Regression Models to Predict the Bio-activities of Different Compounds from the SARS-COVID 19 Database of ChEMBL

Here we are trying to predict the bio activities of different compounds from the SARS-COVID 19 database of ChEMBL. We have fitted the data to five different models and evaluated the fitting of the data in the model using the root mean squared error.
We download the database from https://www.ebi.ac.uk/chembl/ in csv format. Then we store this data as pandas DataFrame.
There are 6900 samples in the dataset with 30 features and corresponding 6900 labels (Bio-activities).

Data Cleaning

Then we go on to clean the dataset.
We drop 15 features that have very low correlation with the labels and also features which have Nan or None entry. We also drop all samples that have molecular weights less than 500. We have also dropped a sample which was an outlier. After cleaning the dataset, we have got 5655 samples with 15 features and 5655 corresponding labels.

Helper Functions

Next we go on to define some helper functions that does data splitting, fitting and visualizing much easier.

split(test_size = 0.2, poly_degree = 1)

This function the dataset after data cleaning and splits the data into four sets using the parameter `test_size`: training_samples, training_labels, testing_samples, tesing_labels using the function `train_test_split()` that Scikit-Learn provides. This function also creates polynomial degrees using the `PolynomialFeatures()` function of Scikit-Learn. The degree of the polynomial features is chosen using the parameter `poly_degree`. This function also scales the dataset using the `StandardScaler()` function of Scikit-Learn.

Parameters

test_size : *float or int, default=0.2*
If float, should be between 0.0 and 1.0 and represent the proportion of the dataset to include in the test split. If int, represents the absolute number of test samples.

poly_degree : int, default=1
The degree of the polynomial features.

model_score(model, data)

This function outputs the root mean squared error of the predicted values to the true values of the training set and test set. This function also outputs the mean of the 5-fold cross validation score done on the training set using the `cross_val_score()` of Scikit-Learn.

Parameters

model : *Scikit-Learn model with .predict() method*
Eg. sklearn.linear_model.LinearRegression()

data: python dictionary containing X_train, y_train, X_test, y_test
Output of split()

plot_train_prediction(model, data)

This function outputs the scatter plot of predictions made by the `model.predict()` method in the testing samples (y-axis) vs the true testing labels. This function also plots an orange y=x line to show the fitting line in case of a perfect fit.

Parameters

model : *Scikit-Learn model with .predict() method*
Eg. sklearn.linear_model.LinearRegression()

data: python dictionary containing X_train, y_train, X_test, y_test
Output of split()

plot_learning_curve(model, data)

This function plots the root mean squared error of both the training data and the cross validation data vs different training set size using the `learning_curve()` function of Scikit-Learn.

Parameters

model : ***Scikit-Learn model with .predict() method***
Eg. sklearn.linear_model.LinearRegression()

data: python dictionary containing X_train, y_train, X_test, y_test
Output of split()

plot(model_name, max_degree)

This function generates `plot_train_prediction()`, `plot_test_prediction()`, `plot_learning_curve()` for a model trained in `max_degree` polynomial features.

Parameters

model_name : ***str***
name of the model to be plotted

max_degree: int
The maximum degree of polynomial features.

