Model Selection

Importing Libraries

In [2]:
```
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
from scipy import stats
```

In [3]:
```
from sklearn.model_selection import train_test_split
from sklearn import neighbors
from sklearn.metrics import mean_squared_error
from math import sqrt
from sklearn.svm import SVR
from sklearn.multioutput import MultiOutputRegressor
```

In [4]:
```
from sklearn.linear_model import LinearRegression
from sklearn.ensemble import RandomForestRegressor
```

In [5]:
```
from sklearn.model_selection import KFold
```

In [6]:
```
from sklearn.preprocessing import StandardScaler
sc = StandardScaler() # Creating instance for standard scaler
```

Reading the Data

In [7]:
```
data = pd.read_excel("Inconel_Compiled_Data_New_elems.xlsx")
```

In [8]:
```
df = data.copy()
```

Splitting the Data into Train and Test Sets

In [9]:
```
train_set, test_set = train_test_split(df, test_size=0.2, random_state=42)
```

Separating X and Y variables from Train Dataset

In [10]:
```
x_tr = train_set.drop(["Type", "Surface Roughness (μm)" , "MRR (mm3/min)"],
                      axis = 1).to_numpy()
y_tr = train_set[["Surface Roughness (μm)" , "MRR (mm3/min)"]].to_numpy()
```

Standardazing X variables

In [11]:
```
x_tr_scaled = sc.fit_transform(x_tr)
```

Creating List of Models to be applied

In [12]:
```
models = [LinearRegression()
          , RandomForestRegressor(n_estimators=20, random_state=42)
          , MultiOutputRegressor(SVR(kernel='rbf'))
          , neighbors.KNeighborsRegressor(n_neighbors = 4)]
```

Applying Models and Generate Initial Results

In [13]:
```
fr = []

for model in models:
    lr = model
    lr.fit(x_tr_scaled,y_tr)
    predict = lr.predict(x_tr_scaled)

    actual = y_tr

    # RMSE Calculation
    sr_p = [i[0] for i in predict]
    sr_a = [i[0] for i in actual]

    mrr_p = [i[1] for i in predict]
    mrr_a = [i[1] for i in actual]


    summation_sr = 0  #variable to store the summation of differences
    summation_mrr = 0

    n = len(sr_a) #finding total number of items in list

    for i in range (0,n):  #looping through each element of the list

        difference_sr = sr_a[i] - sr_p[i]  #finding the difference between observe
        difference_mrr = mrr_a[i] - mrr_p[i]

        squared_difference_sr = difference_sr**2  #taking square of the difference
        squared_difference_mrr = difference_mrr**2

        summation_sr = summation_sr + squared_difference_sr  #taking a sum of all
        summation_mrr = summation_mrr + squared_difference_mrr

        MSE_sr = summation_sr/n
        MSE_mrr = summation_mrr/n

        RMSE_sr = np.sqrt(MSE_sr)
        RMSE_mrr = np.sqrt(MSE_mrr)


    dictionary = {
        "Model" : model,
        "RMSE_SR" : RMSE_sr,
        "RMSE_MRR" : RMSE_mrr,
        }
```

```
    fr.append(dictionary)

results_initial = pd.DataFrame(fr)
a= results_initial.Model.unique()
b = ["Linear Regression", "Random Forest", "SVM", "KNN"]
results_initial.Model = results_initial.Model.map(dict(zip(a,b)))

results_initial.to_csv("Results_initial.csv", index = False)

results_initial
```

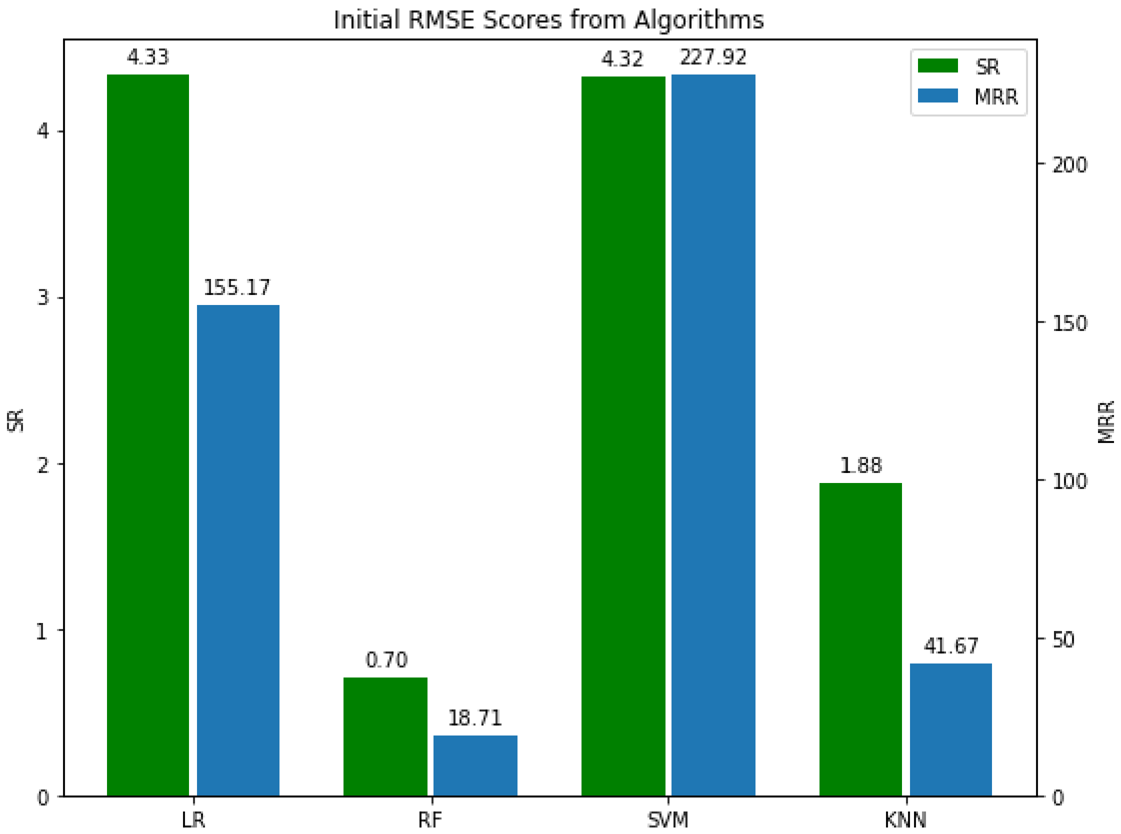
Out[13]:

	Model	RMSE_SR	RMSE_MRR
0	Linear Regression	4.328221	155.169651
1	Random Forest	0.704498	18.708427
2	SVM	4.315385	227.923714
3	KNN	1.878115	41.668207

Vizualizing Initial Results

In [14]:

```
labels = ['LR', 'RF', 'SVM', 'KNN']

sr = results_initial["RMSE_SR"]
mrr = results_initial["RMSE_MRR"]

x = np.arange(len(labels))  # the label locations
width = 0.35 # the width of the bars

fig, ax = plt.subplots(figsize = (8,6))

ax2 = ax.twinx()
rects1 = ax.bar(x - width/1.85, sr, width, label='SR', color = "green")
rects2 = ax2.bar(x + width/1.85, mrr, width, label='MRR')

# Add some text for labels, title and custom x-axis tick labels, etc.
ax.set_ylabel('SR')
ax.set_title('Initial RMSE Scores from Algorithms')
ax.set_xticks(x, labels)

ax.legend(handles=[rects1, rects2])
ax2.set_ylabel('MRR')

ax.bar_label(rects1, padding=4, fmt='%.2f')
ax2.bar_label(rects2, padding=4, fmt='%.2f')

fig.tight_layout()

plt.savefig("Initial RMSE Scores from Algorithms.jpg")

plt.show()
```



It appears that RF is the most suitable among all, but we will apply cross validation on all 4 algorithms to confirm

Applying Cross Validation on all 4 Algorithms

In [15]:
```
kfold = KFold(n_splits = 10, random_state= 42, shuffle = True)
```

Note: A value of k=10 is very common in the field of applied machine learning, and is recommend if you are struggling to choose a value for your dataset.

Ref: https://machinelearningmastery.com/k-fold-cross-validation/#:~:text=Cross%2Dvalidation%20is%20primarily%20used,the%20training%20of%20th

In [16]:
```
fr = []

for train_index, test_index in kfold.split(x_tr_scaled):

    x_train, x_test = x_tr_scaled[train_index], x_tr_scaled[test_index]
    y_train, y_test = y_tr[train_index], y_tr[test_index]

    for model in models:

        lr = model
        lr.fit(x_train,y_train)
        predict = lr.predict(x_test)

        actual = y_test

        # RMSE Calculation
```

```
        sr_p = [i[0] for i in predict]
        sr_a = [i[0] for i in actual]

        mrr_p = [i[1] for i in predict]
        mrr_a = [i[1] for i in actual]


        summation_sr = 0  #variable to store the summation of differences
        summation_mrr = 0

        n = len(sr_a) #finding total number of items in list

        for i in range (0,n):  #looping through each element of the list

            difference_sr = sr_a[i] - sr_p[i]  #finding the difference between obse
            difference_mrr = mrr_a[i] - mrr_p[i]

            squared_difference_sr = difference_sr**2  #taking square of the differe
            squared_difference_mrr = difference_mrr**2

            summation_sr = summation_sr + squared_difference_sr  #taking a sum of a
            summation_mrr = summation_mrr + squared_difference_mrr

            MSE_sr = summation_sr/n
            MSE_mrr = summation_mrr/n

            RMSE_sr = np.sqrt(MSE_sr)
            RMSE_mrr = np.sqrt(MSE_mrr)


        dictionary = {
            "Model" : model,
            "RMSE_SR" : RMSE_sr,
            "RMSE_MRR" : RMSE_mrr,
            }


        fr.append(dictionary)



cross_results = pd.DataFrame(fr)
a= cross_results.Model.unique()
b = ["Linear Regression", "Random Forest", "SVM", "KNN"]
cross_results.Model = cross_results.Model.map(dict(zip(a,b)))
cross_results.sort_values(["Model"], inplace =True)
cross_results.to_csv("Cross_Validation_Results_on_All_Four.csv", index = False)
cross_results
```

