

CODES FOR FINAL ASSIGNMENT

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IRIS DATASET

Listing 1: Matlab Code.

```
1 % Load the data
2 load('IrisDataAnnotated.mat');
3
4 % Set random number generator for reproducibility
5 rng('default');
6 s = rng;
7
8 % Define data matrix X (assuming X is loaded from the .mat file)
9 X = ...; % Load or assign the data matrix X here
10
11 % Dimension and size of the data matrix
12 dim = size(X, 1);
13 [n, m] = size(X);
14 p = m;
15
16 % Distance matrix D using L1 norm
17 D = zeros(p, p);
18 for i = 1:p
19     for j = i:p
20         if i == j
21             D(i, j) = 0;
22         else
23             D(i, j) = norm(X(:, i) - X(:, j), 1); % L1 norm
24         end
25     end
26 end
27 D = D + D'
28
29
30
31 I_m = [33, 99, 101];
32
33
34 figure();
35 plot(X(1, :), X(2, :), 'bo', 'MarkerSize', 8);
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36 hold on;
37 plot(X(1, I_m), X(2, I_m), 'mp', 'MarkerSize', 12, 'LineWidth', 2);
38 legend('Data', 'Random Centroids');
39
40 % Initialize parameters for k-medoids
41 Err = 1;
42 itmax = 100;
43 tol = 1.0e-10;
44 iter = 0;
45
46 % Initial distance to medoids
47 D_m = D(:, I_m);
48 [q, I_assign] = min(D_m, [], 2);
49 Q = sum(q);
50 k = length(I_m);
51 oldI_m = I_m;
52
53 % Main loop for k-medoids algorithm
54 while Err > tol && iter < itmax
55     iter = iter + 1;
56     clear I_m;
57
58     for ell = 1:k
59         I_ell = find(I_assign == ell);
60         D_ell = D(I_ell, I_ell);
61         [~, j] = min(sum(D_ell, 1));
62         I_m(ell) = I_ell(j);
63     end
64
65     newI_m = I_m;
66
67     % Recompute assignments
68     D_m = D(:, I_m);
69     [q, I_assign] = min(D_m, [], 2);
70     Q_new = sum(q);
71
72     % Check for convergence
73     Err = abs(Q_new - Q);
74     Q = Q_new;
75     oldI_m = newI_m;
76 end
77
78 % Assign data to clusters
79 X_l = cell(1, k);
80 for j = 1:k
81     X_l{j} = X(:, I_assign == j);
82 end

```

```

83
84 % Plot final clusters and centroids
85 figure();
86 plot(X(1, :), X(2, :), 'bo', 'MarkerSize', 8);
87 hold on;
88 plot(X(1, I_m), X(2, I_m), 'mp', 'MarkerSize', 12, 'LineWidth', 2);
89 legend('Data', 'Final Centroids');
90
91 % 3D scatter plot of clusters
92 figure();
93 colors = {'cyan', 'red', 'green'};
94 for j = 1:k
95     scatter3(X_l{j}(1, :), X_l{j}(2, :), X_l{j}(3, :), [], colors{j}, '↵
        filled');
96     hold on;
97 end
98 scatter3(X(1, I_m), X(2, I_m), X(3, I_m), 100, 'rx', 'LineWidth', 5);
99 title('Final clustering K Medoids');
100 legend('Cluster 1 (Cyan)', 'Cluster 2 (Red)', 'Cluster 3 (Green)', '↵
    Medoids');
101
102 % Plot each cluster
103 figure();
104 for j = 1:k
105     scatter3(X_l{j}(1, :), X_l{j}(2, :), X_l{j}(3, :), [], colors{j}, '↵
        filled');
106     hold on;
107 end
108 scatter3(X(1, I_m), X(2, I_m), X(3, I_m), 100, 'rx', 'LineWidth', 5);
109 title('Final clustering K Medoids');
110 legend('Cluster 1 (Cyan)', 'Cluster 2 (Blue)', 'Cluster 3 (Green)', '↵
    Medoids');
111
112 % Confusion matrix plot (assuming I is the true label vector)
113 figure();
114 cm = confusionchart(I, I_assign);
115
116 % Load the data
117 load('IrisDataAnnotated.mat');
118
119 % Transpose the data
120 X = X';
121
122 % Perform k-means clustering
123 rng('default'); % For reproducibility
124 [idx, C] = kmeans(X, 3);
125

