# Alzheimer\_classification\_with\_Demographics\_Data\_NestedNonnestedCV

## November 10, 2021

```
[1]: import numpy as np
  import pandas as pd
  import matplotlib
  import matplotlib.pyplot as plt
  import seaborn as sn

from numpy import mean

from sklearn import preprocessing
  from sklearn.metrics import log_loss
  from sklearn.metrics import confusion_matrix
  import sklearn.metrics as metrics
  from sklearn.metrics import plot_confusion_matrix
  from sklearn.metrics import classification_report

from sklearn.model_selection import GridSearchCV, cross_val_score, KFold

%matplotlib inline
```

### Load The data files Display data frame head

```
[2]:
      Subject ID
                        MRI ID
                                     Group
                                            Visit
                                                   MR Delay M/F Hand
                                                                     Age
                                                                         EDUC
    O OAS2_0001 OAS2_0001_MR1
                                Nondemented
                                                         0
                                                             М
                                                                  R.
                                                                      87
                                                                            14
                                                1
    457
                                                                      88
                                Nondemented
                                                2
                                                             Μ
                                                                  R.
                                                                           14
    2 OAS2_0002
                 OAS2_0002_MR1
                                   Demented
                                                1
                                                         0
                                                             М
                                                                  R.
                                                                      75
                                                                           12
    3 OAS2_0002
                 OAS2_0002_MR2
                                                2
                                                             Μ
                                                                  R
                                                                      76
                                                                            12
                                  Demented
                                                       560
    4 OAS2 0002
                 OAS2_0002_MR3
                                                                            12
                                  Demented
                                                3
                                                       1895
                                                             М
                                                                  R.
                                                                      80
       SES MMSE CDR
                             eTIV
                                      nWBV
                                                 ASF
    0 2.0 27.0 0.0
                      1986.550000
                                  0.696106
                                           0.883440
    1 2.0 30.0 0.0 2004.479526
                                  0.681062
                                            0.875539
```

```
2 NaN 23.0 0.5 1678.290000 0.736336 1.045710
3 NaN 28.0 0.5 1737.620000 0.713402 1.010000
4 NaN 22.0 0.5 1697.911134 0.701236 1.033623
```

Data pre-processing and selection Lets first look at columns data types

## [3]: data\_frame.dtypes

[3]: Subject ID object MRI ID object Group object int64 Visit int64 MR Delay M/F object Hand object Age int64 **EDUC** int64 SES float64 MMSE float64 CDR float64 eTIV float64 nWBV float64 ASF float64

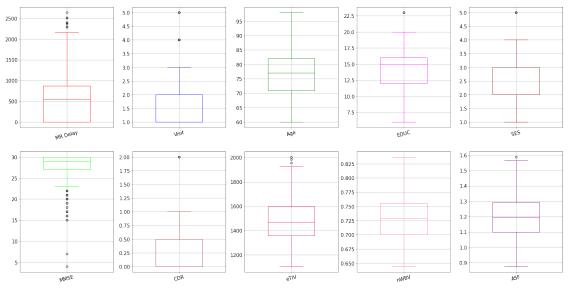
dtype: object

## [4]: data\_frame.info()

<class 'pandas.core.frame.DataFrame'>
RangeIndex: 373 entries, 0 to 372
Data columns (total 15 columns):

#	Column	Non-Null Count	Dtype
0	Subject ID	373 non-null	object
1	MRI ID	373 non-null	object
2	Group	373 non-null	object
3	Visit	373 non-null	int64
4	MR Delay	373 non-null	int64
5	M/F	373 non-null	object
6	Hand	373 non-null	object
7	Age	373 non-null	int64
8	EDUC	373 non-null	int64
9	SES	354 non-null	float64
10	MMSE	371 non-null	float64
11	CDR	373 non-null	float64
12	eTIV	373 non-null	float64
13	nWBV	373 non-null	float64
14	ASF	373 non-null	float64
dtyp	es: float64(	6), int64(4), ob	ject(5)

```
[5]: fig,axs = plt.subplots(2,5,figsize = (30,15))
     boxplot_mrdelay = data_frame.boxplot(column=['MR Delay'], rot=15, widths=.
      \rightarrow5, fontsize=15, color = 'red', ax=axs[0,0])
     boxplot_visit =data_frame.boxplot(column=['Visit'], rot=15, fontsize=15,widths=.
      \hookrightarrow5, color = 'blue', ax=axs[0,1])
     boxplot_Age =data_frame.boxplot(column=['Age'], rot=15, fontsize=15, widths=.
      \rightarrow5,color = 'green',ax=axs[0,2])
     boxplot EDUC = data frame.boxplot(column=['EDUC'], rot=15, fontsize=15, widths=.
      \hookrightarrow5, color = 'magenta', ax=axs[0,3])
     boxplot_SES = data_frame.boxplot(column=['SES'], rot=15, fontsize=15, widths=.
      \hookrightarrow5,color = 'maroon',ax=axs[0,4])
     boxplot_MMSE = data_frame.boxplot(column=['MMSE'], rot=15, fontsize=15, widths=.
      \hookrightarrow5,color = 'lime',ax=axs[1,0])
     boxplot_CDR = data_frame.boxplot(column=['CDR'], rot=15, fontsize=15, widths=.
      \hookrightarrow5,color = 'brown',ax=axs[1,1])
     boxplot_eTIV = data_frame.boxplot(column=['eTIV'], rot=15, fontsize=15, widths=.
      \rightarrow 5, color = 'crimson', ax=axs[1,2])
     boxplot_nWBV = data_frame.boxplot(column=['nWBV'], rot=15, fontsize=15, widths=.
      \rightarrow5,color = 'hotpink',ax=axs[1,3])
     boxplot_ASF = data_frame.boxplot(column=['ASF'], rot=15, fontsize=15, widths=.
      \hookrightarrow5,color = 'purple',ax=axs[1,4])
     plt.show()
```



### Histogram

```
[6]: data_frame.hist(figsize =(14,10))
[6]: array([[<AxesSubplot:title={'center':'Visit'}>,
              <AxesSubplot:title={'center':'MR Delay'}>,
              <AxesSubplot:title={'center':'Age'}>],
             [<AxesSubplot:title={'center':'EDUC'}>,
              <AxesSubplot:title={'center':'SES'}>,
              <AxesSubplot:title={'center':'MMSE'}>],
             [<AxesSubplot:title={'center':'CDR'}>,
              <AxesSubplot:title={'center':'eTIV'}>,
              <AxesSubplot:title={'center':'nWBV'}>],
             [<AxesSubplot:title={'center':'ASF'}>, <AxesSubplot:>,
              <AxesSubplot:>]], dtype=object)
                                                                                Age
                                      150
                                                                    60
          100
                                      100
                                                                    40
           50
                                       50
                                                                    20
           n
                                             500 1000 1500 2000 2500
SES
                      EDUC
          100
                                      100
                                                                   200
                                       75
           50
                                       50
                                                                   100
           25
                                       25
                                        0
                                                                     0
                      15
CDR
                                                                               15 20
nWBV
                                                   eTIV
          200
```

1.5

0.70

## Correlation Heatmap

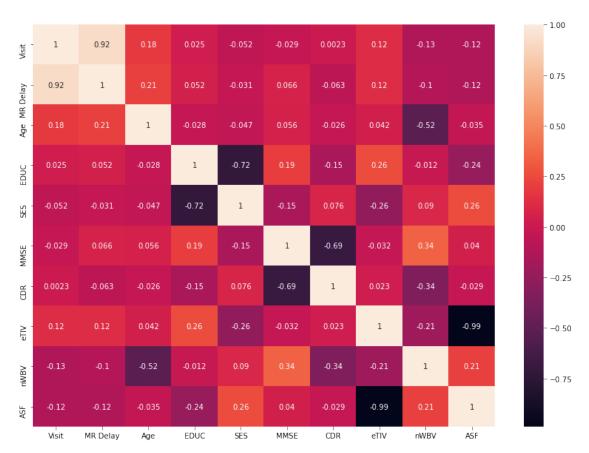
0.0

```
[7]: import matplotlib.pyplot as plt
import seaborn as sns

plt.figure(figsize = (14,10))

sns.heatmap(data_frame[data_frame.columns].corr(), annot=True)
```

## [7]: <AxesSubplot:>



## Dealing the missing values

[8]: missing\_data = data\_frame.isnull()
missing\_data.head()

[8]:	Subjec	t ID 1	MRI ID	Group	Visit	MR Delay	M/F	Hand	Age	EDUC	\
0	F	alse	False	False	False	False	False	False	False	False	
1	F	alse	False	False	False	False	False	False	False	False	
2	F	alse	False	False	False	False	False	False	False	False	
3	F	alse	False	False	False	False	False	False	False	False	
4	F	alse	False	False	False	False	False	False	False	False	
	SES	MMSE	CDR	eTIV	${\tt nWBV}$	ASF					
0	False	False	False	False	False	False					
1	False	False	False	False	False	False					
2	True	False	False	False	False	False					
3	True	False	False	False	False	False					
4	True	False	False	False	False	False					

