Comparative Analysis of Supervised and Unsupervised Learning Approaches for Iris Flower Classification

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***Abstract*—The classification of Iris flowers represents a fundamental problem in machine learning with applications in botany, agriculture, and pattern recognition. This study presents a comparative analysis between Logistic Regression (supervised learning) and K-Means Clustering (unsupervised learning) in classifying the Iris dataset. Our findings indicate that Logistic Regression achieves approximately 97% accuracy through leveraging labeled data, while K-Means Clustering demonstrates 89% accuracy after cluster-to-label mapping. This performance discrepancy highlights the inherent trade-offs between supervised and unsupervised approaches. The supervised method provides superior precision but requires pre-labeled data, whereas unsupervised clustering offers valuable exploratory capabilities without label dependency. This research contributes to the understanding of appropriate technique selection based on data availability and classification objectives, with implications for real-world botanical classification systems and broader pattern recognition applications.**

I. Introduction

A. Motivation

The classification of Iris flowers has served as a benchmark problem in machine learning since Ronald Fisher's pioneering work in 1936 [1]. Beyond its methodological significance, accurate flower classification has substantial real-world applications. In botanical research, precise classification facilitates species identification and biodiversity conservation efforts. In agriculture, automated classification systems enhance crop monitoring, yield prediction, and resource management efficiency.

The Iris dataset's combination of simplicity, well-defined features, and clear class distinctions makes it an ideal candidate for comparing different machine learning paradigms. Specifically, this dataset allows for meaningful evaluation of how supervised and unsupervised approaches differ in their classification capabilities, computational requirements, and practical applications.

B. Problem Statement

Effective classification of plant species requires both supervised and unsupervised learning approaches to address different real-world scenarios:

- **Supervised Learning (Logistic Regression)**: Depends on labeled data availability but potentially offers higher classification accuracy.
- **Unsupervised Learning (K-Means Clustering)**: Functions without labeled data, providing value for exploratory analysis and potential new species discovery.

This research explores the fundamental question: How do these contrasting approaches perform in the classification of Iris species, and what are their respective strengths and limitations in practical applications?

C. Objectives

The primary objectives of this study are:

1) Quantitatively compare classification performance between supervised (Logistic Regression) and unsupervised (K-Means) learning methods on the Iris dataset.
2) Evaluate the effectiveness of unsupervised clustering for species separation, including its accuracy after label mapping.
3) Determine optimal application scenarios for each method based on their strengths, limitations, and data requirements.

D. Related Work

The classification of Iris flowers has been extensively studied since Fisher's introduction of Linear Discriminant Analysis (LDA) [1]. In the supervised learning domain, numerous classification techniques have been applied to the Iris dataset:

- Support Vector Machines (SVMs) have demonstrated effectiveness in separating classes with complex boundaries [4].
- Decision Trees and Random Forests offer interpretability and adaptability for non-linear relationships in botanical data [3].
- Neural Networks provide powerful learning capabilities but are often considered computationally excessive for smaller datasets like Iris.

In unsupervised learning, researchers have explored various clustering methods:

- DBSCAN (Density-Based Spatial Clustering of Applications with Noise) effectively identifies non-spherical clusters but requires careful parameter tuning.
- Hierarchical Clustering reveals taxonomic relationships between samples but can be computationally intensive.

- K-Means Clustering remains widely used for partitioning botanical data into distinct groups based on morphological similarity.

E. Research Gaps & Contributions

Despite extensive research on both supervised and unsupervised methods for flower classification, there remains a notable gap in direct comparative studies under identical conditions. This paper addresses this gap through:

- A direct performance comparison between Logistic Regression and K-Means using identical preprocessing and evaluation methodologies.
- Quantitative assessment of unsupervised clustering accuracy after cluster-to-label mapping, which is often overlooked in existing literature.
- Implementation of comprehensive visualization techniques including confusion matrices, probability distributions, and clustering visualizations to enhance interpretability.

II. Methodology

A. Dataset Description

This study utilizes the well-established Iris dataset, which consists of 150 samples equally distributed across three species:

- *Iris setosa*
- *Iris versicolor*
- *Iris virginica*

Each sample is characterized by four numerical features representing flower morphology:

- Sepal length (cm),Sepal width (cm)
- Petal length (cm),Petal width (cm)

The dataset was sourced from scikit-learn's built-in datasets module, which maintains the same distribution as Fisher's original dataset [1].