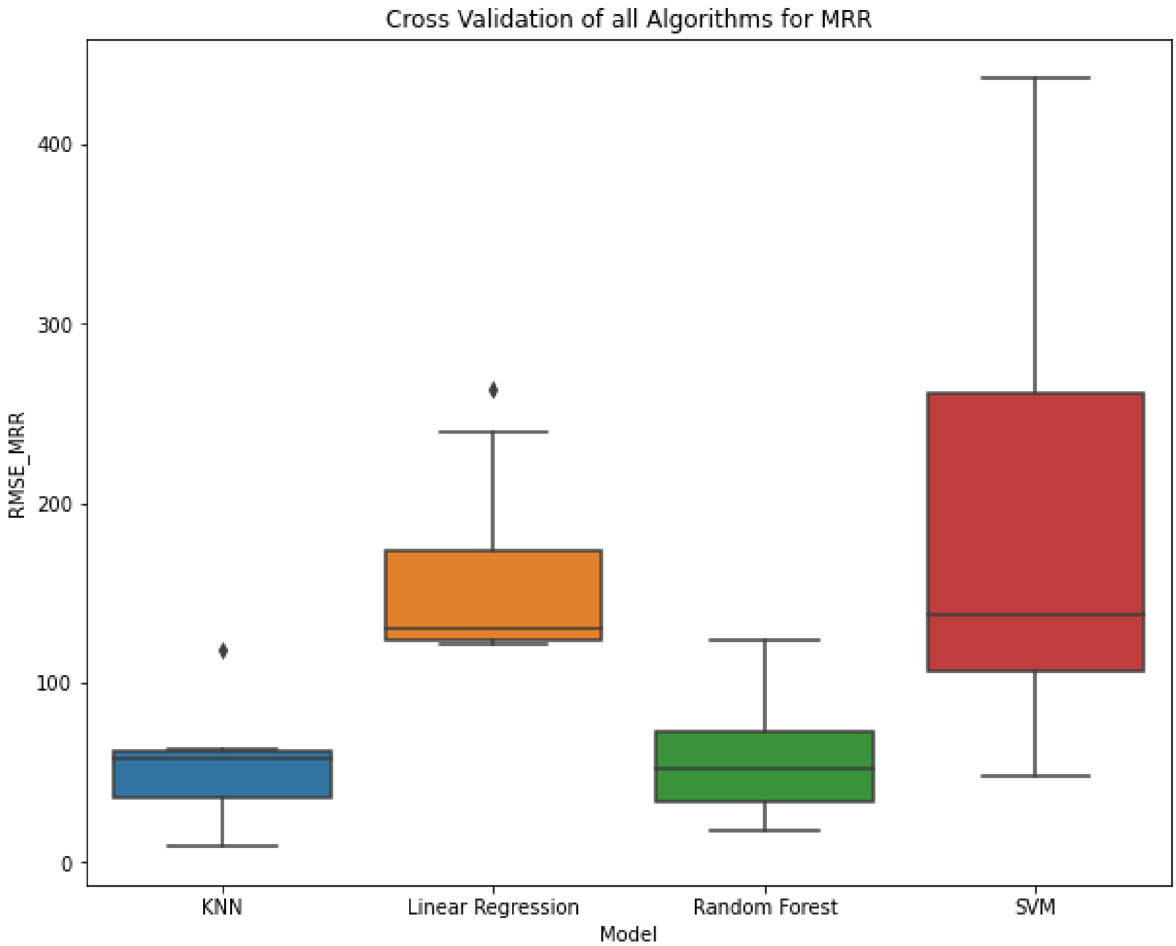
Out[16]:

	Model	RMSE_SR	RMSE_MRR
19	KNN	2.204703	62.346608
35	KNN	1.186280	63.154831
31	KNN	2.252887	55.096145
27	KNN	3.919831	39.932698
23	KNN	1.706416	62.261271
15	KNN	2.289610	61.052642
11	KNN	1.239331	20.629819
39	KNN	3.557879	9.149484
3	KNN	2.475678	34.517297
7	KNN	1.560162	118.725964
8	Linear Regression	3.217647	239.267869
36	Linear Regression	6.211147	123.011728
32	Linear Regression	2.882132	131.324666
28	Linear Regression	5.099496	131.764803
24	Linear Regression	5.542541	130.622724
20	Linear Regression	2.927022	121.524942
4	Linear Regression	3.596408	263.361680
0	Linear Regression	4.777703	127.511665
16	Linear Regression	4.185219	187.306827
12	Linear Regression	4.889825	121.608441
37	Random Forest	2.682070	27.672041
9	Random Forest	0.701950	114.907337
1	Random Forest	2.076529	37.419333
33	Random Forest	1.194282	17.695318
29	Random Forest	1.292987	57.981463
17	Random Forest	1.259070	74.890214
13	Random Forest	3.431464	65.859135
21	Random Forest	1.253960	32.332236
5	Random Forest	1.053744	124.379512
25	Random Forest	2.831058	46.775593
26	SVM	5.943355	79.204586
14	SVM	5.066773	218.787575
22	SVM	2.549555	106.206641
30	SVM	5.325731	158.207672
2	SVM	4.666881	109.535820
10	SVM	2.156337	368.989677

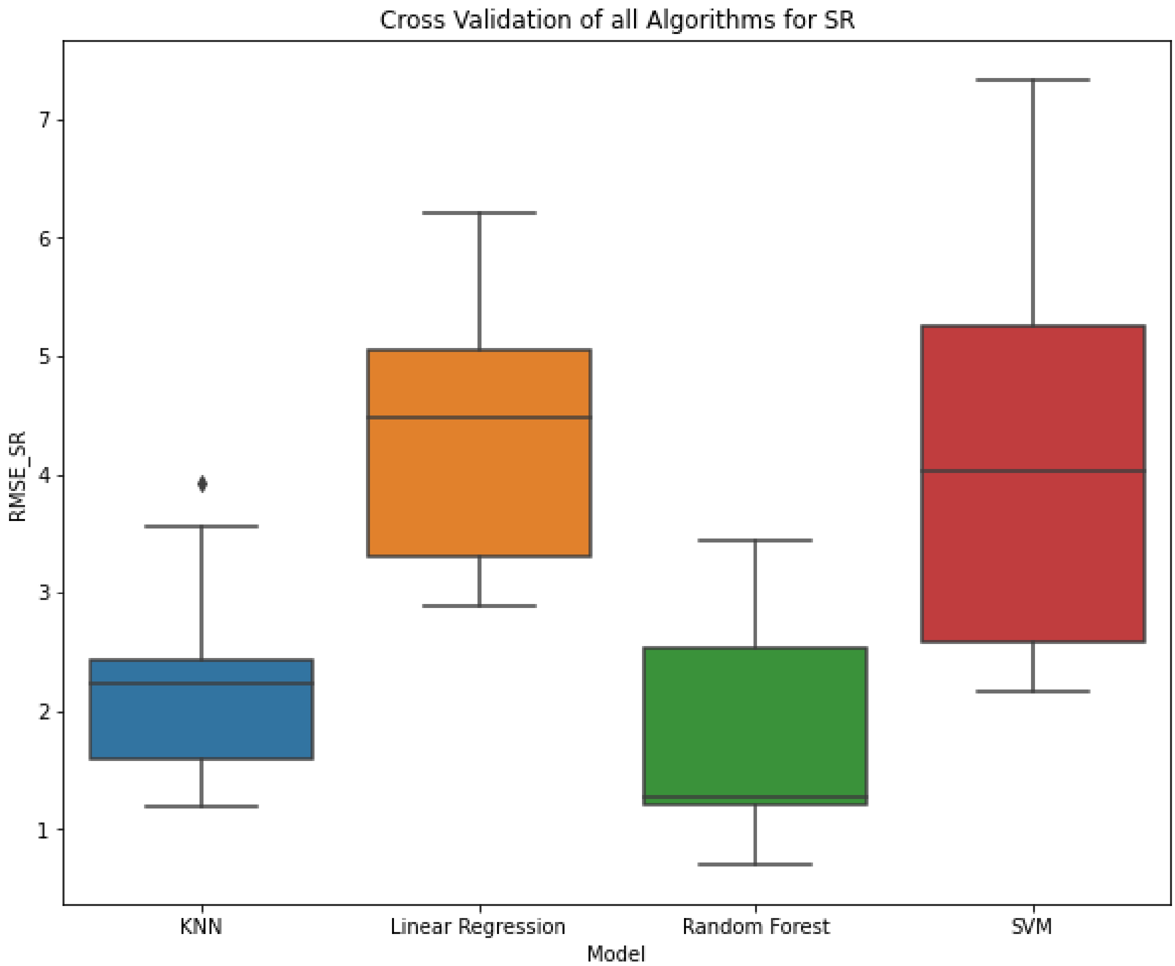
	Model	RMSE_SR	RMSE_MRR
34	SVM	2.284358	116.804266
38	SVM	7.339949	48.483162
18	SVM	3.391829	275.703899
6	SVM	2.667634	437.196573

