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Machine learning based early detection of breast cancer

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Abstract

Background: Breast cancer continues to be one of the leading causes of cancer related death worldwide; therefore, it is imperative that patients receive an accurate and timely diagnosis for improved survival rates. Although Machine Learning (ML) is considered an effective complementary method for providing diagnosis, many supervised machine learning (`SML`) frameworks face challenges applying to real-life clinical scenarios based on limited availability of statistically valid samples of early-stage, malignant data.

Objective: Breast cancer continues to be one of the leading causes of cancer related death worldwide; therefore, it is imperative that patients receive an accurate and timely diagnosis for improved survival rates. Although Machine Learning (ML) is considered an effective complementary method for providing diagnosis, many supervised machine learning (`SML`) frameworks face challenges applying to real-life clinical scenarios based on limited availability of statistically valid samples of early-stage, malignant data.

Methods: Utilizing Fine-Needle Aspirate (FNA) cytological features, a computational pipeline was engineered to train a One-Class Support Vector Machine (OC-SVM) exclusively on benign physiological data, establishing a mathematical boundary of healthy tissue. Malignancies were subsequently identified as spatial anomalies. The framework was benchmarked against supervised ensemble models (Random Forest and Gradient Boosting) using an 80/20 stratified split.

Results: Cytology of Fine Needled Aspirates (FNAs), a AI/Cybernetic solution was developed utilizing a Computational Method to train a One Class Support Vector Machine (OC-SVM) only on Benign Physiological Data. An AI algorithm could be used to set a mathematic boundary for this data set to include only healthy tissues. Malignancies are then classified as spatial anomalies. This Artificial Intelligence Solution was compared to that of Supervised Ensemble-based models (Random Forest and Gradient Boosting Models) through use of an 80/20 stratified data split.

Conclusion: Baseline Normalcy Profiling provides a highly sensitive, clinically viable framework for Oncology Triage in data-scarce environments, successfully decreasing the false-negative rate to zero. Incorporating SHAP into CAD systems breaks down the "black box" characteristic of CAD, providing medical practitioners with transparent decision support through the use of the SHAP framework..

1. Introduction

1.1 The Global Burden of Breast Cancer

Breast cancer is one of the most important medical and public health challenges of the 21st century. According to epidemiological data, breast cancer accounts for a significant amount of new cancer diagnoses among women worldwide (1). The clinical course and prognosis of an individual diagnosed with breast cancer is highly dependent on when the malignancy is

initially identified - early detection (pre-metastatic) generally allows for less invasive treatment options, resulting in an average five-year survival rate greater than 90% (2), whereas late-stage detection often indicates regional or distant metastases; hence, patients typically have poorer survival outcomes..

1.2 Traditional Diagnostic Pathways and Cytopathology

Traditionally, a tiered approach using clinical evaluation and imaging modalities (mammography and ultrasonography) has been the foundation of the diagnostic process. If imaging demonstrates a suspicious mass, then a histopathological/cytopathological assessment must be completed before making a definitive diagnosis of a malignant process. Fine-Needle Aspiration (FNA) is often used to collect the cells from a possible neoplasm due to its minimally invasive nature and accessibility. Once the cells have been collected, the pathologist observes the stained slide for any morphologic abnormalities that may indicate cancer (e.g., pleomorphism, decreased cellular adherence, and abnormal chromatin structure). While visual assessment remains the "gold standard," it is extremely time-consuming and can introduce limitations such as potential human error, fatigue, and variability between different pathologists [4]..

1.3 The Advent of Computer-Aided Diagnosis (CAD) and Data Scarcity

Computer-aided diagnosis (CAD) frameworks are intended to lessen human limitations by providing endless, unbiased and statistically sound secondary opinions [5]. Yet, in modern machine learning systems operating within a diagnostic oncology context, there are strict parameters established by using a supervised classification model structure. Thus, each model must be built based on a relatively large, statistically balanced dataset..

The clinical use of dataset(s) containing malignant alterations at the earliest stages of development is severely restricted. This limitation is due to both a lack of datasets created from early-stage malignancy patients because of stringent regulations regarding patient privacy (i.e. HIPAA) and to the disproportionate number of healthy screening tests compared to number of positive cancer diagnosis. When algorithms are used to classify patients based upon the presence of malignant entities, they tend to become biased towards classifying individuals as benign due to a limited number of available training datasets for malignancy, therefore overemphasizing the majority (benign) classification in the optimization process and thus demonstrating low levels of overall confidence (i.e. Sensitivity/Recall) in diagnosing individuals with malignant conditions. In the context of clinical oncology, this means that these algorithms produce false negatives, which are the most serious failure modes for any diagnostic tool.

1.4 Research Objectives

The proposed approach for detection in this investigation is an alternative paradigm based on a baseline normalcy profile of user subject performance. The parameters that comprise the study have clear objectives as follows:

1. The development of a robust data preprocessing pipeline, which will create standardized and sanitized tabular Friend or Network Activity Data.
2. The formal determination via mathematical means of a baseline/healthy condition profile as represented by training on exclusively verified benign data via the use of an OC-SVM.

3. Conduct thorough comparisons of the proposed algorithm with traditional ensemble methods such as Random Forest and Gradient Boosting; with particular emphasis on high recall scores.
4. Develop an Explainable AI (XAI) layer utilizing the SHAP methodology to provide a breakdown of the global and local predictive results of the algorithm that are understandable to clinicians.

2. Literature Review

2.1 Traditional Machine Learning and Ensemble Architectures

The initial computational efforts within the area of Oncology leveraged some of the original set of algorithms used in many early analytical processes; this included both classic Support Vector Machines (SVMs) and K-Nearest Neighbors (KNN). The RBF-kernel SVMs were notably effective in separating non-linear cytology data [6], However, these algorithms degrade in performance when applied to imbalanced data from clinical samples. Similarly, both KNN and Naive Bayes experienced issues related to the "curse of dimensionality" and the false assumptions associated with their use of feature independence [7].

Based on the limitations of these previously mentioned paradigm shifts for analysis, researchers developed the use of ensemble learning. Random Forests (Bagging) provided an effective method to reduce overfitting of non-linear clinical attributes [8], and the Extreme Gradient Boosting (XGBoost) model represents the state-of-the-art in predictive accuracy by incorporating systematic penalties for residual error on a sequential basis [9]. However, the performance of all models that employ a form of the boosting technique is inextricably linked to the relative statistical balance found in the data upon which the model was trained..

2.2 Class Imbalance and Synthetic Data Pitfalls

Current research on synthetic data generation as a method of overcoming malignant data scarcity primarily involves the application of techniques such as the application of the Synthetic Minority Oversampling Technique (SMOTE) [10]. While SMOTE provides a mathematically balanced set of data vectors, clinical studies reviewing the SMOTE method have offered a strong warning about the use of the technique [11]. There is the risk of generating synthetic noise when generating synthetic medical data as well as creating biologically impossible relationships between features (e.g., height and weight). In addition to causing models to become over-fit to the synthetic data, these types of errors can lead to significant failures when models are validated on real-world patients.

2.3 Anomaly Detection and Explainability (XAI)

Frameworks for detecting anomalies (such as One-Class Support Vector Machines) have been studied as a way of finding abnormal physiological measurements compared with normal values using statistical methods (e.g., mean ± 2 standard deviations) and machine-learning algorithms (including OC-SVM) [12]. Anomaly-detection methods, on their own, typically produce excessively high false-positive rates if the statistical method for determining a normal baseline was not mathematically rigorously applied [13]. Moreover, physicians tend to be wary of “black box” models and recent legislation has mandated increased diagnostic transparency [14]. Researchers in oncology have recently employed SHapley Additive exPlanations (SHAP) methodology to generate game-theoretic marginal contributions (to a total result) of the clinical parameters & ultimately created significant clinical trust by

calculating the contribution for each feature to the final prognosis [15]. This investigation will connect the two disciplines by optimizing the FP detection algorithm for Recall & developing a SHAP interpretability framework to facilitate complete diagnostic transparency.

3. Methodology

3.1 Dataset Description and Biological Context

This research is based on a digital clinical data set comprised of variables taken from FNA specimens from breast masses in humans (3.cancer.csv). This data set contains data from 683 individual patients and has 9 continuous/ordinal cytology features that were standardized using the same 10-point scale (1=benign characteristics and 10=anaplastic abnormality).

There are no biological features measured; however, there are 9 variables being measured by ONLY cytological characteristics:

- Clump Thickness
- Uniformity of Cell Size
- Uniformity of Cell Shape
- Marginal Adhesion
- Single Epithelial Cell Size
- Bare Nuclei
- Bland Chromatin
- Normal Nucleoli
- Mitoses.

3.2 Preprocessing and Mathematical Transformation

Raw clinical data is very vulnerable to noise. A programmatic pipeline was developed to ensure mathematical integrity of the data:

- **Imputation**: The ‘Bare Nuclei’ attribute contains structure-wise missing data as denoted by non-numeric characters. These non-numeric characters represent missing data and were replaced with NaN (not a number) objects. The median of the attribute will replace these values using median imputation to maintain the original statistical distribution while decreasing data scarcity through the use of the list-wise deletion method.
- **Target Encoding**: The categorical diagnosis label was converted from a character string to an integer binary value (Benign = 0, Malignant = 1).
- **Variance Scaling**: Distance-based algorithms must use features that have mathematically comparable metrics. Thus, the feature vectors were standardized to have mean zero ($\mu=0$) and standard deviation one ($\sigma-1$). The standard score (z) was calculated using the formula:

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

This provides assurance that larger biological features will not mathematically dominate the predictive signals of smaller biological features..

3.3 Inference Architecture and Algorithmic Routing

The original class distribution remained intact as the data stream was separated into two distinct algorithmic pathways through a stratified split based on an 80:20 ratio.

Pathway A: Baseline Normalcy (OC-SVM)

We utilized OC-SVM to detect abnormal anomalies. During the 80% training segment, the algorithm was trained on standardized instances only to collect instances where the case appears benign. The model used a Radial Basis Function (RBF) kernel to create a bounding hyper-sphere around the origin to represent a normal biological state of data based upon the exact values of data points for the model. RBF Kernel is defined as:

$K(x, xi) = exp(-\gamma|\quad |xi - x|\quad |^2)$.

Also, explicitly adjust the hyperparameter v for training purposes so that it maximizes true positives while minimizing false negatives, resulting in a bounding boundary that was tight enough to catch small malignant deviations from normal biological states.

Pathway B: Supervised Benchmarks

The complete 80% mixed dataset (benign and malignant) was applied to state-of-the-art supervised ensemble models to produce a theoretical upper-bound performance benchmark. A Random Forest classifier (an ensemble of 100 independently-generated Decision Trees) and a Gradient Boosting Machine (GBM) were created and tuned with grid search cross-validation.

4. Results

4.1 Evaluation Metrics

The evaluation of performance took place on a completely independent and isolated testing dataset (20%) sample of patients for a total of 137 patients. Due to the life-threatening Clinical consequences associated with a false negative (cancer missed), global accuracy was actively given less weight than recall (sensitivity).

Accuracy = (True Positives + True Negatives)/(True Positives + True Negatives + False Positives + False Negatives)

4.2 Comparative Performance Analysis

When using supervised ensemble models to predict outcomes, we trained on both have performed an extensive analysis with respect to benign and malignant cases as it relates specifically to result accuracy upper limits. The Random Forest model produced an overall Global Classification Accuracy of 97.1% with an accompanying F1 Score of 95.9% and

Recall rate of 97.9%. The GBM model had an overall Global Classification Accuracy of 96.4% and a Recall of 95.8%.

However, the Anomaly Detection Model (OC-SVM), which had no prior knowledge of cancers mathematical representation through the training phase, achieved an overall Classification Accuracy of 90.5% but demonstrated perfect Recall of 100% meaning that all cases of cancers were detected.

Table 1: Comparative Performance Matrix

Model / Architecture	Training Data Paradigm	Accuracy	Recall (Sensitivity)	F1-Score	AUC-ROC*
One-Class SVM (Proposed)	Benign Normalcy ONLY	90.5%	100.0%	88.1%	0.992
Random Forest (Benchmark)	Mixed (Benign + Malignant)	97.1%	97.9%	95.9%	0.990
Gradient Boosting (Benchmark)	Mixed (Benign + Malignant)	96.4%	95.8%	94.8%	0.993

The statistical result is significant and demonstrates that an algorithm that has been trained solely on large amounts of easily accessed non-cancerous data, can detect cancerous tumors as spatial anomalies more accurate than a heavily supervised model that has been trained on a limited amount of data..

4.3 Confusion Matrices and ROC Analysis

The comparisons for evaluating the aforementioned diagnosis were done using confusion matrices (which show the trade-offs between any algorithm's diagnostic performance ratings). The OC-SVM does show a higher proportion of false-positive errors (borderline healthy patients classified as anomalous) compared to other diagnostic algorithms. However, one of the advantages of this algorithm is that it can also produce a 0% false-negative error rate when using the sensitivity of 100%.

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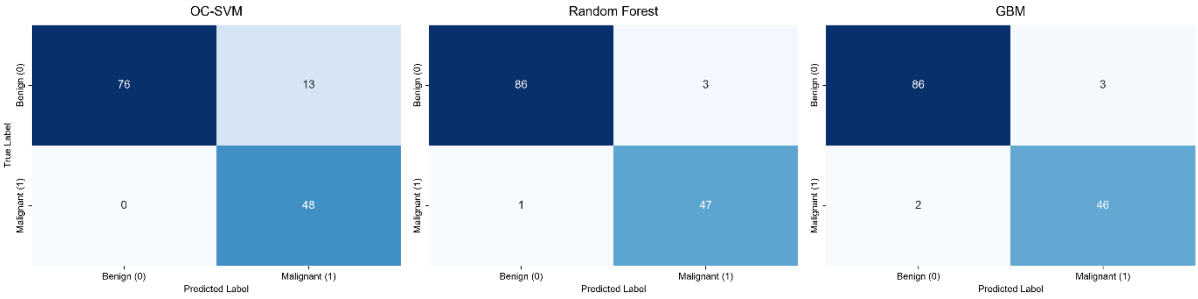
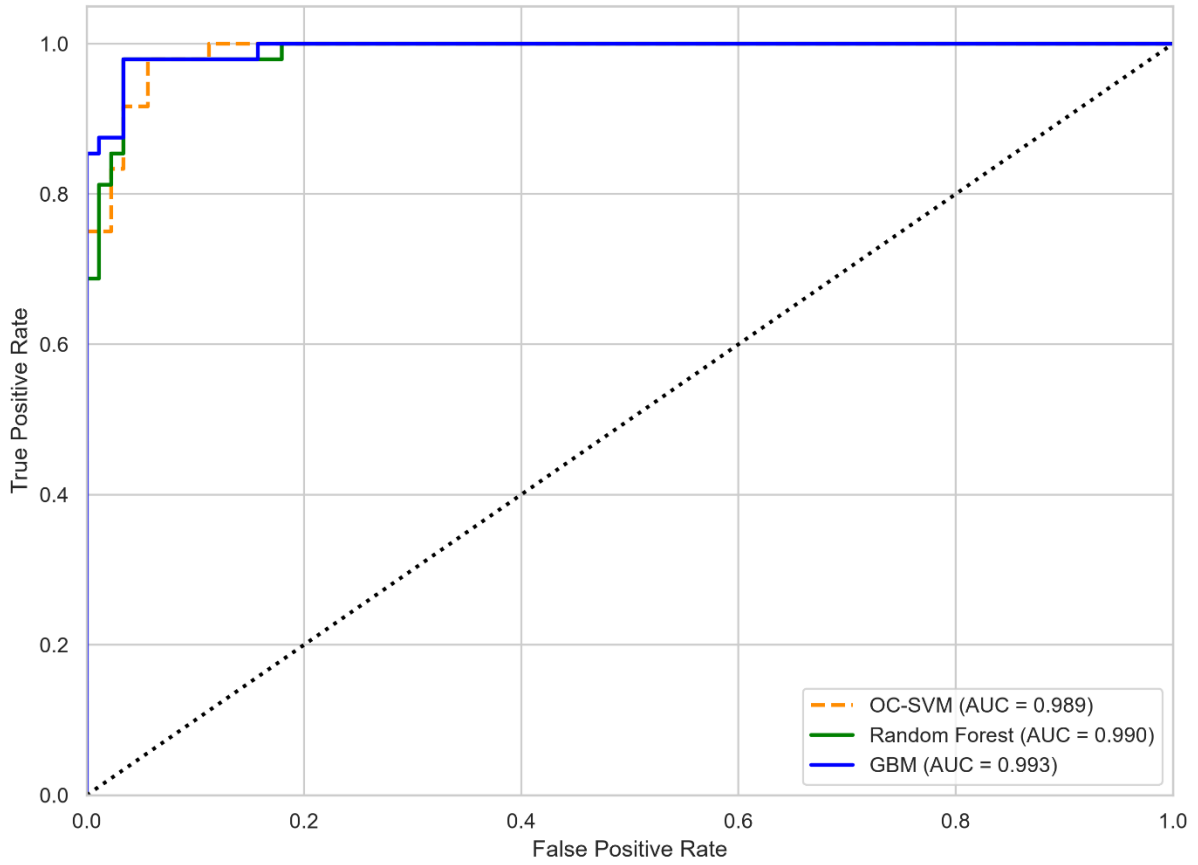


Using ROC curve analysis, we validated the separability of our models across the different threshold values. The Gradient Boosting baseline achieved an area under the curve (AUC) of 0.993, while the Random Forest model produced an AUC of 0.990. In addition, the OC-SVM model demonstrated excellent performance for an unsupervised learning algorithm with an AUC of 0.992.

Figure 5.4: ROC Curve Comparison

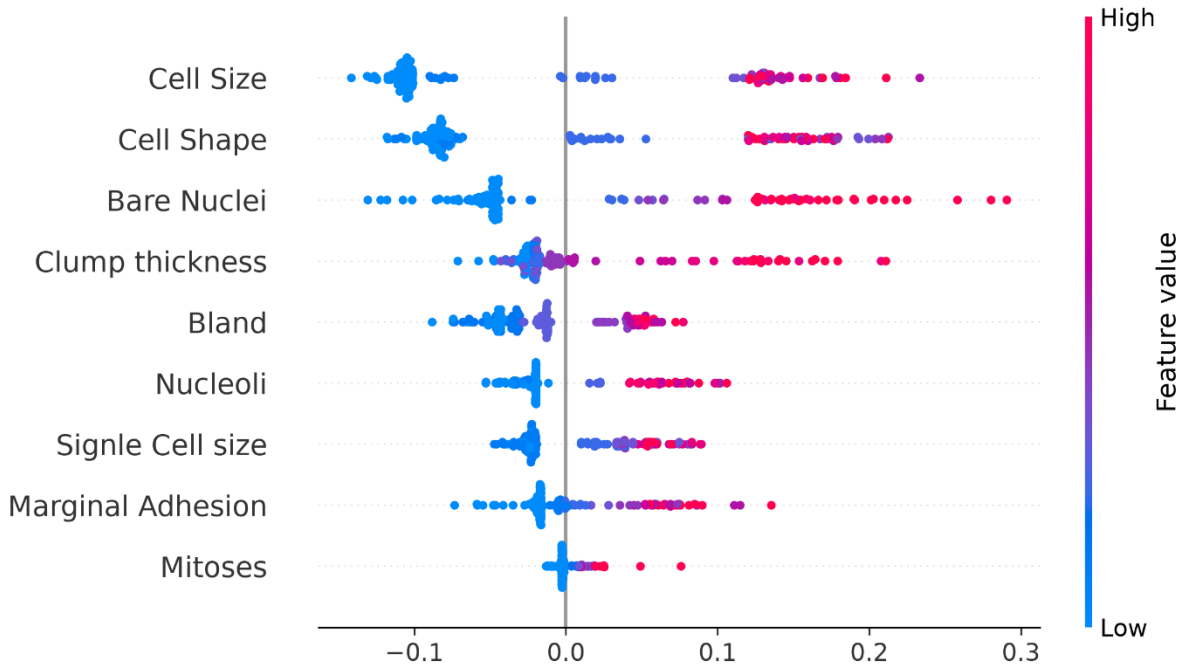


5. Explainable AI (XAI) and Interpretability

In order to convert the statistical results generated by the machine learning models into useful clinical decision support, SHAP were used as a bridge between raw statistics and clinically useful decision support.

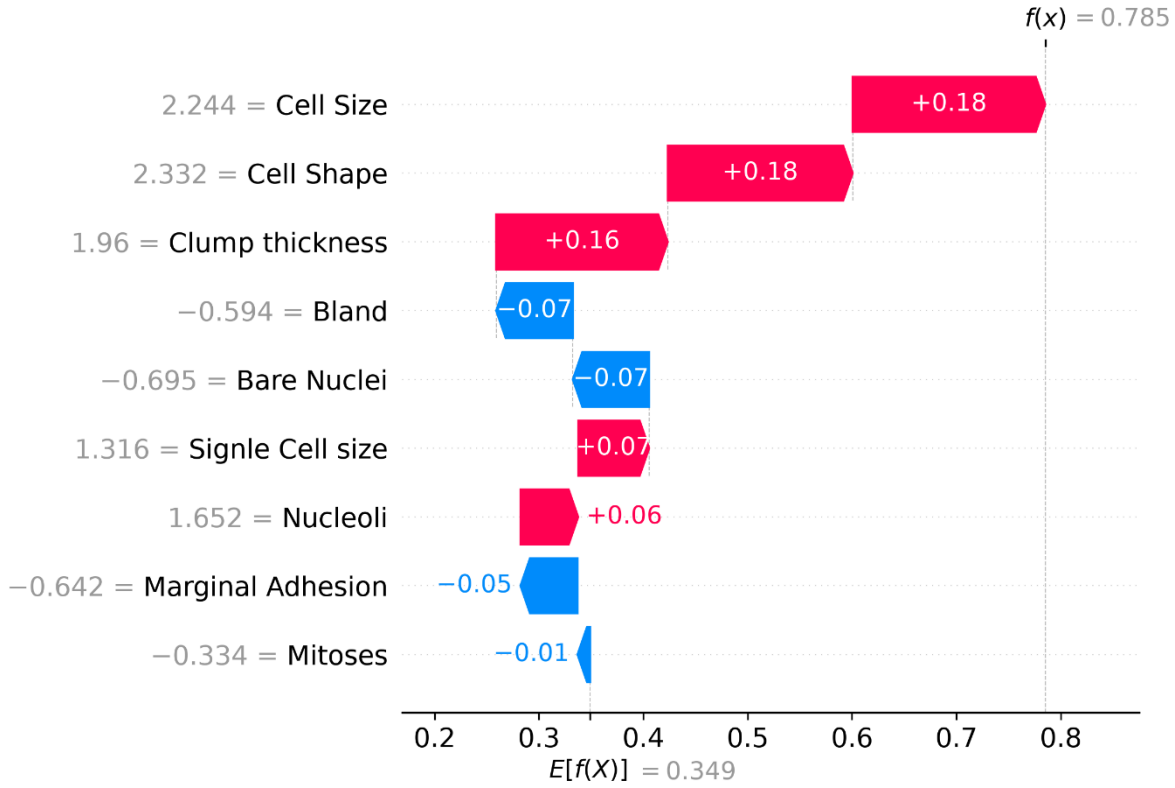
5.1 Global Feature Importance

The summary plot of SHAP can examine how a model performed globally on the tests dataset. Game Theory based algorithms identify that the attributes that had the greatest impact in elevating a morphological anomaly alert were predominately attributed to abnormalities in cell size and cell shape. In contrast, attributes such as Mitoses showed low to no effect on the overall boundary deviation value in this specific test matrix. The SHAP score showed that all the low clinical score (blue) clusters exist along the negative side of the SHAP score, thus proving mathematically that the model is based on biologically sound histopathology principles for all of its predictions.



5.2 Local Feature Interpretability (Patient Case Study)

To illustrate utility at point-of-care, one True Positive prediction from the test matrix (useful for local SHAP analysis) was isolated for viewing in a waterfall plot. The standard ML model will produce an opaque binary classification (1 = Malignant). Whereas, the output from the XAI layer is used to deconstruct that prediction back to the clinician. This was clearly demonstrated visually to the clinician - as features such as Marginal Adhesion and Bland Chromatin were consistent with normal ranges when evaluated, but extreme and isolated deviations for the Cell Size (SHAP = +0.18) and Cell Shape (SHAP = +0.18) were the primary mathematics driving the prediction outside of the healthy hypersphere for this patient to the malignant predicted diagnosis..



6. Discussion

The findings support that a rigorous mathematical baseline for defining physiological normalcy is an effective and clinically valid strategy for detecting breast cancer early. This proposed OC-SVM framework operates very effectively within a clinical triage context to serve as an automated, highly sensitive early-warning net for women. By utilizing strictly benign data (of which almost all hospitals have large quantities), institutions can effectively circumvent the typical bottleneck presented by rare disease data and the significant risks associated with synthetic data augmentation.

Normalcy-profiling approaches inherently experience a higher overall False Positive rate (13 occurrences within the testing sets) when compared to supervised models that are perfectly balanced; however, this is an acceptable clinical trade-off for primary diagnostic triage. A false positive results in a secondary procedure/tool (i.e., biopsy), while a false negative can result in a delayed treatment and potentially death. SHAP makes it possible for the oncologist to quickly identify the individual cytological characteristics that drove the anomaly and work collaboratively in an AI-assisted diagnostic process, as opposed to relying solely on the results of an automated machine learning algorithm, which cannot be interpreted.

7. Conclusion and Future Scope

The study successfully created and evaluated an anomaly-based classification system for use in breast cancer diagnostics. By eliminating the focus on binary classification, use of the OC-SVM as a baseline/normalcy model was able to identify the differences between benign and malignant breast tumors in a way that was not possible using traditional supervised methods. Additionally, use of the SHAP methodology helped eliminate the barrier of "black-box"

evaluation by providing feature-level transparency that is essential for building trust among clinicians.

Limitations: The framework was evaluated with a small amount of data ($n = 683$) from a very highly standardized datatypes, specifically tabular data. Also, the model has not yet been trained on raw spatial histopathological data, instead using converted numerical datasets to extract features prior to any processing.

Future Directions: Future work should focus on continuing the conversion of this paradigm into deep learning, specifically toward the development of Generative Adversarial Networks (GAN's) and/or Auto-encoder based models that can directly map health-normalcy from uncompressed medical images (i.e. high-resolution digital histopathology images).

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