

Breast Cancer Dataset

In [1]:

```
#Import and install the libraries needed for model development
import pandas as pd
from sklearn.tree import DecisionTreeClassifier
from sklearn.model_selection import train_test_split, GridSearchCV
from sklearn.metrics import make_scorer, classification_report, recall_score, roc_auc_score, f1_score
from sklearn.metrics import plot_confusion_matrix
import matplotlib.pyplot as plt
from sklearn import tree
import warnings
warnings.filterwarnings("ignore")
warnings.filterwarnings("ignore", category=UserWarning)
from sklearn.model_selection import KFold, cross_val_score
from sklearn.tree import DecisionTreeClassifier
from sklearn.neighbors import KNeighborsClassifier
from sklearn.linear_model import LogisticRegression
from sklearn.svm import SVC
```

In [2]:

```
#Replacing the space from column names and changing M - 1 and B - 0
df = pd.read_csv('wdbc.csv', header = 0)
df.columns = df.columns.str.replace(' ', '')

def diagnose(x):
    if x == 'M':
        x = 1
    else:
        x = 0
    return x
```

In [3]:

```
df['target'] = df['target'].apply(lambda x :diagnose(x))
```

In [4]:

```
#Check for null values  
df.isnull().sum()
```

Out[4]:

```
id                0  
target           0  
mean_radius      0  
mean_texture     0  
mean_perimeter   0  
mean_area        0  
mean_smoothness  0  
mean_compactness 0  
mean_concavity   0  
mean_concave_points 0  
mean_symmetry    0  
mean_fractal_dimension 0  
std_error_radius 0  
std_error_texture 0  
std_error_perimeter 0  
std_error_area   0  
std_error_smoothness 0  
std_error_compactness 0  
std_error_concavity 0  
std_error_concave_points 0  
std_error_symmetry 0  
std_error_fractal_dimension 0  
worst_radius     0  
worst_texture    0  
worst_perimeter  0  
worst_area       0  
worst_smoothness 0  
worst_compactness 0  
worst_concavity  0  
worst_concave_points 0  
worst_symmetry   0  
worst_fractal_dimension 0  
dtype: int64
```

In [5]:

```
#Get the summary of dataframe  
df.describe()
```

Out[5]:

	id	target	mean_radius	mean_texture	mean_perimeter	mean_area
count	5.690000e+02	569.000000	569.000000	569.000000	569.000000	569.000000
mean	3.037183e+07	0.372583	14.127292	19.289649	91.969033	654.889104
std	1.250206e+08	0.483918	3.524049	4.301036	24.298981	351.914129
min	8.670000e+03	0.000000	6.981000	9.710000	43.790000	143.500000
25%	8.692180e+05	0.000000	11.700000	16.170000	75.170000	420.300000
50%	9.060240e+05	0.000000	13.370000	18.840000	86.240000	551.100000
75%	8.813129e+06	1.000000	15.780000	21.800000	104.100000	782.700000
max	9.113205e+08	1.000000	28.110000	39.280000	188.500000	2501.000000

8 rows × 32 columns

In [6]:

```
#Extracting the independent and target variables  
X = df.iloc[:,2:]  
y = df.iloc[:,1]
```

In [7]:

```
#Print first 5 rows for independent variables  
X.head()
```

Out[7]:

	mean_radius	mean_texture	mean_perimeter	mean_area	mean_smoothness	mean_compa
0	17.99	10.38	122.80	1001.0	0.11840	0
1	20.57	17.77	132.90	1326.0	0.08474	0
2	19.69	21.25	130.00	1203.0	0.10960	0
3	11.42	20.38	77.58	386.1	0.14250	0
4	20.29	14.34	135.10	1297.0	0.10030	0

5 rows × 30 columns

In [8]:

```
#Print first 5 for dependent variables  
y.head()  
y.unique()
```

Out[8]:

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

In [9]:

```
#Splitting the data set into training and testing data in 4:1 ration  
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size = 0.2, random_state  
= 42)
```

Min-Max Scaling is done to avoid dominance of particular variables on the prediction

In [10]:

```
#Using normalisation  
from sklearn import preprocessing  
scaler = preprocessing.MinMaxScaler()  
scaler.fit(X_train)  
X_train = scaler.transform(X_train)  
X_test = scaler.transform(X_test)
```

Nested Cross Validation For Model Selection

With Recall as the performance evaluation metric

In [11]:

```

scoring = 'recall'
dt_cv_score = []
knn_cv_score = []
log_cv_score = []
svc_cv_score = []

N_TRIALS = 10
for i in range(N_TRIALS):
    inner_cv=KFold(n_splits=5,shuffle=True,random_state=100)
    outer_cv=KFold(n_splits=5,shuffle=True,random_state=100)
    dt = DecisionTreeClassifier(random_state=42)
    dt_grid = {'max_depth':list(range(0,10)), 'min_samples_leaf':[2, 3, 4], 'min_samples_
_split':[10, 20, 30],
               'criterion':['entropy', 'gini']}

    knn = KNeighborsClassifier()
    knn_grid = {'n_neighbors':list(range(2,8)), 'p':[1,2,3], 'weights':['uniform', 'dist
ance']}

    log = LogisticRegression(random_state=42, multi_class = 'multinomial')
    lr_grid = {'C': [0.001, 0.01, 0.05, 0.1,0.05, 1, 10, 100], 'penalty' : ['l1','l2'],
'solver': ['lbfgs', 'liblinear', 'sag', 'saga', 'newton-cg']}

    svc = SVC(random_state = 42, probability=True)
    svc_grid = [{'kernel': ['rbf'], 'gamma': [0.1, 0.5], 'C': [1, 10, 100, 1000]},
                {'kernel': ['linear'], 'C': [1, 10, 100, 1000]}]

    dt_clf = GridSearchCV(estimator = dt, param_grid = dt_grid, cv = inner_cv, scoring
= 'recall')
    knn_clf = GridSearchCV(estimator = knn, param_grid = knn_grid, cv = inner_cv, scori
ng = 'recall')
    svc_clf = GridSearchCV(estimator = svc, param_grid = svc_grid, cv=inner_cv, scoring
= 'recall')
    lr_clf = GridSearchCV(estimator = log, param_grid = lr_grid, cv = inner_cv, scoring
= 'recall')

    dt_score=cross_val_score(dt_clf,X_train,y_train, cv = outer_cv)
    dt_score = dt_score.mean()
    dt_cv_score.append(dt_score.mean())

    knn_score=cross_val_score(knn_clf,X_train,y_train, cv = outer_cv)
    knn_score = knn_score.mean()
    knn_cv_score.append(knn_score.mean())

    lr_score=cross_val_score(lr_clf,X_train,y_train, cv = outer_cv)
    lr_score = lr_score.mean()
    log_cv_score.append(lr_score.mean())

    svc_score=cross_val_score(svc_clf,X_train,y_train, cv = outer_cv)
    svc_score = svc_score.mean()
    svc_cv_score.append(svc_score.mean())

# print("Mean accuracy for training data set with cross validations for decision tre
e:",dt_cv_score)
# print("Mean accuracy for training data set with cross validations for KNN:",knn_cv_sc
ore)
# print("Mean accuracy for training data set with cross validations for logistic regres
sion:",log_cv_score)

```

```
# print("Mean accuracy for training data set with cross validations for SVM:",svc_cv_score)
```

In [12]:

```
#Assign a function to calculate the mean of the accuracies
def Average(lst):
    return sum(lst) / len(lst)
```

In [13]:

```
dt_avg = Average(dt_cv_score)
knn_avg = Average(knn_cv_score)
log_avg = Average(log_cv_score)
svc_avg = Average(svc_cv_score)

print("Decision Tree Recall:",dt_avg)
print("KNN Classifier Recall: ",knn_avg)
print("Logistic Regression: ",log_avg)
print("Support Vector Machine Classifier: ",svc_avg)
```

```
Decision Tree Recall: 0.9202306412583182
KNN Classifier Recall: 0.949627192982456
Logistic Regression: 0.9549236237144585
Support Vector Machine Classifier: 0.9471937386569873
```

From the Nested Cross Validation results, it is observed that Logistic Regression performs the best out of all 4 models on "recall" as the scoring metric.

