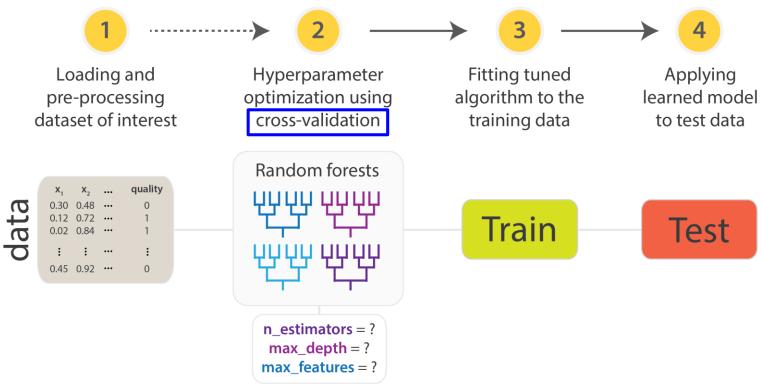
4. Cross Validation

KUBIG 학술부



Hyperparameter tuning



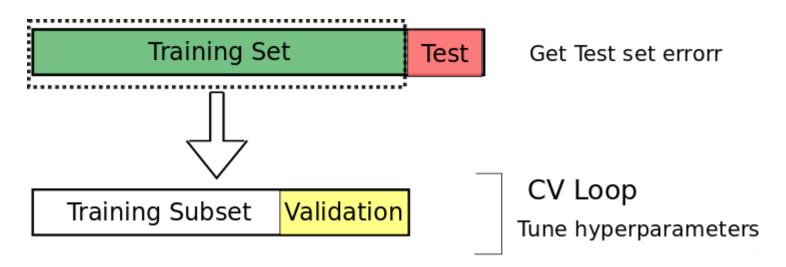


Index

- 1. Hold-out Cross Validation
- 2. LOOCV (leave-one-out-cross-validation)
- 3. K-fold Cross Validation
- 4. Nested Cross Validation



1. Hold-out Cross Validation



- 0. 데이터를 Training set과 Test set으로 나눈다.
- 1. Training set을 다시 Training Subset과 Validation set으로 <u>한번</u> 나눈다.
- 2. Training Subset으로 학습한 모델이 Validation set에서 가장 좋은 성능을 내는 hyperparameter를 선택

```
import pandas as pd
import numpy as np
from sklearn.datasets import load_iris
from sklearn.model_selection import train_test_split,ShuffleSplit,GridSearchCV
from sklearn.tree import DecisionTreeClassifier
from sklearn.metrics import accuracy_score
```

```
In [13]:
      rsf=rs.split(train set X,train set y)
      for iteration, data in enumerate(rsf, start=1):
           print('\n{} {:^61}'.format('Iteration', 'Training subset observations'))
           print('\n{:^9} {}'.format(iteration, data[0]))
           print('\n{:^61}'.format('Validation set observations'))
           print('\n{:^9}'.format(str(data[1])))
                       Training subset observations
                                                              Iris data에는 150개의 관측치가 있다.
      Iteration
                    92 61 111 22 116 79 66 23 13
                               38 91 72 51 55 24 81 41 40 \longrightarrow 150*0.8*0.8=967#
                    16 60 29 90
          9 103 83 99 11 30 26 47 94 57 56 65 2 15 21 37 108
       62 118 80 78 10 8 50 5 4 28 104 14 98 117 42 74 67 54
       48 52 110 82 75 891
                                                              150*0.8*0.2=24개
                 Validation set observations
      [ 25 68 101 44 105 64 100 119 93 85 6 73 27 97 32 20 71 88
                                                              150-(96+24)=150*0.2=30, Test data
       63 3 114 36 70 76]
```



```
In [2]:
     iris=load iris()
     train_set_X, test_set_X,train_set_y, test_set_y=train_test_split(iris.data,
                                                                        iris.target,
                         전체 data를 Training set과 Test set으로 분리
                                                                       test size=0.2,
                                                                       random_state=1
     model=DecisionTreeClassifier()
     param={
                                          Tuning할 hyperparameter
         'max_depth':[1,2,3],
         'min_samples_leaf':[2,3]
     Training set을 training subset과 validation set으로 분리해줄 CV splitter
     rs=ShuffleSplit(n splits=1,test size=0.2)
     Dtr=GridSearchCV(cv=rs,estimator=model,param_grid=param,scoring='accuracy')
     Dtr.fit(train set X,train set y)
     print('Model performance : ',
           accuracy score(test set y, Dtr.predict(test set X)))
     Model performance: 0.8666666666666667
```

