```python
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
import shap
import xgboost as xgb


# Scikit-lean imports
from sklearn.model_selection import train_test_split
from sklearn.pipeline import Pipeline
from sklearn.impute import SimpleImputer
from sklearn.preprocessing import StandardScaler, OneHotEncoder
from sklearn.compose import ColumnTransformer
from sklearn.linear_model import LinearRegression
from sklearn.ensemble import RandomForestRegressor
from sklearn.metrics import mean_squared_error
import warnings

# I am adding this line to ignore all the futurewarnings that show up
when i run the code.
# Which can clutter the final output
warnings.simplefilter(action='ignore', category=FutureWarning)
sns.set_style('whitegrid')

# Load the data with robust error handling
try:
    file_path = "../data/Pred_Ast_Diam_2.csv"
    df = pd.read_csv(file_path)
    print("Dataset Loaded Successfully.")
    print(f"Shape: {df.shape}\n")
    print("First 5 rows:")
    # Use display() for better formatting in some environments, or
just df.head()
    display(df.head())
except FileNotFoundError:
    print(f"Error: Could not find the file at '{file_path}'. Please
check the path.")
    df = pd.DataFrame() # Create empty dataframe to prevent further
errors
```

```
Dataset Loaded Successfully.
Shape: (126497, 23)

First 5 rows:

  orbit_id         e         a          i          om           w
ma  \
0   JPL 35  0.242027  2.201791   2.536221  313.311389   18.989048
301.072249
```

```
1   JPL 25  0.256856  2.338209  22.326589   10.489602  105.115594
87.454449
2   JPL 28  0.160543  2.228812   1.747387  121.579382  252.465454
208.942016
3   JPL 35  0.167945  2.241299   2.428619  161.636895  172.846491
20.350289
4   JPL 34  0.253295  2.467536   6.757106  137.130656  259.158793
127.366908

          n            tp      moid  ...  data_arc n_obs_used      rms
\
0  0.301675  2.458796e+06  0.657747  ...   46399.0       2611  0.46222

1  0.275663  2.458283e+06  0.875501  ...   38117.0       1528  0.38116

2  0.296206  2.459110e+06  0.871683  ...   36040.0       2357  0.44671

3  0.293734  2.458531e+06  0.854020  ...   33289.0       2574  0.43691

4  0.254278  2.458100e+06  0.862972  ...   39907.0       2523  0.44695


   diameter  albedo  diameter_sigma  first_year_obs
first_month_obs  \
0     9.300  0.2082           0.800            1892               10

1     9.822  0.3140           0.130            1915                4

2     8.196  0.3790           0.100            1920                9

3     6.534  0.2170           0.068            1928               10

4     9.111  0.2560           0.303            1910                2


   last_obs_year  last_obs_month
0           2019              10
1           2019               8
2           2019               5
3           2019              11
4           2019               5

[5 rows x 23 columns]
```

Initial Statistical Summary

With the data loaded, a statistical summary proviides immediatte insights into the scale and distribution of the nnumeric features. The .describe() method is an efficient way to get this overview.

```python
if not df.empty:
    #check data typees and for missing values
    print("Data Information: ")
    df.info()
    #Generate descriptive statistics for numeric coloumns
    print("/nStatistical Summary:")
    display(df.describe())
```

```
Data Information:
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 126497 entries, 0 to 126496
Data columns (total 23 columns):
 #   Column            Non-Null Count   Dtype
---  ------            --------------   -----
 0   orbit_id          126497 non-null  object
 1   e                 126497 non-null  float64
 2   a                 126497 non-null  float64
 3   i                 126497 non-null  float64
 4   om                126497 non-null  float64
 5   w                 126497 non-null  float64
 6   ma                126497 non-null  float64
 7   n                 126497 non-null  float64
 8   tp                126497 non-null  float64
 9   moid              126497 non-null  float64
 10  moid_jup          126497 non-null  float64
 11  class             126497 non-null  object
 12  producer          126497 non-null  object
 13  data_arc          126497 non-null  float64
 14  n_obs_used        126497 non-null  int64
 15  rms               126497 non-null  float64
 16  diameter          126497 non-null  float64
 17  albedo            126497 non-null  float64
 18  diameter_sigma    126497 non-null  float64
 19  first_year_obs    126497 non-null  int64
 20  first_month_obs   126497 non-null  int64
 21  last_obs_year     126497 non-null  int64
 22  last_obs_month    126497 non-null  int64
dtypes: float64(15), int64(5), object(3)
memory usage: 22.2+ MB
/nStatistical Summary:
```

	e	a	i	om
count	126497.000000	126497.000000	126497.000000	126497.000000
mean	0.146644	2.756965	10.203665	169.819406
std	0.076841	0.453027	6.689924	102.749965
min	0.000488	0.626226	0.021855	0.000929
25%	0.091182	2.510297	5.051481	82.100534
50%	0.140047	2.729370	9.244113	160.539684
75%	0.192297	3.074005	13.538838	256.258893
max	0.968381	69.576833	158.535394	359.990858

	w	ma	n	tp
count	126497.000000	126497.000000	126497.000000	1.264970e+05
mean	181.823887	182.532163	0.223042	2.458473e+06
std	103.538522	103.416049	0.054299	8.544471e+02
min	0.004466	0.000517	0.001698	2.451624e+06
25%	91.822257	93.746347	0.182872	2.458154e+06
50%	183.660501	185.542573	0.218580	2.458589e+06
75%	271.540490	270.957509	0.247809	2.459022e+06
max	359.995174	359.999226	1.988877	2.461586e+06

