 'price']])
df_x.head()
```

Out[36]:

	carat	depth	price	mahala
0	0.23	61.5	326	3.766898
1	0.21	59.8	326	5.040171
2	0.23	56.9	327	11.473766
3	0.29	62.4	334	3.876022
4	0.31	63.3	335	4.661105

Manual Calculation

In [37]:

```
pd.DataFrame(((df - np.mean(df)).values @ scipy.linalg.inv(df.cov().values)) @ ((df
```

Out[37]: (500, 500)

In [38]:

```
pd.DataFrame(((df - np.mean(df)).values @ scipy.linalg.inv(df.cov().values)) @ ((df
```

Out[38]:

	0	1	2	3	4	5	6	7	8
0	3.766898	3.916408	3.985651	3.509290	3.396797	3.658189	3.682101	3.631782	3.615154
1	3.916408	5.040171	6.724389	3.101321	2.465016	3.068993	3.374325	3.531883	1.749026
2	3.985651	6.724389	11.473766	2.590670	1.152378	1.861321	2.675488	3.354030	-1.915498
3	3.509290	3.101321	2.590670	3.876022	4.122082	3.776873	3.677306	3.664491	4.162841
4	3.396797	2.465016	1.152378	4.122082	4.661105	4.052604	3.808965	3.714524	5.067003
...	...	...	...	...	...	...	...	...	...
495	-1.030892	-1.550898	-2.805898	-1.077694	-0.864771	-0.577531	-0.770679	-1.059940	0.449597
496	-0.963937	-0.695969	-0.526231	-1.356482	-1.546962	-1.124048	-1.076651	-1.143898	-1.233603
497	-0.877226	0.018579	1.250222	-1.610250	-2.134672	-1.516238	-1.285177	-1.208840	-2.467239
498	-0.901139	-0.286753	0.436055	-1.510683	-1.891033	-1.321054	-1.175901	-1.178855	-1.866096
499	-1.741025	-3.158284	-4.643153	-0.159136	0.751059	-0.777156	-1.092296	-1.001465	0.323868

500 rows × 500 columns

So, good here as everything matched!!

CASE-V

Applying Mahalanobis Distance Metric on Breast Cancer

In [40]:
```
cancer = load_breast_cancer()
```

In [41]:
```
cancer_df = pd.DataFrame(cancer.data,columns=cancer.feature_names)
cancer_df.head()
```

Out[41]:

	mean radius	mean texture	mean perimeter	mean area	mean smoothness	mean compactness	mean concavity	mean concave points	mean symmetry	di
0	17.99	10.38	122.80	1001.0	0.11840	0.27760	0.3001	0.14710	0.2419	
1	20.57	17.77	132.90	1326.0	0.08474	0.07864	0.0869	0.07017	0.1812	
2	19.69	21.25	130.00	1203.0	0.10960	0.15990	0.1974	0.12790	0.2069	
3	11.42	20.38	77.58	386.1	0.14250	0.28390	0.2414	0.10520	0.2597	
4	20.29	14.34	135.10	1297.0	0.10030	0.13280	0.1980	0.10430	0.1809	

5 rows × 30 columns

In [42]:
```
y = pd.DataFrame(cancer.target,columns=['Label'])
y.head()
```

Out[42]:

	Label
0	0
1	0
2	0
3	0
4	0

In [43]:
```
cancer_df = pd.concat([cancer_df,y],axis=1).copy(deep=True)
cancer_df.head()
```

Out[43]:

	mean radius	mean texture	mean perimeter	mean area	mean smoothness	mean compactness	mean concavity	mean concave points	mean symmetry	di
0	17.99	10.38	122.80	1001.0	0.11840	0.27760	0.3001	0.14710	0.2419	
1	20.57	17.77	132.90	1326.0	0.08474	0.07864	0.0869	0.07017	0.1812	
2	19.69	21.25	130.00	1203.0	0.10960	0.15990	0.1974	0.12790	0.2069	
3	11.42	20.38	77.58	386.1	0.14250	0.28390	0.2414	0.10520	0.2597	
4	20.29	14.34	135.10	1297.0	0.10030	0.13280	0.1980	0.10430	0.1809	

5 rows × 31 columns

In [44]:
```
from sklearn.model_selection import train_test_split
from sklearn.metrics import accuracy_score, precision_score, recall_score
```

In [45]:
```
X_train, X_test, y_train, y_test = train_test_split(cancer_df.iloc[:, 0:-1],cancer_d
                                                    stratify=cancer_df['Label'])
```

In [46]:
```
X_train.shape, X_test.shape, y_train.shape, y_test.shape
```

Out[46]:
```
((341, 30), (228, 30), (341,), (228,))
```

Seggregating the positive and negative observations

Only positivies

In [47]:
```
train_df = pd.concat([X_train,y_train],axis=1).copy(deep=True)
train_df_pos = train_df[train_df['Label']==1].copy(deep=True)
train_df_pos.shape
```

Out[47]:
```
(214, 31)
```

In [48]:
```
train_df_pos.head()
```

Out[48]:

	mean radius	mean texture	mean perimeter	mean area	mean smoothness	mean compactness	mean concavity	mean concave points	mean symmetry
525	8.571	13.10	54.53	221.3	0.10360	0.07632	0.025650	0.015100	0.1678
