Predictive model for the Lunar albedo based on the chemical composition data from the Lunar Prospector.

Data source - https://github.com/ML4SCI/ML4SCI_GSoC/tree/main/Messenger/Moon (https://github.com/ML4SCI/ML4SCI_GSoC/tree/main/Messenger/Moon)

In [2]:

```
##Importing important python libraries for plotting and data preprocessing¶

import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
import matplotlib as mpl
import pandas as pd
mpl.style.use('classic')
%matplotlib inline

from sklearn import metrics
sns.set()
```

Part 1- Data Preprocessing and Exploratory Data Analysis

The data is stored in a CSV files with 360 rows and 720 columns.

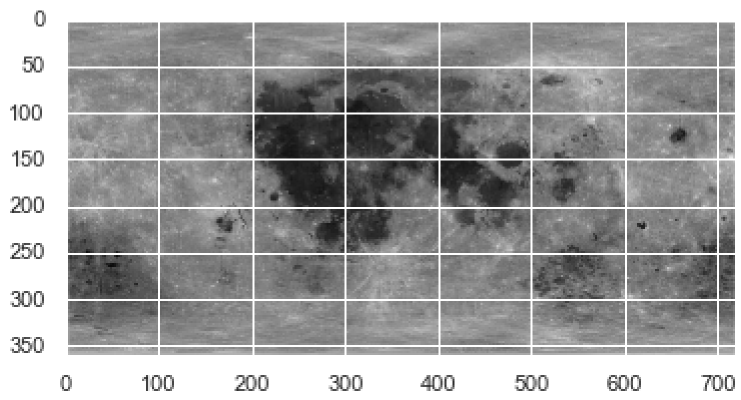
The goal of data preprocessing is to convert the data in a format suitable for training and testing .

In [3]:

```
##Step 1 - > Converting all the data frames into Numpy Matrix to divide the Left Side as Tr


albedo = pd.read_csv('Albedo_Map.csv',header=None);
Ti =  pd.read_csv("LPTi_Map.csv",header=None);
Fe =  pd.read_csv("LPFe_Map.csv",header=None);
K  =  pd.read_csv("LPK_Map.csv",header=None);
Th =  pd.read_csv("LPK_Map.csv",header=None);


alb = albedo.to_numpy()
ti = Ti.to_numpy()
fe = Fe.to_numpy()
k = K.to_numpy()
th = Th.to_numpy()

alb_train = alb[:,:360]
alb_test = alb[:,360:]
ti_train = ti[:,:360]
ti_test = ti[:,360:]
fe_train = fe[:,:360]
fe_test = fe[:,360:]
k_train = k[:,:360]
k_test = k[:,360:]
th_train = th[:,:360]
th_test = th[:,360:]
```

In [4]:

```
##Plotting to the original to check if the above conversion of successful

alb_final = np.concatenate((alb_train,alb_test), axis=1)

plt.imshow(alb_final, cmap="gray")
plt.show()
```



In [5]:

```
##Step 2-> Flatting all the Matrices and stacking the Left side and right side data to thei


flat_alb_train = alb_train.flatten()
flat_alb_test = alb_test.flatten()

flat_ti_train = ti_train.flatten()
flat_ti_test = ti_test.flatten()

flat_fe_train = fe_train.flatten()
flat_fe_test= fe_test.flatten()

flat_k_train = k_train.flatten()
flat_k_test = k_test.flatten()

flat_th_train = th_train.flatten()
flat_th_test = th_test.flatten()

data_train = {'Ti':flat_ti_train,
        'Fe':flat_fe_train,
        'K':flat_k_train,
        'Th':flat_th_train,
        'Albedo':flat_alb_train}
data_test = {'Ti':flat_ti_test,
        'Fe':flat_fe_test,
        'K':flat_k_test,
        'Th':flat_th_test,
        'Albedo':flat_alb_test}

LEFT = pd.DataFrame(data= data_train)
RIGHT = pd.DataFrame(data= data_test)
```

In [6]:

```
##Step 3-> Lets do some EDA
##Top five rows of the Left side Dataframe

LEFT.head()
```

Out[6]:

	Ti	Fe	K	Th	Albedo
0	0.190154	4.04409	788.81	788.81	0.331936
1	0.190154	4.04409	788.81	788.81	0.332611
2	0.190154	4.04409	788.81	788.81	0.332240
3	0.190154	4.04409	788.81	788.81	0.331028
4	0.190154	4.04409	788.81	788.81	0.331094

In [7]:

```
##some insights about the data using info() and describe() methods.

LEFT.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 129600 entries, 0 to 129599
Data columns (total 5 columns):
 #   Column  Non-Null Count   Dtype  
---  ------  --------------   -----  
 0   Ti      129600 non-null  float64
 1   Fe      129600 non-null  float64
 2   K       129600 non-null  float64
 3   Th      129600 non-null  float64
 4   Albedo  129600 non-null  float64
dtypes: float64(5)
memory usage: 4.9 MB
```

In [8]:

```
LEFT.describe()
```

Out[8]:

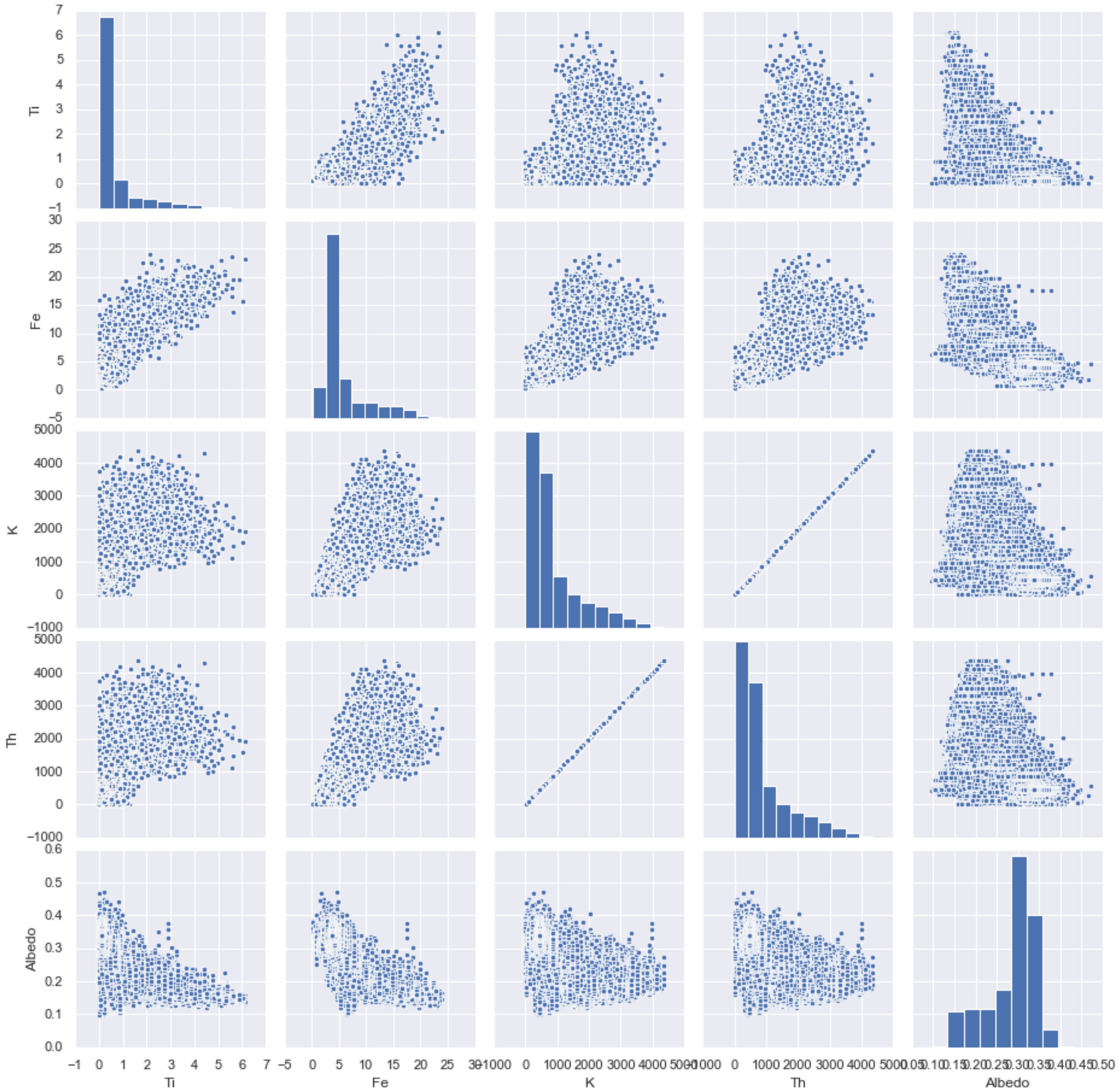
	Ti	Fe	K	Th	Albedo
count	129600.000000	129600.000000	129600.000000	129600.000000	129600.000000
mean	0.604026	5.734629	853.252498	853.252498	0.285794
std	0.904006	4.134721	824.795878	824.795878	0.057578
min	0.000000	0.271907	0.000000	0.000000	0.096897
25%	0.069470	3.306880	310.490000	310.490000	0.258126
50%	0.277718	4.019060	539.460000	539.460000	0.303909
75%	0.626194	6.295210	1116.425000	1116.425000	0.324932
max	6.135470	23.901800	4356.400000	4356.400000	0.470428

