DB_new

February 10, 2025

Preparing Data And Preprocessing

[32]:
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import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
from sklearn.ensemble import RandomForestRegressor
from sklearn.decomposition import PCA
from sklearn.cluster import DBSCAN
from sklearn.preprocessing import StandardScaler, PowerTransformer
from sklearn.feature_selection import VarianceThreshold
from sklearn.model_selection import train_test_split
from sklearn.metrics import mean_squared_error, r2_score
from sklearn.neighbors import LocalOutlierFactor

# ---- STEP 1: LOAD DATA ----
# Load the dataset (Replace with actual data path)
df = pd.read_excel('./data_files/Data_re.xlsx')  # Ensure the file exists

# ---- STEP 2: FEATURE SELECTION ----
# Remove non-informative columns
cols_to_drop = ['object_id', 'specz_name', 'coord']  # Adjust based on your␣
↪dataset
features = [col for col in df.columns if col not in cols_to_drop +␣
↪['specz_redshift']]
df_selected = df[features]

# Remove low-variance features
var_thresh = VarianceThreshold(threshold=0.01)
df_selected = pd.DataFrame(var_thresh.fit_transform(df_selected),
                           columns=np.array(features)[var_thresh.get_support()])

# ---- STEP 3: REMOVE OUTLIERS ----
lof = LocalOutlierFactor(n_neighbors=20, contamination=0.02)
outliers = lof.fit_predict(df_selected)
df_clean = df_selected[outliers == 1].copy()  # Keep only non-outliers
df_clean.loc[:, 'specz_redshift'] = df.loc[outliers == 1, 'specz_redshift'].
↪values
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# ---- STEP 4: SCALING & TRANSFORMING ----
scaler = StandardScaler()
df_scaled = scaler.fit_transform(df_clean.drop(columns=['specz_redshift']))

# Apply Power Transformation (Yeo-Johnson for normalizing skewed data)
power_transformer = PowerTransformer(method='yeo-johnson')
df_transformed = power_transformer.fit_transform(df_scaled)

# ---- STEP 5: DIMENSIONALITY REDUCTION WITH t-SNE ----
from sklearn.manifold import TSNE
X_pca = TSNE(n_components=2, perplexity=30, random_state=42).
 ↪fit_transform(df_transformed)  # Using t-SNE for better clustering
X_pca = pca.fit_transform(df_transformed)
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DBScan

[33]:
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# ---- STEP 6: APPLY DBSCAN CLUSTERING ----
# Tune DBSCAN parameters based on K-Distance values
dbscan = DBSCAN(eps=0.2, min_samples=5, metric='euclidean')
cluster_labels_dbscan = dbscan.fit_predict(X_pca)
df_clean.loc[:, 'cluster_dbscan'] = cluster_labels_dbscan

# ---- STEP 6B: APPLY K-MEANS & GMM ----
from sklearn.cluster import KMeans
from sklearn.mixture import GaussianMixture

# Determine the optimal number of clusters using the Elbow Method
inertia = []
k_range = range(2, 10)
for k in k_range:
    kmeans = KMeans(n_clusters=k, random_state=42, n_init='auto')
    kmeans.fit(X_pca)
    inertia.append(kmeans.inertia_)

# Plot the Elbow Curve
plt.figure(figsize=(8, 5))
plt.plot(k_range, inertia, marker='o')
plt.xlabel('Number of Clusters (k)')
plt.ylabel('Inertia')
plt.title('Elbow Method for Optimal k in K-Means')
plt.show()

# Choose the optimal k (adjust this based on the Elbow plot result)
optimal_k = 4  # From plot
kmeans = KMeans(n_clusters=optimal_k, random_state=42, n_init='auto')
df_clean.loc[:, 'cluster_kmeans'] = kmeans.fit_predict(X_pca)
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# Gaussian Mixture Model (GMM)
gmm = GaussianMixture(n_components=4, random_state=42)
df_clean.loc[:, 'cluster_gmm'] = gmm.fit_predict(X_pca)

