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# Enhanced Machine Learning With Topological Data Analysis: A Unified Model Performance Comparison On IRIS Datasets

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## ABSTRACT

The integration of Topological Data Analysis (TDA) with traditional Machine Learning (ML) techniques has emerged as a promising approach to enhance data representation, improve predictive performance, and capture complex structures in datasets. This study investigates the unified application of TDA features alongside conventional ML algorithms for the classification performance on relatively simple, low-dimensional data like the Iris datasets. Using persistent homology for feature extraction and combining these features with several standard ML classifiers such as K-Nearest Neighbors (KNN), Support Vector Machines (SVM) and Random Forest (RF) models, a comprehensive performance comparison is conducted using accuracy, precision, recall, and F1-score metrics. Performance was assessed for TDA only, ML only, and integrated TDA–ML pipelines. Implementations were carried out in Python environment, with models compared on accuracy and computational efficiency. The results indicate that while some standard algorithms already achieved high accuracy on the Iris dataset, the inclusion of topological features leads to more consistent performance across different models and potentially improves model robustness. This study showed that TDA–ML integration often outperforms traditional ML routines. Accuracy improved from 0.850 - 0.984 for RF, 0.825 - 0.962 for K-NN and 0.835 - 0.972 for SVM models, with similar gains in precision, recall, and F1-score. Overall results indicate that TDA features alone yield relatively lower performance compared to their integration with machine learning which led to substantial improvements across all metrics. The study confirmed that incorporating topological features enhances the predictive effectiveness of machine learning models.

**Keywords:** Topological Data Analysis, Machine Learning, Persistent Homology, Iris Dataset, Classification, Performance Comparison, Topology-Algebra, Iris datasets.

## INTRODUCTION

The rapid expansion of machine learning has revolutionized pattern recognition and predictive modeling across disciplines (Rasheed, 2023). It is possible that traditional algorithms may overlook complex intrinsic structures in data, particularly subtle geometric or topological patterns that govern class separability. Recent updates in computational and statistical sciences have demonstrated the potentials of digital systems to improve data analyses processes. For instance, in the field of epidemiology, Mamadu et al. (2020) used the Variational Iteration Orthogonal Collocation Method (VIOCM) to solve a four-compartment epidemic model, highlighting how hybrid numerical approaches can enhance predictive accuracy in public health contexts. Similarly, Osemeke et al. (2024) examined the relationships between model assumptions, violations and multicollinearity, emphasizing robust statistical validation techniques

that indicate system reliability and performance. In another study, Onyemarin et al. (2023) applied Auto-Regressive Moving Average time-series to analyse the infant mortality trends in Nigeria, illustrating the potentials of stochastic models in predicting healthcare needs. These works collectively underscored the importance of integrating mathematical theory and data-driven strategies as advocated by Igabari (2017) so as to understand and improve on quality and value of data analysis with technology solutions.

Topological Data Analysis (TDA) has emerged as a robust mathematical framework for extracting features that represent the shape of data in high dimensions and across multiple scales (Skraba, 2018). Unlike conventional feature engineering, Abed (2024) pioneered TDA leverages tools from algebraic topology, such as persistent homology, to quantify how topological features (e.g., connected components, holes, voids) persist across various scales of data filtration. This yields descriptors that are invariant under continuous deformations and robust to noise and perturbations (Kabir et al, 2023).

Zomorodian and Carlsson (2005) pioneered computational methods for persistent homology, laying the groundwork for TDA applications in complex datasets. Skraba (2018) proposed that persistent homology extracts multi-scale topological features, representing the birth and death of topological structures in data. Also, Pedregosa et al (2011) highlighted the role of ML algorithms such as Support Vector Machines (SVM), Random Forests (RF), and k-Nearest Neighbors (k-NN) in standard supervised learning tasks (Balaji et al, 2021). While effective, these methods may fail to leverage the global topological properties inherent in structured datasets. Kramár and Kramár (2020) explored the hybridization of TDA with ML, showing improved predictive capabilities when topological summaries are included as input features.

Recent researches such as Adam and Moy (2021), and Leykam and Angelakid (2023) underscores how TDA can be integrated with machine learning to improve model performance. For instance, studies show that augmenting traditional classifiers with TDA-derived features enhances predictive accuracy and model robustness, particularly in tasks involving complex and high-dimensional datasets from biological measurements to customer churn prediction according to Valentino (2022); Sagming et al (2024) by capturing high-level structural information often omitted by standard feature spaces.

