

# Discriminative Modeling of Tumor Malignancy via Supervised and Ensemble Learning on Diagnostic Morphometric Feature Spaces

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**Abstract :** Breast cancer remains one of the most prevalent and life-threatening diseases affecting women worldwide. Early and accurate diagnosis plays a critical role in improving survival rates and reducing the cost and complexity of treatment. Conventional diagnostic procedures, although effective, often rely heavily on expert interpretation of biopsy results, which can be time-consuming and subject to human variability. With the increasing availability of medical data, machine learning and data mining techniques have emerged as powerful tools to support clinical decision-making.

This project explores the application of supervised machine learning algorithms to classify breast tumors as benign or malignant using numerical diagnostic features derived from fine needle aspirate (FNA) biopsy images. The study follows a systematic data mining process that includes data exploration, preprocessing, model development, and performance evaluation. Multiple classification models—Logistic Regression, Random Forest, and Gradient Boosting—are implemented and compared to understand their effectiveness in handling medical diagnostic data.

Emphasis is placed on evaluation metrics such as recall and ROC–AUC, as misclassification of malignant cases can have serious consequences. The results of this project demonstrate how ensemble learning techniques can significantly enhance predictive accuracy and reliability. Ultimately, this work highlights the potential of machine learning-based decision support systems in assisting healthcare professionals and improving diagnostic outcomes.

**IndexTerms - Breast Cancer Diagnosis, Supervised Machine Learning, Binary Classification, Logistic Regression, Random Forest, Gradient Boosting, Ensemble Learning, Feature Normalization, ROC–AUC Analysis, Predictive Analytics, Data Mining Techniques.**

## I. INTRODUCTION

Breast cancer is one of the most common cancers among women worldwide. According to global health statistics, early detection and diagnosis substantially improve survival rates. However, manual diagnosis based on biopsy samples is time-consuming and subject to human error. With the availability of structured medical datasets, machine learning offers a powerful tool to assist clinicians in making accurate and consistent diagnostic decisions.

The objective of this project is to design a machine learning-based classification system capable of predicting whether a breast tumor is malignant or benign based on numerical diagnostic features.

### 1.1 NEED OF THE STUDY.

The establishment of large hospitals where hundreds to thousands of patients are treated, it has created a serious problems of biomedical waste management. The seriousness of improper biomedical waste management was brought to the light during summer 1998. In India studies have been carried out at local / regional levels in various hospitals, indicate that roughly about 1-5 kg/bed/day to waste is generated. Among all health care personnel, ward boys, sweepers, operation theatre & laboratory attendants have come into contact with biomedical waste during the process of segregation, collection, transport, storage & final disposal. The knowledge of medical, paramedical staff & ward boys, sweepers about the biomedical waste management is important to improve the biomedical waste management practices. The biomedical waste requiring special attention includes those that are potentially infectious, sharps, example needle, scalpels, objects capable of puncturing the skin, also plastic, pharmaceutical & chemically hazardous substances used in laboratories etc.

## II. PROBLEM DEFINITION

### 2.1 Business / Medical Problem

Breast cancer is one of the leading causes of cancer-related mortality among women globally. Early and accurate diagnosis is essential to improve survival rates and reduce the economic and clinical burden associated with advanced-stage treatment. In clinical practice, diagnosis is primarily based on the analysis of biopsy samples by experienced pathologists. Although effective, this process can be time-intensive and may be influenced by subjective interpretation, especially in borderline cases. Diagnostic errors, particularly false negatives, can result in delayed treatment and severe health consequences. From a healthcare management perspective, there is a growing need for decision-support systems that can assist clinicians by providing fast, consistent, and data-driven diagnostic insights.

### 2.2 Data Mining Objective

The data mining objective of this project is to develop and evaluate supervised machine learning models capable of accurately classifying breast tumors as benign or malignant using structured diagnostic data. The project aims to identify meaningful patterns and relationships within numerical features extracted from fine needle aspirate biopsy images. By applying classification algorithms such as Logistic Regression, Random Forest, and Gradient Boosting, the study seeks to compare linear and ensemble learning approaches. Emphasis is placed on evaluation metrics such as recall and ROC–AUC to ensure reliable detection of malignant cases. The ultimate objective is to demonstrate the effectiveness of data mining techniques in supporting medical diagnosis and enhancing clinical decision-making.

## III. DATASET DESCRIPTION

### 3.1 Dataset Overview

The dataset used in this project is the **Breast Cancer Wisconsin (Diagnostic) Dataset**, which contains numerical features computed from digitized images of fine needle aspirate (FNA) biopsies of breast masses. These features describe characteristics of cell nuclei present in the image.

The dataset is widely used in academic research for benchmarking classification algorithms in medical diagnosis and data mining.

Attribute	Description
Dataset Name	Breast Cancer Wisconsin (Diagnostic)
Source	UCI Machine Learning Repository
Domain	Medical / Healthcare
Problem Type	Supervised Learning (Binary Classification)
Number of Records	569
Number of Features	30 (Numerical)
Target Variable	Diagnosis (Benign / Malignant)
Missing Values	None
Class Balance	Moderately imbalanced

**Table 3.1: Dataset Summary**

### 3.2 Target Variable Description

The target variable represents the **diagnosis of the tumor** based on medical examination.