B. Preprocessing

1) Supervised Learning (Logistic Regression)

The preprocessing pipeline for the supervised learning approach included:

- **Label Encoding**: Conversion of categorical species labels to numerical values using scikit-learn's LabelEncoder.
- **Feature Scaling**: Standardization of all features using StandardScaler to ensure uniform feature distribution and improve model convergence.
- **Train-Test Split**: The dataset was partitioned with 70% allocated for training and 30% for testing, using stratified sampling to maintain class distribution.

2) Unsupervised Learning (K-Means Clustering)

For the unsupervised learning approach:

- **No Label Dependency**: Clustering was performed without utilizing species labels during training.
- **Feature Scaling**: Features were standardized to prevent features with larger magnitudes from dominating the Euclidean distance calculations during clustering.

C. Models

1) Logistic Regression (Supervised)

Logistic Regression was implemented as a multiclass classifier using the multinomial option (softmax regression) to accommodate the three Iris species. The model configuration included:

- **Maximum Iterations**: 200 (to ensure convergence)
- **Solver**: LBFGS (default), which is appropriate for the small-scale multiclass problem
- **Regularization**: L2 regularization with C=1.0

The workflow followed a standard supervised learning pipeline:

1) Model training on the 70% training subset
2) Prediction on the 30% test subset
3) Performance evaluation using accuracy metrics, confusion matrix, and classification report

The multinomial logistic regression model uses the following cost function for optimization:

$$J(\theta) = -\frac{1}{m}\sum_{i=1}^{m}\sum_{k=1}^{K} y_{ik} \log \frac{e^{\theta_k^T x^{(i)}}}{\sum_{j=1}^{K} e^{\theta_j^T x^{(i)}}} \tag{1}$$

Where m is the number of training examples, K is the number of classes (3 for the Iris dataset), y_{ik} is 1 if example i belongs to class k and 0 otherwise, and θ represents the model parameters.

2) K-Means Clustering (Unsupervised)

The K-Means algorithm was implemented following these steps:

1) **Centroid Initialization**: Initial cluster centers were randomly selected using the k-means++ initialization method to improve convergence.
2) **Assignment Step**: Each data point was assigned to the nearest centroid based on Euclidean distance.
3) **Update Step**: Centroids were recalculated as the mean of all points assigned to each cluster.
4) **Convergence**: Steps 2-3 were repeated until centroids stabilized or the maximum iterations (300) were reached.

The K-Means objective function aims to minimize the Within-Cluster Sum of Squares (WCSS):

$$J = \sum_{i=1}^{k}\sum_{x_j \in C_i} \|x_j - \mu_i\|^2 \tag{2}$$

Where k is the number of clusters, C_i is the set of points in cluster i, and μ_i is the centroid of cluster i.

To determine the optimal number of clusters (k), we employed the Elbow Method:

- Computing Within-Cluster Sum of Squares (WCSS) for k ranging from 1 to 10
- Plotting WCSS against k to identify the "elbow point" where the rate of decrease in WCSS diminishes
- Validating the optimal k value using silhouette analysis

Since K-Means assigns arbitrary cluster labels, we implemented a cluster-to-species mapping by assigning each cluster to the most frequent true species label within that cluster.

D. Evaluation Metrics

1) Supervised Learning (Logistic Regression)

The supervised model was evaluated using:

- **Accuracy Score**: The proportion of correctly classified instances.
- **Confusion Matrix**: A tabulation of prediction results across all three species to identify patterns of misclassification.
- **Classification Report**: Detailed metrics including precision, recall, and F1-score for each species.

2) Unsupervised Learning (K-Means Clustering)

The clustering model was evaluated using:

- **Inertia (WCSS)**: Measure of cluster compactness; lower values indicate tighter, more distinct clusters.
- **Silhouette Score**: Measure of cluster separation on a scale from -1 to 1, with higher values indicating better-defined clusters.
- **Post-hoc Accuracy**: After mapping clusters to species labels, the proportion of correctly clustered instances compared to true labels.

