

3D_SPHERE_CUBE Dataset k=20

```
clc  
clear
```

Load the file

```
sp_cube_mat = load('3d_sphere_cube.mat');  
  
% Display the structure of the file  
disp(sp_cube_mat);
```

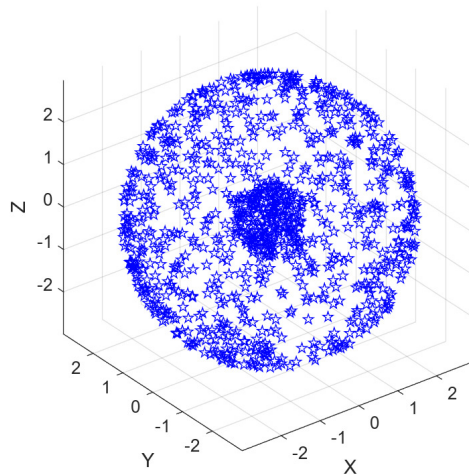
```
X: [1200x3 double]
```

```
% Extract the matrix of points  
X = sp_cube_mat.X;
```

Plot the points

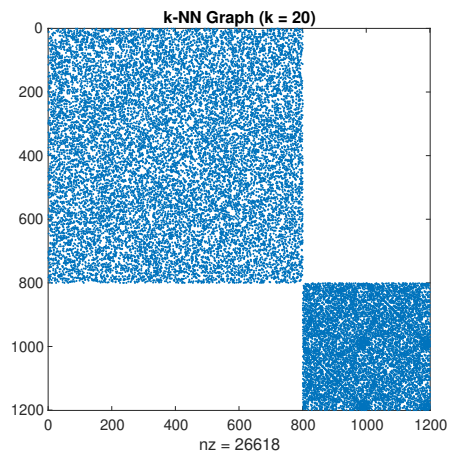
```
figure;  
scatter3(X(:,1), X(:,2), X(:,3), 'b','p');  
xlabel('X');  
ylabel('Y');  
zlabel('Z');  
title('Plot of the points in the 3d\_sphere\_cube.mat dataset');  
grid on;  
axis equal;
```

Plot of the points in the 3d_sphere_cube.mat dataset

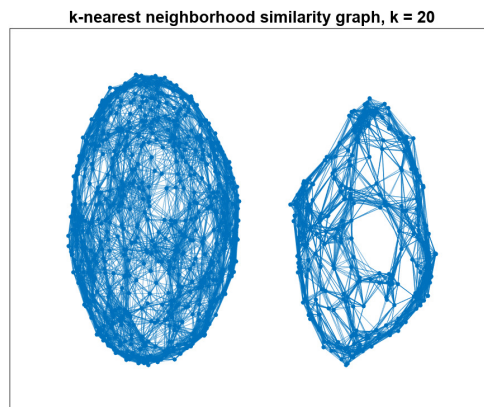


1. Similarity matrix and adjacency matrix

```
k_values = [10, 20, 40];  
k = 20;  
  
% Construct the k-nearest neighborhood similarity graph and its adjacency  
% matrix W  
W = knn_graph(X, k);  
  
% Visualize the graph using its similarity matrix  
figure;  
spy(W);  
title(['k-NN Graph (k = ', num2str(k), ')']);
```



```
% Store W as a sparse matrix  
W = sparse(W);  
% Visualize the graph G corresponding to the adjacency matrix W  
G = graph(W);  
figure;  
plot(G);  
title(['k-nearest neighborhood similarity graph, k = ', num2str(k)]);
```



2. Construct the degree matrix D and the Laplacian matrix L

```
N = size(W, 1);

% Initialize the degree matrix D
D = zeros(N, N);

% The degree of each point is given by the sum of the elements of each row in W
D = diag(sum(W, 2));

% Save D in a sparse format
D = sparse(D);

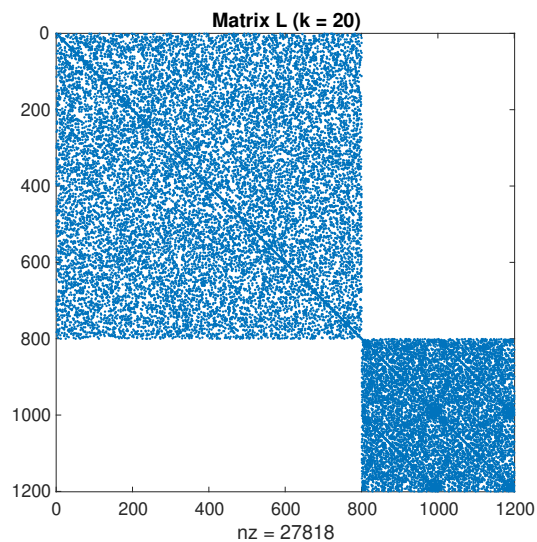
% Compute the Laplacian matrix L
L = D - W;

% Compute the normalized Laplacian matrix L(sym)
D_inv_sqrt = diag(1 ./ sqrt(diag(D)));
L = D_inv_sqrt * L * D_inv_sqrt;

L = sparse(L);
if issparse(L) % issparse(L)==1 means that L is stored in a sparse format
    disp("The matrix L is stored in a sparse format")
end
```