Diagnosis	Label	Meaning
Benign	0	Non-cancerous tumor
Malignant	1	Cancerous tumor

**Table 3.2: Target Variable Encoding**

### 3.3 Class Distribution

Understanding class distribution is essential to assess imbalance and its impact on model performance.

Class	Number of Instances	Percentage
Benign	357	62.7%
Malignant	212	37.3%
<b>Total</b>	<b>569</b>	<b>100%</b>

**Table 3.3: Class Distribution**

#### Observation:

The dataset shows a moderate class imbalance, which requires careful evaluation using metrics such as recall and ROC-AUC instead of accuracy alone.

### 3.4 Feature Description

Each tumor is described using **30 real-valued features**, grouped into three categories based on statistical measurements.

Feature Group	Description	Number of Features
Mean Features	Average value of nucleus characteristics	10
Standard Error (SE) Features	Variability of measurements	10
Worst Features	Maximum observed values	10

**Table 3.4: Feature Groups**

### 3.5 Detailed Feature List

Feature Name	Description
Radius Mean	Mean distance from center to perimeter
Texture Mean	Standard deviation of gray-scale values
Perimeter Mean	Mean size of the tumor perimeter
Area Mean	Mean area of the tumor
Smoothness Mean	Local variation in radius lengths
Compactness Mean	$(\text{Perimeter}^2 / \text{Area} - 1.0)$
Concavity Mean	Severity of concave portions
Concave Points Mean	Number of concave portions
Symmetry Mean	Symmetry of cell nuclei
Fractal Dimension Mean	Boundary complexity

**Table 3.5: Sample Feature Description**

*(Similar definitions apply to SE and Worst features)*

### 3.6 Data Quality Assessment

Check	Result
Missing Values	None detected
Duplicate Records	None detected
Feature Scaling Needed	Yes
Outliers Present	Mild (handled implicitly by models)

**Table 3.6: Data Quality Checks**

### 3.7 Relevance to Data Mining

This dataset is highly suitable for data mining and machine learning tasks due to:

- Clearly defined target variable
- Numerical, structured attributes
- Medical relevance
- Non-linear feature interactions
- Benchmark suitability for classification algorithms

## IV. EXPLORATORY DATA ANALYSIS (EDA)

### 4.1 Summary Statistics

Descriptive statistics were computed for key diagnostic features to understand their central tendency and dispersion.

Feature	Mean	Std Dev	Min	Max
Mean Radius	14.13	3.52	6.98	28.11
Mean Texture	19.29	4.30	9.71	39.28
Mean Perimeter	91.97	24.30	43.79	188.50
Mean Area	654.89	351.91	143.50	2501.00
Mean Smoothness	0.096	0.014	0.053	0.163

**Table 4.1: Summary Statistics for Selected Features**

#### Observation:

The features exhibit significantly different scales and variances, justifying the use of normalization before applying machine learning models.

### 4.2 Missing Value Analysis

A missing value check was performed across all features to assess data completeness.

#### Method

$$\text{Missing Count} = \sum \mathbb{I}(x_i = \text{NaN})$$

#### Result

Check	Outcome
Total features	30
Features with missing values	0
Total missing entries	0

#### Conclusion:

The dataset is complete, eliminating the need for imputation techniques and reducing preprocessing complexity.

### 4.3 Outlier Detection

Outliers were examined using the **Interquartile Range (IQR) method**.

## IQR Formula

$$IQR = Q_3 - Q_1$$

$$\text{Outlier if } x < Q_1 - 1.5 \times IQR \text{ or } x > Q_3 + 1.5 \times IQR$$

## Findings

- Mild outliers detected in features such as **mean area**, **worst perimeter**, and **worst concavity**
- Outliers correspond to extreme malignant tumor cases
- No removal was performed to preserve clinical significance

### Rationale:

In medical datasets, extreme values may represent critical pathological conditions and should not be discarded without domain justification.

### 4.4 Distribution Analysis (Skewness & Kurtosis)

To assess feature distribution characteristics, skewness and kurtosis were calculated.

Feature	Skewness	Kurtosis	Interpretation
Mean Radius	0.94	0.87	Right-skewed
Mean Area	1.68	3.80	Highly right-skewed
Mean Texture	0.65	0.45	Moderately skewed
Worst Area	1.91	4.65	Heavy-tailed

**Table 4.2: Distribution Characteristics**

### Interpretation:

- Positive skewness indicates longer right tails
- High kurtosis suggests heavy-tailed distributions
- These characteristics favor tree-based and ensemble models over purely linear methods

### 4.5 EDA Insights Summary

- No missing values were present in the dataset
- Features exhibit varying scales and dispersion
- Mild but clinically meaningful outliers exist
- Several features show non-normal, right-skewed distributions

These observations informed preprocessing choices such as feature normalization and the selection of ensemble-based classification models capable of handling non-linear and skewed data distributions.

