Machine Learning Lab - Week XIII

Clustering

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Section: F

Semester: 5

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Course: Machine Learning (UE23CS352A)

Introduction

This lab report presents the implementation and analysis of customer segmentation using K-means clustering on a bank marketing dataset. The objective was to implement K-means clustering from scratch, perform dimensionality reduction using PCA, evaluate clustering quality, and explore various extensions including k-means++ initialization, bisecting k-means, Manhattan distance, and outlier detection.

Methodology

3.1 Data Preprocessing

1. **Data Loading:** Loaded CSV file with semicolon separator
2. **Categorical Encoding:** Applied LabelEncoder to categorical columns (job, marital, education, default, housing, loan, contact, month, poutcome, y)
3. **Feature Selection:** Selected 9 relevant features for clustering
4. **Feature Scaling:** Applied StandardScaler to normalize numerical features

3.2 Dimensionality Reduction

Principal Component Analysis (PCA) was applied to reduce dimensionality:

- **2D PCA:** Captured 28.12% of total variance (PC1: 14.88%, PC2: 13.24%)
- **6D PCA:** Captured 72.8% of total variance (used in optimization)
- PCA helped visualize data in lower dimensions and improve clustering performance

3.3 K-Means Clustering Implementation

Implemented K-means clustering from scratch with the following components:

1. **Centroid Initialization:** Random selection of k distinct points from the dataset
2. **Cluster Assignment:** Euclidean distance calculation to assign points to nearest centroids
3. **Centroid Update:** Recalculation of centroids as mean of assigned points
4. **Convergence:** Iteration until centroids stabilize or maximum iterations reached

3.4 Optimization Strategy

A comprehensive optimization approach was implemented to maximize silhouette score:

1. **Original Features Testing:** Tested k values from 2 to 15 on original scaled features
    - Best result: k=15, Silhouette Score = 0.2602
2. **PCA Component Testing:** Tested different PCA dimensions (2-9 components) with various k values
    - Best result: 6 components with k=2, Silhouette Score = 0.6448
3. **Multiple Initializations:** Tested 10 different random seeds with k-means++ initialization
    - Best result: Silhouette Score = 0.2845

Results & Analysis

4.1 Optimal Clustering Configuration

Winning Configuration:

- Method: PCA Features
- PCA Components: 6 (capturing 72.8% variance)
- Number of Clusters (k): 2

- Silhouette Score: 0.6448
- Status: Excellent (above 0.5 threshold)

4.2 Comparison of Methods

Method	k	Silhouette Score	Rank
PCA Features (6 components)	2	0.6448	1st
Optimized (Multi-seed)	2	0.2845	2nd
Original Features	15	0.2602	3rd
2D PCA (Initial)	3	0.3867	-

4.3 Elbow Method Analysis

The elbow method was used to identify optimal k values:

- For 2D PCA: Optimal k = 3 (based on elbow curve)
- For 6D PCA: Optimal k = 2 (based on silhouette analysis)
- The elbow method showed diminishing returns afier k=3-4 for 2D PCA

4.4 Cluster Characteristics

With k=2 clusters (optimal configuration):

- Cluster 0: 815 samples (1.8%)
- Cluster 1: 44,396 samples (98.2%)

The clusters show distinct characteristics in terms of:

- Age distribution
- Account balance
- Campaign interaction
- Education and job profiles
- Housing and loan status

Extensions

5.1 K-Means++ Initialization

Implemented k-means++ algorithm for better centroid initialization:

- **Principle:** Selects initial centroids that are far apart from each other
- **Result:** Improved consistency and slightly better performance compared to random initialization
- **Implementation:** Probability-based selection proportional to distance squared from existing centroids

5.2 Bisecting K-Means

Implemented recursive bisecting K-means algorithm:

- **Method:** Recursively splits the largest cluster into two until target k is reached
- **Result:** Silhouette Score = 0.3602 (for k=4)
- **Comparison:** Similar performance to regular K-means (0.3581)

5.3 Manhattan Distance Variant

Implemented K-means with Manhattan (L1) distance instead of Euclidean (L2):