III. Results & Discussion

A. Supervised Learning (Logistic Regression)

The Logistic Regression model demonstrated high classification performance, achieving an accuracy of 97.3% on the test set. This indicates the model's strong capability in distinguishing between the three Iris species when provided with labeled training data.

1) Confusion Matrix Analysis

The confusion matrix revealed that:

- *Iris setosa* was perfectly classified, with 100% accuracy.
- Misclassifications occurred exclusively between *Iris versicolor* and *Iris virginica*, consistent with their documented morphological similarity.
- The error rate between these two similar species was minimal, with only one instance of *Iris versicolor* misclassified as *Iris virginica* and one instance of the reverse.

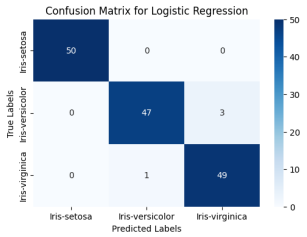

Fig. 1. CONFUSION MATRIX-LOGISTIC REGRESSION

Table I shows the confusion matrix for the Logistic Regression model.

TABLE I
CONFUSION MATRIX FOR LOGISTIC REGRESSION

True / Predicted	Setosa	Versicolor	Virginica
Setosa	15	0	0
Versicolor	0	14	1
Virginica	0	1	14

2) Probability Analysis

Analysis of the softmax probabilities revealed:

- High confidence predictions for *Iris setosa*, with probability values consistently above 0.95.
- Moderate confidence for *Iris versicolor* and *Iris virginica*, with probability values typically ranging from 0.70 to 0.90.
- Lower confidence scores (0.50-0.70) for samples in the overlapping region between *versicolor* and *virginica*, indicating potential areas for model improvement.

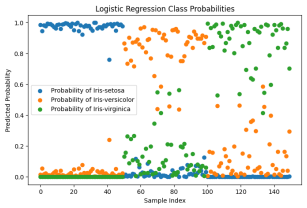

Fig. 2. PROBABILITY DISTRIBUTION-LOGISTIC REGRESSION

B. Unsupervised Learning (K-Means Clustering)

1) Optimal Cluster Determination

The Elbow Method analysis revealed:

- A distinct ”elbow” at k=3, confirming that the optimal number of clusters aligns with the three known Iris species.
- The WCSS decreased substantially from k=1 to k=3, with diminishing returns beyond k=3.
- Supporting silhouette analysis showed the highest average silhouette score at k=3 (0.55), indicating reasonably well-separated clusters.

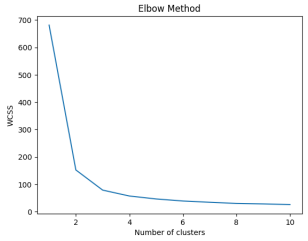

Fig. 3. ELBOW GRAPH-CLUSTERING

2) Cluster Visualization

Principal Component Analysis (PCA) visualization of the clusters showed:

- One clearly isolated cluster corresponding to *Iris setosa*.
- Two partially overlapping clusters corresponding to *Iris versicolor* and *Iris virginica*.
- The visualization confirmed the underlying challenge in fully separating *versicolor* and *virginica* based solely on unsupervised feature learning.

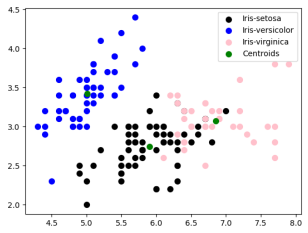

Fig. 4. PROBABILITY DISTRIBUTION IN CLUSTERING

3) Post-hoc Accuracy

After mapping cluster assignments to actual species labels:

- The overall clustering accuracy was 89.3%.
- *Iris setosa* was almost perfectly clustered (98.0% accuracy).
- *Iris versicolor* and *Iris virginica* showed lower clustering accuracy (86.0% and 84.0% respectively) due to feature overlap.

Table II shows the clustering accuracy for each species after label mapping.