Count missing values in each column

```
[9]: for column in missing_data.columns.values.tolist():
         print(column)
         print(missing_data[column].value_counts())
         print(" ")
    Subject ID
    False
             373
    Name: Subject ID, dtype: int64
    MRI ID
    False
             373
    Name: MRI ID, dtype: int64
    Group
    False
             373
    Name: Group, dtype: int64
    Visit
             373
    False
    Name: Visit, dtype: int64
    MR Delay
    False
             373
    Name: MR Delay, dtype: int64
    M/F
    False
             373
    Name: M/F, dtype: int64
    Hand
    False
             373
    Name: Hand, dtype: int64
    Age
    False
             373
    Name: Age, dtype: int64
    EDUC
    False
             373
    Name: EDUC, dtype: int64
    SES
    False
             354
    True
              19
    Name: SES, dtype: int64
    MMSE
```

False

371

```
Name: MMSE, dtype: int64
     CDR
              373
     False
     Name: CDR, dtype: int64
     eTIV
     False
              373
     Name: eTIV, dtype: int64
     nWBV
              373
     False
     Name: nWBV, dtype: int64
     ASF
     False
              373
     Name: ASF, dtype: int64
     SES have 19 missing value and MMSE have 2 missing Value replace missing values
[10]: # check the details value of SES
      data_frame['SES'].value_counts()
[10]: 2.0
             103
      1.0
              88
      3.0
              82
      4.0
              74
      5.0
               7
      Name: SES, dtype: int64
[11]: #Here 2 is most common values. use the ".idxmax()" method to calculate for usu
      → the most common type automatically:
      data_frame['SES'].value_counts().idxmax()
[11]: 2.0
[12]: #replace null with most common values
      data_frame['SES'].fillna(2.0, inplace=True)
[13]: #check the details value of MMSE
      data_frame['MMSE'].value_counts()
[13]: 30.0
              114
      29.0
               91
      28.0
               45
```

True

```
26.0
              20
     25.0
              12
     23.0
              11
     21.0
              11
     20.0
               7
     22.0
               7
     17.0
               5
     24.0
               4
     16.0
               3
     19.0
               3
     18.0
               2
     15.0
               2
     7.0
               1
     4.0
               1
     Name: MMSE, dtype: int64
[14]: #30 is the most common value. We can also use the ".idxmax()" method to,
      →calculate for us the most common type automatically:
     data_frame['MMSE'].value_counts().idxmax()
[14]: 30.0
[15]: #replace null with most common values
     data_frame['MMSE'].fillna(30,inplace=True)
[16]: missing_data = data_frame.isnull()
     missing_data.head()
[16]:
        Subject ID
                   MRI ID
                                  Visit
                                         MR Delay
                                                    M/F
                                                                       EDUC
                           Group
                                                          Hand
                                                                  Age
                                                  False False
     0
             False
                    False False
                                 False
                                            False
                                                               False False
             False
                    False False False
     1
                                            False
                                                  False False
                                                                False
                                                                      False
     2
             False
                    False False False
                                           False
                                                  False False
                                                               False False
     3
                    False False
             False
                                 False
                                           False
                                                  False False
                                                                False False
             False
                    False False False
                                           False
                                                  False False
                                                                False False
                MMSE
                       CDR
                             eTIV
                                            ASF
          SES
                                    nWBV
     O False False False False False
     1 False False False False
                                         False
     2 False False False False False
     3 False False False False False
     4 False False False False False
[17]: missing_data.info()
     <class 'pandas.core.frame.DataFrame'>
     RangeIndex: 373 entries, 0 to 372
     Data columns (total 15 columns):
```

27.0

32

```
#
          Column
                       Non-Null Count
                                       Dtype
          _____
                       _____
      0
          Subject ID
                      373 non-null
                                       bool
      1
          MRI ID
                       373 non-null
                                       bool
      2
          Group
                       373 non-null
                                       bool
      3
          Visit
                       373 non-null
                                       bool
      4
          MR Delay
                       373 non-null
                                       bool
      5
          M/F
                       373 non-null
                                       bool
      6
          Hand
                       373 non-null
                                       bool
      7
                       373 non-null
          Age
                                       bool
      8
          EDUC
                       373 non-null
                                       bool
      9
          SES
                       373 non-null
                                       bool
          MMSE
                       373 non-null
      10
                                       bool
          CDR
                       373 non-null
      11
                                       bool
                       373 non-null
      12
          eTIV
                                       bool
      13
          nWBV
                       373 non-null
                                       bool
      14 ASF
                       373 non-null
                                       bool
     dtypes: bool(15)
     memory usage: 5.6 KB
[18]: for column in missing_data.columns.values.tolist():
          print(column)
          print(missing_data[column].value_counts())
          print(" ")
     Subject ID
     False
              373
     Name: Subject ID, dtype: int64
     MRI ID
     False
              373
     Name: MRI ID, dtype: int64
     Group
     False
              373
     Name: Group, dtype: int64
     Visit
     False
              373
     Name: Visit, dtype: int64
     MR Delay
     False
              373
     Name: MR Delay, dtype: int64
     M/F
     False
              373
     Name: M/F, dtype: int64
```

```
Name: Hand, dtype: int64
     Age
     False
               373
     Name: Age, dtype: int64
     EDUC
     False
               373
     Name: EDUC, dtype: int64
     SES
     False
               373
     Name: SES, dtype: int64
     MMSE
     False
               373
     Name: MMSE, dtype: int64
     CDR
     False
               373
     Name: CDR, dtype: int64
     eTIV
     False
               373
     Name: eTIV, dtype: int64
     nWBV
     False
               373
     Name: nWBV, dtype: int64
     ASF
     False
               373
     Name: ASF, dtype: int64
     Let's see how many of each class is in our data set
[19]: data_frame['Subject ID'].value_counts()
[19]: OAS2_0073
                   5
      OAS2_0070
                   5
                   5
      OAS2_0127
      OAS2_0048
                   5
      OAS2_0036
                   4
                   . .
```

Hand False

373

```
OAS2_0008
                   2
      OAS2_0108
                   2
      OAS2_0029
                   2
      OAS2_0113
      OAS2_0096
                   2
      Name: Subject ID, Length: 150, dtype: int64
[20]: # check the total number of subject
      data_frame['Subject ID'].nunique()
[20]: 150
      data_frame['Group'].value_counts()
[21]: Nondemented
                     190
      Demented
                     146
      Converted
                      37
      Name: Group, dtype: int64
     Check for male and female
[22]: data_frame.groupby(['M/F','Group'])['Subject ID'].nunique()
[22]: M/F
           Group
      F
           Converted
                          10
           Demented
                          28
           Nondemented
                          50
           Converted
                           4
      М
           Demented
                          36
           Nondemented
                          22
      Name: Subject ID, dtype: int64
     Group by Male female and Subject ID
[23]: data_frame_sub =data_frame.groupby(['M/F','Group'])
[24]: data_frame_sub= data_frame_sub.agg({'Subject ID':'nunique'})
[25]: data_frame_sub.head()
[25]:
                       Subject ID
     M/F Group
          Converted
                               10
          Demented
                               28
          Nondemented
                               50
          Converted
                                4
          Demented
                               36
```

```
[26]: # Change M to 1 and F to 0
      data_frame['M/F'] = data_frame['M/F'].replace(['F','M'], [0,1])
[27]: # Hand cloumn value to numaric data R to 1 and L to 0
      data_frame['Hand'] = data_frame['Hand'].replace(['L','R'], [0,1]) # Hand column
[28]: # Group : Replace Converted to Demented
      data_frame['Group'] = data_frame['Group'].replace(['Converted'], ['Demented'])
[29]: data frame.head()
[29]:
        Subject ID
                           MRI ID
                                          Group
                                                 Visit
                                                        MR Delay
                                                                   M/F
                                                                              Age
                                                                        Hand
      0 DAS2_0001
                    OAS2_0001_MR1
                                    Nondemented
                                                     1
                                                                0
                                                                     1
                                                                           1
                                                                               87
      1 OAS2 0001
                    OAS2 0001 MR2
                                    Nondemented
                                                     2
                                                              457
                                                                     1
                                                                           1
                                                                               88
      2 OAS2 0002
                    OAS2 0002 MR1
                                       Demented
                                                     1
                                                                0
                                                                     1
                                                                           1
                                                                               75
      3 OAS2_0002
                    OAS2_0002_MR2
                                       Demented
                                                     2
                                                              560
                                                                           1
                                                                               76
                                                                     1
      4 OAS2_0002
                    OAS2_0002_MR3
                                                                               80
                                       Demented
                                                     3
                                                             1895
                                                                     1
                                                                           1
         EDUC SES MMSE CDR
                                                 nWBV
                                                             ASF
                                       eTIV
               2.0 27.0
      0
           14
                          0.0
                               1986.550000
                                             0.696106
                                                       0.883440
      1
           14
               2.0
                    30.0 0.0
                                2004.479526
                                             0.681062
                                                       0.875539
      2
           12
               2.0
                    23.0
                          0.5
                                1678.290000
                                             0.736336
                                                       1.045710
      3
           12
               2.0
                    28.0
                          0.5
                                1737.620000
                                             0.713402
                                                       1.010000
           12
               2.0
                    22.0
                          0.5
                                1697.911134
                                             0.701236
                                                       1.033623
[30]: data frame.info()
     <class 'pandas.core.frame.DataFrame'>
     RangeIndex: 373 entries, 0 to 372
     Data columns (total 15 columns):
      #
          Column
                       Non-Null Count
                                       Dtype
          _____
                       _____
      0
          Subject ID
                       373 non-null
                                       object
      1
          MRI ID
                       373 non-null
                                       object
      2
          Group
                       373 non-null
                                       object
                       373 non-null
      3
          Visit
                                       int64
      4
          MR Delay
                       373 non-null
                                       int64
      5
          M/F
                       373 non-null
                                       int64
      6
          Hand
                       373 non-null
                                       int64
      7
          Age
                       373 non-null
                                       int64
      8
          EDUC
                       373 non-null
                                       int64
          SES
                       373 non-null
                                       float64
      10
          MMSE
                       373 non-null
                                       float64
      11
          CDR
                       373 non-null
                                       float64
      12
          eTIV
                       373 non-null
                                       float64
      13
          nWBV
                       373 non-null
                                       float64
      14
          ASF
                       373 non-null
```