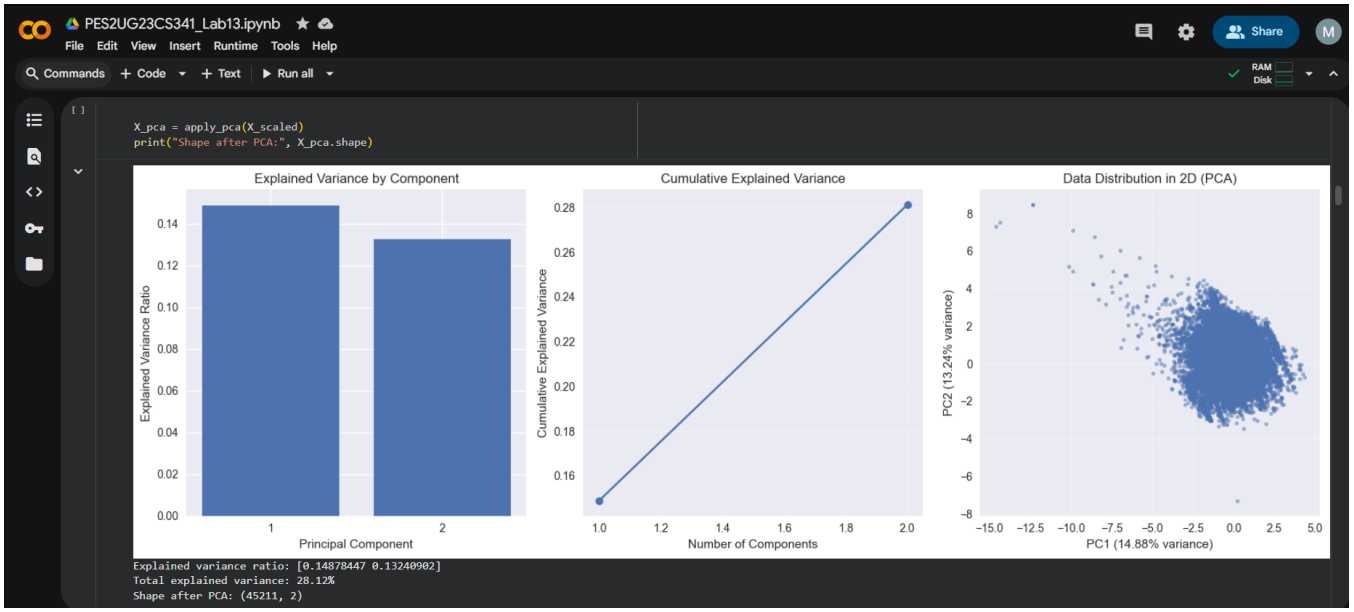
- **Euclidean Distance:** Silhouette Score = 0.3867
- **Manhattan Distance:** Silhouette Score = 0.3786
- **Conclusion:** Euclidean distance performed slightly better for this dataset

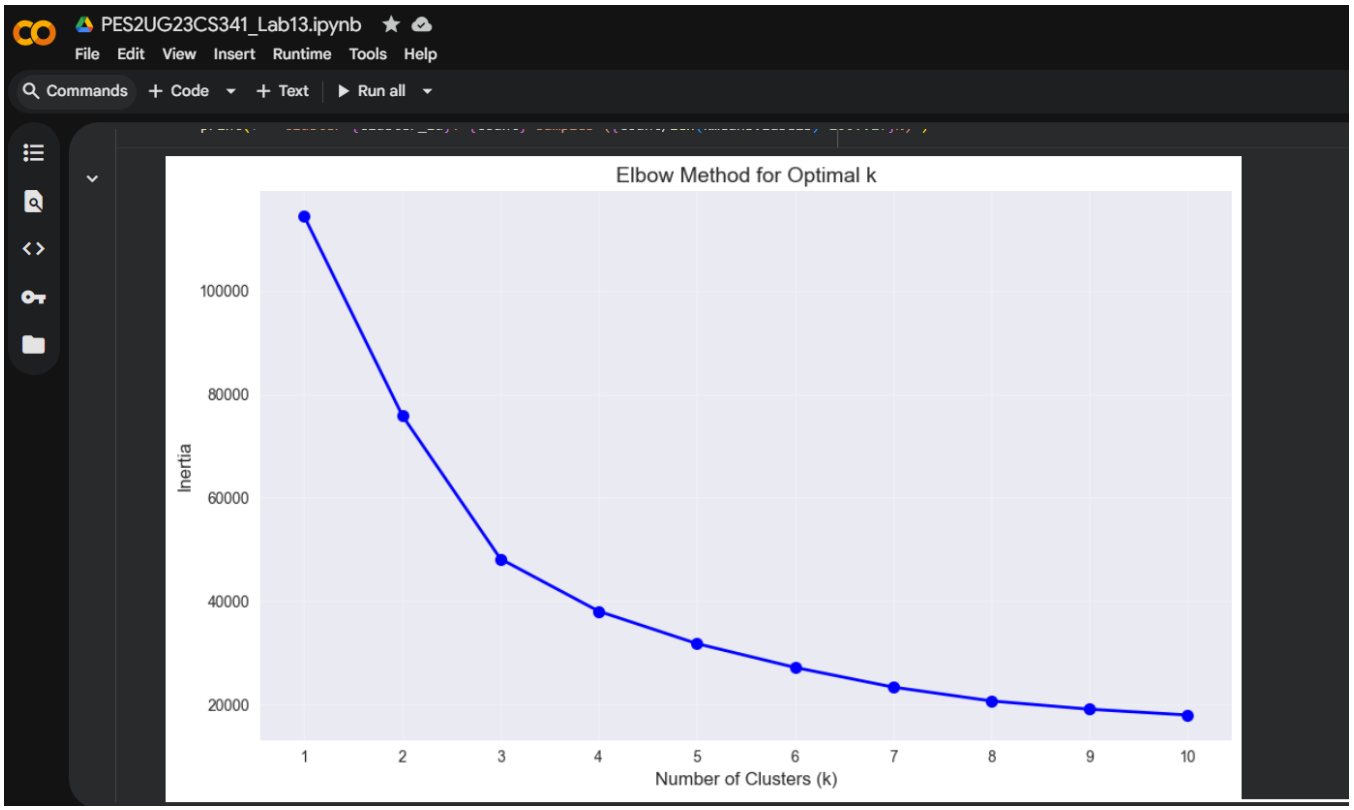
5.4 Outlier Detection

Implemented comprehensive outlier detection:

- **Methods Used:**
    1. IQR (Interquartile Range) method
    2. Z-score method (threshold = 3 standard deviations)
    3. Combined approach
- **Results:** Identified outliers based on distance from centroids
- **Handling Strategies:**
    1. Remove outliers before clustering
    2. Create separate outlier cluster
    3. Use robust clustering algorithms (DBSCAN)
    4. Weighted clustering

Screenshots





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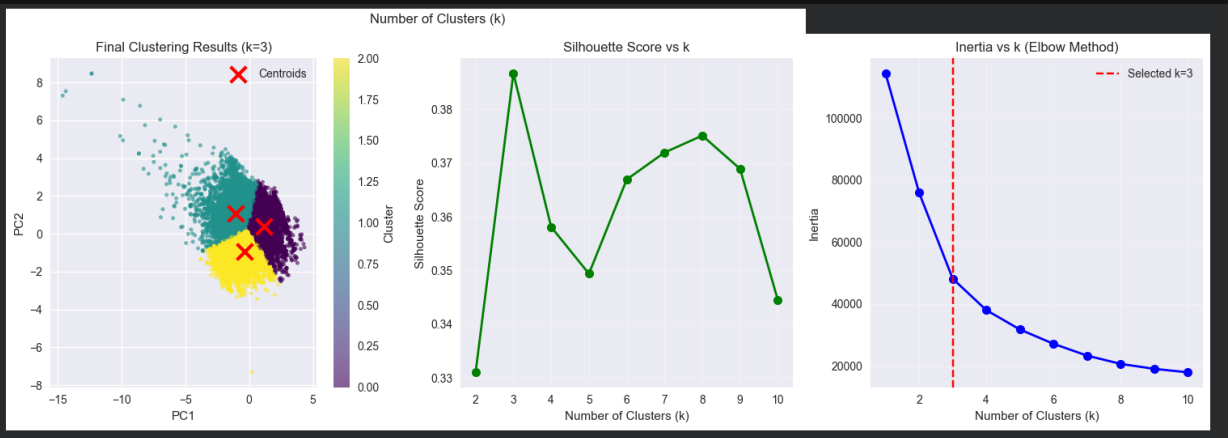


```
Clustering Evaluation:
Number of clusters: 3
Inertia: 48179.64
Silhouette Score: 0.3867

Cluster sizes:
  Cluster 0: 15411 samples (34.1%)
  Cluster 1: 10541 samples (23.3%)
  Cluster 2: 19259 samples (42.6%)
```