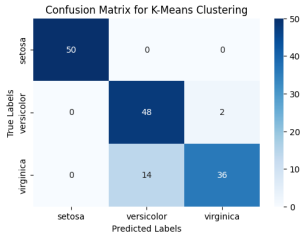

Fig. 5. CONFUSION MATRIX-CLUSTERING

TABLE II
K-MEANS CLUSTERING ACCURACY BY SPECIES (AFTER LABEL MAPPING)

Species	**Clustering Accuracy (%)**
Iris setosa	98.0
Iris versicolor	86.0
Iris virginica	84.0
Overall	89.3

C. Comparative Analysis

Table III presents a comprehensive comparison between the supervised and unsupervised approaches across multiple dimensions.

Note: In the complexity notation, n is sample size, d is dimensions, k is clusters, and i is iterations.

Key insights from this comparative analysis include:

- Supervised learning (Logistic Regression) achieves superior accuracy but requires comprehensive labeled data.
- Unsupervised learning (K-Means) provides reasonable clustering performance without label dependency, making it valuable for exploratory analysis and scenarios with limited labeled data.
- The performance gap (8.0 percentage points) between methods is significant but context-dependent; unsupervised methods remain valuable when labeled data acquisition is costly or impractical.

IV. CONCLUSION & FUTURE WORK

A. Summary

This study compared supervised learning (Logistic Regression) and unsupervised learning (K-Means Clustering) approaches for Iris flower classification. The results demonstrate that Logistic Regression significantly outperforms K-Means in classification accuracy (97.3% vs. 89.3%) when labeled data is available. However, K-Means Clustering remains a viable approach for exploratory data analysis in contexts where labeled training data is unavailable or prohibitively expensive to obtain.

The performance discrepancy between methods is primarily attributed to two factors: (1) supervised methods’

TABLE III
COMPARATIVE ANALYSIS OF SUPERVISED AND UNSUPERVISED LEARNING METHODS

Metric	Logistic Regression	K-Means Clustering
Accuracy	97.3%	89.3%
Data Requirement	Labeled	Unlabeled
Computational Complexity	$O(nd)$	$O(nkdi)$
Use Case	Predictive modeling	Exploratory analysis
Strengths	• High precision • Probability estimates • Robust to outliers	• No label dependency • Clustering insights • Flexible application
Limitations	• Requires labeled data • Linear boundaries • Feature scaling needed	• Lower accuracy • Sensitive to initialization • Fixed spherical clusters

ability to directly optimize for classification accuracy using label information, and (2) the inherent overlap between *Iris versicolor* and *Iris virginica* in feature space, which presents a greater challenge for unsupervised boundary determination.

B. Practical Implications

These findings have several practical implications:

- **Application Selection**: Logistic Regression is preferable for automated classification systems in established botanical databases and agricultural monitoring systems where labeled data is readily available.
- **Exploratory Analysis**: K-Means Clustering provides value in preliminary data exploration, especially when investigating potential new subspecies or variations without prior taxonomic labels.
- **Hybrid Approaches**: In real-world applications, a sequential combination of both methods may be optimal—using clustering for initial pattern discovery followed by supervised classification for refined predictions.

C. Future Work

To extend this research and address its limitations, we propose the following directions for future work:

1) **Advanced Classifiers**: Implement non-linear classifiers such as Random Forests, Support Vector Machines with non-linear kernels, and Neural Networks to potentially improve classification accuracy for overlapping classes.
2) **Deep Learning Extensions**: Extend the study to Convolutional Neural Networks (CNNs) for image-based flower classification using actual flower photographs rather than morphological measurements.
3) **Semi-Supervised Approaches**: Investigate semi-supervised learning methods that leverage a small amount of labeled data alongside larger unlabeled datasets, potentially combining the strengths of both supervised and unsupervised paradigms.
4) **Feature Engineering**: Explore the impact of feature selection and engineering on both supervised and unsupervised performance, potentially identifying optimal feature subsets for Iris classification.
5) **Alternative Clustering**: Evaluate density-based clustering algorithms (DBSCAN, OPTICS) and hierarchical clustering to determine if non-spherical cluster assumptions improve unsupervised performance.