58	13.050	19.31	82.61	527.2	0.08060	0.03789	0.000692	0.004167	0.1819
342	11.060	14.96	71.49	373.9	0.10330	0.09097	0.053970	0.033410	0.1776
413	14.990	22.11	97.53	693.7	0.08515	0.10250	0.068590	0.038760	0.1944
559	11.510	23.93	74.52	403.5	0.09261	0.10210	0.111200	0.041050	0.1388

5 rows × 31 columns

Only negatives

In [49]:
```
train_df_neg = train_df[train_df['Label']==0].copy(deep=True)
train_df_neg.shape
```

Out[49]:
```
(127, 31)
```

In [50]:
```
train_df_neg.head()
```

Out[50]:

	mean radius	mean texture	mean perimeter	mean area	mean smoothness	mean compactness	mean concavity	mean concave points	mean symmetry
39	13.48	20.82	88.40	559.2	0.10160	0.12550	0.1063	0.05439	0.1720
229	12.83	22.33	85.26	503.2	0.10880	0.17990	0.1695	0.06861	0.2123
40	13.44	21.58	86.18	563.0	0.08162	0.06031	0.0311	0.02031	0.1784
172	15.46	11.89	102.50	736.9	0.12570	0.15550	0.2032	0.10970	0.1966
213	17.42	25.56	114.50	948.0	0.10060	0.11460	0.1682	0.06597	0.1308

5 rows × 31 columns

Distance calculation for positive observations

In [51]:
```
train_df_pos_mh_dist = ((train_df_pos.iloc[:,0:-1] - np.mean(train_df_pos.iloc[:,0:-
                        @ scipy.linalg.inv(train_df_pos.iloc[:,0:-1].cov().values))\
@ ((train_df_pos.iloc[:,0:-1] - np.mean(train_df_pos.iloc[:,0:-1])).T).values
```

In [52]:
```
train_df_pos['mahal_dist'] = train_df_pos_mh_dist.diagonal()
```

In [53]:
```
train_df_pos.head()
```

Out[53]:

	mean radius	mean texture	mean perimeter	mean area	mean smoothness	mean compactness	mean concavity	mean concave points	mean symmetry
525	8.571	13.10	54.53	221.3	0.10360	0.07632	0.025650	0.015100	0.1678
58	13.050	19.31	82.61	527.2	0.08060	0.03789	0.000692	0.004167	0.1819
342	11.060	14.96	71.49	373.9	0.10330	0.09097	0.053970	0.033410	0.1776
413	14.990	22.11	97.53	693.7	0.08515	0.10250	0.068590	0.038760	0.1944
559	11.510	23.93	74.52	403.5	0.09261	0.10210	0.111200	0.041050	0.1388

5 rows × 32 columns

Distance calculation for negative observations

In [54]:
```
train_df_neg_mh_dist = ((train_df_neg.iloc[:,0:-1] - np.mean(train_df_neg.iloc[:,0:-
                        @ scipy.linalg.inv(train_df_neg.iloc[:,0:-1].cov().values))\
@ ((train_df_neg.iloc[:,0:-1] - np.mean(train_df_neg.iloc[:,0:-1])).T).values
```

In [55]:
```
train_df_neg['mahal_dist'] = train_df_neg_mh_dist.diagonal()
```

In [56]:
```
train_df_neg.head()
```

Out[56]:

	mean radius	mean texture	mean perimeter	mean area	mean smoothness	mean compactness	mean concavity	mean concave points	mean symmetry
39	13.48	20.82	88.40	559.2	0.10160	0.12550	0.1063	0.05439	0.1720
229	12.83	22.33	85.26	503.2	0.10880	0.17990	0.1695	0.06861	0.2123
40	13.44	21.58	86.18	563.0	0.08162	0.06031	0.0311	0.02031	0.1784
172	15.46	11.89	102.50	736.9	0.12570	0.15550	0.2032	0.10970	0.1966
213	17.42	25.56	114.50	948.0	0.10060	0.11460	0.1682	0.06597	0.1308

5 rows × 32 columns

Hypothesis_Testing

Find Chi-square test Critical Value

In [57]:
```
from scipy.stats import chi2
chi2.ppf((1-0.01), df=2)
```

Out[57]:
```
9.21034037197618
```

Find Chi-square P-Value

In [58]:
```
1 - chi2.cdf(12.7,df=2)
```
Out[58]: 0.0017467471362611064

CASE-1

Only +ve observations

Here, first I'll perform the test on positive observations considering the `null hypothesis` as TRUE or POSITIVE and the `alternate hypothesis` as FALSE or negative.

Means,

- `Ho = All are positive observations`
- `Ha = All are not positive observations`

In [59]:
```
dof = train_df_pos.iloc[:,0:-1].shape[1]-1
dof
```
Out[59]: 30

In [60]:
```
c_val = chi2.ppf((1-0.01), df=dof)
c_val
```
Out[60]: 50.89218131151707

So, above is the critical value and if mahalanobis distance is greater than this value then we will reject the null hypothesis.

In [61]:
```
train_df_pos['p_val'] = 1 - chi2.cdf(train_df_pos['mahal_dist'], df=dof)
```
In [62]:
```
train_df_pos.head()
```
Out[62]:

	mean radius	mean texture	mean perimeter	mean area	mean smoothness	mean compactness	mean concavity	mean concave points	mean symmetry
525	8.571	13.10	54.53	221.3	0.10360	0.07632	0.025650	0.015100	0.1678
58	13.050	19.31	82.61	527.2	0.08060	0.03789	0.000692	0.004167	0.1819
342	11.060	14.96	71.49	373.9	0.10330	0.09097	0.053970	0.033410	0.1776
413	14.990	22.11	97.53	693.7	0.08515	0.10250	0.068590	0.038760	0.1944
559	11.510	23.93	74.52	403.5	0.09261	0.10210	0.111200	0.041050	0.1388

5 rows × 33 columns

In [63]:
```
train_df_pos.shape
```
Out[63]: (214, 33)

In [64]:
```
train_df_pos[train_df_pos['p_val'] < 0.01].shape
```
Out[64]: (26, 33)

In [65]:
```
rej_null_hyp = train_df_pos[train_df_pos['p_val'] < 0.01]['mahal_dist'].values
rej_null_hyp
```

Out[65]:
```
array([ 81.02384852,  72.07114302,  52.08522329,  62.90183841,
        69.0939475 ,  66.10649304,  66.76169799,  76.36211933,
       118.79639287, 145.94310336,  59.52453926,  73.90722389,
        68.33222003,  96.34523381,  54.67357222, 154.13771741,
        76.20390925, 100.12061258,  74.13167215,  58.07212966,
       194.52697533,  54.58637054, 129.41505176,  60.14696292,
        89.70806506,  54.60903334])
```

In [66]:
```
rej_null_hyp.min(), rej_null_hyp.max()
```

Out[66]:
```
(52.085223289182096, 194.5269753331549)
```

In [67]:
```
train_df_pos[train_df_pos['p_val'] >= 0.01]['mahal_dist'].min(), train_df_pos[train_
```

Out[67]:
```
(6.167006044471601, 50.03579960395341)
```

So, the null hypothesis got rejected based on the above 26 observations where the mahalanobis distance is greater than the critical value thus the distance ended up in the rejection region.

CASE-2

Only -ve observations

Now, I'll perform the test on negative observations considering the `null hypothesis` as FALSE or NEGATIVE and the `alternate hypothesis` as TRUE or POSITIVE.

Means,

- `Ho = All are negative observations`
- `Ha = All are not negative observations`

In [68]:
```
train_df_neg['p_val'] = 1 - chi2.cdf(train_df_neg['mahal_dist'], df=dof)
```

In [69]:
```
train_df_neg.head()
```

Out[69]:

	mean radius	mean texture	mean perimeter	mean area	mean smoothness	mean compactness	mean concavity	mean concave points	mean symmetry
39	13.48	20.82	88.40	559.2	0.10160	0.12550	0.1063	0.05439	0.1720
229	12.83	22.33	85.26	503.2	0.10880	0.17990	0.1695	0.06861	0.2123
40	13.44	21.58	86.18	563.0	0.08162	0.06031	0.0311	0.02031	0.1784
172	15.46	11.89	102.50	736.9	0.12570	0.15550	0.2032	0.10970	0.1966
213	17.42	25.56	114.50	948.0	0.10060	0.11460	0.1682	0.06597	0.1308

5 rows × 33 columns

In [70]:
```
train_df_neg.shape
```
Out[70]:
```
(127, 33)
```
In [71]:
```
train_df_neg[train_df_neg['p_val'] < 0.01].shape
```
Out[71]:
```
(14, 33)
```
In [72]:
```
rej_null_hyp_neg = train_df_neg[train_df_neg['p_val'] < 0.01]['mahal_dist'].values
rej_null_hyp_neg
```
Out[72]:
```
array([104.13997248,  65.26593056,  57.53158832,  74.66179609,
        55.42755962,  79.93825875,  52.30118131,  67.52958184,
        58.82178158,  52.2838042 ,  61.00788787, 102.21571179,
        60.01309311,  70.31700251])
```
In [73]:
```
rej_null_hyp_neg.min(), rej_null_hyp_neg.max()
```
Out[73]:
```
(52.28380420063802, 104.13997248029511)
```
In [74]:
```
train_df_neg[train_df_neg['p_val'] >= 0.01]['mahal_dist'].min(), train_df_neg[train_
```
Out[74]:
```
(8.361142675252562, 49.68938504959755)
```

So, the null hypothesis got rejected based on the above 14 observations where the mahalanobis distance is greater than the critical value thus the distance ended up in the rejection region.

Calculate_Euclidean_Distance

Euclidean Distance :: It performs the pairwise difference and not takes the distribution into account.

In [75]:
```
x1 = np.array([1,2,3,4,5])
x2 = np.array([5,6,7,8,9])
```

Case-1

Self implementation

In [97]:
```
def calc_euclidean_dist(vec1, vec2):
    """
    Description: This function is created for calculating the Euclidean Distance bet