Vizualizing Cross Validation Results for All 4 Algorithms

In [17]:
```
plt.figure(figsize = (10,8))
sns.boxplot(data = cross_results, y= "RMSE_MRR", x ="Model").set(
    title = "Cross Validation of all Algorithms for MRR");
plt.savefig("Cross_Val_All_Algo_MRR_boxplot.jpg")
```

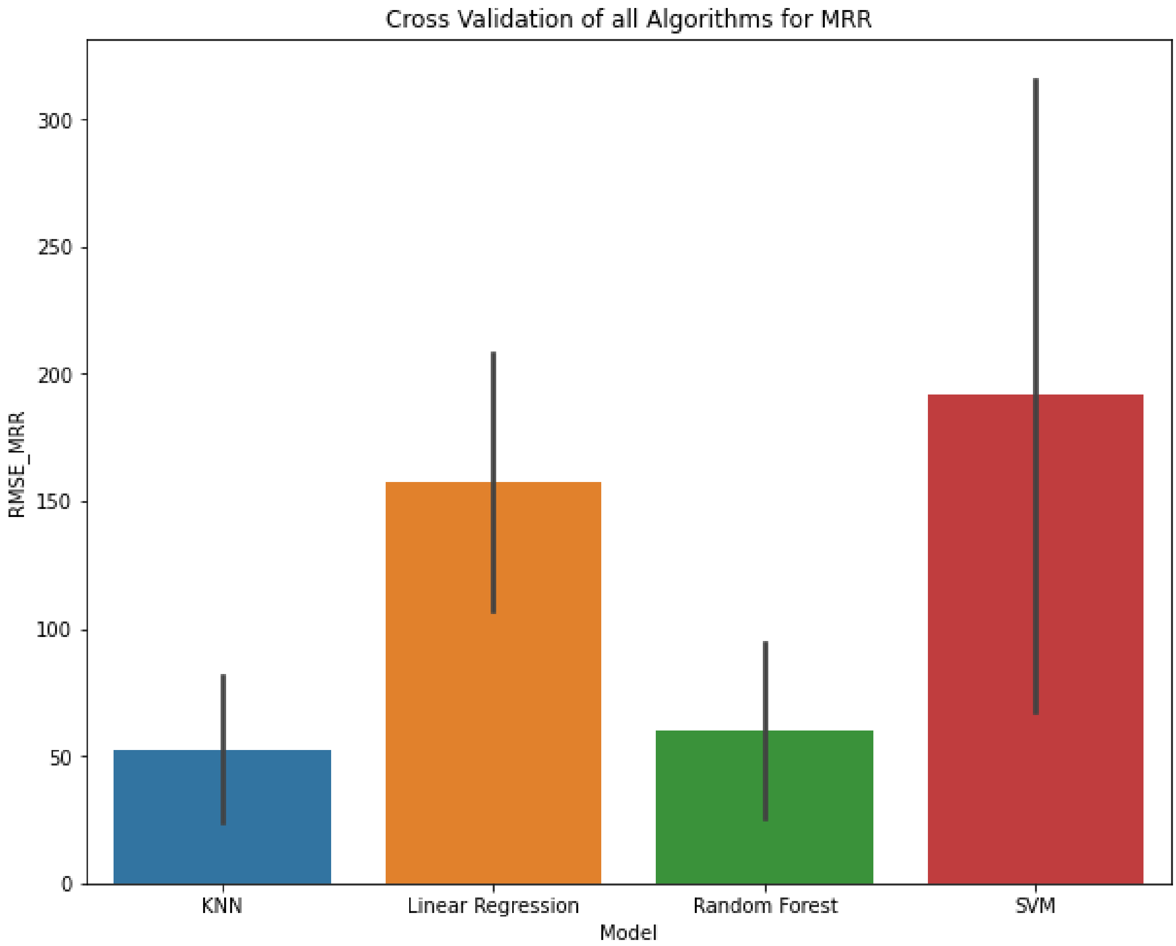


In [18]:
```
plt.figure(figsize = (10,8))
sns.boxplot(data = cross_results, y= "RMSE_SR", x ="Model").set(
    title = "Cross Validation of all Algorithms for SR");
plt.savefig("Cross_Val_All_Algo_SR_boxplot.jpg")
```