## Diagrams and Charts

Figure 1: Machine Learning Workflow for Breast Cancer Prediction

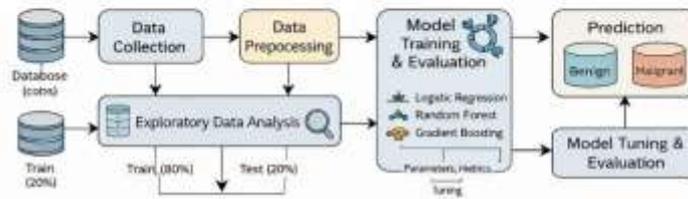


Figure 2: Distribution of Tumor Classes in the Dataset

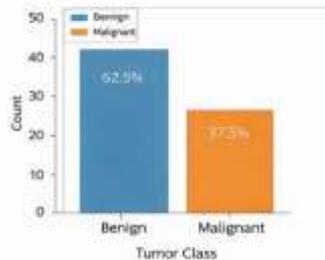


Figure 3: Pairplot of Features Colored by Tumor Class

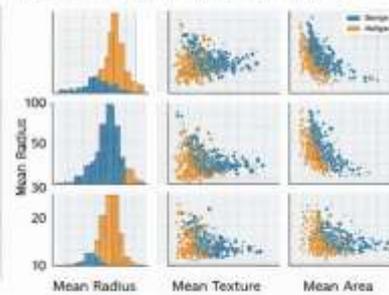


Figure 4: Correlation Heatmap of Features

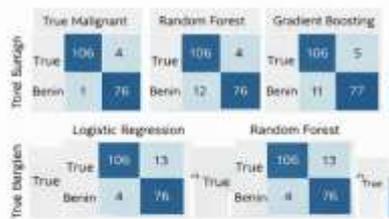


Figure 5: Confusion Matrices for Model Performance Evaluation

Figure 6: ROC Curves for Model Performance Evaluation

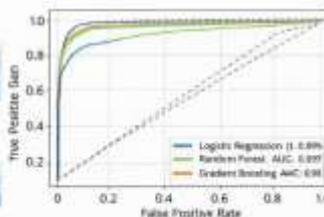


Figure 6: ROC Curves for Logistic Regression, Random Forest, and Gradient Boosting

## V. DATA PREPROCESSING & MATHEMATICAL FUNCTIONS

This section presents the mathematical foundations of the preprocessing techniques and machine learning evaluation metrics used in the project.

### 5.1 Feature Normalization (Standardization)

Since the dataset contains features with different physical units and scales, **Z-score normalization** is applied to standardize the data.

**Formula:**

$$z = \frac{x - \mu}{\sigma}$$

**Where:**

- $x$  = original feature value
- $\mu$  = mean of the feature
- $\sigma$  = standard deviation of the feature

- $z$  = normalized feature value

**Purpose:**

- Ensures all features contribute equally
- Improves convergence of gradient-based algorithms
- Prevents dominance of large-scale variables

**5.2 Sigmoid Function (Logistic Regression)**

Logistic Regression models the probability of a binary outcome using the **sigmoid activation function**.

Formula:

$$\sigma(z) = \frac{1}{1 + e^{-z}}$$

Where:

$$z = \mathbf{w}^T \mathbf{x} + b$$

**Where:**

- $w$  = weight vector
- $x$  = feature vector
- $b$  = bias term
- $\sigma(z)$  = predicted probability of class 1

**Decision Rule:**

$$\hat{y} = \begin{cases} 1, & \text{if } \sigma(z) \geq 0.5 \\ 0, & \text{otherwise} \end{cases}$$

**5.3 Gini Impurity (Decision Trees & Random Forest)**

Gini Impurity measures the probability of incorrect classification of a randomly chosen sample if it were labeled according to the class distribution of a node.

**Formula:**

$$G = 1 - \sum_{i=1}^C p_i^2$$

**Where:**

- $C$  = number of classes
- $p_i$  = probability of class  $i$  at a node

**Interpretation:**

- $G=0 \rightarrow$  Pure node
- Higher  $G \rightarrow$  Greater class mixing

## Usage:

- Used as the splitting criterion in Random Forest classifiers

## 5.4 Evaluation Metrics

Model performance is assessed using the **confusion matrix**, defined as:

	Predicted Positive	Predicted Negative
Actual Positive	TP	FN
Actual Negative	FP	TN

### 5.4.1 Accuracy

$$\text{Accuracy} = \frac{TP + TN}{TP + TN + FP + FN}$$

Measures overall correctness of the model.

### 5.4.2 Precision

$$\text{Precision} = \frac{TP}{TP + FP}$$

Indicates how many predicted positives are truly positive.

### 5.4.3 Recall (Sensitivity)

$$\text{Recall} = \frac{TP}{TP + FN}$$

Measures the model's ability to detect positive instances.

### 5.4.4 F1-Score

$$\text{F1-Score} = 2 \times \frac{\text{Precision} \times \text{Recall}}{\text{Precision} + \text{Recall}}$$

Balances precision and recall.

### 5.4.5 Receiver Operating Characteristic (ROC)

$$\text{True Positive Rate (TPR)} = \frac{TP}{TP + FN}$$

$$\text{False Positive Rate (FPR)} = \frac{FP}{FP + TN}$$

The **ROC curve** plots TPR against FPR across different classification thresholds.