In [9]:

```
##Let's explore some relationships among the variables if any across the entire data set

sns.pairplot(LEFT)
```

Out[9]:

```
<seaborn.axisgrid.PairGrid at 0x1a265a5d3c8>
```

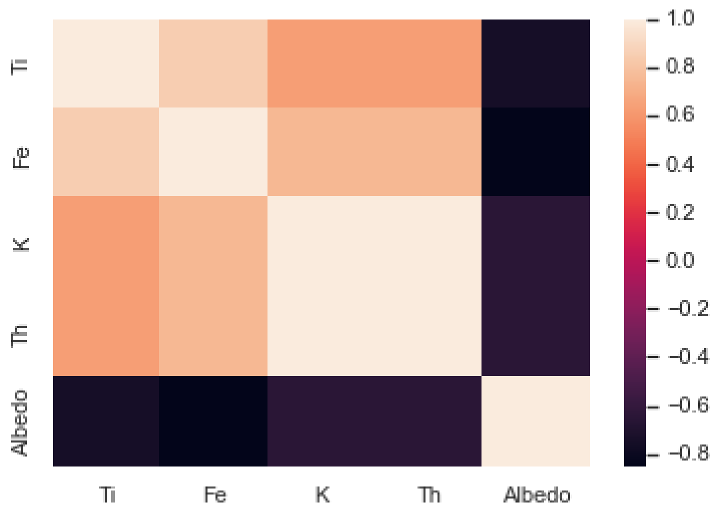


In [10]:

```
##Ingsights from the plots above
#1) Almost all of the variables are heavly skewed.
2#) Some correlation can also be obeserved , so lets plot the correlation matrix to underst

sns.heatmap(LEFT.corr())
```

Out[10]:

```
<matplotlib.axes._subplots.AxesSubplot at 0x1a2685959c8>
```



Part 2- Machine Learning

The goal is to build a regression model using different machine learning algorithms to predict the brightness of each pixel using the left side of the albedo as training data and right side as the test data.

For all the models these steps will be followed :-

1) Fitting the regressor object on the hyperparameters obtained using GridSearch

2) Print the details about the model (Correlation(R) bewtween actual and predicted values, evaluation metrics etc.

3) Plotting the predictions and 2-D image and residuals as 1-D histogram

Note the final peformace would be compared using Mean Square Error(MSE) as its a good evaluation metric for regression models

In [11]:

```
##First and foremost lets divide the data in train and test and do feature scaling


X_train = LEFT.iloc[:, :-1].values
y_train = LEFT.iloc[:, 4].values
X_test = RIGHT.iloc[:, :-1].values
y_test = RIGHT.iloc[:, 4].values
```

In [12]:

```
from sklearn.preprocessing import StandardScaler
sc_X = StandardScaler()
X_train = sc_X.fit_transform(X_train)
X_test = sc_X.transform(X_test)
```

1)Linear Regression¶

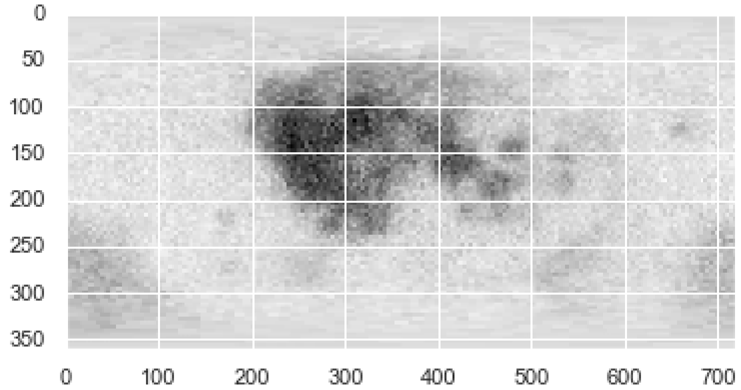
In [13]:

```
from sklearn.linear_model import LinearRegression
regressor = LinearRegression()
regressor.fit(X_train, y_train)

# Predicting the Test set results
y_pred_train = regressor.predict(X_train)
y_pred_test = regressor.predict(X_test)
residuals  = y_test-y_pred_test

print("About Model")
print("R:",regressor.score(X_train, y_train))
print("Adj R^2:",(1 - (1-regressor.score(X_train, y_train))*(len(y_train)-1)/(len(y_train)-

print("Model Evaluation")

print('MAE:', metrics.mean_absolute_error(y_test, y_pred_test))
print('MSE:', metrics.mean_squared_error(y_test, y_pred_test))
print('RMSE:', np.sqrt(metrics.mean_squared_error(y_test, y_pred_test)))
```

```
About Model
R: 0.7269141920289073
Adj R^2: 0.7269057631293983

Model Evaluation
MAE: 0.024634054761986983
MSE: 0.0010251522221398642
RMSE: 0.032017998397755
```

In [14]:

```
y_pred_train= y_pred_train.reshape(360,360)
y_pred_test= y_pred_test.reshape(360,360)
y_img = np.concatenate([y_pred_train,y_pred_test],axis=1)
plt.imshow(y_img, cmap="gray")
plt.show()
```

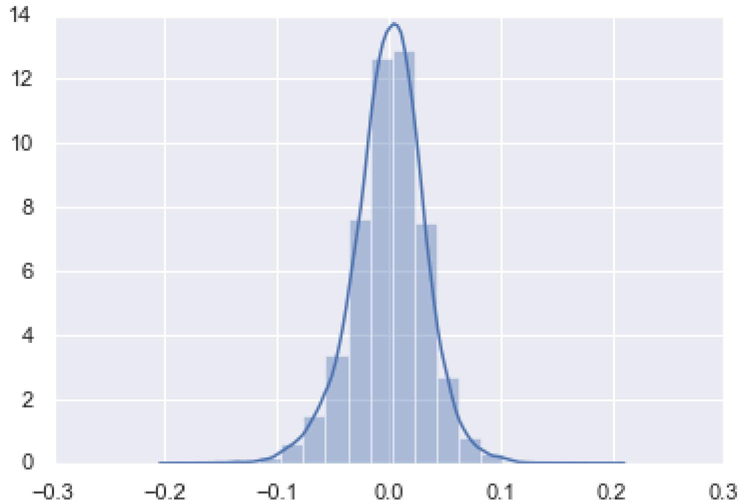


In [15]:

```
sns.distplot(residuals,bins=20)
```

Out[15]:

```
<matplotlib.axes._subplots.AxesSubplot at 0x1a268782d08>
```



The MSE is 0.001025152221398643

Insights As expected the Linear Regression doesnt perform well as the data doesnt seem to be linearly seperable and there is correlation among the features .

2)Support Vector Machine Regressor

In [16]:

```
from sklearn.svm import SVR
```

In [17]:

```
##Note - Many instances of Grid Seach using different values of hyperparameter have been do


from sklearn.model_selection import GridSearchCV
param_grid = {'C': [0.1,1,10,500],
              'gamma': [ 0.003, 0.03,0.3,1],
              'kernel': ['linear']}

grid = GridSearchCV(SVR(), param_grid, refit = True, verbose = 4,cv=3,scoring='neg_mean_squ

# fitting the model for grid search
grid.fit(X_train, y_train)
```

```
Fitting 3 folds for each of 16 candidates, totalling 48 fits
[CV] C=0.1, gamma=0.003, kernel=linear ...............................


[Parallel(n_jobs=1)]: Using backend SequentialBackend with 1 concurrent wo
rkers.

[CV] .. C=0.1, gamma=0.003, kernel=linear, score=-0.001, total=   1.6s
[CV] C=0.1, gamma=0.003, kernel=linear ...............................

[Parallel(n_jobs=1)]: Done   1 out of   1 | elapsed:    1.5s remaining:
0.0s

[CV] .. C=0.1, gamma=0.003, kernel=linear, score=-0.001, total=   1.3s
[CV] C=0.1, gamma=0.003, kernel=linear ...............................

[Parallel(n_jobs=1)]: Done   2 out of   2 | elapsed:    2.8s remaining:
0.0s

[CV] .. C=0.1, gamma=0.003, kernel=linear, score=-0.001, total=   1.3s
[CV] C=0.1, gamma=0.03, kernel=linear ................................
```

In [18]:

```
print(grid.best_params_)
print(grid.best_estimator_)
```

```
{'C': 0.1, 'gamma': 0.003, 'kernel': 'linear'}
SVR(C=0.1, cache_size=200, coef0=0.0, degree=3, epsilon=0.1, gamma=0.003,
    kernel='linear', max_iter=-1, shrinking=True, tol=0.001, verbose=False)
```

In [19]:

```
#The linear model was performing poorly and using gussian kernel gave better results

print(grid.best_params_)
print(grid.best_estimator_)
```

```
{'C': 0.1, 'gamma': 0.003, 'kernel': 'linear'}
SVR(C=0.1, cache_size=200, coef0=0.0, degree=3, epsilon=0.1, gamma=0.003,
    kernel='linear', max_iter=-1, shrinking=True, tol=0.001, verbose=False)
```