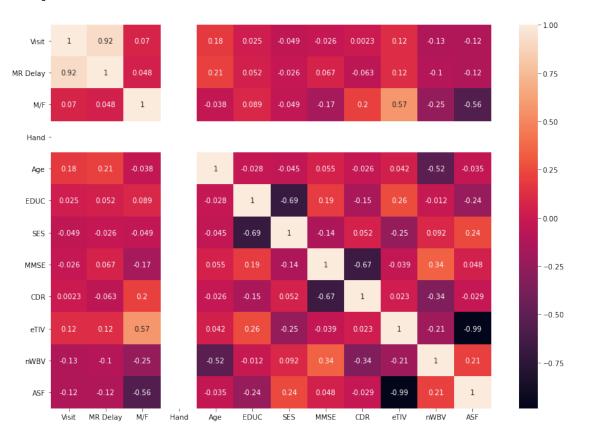
float64

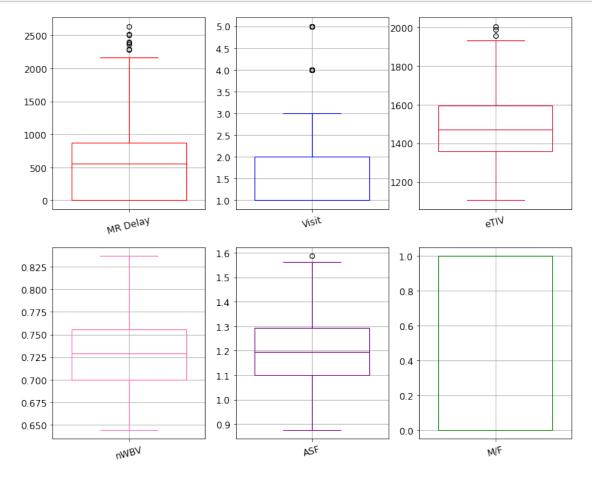
dtypes: float64(6), int64(6), object(3)

### memory usage: 43.8+ KB

```
New dataframe for male female group with Unique Subject ID
[31]:
      data_frame_new = data_frame.groupby(['M/F','Group'])
[32]:
      data_frame_new = data_frame_new.agg({'Subject ID':'nunique'})
[33]:
      data_frame_new.head()
[33]:
                       Subject ID
      M/F Group
          Demented
                               38
          Nondemented
                               50
          Demented
                               40
      1
          Nondemented
                               22
[34]:
      import matplotlib.pyplot as plt
      import seaborn as sns
      plt.figure(figsize = (14,10))
      sns.heatmap(data_frame[data_frame.columns].corr(), annot=True)
```

## [34]: <AxesSubplot:>





```
Target value, response variable or dependent variable
[36]: y_data = data_frame['Group']
[37]: y_data[0:5]
[37]: 0
           Nondemented
           Nondemented
      1
      2
              Demented
      3
              Demented
      4
              Demented
      Name: Group, dtype: object
[38]: # Independent variable or regressor as X
      # drop unrelated values
      X_data = data_frame.drop(['Subject ID', 'MRI ID', 'Group'], axis=1)
      X_data.head()
         Visit
[38]:
                MR Delay M/F
                               Hand
                                     Age
                                         EDUC
                                                SES
                                                     MMSE
                                                           CDR
                                                                        eTIV
                                  1
                                      87
                                                                 1986.550000
      0
             1
                       0
                            1
                                            14
                                                2.0
                                                     27.0
                                                            0.0
      1
             2
                     457
                            1
                                  1
                                      88
                                            14
                                                2.0
                                                     30.0
                                                           0.0
                                                                 2004.479526
                                                     23.0
      2
                                      75
                                            12 2.0
             1
                       0
                            1
                                  1
                                                           0.5
                                                                 1678.290000
      3
             2
                     560
                            1
                                  1
                                      76
                                            12 2.0
                                                     28.0
                                                           0.5
                                                                 1737.620000
             3
                            1
                                  1
                                      80
                                            12 2.0 22.0 0.5
                                                                1697.911134
                    1895
             nWBV
                        ASF
      0 0.696106 0.883440
      1 0.681062 0.875539
      2 0.736336 1.045710
      3 0.713402 1.010000
      4 0.701236 1.033623
     0.0.1 Train and Test Split
[39]: # import train_test_split library
      from sklearn.model_selection import train_test_split
      from sklearn.metrics import accuracy_score
      from sklearn.metrics import roc_auc_score
      from sklearn.metrics import roc_curve, auc
      X_train,X_test, y_train, y_test = train_test_split(X_data, y_data, test_size = __
      →0.33)
```

Train set: (249, 12) (249,) Test set: (124, 12) (124,)

Normalize Data Standardization give data zero mean and unit variance

print ('Train set:', X\_train.shape, y\_train.shape)
print ('Test set:', X\_test.shape, y\_test.shape)

```
[40]: X_data= preprocessing.StandardScaler().fit(X_data).transform(X_data)
     X_data[0:5]
[40]: array([[-0.95706686, -0.93771494, 1.15379808, 0.
                                                              , 1.30873772,
             -0.20813199, -0.3944662, -0.09706416, -0.77765291, 2.83359462,
             -0.90181966, -2.26232493],
             [ 0.12799678, -0.21761337, 1.15379808, 0.
                                                              , 1.43978716,
             -0.20813199, -0.3944662, 0.71958842, -0.77765291, 2.93552502,
             -1.30741435, -2.31961167],
             [-0.95706686, -0.93771494, 1.15379808, 0.
                                                               , -0.26385558,
             -0.90439416, -0.3944662 , -1.18593426, 0.55905002, 1.08111854,
              0.18280374, -1.08577527,
             [ 0.12799678, -0.05531476, 1.15379808, 0.
                                                              , -0.13280614,
             -0.90439416, -0.3944662, 0.17515337, 0.55905002, 1.41841305,
             -0.43550978, -1.34469305],
             [ 1.21306043, 2.04826424, 1.15379808, 0.
                                                             , 0.39139163,
             -0.90439416, -0.3944662 , -1.45815179, 0.55905002, 1.19266583,
             -0.76351198, -1.17341289]])
     0.0.2 Support Vector Machine (SVM)
[41]: # import SVM library
     from sklearn import svm
[42]: | svm_clf = svm.SVC(C=1, kernel='linear').fit(X_train, y_train)
[43]: yhat_svm = svm_clf.predict(X_test)
[44]: SVM_accuracy_score = accuracy_score(y_test,yhat_svm)*100
     print("SVM_accuracy_score:", SVM_accuracy_score)
     SVM accuracy score: 92.74193548387096
[45]: # Number of random trials
     NUM_TRIALS = 10
      # Arrays to store scores
     svm_nested_scores = np.zeros(NUM_TRIALS)
     svm_non_nested_scores = np.zeros(NUM_TRIALS)
      # Set up possible values of parameters to optimize over
     p_grid = {"C": [1, 10, 100], "gamma": [0.01, 0.1]}
[46]: # Loop for each trial
     for i in range(NUM_TRIALS):
```

```
inner_cv = KFold(n_splits=10, shuffle=True, random_state=i)
           outer_cv = KFold(n_splits=10, shuffle=True, random_state=i)
           # Non_nested parameter search and scoring
          nonnes_svm_clf = GridSearchCV(estimator=svm_clf, param_grid=p_grid,__
        →cv=outer cv)
          nonnes_svm_clf.fit(X_data, y_data)
           svm_non_nested_scores[i] = nonnes_svm_clf.best_score_
           # Nested CV with parameter optimization
          Nes_svm_clf = GridSearchCV(estimator=svm_clf, param_grid=p_grid,__
        svm_nested_score = cross_val_score(svm_clf, X=X_data, y=y_data, cv=outer_cv)
          svm_nested_score[i] = svm_nested_score.mean()
[142]: | svm_non_nested_score_mean = svm_non_nested_scores.mean()
      svm_non_nested_score_mean
[142]: 0.9463157894736842
[135]: svm_nested_score_mean = svm_nested_score.mean()
      svm_nested_score_mean
[135]: 0.94649359886202
[49]: SVM_nested_vs_non_nested_score = svm_nested_score - svm_non_nested_scores
      print(
           "Average difference of nested and nonnested {:6f} with std. dev. of {:6f}.".
               SVM nested vs non nested score mean(), SVM nested vs non nested score.
       →std()
          )
      Average difference of nested and nonnested 0.000178 with std. dev. of 0.023795.
[50]: print('SVM Nested Accuracy: %.3f' % (mean(svm_nested_score)*100))
      SVM Nested Accuracy: 94.649
```