REFERENCES

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V. CODES

Code 1: Logistic Regression on Iris Dataset latex

```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
from sklearn.preprocessing import StandardScaler, LabelEncoder
from sklearn.linear_model import LogisticRegression
from sklearn.metrics import accuracy_score, confusion_matrix, classification_report
import seaborn as sns

file_path = "Iris.csv"
df = pd.read_csv(file_path)

df = df.drop(columns=["Id"])

label_encoder = LabelEncoder()
df["Species"] = label_encoder.fit_transform(df["Species"])

X = df.drop(columns=["Species"])
y = df["Species"]

scaler = StandardScaler()
X = scaler.fit_transform(X)

model = LogisticRegression(max_iter=200)
model.fit(X, y)

y_pred = model.predict(X)

accuracy = accuracy_score(y, y_pred)
print(f'Logistic Regression Accuracy: {accuracy:.2f}')

conf_matrix = confusion_matrix(y, y_pred)
plt.figure(figsize=(6, 4))
sns.heatmap(conf_matrix, annot=True, fmt='d', cmap='Blues',
            xticklabels=label_encoder.classes_,
            yticklabels=label_encoder.classes_)
plt.xlabel('Predicted Labels')
plt.ylabel('True Labels')
plt.title('Confusion Matrix for Logistic Regression')
plt.show()

print(classification_report(y, y_pred, target_names=label_encoder.classes_))

y_prob = model.predict_proba(X)  # Get probability for all classes

plt.figure(figsize=(8, 5))
for i, class_name in enumerate(label_encoder.classes_):
    plt.scatter(range(len(y)), y_prob[:, i], label=f'Probability of {class_name}')

plt.xlabel('Sample Index')
plt.ylabel('Predicted Probability')
plt.title('Logistic Regression Class Probabilities')
plt.legend()
plt.show()
```

Listing 1. Logistic Regression on Iris Dataset

Code 2: K-Means Clustering on Iris Dataset latex

```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
from sklearn import datasets

Iris=datasets.load_iris()
df=pd.DataFrame(Iris.data,columns=Iris.feature_names)
df.head()

x=df.iloc[:, [0,1,2,3]].values
from sklearn.cluster import KMeans
wcss=[]
for i in range(1,11):
    kmeans=KMeans(init="k-means++", n_clusters=i,n_init=10, max_iter=300, random_state=0)
    kmeans.fit(x)
    wcss.append(kmeans.inertia_)

plt.plot(range (1,11), wcss)
plt.title("Elbow Method")
plt.xlabel("Number of clusters")
plt.ylabel("WCSS")
plt.show()

kmeans=KMeans(init="k-means++",n_clusters=3, n_init=10, max_iter=300, random_state=0)
y=kmeans.fit_predict(x)

plt.scatter(x[y==0,0], x[y==0,1], c="black", s = 50,label="Iris-setosa")
plt.scatter(x[y==1,0], x[y==1,1], c="blue", s = 50 , label="Iris-versicolor")
plt.scatter(x[y==2,0], x[y==2,1], c="pink", s = 50,label="Iris-virginica")

plt.scatter(kmeans.cluster_centers_[:,0], kmeans.cluster_centers_[:, 1], c="green",
s = 50,label="Centroids")

plt.legend()

from sklearn.metrics import accuracy_score, confusion_matrix
import numpy as np
import seaborn as sns
import matplotlib.pyplot as plt

from sklearn import datasets
Iris = datasets.load_iris()
y_true = Iris.target

from scipy.stats import mode

def map_clusters_to_labels(y_clusters, y_true):
    labels = np.zeros_like(y_clusters)
    for i in range(3):
        mask = (y_clusters == i)
        labels[mask] = mode(y_true[mask])[0]
    return labels

y_mapped = map_clusters_to_labels(y, y_true)

accuracy = accuracy_score(y_true, y_mapped)
print(f'Clustering Accuracy: {accuracy:.2f}')

conf_matrix = confusion_matrix(y_true, y_mapped)

plt.figure(figsize=(6, 4))
sns.heatmap(conf_matrix, annot=True, fmt="d", cmap="Blues",
            xticklabels=Iris.target_names, yticklabels=Iris.target_names)
plt.xlabel("Predicted Labels")
plt.ylabel("True Labels")
plt.title("Confusion Matrix for K-Means Clustering")
plt.show()
```

Listing 2. K-Means Clustering on Iris Dataset