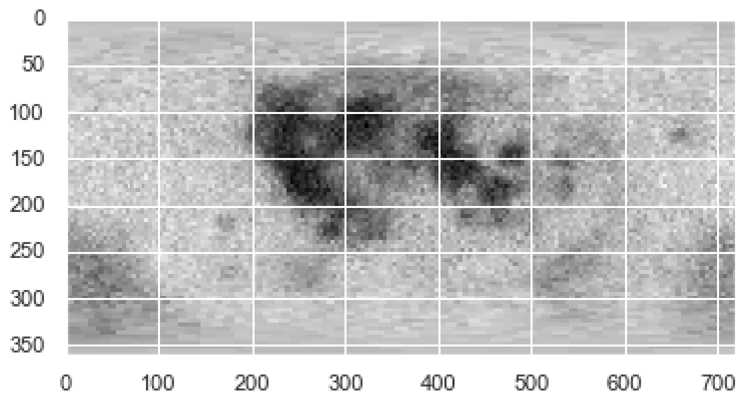
In [20]:

```
##After doing grid search and experimenting with the hyperparameters C=2700 and gamma = 0.0


regressor =SVR(C=2700, gamma=0.00008)
regressor.fit(X_train,y_train)

# Predicting the Test set results

y_pred_train = regressor.predict(X_train)
y_pred_test = regressor.predict(X_test)
residuals  = y_test-y_pred_test


print("About Model")
print("R:",regressor.score(X_train, y_train))
print("Adj R^2:",(1 - (1-regressor.score(X_train, y_train))*(len(y_train)-1)/(len(y_train)-

print("Model Evaluation")

print('MAE:', metrics.mean_absolute_error(y_test, y_pred_test))
print('MSE:', metrics.mean_squared_error(y_test, y_pred_test))
print('RMSE:', np.sqrt(metrics.mean_squared_error(y_test, y_pred_test)))
```

```
About Model
R: 0.7313521137574608
Adj R^2: 0.7313438218361292

Model Evaluation
MAE: 0.02549109407986941
MSE: 0.0010568361978324054
RMSE: 0.03250901717727568
```

In [21]:

```
y_pred_train= y_pred_train.reshape(360,360)
y_pred_test= y_pred_test.reshape(360,360)
y_img = np.concatenate([y_pred_train,y_pred_test],axis=1)
plt.imshow(y_img, cmap="gray")
plt.show()
```

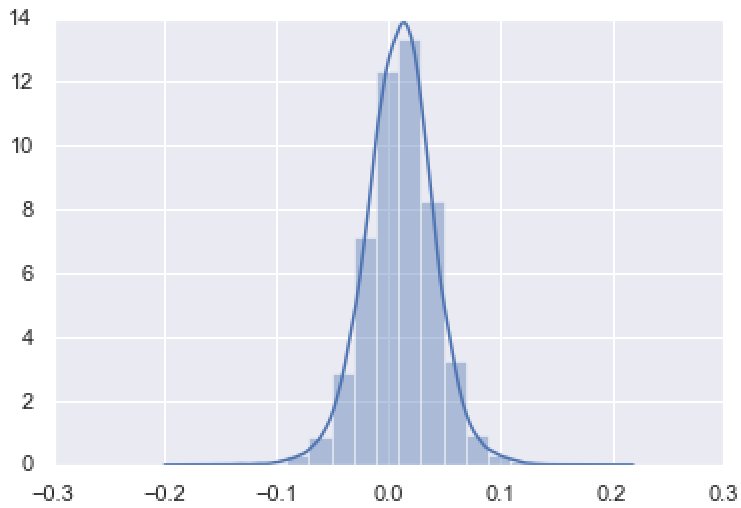


In [22]:

```
sns.distplot(residuals,bins=20)
```

Out[22]:

```
<matplotlib.axes._subplots.AxesSubplot at 0x1a2686471c8>
```



The MSE is 0.0010564847231500207

Insights

The image looks better than the one obtained through Linear Regression even though the MSE is slightly higher , their is scope for improvement

3)Random Forest

In [23]:

```
from sklearn.ensemble import RandomForestRegressor
```

In [24]:

```
##Tuning the hyperparameter n_estimators and plotting the results

rf = RandomForestRegressor(n_estimators=100)
error_rate_test = []
error_rate_train=[]

for iter in range(10):
    rf.fit(X_train, y_train)
    y_train_predicted = rf.predict(X_train)
    y_test_predicted = rf.predict(X_test)
    mse_train = metrics.mean_squared_error(y_train, y_train_predicted)
    mse_test = metrics.mean_squared_error(y_test, y_test_predicted)
    error_rate_train.append( metrics.mean_squared_error(y_train, y_train_predicted))
    error_rate_test.append(metrics.mean_squared_error(y_test, y_test_predicted))
    print("Iteration: {} Train mse: {} Test mse: {}".format(iter, mse_train, mse_test))
    rf.n_estimators += 100
```

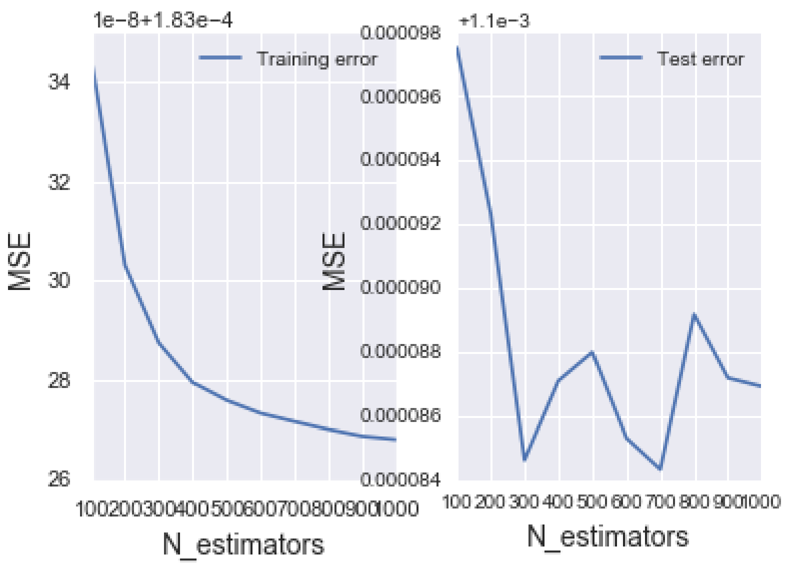
```
Iteration: 0 Train mse: 0.00018334486383259147 Test mse: 0.001197518418827O8
96
Iteration: 1 Train mse: 0.0001833031719271683 Test mse: 0.001192337948347787
4
Iteration: 2 Train mse: 0.00018328752340904304 Test mse: 0.001184617550331З6
38
Iteration: 3 Train mse: 0.00018327951977664867 Test mse: 0.001187091931218З2
22
Iteration: 4 Train mse: 0.00018327594746763196 Test mse: 0.001187985513692Z0
07
Iteration: 5 Train mse: 0.0001832733552385428 Test mse: 0.001185299635983599
9
Iteration: 6 Train mse: 0.000183271698649122 Test mse: 0.0011843275287877122
Iteration: 7 Train mse: 0.00018327011085902587 Test mse: 0.001189173571315999
6
Iteration: 8 Train mse: 0.0001832687456017879 Test mse: 0.001187182645696979
Iteration: 9 Train mse: 0.00018326808630423228 Test mse: 0.001186917564607З6
24
```

In [25]:

```
plt.subplot(1, 2, 1)

plt.style.use('seaborn')
plt.plot(range(100,1100,100),error_rate_train, label = 'Training error')
#plt.plot(range(100,1200,100),error_rate_test, label = 'Validation error')
plt.ylabel('MSE', fontsize = 14)
plt.xlabel('N_estimators', fontsize = 14)
plt.legend()
plt.subplot(1, 2, 2)

plt.style.use('seaborn')
plt.plot(range(100,1100,100),error_rate_test, label = 'Test error')
#plt.plot(range(100,1200,100),error_rate_test, label = 'Validation error')
plt.ylabel('MSE', fontsize = 14)
plt.xlabel('N_estimators', fontsize = 14)
plt.legend()
```