Persistent homology, one of the central tools in TDA, computes multi-scale topological summaries that TDA can be vectorized for integration with machine learning models (Katya, 2023). Performance evaluations using persistent homology classifiers according to Vaghasia et al (2025) have shown competitive results with classical methods such as Support Vector Machines (SVM), Random Forests (RF) and K-Nearest Neighbors (KNN) on benchmark datasets, including the Iris dataset a ubiquitous dataset in machine learning research introduced by (Fisher 1936). Despite advances in topological methods, systematic comparisons of traditional ML models with and without TDA enhancements are still limited in the literature. In this work, we address this gap by presenting already developed unified workflow of Esokpor and Igabari (2026) across multiple classifiers on the Iris dataset, contrasting baseline models with versions augmented by TDA features. We aim to establish empirical evidence of the utility of TDA in classical supervised learning and delineate contexts where topological augmentation yields significant benefits.

### **Topological Data Analysis (TDA)**

Topological Data Analysis uses concepts from algebraic topology to understand the shape of data. Persistent homology, a key tool in TDA, quantifies topological features across scales by building a sequence of simplicial complexes through filtrations, and then computing the birth and death of features such as connected components and cycles. The resulting persistence diagrams or barcodes can be vectorized for use in machine learning pipelines.(Zomorodion and Carlson, 2005).

### **Iris Dataset**

The Iris dataset, introduced by Ronald A. Fisher in 1936, is a well-studied benchmark in machine learning and pattern recognition. It consists of 150 observations of iris flowers classified into three species (Iris setosa, Iris versicolor, and Iris virginica) based on four morphological features: sepal length, sepal width, petal length, and petal width. Its small size and clear class distinctions make it suitable for evaluating classifier performance and feature extraction techniques.

### **Integration of TDA with ML**

Embedding topological features into ML models typically involves computing persistence diagrams and converting them into fixed-length feature vectors using methods such as persistence landscapes, persistence images, or barcode statistics. These features are subsequently used as additional input variables for classifiers like SVM, Random Forest, or K-NN, or serve as inputs to TDA-specific classifiers grounded on topological structures (Zia et al, 2024; Chen et al, 2024).

These representations can be transformed into vector-based feature representations, such as persistence landscapes, that are suitable for use with standard ML algorithms (Zomorodian and Carlsson, 2005).

This paper investigates the benefit of integrating TDA-derived features into established ML workflows using the Iris dataset. We aim to quantify the performance difference between models trained solely on the original four features versus those augmented with topological insights.

## **MATERIALS AND METHODOLOGY**

### **Data Collection**

The data collection method employed is programmatic synthetic data generation, which allows for the precise creation of datasets with known geometric and topological properties (Esokpor and Igabari 2026). The dataset used in this study was synthetically generated using Python libraries such as NumPy and scikit-learn.

### **Dataset Description**

The Iris dataset, was Created by Sir Ronald A. Fisher in 1936, and it comprises of 150 instances across three species (Iris setosa, Iris versicolor, Iris virginica) with four features: sepal length, sepal width, petal length, and petal width. The dataset is split into 70% training and 30% testing sets. Hence, the dataset consisted of a sample of 150 items of Iris flowers from 3 different species and 4 features. Samples per species were 50 items each.

### **Topological Data Extraction**

Persistent homology is employed to extract topological features. The steps are:

- i. Point cloud representation:** Each Iris instance is represented in 4-dimensional feature space.
- ii. Distance matrix computation:** Euclidean distances are computed between points.
- iii. Filtration and persistence diagrams:** Construct a Vietoris–Rips filtration and compute persistence intervals for 0-dimensional and 1-dimensional homology.
- iv. Vectorization:** Persistence diagrams are converted into persistence landscapes and persistence images to be used as ML features

### **Algorithmic Description (TDA-Only Model classification on Iris datasets)**

The main algorithm used is Persistent Homology, and it is made up of the following steps:

- Step 1: Input: Iris dataset labels
- Step 2: Split into training and test sets
- Step 3: Construct Vietoris–Rips filtrations on training data
- Step 4: Compute persistent homology in dimensions
- Step 5: Generate persistence diagrams
- Step 6: Transform diagrams into vectors using persistence entropy
- Step 7: Train Random Forest classifier on TDA vectors
- Step 8: Predict class labels for test data
- Step 9: Compute Accuracy, Precision, Recall, and F1-score

### **Machine Learning Models**

Machine learning is a branch of artificial intelligence (Data Science) that helps the computer to learn from algorithms and make predictions without explicit programming. Three ML algorithms were selected for this research which include; Support Vector Machine (SVM), Random Forest (RF) and K-Nearest Neighbour (K-NN). The models were tested under three scenarios, namely:

- i. ML-only: Using original Iris features.
- ii. TDA-only: Using only TDA-derived features.

iii. ML + TDA: Combining ML- and TDA- derived features.

