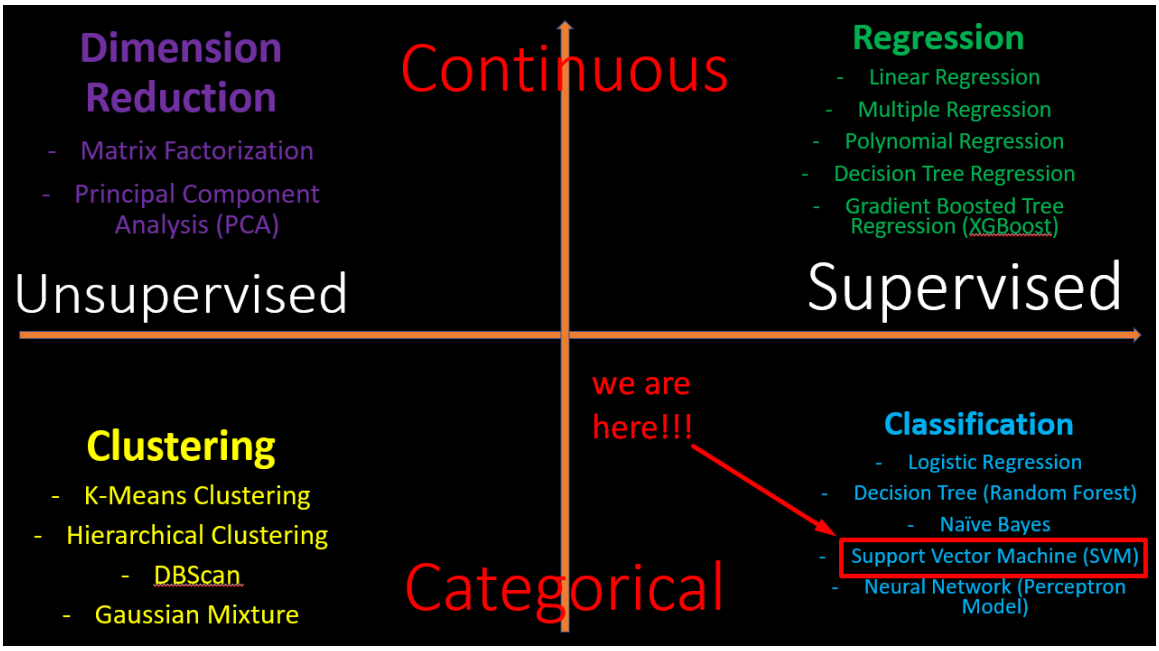
GRID, RANDOM AND BAYES SEARCH

HYPERPARAMETER TUNING ON SVM WITH PYTHON

DR. ALVIN ANG

CONTENTS



This manuscript is the Third Part.

First part is https://www.alvinang.sg/s/Understanding-SVM-with-Python-by-Dr-Alvin-Ang.pdf

The second part is https://www.alvinang.sg/s/Simple-SVM-Applied-to-Iris-Dataset-with-Python-by-Dr-Alvin-Ang.pdf

References

https://towardsdatascience.com/a-practical-introduction-to-grid-search-random-search-and-bayes-search-d5580b1d941d

https://medium.com/grabngoinfo/support-vector-machine-svm-hyperparameter-tuning-in-python-a65586289bcb

II. IMPORT DATA + TRAIN TEST SPLIT

A. IMPORT DATA

1. Import Data

```
import pandas as pd
from sklearn.datasets import load_breast_cancer

cancer = load_breast_cancer()
```

```
df_X = pd.DataFrame(cancer['data'], columns=cancer['feature_names'])
df_X.head()
```

	mean radius	mean texture	mean perimeter	mean area	mean smoothness	mean compactness	mean concavity	mean concave points	mean symmetry	mean fractal dimension	...	worst radius	worst texture	worst perimeter	worst area	worst smoothness	worst compactness	worst concavity	worst concave points	worst symmetry	worst fractal dimension
0	17.99	10.38	122.80	1001.0	0.11840	0.27760	0.3001	0.14710	0.2419	0.07871	...	25.38	17.33	184.60	2019.0	0.1622	0.6656	0.7119	0.2654	0.4601	0.1189
1	20.57	17.77	132.90	1326.0	0.08474	0.07864	0.0869	0.07017	0.1812	0.05667	...	24.99	23.41	158.80	1956.0	0.1238	0.1866	0.2416	0.1860	0.2750	0.0890
2	19.69	21.25	130.00	1203.0	0.10960	0.15990	0.1974	0.12790	0.2069	0.05999	...	23.57	25.53	152.50	1709.0	0.1444	0.4245	0.4504	0.2430	0.3613	0.0875
3	11.42	20.38	77.58	386.1	0.14250	0.28390	0.2414	0.10520	0.2597	0.09744	...	14.91	26.50	98.87	567.7	0.2098	0.8663	0.6869	0.2575	0.6638	0.1730
4	20.29	14.34	135.10	1297.0	0.10030	0.13280	0.1980	0.10430	0.1809	0.05883	...	22.54	16.67	152.20	1575.0	0.1374	0.2050	0.4000	0.1625	0.2364	0.0767

5 rows × 30 columns

```
df_y = pd.DataFrame(cancer['target'], columns=['Cancer'])
df_y.head()
```

	Cancer
0	0
1	0
2	0
3	0
4	0

B. TRAIN TEST SPLIT

2. Train Test Split

```
# Train test split
from sklearn.model_selection import train_test_split
import numpy as np

X_train, X_test, y_train, y_test = train_test_split(df_X, np.ravel(df_y), test_size=0.3)
```

C. IMPORT ML MODEL – SVC

3. Import ML Model - SVC

```
[ ] from sklearn.svm import SVC
```

```
svc = SVC()
params = svc.get_params()
params_df = pd.DataFrame(params, index = [0])
params_df.T
```

	0
C	1.0
break_ties	False
cache_size	200
class_weight	None
coef0	0.0
decision_function_shape	ovr
degree	3
gamma	scale
kernel	rbf
max_iter	-1
probability	False
random_state	None
shrinking	True
tol	0.001
verbose	False

