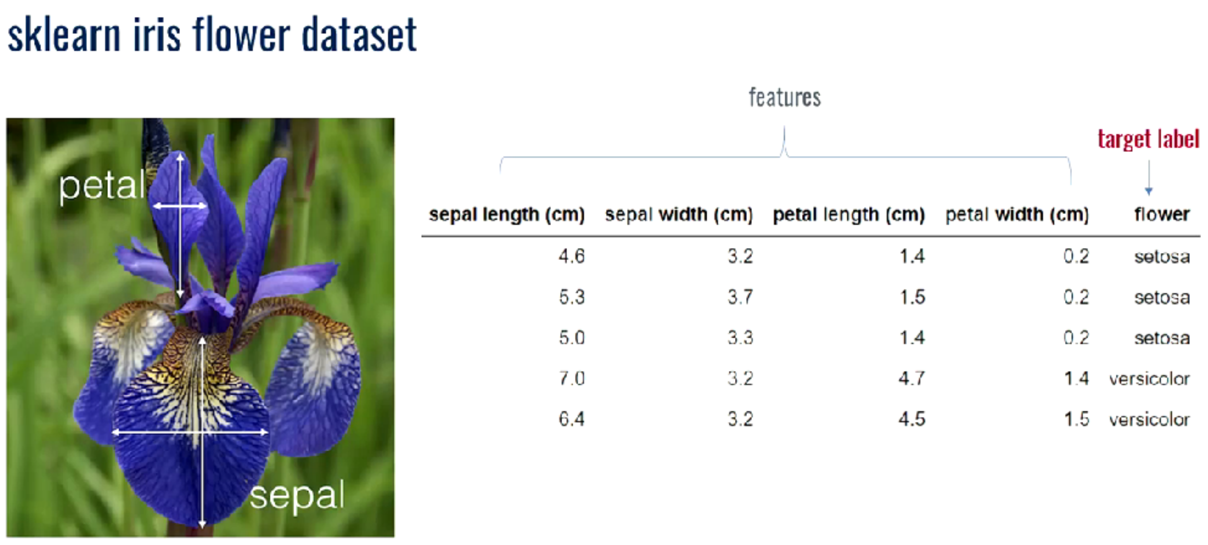
Finding best model and hyper parameter tunning using GridSearchCV

In this tutorial we learn how to choose the best model for machine learning problem and how to do a hyperperameter tuning.

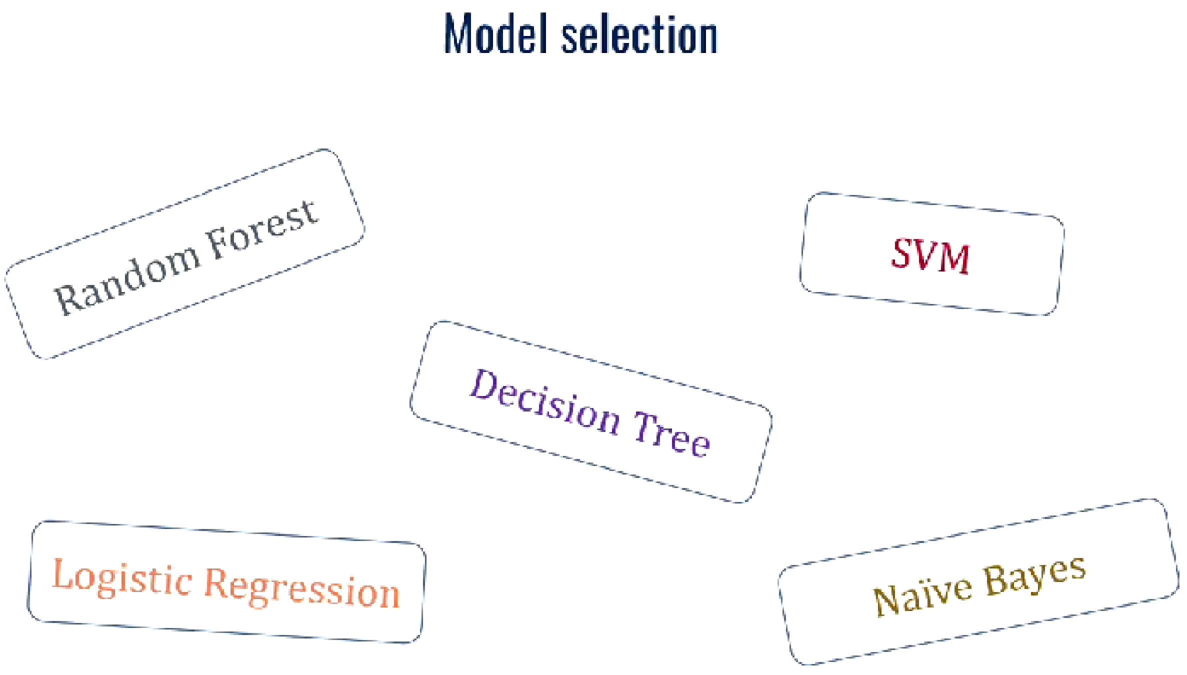
For iris flower dataset in sklearn library, we are going to find out best model and best hyper parameters using GridSearchCV


