In [1]:
```
# Predict asteroid diameter values using 'Asteroid.csv' dataset from Kaggle co
ntributed by Victor Basu
    # Link: https://www.kaggle.com/basu369victor/prediction-of-asteroid-diamet
er
# Model: XGBRegressor
# Notes on data:
    # data is medium size comprising of 839736 entries and 27 columns
    # for a small portion of the data (~ 1/6) the asteroids diameters are know
n -
        # this portion will be used to train and validate the model
    # subsequently the model will be used to predict the diameters for the dat
a in which this information is missing

# Essential updates (6/2020) from previous project version (2/2020)
    # Improvements in data processing and data visualization
    # Comparison between XGBRegressor model and Linear Regression model is dis
carded -->
        # XGBRegressor model optimization via hyperparameter tuning is added i
nstead
    # Statistics of residuals - distribution, mean and standard deviation - re
place absolute error statistics
    # as model performance metrics
```

In [2]:
```
# Import libraries

import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns
%matplotlib inline
sns.set(style = "whitegrid", font_scale = 1.5)
```

In [3]:
```
# Ignore warnings

import warnings
warnings.filterwarnings('ignore')
```

In [4]:
```
# Read data

data = pd.read_csv('Asteroid.csv', low_memory = False)
data.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 839736 entries, 0 to 839735
Data columns (total 27 columns):
 #   Column          Non-Null Count   Dtype  
---  ------          --------------   -----  
 0   full_name       839736 non-null  object 
 1   a               839734 non-null  float64
 2   e               839736 non-null  float64
 3   G               119 non-null     float64
 4   i               839736 non-null  float64
 5   om              839736 non-null  float64
 6   w               839736 non-null  float64
 7   q               839736 non-null  float64
 8   ad              839730 non-null  float64
 9   per_y           839735 non-null  float64
 10  data_arc        823947 non-null  float64
 11  condition_code  838743 non-null  object 
 12  n_obs_used      839736 non-null  int64  
 13  H               837042 non-null  float64
 14  diameter        137681 non-null  object 
 15  extent          18 non-null      object 
 16  albedo          136452 non-null  float64
 17  rot_per         18796 non-null   float64
 18  GM              14 non-null      float64
 19  BV              1021 non-null    float64
 20  UB              979 non-null     float64
 21  IR              1 non-null       float64
 22  spec_B          1666 non-null    object 
 23  spec_T          980 non-null     object 
 24  neo             839730 non-null  object 
 25  pha             822814 non-null  object 
 26  moid            822814 non-null  float64
dtypes: float64(18), int64(1), object(8)
memory usage: 173.0+ MB
```

In [5]:
```
# Print data column names for use in the code below

data.columns
```

Out[5]:
```
Index(['full_name', 'a', 'e', 'G', 'i', 'om', 'w', 'q', 'ad', 'per_y',
       'data_arc', 'condition_code', 'n_obs_used', 'H', 'diameter', 'extent',
       'albedo', 'rot_per', 'GM', 'BV', 'UB', 'IR', 'spec_B', 'spec_T', 'ne
o',
       'pha', 'moid'],
      dtype='object')
```

In [6]:
```
# Select only features with meaningful amount of non-null values -->
    # drop 'G', 'extent', 'GM', 'BV', 'UB', 'IR', 'spec_B', and 'spec_T'
# In addition, drop 'full_name' and 'n_obs_used' which are not meaningful for
 the problem
# Place the target 'diameter' at the end for easier separation of features, X,
and target, y, later on

data = data[['a', 'e', 'i', 'om', 'w', 'q', 'ad', 'per_y', 'data_arc', 'condit
ion_code',
             'H', 'albedo', 'neo', 'pha', 'moid', 'diameter']]
data.head(10)
```

Out[6]:

	a	e	i	om	w	q	ad	per_y	data_ar
0	2.769165	0.076009	10.594067	80.305532	73.597694	2.558684	2.979647	4.608202	8822.
1	2.772466	0.230337	34.836234	173.080063	310.048857	2.133865	3.411067	4.616444	72318.
2	2.669150	0.256942	12.988919	169.852760	248.138626	1.983332	3.354967	4.360814	72684.
3	2.361418	0.088721	7.141771	103.810804	150.728541	2.151909	2.570926	3.628837	24288.
4	2.574249	0.191095	5.366988	141.576604	358.687608	2.082324	3.066174	4.130323	63431.
5	2.425160	0.203007	14.737901	138.640203	239.807490	1.932835	2.917485	3.776755	62329.
6	2.385334	0.231206	5.523651	259.563231	145.265106	1.833831	2.936837	3.684105	62452.
7	2.201764	0.156499	5.886955	110.889330	285.287462	1.857190	2.546339	3.267115	62655.
8	2.385637	0.123114	5.576816	68.908577	6.417369	2.091931	2.679342	3.684806	61821.
9	3.141539	0.112461	3.831560	283.202167	312.315206	2.788240	3.494839	5.568291	62175.

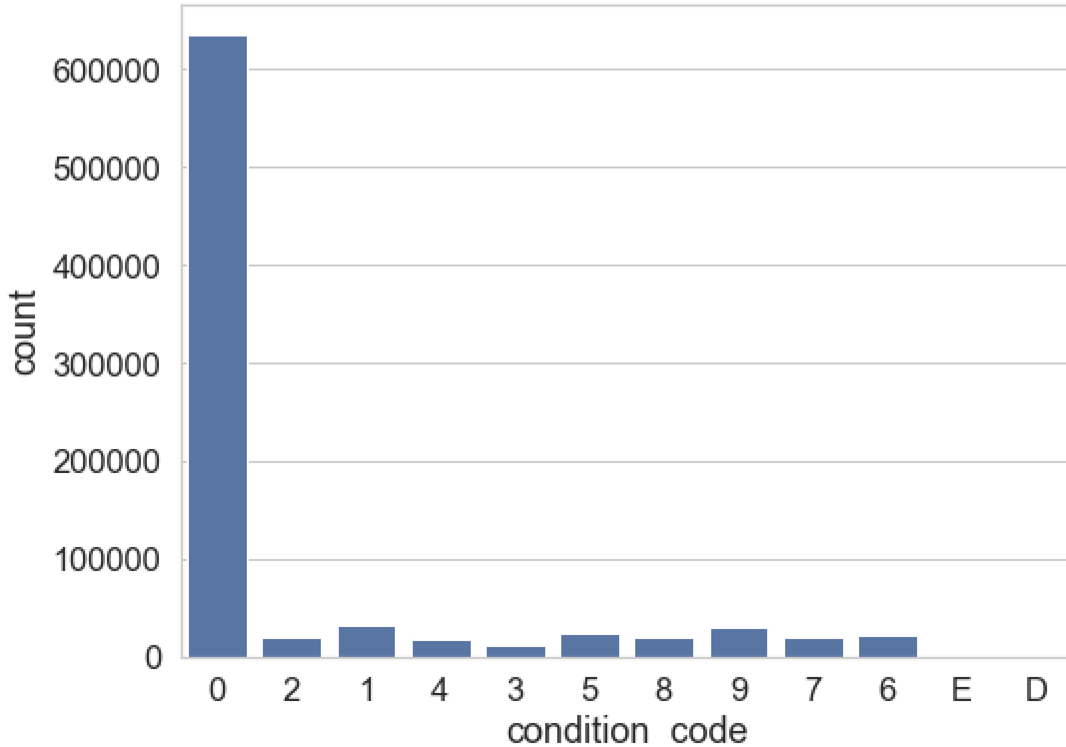
In [7]:
```
# 1) Data Processing and EDA
```

In [8]:
```
data.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 839736 entries, 0 to 839735
Data columns (total 16 columns):
 #   Column          Non-Null Count   Dtype  
---  ------          --------------   -----  
 0   a               839734 non-null  float64
 1   e               839736 non-null  float64
 2   i               839736 non-null  float64
 3   om              839736 non-null  float64
 4   w               839736 non-null  float64
 5   q               839736 non-null  float64
 6   ad              839730 non-null  float64
 7   per_y           839735 non-null  float64
 8   data_arc        823947 non-null  float64
 9   condition_code  838743 non-null  object 
 10  H               837042 non-null  float64
 11  albedo          136452 non-null  float64
 12  neo             839730 non-null  object 
 13  pha             822814 non-null  object 
 14  moid            822814 non-null  float64
 15  diameter        137681 non-null  object 
dtypes: float64(12), object(4)
memory usage: 102.5+ MB
```

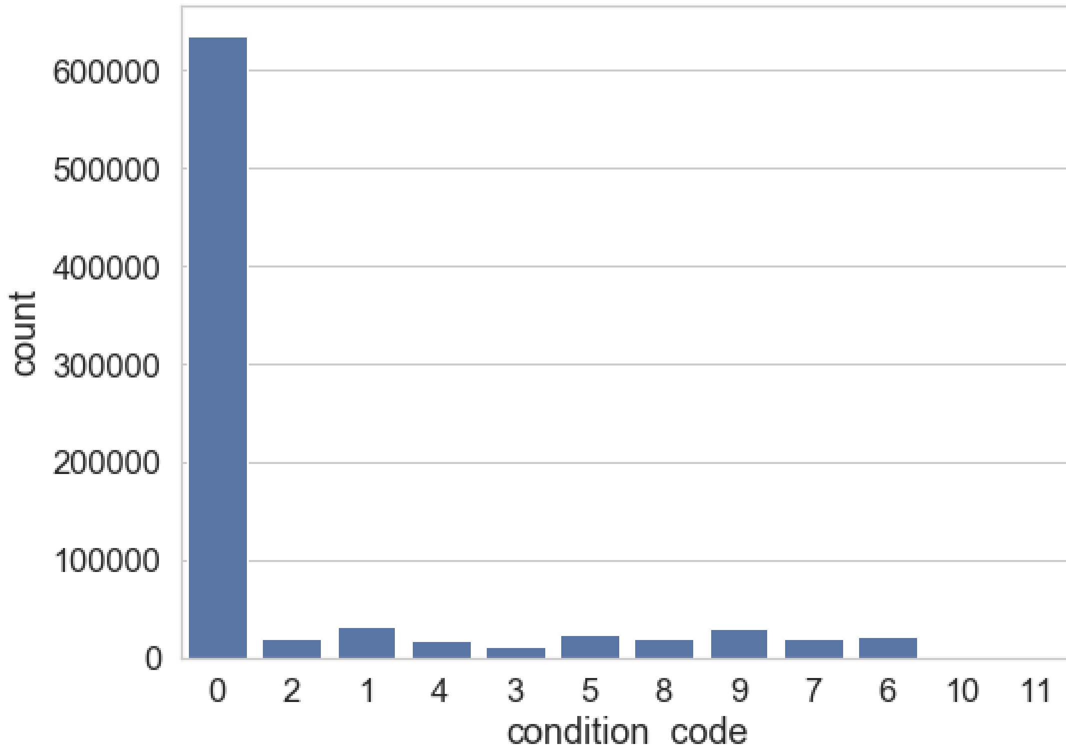
In [9]:
```
# Features 'condition_code', 'neo', and 'pha' appear to be categorical --> exa
mine these features
```

In [10]:
```
# Examine 'condition_code'

plt.figure(figsize = (8, 6))
sns.countplot(data['condition_code'], color = 'b')
plt.show()
```

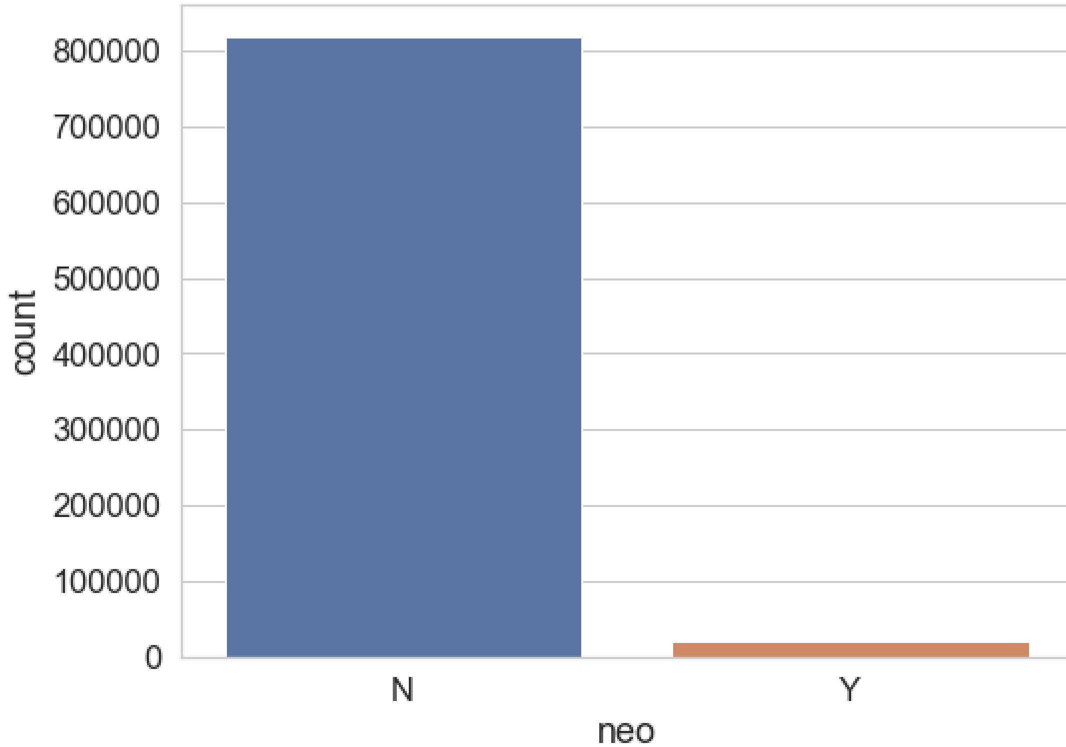


In [11]:
```
# This is a categorical feature with majority of data points having values = 0
# Note that 'condition_code' values includes both numbers and letters
```

In [12]:
```
# Assign numeric values to the categorical values 'E' and 'D'

data['condition_code'].replace({'E': 10, 'D': 11}, inplace=True)

plt.figure(figsize = (8, 6))
sns.countplot(data['condition_code'], color = 'b')
plt.show()
```