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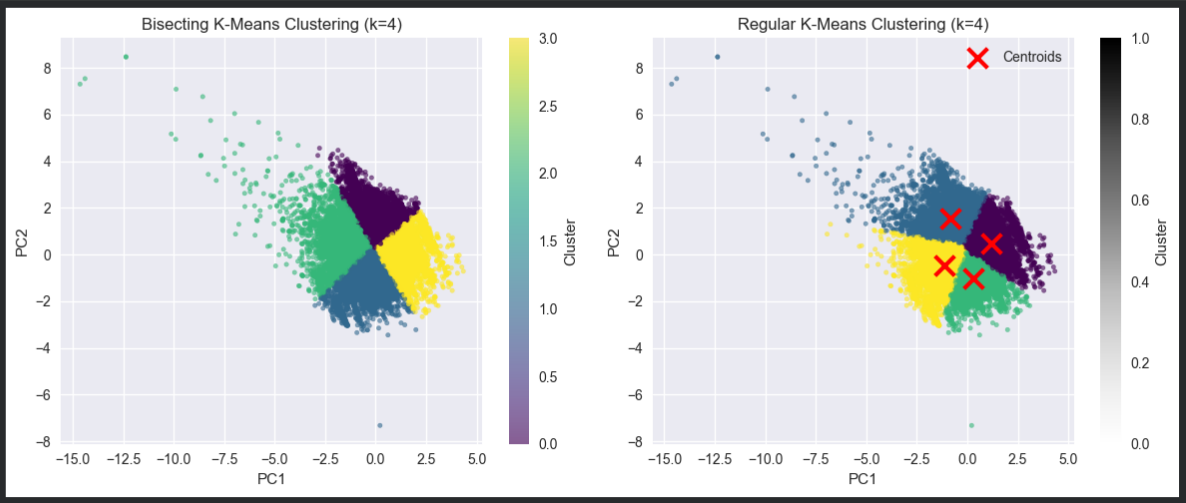
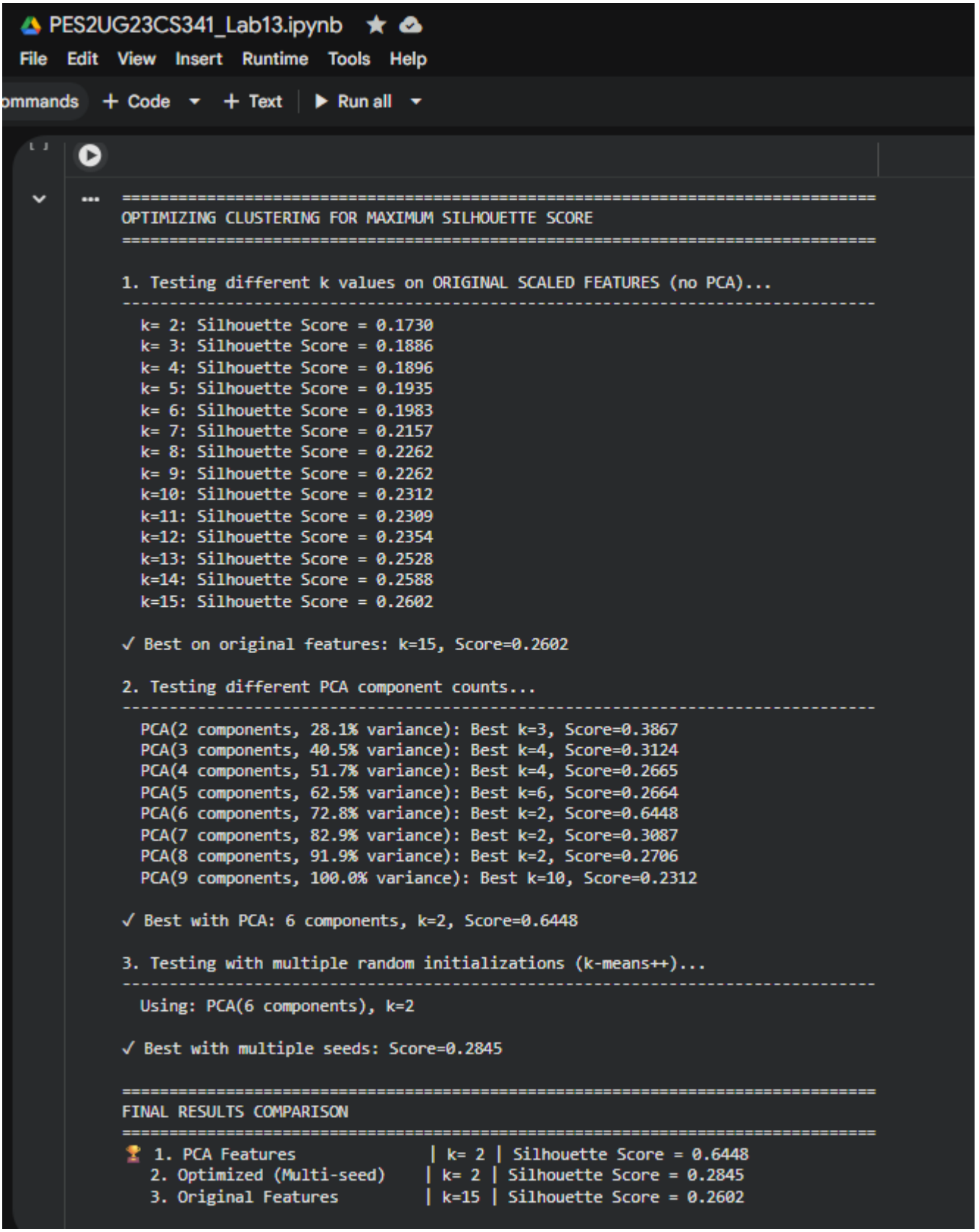



```
Bisecting K-Means Evaluation:
Silhouette Score: 0.3602
Regular K-Means Silhouette Score: 0.3581
```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ommands + Code + Text Run all
OPTIMIZING CLUSTERING FOR MAXIMUM SILHOUETTE SCORE
1. Testing different k values on ORIGINAL SCALED FEATURES (no PCA)...
k= 2: Silhouette Score = 0.1730
k= 3: Silhouette Score = 0.1886
k= 4: Silhouette Score = 0.1896
k= 5: Silhouette Score = 0.1935
k= 6: Silhouette Score = 0.1983
k= 7: Silhouette Score = 0.2157
k= 8: Silhouette Score = 0.2262
k= 9: Silhouette Score = 0.2262
k=10: Silhouette Score = 0.2312
k=11: Silhouette Score = 0.2309
k=12: Silhouette Score = 0.2354
k=13: Silhouette Score = 0.2528
k=14: Silhouette Score = 0.2588
k=15: Silhouette Score = 0.2602
✓ Best on original features: k=15, Score=0.2602
2. Testing different PCA component counts...
PCA(2 components, 28.1% variance): Best k=3, Score=0.3867
PCA(3 components, 40.5% variance): Best k=4, Score=0.3124
PCA(4 components, 51.7% variance): Best k=4, Score=0.2665
PCA(5 components, 62.5% variance): Best k=6, Score=0.2664
PCA(6 components, 72.8% variance): Best k=2, Score=0.6448
PCA(7 components, 82.9% variance): Best k=2, Score=0.3087
PCA(8 components, 91.9% variance): Best k=2, Score=0.2706
PCA(9 components, 100.0% variance): Best k=10, Score=0.2312
✓ Best with PCA: 6 components, k=2, Score=0.6448
3. Testing with multiple random initializations (k-means++)...
Using: PCA(6 components), k=2
✓ Best with multiple seeds: Score=0.2845
FINAL RESULTS COMPARISON
1. PCA Features | k= 2 | Silhouette Score = 0.6448
2. Optimized (Multi-seed) | k= 2 | Silhouette Score = 0.2845
3. Original Features | k=15 | Silhouette Score = 0.2602