Hyper-Parameter Tuning for Logistic Regression Model

In [14]:

```
log = LogisticRegression(random_state=42)
parameters = {'C': [0.001, 0.01, 0.05, 0.1,0.05, 1, 10, 100], 'penalty' : ['l1','l2'],
'solver': ['lbfgs', 'liblinear', 'sag', 'saga', 'newton-cg']}
```

Hyper parameter tuning for precision and recall as scoring metrics separately

In [15]:

```
scores = ['precision', 'recall']
for score in scores:
    print("# Tuning hyper-parameters for %s" % score)
    print()

    clf = GridSearchCV(log, parameters, cv=5, scoring='%s_macro' % score)
    clf.fit(X_train, y_train)
    print("Best parameters set found on development set:")
    print()
    print(clf.best_params_)
    print()
    print("Grid scores on development set:")
    print()
    means = clf.cv_results_['mean_test_score']
    stds = clf.cv_results_['std_test_score']
    for mean, std, params in zip(means, stds, clf.cv_results_['params']):
        print("%0.3f (+/-%0.03f) for %r"
              % (mean, std * 2, params))
    print()

    print("Detailed classification report:")
    print()
    print("The model is trained on the full development set.")
    print("The scores are computed on the full evaluation set.")
    print()
    y_true, y_pred = y_test, clf.predict(X_test)
    print(classification_report(y_true, y_pred))
    print()
```

Tuning hyper-parameters for precision

Best parameters set found on development set:

```
{'C': 10, 'penalty': 'l1', 'solver': 'saga'}
```

Grid scores on development set:

```
nan (+/-nan) for {'C': 0.001, 'penalty': 'l1', 'solver': 'lbfgs'}
0.314 (+/-0.004) for {'C': 0.001, 'penalty': 'l1', 'solver': 'liblinear'}
nan (+/-nan) for {'C': 0.001, 'penalty': 'l1', 'solver': 'sag'}
0.314 (+/-0.004) for {'C': 0.001, 'penalty': 'l1', 'solver': 'saga'}
nan (+/-nan) for {'C': 0.001, 'penalty': 'l1', 'solver': 'newton-cg'}
0.314 (+/-0.004) for {'C': 0.001, 'penalty': 'l2', 'solver': 'lbfgs'}
0.833 (+/-0.011) for {'C': 0.001, 'penalty': 'l2', 'solver': 'liblinear'}
0.314 (+/-0.004) for {'C': 0.001, 'penalty': 'l2', 'solver': 'sag'}
0.314 (+/-0.004) for {'C': 0.001, 'penalty': 'l2', 'solver': 'saga'}
0.314 (+/-0.004) for {'C': 0.001, 'penalty': 'l2', 'solver': 'newton-cg'}
nan (+/-nan) for {'C': 0.01, 'penalty': 'l1', 'solver': 'lbfgs'}
0.314 (+/-0.004) for {'C': 0.01, 'penalty': 'l1', 'solver': 'liblinear'}
nan (+/-nan) for {'C': 0.01, 'penalty': 'l1', 'solver': 'sag'}
0.314 (+/-0.004) for {'C': 0.01, 'penalty': 'l1', 'solver': 'saga'}
nan (+/-nan) for {'C': 0.01, 'penalty': 'l1', 'solver': 'newton-cg'}
0.846 (+/-0.023) for {'C': 0.01, 'penalty': 'l2', 'solver': 'lbfgs'}
0.911 (+/-0.027) for {'C': 0.01, 'penalty': 'l2', 'solver': 'liblinear'}
0.846 (+/-0.023) for {'C': 0.01, 'penalty': 'l2', 'solver': 'sag'}
0.846 (+/-0.023) for {'C': 0.01, 'penalty': 'l2', 'solver': 'saga'}
0.846 (+/-0.023) for {'C': 0.01, 'penalty': 'l2', 'solver': 'newton-cg'}
nan (+/-nan) for {'C': 0.05, 'penalty': 'l1', 'solver': 'lbfgs'}
0.832 (+/-0.023) for {'C': 0.05, 'penalty': 'l1', 'solver': 'liblinear'}
nan (+/-nan) for {'C': 0.05, 'penalty': 'l1', 'solver': 'sag'}
0.886 (+/-0.022) for {'C': 0.05, 'penalty': 'l1', 'solver': 'saga'}
nan (+/-nan) for {'C': 0.05, 'penalty': 'l1', 'solver': 'newton-cg'}
0.936 (+/-0.017) for {'C': 0.05, 'penalty': 'l2', 'solver': 'lbfgs'}
0.935 (+/-0.027) for {'C': 0.05, 'penalty': 'l2', 'solver': 'liblinear'}
0.936 (+/-0.017) for {'C': 0.05, 'penalty': 'l2', 'solver': 'sag'}
0.936 (+/-0.017) for {'C': 0.05, 'penalty': 'l2', 'solver': 'saga'}
0.936 (+/-0.017) for {'C': 0.05, 'penalty': 'l2', 'solver': 'newton-cg'}
nan (+/-nan) for {'C': 0.1, 'penalty': 'l1', 'solver': 'lbfgs'}
0.931 (+/-0.051) for {'C': 0.1, 'penalty': 'l1', 'solver': 'liblinear'}
nan (+/-nan) for {'C': 0.1, 'penalty': 'l1', 'solver': 'sag'}
0.935 (+/-0.044) for {'C': 0.1, 'penalty': 'l1', 'solver': 'saga'}
nan (+/-nan) for {'C': 0.1, 'penalty': 'l1', 'solver': 'newton-cg'}
0.947 (+/-0.016) for {'C': 0.1, 'penalty': 'l2', 'solver': 'lbfgs'}
0.939 (+/-0.028) for {'C': 0.1, 'penalty': 'l2', 'solver': 'liblinear'}
0.947 (+/-0.016) for {'C': 0.1, 'penalty': 'l2', 'solver': 'sag'}
0.947 (+/-0.016) for {'C': 0.1, 'penalty': 'l2', 'solver': 'saga'}
0.947 (+/-0.016) for {'C': 0.1, 'penalty': 'l2', 'solver': 'newton-cg'}
nan (+/-nan) for {'C': 0.05, 'penalty': 'l1', 'solver': 'lbfgs'}
0.832 (+/-0.023) for {'C': 0.05, 'penalty': 'l1', 'solver': 'liblinear'}
nan (+/-nan) for {'C': 0.05, 'penalty': 'l1', 'solver': 'sag'}
0.886 (+/-0.022) for {'C': 0.05, 'penalty': 'l1', 'solver': 'saga'}
nan (+/-nan) for {'C': 0.05, 'penalty': 'l1', 'solver': 'newton-cg'}
0.936 (+/-0.017) for {'C': 0.05, 'penalty': 'l2', 'solver': 'lbfgs'}
0.935 (+/-0.027) for {'C': 0.05, 'penalty': 'l2', 'solver': 'liblinear'}
0.936 (+/-0.017) for {'C': 0.05, 'penalty': 'l2', 'solver': 'sag'}
0.936 (+/-0.017) for {'C': 0.05, 'penalty': 'l2', 'solver': 'saga'}
0.936 (+/-0.017) for {'C': 0.05, 'penalty': 'l2', 'solver': 'newton-cg'}
nan (+/-nan) for {'C': 1, 'penalty': 'l1', 'solver': 'lbfgs'}
0.969 (+/-0.036) for {'C': 1, 'penalty': 'l1', 'solver': 'liblinear'}
nan (+/-nan) for {'C': 1, 'penalty': 'l1', 'solver': 'sag'}
```



```

0.966 (+/-0.034) for {'C': 1, 'penalty': 'l1', 'solver': 'saga'}
nan (+/-nan) for {'C': 1, 'penalty': 'l1', 'solver': 'newton-cg'}
0.969 (+/-0.023) for {'C': 1, 'penalty': 'l2', 'solver': 'lbfgs'}
0.967 (+/-0.010) for {'C': 1, 'penalty': 'l2', 'solver': 'liblinear'}
0.969 (+/-0.023) for {'C': 1, 'penalty': 'l2', 'solver': 'sag'}
0.969 (+/-0.023) for {'C': 1, 'penalty': 'l2', 'solver': 'saga'}
0.969 (+/-0.023) for {'C': 1, 'penalty': 'l2', 'solver': 'newton-cg'}
nan (+/-nan) for {'C': 10, 'penalty': 'l1', 'solver': 'lbfgs'}
0.974 (+/-0.031) for {'C': 10, 'penalty': 'l1', 'solver': 'liblinear'}
nan (+/-nan) for {'C': 10, 'penalty': 'l1', 'solver': 'sag'}
0.979 (+/-0.031) for {'C': 10, 'penalty': 'l1', 'solver': 'saga'}
nan (+/-nan) for {'C': 10, 'penalty': 'l1', 'solver': 'newton-cg'}
0.976 (+/-0.024) for {'C': 10, 'penalty': 'l2', 'solver': 'lbfgs'}
0.979 (+/-0.017) for {'C': 10, 'penalty': 'l2', 'solver': 'liblinear'}
0.976 (+/-0.024) for {'C': 10, 'penalty': 'l2', 'solver': 'sag'}
0.976 (+/-0.024) for {'C': 10, 'penalty': 'l2', 'solver': 'saga'}
0.976 (+/-0.024) for {'C': 10, 'penalty': 'l2', 'solver': 'newton-cg'}
nan (+/-nan) for {'C': 100, 'penalty': 'l1', 'solver': 'lbfgs'}
0.965 (+/-0.047) for {'C': 100, 'penalty': 'l1', 'solver': 'liblinear'}
nan (+/-nan) for {'C': 100, 'penalty': 'l1', 'solver': 'sag'}
0.978 (+/-0.027) for {'C': 100, 'penalty': 'l1', 'solver': 'saga'}
nan (+/-nan) for {'C': 100, 'penalty': 'l1', 'solver': 'newton-cg'}
0.972 (+/-0.038) for {'C': 100, 'penalty': 'l2', 'solver': 'lbfgs'}
0.976 (+/-0.037) for {'C': 100, 'penalty': 'l2', 'solver': 'liblinear'}
0.979 (+/-0.031) for {'C': 100, 'penalty': 'l2', 'solver': 'sag'}
0.978 (+/-0.027) for {'C': 100, 'penalty': 'l2', 'solver': 'saga'}
0.972 (+/-0.038) for {'C': 100, 'penalty': 'l2', 'solver': 'newton-cg'}