Out[25]:

```
<matplotlib.legend.Legend at 0x1a269404108>
```



In [26]:

```
##Note - Many instances of Grid Seach using different values of hyperparameter have been do

from sklearn.model_selection import GridSearchCV

param_grid = [
{'n_estimators': [50,250,500,1000],
 'max_depth': [5,10],
 'max_features' :["sqrt"],
'min_samples_leaf':[5,10]}
]

grid_search_forest = GridSearchCV(regressor, param_grid, cv=10, scoring='neg_mean_squared_e
grid_search_forest.fit(X_train, y_train)

grid_search_forest.best_params_
```

```
Fitting 10 folds for each of 16 candidates, totalling 160 fits
[CV] max_depth=5, max_features=sqrt, min_samples_leaf=5, n_estimators=50

[Parallel(n_jobs=1)]: Using backend SequentialBackend with 1 concurrent work
ers.

---------------------------------------------------------------------------
ValueError                                Traceback (most recent call last)
<ipython-input-26-0b6cd933e04d> in <module>
     11 
     12 grid_search_forest = GridSearchCV(regressor, param_grid, cv=10, scor
ing='neg_mean_squared_error',verbose=5)
---> 13 grid_search_forest.fit(X_train, y_train)
     14 
     15 grid_search_forest.best_params_

E:\anxe\lib\site-packages\sklearn\model_selection\_search.py in fit(self, X,
y, groups, **fit_params)
    708                 return results
    709 
--> 710             self._run_search(evaluate_candidates)
    711 
    712         # For multi-metric evaluation, store the best_index_, best_p
arams_ and

E:\anxe\lib\site-packages\sklearn\model_selection\_search.py in _run_search
(self, evaluate_candidates)
   1149     def _run_search(self, evaluate_candidates):
   1150         """Search all candidates in param_grid"""
-> 1151         evaluate_candidates(ParameterGrid(self.param_grid))
   1152 
   1153 

E:\anxe\lib\site-packages\sklearn\model_selection\_search.py in evaluate_can
didates(candidate_params)
    687                                for parameters, (train, test)
    688                                in product(candidate_params,
--> 689                                           cv.split(X, y, groups)))
    690 
    691                 if len(out) < 1:

E:\anxe\lib\site-packages\joblib\parallel.py in __call__(self, iterable)
   1002             # remaining jobs.
```

```
   1003             self._iterating = False
-> 1004             if self.dispatch_one_batch(iterator):
   1005                 self._iterating = self._original_iterator is not Non
e
   1006 

E:\anxe\lib\site-packages\joblib\parallel.py in dispatch_one_batch(self, ite
rator)
    833                 return False
    834             else:
--> 835                 self._dispatch(tasks)
    836                 return True
    837 

E:\anxe\lib\site-packages\joblib\parallel.py in _dispatch(self, batch)
    752         with self._lock:
    753             job_idx = len(self._jobs)
--> 754             job = self._backend.apply_async(batch, callback=cb)
    755             # A job can complete so quickly than its callback is
    756             # called before we get here, causing self._jobs to

E:\anxe\lib\site-packages\joblib\_parallel_backends.py in apply_async(self,
 func, callback)
    207     def apply_async(self, func, callback=None):
    208         """Schedule a func to be run"""
--> 209         result = ImmediateResult(func)
    210         if callback:
    211             callback(result)

E:\anxe\lib\site-packages\joblib\_parallel_backends.py in __init__(self, bat
ch)
    588         # Don't delay the application, to avoid keeping the input
    589         # arguments in memory
--> 590         self.results = batch()
    591 
    592     def get(self):

E:\anxe\lib\site-packages\joblib\parallel.py in __call__(self)
    254         with parallel_backend(self._backend, n_jobs=self._n_jobs):
    255             return [func(*args, **kwargs)
--> 256                     for func, args, kwargs in self.items]
    257 
    258     def __len__(self):

E:\anxe\lib\site-packages\joblib\parallel.py in <listcomp>(.0)
    254         with parallel_backend(self._backend, n_jobs=self._n_jobs):
    255             return [func(*args, **kwargs)
--> 256                     for func, args, kwargs in self.items]
    257 
    258     def __len__(self):

E:\anxe\lib\site-packages\sklearn\model_selection\_validation.py in _fit_and
_score(estimator, X, y, scorer, train, test, verbose, parameters, fit_param
s, return_train_score, return_parameters, return_n_test_samples, return_time
s, return_estimator, error_score)
    502             cloned_parameters[k] = clone(v, safe=False)
    503 
--> 504         estimator = estimator.set_params(**cloned_parameters)
    505 
    506     start_time = time.time()
```

```
E:\anxe\lib\site-packages\sklearn\base.py in set_params(self, **params)
    234                                  'Check the list of available parame
ters '
    235                                  'with `estimator.get_params().keys
()`.' %
--> 236                                  (key, self))
    237
    238             if delim:

ValueError: Invalid parameter max_depth for estimator SVR(C=2700, cache_size
=200, coef0=0.0, degree=3, epsilon=0.1, gamma=8e-05,
    kernel='rbf', max_iter=-1, shrinking=True, tol=0.001, verbose=False). Ch
eck the list of available parameters with `estimator.get_params().keys()`.
```

In [27]:

```
# create regressor object
regressor = RandomForestRegressor(max_features='sqrt',max_depth=10,min_samples_leaf=5,n_est

# fit the regressor with x and y data
regressor.fit(X_train, y_train)
y_pred = regressor.predict(X_test)
y_pred_train = regressor.predict(X_train)
y_pred_test = regressor.predict(X_test)
```

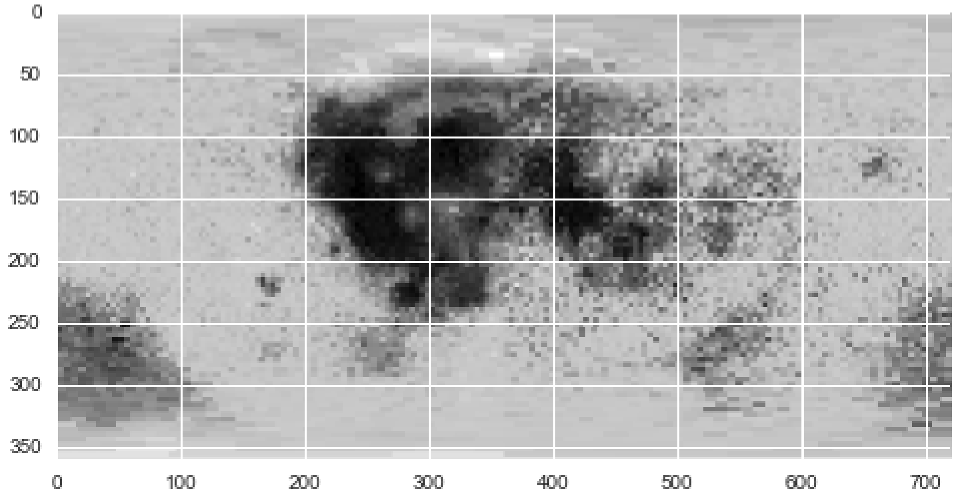
In [28]:

```
print("About Model")
print("R:",regressor.score(X_train, y_train))
print("Adj R^2:",(1 - (1-regressor.score(X_train, y_train))*(len(y_train)-1)/(len(y_train)-

print("Model Evaluation")

print('MAE:', metrics.mean_absolute_error(y_test, y_pred_test))
print('MSE:', metrics.mean_squared_error(y_test, y_pred_test))
print('RMSE:', np.sqrt(metrics.mean_squared_error(y_test, y_pred_test)))
```

```
About Model
R: 0.8648975622181015
Adj R^2: 0.8648933922288957

Model Evaluation
MAE: 0.023970223129863494
MSE: 0.000986058268347703
RMSE: 0.03140156474361911
```

In [29]:

```
y_pred_train= y_pred_train.reshape(360,360)
y_pred_test= y_pred_test.reshape(360,360)
y_img = np.concatenate([y_pred_train,y_pred_test],axis=1)
plt.imshow(y_img, cmap="gray")
plt.show()
```

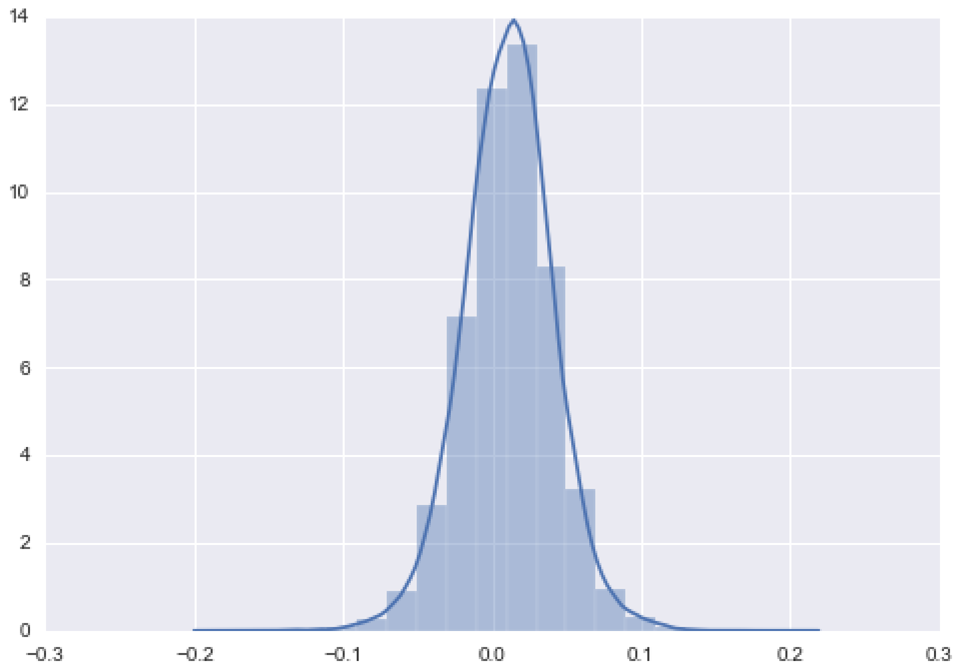


In [30]:

```
sns.distplot(residuals,bins=20)
```

Out[30]:

```
<matplotlib.axes._subplots.AxesSubplot at 0x1a26a515688>
```



The MSE is 0.000986584356014296

Insights

The Model perform better than all the above ones wrt MSE but even after doing hours of grid search and hyperparameter tuning it has overfitted to the left portion as its clearly visible from the image .