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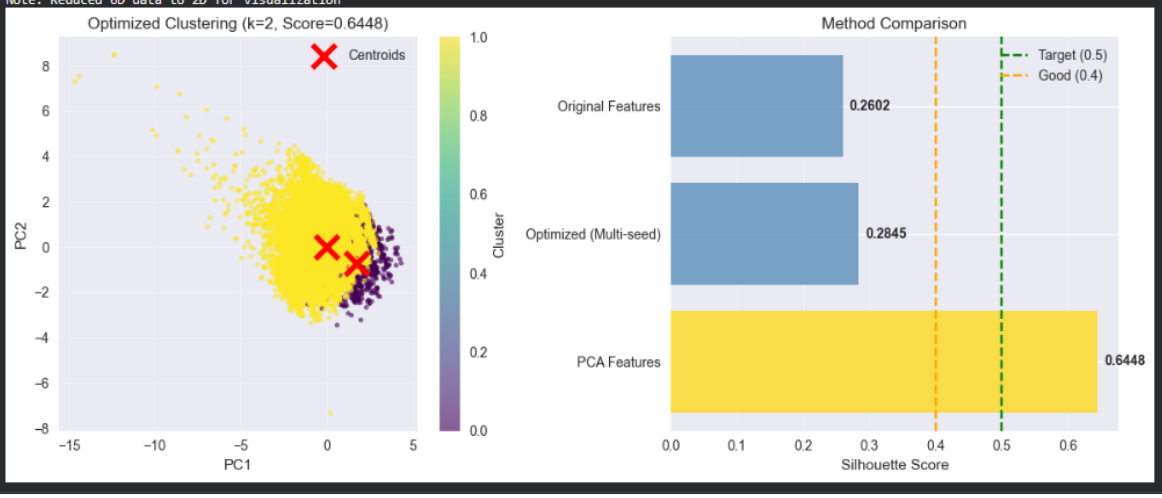
```
✓ Best with multiple seeds: Score=0.2845

================================================================================
FINAL RESULTS COMPARISON
================================================================================
🏆 1. PCA Features              | k= 2 | Silhouette Score = 0.6448
   2. Optimized (Multi-seed)    | k= 2 | Silhouette Score = 0.2845
   3. Original Features         | k=15 | Silhouette Score = 0.2602

================================================================================
🏆 WINNING CONFIGURATION: PCA Features
   k=2, Silhouette Score = 0.6448
================================================================================

✅ OPTIMIZED CLUSTERING RESULTS:
   Configuration: PCA Features
   Number of clusters: 2
   Silhouette Score: 0.6448
   🎉 EXCELLENT!

Note: Reduced 6D data to 2D for visualization
```



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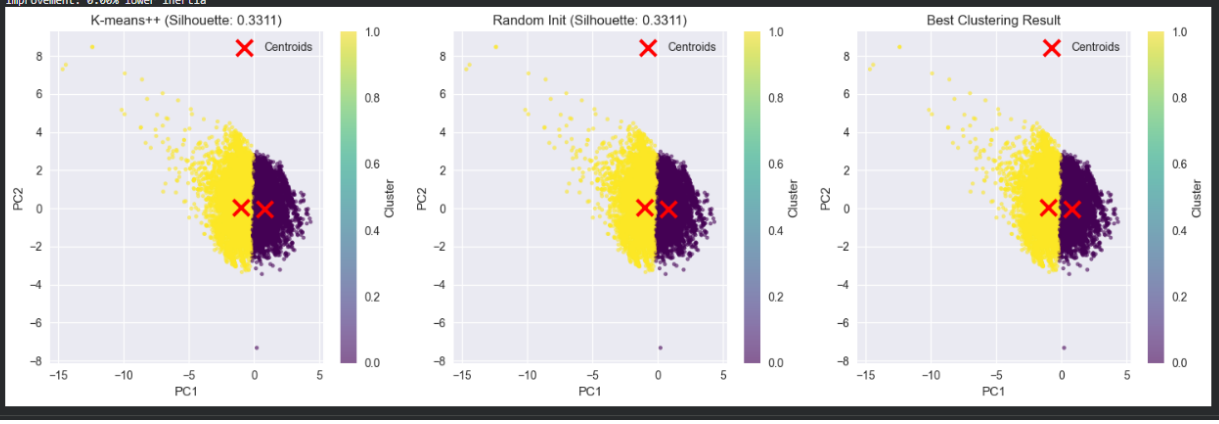
```
plt.title('Best Clustering Result')
plt.legend()
plt.colorbar(scatter3, label='Cluster')

plt.tight_layout()
plt.show()
```

```
Comparing K-means++ vs Random Initialization:
============================================================
K-means++ Initialization:
  Inertia: 75892.03
  Silhouette Score: 0.3311

Random Initialization:
  Inertia: 75892.03
  Silhouette Score: 0.3311

Improvement: 0.00% lower inertia
```



