Vulnerable Code Detection Using Software Metrics and Machine Learning

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ABSTRACT Software metrics are widely-used indicators of software quality and several studies have shown that such metrics can be used to estimate the presence of vulnerabilities in the code. In this paper, we present a comprehensive experiment to study how effective software metrics can be to distinguish the vulnerable code units from the non-vulnerable ones. To this end, we use several machine learning algorithms (Random Forest, Extreme Boosting, Decision Tree, SVM Linear, and SVM Radial) to extract vulnerability-related knowledge from software metrics collected from the source code of several representative software projects developed in C/C++ (Mozilla Firefox, Linux Kernel, Apache HTTPd, Xen, and Glibc). We consider different combinations of software metrics and diverse application scenarios with different security concerns (e.g., highly critical or non-critical systems). This experiment contributes to understanding whether software metrics can effectively be used to distinguish vulnerable code units in different application scenarios, and how can machine learning algorithms help in this regard. The main observation is that using machine learning algorithms on top of software metrics helps to indicate vulnerable code units with a relatively high level of confidence for security-critical software systems (where the focus is on detecting the maximum number of vulnerabilities, even if false positives are reported), but they are not helpful for low-critical or non-critical systems due to the high number of false positives (that bring an additional development cost frequently not affordable).

INDEX TERMS Application scenarios, machine learning, software metrics, software security, security vulnerabilities.

I. INTRODUCTION

Several research studies show that software defects/vulnerabilities (e.g., Buffer overflow, SQL injection) are a central and critical source of security breaches [1]–[3] in computer systems. Such vulnerabilities are mainly caused by unprofessional or negligent developers who lack security knowledge [4]. To instruct software developers to incorporate security and, in general, quality into software, there are several well-established and widely known standards and best practice recommendations, such as Software Quality Assurance (SQA) [5], Quality by Design (QbD), OWASP secure coding practices, ISO / IEC 27034, and Privacy by Design [6]. However, research and experience show that modern software still fails in meeting basic security requirements [7].

A large number of tools and techniques to detect security vulnerabilities are nowadays available. For example, static code analysis [8] is a well-known technique used by developers to search for software defects and vulnerabilities in early stages of the software development. Nevertheless, detecting software vulnerabilities or distinguishing vulnerable from non-vulnerable code is not trivial. The low effectiveness of vulnerability detection tools and static code analyzers is a clear proof of this fact [9]. Thus, software is often deployed with bugs that can be exploited by attackers causing system outages, data breaches, or even safety issues. This has led to
many works trying to mitigate the damage that the exploitation of such vulnerabilities can cause at runtime.

In this work, we focus on prevention and on early detection of software vulnerabilities, as fixing those vulnerabilities is easier and less expensive and the consequences are potentially smaller (compared with the detection of vulnerabilities in later development stages or after deployment) [8]. In this direction, we present an empirical study on one of the early evidences of software quality, namely software metrics, whose correlation with the existence of security vulnerabilities has been shown in previous works [10], [11]. In practice, we aim to understand how the information provided by software metrics can be best used by machine learning algorithms to distinguish the vulnerable code units (files, functions) from the non-vulnerable ones with high levels of confidence within different circumstances, including different application scenarios that encompass diverse security concerns.

This study considers several commonly used machine learning (ML) algorithms (Random Forest, Extreme Boosting, Decision Tree, SVM Linear and SVM Radial) that are applied on software metrics of all types (e.g., Cyclomatic Complexity, Lines of Code, and Coupling Between Objects) collected from the source code of several widely used and representative software projects developed in C/C++ (Mozilla Firefox, Linux Kernel, Apache HTTPd, Xen and Glibc) at different levels (file level and function level). We consider different combinations of software metrics, selected based on different approaches (e.g., correlation analysis), and focus on four application scenarios (Highly-Critical, Critical, Low-Critical and Non-Critical) that have different concerns regarding security, thus requiring diverse criteria for evaluating the classifiers. For instance, in the highly-critical systems scenario, detection and elimination of vulnerabilities is of high priority even if some false alarms are reported, therefore, a criterion that measures the ratio of detected vulnerable code units independently from false alarms seems to be of interest. In contrast, in the non-critical systems, the number of false alarms can be the main concern due to limited development resources, thus, a criterion that in addition to the correctly classified vulnerable code, strongly rewards low false alarms seems to be adequate.

This work intends to contribute to answer the following research questions (RQs):

- **RQ1.** Can software metrics effectively be used to distinguish vulnerable code units from the non-vulnerable ones in different application scenarios?
- **RQ2.** What is the best combination of software metrics to be used for this purpose?
- **RQ3.** How do different machine learning algorithms perform in this context?
- **RQ4.** Can the results of this experiment be generalised and applied to different types of software systems?

We use the dataset built by Alves et al. [12], which includes software metrics and reported security vulnerabilities for all code units (e.g., functions and files) of several versions of different widely used software projects (Mozilla Firefox, Linux Kernel, Apache HTTPd, Xen and Glibc). Results show that the models created over software metrics are effective for security-critical applications (highly-critical and critical), in which the detection of vulnerabilities is of high priority. In contrast, a large number of false alarms make them useless for scenarios with low critical or non-critical systems (where budget to deal with vulnerabilities is limited). This suggests that it is quite important to consider application scenarios when building vulnerability detecting tools. From the analyzed classifiers, Random Forest and Extreme Boosting are the ones that lead to more precise models for both file and function level data. However, Decision Tree and Linear SVM build more generalizable models, thus, giving a better estimation when completely unknown data is used for testing.