4)XGBOOST

In [31]:

```
conda install -c conda-forge xgboost
```

```
Collecting package metadata (current_repodata.json): ...working... done
Solving environment: ...working... done

# All requested packages already installed.


Note: you may need to restart the kernel to use updated packages.
```

In [32]:

```
import pickle
import xgboost
regressor=xgboost.XGBRegressor()
```

In [33]:

```
##Hyperparameter tuning using RandomizedSearchCV

# Hyper Parameter Optimization

booster=['gbtree','gblinear']
base_score=[0.25,0.5,0.75,1]

n_estimators = [100, 500, 900, 1100, 1500]
max_depth = [2, 3, 5, 10, 15]
booster=['gbtree','gblinear']
learning_rate=[0.05,0.1,0.15,0.20]
min_child_weight=[1,2,3,4]

# Defineing the grid of hyperparameters to search
hyperparameter_grid = {
    'n_estimators': n_estimators,
    'max_depth':max_depth,
    'learning_rate':learning_rate,
    'min_child_weight':min_child_weight,
    'booster':booster,
    'base_score':base_score
    }

# Using RandomizedSearchCV for creating model

from sklearn.model_selection import RandomizedSearchCV

# Set up the random search with 5-fold cross validation
random_cv = RandomizedSearchCV(estimator=regressor,
            param_distributions=hyperparameter_grid,
            cv=5, n_iter=50,
            scoring = 'neg_mean_absolute_error',n_jobs = 4,
            verbose = 5,
            return_train_score = True,
            random_state=42)

random_cv.fit(X_train,y_train)
```

```
Fitting 5 folds for each of 50 candidates, totalling 250 fits


[Parallel(n_jobs=4)]: Using backend LokyBackend with 4 concurrent workers.
[Parallel(n_jobs=4)]: Done  10 tasks      | elapsed:   53.6s
[Parallel(n_jobs=4)]: Done  64 tasks      | elapsed:  7.4min
[Parallel(n_jobs=4)]: Done 154 tasks      | elapsed: 12.1min
[Parallel(n_jobs=4)]: Done 250 out of 250 | elapsed: 17.5min finished
```

Out[33]:

```
RandomizedSearchCV(cv=5, error_score=nan,
                   estimator=XGBRegressor(base_score=None, booster=None,
                                          colsample_bylevel=None,
                                          colsample_bynode=None,
                                          colsample_bytree=None, gamma=None,
                                          gpu_id=None, importance_type='gai
n',
```

```
                                          interaction_constraints=None,
                                          learning_rate=None,
                                          max_delta_step=None, max_depth=Non
e,
                                          min_child_weight=None, missing=na
n,
                                          monotone_constraints=None,
                                          n_...
                   iid='deprecated', n_iter=50, n_jobs=4,
                   param_distributions={'base_score': [0.25, 0.5, 0.75, 1],
                                        'booster': ['gbtree', 'gblinear'],
                                        'learning_rate': [0.05, 0.1, 0.15,
0.2],
                                        'max_depth': [2, 3, 5, 10, 15],
                                        'min_child_weight': [1, 2, 3, 4],
                                        'n_estimators': [100, 500, 900, 110
0,
                                                         1500]},
                   pre_dispatch='2*n_jobs', random_state=42, refit=True,
                   return_train_score=True, scoring='neg_mean_absolute_erro
r',
                   verbose=5)
```

In [34]:

```
random_cv.best_estimator_
```

Out[34]:

```
XGBRegressor(base_score=0.5, booster='gbtree', colsample_bylevel=1,
             colsample_bynode=1, colsample_bytree=1, gamma=0, gpu_id=-1,
             importance_type='gain', interaction_constraints='',
             learning_rate=0.1, max_delta_step=0, max_depth=2,
             min_child_weight=1, missing=nan, monotone_constraints='()',
             n_estimators=100, n_jobs=8, num_parallel_tree=1,
             objective='reg:squarederror', random_state=0, reg_alpha=0,
             reg_lambda=1, scale_pos_weight=1, subsample=1, tree_method='exa
ct',
             validate_parameters=1, verbosity=None)
```

In [35]:

```
##The hyperparameters obtained using the above method gave the best results

regressor=xgboost.XGBRegressor(base_score=0.5, booster='gbtree', colsample_bylevel=1,
             colsample_bynode=1, colsample_bytree=1, gamma=0, gpu_id=-1,
             importance_type='gain', interaction_constraints='',
             learning_rate=0.1, max_delta_step=0, max_depth=2,
             min_child_weight=1, missing=None, monotone_constraints='()',
             n_estimators=100, n_jobs=8, num_parallel_tree=1, random_state=0,
             reg_alpha=0, reg_lambda=1, scale_pos_weight=1, subsample=1,
             tree_method='exact', validate_parameters=1, verbosity=None)

regressor.fit(X_train,y_train)
# Predicting the Test set results
y_pred_train = regressor.predict(X_train)
y_pred_test = regressor.predict(X_test)
residuals  = y_test-y_pred_test
```

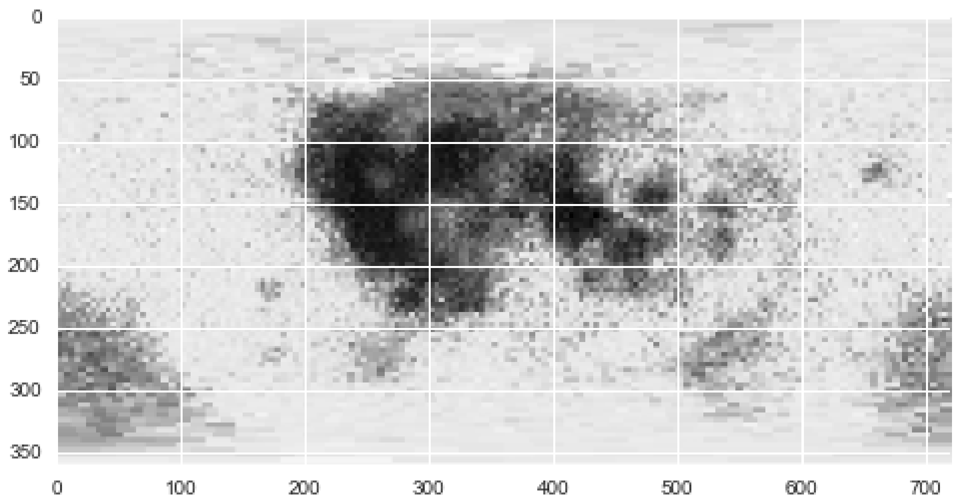
In [36]:

```
print("R:",regressor.score(X_train, y_train))
print("Adj R^2:",(1 - (1-regressor.score(X_train, y_train))*(len(y_train)-1)/(len(y_train)-

print("Model Evaluation")

print('MAE:', metrics.mean_absolute_error(y_test, y_pred_test))
print('MSE:', metrics.mean_squared_error(y_test, y_pred_test))
print('RMSE:', np.sqrt(metrics.mean_squared_error(y_test, y_pred_test)))
```

```
R: 0.7903649932835797
Adj R^2: 0.7903585228176908

Model Evaluation
MAE: 0.02334789735875415
MSE: 0.0009304179266331601
RMSE: 0.03050275277140016
```

In [37]:

```
y_pred_train= y_pred_train.reshape(360,360)
y_pred_test= y_pred_test.reshape(360,360)
y_img = np.concatenate([y_pred_train,y_pred_test],axis=1)
plt.imshow(y_img, cmap="gray")
plt.show()
```

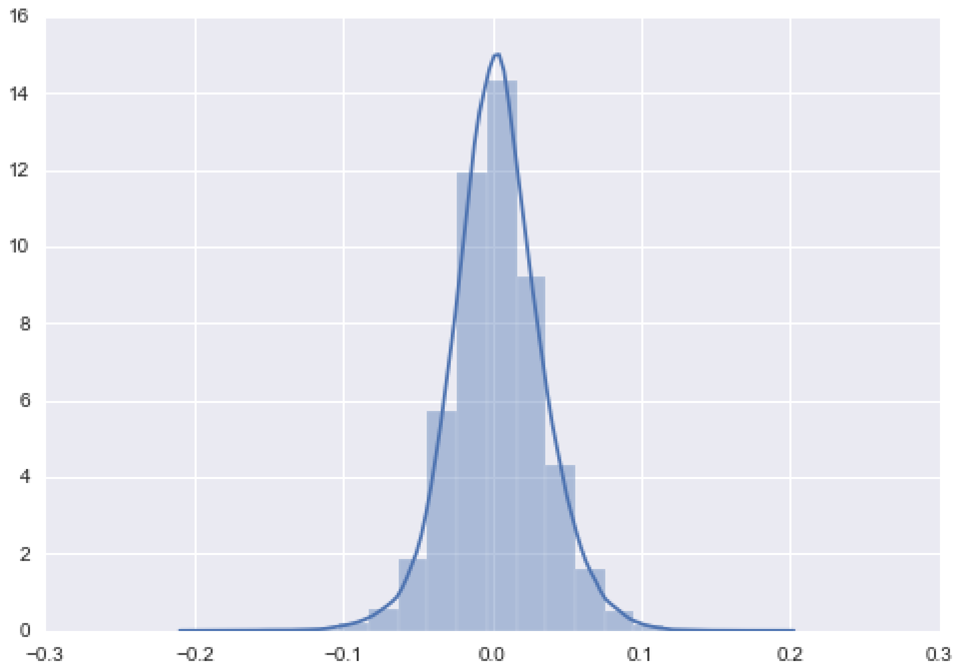


In [38]:

```
sns.distplot(residuals,bins=20)
```

Out[38]:

```
<matplotlib.axes._subplots.AxesSubplot at 0x1a26d4c6dc8>
```



Insights

Looks like we have a winner here, as the MSE is the lowest obtained will now and Image also looks good on both the sides XGBoost is one of the most powerful ML algorithm