    Input parameters : It accepts below 2 parameters:
        1. vec1 : np.array
            First vector
        2. vec2 : np.array
            Second vector

    Output : It returns the pandas dataframe with the input vectors and calculated E
    """
    data_points = list(zip(x1,x2))
    point_a = data_points[0]
    distances = []
    for i in range(len(data_points)):
        euc_dist = np.sqrt(np.sum(np.square(np.array(data_points[0]) - np.array(data
        distances.append(euc_dist)
    euc_df = pd.DataFrame({'vec1':vec1,'vec2':vec2,'euclidean_dist':distances})
    return euc_df
```
In [98]:
```
calc_euclidean_dist(x1,x2)
```

Out[98]:

	vec1	vec2	euclidean_dist
0	1	5	0.000000
1	2	6	1.414214
2	3	7	2.828427
3	4	8	4.242641
4	5	9	5.656854

Case-2

Using Scipy

In [99]:
```
from scipy.spatial.distance import pdist, squareform
```

In [100…
```
distances = pdist(pd.DataFrame({'x1':x1,'x2':x2}), metric='euclidean')
dist_matrix = pd.DataFrame(squareform(distances))
```

In [101…
```
pd.DataFrame(dist_matrix.iloc[0:5,0])
```

Out[101…

	0
0	0.000000
1	1.414214
2	2.828427
3	4.242641
4	5.656854

So, good here as the results matched!!

Radius_Neighbors

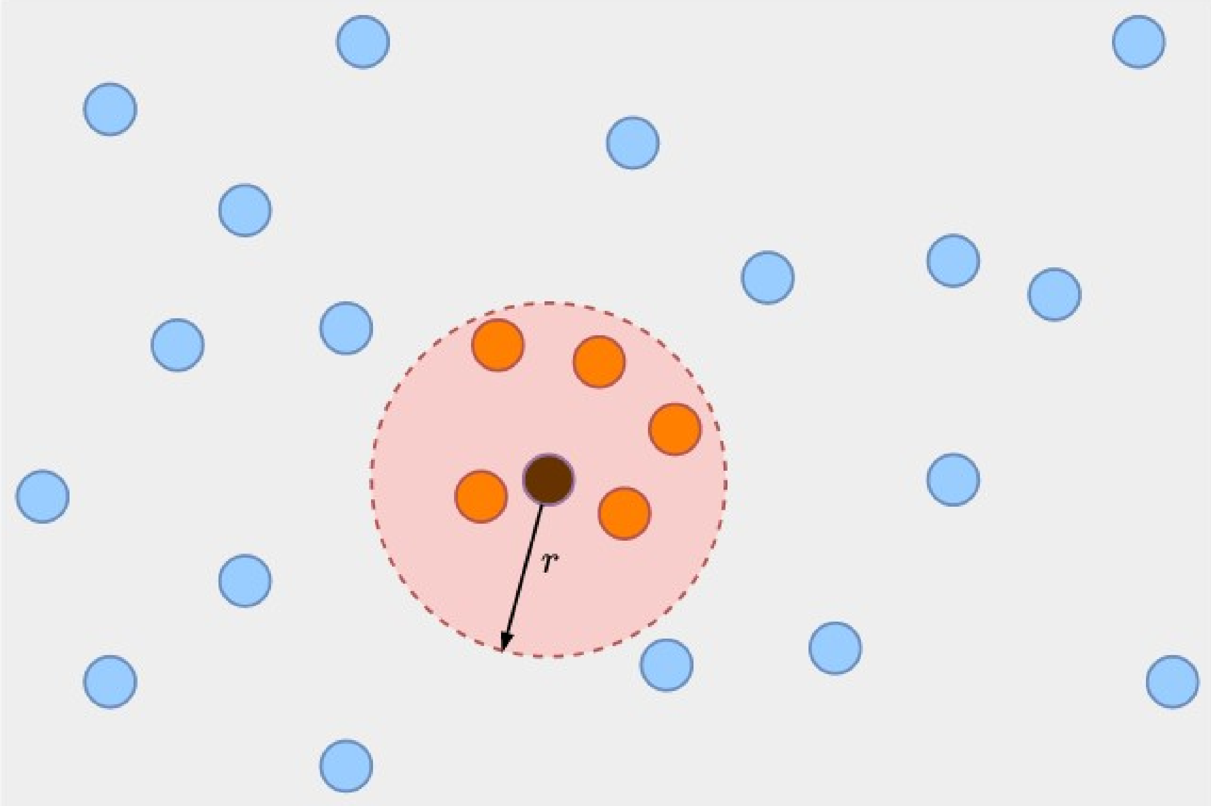
Reference Link of Fixed Nearest Neighbors ::

- https://machinelearningmastery.com/radius-neighbors-classifier-algorithm-with-python/
- **Julia Blog** :: https://jaantollander.com/post/searching-for-fixed-radius-near-neighbors-with-cell-lists-algorithm/

In [688…
```
from IPython.display import Image
from IPython.core.display import HTML