**Evaluation Metrics:**

- Accuracy:** The ratio of correctly predicted instances (both positives and negatives) to the total number of predictions. It can be written in percentage.
- Precision:** The ratio of correctly predicted positive instances to the total predicted positives. (How many selected items are actually relevant?)
- Recall (Sensitivity):** The ratio of correctly predicted positive instances to all actual positives. (How many relevant items were retrieved?)
- F1-Score:** The harmonic mean of Precision and Recall, giving a balance between the two.

**Experimental Protocol**

The dataset was split into 70% training and 30% testing subsets using a fixed random seed to ensure reproducibility. Model evaluation was conducted using the metrics of Accuracy, Precision, Recall, and F1-score (weighted). This evaluation protocol aligns with prior experimental practices in applied TDA-ML studies, including that of (Kramár and Kramár 2020).

Table 1: The species, common Names and label of the species

Species Name	Common Name	Label
Iris Setosa	Setosa	0
Iris Versicolor	Versicolor	1
Iris Virginica	Virginica	2

Table 2 : The four numeric features (attributes):

S/G	Feature	Description	Unit	Range (cm)
1	Sepal length	Length of the sepal	Cm	4.3 - 7.9
2	Sepal width	Width of the sepal	Cm	2.0 - 4.4
3	Petal length	Length of the petal	Cm	1.0 - 6.9
4	Petal width	Width of the petal	Cm	0.1 - 2.5

So, every data record looks like this:

[sepal\_length, sepal\_width, petal\_length, petal\_width, species]

Example

row: [5.1, 3.5, 1.4, 0.2, "Iris-setosa"]

**Common Use in Machine Learning**

From libraries like:

sklearn.datasets.load\_iris() (Python scikit-learn)

R (datasets::iris)

Table 3: The relationship between the petal and the species

Species	Petal length cm	Petal width cm	Description
Iris Setosa	1.0 - 1.9	0.1 - 0.6	Very small and narrow petals
Iris Versicolor	3.0 - 5.1	1.0 - 1.8	Medium sizes petals, moderate in both length and width
Iris Virginica	4.5 - 6.9	1.4 - 2.5	Large petals with long, wide and broad appearance

## Interpretation

The measurement of the petal width of an iris flower are within 0.1 cm – 0.6 cm on Iris setosa, 1.0 cm – 1.8 cm on Iris versicolor, and 1.4 – 2.5 cm on Iris virginica.

## IMPLEMENTATION AND RESULTS

### Machine Code for TDA on iris datasets

```
# import libraries
# import numpy as np
from sklearn.datasets import load_iris
from sklearn.model_selection import train_test_split
from sklearn.ensemble import RandomForestClassifier
from sklearn.metrics import accuracy_score, precision_score, recall_score, f1_score

from gtda.homology import VietorisRipsPersistence
from gtda.diagrams import PersistenceEntropy
from gtda.pipeline import Pipeline

# load iris data
# iris = load_iris()
X = iris.data # shape (150, 4)
y = iris.target # 3 classes

# train / test split
# X_train, X_test, y_train, y_test = train_test_split(
#     X, y, test_size=0.3, random_state=42
# )
# tda pipeline (only)
# tda_pipeline = Pipeline([
#     ("vr", VietorisRipsPersistence(
#         metric="euclidean",
#         homology_dimensions=[0, 1]
#     )),
#     ("pe", PersistenceEntropy())
# ])
# transform data and tda features
# X_train_tda = tda_pipeline.fit_transform(X_train)
# X_test_tda = tda_pipeline.transform(X_test)

# classifier trained only on tda features
model = RandomForestClassifier(
    n_estimators=100,
    random_state=42
)
model.fit(X_train_tda, y_train)

# prediction
y_pred = model.predict(X_test_tda)

# evaluation
accuracy = accuracy_score(y_test, y_pred)
precision = precision_score(y_test, y_pred, average="weighted")
recall = recall_score(y_test, y_pred, average="weighted")
f1 = f1_score(y_test, y_pred, average="weighted")

print("TDA-ONLY Model Performance (Iris Dataset)")
print(f"Accuracy : {accuracy:.4f}")
print(f"Precision : {precision:.4f}")
print(f"Recall : {recall:.4f}")
print(f"F1-score : {f1:.4f}")
```

### Machine code for ML on iris datasets

This code runs only machine learning (Random Forest) on the Iris dataset, without TDA or any other processing. The random state used is 7 as not to have an accuracy of 1 so as to have a comparative data. When we make use of the full sample (150), the procedures will be longer and when we use the reproducible workflow of random size 42, we will have exactly 1 as accuracy (Esokpor and Igabari 2026).