Models

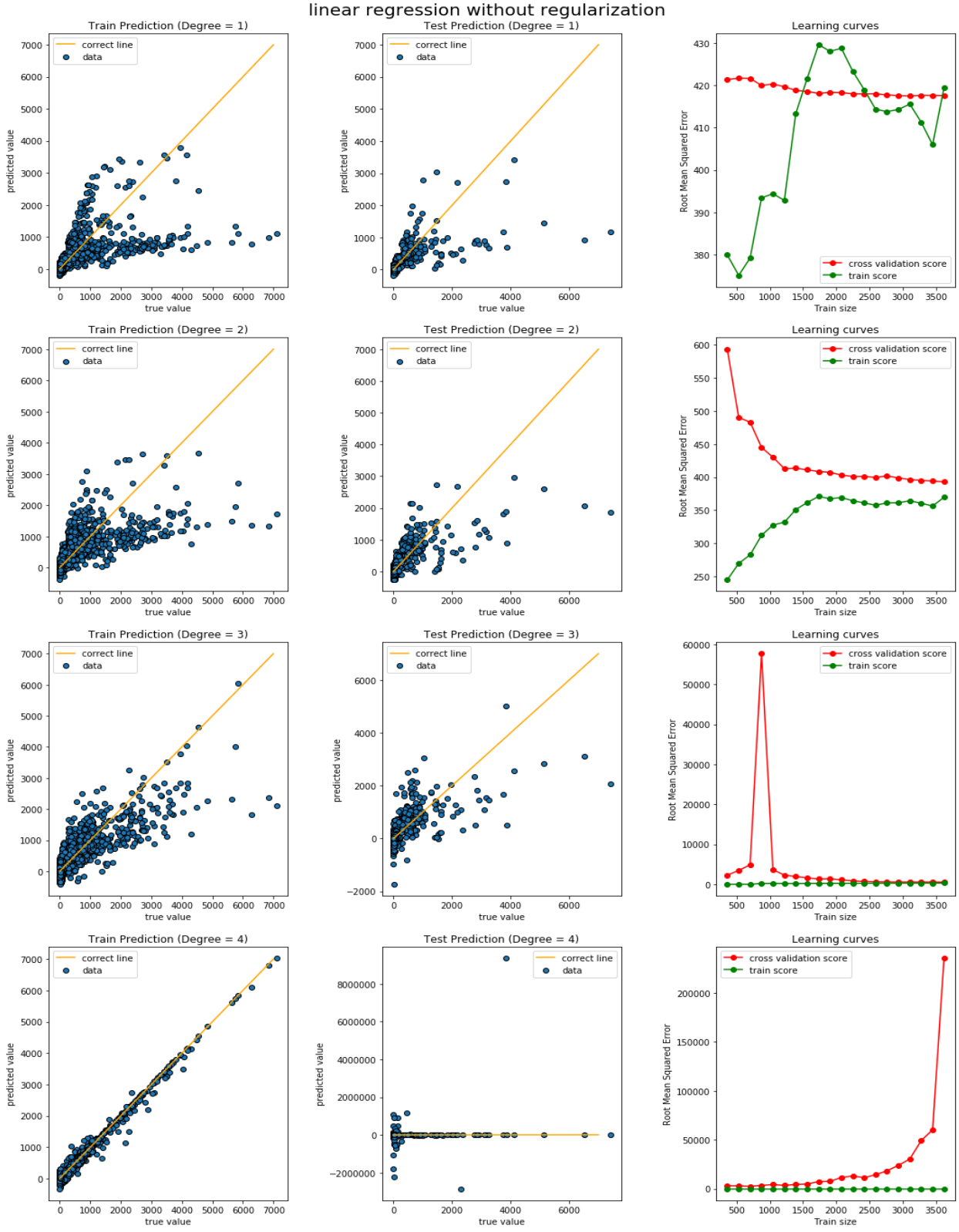
Here we fit the data (with polynomial degrees upto 4 degrees) into five different models and compare their scores.

- Linear regression without regularization
- Linear regression with regularization or Ridge regression
- Decision tree
- Bayesian Regression

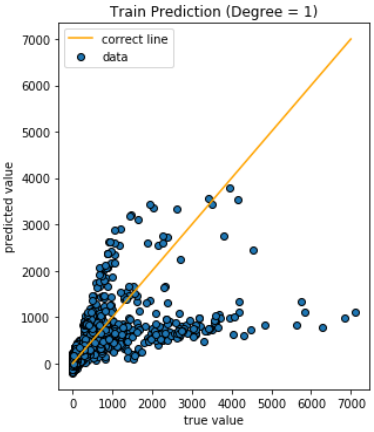
Training fit, testing fit and the learning curve has been plotted for all five models fitted in upto 4 degrees of polynomial features.