path = 'E:\STUDY\PROJECTS\AAIC_Practice\MODULES\Module_3\Mod_3_KNN\Refer_Notes\\'
Image(filename = path + "Fixed_NN.jpg", width=700, height=700)
```

Out[688…



- **RadiusNN is an extension of KNN and both are similar in a way of storing the entire train dataset in the training phase, however, they both uses the training dataset for prediction in a different manner.**

- `Instead of locating the k-neighbors, the Radius Neighbors Classifier locates all examples in the training dataset that are within a given radius of the new example. The radius neighbors are then used to make a prediction for the new example.`

- **The radius is defined in the feature space and generally assumes that the input variables are numeric and scaled to the range 0-1, e.g. normalized.**

- **Given a fixed radius, dense regions of the feature space will contribute more information and sparse regions will contribute less information. It is this latter case that is most desirable and it prevents examples very far in feature space from the new example from contributing to the prediction.**

- **The radius-based approach to locating neighbors is appropriate for those datasets where it is desirable for the contribution of neighbors to be proportional to the density of examples in the feature space.**

- **The Radius Neighbors Classifier may be more appropriate for prediction problems where there are sparse regions of the feature space.**

- **Given that the radius is fixed in all dimensions of the feature space, it will become less effective as the number of input features is increased, which causes examples in the feature space to spread further and further apart. This property is referred to as the curse of dimensionality.**

```
X_train, X_test, y_train, y_test = train_test_split(cancer_df.iloc[:,0:-1], cancer_d
```

In [170…

```

```

In [171…

```
X_train.shape, X_test.shape, y_train.shape, y_test.shape
```

Out[171…

```
((426, 30), (143, 30), (426,), (143,))
```

In [205…

```
from sklearn.preprocessing import MinMaxScaler
```

In [194…

```
mms = MinMaxScaler()
mms.fit(X_train)
X_train_mms = mms.transform(X_train)
X_test_mms = mms.transform(X_test)
```

In [195…

```
pd.DataFrame(X_train_mms).head()
```

Out[195…

	0	1	2	3	4	5	6	7	8	9
0	0.636992	0.408184	0.622003	0.487593	0.287343	0.287467	0.229808	0.406952	0.281818	0.118155
1	0.284869	0.409537	0.302052	0.159618	0.642185	0.533157	0.435976	0.488918	0.651515	0.504002
2	0.108240	0.106865	0.122314	0.044624	1.000000	0.627323	0.228189	0.274543	0.665657	0.949031
3	0.334091	0.212039	0.317808	0.198388	0.218753	0.121373	0.082880	0.153894	0.330303	0.189975
4	0.519144	0.348326	0.486559	0.355673	0.213202	0.146739	0.171037	0.292525	0.539899	0.006108

5 rows × 30 columns

In [200…

```
np.unique(y_train), np.bincount(y_train)
```

Out[200…

```
(array([0, 1]), array([158, 268], dtype=int64))
```

In [196…

```
pd.DataFrame(X_test_mms).head()
```

Out[196…

	0	1	2	3	4	5	6	7	8	9
0	0.550381	0.356442	0.541151	0.403181	0.316087	0.267530	0.349437	0.404130	0.321717	0.148062
1	0.210564	0.257017	0.206413	0.107953	0.462781	0.231520	0.047631	0.097282	0.295455	0.329823
2	0.197785	0.395671	0.187686	0.100445	0.389434	0.123919	0.021001	0.056247	0.280303	0.241786
3	0.373373	0.355090	0.361620	0.227953	0.330657	0.196522	0.160038	0.258808	0.215657	0.158382
4	0.375740	0.176530	0.363900	0.230498	0.183071	0.202779	0.129902	0.168374	0.316667	0.141744

5 rows × 30 columns

Case:1

Radius is larger than 1

In [257…

```
rnc1 = RadiusNeighborsClassifier(radius=3,n_neighbors=5,weights='uniform',algorithm=
                                 leaf_size=30,p=2,metric='minkowski',outlier_label=0)
rnc1.fit(X_train_mms, y_train)
print(rnc1.predict(pd.DataFrame(X_test_mms)))
print(rnc1.score(pd.DataFrame(X_test_mms),y_test))
```

```
[1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
```

```
 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1]
0.6223776223776224
```

Here, as the dominating class is 1 thus with a radius of 3 we are considering the entire training dataset to label the test dataset. Hence, all are labelled as 1 because all the training points are inside the radius of 3.

Case:2

Different values of Radius and Nearest Neighbors

NOTE :: I'm making an assumption here that is if the nearest neighbors of a point are not found within the given radius then it will be marked as -ve i.e. 0.

In [288…

```
k = [7,9,11,13,15]
radius = [0.8,0.9,1.0,1.2,1.5]
for idx,(n,r) in enumerate(list(zip(k,radius))):
    print("\n### Run -- {} with Nearest Neighbors -- {} and Radius -- {} ###".format
    rnc1 = RadiusNeighborsClassifier(radius=r,n_neighbors=n,weights='uniform',algori
                                leaf_size=15,p=2,metric='minkowski',outlier_label=0)
    rnc1.fit(X_train_mms, y_train)
    print(rnc1.predict(pd.DataFrame(X_test_mms)))
    print("Accuracy Score is {}".format(np.round(rnc1.score(pd.DataFrame(X_test_mms)
```

