Machine Learning techniques for malicious PDF detection

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ABSTRACT

This project presents an exhaustive analysis of machine learning techniques for detecting malicious PDF files. By comparing the performance of four binary classification models - Support Vector Machines (SVM), K-Nearest Neighbors (KNN), Decision Trees and Random Forests - we demonstrate the effectiveness of these approaches in achieving high accuracy and low false negative rates. What makes this project stand out is its focus on the machine learning models themselves, including the careful selection of hyperparameters to optimize their performance. Additionally, the inclusion of KNN as a valid model is rare in the field, and the analysis of evasion techniques adds another layer of depth to the study. Overall this paper, realized for the MALIS course at EURECOM (year 2022/2023), offers a comprehensive look at the use of machine learning for malicious PDF detection and the potential vulnerabilities of these models.

1 Introduction

PDF (Portable Document Format) is a file format used for exchanging and sharing documents. It can contain various types of elements, such as text, images, multimedia, and executable code. Keywords, also known as actions or triggers, specify the different types of contents and they can be used to detect whether the file is malicious or Benign. In addition, PDF files may include also fonts, annotations, and form fields, which can be exploited for malicious purposes. We implemented four different binary classifiers to analyze their performances and to prove which one achieves the best results in terms of Accuracy and False Negative Rate. The task is a binary classification, with malicious PDFs labelled as Positive and Benign PDFs labelled as Negative. We also investigated evasion techniques against our classifiers concluding the work with the implementation of a countermeasure algorithm known as Adversarial Learning.

2 Related work

Most of the publications on this topic makes use of the Contagio dataset [1] that is the one we have adopted as benchmark. We have considered some of them. Maiorca et al. [2] preprocesses data with PDFiD [3] and uses SVM and Random Forest, Cuan et al. [4] uses both PDFiD as preprocessing and train a RBF SVM, they also explain how to perform evasion attacks and relative countermeasures. In [5] Li et al. explain the iterative Gradient Descent attack algorithm against RBF SVM.

3 Datasets and features

As first step in building our model, we needed to obtain a dataset of PDFs to use for training and evaluation and we went for the Contagio dataset. It is a collection of malicious PDF files that has been widely used for research and testing purposes. The dataset contains about 20000 PDF samples (almost balanced between Malicious and Benign), including malware, phishing attacks, and other types of malicious contents. The samples in the dataset are representative of the types of threats that are commonly encountered.

We chose to perform a static analysis, which does not require opening the PDFs in a reader. Indeed, we used a tool called PDFiD to extract relevant information from the PDFs. PDFiD characterizes each PDF by extracting the number of occurrences of specific keywords. This allowed us to map each PDF into an array of 21 elements that became our features vector.

Among the keywords that we selected, some are related to the structure of the PDF file, such as obj and endobj, which mark the beginning and end of an object, stream and endstream, which mark the beginning and end of a stream of data. We also included xref, trailer, and startxref, which pertain to the organization of the file. Next, there are features related to the content of the PDF: we added /Page, which specifies a page object in the file, and /Encrypt. We also included /ObjStm, which denotes an object stream, /JS and /JavaScript, which indicate the presence of JavaScript code. Additionally, we selected features related to actions that can be triggered by the PDF, such as /AA, /OpenAction, /XFA and /AcroForm, that could potentially exfiltrate information from users. We also included the features related to the types of data that may be present in the file, such as /JBIG2Decode, /RichMedia, /Launch and /EmbeddedFile. Finally we also chose /Colors, which specifies the presence of more than 16 million colors.

The output of PDFiD is then converted into a CSV file, which can be easily accessed using the numpy and pandas Python libraries. This CSV file serves as the basis for our data extraction pipeline, which we have implemented using the functions provided by PDFiD. It is important to note that the keywords we selected are well known to be discriminant for PDF malware analysis but they do not represent the full set that may appear in a PDF file.

The plot in Fig. 2 shows that the features distribution is much different between Benign and Malicious PDFs.

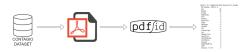


Figure 1: Features extraction pipeline.