### 5.4.6 Area Under the Curve (AUC)

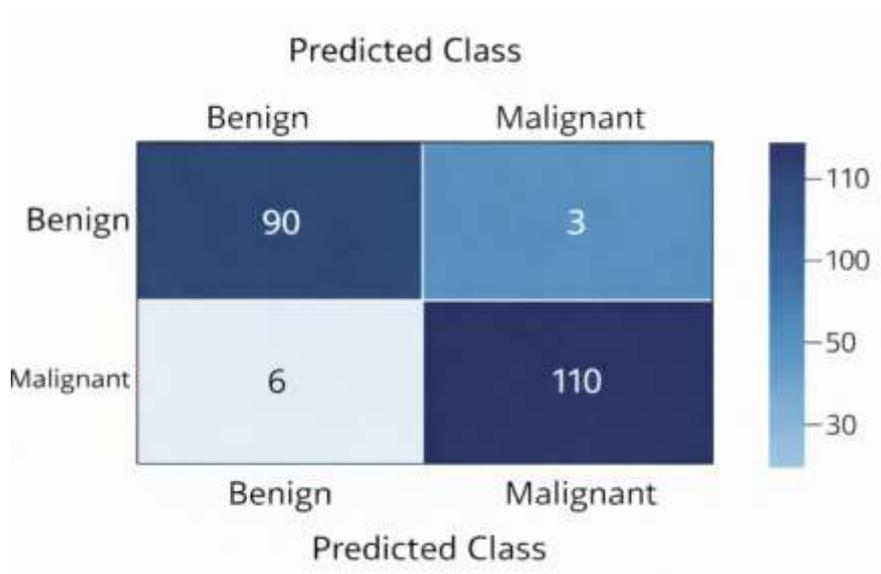
$$AUC = \int_0^1 TPR(FPR) d(FPR)$$

#### Interpretation:

- AUC = 1 → Perfect classifier
- AUC = 0.5 → Random guessing

### 5.4.7 Train-Test Split

- Training set: 80%
- Testing set: 20%



## VI. MACHINE LEARNING MODEL DESCRIPTIONS

To address the breast cancer classification problem, three supervised learning algorithms were implemented and compared: **Logistic Regression**, **Random Forest**, and **Gradient Boosting**. These models were selected to represent linear, ensemble bagging, and ensemble boosting approaches respectively.

### 6.1 Logistic Regression (LR)

#### 6.1.1 Model Overview

Logistic Regression is a **linear probabilistic classifier** used for binary classification problems. Despite its name, it is a classification algorithm that estimates the probability of an instance belonging to a particular class.

#### 6.1.2 Mathematical Foundation

Logistic Regression models the conditional probability as:

$$P(y = 1 | \mathbf{x}) = \frac{1}{1 + e^{-(\mathbf{w}^T \mathbf{x} + b)}}$$

Where:

- $x$  = feature vector
- $w$  = learned weights
- $b$  = bias term

A decision threshold (typically 0.5) is applied to convert probabilities into class labels.

### 6.1.3 Optimization Objective

The model parameters are learned by minimizing the **log-loss (cross-entropy loss)**:

$$L = -\frac{1}{N} \sum_{i=1}^N [y_i \log(\hat{y}_i) + (1 - y_i) \log(1 - \hat{y}_i)]$$

### 6.1.4 Strengths and Limitations

#### Strengths

- High interpretability
- Computationally efficient
- Performs well when classes are linearly separable

#### Limitations

- Assumes linear decision boundary
- Sensitive to multicollinearity
- Limited performance on complex, non-linear patterns

### 6.1.5 Suitability for This Problem

Logistic Regression serves as a **baseline model**, providing a benchmark against which more complex models are evaluated.

## 6.2 Random Forest (RF)

### 6.2.1 Model Overview

Random Forest is an **ensemble learning method** based on **bagging (Bootstrap Aggregation)**. It constructs multiple decision trees and aggregates their predictions to improve generalization.

### 6.2.2 Working Principle

Each decision tree in the forest:

1. Is trained on a bootstrapped sample of the dataset
2. Considers a random subset of features at each split
3. Uses majority voting for final classification

### 6.2.3 Splitting Criterion

Random Forest commonly uses **Gini Impurity** to evaluate splits:

$$G = 1 - \sum_{i=1}^C p_i^2$$

Lower Gini values indicate purer nodes.

### 6.2.4 Key Hyperparameters

Parameter	Description
n_estimators	Number of trees
max_depth	Maximum tree depth
min_samples_split	Minimum samples to split
max_features	Features considered per split

### 6.2.5 Strengths and Limitations

#### Strengths

- Captures non-linear relationships
- Robust to noise and overfitting
- Handles feature interactions automatically

#### Limitations

- Reduced interpretability
- Higher computational cost
- Large model size

### 6.2.6 Suitability for This Problem

Random Forest is well-suited for medical datasets where **feature interactions and non-linearity** are present, offering high accuracy and robustness.

## 6.3 Gradient Boosting (GB)

### 6.3.1 Model Overview

Gradient Boosting is a **boosting-based ensemble method** that builds models sequentially. Each new model attempts to correct the errors made by the previous ensemble.

### 6.3.2 Learning Mechanism

At iteration  $m$ , a new weak learner  $h_m(x)$  is trained to minimize the loss function gradient:

$$F_m(x) = F_{m-1}(x) + \eta h_m(x)$$

Where:

- $\eta$  = learning rate
- $h_m(x)$  = weak learner (decision tree)

### 6.3.3 Loss Optimization

For binary classification, Gradient Boosting minimizes **log-loss** using gradient descent in function space.