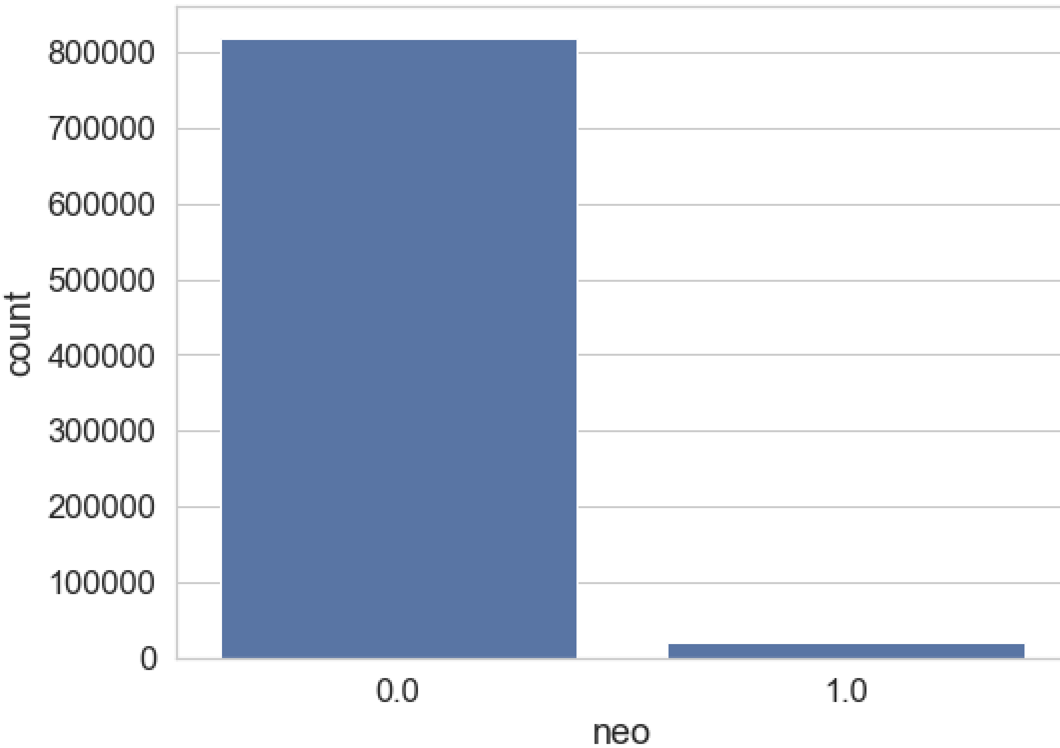


In [13]:
```
# Examine 'neo'

plt.figure(figsize = (8, 6))
sns.countplot(data['neo'])
plt.show()
```

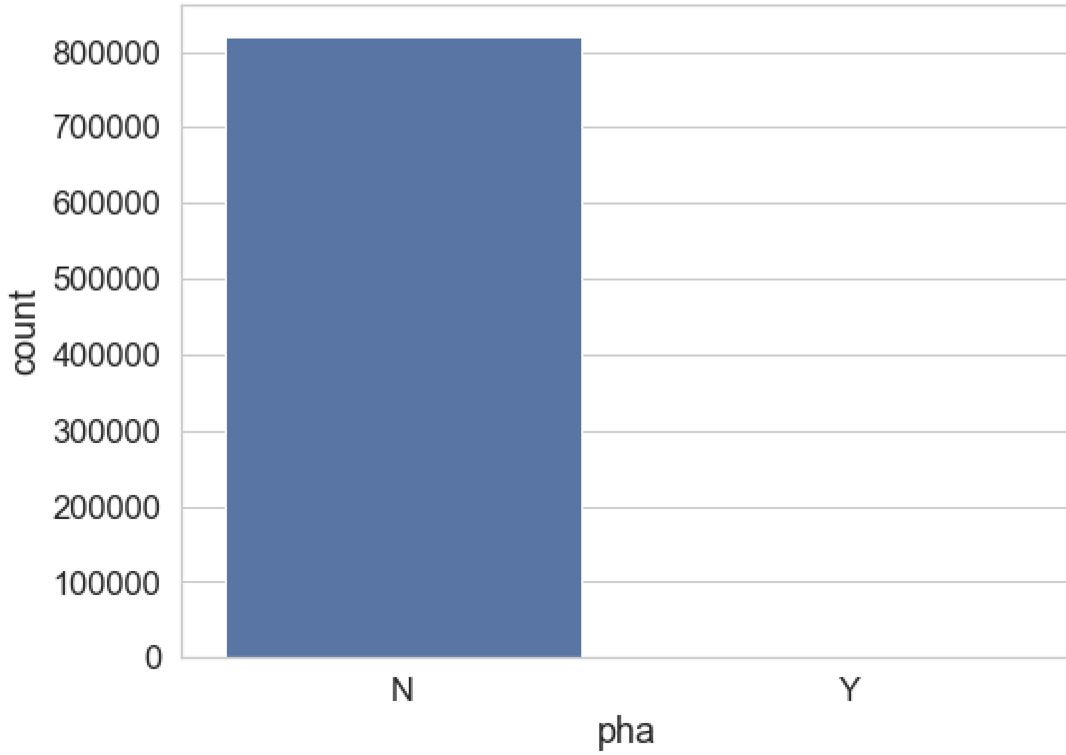


In [14]:
```
# Categorical feature --> majority of data points = N
```

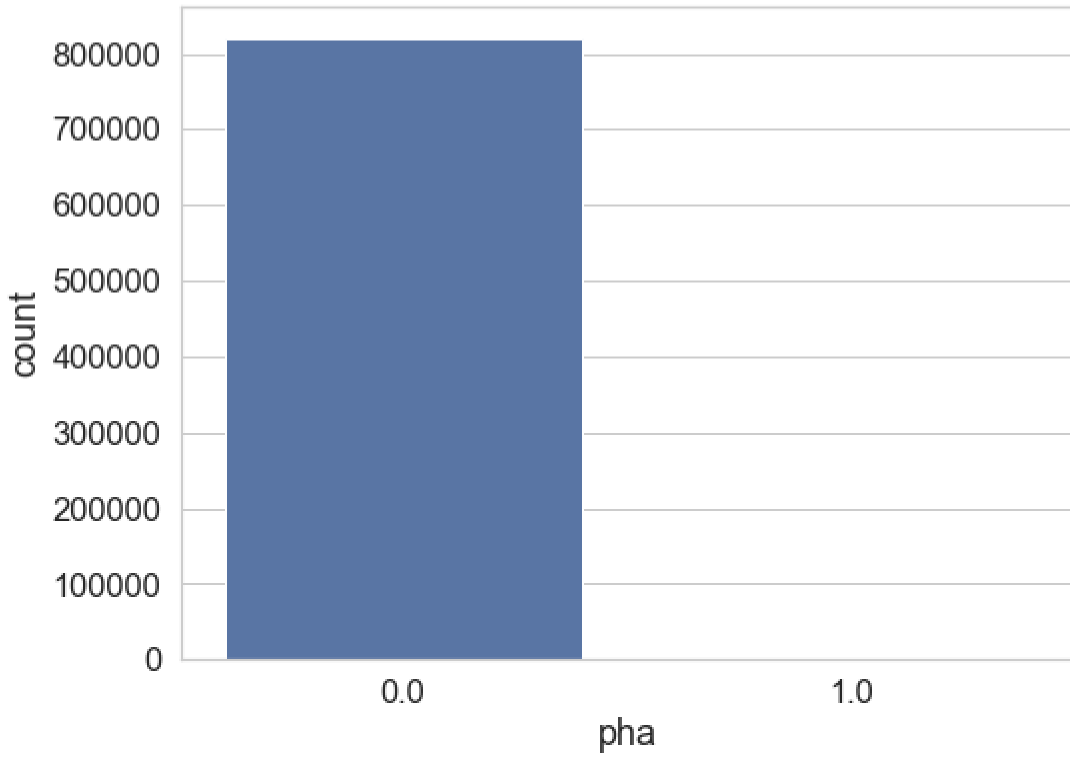
In [15]:
```
# Replace categorical values, N and Y, with numerical values of 0 and 1, respe
ctively

data['neo'].replace({'N': 0, 'Y': 1}, inplace=True)

plt.figure(figsize = (8, 6))
sns.countplot(data['neo'], color = 'b')
plt.show()
```



In [16]:
```
# Examine 'pha'

plt.figure(figsize = (8, 6))
sns.countplot(data['pha'])
plt.show()
```



In [17]:
```
# Categorical feature --> majority of data points = N

# Replace the categorical values, N and Y, with numerical values of 0 and 1, r
espectively

data['pha'].replace({'N': 0, 'Y': 1}, inplace=True)

plt.figure(figsize = (8, 6))
sns.countplot(data['pha'], color = 'b')
plt.show()
```



In [18]:
```
# Examine target, 'diameter'

data.head(10)
```

Out[18]:

	a	e	i	om	w	q	ad	per_y	data_ar
0	2.769165	0.076009	10.594067	80.305532	73.597694	2.558684	2.979647	4.608202	8822.
1	2.772466	0.230337	34.836234	173.080063	310.048857	2.133865	3.411067	4.616444	72318.
2	2.669150	0.256942	12.988919	169.852760	248.138626	1.983332	3.354967	4.360814	72684.
3	2.361418	0.088721	7.141771	103.810804	150.728541	2.151909	2.570926	3.628837	24288.
4	2.574249	0.191095	5.366988	141.576604	358.687608	2.082324	3.066174	4.130323	63431.
5	2.425160	0.203007	14.737901	138.640203	239.807490	1.932835	2.917485	3.776755	62329.
6	2.385334	0.231206	5.523651	259.563231	145.265106	1.833831	2.936837	3.684105	62452.
7	2.201764	0.156499	5.886955	110.889330	285.287462	1.857190	2.546339	3.267115	62655.
8	2.385637	0.123114	5.576816	68.908577	6.417369	2.091931	2.679342	3.684806	61821.
9	3.141539	0.112461	3.831560	283.202167	312.315206	2.788240	3.494839	5.568291	62175.

In [19]:
```
data.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 839736 entries, 0 to 839735
Data columns (total 16 columns):
 #   Column          Non-Null Count   Dtype  
---  ------          --------------   -----  
 0   a               839734 non-null  float64
 1   e               839736 non-null  float64
 2   i               839736 non-null  float64
 3   om              839736 non-null  float64
 4   w               839736 non-null  float64
 5   q               839736 non-null  float64
 6   ad              839730 non-null  float64
 7   per_y           839735 non-null  float64
 8   data_arc        823947 non-null  float64
 9   condition_code  838743 non-null  object 
 10  H               837042 non-null  float64
 11  albedo          136452 non-null  float64
 12  neo             839730 non-null  float64
 13  pha             822814 non-null  float64
 14  moid            822814 non-null  float64
 15  diameter        137681 non-null  object 
dtypes: float64(14), object(2)
memory usage: 102.5+ MB
```

In [20]:
```
# Columns 'diameter' and 'albedo' have only about 1/6 of non-null values compa
red to other features
# Although 'diameter' has numerical values in the table, it appears that it is
in string format - data type 'object'
# Convert data to numeric format 'float64'

data = data.astype('float64')

data.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 839736 entries, 0 to 839735
Data columns (total 16 columns):
 #   Column          Non-Null Count   Dtype  
---  ------          --------------   -----  
 0   a               839734 non-null  float64
 1   e               839736 non-null  float64
 2   i               839736 non-null  float64
 3   om              839736 non-null  float64
 4   w               839736 non-null  float64
 5   q               839736 non-null  float64
 6   ad              839730 non-null  float64
 7   per_y           839735 non-null  float64
 8   data_arc        823947 non-null  float64
 9   condition_code  838743 non-null  float64
 10  H               837042 non-null  float64
 11  albedo          136452 non-null  float64
 12  neo             839730 non-null  float64
 13  pha             822814 non-null  float64
 14  moid            822814 non-null  float64
 15  diameter        137681 non-null  float64
dtypes: float64(16)
memory usage: 102.5 MB
```

In [21]:
```
# Replace all missing values with 0 which is the sparse value expected by XGBo
ost

data.fillna(0, inplace = True)

data.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 839736 entries, 0 to 839735
Data columns (total 16 columns):
 #   Column          Non-Null Count   Dtype  
---  ------          --------------   -----  
 0   a               839736 non-null  float64
 1   e               839736 non-null  float64
 2   i               839736 non-null  float64
 3   om              839736 non-null  float64
 4   w               839736 non-null  float64
 5   q               839736 non-null  float64
 6   ad              839736 non-null  float64
 7   per_y           839736 non-null  float64
 8   data_arc        839736 non-null  float64
 9   condition_code  839736 non-null  float64
 10  H               839736 non-null  float64
 11  albedo          839736 non-null  float64
 12  neo             839736 non-null  float64
 13  pha             839736 non-null  float64
 14  moid            839736 non-null  float64
 15  diameter        839736 non-null  float64
dtypes: float64(16)
memory usage: 102.5 MB
```

In [22]:
```
# Create data set, data_1, where diameter is known

data_1 = data[data['diameter'] > 0] # values greater than 0 correspond to data
with known diameter
data_1.info()
```

```
<class 'pandas.core.frame.DataFrame'>
Int64Index: 137681 entries, 0 to 810411
Data columns (total 16 columns):
 #   Column          Non-Null Count   Dtype  
---  ------          --------------   -----  
 0   a               137681 non-null  float64
 1   e               137681 non-null  float64
 2   i               137681 non-null  float64
 3   om              137681 non-null  float64
 4   w               137681 non-null  float64
 5   q               137681 non-null  float64
 6   ad              137681 non-null  float64
 7   per_y           137681 non-null  float64
 8   data_arc        137681 non-null  float64
 9   condition_code  137681 non-null  float64
 10  H               137681 non-null  float64
 11  albedo          137681 non-null  float64
 12  neo             137681 non-null  float64
 13  pha             137681 non-null  float64
 14  moid            137681 non-null  float64
 15  diameter        137681 non-null  float64
dtypes: float64(16)
memory usage: 17.9 MB
```

In [23]:
```
# Data with known asteroid diameter have total of 137681 entries
```

In [24]:
```
# Check data_1

data_1.head(10)
```

Out[24]:

	a	e	i	om	w	q	ad	per_y	data_ar
0	2.769165	0.076009	10.594067	80.305532	73.597694	2.558684	2.979647	4.608202	8822.
1	2.772466	0.230337	34.836234	173.080063	310.048857	2.133865	3.411067	4.616444	72318.
2	2.669150	0.256942	12.988919	169.852760	248.138626	1.983332	3.354967	4.360814	72684.
3	2.361418	0.088721	7.141771	103.810804	150.728541	2.151909	2.570926	3.628837	24288.
4	2.574249	0.191095	5.366988	141.576604	358.687608	2.082324	3.066174	4.130323	63431.
5	2.425160	0.203007	14.737901	138.640203	239.807490	1.932835	2.917485	3.776755	62329.
6	2.385334	0.231206	5.523651	259.563231	145.265106	1.833831	2.936837	3.684105	62452.
7	2.201764	0.156499	5.886955	110.889330	285.287462	1.857190	2.546339	3.267115	62655.
8	2.385637	0.123114	5.576816	68.908577	6.417369	2.091931	2.679342	3.684806	61821.
9	3.141539	0.112461	3.831560	283.202167	312.315206	2.788240	3.494839	5.568291	62175.