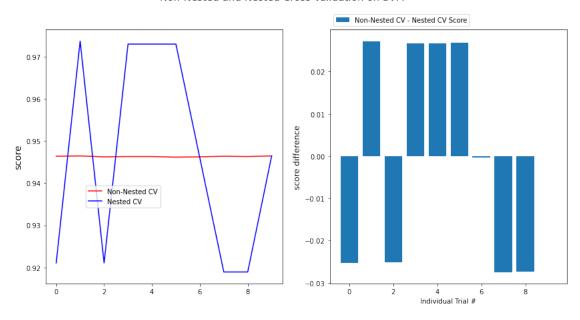
17

```
[51]: print('SVM Nonnested Accuracy: %.3f ' % (mean(svm_non_nested_scores)*100))
```

SVM Nonnested Accuracy: 94.632

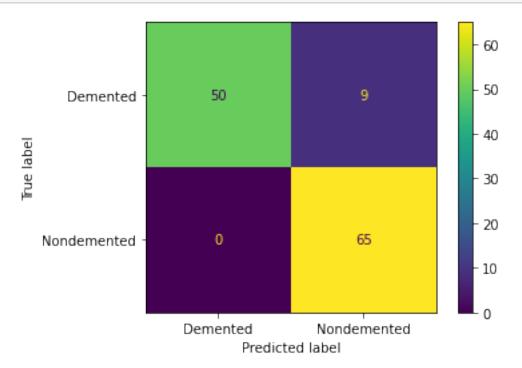
```
[52]: # Plot scores for nested and non-nested CV
      plt.figure(figsize=(14, 7))
      plt.subplot(1,2,1)
      (non_nested_line,) = plt.plot(svm_non_nested_scores, color="r")
      (nested_line,) = plt.plot(svm_nested_score, color="b")
      plt.ylabel("score", fontsize="14")
      plt.legend(
          [non_nested_line, nested_line],
          ["Non-Nested CV", "Nested CV"],
          bbox_to_anchor=(0, 0.4, 0.5, 0),
      )
      plt.title( "Non-Nested and Nested Cross Validation on SVM", x=1.0, y=1.1, u
       →fontsize="15" )
      # Plot bar chart of the difference.
      plt.subplot(1,2,2)
      difference_plot = plt.bar(range(NUM_TRIALS), SVM_nested_vs_non_nested_score)
      plt.xlabel("Individual Trial #")
      plt.legend(
          [difference_plot],
          ["Non-Nested CV - Nested CV Score"],
          bbox_to_anchor=(0, 1, 0.8, 0),
      plt.ylabel("score difference", fontsize="12")
      plt.show()
```

### Non-Nested and Nested Cross Validation on SVM

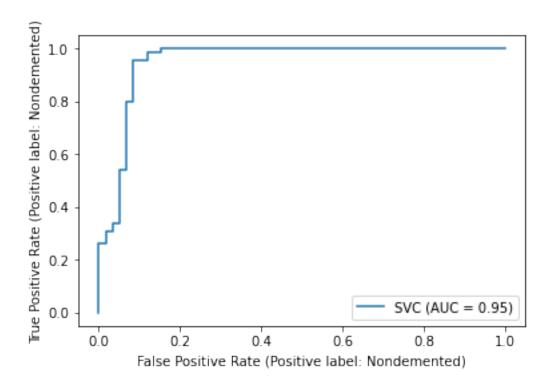


## SVM Confusion matrix

[53]: #confusion\_matrix(y\_test,yhat\_svm)
from sklearn.metrics import confusion\_matrix
plot\_confusion\_matrix(svm\_clf, X\_test, y\_test)
plt.show()

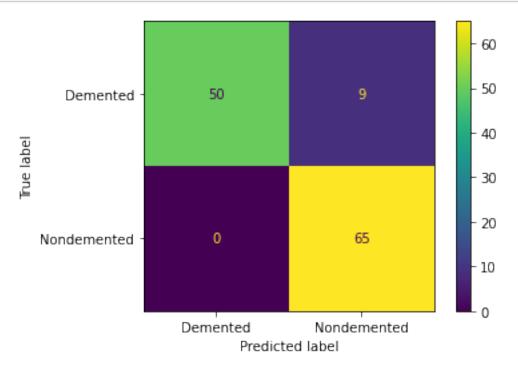


```
[54]: # Confusion matrix using crosstab method of pandas.
      svm_pd = pd.crosstab(y_test, yhat_svm, rownames=['True'],__
       →colnames=['Predicted'], margins=True)
      svm_pd
[54]: Predicted
                   Demented Nondemented All
      True
      Demented
                         50
                                           59
      Nondemented
                                           65
                          0
                                      65
      All
                         50
                                      74 124
     SVM Classification Report
[55]: #print(classification_report(y_test,yhat_svm))
      print("confusion matrix\n",confusion_matrix(y_test,yhat_svm))
      print("\nclassification report\n", classification_report(y_test, yhat_svm))
      print("Accuracy: ",accuracy_score(y_test, yhat_svm)*100)
     confusion matrix
      [[50 9]
      [ 0 65]]
     classification report
                    precision
                                 recall f1-score
                                                     support
         Demented
                        1.00
                                  0.85
                                             0.92
                                                         59
                        0.88
                                             0.94
      Nondemented
                                   1.00
                                                         65
                                             0.93
                                                        124
         accuracy
        macro avg
                                             0.93
                                                        124
                        0.94
                                  0.92
                                             0.93
     weighted avg
                        0.94
                                  0.93
                                                        124
     Accuracy: 92.74193548387096
[56]: SVM_roc_auc_score = roc_auc_score(y_test, svm_clf.decision_function(X_test),__
      →average=None)
      print("SVM_roc_auc_score:", SVM_roc_auc_score)
     SVM_roc_auc_score: 0.951238591916558
      metrics.plot_roc_curve(svm_clf, X_test, y_test)
[57]: l
       plt.show()
```



### 0.0.3 Logistic Regression

```
plot_confusion_matrix(lr_clf, X_test, y_test)
plt.show()
```



```
[63]: # Confusion matrix using crosstab method of pandas.

LR_pd = pd.crosstab(y_test, yhat_lr, rownames=['True'], colnames=['Predicted'], 

→margins=True)

LR_pd
```

```
[63]: Predicted Demented Nondemented All
True
Demented 50 9 59
Nondemented 0 65 65
All 50 74 124
```

### LR Classification Report

```
[64]: #print(classification_report(y_test,yhat_lr))

print("confusion matrix\n",confusion_matrix(y_test,yhat_lr))

print("\nclassification_report\n",classification_report(y_test,yhat_lr))

print("Accuracy: ",accuracy_score(y_test, yhat_lr)*100)

confusion matrix
```

```
[[50 9]
[ 0 65]]
```

classification report

	precision	recall	f1-score	support
Demented	1.00	0.85	0.92	59
Nondemented	0.88	1.00	0.94	65
accuracy			0.93	124
macro avg	0.94	0.92	0.93	124
weighted avg	0.94	0.93	0.93	124

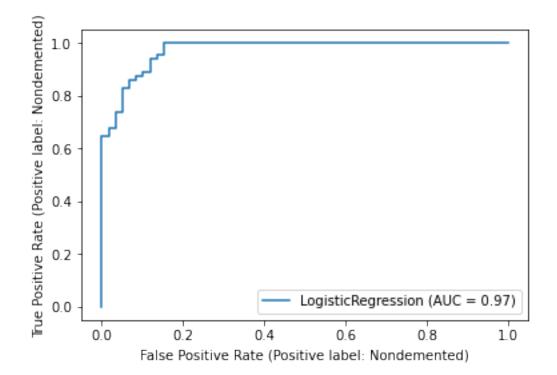
Accuracy: 92.74193548387096

```
[65]: LR_roc_auc_score= roc_auc_score(y_test, lr_clf.decision_function(X_test), 

→average=None)
print("LR_roc_auc_score:", LR_roc_auc_score)
```

LR\_roc\_auc\_score : 0.9731421121251629

```
[66]: metrics.plot_roc_curve(lr_clf, X_test, y_test)
    plt.show()
```