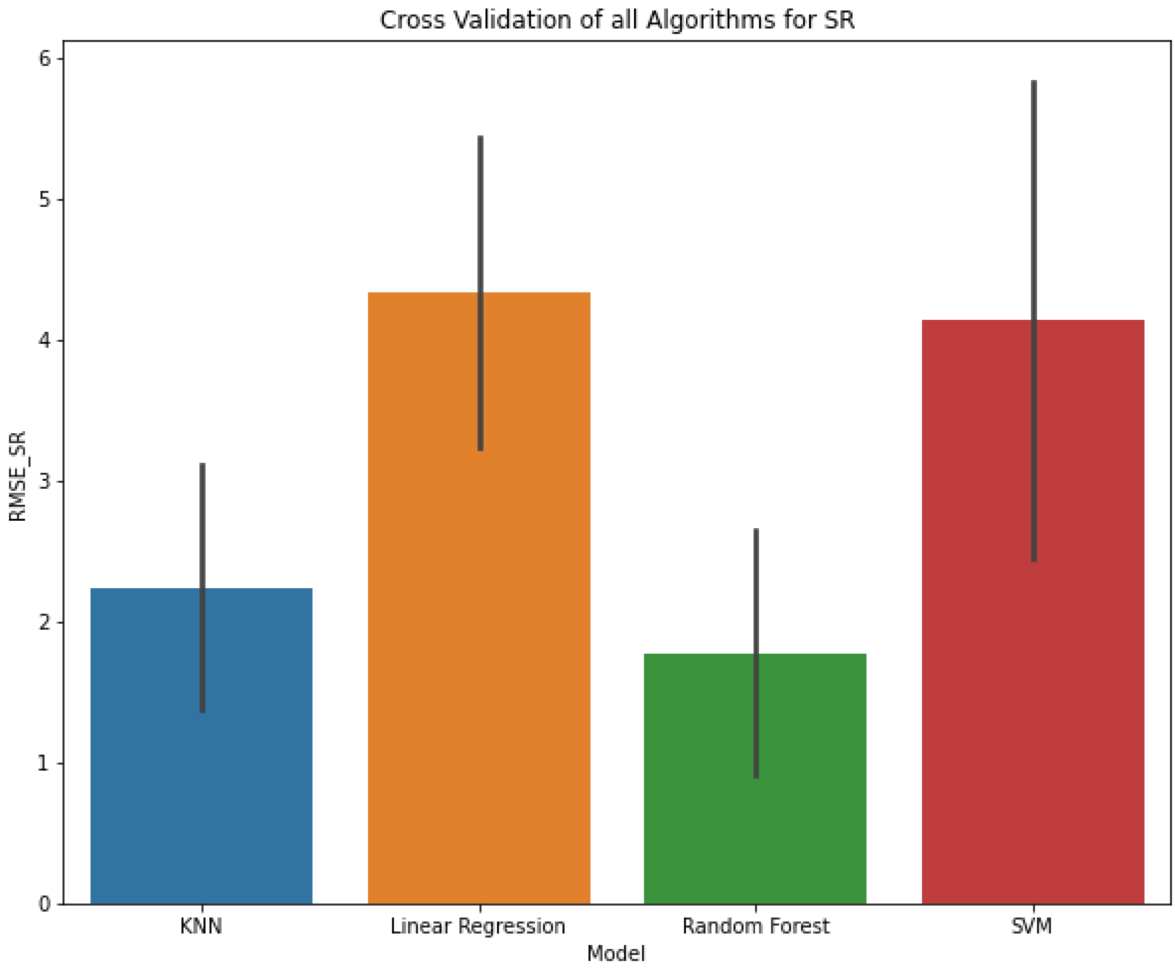


In [19]:

```
plt.figure(figsize = (10,8))
sns.barplot(x = "Model", y = "RMSE_MRR",data = cross_results, ci = "sd").set(
    title = "Cross Validation of all Algorithms for MRR")
plt.savefig("Cross_Val_All_Algo_MRR_barplot.jpg")
```



In [20]:
```
plt.figure(figsize = (10,8))
sns.barplot(x = "Model", y = "RMSE_SR",data = cross_results, ci = "sd").set(
    title = "Cross Validation of all Algorithms for SR")
plt.savefig("Cross_Val_All_Algo_SR_barplot.jpg")
```



In [21]:

```
r_sr = cross_results.groupby("Model")["RMSE_SR"].agg(["mean", "std"])
r_sr.rename(columns = {'mean' : "RMSE_SR_Mean", "std": "RMSE_SR_Std"}, inplace= Tru
r_mrr = cross_results.groupby("Model")["RMSE_MRR"].agg(["mean", "std"])
r_mrr.rename(columns = {'mean' : "RMSE_MRR_Mean", "std": "RMSE_MRR_Std"}, inplace=
comp = pd.concat([r_sr, r_mrr], axis =1)
comp.to_csv("Cross_Validation_Mean_ALl_Algo.csv")
comp
```

Out[21]:

Model	RMSE_SR_Mean	RMSE_SR_Std	RMSE_MRR_Mean	RMSE_MRR_Std
KNN	2.239278	0.911446	52.686676	30.087782
Linear Regression	4.332914	1.153544	157.730534	53.251585
Random Forest	1.777711	0.916008	59.991218	36.062783
SVM	4.139240	1.784803	191.911987	130.574625

Random Forest performs best for SR, whereas KNN performs best for MRR

First we will find parameters for Random Forest, then for KNN

Parameter Tunning for RF

In [22]:

```
fr = []

estimators = range(1,21)
```

```
for est in estimators:

    lr = RandomForestRegressor(n_estimators=est, random_state=42)
    lr.fit(x_tr_scaled,y_tr)

    predict = lr.predict(x_tr_scaled)

    actual = y_tr

    # RMSE Calculation
    sr_p = [i[0] for i in predict]
    sr_a = [i[0] for i in actual]

    mrr_p = [i[1] for i in predict]
    mrr_a = [i[1] for i in actual]


    summation_sr = 0  #variable to store the summation of differences
    summation_mrr = 0

    n = len(sr_a) #finding total number of items in list

    for i in range (0,n):  #looping through each element of the list

        difference_sr = sr_a[i] - sr_p[i]  #finding the difference between observed
        difference_mrr = mrr_a[i] - mrr_p[i]

        squared_difference_sr = difference_sr**2  #taking square of the differences
        squared_difference_mrr = difference_mrr**2

        summation_sr = summation_sr + squared_difference_sr  #taking a sum of all 
        summation_mrr = summation_mrr + squared_difference_mrr

    MSE_sr = summation_sr/n
    MSE_mrr = summation_mrr/n

    RMSE_sr = np.sqrt(MSE_sr)
    RMSE_mrr = np.sqrt(MSE_mrr)


    dictionary = {
        "Estimators" : est,
        "RMSE_SR" : RMSE_sr,
        "RMSE_MRR" : RMSE_mrr
        }


    fr.append(dictionary)

rf = pd.DataFrame(fr)
rf.to_csv("RF_Parameter_Tuning.csv", index = False)

rf
```