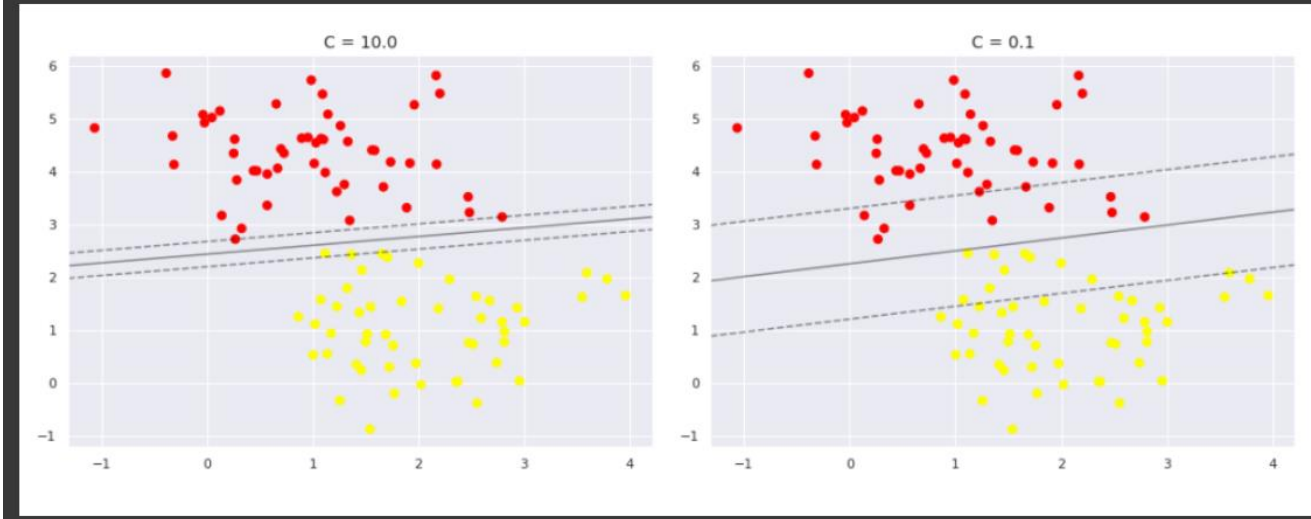
D. UNDERSTANDING C

https://medium.com/all-things-ai/in-depth-parameter-tuning-for-svc-758215394769#:~:text=gamma,.fit(X%2C%20y)

1. FOR LINEAR KERNEL

3a) Understanding C

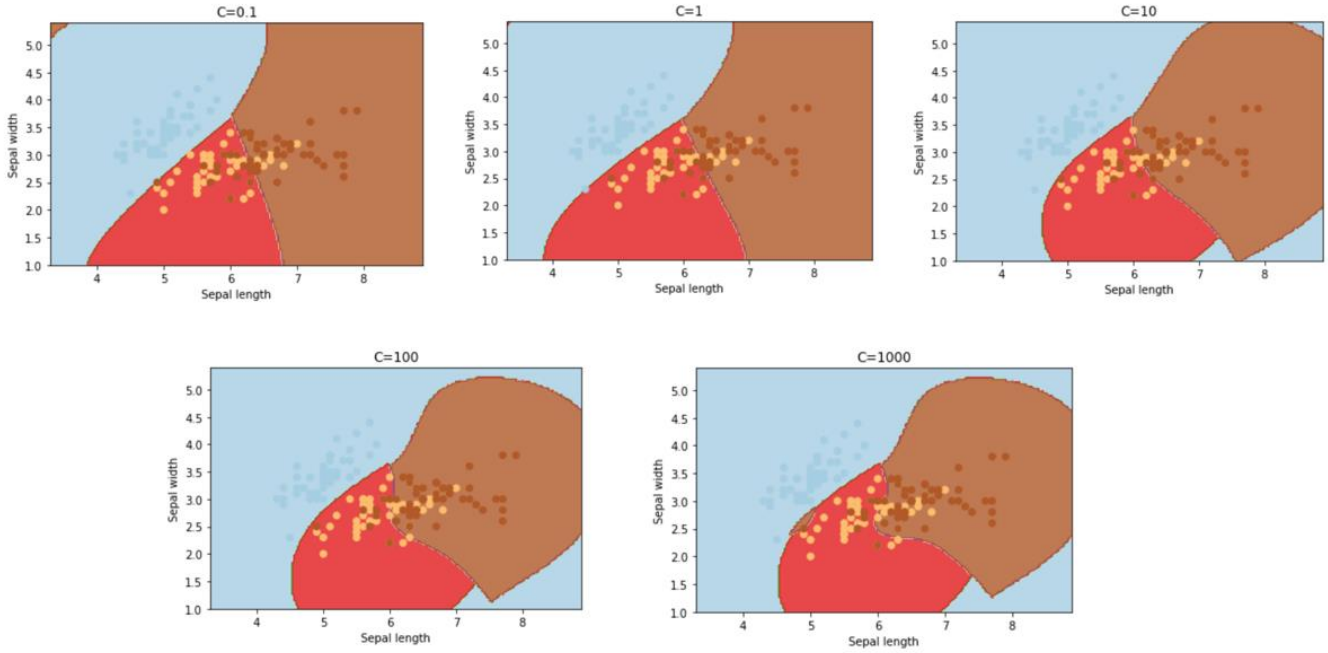
For Linear Kernel




```
#For very large  C , the margin is hard, and points cannot lie in it.
#For smaller  C , the margin is softer, and can grow to encompass some points.
```