The matrix L is stored in a sparse format

```
% Plot the Laplacian matrix L
figure;
spy(L);
title(['Matrix L (k = ', num2str(k), ')']);
```



3. Compute the number of connected components of the similarity graph

```
% The points with the same number belong to the same connected component
bins = conncomp(G);

% Number of connected components
num_components = max(bins);

% Display the result
disp(['Number of connected components: ', num2str(num_components)]);
```

Number of connected components: 2

4 - 5. Compute eigenvalues and eigenvectors

```
% Set a number M of values to be computed (later it will be changed)
M = 5;

% Initialize the eigenvalues vector and the eigenvectors matrix
eigvalues = zeros(M, 1);
eigvects = zeros(N, M);

% Choose the vector v that will be used for the inverse power method
v = 0.5 * ones(N, 1);
v(1:2:N) = -0.5;

% Max iterations in the power method
maxIter = 1000;
% Relative tolerance
relTol = 1e-10;

% A known fact from theory is that L is semi pos def and has at least one
% eigenvalue = 0 and that the vector of all ones is a corresponding
% eigvalues(1) = 0;
% eigvects(:, 1) = ones(N,1)/ norm(ones(N,1));

% Or use the inverse power method to compute them (if L_sym, use this)
[eigvalues(1), eigvects(:, 1)] = invpower_method(L, v(1:end), maxIter, relTol);
% Compute the remaining eigenvectors and eigenvalues
[eigvalues, eigvects, residualnorms] =
    deflation_method(L, v, eigvects, eigvalues, M, maxIter, relTol);
```

Warning: Matrix is close to singular or badly scaled. Results may be inaccurate.
RCOND = 1.165223e-16.

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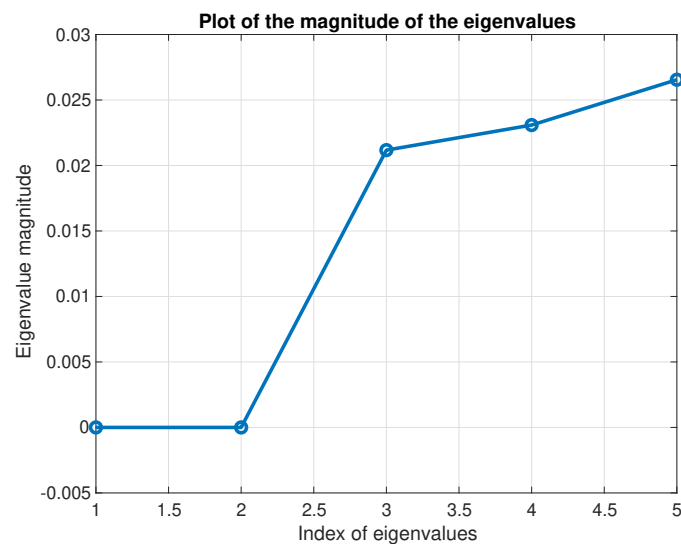
Warning: Matrix is close to singular or badly scaled. Results may be inaccurate.
RCOND = 1.165223e-16.

```
% Check how good the approximation is by comparing with eigs function of
% Matlab
[mat_eigvects, mat_eigs] = eigs(L, M, 'smallestabs');
norm(eigvalues - diag(mat_eigs))
```

```
ans = 1.1243e-11
```

Now, find the actual number M of eigenvalues that will be used for the clustering algorithm

```
% Plot the computed eigenvalues
x = 1:M;
figure;
plot(x, eigvalues, '-o', 'LineWidth', 2);
xlabel('Index of eigenvalues');
ylabel('Eigenvalue magnitude');
title('Plot of the magnitude of the eigenvalues');
grid on;
```