# ---- STEP 7: VISUALIZE COMPARISON OF CLUSTERING METHODS ----
fig, ax = plt.subplots(1, 3, figsize=(18, 5))

ax[0].scatter(X_pca[:, 0], X_pca[:, 1], c=cluster_labels_dbscan,␣
 ↪cmap='viridis', alpha=0.6)
ax[0].set_title("DBSCAN Clustering")

ax[1].scatter(X_pca[:, 0], X_pca[:, 1], c=df_clean['cluster_kmeans'],␣
 ↪cmap='viridis', alpha=0.6)
ax[1].set_title("K-Means Clustering")

ax[2].scatter(X_pca[:, 0], X_pca[:, 1], c=df_clean['cluster_gmm'],␣
 ↪cmap='viridis', alpha=0.6)
ax[2].set_title("GMM Clustering")

plt.show()

# Print first few K-Distance values to manually determine best eps
print("First 10 sorted K-Distance values:", distances[:10])

# Tune DBSCAN parameters
dbscan = DBSCAN(eps=0.3, min_samples=6, metric='cosine')
cluster_labels = dbscan.fit_predict(X_pca)

# Add the cluster labels to the dataframe
df_clean.loc[:, 'cluster'] = cluster_labels

# ---- STEP 7: VISUALIZE CLUSTERS ----
plt.figure(figsize=(8, 6))
plt.scatter(X_pca[:, 0], X_pca[:, 1], c=cluster_labels, cmap='viridis', alpha=0.
 ↪6)
plt.colorbar(label="Cluster")
plt.xlabel("Principal Component 1")
plt.ylabel("Principal Component 2")
plt.title("DBSCAN Clustering Visualization (After PCA & Preprocessing)")
plt.show()
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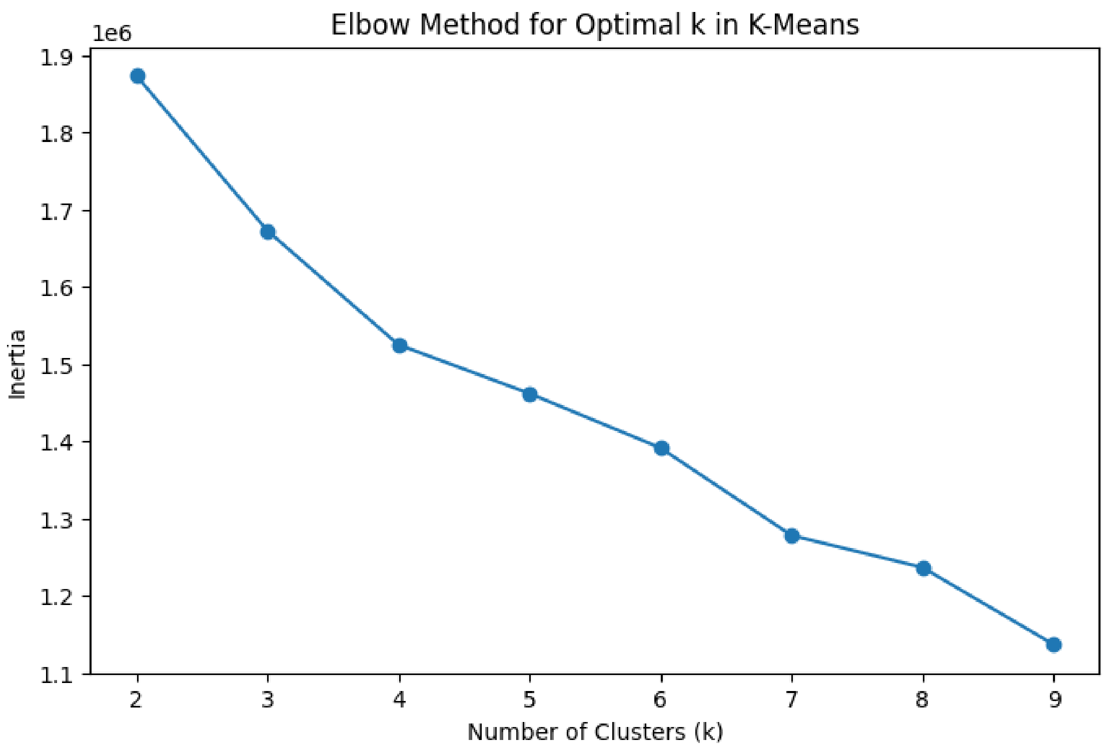