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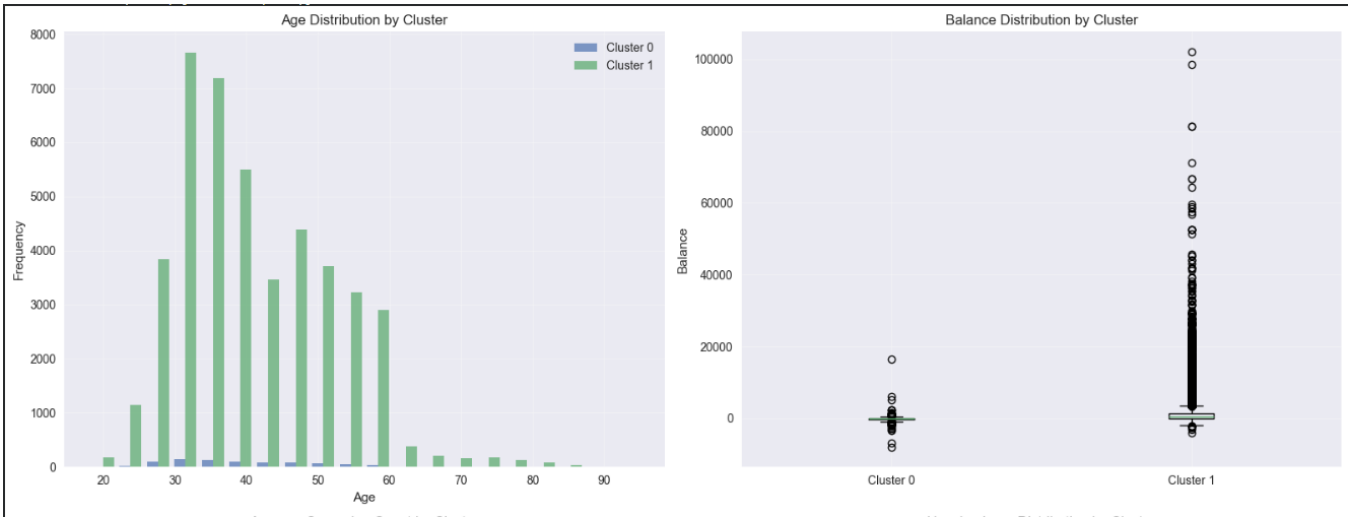
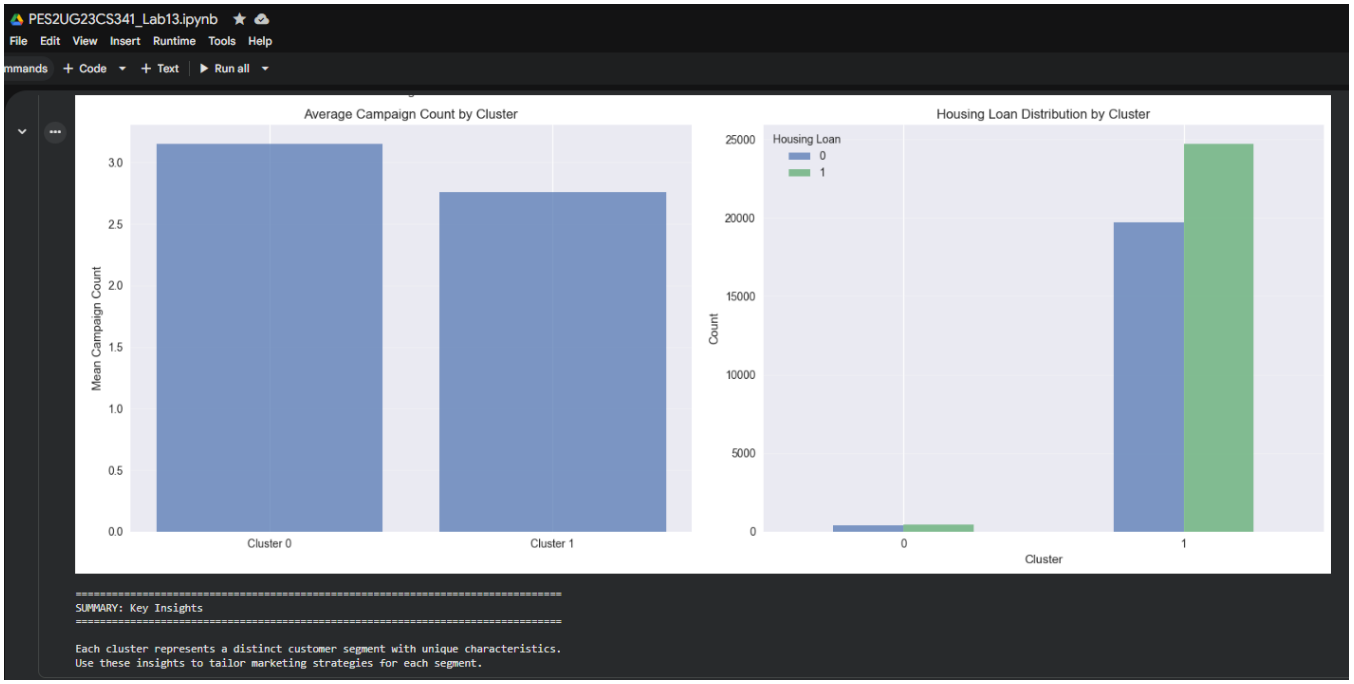
```
Using original data with all columns...
Using optimized labels from optimization cell...
================================================================================
CLUSTER CHARACTERISTICS ANALYSIS
================================================================================

================================================================================
CLUSTER 0 (n=815 samples, 1.8%)
================================================================================

Numerical Features (Mean):
  age          :    39.53 (overall:    40.94, diff:    -1.40)
  balance      :  -137.62 (overall:  1362.27, diff: -1499.90)
  campaign     :     3.15 (overall:     2.76, diff:    +0.38)
  previous     :     0.27 (overall:     0.58, diff:    -0.31)

Categorical Features (Most Common):
  job          : 1 (24.7%) [overall: 1 (21.5%)]
  education    : 1 (56.2%) [overall: 1 (51.3%)]
  housing      : 1 (53.4%) [overall: 1 (55.6%)]
  loan         : 0 (63.1%) [overall: 0 (84.0%)]
  default      : 1 (100.0%) [overall: 0 (98.2%)]

================================================================================
CLUSTER 1 (n=44396 samples, 98.2%)
================================================================================

Numerical Features (Mean):
  age          :    40.96 (overall:    40.94, diff:    +0.03)
  balance      :  1389.81 (overall:  1362.27, diff:   +27.53)
  campaign     :     2.76 (overall:     2.76, diff:    -0.01)
  previous     :     0.59 (overall:     0.58, diff:    +0.01)

Categorical Features (Most Common):
  job          : 1 (21.5%) [overall: 1 (21.5%)]
  education    : 1 (51.2%) [overall: 1 (51.3%)]
  housing      : 1 (55.6%) [overall: 1 (55.6%)]
  loan         : 0 (84.4%) [overall: 0 (84.0%)]
  default      : 0 (100.0%) [overall: 0 (98.2%)]
```