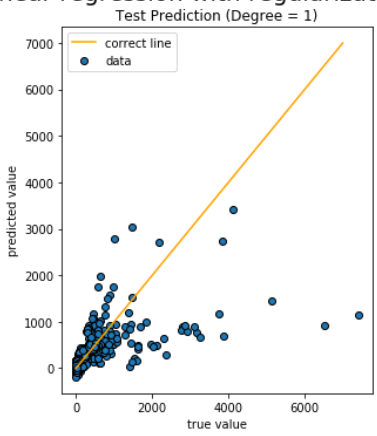
Results

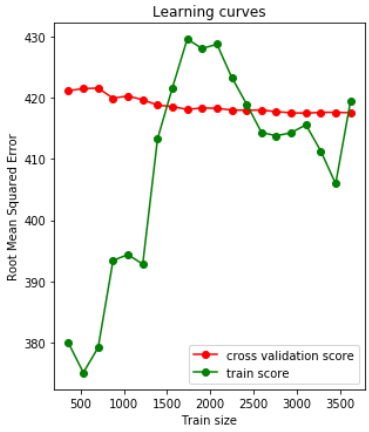
linear regression without regularization

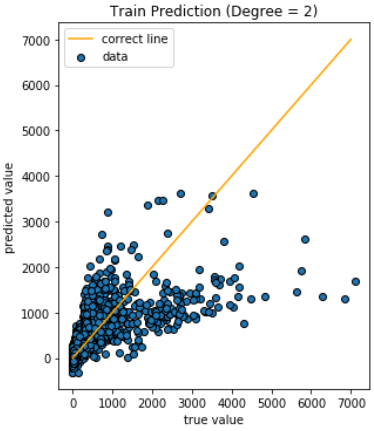


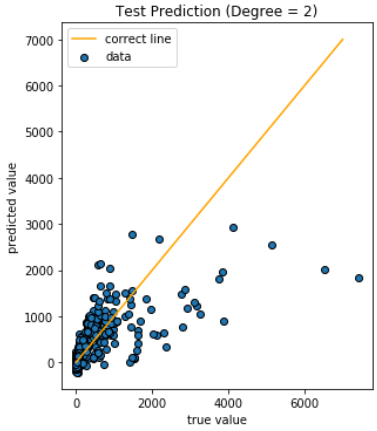
linear regression with regularization

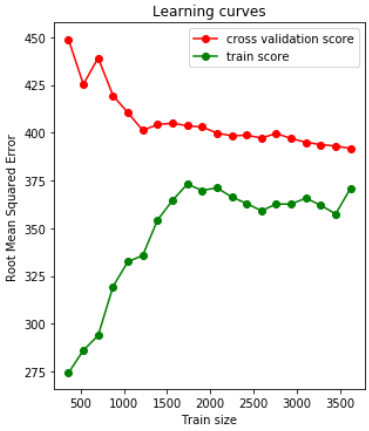


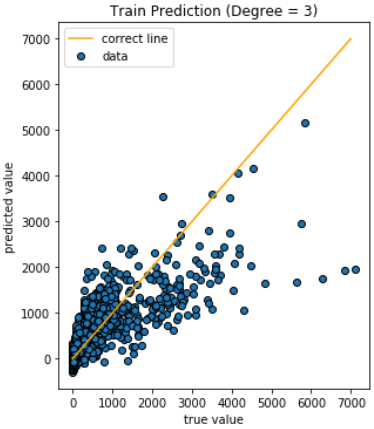


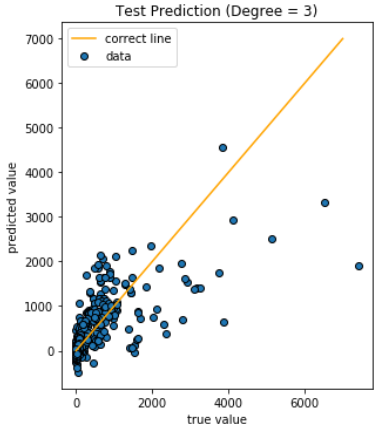


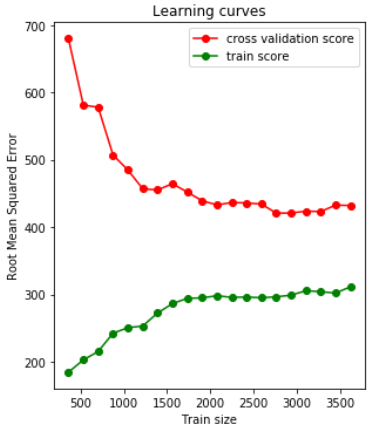


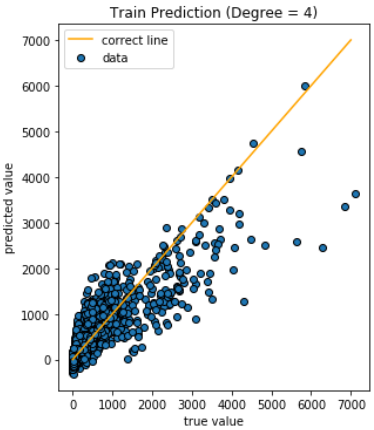


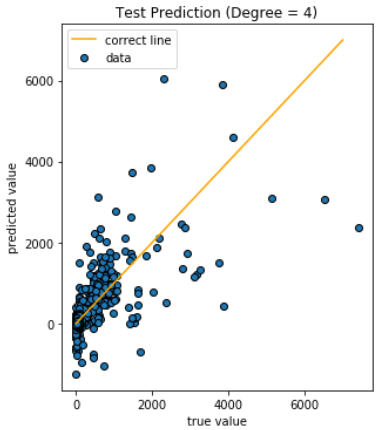


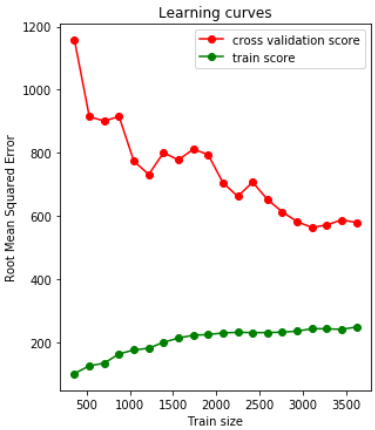