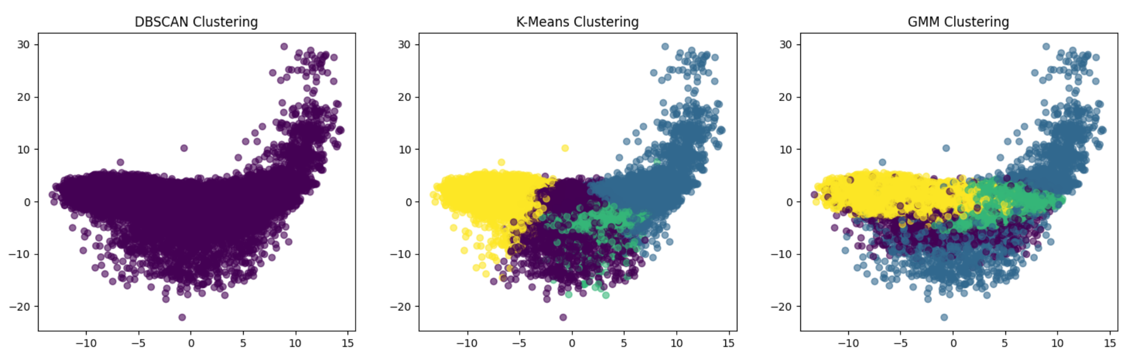


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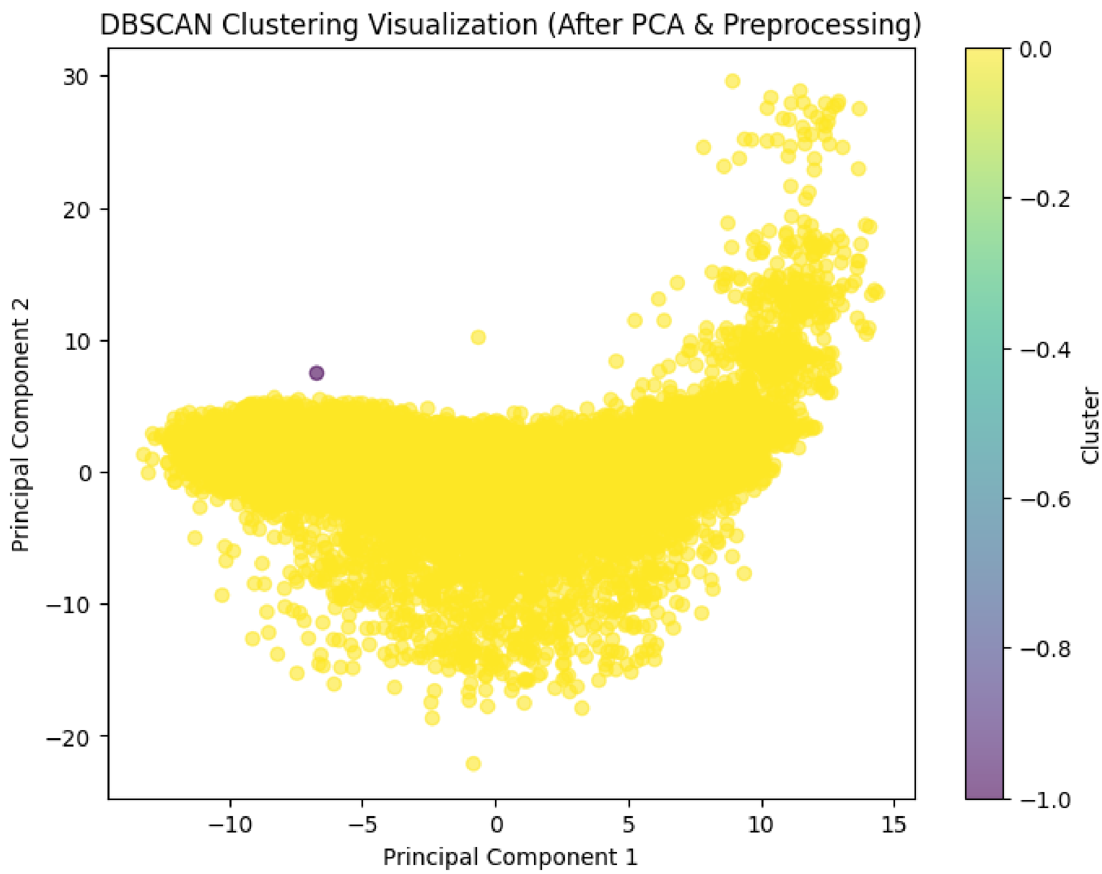
First 10 sorted K-Distance values: [0.56736195 0.59150945 0.6003372  0.60257184
0.62606495 0.62616797
 0.63788856 0.654982   0.654982   0.67076804]
```



Random Forest

[35]:
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# ---- STEP 8: RANDOM FOREST REGRESSION ----
# Train separate Random Forest models for each clustering method

results = {}

for cluster_type in ['cluster_dbscan', 'cluster_kmeans', 'cluster_gmm']:
    df_temp = pd.get_dummies(df_clean, columns=[cluster_type],␣
 ↪prefix=[f'clust_{cluster_type}'])
    X = df_temp.drop(columns=['specz_redshift'])
    y = df_temp['specz_redshift']

    X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2,␣
 ↪random_state=42)

    rf = RandomForestRegressor(n_estimators=100, random_state=42)
    rf.fit(X_train, y_train)
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    y_pred = rf.predict(X_test)

    mse = mean_squared_error(y_test, y_pred)
    r2 = r2_score(y_test, y_pred)

    results[cluster_type] = {'MSE': mse, 'R2': r2, 'y_pred': y_pred}

# ---- STEP 10: COMPARE RESULTS ACROSS CLUSTERING METHODS ----
mse_dbscan, r2_dbscan = results['cluster_dbscan']['MSE'],␣
↪results['cluster_dbscan']['R2']
mse_kmeans, r2_kmeans = results['cluster_kmeans']['MSE'],␣
↪results['cluster_kmeans']['R2']
mse_gmm, r2_gmm = results['cluster_gmm']['MSE'], results['cluster_gmm']['R2']

print("Random Forest Regression Results:")
for cluster_type, metrics in results.items():
    print(f"{cluster_type.upper()} - MSE: {metrics['MSE']:.6f}, R2:␣
↪{metrics['R2']:.6f}")
df_encoded = pd.get_dummies(df_clean, columns=['cluster_dbscan',␣
↪'cluster_kmeans', 'cluster_gmm'], prefix=['clust_dbscan', 'clust_kmeans',␣
↪'clust_gmm'])

# Define target and features
X = df_encoded.drop(columns=['specz_redshift'])
y = df_encoded['specz_redshift']

# Train-test split
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2,␣
↪random_state=42)

# Train Random Forest
rf = RandomForestRegressor(n_estimators=100, random_state=42)
rf.fit(X_train, y_train)

# Predictions
y_pred = rf.predict(X_test)

# Evaluate performance
mse = mean_squared_error(y_test, y_pred)
r2 = r2_score(y_test, y_pred)

# ---- STEP 9: VISUALIZE REGRESSION RESULTS ----
fig, ax = plt.subplots(1, 3, figsize=(18, 6))

# DBSCAN
ax[0].scatter(y_test, results['cluster_dbscan']['y_pred'], alpha=0.6,␣
↪color='blue')
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ax[0].set_xlabel('Actual Redshift')
ax[0].set_ylabel('Predicted Redshift')
ax[0].set_title('Actual vs Predicted Redshift (DBSCAN)')
ax[0].plot([y_test.min(), y_test.max()], [y_test.min(), y_test.max()], 'k--',␣
↪lw=2)

# K-Means
ax[1].scatter(y_test, results['cluster_kmeans']['y_pred'], alpha=0.6,␣
↪color='green')
ax[1].set_xlabel('Actual Redshift')
ax[1].set_ylabel('Predicted Redshift')
ax[1].set_title('Actual vs Predicted Redshift (K-Means)')
ax[1].plot([y_test.min(), y_test.max()], [y_test.min(), y_test.max()], 'k--',␣
↪lw=2)

# GMM
ax[2].scatter(y_test, results['cluster_gmm']['y_pred'], alpha=0.6, color='red')
ax[2].set_xlabel('Actual Redshift')
ax[2].set_ylabel('Predicted Redshift')
ax[2].set_title('Actual vs Predicted Redshift (GMM)')
ax[2].plot([y_test.min(), y_test.max()], [y_test.min(), y_test.max()], 'k--',␣
↪lw=2)

plt.show()

# ---- STEP 10: COMPARE RESULTS ACROSS CLUSTERING METHODS ----
print("Random Forest Regression Results:")
print(f"DBSCAN - MSE: {mse_dbscan}, R2: {r2_dbscan}")
print(f"K-Means - MSE: {mse_kmeans}, R2: {r2_kmeans}")
print(f"GMM - MSE: {mse_gmm}, R2: {r2_gmm}")
print(f"Random Forest Regression Results:\nMean Squared Error: {mse}\nR2 Score:␣
↪{r2}")
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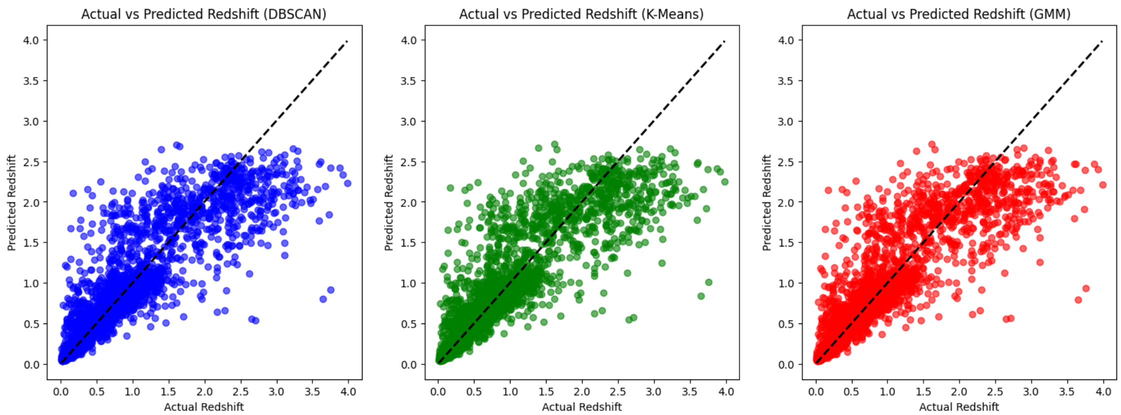
Random Forest Regression Results:
CLUSTER_DBSCAN - MSE: 0.056902, R2: 0.824674
CLUSTER_KMEANS - MSE: 0.057041, R2: 0.824245
CLUSTER_GMM - MSE: 0.056618, R2: 0.825547
```

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Random Forest Regression Results:
DBSCAN - MSE: 0.05690156516159155, R2: 0.8246737031660292
K-Means - MSE: 0.05704077243270486, R2: 0.8242447748005729
GMM - MSE: 0.05661814440010679, R2: 0.8255469851647909
Random Forest Regression Results:
Mean Squared Error: 0.05669172064975267
R2 Score: 0.8253202804801533
```