```

```

126 % Visualize the clusters and centroids in 2D
127 figure;
128 plot(X(idx == 1, 1), X(idx == 1, 2), 'r.', 'MarkerSize', 9);
129 hold on;
130 plot(X(idx == 2, 1), X(idx == 2, 2), 'b.', 'MarkerSize', 9);
131 plot(X(idx == 3, 1), X(idx == 3, 2), 'g.', 'MarkerSize', 9);
132 plot(C(:, 1), C(:, 2), 'mp', 'MarkerSize', 10, 'LineWidth', 1.5);
133 legend('Cluster 1', 'Cluster 2', 'Cluster 3', 'Centroids', 'Location', 'NW↵
    ');
134 title('Cluster Assignments and Centroids');
135 hold off;
136
137 % Visualize the clusters and centroids in 3D
138 figure;
139 scatter3(X(idx == 1, 1), X(idx == 1, 2), X(idx == 1, 3), 'r. ');
140 hold on;
141 scatter3(X(idx == 2, 1), X(idx == 2, 2), X(idx == 2, 3), 'b. ');
142 scatter3(X(idx == 3, 1), X(idx == 3, 2), X(idx == 3, 3), 'g. ');
143 scatter3(C(:, 1), C(:, 2), C(:, 3), 200, 'mp', 'filled');
144 legend('Cluster 1', 'Cluster 2', 'Cluster 3', 'Cluster Mean', 'Location', '↵
    'NW');
145 title('K-means Clusters and Centroids');
146 xlabel('Feature 1');
147 ylabel('Feature 2');
148 zlabel('Feature 3');
149 hold off;
150
151 % Plot the confusion matrix
152 figure;
153 cm = confusionchart(I, idx);
154 cm.Title = 'Confusion Matrix for K-means Clustering';
155 cm.RowSummary = 'row-normalized';
156 cm.ColumnSummary = 'column-normalized';
157
158
159 load('IrisDataAnnotated.mat'); % X = data matrix, I = annotation vector
160
161 % Center the data within each class
162 X1_centered = X(:, I == 1) - mean(X(:, I == 1), 2);
163 X2_centered = X(:, I == 2) - mean(X(:, I == 2), 2);
164 X3_centered = X(:, I == 3) - mean(X(:, I == 3), 2);
165
166 % Calculate the within-class scatter matrix
167 Sw = X1_centered * X1_centered' + X2_centered * X2_centered' + X3_centered↵
    * X3_centered';
168
169 % Compute the between-class scatter matrix

```

```

170 mu = mean(X, 2);
171 Sb = length(find(I == 1)) * (mean(X(:, I == 1), 2) - mu) * (mean(X(:, I == 1), 2) - mu)' + ...
172     length(find(I == 2)) * (mean(X(:, I == 2), 2) - mu) * (mean(X(:, I == 2), 2) - mu)' + ...
173     length(find(I == 3)) * (mean(X(:, I == 3), 2) - mu) * (mean(X(:, I == 3), 2) - mu)';
174
175 % Perform eigenvalue decomposition to find the LDA directions
176 [V, D] = eig(pinv(Sw) * Sb);
177 [~, indices] = sort(diag(D), 'descend');
178 eigenvectors_lda = V(:, indices);
179
180 % Project the data onto the first two LDA directions
181 LDA_projection = eigenvectors_lda(:, 1:2)' * X;
182
183 % Perform PCA on the data matrix
184 [coeff, score, ~, ~, explained] = pca(X');
185
186 % Project the data onto the first two PCA directions
187 PCA_projection = coeff(:, 1:2)' * X;
188
189 % Plot the data projected on the first two LDA directions
190 figure;
191 subplot(1, 2, 1);
192 scatter(LDA_projection(1, I == 1), LDA_projection(2, I == 1), 100, 'r.', 'DisplayName', 'Iris setosa');
193 hold on;
194 scatter(LDA_projection(1, I == 2), LDA_projection(2, I == 2), 100, 'g.', 'DisplayName', 'Iris versicolor');
195 scatter(LDA_projection(1, I == 3), LDA_projection(2, I == 3), 100, 'b.', 'DisplayName', 'Iris virginica');
196 title('LDA Projection');
197 xlabel('LDA Component 1');
198 ylabel('LDA Component 2');
199 legend('Location', 'best');
200 grid on;
201 set(gca, 'FontSize', 12);
202
203 % Plot the data projected on the first two PCA directions
204 subplot(1, 2, 2);
205 scatter(PCA_projection(1, I == 1), PCA_projection(2, I == 1), 100, 'r.', 'DisplayName', 'Iris setosa');
206 hold on;
207 scatter(PCA_projection(1, I == 2), PCA_projection(2, I == 2), 100, 'g.', 'DisplayName', 'Iris versicolor');
208 scatter(PCA_projection(1, I == 3), PCA_projection(2, I == 3), 100, 'b.', 'DisplayName', 'Iris virginica');

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        DisplayName', 'Iris virginica');
209 title('PCA Projection');
210 xlabel('PCA Component 1');
211 ylabel('PCA Component 2');
212 legend('Location', 'best');
213 grid on;
214 set(gca, 'FontSize', 12);
215
216 % Classification using LDA projection
217 class_means_lda = [mean(LDA_projection(:, I == 1), 2), mean(LDA_projection↵
        (:, I == 2), 2), mean(LDA_projection(:, I == 3), 2)];
218 predicted_labels_lda = zeros(1, size(X, 2));
219
220 for i = 1:size(X, 2)
221     distances = sum((LDA_projection(:, i) - class_means_lda).^2, 1);
222     [~, predicted_labels_lda(i)] = min(distances);
223 end
224
225 % Classification using PCA projection
226 class_means_pca = [mean(PCA_projection(:, I == 1), 2), mean(PCA_projection↵
        (:, I == 2), 2), mean(PCA_projection(:, I == 3), 2)];
227 predicted_labels_pca = zeros(1, size(X, 2));
228
229 for i = 1:size(X, 2)
230     distances = sum((PCA_projection(:, i) - class_means_pca).^2, 1);
231     [~, predicted_labels_pca(i)] = min(distances);
232 end
233
234 % Add confusion charts
235 figure;
236 subplot(1, 2, 1);
237 confusionchart(I, predicted_labels_lda);
238 title('Confusion Matrix for LDA Classification');
239
240 subplot(1, 2, 2);
241 confusionchart(I, predicted_labels_pca);
242 title('Confusion Matrix for PCA Classification');