```

Detailed classification report:

The model is trained on the full development set.

The scores are computed on the full evaluation set.

	precision	recall	f1-score	support
0	0.97	0.99	0.98	71
1	0.98	0.95	0.96	43
accuracy			0.97	114
macro avg	0.97	0.97	0.97	114
weighted avg	0.97	0.97	0.97	114

Tuning hyper-parameters for recall

Best parameters set found on development set:

```
{'C': 10, 'penalty': 'l1', 'solver': 'saga'}
```

Grid scores on development set:

```

nan (+/-nan) for {'C': 0.001, 'penalty': 'l1', 'solver': 'lbfgs'}
0.500 (+/-0.000) for {'C': 0.001, 'penalty': 'l1', 'solver': 'liblinear'}
nan (+/-nan) for {'C': 0.001, 'penalty': 'l1', 'solver': 'sag'}
0.500 (+/-0.000) for {'C': 0.001, 'penalty': 'l1', 'solver': 'saga'}
nan (+/-nan) for {'C': 0.001, 'penalty': 'l1', 'solver': 'newton-cg'}
0.500 (+/-0.000) for {'C': 0.001, 'penalty': 'l2', 'solver': 'lbfgs'}
0.577 (+/-0.035) for {'C': 0.001, 'penalty': 'l2', 'solver': 'liblinear'}
0.500 (+/-0.000) for {'C': 0.001, 'penalty': 'l2', 'solver': 'sag'}
0.500 (+/-0.000) for {'C': 0.001, 'penalty': 'l2', 'solver': 'saga'}
0.500 (+/-0.000) for {'C': 0.001, 'penalty': 'l2', 'solver': 'newton-cg'}

```

```
nan (+/-nan) for {'C': 0.01, 'penalty': 'l1', 'solver': 'lbfgs'}
0.500 (+/-0.000) for {'C': 0.01, 'penalty': 'l1', 'solver': 'liblinear'}
nan (+/-nan) for {'C': 0.01, 'penalty': 'l1', 'solver': 'sag'}
0.500 (+/-0.000) for {'C': 0.01, 'penalty': 'l1', 'solver': 'saga'}
nan (+/-nan) for {'C': 0.01, 'penalty': 'l1', 'solver': 'newton-cg'}
0.622 (+/-0.073) for {'C': 0.01, 'penalty': 'l2', 'solver': 'lbfgs'}
0.821 (+/-0.087) for {'C': 0.01, 'penalty': 'l2', 'solver': 'liblinear'}
0.622 (+/-0.073) for {'C': 0.01, 'penalty': 'l2', 'solver': 'sag'}
0.622 (+/-0.073) for {'C': 0.01, 'penalty': 'l2', 'solver': 'saga'}
0.622 (+/-0.073) for {'C': 0.01, 'penalty': 'l2', 'solver': 'newton-cg'}
nan (+/-nan) for {'C': 0.05, 'penalty': 'l1', 'solver': 'lbfgs'}
0.571 (+/-0.071) for {'C': 0.05, 'penalty': 'l1', 'solver': 'liblinear'}
nan (+/-nan) for {'C': 0.05, 'penalty': 'l1', 'solver': 'sag'}
0.762 (+/-0.057) for {'C': 0.05, 'penalty': 'l1', 'solver': 'saga'}
nan (+/-nan) for {'C': 0.05, 'penalty': 'l1', 'solver': 'newton-cg'}
0.880 (+/-0.050) for {'C': 0.05, 'penalty': 'l2', 'solver': 'lbfgs'}
0.884 (+/-0.066) for {'C': 0.05, 'penalty': 'l2', 'solver': 'liblinear'}
0.880 (+/-0.050) for {'C': 0.05, 'penalty': 'l2', 'solver': 'sag'}
0.880 (+/-0.050) for {'C': 0.05, 'penalty': 'l2', 'solver': 'saga'}
0.880 (+/-0.050) for {'C': 0.05, 'penalty': 'l2', 'solver': 'newton-cg'}
nan (+/-nan) for {'C': 0.1, 'penalty': 'l1', 'solver': 'lbfgs'}
0.901 (+/-0.051) for {'C': 0.1, 'penalty': 'l1', 'solver': 'liblinear'}
nan (+/-nan) for {'C': 0.1, 'penalty': 'l1', 'solver': 'sag'}
0.903 (+/-0.049) for {'C': 0.1, 'penalty': 'l1', 'solver': 'saga'}
nan (+/-nan) for {'C': 0.1, 'penalty': 'l1', 'solver': 'newton-cg'}
0.904 (+/-0.049) for {'C': 0.1, 'penalty': 'l2', 'solver': 'lbfgs'}
0.904 (+/-0.055) for {'C': 0.1, 'penalty': 'l2', 'solver': 'liblinear'}
0.904 (+/-0.049) for {'C': 0.1, 'penalty': 'l2', 'solver': 'sag'}
0.904 (+/-0.049) for {'C': 0.1, 'penalty': 'l2', 'solver': 'saga'}
0.904 (+/-0.049) for {'C': 0.1, 'penalty': 'l2', 'solver': 'newton-cg'}
nan (+/-nan) for {'C': 0.05, 'penalty': 'l1', 'solver': 'lbfgs'}
0.571 (+/-0.071) for {'C': 0.05, 'penalty': 'l1', 'solver': 'liblinear'}
nan (+/-nan) for {'C': 0.05, 'penalty': 'l1', 'solver': 'sag'}
0.762 (+/-0.057) for {'C': 0.05, 'penalty': 'l1', 'solver': 'saga'}
nan (+/-nan) for {'C': 0.05, 'penalty': 'l1', 'solver': 'newton-cg'}
0.880 (+/-0.050) for {'C': 0.05, 'penalty': 'l2', 'solver': 'lbfgs'}
0.884 (+/-0.066) for {'C': 0.05, 'penalty': 'l2', 'solver': 'liblinear'}
0.880 (+/-0.050) for {'C': 0.05, 'penalty': 'l2', 'solver': 'sag'}
0.880 (+/-0.050) for {'C': 0.05, 'penalty': 'l2', 'solver': 'saga'}
0.880 (+/-0.050) for {'C': 0.05, 'penalty': 'l2', 'solver': 'newton-cg'}
nan (+/-nan) for {'C': 1, 'penalty': 'l1', 'solver': 'lbfgs'}
0.960 (+/-0.044) for {'C': 1, 'penalty': 'l1', 'solver': 'liblinear'}
nan (+/-nan) for {'C': 1, 'penalty': 'l1', 'solver': 'sag'}
0.955 (+/-0.037) for {'C': 1, 'penalty': 'l1', 'solver': 'saga'}
nan (+/-nan) for {'C': 1, 'penalty': 'l1', 'solver': 'newton-cg'}
0.948 (+/-0.045) for {'C': 1, 'penalty': 'l2', 'solver': 'lbfgs'}
0.949 (+/-0.017) for {'C': 1, 'penalty': 'l2', 'solver': 'liblinear'}
0.948 (+/-0.045) for {'C': 1, 'penalty': 'l2', 'solver': 'sag'}
0.948 (+/-0.045) for {'C': 1, 'penalty': 'l2', 'solver': 'saga'}
0.948 (+/-0.045) for {'C': 1, 'penalty': 'l2', 'solver': 'newton-cg'}
nan (+/-nan) for {'C': 10, 'penalty': 'l1', 'solver': 'lbfgs'}
0.969 (+/-0.035) for {'C': 10, 'penalty': 'l1', 'solver': 'liblinear'}
nan (+/-nan) for {'C': 10, 'penalty': 'l1', 'solver': 'sag'}
0.974 (+/-0.037) for {'C': 10, 'penalty': 'l1', 'solver': 'saga'}
nan (+/-nan) for {'C': 10, 'penalty': 'l1', 'solver': 'newton-cg'}
0.968 (+/-0.027) for {'C': 10, 'penalty': 'l2', 'solver': 'lbfgs'}
0.970 (+/-0.030) for {'C': 10, 'penalty': 'l2', 'solver': 'liblinear'}
0.968 (+/-0.027) for {'C': 10, 'penalty': 'l2', 'solver': 'sag'}
0.968 (+/-0.027) for {'C': 10, 'penalty': 'l2', 'solver': 'saga'}
0.968 (+/-0.027) for {'C': 10, 'penalty': 'l2', 'solver': 'newton-cg'}
nan (+/-nan) for {'C': 100, 'penalty': 'l1', 'solver': 'lbfgs'}
```

```

0.960 (+/-0.046) for {'C': 100, 'penalty': 'l1', 'solver': 'liblinear'}
nan (+/-nan) for {'C': 100, 'penalty': 'l1', 'solver': 'sag'}
0.971 (+/-0.031) for {'C': 100, 'penalty': 'l1', 'solver': 'saga'}
nan (+/-nan) for {'C': 100, 'penalty': 'l1', 'solver': 'newton-cg'}
0.968 (+/-0.047) for {'C': 100, 'penalty': 'l2', 'solver': 'lbfgs'}
0.972 (+/-0.040) for {'C': 100, 'penalty': 'l2', 'solver': 'liblinear'}
0.974 (+/-0.037) for {'C': 100, 'penalty': 'l2', 'solver': 'sag'}
0.971 (+/-0.031) for {'C': 100, 'penalty': 'l2', 'solver': 'saga'}
0.968 (+/-0.047) for {'C': 100, 'penalty': 'l2', 'solver': 'newton-cg'}