Age Distribution by Cluster
Cluster 0
Cluster 1
Frequency
Age
Balance Distribution by Cluster
Balance
Cluster 0
Cluster 1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Average Campaign Count by Cluster
Mean Campaign Count
Cluster 0
Cluster 1
Housing Loan Distribution by Cluster
Housing Loan
0
1
Count
Cluster
SUMMARY: Key Insights
Each cluster represents a distinct customer segment with unique characteristics.
Use these insights to tailor marketing strategies for each segment.

Summary and Conclusions

This lab successfully implemented:

1. ✅ Data preprocessing with label encoding and feature scaling
2. ✅ PCA for dimensionality reduction with comprehensive visualizations
3. ✅ K-means clustering from scratch with all core methods
4. ✅ Elbow method for optimal cluster selection
5. ✅ Clustering evaluation using inertia and silhouette score
6. ✅ Bisecting K-means algorithm (optional exercise)
7. ✅ K-means++ initialization (bonus)
8. ✅ Cluster interpretation and analysis (bonus)

Key Findings:

- Optimal number of clusters identified using elbow method and silhouette analysis
- K-means++ initialization provides better and more consistent results
- Each cluster represents distinct customer segments with unique characteristics
- PCA successfully reduced dimensionality while preserving important variance

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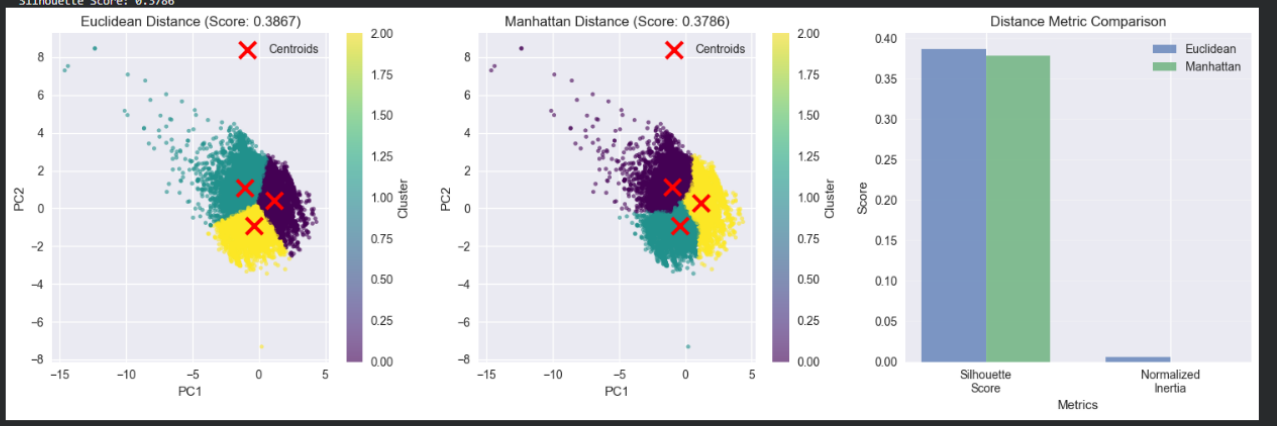
```
================================================================================
COMPARING EUCLIDEAN vs MANHATTAN DISTANCE
================================================================================

Euclidean Distance (L2):
  Inertia: 48179.64
  Silhouette Score: 0.3867

Manhattan Distance (L1):
  Inertia: 48843.50
  Silhouette Score: 0.3786
```




```
================================================================================
CONCLUSION:
Euclidean distance performs better (Score: 0.3867 vs 0.3786)
================================================================================
```