The MSE is 0.0009304179266331601

In [39]:

```
filename = 'Best_Model_XG_boost.sav'
pickle.dump(regressor, open(filename, 'wb'))
```

5) Neural Network

Lets wrap things up by trying a Neural Network

In [54]:

```
!pip install tensorflow
import tensorflow as tf
from tensorflow.keras.layers import Input, Dense, Activation,Dropout
from tensorflow.keras.models import Model
from tensorflow import keras
```

```
Collecting tensorflow
  Using cached tensorflow-2.4.1-cp37-cp37m-win_amd64.whl (370.7 MB)
Collecting google-pasta~=0.2
  Using cached google_pasta-0.2.0-py3-none-any.whl (57 kB)
Requirement already satisfied: numpy~=1.19.2 in e:\anxe\lib\site-packages (f
rom tensorflow) (1.19.5)
Processing c:\users\ritika saxena\appdata\local\pip\cache\wheels\3f\e3\ec\8a
8336ff196023622fbcb36de0c5a5c218cbb24111d1d4c7f2\termcolor-1.1.0-py3-none-an
y.whl
Collecting grpcio~=1.32.0
  Using cached grpcio-1.32.0-cp37-cp37m-win_amd64.whl (2.5 MB)
Collecting typing-extensions~=3.7.4
  Using cached typing_extensions-3.7.4.3-py3-none-any.whl (22 kB)
Collecting protobuf>=3.9.2
  Using cached protobuf-3.15.8-cp37-cp37m-win_amd64.whl (904 kB)
Collecting tensorboard~=2.4
  Using cached tensorboard-2.4.1-py3-none-any.whl (10.6 MB)
Collecting tensorflow-estimator<2.5.0,>=2.4.0
  Using cached tensorflow_estimator-2.4.0-py2.py3-none-any.whl (462 kB)
Requirement already satisfied: wheel~=0.35 in e:\anxe\lib\site-packages (fro
m tensorflow) (0.36.2)
Requirement already satisfied: gast==0.3.3 in e:\anxe\lib\site-packages (fro
m tensorflow) (0.3.3)
Requirement already satisfied: h5py~=2.10.0 in e:\anxe\lib\site-packages (fr
om tensorflow) (2.10.0)
Collecting flatbuffers~=1.12.0
  Using cached flatbuffers-1.12-py2.py3-none-any.whl (15 kB)
Requirement already satisfied: six~=1.15.0 in e:\anxe\lib\site-packages (fro
m tensorflow) (1.15.0)
Processing c:\users\ritika saxena\appdata\local\pip\cache\wheels\62\76\4c\aa
25851149f3f6d9785f6c869387ad82b3fd37582fa8147ac6\wrapt-1.12.1-cp37-cp37m-win
_amd64.whl
Collecting opt-einsum~=3.3.0
  Using cached opt_einsum-3.3.0-py3-none-any.whl (65 kB)
Requirement already satisfied: absl-py~=0.10 in e:\anxe\lib\site-packages (f
rom tensorflow) (0.12.0)
Requirement already satisfied: astunparse~=1.6.3 in e:\anxe\lib\site-package
s (from tensorflow) (1.6.3)
Collecting keras-preprocessing~=1.1.2
  Using cached Keras_Preprocessing-1.1.2-py2.py3-none-any.whl (42 kB)
Requirement already satisfied: setuptools>=41.0.0 in e:\anxe\lib\site-packag
es (from tensorboard~=2.4->tensorflow) (45.2.0.post20200210)
Requirement already satisfied: google-auth-oauthlib<0.5,>=0.4.1 in e:\anxe\l
ib\site-packages (from tensorboard~=2.4->tensorflow) (0.4.4)
Requirement already satisfied: google-auth<2,>=1.6.3 in e:\anxe\lib\site-pac
kages (from tensorboard~=2.4->tensorflow) (1.28.1)
Requirement already satisfied: werkzeug>=0.11.15 in e:\anxe\lib\site-package
s (from tensorboard~=2.4->tensorflow) (1.0.0)
Requirement already satisfied: requests<3,>=2.21.0 in e:\anxe\lib\site-packa
ges (from tensorboard~=2.4->tensorflow) (2.22.0)
Requirement already satisfied: markdown>=2.6.8 in e:\anxe\lib\site-packages
(from tensorboard~=2.4->tensorflow) (3.3.4)
Collecting tensorboard-plugin-wit>=1.6.0
```

```
  Using cached tensorboard_plugin_wit-1.8.0-py3-none-any.whl (781 kB)
Requirement already satisfied: requests-oauthlib>=0.7.0 in e:\anxe\lib\site-
packages (from google-auth-oauthlib<0.5,>=0.4.1->tensorboard~=2.4->tensorflo
w) (1.3.0)
Requirement already satisfied: cachetools<5.0,>=2.0.0 in e:\anxe\lib\site-pa
ckages (from google-auth<2,>=1.6.3->tensorboard~=2.4->tensorflow) (4.2.1)
Requirement already satisfied: pyasn1-modules>=0.2.1 in e:\anxe\lib\site-pac
kages (from google-auth<2,>=1.6.3->tensorboard~=2.4->tensorflow) (0.2.8)
Requirement already satisfied: rsa<5,>=3.1.4; python_version >= "3.6" in
e:\anxe\lib\site-packages (from google-auth<2,>=1.6.3->tensorboard~=2.4->ten
sorflow) (4.7.2)
Requirement already satisfied: urllib3!=1.25.0,!=1.25.1,<1.26,>=1.21.1 in
e:\anxe\lib\site-packages (from requests<3,>=2.21.0->tensorboard~=2.4->tenso
rflow) (1.25.8)
Requirement already satisfied: idna<2.9,>=2.5 in e:\anxe\lib\site-packages
(from requests<3,>=2.21.0->tensorboard~=2.4->tensorflow) (2.8)
Requirement already satisfied: chardet<3.1.0,>=3.0.2 in e:\anxe\lib\site-pac
kages (from requests<3,>=2.21.0->tensorboard~=2.4->tensorflow) (3.0.4)
Requirement already satisfied: certifi>=2017.4.17 in e:\anxe\lib\site-packag
es (from requests<3,>=2.21.0->tensorboard~=2.4->tensorflow) (2019.11.28)
Requirement already satisfied: importlib-metadata; python_version < "3.8" in
e:\anxe\lib\site-packages (from markdown>=2.6.8->tensorboard~=2.4->tensorflo
w) (1.5.0)
Requirement already satisfied: oauthlib>=3.0.0 in e:\anxe\lib\site-packages
(from requests-oauthlib>=0.7.0->google-auth-oauthlib<0.5,>=0.4.1->tensorboar
d~=2.4->tensorflow) (3.1.0)
Requirement already satisfied: pyasn1<0.5.0,>=0.4.6 in e:\anxe\lib\site-pack
ages (from pyasn1-modules>=0.2.1->google-auth<2,>=1.6.3->tensorboard~=2.4->t
ensorflow) (0.4.8)
Requirement already satisfied: zipp>=0.5 in e:\anxe\lib\site-packages (from
importlib-metadata; python_version < "3.8"->markdown>=2.6.8->tensorboard~=2.
4->tensorflow) (2.2.0)
Installing collected packages: google-pasta, termcolor, grpcio, typing-exten
sions, protobuf, tensorboard-plugin-wit, tensorboard, tensorflow-estimator,
flatbuffers, wrapt, opt-einsum, keras-preprocessing, tensorflow
  Attempting uninstall: wrapt
    Found existing installation: wrapt 1.11.2
    Uninstalling wrapt-1.11.2:
      Successfully uninstalled wrapt-1.11.2
Successfully installed flatbuffers-1.12 google-pasta-0.2.0 grpcio-1.32.0 ker
as-preprocessing-1.1.2 opt-einsum-3.3.0 protobuf-3.15.8 tensorboard-2.4.1 te
nsorboard-plugin-wit-1.8.0 tensorflow-2.4.1 tensorflow-estimator-2.4.0 termc
olor-1.1.0 typing-extensions-3.7.4.3 wrapt-1.12.1

ERROR: astroid 2.3.3 requires typed-ast<1.5,>=1.4.0; implementation_name ==
"cpython" and python_version < "3.8", which is not installed.
ERROR: astroid 2.3.3 has requirement wrapt==1.11.*, but you'll have wrapt 1.
12.1 which is incompatible.
```