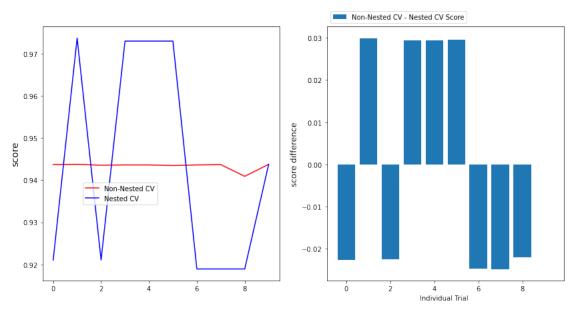
```
[67]: NUM_TRIALS = 10
```

```
lr_non_nested_scores = np.zeros(NUM_TRIALS)
      p_grid = {"C": [1, 10, 100]}
      # Loop for each trial
      for i in range(NUM_TRIALS):
          inner_cv = KFold(n_splits=10, shuffle=True, random_state=i)
         outer_cv = KFold(n_splits=10, shuffle=True, random_state=i)
         nonnes_lr_clf = GridSearchCV(estimator=lr_clf, param_grid=p_grid,_
      nonnes_lr_clf.fit(X_data, y_data)
         lr_non_nested_scores[i] = nonnes_lr_clf.best_score_
         # Nested CV with parameter optimization
         Nes_lrclf = GridSearchCV(estimator=lr_clf, param_grid=p_grid, cv=inner_cv)
         lr_nested_score = cross_val_score(lr_clf, X=X_data, y=y_data, cv=outer_cv)
         lr_nested_score[i] = lr_nested_score.mean()
[68]: LR_nested_vs_non_nested_score = lr_nested_score - lr_non_nested_scores
      print(
         "Average difference of nested and nonnested {:6f} with std. dev. of {:6f}.".
             LR_nested_vs_non_nested_score.mean(), LR_nested_vs_non_nested_score.
      →std()
         )
     Average difference of nested and nonnested 0.000171 with std. dev. of 0.024929.
[69]: print('LR Nested Accuracy: %.3f' % (mean(lr_nested_score)*100))
      print('LR Nonnested Accuracy: %.3f ' % (mean(lr_non_nested_scores)*100))
     LR Nested Accuracy: 94.352
     LR Nonnested Accuracy: 94.335
```

lr\_nested\_scores = np.zeros(NUM\_TRIALS)

```
[70]: # Plot scores for nested and non-nested CV
      plt.figure(figsize=(14, 7))
      plt.subplot(1,2,1)
      (non_nested_line,) = plt.plot(lr_non_nested_scores, color="r")
      (nested_line,) = plt.plot(lr_nested_score, color="b")
      plt.ylabel("score", fontsize="14")
      plt.legend(
          [non_nested_line, nested_line],
          ["Non-Nested CV", "Nested CV"],
          bbox_to_anchor=(0, 0.4, 0.5, 0),
      )
      plt.title( "Non-Nested and Nested Cross Validation on Logistic Regression", x=1.
      \hookrightarrow 0, y=1.1, fontsize="15")
      # Plot bar chart of the difference.
      plt.subplot(1,2,2)
      difference_plot = plt.bar(range(NUM_TRIALS), LR_nested_vs_non_nested_score)
      plt.xlabel("Individual Trial ")
      plt.legend(
          [difference_plot],
          ["Non-Nested CV - Nested CV Score"],
          bbox_to_anchor=(0, 1, 0.8, 0),
      plt.ylabel("score difference", fontsize="12")
      plt.show()
```

### Non-Nested and Nested Cross Validation on Logistic Regression



```
[127]: lr_nested_score_mean = lr_nested_score.mean() lr_nested_score_mean
```

[127]: 0.943520625889047

```
[136]: lr_non_nested_score_mean = lr_non_nested_scores.mean() lr_non_nested_score_mean
```

[136]: 0.9433499288762446

### 0.0.4 Random Forest Classifier

```
[71]: from sklearn.ensemble import RandomForestClassifier

rf_clf = RandomForestClassifier().fit(X_train, y_train)

rf_pred = rf_clf.predict(X_test)

rf_yhat_prob = rf_clf.predict_proba(X_test)
```

```
[72]: from sklearn.metrics import classification_report, confusion_matrix,

→accuracy_score

print("confusion matrix\n",confusion_matrix(y_test,rf_pred))

print("\nclassification report\n",classification_report(y_test,rf_pred))

print("Accuracy: ",accuracy_score(y_test, rf_pred)*100)
```

```
confusion matrix [[51 8]
```

[ 0 65]]

classification report

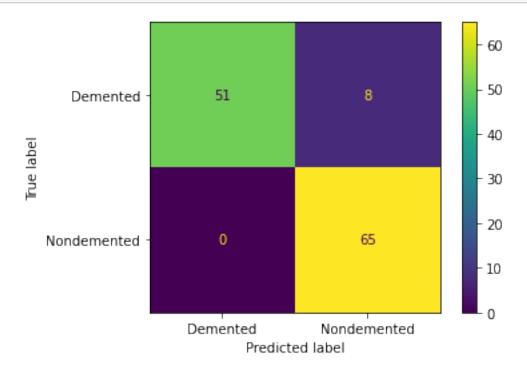
	precision	recall	f1-score	support
Demented	1.00	0.86	0.93	59
Nondemented	0.89	1.00	0.94	65
accuracy			0.94	124
macro avg	0.95	0.93	0.93	124
weighted avg	0.94	0.94	0.94	124

Accuracy: 93.54838709677419

```
[73]: RF_accuracy_score = accuracy_score(y_test,rf_pred)*100 print("RF_accuracy_score:",RF_accuracy_score)
```

RF\_accuracy\_score : 93.54838709677419

[74]: plot\_confusion\_matrix(rf\_clf, X\_test, y\_test) plt.show()



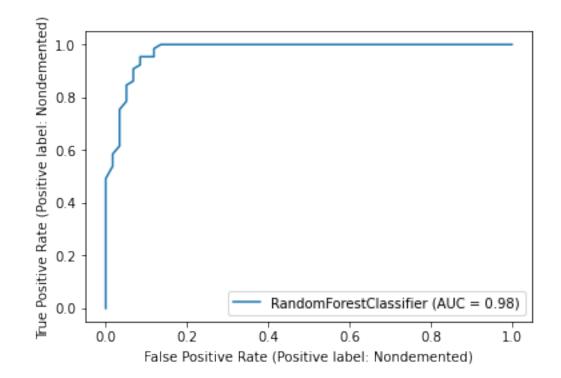
[75]: # Confusion matrix using crosstab method of pandas.

RF\_pd = pd.crosstab(y\_test, rf\_pred, rownames=['True'], colnames=['Predicted'],

→margins=True)

### RF\_pd [75]: Predicted Demented Nondemented True Demented 59 51 8 Nondemented 0 65 65 All 51 73 124 [76]: RF\_roc\_auc\_score= roc\_auc\_score(y\_test, rf\_clf.predict\_proba(X\_test)[:,1],\_\_ →average=None) print("RF roc\_auc score :",RF\_roc\_auc\_score ) RF roc\_auc score : 0.9754889178617991 [77]: metrics.plot\_roc\_curve(rf\_clf, X\_test, y\_test)

plt.show()



```
[78]: NUM_TRIALS = 10

rf_nested_scores = np.zeros(NUM_TRIALS)

rf_non_nested_scores = np.zeros(NUM_TRIALS)
```

```
p_grid = {
    'n_estimators': [200, 300],
    'max_features': ['auto', 'sqrt', 'log2'],
    'max_depth' : [3,5,10],
    'min_samples_split': [2, 5, 10],
    'criterion' :['gini', 'entropy']
}
# Loop for each trial
for i in range(NUM_TRIALS):
    inner_cv = KFold(n_splits=10, shuffle=True, random_state=i)
   outer_cv = KFold(n_splits=10, shuffle=True, random_state=i)
   nonnes_rf_clf = GridSearchCV(estimator=rf_clf, param_grid=p_grid,_u
 nonnes_rf_clf.fit(X_data, y_data)
   rf_non_nested_scores[i] = nonnes_rf_clf.best_score_
   # Nested CV with parameter optimization
   Nes_rfclf = GridSearchCV(estimator=rf_clf, param_grid=p_grid, cv=inner_cv)
   rf_nested_score = cross_val_score(rf_clf, X=X_data, y=y_data, cv=outer_cv)
   rf_nested_score[i] = rf_nested_score.mean()
```

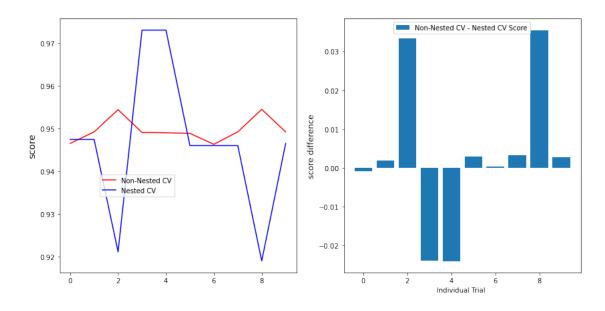
```
[]:
```

```
[79]: RF_nested_vs_non_nested_score = rf_non_nested_scores- rf_nested_score
      print(
          "Average difference of nested and nonnested {:6f} with std. dev. of {:6f}.".
              RF_nested_vs_non_nested_score.mean(), RF_nested_vs_non_nested_score.
      ⇔std()
          )
```