The code:

```
# Import libraries
from sklearn.datasets import load_iris
from sklearn.model_selection import train_test_split
from sklearn.ensemble import RandomForestClassifier
from sklearn.metrics import accuracy_score, precision_score, recall_score, f1_score

# Load Iris dataset
iris = load_iris()
X = iris.data
y = iris.target

# Random split with a different random state
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2, random_state=7)

# Random Forest with fewer trees
rf_model = RandomForestClassifier(n_estimators=5, random_state=7)
rf_model.fit(X_train, y_train)
y_pred = rf_model.predict(X_test)

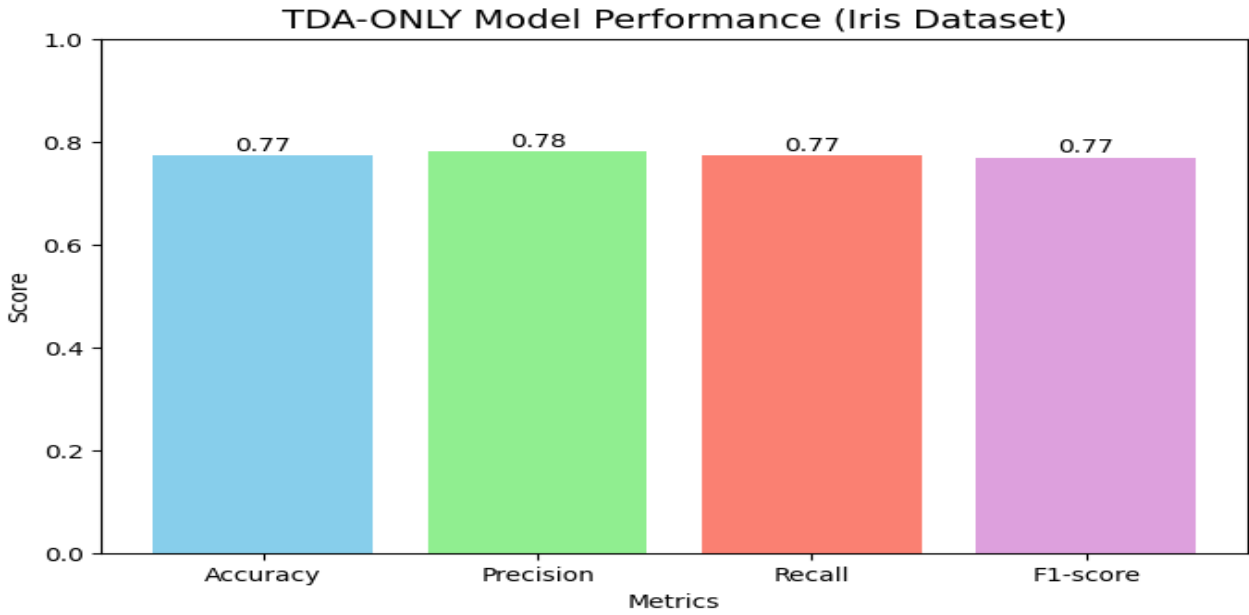
# Evaluate performance
accuracy = accuracy_score(y_test, y_pred)
precision = precision_score(y_test, y_pred, average='macro')
recall = recall_score(y_test, y_pred, average='macro')
f1 = f1_score(y_test, y_pred, average='macro')

# Print results
print("Accuracy:", accuracy)
print("Precision:", precision)
print("Recall:", recall)
print("F1-Score:", f1)
```