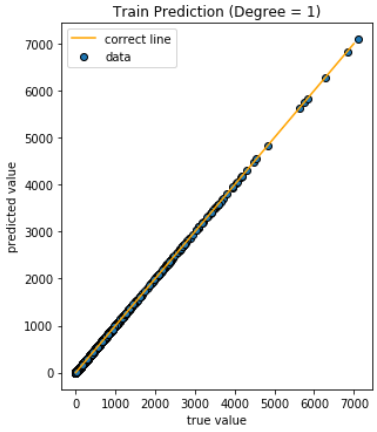


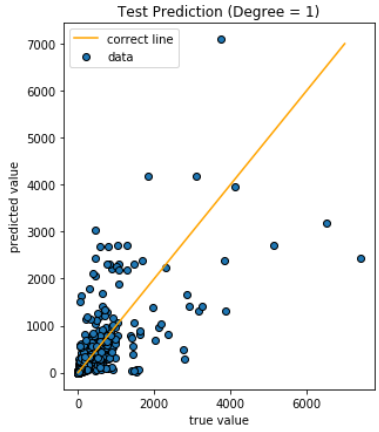


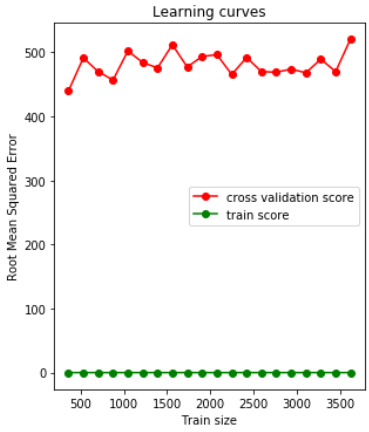


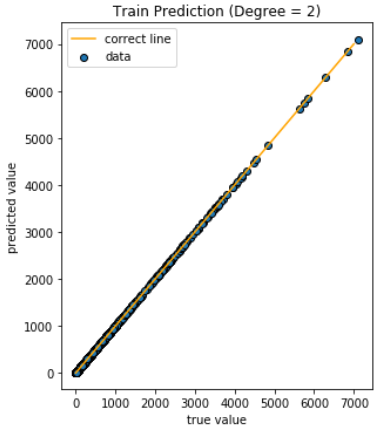


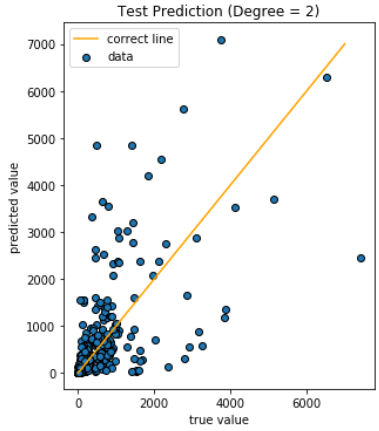
decision tree

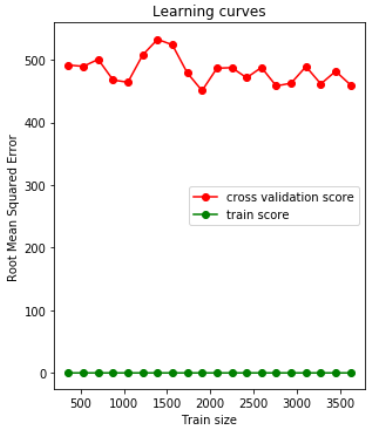


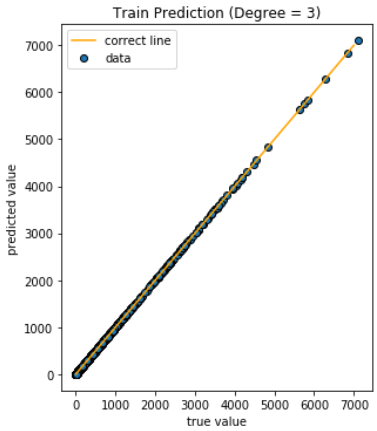


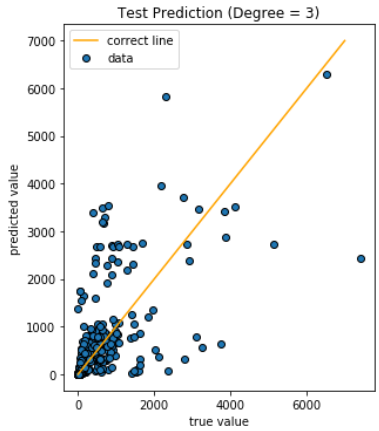


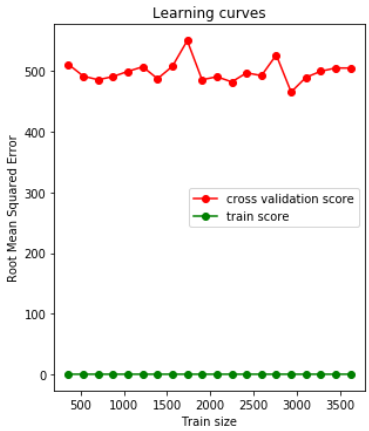


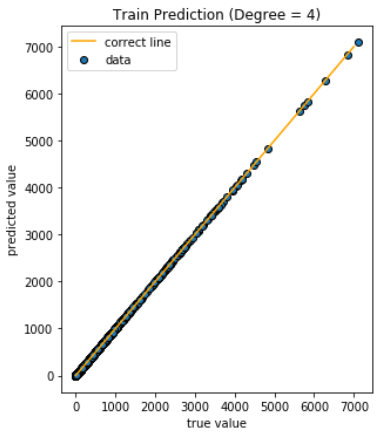


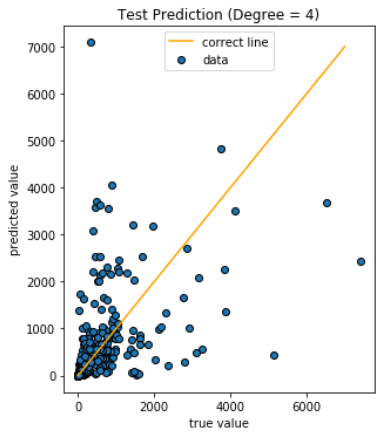


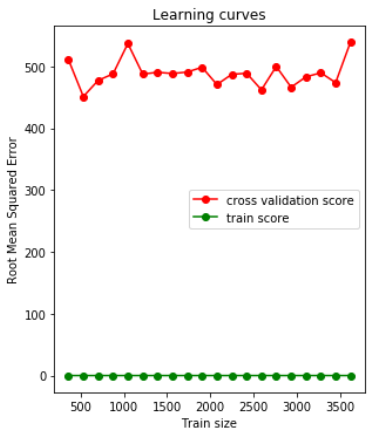




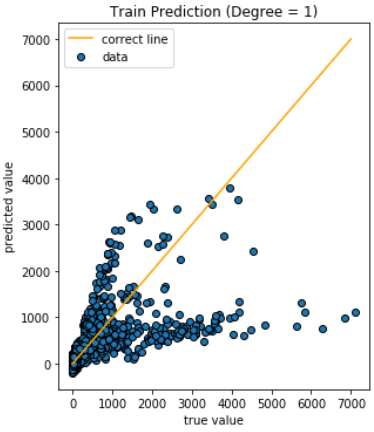