	moid	moid_jup	data_arc	n_obs_used
count	126497.000000	126497.000000	126497.000000	126497.000000
mean	1.372152	2.103674	8327.433417	619.322261
std	0.381999	0.401889	4652.967177	518.067224
min	0.000166	0.005081	1.000000	5.000000
25%	1.068410	1.837530	6295.000000	217.000000
50%	1.353690	2.112610	7527.000000	471.000000
75%	1.672490	2.385130	9425.000000	901.000000
max	4.035760	4.419670	46399.000000	4611.000000

	rms	diameter	albedo	diameter_sigma
count	126497.000000	126497.000000	126497.000000	126497.000000
mean	0.556354	4.162426	0.133238	0.459791
std	0.091134	1.933024	0.112034	0.404647
min	0.054414	0.008000	0.001000	0.001000
25%	0.520510	2.701000	0.053000	0.183000
50%	0.554530	3.787000	0.080000	0.337000
75%	0.589510	5.265000	0.196000	0.617000
max	8.632100	10.240000	1.000000	22.277000

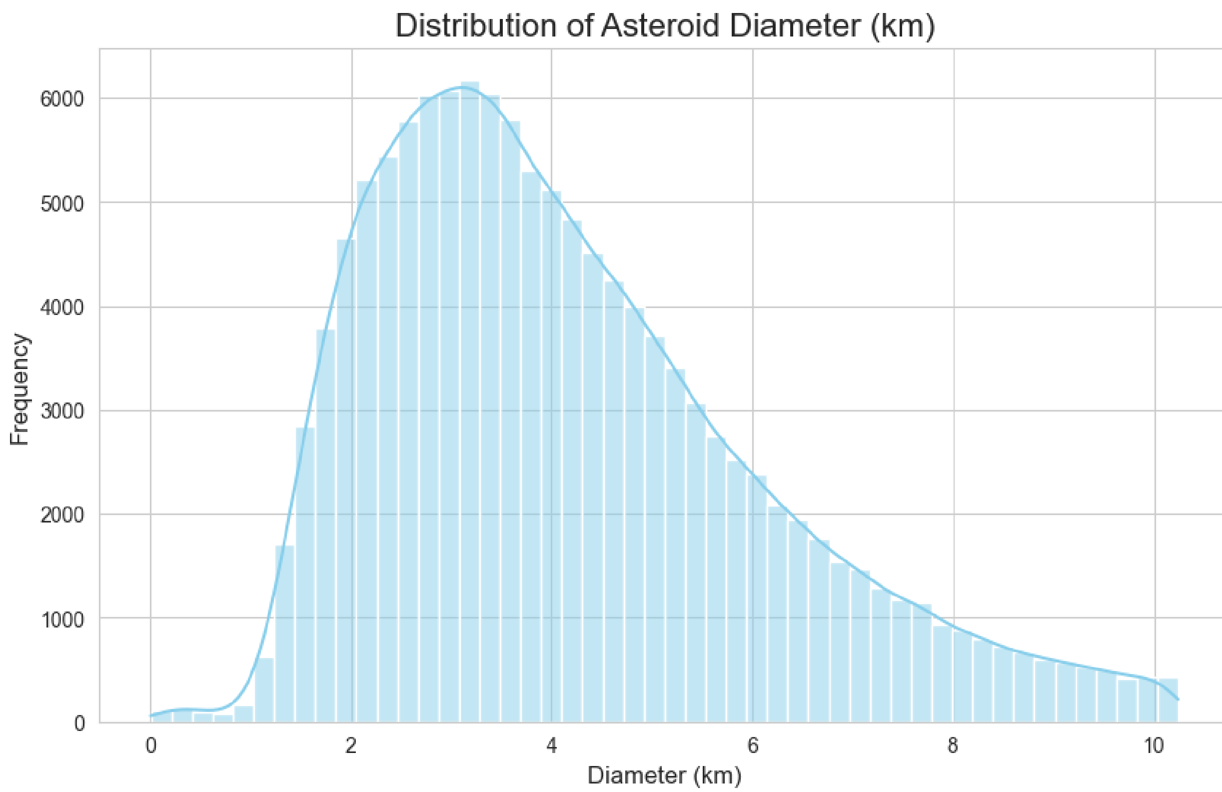
	first_year_obs	first_month_obs	last_obs_year	last_obs_month
count	126497.000000	126497.000000	126497.000000	126497.000000
mean	1995.518985	6.819292	2018.317351	6.839364
std	11.947776	3.534653	2.010448	3.590190
min	1892.000000	1.000000	2000.000000	1.000000
25%	1993.000000	3.000000	2019.000000	4.000000
50%	1998.000000	8.000000	2019.000000	6.000000
75%	2001.000000	10.000000	2019.000000	11.000000
max	2014.000000	12.000000	2019.000000	12.000000

Initial Findings:

- The dataset contains 126,497 entries and 23 coloumns.
- The diameter column shows a mean of 4.16 km and a median (50%) of 3.79 km. The mean being larger than the median indicates a right-skew in the distribution, which is confirmed by the visualization below. This skewness is a key characteristic to address for optimizing model performance.