2. FOR RBF (NON LINEAR) KERNEL

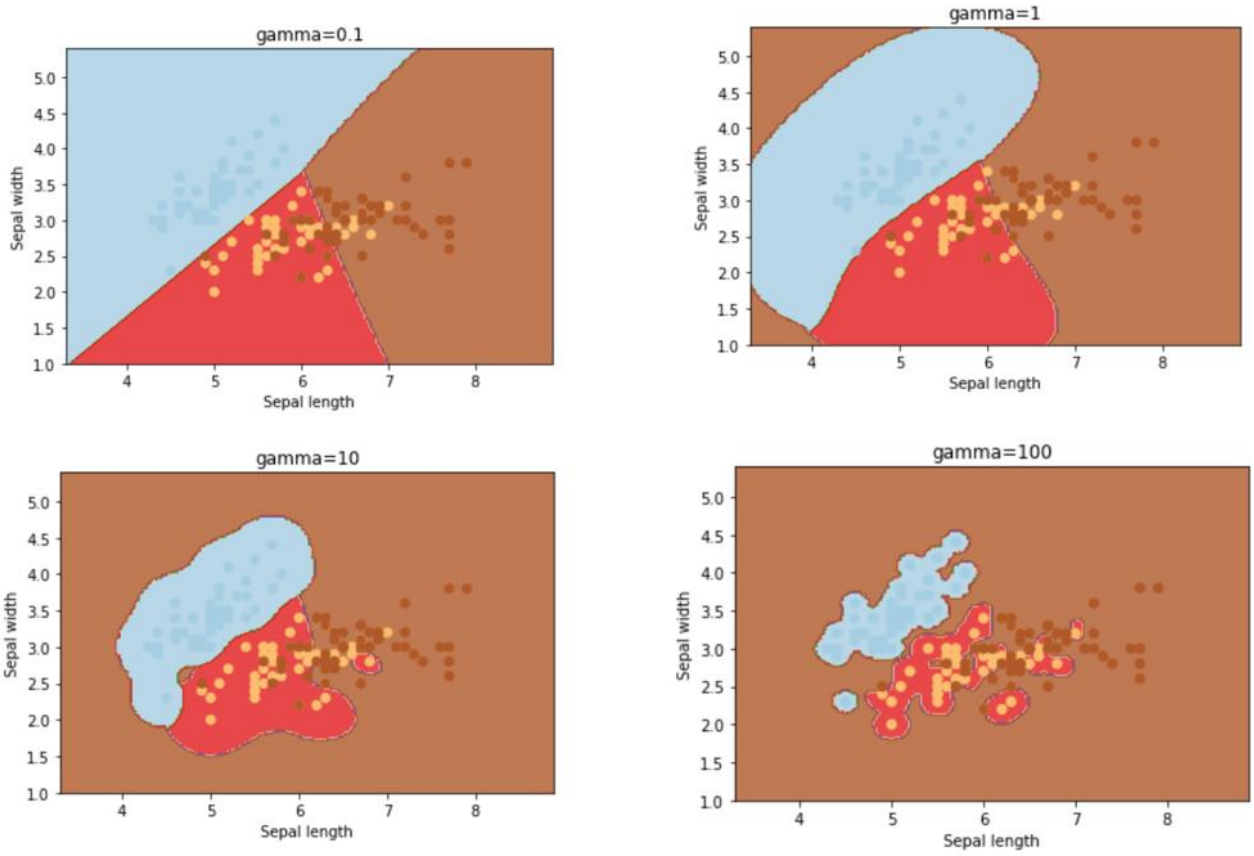
For RBF Kernel




```
#As C increases above, you notice the brown area shrinking
#You also notice that the brown area is trying to get more and more stringent
#Its trying to include browns (strictly) and trying to exclude the yellow

# C is the strength of the regularization (the penalty term)
#It controls the trade off between smooth decision boundary
#and classifying the training points correctly.

#In other words, increasing C means increasing the Penalty by making
#the model very stringent on the boundaries.

#However, increasing C values may lead to overfitting the training data.
```

E. UNDERSTANDING GAMMA

3b) Understanding Gamma



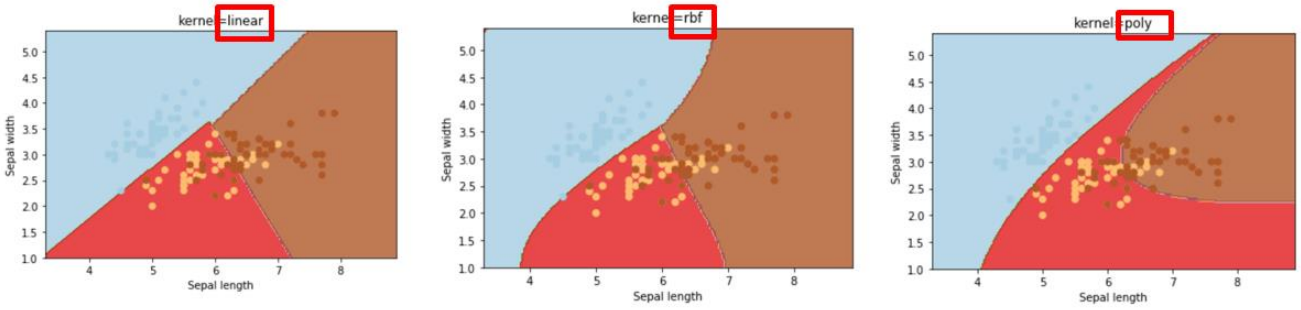
```
#Gamma is a parameter for non linear hyperplanes.
#The higher the gamma value it tries to exactly fit the training data set
#We can see that increasing gamma leads to overfitting
#as the classifier tries to perfectly fit the training data

#Gamma controls the width of the kernel.

#Gamma = {‘scale’, ‘auto’} or float, default=’scale’
#Gamma is the Kernel coefficient for ‘rbf’, ‘poly’ and ‘sigmoid’.

#if gamma='scale' (default) is passed then it uses 1 / (n_features * X.var())
#as value of gamma,

#if ‘auto’, uses 1 / n_features.
```