In [25]:
```
# Everything looks fine
```

In [26]:
```
# Create dataset, data_2, where diameter is unknown

data_2 = data[data['diameter'] < data_1['diameter'].min()] # this leaves only
 0s which correspond to unknown diameter
data_2.info()
```

```
<class 'pandas.core.frame.DataFrame'>
Int64Index: 702055 entries, 681 to 839735
Data columns (total 16 columns):
 #   Column          Non-Null Count   Dtype
---  ------          --------------   -----
 0   a               702055 non-null  float64
 1   e               702055 non-null  float64
 2   i               702055 non-null  float64
 3   om              702055 non-null  float64
 4   w               702055 non-null  float64
 5   q               702055 non-null  float64
 6   ad              702055 non-null  float64
 7   per_y           702055 non-null  float64
 8   data_arc        702055 non-null  float64
 9   condition_code  702055 non-null  float64
 10  H               702055 non-null  float64
 11  albedo          702055 non-null  float64
 12  neo             702055 non-null  float64
 13  pha             702055 non-null  float64
 14  moid            702055 non-null  float64
 15  diameter        702055 non-null  float64
dtypes: float64(16)
memory usage: 91.1 MB
```

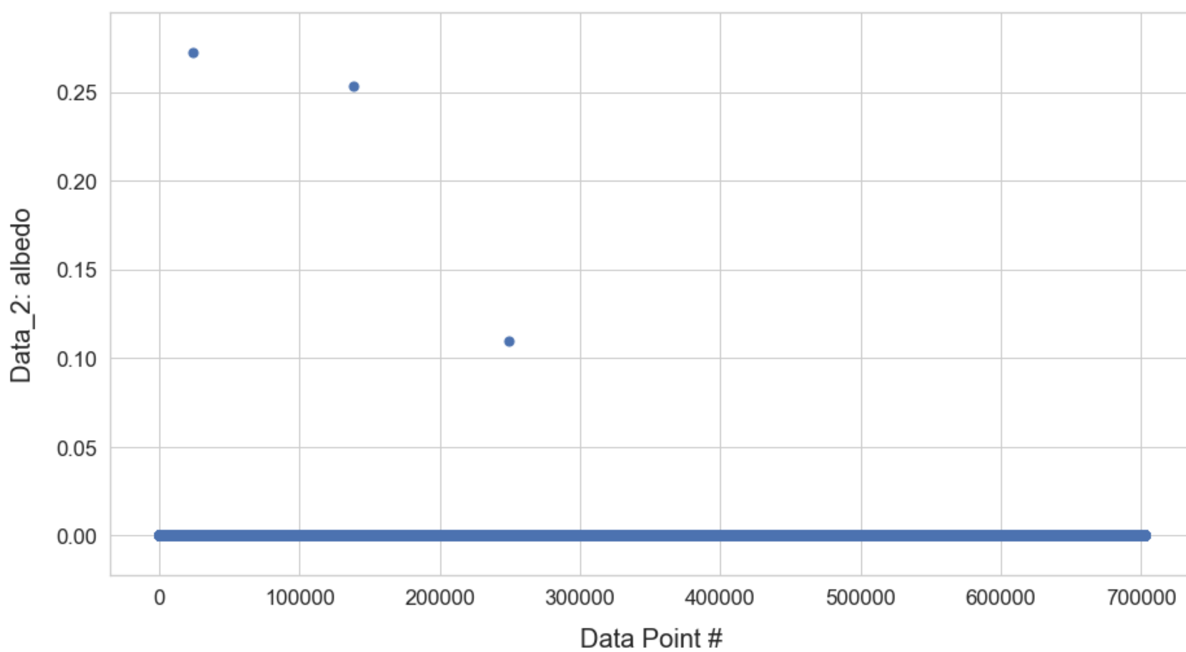
In [27]:
```
# Data with unknown asteroid diameter have total of 702055 entries (more than
 5 x that of data_1)
```

In [28]:
```
# Check data_2

data_2.head(10)
```

Out[28]:

	a	e	i	om	w	q	ad	per_y	data
681	2.654040	0.171983	11.505648	190.799958	104.993826	2.197591	3.110489	4.323837	40(
698	2.610998	0.410284	15.299180	242.551766	91.399514	1.539746	3.682249	4.219081	42
718	2.638780	0.546301	11.564845	183.887287	156.163668	1.197212	4.080348	4.286601	39
729	2.243362	0.177505	4.234895	95.073806	123.549777	1.845154	2.641570	3.360139	39
842	2.279598	0.209766	7.997717	4.071363	316.957206	1.801415	2.757780	3.441878	37
961	2.908998	0.097329	2.602636	145.481660	223.473847	2.625868	3.192128	4.961619	37
984	2.299979	0.277462	4.056565	290.307048	59.553605	1.661822	2.938137	3.488142	35
1008	2.625175	0.455500	15.769676	229.461495	186.428747	1.429408	3.820942	4.253492	34
1010	2.391976	0.350864	5.494744	132.525452	353.279770	1.552718	3.231235	3.699504	34
1064	2.360276	0.297141	8.362855	330.324142	353.652287	1.658942	3.061610	3.626205	33

In [29]:
```
# It appears 'albedo' is also unknown in data_2 --> only 0s are shown in table

# Check by plotting data_2['albedo']

plt.figure(figsize = (15, 8))
plt.scatter(np.arange(1, len(data_2) + 1), data_2['albedo'], s = 50, c = 'b')
plt.xlabel('Data Point #', fontsize = 20, labelpad = 15)
plt.ylabel('Data_2: albedo', fontsize = 20, labelpad = 15)
plt.show()
```



In [30]:
```
# Indeed, almost all ‘albedo’ data points in data_2 are 0s and it cannot be us
ed in predictions -->
    # remove ‘albedo’ from both data_1 and data_2
```

In [31]:
```
data_1.columns
```

Out[31]:
```
Index(['a', 'e', 'i', 'om', 'w', 'q', 'ad', 'per_y', 'data_arc',
       'condition_code', 'H', 'albedo', 'neo', 'pha', 'moid', 'diameter'],
      dtype='object')
```

In [32]:
```
# Keep all features in data_1 except 'albedo'

data_1 = data_1[['a', 'e', 'i', 'om', 'w', 'q', 'ad', 'per_y', 'data_arc',
                 'condition_code', 'H', 'neo', 'pha', 'moid', 'diameter']]
data_1.head(10)
```

Out[32]:

	a	e	i	om	w	q	ad	per_y	data_ar
0	2.769165	0.076009	10.594067	80.305532	73.597694	2.558684	2.979647	4.608202	8822.
1	2.772466	0.230337	34.836234	173.080063	310.048857	2.133865	3.411067	4.616444	72318.
2	2.669150	0.256942	12.988919	169.852760	248.138626	1.983332	3.354967	4.360814	72684.
3	2.361418	0.088721	7.141771	103.810804	150.728541	2.151909	2.570926	3.628837	24288.
4	2.574249	0.191095	5.366988	141.576604	358.687608	2.082324	3.066174	4.130323	63431.
5	2.425160	0.203007	14.737901	138.640203	239.807490	1.932835	2.917485	3.776755	62329.
6	2.385334	0.231206	5.523651	259.563231	145.265106	1.833831	2.936837	3.684105	62452.
7	2.201764	0.156499	5.886955	110.889330	285.287462	1.857190	2.546339	3.267115	62655.
8	2.385637	0.123114	5.576816	68.908577	6.417369	2.091931	2.679342	3.684806	61821.
9	3.141539	0.112461	3.831560	283.202167	312.315206	2.788240	3.494839	5.568291	62175.

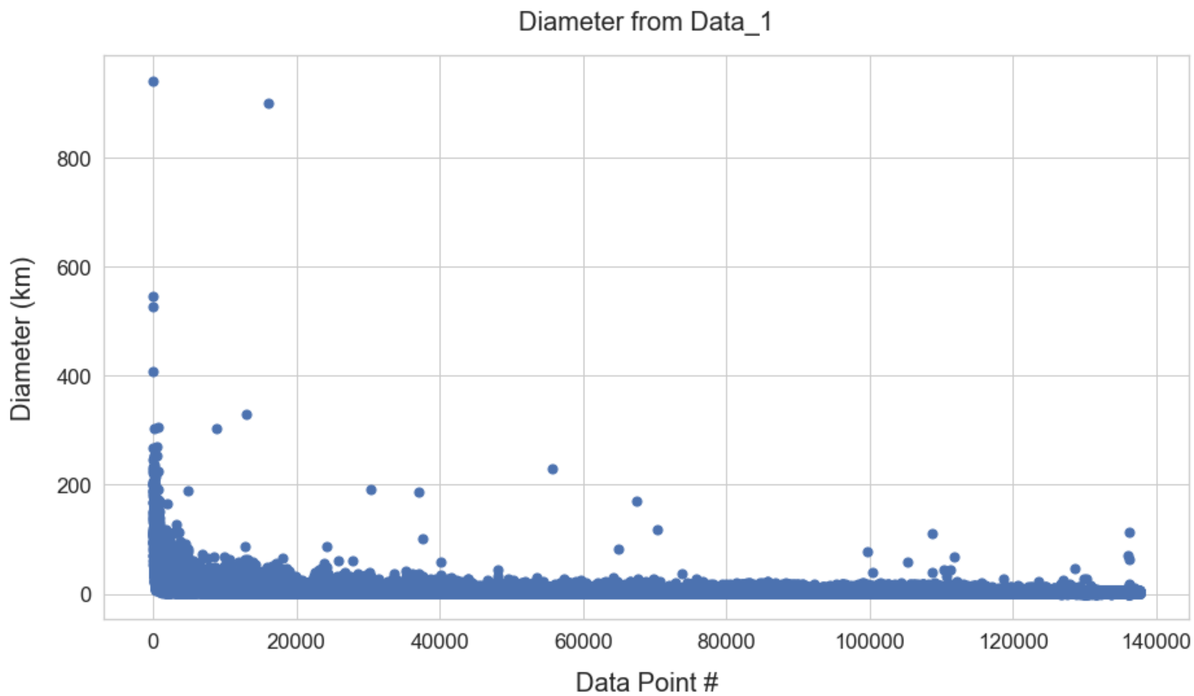
In [33]:
```
# Keep all features in data_2 except 'albedo' and 'diameter' which is unknown

data_2 = data_2[['a', 'e', 'i', 'om', 'w', 'q', 'ad', 'per_y', 'data_arc', 'co
ndition_code', 'H', 'neo', 'pha', 'moid']]

data_2.head(10)
```

Out[33]:

	a	e	i	om	w	q	ad	per_y	data
681	2.654040	0.171983	11.505648	190.799958	104.993826	2.197591	3.110489	4.323837	400
698	2.610998	0.410284	15.299180	242.551766	91.399514	1.539746	3.682249	4.219081	425
718	2.638780	0.546301	11.564845	183.887287	156.163668	1.197212	4.080348	4.286601	394
729	2.243362	0.177505	4.234895	95.073806	123.549777	1.845154	2.641570	3.360139	391
842	2.279598	0.209766	7.997717	4.071363	316.957206	1.801415	2.757780	3.441878	375
961	2.908998	0.097329	2.602636	145.481660	223.473847	2.625868	3.192128	4.961619	374
984	2.299979	0.277462	4.056565	290.307048	59.553605	1.661822	2.938137	3.488142	353
1008	2.625175	0.455500	15.769676	229.461495	186.428747	1.429408	3.820942	4.253492	349
1010	2.391976	0.350864	5.494744	132.525452	353.279770	1.552718	3.231235	3.699504	349
1064	2.360276	0.297141	8.362855	330.324142	353.652287	1.658942	3.061610	3.626205	338

In [34]:
```
# Data_1 has 14 features and target, 'diameter', left
# Data_2 consists of the same 14 features only -- no 'diameter'
```

In [35]:
```
# Visualize 'diameter' from data_1 using scatterplot

plt.figure(figsize = (15, 8))
plt.scatter(np.arange(1, len(data_1) + 1), data_1['diameter'], s = 50, c = 'b'
)
plt.title('Diameter from Data_1', fontsize = 20, pad = 20)
plt.xlabel('Data Point #', fontsize = 20, labelpad = 15)
plt.ylabel('Diameter (km)', fontsize = 20, labelpad = 15)
plt.show()
```



In [36]:
```
# It appears 'diameter' has great number of small values and only small portio
n of large values
# Get some insights from min, max, median and mean of diameter in data_1
```

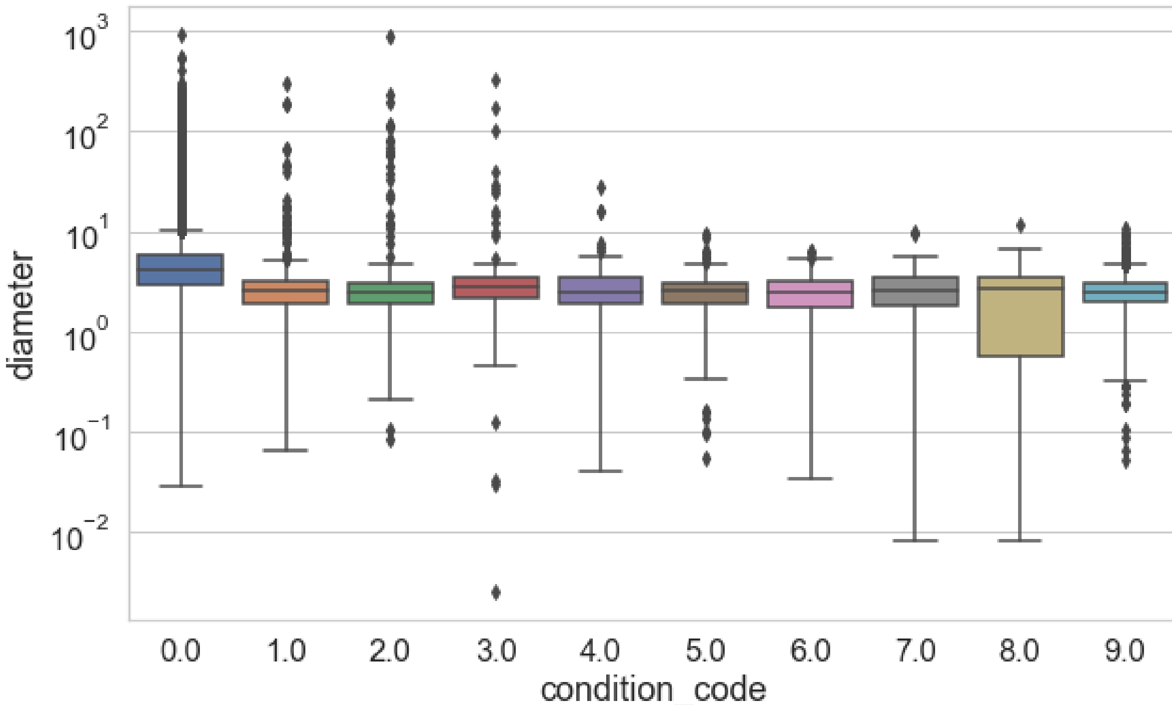
In [37]:
```
# Min, max, median and mean of diameter in data_1

print("Min diameter in km -->", round(data_1['diameter'].min(), 4))
print("Max diameter in km -->", round(data_1['diameter'].max(), 4))
print("Median diameter in km -->", round(data_1['diameter'].median(), 4))
print("Mean diameter in km -->", round(data_1['diameter'].mean(), 4))
```

```
Min diameter in km --> 0.0025
Max diameter in km --> 939.4
Median diameter in km --> 3.956
Mean diameter in km --> 5.4825
```