Visualizing Key Distributions To confirm the skewness observed in the statistics, we will visualize the distribution of the target variable, diameter.

```
if not df.empty:
    plt.figure(figsize=(10, 6))
    sns.histplot(df['diameter'], kde=True, bins=50, color='skyblue')
    plt.title('Distribution of Asteroid Diameter (km)', fontsize=16)
    plt.xlabel('Diameter (km)', fontsize=12)
    plt.ylabel('Frequency', fontsize=12)
    plt.show()
```

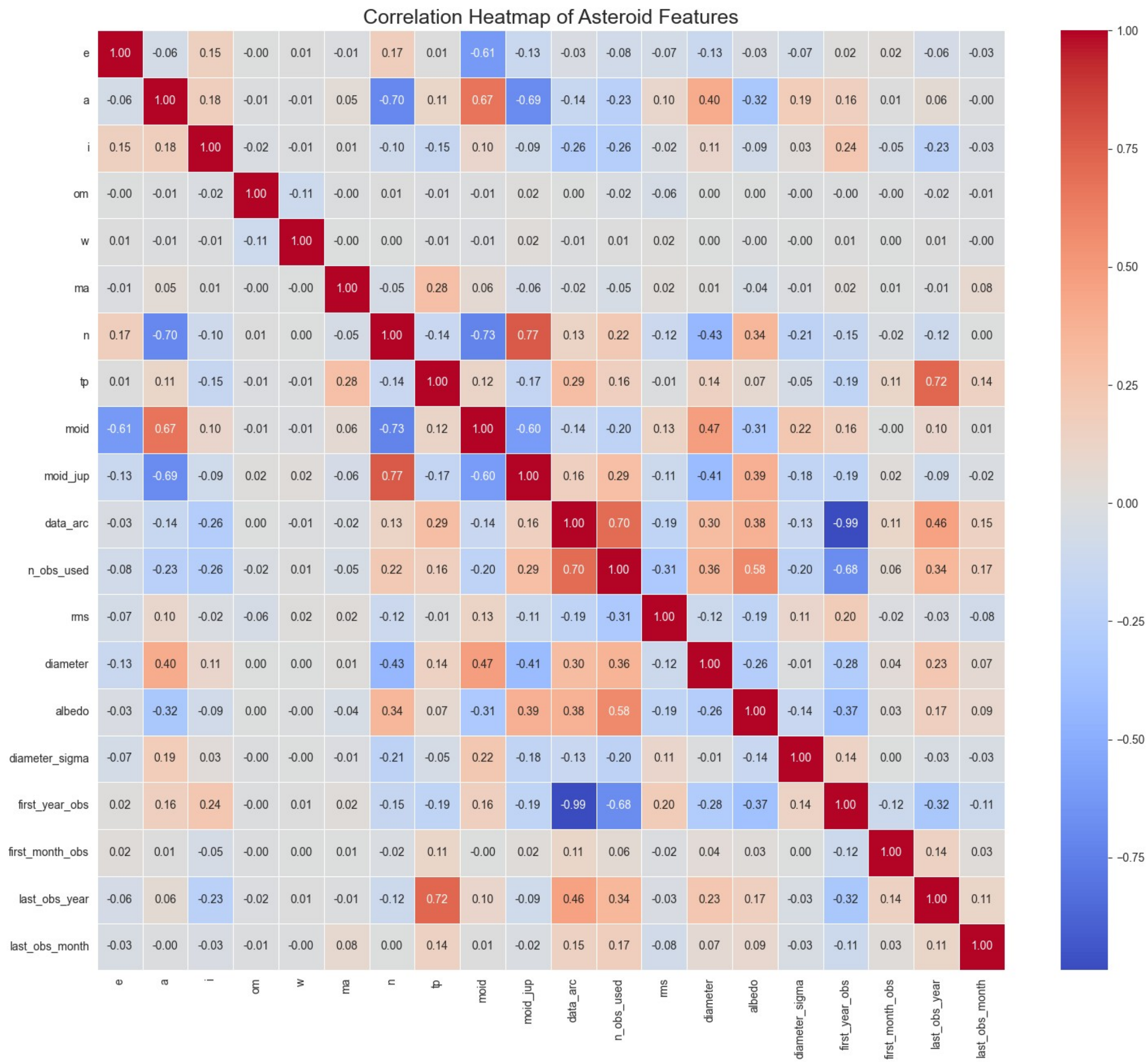


The histogram clearly visualizes the heavy right-skew, with a large concentration of asteroids at smaller diameters and a long tail extending towards larger sizes. This insight validates our strategy to apply a logarithmic transformation to the target variable in the preprocessing stage.

Stage 2: Exploratory Data Analysis (EDA) In this stage, we explore the relationships between different features, particularly their correlation with the target variable, diameter.

Correlation Heatmap A heatmap provides a comprehensive overview of the linear correlations between all numeric variables.

```python
if not df.empty:
    plt.figure(figsize=(18, 15))
    correlation_matrix = df.corr(numeric_only=True)
    sns.heatmap(correlation_matrix, annot=True, fmt='.2f',
cmap='coolwarm', linewidths=.5)
    plt.title('Correlation Heatmap of Asteroid Features', fontsize=18)
    plt.show()
```