F. UNDERSTANDING KERNEL

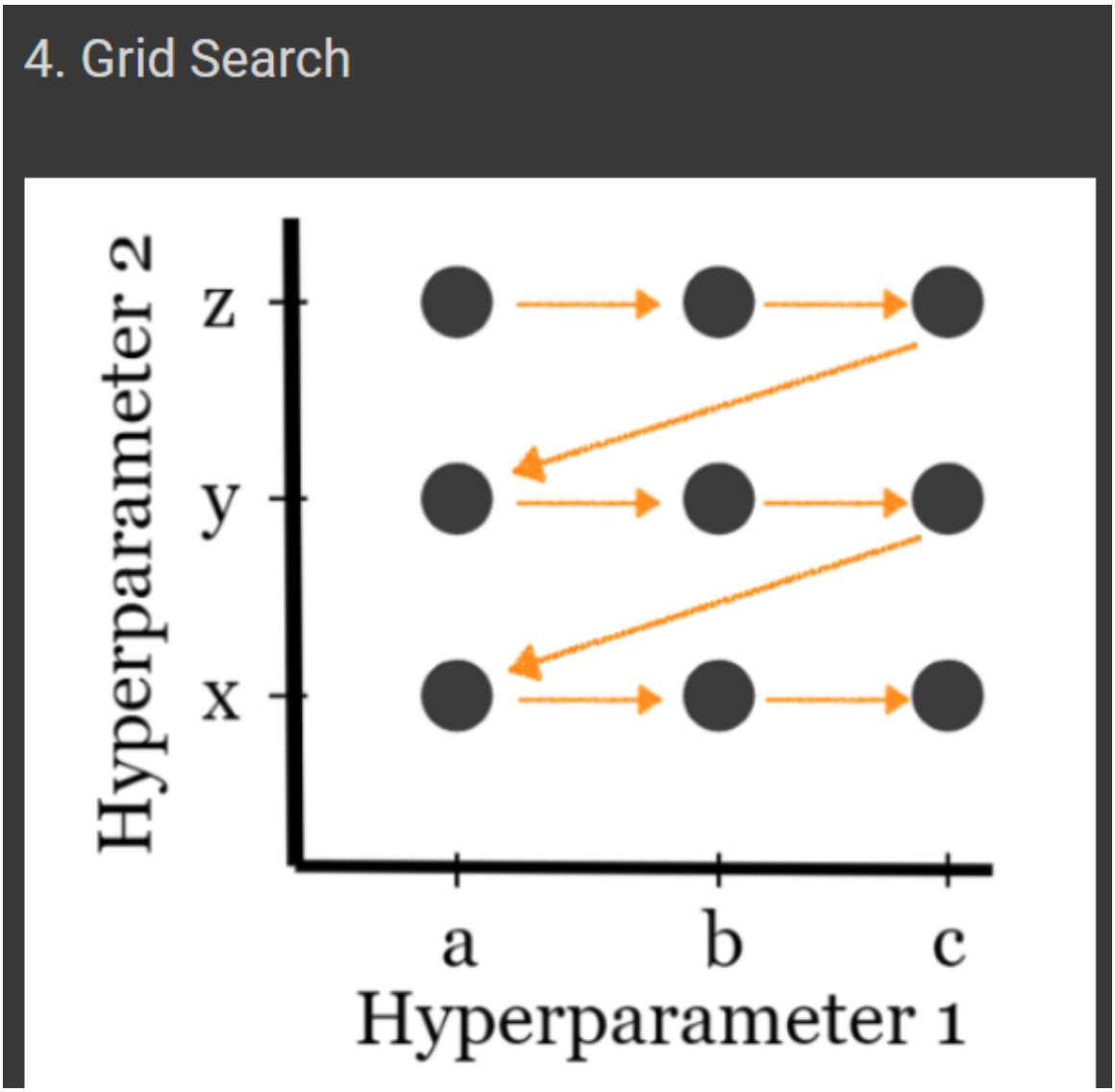
3c) Understanding Kernel

https://www.alvinang.sg/s/Understanding-SVM-with-Python-by-Dr-Alvin-Ang.pdf

https://www.alvinang.sg/s/Understanding-SVM-with-Python-by-Dr-Alvin-Ang.pdf




```
#Default kernel = 'rbf'
# SVC uses radial basis function(RBF) kernel by default (also known as the Gaussian kernel).
#this parameter selects the type of hyperplane used to separate the data.

#Using ‘linear’ will use a linear hyperplane (a line in the case of 2D data).
#‘rbf’ and ‘poly’ uses a non linear hyper-plane
```



A. DEFINING THE PARAMETER GRID

4a) Defining the Parameter Grid

```
[ ] #defining the Parameter Grid
    #basically defining the values of C and gamma

    param_grid = {
        'C': [0.1, 1, 10, 100, 1000],
        'gamma': [1, 0.1, 0.01, 0.001, 0.0001]
    }
```

B. IMPORTING GRIDSEARCHCV

4b) Importing GridSearchCV

```
from sklearn.model_selection import GridSearchCV
from sklearn.svm import SVC

grid = GridSearchCV(
    SVC(),
    param_grid,
    refit=True,
    verbose=3
)
```

C. DEFAULT VALUES FOR GRIDSEARCH

4c) Default Values for GridSearch

```
#Default Values

#GridSearchCV(
            #estimator, = the ML model chosen = here is SVC()
            #param_grid, = the search space = your predefined C and gamma

            #scoring=None, = used to measure the model's performance.
            #For classification, we generally use 'accuracy' or 'roc_auc'.
            #For regression, 'r2' or 'neg_mean_squared_error' is preferred.
            #default here = none

            #fit_params=None, (ignore)
```

```
            #n_jobs=1, = number of parallel jobs to run when executing grid search
            #If your computer processor has many cores,
            #set a higher value for this.
            #The -1 value uses all available cores.
            #This will speed up the execution process.

            #iid=True, = If True,
            #the data is assumed to be identically distributed across the folds

            #refit=True, = refits the the best estimator (SVC)
            #across the whole dataset
            #If "False", it is impossible to make predictions
            #using this GridSearchCV instance after fitting.

            #cv=None, = number of folds for cross-validation.
            #The standard numbers are 5, 10.
            #If 5, then each hyperparameter combination is repeated 5 times.

            #verbose=0, = the higher, the more messages...
            # we will try this out later to see the effect....

            #pre_dispatch='2*n_jobs', (ignore)
            #error_score='raise') (ignore)
```

D. TRAINING THE GRID SEARCH

4d) Training the Grid Search

```
[13] grid.fit(X_train,y_train)

     #if verbose is set to =0, you won't see any messages appear below
     #if verbose is set to >0, lots of messages will appear below
```

```
Fitting 5 folds for each of 25 candidates, totalling 125 fits
[CV 1/5] END .....................C=0.1, gamma=1;, score=0.637 total time=   0.0s
[CV 2/5] END .....................C=0.1, gamma=1;, score=0.637 total time=   0.0s
[CV 3/5] END .....................C=0.1, gamma=1;, score=0.637 total time=   0.0s
[CV 4/5] END .....................C=0.1, gamma=1;, score=0.646 total time=   0.0s
[CV 5/5] END .....................C=0.1, gamma=1;, score=0.646 total time=   0.0s
[CV 1/5] END ...................C=0.1, gamma=0.1;, score=0.637 total time=   0.0s
[CV 2/5] END ...................C=0.1, gamma=0.1;, score=0.637 total time=   0.0s
[CV 3/5] END ...................C=0.1, gamma=0.1;, score=0.637 total time=   0.0s
[CV 4/5] END ...................C=0.1, gamma=0.1;, score=0.646 total time=   0.0s
[CV 5/5] END ...................C=0.1, gamma=0.1;, score=0.646 total time=   0.0s
[CV 1/5] END ..................C=0.1, gamma=0.01;, score=0.637 total time=   0.0s
[CV 2/5] END ..................C=0.1, gamma=0.01;, score=0.637 total time=   0.0s
[CV 3/5] END ..................C=0.1, gamma=0.01;, score=0.637 total time=   0.0s
[CV 4/5] END ..................C=0.1, gamma=0.01;, score=0.646 total time=   0.0s
[CV 5/5] END ..................C=0.1, gamma=0.01;, score=0.646 total time=   0.0s
[CV 1/5] END .................C=0.1, gamma=0.001;, score=0.637 total time=   0.0s
[CV 2/5] END .................C=0.1, gamma=0.001;, score=0.637 total time=   0.0s
[CV 3/5] END .................C=0.1, gamma=0.001;, score=0.637 total time=   0.0s
[CV 4/5] END .................C=0.1, gamma=0.001;, score=0.646 total time=   0.0s
[CV 5/5] END .................C=0.1, gamma=0.001;, score=0.646 total time=   0.0s
[CV 1/5] END ................C=0.1, gamma=0.0001;, score=0.912 total time=   0.0s
[CV 2/5] END ................C=0.1, gamma=0.0001;, score=0.925 total time=   0.0s
[CV 3/5] END ................C=0.1, gamma=0.0001;, score=0.900 total time=   0.0s
```