In [38]:
```
# Key observations:
    # 1) Max value is much larger than mean (almost 3 orders of magnitude)
    # 2) Despite that, mean and median are very close --> large values are sma
ll portion of the total number of observations
```

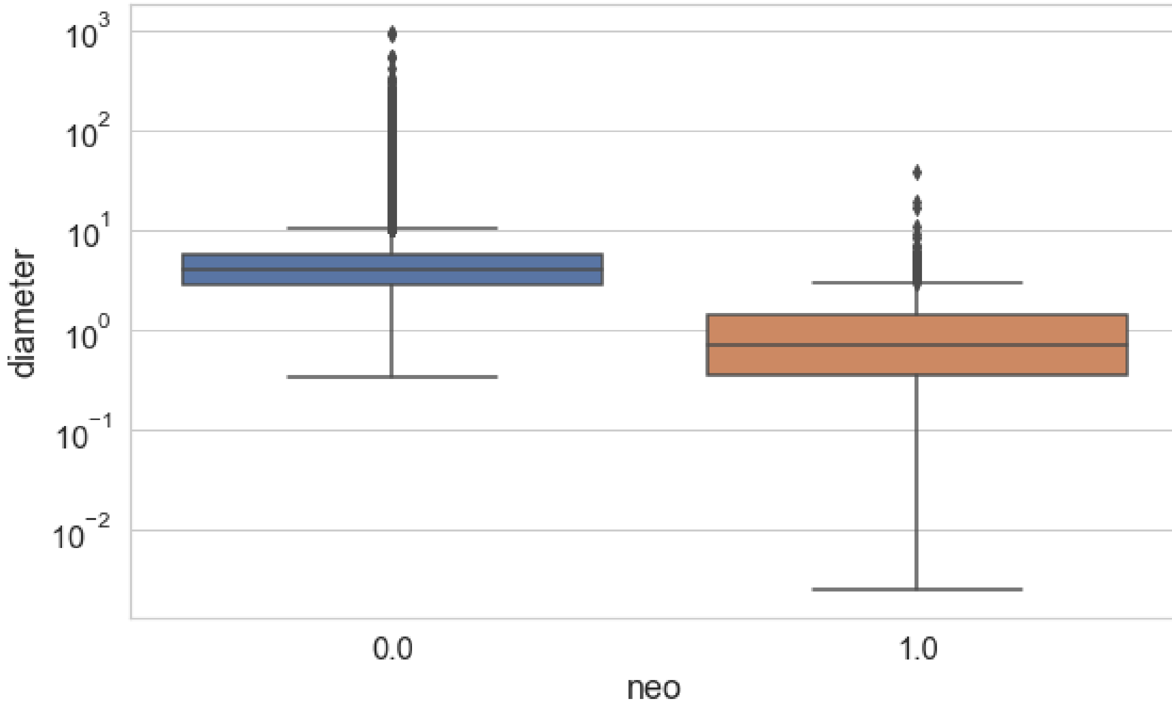
In [39]:
```
# Explore further by using boxplots
# Important note:
    # use log scale due to large spread and disparity between the number of sm
all (majority) and large diameter values
```

In [40]:
```
# Boxplot of 'diameter' in data_1 vs. 'condition_code' classes

plt.figure(figsize = (10, 6))
sns.boxplot(x = 'condition_code', y = 'diameter', data = data_1)
plt.yscale('log')
plt.show()
```

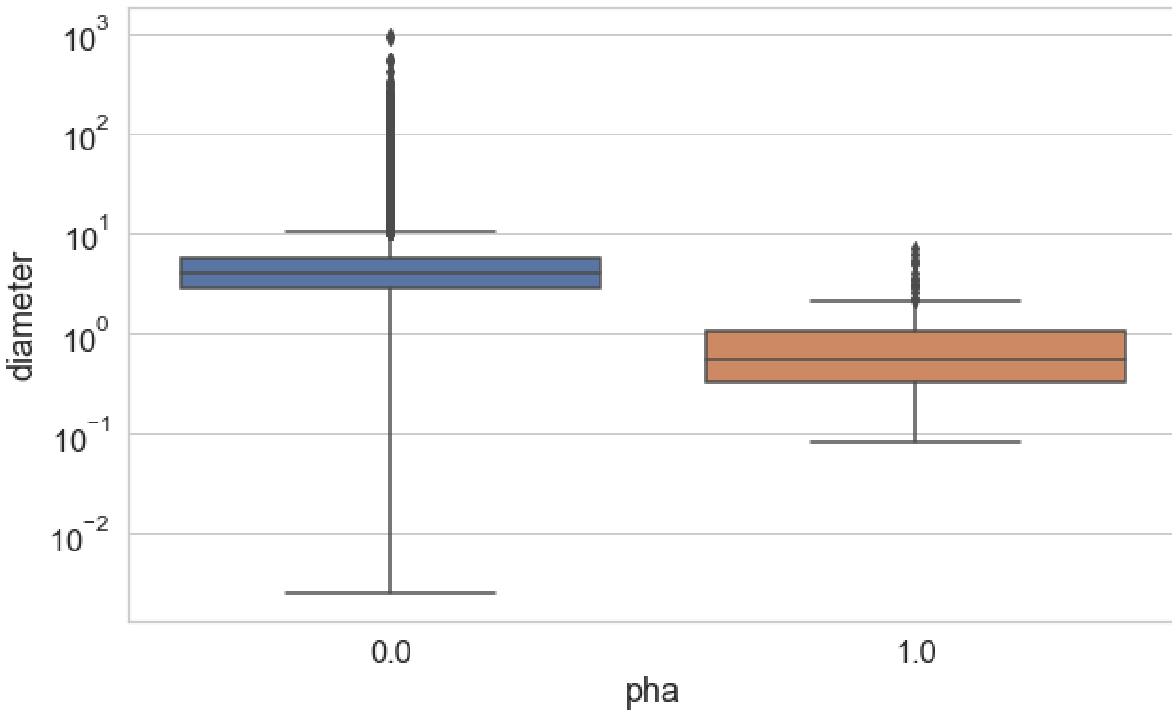


In [41]:
```
# Boxplot confirms that most of the diameter values are small -- between 0 and
10 km
# Everything above 10 km is considered outliers
```

In [42]:
```
# Boxplot of 'diameter' in data_1 vs. 'neo' classes

plt.figure(figsize = (10, 6))
sns.boxplot(x = 'neo', y = 'diameter', data = data_1)
plt.yscale('log')
plt.show()
```



In [43]:
```
# Boxplot of 'diameter' in data_1 vs. 'pha' classes

plt.figure(figsize = (10, 6))
sns.boxplot(x = 'pha', y = 'diameter', data = data_1)
plt.yscale('log')
plt.show()
```



In [44]:
```
# The distribution of values by 'neo' and 'pha' classes is similar to that by
 'condition_code' classes -->
    # Everything greater than 10 km is considered outlier
```

In [45]:
```
# This concludes Data Processing and EDA section
```

In [46]:
```
# 2) Apply XGBRegressor
```

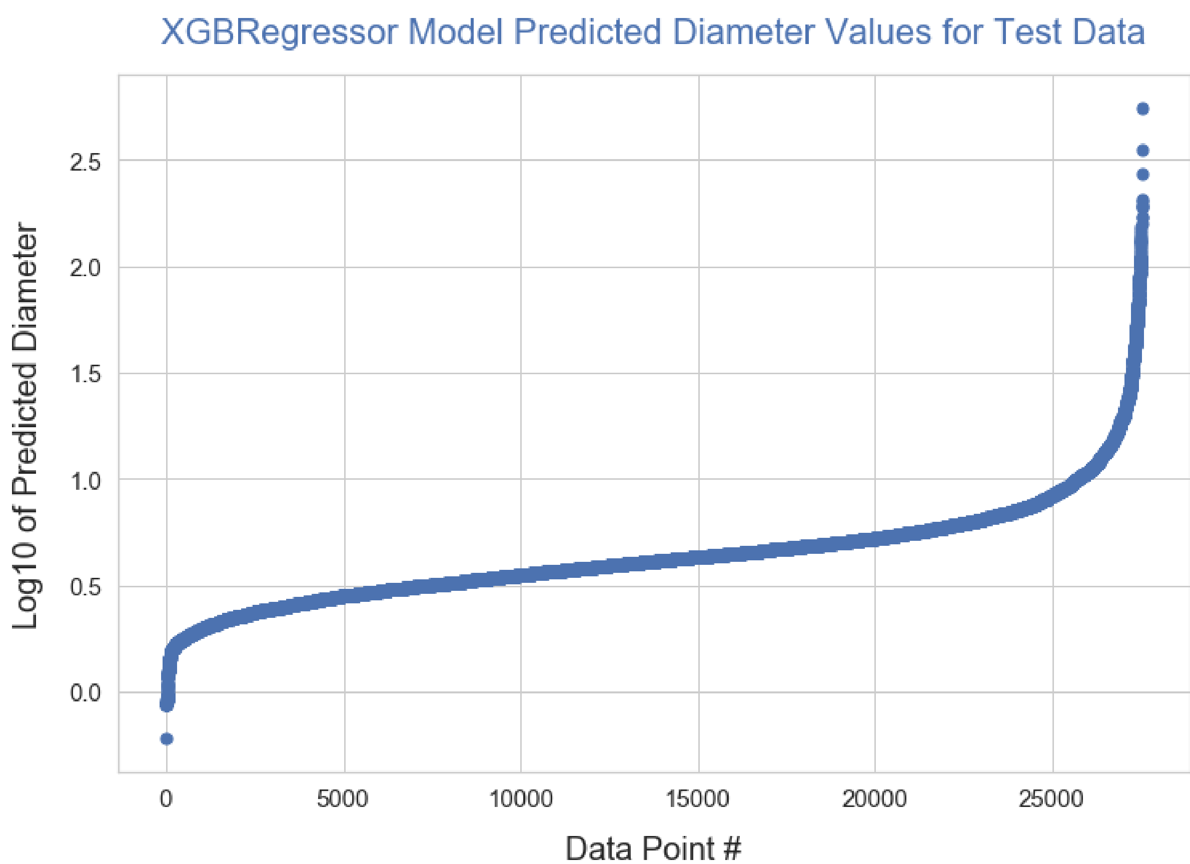
In [47]:
```
# Separate features and target from data_1 which we will use with the xgb mode
l

X_1 = data_1.iloc[:, :-1].values # all columns, but last
y_1 = data_1.iloc[:, -1].values # last column

X_2 = data_2.values # data_2 has only features
```

In [48]:
```
# Split X_1 and y_1 in train/test sets

from sklearn.model_selection import train_test_split

X_train, X_test, y_train, y_test = train_test_split(X_1, y_1, test_size = 0.2,
random_state = 0)
```

In [49]:
```
# Create XGBRegressor model

from xgboost import XGBRegressor

xgb_ini = XGBRegressor(objective = 'reg:squarederror') # denote model as'ini"
 to distinguish from optimized model later on
```

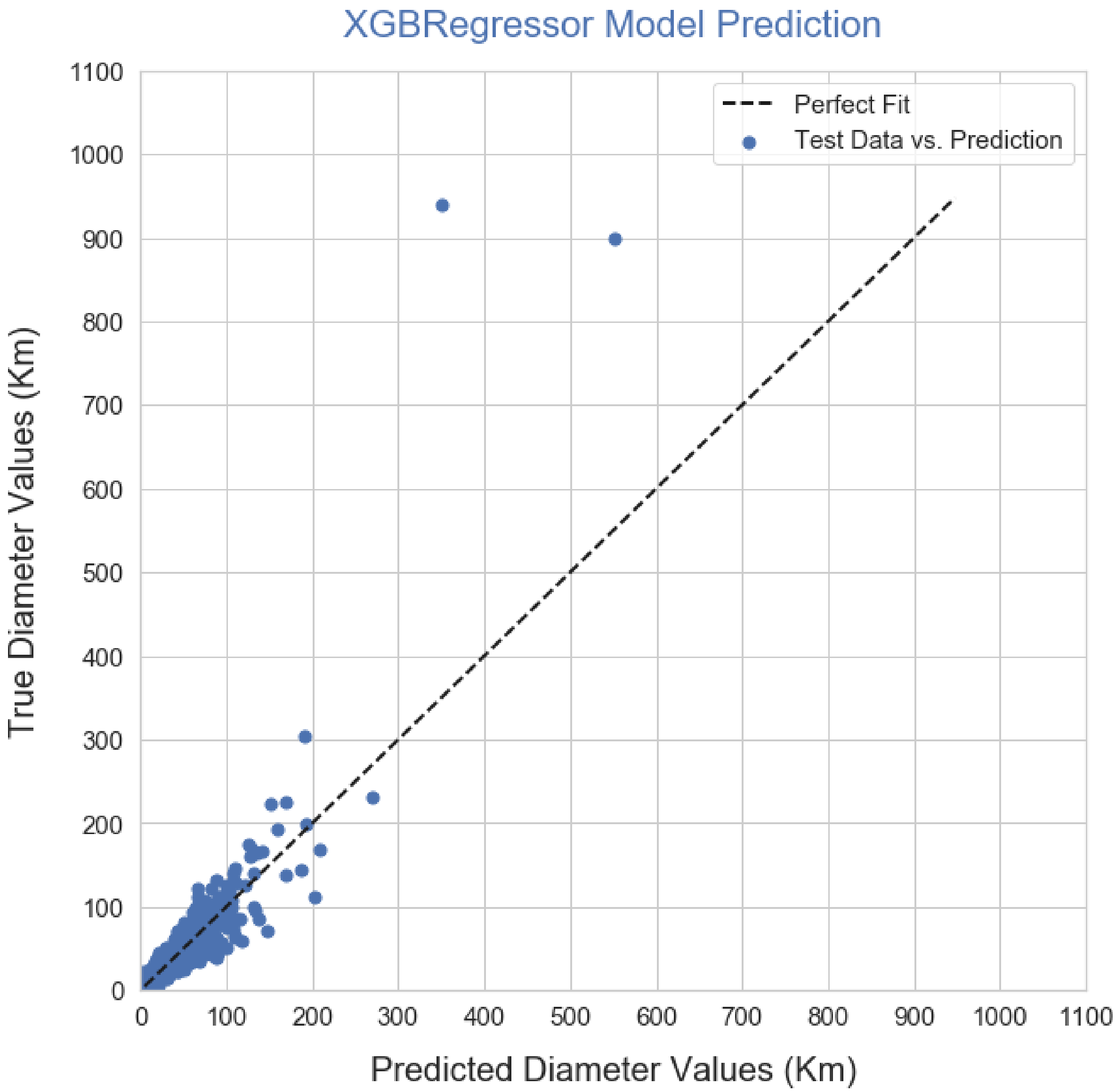
In [50]:
```
# Fit & predict

xgb_ini.fit(X_train, y_train)

y_pred_1a = xgb_ini.predict(X_test) # use indexing '_1a' for comparison with l
ater predictions
```