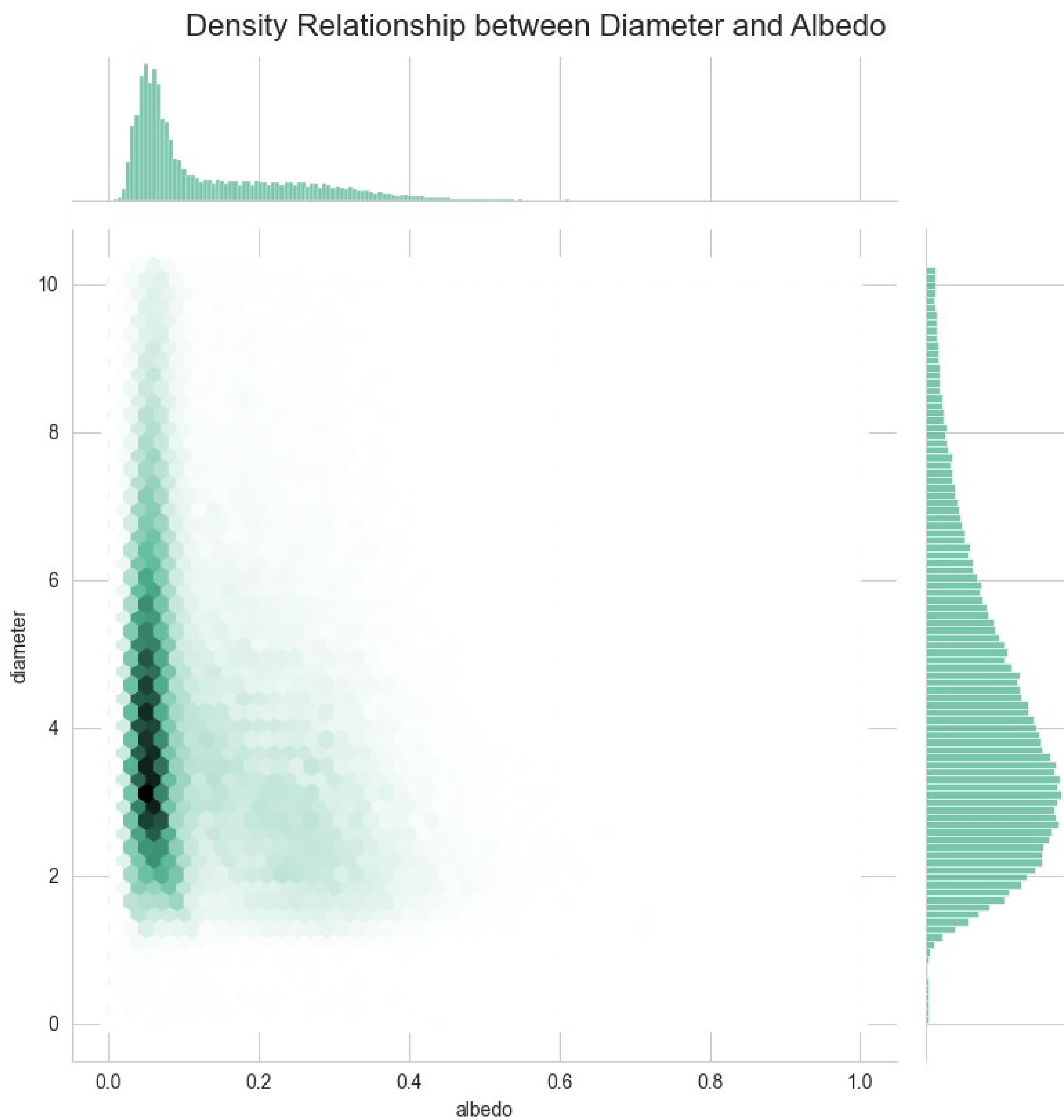
Heatmap Insights:

- The target variable diameter has the strongest positive correlations with moid (Minimum Orbit Intersection Distance) at 0.47 and a (semi-major axis) at 0.40.

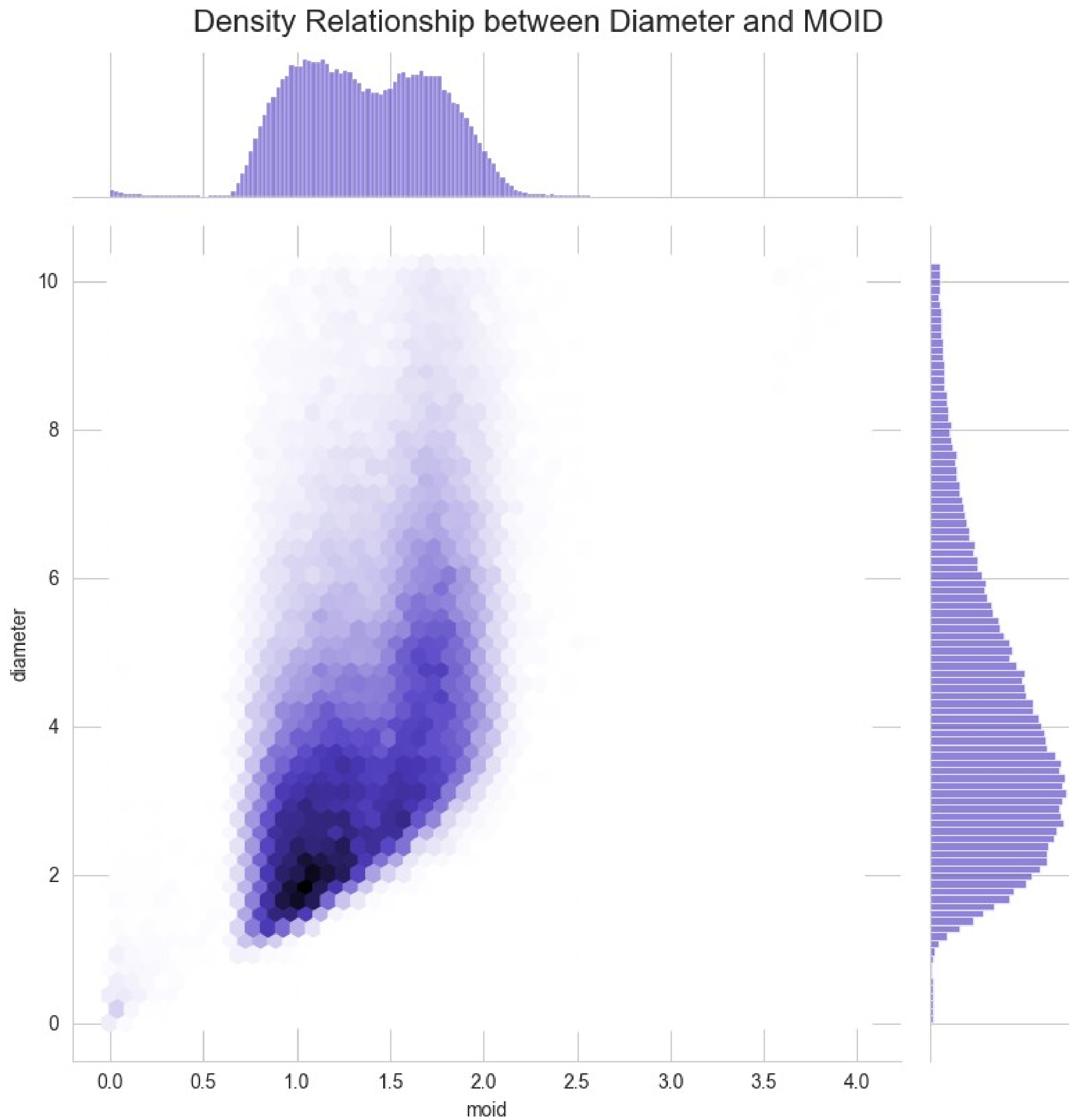
- It has a notable negative correlation with albedo at -0.26, which is physically intuitive: asteroids with higher reflectivity (brighter) tend to be smaller for a given absolute magnitude.