sklearn iris flower dataset

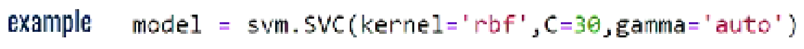
petal
sepal
features
target label

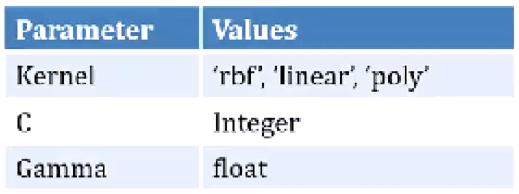
sepal length (cm)	sepal width (cm)	petal length (cm)	petal width (cm)	flower
4.6	3.2	1.4	0.2	setosa
5.3	3.7	1.5	0.2	setosa
5.0	3.3	1.4	0.2	setosa
7.0	3.2	4.7	1.4	versicolor
6.4	3.2	4.5	1.5	versicolor

Which Model Should I choose?



After choosing the model now you have hyperparameters to choose?!? (e.g. SVM: Kernel, C, Gamma)


example
```
model = svm.SVC(kernel='rbf',C=30,gamma='auto')
```



Parameter	Values
Kernel	'rbf', 'linear', 'poly'
C	Integer
Gamma	float

The process of choosing the optimal parameter is called Hyperparameter Tunning.

Load iris flower dataset

In [1]:
```
from sklearn import svm, datasets
iris = datasets.load_iris()
```

In [2]:
```
import pandas as pd
df = pd.DataFrame(iris.data,columns=iris.feature_names)
df['flower'] = iris.target
df['flower'] = df['flower'].apply(lambda x: iris.target_names[x])
df[47:150]
```

Out[2]:

	sepal length (cm)	sepal width (cm)	petal length (cm)	petal width (cm)	flower
47	4.6	3.2	1.4	0.2	setosa
48	5.3	3.7	1.5	0.2	setosa
49	5.0	3.3	1.4	0.2	setosa
50	7.0	3.2	4.7	1.4	versicolor
51	6.4	3.2	4.5	1.5	versicolor
...	...	...	...	...	...
145	6.7	3.0	5.2	2.3	virginica
146	6.3	2.5	5.0	1.9	virginica
147	6.5	3.0	5.2	2.0	virginica
148	6.2	3.4	5.4	2.3	virginica
149	5.9	3.0	5.1	1.8	virginica

103 rows × 5 columns

Approach 1: Use train_test_split and manually tune parameters by trial and error

```
In [3]: from sklearn.model_selection import train_test_split
        X_train, X_test, y_train, y_test = train_test_split(iris.data, iris.target, test_
```