```

Detailed classification report:

The model is trained on the full development set.

The scores are computed on the full evaluation set.

	precision	recall	f1-score	support
0	0.97	0.99	0.98	71
1	0.98	0.95	0.96	43
accuracy			0.97	114
macro avg	0.97	0.97	0.97	114
weighted avg	0.97	0.97	0.97	114

It is observed from above GridSearchCV hyper-parameter tuning the best parameters available for Logistic Regression are: {'C': 10, 'penalty': 'l1', 'solver': 'saga'}.

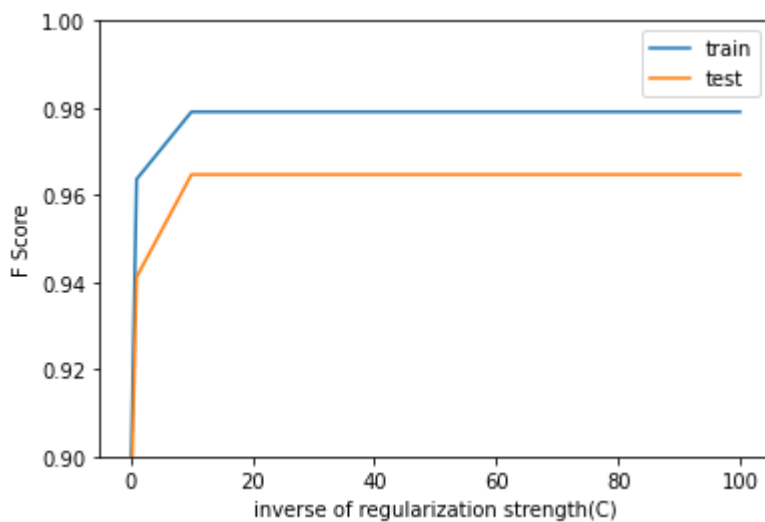
Plotting the performance of Logistic Regression model on various C inputs to understand the overfitting threshold and selecting the best value for hyper-parameter.

F_score for malignant class is 0.96 and f1_score for benign is 0.98 from the logistic regression model.

Inverse of regularization strength(C) vs Recall, f_score and AUC Score Curve

In [16]:

```
import matplotlib.pyplot as plt
C = [0.001, 0.01, 0.1, 1, 10, 100]
train_f_score = []
test_f_score = []
for i in C:
    clf = LogisticRegression(C=i, penalty='l1', random_state=42, solver='saga')
    clf.fit(X_train, y_train)
    train_f_score.append(f1_score(y_train, clf.predict(X_train)))
    test_f_score.append(f1_score(y_test, clf.predict(X_test)))
    #print(classification_report(y_test, clf.predict(X_test_N)))
plt.plot(C, train_f_score, label = 'train')
plt.plot(C, test_f_score, label = 'test')
plt.axis([-5,105,0.9,1])
plt.xlabel('inverse of regularization strength(C)')
plt.ylabel('F Score')
plt.legend()
plt.show()
```

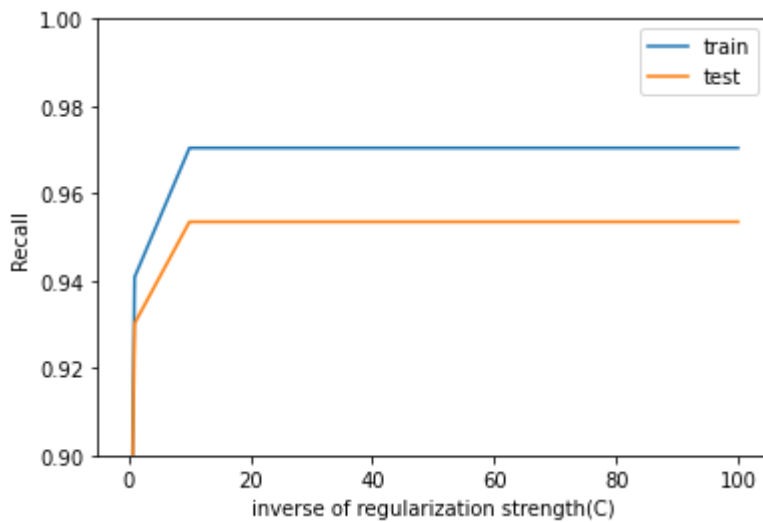


In [17]:

```

import matplotlib.pyplot as plt
C = [0.001, 0.01, 0.1, 1, 10, 100]
train_recall_score = []
test_recall_score = []
for i in C:
    clf = LogisticRegression(C=i, penalty='l1', random_state=42, solver='saga')
    clf.fit(X_train, y_train)
    train_recall_score.append(recall_score(y_train, clf.predict(X_train)))
    test_recall_score.append(recall_score(y_test, clf.predict(X_test)))
    #print(classification_report(y_test, clf.predict(X_test_N)))
plt.plot(C, train_recall_score, label = 'train')
plt.plot(C, test_recall_score, label = 'test')
plt.axis([-5,105,0.9,1])
plt.xlabel('inverse of regularization strength(C)')
plt.ylabel('Recall')
plt.legend()
plt.show()

```

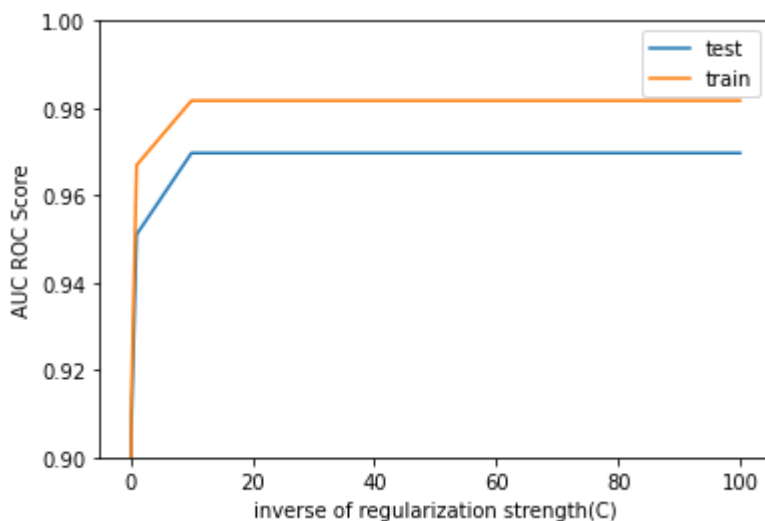


In [18]:

```

import matplotlib.pyplot as plt
from sklearn.metrics import recall_score, roc_auc_score
C = [0.001, 0.01, 0.1, 1, 10, 100]
train_auc_score = []
test_auc_score = []
for i in C:
    clf = LogisticRegression(C=i, penalty='l1', random_state=42, solver='saga')
    clf.fit(X_train, y_train)
    train_auc_score.append(roc_auc_score(y_train, clf.predict(X_train)))
    test_auc_score.append(roc_auc_score(y_test, clf.predict(X_test)))
    #print(classification_report(y_test, clf.predict(X_test_N)))
plt.plot(C, test_auc_score, label = 'test')
plt.plot(C, train_auc_score, label = 'train')
plt.xlabel('inverse of regularization strength(C)')
plt.ylabel('AUC ROC Score')
plt.axis([-5,105,0.9,1])
plt.legend()
plt.show()

```



From the f_{score} , recall and AUC curve, we can see that the model performance on testing is improving until $C = 10$ beyond which there is no improvement, hence to avoid model overfitting, the C value is taken as 10.