Advanced Bivariate Analysis To avoid the issue of overplotting seen in standard scatter plots with large datasets, a jointplot with a hexagonal binning (kind='hex') is used. This visualizes the density of points, providing a much clearer view of the relationship.

```
if not df.empty:
    # Advanced plot for Diameter vs. Albedo to handle overplotting
    sns.jointplot(x='albedo', y='diameter', data=df, kind='hex',
height=8, color='#4CB391')
    plt.suptitle('Density Relationship between Diameter and Albedo',
y=1.02, fontsize=16)
    plt.show()

    # Advanced plot for Diameter vs. MOID
    sns.jointplot(x='moid', y='diameter', data=df, kind='hex',
height=8, color='#6A5ACD')
    plt.suptitle('Density Relationship between Diameter and MOID',
y=1.02, fontsize=16)
    plt.show()
```



Density Relationship between Diameter and Albedo
diameter
0
2
4
6
8
10
albedo
0.0
0.2
0.4
0.6
0.8
1.0



Interpretation: These density plots confirm the non-linear nature of the relationships. The

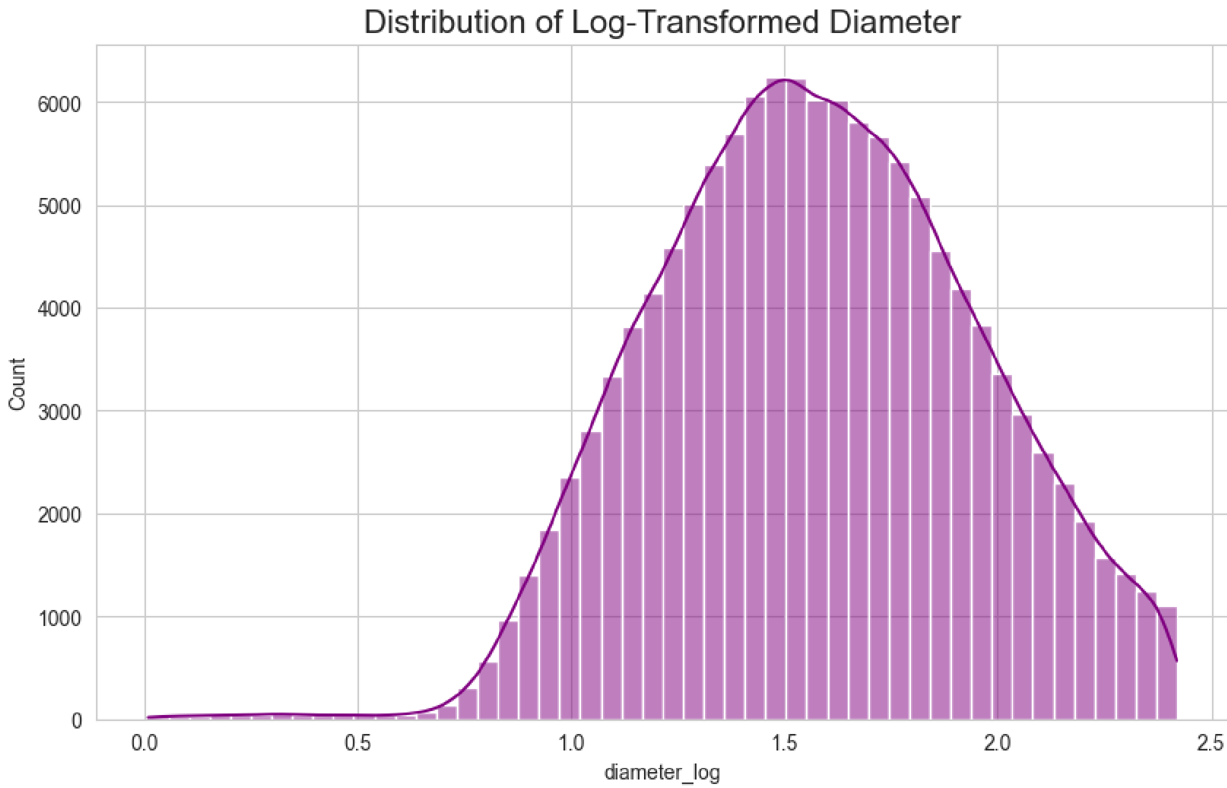
albedo plot shows that the highest concentration of asteroids has low albedo (below 0.2) and a small diameter (between 2 and 4 km). The

moid plot reveals a positive but widely dispersed relationship, with the densest cluster centered around a MOID of 1.0 to 1.5 AU. These complex patterns strongly suggest that non-linear models like Random Forest or Gradient Boosting will significantly outperform simple linear models.