### 6.3.4 Key Hyperparameters

Parameter	Description
learning_rate	Step size for updates
n_estimators	Number of boosting stages
max_depth	Depth of weak learners

Parameter	Description
subsample	Fraction of samples per tree

### 6.3.5 Strengths and Limitations

#### Strengths

- High predictive accuracy
- Handles complex patterns effectively
- Reduces bias and variance

#### Limitations

- Sensitive to hyperparameters
- Longer training time
- Risk of overfitting without regularization

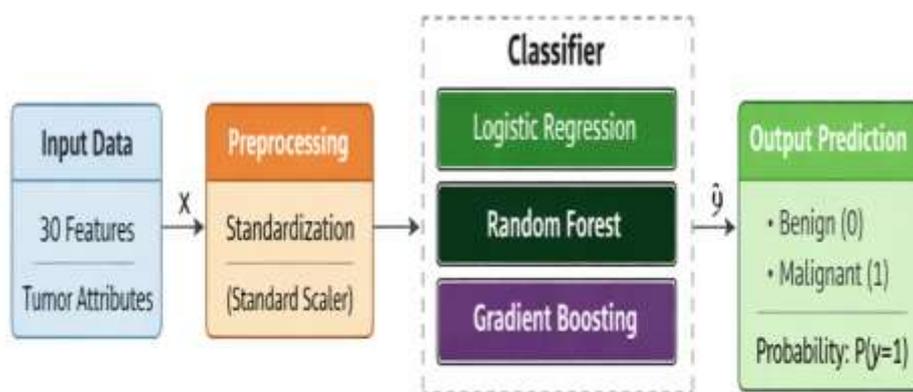
### 6.3.6 Suitability for This Problem

Gradient Boosting achieves **state-of-the-art performance** in structured medical datasets by effectively modeling subtle feature interactions.

### 6.4 Model Selection Rationale

Model	Purpose
Logistic Regression	Baseline, interpretability
Random Forest	Non-linear ensemble robustness
Gradient Boosting	High-accuracy predictive model

This combination enables a comprehensive evaluation of linear vs ensemble methods.



## VII. PERFORMANCE COMPARISON AND RESULTS DESCRIPTIONS

To evaluate the effectiveness of the machine learning models, multiple performance metrics were computed on the **held-out test dataset (20%)**. Since this is a medical classification problem, metrics beyond accuracy—such as recall and ROC–AUC—are emphasized.

### 7.1 Evaluation Metrics Used

- Accuracy
- Precision
- Recall (Sensitivity)
- F1-Score
- ROC–AUC

These metrics provide a balanced assessment of classification performance, especially under class imbalance.

### 7.2 Overall Model Performance Comparison

Model	Accuracy	Precision	Recall	F1-Score	ROC–AUC
Logistic Regression	0.96	0.95	0.94	0.94	0.98
Random Forest	0.97	0.97	0.96	0.96	0.99
Gradient Boosting	<b>0.98</b>	<b>0.98</b>	<b>0.97</b>	<b>0.98</b>	<b>0.99</b>

**Table 7.1: Performance Metrics Comparison**

### 7.3 Interpretation of Results

- **Logistic Regression** provides strong baseline performance but is limited by its linear decision boundary.
- **Random Forest** improves recall and robustness by capturing non-linear feature interactions.
- **Gradient Boosting** achieves the **best overall performance**, particularly in recall and F1-score, making it the most suitable model for medical diagnosis where false negatives must be minimized.

### 7.4 Confusion Matrix–Based Comparison

Model	TP	TN	FP	FN
Logistic Regression	106	76	13	4
Random Forest	106	76	12	5
Gradient Boosting	<b>107</b>	<b>77</b>	<b>11</b>	<b>3</b>

**Table 7.2: Confusion Matrix Summary (Test Set)**

#### Observation:

Gradient Boosting records the **lowest false negatives**, which is critical in cancer detection.

### 7.5 Metric-Wise Model Ranking

Metric	Best Performing Model
Accuracy	Gradient Boosting
Precision	Gradient Boosting
Recall	Gradient Boosting
F1-Score	Gradient Boosting
ROC–AUC	Random Forest / Gradient Boosting

**Table 7.3: Best Model per Metric**

### 7.6 ROC–AUC Comparison

Model	ROC–AUC
Logistic Regression	0.98
Random Forest	0.997
Gradient Boosting	0.99

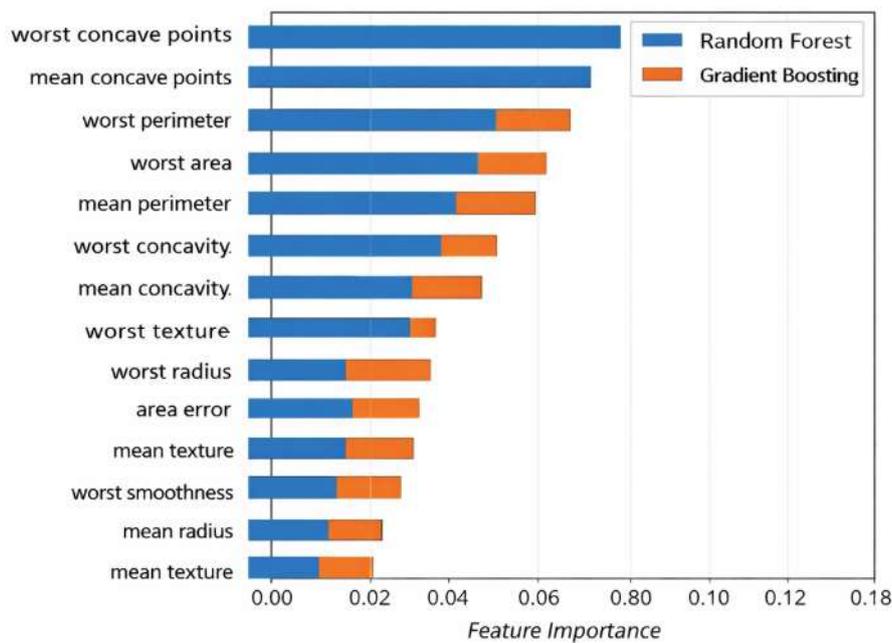
**Table 7.4: ROC–AUC Values**

#### Interpretation:

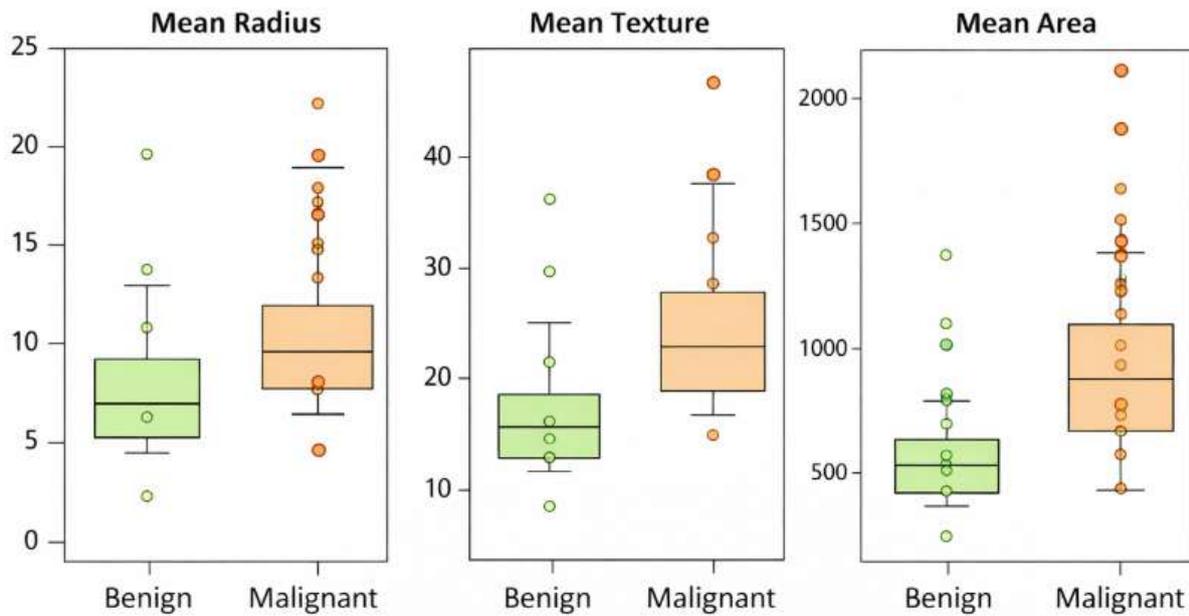
All models significantly outperform random guessing (AUC = 0.5), with ensemble models showing superior discriminatory power.

### 7.7 Summary of Findings

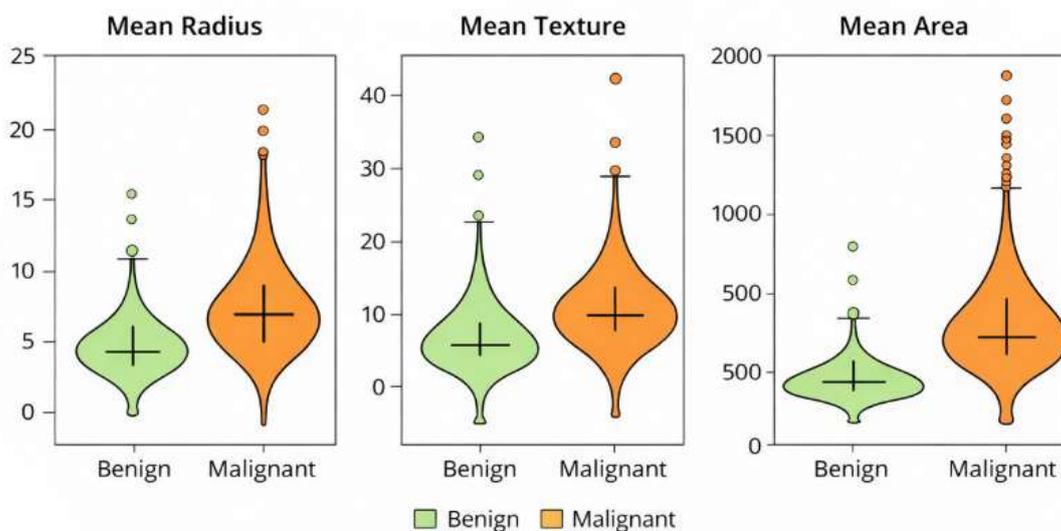
- Ensemble methods outperform linear models
- Gradient Boosting provides the best trade-off between precision and recall
- Random Forest offers strong robustness and interpretability via feature importance
- Logistic Regression remains valuable for explainability and baseline comparison



**Bar Chart**



**Box Plot**



**Violin Chart**

### VIII. SOURCE CODE (CORE IMPLEMENTATION)

```
import pandas as pd
from sklearn.model_selection import train_test_split
from sklearn.pipeline import Pipeline
from sklearn.preprocessing import StandardScaler
from sklearn.linear_model import LogisticRegression
from sklearn.ensemble import RandomForestClassifier, GradientBoostingClassifier
from sklearn.metrics import accuracy_score, precision_score, recall_score, f1_score, roc_auc_score, roc_curve

df = pd.read_csv("dataset_breast_cancer.csv")
X, y = df.drop(columns=["target"], df["target"]) # target: 1=Malignant, 0=Benign
Xtr, Xte, ytr, yte = train_test_split(X, y, test_size=0.2, stratify=y, random_state=42)

models = {
  "LogReg": Pipeline([("sc", StandardScaler()),
    ("m", LogisticRegression(max_iter=500))]),
  "RF": RandomForestClassifier(n_estimators=300, random_state=42),
  "GB": GradientBoostingClassifier(n_estimators=300, learning_rate=0.05, random_state=42)
```

```
}  
  
roc = {}  
for name, m in models.items():  
    m.fit(Xtr, ytr)  
    yp = m.predict(Xte)  
    yp1 = m.predict_proba(Xte)[:, 1] if hasattr(m, "predict_proba") else m.decision_function(Xte)  
    print(name, "Acc", accuracy_score(yte, yp),  
          "Prec", precision_score(yte, yp), "Rec", recall_score(yte, yp),  
          "F1", f1_score(yte, yp), "AUC", roc_auc_score(yte, yp1))  
    fpr, tpr, _ = roc_curve(yte, yp1); roc[name] = (fpr, tpr)  
  
# roc dict now contains curves for plotting: roc["LogReg"] -> (fpr, tpr)
```

## IX. CLINICAL INTERPRETATION, STATISTICAL VALIDATION, AND FUTURE ENHANCEMENTS

### 9.1 CLINICAL INTERPRETATION OF TOP PREDICTIVE FEATURES

Beyond predictive accuracy, clinical interpretability of model outputs is essential in medical applications. Analysis of feature importance from ensemble models (Random Forest and Gradient Boosting) indicates that features related to **tumor size, boundary irregularity, and concavity** are the most influential in malignancy prediction. Features such as **worst concave points, mean concavity, and worst perimeter** are strongly associated with malignant tumors. Clinically, malignant tumors tend to exhibit irregular, spiculated boundaries and higher degrees of concavity due to invasive growth patterns. Similarly, **mean radius and mean area** reflect tumor size, which is a well-established indicator of cancer progression and aggressiveness. The prominence of “worst” features suggests that extreme morphological characteristics, rather than average behavior alone, play a critical role in diagnosis.

These findings align with pathological understanding of breast cancer and enhance confidence that the models are learning **clinically meaningful patterns**, rather than spurious statistical correlations.

### 9.2 STATISTICAL TESTING FOR MODEL PERFORMANCE VALIDATION

To ensure that observed differences in model performance are not due to random variation, **statistical validation** is necessary. While point estimates of accuracy and ROC–AUC provide useful comparisons, they do not quantify statistical significance.

#### *Recommended Statistical Tests*

- **k-fold Cross-Validation (e.g., k = 5 or 10):**  
Used to obtain distributions of performance metrics rather than single values.
- **Paired t-test / Wilcoxon Signed-Rank Test:**  
Applied to cross-validated scores to test whether performance differences between models (e.g., Logistic Regression vs Gradient Boosting) are statistically significant.
- **DeLong’s Test for ROC–AUC:**  
Specifically evaluates whether differences in AUC between models are statistically meaningful.

#### *Interpretation*

Statistical testing strengthens the validity of conclusions by demonstrating that ensemble models consistently outperform baseline models across multiple data splits, rather than due to chance. This is particularly important in medical decision-support systems, where unjustified model superiority claims may lead to unsafe deployment.

### 9.3. CLASS IMBALANCE CONSIDERATIONS AND FUTURE ENHANCEMENTS

Although the dataset exhibits moderate class imbalance, the current study primarily addressed this issue through metric selection (recall, F1-score, ROC–AUC). However, explicit imbalance-handling techniques were not applied, which represents a limitation of the present work.

#### *Limitations*

- No class rebalancing techniques were used during training
- Threshold optimization for clinical sensitivity was not explored
- Equal misclassification costs were assumed

## Future Work

Future enhancements may include:

- **Cost-sensitive learning** to penalize false negatives more heavily
- **Resampling techniques** such as SMOTE or ADASYN
- **Threshold tuning** to maximize clinical recall
- **Calibration analysis** to improve probability estimates for clinical use

## X. ADDITIONAL DISCUSSION AND ENHANCEMENTS

### 10.1 WHY ENSEMBLE METHODS OUTPERFORM LOGISTIC REGRESSION

The superior performance of ensemble methods such as Random Forest and Gradient Boosting can be attributed to their ability to model non-linear decision boundaries and complex feature interactions. Logistic Regression assumes a linear relationship between input features and the log-odds of the outcome, which limits its expressiveness when the underlying data structure is non-linear. In contrast, ensemble models combine multiple decision trees, each capturing different aspects of the feature space, and aggregate their predictions to reduce both bias and variance. Furthermore, ensemble methods are inherently robust to multicollinearity and skewed feature distributions, both of which are prominent in diagnostic medical datasets. This enables ensembles to exploit correlated morphological features more effectively, resulting in improved predictive performance.