E. DISPLAYING THE BEST OPTIMAL PARAMETERS FROM GRID SEARCH

4e) Displaying the BEST Optimal Parameters from GridSearch

```
[14] # Find the best parameter
     grid.best_params_
```

```
     {'C': 10, 'gamma': 0.0001}
```

```
[15] # Find the best estimator
     grid.best_estimator_
```

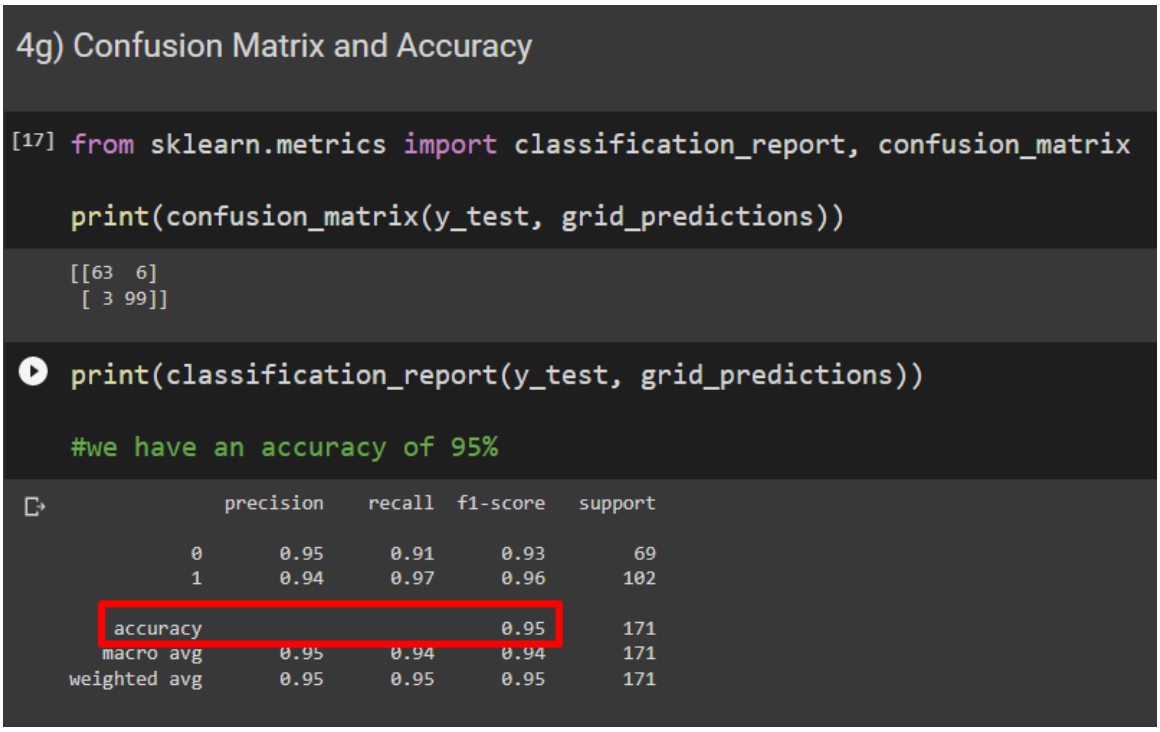
```
     SVC(C=10, gamma=0.0001)
```

F. USING GRIDSEARCH TO PREDICT X_TEST

4f) Using GridSearch to Predict X_test

```
[16] grid_predictions = grid.predict(X_test)

    #grid_predictions are exactly the same as below:
    #-----------------------------------------------------------

    #from sklearn import svm
    #from sklearn.svm import SVC

    #svc = svm.SVC(C = 1, gamma = 0.0001).fit(X_train,y_train)
    #y_pred = svc.predict(X_test)
    #-----------------------------------------------------------

    #both yield the same results

    #in other words, whether you use "grid.predict()"
    #or "svc.predict()" .... is the same....
    #but "grid.predict()" simply uses back the best optimal parameters
    #(C = 1, gamma = 0.0001), you don't have to specify them

    #like as in svm.SVC(C=1, gamma=0.0001) you need to specify....
```