```

BIOPSY DATASET

Listing 2: Matlab Code.

```

1
2 % Load the data

```

```

3 load('BiopsyData.mat');
4
5 % Clean the data by removing columns with any NaN values
6 X_clean = X(:, all(~isnan(X)));
7
8 % Set random number generator for reproducibility
9 rng(1);
10
11 % Get the size of the cleaned data
12 [n, m] = size(X_clean);
13
14 % Initialize distance matrix
15 D = zeros(m, m);
16
17 % Define the norm type (Euclidean norm)
18 norm_type = 2;
19
20 % Compute the pairwise distance matrix using the specified norm
21 for i = 1:m
22     for j = i:m
23         if i == j
24             D(i, j) = 0;
25         else
26             D(i, j) = norm(X_clean(:, i) - X_clean(:, j), norm_type);
27         end
28     end
29 end
30 D = D + D'; % Make the distance matrix symmetric
31
32 % Initial random medoid indices
33 I_m = [180, 356];
34
35 % Plot initial data and random centroids in 2D
36 figure;
37 plot(X_clean(1, :), X_clean(2, :), 'bo', 'MarkerSize', 8);
38 hold on;
39 plot(X_clean(1, I_m), X_clean(2, I_m), 'mp', 'MarkerSize', 12, 'LineWidth'↵
    , 2);
40 legend('Data', 'Random Centroids');
41 title('Initial Random Centroids');
42 hold off;
43
44 % Parameters for k-medoids
45 Err = 1;
46 itmax = 100;
47 tol = 1.0e-10;
48 iter = 0;

```

```

49
50 % Compute initial distance matrix for medoids
51 D_m = D(:, I_m);
52 [q, I_assign] = min(D_m, [], 2);
53 Q = sum(q);
54
55 k = length(I_m);
56 oldI_m = I_m;
57 clear I_m;
58
59 % Main loop for k-medoids algorithm
60 while Err > tol && iter < itmax
61     iter = iter + 1;
62
63     for ell = 1:k
64         I_ell = find(I_assign == ell);
65         D_ell = D(I_ell, I_ell);
66         s = sum(D_ell, 2);
67         [qq(ell), j] = min(s);
68         I_m(ell) = I_ell(j);
69     end
70
71     D_m = D(:, I_m);
72     [q, I_assign] = min(D_m, [], 2);
73     Q_new = sum(q);
74
75     Err = abs(Q - Q_new);
76     Q = Q_new;
77 end
78
79 % Assign data to clusters
80 X_l = cell(1, k);
81 for j = 1:k
82     X_l{j} = X_clean(:, I_assign == j);
83 end
84
85 % Plot final medoids in 2D
86 figure;
87 plot(X_clean(1, :), X_clean(2, :), 'bo', 'MarkerSize', 8);
88 hold on;
89 plot(X_clean(1, I_m), X_clean(2, I_m), 'mp', 'MarkerSize', 12, 'LineWidth'↵
    , 2);
90 legend('Data', 'Final Medoids (Euclidean Norm)');
91 title('Final Medoids');
92 hold off;
93
94 % Plot final clusters in 2D

```



```

95 figure;
96 hold on;
97 scatter(X_l{1}(1, :), X_l{1}(2, :), 'blue', 'filled');
98 scatter(X_l{2}(1, :), X_l{2}(2, :), 'red', 'filled');
99 plot(X_clean(1, I_m), X_clean(2, I_m), 'mp', 'MarkerSize', 12, 'LineWidth'↵
    , 2);
100 title('Final Clustering K-Medoids (Euclidean Norm)');
101 legend('Cluster 1', 'Cluster 2', 'Medoids');
102 hold off;
103
104 % Plot each cluster in 3D
105 figure;
106 hold on;
107 colors = {'blue', 'red', 'green'}; % Update the colors if more clusters
108 for j = 1:k
109     scatter3(X_l{j}(1, :), X_l{j}(2, :), X_l{j}(3, :), 36, colors{j}, '↵
        filled');
110 end
111 % Plot medoids in 3D
112 scatter3(X_clean(1, I_m), X_clean(2, I_m), X_clean(3, I_m), 100, 'kx', '↵
    LineWidth', 5);
113 title('Final Clustering K-Medoids (3D Visualization)');
114 legend('Cluster 1', 'Cluster 2', 'Medoids'); % Update legend for more ↵
    clusters
115 grid on;
116 view(3);
117 hold off;
118
119 % Assuming I is the true label vector
120 figure;
121 cm = confusionchart(I, I_assign);
122 cm.Title = 'Confusion Matrix for K-medoids Clustering';
123 cm.RowSummary = 'row-normalized';
124 cm.ColumnSummary = 'column-normalized';

```

CONGRESSVOTE DATASET

Listing 3: Matlab Code.

```

1 % Load the data
2 load('CongressionalVote.mat');
3
4 % Remove rows with all zero values
5 X(sum(X ~= 0, 2) == 0, :) = [];