Final Logistic Regression Model

In [19]:

```

log_final = LogisticRegression(C=10, penalty='l1', random_state=42, solver='saga')
log_final.fit(X_train, y_train)

best_train = log_final.predict(X_train)
best_test = log_final.predict(X_test)

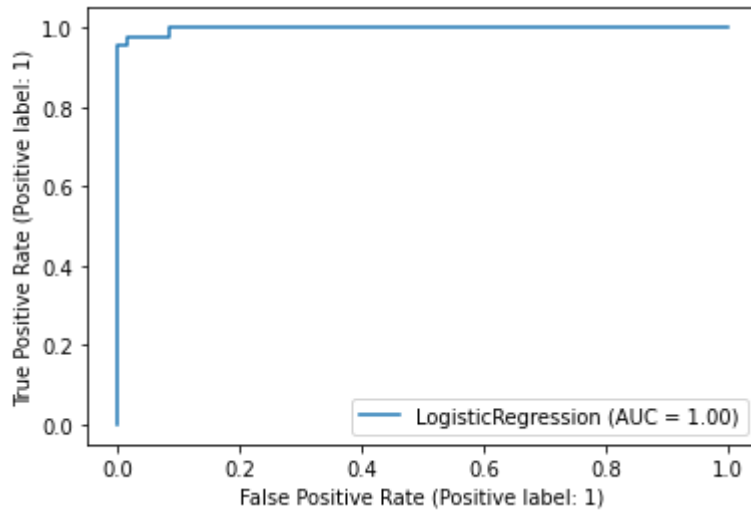
```

Lift Curve, ROC Curve and Cumulative Gains Curve

In [20]:

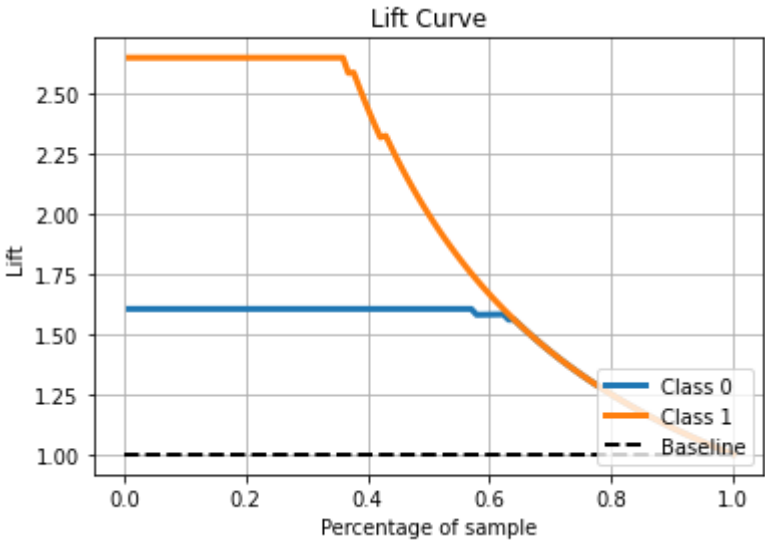
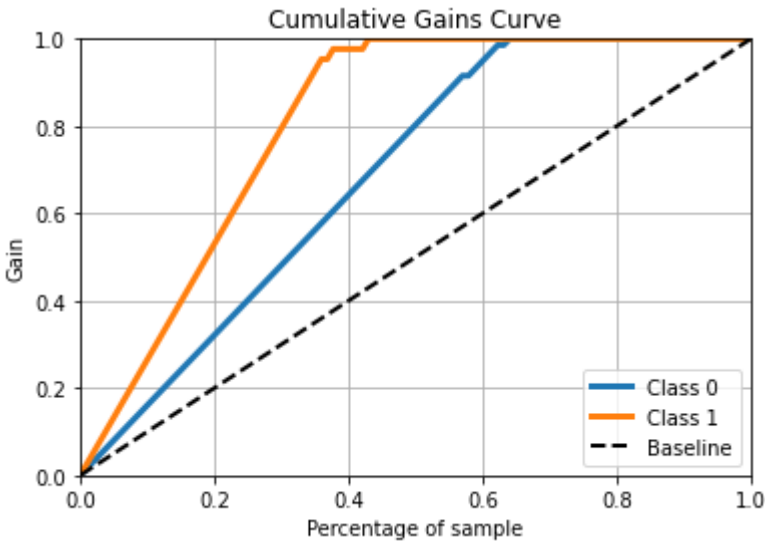
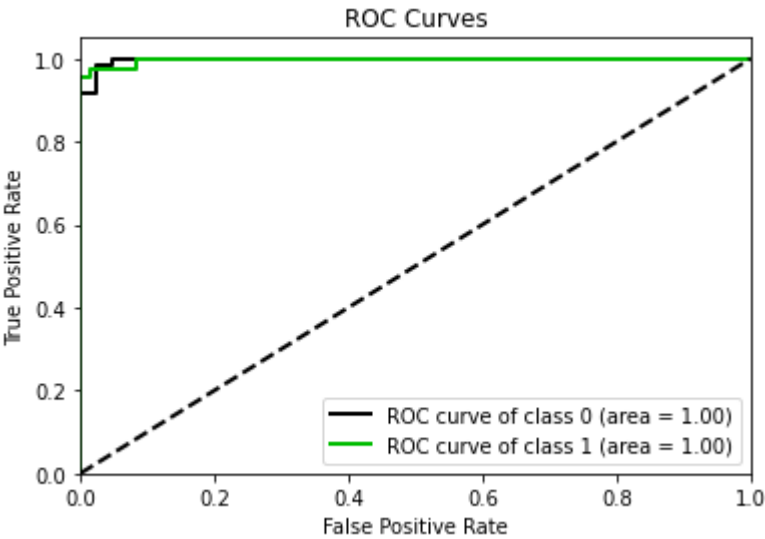
```
from sklearn.metrics import plot_roc_curve
print("The AUC score is ", roc_auc_score(y_test, log_final.predict(X_test)))
plot_roc_curve(log_final, X_test, y_test)
plt.show()
```

The AUC score is 0.9697019325253848



In [21]:

```
import scikitplot as skplt
skplt.metrics.plot_roc(y_test, log_final.predict_proba(X_test), plot_micro =False, plot_macro = False)
skplt.metrics.plot_cumulative_gain(y_test, log_final.predict_proba(X_test))
skplt.metrics.plot_lift_curve(y_test, log_final.predict_proba(X_test))
plt.show()
```

In [22]:

```
roc_auc_score(y_test, log_final.predict(X_test))
```

Out[22]:

0.9697019325253848

Interpreting the ROC, AUC and Lift Curve

ROC Curve - From the ROC Curve, we obtained area under the curve value of 0.9697 which measures the probability that a randomly chosen malignant instance will have a higher predicted probability of being malignant by the model than a randomly chosen benign instance.

Lift Curve - The lift ratio indicates how better the model performs compared to a random guess. For Malignant classification (Class 1), at 30% of sample, the lift ratio is approximately 2.65 meaning that model's top 30% predictions are 2.65X as good at predicting the outcome than as random guess. For Benign classification (Class 0), at 30% of sample, the lift ratio is approximately 1.60 meaning that model's top 30% predictions are 1.60X as good at predicting the outcome than as random guess.