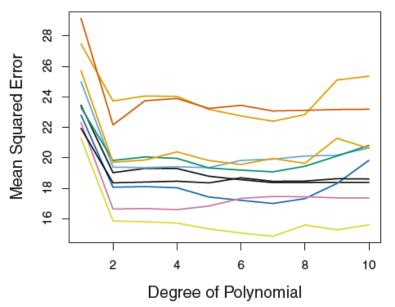


```
iris=load iris()
model=DecisionTreeClassifier()
param={
    'max depth':[1.2.3].
    'min samples leaf':[2,3]
for i in range(10):
    train set X, test set X,train set y, test set y=train test split(iris.data
                                                                  iris.target,
                                                                 test size=0.2)
    rs=ShuffleSplit(n splits=1,test size=0.2)
    Dtr=GridSearchCV(cv=rs,estimator=model,param grid=param,scoring='accuracy'
    Dtr.fit(train_set_X,train_set_y)
    print('Model performance : ',
      accuracy score(test set v, Dtr.predict(test set X)),
      'Best parameter : '.
       Dtr.best params )
Model performance: 0.8866868668668667 Best parameter: {'max_depth': 2, 'min_samples_leaf': 2}
Model performance : 0.9333333333333333 Best parameter : {'max_depth': 3, 'min_samples_leaf': 2}
Model performance: 0.9 Best parameter: {'max_depth': 2, 'min_samples_leaf': 2}
Model performance: 0.9868868868686867 Best parameter: {'max_depth': 3, 'min_samples_leaf': 3}
Model performance: 1.0 Best parameter: {'max_depth': 3. 'min_samples_leaf': 3}
Model performance: 0.93333333333333333 Best parameter: {'max depth': 2, 'min samples leaf': 2}
```



```
In [17]:
     iris=load iris()
     model=DecisionTreeClassifier()
     param={
          'max depth':[1,2,3],
          'min samples leaf':[2,3]
     for i in range(10):
          train_set_X, test_set_X,train_set_y, test_set_y=train test split(iris.data
                                                                         iris.target,
                                                                        test size=0.2)
          rs=ShuffleSplit(n splits=1,test size=0.2)
          Dtr=GridSearchCV(cv=rs,estimator=model,param grid=param,scoring='accuracy'
          Dtr.fit(train_set_X,train_set_y)
                                             Random한 split이 어떻게 이뤄지느냐에 따라 추정값이 크게 달라짐.
          print('Model performance : ',
            accuracy score(test set y, Dtr.predict(test set X)),
                                                   0.866666666666667 Best parameter : {'max_depth': 2, 'min_samples_leaf': 2}
            'Best parameter :
                               Model performance:
                                                   0.933333333333333 Best parameter : {'max depth': 3, 'min samples leaf': 2}
                               Model performance:
             Dtr.best params
                               Model performance: 0.9 Best parameter: {'max depth': 2. 'min samples leaf': 2}
                                                   0.93333333333333333 Best parameter : {'max depth': 2. 'min samples leaf': 2}
                               Model performance:
     Model performance:
                                                   0.93333333333333 Best parameter : {'max depth': 2, 'min samples leaf': 2}
     Model performance : 0.9 Best parameter
                                                   0.966666666666667 Best parameter : {'max depth': 2, 'min samples leaf': 2}
                               Model performance:
                                                   0.966666666666667 Best parameter : {'max depth': 3, 'min samples leaf': 3}
                               Model performance:
         performance : 0.9868668666666667 Be
         Model performance:
                                                   1.0 Best parameter : {'max_depth': 3, 'min_samples_leaf': 3}
     Model performance : 1.0 Best parameter
                               Model performance:
                                                   0.93333333333333 Best parameter : {'max depth': 2, 'min samples leaf': 2}
         performance : 0,9333333333333333 Bes
     Model performance : 0.933333333333333
                               Model performance:
                                                   0.93333333333333 Best parameter : {'max depth': 2, 'min samples leaf': 2}
```