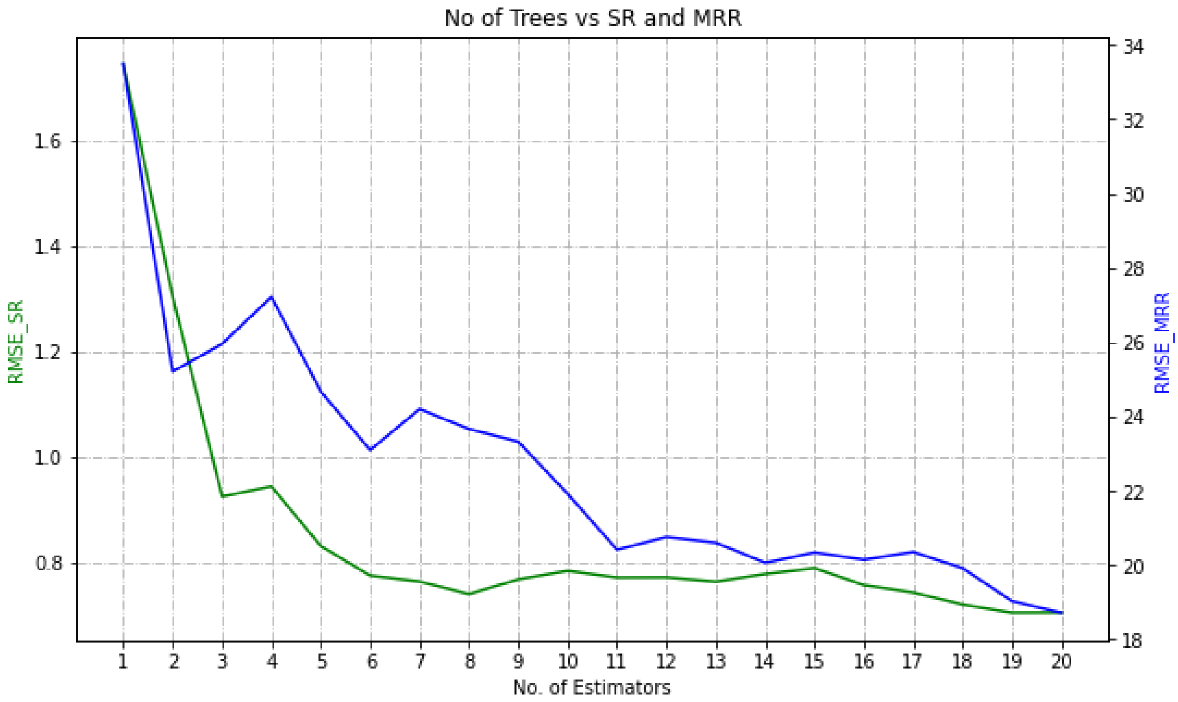
Out[22]:

	Estimators	RMSE_SR	RMSE_MRR
0	1	1.744588	33.494527
1	2	1.304265	25.205571
2	3	0.924497	25.951893
3	4	0.943693	27.219166
4	5	0.830706	24.667806
5	6	0.774644	23.090775
6	7	0.763482	24.197440
7	8	0.739802	23.658888
8	9	0.767500	23.316622
9	10	0.783856	21.910707
10	11	0.770945	20.408666
11	12	0.771259	20.750857
12	13	0.763152	20.597124
13	14	0.777739	20.056339
14	15	0.788892	20.329991
15	16	0.756647	20.140031
16	17	0.742714	20.343568
17	18	0.719861	19.909184
18	19	0.704225	19.022222
19	20	0.704498	18.708427

Vizualizing Number of Trees vs RMSE of SR and MRR

In [23]:

```
fig, ax1 = plt.subplots(figsize = (10,6))

ax2 = ax1.twinx()
ax1.plot(estimators, rf["RMSE_SR"], 'g-')
ax2.plot(estimators, rf["RMSE_MRR"], 'b-')

ax1.set_xlabel('No. of Estimators')
ax1.set_ylabel('RMSE_SR', color='g')
ax2.set_ylabel('RMSE_MRR', color='b')

ax1.grid(True, linestyle='-.')

tickpos = list(estimators)

plt.xticks(tickpos,tickpos)
plt.title("No of Trees vs SR and MRR")

plt.savefig("No of Trees vs SR and MRR.jpg")
plt.show()
```



20 number of trees yield best results, So we will cross validate Random Forest with 20 number of Trees