```

```

6 I(sum(X ~= 0, 2) == 0) = [];
7
8 % Handle missing data by replacing zeros with NaN
9 X(X == 0) = NaN;
10
11 % Replace NaN values with the mean of the respective feature
12 for i = 1:size(X, 2)
13     nan_idx = isnan(X(:, i));
14     X(nan_idx, i) = mean(X(~nan_idx, i));
15 end
16
17 % Perform Linear Discriminant Analysis (LDA)
18 lda = fitcdiscr(X, I);
19
20 % Predict using LDA
21 lda_pred = predict(lda, X);
22
23 % Plot the confusion matrix for LDA
24 figure();
25 cm_lda = confusionchart(I, lda_pred);
26 title('Confusion Chart (LDA)');
27
28 % Transform the data using LDA coefficients for visualization
29 X_lda = X * lda.Coeffs(1, 2).Linear;
30
31 % Since LDA reduces to a single dimension, plot in 2D for clarity
32 X_lda_2D = [X_lda X_lda];
33
34 % Plot the LDA transformed data
35 figure;
36 gscatter(X_lda_2D(:,1), X_lda_2D(:,2), I);
37 title('LDA of Congressional Vote Data');
38 xlabel('LDA Dimension 1');
39 ylabel('LDA Dimension 2');
40 grid on;
41
42 % Customize the plot for clarity
43 legend('Democrat', 'Republican');
44
45 % Calculate and display sensitivity and specificity
46 sensitivity = sum((I == 1) & (lda_pred == 1)) / sum(I == 1);
47 specificity = sum((I == 0) & (lda_pred == 0)) / sum(I == 0);
48
49 disp(['Sensitivity (Recall): ', num2str(sensitivity)]);
50 disp(['Specificity (True Negative Rate): ', num2str(specificity)]);

```

WINE DATASET

Listing 4: Matlab Code.

```
51 % Load the data
52 load("WineData.mat")
53
54 % Initialize random seed for reproducibility
55 rng(1);
56
57 % Get dimensions of the data matrix
58 [n, m] = size(X);
59 p = m;
60
61 % Compute the distance matrix using norm 1 (Manhattan distance)
62 D = zeros(p);
63 for i = 1:p
64     for j = i:p
65         if i == j
66             D(i, j) = 0;
67         else
68             D(i, j) = norm(X(:, i) - X(:, j), 2);
69         end
70     end
71 end
72 D = D + D';
73
74 % Initial medoids
75 I_m = [1, 100, 150];
76
77 % Plot initial data and medoids
78 figure()
79 plot(X(1,:), X(2,:), 'o', 'MarkerSize', 8, 'MarkerFaceColor', 'c', '↵
    MarkerEdgeColor', 'k');
80 hold on;
81 plot(X(1, I_m), X(2, I_m), 'p', 'MarkerSize', 12, 'LineWidth', 2, '↵
    MarkerEdgeColor', 'm', 'MarkerFaceColor', 'm');
82 legend('Data', 'Random Centroids', 'Location', 'best')
83 title('Initial Data and Random Centroids');
84 hold off;
85
86 % K-medoids algorithm
87 Err = 1;
88 itmax = 100;
89 tol = 1.0e-10;
90 iter = 0;
```

```

91
92 D_m = D(1:end, I_m);
93 [q, I_assign] = min(D_m');
94 Q = sum(q);
95 k = length(I_m);
96 oldI_m = I_m;
97 clear I_m;
98
99 % Iteratively refine medoids
100 while Err > tol && iter < itmax
101     iter = iter + 1;
102     for ell = 1:k
103         I_ell = find(I_assign == ell);
104         D_ell = D(I_ell, I_ell);
105         s = sum(D_ell);
106         [~, j] = min(s);
107         I_m(ell) = I_ell(j);
108     end
109     D_m = D(1:end, I_m);
110     [q, I_assign] = min(D_m');
111     Qnew = sum(q);
112     Err = abs(Q - Qnew);
113     Q = Qnew;
114 end
115
116 % Plot final data and medoids
117 figure()
118 plot(X(1,:), X(2,:), 'o', 'MarkerSize', 8, 'MarkerFaceColor', 'y', '↵
    MarkerEdgeColor', 'k');
119 hold on;
120 plot(X(1, I_m), X(2, I_m), 'p', 'MarkerSize', 12, 'LineWidth', 2, '↵
    MarkerEdgeColor', 'r', 'MarkerFaceColor', 'r');
121 legend('Data', 'Final Centroids', 'Location', 'best')
122 title('Final Data and Medoids');
123 hold off;
124
125 % Separate data points into clusters
126 for j = 1:k
127     X_l{j} = X(:, find(I_assign == j));
128 end
129
130 % 3D scatter plot of clusters with different colors
131 figure()
132 hold on;
133 scatter3(X_l{1}(1,:), X_l{1}(2,:), X_l{1}(3,:), 36, 'g', 'filled');
134 scatter3(X_l{2}(1,:), X_l{2}(2,:), X_l{2}(3,:), 36, 'b', 'filled');
135 scatter3(X_l{3}(1,:), X_l{3}(2,:), X_l{3}(3,:), 36, 'm', 'filled');