Hold-out Cross Validation의 단점



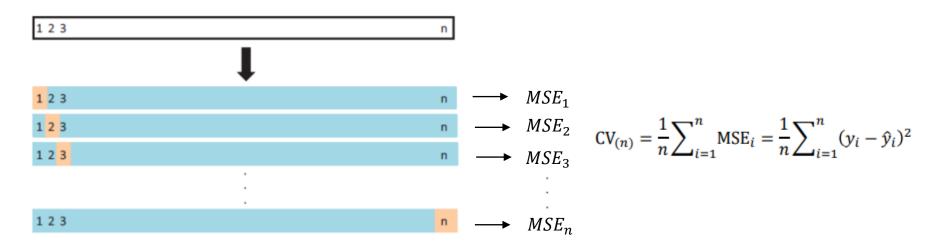
'Auto' dataset으로 Hold-out Cross Validation을 반복적으로 적용해 봄

동일한 데이터로 10번 해본 결과 매번 결과가 다름을 알 수 있음.

Split에 randomness가 있고 random한 split을 한번만 하기 때문

출처 : An introduction to statistical learning with Applications in R

2. LOOCV(leave-one-out-cross validation)



- 1. 관측치가 n개인 training set을 관측치가 1개인 validation set과 관측치가 (n-1)개인 training subset으로 나눈다.
- 2. 각각의 관측치들이 한번씩 validation set이 되도록 1번 과정을 n번 반복하며 metric을 구한다.
- 3. 이 n개 metric의 평균을 기준으로 가장 좋은 성능을 보여주는 hyper parameter를 선택한다.

```
import pandas as pd
 import numpy as np
 from sklearn.datasets import load iris
from sklearn.model_selection import train_test_split,LeaveOneOut,GridSearchCV
 from sklearn.tree import DecisionTreeClassifier
from sklearn.metrics import accuracy score
loof=loo.split(train set X,train set y)
for iteration, data in enumerate(loof, start=1):
    print('\n{} {:^61}'.format('Iteration', 'Training subset observations'))
    print('\n{:^9} {}'.format(iteration, data[0]))
    print('\n{:^70}'.format('Validation set observations'))
    print('\n{:^70}'.format(str(data[1])))
                                                             Iris data에는 150개의 관측치가 있다.
Iteration
                Training subset observations
                                                           ➡ (150*0.8)-1=119개
 55 56 57 58 59 60 61 62 63 64 65 66 67
 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88
 91 92 93 94 95 96 97 98 99 100 101 102 103 104 105 106 107 108
109 110 111 112 113 114 115 116 117 118 119]
             Validation set observations
                                                             150-119-1=150*0.2=30,
                                                                                         Test data
```

```
Iteration
                          Training subset observations
                                                10 11 12 13 14
                                                                   15
                          25
                              26
                                                  31
                                  45
                                          47
                                                       50
                          61
                              62
                                  63
                                      64 65
                                              66
                                                  67
                                                      68 69
                                  81
                                      82
                                          83
                                                  85
                                  99 100 101 102 103 104 105 106 107 108
 109 110 111 112 113 114 115 116 117 118 119]
                     Validation set observations
                                                                                 Iteration
                                                                                                        Training subset observations
                                 [1]
Iteration
                          Training subset observations
                                                                                                                   99 100 101 102 103 104 105 106 107
                                                                                  108 109 110 111 112 113 114 115 116 117 118]
                      24
                          25
                              26
                                  27
                                      28
                                          29
                                               30
                                                   31
                                                                                                    Validation set observations
                                          47
                                                           51
                              62
                                  63
                                      64
                                          65
                                              66
                                                   67
                                                                                                              [119]
                              80
                                  81
                                      82 83
                                              84
                                                  85
                              98
                                  99 100 101 102 103 104 105 106 107 108
109 110 111 112 113 114 115 116 117 118 119]
                     Validation set observations
```