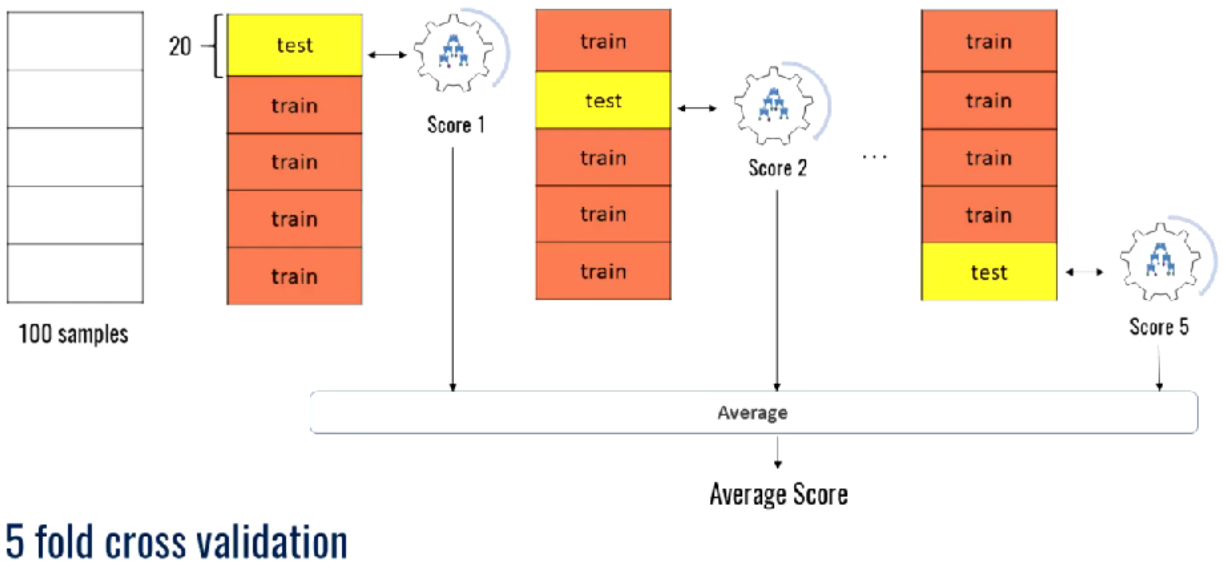
```
In [4]: model = svm.SVC(kernel='rbf',C=30,gamma='auto')
        model.fit(X_train,y_train)
        model.score(X_test, y_test)

Out[4]: 0.9777777777777777
```

The problem with this method is that by doing it again the score is changing.

Approach 2: Use K Fold Cross validation

In K Fold Cross Validation, we divide datasamples into n number of folds(here n=5). Then we take 5 iterations and in each iteration 1 Fold is test set and the other 4 is training test, we find a score in that iteration and make an average for scores.



Manually try suppling models with different parameters to cross_val_score function with 5 fold cross validation

```
In [6]: from sklearn.model_selection import cross_val_score
        cross_val_score(svm.SVC(kernel='linear',C=10,gamma='auto'),iris.data, iris.target

Out[6]: array([1.        , 1.        , 0.9       , 0.96666667, 1.        ])
```

```
In [7]: cross_val_score(svm.SVC(kernel='rbf',C=10,gamma='auto'),iris.data, iris.target, c

Out[7]: array([0.96666667, 1.        , 0.96666667, 0.96666667, 1.        ])
```

In [8]:
```
cross_val_score(svm.SVC(kernel='rbf',C=20,gamma='auto'),iris.data, iris.target, c
```

Out[8]:
```
array([0.96666667, 1.        , 0.9       , 0.96666667, 1.        ])
```

Above approach is tiresome and very manual. We can use for loop as an alternative

In [10]:
```
import numpy as np
kernels = ['rbf', 'linear']
C = [1,10,20]
avg_scores = {}
for kval in kernels:
    for cval in C:
        cv_scores = cross_val_score(svm.SVC(kernel=kval,C=cval,gamma='auto'),iris
        avg_scores[kval + '_' + str(cval)] = np.average(cv_scores)

avg_scores
```

Out[10]:
```
{'rbf_1': 0.9800000000000001,
 'rbf_10': 0.9800000000000001,
 'rbf_20': 0.9666666666666668,
 'linear_1': 0.9800000000000001,
 'linear_10': 0.9733333333333334,
 'linear_20': 0.9666666666666666}
```

From above results we can say that rbf with C=1 or 10 or linear with C=1 will give best performance. So this way I can find the optimal score.