In [51]:
```
# Plot predicted diameter values in ascending order
# Log10 is used in order to display well all values

plt.figure(figsize = (12, 8))

plt.scatter(np.arange(1, len(y_test) + 1), np.sort(np.log10(y_pred_1a)), s = 5
0, color = 'b')

plt.xlabel('Data Point #', fontsize = 20, labelpad = 15)
plt.ylabel('Log10 of Predicted Diameter', fontsize = 20, labelpad = 15)
plt.title('XGBRegressor Model Predicted Diameter Values for Test Data', fontsi
ze = 22, c = 'b', pad = 20)
plt.tick_params(labelsize = 15)
plt.show()
```



In [52]:
```
# Main observations from plot
    # 1) small portion of predicted values are smaller than 1 km -- shown as n
egative values on the plot
    # 2) largest value is approximately 500 km (10 ** 2.7)
    # 3) plot shows that vast majority of predicted values are less than 10 Km
(10 ** 1)
```

In [53]:
```
# Compare predictions, y_pred_1a, to test values, y_test, using scatterplot

# create line to represent perfect fit to y_test

y_line = np.arange(int(y_test.min()) - 10, int(y_test.max()) + 10)

# set axes limits - adjust if necessary
x_min = 0
x_max = y_test.max() + 100
d_x = 100

y_min = 0
y_max = y_test.max() + 100
d_y = 100

plt.figure(figsize = (10, 10))
ax = plt.axes()

ax.set_xlim(x_min, x_max)
ax.set_xticks(np.arange(x_min, x_max + d_x, d_x))

ax.set_ylim(y_min, y_max)
ax.set_yticks(np.arange(y_min, y_max + d_y, d_y))

plt.scatter(y_pred_1a, y_test, s = 50, c = 'b', label = 'Test Data vs. Predict
ion')
plt.plot(y_line, y_line, 'k--', lw = 2, label = 'Perfect Fit')
plt.xlabel('Predicted Diameter Values (Km)', fontsize = 20, labelpad = 15)
plt.ylabel('True Diameter Values (Km)', fontsize = 20, labelpad = 15)
plt.title('XGBRegressor Model Prediction', fontsize = 22, c = 'b', pad = 20)
plt.legend(fontsize = 15)
plt.tick_params(labelsize = 15)
plt.show()
```



In [54]:
```
# Except for two "outliers", predictions are closely grouped around the perfec
t fit line
# Note: this will be discussed again later, but we would like to mention it he
re regarding the perceived "outliers".
    # Perhaps the only limitation of XGBoost is that its predictions are cappe
d by the data used for training
    # From the scatter plot of all diameter values in the EDA secton and the c
urrent plot,
    # it is clear that the training data contained only points with diameter s
maller than 600 km.
    # That's why the predictions with the test data could not capture well the
two points with diameter greater than 800 km
```

In [55]:
```
# Examine model predictions in a more quantitative way --> view statistics of
 residuals
```

In [56]:
```
# Get residuals

residuals_1a = y_test - y_pred_1a
residuals_1a
```

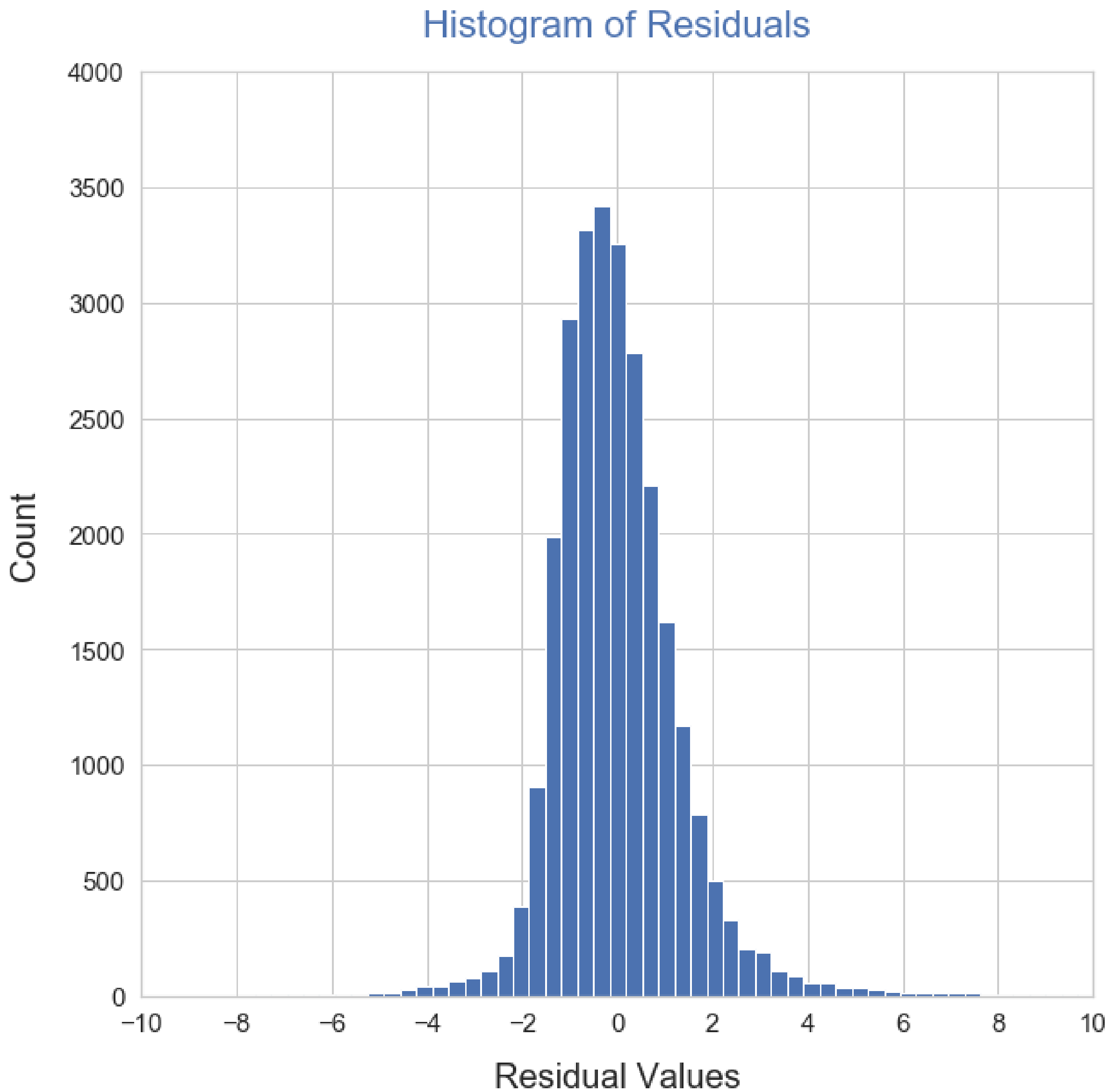
Out[56]:
```
array([-0.91383727, -1.68171666, -0.20006578, ...,  0.16652586,
       -0.47324387,  0.01414502])
```

In [57]:
```
# Get residuals mean and standard deviation, sigma

print("Residuals_ini Mean:", round(residuals_1a.mean(),4))
print("Residuals_ini Sigma:", round(residuals_1a.std(),4))
```

```
Residuals_ini Mean: 0.0187
Residuals_ini Sigma: 4.9317
```

In [58]:
```
# Mean is close to zero and sigma is small compared to the test diameter value
s, y_test -->
    # indicates good model accuracy
```

In [59]:
```
# Examine further: plot the histograms of the residuals -->
    # for better visualization plot histogram only for values within two sigma
s from the mean (~ 95% of all data points)

# Set axes limits - adjust if necessary
x_min = -10
x_max = 10
d_x = 2

y_min = 0
y_max = 4000
d_y = 500

plt.figure(figsize = (10, 10))
ax = plt.axes()

ax.set_xlim(x_min, x_max)
ax.set_xticks(np.arange(x_min, x_max + d_x, d_x))

ax.set_ylim(y_min, y_max)
ax.set_yticks(np.arange(y_min, y_max + d_y, d_y))

plt.hist(residuals_1a, bins = 2000, color = 'b')
plt.xlabel('Residual Values', fontsize = 20, labelpad = 15)
plt.ylabel('Count', fontsize = 20, labelpad = 15)
plt.title('Histogram of Residuals', fontsize = 22, c = 'b', pad = 20)
plt.tick_params(labelsize = 15)
plt.show()
```

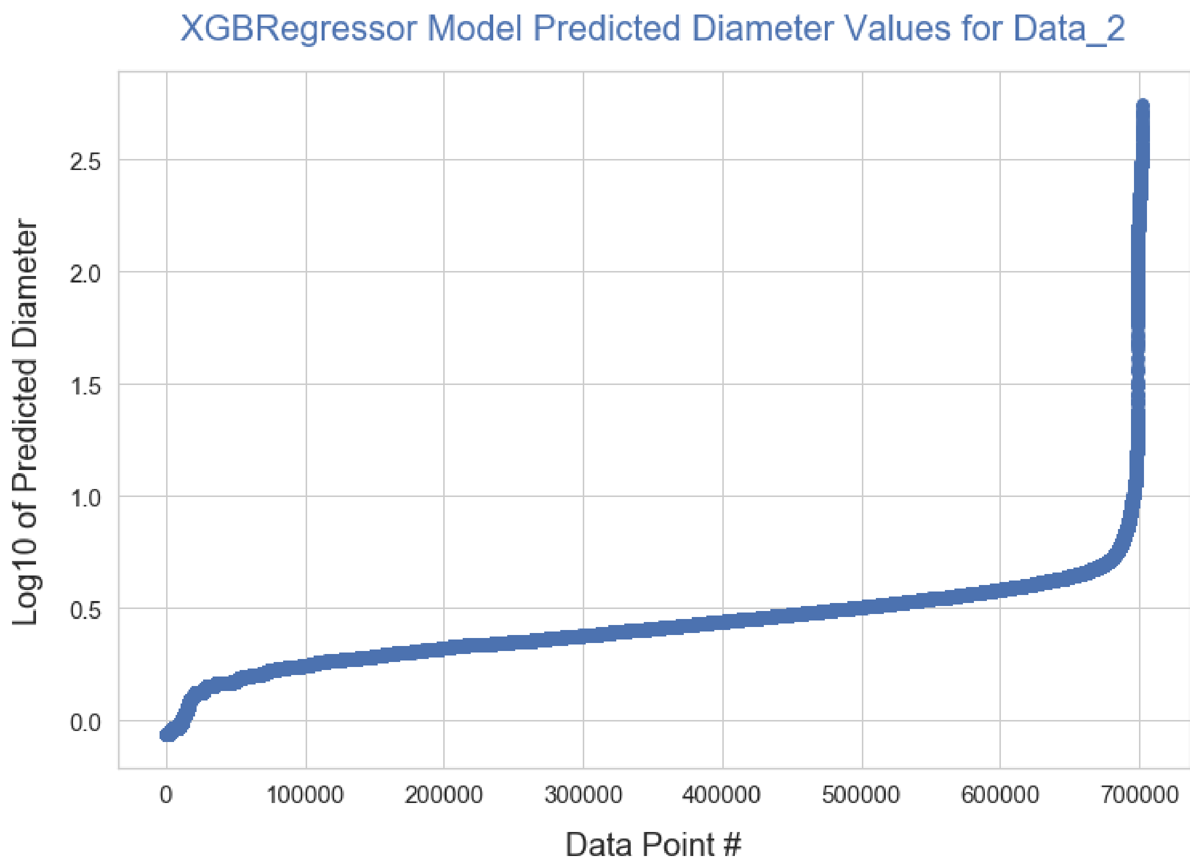


In [60]:
```
# Visually the histogram appears close to normal distribution -->
    # it is skewed slightly towards positive values which means that model is
 slightly underevaluating
    # this can also be seen from the scatter plot of y_test vs y_pred
```

In [61]:
```
# Predict the asteroid diameter values for the asteroids with unknown diamete
r, data_2, using model xgb_ini

y_pred_2a = xgb_ini.predict(X_2)
```

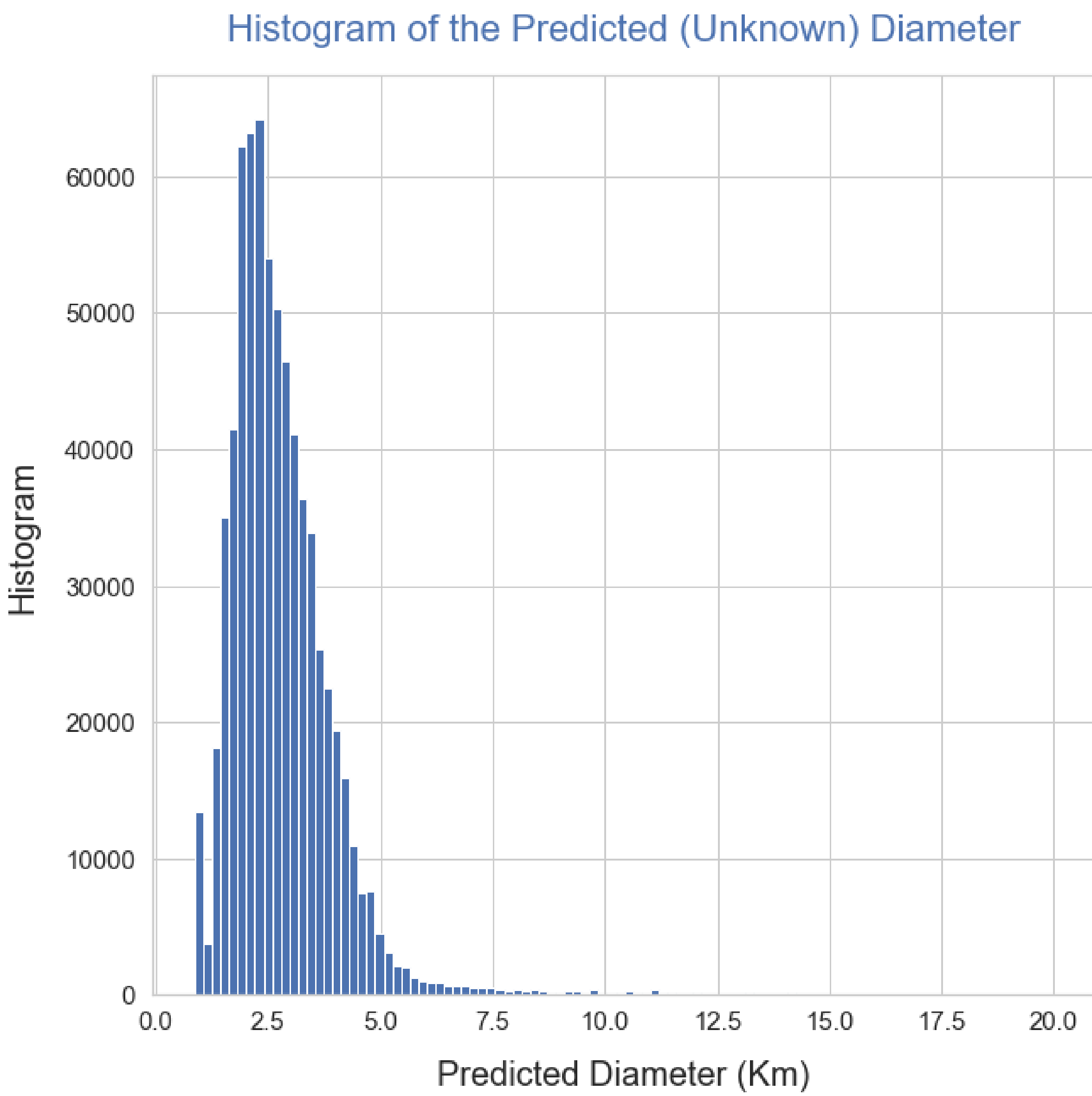
In [62]:
```
# Examine properties of predicted values by creating few simple plots
```