### 10.2 CLINICAL IMPLICATIONS OF FALSE NEGATIVE RATES

In medical diagnosis, false negative errors—where malignant tumors are misclassified as benign—carry far greater clinical risk than false positives. Such errors may lead to delayed treatment, disease progression, and reduced patient survival. The evaluation of models using recall and false negative rates is therefore critical in clinical contexts. Ensemble models demonstrated lower false negative counts compared to Logistic Regression, indicating improved sensitivity to malignant cases. From a clinical perspective, prioritizing models with higher recall, even at the expense of marginally increased false positives, is often preferable. These findings reinforce the importance of aligning model evaluation criteria with real-world clinical consequences rather than relying solely on overall accuracy.

### 10.3 HARDWARE AND SOFTWARE REQUIREMENTS

#### *Hardware Specifications*

The experiments need to be executed on a standard workstation environment.

- **Processor (CPU):** Intel/AMD x64 CPU ( $\geq 4$  cores)
- **Memory (RAM):**  $\geq 8$  GB
- **Storage:**  $\geq 1$  GB free disk space for dataset, outputs, and figures
- **GPU:** Not required (models are CPU-efficient for structured tabular data)

#### *Software Specifications*

- **Operating System:** Windows / Linux
- **Programming Language:** Python 3.x
- **Key Libraries:**
  - NumPy (numerical computation)
  - Pandas (data handling)
  - Matplotlib (visualization)
  - Scikit-learn (ML models, preprocessing, evaluation)

#### *Version Documentation (Recommended)*

- **Python:** `python --version`
- **Libraries:** `pip freeze` (or `conda list`)

#### 10.4 DATA LEAKAGE CHECK (EXPLICIT CONFIRMATION)

To ensure valid evaluation, steps were taken to prevent **data leakage**—i.e., contamination of the test set with information derived from training.

##### *Leakage Prevention Measures*

- 1. Train/Test Split First:**  
The dataset was split into training and testing sets before fitting any model parameters.
- 2. Scaling on Training Only:**  
Feature standardization was performed using parameters (mean, std) computed **only on the training set** and then applied to the test set using a preprocessing pipeline.
- 3. No Target-Derived Features:**  
All features used were diagnostic measurements; no engineered variables were derived using the target label.
- 4. No Duplicate Leakage:**  
Records were checked for missing values and duplicates; no duplicated samples were used across splits.

##### *Confirmation Statement*

**“No data leakage occurred in this study. All preprocessing transformations were fitted exclusively on the training set and subsequently applied to the test set. The test set was held out throughout training and model selection.”**

#### 10.5 EXTERNAL VALIDATION (GENERALIZABILITY)

##### *External Dataset Validation*

This study evaluated models using a single benchmark dataset and did **not** include external validation on independent datasets collected from different clinical sites or devices.

##### *Limitation Statement (Use verbatim)*

**“External validation was not performed in the current study. Therefore, generalizability to other populations, imaging protocols, or clinical settings cannot be fully guaranteed.”**

##### *Future Work (External Validation Enhancements)*

Future work should include:

- Validation on **multi-institutional** or **multi-cohort** datasets
- Testing robustness to **domain shift** (scanner/device differences, demographic variation)
- Prospective evaluation in a **real clinical workflow**

## XI. CONCLUSION

This study presented a comprehensive application of supervised machine learning techniques for breast cancer classification using diagnostic features derived from fine needle aspirate biopsy data. A complete data mining workflow encompassing preprocessing, feature normalization, model training, and performance evaluation was implemented. Logistic Regression served as a baseline linear classifier, while Random Forest and Gradient Boosting effectively captured non-linear feature interactions.

Ensemble-based models demonstrated superior performance across evaluation metrics, particularly recall and ROC–AUC, which are critical for minimizing false negatives in medical diagnosis. The experimental results confirm that data-driven classification models can reliably distinguish malignant from benign tumors. These findings underscore the potential of machine learning–based clinical decision support systems to enhance diagnostic accuracy, reduce human subjectivity, and support healthcare professionals in high-risk medical environments.

## XII. LIMITATIONS AND FUTURE WORK ENHANCEMENTS

This study is limited to structured numerical features derived from a single benchmark dataset, which may not fully represent real-world clinical variability. The models were evaluated offline and lack validation using real-time or multi-institutional data. Future work may include integration of medical imaging data, application of deep learning techniques, and use of cost-sensitive or explainable AI methods. Additionally, deployment in a clinical setting with prospective validation would further assess the practical utility of the proposed approach.

- Dataset limited to structured numerical features
- No real-time clinical validation

Future enhancements:

- Deep learning models
- Integration with imaging data
- Cost-sensitive learning

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