In [23]:

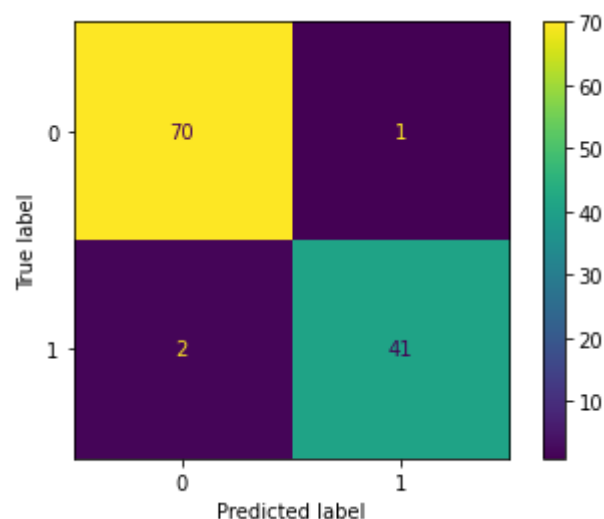
```
# Calculate the f1_score of the new model.
print('The training F1 Score is', recall_score(best_train, y_train))
print('The testing F1 Score is', recall_score(best_test, y_test))
print('\n')
print("-----")

from sklearn.metrics import plot_confusion_matrix
plot_confusion_matrix(log_final, X_test, y_test)
plt.show()

print("-----")
print(classification_report(y_test, log_final.predict(X_test)))
```

The training F1 Score is 0.9879518072289156

The testing F1 Score is 0.9761904761904762



	precision	recall	f1-score	support
0	0.97	0.99	0.98	71
1	0.98	0.95	0.96	43
accuracy			0.97	114
macro avg	0.97	0.97	0.97	114
weighted avg	0.97	0.97	0.97	114

With F_Score as Performance Evaluation Metric

In [24]:

```

scorer = make_scorer(f1_score)
dt_cv_score = []
knn_cv_score = []
log_cv_score = []
svc_cv_score = []

N_TRIALS = 10
for i in range(N_TRIALS):
    inner_cv=KFold(n_splits=5,shuffle=True,random_state=100)
    outer_cv=KFold(n_splits=5,shuffle=True,random_state=100)
    dt = DecisionTreeClassifier(random_state=42)
    dt_grid = {'max_depth':list(range(0,10)), 'min_samples_leaf':[2, 3, 4], 'min_samples
_split':[10, 20, 30],
               'criterion':['entropy', 'gini']}

    knn = KNeighborsClassifier()
    knn_grid = {'n_neighbors':list(range(2,8)), 'p':[1,2,3], 'weights':['uniform', 'dist
ance']}

    log = LogisticRegression(random_state=42, multi_class = 'multinomial')
    lr_grid = {'C': [0.001, 0.01, 0.05, 0.1,0.05, 1, 10, 100], 'penalty' : ['l1','l2'],
'solver': ['lbfgs', 'liblinear', 'sag', 'saga', 'newton-cg']}

    svc = SVC(random_state = 42, probability=True)
    svc_grid = [{'kernel': ['rbf'], 'gamma': [0.1, 0.5], 'C': [1, 10, 100, 1000]},
                {'kernel': ['linear'], 'C': [1, 10, 100, 1000]}]

    dt_clf = GridSearchCV(estimator = dt, param_grid = dt_grid, cv = inner_cv, scoring
= scorer)
    knn_clf = GridSearchCV(estimator = knn, param_grid = knn_grid, cv = inner_cv, scori
ng = scorer)
    svc_clf = GridSearchCV(estimator = svc, param_grid = svc_grid, cv=inner_cv, scoring
= scorer)
    lr_clf = GridSearchCV(estimator = log, param_grid = lr_grid, cv = inner_cv, scoring
= scorer)

    dt_score=cross_val_score(dt_clf,X_train,y_train, cv = outer_cv)
    dt_score = dt_score.mean()
    dt_cv_score.append(dt_score.mean())

    knn_score=cross_val_score(knn_clf,X_train,y_train, cv = outer_cv)
    knn_score = knn_score.mean()
    knn_cv_score.append(knn_score.mean())

    lr_score=cross_val_score(lr_clf,X_train,y_train, cv = outer_cv)
    lr_score = lr_score.mean()
    log_cv_score.append(lr_score.mean())

    svc_score=cross_val_score(svc_clf,X_train,y_train, cv = outer_cv)
    svc_score = svc_score.mean()
    svc_cv_score.append(svc_score.mean())

```

In [26]:

```
dt_avg = Average(dt_cv_score)
knn_avg = Average(knn_cv_score)
log_avg = Average(log_cv_score)
svc_avg = Average(svc_cv_score)

print("Mean f_score for training data set with cross validations for decision tree: ",dt_avg)
print("Mean f_score for training data set with cross validations for KNN: ",knn_avg)
print("Mean f_score for training data set with cross validations for logistic regression: ",log_avg)
print("Mean f_score for training data set with cross validations for SVM: ",svc_avg)
```

Mean f_score for training data set with cross validations for decision tree: 0.9321501574081574

Mean f_score for training data set with cross validations for KNN: 0.9679211727950012

Mean f_score for training data set with cross validations for logistic regression: 0.9657489938027636

Mean f_score for training data set with cross validations for SVM: 0.9718631611335911

It is observed that SVM performs the best from Nested CV results with f_score as the performance metric

Hyper-Parameter Tuning for SVC Classifier

In [27]:

```
parameters = [{'kernel': ['rbf'], 'gamma': [0.1, 0.5], 'C': [1, 10, 100, 1000]},
               {'kernel': ['linear'], 'C': [1, 10, 100, 1000]}]

scores = ['precision', 'recall']
for score in scores:
    print("# Tuning hyper-parameters for %s" % score)
    print()

    clf = GridSearchCV(SVC(), parameters, cv=5, scoring='%s_macro' % score)
    clf.fit(X_train, y_train)
    print("Best parameters set found on development set:")
    print()
    print(clf.best_params_)
    print()
    print("Grid scores on development set:")
    print()
    means = clf.cv_results_['mean_test_score']
    stds = clf.cv_results_['std_test_score']
    for mean, std, params in zip(means, stds, clf.cv_results_['params']):
        print("%0.3f (+/-%0.03f) for %r"
              % (mean, std * 2, params))
    print()

    print("Detailed classification report:")
    print()
    print("The model is trained on the full development set.")
    print("The scores are computed on the full evaluation set.")
    print()
    y_true, y_pred = y_test, clf.predict(X_test)
    print(classification_report(y_true, y_pred))
    print()
```

Tuning hyper-parameters for precision

Best parameters set found on development set:

```
{'C': 1, 'kernel': 'linear'}
```

Grid scores on development set:

```
0.964 (+/-0.022) for {'C': 1, 'gamma': 0.1, 'kernel': 'rbf'}
0.979 (+/-0.022) for {'C': 1, 'gamma': 0.5, 'kernel': 'rbf'}
0.977 (+/-0.029) for {'C': 10, 'gamma': 0.1, 'kernel': 'rbf'}
0.973 (+/-0.026) for {'C': 10, 'gamma': 0.5, 'kernel': 'rbf'}
0.972 (+/-0.034) for {'C': 100, 'gamma': 0.1, 'kernel': 'rbf'}
0.968 (+/-0.038) for {'C': 100, 'gamma': 0.5, 'kernel': 'rbf'}
0.966 (+/-0.035) for {'C': 1000, 'gamma': 0.1, 'kernel': 'rbf'}
0.962 (+/-0.017) for {'C': 1000, 'gamma': 0.5, 'kernel': 'rbf'}
0.980 (+/-0.009) for {'C': 1, 'kernel': 'linear'}
0.979 (+/-0.020) for {'C': 10, 'kernel': 'linear'}
0.971 (+/-0.034) for {'C': 100, 'kernel': 'linear'}
0.958 (+/-0.045) for {'C': 1000, 'kernel': 'linear'}
```

Detailed classification report:

The model is trained on the full development set.