```

```

136 scatter3(X(1, I_m), X(2, I_m), X(3, I_m), 100, 'kx', 'LineWidth', 5);
137 title('Final clustering K Medoids');
138 legend('Cluster 1', 'Cluster 2', 'Cluster 3', 'Medoids', 'Location', 'best↔
    ');
139 hold off;
140
141 % Confusion matrix chart
142 figure()
143 cm = confusionchart(I, I_assign);
144 title('Confusion Matrix for K-Medoids');
145 % Load the data
146 load("WineData.mat")
147
148 % Transpose the data
149 X = X';
150
151 % Perform k-means clustering
152 rng('default'); % For reproducibility
153 [idx, C] = kmeans(X, 3);
154
155 % Visualize the clusters and centroids with larger data point size
156 figure;
157 scatter(X(idx==1, 1), X(idx==1, 2), 100, 'r.', 'MarkerFaceColor', 'r');
158 hold on;
159 scatter(X(idx==2, 1), X(idx==2, 2), 100, 'b.', 'MarkerFaceColor', 'b');
160 scatter(X(idx==3, 1), X(idx==3, 2), 100, 'g.', 'MarkerFaceColor', 'g');
161 plot(C(:, 1), C(:, 2), 'mp', 'MarkerSize', 12, 'LineWidth', 2);
162 legend('Cluster 1', 'Cluster 2', 'Cluster 3', 'Centroids', 'Location', 'NW↔
    ');
163 title('Cluster Assignments and Centroids');
164 hold off;
165
166 % 3D scatter plot of clusters and centroids with larger data point size
167 figure;
168 scatter3(X(idx==1, 1), X(idx==1, 2), X(idx==1, 3), 100, 'r.');
```

```

180 % Confusion matrix chart
181 figure;
182 cm = confusionchart(I, idx);
183 title('Confusion Matrix for K-means');
184
185 % Load the data
186 load("WineData.mat");
187
188 % Separate data into subsets based on cluster annotation
189 I1 = find(I == 1);
190 I2 = find(I == 2);
191 I3 = find(I == 3);
192
193 % Compute class means
194 mu1 = mean(X(:, I1), 2);
195 mu2 = mean(X(:, I2), 2);
196 mu3 = mean(X(:, I3), 2);
197
198 % Compute within-class scatter matrix
199 Sw = cov(X(:, I1)', 1) + cov(X(:, I2)', 1) + cov(X(:, I3)', 1);
200
201 % Compute between-class scatter matrix
202 Sb = length(I1) * (mu1 - mean(X, 2)) * (mu1 - mean(X, 2))' + ...
203     length(I2) * (mu2 - mean(X, 2)) * (mu2 - mean(X, 2))' + ...
204     length(I3) * (mu3 - mean(X, 2)) * (mu3 - mean(X, 2))';
205
206 % Solve the generalized eigenvalue problem
207 [V, D] = eig(Sb, Sw);
208
209 % Sort eigenvectors and eigenvalues in descending order
210 [D_sorted, idx] = sort(diag(D), 'descend');
211 V_sorted = V(:, idx);
212
213 % Project the data onto the LDA directions
214 LDA_projection = V_sorted(:, 1:3)' * X;
215
216 % Plot two-dimensional projections for each LDA direction
217 for i = 1:size(LDA_projection, 1)
218     figure;
219     scatter(LDA_projection(i, I1), LDA_projection(i, I1), 100, 'r.');
```

```

227 end
228
229 % Histogram of LDA Components
230 figure;
231 for i = 1:size(LDA_projection, 1)
232     subplot(size(LDA_projection, 1), 1, i);
233     histogram(LDA_projection(i, I1), 'FaceColor', 'r', 'EdgeColor', 'none'↵
        );
234     hold on;
235     histogram(LDA_projection(i, I2), 'FaceColor', 'b', 'EdgeColor', 'none'↵
        );
236     histogram(LDA_projection(i, I3), 'FaceColor', 'g', 'EdgeColor', 'none'↵
        );
237     title(['Histogram of LDA Component ' num2str(i)]);
238     legend('Cluster 1', 'Cluster 2', 'Cluster 3');
239     ylabel('Frequency');
240     xlabel(['LDA Component ' num2str(i)]);
241     hold off;
242 end
243
244 % Perform PCA
245 [coeff, score, ~, ~, explained] = pca(X');
246
247 % Project the data onto the first three PCA directions
248 PCA_projection = coeff(:, 1:3)' * X;
249
250 % Plot two-dimensional projections for each PCA direction
251 for i = 1:size(PCA_projection, 1)
252     figure;
253     scatter(PCA_projection(i, I1), PCA_projection(i, I1), 100, 'r. ');
254     hold on;
255     scatter(PCA_projection(i, I2), PCA_projection(i, I2), 100, 'b. ');
256     scatter(PCA_projection(i, I3), PCA_projection(i, I3), 100, 'g. ');
257     title(['PCA Projection ' num2str(i)]);
258     xlabel(['PCA Component ' num2str(i)]);
259     ylabel(['PCA Component ' num2str(i)]);
260     legend('Cluster 1', 'Cluster 2', 'Cluster 3');
261 end
262
263 % Histogram of PCA Components
264 figure;
265 for i = 1:size(PCA_projection, 1)
266     subplot(size(PCA_projection, 1), 1, i);
267     histogram(PCA_projection(i, I1), 'FaceColor', 'r', 'EdgeColor', 'none'↵
        );
268     hold on;
269     histogram(PCA_projection(i, I2), 'FaceColor', 'b', 'EdgeColor', 'none'↵

```

```

    );
270     histogram(PCA_projection(i, I3), 'FaceColor', 'g', 'EdgeColor', 'none'↵
    );
271     title(['Histogram of PCA Component ' num2str(i)]);
272     legend('Cluster 1', 'Cluster 2', 'Cluster 3');
273     ylabel('Frequency');
274     xlabel(['PCA Component ' num2str(i)]);
275     hold off;
276 end
277
278 % Confusion Matrix for LDA
279 LDA_labels = classify(LDA_projection(1:2, :)', LDA_projection(1:2, :)', I'↵
    ); % Use first two LDA components
280 confMat_LDA = confusionmat(I, LDA_labels);
281
282 % Plot the confusion matrix for LDA
283 figure;
284 confusionchart(confMat_LDA, {'Cluster 1', 'Cluster 2', 'Cluster 3'});
285 title('Confusion Matrix for LDA Classification of Wine Data');
286
287 % Confusion Matrix for PCA
288 PCA_labels = classify(PCA_projection(1:2, :)', PCA_projection(1:2, :)', I'↵
    ); % Use first two PCA components
289 confMat_PCA = confusionmat(I, PCA_labels);
290
291 % Plot the confusion matrix for PCA
292 figure;
293 confusionchart(confMat_PCA, {'Cluster 1', 'Cluster 2', 'Cluster 3'});
294 title('Confusion Matrix for PCA Classification of Wine Data');