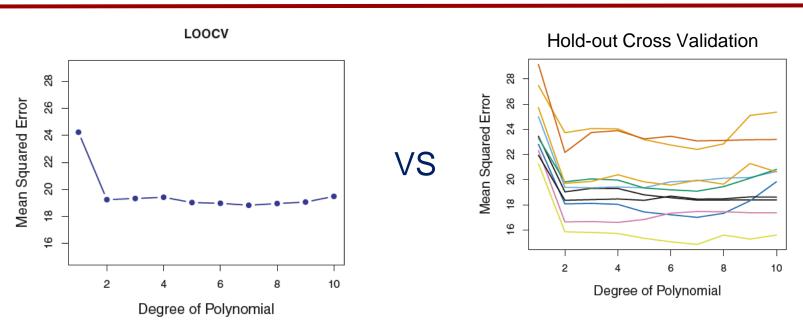


[2]

```
In [3]:
     iris=load_iris()
     train set X, test set X, train set y, test set y=train test split(iris.data,
                                                                       iris.target,
                           전체 data를 Training set과 Test set으로 분리
                                                                      test size=0.2,
                                                                      random state=4
     model=DecisionTreeClassifier()
     param={
                                           Tuning할 hyperparameter
         'max_depth':[1,2,3],
         'min samples leaf':[2,3]
        Training set을 training subset과 validation set으로 분리해줄 CV splitter
     loo=LeaveOneOut()
     Dtr=GridSearchCV(cv=loo,estimator=model,param_grid=param,scoring='accuracy')
     Dtr.fit(train set X,train set y)
     print('Model performance : ',
           accuracy score(test set y, Dtr.predict(test set X)))
```

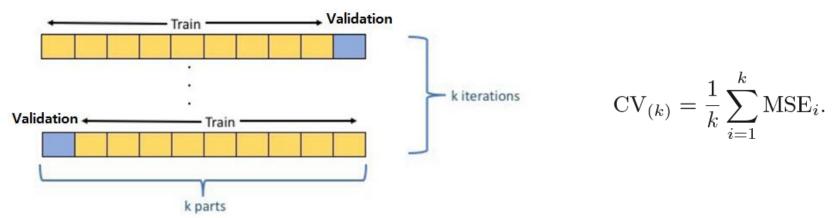


LOOCV의 장점



LOOCV는 Training set이 어떻게 Training subset과 validation set으로 나눠지는지에 randomness가 없음. 따라서, Training set이 동일하다면 항상 같은 결과를 반환함.

3. k-fold cross validation



- 1. Training set을 동일한 크기의 k개의 그룹으로 나눈다.
- 2. K개의 그룹 중 (k-1)개의 그룹에 해당하는 data들을 training subset으로 하고 나머지 1개의 그룹에 해당하는 data들을 validation set으로 한다.
- 3. 모든 그룹이 한번씩 validation set이 되도록 2번 과정을 k번 반복하며 K개의 metric을 구한 후 평균을 내서 가장 좋은 성능을 보여주는 hyperparameter를 선택한다.

```
from sklearn.datasets import load_iris
      from sklearn.tree import DecisionTreeClassifier
      from sklearn.model_selection import train_test_split, KFold, GridSearchCV
      from sklearn.metrics import accuracy_score
In [65]:
     kf = KFold(n splits=5, shuffle=False).split(train_set_X,train_set_y)
     for iteration, data in enumerate(kf, start=1):
          print('\n{} {:^61}'.format('Iteration', 'Training subset observations'))
          print('\n{:^9} {}'.format(iteration, data[0]))
          print('\n{:^61}'.format('Validation set observations'))
```

print('\n{:^9}'.format(str(data[1])))

print('\n{:^61}'.format("Test set observations"))



print('\n',np.arange(iris.data.shape[0]-test set X.shape[0],

iris.data.shape[0],1))