In [63]:
```
# Plot predicted diameter values in ascending order

# Log10 is used in order to display well all values

plt.figure(figsize = (12, 8))

plt.scatter(np.arange(1, len(X_2) +1), np.sort(np.log10(y_pred_2a)), s = 50, c
olor = 'b')

plt.xlabel('Data Point #', fontsize = 20, labelpad = 15)
plt.ylabel('Log10 of Predicted Diameter', fontsize = 20, labelpad = 15)
plt.title('XGBRegressor Model Predicted Diameter Values for Data_2', fontsize
= 22, c = 'b', pad = 20)
plt.tick_params(labelsize = 15)
plt.show()
```

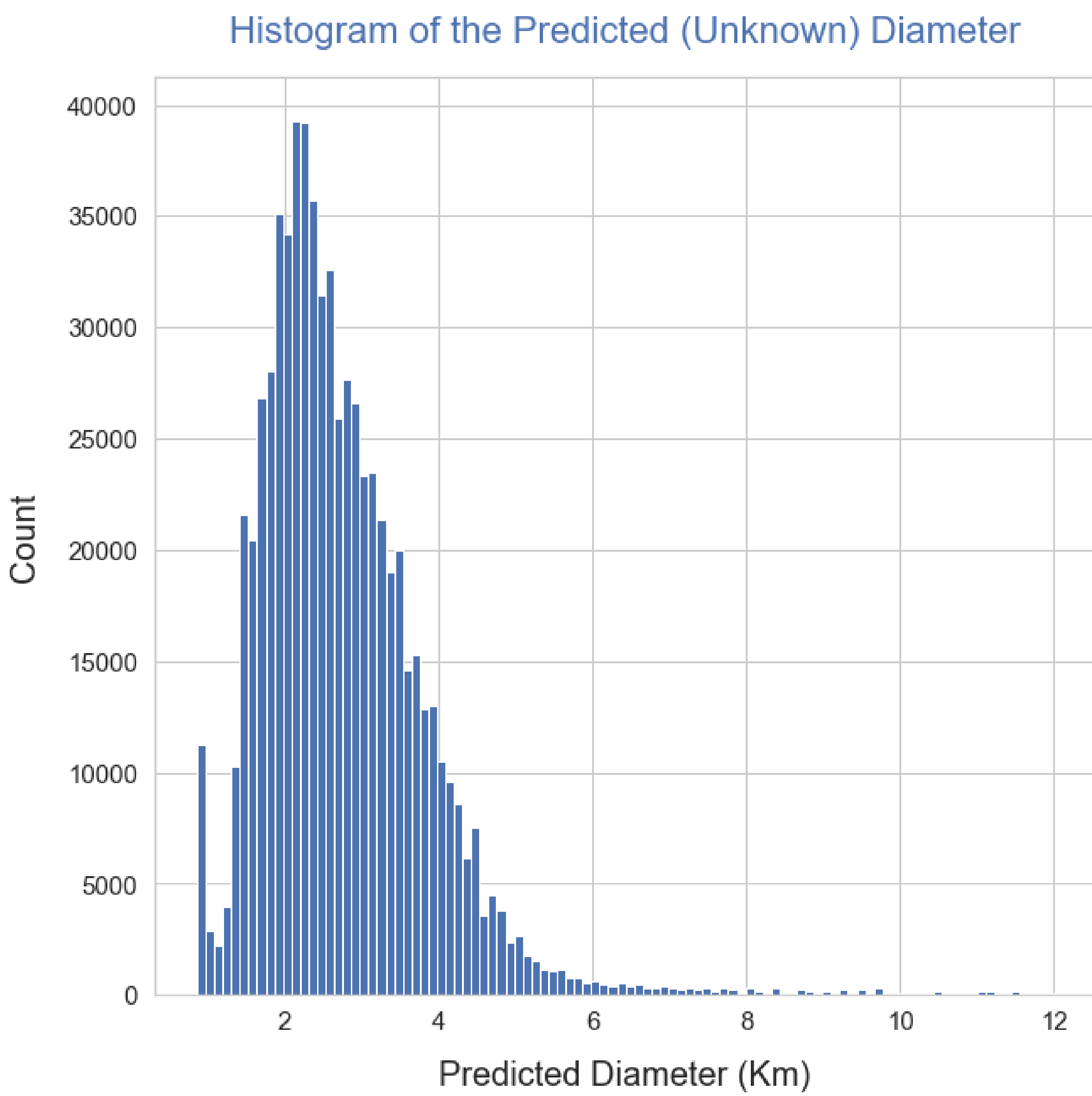


In [64]:
```
# The range of the predicted unknown diameter values is similar to that of the
predicted test values
```

In [65]:
```
# Plot histogram of predicted diameter values
# For better visualization, limit histogram to diameter values smaller than 20
Km

plt.figure(figsize = (10, 10))

plt.hist(y_pred_2a[y_pred_2a < 20], bins = 100, color = 'b') # limit predictio
n values to 20 Km
plt.xlabel('Predicted Diameter (Km)', fontsize = 20, labelpad = 15)
plt.ylabel('Histogram', fontsize = 20, labelpad = 15)
plt.title('Histogram of the Predicted (Unknown) Diameter', fontsize = 22, c =
'b', pad = 20)
plt.tick_params(labelsize = 15)
plt.show()
```

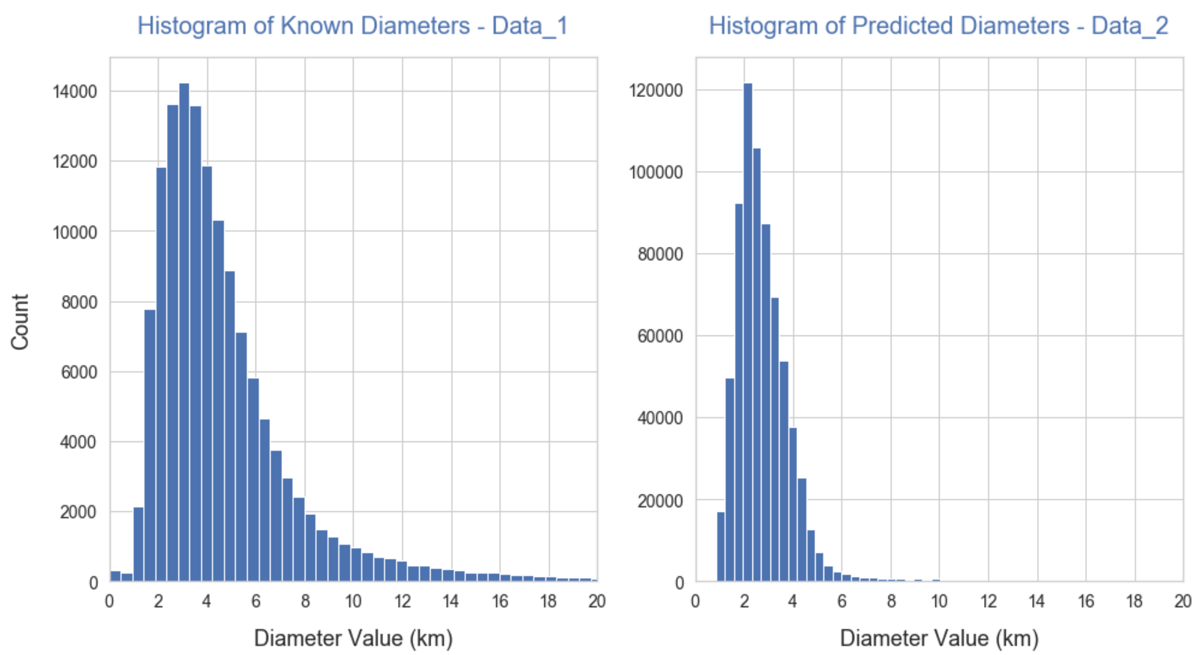


In [66]:
```
# Majority of predicted diameter values are capped by 12 km --> use this numbe
r as upper limit for histogram

plt.figure(figsize = (10, 10))

plt.hist(y_pred_2a[y_pred_2a < 12], bins = 100, color = 'b') # limit predicted
values to 12 Km
plt.xlabel('Predicted Diameter (Km)', fontsize = 20, labelpad = 15)
plt.ylabel('Count', fontsize = 20, labelpad = 15)
plt.title('Histogram of the Predicted (Unknown) Diameter', fontsize = 22, c =
'b', pad = 20)
plt.tick_params(labelsize = 15)
plt.show()
```



In [67]:
```
# Predicted values for unknown diameter (data_2) have Poisson-like distributio
n with most of the values between 1.5 and 4 km
```

In [68]:
```
# Examine if distribution is similar to distribution of known diameter values
 -->
    # for adequate comparison set x-axis limit to 20 km

# set axes limits - adjust if necessary
x_min = 0
x_max = 20
d_x = 2

fig, axes = plt.subplots(1, 2, sharey = False, figsize=(16,8))

# known diameter values
axes[0].hist(y_1, bins = 2000, color = 'b')
axes[0].set_title('Histogram of Known Diameters - Data_1', fontsize = 20, c =
'b', pad = 20)
axes[0].set_xlabel('Diameter Value (km)', fontsize = 18, labelpad = 15)
axes[0].set_ylabel('Count', fontsize = 18, labelpad = 15)
axes[0].set_xlim(x_min, x_max)
axes[0].set_xticks(np.arange(x_min, x_max + d_x, d_x))
axes[0].tick_params(labelsize = 14)


# predicted unknown diameter values
axes[1].hist(y_pred_2a, bins = 1500, color = 'b')
axes[1].set_title('Histogram of Predicted Diameters - Data_2', fontsize = 20,
c = 'b', pad = 20)
axes[1].set_xlabel('Diameter Value (km)', fontsize = 18, labelpad = 15)
axes[1].set_xlim(x_min, x_max)
axes[1].set_xticks(np.arange(x_min, x_max + d_x, d_x))
axes[1].tick_params(labelsize = 14)

plt.show()
```



In [69]:
```
# It appears that predicted diameter values have significantly narrower distri
bution encompassing smaller values

# Couple of comments regarding this observation:

# 1) We do not know how the data with known and unknown asteroid diameter were
collected -->
    # Thus, comparison between these two histograms may not be fully justified

# 2) However, assuming that the two sets of data are derived from the same ast
ronomical observation and taking into account
# that the number of observation for asteroids with unknown diameter is ~ 5 ti
mes greater than that of known diameter
# one would expect that the predicted values should have similar or even wider
distribution -->
    # Based on item #2, the question whether an optimized model would provide
 different results arises
```

In [70]:
```
# 3) Model optimization via hyperparameter tuning
```

In [71]:
```
# For tuning use 'max_depth', 'min_child_weight', 'gamma', 'n_estimators', 'le
arning_rate', and 'subsample' with Randomized Search

# Note: It is important to select appropriate ranges for each of these paramet
ers

grid_random = {'max_depth': [3, 6, 10, 20],
              'min_child_weight': np.arange(1, 10, 1),
              'gamma': np.arange(0, 10, 1),
               'n_estimators': [50, 100, 150],
              'learning_rate': [0.001, 0.01, 0.1, 0.2],
              'subsample': np.arange(0.5, 1.0, 0.1)}

from sklearn.model_selection import RandomizedSearchCV

xgb = XGBRegressor(objective = 'reg:squarederror')

xgb_random = RandomizedSearchCV(estimator = xgb, param_distributions = grid_ra
ndom, n_iter = 100, cv = 5, verbose = 2,
                                random_state = 42, n_jobs = -1)
```

In [72]:
```
# Fit xgb_random with X_train, y_train (using same data as with xgb_ini)

xgb_random.fit(X_train, y_train)
```

```
Fitting 5 folds for each of 100 candidates, totalling 500 fits

[Parallel(n_jobs=-1)]: Using backend LokyBackend with 12 concurrent workers.
[Parallel(n_jobs=-1)]: Done  17 tasks      | elapsed:  1.8min
[Parallel(n_jobs=-1)]: Done 138 tasks      | elapsed:  9.2min
[Parallel(n_jobs=-1)]: Done 341 tasks      | elapsed: 25.5min
[Parallel(n_jobs=-1)]: Done 500 out of 500 | elapsed: 38.8min finished
```

Out[72]:
```
RandomizedSearchCV(cv=5, error_score=nan,
                   estimator=XGBRegressor(base_score=0.5, booster='gbtree',
                                          colsample_bylevel=1,
                                          colsample_bynode=1,
                                          colsample_bytree=1, gamma=0,
                                          importance_type='gain',
                                          learning_rate=0.1, max_delta_step=
0,
                                          
                                          max_depth=3, min_child_weight=1,
                                          missing=None, n_estimators=100,
                                          n_jobs=1, nthread=None,
                                          objective='reg:squarederror',
                                          random_state=0, reg_...
                   iid='deprecated', n_iter=100, n_jobs=-1,
                   param_distributions={'gamma': array([0, 1, 2, 3, 4, 5, 6,
7, 8, 9]),
                                        'learning_rate': [0.001, 0.01, 0.1,
                                                          0.2],
                                        'max_depth': [3, 6, 10, 20],
                                        'min_child_weight': array([1, 2, 3,
4, 5, 6, 7, 8, 9]),
                                        'n_estimators': [50, 100, 150],
                                        'subsample': array([0.5, 0.6, 0.7, 0.
8, 0.9])},
                   pre_dispatch='2*n_jobs', random_state=42, refit=True,
                   return_train_score=False, scoring=None, verbose=2)
```