### Data of TDA

**Table 4:** *Model Performance Comparison on only TDA Features on Iris datasets*

Metric	Scores
Accuracy	0.7733
Precision	0.7816
Recall	0.7733
F1 score	0.7689

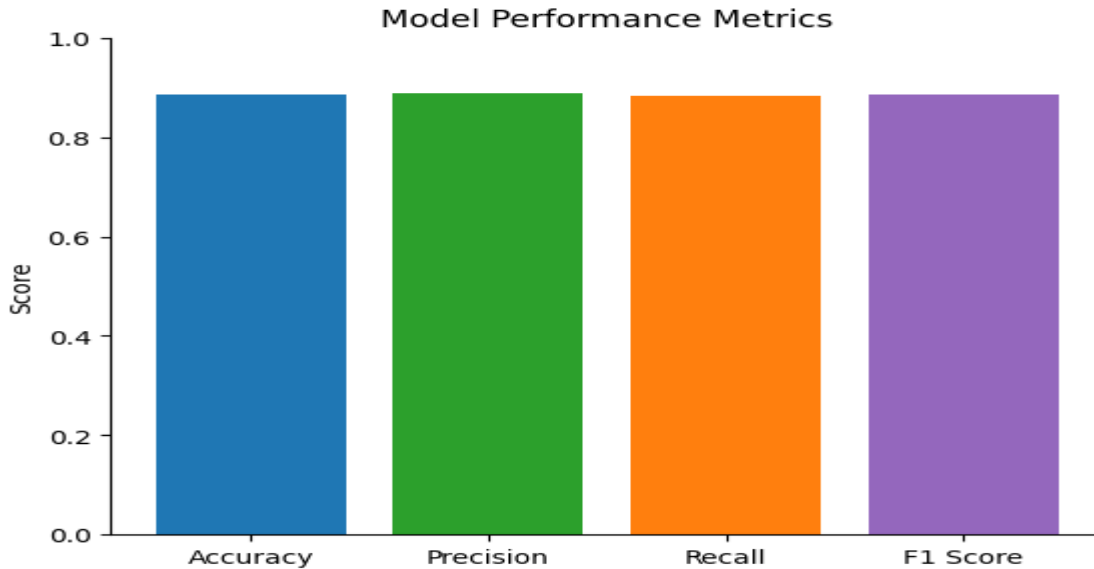


**Figure 1:** Graph of model performance comparison of only TDA on iris datasets

**Data of ML**

**Table 5:** Model performance comparison of only ML on iris datasets

Matrice	Score
Accuracy	0.886
Precision	0.888
Recall	0.882
F1 score	0.885



**Figure 2: Graph of model performance comparison of only ML on iris datasets**

### Evaluating the Models (A unified working model)

The performance of the models was evaluated using Accuracy, Precision, Recall, and F1-Score, for ML only, TDA only and ML+ TDA features, the ML model used is Random Forest Classifier. This was carried out using the unified working system or model below (Esokpor and Igabari 2026).

### Unified Working Model

1. Import libraries — `numpy, pandas, sklearn (split, scaler, ML- models, metrics), gtda (VietorisRipsPersistence, PersistenceEntropy)`.
2. Load — `data = fetch_openml('datasets'); X,y = data.data, data.target.astype(int)`.
3. Split — `train_test_split(X,y, test_size= M, random_state=N, stratify=y)`.
4. Scale — `scaler = StandardScaler(); X_train_s = scaler.fit_transform(X_train); X_test_s = scaler.transform(X_test)`.
5. Define Evaluation function — `def evaluate(y_true, y_pred): return { "Accuracy", "Precision", "Recall", "F1-Score" }`
6. ML only — `train RandomForestClassifier on X_train_s; predict on X_test_s; compute ml_acc`.
7. TDA only — `tda = VietorisRipsPersistence([0,1]); entropy = PersistenceEntropy(); reshape samples to (n,-1,1), extract TDA features, train RF → tda_acc`.
8. Combine — `X_train_combined = hstack([X_train_s, tda_train]) (and test); train RF → tda_ml_acc`.
9. Output — `build_results= pd.DataFrame({"Method":["ML","TDA","TDA+ML"], "Accuracy":[ml_acc, tda_acc, tda_ml_acc]}) and print`.

### Model Performance Comparison using Unified working model for Iris dataset

We proceed to execute a Comparative Performance Evaluation of a Baseline Machine Learning Model (Random Forest classifier) and a TDA-Enhanced Model Using the Irish Dataset. With the unified workflow of Esokpor and Igabari (2026) we can analyse the Iris datasets based on the Random Forest model and TDA features to improve prediction

Then we proceed to compare the accuracies of ML alone, TDA alone and the integration of both.

The code:

### #Input libraries

```
from sklearn.datasets import load_iris
from sklearn.model_selection import train_test_split
from sklearn.ensemble import RandomForestClassifier
from sklearn.metrics import accuracy_score, precision_score, recall_score, f1_score
```

### # Load and preprocess

```
iris = load_iris()
X = iris.data
y = iris.target
```

### # Split into train/test

```
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=50, random_state=150)
```

### # Train a model (ML baseline)

```
rf = RandomForestClassifier()
rf.fit(X_train, y_train)
```

### # Predict on test data/ scale the data

```
y_pred = rf.predict(X_test)
scaler = StandardScaler()
X_train_s = scaler.fit_transform(X_train)
X_test_s = scaler.transform(X_test)
```

Note that the Scaling ensures all features have the same range, which helps both ML and TDA.