Iteration

Training subset observations

1 [24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95 96 97 98 99 100 101 102 103 104 105 106 107 108 109 110 111 112 113 114 115 116 117 118 119]

Validation set observations

[0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23]

Test set observations

[120 121 122 123 124 125 126 127 128 129 130 131 132 133 134 135 136 137 138 139 140 141 142 143 144 145 146 147 148 149]

Iteration

Training subset observations

2 [0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 1 18 19 20 21 22 23 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95 96 97 98 99 100 101 102 103 104 105 106 107 108 109 110 111 112 113 114 115 116 117 118 119]

Validation set observations

[24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47]

Test set observations

[120 121 122 123 124 125 126 127 128 129 130 131 132 133 134 135 136 137 138 139 140 141 142 143 144 145 146 147 148 149]

Iteration

Training subset observations

5 [0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95]

Validation set observations

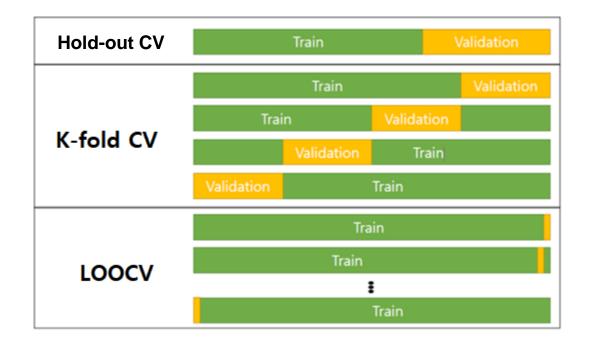
[96 97 98 99 100 101 102 103 104 105 106 107 108 109 110 111 112 113 114 115 116 117 118 119]

Test set observations

[120 121 122 123 124 125 126 127 128 129 130 131 132 133 134 135 136 137 138 139 140 141 142 143 144 145 146 147 148 149]



Hold-out CV, K-fold CV, LOOCV



Time series data를 위한 Cross Validation

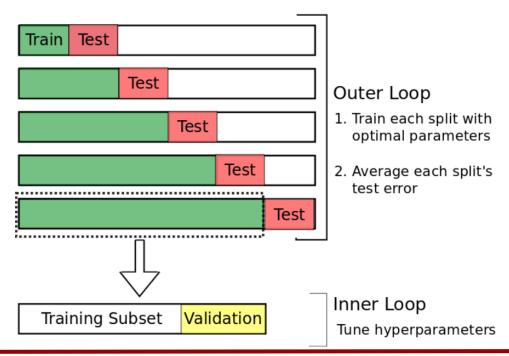
- 1. Temporal dependence
 - -시간 순서가 있는 time series data를 random하게 training subset, validation set으로 나눌 수 없다.
 - 어느 시점부터를 test data로 나눌지가 자의적임. Biased estimator가 될 가능성이 높음

- 2. 과거의 데이터를 이용해 미래를 예측해야 함.
 - 미래의 데이터로 과거의 데이터를 예측하는 상황을 원하지 않음.