Average difference of nested and nonnested 0.003065 with std. dev. of 0.018590.

```
[80]: print('RF Nested Accuracy: %.3f' % (mean(rf_nested_score)*100))
      print('RF Nonnested Accuracy: %.3f ' % (mean(rf_non_nested_scores)*100))
     RF Nested Accuracy: 94.649
     RF Nonnested Accuracy: 94.956
[81]: plt.figure(figsize=(14, 7))
      plt.subplot(1,2,1)
      (non_nested_line,) = plt.plot(rf_non_nested_scores, color="r")
      (nested_line,) = plt.plot(rf_nested_score, color="b")
      plt.ylabel("score", fontsize="14")
      plt.legend(
          [non_nested_line, nested_line],
          ["Non-Nested CV", "Nested CV"],
          bbox_to_anchor=(0, 0.4, 0.5, 0),
      plt.title( "Non-Nested and Nested Cross Validation on RandomForest", x=1.0, y=1.
       \hookrightarrow1, fontsize="15")
      # Plot bar chart of the difference.
      plt.subplot(1,2,2)
      difference_plot = plt.bar(range(NUM_TRIALS), RF_nested_vs_non_nested_score)
      plt.xlabel("Individual Trial ")
      plt.legend(
          [difference_plot],
          ["Non-Nested CV - Nested CV Score"],
          bbox_to_anchor=(0, 1, 0.8, 0),
      plt.ylabel("score difference", fontsize="12")
      plt.show()
```

#### Non-Nested and Nested Cross Validation on RandomForest



```
[128]: rf_nested_score_mean = rf_nested_score.mean()
rf_nested_score_mean
```

[128]: 0.9464935988620198

```
[137]: rf_non_nested_score_mean = rf_non_nested_scores.mean()
rf_non_nested_score_mean
```

[137]: 0.9495590327169274

### 0.0.5 Naive Bayes

[86]: 93.54838709677419

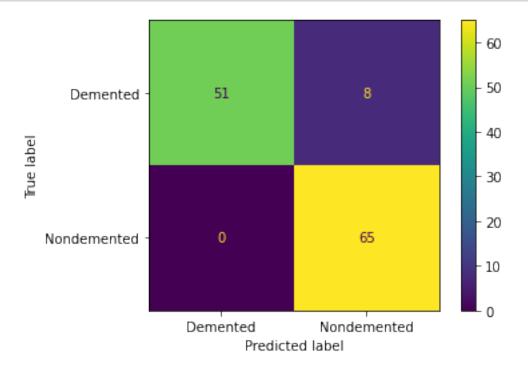
```
[87]: print("confusion matrix\n",confusion_matrix(y_test,y_pred_gnb))
print("\nclassification report\n",classification_report(y_test,y_pred_gnb))
print("Accuracy: ",accuracy_score(y_test, y_pred_gnb)*100)
```

confusion matrix
[[51 8]
[ 0 65]]

classification report

	precision	recall	f1-score	support
Demented	1.00	0.86	0.93	59
Nondemented	0.89	1.00	0.94	65
accuracy			0.94	124
macro avg	0.95	0.93	0.93	124
weighted avg	0.94	0.94	0.94	124

Accuracy: 93.54838709677419



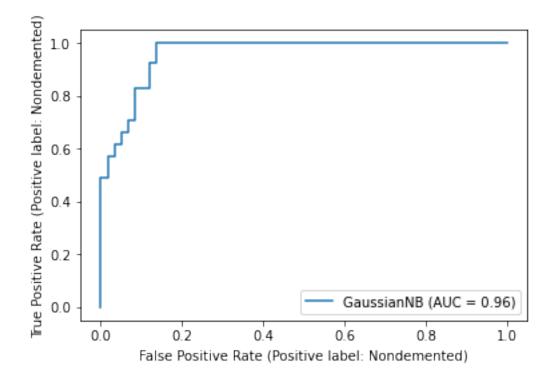
[89]: # Confusion matrix using crosstab method of pandas.

```
GNV_pd = pd.crosstab(y_test, y_pred_gnb, rownames=['True'],

colnames=['Predicted'], margins=True)
GNV_pd
```

```
[89]: Predicted
                   Demented Nondemented
                                            All
      True
      Demented
                          51
                                         8
                                             59
      Nondemented
                           0
                                        65
                                             65
      All
                          51
                                        73
                                           124
```

```
[90]: metrics.plot_roc_curve(gnb_clf, X_test, y_test)
plt.show()
```



```
[93]: NUM_TRIALS = 10
      gnb_nested_scores = np.zeros(NUM_TRIALS)
      gnb_non_nested_scores = np.zeros(NUM_TRIALS)
      p_grid = { }
      #"priors" : "None", "var_smoothing" : 1e-9
      # Loop for each trial
      for i in range(NUM TRIALS):
           # Choose cross-validation techniques for the inner and outer loops,
           # independently of the dataset.
           # E.q "GroupKFold", "LeaveOneOut", "LeaveOneGroupOut", etc.
          inner_cv = KFold(n_splits=10, shuffle=True, random_state=i)
           outer_cv = KFold(n_splits=10, shuffle=True, random_state=i)
            # Non_nested parameter search and scoring
          nonnes_gnb_clf = GridSearchCV(estimator=gnb_clf, param_grid=p_grid,_
       nonnes_gnb_clf.fit(X_data, y_data)
           gnb_non_nested_scores[i] = nonnes_gnb_clf.best_score_
           # Nested CV with parameter optimization
          Nes_gnbclf = GridSearchCV(estimator=gnb_clf, param_grid=p_grid, cv=inner_cv)
           gnb_nested_score = cross_val_score(gnb_clf, X=X_data, y=y_data, cv=outer_cv)
          gnb_nested_score[i] = gnb_nested_score.mean()
[129]: | gnb_nested_score_mean = gnb_nested_score.mean()
      gnb_nested_score_mean
[129]: 0.9464153627311523
[138]: | gnb_non_nested_score_mean = gnb_non_nested_scores.mean()
      gnb_non_nested_score_mean
[138]: 0.9449573257467995
[95]: GNB_nested_vs_non_nested_score = gnb_nested_score - gnb_non_nested_scores
```

Average difference of nested and nonnested 0.001458 with std. dev. of 0.026971.

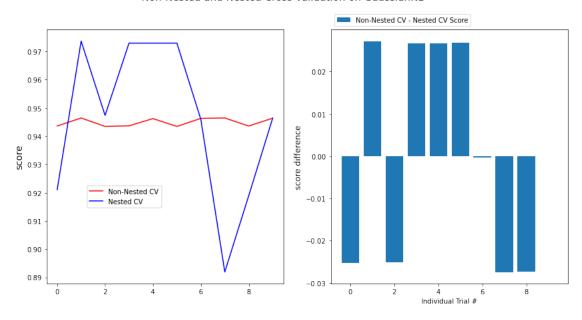
```
[96]: print('GNB Nested Accuracy: %.3f' % (mean(gnb_nested_score)*100))

print('GNB Nonnested Accuracy: %.3f' % (mean(gnb_non_nested_scores)*100))
```

GNB Nested Accuracy: 94.642 GNB Nonnested Accuracy: 94.496

```
[97]: # Plot scores for nested and non-nested CV
      plt.figure(figsize=(14, 7))
      plt.subplot(1,2,1)
      (non_nested_line,) = plt.plot(gnb_non_nested_scores, color="r")
      (nested_line,) = plt.plot(gnb_nested_score, color="b")
      plt.ylabel("score", fontsize="14")
      plt.legend(
          [non_nested_line, nested_line],
          ["Non-Nested CV", "Nested CV"],
          bbox_to_anchor=(0, 0.4, 0.5, 0),
      )
      plt.title( "Non-Nested and Nested Cross Validation on GaussianNB", x=1.0, y=1.
      \rightarrow 1, fontsize="15")
      # Plot bar chart of the difference.
      plt.subplot(1,2,2)
      difference_plot = plt.bar(range(NUM_TRIALS), SVM_nested_vs_non_nested_score)
      plt.xlabel("Individual Trial #")
      plt.legend(
          [difference_plot],
          ["Non-Nested CV - Nested CV Score"],
          bbox_to_anchor=(0, 1, 0.8, 0),
      plt.ylabel("score difference", fontsize="12")
      plt.show()
```

#### Non-Nested and Nested Cross Validation on GaussianNB



```
[]:
```

## 0.0.6 Ada Boosting

```
[98]: from sklearn.ensemble import AdaBoostClassifier

ada_clf = AdaBoostClassifier(n_estimators=100, random_state=42)
ada_clf.fit(X_train, y_train)
```