```

CARDIAC DATASET

Listing 5: Matlab Code.

```

298 % Load the data
299 clear;
300 close all;
301 load CardiacSPECT.mat
302
303 % Get the size of the data matrix
304 [n, p] = size(X);
305
306 % Initialize the distance matrix
307 D = zeros(p);

```



```

308
309 % Compute the distance matrix by comparing columns of X
310 for i = 1:(p-1)
311     for j = (i+1):p
312         D(i, j) = sum(X(:, i) ~= X(:, j)) / n;
313     end
314 end
315
316 % Make the distance matrix symmetric
317 D = D + D';
318
319 % Set the random number generator seed for reproducibility
320 rng('default');
321
322 % Number of clusters
323 k = 2;
324
325 % Number of trials for k-medoids
326 n_init = 20;
327
328 % Initialize variables for storing results
329 I_m_ni = cell(1, n_init);
330 I_assign_ni = cell(1, n_init);
331 Q_ni = zeros(1, n_init);
332
333 % Run k-medoids algorithm with multiple initializations
334 for ni = 1:n_init
335     % Random initial medoids
336     I_m_ni{ni} = sort(randperm(length(D), k));
337     D_m = D(:, I_m_ni{ni});
338     [~, I_assign_ni{ni}] = min(D_m');
339     Q_ni(ni) = sum(min(D_m'));
340 end
341
342 % Find the best clustering with minimum tightness (coherence)
343 [~, ni_min_tightness] = min(Q_ni);
344 I_m = I_m_ni{ni_min_tightness};
345 I_assign = I_assign_ni{ni_min_tightness};
346
347 % Refine the clustering iteratively
348 Err = 1;
349 itmax = 100;
350 iter = 0;
351 tol = 1.0e-10;
352 Q = sum(min(D(:, I_m)));
353
354 while (Err >= tol && iter < itmax)

```

```

355     [~, I_assign] = min(D(:, I_m)');
356     Qnew = Q;
357     Q = sum(min(D(:, I_m)));
358
359     for ell = 1:k
360         I_ell = find(I_assign == ell);
361         D_ell = D(I_ell, I_ell);
362         s = sum(D_ell);
363         [~, j] = min(s);
364         I_m(ell) = I_ell(j);
365     end
366
367     Err = abs(Q - Qnew);
368     iter = iter + 1;
369 end
370
371 % Final medoids
372 I_bar = I_m;
373 flag = Err < tol;
374
375 disp('flag');
376 disp(flag);
377 disp('final medoids');
378 disp(I_m);
379
380 % Change I_assign to become 0 and 1 as the I vector
381 I_assign = I_assign - 1;
382
383 % Perform k-means clustering
384 [idx_kmeans, ~] = kmeans(X', k, 'Replicates', 20);
385
386 % Create confusion matrix chart for k-medoids
387 figure();
388 cm_medoids = confusionchart(I, I_assign);
389 title('Confusion Matrix for K-medoids');
390
391 % Create confusion matrix chart for k-means
392 figure();
393 cm_kmeans = confusionchart(I, idx_kmeans - 1);
394 title('Confusion Matrix for K-means');
395
396 % Perform PCA for 2D visualization
397 [coeff, score] = pca(X');
398
399 % Scatter plot of the first two principal components for k-medoids
400 figure();
401 gscatter(score(:, 1), score(:, 2), I_assign, 'rb', 'ox');

```

```

402 xlabel('Principal Component 1');
403 ylabel('Principal Component 2');
404 title('PCA of K-medoids Clustering Results');
405 legend('Cluster 0', 'Cluster 1');
406
407 % Scatter plot of the first two principal components for k-means
408 figure();
409 gscatter(score(:, 1), score(:, 2), idx_kmeans - 1, 'gb', 'ox');
410 xlabel('Principal Component 1');
411 ylabel('Principal Component 2');
412 title('PCA of K-means Clustering Results');
413 legend('Cluster 0', 'Cluster 1');
414
415 % Create matrix C for k-medoids
416 c11_medoids = length(find(I_assign == 1 & I == 1));
417 c12_medoids = length(find(I_assign == 0 & I == 1));
418 c21_medoids = length(find(I_assign == 1 & I == 0));
419 c22_medoids = length(find(I_assign == 0 & I == 0));
420 C_medoids = [c11_medoids c12_medoids; c21_medoids c22_medoids];
421
422 % Create matrix C for k-means
423 c11_kmeans = length(find(idx_kmeans - 1 == 1 & I == 1));
424 c12_kmeans = length(find(idx_kmeans - 1 == 0 & I == 1));
425 c21_kmeans = length(find(idx_kmeans - 1 == 1 & I == 0));
426 c22_kmeans = length(find(idx_kmeans - 1 == 0 & I == 0));
427 C_kmeans = [c11_kmeans c12_kmeans; c21_kmeans c22_kmeans];
428
429 % Display matrices for k-medoids
430 disp('Matrix C for K-medoids:');
431 disp(C_medoids);
432
433 % Display matrices for k-means
434 disp('Matrix C for K-means:');
435 disp(C_kmeans);
436
437 % Additional visualization: Clustering in the original feature space for k↔
    -medoids
438 figure;
439 hold on;
440 for i = 1:p
441     cluster = I_assign(i) + 1; % 1 or 2
442     scatter(1:n, X(:, i), 36);
443 end
444 xlabel('Feature Index');
445 ylabel('Binary Value');
446 title('K-medoids Clustering in Original Feature Space');
447 legend('Cluster 0', 'Cluster 1');