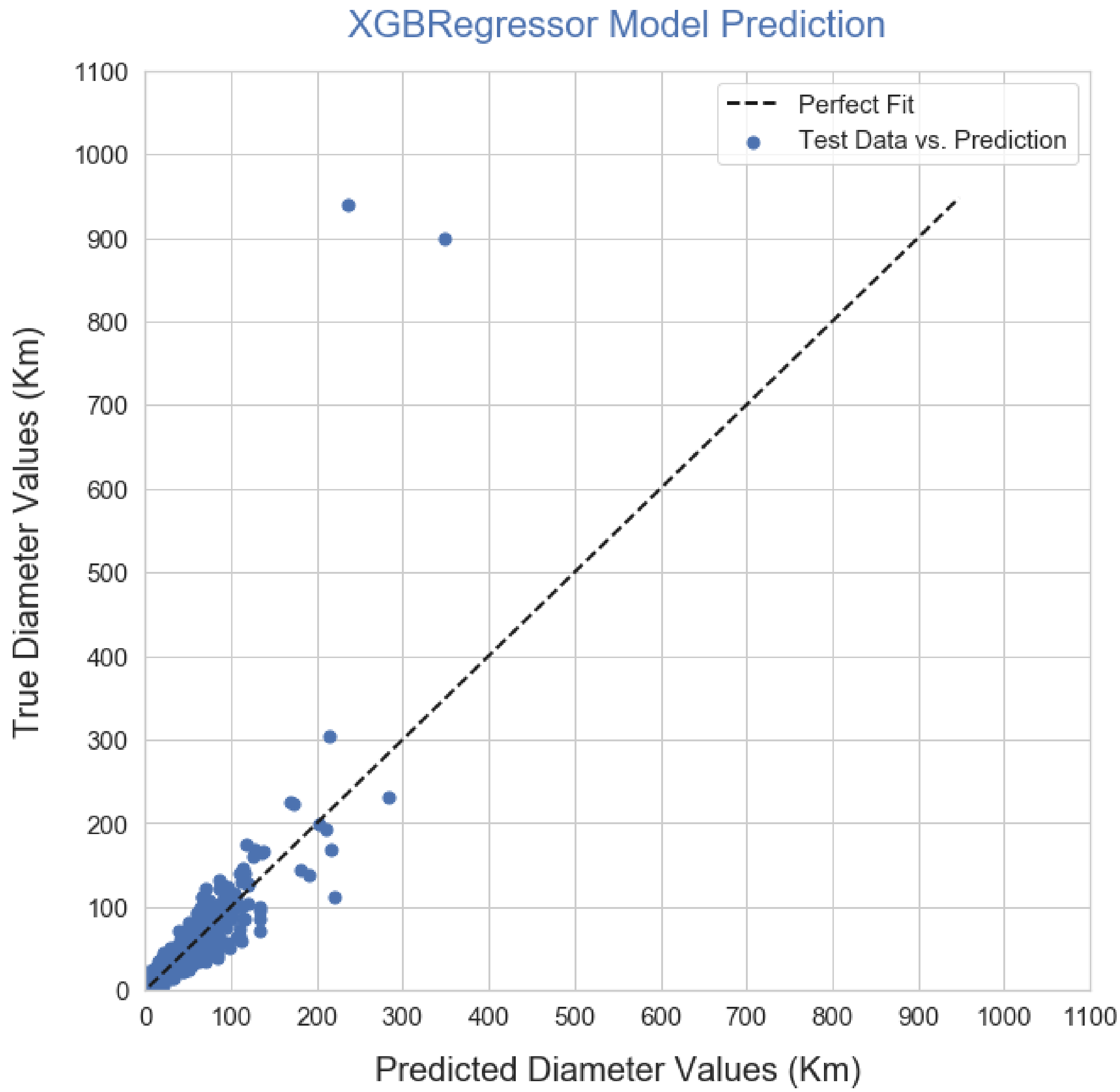
In [73]:
```
# Print best score and best model parameters

print("Best score: %f with %s" % (xgb_random.best_score_, xgb_random.best_para
ms_))
```

```
Best score: 0.866256 with {'subsample': 0.8999999999999999, 'n_estimators': 1
00, 'min_child_weight': 6, 'max_depth': 3, 'learning_rate': 0.1, 'gamma': 5}
```

In [74]:
```
# Get best_estimator_

xgb_opt = xgb_random.best_estimator_
```

In [75]:
```
# Use xgb_opt to predict for X_test data and compare with the true values, y_t
est

y_pred_1b = xgb_opt.predict(X_test)
```

In [76]:
```
# Compare predictions, y_pred_1b, to test values, y_test

# create line to represent perfect fit to data test values, y_test

y_line = np.arange(int(y_test.min()) - 10, int(y_test.max()) + 10)

# set axes limits - adjust if necessary
x_min = 0
x_max = y_test.max() + 100
d_x = 100

y_min = 0
y_max = y_test.max() + 100
d_y = 100

plt.figure(figsize = (10, 10))
ax = plt.axes()

ax.set_xlim(x_min, x_max)
ax.set_xticks(np.arange(x_min, x_max + d_x, d_x))

ax.set_ylim(y_min, y_max)
ax.set_yticks(np.arange(y_min, y_max + d_y, d_y))

plt.scatter(y_pred_1b, y_test, s = 50, c = 'b', label = 'Test Data vs. Predict
ion')
plt.plot(y_line, y_line, 'k--', lw = 2, label = 'Perfect Fit')
plt.xlabel('Predicted Diameter Values (Km)', fontsize = 20, labelpad = 15)
plt.ylabel('True Diameter Values (Km)', fontsize = 20, labelpad = 15)
plt.title('XGBRegressor Model Prediction', fontsize = 22, c = 'b', pad = 20)
plt.legend(fontsize = 15)
plt.tick_params(labelsize = 15)
plt.show()
```



In [77]:
```
# Predictions from  Optimized model have similar behavior to those from Initia
l model
```

In [78]:
```
# Get residuals

residuals_1b = y_test - y_pred_1b
residuals_1b
```

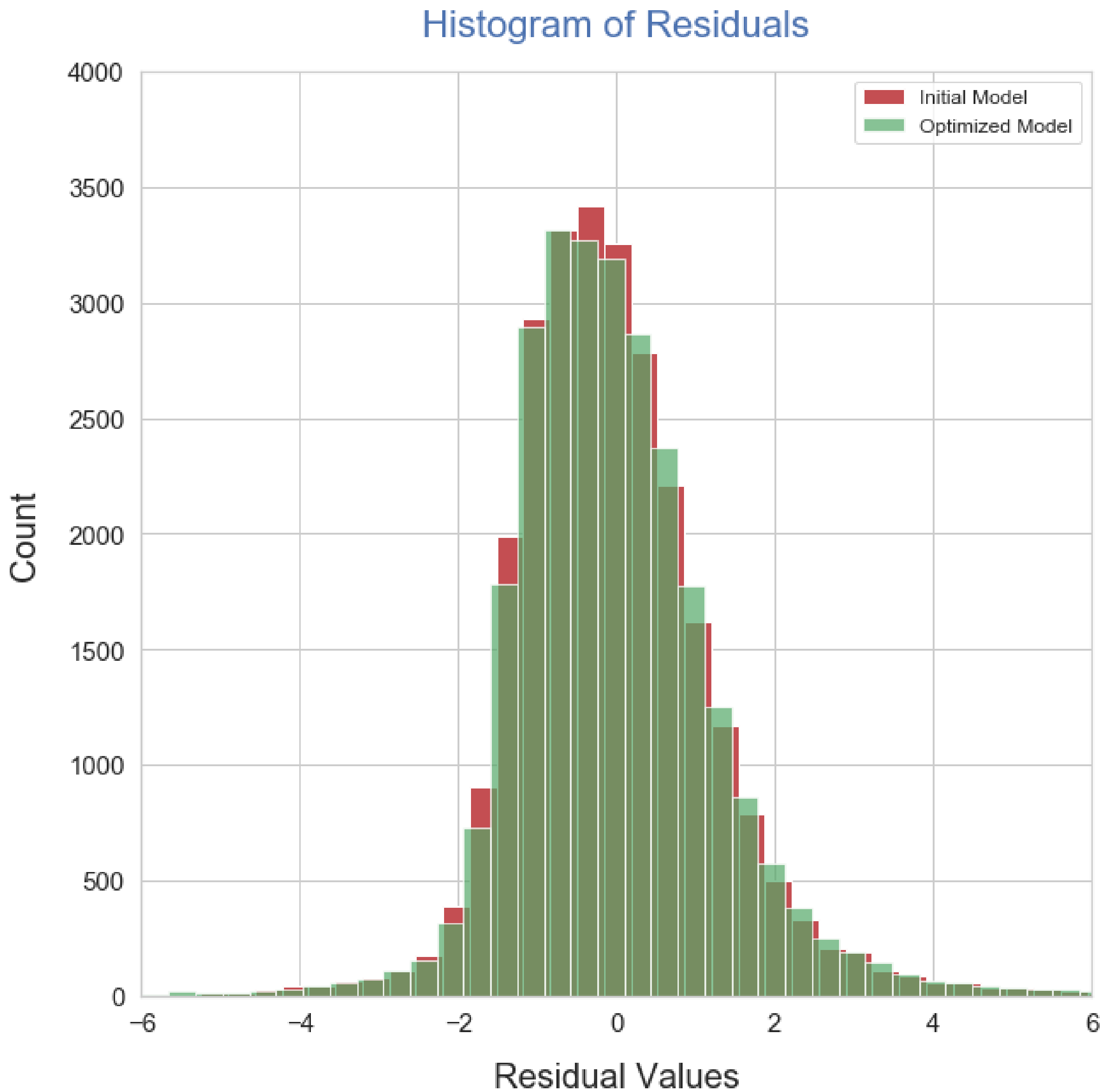
Out[78]:
```
array([-1.05671079, -1.6761534 , -0.22539156, ...,  0.15230133,
       -0.62706057, -0.06124246])
```

In [79]:
```
# Compare residuals mean and standard deviation, sigma, from Initial and Optim
ized models

print("Residuals_ini Mean:", round(residuals_1a.mean(),4))
print("Residuals_ini Sigma:", round(residuals_1a.std(),4))
print('\n')
print("Residuals_opt Mean:", round(residuals_1b.mean(),4))
print("Residuals_opt Sigma:", round(residuals_1b.std(),4))
```

```
Residuals_ini Mean: 0.0187
Residuals_ini Sigma: 4.9317


Residuals_opt Mean: 0.0292
Residuals_opt Sigma: 6.0209
```

In [80]:
```
# Although numbers are close, Initial model has slightly better residuals mean
and sigma
# Thus, we should consider changing the number of hyperparameter, their ranges
and the optimization method used -->
    # Perhaps, use Bayesian optimization instead of Randomized Search
    # This goes beyond the scope of this project and will be explored in subse
quent project
```

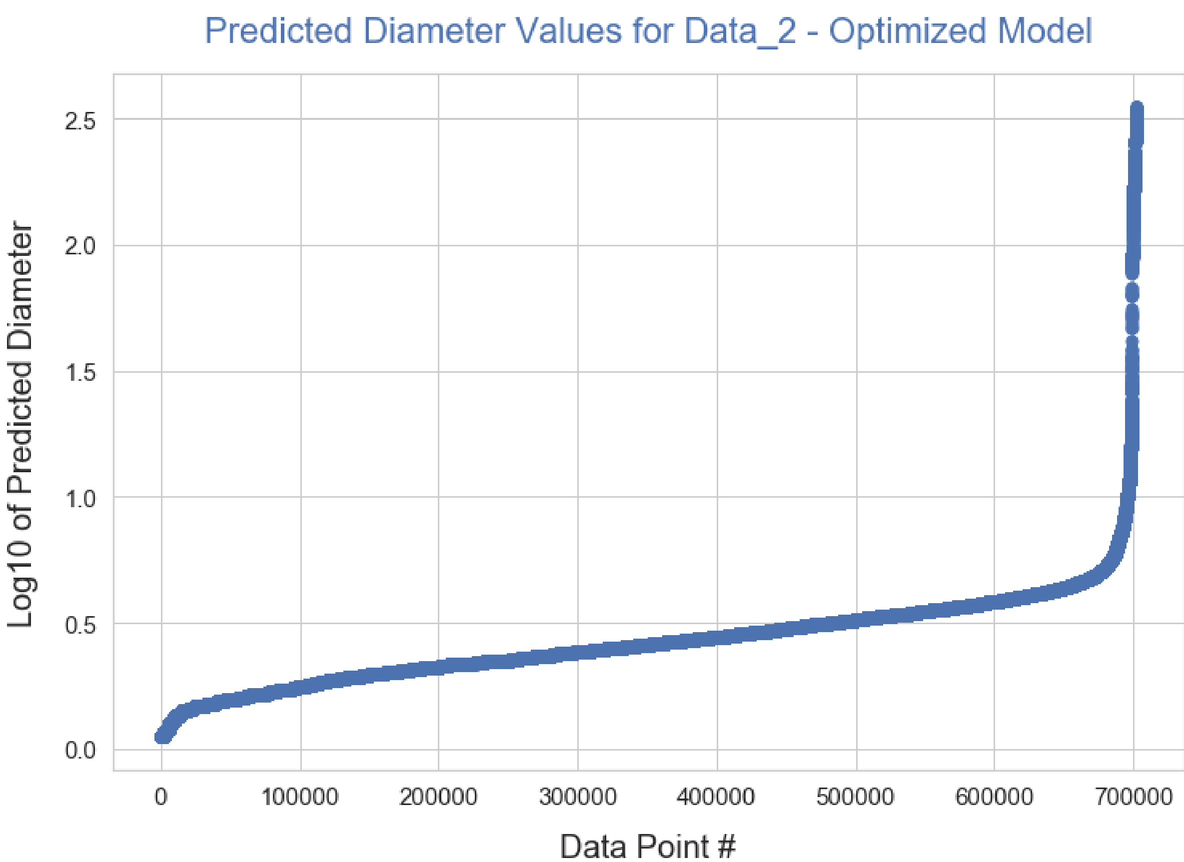
In [81]:
```
# Compare histograms of residuals from Initial and Optimized models --> for be
tter comparison plot histograms on same graph

# Set axes limits - adjust if necessary
x_min = -6
x_max = 6
d_x = 2

y_min = 0
y_max = 4000
d_y = 500

plt.figure(figsize = (10, 10))
ax = plt.axes()

ax.set_xlim(x_min, x_max)
ax.set_xticks(np.arange(x_min, x_max + d_x, d_x))

ax.set_ylim(y_min, y_max)
ax.set_yticks(np.arange(y_min, y_max + d_y, d_y))

plt.hist(residuals_1a, bins = 2000, color = 'r', label = 'Initial Model')
plt.hist(residuals_1b, bins = 2400, color = 'g', alpha = 0.7, label = 'Optimiz
ed Model')
plt.xlabel('Residual Values', fontsize = 20, labelpad = 15)
plt.ylabel('Count', fontsize = 20, labelpad = 15)
plt.title('Histogram of Residuals', fontsize = 22, c = 'b', pad = 20)
plt.tick_params(labelsize = 15)
plt.legend(fontsize = 12)
plt.show()
```