The scores are computed on the full evaluation set.

	precision	recall	f1-score	support
0	0.97	1.00	0.99	71
1	1.00	0.95	0.98	43
accuracy			0.98	114
macro avg	0.99	0.98	0.98	114
weighted avg	0.98	0.98	0.98	114

Tuning hyper-parameters for recall

Best parameters set found on development set:

```
{'C': 10, 'kernel': 'linear'}
```

Grid scores on development set:

```
0.939 (+/-0.033) for {'C': 1, 'gamma': 0.1, 'kernel': 'rbf'}
0.966 (+/-0.046) for {'C': 1, 'gamma': 0.5, 'kernel': 'rbf'}
0.967 (+/-0.043) for {'C': 10, 'gamma': 0.1, 'kernel': 'rbf'}
0.962 (+/-0.045) for {'C': 10, 'gamma': 0.5, 'kernel': 'rbf'}
0.968 (+/-0.039) for {'C': 100, 'gamma': 0.1, 'kernel': 'rbf'}
0.967 (+/-0.034) for {'C': 100, 'gamma': 0.5, 'kernel': 'rbf'}
0.965 (+/-0.029) for {'C': 1000, 'gamma': 0.1, 'kernel': 'rbf'}
0.964 (+/-0.005) for {'C': 1000, 'gamma': 0.5, 'kernel': 'rbf'}
0.969 (+/-0.026) for {'C': 1, 'kernel': 'linear'}
0.974 (+/-0.025) for {'C': 10, 'kernel': 'linear'}
0.969 (+/-0.034) for {'C': 100, 'kernel': 'linear'}
0.958 (+/-0.044) for {'C': 1000, 'kernel': 'linear'}
```

Detailed classification report:

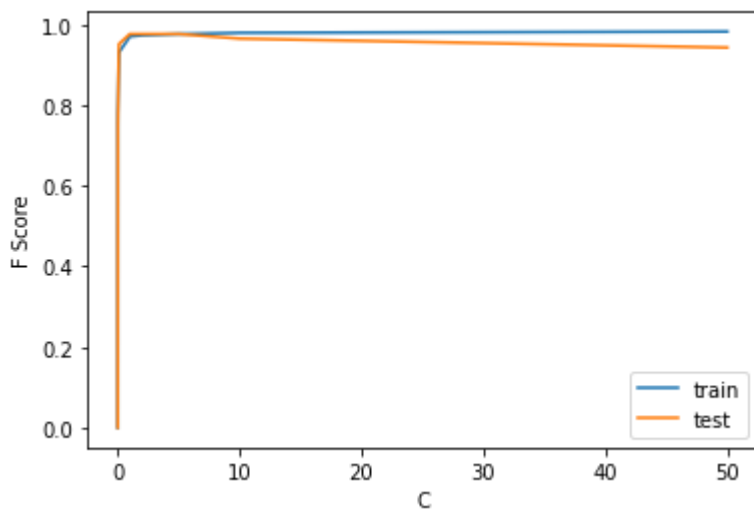
The model is trained on the full development set.

The scores are computed on the full evaluation set.

	precision	recall	f1-score	support
0	0.97	0.99	0.98	71
1	0.98	0.95	0.96	43
accuracy			0.97	114
macro avg	0.97	0.97	0.97	114
weighted avg	0.97	0.97	0.97	114

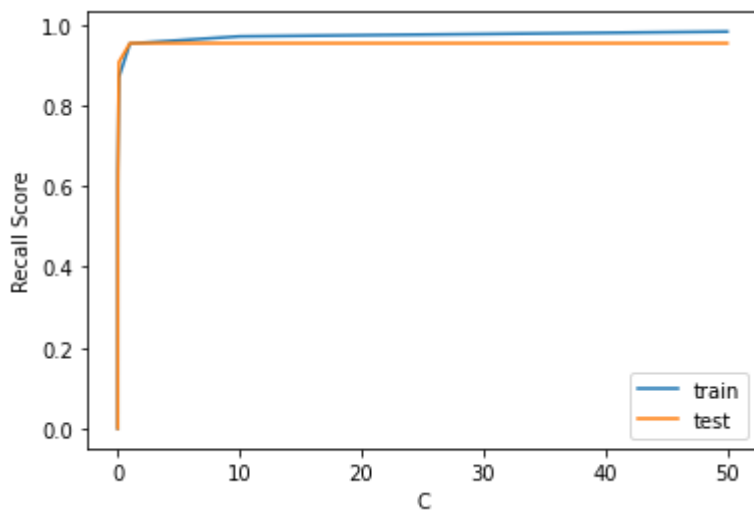
In [28]:

```
import matplotlib.pyplot as plt
from sklearn.metrics import make_scorer, recall_score, f1_score
C = [0.001, 0.01, 0.1, 1, 2, 5, 10, 50]
train_f_score = []
test_f_score = []
for i in C:
    clf = SVC(C=i, kernel= 'linear', random_state = 42, probability=True)
    clf.fit(X_train, y_train)
    train_f_score.append(f1_score(y_train, clf.predict(X_train)))
    test_f_score.append(f1_score(y_test, clf.predict(X_test)))
plt.plot(C, train_f_score, label = 'train')
plt.plot(C, test_f_score, label = 'test')
plt.xlabel('C')
plt.ylabel('F Score')
plt.legend()
plt.show()
```



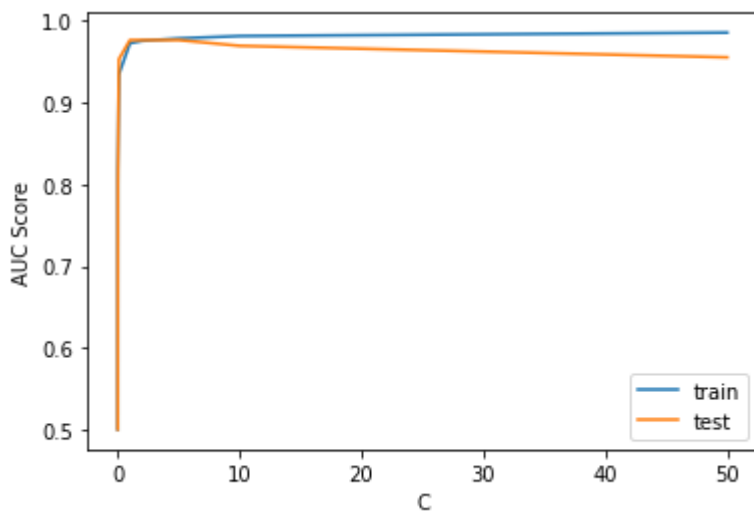
In [29]:

```
import matplotlib.pyplot as plt
from sklearn.metrics import make_scorer, recall_score, f1_score
C = [0.001, 0.01, 0.1, 1, 10, 50]
train_recall_score = []
test_recall_score = []
for i in C:
    clf = SVC(C=i, kernel = 'linear', random_state = 42, probability=True)
    clf.fit(X_train, y_train)
    train_recall_score.append(recall_score(y_train, clf.predict(X_train)))
    test_recall_score.append(recall_score(y_test, clf.predict(X_test)))
plt.plot(C, train_recall_score, label = 'train')
plt.plot(C, test_recall_score, label = 'test')
plt.xlabel('C')
plt.ylabel('Recall Score')
plt.legend()
plt.show()
```



In [30]:

```
import matplotlib.pyplot as plt
from sklearn.metrics import recall_score, roc_auc_score
from sklearn.metrics import make_scorer, recall_score, f1_score
C = [0.001, 0.01, 0.1, 1, 2, 5, 10, 50]
train_auc_score = []
test_auc_score = []
for i in C:
    clf = SVC(C=i, kernel = 'linear', random_state = 42, probability=True)
    clf.fit(X_train, y_train)
    train_auc_score.append(roc_auc_score(y_train, clf.predict(X_train)))
    test_auc_score.append(roc_auc_score(y_test, clf.predict(X_test)))
plt.plot(C, train_auc_score, label = 'train')
plt.plot(C, test_auc_score, label = 'test')
plt.xlabel('C')
plt.ylabel('AUC Score')
plt.legend()
plt.show()
```



From the f_score , recall and AUC curve, we can see that the model performance on testing is improving until $C = 1$ beyond which there is no improvement, hence to avoid model overfitting, the C value is taken as 1.

In [31]:

```

clf_svc = SVC(C=1, kernel = 'linear', random_state = 42, probability=True)
clf_svc.fit(X_train, y_train)
best_train_predictions_new = clf_svc.predict(X_train)
print(classification_report(y_test, clf_svc.predict(X_test)))

```

	precision	recall	f1-score	support
0	0.97	1.00	0.99	71
1	1.00	0.95	0.98	43
accuracy			0.98	114
macro avg	0.99	0.98	0.98	114
weighted avg	0.98	0.98	0.98	114

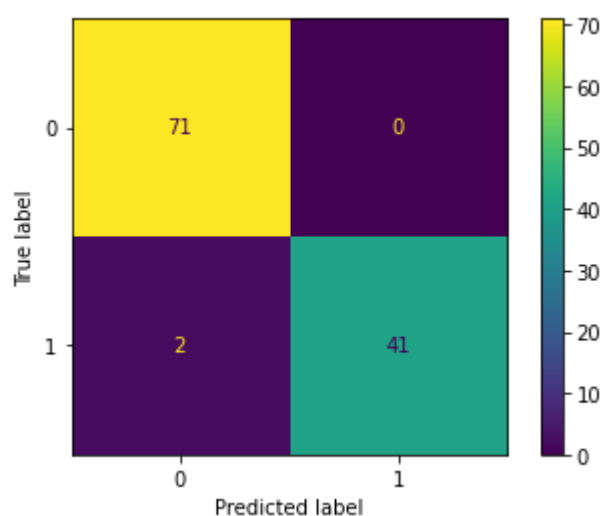
F_score for malignant class is 0.95 and f1_score for benign is 1.0 for the Support Vector Machine Classifier.