But this approcah has some issues, because if I have 4 parameters then I have to run 4 for loops then it will be too iterations and it is not convinient.

Approach 3: Use GridSearchCV

GridSearchCV does exactly same thing as for loop above but in a single line of code

```
In [11]: from sklearn.model_selection import GridSearchCV
         clf = GridSearchCV(svm.SVC(gamma='auto'), {
             'C': [1,10,20],
             'kernel': ['rbf','linear']
         }, cv=5, return_train_score=False)
         clf.fit(iris.data, iris.target)
         clf.cv_results_
```

```
Out[11]: {'mean_fit_time': array([0.00100017, 0.00140014, 0.0012001 , 0.0006    , 0.0010
         0017,
                 0.00080004]),
          'std_fit_time': array([1.50789149e-07, 1.35650829e-03, 7.48353720e-04, 4.89901
         382e-04,
                 1.50789149e-07, 4.00018706e-04]),
          'mean_score_time': array([0.        , 0.00039997, 0.00040002, 0.00040007, 0.00
         019999,
                 0.00020003]),
          'std_score_time': array([0.        , 0.00048986, 0.00048992, 0.00048998, 0.000
         39997,
                 0.00040007]),
          'param_C': masked_array(data=[1, 1, 10, 10, 20, 20],
                       mask=[False, False, False, False, False, False],
                 fill_value='?',
                      dtype=object),
          'param_kernel': masked_array(data=['rbf', 'linear', 'rbf', 'linear', 'rbf', 'l
         inear'],
                       mask=[False, False, False, False, False, False],
                 fill_value='?',
                      dtype=object),
          'params': [{'C': 1, 'kernel': 'rbf'},
           {'C': 1, 'kernel': 'linear'},
           {'C': 10, 'kernel': 'rbf'},
           {'C': 10, 'kernel': 'linear'},
           {'C': 20, 'kernel': 'rbf'},
           {'C': 20, 'kernel': 'linear'}],
          'split0_test_score': array([0.96666667, 0.96666667, 0.96666667, 1.        , 0.
         96666667,
                 1.        ]),
          'split1_test_score': array([1., 1., 1., 1., 1., 1.]),
          'split2_test_score': array([0.96666667, 0.96666667, 0.96666667, 0.9       , 0.
         9        ,
                 0.9       ]),
          'split3_test_score': array([0.96666667, 0.96666667, 0.96666667, 0.96666667, 0.
         96666667,
                 0.93333333]),
          'split4_test_score': array([1., 1., 1., 1., 1., 1.]),
          'mean_test_score': array([0.98      , 0.98      , 0.98      , 0.97333333, 0.96
         666667,
                 0.96666667]),
          'std_test_score': array([0.01632993, 0.01632993, 0.01632993, 0.03887301, 0.036
         51484,
                 0.0421637 ]),
          'rank_test_score': array([1, 1, 1, 4, 5, 6])}
```

CV results are not easy to view, but sklearn provides a way to download these results into a

dataframe.