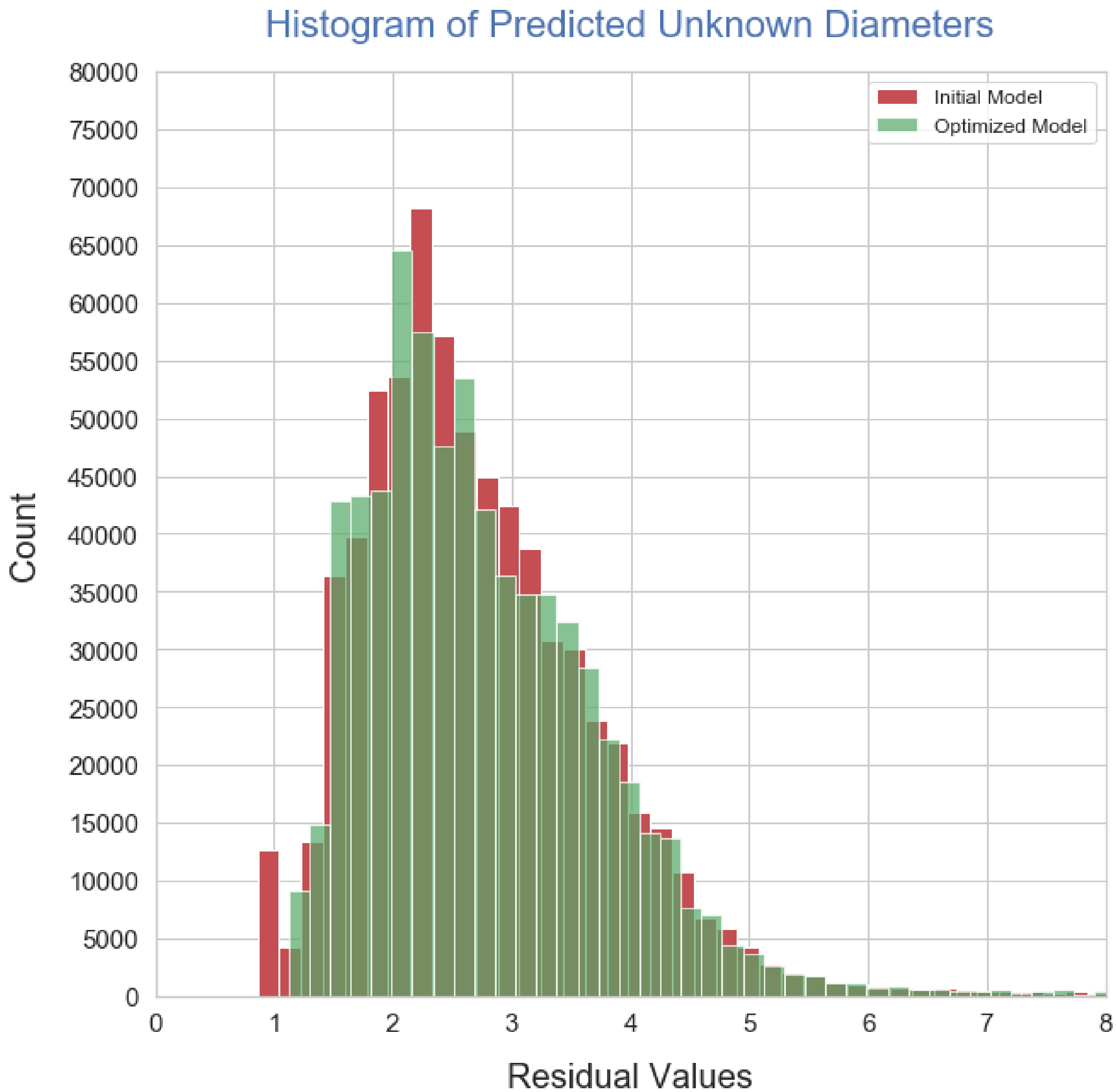
In [82]:
```
# Histograms are nearly identical --> difficult to make the case for one model over the other
```

In [83]:
```
# Use xgb_opt to predict diameters for the set with unknown diameter, X_2

y_pred_2b = xgb_opt.predict(X_2)
```

In [84]:
```
# Plot predicted diameter values in ascending order
# Log10 is used in order to display well all values

plt.figure(figsize = (12, 8))

plt.scatter(np.arange(1, len(X_2) +1), np.sort(np.log10(y_pred_2b)), s = 50, c
olor = 'b')

plt.xlabel('Data Point #', fontsize = 20, labelpad = 15)
plt.ylabel('Log10 of Predicted Diameter', fontsize = 20, labelpad = 15)
plt.title('Predicted Diameter Values for Data_2 - Optimized Model', fontsize =
22, c = 'b', pad = 20)
plt.tick_params(labelsize = 15)
plt.show()
```



In [85]:
```
# Compare histograms of predicted diameters from Initial and Optimized models
 -->
    # for better comparison plot histograms on same graph

# Set axes limits - adjust if necessary
x_min = 0
x_max = 8
d_x = 1

y_min = 0
y_max = 80000
d_y = 5000

plt.figure(figsize = (10, 10))
ax = plt.axes()

ax.set_xlim(x_min, x_max)
ax.set_xticks(np.arange(x_min, x_max + d_x, d_x))

ax.set_ylim(y_min, y_max)
ax.set_yticks(np.arange(y_min, y_max + d_y, d_y))

plt.hist(y_pred_2a, bins = 3000, color = 'r', label = 'Initial Model')
plt.hist(y_pred_2b, bins = 2000, color = 'g', alpha = 0.7, label = 'Optimized
 Model')
plt.xlabel('Residual Values', fontsize = 20, labelpad = 15)
plt.ylabel('Count', fontsize = 20, labelpad = 15)
plt.title('Histogram of Predicted Unknown Diameters', fontsize = 22, c = 'b',
pad = 20)
plt.tick_params(labelsize = 15)
plt.legend(fontsize = 12)
plt.show()
```

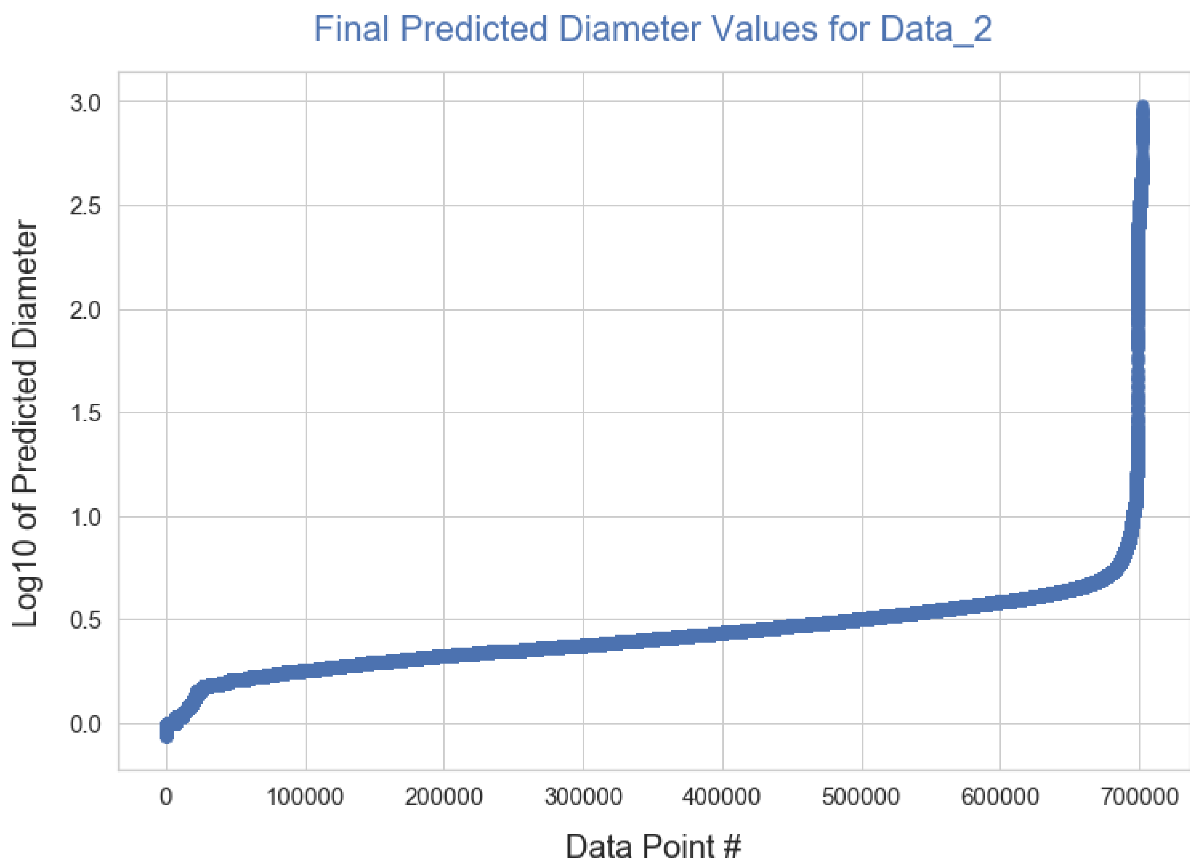


In [86]:
```
# As with the residuals, the predicted unknown diameters distributions are nea
rly identical for both models
# Indicates that difference in distributions between known and predicted unkno
wn diameters is not an issue of model optimization
# Because of the slightly better residual parameters we will use Initial model
for final predictions
```

In [87]:
```
# 4) Final Predictions of Unknown Diameter
```

In [88]:
```
# Train Initial model with entire X_1, y_1 dataset and use that model to predi
ct unknown diameters for X_2
# Reason: XGBoost predictions are capped by the training data and the max valu
es might be missing there (as in our case)
# By using the entire 'data_1' dataset model should achieve the most accurate
 predictions possible

xgb_ini.fit(X_1, y_1)
y_pred_fin = xgb_ini.predict(X_2)
```

In [89]:
```
# Plot final predicted diameter values in ascending order
# Log10 is used in order to display well all values

plt.figure(figsize = (12, 8))

plt.scatter(np.arange(1, len(X_2) +1), np.sort(np.log10(y_pred_fin)), s = 50,
color = 'b')

plt.xlabel('Data Point #', fontsize = 20, labelpad = 15)
plt.ylabel('Log10 of Predicted Diameter', fontsize = 20, labelpad = 15)
plt.title('Final Predicted Diameter Values for Data_2', fontsize = 22, c = 'b'
, pad = 20)
plt.tick_params(labelsize = 15)
plt.show()
```



In [90]:
```
# As expected, the maximum predicted value is now capped at 1000 km (10 ** 3)
```

In [91]:
```
# Finally, combine the predicted diameter values with features from data_2 to
 complete the data as our final delivarable

data_2.head(10)
```

Out[91]:

	a	e	i	om	w	q	ad	per_y	data
681	2.654040	0.171983	11.505648	190.799958	104.993826	2.197591	3.110489	4.323837	40(
698	2.610998	0.410284	15.299180	242.551766	91.399514	1.539746	3.682249	4.219081	425
718	2.638780	0.546301	11.564845	183.887287	156.163668	1.197212	4.080348	4.286601	394
729	2.243362	0.177505	4.234895	95.073806	123.549777	1.845154	2.641570	3.360139	39
842	2.279598	0.209766	7.997717	4.071363	316.957206	1.801415	2.757780	3.441878	375
961	2.908998	0.097329	2.602636	145.481660	223.473847	2.625868	3.192128	4.961619	374
984	2.299979	0.277462	4.056565	290.307048	59.553605	1.661822	2.938137	3.488142	353
1008	2.625175	0.455500	15.769676	229.461495	186.428747	1.429408	3.820942	4.253492	349
1010	2.391976	0.350864	5.494744	132.525452	353.279770	1.552718	3.231235	3.699504	349
1064	2.360276	0.297141	8.362855	330.324142	353.652287	1.658942	3.061610	3.626205	338

In [92]:
```
# Reset data_2 indices before adding the predicted diameter values

data_2 = data_2.reset_index(drop = True)

data_2.head(10)
```

Out[92]:

	a	e	i	om	w	q	ad	per_y	data_ar
0	2.654040	0.171983	11.505648	190.799958	104.993826	2.197591	3.110489	4.323837	40087.
1	2.610998	0.410284	15.299180	242.551766	91.399514	1.539746	3.682249	4.219081	42540.
2	2.638780	0.546301	11.564845	183.887287	156.163668	1.197212	4.080348	4.286601	39478.
3	2.243362	0.177505	4.234895	95.073806	123.549777	1.845154	2.641570	3.360139	39112.
4	2.279598	0.209766	7.997717	4.071363	316.957206	1.801415	2.757780	3.441878	37579.
5	2.908998	0.097329	2.602636	145.481660	223.473847	2.625868	3.192128	4.961619	37450.
6	2.299979	0.277462	4.056565	290.307048	59.553605	1.661822	2.938137	3.488142	35366.
7	2.625175	0.455500	15.769676	229.461495	186.428747	1.429408	3.820942	4.253492	34990.
8	2.391976	0.350864	5.494744	132.525452	353.279770	1.552718	3.231235	3.699504	34919.
9	2.360276	0.297141	8.362855	330.324142	353.652287	1.658942	3.061610	3.626205	33882.

In [93]:
```
# Transform y_pred_1b array into series with name 'diameter'

y_pred_fin = pd.Series(y_pred_fin, name = 'diameter')
y_pred_fin.head(10)
```

Out[93]:
```
0    12.809157
1    15.107341
2     7.265679
3     6.928519
4     7.174271
5    16.591328
6     8.169825
7     7.139175
8     8.464670
9    11.164869
Name: diameter, dtype: float32
```

In [94]:
```
# Combine features with predicted diameter values

data_2 = pd.concat([data_2, y_pred_fin], axis = 1)
data_2.head(10)
```

Out[94]:

	a	e	i	om	w	q	ad	per_y	data_ar
0	2.654040	0.171983	11.505648	190.799958	104.993826	2.197591	3.110489	4.323837	40087.
1	2.610998	0.410284	15.299180	242.551766	91.399514	1.539746	3.682249	4.219081	42540.
2	2.638780	0.546301	11.564845	183.887287	156.163668	1.197212	4.080348	4.286601	39478.
3	2.243362	0.177505	4.234895	95.073806	123.549777	1.845154	2.641570	3.360139	39112.
4	2.279598	0.209766	7.997717	4.071363	316.957206	1.801415	2.757780	3.441878	37579.
5	2.908998	0.097329	2.602636	145.481660	223.473847	2.625868	3.192128	4.961619	37450.
6	2.299979	0.277462	4.056565	290.307048	59.553605	1.661822	2.938137	3.488142	35366.
7	2.625175	0.455500	15.769676	229.461495	186.428747	1.429408	3.820942	4.253492	34990.
8	2.391976	0.350864	5.494744	132.525452	353.279770	1.552718	3.231235	3.699504	34919.
9	2.360276	0.297141	8.362855	330.324142	353.652287	1.658942	3.061610	3.626205	33882.

In [95]:
```
# Data is complete, predicted asteroid diameter values are included, and we ha
ve accomplished project's objective
```