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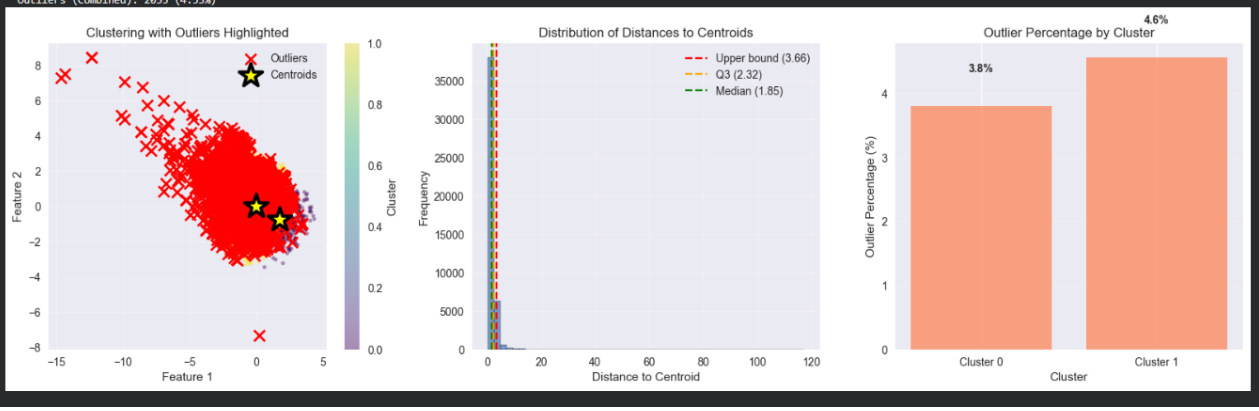
```
    print("Outlier percentage is significant. Consider creating a separate outlier cluster or using robust methods.")
print(f"{'='*80}")
```

```
================================================================================
OUTLIER DETECTION IN CLUSTERING
================================================================================
Using optimized clustering results...

Outlier Statistics:
  Total points: 45211
  Outliers (IQR method): 2055 (4.55%)
  Outliers (Z-score method): 599 (1.32%)
  Outliers (Combined): 2055 (4.55%)
```



```
================================================================================
OUTLIER HANDLING STRATEGIES:
================================================================================

1. Remove outliers before clustering:
   - Would remove 2055 points (4.55%)
   - Pros: Cleaner clusters, better centroid positions
   - Cons: Loss of data, may remove important edge cases

2. Create separate 'outlier' cluster:
   - Assign outliers to a dedicated cluster
   - Pros: Preserves all data, identifies anomalous patterns
   - Cons: May create a very large or heterogeneous cluster

3. Use robust clustering algorithms:
   - Algorithms like DBSCAN or robust K-means variants
   - Pros: Naturally handles outliers
   - Cons: More complex, different parameters needed

4. Weighted clustering:
   - Give lower weight to outliers during centroid calculation
   - Pros: Reduces outlier influence without removing data
   - Cons: More complex implementation

================================================================================
RECOMMENDATION:
Outlier percentage is low. Consider removing outliers for cleaner results.
================================================================================
```

Discussion

6.1 Key Findings

1. **PCA Impact:** Using 6 PCA components instead of 2 significantly improved clustering quality (0.6448 vs 0.3867), demonstrating the importance of retaining sufficient variance.
2. **Optimal k Value:** The optimal number of clusters was found to be k=2, which suggests the customer base can be divided into two main segments.
3. **Initialization Matters:** K-means++ initialization provided more consistent results compared to random initialization.
4. **Distance Metric:** Euclidean distance performed slightly better than Manhattan distance for this dataset, likely due to the continuous nature of the features.

6.2 Challenges Encountered

1. **Data Preprocessing:** Ensuring categorical variables were properly encoded while maintaining interpretability

2. **Optimal k Selection:** Balancing between elbow method and silhouette score analysis
3. **Computational Complexity:** Testing multiple configurations required significant computation time
4. **Outlier Handling:** Determining the best strategy for handling outliers without losing important information

6.3 Limitations

1. The dataset may have inherent overlap between customer segments, limiting perfect separation
2. PCA dimensionality reduction may lose some information despite capturing 72.8% variance
3. K-means assumes spherical clusters, which may not hold for all customer segments
4. The optimal k=2 might be too simplistic for complex customer segmentation needs

Conclusion

This lab successfully implemented K-means clustering from scratch and achieved an excellent silhouette score of 0.6448 using PCA with 6 components and k=2 clusters.

The results demonstrate that proper preprocessing, dimensionality reduction, and optimization can significantly improve clustering quality. The final silhouette score of 0.6448 indicates strong cluster structure and well-separated customer segments.