In [55]:

```
def create_model(learn_rate=0.01):
    model = tf.keras.Sequential()
    model.add(tf.keras.layers.Dense(4))
    # model.add(tf.keras.layers.Dropout(0.2))
    model.add(tf.keras.layers.Dense(4))
    model.add(tf.keras.layers.Dense(4))
    model.add(tf.keras.layers.Dense(1))

    opt = keras.optimizers.Adam(learning_rate=learn_rate)
    model.compile(loss='mse', optimizer=opt)
    return model
```

In [63]:

```
from keras.wrappers.scikit_learn import KerasRegressor
model = KerasRegressor(build_fn=create_model)
learn_rate = [0.001]
batch_size = [10,32]
epochs = [10, 50]
param_grid = dict(learn_rate=learn_rate,batch_size=batch_size,epochs=epochs)

grid = GridSearchCV(estimator=model, param_grid=param_grid, n_jobs=4, cv=5,verbose=10)
grid_result = grid.fit(X_train, y_train)
```

```
Fitting 5 folds for each of 4 candidates, totalling 20 fits

[Parallel(n_jobs=4)]: Using backend LokyBackend with 4 concurrent workers.
[Parallel(n_jobs=4)]: Done   5 tasks      | elapsed:  6.4min
[Parallel(n_jobs=4)]: Done  10 tasks      | elapsed: 19.9min
[Parallel(n_jobs=4)]: Done  16 out of  20 | elapsed: 26.2min remaining:  6.5
min
[Parallel(n_jobs=4)]: Done  20 out of  20 | elapsed: 33.1min finished

Epoch 1/10
4050/4050 [==============================] - 8s 2ms/step - loss: 0.1141
Epoch 2/10
4050/4050 [==============================] - 7s 2ms/step - loss: 9.3862e-04
Epoch 3/10
4050/4050 [==============================] - 8s 2ms/step - loss: 9.6394e-04
Epoch 4/10
4050/4050 [==============================] - 8s 2ms/step - loss: 9.5172e-04
Epoch 5/10
4050/4050 [==============================] - 7s 2ms/step - loss: 9.4647e-04
Epoch 6/10
4050/4050 [==============================] - 8s 2ms/step - loss: 9.3301e-04
Epoch 7/10
4050/4050 [==============================] - 7s 2ms/step - loss: 9.3517e-04
Epoch 8/10
4050/4050 [==============================] - 7s 2ms/step - loss: 9.3295e-04
Epoch 9/10
4050/4050 [==============================] - 7s 2ms/step - loss: 9.2471e-04
Epoch 10/10
4050/4050 [==============================] - 7s 2ms/step - loss: 9.2251e-04
```

In [64]:

```
print("Best: %f using %s" % (grid_result.best_score_, grid_result.best_params_))
```

```
Best: -0.000989 using {'batch_size': 32, 'epochs': 10, 'learn_rate': 0.001}
```

After doing grid search and experimenting with the hyperparameters 'batch_size': 10, 'epochs': 10, 'learn_rate': 0.001 gave the best MSE

In [65]:

```
model = tf.keras.Sequential()
model.add(tf.keras.layers.Dense(4))
# model.add(tf.keras.layers.Dropout(0.2))
model.add(tf.keras.layers.Dense(4))
model.add(tf.keras.layers.Dense(4))

model.add(tf.keras.layers.Dense(1))
opt = keras.optimizers.Adam(learning_rate=0.001)

model.compile(optimizer=opt, loss='mse')
# This builds the model for the first time:
history  = model.fit(X_train, y_train, batch_size=10, epochs=10, validation_data=(X_test,y_
```

```
Epoch 1/10
12960/12960 [==============================] - 39s 3ms/step - loss: 0.0066 -
val_loss: 9.7876e-04
Epoch 2/10
12960/12960 [==============================] - 37s 3ms/step - loss: 9.6283e-
04 - val_loss: 9.9579e-04
Epoch 3/10
12960/12960 [==============================] - 38s 3ms/step - loss: 9.3112e-
04 - val_loss: 0.0010
Epoch 4/10
12960/12960 [==============================] - 38s 3ms/step - loss: 9.2420e-
04 - val_loss: 0.0010
Epoch 5/10
12960/12960 [==============================] - 38s 3ms/step - loss: 9.2267e-
04 - val_loss: 0.0010
Epoch 6/10
12960/12960 [==============================] - 38s 3ms/step - loss: 9.1565e-
04 - val_loss: 0.0010
Epoch 7/10
12960/12960 [==============================] - 38s 3ms/step - loss: 9.1141e-
04 - val_loss: 0.0010
Epoch 8/10
12960/12960 [==============================] - 38s 3ms/step - loss: 9.1227e-
04 - val_loss: 0.0010
Epoch 9/10
12960/12960 [==============================] - 36s 3ms/step - loss: 9.1555e-
04 - val_loss: 0.0010
Epoch 10/10
12960/12960 [==============================] - 36s 3ms/step - loss: 9.1818e-
04 - val_loss: 0.0010
```

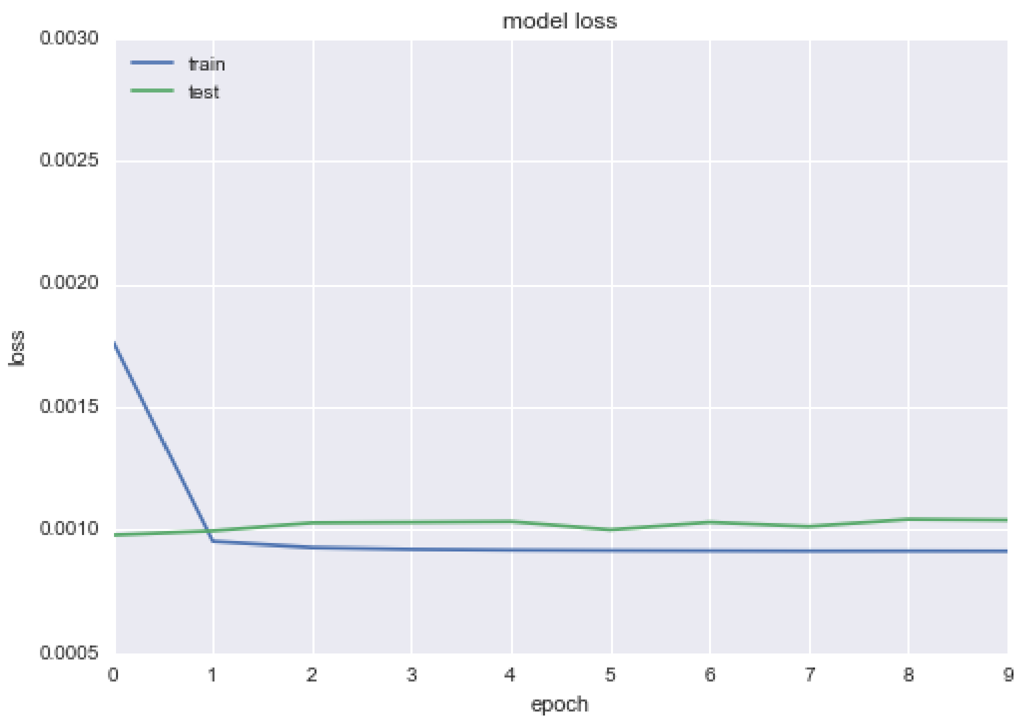
In [66]:

```
model.summary()
```

```
Model: "sequential_1"
_________________________________________________________________
Layer (type)                 Output Shape              Param #   
=================================================================
dense_4 (Dense)              (10, 4)                   20        
_________________________________________________________________
dense_5 (Dense)              (10, 4)                   20        
_________________________________________________________________
dense_6 (Dense)              (10, 4)                   20        
_________________________________________________________________
dense_7 (Dense)              (10, 1)                   5         
=================================================================
Total params: 65
Trainable params: 65
Non-trainable params: 0
_________________________________________________________________
```

In [67]:

```
plt.plot(history.history['loss'])
plt.plot(history.history['val_loss'])
plt.title('model loss')
plt.ylim(0.0005,0.003)
plt.ylabel('loss')
plt.xlabel('epoch')
plt.legend(['train', 'test'], loc='upper left')
plt.show()
```



In [68]:

```
y_pred = model.predict(X_test)
y_pred_train = model.predict(X_train)
y_pred_train = y_pred_train.flatten()
y_pred_test = model.predict(X_test)
y_pred_test = y_pred_test.flatten()
residuals  = y_test-y_pred_test
```