```
### Run -- 1 with Nearest Neighbors -- 7 and Radius -- 0.8 ###
[0 1 1 1 1 1 1 1 1 1 1 1 0 1 1 1 0 1 1 1 1 0 1 1 1 0 0 0 1 1 1 1 1 1 1 1 0 0
 1 1 1 1 1 1 1 1 1 1 1 1 1 1 0 1 1 1 1 1 0 1 1 0 0 1 0 1 1 1 1 1 0 1 1 1 0
 0 0 0 0 0 1 0 1 1 0 1 0 1 0 1 1 1 0 0 1 0 1 1 0 1 1 0 1 1 1 1 0 1 0 1 0 1
 0 1 0 1 1 0 1 0 0 1 0 1 1 0 0 1 1 0 1 1 1 1 1 1 0 1 0 1 1 1 0 0]
Accuracy Score is 0.944

### Run -- 2 with Nearest Neighbors -- 9 and Radius -- 0.9 ###
[0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 0 1 1 1 1 0 1 1 1 0 0 0 1 1 1 1 1 1 1 1 1 0
 1 1 1 1 1 1 1 1 1 1 1 1 1 1 0 1 1 1 1 1 0 1 1 0 0 1 0 1 1 1 1 1 0 1 1 1 0
 0 0 0 0 0 1 0 1 1 0 1 0 1 0 1 1 1 0 0 1 0 1 1 0 1 1 0 1 1 1 1 0 1 0 1 0 1
 0 1 0 1 1 0 1 0 0 1 1 1 1 0 0 1 1 0 1 1 1 1 1 1 0 1 0 1 1 1 0 0]
Accuracy Score is 0.923

### Run -- 3 with Nearest Neighbors -- 11 and Radius -- 1.0 ###
[0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 0 0 0 1 1 1 1 1 1 1 1 1 0
 1 1 1 1 1 1 1 1 1 1 1 1 1 1 0 1 1 1 1 1 0 1 1 0 0 1 0 1 1 1 1 1 0 1 1 1 0
 0 1 0 1 0 1 0 1 1 0 1 0 1 0 1 1 1 0 1 1 1 1 1 0 1 1 0 1 1 1 1 0 1 0 1 0 1
 0 1 1 1 1 0 1 0 0 1 1 1 1 0 0 1 1 0 1 1 1 1 1 1 0 1 0 1 1 1 0 0]
Accuracy Score is 0.874

### Run -- 4 with Nearest Neighbors -- 13 and Radius -- 1.2 ###
[1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 0 1 1 1 1 1 1 1 1 1 1 1 0
 1 1 1 1 1 1 1 1 1 1 1 1 1 1 0 1 1 1 1 1 0 1 1 1 0 1 0 1 1 1 1 1 0 1 1 1 0
 1 1 0 1 0 1 1 1 1 0 1 0 1 0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 0 1 1 1 0 1
 0 1 1 1 1 0 1 0 0 1 1 1 1 1 0 1 1 0 1 1 1 1 1 1 1 1 1 1 1 1 0 0]
Accuracy Score is 0.783

### Run -- 5 with Nearest Neighbors -- 15 and Radius -- 1.5 ###
[1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 0 1 1 1 1 1 1 1 1 1 1 1 1
 1 1 1 1 1 1 1 1 1 1 1 1 1 1 0 1 1 1 1 1 0 1 1 1 1 1 0 1 1 1 1 1 1 1 1 1 0
 1 1 0 1 1 1 1 1 1 0 1 1 1 0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 0 1 1 1 0 1
 1 1 1 1 1 1 1 1 1 1 1 1 1 1 0 1 1 0 1 1 1 1 1 1 1 1 1 1 1 1 1 0]
Accuracy Score is 0.713
```

So, the accuracy is clearly dropping down with the increase in radius.

NN_Distances_and_Indices

Distance to every Nearest Neighbor and their indices

- **The `Radius Neighbors` function finds the neighbors within a given radius of a point or points.**
- **It return the indices and distances of each point from the dataset lying in a ball with size `radius` around the points of the query array. Points lying on the boundary are included in the results.**
- **The result points are *not* necessarily sorted by distance to their query point.**

In [292…
```
distances_to_each_nn, indices_of_nn = rnc1.radius_neighbors(X_test_st,radius=0.8)
```

In [293…
```
distances_to_each_nn.shape, indices_of_nn.shape
```

Out[293…
```
((143,), (143,))
```

So, till now we are good because 143 data points exist in the test dataset.

In [294…
```
X_test_st[0]
```

Out[294…
```
array([0.55038099, 0.35644234, 0.54115127, 0.40318134, 0.31608683,
       0.2675296 , 0.34943715, 0.40412964, 0.32171717, 0.14806234,
       0.26847728, 0.32903112, 0.22970362, 0.16133929, 0.30720332,
       0.18752065, 0.12830808, 0.36200038, 0.18815124, 0.11477551,
       0.47598719, 0.40618337, 0.44568953, 0.29930201, 0.41359044,
       0.1789155 , 0.27523962, 0.51202749, 0.15279968, 0.12476197])
```

In [297…
```
len(distances_to_each_nn[0])
```

Out[297…
```
107
```

Here, the first point in the test dataset has 107 Radius Nearest Neighbors.

In [298…
```
distances_to_each_nn[0]
```

Out[298…
```
array([0.77485119, 0.79928181, 0.75381767, 0.70104903, 0.78250427,
       0.66317849, 0.663835  , 0.59951726, 0.73479384, 0.63464298,
       0.68966113, 0.73084904, 0.75086833, 0.76285138, 0.60855405,
       0.7042115 , 0.65302504, 0.77355881, 0.7643015 , 0.69141421,
       0.50073962, 0.64050169, 0.72027237, 0.72954823, 0.7175256 ,
       0.70404708, 0.56169357, 0.61452768, 0.62009898, 0.61641988,
       0.7451911 , 0.63563298, 0.58947877, 0.6019377 , 0.52353405,
       0.53506146, 0.61081914, 0.62331693, 0.52414384, 0.52262196,
       0.72080903, 0.46332191, 0.60930924, 0.44142947, 0.60589131,
       0.45932364, 0.6261524 , 0.40951519, 0.60013706, 0.44445524,
       0.74071954, 0.43127356, 0.49096904, 0.77621701, 0.56782249,
       0.66669249, 0.6931883 , 0.55817302, 0.62487651, 0.78417201,
       0.56344947, 0.77031498, 0.73625407, 0.72129064, 0.72113906,
       0.63343834, 0.78740412, 0.57786836, 0.74541704, 0.7393466 ,
       0.39731962, 0.77010967, 0.74216385, 0.68700304, 0.72430201,
       0.66556779, 0.58060416, 0.40485425, 0.61051576, 0.68552695,
       0.5759053 , 0.64410966, 0.4960889 , 0.52578606, 0.48918407,
       0.79324096, 0.48277944, 0.75340673, 0.5322959 , 0.72316033,
       0.68425833, 0.69591922, 0.389545  , 0.58881879, 0.44132117,
       0.78901245, 0.7205242 , 0.54556867, 0.6572326 , 0.46841819,
       0.68788622, 0.48553522, 0.73903593, 0.79735253, 0.54686117,
       0.58888114, 0.51697856])
```

Above are the distances of first test point to its 107 Radius Nearest Neighbors.

In [296…
```
indices_of_nn[0]
```