```

```

448 hold off;
449
450 % Additional visualization: Clustering in the original feature space for k↔
    -means
451 figure;
452 hold on;
453 for i = 1:p
454     cluster = idx_kmeans(i); % 1 or 2
455     scatter(1:n, X(:, i), 36, colors(cluster), markers(cluster));
456 end
457 xlabel('Feature Index');
458 ylabel('Binary Value');
459 title('K-means Clustering in Original Feature Space');
460 legend('Cluster 0', 'Cluster 1');
461 hold off;
462 % Load the dataset
463 load CardiacSPECT.mat;
464
465 % Perform LDA
466 classLabels = unique(I);
467 numClasses = numel(classLabels);
468 numFeatures = size(X, 1);
469 meanVecs = zeros(numFeatures, numClasses);
470 Sw = zeros(numFeatures, numFeatures);
471 Sb = zeros(numFeatures, numFeatures);
472
473 % Calculate class means
474 for i = 1:numClasses
475     meanVecs(:, i) = mean(X(:, I == classLabels(i)), 2);
476 end
477
478 % Calculate within-class scatter matrix
479 for i = 1:numClasses
480     Xi = X(:, I == classLabels(i));
481     Sw = Sw + (Xi - meanVecs(:, i)) * (Xi - meanVecs(:, i))';
482 end
483
484 % Calculate between-class scatter matrix
485 meanOverall = mean(X, 2);
486 for i = 1:numClasses
487     Ni = sum(I == classLabels(i));
488     Sb = Sb + Ni * (meanVecs(:, i) - meanOverall) * (meanVecs(:, i) - ↵
        meanOverall)';
489 end
490
491 % Solve the generalized eigenvalue problem
492 [V, D] = eig(Sb, Sw);

```

```

493
494 % Sort eigenvectors by eigenvalues in descending order
495 [~, indices] = sort(diag(D), 'descend');
496 W = V(:, indices);
497
498 % Project the data onto the first two LDA directions
499 LDA_projection = W(:, 1:2)' * X;
500
501 % Plot the data projected on the first two LDA directions
502 figure;
503 scatter(LDA_projection(1, I == 0), LDA_projection(2, I == 0), 100, 'b.', '↵
    DisplayName', 'Normal');
504 hold on;
505 scatter(LDA_projection(1, I == 1), LDA_projection(2, I == 1), 100, 'r.', '↵
    DisplayName', 'Abnormal');
506 title('LDA Projection for Cardiac SPECT Dataset');
507 xlabel('LDA Component 1');
508 ylabel('LDA Component 2');
509 legend('Location', 'best');
510 grid on;
511 set(gca, 'FontSize', 12);
512
513 % Classification using LDA projection
514 class_means_lda = [mean(LDA_projection(:, I == 0), 2), mean(LDA_projection↵
    (:, I == 1), 2)];
515 predictedLabels_lda = zeros(1, size(X, 2));
516
517 for i = 1:size(X, 2)
518     distances = sum((LDA_projection(:, i) - class_means_lda).^2, 1);
519     [~, predictedLabels_lda(i)] = min(distances);
520 end
521
522 % Convert 1-based index to original labels
523 predictedLabels_lda = predictedLabels_lda - 1;
524
525 % Create a confusion matrix for LDA
526 confMat_lda = confusionmat(I, predictedLabels_lda);
527
528 % Plot the confusion matrix for LDA
529 figure;
530 confusionchart(confMat_lda, {'Normal', 'Abnormal'});
531 title('Confusion Matrix for LDA Classification of Cardiac SPECT Dataset');
532
533 % Perform PCA
534 [coeff, score, ~, ~, explained] = pca(X');
535
536 % Project the data onto the first two PCA directions

```

```

537 PCA_projection = coeff(:, 1:2)' * X;
538
539 % Plot the data projected on the first two PCA directions
540 figure;
541 scatter(PCA_projection(1, I == 0), PCA_projection(2, I == 0), 100, 'b.', '↵
    DisplayName', 'Normal');
542 hold on;
543 scatter(PCA_projection(1, I == 1), PCA_projection(2, I == 1), 100, 'r.', '↵
    DisplayName', 'Abnormal');
544 title('PCA Projection for Cardiac SPECT Dataset');
545 xlabel('PCA Component 1');
546 ylabel('PCA Component 2');
547 legend('Location', 'best');
548 grid on;
549 set(gca, 'FontSize', 12);
550
551 % Classification using PCA projection
552 class_means_pca = [mean(PCA_projection(:, I == 0), 2), mean(PCA_projection↵
   (:, I == 1), 2)];
553 predictedLabels_pca = zeros(1, size(X, 2));
554
555 for i = 1:size(X, 2)
556     distances = sum((PCA_projection(:, i) - class_means_pca).^2, 1);
557     [~, predictedLabels_pca(i)] = min(distances);
558 end
559
560 % Convert 1-based index to original labels
561 predictedLabels_pca = predictedLabels_pca - 1;
562
563 % Create a confusion matrix for PCA
564 confMat_pca = confusionmat(I, predictedLabels_pca);
565
566 % Plot the confusion matrix for PCA
567 figure;
568 confusionchart(confMat_pca, {'Normal', 'Abnormal'});
569 title('Confusion Matrix for PCA Classification of Cardiac SPECT Dataset');

```

HANDWRITTENDIGITS DATASET

Listing 6: Matlab Code.

```

571 % Load the dataset
572 load HandwrittenDigits.mat % X = data matrix, I = annotation vector
573