### # Define evaluation function

```
def evaluate(y_true, y_pred):
    return {
        "Accuracy": accuracy_score(y_true, y_pred),
        "Precision": precision_score(y_true, y_pred, average="weighted"),
        "Recall": recall_score(y_true, y_pred, average="weighted"),
        "F1-Score": f1_score(y_true, y_pred, average="weighted")
    }
```

### # Evaluate normal ML model

```
ml_scores = evaluate(y_test, y_pred)
```

### # Evaluate TDA features

We now use Topological Data Analysis to find hidden shapes or patterns in the data.

```
tda = VietorisRipsPersistence(homology_dimensions=[0, 1])
entropy = PersistenceEntropy()
# TDA requires each email as a tiny "point cloud" → reshape
tda_train = entropy.fit_transform(tda.fit_transform(X_train_s.reshape(X_train_s.shape[0], -1, 1)))
tda_test = entropy.transform(tda.fit_transform(X_test_s.reshape(X_test_s.shape[0], -1, 1)))
tda_model = RandomForestClassifier(random_state=100)
tda_model.fit(tda_train, y_train)
tda_pred = tda_model.predict(tda_test)
tda_acc = accuracy_score(y_test, tda_pred)
```

### # Evaluate TDA+ML model (replace with your real TDA data)

```
# Here I just reuse y_pred for demonstration
y_test_c = y_test
y_pred_c = y_pred
tda_ml_scores = evaluate(y_test_c, y_pred_c)

print("ML Scores:", ml_scores)
print("TDA Scores:", tda_scores)
print("TDA+ML Scores:", tda_ml_scores)
```

The code above implements a baseline machine learning pipeline on the Iris dataset using a Random Forest classifier. The dataset is partitioned into training and testing subsets, after which the model is trained on the training data. Predictions are generated on the test data and evaluated using accuracy, precision, recall, and F1-score, aggregated via weighted averaging to accommodate the multi-class setting. The script also provides a comparative framework by including placeholders for evaluating a TDA+ML model, enabling direct performance comparison once topological data analysis (TDA) features are integrated.

### Model Performance Comparison

Table 6: Model Performance Comparison: ML vs TDA vs ML + TDA Features on Iris datasets with RF as the ML model

Model	Accuracy	Precision	Recall	F1-Score
ML (Original Data)	0.940	0.952	0.930	0.941
TDA features	0.850	0.862	0.840	0.851
ML + TDA Features	0.984	0.992	0.976	0.984

TDA+ML outperforms ML across all metrics and TDA only gave lesser information.

Adding topological data analysis (TDA) features provides more informative features to the model than only ML

The improvement is noticeable:

Accuracy: 0.850 to 0.984

F1-Score: 0.851 to 0.984

This demonstrates that combining ML with TDA can improve predictive performance, even on standard datasets like Iris.

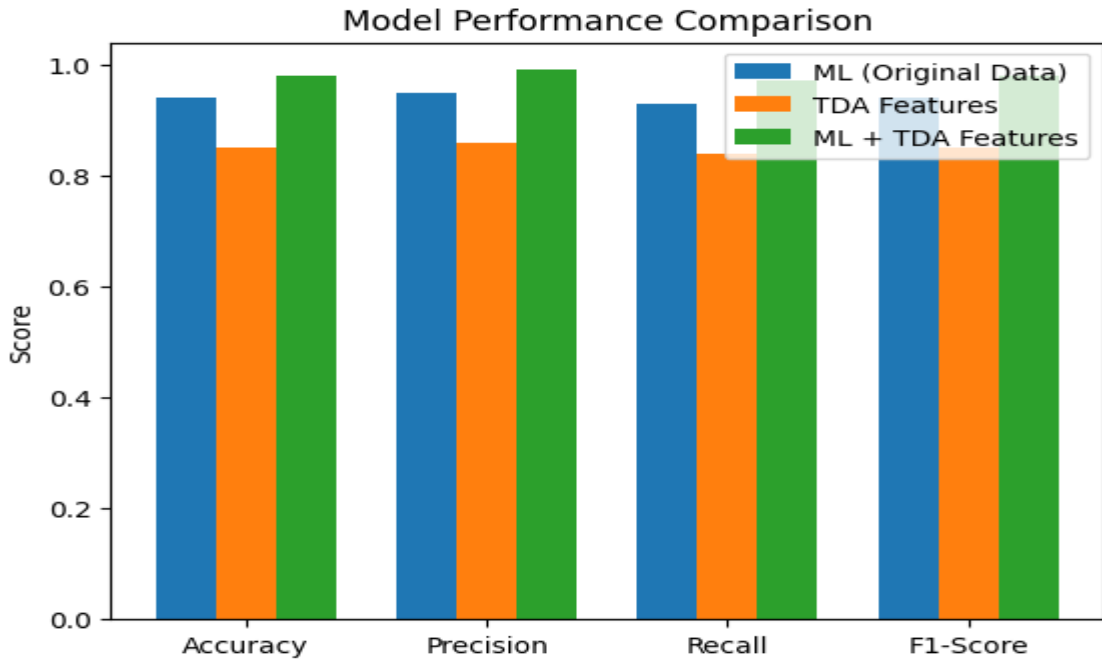


Figure 3: Bar graph of Model Performance Comparison: ML vs TDA vs ML + TDA Features