```
array([ 35,  93, 168, 294, 298,  27,  98, 354, 193, 407, 166, 151, 109,
```

Out[296...

```
        59,  14,  26,  57, 148, 248,  44, 423, 130, 323, 310, 341, 165,
       378, 229, 351,  30,  52, 223, 270, 120, 226, 283,  78,  94, 140,
        54, 314, 333, 318, 102, 107,   0, 144,  43,  36, 312, 376, 306,
        58, 234, 345, 297, 254, 338, 179, 105, 260, 128, 125, 370, 220,
       307, 422, 377, 389, 143, 126,  15, 190,  18, 204,  45, 295, 189,
        74, 181, 369, 374, 121,  28, 247,  75,  24, 340, 394, 324, 408,
       208, 316, 116, 327,  95, 183, 246, 110, 404,  13, 343, 360,  37,
       170, 296, 319], dtype=int64)
```

Above are the training data points indices of first test point 107 Radius Nearest Neighbors.

In [302...

```
pd.DataFrame(X_train_mms[indices_of_nn[0],:])
```

Out[302...

	0	1	2	3	4	5	6	7	8	
0	0.291495	0.373013	0.291549	0.166872	0.240262	0.274584	0.254456	0.183481	0.253535	0.2156
1	0.385205	0.235712	0.380001	0.243097	0.260184	0.234648	0.177064	0.213225	0.269697	0.2085
2	0.441053	0.202570	0.420911	0.286872	0.314798	0.146433	0.129597	0.238526	0.328788	0.1392
3	0.413129	0.142712	0.402253	0.262227	0.318267	0.230783	0.167331	0.310141	0.381818	0.1531
4	0.381419	0.237741	0.379656	0.231559	0.359996	0.358935	0.181074	0.321066	0.307071	0.3944
...	...	...	...	...	...	...	...	...	...	
102	0.475129	0.482584	0.476885	0.320594	0.566855	0.399423	0.566839	0.628855	0.600000	0.2919
103	0.364854	0.144403	0.376132	0.217434	0.402319	0.503711	0.340056	0.329326	0.518182	0.5075
104	0.383312	0.542103	0.374611	0.243097	0.395381	0.240200	0.289634	0.342551	0.296465	0.3091
105	0.439159	0.411566	0.440260	0.289841	0.535137	0.334090	0.421904	0.417198	0.408586	0.3235
106	0.594870	0.456544	0.588142	0.437116	0.381505	0.344825	0.435272	0.533717	0.469192	0.1870

107 rows × 30 columns

Above are the 107 Radius Nearest Neighbors of first test point from training data.

KNN

Using pre-computed Mahalanobis Distance

NOTE :: Sklearn implementation expects the distances to be +ve valued when using metric as 'precomputed' and algorithm also should be set as 'auto' or 'ball_tree'.

In [643...