```

```

574 % Create a data matrix X04 containing images of digits '0' and '4'
575 I0 = find(I == 0); % Indices of digit '0'
576 I4 = find(I == 4); % Indices of digit '4'
577 X04 = [X(:, I0), X(:, I4)]; % Combine images of digits '0' and '4'
578
579 % Calculate centered matrices for within-class scatter
580 X0_centered = X(:, I0) - mean(X(:, I0), 2);
581 X4_centered = X(:, I4) - mean(X(:, I4), 2);
582
583 % Calculate within-class scatter matrix
584 Sw = X0_centered * X0_centered' + X4_centered * X4_centered';
585
586 % Compute between-class scatter matrix
587 Sb = length(I0) * (mean(X(:, I0), 2) - mean(X04, 2)) * (mean(X(:, I0), 2) ←
    - mean(X04, 2))' + ...
588     length(I4) * (mean(X(:, I4), 2) - mean(X04, 2)) * (mean(X(:, I4), 2) ←
    mean(X04, 2))';
589
590 % Perform eigenvalue decomposition for LDA
591 [V, D] = eig(pinv(Sw) * Sb);
592 [~, indices] = sort(diag(D), 'descend');
593 eigenvectors = V(:, indices);
594
595 % Project data onto first two LDA directions
596 LDA_projection = eigenvectors(:, 1:2)' * X04;
597
598 % Plot LDA projection
599 figure;
600 scatter(LDA_projection(1, 1:length(I0)), LDA_projection(2, 1:length(I0)), ←
    100, 'b.', 'DisplayName', 'Digit ''0''');
601 hold on;
602 scatter(LDA_projection(1, length(I0)+1:end), LDA_projection(2, length(I0)←
    +1:end), 100, 'r.', 'DisplayName', 'Digit ''4''');
603 title('Projection of Digits ''0'' and ''4'' on LDA Directions');
604 xlabel('LDA Component 1');
605 ylabel('LDA Component 2');
606 legend('Location', 'best');
607 grid on;
608 set(gca, 'FontSize', 12);
609
610 % NMF algorithm
611 k_values = [5, 10, 20];
612
613 for k = k_values
614     disp(['Running NMF for k = ', num2str(k)]);
615     rng(1);
616     W = rand(size(X04, 1), k);

```

```

617     H = rand(k, size(X04, 2));
618     nmax = 100;
619     tau = 0.01;
620     ch = NaN(1, nmax);
621
622     for t = 1:nmax
623         H = max(0, H .* (W' * X04) ./ (W' * W * H + eps));
624         W = max(0, W .* (X04 * H') ./ (W * H * H' + eps));
625         ch(t) = norm(X04 - W * H, 'fro') / norm(X04, 'fro');
626         if ch(t) < tau
627             disp(['Converged at iteration ', num2str(t)]);
628             break;
629         end
630     end
631
632     % Plot convergence diagnostics
633     figure;
634     plot(1:t, ch(1:t), 'b-', 'LineWidth', 2);
635     title(['Convergence Diagnostics (k = ', num2str(k), ')']);
636     xlabel('Iteration');
637     ylabel('Relative Change');
638     grid on;
639     set(gca, 'FontSize', 12);
640
641     % Plot feature vectors as images
642     figure;
643     for j = 1:k
644         subplot(ceil(sqrt(k)), ceil(sqrt(k)), j);
645         imagesc(reshape(W(:, j), 16, 16));
646         colormap(gray);
647         axis('square');
648         axis('off');
649         title(['Feature ', num2str(j)]);
650     end
651 end
652
653 % Identify specific feature vector
654 [~, idx] = max(H(:));
655 [idx_row, idx_col] = ind2sub(size(H), idx);
656 feature_vector = H(:, idx_col);
657 digit_classification = I0(idx_row);
658
659 if digit_classification == 0
660     disp('The feature vector represents a ''0''.');
661 elseif digit_classification == 4
662     disp('The feature vector represents a ''4''.');
663 else

```



```

664     disp('The digit classification is different from ''0'' and ''4''.');
665 end
666
667 % Perform PCA for comparison
668 [coeff, score, ~, ~, explained] = pca(X04');
669 PCA_projection = coeff(:, 1:2)' * X04;
670
671 % Plot PCA and LDA projections
672 figure;
673 subplot(1, 2, 1);
674 scatter(LDA_projection(1, 1:length(I0)), LDA_projection(2, 1:length(I0)), ←
        100, 'b.', 'DisplayName', 'Digit ''0''');
675 hold on;
676 scatter(LDA_projection(1, length(I0)+1:end), LDA_projection(2, length(I0)←
        +1:end), 100, 'r.', 'DisplayName', 'Digit ''4''');
677 title('LDA Projection');
678 xlabel('LDA Component 1');
679 ylabel('LDA Component 2');
680 legend('Location', 'best');
681 grid on;
682 set(gca, 'FontSize', 12);
683
684 subplot(1, 2, 2);
685 scatter(PCA_projection(1, 1:length(I0)), PCA_projection(2, 1:length(I0)), ←
        100, 'b.', 'DisplayName', 'Digit ''0''');
686 hold on;
687 scatter(PCA_projection(1, length(I0)+1:end), PCA_projection(2, length(I0)←
        +1:end), 100, 'r.', 'DisplayName', 'Digit ''4''');
688 title('PCA Projection');
689 xlabel('PCA Component 1');
690 ylabel('PCA Component 2');
691 legend('Location', 'best');
692 grid on;
693 set(gca, 'FontSize', 12);

```
