Hybrid_Model

February 24, 2025

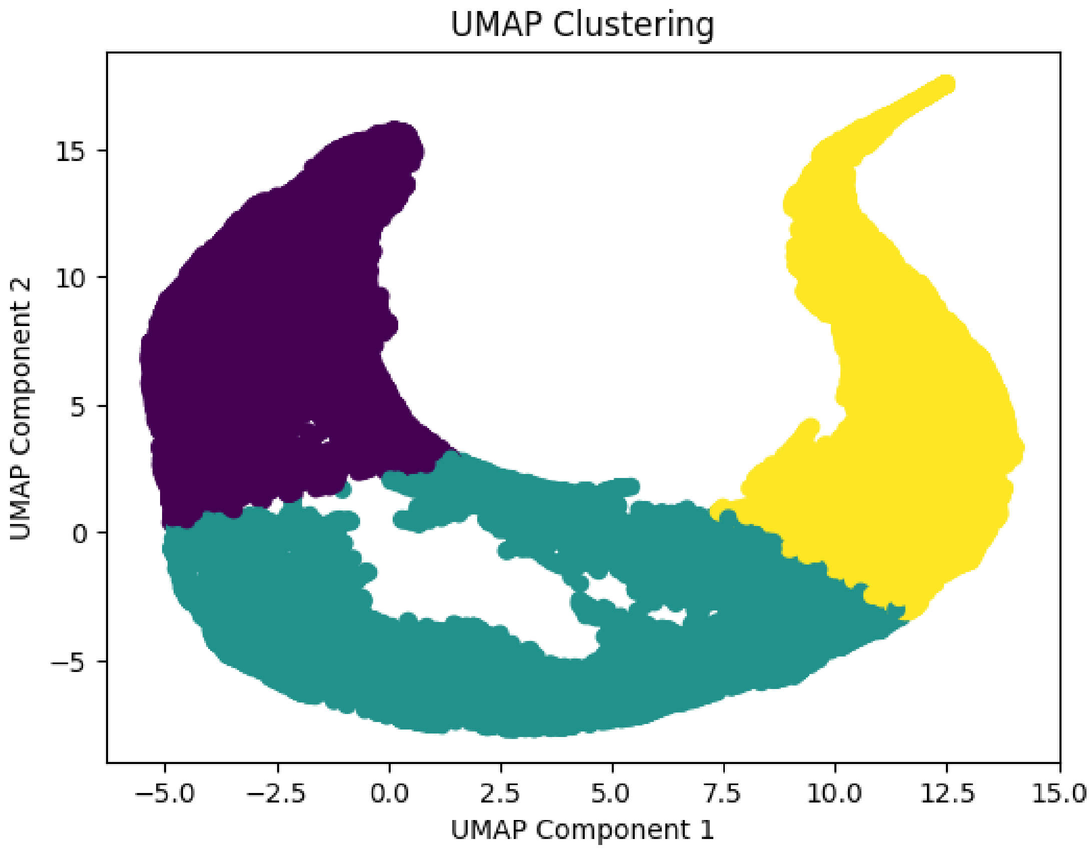
Preparing Data And Preprocessing

[2]:
```
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
from kneed import KneeLocator
from sklearn.cluster import KMeans
from sklearn.mixture import GaussianMixture
import umap.umap_ as umap

# ---- STEP 1: LOAD DATA ----
df = pd.read_excel('./data_files/Data_re.xlsx')  # Ensure the file exists

# ---- STEP 2: FEATURE SELECTION ----
cols_to_keep = ['g_flux', 'r_flux', 'i_flux', 'y_flux', 'z_flux',␣
 ↪'specz_redshift']
df_selected = df[cols_to_keep].copy()

# Compute Flux Color Indices
df_selected['g_r'] = df_selected['g_flux'] - df_selected['r_flux']
df_selected['r_i'] = df_selected['r_flux'] - df_selected['i_flux']
df_selected['i_y'] = df_selected['i_flux'] - df_selected['y_flux']
df_selected['y_z'] = df_selected['y_flux'] - df_selected['z_flux']

# ---- STEP 3: REMOVE OUTLIERS ----
lof = LocalOutlierFactor(n_neighbors=20, contamination=0.02)
outlier_scores = lof.fit_predict(df_selected.drop(columns=['specz_redshift']))
df_clean = df_selected[outlier_scores == 1].copy()
```

```python
# ---- 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 UMAP ----
reducer = umap.UMAP(n_components=2, n_neighbors=15, min_dist=0.1,␣
↪random_state=42)
X_umap = reducer.fit_transform(df_transformed)

# ---- STEP 6: OPTIONAL PCA FOR EXPLORATION ----
pca = PCA(n_components=3)
X_pca = pca.fit_transform(df_transformed)

# ---- STEP 7: CLUSTERING ----
kmeans = KMeans(n_clusters=3, random_state=42)
df_clean['Cluster'] = kmeans.fit_predict(X_umap)

# ---- PLOT RESULTS ----
plt.scatter(X_umap[:, 0], X_umap[:, 1], c=df_clean['Cluster'], cmap='viridis')
plt.xlabel('UMAP Component 1')
plt.ylabel('UMAP Component 2')
plt.title('UMAP Clustering')
plt.show()
```

```
2025-02-24 21:14:13.144587: E
external/local_xla/xla/stream_executor/cuda/cuda_fft.cc:477] Unable to register
cuFFT factory: Attempting to register factory for plugin cuFFT when one has
already been registered
WARNING: All log messages before absl::InitializeLog() is called are written to
STDERR
E0000 00:00:1740411853.199942    3391 cuda_dnn.cc:8310] Unable to register cuDNN
factory: Attempting to register factory for plugin cuDNN when one has already
been registered
E0000 00:00:1740411853.215569    3391 cuda_blas.cc:1418] Unable to register
cuBLAS factory: Attempting to register factory for plugin cuBLAS when one has
already been registered
2025-02-24 21:14:13.331174: I tensorflow/core/platform/cpu_feature_guard.cc:210]
This TensorFlow binary is optimized to use available CPU instructions in
performance-critical operations.
To enable the following instructions: AVX2 FMA, in other operations, rebuild
TensorFlow with the appropriate compiler flags.
/home/chloy/miniconda3/lib/python3.10/site-
packages/sklearn/utils/deprecation.py:151: FutureWarning: 'force_all_finite' was
renamed to 'ensure_all_finite' in 1.6 and will be removed in 1.8.
```

```
  warnings.warn(
/home/chloy/miniconda3/lib/python3.10/site-packages/umap/umap_.py:1952:
UserWarning: n_jobs value 1 overridden to 1 by setting random_state. Use no seed
for parallelism.
  warn(
```



checking

[3]:
```python
print(df.head())
print(df.info())
print(df.describe())
```

```
                                                coord        dec  \
0   b'(179325.3125, 99694.8046875, -21178.96484375)' -5.893433
1  b'(179236.609375, 99349.8203125, -23431.181640… -6.522742
2     b'(179281.5, 99283.5078125, -23368.759765625)' -6.505290
3  b'(179365.171875, 99158.046875, -23259.0839843… -6.474628
4      b'(179366.421875, 99172.25, -23188.84765625)' -6.454993

   g_central_image_pop_10px_rad  g_central_image_pop_15px_rad  \
0                             1                             1
```

```
1                            1                              1
2                            1                              1
3                            1                              1
4                            1                              1

   g_central_image_pop_5px_rad  g_cmodel_mag  g_cmodel_magsigma  \
0                            1     20.314907           0.002624
1                            1     22.217360           0.010902
2                            1     21.148739           0.008013
3                            1     18.464205           0.001740
4                            1     20.998287           0.006011

   g_ellipticity  g_half_light_radius  g_isophotal_area  …  z_minor_axis  \
0          0.147                6.047               603  …         4.938
1          0.130                3.430                93  …         2.713
2          0.209                6.597               254  …         4.351
3          0.525               10.855              1064  …         4.815
4          0.738                8.261               386  …         2.279

   z_peak_surface_brightness  z_petro_rad  z_pos_angle  z_sersic_index  \
0                    -8.2933         5.28        36.15           2.193
1                    -7.3657         5.94       -61.78           1.649
2                    -7.6539         9.24        32.76           2.364
3                    -8.5825         6.60        53.15           1.494
4                    -6.8798         5.94        21.16           1.063

         g_flux        r_flux        i_flux        y_flux        z_flux
0  7.482335e-09  2.987891e-08  5.117533e-08  8.117985e-08  6.737572e-08
1  1.297347e-09  5.643225e-09  1.319162e-08  2.141019e-08  1.828079e-08
2  3.471398e-09  1.571304e-08  3.743521e-08  6.504857e-08  5.585498e-08
3  4.114510e-08  1.090914e-07  1.841788e-07  3.080686e-07  2.402212e-07
4  3.987357e-09  1.373544e-08  2.634882e-08  4.449762e-08  3.527128e-08

[5 rows x 89 columns]
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 40914 entries, 0 to 40913
Data columns (total 89 columns):
 #   Column                       Non-Null Count  Dtype
---  ------                       --------------  -----
 0   coord                        40914 non-null  object
 1   dec                          40914 non-null  float64
 2   g_central_image_pop_10px_rad 40914 non-null  int64
 3   g_central_image_pop_15px_rad 40914 non-null  int64
 4   g_central_image_pop_5px_rad  40914 non-null  int64
 5   g_cmodel_mag                 40914 non-null  float64
 6   g_cmodel_magsigma            40914 non-null  float64
 7   g_ellipticity                40914 non-null  float64
 8   g_half_light_radius          40914 non-null  float64
```

```
9   g_isophotal_area              40914 non-null  int64
10  g_major_axis                  40914 non-null  float64
11  g_minor_axis                  40914 non-null  float64
12  g_peak_surface_brightness     40914 non-null  float64
13  g_petro_rad                   40914 non-null  float64
14  g_pos_angle                   40914 non-null  float64
15  g_sersic_index                40914 non-null  float64
16  i_central_image_pop_10px_rad  40914 non-null  int64
17  i_central_image_pop_15px_rad  40914 non-null  int64
18  i_central_image_pop_5px_rad   40914 non-null  int64
19  i_cmodel_mag                  40914 non-null  float64
20  i_cmodel_magsigma             40914 non-null  float64
21  i_ellipticity                 40914 non-null  float64
22  i_half_light_radius           40914 non-null  float64
23  i_isophotal_area              40914 non-null  int64
24  i_major_axis                  40914 non-null  float64
25  i_minor_axis                  40914 non-null  float64
26  i_peak_surface_brightness     40914 non-null  float64
27  i_petro_rad                   40914 non-null  float64
28  i_pos_angle                   40914 non-null  float64
29  i_sersic_index                40914 non-null  float64
30  object_id                     40914 non-null  int64
31  r_central_image_pop_10px_rad  40914 non-null  int64
32  r_central_image_pop_15px_rad  40914 non-null  int64
33  r_central_image_pop_5px_rad   40914 non-null  int64
34  r_cmodel_mag                  40914 non-null  float64
35  r_cmodel_magsigma             40914 non-null  float64
36  r_ellipticity                 40914 non-null  float64
37  r_half_light_radius           40914 non-null  float64
38  r_isophotal_area              40914 non-null  int64
39  r_major_axis                  40914 non-null  float64
40  r_minor_axis                  40914 non-null  float64
41  r_peak_surface_brightness     40914 non-null  float64
42  r_petro_rad                   40914 non-null  float64
43  r_pos_angle                   40914 non-null  float64
44  r_sersic_index                40914 non-null  float64
45  ra                            40914 non-null  float64
46  skymap_id                     40914 non-null  int64
47  specz_dec                     40914 non-null  float64
48  specz_flag_homogeneous        40914 non-null  bool
49  specz_mag_i                   40914 non-null  float64
50  specz_name                    40914 non-null  object
51  specz_ra                      40914 non-null  float64
52  specz_redshift                40914 non-null  float64
53  specz_redshift_err            40914 non-null  float64
54  x_coord                       40914 non-null  float64
55  y_central_image_pop_10px_rad  40914 non-null  int64
56  y_central_image_pop_15px_rad  40914 non-null  int64
```

```
 57  y_central_image_pop_5px_rad   40914 non-null  int64
 58  y_cmodel_mag                  40914 non-null  float64
 59  y_cmodel_magsigma             40914 non-null  float64
 60  y_coord                       40914 non-null  float64
 61  y_ellipticity                 40914 non-null  float64
 62  y_half_light_radius           40914 non-null  float64
 63  y_isophotal_area              40914 non-null  int64
 64  y_major_axis                  40914 non-null  float64
 65  y_minor_axis                  40914 non-null  float64
 66  y_peak_surface_brightness     40914 non-null  float64
 67  y_petro_rad                   40914 non-null  float64
 68  y_pos_angle                   40914 non-null  float64
 69  y_sersic_index                40914 non-null  float64
 70  z_central_image_pop_10px_rad  40914 non-null  int64
 71  z_central_image_pop_15px_rad  40914 non-null  int64
 72  z_central_image_pop_5px_rad   40914 non-null  int64
 73  z_cmodel_mag                  40914 non-null  float64
 74  z_cmodel_magsigma             40914 non-null  float64
 75  z_ellipticity                 40914 non-null  float64
 76  z_half_light_radius           40914 non-null  float64
 77  z_isophotal_area              40914 non-null  int64
 78  z_major_axis                  40914 non-null  float64
 79  z_minor_axis                  40914 non-null  float64
 80  z_peak_surface_brightness     40914 non-null  float64
 81  z_petro_rad                   40914 non-null  float64
 82  z_pos_angle                   40914 non-null  float64
 83  z_sersic_index                40914 non-null  float64
 84  g_flux                        40914 non-null  float64
 85  r_flux                        40914 non-null  float64
 86  i_flux                        40914 non-null  float64
 87  y_flux                        40914 non-null  float64
 88  z_flux                        40914 non-null  float64
dtypes: bool(1), float64(64), int64(22), object(2)
memory usage: 27.5+ MB
None
                dec  g_central_image_pop_10px_rad  \
count  40914.000000                  40914.000000
mean       4.772650                      1.016278
std       14.789896                      0.202830
min       -7.217183                      0.000000
25%       -0.960840                      1.000000
50%        0.311508                      1.000000
75%        1.712535                      1.000000
max       53.260936                      3.000000

       g_central_image_pop_15px_rad  g_central_image_pop_5px_rad  \
count                  40914.000000                 40914.000000
mean                       1.032141                     0.998142
```

std	0.240109	0.160037
min	0.000000	0.000000
25%	1.000000	1.000000
50%	1.000000	1.000000
75%	1.000000	1.000000
max	4.000000	3.000000

	g_cmodel_mag	g_cmodel_magsigma	g_ellipticity	g_half_light_radius \
count	40914.000000	40914.000000	40914.000000	40914.000000
mean	21.260192	0.010414	0.230579	6.509069
std	1.882030	0.091981	0.171495	3.625851
min	14.753462	0.000149	0.000000	0.000000
25%	19.733286	0.001531	0.095000	3.905000
50%	21.492703	0.004890	0.190000	5.679000
75%	22.614446	0.011530	0.328000	7.976000
max	30.276308	17.593214	0.896000	26.335000

	g_isophotal_area	g_major_axis	…	z_minor_axis \
count	40914.000000	40914.000000	…	40914.000000
mean	694.781786	5.523996	…	4.064275
std	905.508200	4.095328	…	2.145741
min	0.000000	0.000000	…	0.000000
25%	122.000000	2.706250	…	2.308250
50%	262.000000	3.938000	…	3.740000
75%	947.000000	7.249000	…	5.250000
max	6434.000000	33.320000	…	16.530000

	z_peak_surface_brightness	z_petro_rad	z_pos_angle	z_sersic_index \
count	40914.000000	40914.000000	40914.000000	40914.000000
mean	-6.819224	6.249483	1.738910	1.664449
std	1.418684	1.392911	52.237031	0.870328
min	-10.477100	0.000000	-89.990000	0.000000
25%	-7.830100	5.280000	-43.900000	1.037000
50%	-7.000600	5.940000	3.525000	1.523000
75%	-5.935925	6.600000	46.870000	2.095000
max	0.000000	10.560000	90.000000	9.974000

	g_flux	r_flux	i_flux	y_flux	z_flux
count	4.091400e+04	4.091400e+04	4.091400e+04	4.091400e+04	4.091400e+04
mean	1.210340e-08	2.768307e-08	4.473075e-08	6.989669e-08	5.870488e-08
std	2.736938e-08	5.694149e-08	8.773860e-08	1.366205e-07	1.134256e-07
min	7.753125e-13	1.954729e-12	8.507724e-12	3.916208e-11	3.854886e-11
25%	8.999569e-10	2.390220e-09	4.067133e-09	6.001859e-09	5.229988e-09
50%	2.528826e-09	7.571469e-09	1.592592e-08	2.686640e-08	2.237941e-08
75%	1.278456e-08	3.078038e-08	4.926195e-08	7.639837e-08	6.444087e-08
max	1.254918e-06	2.506786e-06	3.731277e-06	5.268088e-06	4.333962e-06

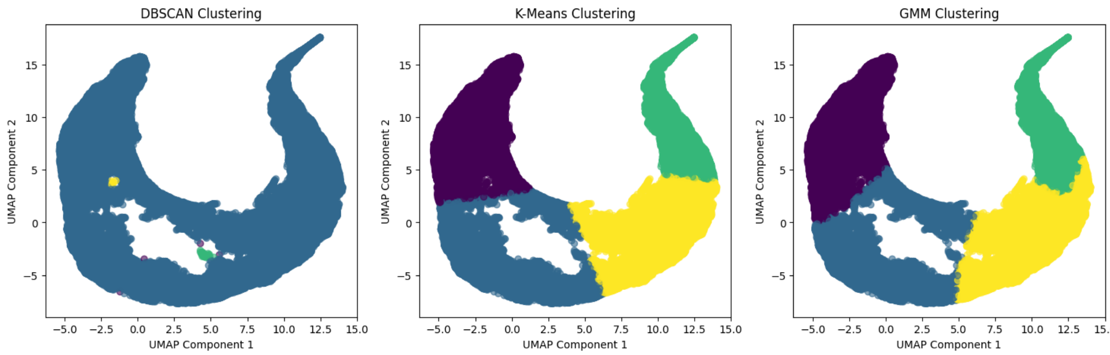
[8 rows x 86 columns]

Clustering (DBScan, K means and Gaussian Mixture Method)

[4]:
```
from sklearn.cluster import DBSCAN, KMeans
from sklearn.mixture import GaussianMixture
from sklearn.neighbors import NearestNeighbors
from sklearn.metrics import silhouette_score
import matplotlib.pyplot as plt
import numpy as np
from kneed import KneeLocator

# ---- STEP 6: DETERMINE OPTIMAL DBSCAN EPS ----
k = 5  # Typically, min_samples value
nearest_neighbors = NearestNeighbors(n_neighbors=k)
nearest_neighbors.fit(X_umap)
distances, indices = nearest_neighbors.kneighbors(X_umap)

# Sort distances to find the "knee" point
distances = np.sort(distances[:, -1])

# Use KneeLocator to find optimal epsilon
knee_locator = KneeLocator(range(len(distances)), distances, curve="convex",␣
 ↪direction="increasing")
optimal_eps = distances[knee_locator.elbow]
print(f"Optimal eps for DBSCAN: {optimal_eps:.3f}")

# ---- STEP 6A: APPLY DBSCAN CLUSTERING WITH OPTIMAL EPS ----
dbscan = DBSCAN(eps=optimal_eps, min_samples=k, metric='euclidean')
cluster_labels_dbscan = dbscan.fit_predict(X_umap)
df_clean.loc[:, 'cluster_dbscan'] = cluster_labels_dbscan

# ---- STEP 6B: APPLY K-MEANS & GMM ----
inertia = []
silhouette_scores = []
k_range = range(2, 10)

for k in k_range:
    kmeans = KMeans(n_clusters=k, random_state=42, n_init='auto')
    labels = kmeans.fit_predict(X_umap)
    inertia.append(kmeans.inertia_)
    score = silhouette_score(X_umap, labels)
    silhouette_scores.append(score)

knee_locator = KneeLocator(k_range, inertia, curve="convex",␣
 ↪direction="decreasing")
optimal_k = knee_locator.elbow
print(f"Optimal k for K-Means/GMM: {optimal_k}")
```

```
# Apply K-Means with the optimal k
kmeans = KMeans(n_clusters=optimal_k, random_state=42, n_init='auto')
df_clean.loc[:, 'cluster_kmeans'] = kmeans.fit_predict(X_umap)

# Apply Gaussian Mixture Model (GMM)
gmm = GaussianMixture(n_components=optimal_k, random_state=42)
df_clean.loc[:, 'cluster_gmm'] = gmm.fit_predict(X_umap)

# ---- STEP 7: COMPUTE SILHOUETTE SCORES ----
silhouette_kmeans = silhouette_score(X_umap, df_clean['cluster_kmeans'])
silhouette_gmm = silhouette_score(X_umap, df_clean['cluster_gmm'])
silhouette_dbscan = silhouette_score(X_umap[df_clean['cluster_dbscan'] != -1],
 ␣
 ↪df_clean['cluster_dbscan'][df_clean['cluster_dbscan'] != -1])

print(f"Silhouette Scores - KMeans: {silhouette_kmeans:.3f}, GMM:␣
 ↪{silhouette_gmm:.3f}, DBSCAN: {silhouette_dbscan:.3f}")

# ---- STEP 8: VISUALIZE CLUSTERING METHODS (2D PLOTS) ----
fig, ax = plt.subplots(1, 3, figsize=(18, 5))

# DBSCAN 2D Plot
ax[0].scatter(X_umap[:, 0], X_umap[:, 1], c=cluster_labels_dbscan,␣
 ↪cmap='viridis', alpha=0.6)
ax[0].set_title("DBSCAN Clustering")
ax[0].set_xlabel("UMAP Component 1")
ax[0].set_ylabel("UMAP Component 2")

# K-Means 2D Plot
ax[1].scatter(X_umap[:, 0], X_umap[:, 1], c=df_clean['cluster_kmeans'],␣
 ↪cmap='viridis', alpha=0.6)
ax[1].set_title("K-Means Clustering")
ax[1].set_xlabel("UMAP Component 1")
ax[1].set_ylabel("UMAP Component 2")

# GMM 2D Plot
ax[2].scatter(X_umap[:, 0], X_umap[:, 1], c=df_clean['cluster_gmm'],␣
 ↪cmap='viridis', alpha=0.6)
ax[2].set_title("GMM Clustering")
ax[2].set_xlabel("UMAP Component 1")
ax[2].set_ylabel("UMAP Component 2")

plt.show()
```

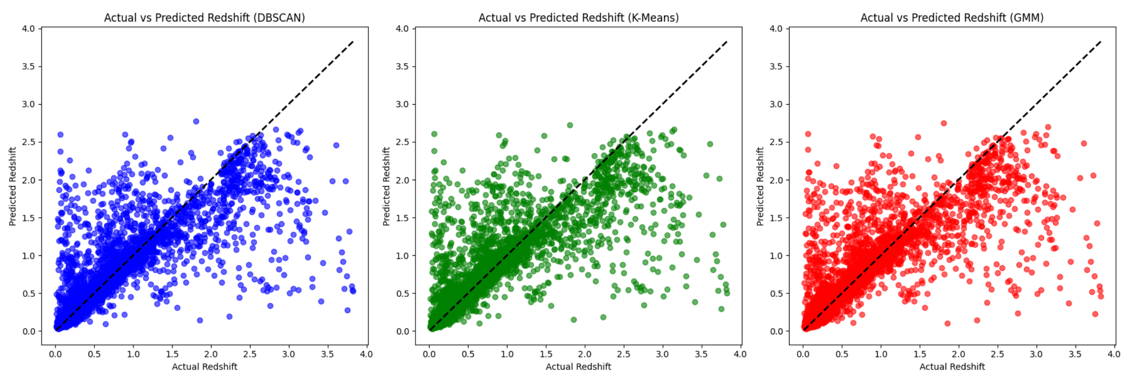
```
Optimal eps for DBSCAN: 0.323
Optimal k for K-Means/GMM: 4
Silhouette Scores - KMeans: 0.486, GMM: 0.455, DBSCAN: -0.422
```



Random Forest

[5]:
```python
# ---- STEP 8: RANDOM FOREST REGRESSION ----
# Train separate Random Forest models for each clustering method using flux features

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[['g_flux', 'r_flux', 'i_flux', 'y_flux', 'z_flux'] +
                [col for col in df_temp.columns if col.startswith(f'clust_{cluster_type}')]]
    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)

    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 9: VISUALIZE REGRESSION RESULTS ----
fig, ax = plt.subplots(1, 3, figsize=(18, 6))
titles = ['DBSCAN', 'K-Means', 'GMM']
colors = ['blue', 'green', 'red']
```

```python
for i, cluster_type in enumerate(results.keys()):
    ax[i].scatter(y_test, results[cluster_type]['y_pred'], alpha=0.6, color=colors[i])
    ax[i].set_xlabel('Actual Redshift')
    ax[i].set_ylabel('Predicted Redshift')
    ax[i].set_title(f'Actual vs Predicted Redshift ({titles[i]})')
    ax[i].plot([y_test.min(), y_test.max()], [y_test.min(), y_test.max()], 'k--', lw=2)

plt.tight_layout()
plt.show()

# ---- STEP 10: COMPARE RESULTS ACROSS CLUSTERING METHODS ----
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}")
```




```
Random Forest Regression Results:
CLUSTER_DBSCAN - MSE: 0.103494, R2: 0.673538
CLUSTER_KMEANS - MSE: 0.103177, R2: 0.674537
CLUSTER_GMM - MSE: 0.103596, R2: 0.673214
```

Checking

[6]:
```python
print(df_clean.head())
print(df_clean.columns)
```

```
         g_flux        r_flux        i_flux        y_flux        z_flux  \
0  7.482335e-09  2.987891e-08  5.117533e-08  8.117985e-08  6.737572e-08
1  1.297347e-09  5.643225e-09  1.319162e-08  2.141019e-08  1.828079e-08
2  3.471398e-09  1.571304e-08  3.743521e-08  6.504857e-08  5.585498e-08
3  4.114510e-08  1.090914e-07  1.841788e-07  3.080686e-07  2.402212e-07
4  3.987357e-09  1.373544e-08  2.634882e-08  4.449762e-08  3.527128e-08
```

```
   specz_redshift           g_r           r_i           i_y           y_z  \
0         0.31652 -2.239657e-08 -2.129643e-08 -3.000452e-08  1.380413e-08
1         0.56769 -4.345878e-09 -7.548391e-09 -8.218576e-09  3.129404e-09
2         0.53428 -1.224164e-08 -2.172218e-08 -2.761336e-08  9.193588e-09
3         0.11878 -6.794635e-08 -7.508739e-08 -1.238898e-07  6.784739e-08
4         0.23497 -9.748082e-09 -1.261338e-08 -1.814880e-08  9.226337e-09

   Cluster  cluster_dbscan  cluster_kmeans  cluster_gmm
0        2               0               3            3
1        1               0               1            1
2        1               0               3            3
3        2               0               2            2
4        1               0               3            3
Index(['g_flux', 'r_flux', 'i_flux', 'y_flux', 'z_flux', 'specz_redshift',
       'g_r', 'r_i', 'i_y', 'y_z', 'Cluster', 'cluster_dbscan',
       'cluster_kmeans', 'cluster_gmm'],
      dtype='object')
```

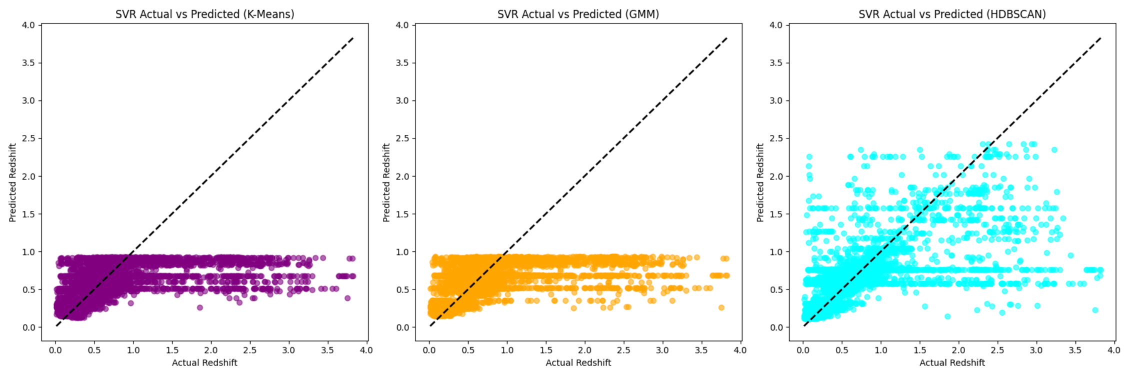
SVR and UMAP

[7]:
```python
# Add-Ons for Photometric Redshift Estimation
# Fixing UMAP Import Issue and Enhancing Preprocessing

# ---- STEP 11: Install and Import UMAP Properly ----
# Ensure proper UMAP installation: pip install umap-learn
from umap import UMAP

umap = UMAP(n_neighbors=15, min_dist=0.1, n_components=2, random_state=42)
X_umap = umap.fit_transform(df_transformed)

# ---- STEP 12: Add More Color Indices (Using Flux Values) ----
df_clean['u_g'] = df_clean['g_flux'] - df_clean['r_flux']
df_clean['g_r'] = df_clean['r_flux'] - df_clean['i_flux']
df_clean['r_i'] = df_clean['i_flux'] - df_clean['y_flux']
df_clean['i_z'] = df_clean['y_flux'] - df_clean['z_flux']

# ---- STEP 13: Additional Clustering (HDBSCAN) for SVR Comparison ----
try:
    from hdbscan import HDBSCAN
except ImportError:
    print("HDBSCAN not installed. Use: pip install hdbscan")
    raise

hdbscan = HDBSCAN(min_cluster_size=8)
df_clean['cluster_hdbscan'] = hdbscan.fit_predict(X_umap)

# ---- STEP 14: SVR Regression for Redshift Estimation ----
from sklearn.svm import SVR
```

```python
svr_results = {}

for cluster_type in ['cluster_kmeans', 'cluster_gmm', 'cluster_hdbscan']:
    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)

    svr = SVR(kernel='rbf', C=1.0, epsilon=0.1)
    svr.fit(X_train, y_train)
    y_pred = svr.predict(X_test)

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

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

# ---- STEP 15: Plot SVR Results ----
fig, ax = plt.subplots(1, 3, figsize=(18, 6))
titles = ['K-Means', 'GMM', 'HDBSCAN']
colors = ['purple', 'orange', 'cyan']

for i, cluster_type in enumerate(svr_results.keys()):
    ax[i].scatter(y_test, svr_results[cluster_type]['y_pred'], alpha=0.6,␣
 ↪color=colors[i])
    ax[i].set_title(f'SVR Actual vs Predicted ({titles[i]})')
    ax[i].set_xlabel('Actual Redshift')
    ax[i].set_ylabel('Predicted Redshift')
    ax[i].plot([y_test.min(), y_test.max()], [y_test.min(), y_test.max()],␣
 ↪'k--', lw=2)

plt.tight_layout()
plt.show()

# ---- Print SVR Performance Metrics ----
print('SVR Regression Results:')
for cluster_type, metrics in svr_results.items():
    print(f"{cluster_type.upper()} - MSE: {metrics['MSE']:.6f}, R2:␣
 ↪{metrics['R2']:.6f}")
```

```
/home/chloy/miniconda3/lib/python3.10/site-
packages/sklearn/utils/deprecation.py:151: FutureWarning: 'force_all_finite' was
renamed to 'ensure_all_finite' in 1.6 and will be removed in 1.8.
  warnings.warn(
```

```
/home/chloy/miniconda3/lib/python3.10/site-packages/umap/umap_.py:1952:
UserWarning: n_jobs value 1 overridden to 1 by setting random_state. Use no seed
for parallelism.
  warn(
/home/chloy/miniconda3/lib/python3.10/site-
packages/sklearn/utils/deprecation.py:151: FutureWarning: 'force_all_finite' was
renamed to 'ensure_all_finite' in 1.6 and will be removed in 1.8.
  warnings.warn(
/home/chloy/miniconda3/lib/python3.10/site-
packages/sklearn/utils/deprecation.py:151: FutureWarning: 'force_all_finite' was
renamed to 'ensure_all_finite' in 1.6 and will be removed in 1.8.
  warnings.warn(
```




```
SVR Regression Results:
CLUSTER_KMEANS - MSE: 0.227899, R2: 0.281111
CLUSTER_GMM - MSE: 0.226127, R2: 0.286701
CLUSTER_HDBSCAN - MSE: 0.167378, R2: 0.472019
```

XGBoost , Gradient boosting and MLP NN

[8]:
```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
from sklearn.model_selection import train_test_split
from sklearn.metrics import mean_squared_error, r2_score
from sklearn.ensemble import GradientBoostingRegressor
from xgboost import XGBRegressor
from sklearn.neural_network import MLPRegressor
import faiss  # Faster nearest neighbor search

# ---- STEP 1: ADD MORE COLOR INDICES ----
# Verify flux columns exist before calculating new features
if all(col in df_clean.columns for col in ['g_flux', 'r_flux', 'i_flux',␣
↪'y_flux', 'z_flux']):
    df_clean['g_i'] = df_clean['g_flux'] - df_clean['i_flux']
```

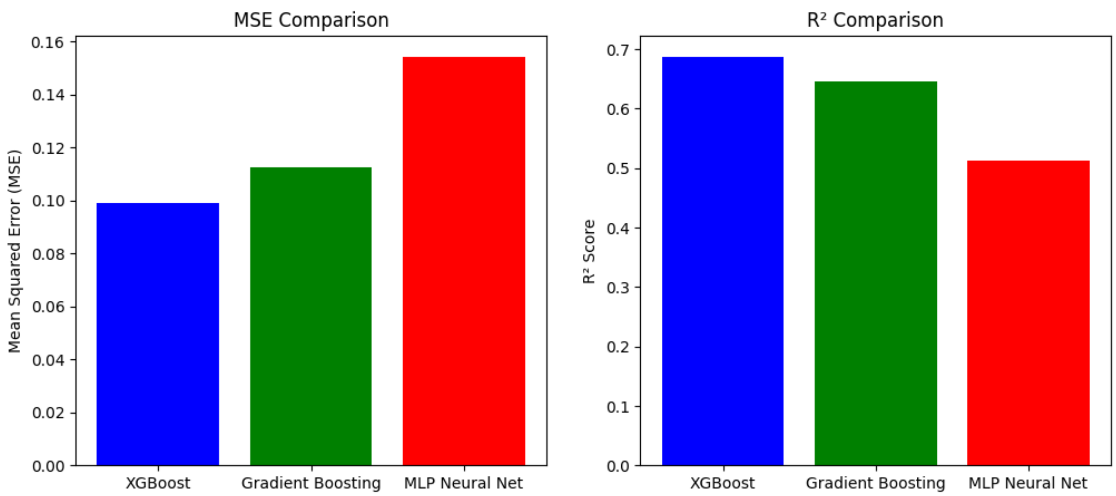
```python
    df_clean['r_z'] = df_clean['r_flux'] - df_clean['z_flux']
    df_clean['i_y_z'] = df_clean['i_flux'] - df_clean['y_flux'] -␣
 ↪df_clean['z_flux']
else:
    raise ValueError("Missing required flux columns in df_clean.")

# ---- STEP 2: DEFINE FEATURES & TARGET ----
features = ['g_flux', 'r_flux', 'i_flux', 'y_flux', 'z_flux',
            'g_r', 'r_i', 'i_y', 'y_z', 'g_i', 'r_z', 'i_y_z']

# Include cluster one-hot encoding for different clustering techniques
if 'cluster_kmeans' in df_clean.columns and 'cluster_gmm' in df_clean.columns␣
 ↪and 'cluster_hdbscan' in df_clean.columns:
    df_encoded = pd.get_dummies(df_clean, columns=['cluster_kmeans',␣
 ↪'cluster_gmm', 'cluster_hdbscan'],
                                prefix=['clust_kmeans', 'clust_gmm',␣
 ↪'clust_hdbscan'])
else:
    raise ValueError("Cluster columns are missing in df_clean.")

X = df_encoded[features + [col for col in df_encoded.columns if col.
 ↪startswith('clust_')]]
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)

# ---- STEP 3: APPLY XGBOOST ----
xgb = XGBRegressor(n_estimators=200, learning_rate=0.1, random_state=42)
xgb.fit(X_train, y_train)
y_pred_xgb = xgb.predict(X_test)

mse_xgb = mean_squared_error(y_test, y_pred_xgb)
r2_xgb = r2_score(y_test, y_pred_xgb)

print(f"XGBoost - MSE: {mse_xgb:.6f}, R2: {r2_xgb:.6f}")

# ---- STEP 4: APPLY GRADIENT BOOSTING ----
gbr = GradientBoostingRegressor(n_estimators=150, learning_rate=0.05,␣
 ↪random_state=42)
gbr.fit(X_train, y_train)
y_pred_gbr = gbr.predict(X_test)

mse_gbr = mean_squared_error(y_test, y_pred_gbr)
r2_gbr = r2_score(y_test, y_pred_gbr)
```

```python
print(f"Gradient Boosting - MSE: {mse_gbr:.6f}, R2: {r2_gbr:.6f}")

# ---- STEP 5: TRY MLP NEURAL NETWORK ----
mlp = MLPRegressor(hidden_layer_sizes=(64, 32), max_iter=500, random_state=42)
mlp.fit(X_train, y_train)
y_pred_mlp = mlp.predict(X_test)

mse_mlp = mean_squared_error(y_test, y_pred_mlp)
r2_mlp = r2_score(y_test, y_pred_mlp)

print(f"MLP Neural Net - MSE: {mse_mlp:.6f}, R2: {r2_mlp:.6f}")

# ---- STEP 6: OPTIONAL - FASTER NEAREST NEIGHBOR SEARCH FOR DBSCAN ----
index = faiss.IndexFlatL2(X_train.shape[1])  # L2 distance (Euclidean)
index.add(X_train.astype('float32'))  # FAISS requires float32
_, indices = index.search(X_train.astype('float32'), k=5)  # Find 5 nearest␣
↪neighbors
```

```
XGBoost - MSE: 0.099036, R2: 0.687598
Gradient Boosting - MSE: 0.112597, R2: 0.644823
MLP Neural Net - MSE: 0.154431, R2: 0.512862
```

[9]:

```python
# ---- PLOT COMPARISON ----
models = ['XGBoost', 'Gradient Boosting', 'MLP Neural Net']
mse_scores = [mse_xgb, mse_gbr, mse_mlp]
r2_scores = [r2_xgb, r2_gbr, r2_mlp]

fig, ax = plt.subplots(1, 2, figsize=(12, 5))

# MSE Plot
ax[0].bar(models, mse_scores, color=['blue', 'green', 'red'])
ax[0].set_ylabel("Mean Squared Error (MSE)")
ax[0].set_title("MSE Comparison")

# R2 Score Plot
ax[1].bar(models, r2_scores, color=['blue', 'green', 'red'])
ax[1].set_ylabel("R² Score")
ax[1].set_title("R² Comparison")

plt.show()
```



Fine Tuning XGBoost Hyper-Parameters

[10]:
```
from xgboost import XGBRegressor
from sklearn.model_selection import GridSearchCV

# ---- XGBOOST HYPERPARAMETER TUNING ----
xgb_params = {
    'n_estimators': [200, 300, 500],  # More trees → better accuracy, but slower
    'learning_rate': [0.01, 0.05, 0.1],  # Lower = slower but more stable
    'max_depth': [5, 7, 9],  # Deeper trees can learn more but risk overfitting
    'subsample': [0.8, 1.0],  # Prevents overfitting by using a fraction of␣
 ↪data per tree
    'colsample_bytree': [0.8, 1.0]  # Randomly selects features per tree to␣
 ↪prevent overfitting
}

xgb = XGBRegressor(random_state=42)
xgb_grid = GridSearchCV(xgb, xgb_params, cv=3, scoring='r2', verbose=2,␣
 ↪n_jobs=-1)
xgb_grid.fit(X_train, y_train)

# Best model
best_xgb = xgb_grid.best_estimator_
y_pred_xgb = best_xgb.predict(X_test)

# Evaluate
mse_xgb = mean_squared_error(y_test, y_pred_xgb)
r2_xgb = r2_score(y_test, y_pred_xgb)

print(f"Tuned XGBoost - Best Params: {xgb_grid.best_params_}")
```

```python
print(f"Tuned XGBoost - MSE: {mse_xgb:.6f}, R2: {r2_xgb:.6f}")
```

```
Fitting 3 folds for each of 108 candidates, totalling 324 fits
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=5,
n_estimators=200, subsample=0.8; total time=  19.7s
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=5,
n_estimators=200, subsample=0.8; total time=  19.9s
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=5,
n_estimators=200, subsample=0.8; total time=  20.1s
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=5,
n_estimators=200, subsample=1.0; total time=  20.0s
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=5,
n_estimators=200, subsample=1.0; total time=  20.3s
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=5,
n_estimators=200, subsample=1.0; total time=  21.1s
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=5,
n_estimators=300, subsample=0.8; total time=  27.2s
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=5,
n_estimators=300, subsample=1.0; total time=  27.0s
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=5,
n_estimators=300, subsample=0.8; total time=  27.8s
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=5,
n_estimators=300, subsample=1.0; total time=  27.9s
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=5,
n_estimators=300, subsample=0.8; total time=  28.3s
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=5,
n_estimators=300, subsample=1.0; total time=  28.4s
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=7,
n_estimators=200, subsample=0.8; total time=  24.8s
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=7,
n_estimators=200, subsample=1.0; total time=  25.3s
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=7,
n_estimators=200, subsample=0.8; total time=  25.6s
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=7,
n_estimators=200, subsample=1.0; total time=  25.6s
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=7,
n_estimators=200, subsample=1.0; total time=  26.4s
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=7,
n_estimators=200, subsample=0.8; total time=  29.1s
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=5,
n_estimators=500, subsample=1.0; total time=  37.7s
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=5,
n_estimators=500, subsample=0.8; total time=  38.7s
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=5,
n_estimators=500, subsample=0.8; total time=  38.6s
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=5,
n_estimators=500, subsample=0.8; total time=  39.2s
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=5,
```

```
n_estimators=500, subsample=1.0; total time=  38.8s
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=5,
n_estimators=500, subsample=1.0; total time=  40.4s
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=7,
n_estimators=300, subsample=0.8; total time=  35.3s
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=7,
n_estimators=300, subsample=0.8; total time=  35.6s
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=7,
n_estimators=300, subsample=0.8; total time=  36.2s
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=7,
n_estimators=300, subsample=1.0; total time=  36.8s
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=7,
n_estimators=300, subsample=1.0; total time=  37.8s
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=7,
n_estimators=300, subsample=1.0; total time=  36.7s
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=7,
n_estimators=500, subsample=0.8; total time=  49.8s
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=7,
n_estimators=500, subsample=0.8; total time=  49.8s
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=7,
n_estimators=500, subsample=1.0; total time=  50.2s
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=7,
n_estimators=500, subsample=0.8; total time=  51.2s
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=7,
n_estimators=500, subsample=1.0; total time=  50.6s
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=7,
n_estimators=500, subsample=1.0; total time=  51.6s
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=9,
n_estimators=200, subsample=0.8; total time=  33.4s
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=9,
n_estimators=200, subsample=0.8; total time=  33.6s
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=9,
n_estimators=200, subsample=0.8; total time=  33.4s
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=9,
n_estimators=200, subsample=1.0; total time=  34.6s
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=9,
n_estimators=200, subsample=1.0; total time=  35.0s
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=9,
n_estimators=200, subsample=1.0; total time=  34.3s
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=9,
n_estimators=300, subsample=0.8; total time=  47.3s
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=9,
n_estimators=300, subsample=0.8; total time=  48.0s
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=9,
n_estimators=300, subsample=0.8; total time=  47.4s
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=9,
n_estimators=300, subsample=1.0; total time=  49.3s
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=9,
```

```
n_estimators=300, subsample=1.0; total time=  48.1s
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=9,
n_estimators=300, subsample=1.0; total time=  48.6s
[CV] END colsample_bytree=0.8, learning_rate=0.05, max_depth=5,
n_estimators=200, subsample=0.8; total time=  15.7s
[CV] END colsample_bytree=0.8, learning_rate=0.05, max_depth=5,
n_estimators=200, subsample=0.8; total time=  15.8s
[CV] END colsample_bytree=0.8, learning_rate=0.05, max_depth=5,
n_estimators=200, subsample=0.8; total time=  15.8s
[CV] END colsample_bytree=0.8, learning_rate=0.05, max_depth=5,
n_estimators=200, subsample=1.0; total time=  15.4s
[CV] END colsample_bytree=0.8, learning_rate=0.05, max_depth=5,
n_estimators=200, subsample=1.0; total time=  15.9s
[CV] END colsample_bytree=0.8, learning_rate=0.05, max_depth=5,
n_estimators=200, subsample=1.0; total time=  15.3s
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=9,
n_estimators=500, subsample=0.8; total time= 1.1min
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=9,
n_estimators=500, subsample=0.8; total time= 1.1min
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=9,
n_estimators=500, subsample=0.8; total time= 1.1min
[CV] END colsample_bytree=0.8, learning_rate=0.05, max_depth=5,
n_estimators=300, subsample=0.8; total time=  20.6s
[CV] END colsample_bytree=0.8, learning_rate=0.05, max_depth=5,
n_estimators=300, subsample=0.8; total time=  20.2s
[CV] END colsample_bytree=0.8, learning_rate=0.05, max_depth=5,
n_estimators=300, subsample=0.8; total time=  20.4s
[CV] END colsample_bytree=0.8, learning_rate=0.05, max_depth=5,
n_estimators=300, subsample=1.0; total time=  20.9s
[CV] END colsample_bytree=0.8, learning_rate=0.05, max_depth=5,
n_estimators=300, subsample=1.0; total time=  21.1s
[CV] END colsample_bytree=0.8, learning_rate=0.05, max_depth=5,
n_estimators=300, subsample=1.0; total time=  20.8s
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=9,
n_estimators=500, subsample=1.0; total time= 1.2min
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=9,
n_estimators=500, subsample=1.0; total time= 1.2min
[CV] END colsample_bytree=0.8, learning_rate=0.01, max_depth=9,
n_estimators=500, subsample=1.0; total time= 1.2min
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[CV] END colsample_bytree=0.8, learning_rate=0.05, max_depth=7,
```

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n_estimators=200, subsample=1.0; total time=  18.5s
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n_estimators=500, subsample=0.8; total time=  31.1s
[CV] END colsample_bytree=0.8, learning_rate=0.05, max_depth=5,
n_estimators=500, subsample=0.8; total time=  31.4s
[CV] END colsample_bytree=0.8, learning_rate=0.05, max_depth=5,
n_estimators=500, subsample=1.0; total time=  30.3s
[CV] END colsample_bytree=0.8, learning_rate=0.05, max_depth=5,
n_estimators=500, subsample=0.8; total time=  32.2s
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n_estimators=500, subsample=1.0; total time=  31.6s
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n_estimators=300, subsample=0.8; total time=  23.6s
[CV] END colsample_bytree=0.8, learning_rate=0.05, max_depth=7,
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n_estimators=300, subsample=1.0; total time=  26.1s
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n_estimators=500, subsample=0.8; total time=  37.7s
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n_estimators=500, subsample=0.8; total time=  41.8s
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n_estimators=200, subsample=0.8; total time=  23.0s
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n_estimators=200, subsample=1.0; total time=  23.1s
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n_estimators=200, subsample=1.0; total time=  22.5s
[CV] END colsample_bytree=0.8, learning_rate=0.05, max_depth=9,
```

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n_estimators=200, subsample=1.0; total time=  23.7s
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n_estimators=300, subsample=0.8; total time=  28.7s
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n_estimators=300, subsample=0.8; total time=  29.1s
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n_estimators=300, subsample=1.0; total time=  29.9s
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n_estimators=300, subsample=1.0; total time=  29.7s
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n_estimators=500, subsample=1.0; total time=  41.1s
[CV] END colsample_bytree=0.8, learning_rate=0.05, max_depth=9,
n_estimators=500, subsample=0.8; total time=  42.7s
[CV] END colsample_bytree=0.8, learning_rate=0.1, max_depth=5, n_estimators=200,
subsample=1.0; total time=  14.9s
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n_estimators=500, subsample=0.8; total time=  42.8s
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n_estimators=500, subsample=1.0; total time=  42.1s
[CV] END colsample_bytree=0.8, learning_rate=0.05, max_depth=9,
n_estimators=500, subsample=1.0; total time=  42.4s
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subsample=0.8; total time=  20.0s
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subsample=0.8; total time=  19.8s
[CV] END colsample_bytree=0.8, learning_rate=0.1, max_depth=5, n_estimators=300,
subsample=1.0; total time=  19.8s
[CV] END colsample_bytree=0.8, learning_rate=0.1, max_depth=5, n_estimators=300,
```

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subsample=0.8; total time=  16.7s
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subsample=0.8; total time=  31.4s
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subsample=0.8; total time=  31.9s
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subsample=0.8; total time=  16.3s
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subsample=0.8; total time=  23.1s
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subsample=0.8; total time=  36.3s
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```

```
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subsample=0.8; total time=  18.8s
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subsample=0.8; total time=  19.1s
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```

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n_estimators=500, subsample=0.8; total time=  42.4s
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n_estimators=500, subsample=0.8; total time=  43.0s
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n_estimators=200, subsample=0.8; total time=  28.1s
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n_estimators=200, subsample=1.0; total time=  27.9s
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n_estimators=200, subsample=1.0; total time=  28.7s
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n_estimators=200, subsample=1.0; total time=  29.1s
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```

```
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```

```
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n_estimators=500, subsample=0.8; total time= 1.2min
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n_estimators=500, subsample=0.8; total time= 1.2min
[CV] END colsample_bytree=1.0, learning_rate=0.05, max_depth=5,
n_estimators=300, subsample=0.8; total time=  21.5s
[CV] END colsample_bytree=1.0, learning_rate=0.01, max_depth=9,
n_estimators=500, subsample=1.0; total time= 1.3min
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[CV] END colsample_bytree=1.0, learning_rate=0.05, max_depth=5,
n_estimators=300, subsample=0.8; total time=  21.5s
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n_estimators=200, subsample=1.0; total time=  19.2s
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```

```
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n_estimators=300, subsample=1.0; total time=  26.3s
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```

```
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subsample=1.0; total time=  20.6s
[CV] END colsample_bytree=1.0, learning_rate=0.1, max_depth=5, n_estimators=300,
subsample=1.0; total time=  20.7s
[CV] END colsample_bytree=1.0, learning_rate=0.1, max_depth=5, n_estimators=300,
subsample=1.0; total time=  21.1s
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subsample=0.8; total time=  32.3s
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```

```
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[CV] END colsample_bytree=1.0, learning_rate=0.1, max_depth=7, n_estimators=300,
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subsample=1.0; total time=  36.7s
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subsample=0.8; total time=  20.3s
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subsample=1.0; total time=  19.8s
[CV] END colsample_bytree=1.0, learning_rate=0.1, max_depth=9, n_estimators=200,
```

```
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[CV] END colsample_bytree=1.0, learning_rate=0.1, max_depth=9, n_estimators=200,
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subsample=0.8; total time=  26.4s
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subsample=0.8; total time=  31.8s
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subsample=0.8; total time=  33.4s
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subsample=0.8; total time=  31.6s
[CV] END colsample_bytree=1.0, learning_rate=0.1, max_depth=9, n_estimators=500,
subsample=1.0; total time=  30.8s
[CV] END colsample_bytree=1.0, learning_rate=0.1, max_depth=9, n_estimators=500,
subsample=1.0; total time=  30.1s
Tuned XGBoost - Best Params: {'colsample_bytree': 0.8, 'learning_rate': 0.01,
'max_depth': 9, 'n_estimators': 500, 'subsample': 0.8}
Tuned XGBoost - MSE: 0.093542, R2: 0.704931
```
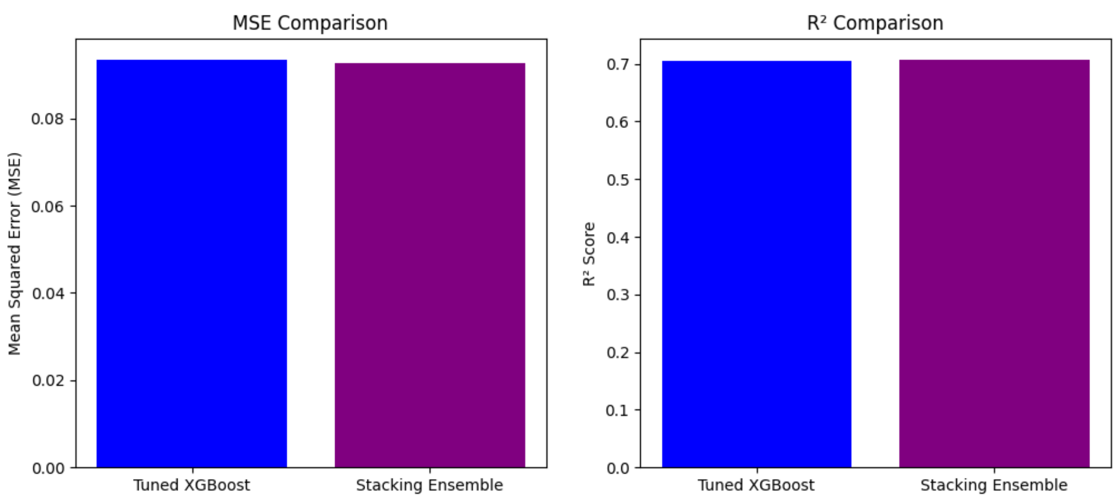

Emsemble (XGBoost + RF)

[11]:
```python
from sklearn.ensemble import StackingRegressor, RandomForestRegressor,␣
 ↪GradientBoostingRegressor
from sklearn.linear_model import Ridge  # Final meta-learner

# Define base models
base_models = [
    ('xgb', best_xgb),  # Best tuned XGBoost
    ('rf', RandomForestRegressor(n_estimators=200, random_state=42)),
    ('gbr', GradientBoostingRegressor(n_estimators=150, learning_rate=0.05,␣
 ↪random_state=42))
]

# Stacking Ensemble
stacking_model = StackingRegressor(estimators=base_models,␣
 ↪final_estimator=Ridge())
```

```python
# Train Stacking Model
stacking_model.fit(X_train, y_train)
y_pred_stack = stacking_model.predict(X_test)

# Evaluate
mse_stack = mean_squared_error(y_test, y_pred_stack)
r2_stack = r2_score(y_test, y_pred_stack)

print(f"Stacking Ensemble - MSE: {mse_stack:.6f}, R2: {r2_stack:.6f}")


# ---- PLOT COMPARISON ----
models = ['Tuned XGBoost', 'Stacking Ensemble']
mse_scores = [mse_xgb, mse_stack]
r2_scores = [r2_xgb, r2_stack]

fig, ax = plt.subplots(1, 2, figsize=(12, 5))

# MSE Plot
ax[0].bar(models, mse_scores, color=['blue', 'purple'])
ax[0].set_ylabel("Mean Squared Error (MSE)")
ax[0].set_title("MSE Comparison")

# R2 Score Plot
ax[1].bar(models, r2_scores, color=['blue', 'purple'])
ax[1].set_ylabel("R² Score")
ax[1].set_title("R² Comparison")

plt.show()
```

```
Stacking Ensemble - MSE: 0.092646, R2: 0.707756
```



Graph Based learning

[12]:
```
import networkx as nx
from sklearn.kernel_ridge import KernelRidge
from sklearn.neighbors import kneighbors_graph
from sklearn.metrics import mean_squared_error, r2_score

# ---- CREATE A KNN GRAPH ----
knn_graph = kneighbors_graph(X_train, n_neighbors=5, mode='connectivity',␣
↪include_self=False)

# Convert to NetworkX Graph
G = nx.from_scipy_sparse_array(knn_graph)

# Visualize Graph Structure
nx.draw(G, node_size=10)

# ---- GRAPH-BASED REDSHIFT ESTIMATION ----
kr = KernelRidge(alpha=1.0, kernel='rbf')  # RBF kernel smooths over the graph
kr.fit(X_train, y_train)  # Train using photometric data

y_pred_graph = kr.predict(X_test)  # Predict redshift

# Evaluate Performance
mse_graph = mean_squared_error(y_test, y_pred_graph)
r2_graph = r2_score(y_test, y_pred_graph)

print(f"Graph-Based Kernel Ridge Regression - MSE: {mse_graph:.6f}, R2:␣
↪{r2_graph:.6f}")
```

```
Graph-Based Kernel Ridge Regression - MSE: 0.200561, R2: 0.367346
```

Hybrid Graph based and XG Boost

[13]:
```
# ---- USE GRAPH-BASED REDSHIFT AS A FEATURE ----
df_clean['graph_pred_redshift'] = kr.predict(X)  #  FIXED: Use Kernel Ridge␣
↪Regression Predictions

# Retrain XGBoost with Graph-Enhanced Features
X_new = df_clean.drop(columns=['specz_redshift'])  # Keep everything except␣
↪actual redshift
y_new = df_clean['specz_redshift']

X_train_new, X_test_new, y_train_new, y_test_new = train_test_split(X_new,␣
↪y_new, test_size=0.2, random_state=42)

xgb = XGBRegressor(n_estimators=300, learning_rate=0.05, max_depth=7,␣
↪random_state=42)
xgb.fit(X_train_new, y_train_new)

y_pred_xgb_new = xgb.predict(X_test_new)
```

```
mse_xgb_new = mean_squared_error(y_test_new, y_pred_xgb_new)
r2_xgb_new = r2_score(y_test_new, y_pred_xgb_new)

print(f"Hybrid Graph + XGBoost Model - MSE: {mse_xgb_new:.6f}, R2: {r2_xgb_new:.
 ↪6f}")

# ---- PLOT COMPARISON ----
models = ['Stacking Ensemble', 'Graph-Based Model', 'Hybrid Graph + XGBoost']
mse_scores = [mse_stack, mse_graph, mse_xgb_new]
r2_scores = [r2_stack, r2_graph, r2_xgb_new]

fig, ax = plt.subplots(1, 2, figsize=(12, 5))

# MSE Plot
ax[0].bar(models, mse_scores, color=['purple', 'orange', 'blue'])
ax[0].set_ylabel("Mean Squared Error (MSE)")
ax[0].set_title("MSE Comparison")

# R2 Score Plot
ax[1].bar(models, r2_scores, color=['purple', 'orange', 'blue'])
ax[1].set_ylabel("R² Score")
ax[1].set_title("R² Comparison")

plt.show()
```

```
Hybrid Graph + XGBoost Model - MSE: 0.095564, R2: 0.698550
```