```
cancer_pre_comp = pd.DataFrame(cancer.data,columns=cancer.feature_names)
cancer_pre_comp_y = cancer.target
cancer_pre_comp.head()
```

Out[643...

	mean radius	mean texture	mean perimeter	mean area	mean smoothness	mean compactness	mean concavity	mean concave points	mean symmetry	di
0	17.99	10.38	122.80	1001.0	0.11840	0.27760	0.3001	0.14710	0.2419	
1	20.57	17.77	132.90	1326.0	0.08474	0.07864	0.0869	0.07017	0.1812	
2	19.69	21.25	130.00	1203.0	0.10960	0.15990	0.1974	0.12790	0.2069	

	mean radius	mean texture	mean perimeter	mean area	mean smoothness	mean compactness	mean concavity	mean concave points	mean symmetry	di
3	11.42	20.38	77.58	386.1	0.14250	0.28390	0.2414	0.10520	0.2597	
4	20.29	14.34	135.10	1297.0	0.10030	0.13280	0.1980	0.10430	0.1809	

5 rows × 30 columns

In [644…
```
cancer_pre_comp.shape, cancer_pre_comp_y.shape
```
Out[644…
```
((569, 30), (569,))
```

In [645…
```
cancer_pre_comp_mahala = np.dot(np.dot((cancer_pre_comp - cancer_pre_comp.mean()),sc
                                (cancer_pre_comp - cancer_pre_comp.mean()).T)

cancer_pre_comp_mahala = np.square(pd.DataFrame(cancer_pre_comp_mahala))
cancer_pre_comp_mahala.shape
```
Out[645…
```
(569, 569)
```

In [577…
```
cancer_pre_comp_mahala.head()
```
Out[577…

	0	1	2	3	4	5	6	
0	8546.335317	217.013675	44.919530	221.166696	38.085944	78.517852	1.480728	0.0017
1	217.013675	1320.319427	13.357036	30.453245	27.211435	44.175538	144.354281	117.8559
2	44.919530	13.357036	555.204880	340.240745	8.547820	17.050733	17.587972	0.7608
3	221.166696	30.453245	340.240745	12586.119449	347.417854	370.360081	32.206953	162.9459
4	38.085944	27.211435	8.547820	347.417854	717.905001	3.477353	9.061761	1.9782

5 rows × 569 columns

In [674…
```
knc = KNeighborsClassifier(n_neighbors=9,weights='distance',algorithm='brute',metric
```
In [675…
```
knc.fit(cancer_pre_comp_mahala,cancer_pre_comp_y)
```
Out[675…
```
KNeighborsClassifier(algorithm='brute', metric='precomputed', n_neighbors=9,
                     weights='distance')
```

In [676…
```
dists, indxs = knc.kneighbors(cancer_pre_comp_mahala,n_neighbors=9)
```
In [677…
```
dists[34], indxs[34]
```
Out[677…
```
(array([2.79474991e-05, 1.65500188e-04, 2.62864771e-04, 5.28682818e-04,
        5.34360407e-04, 5.62853142e-04, 6.25889956e-04, 1.91934304e-03,
        2.30086972e-03]),
 array([173, 271, 144, 334, 331,  28, 475, 359, 153], dtype=int64))
```

In [678…
```
cancer_pre_comp_mahala.iloc[34,173],cancer_pre_comp_mahala.iloc[34,271],cancer_pre_c
cancer_pre_comp_mahala.iloc[34,331],cancer_pre_comp_mahala.iloc[34,28],cancer_pre_co
```
Out[678…
```
(2.7947499113078438e-05,
 0.00016550018833273196,
 0.0002628647705171907,
```

```
 0.0005286828181794098,
 0.0005343604065472748,
 0.0005628531423005402,
 0.0006258899556841858)
```

In [679…

```
cnts = []
for idx in indxs[34]:
    cnts.append(cancer_pre_comp_y[idx])

print(cnts)
if cnts.count(0) > cnts.count(1):
    print("Prediction is :: Non Cancerous")
else:
    print("Prediction is :: Cancerous")
```

```
[1, 1, 1, 1, 1, 0, 1, 1, 1]
Prediction is :: Cancerous
```

In [680…

```
knc.predict(np.array(cancer_pre_comp_mahala.iloc[34,:]).reshape(1,-1))
```

Out[680…

```
array([1])
```

In [681…

```
knc.predict_proba(np.array(cancer_pre_comp_mahala.iloc[34,:]).reshape(1,-1))
```

Out[681…

```
array([[0.03307214, 0.96692786]])
```

When we are using the precomputed distance matrix then 'predict' and 'predict_proba' function accepts test data input in the shape of (number of test observations, number of train data observations). For example, if we are trying ot test only 1 new unseen observation and used 569 training observations then the expected shape is (1,569).

Conclusion

1. **We can use Radius or Fixed Neighbors when we want to give weightage only to the nearby points within fixed distance.**
2. **We can use Radius or Fixed Neighbors to find the outliers if we are sure that points outside of a particular radius are outliers. This can give better results with data of high sparcity.**
3. **With Radius NN the features needs to be normalized. And, we can calculate the distances and indices of NN using `Nearest_neighbors` function.**
4. **The time and space complexity looks to be same for both Radius NN and KNN, its just that we can get better results using Radius NN if we want to find the neighbors only in close proximity.**
5. **If we are using `metric == 'precomputed'` then in sklearn only `'brute'` algorithm is supported otherwise select `'auto'` . Make sure the shape of test set would be (n_test , n_train).**
6. **With KNN we can compute the NN distances and their indices using `kneighbors` function.**