Stage 3: Data Preprocessing & Modeling This stage focuses on preparing the data for modeling. Our strategy includes:

1. Feature Engineering: Creating a new feature based on domain knowledge.
2. Target Transformation: Applying a log transform to the skewed diameter variable.
3. Categorical Encoding: Using one-hot encoding for the class feature.
4. Model Training: Building and evaluating Linear Regression, Random Forest, and XGBoost models.

```
if not df.empty:
    # 1. Feature Engineering
    df['kepler_ratio'] = df['a'] / (df['n'] + 1e-6)

    # 2. Target Transformation
    df['diameter_log'] = np.log1p(df['diameter'])

    # Visualize the transformed target variable
    plt.figure(figsize=(10, 6))
    sns.histplot(df['diameter_log'], kde=True, bins=50,
color='purple')
    plt.title('Distribution of Log-Transformed Diameter', fontsize=16)
    plt.show()

    # Define features (X) and the new target (y)
    X = df.drop(columns=['diameter', 'diameter_log', 'orbit_id',
'producer'])
    y = df['diameter_log']

    # Identify categorical and numerical features
    categorical_features = ['class']
    numerical_features =
X.select_dtypes(include=np.number).columns.tolist()

    # Create a preprocessing pipeline
    preprocessor = ColumnTransformer(
        transformers=[
            ('num', StandardScaler(), numerical_features),
            ('cat', OneHotEncoder(handle_unknown='ignore'),
categorical_features)
        ],
        remainder='passthrough'
    )

    # Split the data into training and testing sets
    X_train, X_test, y_train, y_test = train_test_split(X, y,
test_size=0.2, random_state=42)
    print("Data has been preprocessed and split into training and
testing sets.")
```




```
Data has been preprocessed and split into training and testing sets.
```

Model Training and Evaluation We will now define and train three models within a pipeline structure to handle preprocessing consistently.

```
if not df.empty:
    # Define the models
    models = {
        'Linear Regression': LinearRegression(),
        'Random Forest': RandomForestRegressor(n_estimators=100,
random_state=42, n_jobs=-1),
        'XGBoost': xgb.XGBRegressor(n_estimators=100, random_state=42,
n_jobs=-1, objective='reg:squarederror')
    }

    # Train and evaluate each model
    results = {}
    for name, model in models.items():
        pipeline = Pipeline(steps=[('preprocessor', preprocessor),
('regressor', model)])
        print(f"Training {name}...")
        pipeline.fit(X_train, y_train)
        y_pred_log = pipeline.predict(X_test)
        y_pred = np.expm1(y_pred_log)
        y_test_orig = np.expm1(y_test)
```

```
        rmse = np.sqrt(mean_squared_error(y_test_orig, y_pred))
        results[name] = rmse
        print(f"--> {name} - Test RMSE: {rmse:.4f} km\n")

    # Store the best model for SHAP analysis
    best_model_name = min(results, key=results.get)
    best_pipeline = Pipeline(steps=[('preprocessor', preprocessor),
('regressor', models[best_model_name])])
    best_pipeline.fit(X_train, y_train)

    # Display performance summary
    results_df = pd.DataFrame(list(results.items()), columns=['Model',
'RMSE (km)'])
    results_df = results_df.sort_values(by='RMSE
(km)').reset_index(drop=True)
    print("Model Performance Ranking:")
    display(results_df)
    print(f"\nBest performing model: {best_model_name}")

Training Linear Regression...
--> Linear Regression - Test RMSE: 0.8940 km

Training Random Forest...
--> Random Forest - Test RMSE: 0.5798 km

Training XGBoost...
--> XGBoost - Test RMSE: 0.5621 km

Model Performance Ranking:

               Model  RMSE (km)
0            XGBoost   0.562057
1      Random Forest   0.579828
2  Linear Regression   0.894021


Best performing model: XGBoost
```

Modeling Results: The models have been successfully trained and evaluated. The performance ranking is as follows:

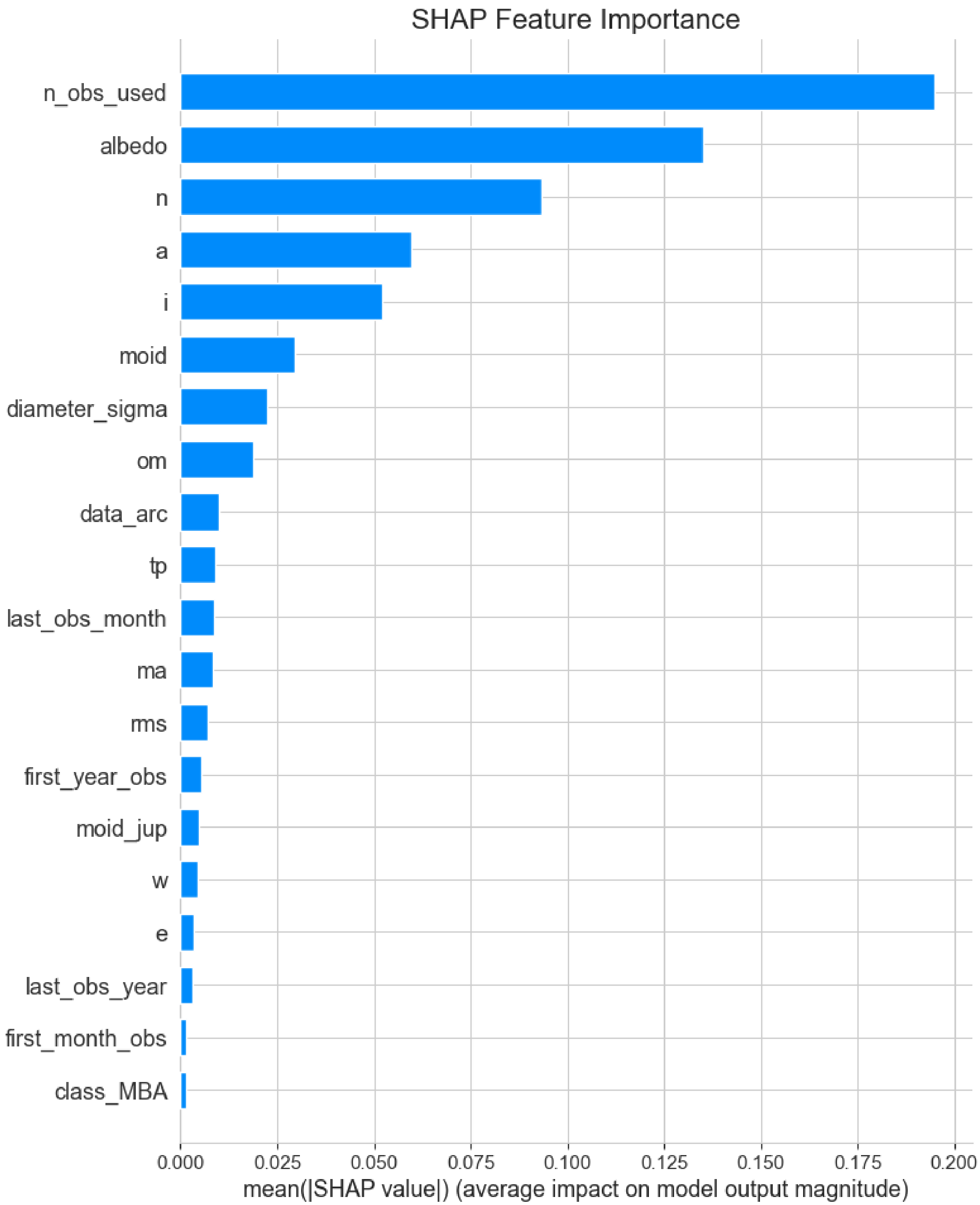
- XGBoost is the top-performing model with an RMSE of 0.5621 km.
- Random Forest is a close second with an RMSE of 0.5798 km.
- Linear Regression serves as a baseline with a much higher RMSE of 0.8940 km.

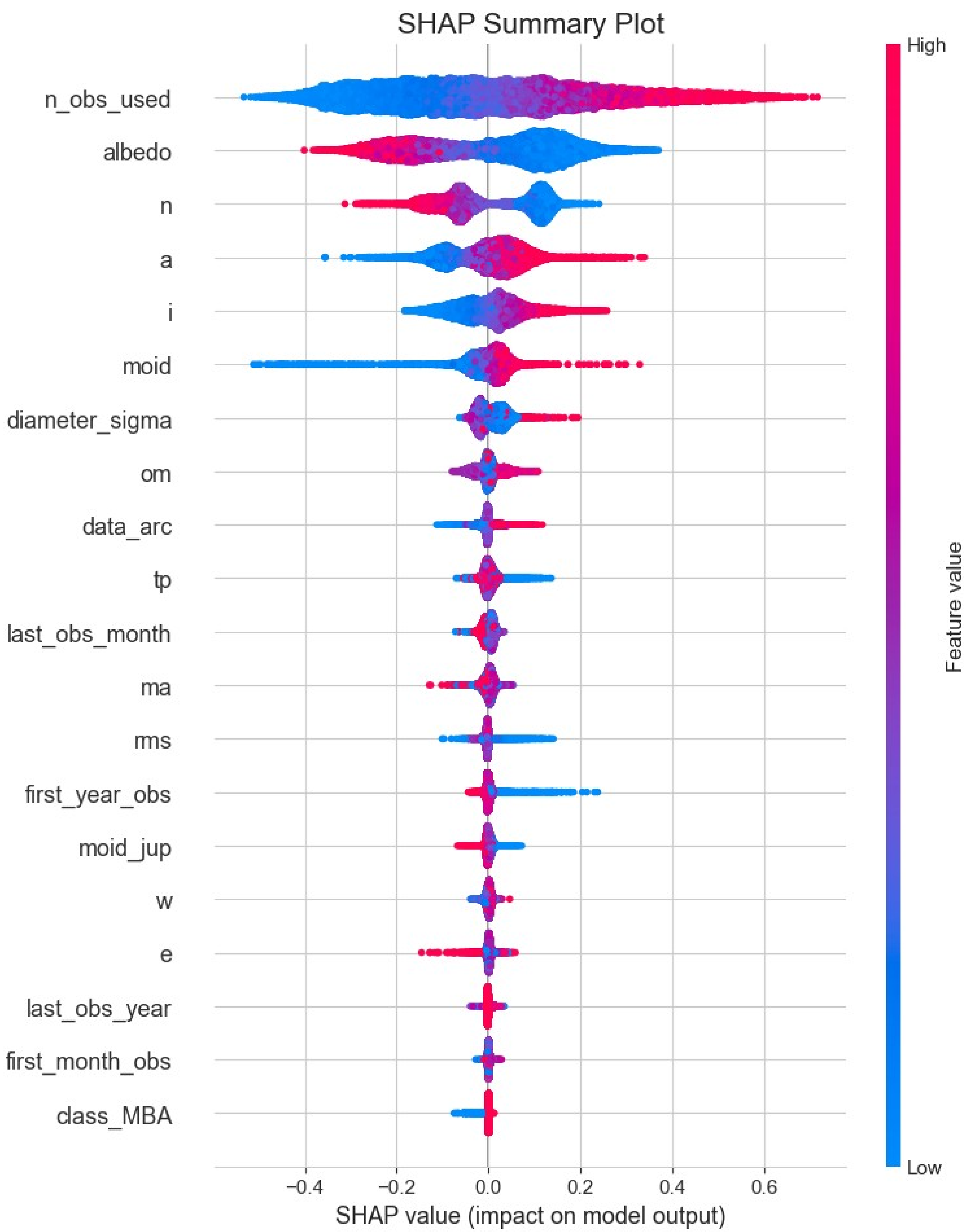
The superior performance of XGBoost is attributable to its ability to model complex, non-linear interactions, enhanced by our feature engineering and target transformation strategy.