G. CONFUSION MATRIX AND ACCURACY



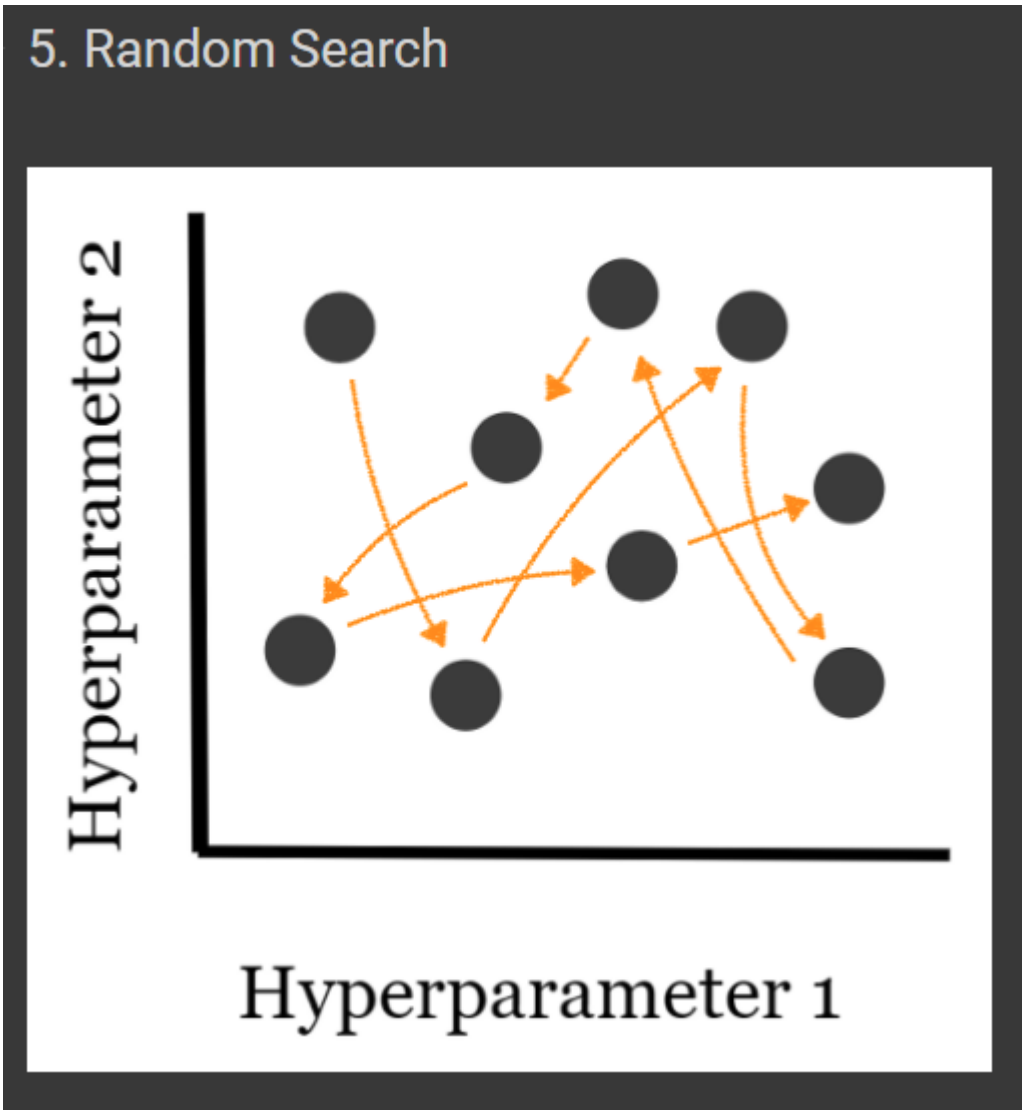
4g) Confusion Matrix and Accuracy

```
[17] from sklearn.metrics import classification_report, confusion_matrix

     print(confusion_matrix(y_test, grid_predictions))
```

```
[[63  6]
 [ 3 99]]
```

```
print(classification_report(y_test, grid_predictions))

#we have an accuracy of 95%
```

```
              precision    recall  f1-score   support

           0       0.95      0.91      0.93        69
           1       0.94      0.97      0.96       102

    accuracy                           0.95       171
   macro avg       0.95      0.94      0.94       171
weighted avg       0.95      0.95      0.95       171
```



- Grid Search tries all combinations of hyperparameters
- hence increasing the time complexity of the computation and could result in an unfeasible computing cost.
- But Random Search tests only combinations preset by you.
- The selection of the hyperparameter values is completely random.

A. DEFINING THE PARAMETER DISTRIBUTIONS

5a) Defining the Parameter Distributions

```
[19] import scipy.stats as stats
     from sklearn.utils.fixes import loguniform

     # Specify parameters and distributions to sample from
     param_dist = {
       'C': stats.uniform(0.1, 1e4),
       'gamma': loguniform(1e-6, 1e+1),
     }
```

B. IMPORTING RANDOMIZED SEARCH CV

5b) Importing RandomizedSearchCV

```
[20] from sklearn.model_selection import RandomizedSearchCV

     n_iter_search = 20

     random_search = RandomizedSearchCV(
         SVC(),
         param_distributions=param_dist,
         n_iter=n_iter_search,
         refit=True,
         verbose=3
     )
```

C. UNDERSTANDING "N_ITER_SEARCH"

5c) Understanding "n_iter_search"

```
[21] #n_iter – Number of hyperparameter combinations to be selected randomly.
     #Random search does NOT check ALL hyperparameter combinations defined in the search space.
     #It considers only a random sample of combinations.

     #Here, n_iter=20 means that it tasks a random sample of
     #size 20 which contain 20 different hyperparameter combinations.
```

D. TRAINING THE RANDOMIZED SEARCH

5d) Training the Randomized Search

```
[22] random_search.fit(X_train, y_train)
```

```
Fitting 5 folds for each of 20 candidates, totalling 100 fits
[CV 1/5] END C=5950.995199765279, gamma=0.06566997154871626;, score=0.637 total time=   0.0s
[CV 2/5] END C=5950.995199765279, gamma=0.06566997154871626;, score=0.637 total time=   0.0s
[CV 3/5] END C=5950.995199765279, gamma=0.06566997154871626;, score=0.637 total time=   0.0s
[CV 4/5] END C=5950.995199765279, gamma=0.06566997154871626;, score=0.646 total time=   0.0s
[CV 5/5] END C=5950.995199765279, gamma=0.06566997154871626;, score=0.646 total time=   0.0s
[CV 1/5] END C=8902.96022978013, gamma=5.478682989333769e-06;, score=0.938 total time=   0.0s
[CV 2/5] END C=8902.96022978013, gamma=5.478682989333769e-06;, score=0.938 total time=   0.0s
[CV 3/5] END C=8902.96022978013, gamma=5.478682989333769e-06;, score=0.938 total time=   0.0s
[CV 4/5] END C=8902.96022978013, gamma=5.478682989333769e-06;, score=0.937 total time=   0.0s
[CV 5/5] END C=8902.96022978013, gamma=5.478682989333769e-06;, score=0.987 total time=   0.0s
[CV 1/5] END C=2055.2077071588164, gamma=0.4242392383012549;, score=0.637 total time=   0.0s
[CV 2/5] END C=2055.2077071588164, gamma=0.4242392383012549;, score=0.637 total time=   0.0s
[CV 3/5] END C=2055.2077071588164, gamma=0.4242392383012549;, score=0.637 total time=   0.0s
```

E. DISPLAYING THE BEST OPTIMAL PARAMETERS FROM RANDOMIZED SEARCH

```
5e) Displaying the BEST Optimal Parameters from Randomized Search

[23] random_search.best_params_

     {'C': 8902.96022978013, 'gamma': 5.478682989333769e-06}

[24] random_search.best_estimator_

     SVC(C=8902.96022978013, gamma=5.478682989333769e-06)
```

F. USING RANDOMIZED SEARCH TO PREDICT X_TEST

```
5f) Using Randomized Search to Predict X_test

[25] # Run prediction using the best estimator
     random_predictions = random_search.predict(X_test)
```