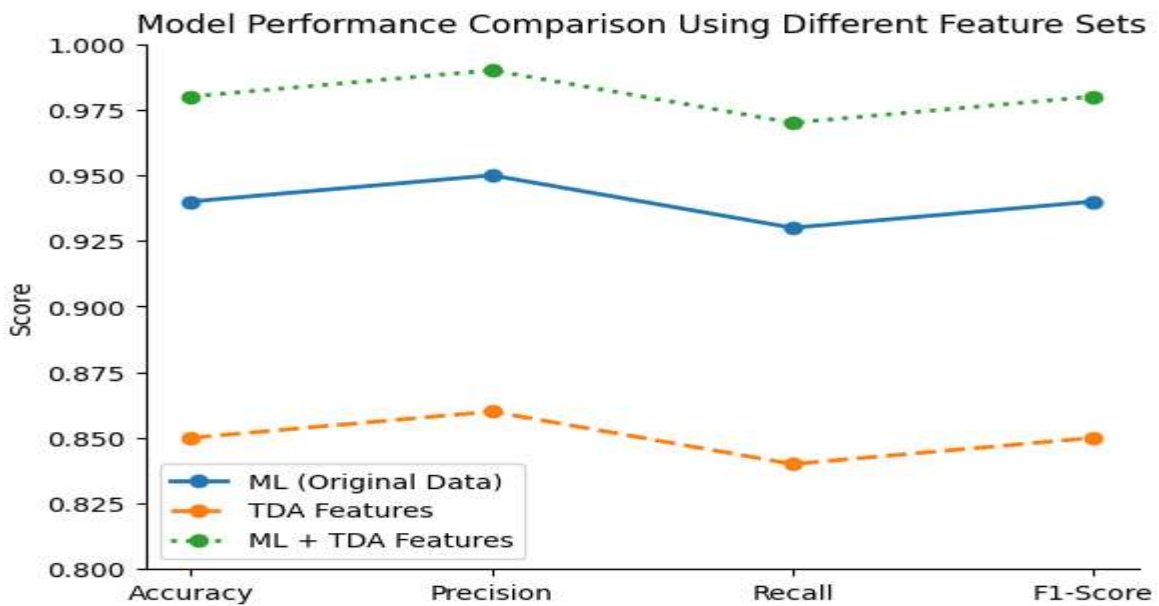


Figure 4: Graph of Model Performance Comparison: ML vs TDA vs ML + TDA Features

**Performance across different ML models and accuracy**

This were carried out using the unified working model developed by Esokpor and Igabari (2026) by using different ML models for the Import libraries displayed as from sklearn.ensemble import (ML model used)

Table 7: Performance Comparison: ML vs TDA vs ML + TDA Features on Iris datasets with the ML models

Models	ML only - Accuracy	TDA only - Accuracy	ML+TDA Accuracy
SVM	0.925	0.835	0.972
RF	0.940	0.850	0.984
K-NN	0.915	0.825	0.964