3.0.1 Model Validation

We statically split the dataset in Train and Test using a stratified approach supplied by the sklearn library [6]. The Training Set, which consists of 80% of the samples, is used to train and validate the models with a k-fold cross validation approach. The Test Set, which consists of 20% of the entire dataset, is used to make final considerations about the performance of the models

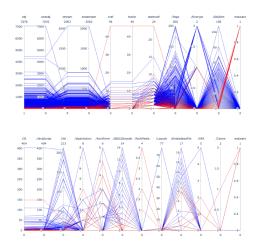


Figure 2: The parallel plot highlights the difference between the features of Benign PDFs (Blue) and Malicious PDFs (Red).

trained with the best parameters/hyperparameters. To evaluate our models, we used two metrics: the False Negative Rate (FNR) and the Accuracy defined as: We aimed to minimize the FNR,

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

Where FN: Malicious predicted Benign, FP: Benign predicted Malicious, TP: Malicious predicted Malicious, TN: Benign predicted Benign.

as False Negatives (Malicious PDFs classified as Benign) can be particularly damaging in this context. At the same time, we also took into consideration the value of the Accuracy, as the penalization of False Negative errors should not result in an excessively high number of False Positives that may lead to unnecessary alerts.

4 SUPPORT VECTOR MACHINES

Support Vector Machines are linear classifiers that look for maximum margin separation hyperplanes. The soft margin SVM problem adds a penalty term $C \sum_{i=1}^{n} \xi_i$ to the hard margin SVM to relax the constraint of having points inside the margin. The hyperparameter C is meant to define the strength of this penalization.

4.1 Linear SVM

We implemented a linear SVM classifier using the sklearn library [6].

4.1.1 Experiments

We have cross-validated the linear model by trying 10 different values for the C hyperparameter in the range [10^{-6} , 10]. As explained in Section 3 we optimized for the False Negative Rate (FNR) with the constraint of obtaining a high accuracy anyway.

The plot in Fig. 3 shows that the variations in terms of Accuracy and FNR when different values of C are used to train the linear SVM are not that evident. Here the results obtained with $C = 10^{-6}$ were not reported because of the significantly worse results (88.67% of Accuracy and 2.94% of FNR).

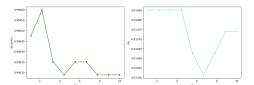


Figure 3: The plots show the change of the Accuracy (left) and the FNR (right) when the value of *C* hyperparameter increases.

C	Accuracy	FNR
2.22	99.06%	1.38%
6.67	99.03%	1.35%

Table 1: Best model parameters for Linear SVM

Optimizing for the FNR we have selected C = 6.67.

4.2 Kernel SVM

What makes the SVM particularly powerful is the way the dual problem is defined since it allows to easily introduce a kernel function to express the problem in a higher dimensional features space. Thus, we implemented a Radial Basis Function (RBF) kernel defined as:

$$k(x, y) = e^{-\gamma ||x-y||^2}$$

4.2.1 Experiments

The cross-validation of the model took into account two different hyperparameters (γ of the RBF kernel and C of the dual SVM problem). This time we exploited a grid search k-fold cross-validation that trains the model with each possible combinations of hyperparameters. The values we tried are:

- γ : 10 values in [10⁻⁶, 1]
- C: 10 values in $[10^{-6}, 10]$

We investigated the influence of both hyperparameters. What it is not displayed and analyzed in the plots is what happens with $C=10^{-6}$ and $\gamma=10^{-6}$, values under which the classifier performs very poorly in terms of Accuracy (around 54%) despite achieving a FPR equal to 0%. However, this is not better than a dummy classifier that safely detects every PDF as Malicious, hence it is not of interest in this project.

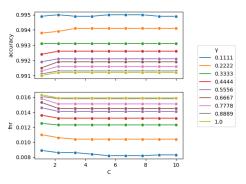


Figure 4: Accuracy (top) and FNR (bottom) when γ (colored lines) and C changes.

From Fig. 4 it is clear that smaller values of γ lead to obtain better results both in terms of Accuracy and FNR. The γ parameter of the RBF kernel controls its width and the shape of

the decision boundary. A lower value of gamma means a larger, less concentrated kernel, which can lead to smoother decision boundaries.