In [32]:

```

from sklearn.metrics import plot_confusion_matrix
plot_confusion_matrix(clf_svc, X_test, y_test)
plt.show()

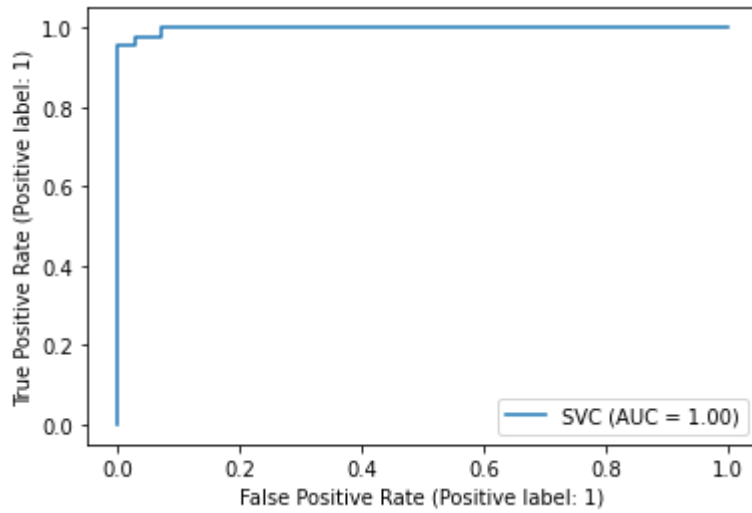
```



In [33]:

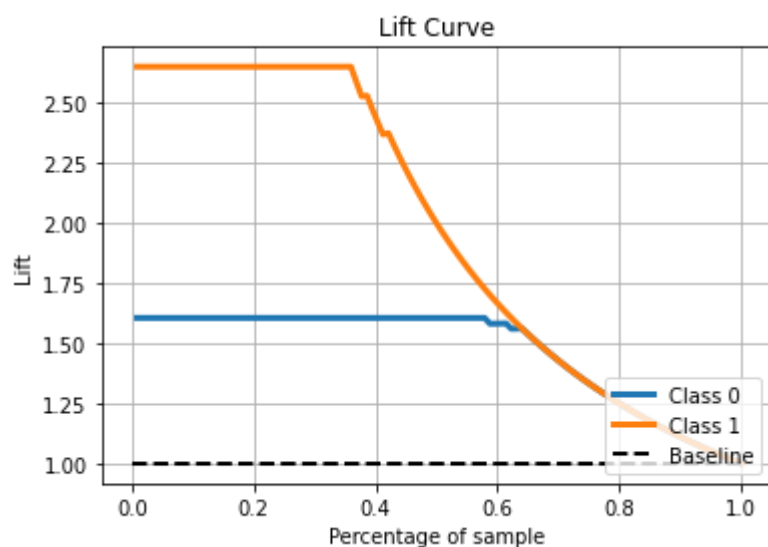
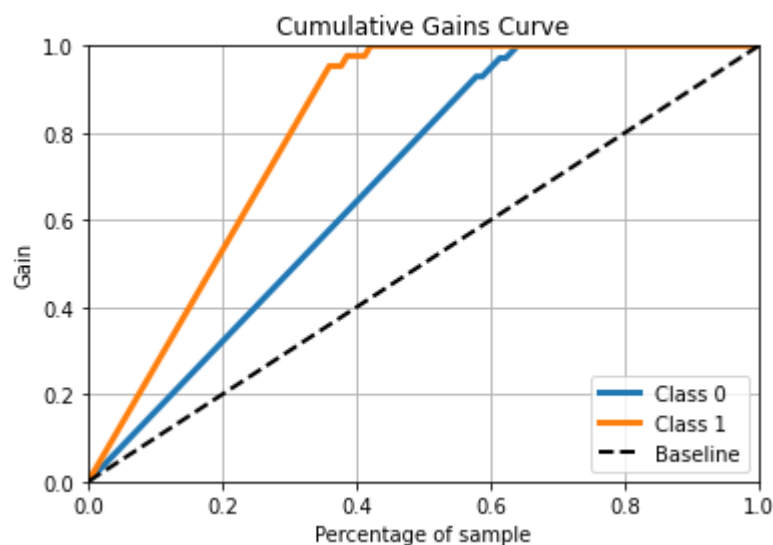
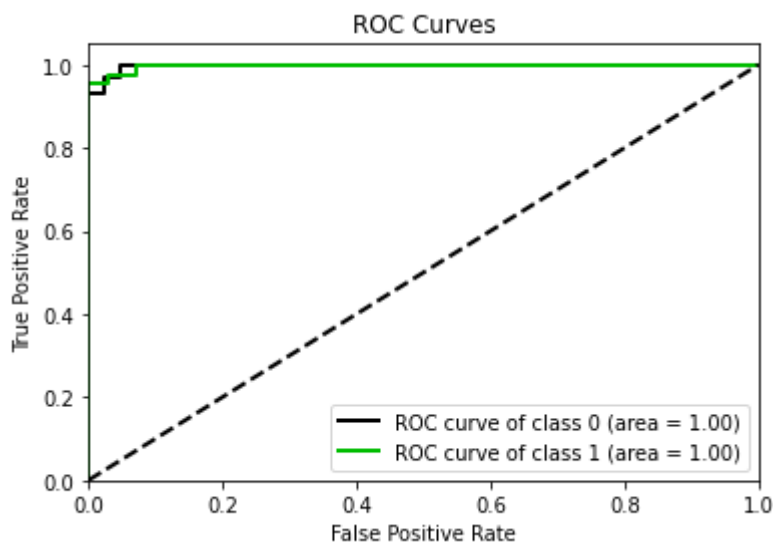
```
from sklearn.metrics import plot_roc_curve
print("The AUC score is ", roc_auc_score(y_test, clf_svc.predict(X_test)))
plot_roc_curve(clf_svc, X_test, y_test)
plt.show()
```

The AUC score is 0.9767441860465116



In [34]:

```
import scikitplot as skplt
skplt.metrics.plot_roc(y_test, clf_svc.predict_proba(X_test), plot_micro=False, plot_macro=False)
skplt.metrics.plot_cumulative_gain(y_test, clf_svc.predict_proba(X_test))
skplt.metrics.plot_lift_curve(y_test, clf_svc.predict_proba(X_test))
plt.show()
```



In [35]:

```
roc_auc_score(y_test, clf_svc.predict(X_test))
```

Out[35]:

0.9767441860465116

Interpreting ROC Curve and Lift Curve

ROC Curve - From the ROC Curve, we obtained area under the curve value of 0.9767 which measures the probability that a randomly chosen malignant instance will have a higher predicted probability of being malignant by the model than a randomly chosen benign instance.

Lift Curve - The lift ratio indicates how better the model performs compared to a random guess. For Malignant classification (Class 1), at 30% of sample, the lift ratio is approximately 2.65 meaning that model's top 30% predictions are 2.65X as good at predicting the outcome than as random guess. For Benign classification (Class 0), at 30% of sample, the lift ratio is approximately 1.60 meaning that model's top 30% predictions are 1.60X as good at predicting the outcome than as random guess.

Conclusion:

It has been observed from the above analysis that best model performance depends on performance evaluation metric and changing the evaluation metric also changes the best model choice. Both recall and f_score have been used separately as performance metrics to get model choice for each of the evaluation metrics and nested cross validation was leveraged for model selection. The findings are summarized below:

Recall as the performance Metric:

- Logistic Regression performs the best out of all 4 models with the below results:

	precision	recall	f1-score	support
0	0.97	0.99	0.98	71
1	0.98	0.95	0.96	43

F_score as the performance Metric:

- SVC performs the best out of all 4 models with the below results:

	precision	recall	f1-score	support
0	0.97	1.00	0.99	71
1	1.00	0.95	0.98	43

In []: