3_Short_list_promising_models

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Completed by:

Name: Adarsh Ghimire Student ID: 100058927

MSc in Electrical and Computer Engineering

```
[]: from google.colab import drive drive.mount('/content/drive')
```

Drive already mounted at /content/drive; to attempt to forcibly remount, call drive.mount("/content/drive", force_remount=True).

```
[]: try:
    import os
    os.chdir('drive/MyDrive/COSC 606 Machine learning/Project/notebooks/')
    except:
    print("Already in working directory")
```

```
[]: import pandas as pd
  import matplotlib.pyplot as plt
  import seaborn as sns
  from sklearn.linear_model import LinearRegression
  from sklearn.preprocessing import PolynomialFeatures
  from sklearn.model_selection import train_test_split
  from sklearn.model_selection import KFold
  from sklearn.metrics import mean_squared_error
  from sklearn.metrics import r2_score
```

```
[]: # Training and test data were made in second notebook, and were saved to make

→ future use easier

training_dataset_path = "../final_dataset/train.csv"

test_dataset_path = "../final_dataset/test.csv"

train_df = pd.read_csv(training_dataset_path)

test_df = pd.read_csv(test_dataset_path)

train_df.head()
```

```
[]: Report Date Route
                             Time ... Direction Min Delay Min Gap
    0 2014-01-02
                    505 06:31:00 ...
                                           E/B
                                                    4.0
                                                            8.0
    1 2014-01-02
                    504 12:43:00 ...
                                           E/B
                                                   20.0
                                                           22.0
    2 2014-01-02 501 14:01:00 ...
                                           W/B
                                                   13.0
                                                           19.0
    3 2014-01-02
                                                    7.0
                    504 14:22:00 ...
                                          W/B
                                                           11.0
    4 2014-01-02
                    504 16:42:00 ...
                                           E/B
                                                    3.0
                                                            6.0
```

[5 rows x 8 columns]

0.1 Data Manipulations functions

```
[]: # Since our target is Min Delay so the function below cleans the Min Delay rows⊔

→ if they are nan values

def clean_delay(df):

df = df[df['Min Delay'].notna()]

return df
```

```
[]: # This function checks for valid routes only
     def check_route(x):
       # load the valid list of TTC Streetcar routes
      valid_routes = [501, 502, 503, 504, 505, 506, 509, 510, 511, 512, 301, 304, ___
      →306, 310]
       if x in valid_routes:
         return x
       else:
         return "bad route"
     # This function cleans the data based on valid routes
     def clean route(df):
       # This function takes dataframe as input
       # cleans the route column based on the validity of the route of street car
       # returns the cleaned dataframe
       df['Route'] = df['Route'].apply(lambda x:check_route(x))
       df = df[df.Route != "bad route"]
       df['Route'] = df['Route'].astype('int64')
       return df
```

```
[]: # This function drops the Location column
def drop_location(df):
    df = df.drop(["Location"], axis=1)
    return df
```

```
[]: def create_date_time_column(df):
    # This function takes dataframe, then merges the date and time
    # Then convert that column into datetime datatype
```

```
# Such that it can be further used in time series easily
       try:
         new = pd.to_datetime(df["Report Date"] + " "+ df["Time"], utc=True)
         df["Date Time"] = new
         df = df.drop(["Report Date", "Time"], axis=1)
         return df
       except:
         return df
[]: # This function divides a day into different period
     def day_divider(hour):
       if hour > 5 and hour < 12:</pre>
         return "morning"
       elif hour >= 12 and hour < 17:
         return "afternoon"
       elif hour >= 17 and hour < 21:
         return "evening"
       else:
         return "night"
[]: def clean_gap(df):
       # This function will help to clean the Min Gap column feature with training
      →data Min Gap mean value
       df["Min Gap"] = df["Min Gap"].fillna(train_df['Min Gap'].mean())
       return df
[]: # These function help to filter the Direction values and clean them
     valid_directions = ['eb','wb','nb','sb','bw']
     def check_direction (x):
         if x in valid directions:
             return(x)
         else:
             return("bad direction")
     def direction cleanup(df):
         df['Direction'] = df['Direction'].str.lower()
         df['Direction'] = df['Direction'].str.replace('/','')
         df['Direction'] = df['Direction'].replace({'eastbound':'eb','westbound':
     →'wb','southbound':'sb','northbound':'nb'})
         df['Direction'] = df['Direction'].apply(lambda x:check_direction(x))
         return(df)
[]: def complete_cleaner(df):
       df = clean_delay(df) # drops the nan Min delay rows
       df = clean_route(df) # cleans the unwanted route from the dataset
       df = drop_location(df) # drops the location column from the dataset
```

df = create_date_time_column(df) # creates Date Time column in the dataset

```
df["Part of Day"] = df.apply(lambda x: day_divider(x["Date Time"].

→hour),axis=1) # Creates Part of Day column in the dataset

df = clean_gap(df) # cleans gap based on the mean of gap values

df = direction_cleanup(df) # cleans the direction column to 5

→directions(eb,wb,nb,sb,bw)

df = df[df["Direction"] != "bad direction"]

df.reset_index(inplace=True, drop=True)

df.drop(['Date Time'], axis=1, inplace=True)

return df
```

```
[]: # Creating a copy of training data to work on df = train_df.copy(deep=True)
```

[]: df = complete_cleaner(df)

/usr/local/lib/python3.7/dist-packages/ipykernel_launcher.py:16: SettingWithCopyWarning:

A value is trying to be set on a copy of a slice from a DataFrame. Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy app.launch_new_instance()

/usr/local/lib/python3.7/dist-packages/ipykernel_launcher.py:18: SettingWithCopyWarning:

A value is trying to be set on a copy of a slice from a DataFrame. Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy

[]: df.sample(10)

	_	_				
	Route	Day	Direction	Min Delay	Min Gap	Part of Day
11615	512	Monday	eb	4.0	8.0	morning
25712	509	Saturday	wb	18.0	36.0	night
61661	506	Tuesday	wb	6.0	12.0	afternoon
57689	506	Thursday	wb	5.0	10.0	evening
17206	501	Monday	eb	10.0	20.0	afternoon
57370	504	Wednesday	eb	11.0	21.0	night
27191	504	Monday	eb	4.0	8.0	morning
51570	501	Friday	eb	60.0	67.0	night
64756	509	Saturday	eb	13.0	26.0	evening
22315	504	Wednesday	wb	7.0	11.0	evening
	25712 61661 57689 17206 57370 27191 51570 64756	25712 509 61661 506 57689 506 17206 501 57370 504 27191 504 51570 501 64756 509	11615 512 Monday 25712 509 Saturday 61661 506 Tuesday 57689 506 Thursday 17206 501 Monday 57370 504 Wednesday 27191 504 Monday 51570 501 Friday 64756 509 Saturday	11615 512 Monday eb 25712 509 Saturday wb 61661 506 Tuesday wb 57689 506 Thursday wb 17206 501 Monday eb 57370 504 Wednesday eb 27191 504 Monday eb 51570 501 Friday eb 64756 509 Saturday eb	11615 512 Monday eb 4.0 25712 509 Saturday wb 18.0 61661 506 Tuesday wb 6.0 57689 506 Thursday wb 5.0 17206 501 Monday eb 10.0 57370 504 Wednesday eb 11.0 27191 504 Monday eb 4.0 51570 501 Friday eb 60.0 64756 509 Saturday eb 13.0	11615 512 Monday eb 4.0 8.0 25712 509 Saturday wb 18.0 36.0 61661 506 Tuesday wb 6.0 12.0 57689 506 Thursday wb 5.0 10.0 17206 501 Monday eb 10.0 20.0 57370 504 Wednesday eb 11.0 21.0 27191 504 Monday eb 4.0 8.0 51570 501 Friday eb 60.0 67.0 64756 509 Saturday eb 13.0 26.0

1 Now doing one hot encoding for the categorical data

- 1. Route is categorical
- 2. Day is categorical
- 3. Direction is categorical
- 4. Part of Day is categorical

```
[]: # One hot encoder object made using training data, so that it can be used for
      \hookrightarrow testing later on.
     from sklearn.preprocessing import OneHotEncoder
     import numpy as np
     day_enc = OneHotEncoder()
     route_enc = OneHotEncoder()
     dir_enc = OneHotEncoder()
     part_enc = OneHotEncoder()
     day_enc.fit(np.array(df["Day"]).reshape(-1,1))
     route_enc.fit(np.array(df["Route"]).reshape(-1,1))
     dir_enc.fit(np.array(df["Direction"]).reshape(-1,1))
     part_enc.fit(np.array(df["Part of Day"]).reshape(-1,1))
[]: OneHotEncoder(categories='auto', drop=None, dtype=<class 'numpy.float64'>,
                   handle_unknown='error', sparse=True)
[]: def one hot encoder(df):
       df[day_enc.categories_[0]] = day_enc.transform(np.array(df["Day"]).
      \rightarrowreshape(-1,1)).toarray()
       df[route_enc.categories_[0]] = route_enc.transform(np.array(df["Route"]).
      \rightarrowreshape(-1,1)).toarray()
       df[dir_enc.categories_[0]] = dir_enc.transform(np.array(df["Direction"]).
      \rightarrowreshape(-1,1)).toarray()
       df[part_enc.categories_[0]] = part_enc.transform(np.array(df["Part of Day"]).
      \rightarrowreshape(-1,1)).toarray()
       df.drop(['Day', 'Route', 'Direction', 'Part of Day'], axis=1, inplace=True)
       return df
[]: df = one_hot_encoder(df)
[]: df
            Min Delay Min Gap Friday Monday ... afternoon evening morning
[]:
     night
                  4.0
                            8.0
                                    0.0
                                            0.0 ...
     0
                                                           0.0
                                                                     0.0
                                                                              1.0
     0.0
                                            0.0 ...
                 20.0
                           22.0
                                    0.0
                                                           1.0
                                                                     0.0
                                                                              0.0
     1
```

0.0							
2	13.0	19.0	0.0	0.0	1.0	0.0	0.0
0.0							
3	7.0	11.0	0.0	0.0	1.0	0.0	0.0
0.0							
4	3.0	6.0	0.0	0.0	1.0	0.0	0.0
0.0							
•••	•••			•••	•••		
71507	8.0	16.0	0.0	0.0	0.0	0.0	1.0
0.0							
71508	7.0	14.0	0.0	0.0	0.0	0.0	1.0
0.0							
71509	5.0	10.0	0.0	0.0	0.0	0.0	1.0
0.0							
71510	5.0	10.0	0.0	0.0	0.0	0.0	1.0
0.0							
71511	9.0	16.0	0.0	0.0	0.0	0.0	1.0
0.0							

[71512 rows x 32 columns]

1.1 Need to do feature scaling for Min Gap column feature

```
[]: # Feature Standardization, which means changing between -1 and 1, such that
     →algorithm can coverge swiftly
     min_gap_train_mean = np.mean(df["Min Gap"])
     min_gap_train_std = np.std(df["Min Gap"])
     print(min_gap_train_mean)
     print(min_gap_train_std)
     def min_gap_scaler(df):
       df["Min Gap"] = (df["Min Gap"]-min_gap_train_mean)/min_gap_train_std
       return df
    18.13560073354417
    33.68768666213863
[]: df = min_gap_scaler(df)
[]: df.head()
[]:
       Min Delay
                   Min Gap Friday Monday ...
                                                afternoon
                                                           evening morning night
             4.0 -0.300870
                                0.0
                                        0.0 ...
                                                      0.0
                                                               0.0
                                                                        1.0
                                                                               0.0
     1
            20.0 0.114713
                                0.0
                                        0.0 ...
                                                      1.0
                                                               0.0
                                                                        0.0
                                                                               0.0
     2
            13.0 0.025659
                                0.0
                                        0.0 ...
                                                      1.0
                                                               0.0
                                                                        0.0
                                                                               0.0
                                        0.0 ...
             7.0 -0.211816
                                0.0
                                                      1.0
                                                               0.0
                                                                        0.0
                                                                               0.0
```

```
4 3.0 -0.360238 0.0 0.0 ... 1.0 0.0 0.0 0.0
```

[5 rows x 32 columns]

2 The data is ready for training

```
[]: def complete_data_preprocessing(df):
    # This function is for test set
    df = complete_cleaner(df)
    df = one_hot_encoder(df) # one hot encoder based on training samples
    df = min_gap_scaler(df) # feature scaler based on training sample
    print("-----")
    if df.isnull().values.any():
        print("There are some null values")
    else:
        print("Data is ready for testing")
    return df
```

```
[]: processed_test_data = complete_data_preprocessing(test_df)
```

```
Data is ready for testing

/usr/local/lib/python3.7/dist-packages/ipykernel_launcher.py:16:
SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy app.launch_new_instance()
/usr/local/lib/python3.7/dist-packages/ipykernel_launcher.py:18:
SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
```

2.0.1 The regression results function computes the different metrics like r2 score, MAE, and RMSE.

```
[]: import sklearn.metrics as metrics
def regression_results(y_true, y_pred):
    # Regression metrics
    mean_absolute_error=metrics.mean_absolute_error(y_true, y_pred)
    mse=metrics.mean_squared_error(y_true, y_pred)
```

```
r2 = metrics.r2_score(y_true, y_pred)
print("R2:", round(r2, 4))
print('MAE: ', round(mean_absolute_error,4))
print('RMSE: ', round(np.sqrt(mse),4))
]: # Selected features for model training
```

```
[]: # Selected features for model training
selected_features = list(df.columns)
selected_features.remove("Min Delay")
target = "Min Delay"
```

Training and validation dataset will be used throughout the model selection and fine tuning process Final test set has been kept seperate, it will be used only after the model is finalized.

```
[]: def evaluate_model(model):
    print("Training Regression results:")
    regression_results(y_train, model.predict(X_train))
    print("\n")
    print("Validation Regression results")
    regression_results(y_val, model.predict(X_val))
```

Model 1 - Simple linear regression

```
[]: lin_reg = LinearRegression()
    lin_reg.fit(X_train, y_train)
    print("Linear regression results")
    evaluate_model(lin_reg)
```

Linear regression results
Training Regression results:

R2: 0.6239 MAE: 3.9846 RMSE: 18.5552

Validation Regression results

R2: 0.8012 MAE: 3.799 RMSE: 11.0773

Model 2 - Polynomial regression of degree 2

```
[]: poly_2 = PolynomialFeatures(degree = 2)
     X_poly_2 = poly_2.fit_transform(X)
     poly_2.fit(X_poly_2, y)
     X_poly_2_train, X_poly_2_val, y_train_poly_2, y_val_poly_2 = train_test_split(
         X_poly_2,
         у,
         test_size=0.1,
         random_state=42)
     reg 2 = LinearRegression()
     reg_2.fit(X_poly_2_train, y_train_poly_2)
     print("Training polynomial Regression of degree 2 results:")
     regression_results(y_train_poly_2, reg_2.predict(X_poly_2_train))
     print("\n")
     print("Validation polynomial Regression of degree 2 results")
     regression_results(y_val_poly_2, reg_2.predict(X_poly_2_val))
    Training polynomial Regression of degree 2 results:
    R2: 0.8298
    MAE: 2.9791
    RMSE: 12.4826
    Validation polynomial Regression of degree 2 results
    R2: 0.852
    MAE: 2.9469
    RMSE: 9.558
    Model 3 - Bayesian regression
[]: from sklearn import linear_model
```

```
[]: from sklearn import linear_model
X_train, X_val, y_train, y_val = train_test_split(X, y, test_size=0.1, u → random_state=42)

BayReg = linear_model.BayesianRidge()
BayReg.fit(X_train, y_train)
print("Bayesian regression results")
evaluate_model(BayReg)
```

Bayesian regression results Training Regression results:

R2: 0.6239 MAE: 3.9854 RMSE: 18.5552 Validation Regression results

R2: 0.8011 MAE: 3.7998 RMSE: 11.0804

Model 4 - SVM Regressor

Model 5 - Random Forest

```
[]: from sklearn.ensemble import RandomForestRegressor
X_train, X_val, y_train, y_val = train_test_split(X, y, test_size=0.1, u → random_state=42)
rf = RandomForestRegressor(random_state=42)
rf.fit(X_train, y_train)
print("Random Forest regression results")
evaluate_model(rf)
```

Random Forest regression results

Training Regression results:

R2: 0.9382 MAE: 1.3267 RMSE: 7.523

Validation Regression results

R2: 0.7878 MAE: 2.3279 RMSE: 11.4465

10

Model 6 - Neural Network

MAE: 2.1503 RMSE: 8.9268

```
[]: from sklearn.neural_network import MLPRegressor
     X_train, X_val, y_train, y_val = train_test_split(X, y, test_size=0.1,_
     →random_state=42)
     nn = MLPRegressor(random_state=1, max_iter=500).fit(X_train, y_train)
     print("Neural network regression results")
     evaluate_model(nn)
    Neural network regression results
    Training Regression results:
    R2: 0.8424
    MAE: 2.7425
    RMSE: 12.0125
    Validation Regression results
    R2: 0.8636
    MAE: 2.6741
    RMSE: 9.177
    Model 7 - XGBoost
[]: from sklearn.ensemble import GradientBoostingRegressor
     X_train, X_val, y_train, y_val = train_test_split(X, y, test_size=0.1,_
     →random state=42)
     boost = GradientBoostingRegressor().fit(X_train, y_train)
     print("Gradient Boosting network regression results")
     evaluate_model(boost)
    Gradient Boosting network regression results
    Training Regression results:
    R2: 0.876
    MAE: 2.1704
    RMSE: 10.6554
    Validation Regression results
    R2: 0.8709
```

3 K-Fold Cross validation

3.1 Cross validation function for model training

```
[]: def cross_validation(model, X, y, n=10): # default 10 splits
      from sklearn.model selection import KFold
      kf = KFold(n splits=n)
      kf.get_n_splits(X)
      train_scores = {}
      val_scores = {}
      train_scores["R2"], train_scores["MAE"] ,train_scores["RMSE"] = [], [], []
      val_scores["R2"], val_scores["MAE"], val_scores["RMSE"] = [], [], []
      model_count = 1
      for train_index, val_index in kf.split(X):
        X_train, X_val = X.loc[train_index], X.loc[val_index]
        y_train, y_val = y[train_index], y[val_index]
        model.fit(X_train, y_train)
        print("Model {} trained".format(model_count))
        print("Training Scores")
        print("R2 Score : {} \t MAE : {} \t RMSE : {}".format(round(metrics.
     →r2_score(y_train, model.predict(X_train)),4),
                                                             round(metrics.
     →mean_absolute_error(y_train, model.predict(X_train)),4),
                                                             round(np.sqrt(metrics.
     →mean_squared_error(y_train, model.predict(X_train))),4)
                                                             ))
        print("Validation Scores")
        print("R2 Score : {} \t MAE : {} \t RMSE : {}".format(round(metrics.
     →r2_score(y_val, model.predict(X_val)),4),
                                                             round(metrics.
     →mean_absolute_error(y_val, model.predict(X_val)),4),
                                                             round(np.sqrt(metrics.
     →mean_squared_error(y_val, model.predict(X_val))),4)
        train_scores["R2"].append(round(metrics.r2_score(y_train, model.
     →predict(X_train)),4))
        train_scores["MAE"].append(round(metrics.mean_absolute_error(y_train, model.
     →predict(X_train)),4))
        train scores["RMSE"].append(round(np.sqrt(metrics.
     →mean_squared_error(y_train, model.predict(X_train))),4))
        val_scores["R2"].append(round(metrics.r2_score(y_val, model.
      →predict(X_val)),4))
```

```
[]: def print_results(train_scores, val_scores):
         train\_scores, and val\_scores should be a dictionary containing R2, MAE and
     \hookrightarrow RMSE
      11 11 11
      print("\n")
      print("Mean and standard deviation of {}-fold cross validation results".
     →format(len(train scores["R2"])))
      print("-----
      print("Train Mean R2 Score: \t {} \t\t Validation Mean R2 Score: \t {}".

→format(round(np.mean(train_scores["R2"]),4), round(np.
     →mean(val_scores["R2"]),4)))
      print("Train Std R2 Score: \t {} \t\t Validation Std R2 Score: \t {}".

→format(round(np.std(train scores["R2"]),4), round(np.

std(val_scores["R2"]),4)))
      print("\n")
      print("Train Mean MAE Score: \t {} \t\t Validation Mean MAE Score: \t {}".

→format(round(np.mean(train_scores["MAE"]),4), round(np.
     →mean(val_scores["MAE"]),4)))
      print("Train Std MAE Score: \t {} \t\t Validation Std MAE Score: \t {}".

→format(round(np.std(train_scores["MAE"]),4), round(np.

std(val_scores["MAE"]),4)))
      print("\n")
      print("Train Mean RMSE Score: \t {} \t\t Validation Mean RMSE Score: \t {}".

→format(round(np.mean(train_scores["RMSE"]),4), round(np.
     →mean(val_scores["RMSE"]),4)))
      print("Train Std RMSE Score: \t {} \t\t Validation Std RMSE Score: \t {}".

→format(round(np.std(train_scores["RMSE"]),4), round(np.
```

3.2 Linear regression

```
[]: train_scores, val_scores = cross_validation(LinearRegression(), X, y, 10)
```

Model 1 trained			
Training Scores			
R2 Score : 0.6216	MAE : 3.9786	RMSE :	18.4698
Validation Scores			
R2 Score : 0.7948	MAE : 3.8018	RMSE :	12.3318
********	******	*****	
Model 2 trained			
Training Scores			
R2 Score : 0.6201	MAE : 3.9552	RMSE :	18.1851
Validation Scores			
R2 Score : 0.756	MAE : 4.2323	RMSE :	15.7741
*******	******	*****	
Model 3 trained			
Training Scores			
R2 Score : 0.6266	MAE : 3.8001	RMSE :	17.9763
Validation Scores			
R2 Score : 0.7073	MAE : 4.2025	RMSE :	17.6362
*******	******	*****	
Model 4 trained			
Training Scores			
R2 Score : 0.6221	MAE : 3.9856	RMSE :	18.3186
Validation Scores			
R2 Score : 0.7646	MAE : 4.0355	RMSE :	14.2505
*******	******	*****	
Model 5 trained			
Training Scores			
R2 Score : 0.8285	MAE : 2.6946	RMSE :	12.3923
Validation Scores			
R2 Score : -1.8484	MAE : 3.417	RMSE :	47.584
*******	******	*****	
Model 6 trained			
Training Scores			
R2 Score : 0.6222	MAE : 4.0218	RMSE :	17.8355
Validation Scores			
R2 Score : 0.7146	MAE : 4.407	RMSE :	19.0997

Model 7 trained			
Training Scores			
R2 Score : 0.6267	MAE : 4.03	RMSE :	18.7283
Validation Scores			
R2 Score : 0.8398	MAE : 3.563	RMSE :	7.9691

Model 8 trained			
Training Scores			
R2 Score : 0.6207	MAE : 4.0756	RMSE :	18.3995
Validation Scores			
R2 Score : 0.7859	MAE : 3.4817	RMSE :	13.2421

Model 9 trained

Training Scores

R2 Score : 0.6175 MAE : 4.0498 RMSE : 18.5795

Validation Scores

R2 Score : 0.8417 MAE : 3.6346 RMSE : 10.7612

Model 10 trained Training Scores

R2 Score : 0.5989 MAE : 4.0737 RMSE : 18.5448

Validation Scores

R2 Score : 0.8809 MAE : 4.2483 RMSE : 11.6323

[]: print("Linear Regression results : ") print_results(train_scores, val_scores)

Linear Regression results :

Mean and standard deviation of 10-fold cross validation results

Train Mean R2 Score: 0.6405 Validation Mean R2 Score:

0.5237

Train Std R2 Score: 0.0631 Validation Std R2 Score:

0.7925

Train Mean MAE Score: 3.8665 Validation Mean MAE Score:

3.9024

Train Std MAE Score: 0.3979 Validation Std MAE Score:

0.3465

Train Mean RMSE Score: 17.743 Validation Mean RMSE Score:

17.0281

Train Std RMSE Score: 1.8026 Validation Std RMSE Score:

10.6511

3.3 Bayesian regression

[]: train_scores, val_scores = cross_validation(linear_model.BayesianRidge(), X, y, ⊔ →10)

Model 1 trained Training Scores

R2 Score : 0.6216 MAE : 3.9792 RMSE : 18.4699

Validation Scores

R2 Score : 0.7947 MAE : 3.8023 RMSE : 12.3347

********	*******	*****				
Model 2 trained						
Training Scores						
R2 Score : 0.6201	MAF · 3 9595	RMSF · 18 1852				
Validation Scores	IME . 0.0000	18.10.1002				
	MAE : 4.2339	RMSF · 15 7749				

Model 3 trained						
Training Scores						
R2 Score : 0.6266	MAE . 2 001	DMCE . 17 0762				
Validation Scores	MAE . 5.001	WISE . 17.9703				
R2 Score: 0.7073	MAE . 4 0020	DMCE . 17 6262				
	MAE: 4.2038					
**************************************	*****	*****				
Model 4 trained						
Training Scores	MAT . 2 OOCE	DMGE . 10 0100				
	MAE : 3.9865	RMSE : 18.3186				
Validation Scores	MAR 4 0055	DVGD 44 0507				
R2 Score : 0.7645						
*********	******	*****				
Model 5 trained						
Training Scores						
R2 Score : 0.8285	MAE : 2.6946	RMSE : 12.3923				
Validation Scores						
R2 Score : -1.8479	MAE : 3.4173	RMSE : 47.5796				
*********	******	*****				
Model 6 trained						
Training Scores						
R2 Score : 0.6222	MAE : 4.0227	RMSE : 17.8356				
Validation Scores						
R2 Score : 0.7145	MAE : 4.4076	RMSE : 19.1025				

Model 7 trained						
Training Scores						
R2 Score : 0.6267	MAE : 4.0309	RMSE : 18.7284				
R2 Score : 0.6267 Validation Scores	MAE : 4.0309	RMSE : 18.7284				
Validation Scores	MAE : 3.5633	RMSE : 7.9706				
Validation Scores R2 Score : 0.8397	MAE : 3.5633	RMSE : 7.9706				
Validation Scores R2 Score: 0.8397 *********** Model 8 trained Training Scores	MAE : 3.5633 *******	RMSE : 7.9706				
Validation Scores R2 Score: 0.8397 ************************************	MAE : 3.5633 *******	RMSE : 7.9706				
Validation Scores R2 Score: 0.8397 *********** Model 8 trained Training Scores	MAE : 3.5633 *******	RMSE : 7.9706				
Validation Scores R2 Score: 0.8397 ************************** Model 8 trained Training Scores R2 Score: 0.6207	MAE : 3.5633 ******** MAE : 4.0764	RMSE : 7.9706 ****** RMSE : 18.3996				
Validation Scores R2 Score: 0.8397 ************** Model 8 trained Training Scores R2 Score: 0.6207 Validation Scores	MAE : 3.5633 ******* MAE : 4.0764 MAE : 3.4828	RMSE : 7.9706 ****** RMSE : 18.3996 RMSE : 13.2443				
Validation Scores R2 Score: 0.8397 ************************** Model 8 trained Training Scores R2 Score: 0.6207 Validation Scores R2 Score: 0.7859	MAE : 3.5633 ******* MAE : 4.0764 MAE : 3.4828	RMSE : 7.9706 ****** RMSE : 18.3996 RMSE : 13.2443				
Validation Scores R2 Score: 0.8397 ************************** Model 8 trained Training Scores R2 Score: 0.6207 Validation Scores R2 Score: 0.7859 ************************************	MAE : 3.5633 ******* MAE : 4.0764 MAE : 3.4828	RMSE : 7.9706 ****** RMSE : 18.3996 RMSE : 13.2443				
Validation Scores R2 Score: 0.8397 ************************** Model 8 trained Training Scores R2 Score: 0.6207 Validation Scores R2 Score: 0.7859 ************************************	MAE : 3.5633 ******* MAE : 4.0764 MAE : 3.4828 *****	RMSE: 7.9706 ****** RMSE: 18.3996 RMSE: 13.2443 ******				
Validation Scores R2 Score: 0.8397 ************************** Model 8 trained Training Scores R2 Score: 0.6207 Validation Scores R2 Score: 0.7859 ************************************	MAE : 3.5633 ******* MAE : 4.0764 MAE : 3.4828 *****	RMSE: 7.9706 ****** RMSE: 18.3996 RMSE: 13.2443 ******				
Validation Scores R2 Score: 0.8397 ************************************	MAE : 3.5633 ******* MAE : 4.0764 MAE : 3.4828 ****** MAE : 4.0507	RMSE: 7.9706 ****** RMSE: 18.3996 RMSE: 13.2443 ******* RMSE: 18.5795				

Model 10 trained Training Scores

R2 Score : 0.5989 MAE : 4.0748 RMSE : 18.5448

Validation Scores

R2 Score : 0.8808 MAE : 4.2496 RMSE : 11.635

[]: print("Bayesian Regression results : ") print_results(train_scores, val_scores)

Bayesian Regression results :

Mean and standard deviation of 10-fold cross validation results

Train Mean R2 Score: 0.6405 Validation Mean R2 Score:

0.5237

Train Std R2 Score: 0.0631 Validation Std R2 Score:

0.7923

Train Mean MAE Score: 3.8676 Validation Mean MAE Score:

3.9032

Train Std MAE Score: 0.3983 Validation Std MAE Score:

0.3467

Train Mean RMSE Score: 17.743 Validation Mean RMSE Score:

17.0293

Train Std RMSE Score: 1.8026 Validation Std RMSE Score:

10.6492

3.4 Random Forest regression

3.4.1 With default parameters

Model 1 trained Training Scores

R2 Score: 0.936 MAE: 1.3269 RMSE: 7.5963

Validation Scores

R2 Score : 0.8438 MAE : 2.5018 RMSE : 10.758

Model 2 trained

Training Scores R2 Score : 0.9392 MAE : 1.3003 RMSE : 7.2726 Validation Scores R2 Score : 0.7908 MAE : 2.7948 RMSE: 14.6076 ************** Model 3 trained Training Scores MAE : 1.3428 RMSE : 7.7094 R2 Score : 0.9313 Validation Scores R2 Score : 0.8554 MAE : 2.4851 RMSE: 12.3964 ************** Model 4 trained Training Scores R2 Score : 0.942 MAE : 1.3253 RMSE: 7.1799 Validation Scores R2 Score : 0.8146 MAE : 2.1795 RMSE : 12.6465 ************ Model 5 trained Training Scores R2 Score : 0.9398 MAE : 1.301 RMSE : 7.3453 Validation Scores R2 Score : 0.5226 MAE : 2.8284 RMSE: 19.481 ************* Model 6 trained Training Scores R2 Score : 0.9434 MAE : 1.2755 RMSE : 6.9034 Validation Scores R2 Score : 0.736 MAE : 2.9011 RMSE: 18.3674 ************* Model 7 trained Training Scores R2 Score : 0.934 MAE : 1.3915 RMSE: 7.8732 Validation Scores R2 Score : 0.8035 MAE : 1.9532 RMSE: 8.8249 ************* Model 8 trained Training Scores R2 Score : 0.9353 MAE : 1.3866 RMSE : 7.5979 Validation Scores R2 Score : 0.8439 MAE : 1.6439 RMSE: 11.306 ************** Model 9 trained Training Scores R2 Score : 0.9309 MAE : 1.3724 RMSE: 7.8973 Validation Scores R2 Score : 0.8997 MAE : 2.0552 RMSE: 8.5652 ************* Model 10 trained

Training Scores

R2 Score : 0.9261 MAE : 1.3753 RMSE : 7.9614

Validation Scores

R2 Score : 0.9374 MAE : 2.2813 RMSE : 8.4341

[]: print("Random Forest regression results") print_results(train_scores, val_scores)

Random Forest regression results

Mean and standard deviation of 10-fold cross validation results

Train Mean R2 Score: 0.9358 Validation Mean R2 Score:

0.8048

Train Std R2 Score: 0.0052 Validation Std R2 Score:

0.1081

Train Mean MAE Score: 1.3398 Validation Mean MAE Score:

2.3624

Train Std MAE Score: 0.0384 Validation Std MAE Score:

0.3933

Train Mean RMSE Score: 7.5337 Validation Mean RMSE Score:

12.5387

Train Std RMSE Score: 0.331 Validation Std RMSE Score: 3.7095

3.5 Gradient Boosting regression

3.5.1 With default parameters

[]: from sklearn.ensemble import GradientBoostingRegressor train_scores, val_scores = cross_validation(GradientBoostingRegressor(), X, y, ⊔ →10)

Model 1 trained Training Scores

R2 Score : 0.8717 MAE : 2.1268 RMSE : 10.755

Validation Scores

R2 Score : 0.8678 MAE : 2.4526 RMSE : 9.8983

Model 2 trained Training Scores

R2 Score : 0.8795 MAE : 2.0974 RMSE : 10.2405

Validation Scores

R2 Score : 0.827	MAE :	2.6866	RMSE :	13.2818
********	*****	******	*****	
Model 3 trained				
Training Scores				
R2 Score : 0.8629	MAE :	2.159	RMSE :	10.8944
Validation Scores				
R2 Score : 0.8872		2.5061		10.9496
*********	*****	*******	*****	
Model 4 trained				
Training Scores				
R2 Score : 0.8764	MAE :	2.1553	RMSE :	10.4759
Validation Scores				
R2 Score : 0.8327		2.2145		12.0133
*********	*****	*******	*****	
Model 5 trained				
Training Scores				
R2 Score : 0.8876	MAE :	2.1058	RMSE :	10.0339
Validation Scores				
R2 Score : 0.6278		2.6106		17.2006
********	*****	********	*****	
Model 6 trained				
Training Scores				
R2 Score : 0.8899	MAE :	2.0705	RMSE :	9.6293
Validation Scores				
R2 Score : 0.7867	MAE :	2.6321	RMSE :	16.5122
********	*****	********	*****	
Model 7 trained				
Training Scores				
R2 Score : 0.8716	MAE :	2.2348	RMSE :	10.9837
Validation Scores				
R2 Score : 0.8654	MAE :	1.8158	RMSE :	7.3045
********	*****	********	*****	
Model 8 trained				
Training Scores				
R2 Score : 0.8734	MAE :	2.2182	RMSE :	10.629
Validation Scores				
R2 Score : 0.8581	MAE :	1.6427	RMSE :	10.7821
********	*****	******	*****	
Model 9 trained				
Training Scores				
R2 Score : 0.8628	MAE :	2.2012	RMSE :	11.1295
Validation Scores				
R2 Score : 0.9203	MAE :	1.9805	RMSE :	7.6348
********	*****	*******	*****	
Model 10 trained				
Training Scores				
R2 Score : 0.8565	MAE :	2.1976	RMSE :	11.0939
Validation Scores				

R2 Score : 0.9683 MAE : 2.1003 RMSE : 6.0022

[]: print("XGBoost regression results")
print_results(train_scores, val_scores)

XGBoost regression results

Mean and standard deviation of 10-fold cross validation results

Train Mean R2 Score: 0.8732 Validation Mean R2 Score:

0.8441

Train Std R2 Score: 0.0102 Validation Std R2 Score:

0.0865

Train Mean MAE Score: 2.1567 Validation Mean MAE Score:

2.2642

Train Std MAE Score: 0.0529 Validation Std MAE Score:

0.35

Train Mean RMSE Score: 10.5865 Validation Mean RMSE Score:

11.1579

Train Std RMSE Score: 0.4678 Validation Std RMSE Score:

3.5502

3.6 Neural Network regression

3.6.1 Default is 1 hidden layer with 100 neurons

Model 1 trained

Training Scores

R2 Score : 0.8442 MAE : 2.6132 RMSE : 11.8528

Validation Scores

R2 Score : 0.844 MAE : 2.8365 RMSE : 10.7524

Model 2 trained Training Scores

R2 Score : 0.8553 MAE : 2.0893 RMSE : 11.2233

Validation Scores

R2 Score : 0.8328 MAE : 2.4967 RMSE : 13.0572

Model 3 trained

Training Scores

R2 Score : 0.8337 MAE : 2.6943 RMSE : 11.9967

Validation Scores

R2 Score : 0.9152 MAE : 2.7922 RMSE : 9.4942

Model 4 trained Training Scores

R2 Score : 0.8565 MAE : 2.3367 RMSE : 11.2896

Validation Scores

R2 Score : 0.8268 MAE : 2.4525 RMSE : 12.2233

/usr/local/lib/python3.7/dist-

packages/sklearn/neural_network/_multilayer_perceptron.py:571:

ConvergenceWarning: Stochastic Optimizer: Maximum iterations (500) reached and the optimization hasn't converged yet.