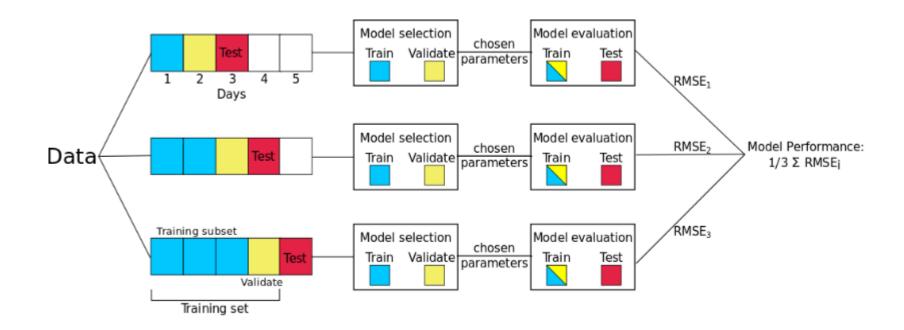
따라서, k-fold cross validation 사용이 곤란

4. Nested Cross Validation

Nested Cross-Validation



Day forward chaining



```
import pandas as pd
       import numpy as np
       from sklearn.model_selection import TimeSeriesSplit,GridSearchCV
       from sklearn.linear_model import ElasticNet
       from sklearn.metrics import mean absolute error
       df=pd.read csv("C:/Users/jjw11/Desktop/고려대학교/학회/data/Gemini ETHUSD d.csv'
       df.head()
Out[1]:
                                     Low Close Volume ETH Volume USD
       0 2019-09-14 ETHUSD 181.55 181.55 181.43 181.43
                                                    0.00
                                                              0.00
       1 2019-09-13 ETHUSD 180.88 181.80 177.70 181.55
                                                  4447.19
                                                          798113.88
       2 2019-09-12 ETHUSD 178.47 182.60 176.45 180.88
                                                  2749.15
                                                          491636.33
       3 2019-09-11 ETHUSD 179.61 182.70 173.70 178.47
                                                  12741.56
                                                         2270428.10
       4 2019-09-10 ETHUSD 181.04 184.35 176.68 179.61
                                                         1544625.31
                                                  8576.85
         df=df.drop(['Symbol'],axis=1)
         df=df.sort values(by='Date').set index('Date')
         df2=df.iloc[:100,:]
         df2.head()
  Out[2]:
                         Low Close Volume ETH Volume USD
             Date
         2016-05-09 12.00 12.00 9.36 9.98
                                      1317.90
                                              12885.06
         2016-05-10 9.98 9.98 9.36 9.68
                                       672.06
                                               6578.20
         2016-05-11 9.68 10.47 9.68 10.43
                                      3052.51
                                              30978.11
         2016-05-12 10.43 12.00 9.92 10.20
                                      2072.56
                                              22183.39
         2016-05-13 10.20 11.59 10.20 10.69
                                      1769.71
                                              18923.55
```



```
In [32]:
       model=ElasticNet()
       param={'alpha':np.arange(0.1,10,0.1)}
       tscv=TimeSeriesSplit(n_splits=95)
In [33]:
     mae=[]
     X=df2[['Open','High','Low','Volume ETH','Volume USD','Close']]
     X=X.iloc[:-1,]
     y=df2['Close'].shift(periods=-1)
     y=y.iloc[:-1,]
     Els=GridSearchCV(cv=tscv, estimator=model, param_grid=param,
                      scoring='neg mean absolute error')
     Els.fit(X,y)
     for train_index, Validation_index in tscv.split(df2):
         if Validation index==df2.shape[0]-2:
             break
         print("TRAIN subset:", train index, "\nValidation set:",
               Validation index,"\ntest set:", Validation index+1)
         X_test=X.iloc[Validation_index+1,:]
         y test=y.iloc[Validation index+1]
         mae.append(mean absolute error(y test,Els.predict(X test)))
     print(' Model performance : ',np.mean(mae))
```

```
TRAIN subset: [0 1 2 3 4 5]
               Validation set: [6]
               test set: [7]
               TRAIN subset: [0 1 2 3 4 5 6]
               Validation set: [7]
               test set: [8]
               TRAIN subset: [0 1 2 3 4 5 6 7]
               Validation set: [8]
               test set: [9]
                                 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71
72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95]
Validation set: [96]
                                 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47
48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71
72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95
```

TRAIN subset: [0 1 2 3 4]

Validation set: ([5])

: 0.6953183352916578

test set: (6)

test set: [97]

Validation 🕰

961

```
In [32]:
       model=ElasticNet()
       param={'alpha':np.arange(0.1,10,0.1)}
       tscv=TimeSeriesSplit(n_splits=95)
In [33]:
     mae=[]
     X=df2[['Open','High','Low','Volume ETH','Volume USD','Close']]
     X=X.iloc[:-1,]
     y=df2['Close'].shift(periods=-1)
     y=y.iloc[:-1,]
     Els=GridSearchCV(cv=tscv, estimator=model, param_grid=param,
                      scoring='neg mean absolute error')
     Els.fit(X,y)
                      Inner Loop??
     for train_index, Validation_index in tscv.split(df2):
         if Validation index==df2.shape[0]-2:
             break
         print("TRAIN subset:", train index, "\nValidation set:",
               Validation index,"\ntest set:", Validation index+1)
         X_test=X.iloc[Validation_index+1,:]
         y test=y.iloc[Validation index+1]
         mae.append(mean absolute error(y test,Els.predict(X test)))
     print(' Model performance : ',np.mean(mae))
```

```
test set: (6)
               TRAIN subset: [0 1 2 3 4 5]
               Validation set: [6]
               test set: [7]
               TRAIN subset: [0 1 2 3 4 5 6]
               Validation set: [7]
               test set: [8]
               TRAIN subset: [0 1 2 3 4 5 6 7]
               Validation set: [8]
               test set: [9]
                                 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71
72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95]
Validation set: [96]
                                 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47
48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71
72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95
```

TRAIN subset: [0 1 2 3 4]

Validation set: ([5])

: 0.6953183352916578

test set: [97]

Validation 🕰

961

```
model=ElasticNet()
 tscv=TimeSeriesSplit(n splits=95)
model performance mae=[]
for train_index, Validation_index in tscv.split(df2):
   if Validation index==df2.shape[0]-2:
        break
   mae=[]
   model_set={}
   print("TRAIN subset:", train index, "\nValidation set:", Validation index,
   df2 train, df2 validation,df2 test = df2.iloc[train index,:],df2.iloc[Vali
   X train=df2 train[['Open', 'High', 'Low', 'Volume ETH', 'Volume USD', 'Close']]
   X train=X train.iloc[:-1,]
   y train=df2 train['Close'].shift(periods=-1)
   y_train=y_train.iloc[:-1,]
   X validation=df2 validation[['Open', 'High', 'Low', 'Volume ETH', 'Volume USD'
   v validation=df2.iloc[Validation index+1,3]
   X_test=df2_test[['Open','High','Low','Volume ETH','Volume USD','Close']]
   y test=df2.iloc[Validation index+2,3]
   for i in np.arange(0.1,10,0.1):
       model set[round((i/0.1)-1)]=ElasticNet(alpha=i)
       mae.append(mean_absolute_error(y_validation,model_set[round((i/0.1)-1)
   idx least mae=np.argmin(np.array(mae))
   model to fit=model set[idx least mae]
   df2 final train=df2.iloc[:int(Validation index+1),:]
   X final train=df2 final train[['Open', 'High', 'Low', 'Volume ETH', 'Volume US
   X final train=X train.append(X validation)
   y final train=y train.append(y validation)
   model_to_fit.fit(X_final_train,y_final_train)
   model performance mae.append(mean absolute error(y test,
                                                     model to fit.predict(X te
print(' Model performance : ',np.mean(model performance mae))
```

Inner loop, hyperparameter tuning

```
TRAIN subset: [ O
                                    7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47
 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71
 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95]
Validation set: [96]
test set: [97]
TRAIN subset: [ 0
                                        8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47
 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71
 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95
 961
Validation set: [97]
test set: [98]
 Model performance: 1.064419068751438
                                                                                 KU-BIG
```

Thank you!

• Q&A Time!