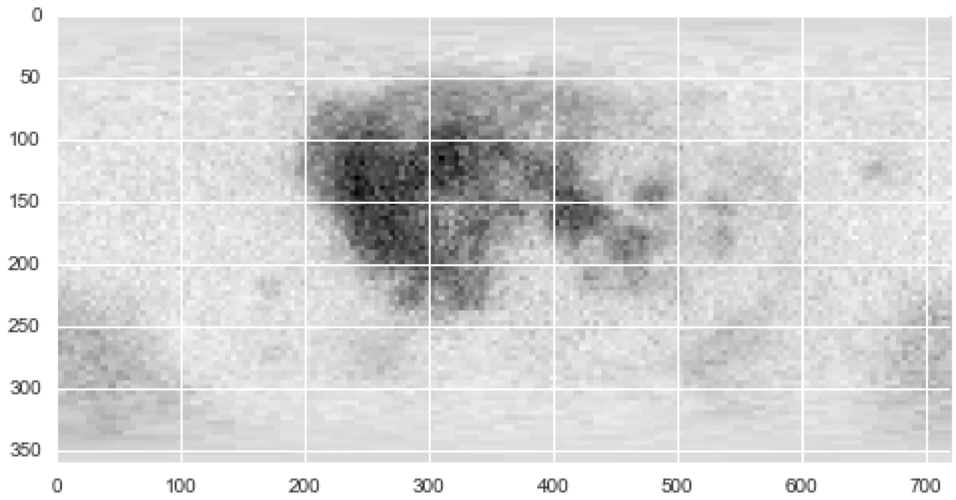
In [69]:

```
print("Model Evaluation")

print('MAE:', metrics.mean_absolute_error(y_test, y_pred_test))
print('MSE:', metrics.mean_squared_error(y_test, y_pred_test))
print('RMSE:', np.sqrt(metrics.mean_squared_error(y_test, y_pred_test)))
```

```
Model Evaluation
MAE: 0.02467982976373349
MSE: 0.0010398941698222788
RMSE: 0.03224739012419887
```

In [70]:

```
y_pred_train= y_pred_train.reshape(360,360)
y_pred_test= y_pred_test.reshape(360,360)
y_img = np.concatenate([y_pred_train,y_pred_test],axis=1)
plt.imshow(y_img, cmap="gray")
plt.show()
```

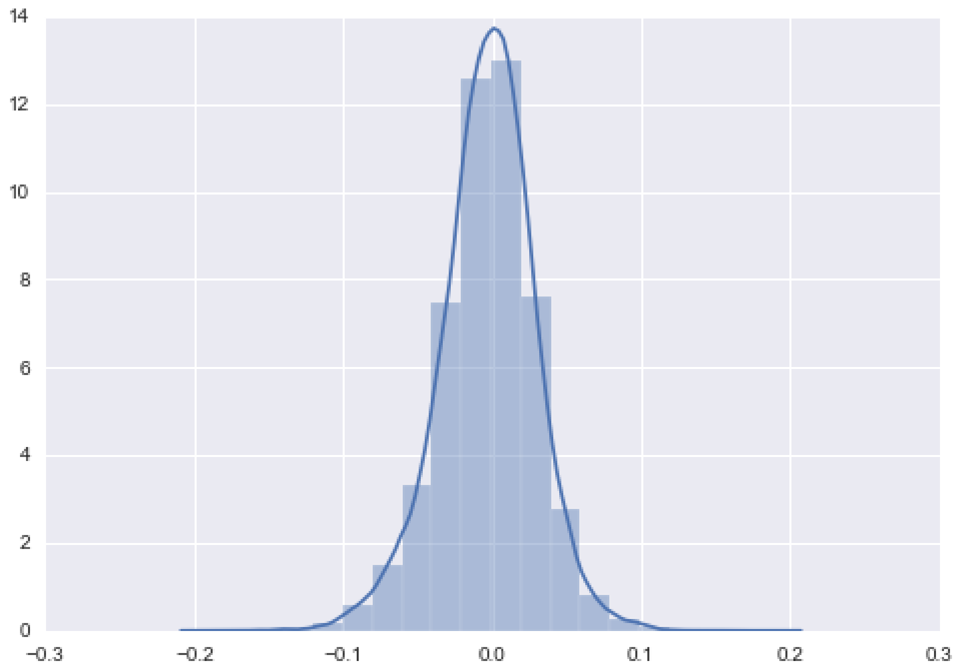


In [71]:

```
sns.distplot(residuals,bins=20)
```

Out[71]:

```
<matplotlib.axes._subplots.AxesSubplot at 0x1a22bf003c8>
```



Insights

Surprisingly even after tuning and experting with a bigger and deeper nn ,the results were still poor. This may have to do with the less no. of input features and also lack of computional resourecs for doing a extensive grid with more hyperparameter tuning

The MSE is 0.0010610954305026602

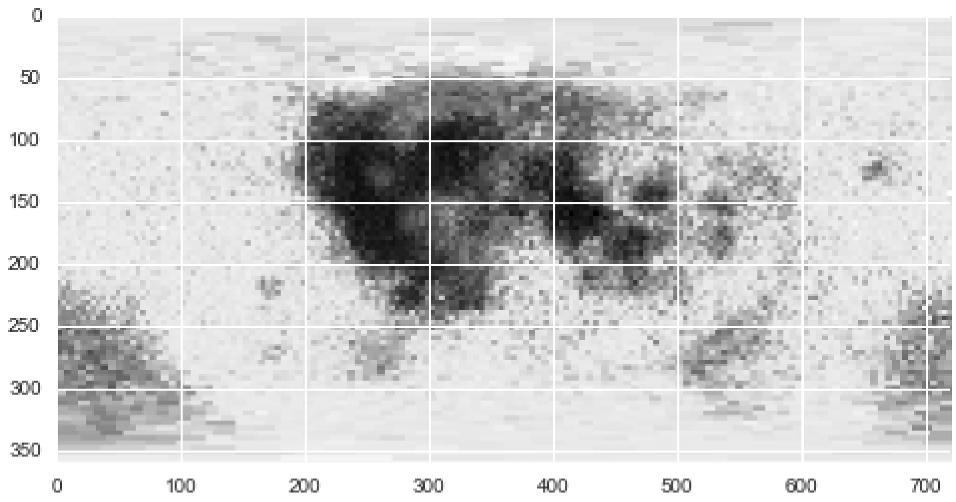
Final Results and Insights

The best image and lowest MSE obtained was with the tuned XGBOOST model

In [72]:

```
filename = 'Best_Model_XG_boost.sav'
loaded_model = pickle.load(open(filename, 'rb'))
y_pred_train = loaded_model.predict(X_train)
y_pred_test = loaded_model.predict(X_test)
residuals  = y_test-y_pred_test
print('MSE:', metrics.mean_squared_error(y_test, y_pred_test))

y_pred_train= y_pred_train.reshape(360,360)
y_pred_test= y_pred_test.reshape(360,360)
y_img = np.concatenate([y_pred_train,y_pred_test],axis=1)

plt.imshow(y_img, cmap="gray")

plt.show()
```

```
MSE: 0.0009304179266331601
```

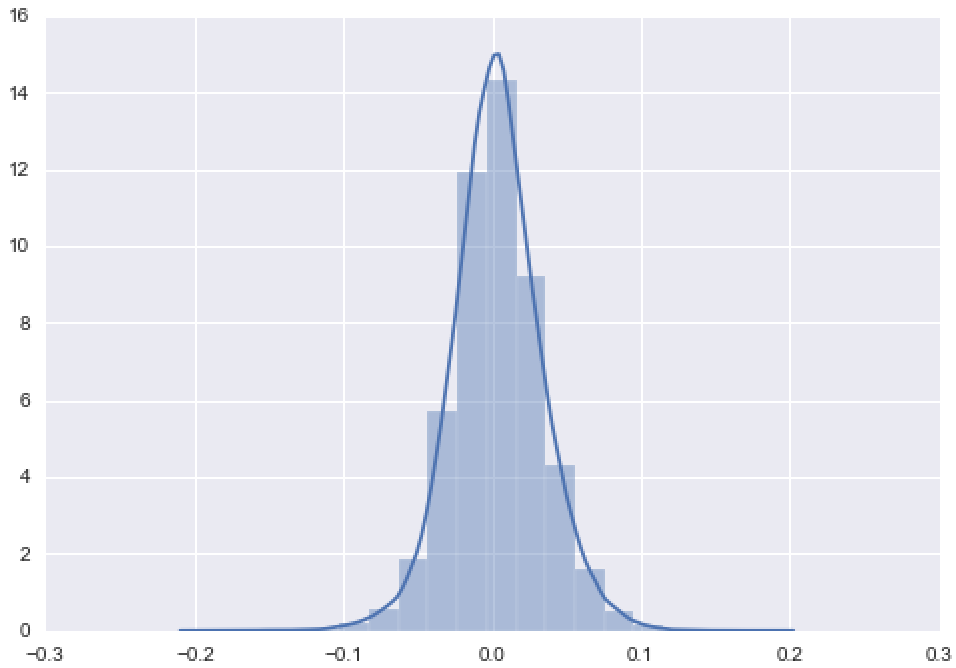


In [73]:

```
sns.distplot(residuals,bins=20)
```

Out[73]:

<matplotlib.axes._subplots.AxesSubplot at 0x1a22bfa0048>



Insights

Best results were obtained using XGBOOST, a decision-tree-based ensemble Machine Learning algorithm that uses a gradient boosting framework.

Neural Networks surprisingly didnt perform as well as expected even after basic hyper parameter tuning , but their maybe a scope of improvement.

Only having 4 features for prediction may also be a reason that most models fail to perform well.

In [ ]:

```
```