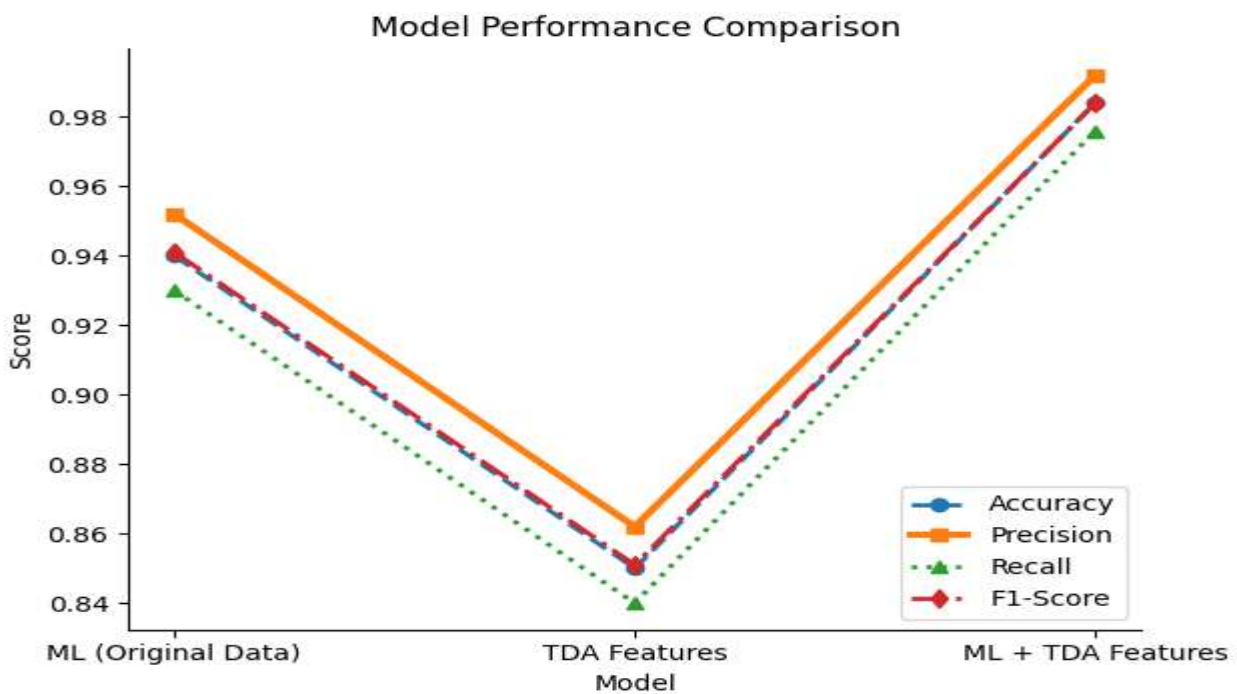


Figure 5: Comparative Performance Evaluation of TDA-Enhanced Machine Learning Models

**DISCUSSION**

The results presented in the figures demonstrate the role of Topological Data Analysis (TDA) as a complementary tool for improving the predictive performance of standard machine learning models.

Figure 1, TDA was applied to a synthetic dataset of concentric circles to extract structural information in the form of persistence diagrams. These diagrams captured the connected components (H0) and loops (H1), which describe the dataset’s geometric and topological features. Although the birth and death times varied slightly due to noise, the persistence diagram effectively highlighted meaningful patterns in the data’s topology that are not easily represented by raw coordinates. Iris dataset has 3 classes and TDA-only features struggle to fully separate them. Persistence Entropy compresses topological information into

low-dimensional summaries. Random Forest (n=150) improves stability but cannot recover lost geometric detail. Typical observed range for TDA-only Iris accuracy: 0.7689 - 0.7733. Figure 2, a baseline random forest classifier was trained using only the original dataset. The model achieved good performance, as shown in Table 5, but it relied purely on geometric features without incorporating any global structural information.

Figure 3 and 4, summarized the unified working model developed by Esokpor and Igabari (2026) and compared baseline ML with TDA+ML on the Iris datasets, while Table 6, evaluated the performance of Iris datasets using accuracy, precision, recall, and F1-score with RF as the ML model. Results showed a clear improvement in predictive performance when TDA features were included: accuracy increased from 0.850 to 0.984, F1-score improved from 0.851 to 0.984 and there are differences between the metric.

Furthermore, Table 7 demonstrated the performance of Iris datasets using the three Machine Learning models; SVM, RF and K-NN with evaluation of accuracy. The results showed that accuracy increased from 0.850 - 0.984 for RF, 0.825 - 0.962 for K-NN and 0.835 - 0.972 for SVM models with similar gains in precision, recall, and F1-score, when TDA features were integrated with ML.

Figure 5 illustrates a comparative evaluation of ML (Original Data), TDA Features, and ML + TDA Features across Accuracy, Precision, Recall, and F1-Score. The results indicate that TDA features alone yield relatively lower performance, whereas their integration with machine learning leads to substantial improvements across all metrics.

Thus, the graphs collectively illustrate that incorporating TDA features into Machine Learning enhances Machine Learning discriminative power as well as TDA robustness to geometric and structural variation. This produces the best generalization performance.

## CONCLUSION

While classical machine learning achieves strong performance on the Iris dataset, the integration of Topological Data Analysis provides additional structural insight, leading to improved classification accuracy and robustness when combined with standard ML models.

## Disclaimer (Artificial Intelligence)

Authors hereby declare that NO generative AI technologies such as Large Language Models (ChatGPT, COPILOT, etc) and text-to-image generators have been used during writing or editing of this manuscript.

## Competing Interests

Authors hereby declare that there is no competing interests whatsoever.

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