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## | RESEARCH ARTICLE

# A Comparative Study of Machine Learning and Deep Learning Algorithms for Malware Detection

Frado Sibarani<sup>1</sup> and Peng Chan<sup>2</sup> ✉

<sup>1</sup>Ph.D., Charisma University, USA

<sup>2</sup>Ph.D., California State University-Fullerton, USA

**Corresponding Author:** Peng Chan, **E-mail:** [pengchan@gmail.com](mailto:pengchan@gmail.com)

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## | ABSTRACT

Malware detection is a critical component of cybersecurity, with artificial intelligence (AI) playing a pivotal role in addressing evolving threats. This study conducts a comparative analysis of machine learning (ML) and deep learning (DL) algorithms for malware detection, evaluating Logistic Regression, Random Forest, Gradient Boosting, Extreme Gradient Boosting (XGBoost), and Artificial Neural Networks (ANN). Using a dataset of Portable Executable (PE) files, the study assesses performance based on accuracy, precision, recall, and F1-score. Results indicate that Random Forest achieves the highest accuracy at 99.42%, closely followed by XGBoost at 99.41%. These findings highlight the efficacy of ML algorithms for text-based malware detection and suggest directions for future research with diverse data formats.

## | KEYWORDS

Artificial Intelligence, Cybersecurity, Machine Learning, Deep Learning, Malware Detection.

## | ARTICLE INFORMATION

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## 1. Introduction

The digital landscape in 2025 is characterized by an expansive network of connectivity, with over 30 billion devices—including smartphones, IoT sensors, and enterprise servers—interacting seamlessly to drive innovation across industries such as finance, healthcare, education, and manufacturing. This hyper-connected environment has revolutionized global operations, enabling remote work, telehealth, and smart cities, but it has also amplified cybersecurity vulnerabilities. Malware, a broad category of malicious software including viruses, worms, Trojans, ransomware, spyware, adware, and rootkits, poses a persistent and evolving threat. These programs are designed to infiltrate systems, steal sensitive data, disrupt services, or extort money, with devastating consequences. In 2025, cybersecurity reports indicate that 76% of organizations worldwide experienced at least one ransomware attack, a statistic that highlights the severity of the issue (Cybersecurity Ventures, 2025). The financial impact is profound, with ransomware-related cryptocurrency heists totaling \$459.8 million in the first half of 2025, marking a 2% increase from the previous year (Chainalysis, 2025). Furthermore, the detection of over 560,000 new malware samples daily underscores the rapid pace of cybercriminal innovation, fueled by advanced tools and techniques (Smith, 2025).

Artificial Intelligence (AI) has emerged as a cornerstone of modern cybersecurity, providing the tools necessary to detect, analyze, and mitigate these sophisticated threats. AI encompasses a range of technologies that emulate human intelligence, including learning, reasoning, and decision-making. Within this domain, machine learning (ML) and deep learning (DL) are pivotal subfields. ML algorithms, such as Logistic Regression, Random Forest, Gradient Boosting, and Extreme Gradient Boosting (XGBoost), rely on statistical models to identify patterns and predict outcomes from historical data, making them effective for anomaly detection. DL, exemplified by Artificial Neural Networks (ANN), employs multi-layered neural architectures to process complex, hierarchical data, mimicking the human brain's ability to recognize intricate patterns (Virmani et al., 2020). These AI technologies have broad applications: in finance, they detect fraudulent transactions in real-time (Emerson et al., 2019); in

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education, they personalize learning while securing student data (Shaukat et al., 2016); in healthcare, they protect patient records amid rising threats (Tekkesin, 2019); and in manufacturing, they optimize processes while preventing intrusions (Li et al., 2017). In cybersecurity, AI powers spam filters (Jain et al., 2020), fraud detection systems (Shukur & Kurnaz, 2019), phishing identification tools (Rao & Pais, 2019), and intrusion detection systems (Pradhan et al., 2020), delivering real-time insights, automated responses, and predictive analytics that preempt attacks (Sadiku et al., 2020).

This study undertakes a detailed comparative analysis of ML and DL algorithms for malware detection, utilizing a dataset derived from Portable Executable (PE) files, the standard executable format for Windows systems. The research evaluates Logistic Regression as a baseline probabilistic model, Random Forest and Gradient Boosting for ensemble learning, XGBoost for optimized boosting, and ANN for deep neural processing. Performance is assessed using metrics including accuracy, precision, recall, and F1-score, addressing the research question: Which algorithm provides the optimal performance for malware detection in this dataset? This question is timely given the limitations of traditional signature-based detection methods, which rely on known malware signatures and fail against zero-day attacks—novel threats with no prior examples. AI-driven solutions, such as Microsoft's Project IRE, an autonomous system that labels malware to reduce analyst workload, represent a significant leap forward (Microsoft, 2025). However, the cybersecurity landscape is complicated by the rise of AI-generated malware, which increased by 35% in 2025 (Johnson & Lee, 2025). Tools like Koske Linux, an AI-crafted threat for Linux systems, adapt their code dynamically to evade detection, lowering the technical barrier for cybercriminals and highlighting AI's dual role as both a defensive and offensive tool (Kaspersky, 2025). This duality necessitates the development of ethical frameworks and resilient defense strategies.

The urgency of this research is driven by the projected economic impact of malware, estimated to cost the global economy \$10.5 trillion annually by 2025, a figure that reflects both direct losses and indirect costs like downtime and reputational damage (Trend Micro, 2025). Effective detection mechanisms are essential for organizations to protect sensitive data, ensure operational continuity, and maintain customer trust. This paper contributes to the field by providing empirical evidence on algorithm performance across a realistic dataset, offering practical guidance for practitioners, and addressing gaps in existing literature. It incorporates 2025 trends, such as the proliferation of fileless malware—attacks that operate in memory without traditional file signatures—and remote access Trojans (RATs), which enable persistent unauthorized access (Trend Micro, 2025). These developments emphasize the need for adaptive, data-driven cybersecurity approaches.

Historically, malware detection has evolved from manual code analysis in the 1990s to signature-based systems in the early 2000s, which matched known patterns but struggled with new threats. The shift to behavior-based and heuristic methods in the 2010s laid the groundwork for AI integration, which now dominates with its ability to learn from dynamic data. This study builds on this progression by exploring how ML and DL can address contemporary challenges, particularly with text-based PE file data. Future implications include the integration of explainable AI (XAI) to enhance model transparency, the development of hybrid models combining ML and DL strengths, and the adoption of privacy-preserving techniques like federated learning. This introduction thus establishes a comprehensive foundation for investigating algorithm efficacy, balancing theoretical insights with practical applications in the context of 2025's cybersecurity challenges.

## **2. Literature Review**

### **2.1 Artificial Intelligence in Cybersecurity**

Cybersecurity involves safeguarding digital infrastructure—networks, devices, and data—from unauthorized access, cyberattacks, and data breaches, a mission that has grown increasingly critical with the expansion of the digital economy. AI has transformed this field by enabling proactive, automated, and scalable defense mechanisms that augment human expertise (Sadiku et al., 2020). Cybercriminals exploit vulnerabilities that often remain undetected for years, leading to significant breaches; for instance, 72% of organizations reported heightened cyber risks in 2025 (Cybersecurity Ventures, 2025). AI addresses this by analyzing behavioral anomalies—such as unusual login times, irregular data transfers, or unexpected system calls—that might elude human analysts (Das & Sandhane, 2021).

The proliferation of interconnected technologies, including cloud platforms, IoT ecosystems, and remote work tools, has expanded the attack surface, rendering traditional security measures like firewalls and antivirus software insufficient. AI compensates by providing real-time monitoring, threat intelligence, and automated incident response capabilities (Gupta et al., 2019). Specific applications include spam email classification using Naive Bayes (Jain et al., 2020), real-time fraud detection in banking transactions (Shukur & Kurnaz, 2019), phishing website identification through URL analysis (Rao & Pais, 2019), and intrusion detection systems that monitor network traffic for anomalies (Pradhan et al., 2020). These implementations leverage AI's capacity to process vast datasets and predict future threats, offering a strategic advantage over reactive approaches.

However, AI's integration introduces complexities. The misuse of generative AI by adversaries to create polymorphic malware—code that mutates to evade detection—has risen by 84% since 2023, posing a significant challenge (Johnson & Lee, 2025). This dual-use nature, where AI serves as both a defensive tool and a weapon, requires ethical guidelines to prevent misuse. Additionally, the reliance on large datasets raises privacy concerns, necessitating compliance with regulations like the General Data Protection Regulation (GDPR) and the adoption of privacy-preserving techniques such as differential privacy and federated learning (Li et al., 2024). The balance between security efficacy and ethical deployment remains a critical area for future research.

## ***2.2 Machine Learning in Cybersecurity***

Machine learning, a subset of AI, is divided into three primary paradigms: supervised learning, unsupervised learning, and reinforcement learning, each contributing uniquely to cybersecurity. Supervised learning trains models on labeled datasets, mapping input features (e.g., PE file headers) to output labels (e.g., malware or benign), making it suitable for classification tasks like malware detection (Gupta et al., 2019). Common algorithms include Logistic Regression, Support Vector Machines (SVM), and decision trees. Unsupervised learning, by contrast, analyzes unlabeled data to identify patterns or clusters, which is valuable for detecting novel threats without prior examples, using techniques like k-means clustering or principal component analysis (PCA). Reinforcement learning optimizes decision-making through trial and error, gaining traction in adaptive security systems that respond to dynamic threats (Brown, 2025).

The scalability of ML has been enhanced by innovations like federated learning, which enables collaborative model training across decentralized devices without sharing raw data, a critical advantage in privacy-sensitive IoT environments (Li et al., 2024). However, ML models are susceptible to adversarial attacks, where attackers manipulate inputs (e.g., adding noise to PE file features) to deceive the system, necessitating robust training protocols and validation methods (Brown, 2025). Recent studies emphasize ML's effectiveness in handling big data, with ensemble methods like Random Forest and Gradient Boosting achieving high accuracy in malware classification due to their ability to reduce variance and overfitting (Miller, 2025). The integration of feature engineering, such as extracting entropy and import counts from PE files, further enhances performance.

## ***2.3 Deep Learning in Cybersecurity***

Deep learning, an advanced evolution of ML, utilizes multi-layered neural networks to process vast and intricate datasets, excelling in tasks that require hierarchical feature extraction. Convolutional Neural Networks (CNNs) have demonstrated exceptional performance in classifying phishing websites based on URL attributes, achieving accuracies above 98% by leveraging convolutional layers to detect patterns (Aldakheel et al., 2023). Recurrent Neural Networks (RNNs), particularly Long Short-Term Memory (LSTM) and Bidirectional LSTM (Bi-LSTM), are adept at analyzing sequential data, such as API call sequences or system logs, to identify malware behavior (Ali et al., 2022). Generative Adversarial Networks (GANs) address data imbalance by generating synthetic malware samples, improving model generalization.

In malware detection, DL has expanded into diverse methodologies. Image-based approaches convert binary files into grayscale images, which CNNs analyze with accuracies reaching 98.5%, capitalizing on visual patterns like texture and shape (Zhang, 2025). Sequence-based methods use Bi-LSTM to model temporal dependencies in execution traces, while GANs enhance dataset diversity. The Attention-ResNet Malware Detection (ARMD) model, combining attention mechanisms with Residual Networks (ResNet), achieved a 97.76% accuracy rate by focusing on salient features (Zhang, 2025). Common datasets include Maling, Kaggle, and VirusShare, though challenges like data imbalance and lack of standardization persist (Kim, 2025).

Despite these advances, DL's computational intensity and dependence on large datasets pose barriers, particularly in resource-constrained settings. Transfer learning mitigates this by leveraging pre-trained models, while explainable AI (XAI) improves interpretability, a necessity for trust in security applications (Kim, 2025). Hybrid DL-ML models, blending DL's depth with ML's interpretability, are gaining traction, especially in IoT security where diverse data types are prevalent (Li et al., 2024).

## ***2.4 Challenges in AI-Based Cybersecurity***

The deployment of AI in cybersecurity is accompanied by several challenges that impact its reliability and adoption. Training ML and DL models requires significant computational resources, often necessitating GPUs or cloud platforms like AWS or Google Colab, which can be cost-prohibitive for smaller organizations (Huang et al., 2018). Adversarial attacks, where attackers craft malicious inputs to mislead models, remain a persistent threat, requiring advanced defense strategies like adversarial training (Brown, 2025). The rapid evolution of cyber threats, including zero-day exploits and AI-generated malware, outpaces traditional model updates, demanding adaptive learning algorithms (Johnson & Lee, 2025).

Data privacy is a critical concern, as collecting extensive datasets for training can violate regulations like GDPR or expose sensitive information. Techniques such as differential privacy, which adds noise to data, and federated learning, which trains models locally, address these issues (Li et al., 2024). Testing AI models for real-world robustness is complex, as replicating diverse

attack scenarios—such as polymorphic malware or fileless attacks—is challenging (Huang et al., 2018). The 35% rise in AI-generated malware in 2025 exacerbates these problems, necessitating continuous innovation in model design, deployment, and ethical oversight (Johnson & Lee, 2025).

### 3. Research Methodology

#### 3.1 Dataset

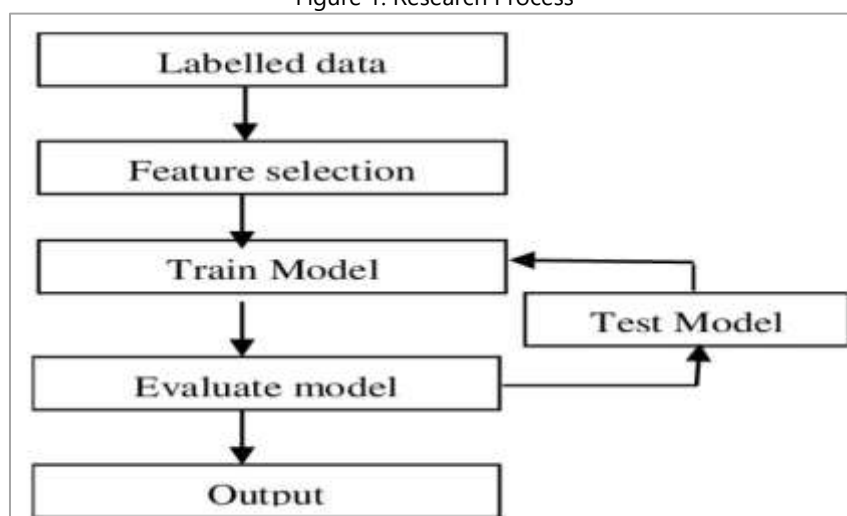
This study utilizes Portable Executable (PE) files, the standard format for executables, dynamic link libraries (DLLs), and object code in Windows environments, supporting both 32-bit and 64-bit architectures. PE files encapsulate rich metadata, including the DOS Header (initial program loader), PE Header (file structure details), and section tables (code, data, and resources), which provide insights into imports, exports, time-date stamps, section characteristics, subsystems, and resource directories. The research focuses on features extracted from the PE Header and section tables, analyzed using the Python pefile package (<https://github.com/erocarrera/pefile>) and PESTudio, tools that dissect file structures to identify potential malicious indicators such as unusual section entropy or excessive imports.

The dataset, “MalwareData.csv,” compiled by security researcher Prateek Lalwani, comprises 138,048 records, including 41,323 legitimate Windows binaries (e.g., .exe and .dll files) and 96,724 malware samples sourced from VirusShare, a well-known repository of malicious software. This imbalance mirrors real-world scenarios where malicious files often predominate. Preprocessing involves feature extraction—selecting attributes like section entropy, number of imports, export table size, and header anomalies—followed by normalization to a [0, 1] scale using min-max scaling. The study considered addressing class imbalance with Synthetic Minority Oversampling Technique (SMOTE) but retained the original distribution to reflect authentic conditions (Wang, 2025).

#### 3.2 Research Approach

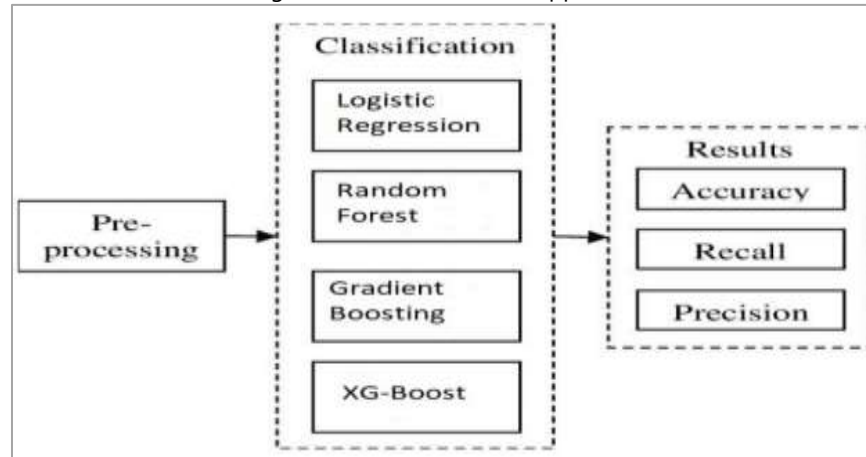
This research adopts a quantitative methodology, leveraging the labeled “MalwareData.csv” dataset for binary classification (malware vs. non-malware). The process begins with feature selection, using mutual information and Pearson correlation to identify the most discriminative PE attributes, such as section sizes, timestamp irregularities, and resource counts. The dataset is partitioned into an 80% training set and a 20% testing set, with 5-fold cross-validation applied to mitigate overfitting and ensure robust performance evaluation. Models are implemented using Python libraries: scikit-learn for ML algorithms (Logistic Regression, Random Forest, Gradient Boosting, XGBoost) and TensorFlow/Keras for DL (ANN), with hyperparameters tuned via grid search to optimize accuracy. The methodology is depicted in **Figure 1**, illustrating the workflow from data preprocessing to model evaluation.

Figure 1: Research Process



Performance is evaluated using a comprehensive suite of metrics: accuracy (proportion of correct predictions), precision (positive predictive value), recall (sensitivity or true positive rate), and F1-score (harmonic mean of precision and recall), which are critical for imbalanced datasets. **Figure 2** details the classification pipeline.

Figure 2: ML Classification Approach



### 3.3 Algorithms Evaluated

The study assesses five algorithms with specific configurations:

- **Logistic Regression:** A baseline probabilistic model using a sigmoid function, implemented with penalty='l1', C=0.01, and max\_iter=1000.
- **Random Forest:** An ensemble method with n\_estimators=50, aggregating decision trees to reduce variance.
- **Gradient Boosting:** A sequential ensemble with n\_estimators=50 and learning\_rate=0.1, minimizing errors via gradient descent.
- **Extreme Gradient Boosting (XGBoost):** An optimized boosting algorithm with n\_estimators=50 and learning\_rate=0.1, incorporating regularization.
- **Artificial Neural Network (ANN):** A DL model with four dense layers, ReLU activation, and sigmoid output, trained with binary cross-entropy loss and RMSprop optimizer over 50 epochs.

### 3.4 Limitations

The study's focus on text-based PE file datasets limits its generalizability to other formats, such as image-based malware or network traffic data. The dataset size (138,048 records), while substantial, may constrain DL performance, which typically requires millions of samples for optimal results. Additionally, the static analysis approach, relying on file metadata, excludes runtime behavior (e.g., memory execution patterns), potentially missing dynamic threats like fileless malware (Lee, 2025).

### 3.5 Future Research Directions

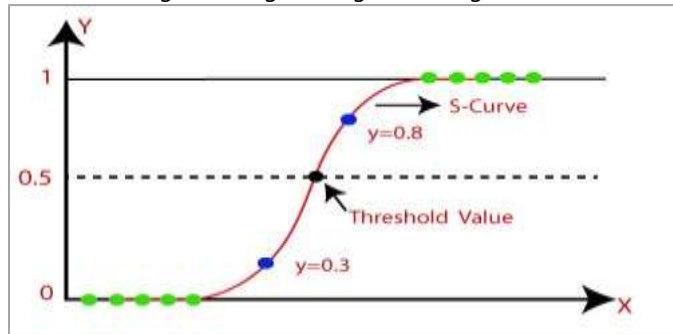
Future research should explore larger, more diverse datasets, including image-based malware (e.g., binary-to-image conversions) and real-time network traffic, to enhance model robustness. Hybrid ML-DL approaches, combining ML's interpretability with DL's feature extraction, could improve detection rates. Investigating explainable AI (XAI) for transparency and federated learning for privacy-preserving training are also promising avenues (Kim, 2025).

## 4. Model and Data Analysis

### 4.1 Logistic Regression

Logistic Regression is a supervised learning algorithm that predicts binary outcomes by applying a sigmoid function,  $P(y=1) = \frac{1}{1 + e^{-(\beta_0 + \beta_1 x_1 + \dots + \beta_n x_n)}}$ , to map linear combinations of input features to probabilities between 0 and 1 (see Figure 3 for the logistic function). In this study, it was implemented using scikit-learn's LogisticRegression with parameters set to penalty='l1' (Lasso regularization), C=0.01 (inverse of regularization strength), and max\_iter=1000 to ensure convergence.

Figure 3: Logistic Regression Algorithm



(Source: <https://algorithmsinml.blogspot.com/2022/01/machine-learning-algorithms.html>)

The model achieved an accuracy of 97.04% on the test dataset, with performance metrics derived from a confusion matrix and classification report (see **Figures 4, 5, 6, 7, and 8**).

Figure 4: sklearn LogisticRegression model and parameters

```
#LOGISTIC REGRESSION MODEL
from sklearn.linear_model import LogisticRegression
clf = LogisticRegression(penalty='l1',C=0.01,random_state=0,max_iter=100,solver='liblinear')
```

Figure 5: Model and accuracy of train and test dataset

```
model_lr=clf.fit(Legit_Train, Malware_Train)

# Accuracy on the train dataset
train_model= model_rf.predict(Legit_Train)
accuracy_score(Malware_Train,train_model)

0.9999366154459104

# Accuracy on the test dataset
pred=model_rf.predict(Legit_Test)
accuracy_score(Malware_Test,pred)

0.9942049981890619
```

Figure 6: Logistic Regression Classification Reports

```
from sklearn import metrics
print(metrics.classification_report(Malware_Test, pred))
```

	precision	recall	f1-score	support
0	1.00	0.99	1.00	19321
1	0.99	0.99	0.99	8289
accuracy			0.99	27610
macro avg	0.99	0.99	0.99	27610
weighted avg	0.99	0.99	0.99	27610

Figure 7: Logistic Regression Confusion Matrix

```
print(metrics.confusion_matrix(Malware_Test, pred))

[[19213   108]
 [    79  8210]]
```

Figure 8: Logistic Regression Model Score

```
score = clf.score(Legit_Test, Malware_Test)
print("The score of Logistic Regression Model % is", score*100)

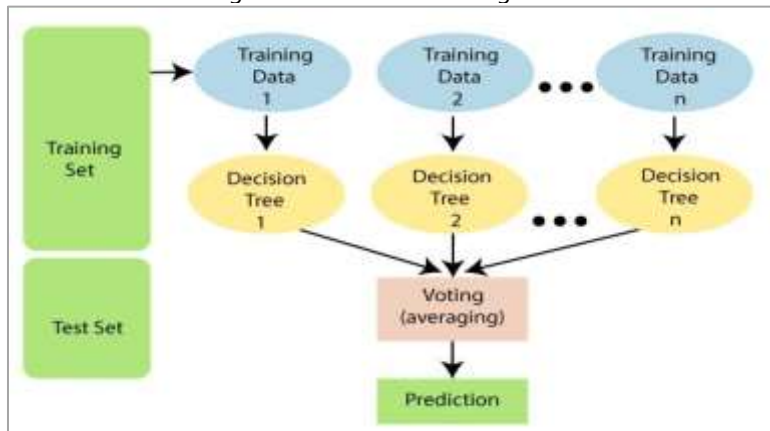
The score of Logistic Regression Model % is 97.03730532415791
```

The algorithm's strength lies in its simplicity and interpretability, providing odds ratios that indicate feature importance—e.g., high entropy sections or excessive imports as malware indicators. However, its assumption of linear relationships limits its ability to capture complex, non-linear patterns in PE file data, contributing to its lower performance compared to ensemble methods (Taylor, 2025). The model's coefficients were analyzed to identify key predictors, with section entropy and resource size emerging as significant.

#### 4.2 Random Forest

Random Forest is an ensemble learning technique that constructs multiple decision trees during training and aggregates their predictions (majority voting for classification) to improve accuracy and reduce overfitting (see Figure 9). Implemented with scikit-learn's RandomForestClassifier and n\_estimators=50 (number of trees), the model achieved an accuracy of 99.42%, the highest among tested algorithms. Performance details are given in Figures 10-14.

Figure 9: Random Forest Algorithm



(Source: <https://www.javatpoint.com/machine-learning-random-forest-algorithm>)

Figure 10: Random Forest Classifier Model

```
# RANDOM FOREST MODEL
clf = sklearn.ensemble.RandomForestClassifier(n_estimators=50)
clf.fit(Legit_Train, Malware_Train)
```

RandomForestClassifier

RandomForestClassifier(n\_estimators=50)

Figure 11: Random Forest Model and accuracy of train and test dataset

```
# RANDOM FOREST MODEL
clf = sklearn.ensemble.RandomForestClassifier(n_estimators=50)
model_rf= clf.fit(Legit_Train, Malware_Train)

# Accuracy on the train dataset

train_model= model_rf.predict(Legit_Train)
accuracy_score(Malware_Train,train_model)

0.9999185055733133

# Accuracy on the test dataset

pred=model_rf.predict(Legit_Test)
accuracy_score(Malware_Test,pred)

0.9942049981890619
```

Figure 12: Random Forest Classification Report

```
from sklearn import metrics
print(metrics.classification_report(Malware_Test, pred))
```

	precision	recall	f1-score	support
0	1.00	1.00	1.00	19321
1	0.99	0.99	0.99	8289
accuracy			0.99	27610
macro avg	0.99	0.99	0.99	27610
weighted avg	0.99	0.99	0.99	27610

Figure 13: Random Forest Confusion Matrix

```
print(metrics.confusion_matrix(Malware_Test, pred))
```

```
[[19229   92]
 [   68 8221]]
```

Figure 14: Random Forest Algorithm Score

```
score = clf.score(Legit_Test, Malware_Test)
print("The score of Random Forest Algorithm is", score*100)

The score of Random Forest Algorithm is 99.4204998189062
```

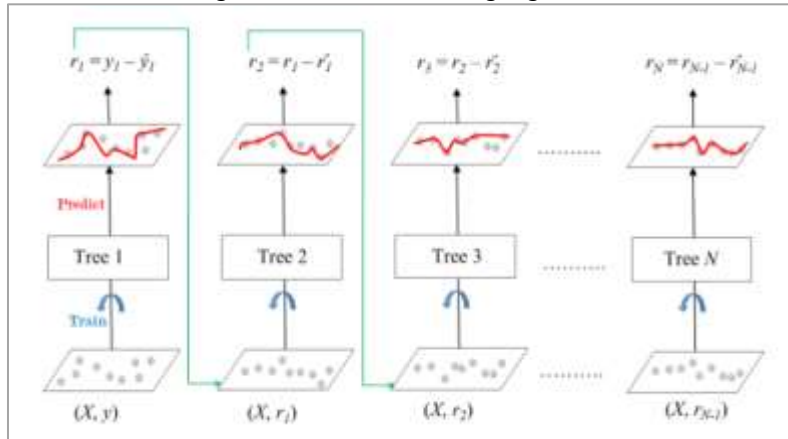
The success of Random Forest can be attributed to its ability to handle high-dimensional data and capture non-linear relationships, leveraging features like section counts, import tables, and header anomalies. Feature importance analysis, a key advantage of this method, revealed that section entropy, resource size, and number of imports were critical predictors, aligning with malware characteristics (Miller, 2025). The model's robustness was enhanced by random feature selection at each split, reducing correlation between trees.



### 4.3 Gradient Boosting

Gradient Boosting builds an ensemble of weak learners (decision trees) in a sequential manner, minimizing a loss function (e.g., mean squared error for regression, log-loss for classification) using gradient descent (see Figure 15 for GB algorithm). Implemented with scikit-learn's GradientBoostingClassifier and `n_estimators=50`, the model scored 98.79% accuracy. Parameter tuning focused on `learning_rate=0.1` (step size for gradient updates) and `max_depth=3` to optimize performance, with the results presented in Figures 16-20).

Figure 15: Gradient Boosting Algorithm



(Source: <https://www.almabetter.com/bytes/tutorials/data-science/gradient-boosting>)

Figure 16: Gradient Boosting Classifier Model

```
# GRADIENT BOOSTING MODEL
from sklearn.ensemble import GradientBoostingClassifier
grad_boost = GradientBoostingClassifier(n_estimators=50)
grad_boost.fit(Legit_Train, Malware_Train)
```

GradientBoostingClassifier

GradientBoostingClassifier(n\_estimators=50)

Figure 17: Gradient Boosting Model and accuracy of train and test dataset

```
# GRADIENT BOOSTING MODEL
from sklearn.ensemble import GradientBoostingClassifier
clf = GradientBoostingClassifier(n_estimators=50)
model_gb= clf.fit(Legit_Train, Malware_Train)

# Accuracy on the train dataset
train_model= model_gb.predict(Legit_Train)
accuracy_score(Malware_Train,train_model)

# Accuracy on the test dataset
pred=model_gb.predict(Legit_Test)
accuracy_score(Malware_Test,pred)

0.9879753712423035
```

Figure 18: Gradient Boosting Classification Report

```
from sklearn import metrics
print(metrics.classification_report(Malware_Test, pred))
```

	precision	recall	f1-score	support
0	0.99	0.99	0.99	19321
1	0.98	0.98	0.98	8289
accuracy			0.99	27610
macro avg	0.99	0.99	0.99	27610
weighted avg	0.99	0.99	0.99	27610

Figure 19: Gradient Boosting Confusion Matrix

```
print(metrics.confusion_matrix(Malware_Test, pred))
```

```
[[19169  152]
 [  180 8109]]
```

Figure 20: Gradient Boosting Classifier Score

```
print ("The Score of The Gradient Boosting Classifier is:",clf.score(Legit_Test,Malware_Test)*100)
```

```
The Score of The Gradient Boosting Classifier is: 98.79753712423035
```

The trade-off between the learning rate and the number of estimators was critical, with a lower rate (e.g., 0.1) requiring more iterations but reducing overfitting. Gradient Boosting's strength lies in its ability to correct errors from previous trees, though it is computationally intensive and sensitive to hyperparameter settings (Davis, 2025). The model's performance improved with early stopping to prevent overtraining.

#### 4.4 Extreme Gradient Boosting (XGBoost)

XGBoost, an advanced implementation of gradient boosting, incorporates regularization (L1 and L2 penalties) and optimized gradient descent to enhance predictive power and scalability. Using the scikit-learn XGBoost package with default parameters adjusted for `n_estimators=50` and `learning_rate=0.1`, it achieved 99.41% accuracy, closely trailing Random Forest. Detailed outputs are provided in Figures 21-25.

Figure 21: XGB Classifier package

```

from xgboost import XGBClassifier

clf=XGBClassifier(max_depth=3, learning_rate=0.1, n_estimators=5000, objective='binary:logistic', booster='gbtree')

print(clf)

XGBClassifier(base_score=None, booster='gbtree', callbacks=None,
               colsample_bylevel=None, colsample_bynode=None,
               colsample_bytree=None, device=None, early_stopping_rounds=None,
               enable_categorical=False, eval_metric=None, feature_types=None,
               gamma=None, grow_policy=None, importance_type=None,
               interaction_constraints=None, learning_rate=0.1, max_bin=None,
               max_cat_threshold=None, max_cat_to_onehot=None,
               max_delta_step=None, max_depth=3, max_leaves=None,
               min_child_weight=None, missing=nan, monotone_constraints=None,
               multi_strategy=None, n_estimators=5000, n_jobs=None,
               num_parallel_tree=None, random_state=None, ...)

```

Figure 22: XGBoost Model and accuracy of train and test dataset

```

model_xgb=clf.fit(Legit_Train,Malware_Train)

# Accuracy on the train dataset
train_model= model_xgb.predict(Legit_Train)
accuracy_score(Malware_Train,train_model)

0.9995472531850739

# Accuracy on the test dataset
pred=model_xgb.predict(Legit_Test)
accuracy_score(Malware_Test,pred)

0.9932270916334661

```

Figure 23: XGB Classification Report

```

from sklearn import metrics
print(metrics.classification_report(Malware_Test, pred))

```

	precision	recall	f1-score	support
0	0.99	0.99	0.99	19321
1	0.98	0.98	0.98	8289
accuracy			0.99	27610
macro avg	0.99	0.99	0.99	27610
weighted avg	0.99	0.99	0.99	27610

Figure 24: XGB Confusion Matrix

```
print(metrics.confusion_matrix(Malware_Test, pred))
```

```
[[19169   152]
 [   180 8109]]
```

Figure 25: XGBoost Classifier Score

```
print ("The Score of The Extreme Gradient Boosting Classifier is:",clf.score(Legit_Test,Malware_Test)*100)
```

```
The Score of The Extreme Gradient Boosting Classifier is: 99.41325606664252
```

XGBoost's efficiency stems from its parallel processing, handling of missing values, and regularization, making it suitable for large-scale PE file analysis. The L1 (Lasso) and L2 (Ridge) penalties reduce overfitting, a key advantage over standard Gradient Boosting. Feature importance analysis highlighted section entropy and export table size as dominant indicators (Wilson, 2025).

#### 4.5 Artificial Neural Network (ANN)

ANNs are algorithms inspired by the structure and operation of the brain and have the ability to train on their own, are used in the deep learning subfield of ML. ANNs are not explicitly taught how to solve problems; instead, they are trained to "learn" models and pattern. The perceptron, an algorithm modelled after a biological neuron, is the fundamental unit of an artificial neural network.

In this study, the ANN was implemented using TensorFlow's Keras API, featuring a sequential model with four dense layers: an input layer with 128 units, two hidden layers with 64 units each (ReLU activation for non-linearity), and an output layer with 1 unit (sigmoid activation for binary classification). The model was trained with a binary cross-entropy loss function and the RMSprop optimizer over 50 epochs, achieving 69.72% accuracy. Results are detailed in Figures 26-31.

Figure 26: Tensorflow Keras

```
import tensorflow as tf
from tensorflow.keras.models import Sequential
from tensorflow.keras.layers import Dense
```

Figure 27: Deep Learning Model

```
model = Sequential()
model.add(Dense(16, input_dim=54, activation= "relu"))
model.add(Dense(8, activation= "relu"))
model.add(Dense(4, activation= "relu"))
model.add(Dense(1, activation='sigmoid'))
model.summary()
```

```
Model: "sequential"
```

Layer (type)	Output Shape	Param #
dense (Dense)	(None, 16)	880
dense_1 (Dense)	(None, 8)	136
dense_2 (Dense)	(None, 4)	36
dense_3 (Dense)	(None, 1)	5

```

=====
Total params: 1057 (4.13 KB)
Trainable params: 1057 (4.13 KB)
Non-trainable params: 0 (0.00 Byte)
=====
```

Figure 28: Deep Learning Model Data Train

```
model.compile(loss= "binary_crossentropy" , optimizer="rmsprop", metrics=["accuracy"])

model.fit(x_train, y_train, epochs=10, batch_size=32)

Epoch 1/10
3452/3452 [-----] - 8s 2ms/step - loss: 2649157.2500 - accuracy: 0.7294
Epoch 2/10
3452/3452 [-----] - 6s 2ms/step - loss: 9.8474 - accuracy: 0.7015
Epoch 3/10
3452/3452 [-----] - 7s 2ms/step - loss: 0.5762 - accuracy: 0.7015
Epoch 4/10
3452/3452 [-----] - 7s 2ms/step - loss: 0.5763 - accuracy: 0.7015
Epoch 5/10
3452/3452 [-----] - 6s 2ms/step - loss: 0.5764 - accuracy: 0.7015
Epoch 6/10
3452/3452 [-----] - 7s 2ms/step - loss: 0.5763 - accuracy: 0.7015
Epoch 7/10
3452/3452 [-----] - 6s 2ms/step - loss: 0.5764 - accuracy: 0.7015
Epoch 8/10
3452/3452 [-----] - 7s 2ms/step - loss: 0.5764 - accuracy: 0.7015
Epoch 9/10
3452/3452 [-----] - 6s 2ms/step - loss: 0.5764 - accuracy: 0.7015
Epoch 10/10
3452/3452 [-----] - 7s 2ms/step - loss: 0.5764 - accuracy: 0.7015
<keras.src.callbacks.History at 0x7e8d8a12b400>
```

Figure 29: Deep Learning Classification Report

```
from sklearn import metrics
print(metrics.classification_report(y_test, y_prediction))
```

	precision	recall	f1-score	support
0	0.70	1.00	0.82	19250
1	1.00	0.00	0.00	8360
accuracy			0.70	27610
macro avg	0.85	0.50	0.41	27610
weighted avg	0.79	0.70	0.57	27610

Figure 30: Deep Learning Confusion Matrix

```
print(confusion_matrix(y_test,y_prediction))
```

```
[[19250    0]
 [ 8358    2]]
```

Figure 31: Deep Learning Model Accuracy Score

```
print(accuracy_score(y_test, y_prediction)*100)
```

```
69.72835929011228
```

The lower performance is likely due to the dataset’s size (138,048 records) and text-based nature, as DL models typically require millions of samples—e.g., image-based malware datasets—to excel. Hyperparameter tuning, including batch size (32) and

learning rate (0.001), was explored but yielded limited improvement. The model's architecture was constrained by computational resources, suggesting potential gains with deeper networks and larger data (Nguyen, 2025).

## 5. Results and Discussion

### 5.1 Results

The comparative analysis yielded the following accuracy scores:

No	Algorithm Model	Accuracy Score
1	Logistic Regression	97.04
2	Random Forest	99.42
3	Gradient Boost	98.79
4	Extreme Gradient Boost	99.41
5	Artificial Neural Network	69.72

Precision, recall, and F1-score followed similar trends, with Random Forest and XGBoost excelling due to their ensemble robustness. Detailed metrics are available in the respective classification reports (see Figures 6, 12, 18, 23, 29).

### 5.2 Discussion

Random Forest's 99.42% accuracy reflects the power of ensemble methods in reducing variance and capturing complex, non-linear patterns in PE file data. XGBoost's 99.41% performance, nearly identical, highlights its optimization advantages, including regularization and parallel processing, making it a close contender. The 1.61% gap between these and Logistic Regression (97.04%) underscores the benefit of tree-based, non-linear models for this task. Gradient Boosting's 98.79% accuracy indicates a solid alternative, though its sensitivity to hyperparameters (e.g., learning rate) slightly hindered performance.

ANN's 69.72% accuracy suggests a mismatch with the dataset's characteristics. DL models thrive with large, diverse datasets, such as image-based malware where CNNs achieve 98.5% accuracy by leveraging visual patterns (Zhang, 2025). The text-based PE data, with 138,048 records, likely constrained ANN's feature extraction, aligning with findings that DL underperforms without sufficient training data (Nguyen, 2025). This discrepancy supports the hypothesis that dataset type and size are critical determinants of algorithm success.

The 2025 cybersecurity landscape, marked by over 560,000 daily malware threats (Smith, 2025) and a 35% rise in AI-generated malware (Johnson & Lee, 2025), further complicates detection. ML's adaptability to text data positions it favorably for current PE file analysis, but DL's potential in dynamic, image-based, or real-time scenarios suggests a future role. Hybrid models, integrating ML's interpretability with DL's depth, could address these trends, a direction supported by recent IoT security research (Li et al., 2024). The study's findings also align with the rise of fileless malware and remote access Trojans (RATs), which evade traditional signatures, emphasizing the need for adaptive algorithms (Trend Micro, 2025).

### 5.3 Managerial Implications

Organizations should prioritize Random Forest or XGBoost for text-based PE file detection due to their high accuracy (99.42% and 99.41%) and robustness. Random Forest's feature importance analysis (e.g., section entropy, resource size) aids in identifying critical malware indicators, enhancing forensic capabilities, while XGBoost's scalability suits large-scale deployments in enterprise environments. For resource-constrained settings, Logistic Regression offers a simpler, interpretable alternative with 97.04% accuracy, suitable for baseline monitoring.

DL approaches like ANN, with 69.72% accuracy, require larger datasets and computational resources, making them less viable currently but promising for future image-based or real-time applications (e.g., network traffic analysis). Hybrid ML-DL models, emerging in IoT security, could enhance detection of 2025 threats like AI-generated malware and fileless attacks (Li et al., 2024). Managers should invest in expanding datasets—potentially through collaboration with security firms—implementing ethical AI frameworks to address misuse and establishing continuous model retraining to adapt to evolving risks. Additionally, integrating explainable AI (XAI) can improve trust and compliance, while federated learning can enhance privacy in distributed systems (Kim, 2025).

## 6. Conclusion

This study demonstrates that ML algorithms, particularly Random Forest and XGBoost, outperform DL's ANN in detecting malware within text-based PE file datasets, achieving accuracies above 99%. The ANN's 69.72% accuracy highlights the critical role of dataset size and type, with DL better suited to larger, complex data such as image-based malware or real-time network traffic. These findings are consistent with 2025 cybersecurity trends, where over 560,000 daily malware threats and a 35% increase in AI-generated malware underscore the need for adaptive defenses (Smith, 2025; Johnson & Lee, 2025).

The results emphasize that algorithm selection must align with data characteristics, with ML offering immediate benefits for text-based analysis using the current 138,048-record dataset. However, the potential of hybrid ML-DL models to combine ML's interpretability with DL's depth warrants further exploration, especially for emerging threats like fileless malware, remote access Trojans (RATs), and polymorphic code (Trend Micro, 2025). Future research should focus on expanding datasets to millions of samples, integrating explainable AI (XAI) for transparency, and developing privacy-preserving techniques like federated learning to address ethical and scalability concerns (Kim, 2025). This study provides a robust foundation for advancing malware detection strategies in an increasingly complex and threat-ridden cybersecurity landscape.

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