% self.max_iter, ConvergenceWarning)

Model 5 trained

Training Scores

R2 Score : 0.8811 MAE : 2.6773 RMSE : 10.3188

Validation Scores

R2 Score : 0.6288 MAE : 3.0712 RMSE : 17.177

Model 6 trained

Training Scores

R2 Score : 0.8545 MAE : 2.7583 RMSE : 11.0693

Validation Scores

R2 Score: 0.7661 MAE: 3.2038 RMSE: 17.2891

Model 7 trained

Training Scores

R2 Score : 0.8517 MAE : 2.6029 RMSE : 11.8045

Validation Scores

R2 Score : 0.8762 MAE : 2.3416 RMSE : 7.004

Model 8 trained

Training Scores

R2 Score : 0.8421 MAE : 3.4655 RMSE : 11.8719

Validation Scores

R2 Score : 0.8178 MAE : 3.0049 RMSE : 12.2158

Model 9 trained

Training Scores

R2 Score : 0.839 MAE : 2.7145 RMSE : 12.0548

Validation Scores

R2 Score : 0.9034 MAE : 2.6728 RMSE : 8.4049

Model 10 trained Training Scores

R2 Score : 0.8261 MAE : 2.698 RMSE : 12.2111

Validation Scores

R2 Score : 0.971 MAE : 2.6819 RMSE : 5.741

[]: print("Neural network regression results") print_results(train_scores, val_scores)

Neural network regression results

Mean and standard deviation of 10-fold cross validation results

Train Mean R2 Score: 0.8484 Validation Mean R2 Score:

0.8382

Train Std R2 Score: 0.0145 Validation Std R2 Score:

0.0888

Train Mean MAE Score: 2.665 Validation Mean MAE Score: 2.7554

Train Std MAE Score: 0.3316 Validation Std MAE Score:

0.267

Train Mean RMSE Score: 11.5693 Validation Mean RMSE Score:

11.3359

Train Std RMSE Score: 0.554 Validation Std RMSE Score: 3.6943

3.7 Neural Network regression

3.7.1 2 hidden layer with 64 neurons and 32 neurons

Model 1 trained Training Scores

R2 Score : 0.8537 MAE : 2.4604 RMSE : 11.4837

Validation Scores

R2 Score : 0.8638 MAE : 2.7862 RMSE : 10.0478

Model 2 trained

Training Scores

R2 Score : 0.8425 MAE : 3.1197 RMSE : 11.7073

Validation Scores R2 Score : 0.8267 MAE : 3.4537 RMSE: 13.2953 ************* Model 3 trained Training Scores R2 Score : 0.8329 MAE : 2.6483 RMSE : 12.0261 Validation Scores R2 Score : 0.9025 MAE : 2.8511 RMSE: 10.1812 ************** Model 4 trained Training Scores R2 Score : 0.8446 MAE : 3.3345 RMSE: 11.7464 Validation Scores R2 Score : 0.8172 MAE : 3.3833 RMSE: 12.5576 ************** Model 5 trained Training Scores R2 Score : 0.8849 MAE: 2.3674 RMSE: 10.1522 Validation Scores R2 Score : 0.592 MAE : 2.8878 RMSE: 18.0079 ************ Model 6 trained Training Scores RMSE : 10.7184 R2 Score : 0.8635 MAE : 2.456 Validation Scores R2 Score : 0.7768 MAE : 3.0608 RMSE: 16.889 ************** Model 7 trained Training Scores R2 Score : 0.8505 MAE : 2.8334 RMSE: 11.8505 Validation Scores R2 Score : 0.8768 MAE : 2.6092 RMSE: 6.9869 ************** Model 8 trained Training Scores R2 Score : 0.8533 MAE : 2.7682 RMSE: 11.4416 Validation Scores R2 Score : 0.8308 MAE : 2.4281 RMSE: 11.7737 ************** Model 9 trained Training Scores R2 Score : 0.8372 MAE : 3.972 RMSE: 12.1236 Validation Scores R2 Score : 0.8973 MAE : 3.7011 RMSE: 8.6678 ************** Model 10 trained Training Scores R2 Score : 0.833 MAE : 3.017 RMSE: 11.9659

Validation Scores

R2 Score : 0.9709 MAE : 2.8536 RMSE : 5.7455

[71]: print("Neural network regression results")

print_results(train_scores, val_scores)

Neural network regression results

Mean and standard deviation of 10-fold cross validation results

Train Mean R2 Score: 0.8496 Validation Mean R2 Score:

0.8355

Train Std R2 Score: 0.015 Validation Std R2 Score: 0.0961

Train Mean MAE Score: 2.8977 Validation Mean MAE Score:

3.0015

Train Std MAE Score: 0.4647 Validation Std MAE Score:

0.3781

Train Mean RMSE Score: 11.5216 Validation Mean RMSE Score:

11.4153

Train Std RMSE Score: 0.5946 Validation Std RMSE Score:

3.7562