In contrast, the value of the C hyperparameter has clearly less influence on the model than γ , as we can observe in Fig. 4. It controls the trade-off between the simplicity of the model (low bias, high variance) and the training error (low variance, high bias). A higher value of C means a higher penalty for misclassification. When γ is sufficiently small, the Accuracy reaches the best values and the same happens for the FNR. Overall the best values we have found from cross validation are:

$$C = 5.56$$
 $\gamma = 0.11$ Accuracy = 99.50% $FNR = 0.82\%$

4.3 Performances on Test Set

Finally, given the best hyperparameters found in Section 4.2.1, we assessed the performances achieved on the Test Set.

4.3.1 Linear SVM

The obtained results are:

$$C = 6.67$$
 Accuracy = 99.06% $FNR = 1.58\%$

The scores obtained are comparable with the ones achieved on the Training Set. Despite a smaller improvement in the Accuracy, a slightly worse FNR has been obtained.

4.3.2 Kernel SVM

The RBF SVM on the entire Test Set achieves these results:

$$C = 5.56$$
 $\gamma = 0.11$ Accuracy = 99.73% $FNR = 0.36\%$

Here, in constrast with the linear model, we obtained better results both in terms of Accuracy and FNR.

5 Decision Trees and Random Forests

5.1 Decision Trees

The Decision Tree is a classification technique in which predictions are made in a sequence of single-attribute tests. Each internal node represents a test on an attribute and each branch represents the outcome of the test. The paths from the root to the leaf nodes represent the classification rules, and the leaf nodes represent the class labels.

5.1.1 Experiments

We performed a k-fold cross-validation with 5 folds in order to learn the best model parameters on the Training Set with more focus on *max depth*. To summarize, the results we have

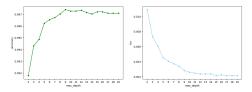


Figure 5: Accuracy (left) and FNR (right) when *max_depth* changes.

obtained are reported in Tab. 2. Despite the model achieves the best Accuracy with $max_depth = 9$, we chose $max_depth = 15$ that achieves the lowest FNR.

max depth	Accuracy	FNR
15	99.72%	0.21%
9	99.74%	0.28%

Table 2: Decision Tree - Optimal depths from cross-validation.

5.2 Random Forests

Random Forests is an ensemble method that combines the predictions of multiple Decision Trees models to make more accurate and stable predictions. To train a Random Forests model, multiple Decision Trees are trained on different samples of the data and their predictions are combined. This helps to reduce overfitting and improve the model's generalization ability.

5.2.1 Experiments

We performed a k-fold cross-validation with 5 folds in order to learn the best model parameters on the Training Set with more focus on *max_depth*. The plot in Fig. 6 shows how both the Accuracy and the FNR improve as the depth increases. Choosing a not too high value of depth is crucial to avoid overfitting.

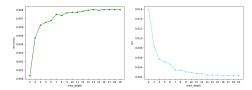


Figure 6: Accuracy (left) and FNR (right) when max_depth increases.

The best obtained result is:

$$max_depth = 16$$
 $Accuracy = 99.80\%$ $FNR = 0.22\%$

5.2.2 Performances on Test Set

The results obtained on the Test Set of both Decision Trees and Random Forests using the best model parameters discussed in 5.1.1 and 5.2.1 are:

$$max_depth = 15 \quad Accuracy = 99.75\% \quad FNR = 0.22\%$$

$$Random Forests$$

$$max_depth = 16 \quad Accuracy = 99.90\% \quad FNR = 0.13\%$$

6 K-Nearest Neighbors

K-Nearest Neighbors (KNN) works by identifying the K number of training samples that are closest in distance to the input sample and then assigning the input sample to the class of the majority of the K nearest neighbors. We implemented it with sklearn [6] using the default Euclidean distance.

6.1 Experiments

We performed a k-fold cross-validation with 5 folds. To determine the optimal value of K (the number of nearest neighbors to consider), we conducted a grid search over a range of possible values ($K \in [1,8]$). The results of this search shows, as expected, that the best performances were achieved with K=1. Since we have selected very discriminant features and we dispose of a large and diverse dataset, we expect that the possible overfitting effect is not really high. To visualize the effect of increasing

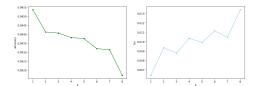


Figure 7: Accuracy (left) and FNR (right) when *K* increases.