G. CONFUSION MATRIX AND ACCURACY

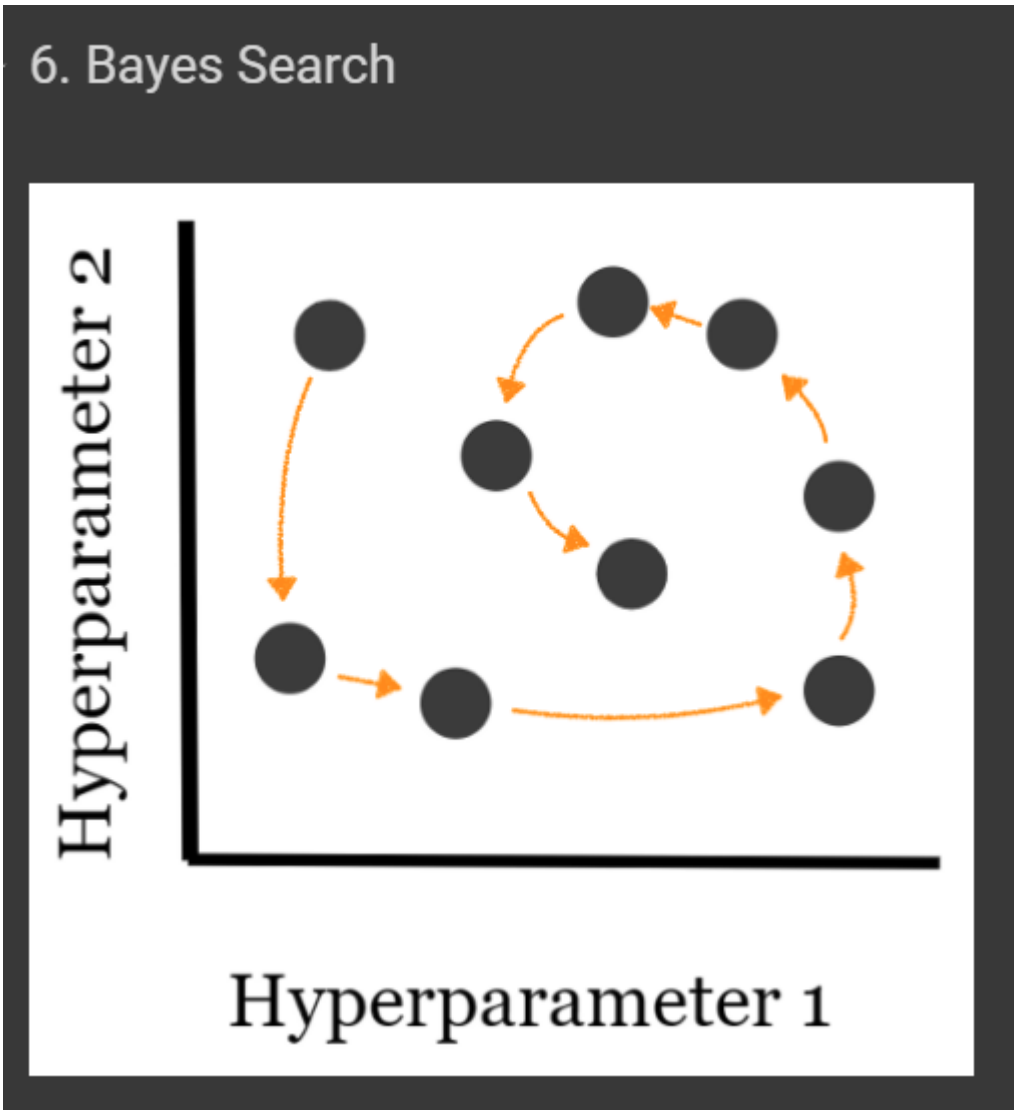
5g) Confusion Matrix and Accuracy

```
[26] from sklearn.metrics import classification_report, confusion_matrix

     print(confusion_matrix(y_test, random_predictions))
```

```
[[64  5]
 [ 5 97]]
```

```
print(classification_report(y_test, random_predictions))

#we have an accuracy of 94%
```

```
              precision    recall  f1-score   support

           0       0.93      0.93      0.93        69
           1       0.95      0.95      0.95       102

    accuracy                           0.94       171
   macro avg       0.94      0.94      0.94       171
weighted avg       0.94      0.94      0.94       171
```



- Bayes Search uses the Bayesian optimization technique to model the search space to arrive at optimized parameter values as soon as possible.
- It uses the structure of search space to optimize the search time.
- Bayes Search approach uses the past evaluation results to sample new candidates that are most likely to give better results (shown in the figure below).

```
[28] pip install scikit_optimize

Looking in indexes: https://pypi.org/simple, https://us-python.pkg.dev/colab-wheels/public/simple/
Collecting scikit_optimize
  Downloading scikit_optimize-0.9.0-py2.py3-none-any.whl (100 kB)
     |████████████████████████████████| 100 kB 3.3 MB/s
Requirement already satisfied: scikit-learn>=0.20.0 in /usr/local/lib/python3.7/dist-packages (from scikit_optimize) (1.0.2)
Collecting pyaml>=16.9
  Downloading pyaml-21.10.1-py2.py3-none-any.whl (24 kB)
Requirement already satisfied: joblib>=0.11 in /usr/local/lib/python3.7/dist-packages (from scikit_optimize) (1.1.0)
Requirement already satisfied: numpy>=1.13.3 in /usr/local/lib/python3.7/dist-packages (from scikit_optimize) (1.21.6)
Requirement already satisfied: scipy>=0.19.1 in /usr/local/lib/python3.7/dist-packages (from scikit_optimize) (1.7.3)
Requirement already satisfied: PyYAML in /usr/local/lib/python3.7/dist-packages (from pyaml>=16.9->scikit_optimize) (6.0)
Requirement already satisfied: threadpoolctl>=2.0.0 in /usr/local/lib/python3.7/dist-packages (from scikit-learn>=0.20.0->scikit_optimize) (3.1.0)
```