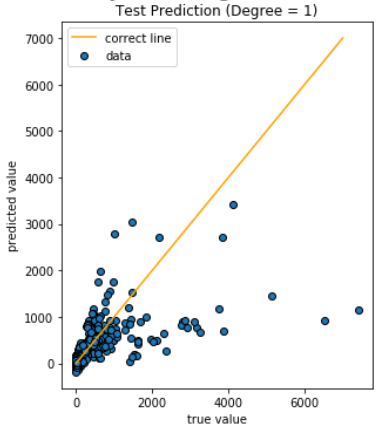


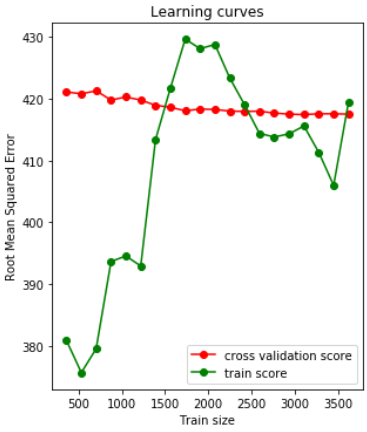


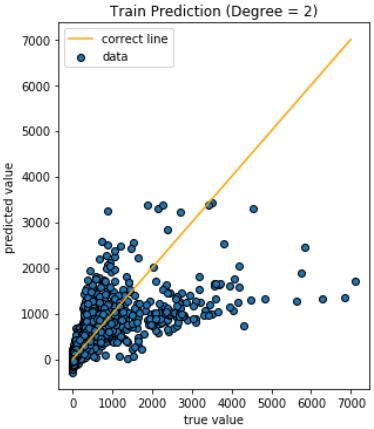


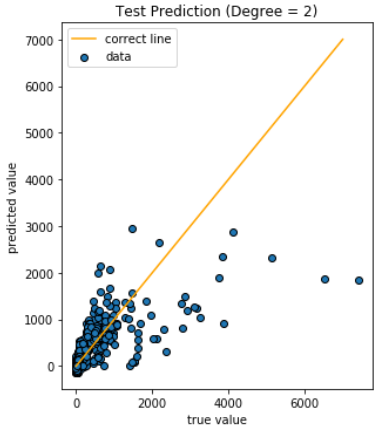
bayesian regression

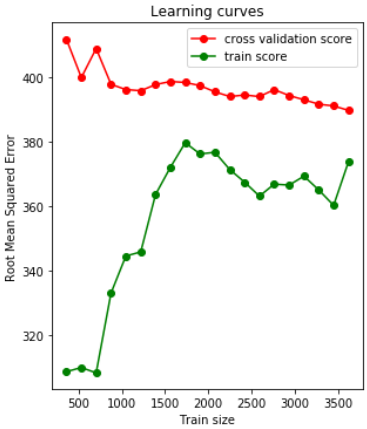


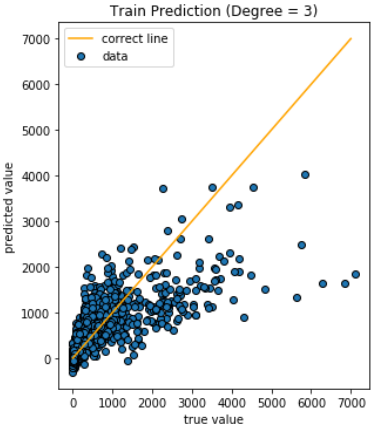


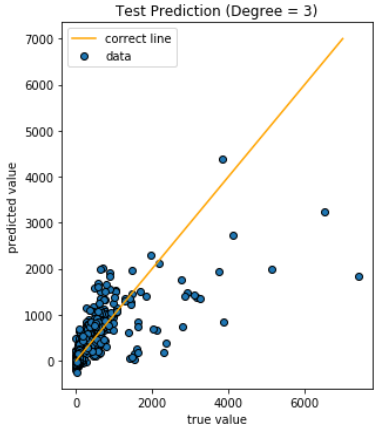


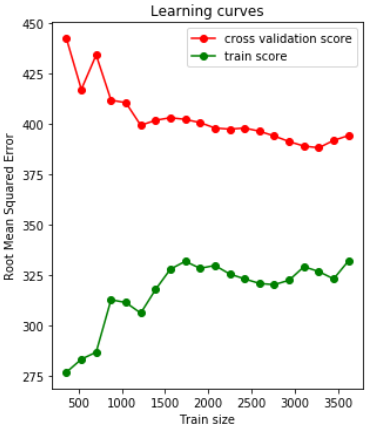


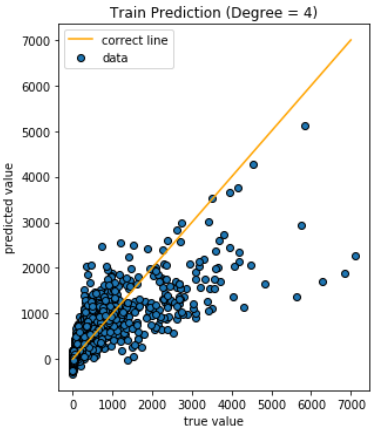


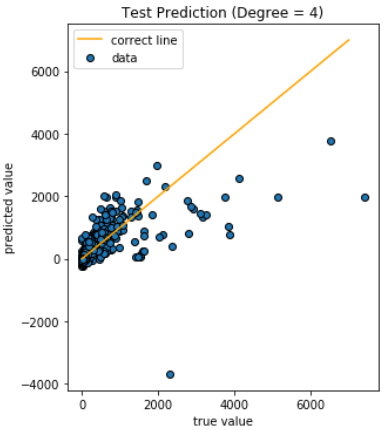


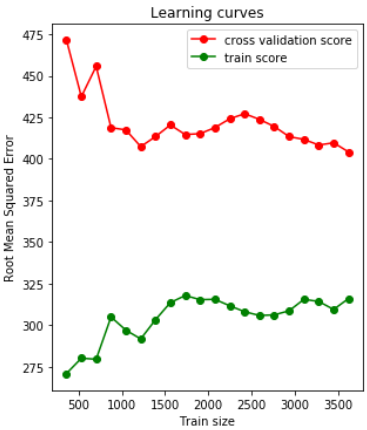








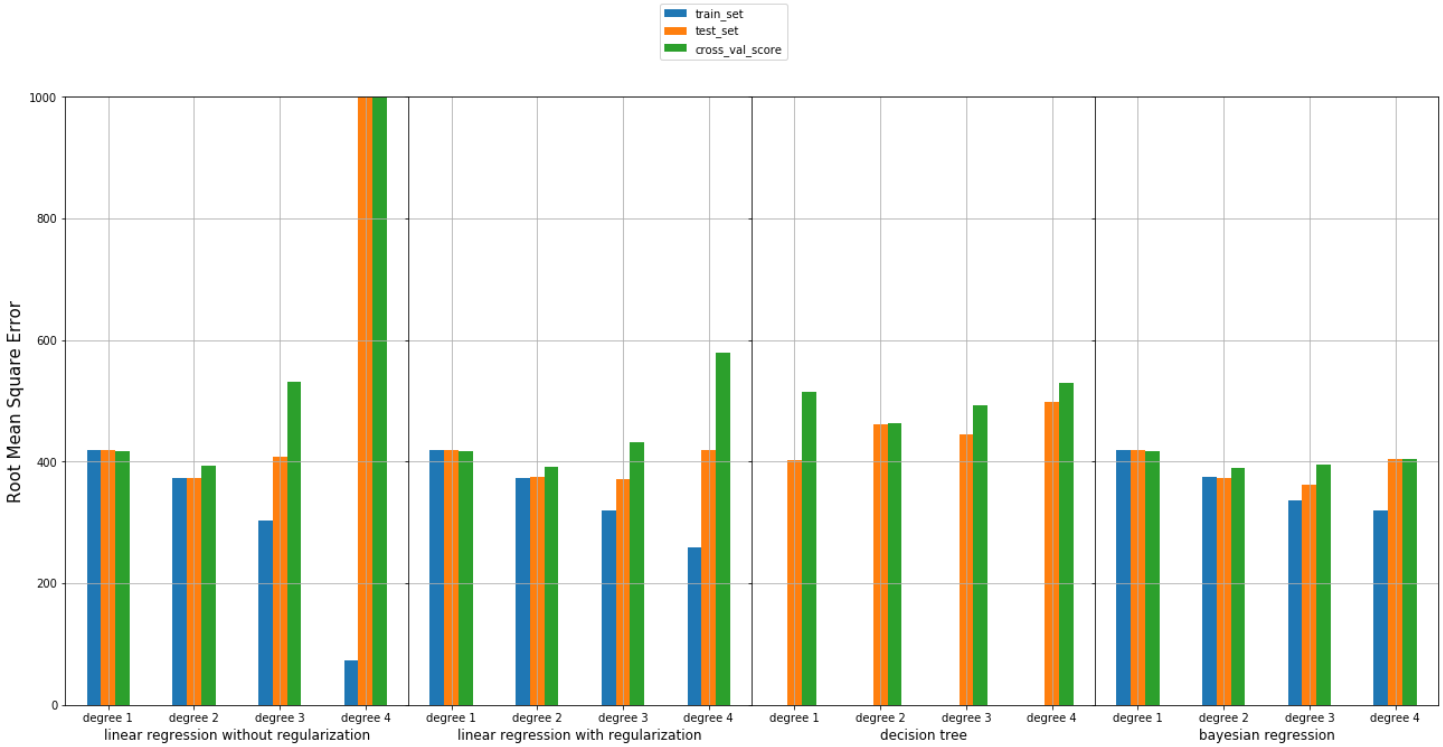