The suitable number of eigenvalues is either 2 since eig3 is much larger than eig2 for $k=20$

```
M = 2;

% Define the matrix U that will be used for the spectral clustering
U = eigvects(:, 1:M);
```

6 - 7 - 8. Spectral clustering, k means

```
% Clusterize using k means and obtain the indices (and the centroids)
% inside the clusters of each point
[idx, C] = kmeans(U, M);
```

```

% Assing the original data to the corresponding clusters
A = cell(M, 1);

for i = 1:N
    % Find the cluster of y_i
    cluster_idx = idx(i);

    % Assing it to x_i
    A{cluster_idx} = [A{cluster_idx}; X(i, :)];
end

% Plot of the clusterized data in the original space
X_spect_clust = zeros(N, 4);
X_spect_clust(:, 1: 3) = X;
X_spect_clust(:, 4) = idx;

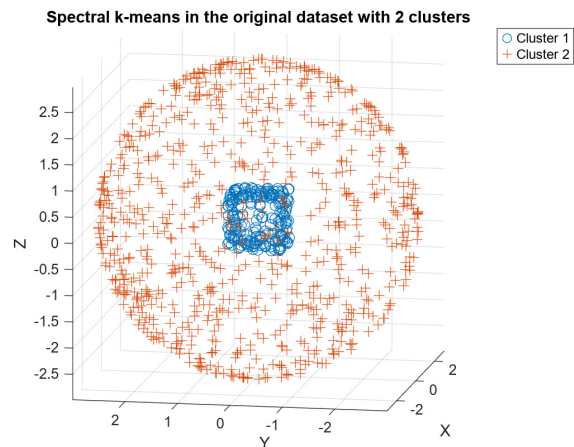
markers = ['o', '+', 's'];
figure;

for k = 1:M
    cluster_points = X_spect_clust(X_spect_clust(:, 4) == k, :);

    scatter3(cluster_points(:,1), cluster_points(:,2), cluster_points(:,3), ...
        50, 'Marker', markers(k), 'DisplayName', ['Cluster ' num2str(k)]);
    hold on
end

title(['Spectral k-means in the original dataset with ', num2str(M), ' clusters']);
xlabel('X');
ylabel('Y');
zlabel('Z');
legend show;
grid on;
axis equal;

```



9.a K MEANS TO THE ORIGINAL DATA

```
k_value = 2;

% Clusterize the original data
[idx_k, C_k] = kmeans(X, k_value);

% Add the index to X_kmeans
X_kmeans = zeros(N, 4);
X_kmeans(:, 1: 3) = X;
X_kmeans(:, 4) = idx_k;

markers = ['o', '+', 's'];
figure;

for k = 1:M
    cluster_points_k = X_kmeans(X_kmeans(:, 4) == k, :);
    scatter3(cluster_points_k(:,1), cluster_points_k(:,2), cluster_points_k(:,3), ...
        50, 'Marker', markers(k), 'DisplayName', ['Cluster ' num2str(k)]);
    hold on
end

title(['K means in the original dataset with ', num2str(M), ' clusters']);
xlabel('X');
ylabel('Y');
zlabel('Z');
legend show;
grid on;
```



9.b DBSCAN TO THE ORIGINAL DATA

Apply the DBSCAN algorithm

```
% Neighborhood radius
epsilon = 0.6;
```

```

% Minimum points for a cluster
minPts = 6;

idx_d = dbscan(X, epsilon, minPts);

X_dbscan = zeros(N, 4);
X_dbscan(:, 1: 3) = X;
X_dbscan(:, 4) = idx_d;

% Only the different clusters (-1 are put together as outliers)
cluster_ids = unique(X_dbscan(:, 4));

figure;
colors = hsv(length(cluster_ids));
for k_idx = 1:length(cluster_ids)
    k = cluster_ids(k_idx);
    cluster_points_d = X_dbscan(X_dbscan(:, 4) == k, :);
    scatter3(cluster_points_d(:, 1), cluster_points_d(:, 2), cluster_points_d(:, 3), ...
        50, colors(k_idx, :), '*');
    hold on
end

title('DBSCAN in the original dataset');
xlabel('X');
ylabel('Y');
zlabel('Z');
legend show; grid on;

```