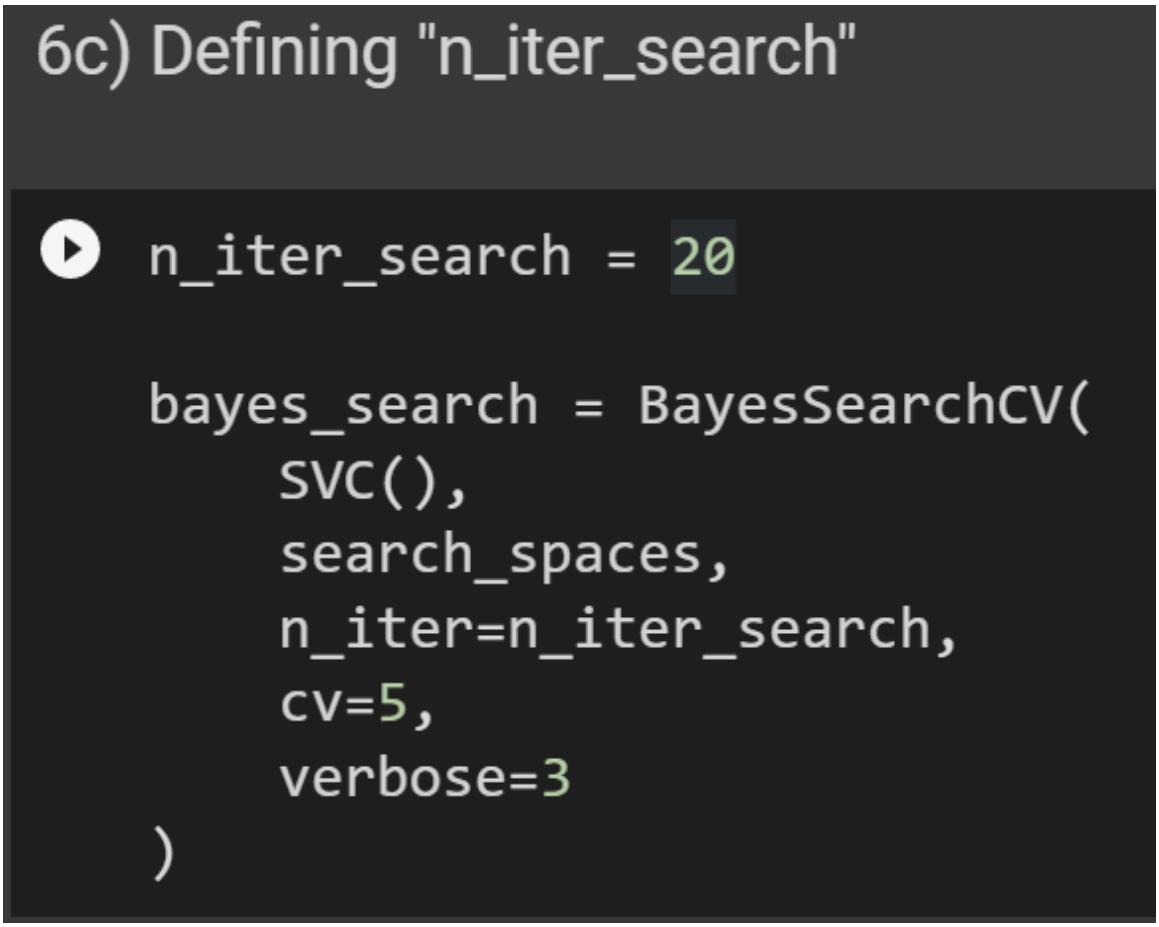
A. IMPORTING BAYES SEARCH CV

```
6a) Importing Bayes Search CV

0s
from skopt import BayesSearchCV
# parameter ranges are specified by one of below
from skopt.space import Real, Categorical, Integer
```

B. DEFINING THE SEARCH SPACE

```
6b) Defining the Search Space

search_spaces = {
    'C': Real(0.1, 1e+4),
    'gamma': Real(1e-6, 1e+1, 'log-uniform'),
}
```

C. DEFINING "N_ITER_SEARCH"



D. TRAINING THE BAYES SEARCH

```
6d) Training the Bayes Search

[32] bayes_search.fit(X_train, y_train)

     Fitting 5 folds for each of 1 candidates, totalling 5 fits
     [CV 1/5] END C=9868.145949252299, gamma=0.017924236378480632;, score=0.637 total time=   0.0s
     [CV 2/5] END C=9868.145949252299, gamma=0.017924236378480632;, score=0.637 total time=   0.0s
     [CV 3/5] END C=9868.145949252299, gamma=0.017924236378480632;, score=0.637 total time=   0.0s
     [CV 4/5] END C=9868.145949252299, gamma=0.017924236378480632;, score=0.646 total time=   0.0s
     [CV 5/5] END C=9868.145949252299, gamma=0.017924236378480632;, score=0.646 total time=   0.0s
     Fitting 5 folds for each of 1 candidates, totalling 5 fits
     [CV 1/5] END C=1024.706571755016, gamma=3.1841789671432383e-06;, score=0.963 total time=   0.0s
     [CV 2/5] END C=1024.706571755016, gamma=3.1841789671432383e-06;, score=0.950 total time=   0.0s
     [CV 3/5] END C=1024.706571755016, gamma=3.1841789671432383e-06;, score=0.938 total time=   0.0s
     [CV 4/5] END C=1024.706571755016, gamma=3.1841789671432383e-06;, score=0.924 total time=   0.0s
     [CV 5/5] END C=1024.706571755016, gamma=3.1841789671432383e-06;, score=0.975 total time=   0.0s
     Fitting 5 folds for each of 1 candidates, totalling 5 fits
     [CV 1/5] END C=9715.273733663513, gamma=0.0022159372686204907;, score=0.900 total time=   0.0s
```

E. DISPLAYING THE BEST OPTIMAL PARAMETERS FROM BAYES SEARCH

```
6e) Displaying the BEST Optimal Parameters from Bayes Search

[33] bayes_search.best_params_

     OrderedDict([('C', 10000.0), ('gamma', 1e-06)])

[34] bayes_search.best_estimator_

     SVC(C=10000.0, gamma=1e-06)
```

F. USING BAYES SEARCH TO PREDICT X_TEST

```
6f) Using Bayes Search to Predict X_test

[35] bayes_predictions = bayes_search.predict(X_test)
```

G. CONFUSION MATRIX AND ACCURACY

6g) Confusion Matrix and Accuracy

```
[36] from sklearn.metrics import classification_report,confusion_matrix

     print(confusion_matrix(y_test, bayes_predictions))
```

```
[[65  4]
 [ 3 99]]
```

```
[37] print(classification_report(y_test, bayes_predictions))

     #accuracy of 96%!
```

```
              precision    recall  f1-score   support

           0       0.96      0.94      0.95        69
           1       0.96      0.97      0.97       102

    accuracy                           0.96       171
   macro avg       0.96      0.96      0.96       171
weighted avg       0.96      0.96      0.96       171
```

ABOUT DR. ALVIN ANG

Dr. Alvin Ang earned his Ph.D., Masters and Bachelor degrees from NTU, Singapore. He is a scientist, entrepreneur, as well as a personal/business advisor. More about him at www.AlvinAng.sg.