[98]: AdaBoostClassifier(n\_estimators=100, random\_state=42)

```
[99]: yhat_ada = ada_clf.predict(X_test)
#yhat_ada
```

```
[100]: ada_yhat_prob = ada_clf.predict_proba(X_test)
#ada_yhat_prob
```

```
[101]: ada_accuracy_score =accuracy_score(y_test, yhat_ada)*100 print("ada_accuracy_score:", ada_accuracy_score)
```

ada\_accuracy\_score : 93.54838709677419

```
print("\nclassification report\n",classification_report(y_test,yhat_ada))
print("Accuracy: ",accuracy_score(y_test, yhat_ada)*100)
```

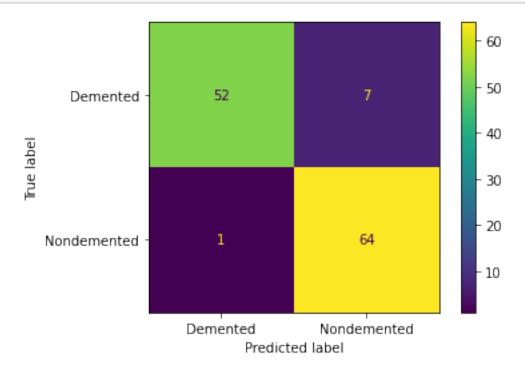
confusion matrix
 [[52 7]
 [ 1 64]]

classification report

	precision	recall	f1-score	support
Demented	0.98	0.88	0.93	59
Nondemented	0.90	0.98	0.94	65
accuracy			0.94	124
macro avg	0.94	0.93	0.93	124
weighted avg	0.94	0.94	0.94	124

Accuracy: 93.54838709677419

[103]: plot\_confusion\_matrix(ada\_clf, X\_test, y\_test) plt.show()



```
[104]: # Confusion matrix using crosstab method of pandas.

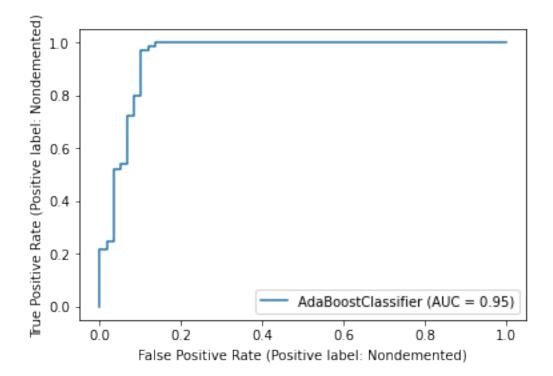
ada_pd = pd.crosstab(y_test, yhat_ada, rownames=['True'],

→colnames=['Predicted'], margins=True)
```

```
ada_pd
```

```
[104]: Predicted Demented Nondemented All
True
Demented 52 7 59
Nondemented 1 64 65
All 53 71 124
```

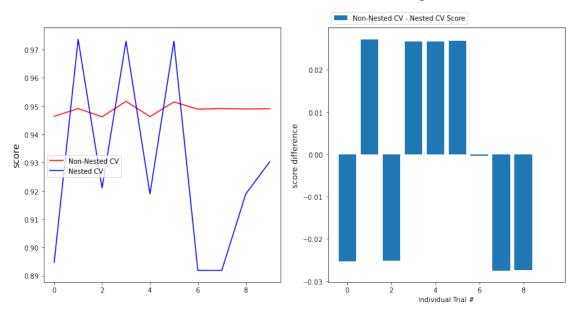
```
[105]: metrics.plot_roc_curve(ada_clf, X_test, y_test)
    plt.show()
```



```
p grid={'n estimators':[100,200,500],'learning rate':[.001,0.01,.1]}
      # Loop for each trial
      for i in range(NUM_TRIALS):
           inner_cv = KFold(n_splits=10, shuffle=True, random_state=i)
          outer_cv = KFold(n_splits=10, shuffle=True, random_state=i)
           # Non_nested parameter search and scoring
          nonnes_ada_clf = GridSearchCV(estimator=ada_clf, param_grid=p_grid,_
       nonnes_ada_clf.fit(X_data, y_data)
          ada_non_nested_scores[i] = nonnes_ada_clf.best_score_
           # Nested CV with parameter optimization
          Nes_adaclf = GridSearchCV(estimator=ada_clf, param_grid=p_grid, cv=inner_cv)
          ada_nested_score = cross_val_score(ada_clf, X=X_data, y=y_data, cv=outer_cv)
           ada_nested_score[i] = ada_nested_score.mean()
[108]: ADA_nested_vs_non_nested_score = ada_non_nested_scores - ada_nested_score
      print(
           "Average difference of nested and nonnested {:6f} with std. dev. of {:6f}.".
       →format(
               ADA_nested_vs_non_nested_score.mean(), ADA_nested_vs_non_nested_score.
       ⇒std()
          )
      )
      Average difference of nested and nonnested 0.020007 with std. dev. of 0.030582.
[109]: print('ADA Nested Accuracy: %.3f' % (mean(ada_nested_score)*100))
      print('ADA Nonnested Accuracy: %.3f ' % (mean(ada_non_nested_scores)*100))
      ADA Nested Accuracy: 92.873
      ADA Nonnested Accuracy: 94.874
[146]: # Plot scores for nested and non-nested CV
      plt.figure(figsize=(14, 7))
```

```
plt.subplot(1,2,1)
(non_nested_line,) = plt.plot(ada_non_nested_scores, color="r")
(nested_line,) = plt.plot(ada_nested_score, color="b")
plt.ylabel("score", fontsize="14")
plt.legend(
    [non_nested_line, nested_line],
    ["Non-Nested CV", "Nested CV"],
    bbox_to_anchor=(0, 0.4, 0.5, 0),
)
plt.title( "Non-Nested and Nested Cross Validation on Ada Boosting", x=1.0, y=1.
 \hookrightarrow1, fontsize="15")
# Plot bar chart of the difference.
plt.subplot(1,2,2)
difference_plot = plt.bar(range(NUM_TRIALS), SVM_nested_vs_non_nested_score)
plt.xlabel("Individual Trial #")
plt.legend(
    [difference_plot],
    ["Non-Nested CV - Nested CV Score"],
    bbox_to_anchor=(0, 1, 0.8, 0),
plt.ylabel("score difference", fontsize="12")
plt.show()
```

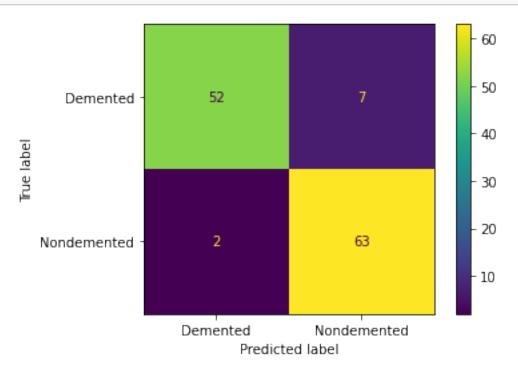
## Non-Nested and Nested Cross Validation on Ada Boosting



```
[130]: ada_nested_score_mean = ada_nested_score.mean()
       ada_nested_score_mean
[130]: 0.9287339971550498
[139]: ada_non_nested_score_mean = ada_non_nested_scores.mean()
       ada_non_nested_score_mean
[139]: 0.9487411095305832
      0.0.7 Gradient boosting
[111]: from sklearn.ensemble import GradientBoostingClassifier
[112]: Gra_clf = GradientBoostingClassifier(n_estimators=100, learning_rate=1.0,
                                             max_depth=1, random_state=0).fit(X_train,__
        →y_train)
[113]: Gra_clf.score(X_test, y_test)
[113]: 0.9274193548387096
[114]: yhat_Gra_cl = Gra_clf.predict(X_test)
       Gra_yhat_prob = Gra_clf.predict_proba(X_test)
[115]: gra_accuracy_score = Gra_clf.score(X_test, y_test)*100
       print("gra_accuracy_score :", gra_accuracy_score )
      gra_accuracy_score : 92.74193548387096
[116]: print("confusion matrix\n", confusion matrix(y_test, yhat_Gra_cl))
       print("\nclassification report\n", classification_report(y_test, yhat_Gra_cl))
       print("Accuracy: ",accuracy_score(y_test, yhat_Gra_cl)*100)
      confusion matrix
       [[52 7]
       [ 2 63]]
      classification report
                     precision
                                  recall f1-score
                                                      support
          Demented
                          0.96
                                    0.88
                                              0.92
                                                          59
       Nondemented
                          0.90
                                    0.97
                                              0.93
                                                          65
                                              0.93
                                                         124
          accuracy
         macro avg
                         0.93
                                    0.93
                                              0.93
                                                         124
      weighted avg
                                    0.93
                                              0.93
                                                         124
                          0.93
```

Accuracy: 92.74193548387096

```
[117]: plot_confusion_matrix(Gra_clf, X_test, y_test)
plt.show()
```



```
[118]: # Confusion matrix using crosstab method of pandas.

Gra_pd = pd.crosstab(y_test, yhat_Gra_cl, rownames=['True'],

colnames=['Predicted'], margins=True)

Gra_pd
```