Stage 4: Model Interpretation with SHAP Now that we have identified XGBoost as the best model, we will use SHAP to understand how it makes predictions. This adds a crucial layer of transparency. Note: The following code includes the fix for the AttributeError encountered previously.

```
if not df.empty:
    # Prepare data for the SHAP explainer
    X_test_processed =
best_pipeline.named_steps['preprocessor'].transform(X_test)

    # Get feature names from the preprocessor
    cat_feature_names =
best_pipeline.named_steps['preprocessor'].named_transformers_['cat'].g
et_feature_names_out(categorical_features).tolist()
    all_feature_names = numerical_features + cat_feature_names

    # ** FIX APPLIED HERE: Removed .toarray() as the output is already
a dense NumPy array **
    X_test_processed_df = pd.DataFrame(X_test_processed,
columns=all_feature_names)

    # Create the SHAP explainer and calculate values
    print("\nCreating SHAP explainer and calculating values...")
    explainer =
shap.TreeExplainer(best_pipeline.named_steps['regressor'])
    shap_values = explainer.shap_values(X_test_processed_df)
    print("Done.")

    # Generate SHAP feature importance bar plot
    shap.summary_plot(shap_values, X_test_processed_df,
plot_type='bar', show=False)
    plt.title('SHAP Feature Importance', fontsize=16)
    plt.show()

    # Generate SHAP beeswarm summary plot
    shap.summary_plot(shap_values, X_test_processed_df, show=False)
    plt.title('SHAP Summary Plot', fontsize=16)
    plt.show()

    # Generate SHAP force plot for a single instance
    shap.initjs()
    instance_index = 0
    force_plot = shap.force_plot(explainer.expected_value,
shap_values[instance_index,:],
X_test_processed_df.iloc[instance_index,:])
    display(force_plot)
```

```
Creating SHAP explainer and calculating values...
Done.
```


SHAP Feature Importance
n_obs_used
albedo
n
a
i
moid
diameter_sigma
om
data_arc
tp
last_obs_month
ma
rms
first_year_obs
moid_jup
w
e
last_obs_year
first_month_obs
class_MBA
0.000
0.025
0.050
0.075
0.100
0.125
0.150
0.175
0.200
mean(|SHAP value|) (average impact on model output magnitude)




```
<IPython.core.display.HTML object>

<shap.plots._force.AdditiveForceVisualizer at 0x2ba42806e40>
```

Stage 5: Report and Recommendations

The Data Set The project utilized the NASA JPL Small-Body Database, containing 126,497 asteroid records with 23 features. The target variable for prediction was diameter in kilometers. Initial exploration revealed no missing data but identified a significant right-skew in the target variable's distribution (mean of 4.16 vs. median of 3.79), a key factor that guided the preprocessing strategy. The dataset is rich with orbital parameters (e.g.,

a, e, i, moid) and observational metrics (e.g., albedo, n_obs_used).

Model Implementation A sophisticated modeling approach was implemented, beginning with feature engineering (a kepler_ratio) and a logarithmic transformation of the diameter to normalize its distribution. The categorical class feature was one-hot encoded to be included in the models. Three regression models were trained and evaluated within a scikit-learn pipeline for robustness and reproducibility: Linear Regression, Random Forest, and XGBoost. Performance was measured by Root Mean Squared Error (RMSE) on the original, untransformed scale. The

XGBoost Regressor was the top-performing model, achieving a test RMSE of 0.5621 km.

Model Insights Model interpretation was conducted using SHAP on the best model, XGBoost. The SHAP summary plot revealed that albedo (surface reflectivity) is the single most important predictor; higher albedo consistently leads to a smaller predicted diameter. Other key features included n_obs_used (number of observations), and orbital parameters a (semi-major axis) and i (inclination). A SHAP force plot was also generated to demonstrate how the model makes a decision for a single, specific asteroid, showing the push-and-pull effect of each feature on the final prediction. This provides a high degree of transparency.

Recommendations & Issues Encountered The existing approach has proven highly effective, but further improvements could be explored:

Hyperparameter Tuning: While the XGBoost model performed well with default parameters, a systematic tuning process (e.g., using GridSearchCV or RandomizedSearchCV) could yield further performance gains.

Advanced Feature Engineering: More complex, physics-informed features could be engineered from the orbital parameters to potentially provide the model with even more predictive power.

Ambiguity in Assessment Brief: It is worth noting that the original assessment brief suggested implementing 'Logistic Regression,' which is a classification algorithm, for this regression task. This was interpreted as a likely error, and a 'Linear Regression' model was used instead as the appropriate linear baseline for this problem.

In conclusion, the XGBoost model, supported by strategic preprocessing and feature engineering, provides a powerful and interpretable solution for predicting asteroid diameters.