Cross Validation on RF based by keeping no. of trees = 20

In [24]:
```
fr = []

k = 1

for train_index, test_index in kfold.split(x_tr_scaled):

    x_train, x_test = x_tr_scaled[train_index], x_tr_scaled[test_index]
    y_train, y_test = y_tr[train_index], y_tr[test_index]

    lr = RandomForestRegressor(n_estimators=20, random_state=42)
    lr.fit(x_train,y_train)
    predict = lr.predict(x_test)

    actual = y_test

    # RMSE Calculation
    sr_p = [i[0] for i in predict]
    sr_a = [i[0] for i in actual]

    mrr_p = [i[1] for i in predict]
    mrr_a = [i[1] for i in actual]


    summation_sr = 0  #variable to store the summation of differences
    summation_mrr = 0

    n = len(sr_a) #finding total number of items in list

    for i in range (0,n):  #looping through each element of the list
```

```
        difference_sr = sr_a[i] - sr_p[i]  #finding the difference between observed
        difference_mrr = mrr_a[i] - mrr_p[i]

        squared_difference_sr = difference_sr**2  #taking square of the differences
        squared_difference_mrr = difference_mrr**2

        summation_sr = summation_sr + squared_difference_sr  #taking a sum of all t
        summation_mrr = summation_mrr + squared_difference_mrr

        MSE_sr = summation_sr/n
        MSE_mrr = summation_mrr/n

        RMSE_sr = np.sqrt(MSE_sr)
        RMSE_mrr = np.sqrt(MSE_mrr)


    dictionary = {
        "Model" : "RF",
        "RMSE_SR" : RMSE_sr,
        "RMSE_MRR" : RMSE_mrr,
        "Fold No." : k
        }


    fr.append(dictionary)

    k+=1

rf_20 = pd.DataFrame(fr)
rf_20_sr = rf_20.groupby("Model")["RMSE_SR"].agg(["mean", "std"])
rf_20_sr.rename(columns = {'mean' : "RMSE_SR_Mean", "std": "RMSE_SR_Std"}, inplace=

rf_20_mrr = rf_20.groupby("Model")["RMSE_MRR"].agg(["mean", "std"])
rf_20_mrr.rename(columns = {'mean' : "RMSE_SR_Mean", "std": "RMSE_SR_Std"}, inplace

rf_20_cross_val = pd.concat([rf_20_sr, rf_20_mrr], axis=1)
rf_20_cross_val.to_csv("RF_20_Cross_Val_Results.csv")
rf_20_cross_val
```

Out[24]:

	RMSE_SR_Mean	RMSE_SR_Std	RMSE_SR_Mean	RMSE_SR_Std
Model				
RF	1.777711	0.916008	59.991218	36.062783

Parameter Tunning for KNN

In [25]:

```
fr = []

estimators = range(1,21)

for est in estimators:

    lr = neighbors.KNeighborsRegressor(n_neighbors = est)
    lr.fit(x_tr_scaled,y_tr)

    predict = lr.predict(x_tr_scaled)

    actual = y_tr

    # RMSE Calculation
```

```
    sr_p = [i[0] for i in predict]
    sr_a = [i[0] for i in actual]

    mrr_p = [i[1] for i in predict]
    mrr_a = [i[1] for i in actual]


    summation_sr = 0  #variable to store the summation of differences
    summation_mrr = 0

    n = len(sr_a) #finding total number of items in list

    for i in range (0,n):  #looping through each element of the list

        difference_sr = sr_a[i] - sr_p[i]  #finding the difference between observed
        difference_mrr = mrr_a[i] - mrr_p[i]

        squared_difference_sr = difference_sr**2  #taking square of the differences
        squared_difference_mrr = difference_mrr**2

        summation_sr = summation_sr + squared_difference_sr  #taking a sum of all
        summation_mrr = summation_mrr + squared_difference_mrr

    MSE_sr = summation_sr/n
    MSE_mrr = summation_mrr/n

    RMSE_sr = np.sqrt(MSE_sr)
    RMSE_mrr = np.sqrt(MSE_mrr)


    dictionary = {
        "Estimators" : est,
        "RMSE_SR" : RMSE_sr,
        "RMSE_MRR" : RMSE_mrr
        }


    fr.append(dictionary)

knn = pd.DataFrame(fr)
knn.to_csv("KNN_Parameter_Tuning.csv", index = False)

knn
```

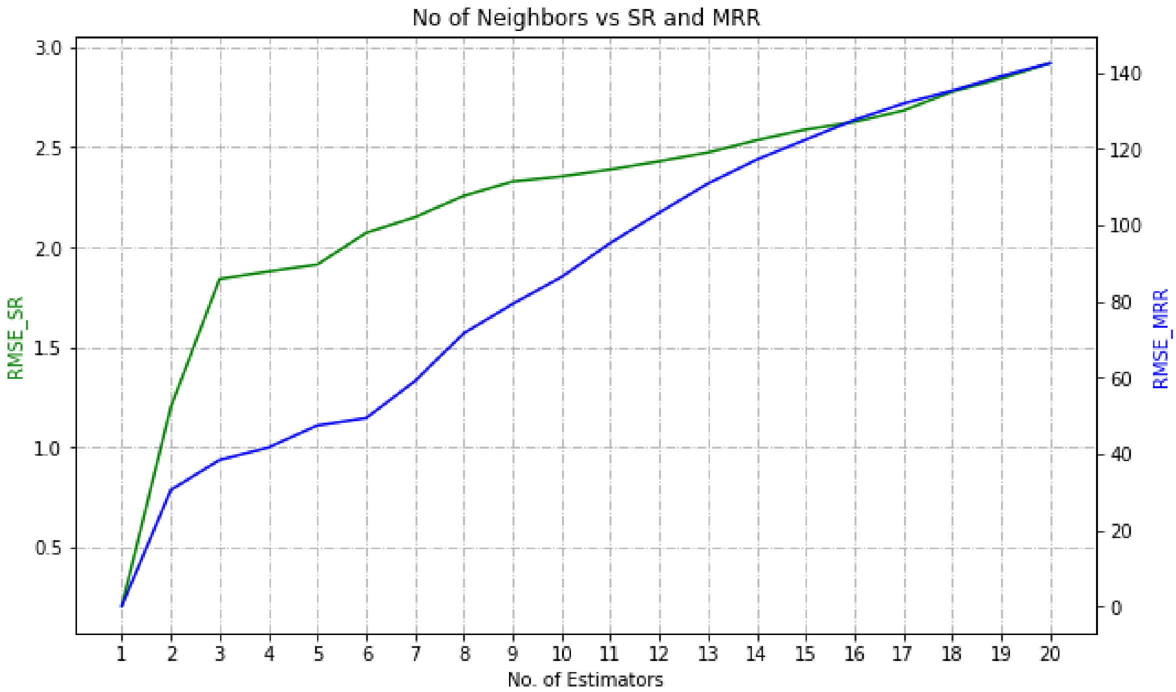
Out[25]:

	Estimators	RMSE_SR	RMSE_MRR
0	1	0.205198	0.150360
1	2	1.199465	30.546262
2	3	1.840616	38.401000
3	4	1.878115	41.668207
4	5	1.912881	47.443957
5	6	2.071054	49.360603
6	7	2.149581	59.081334
7	8	2.256224	71.634935
8	9	2.327642	79.314669
9	10	2.353073	86.369789
10	11	2.387875	95.266835
11	12	2.428913	103.210939
12	13	2.472726	110.851030
13	14	2.534710	117.127376
14	15	2.587898	122.349423
15	16	2.625480	127.528955
16	17	2.683062	131.862948
17	18	2.777623	135.218682
18	19	2.842907	139.003982
19	20	2.920188	142.420124

Vizualizing Number of Neighbors vs RMSE of SR and MRR

In [26]:

```
fig, ax1 = plt.subplots(figsize = (10,6))

ax2 = ax1.twinx()
ax1.plot(estimators, knn["RMSE_SR"], 'g-')
ax2.plot(estimators, knn["RMSE_MRR"], 'b-')

ax1.set_xlabel('No. of Estimators')
ax1.set_ylabel('RMSE_SR', color='g')
ax2.set_ylabel('RMSE_MRR', color='b')

ax1.grid(True, linestyle='-.')

tickpos = list(estimators)

plt.xticks(tickpos,tickpos)
plt.title("No of Neighbors vs SR and MRR")

plt.savefig("No of Neighbors vs SR and MRR.jpg")
plt.show()
```



Note: We can not go further with KNN because as the no. of neigbors increases, the RMSE scores also increase, which we have to avoid.

Why we cant use n=1 in KNN

https://stats.stackexchange.com/questions/440064/is-k-1-is-good-for-knn-when-error-is-min-accuracy-is-max-and-even-auroc-is-m#:~:text=The%20error%20rate%20at%20K,and%20plot%20the%20validation%20error.

Finally we are selecting RF Model, with no. of trees = 20. With this Model we will test our dataset

Separating x and y variables from the Test dataset

In [27]:
```
x_ts = test_set.drop(["Type", "Surface Roughness (μm)" , "MRR (mm3/min)"],
                     axis = 1).to_numpy()
y_ts = test_set[["Surface Roughness (μm)" , "MRR (mm3/min)"]].to_numpy()
```

Standardazing X variables

In [28]:
```
x_ts_scaled = sc.transform(x_ts)
```

Running Random Forest with 20 number of trees and taking predictions on Test

dataset

In [29]:
```
fr_20 = []

# Model Training and Prediction
lr = RandomForestRegressor(n_estimators=20, random_state=42)
lr.fit(x_tr_scaled,y_tr)

predict = lr.predict(x_ts_scaled)

actual = y_ts

# RMSE Calculation
sr_p_20 = [i[0] for i in predict]
sr_a_20 = [i[0] for i in actual]

mrr_p_20 = [i[1] for i in predict]
mrr_a_20 = [i[1] for i in actual]


summation_sr_20 = 0  #variable to store the summation of differences
summation_mrr_20 = 0

n = len(sr_a_20) #finding total number of items in list

for i in range (0,n):  #looping through each element of the list

    difference_sr_20 = sr_a_20[i] - sr_p_20[i]  #finding the difference between obs
    difference_mrr_20 = mrr_a_20[i] - mrr_p_20[i]

    squared_difference_sr_20 = difference_sr_20**2  #taking square of the differen
    squared_difference_mrr_20 = difference_mrr_20**2

    summation_sr_20 = summation_sr_20 + squared_difference_sr_20  #taking a sum of
    summation_mrr_20 = summation_mrr_20 + squared_difference_mrr_20

MSE_sr_20 = summation_sr_20/n
MSE_mrr_20 = summation_mrr_20/n

RMSE_sr_20 = np.sqrt(MSE_sr_20)
RMSE_mrr_20 = np.sqrt(MSE_mrr_20)


dictionary = {
    "Estimators" : 20,
    "RMSE_SR" : RMSE_sr_20,
    "RMSE_MRR" : RMSE_mrr_20
    }


fr_20.append(dictionary)

final_rf_20 = pd.DataFrame(fr_20)

final_rf_20.to_csv("Final_RF_20_Results.csv", index =False)

final_rf_20
```

Out[29]:

	Estimators	RMSE_SR	RMSE_MRR
0	20	1.570611	73.938661

Calculating Confidence Intervals

Ref from Book: Hands-On Machine Learning with Scikit-Learn, Keras, and TensorFlow (2019), Page 110

In [30]:
```
confidence = 0.95
```

In [31]:
```
squared_errors = (np.array(mrr_a_20) - np.array(mrr_p_20)) ** 2
se_mrr = np.sqrt(stats.t.interval(confidence,
                                  len(squared_errors) - 1,
                                  loc=squared_errors.mean(),
                                  scale = stats.sem(squared_errors)/2))
```

In [32]:
```
print("95% Confidence Interval for RMSE MRR is:", se_mrr[0], "to", se_mrr[1])
```

```
95% Confidence Interval for RMSE MRR is: 51.91782574832816 to 90.76557942303033
```

In [33]:
```
squared_errors = (np.array(sr_a_20) - np.array(sr_p_20)) ** 2
se_sr = np.sqrt(stats.t.interval(confidence,
                                 len(squared_errors) - 1,
                                 loc=squared_errors.mean(),
                                 scale = stats.sem(squared_errors) ))
```

In [34]:
```
print("95% Confidence Interval for RMSE SR is:", se_sr[0], "to", se_sr[1])
```

```
95% Confidence Interval for RMSE SR is: 0.5999948932051761 to 2.13860754088344
```