In [12]:

```
df = pd.DataFrame(clf.cv_results_)
df
```

Out[12]:

	mean_fit_time	std_fit_time	mean_score_time	std_score_time	param_C	param_kernel	params
0	0.0010	1.507891e-07	0.0000	0.00000	1	rbf	{'C': 1, 'kernel': 'rbf'}
1	0.0014	1.356508e-03	0.0004	0.00049	1	linear	{'C': 1, 'kernel': 'linear'}
2	0.0012	7.483537e-04	0.0004	0.00049	10	rbf	{'C': 10, 'kernel': 'rbf'}
3	0.0006	4.899014e-04	0.0004	0.00049	10	linear	{'C': 10, 'kernel': 'linear'}
4	0.0010	1.507891e-07	0.0002	0.00040	20	rbf	{'C': 20, 'kernel': 'rbf'}
5	0.0008	4.000187e-04	0.0002	0.00040	20	linear	{'C': 20, 'kernel': 'linear'}

In [13]:

```
df[['param_C','param_kernel','mean_test_score']]
```

Out[13]:

	param_C	param_kernel	mean_test_score
0	1	rbf	0.980000
1	1	linear	0.980000
2	10	rbf	0.980000
3	10	linear	0.973333
4	20	rbf	0.966667
5	20	linear	0.966667

In [14]:
```
dir(clf)
```
```
 '__le__',
 '__lt__',
 '__module__',
 '__ne__',
 '__new__',
 '__reduce__',
 '__reduce_ex__',
 '__repr__',
 '__setattr__',
 '__setstate__',
 '__sizeof__',
 '__str__',
 '__subclasshook__',
 '__weakref__',
 '_abc_impl',
 '_check_is_fitted',
 '_check_n_features',
 '_estimator_type',
 '_format_results',
 '_get_param_names',
```

In [15]:
```
clf.best_params_
```
Out[15]:
```
{'C': 1, 'kernel': 'rbf'}
```

In [16]:
```
clf.best_score_
```
Out[16]:
```
0.9800000000000001
```

One issue that can happen with GraiSearchCV is the computation cost. Our dataset is very limited in this tutorial but imagine a big dataset for parameters you have so many values. Right now C values are 1,10,20; what if I want to try a range like 1 to 50, the cost will go really high.

To tackle this priblem use RandomizedSearchCV to reduce number of iterations and with random combination of parameters. It helps reduce the cost of computation.

In [17]:
```
from sklearn.model_selection import RandomizedSearchCV
rs = RandomizedSearchCV(svm.SVC(gamma='auto'), {
        'C': [1,10,20],
        'kernel': ['rbf','linear']
    },
    cv=5,
    return_train_score=False,
    n_iter=2
)
rs.fit(iris.data, iris.target)
pd.DataFrame(rs.cv_results_)[['param_C','param_kernel','mean_test_score']]
```

Out[17]:

	param_C	param_kernel	mean_test_score
0	10	linear	0.973333
1	1	rbf	0.980000

This works well in practical life, because if you don't have too much comutation power and you want to try random values of parameters.

Choose a best model:

In [18]:
```
from sklearn import svm
from sklearn.ensemble import RandomForestClassifier
from sklearn.linear_model import LogisticRegression
```

In [19]:
```
model_params = {
    'svm': {
        'model': svm.SVC(gamma='auto'),
        'params' : {
            'C': [1,10,20],
            'kernel': ['rbf','linear']
        }
    },
    'random_forest': {
        'model': RandomForestClassifier(),
        'params' : {
            'n_estimators': [1,5,10]
        }
    },
    'logistic_regression' : {
        'model': LogisticRegression(solver='liblinear',multi_class='auto'),
        'params': {
            'C': [1,5,10]
        }
    }
}
```

In [20]:
```
scores = []

for model_name, mp in model_params.items():
    clf =  GridSearchCV(mp['model'], mp['params'], cv=5, return_train_score=False
    clf.fit(iris.data, iris.target)
    scores.append({
        'model': model_name,
        'best_score': clf.best_score_,
        'best_params': clf.best_params_
    })

df = pd.DataFrame(scores,columns=['model','best_score','best_params'])
df
```

Out[20]:

	model	best_score	best_params
0	svm	0.980000	{'C': 1, 'kernel': 'rbf'}
1	random_forest	0.966667	{'n_estimators': 10}
2	logistic_regression	0.966667	{'C': 5}

Based on above, I can conclude that SVM with C=1 and kernel='rbf' is the best model for solving my problem of iris flower classification.

Date	Author
2021-10-15	**Ehsan Zia**