Scores of different models:

Model	Degree	train_set	test_set	cross_val_score
Linear Regression Without Regularization	degree 1	419.866307	418.615324	417.576640
	degree 2	372.359705	373.617408	392.908943
	degree 3	302.323809	408.804532	530.672084
	degree 4	73.435118	315326.589993	234891.759073
Linear Regression With Regularization	degree 1	419.866345	418.620364	417.572391
	degree 2	373.331604	374.237336	391.771967
	degree 3	319.505548	371.551272	431.990171
	degree 4	259.533636	419.349684	579.059199
Decision Tree	degree 1	0.010513	402.316586	515.481392
	degree 2	0.010513	460.950956	463.807661
	degree 3	0.010513	445.487777	491.780578
	degree 4	0.010513	499.054130	529.658289
Bayesian Regression	degree 1	419.876959	418.721758	417.520349
	degree 2	375.652153	372.505208	389.671285
	degree 3	337.025040	362.046311	394.414341
	degree 4	320.420003	403.531846	404.180608

A bar plot of the root mean squared error of all the models fitted to 4 degrees of polynomial features has been plotted to compare the fitting of the data.



Conclusions

While comparing different model scores we observe that

- **Overfitting** is seen in **linear regression without regularization** for higher degrees of polynomial features as there is low training set error and high cross validation and test set errors.
- **Overfitting** is also observed in **Decision Tree** as there is a significant difference between the training set error and cross validation and test set errors even though they are comparable with other models cross validation and test set errors.
- **Bayesian Regression** and **Ridge Regression** gives a good score in all training set, test set and cross validation set.