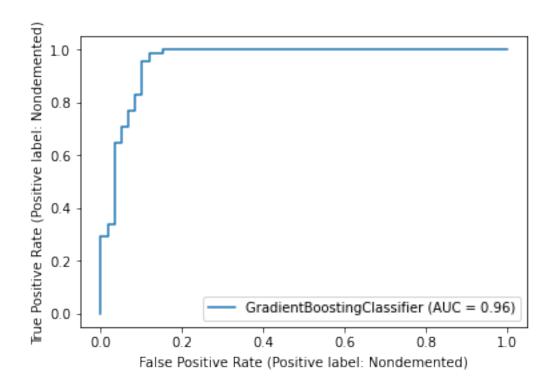
```
[118]: Predicted Demented Nondemented All True

Demented 52 7 59

Nondemented 2 63 65

All 54 70 124
```

```
[119]: metrics.plot_roc_curve(Gra_clf, X_test, y_test)
    plt.show()
```

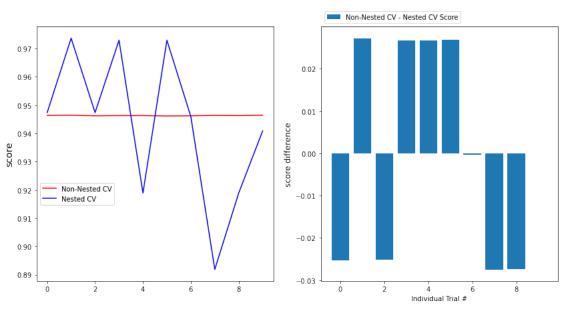


```
[120]: gra_roc_auc_score= roc_auc_score(y_test, Gra_clf.decision_function(X_test),__
        →average=None)
       print("gra_roc_auc_score :",gra_roc_auc_score )
      gra_roc_auc_score : 0.9577574967405476
[121]: NUM_TRIALS = 10
       gra_nested_scores = np.zeros(NUM_TRIALS)
       gra_non_nested_scores = np.zeros(NUM_TRIALS)
       p_grid = {
           "loss":["deviance"],
           "learning_rate": [0.01, 0.025, 0.05, 0.075, 0.1, 0.15, 0.2],
           "min_samples_split": np.linspace(0.1, 0.5, 12),
           "min_samples_leaf": np.linspace(0.1, 0.5, 12),
           "max_depth": [3,5,8],
           "max_features":["log2","sqrt"],
           "criterion": ["friedman_mse"],
           "subsample":[0.5, 0.618, 0.8, 0.85, 0.9, 0.95, 1.0],
           "n estimators":[10]
           }
```

```
for i in range(NUM_TRIALS):
           inner_cv = KFold(n_splits=10, shuffle=True, random_state=i)
          outer_cv = KFold(n_splits=10, shuffle=True, random_state=i)
           # Non nested parameter search and scoring
          nonnes_gra_clf = GridSearchCV(estimator=Gra_clf, param_grid=p_grid,_
       ⇔cv=outer cv)
          nonnes_gra_clf.fit(X_data, y_data)
          gra_non_nested_scores[i] = nonnes_gra_clf.best_score_
          # Nested CV with parameter optimization
          Nes_graclf = GridSearchCV(estimator=Gra_clf, param_grid=p_grid, cv=inner_cv)
          gra_nested_scores = cross_val_score(Gra_clf, X=X_data, y=y_data,_u
        →cv=outer cv)
          gra_nested_scores[i] = gra_nested_scores.mean()
[122]: GRA_nested_vs_non_nested_score = gra_nested_scores - gra_non_nested_scores
       print(
           "Average difference of nested and nonnested {:6f} with std. dev. of {:6f}.".
               GRA_nested_vs_non_nested_score.mean(), GRA_nested_vs_non_nested_score.
       →std()
          )
      Average difference of nested and nonnested -0.003222 with std. dev. of 0.025631.
[123]: print('Gradient Nested Accuracy: %.3f' % (mean(gra_nested_scores)*100))
       print('Gradient Nonnested Accuracy: %.3f ' % (mean(gra_non_nested_scores)*100))
      Gradient Nested Accuracy: 94.309
      Gradient Nonnested Accuracy: 94.632
[124]: # Plot scores for nested and non-nested CV
       plt.figure(figsize=(14, 7))
       plt.subplot(1,2,1)
```

```
(non_nested_line,) = plt.plot(gra_non_nested_scores, color="r")
(nested_line,) = plt.plot(gra_nested_scores, color="b")
plt.ylabel("score", fontsize="14")
plt.legend(
    [non_nested_line, nested_line],
    ["Non-Nested CV", "Nested CV"],
    bbox_to_anchor=(0, 0.4, 0.5, 0),
)
plt.title( "Non-Nested and Nested Cross Validation on Gradient boosting", x=1.
\rightarrow 0, y=1.1, fontsize="15")
# Plot bar chart of the difference.
plt.subplot(1,2,2)
difference_plot = plt.bar(range(NUM_TRIALS), SVM_nested_vs_non_nested_score)
plt.xlabel("Individual Trial #")
plt.legend(
    [difference_plot],
    ["Non-Nested CV - Nested CV Score"],
    bbox_to_anchor=(0, 1, 0.8, 0),
plt.ylabel("score difference", fontsize="12")
plt.show()
```

## Non-Nested and Nested Cross Validation on Gradient boosting



```
[131]: gra_nested_score_mean = gra_nested_scores.mean()
    gra_nested_score_mean

[131]: 0.9430938833570414

[140]: gra_non_nested_score_mean = gra_non_nested_scores.mean()
    gra_non_nested_score_mean
```

[140]: 0.9463157894736842

## 0.0.8 Results

Accuracy score report dataframe

```
[144]: # create a accuracy list
       accuracy_score = [__
       →SVM accuracy score, LR accuracy score, RF accuracy score, gnb Accuracy score,
                         ada_accuracy_score,gra_accuracy_score]
       # create a AUC-score list
       auc score =
       → [SVM_roc_auc_score,LR_roc_auc_score,RF_roc_auc_score,gnb_roc_auc_score,
                    ada_roc_auc_score,gra_roc_auc_score,]
       # create a nested-score list
       Nested score = [svm nested score mean, lr nested score mean, rf nested score mean,
       →gnb_nested_score_mean,ada_nested_score_mean,gra_nested_score_mean]
       # create a non nested-score list
       Non_Nested_score =
        → [svm non_nested_score_mean, lr_non_nested_score_mean, rf_non_nested_score_mean,
       ⇒gnb non nested score mean, ada non nested score mean, gra non nested score mean]
       # fomulate the report format
       df_report = pd.DataFrame(accuracy_score, index=['SVM', 'Logistic_
       →Regression', 'Random Forest',
                                                       'Naive Bayes', 'Ada
       →Boosting','Gradient boosting'])
       df_report.columns = ['Accuracy Score']
       df_report.insert(loc=1, column='ROC AUC Score', value= auc_score)
       df_report.insert(loc=2, column='Nested Score (mean)', value= Nested_score)
       df_report.insert(loc=3, column='Non Nested Score (mean)', value=__
        →Non_Nested_score)
       df report.columns.name = 'Algorithm'
```

```
df_report
[144]: Algorithm
                            Accuracy Score ROC AUC Score Nested Score (mean)
      SVM
                                 92.741935
                                                  0.951239
                                                                       0.946494
      Logistic Regression
                                 92.741935
                                                  0.973142
                                                                       0.943521
       Random Forest
                                 93.548387
                                                  0.975489
                                                                       0.946494
       Naive Bayes
                                 93.548387
                                                  0.959844
                                                                       0.946415
       Ada Boosting
                                 93.548387
                                                  0.949153
                                                                       0.928734
       Gradient boosting
                                 92.741935
                                                  0.957757
                                                                       0.943094
      Algorithm
                            Non Nested Score (mean)
       SVM
                                           0.946316
      Logistic Regression
                                           0.943350
       Random Forest
                                           0.949559
       Naive Bayes
                                           0.944957
       Ada Boosting
                                           0.948741
       Gradient boosting
                                           0.946316
[126]: | fig = metrics.plot_roc_curve(rf_clf, X_test, y_test)
       fig = metrics.plot_roc_curve(Gra_clf, X_test, y_test,ax = fig.ax_)
       fig = metrics.plot_roc_curve(ada_clf, X_test, y_test,ax = fig.ax_ )
       fig = metrics.plot_roc_curve(gnb_clf, X_test, y_test,ax = fig.ax_ )
       #metrics.plot_roc_curve(rf_regressor, X_test, y_test)
       fig = metrics.plot_roc_curve(lr_clf, X_test, y_test,ax = fig.ax_ )
       fig = metrics.plot_roc_curve(svm_clf, X_test, y_test,ax = fig.ax_ )
       fig.figure_.suptitle("ROC curve comparison")
       fig.figure_.set_size_inches(14,10)
```

plt.show()