K on the performance of our model, we plotted in Fig. 7 the Accuracy and FNR as a function of *K*. The performance of the model slightly decreases as *K* increases. This is to be expected, as increasing *K* allows the model to consider more neighbors, which can introduce more noise and reduce the model's ability to accurately classify samples. The best result obtained is:

$$K = 1$$
 Accuracy = 99.67% $FNR = 0.82\%$

6.2 Performances on Test Set

The results on the Test Set are:

$$K = 1$$
 Accuracy = 99.68% $FNR = 0.36\%$

We also obtained excellent results on the Test Set. We could explain the fact that K=1 is still the best model parameter by noticing that, despite the dataset is made of PDFs that are unique, PDFiD is able to extract such discriminant features that different PDFs result to be equal in terms of the extracted features vector. Having overlapped samples in the features space is really helpful for the way KNN classifies because the nearest neighbor of a test sample will probably consist in different overlapped samples, most of them belonging to the same class. Our results demonstrate that KNN is an effective technique for detecting malicious PDFs and that it can achieve high level performances with relatively little tuning.

7 Final results

We have summarized the results of all our classifiers in Tab. 3. The table shows that, as widely discussed in the previous sections, the model that achieves the best results is the Random Forests. Actually, all of them reach an impressively high Accuracy and low FNR. This is also coherent with the results obtained in Corona et al. [2] that proved Random Forests to be the best performing model. Also the other works cited achieve comparable results.

	Train		Test	
Model	Accuracy	FNR	Accuracy	FNR
Tree $depth = 15$	99.72%	0.21%	99.75%	0.22%
Forest $depth = 16$	99.80%	0.22%	99.90%	0.13%
KNN $k = 1$	99.67%	0.82%	99.68%	0.36%
LSVM C = 6.67	99.03%	1.35%	99.06%	1.58%
KSVM $C = 5.56$ $\gamma = 0.11$	99.50%	0.82%	99.73%	0.36%

Table 3: Overall results of all the models (LSVM: linear SVM, KSVM: RBF Kernel SVM). Results on Training Set are the ones obtained through k-fold cross-validation.

Finally we also plotted the ROC curves for all the models. In Fig. 8 we can confirm the results showed in Tab. 3.

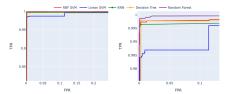


Figure 8: ROC curves comparing all the models.

8 ATTACKING THE CLASSIFIERS

In this Section, we present two evasion attacks against the classifiers we built and a countermeasure. We increased the number of objects in Malicious PDFs so that they will be detected as Benign by the classifiers (still preserving their malicious behaviour). We operated in a condition in which the attacker is equipped with the Training Set, the type of classifier and the model parameters used to train it.

8.1 Attack against SVM

We have studied an evasion attack based on the Gradient Descent algorithm following the idea of Cuan et al. in [4]. Given a feature vector x characterizing a Malicious PDF correctly classified, our goal is to find a x' that will be detected as Benign. The constraint is that x' is obtained with a minimal perturbation over x. The function to be minimized is the L1 distance between x' and x:

$$||x - x'||_1 = \sum_{i=1}^d x_i - x'_i$$

The Gradient Descent attack converges to the minimum iteratively. Following the approach of Li et al. in [5] the feature vector is moved in the negative direction of the vector normal to the decision boundary, that means that the Gradient Descent update step becomes:

$$x_{t+1} = x_t - \mu_t \nabla_x f_{\Phi}(x_t)$$

By recovering that $w = \nabla_x (w^T x_t + w_0)$ for a linear SVM it can be derived that $w = \nabla_x f_{\Phi}(x_t)$ in a kernel SVM. We obtained the expression for a RBF kernel SVM from the dual problem definition:

$$\nabla_x f_{\Phi}(x_t) = \sum_{i \in SV} \alpha_i z_i \nabla_x k(x_i, x_t) \text{ where}$$

$$\nabla_x k(x_i, x_t) = \nabla_{x_t} e^{-\gamma ||x_i - x_t||^2} = -2\gamma \alpha_i z_i (x_i - x_t) e^{-\gamma ||x_i - x_t||^2}$$

To better get the idea behind the attack we trained a RBF SVM $(C=1, \gamma=0.1)$ on the dataset preprocessing it with PCA (with 2 components) just to visualize it. In Fig. 9 a random Malicious PDF is perturbated iteratively (using a learning rate for the Gradient Descent of $\mu=0.03$) and it is successfully attacked. We only inspected the working mechanism of this evasion attack by trying to successfully craft Benign PDFs from malicious ones.

8.2 Attack against Decision Trees

We also investigated an attack against the Decision Trees classifier. Firstly we found a way to craft Malicious PDFs that are

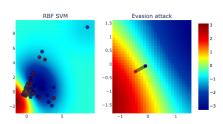


Figure 9: Decision boundary of RBF SVM (C = 1, $\gamma = 0.1$) on PCA = 2 dataset (left), Gradient Descent attack on a random Malicious PDF (right). (Blue: Benign, Red: Malicious).

detected as Benign (using a different approach with respect to the one used in 8.1 that is explained in the Pseudocode 1).

Algorithm 1 Evasion Attack

```
Require: Train DecisionTree using X_{train}
   M \leftarrow X_{train}[malicious]
   t \leftarrow 50
  for m_i \in M do
       for feature_i \in m_i do
           while feature_i < t do
                feature_i \leftarrow feature_i + 1
               m_i[j] \leftarrow feature_i
                Benign \leftarrow predict(m_i)
                if Benign is True then
                                                                 ▶ PDF evaded
                    break
                end if
           end while
                                                            > PDF not evaded
       end for
   end for
```

With a threshold t = 50 we obtained a success rate of evasion attack on the Training Set equal to 91.28%.

8.3 Adversarial Learning

In order to improve the strenght of the Decision Trees classifier against the attack procedure in 8.2 we implemented a defense mechanism similar to what has been implemented by Cuan et al. in [4]. It is called Adversarial Learning and the algorithm is shown in Pseudocode 2.

Algorithm 2 Adversarial Learning

```
Require: Train DecisionTree using X_{train}

t \leftarrow 50

X_{train}^{imp} \leftarrow X_{train}

M \leftarrow X_{train}[malicious]

while \#PDFevaded > 0 do

evaded, X_{train}^{evaded} \leftarrow evade(M, t)

if evaded is True then

X_{train}^{imp} \leftarrow X_{train}^{imp} + X_{train}^{evaded}

end if

train(X_{train}^{imp})

end while
```

The results we obtained are overall satisfying because the classifier is able to defend perfectly against our evasion algorithm.

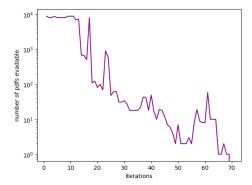


Figure 10: Adversarial Learning defense effectivness in different iterations: although the different spikes, the number of evadable PDFs of Training Set reduces progressively.

The plot in Fig. 10 shows that the number of PDFs that can be evaded in the Training Set reaches 0 at iteration 69.

We can also see in Fig. 11 how the features of the improved dataset (the ones obtained adding the crafted PDFs to the original Training Dataset) have been modified to defend against this attack.



Figure 11: Difference of features frequencies between X_{train} and X_{train}^{imp} (logarithmic scale).

9 Conclusions and future works

Classifiers To conclude, the model that performs better is the Random Forests, both in terms of Accuracy and FNR. Comparable results are achieved by the other models and the use of PDFiD makes all the algorithms efficient in detecting patters using the most discriminant features. Further improvement could be done in order to achieve even lower values of FNR. Dimensionality reduction techniques could be exploited toghether with other types of metrics that take into account both the Accuracy and the FNR.

Evasion Attacks The evasion attack against the Decision Trees showed a really high success rate on the Training Set. We thus implemented the defense mechanism that proved to be very effective using Adversarial Learning. We could investigate more the size of the improved training dataset nedded to mitigate the attack.

10 Contributions

These are the contributions of each member:

- L. Ippolito worked on Decision Trees and Random Forests classifiers carefully exploring all the model parameters and the presence of overfitting.
- M. Picasso studied the KNN classifier to better understand the reason why K = 1 is the best performing parameter.
- M. Rosso worked on SVM classifiers investigating the role of the different hyperparameters and the formulation of the dual soft margin SVM problem to be used in the evasion attacks.

We collaborated as a team both in the features extraction phase and on the choice of the model validation approach. After having assessed the performances of all the models we worked toghether on designing the evasion attacks algorithms and the countermeasures.

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