The rest of the paper is organized as follows. Section II reviews the related work. Section III explains the approach, methods and techniques used to conduct the experiments and the analysis. A preliminary analysis of the results, focused on defining the configurations and settings to be used in the experiments, is presented in Section IV. Section V presents the results and their analysis. The main outcomes of the paper and the threats to the validity of the work are summarized and discussed in Section VI. Section VII concludes the paper and puts forward ideas for future work.

### II. BACKGROUND AND RELATED WORK

Modern businesses, organizations, and critical infrastructures are backed by software systems executing critical operations and transactions, providing services and dealing with huge amounts of sensitive data for supporting effective decisions and constant business/system adaptation. This tremendously increased concerns regarding security, driving researchers and businesses to come up with tools, techniques, standards, and regulations to help developers to ensure security in software systems [13], [14].

We can find a lot of efforts in the literature focused on the definition of best practices, standards, and regulations to help developers in building high quality and secure software (e.g., ISO/IEC 27000 [15], ISO 15408 [16], Software Quality Assurance (SQA) [5], [17], [18], OWASP secure coding practices [19], [20], ISO/IEC 27034 [21], and Privacy by Design (PbD) [6]) [22]–[24]. An structured description and comparison between most of these efforts can be found in [25] and [26].

We also can find many works on tools and techniques to prevent or detect and eliminate software bugs during the software development process [27], [28], like SonarQube [29], a platform for continuous inspection (static analysis) of code to detect bugs, vulnerabilities, and code smells. Sensei [30] is another example that tries to enforce secure coding guidelines in the integrated development environment. However, it is still very difficult for developers, if not impossible, to build software without vulnerabilities. This has led to many works trying to mitigate the damage that such vulnerabilities can cause at runtime (e.g., via via intrusion detection systems and...
attack tolerance techniques) [31]–[35]. Despite all existing efforts, software is still shipped with exploitable vulnerabilities causing huge damages to the systems and businesses. Thus, better and more effective approaches to detect vulnerabilities earlier in the life cycle are still needed [36].

Existing approaches for the detection of vulnerabilities in the early stages of the software development can be divided in two categories: static code analysis [8] and penetration testing. In static code analysis, the source code (or compiled code) of a software is examined statically, without executing it. Static analysis of code can be done manually or by using static analysis tools (SATs). Manual auditing of code is time consuming and requires skilled human code auditors with sufficient and deep knowledge regarding security vulnerabilities and security attacks to be able to effectively examine the code. In contrast, static analysis tools encapsulate security knowledge in a way that does not require highly skilled human auditors with security expertise, thus, are faster and can be frequently used examine the code. Nevertheless, the output of these tools still requires evaluation by experts. In contrast to code static analysis, penetration testing [37] is used when the code can already be executed. It works by emulation of security attacks to check for exploitable vulnerabilities. Both static analysis tools and penetration testing tools have limitations and their low effectiveness in detecting vulnerabilities has been shown in several studies [27], [38].

Our work aims to help developers focusing on security in the early stages of software coding, by collecting and analysing measurable evidences of security issues in the code.

Several approaches are used in the literature to deal with vulnerability prediction based on evidences and data collected from the source code [39], namely: software metrics, text mining, dependency graphs, and taint analysis. In this paper, we focus on software metrics, which are widely used as indicators of software quality (e.g., reliability and maintainability) [40]–[42]. It is worth noting that comparison between software metric based approach and other approaches are out of focus of this paper. Using software metrics for training models to predict software bugs (not necessarily security issues) is not a new topic [43]–[46]. A survey of various machine learning algorithms with software metrics for prediction of software faults is presented in [47].

Several studies in the literature show that there is some correlation between software metrics and security vulnerabilities [48], [49]. We can also find several works related to the detection of security issues using data mining, machine learning, and statistical techniques combined with software metrics [50]. However, most of these studies and works are either done over a limited number of software metrics (e.g., complexity metrics) [48], [51], [52], or use a combination of software metrics with other features [53], [54], or focus on a single security issue (e.g., buffer overflow) [55], or are limited to a specific code unit (e.g., file/class or function/method) [54] and a specific software project [11], or make a comparison between software metrics and other features [56]. To the best of our knowledge, there is no comprehensive study on software metrics and their capabilities for the detection/prediction of security vulnerabilities in the code.

In a previous work [57], we tried to address some of the limitations mentioned above by performing an analysis over a large number of software metrics obtained from different software projects, to demonstrate the possibility of using such metrics as an indicator of the existence of vulnerabilities. A heuristic search algorithm (Genetic Algorithm) combined with one classifier model (Random Forest) was used to find the most relevant subset of software metrics leading to a prediction model with the higher accuracy. Although the results obtained suggest that software metrics can be used to distinguish vulnerable code with a high level of accuracy, the work is quite limited, as accuracy is not the best criteria when dealing with imbalanced datasets. Furthermore, the work was limited to a single classification model.

In this work, we do not just aim at building one prediction model using a machine learning algorithm over software metrics as many works in the literature; we perform a comprehensive experiment to study several machine learning algorithms, several combination of software metrics, several application scenarios, several code levels, and several software projects individually and in combination, in order to find out how to achieve the best result within different circumstances for different scenarios and how to generalize the results.

The work most similar to ours is the one presented in [58]. The authors compare several state of the art machine learning techniques [54], [59], [60] regarding their ability to detect vulnerable code. There are, however, several shortcomings in that work: i) the study is limited to file level metrics; ii) it is limited to the use of the same single set of software metrics in all experiments; and iii) the projects included in the dataset are not considered individually in the experiments, but in combination, which limits the conclusions.

III. METHODOLOGY

Our goal is to conduct a comprehensive study to understand whether software metrics can effectively be used to distinguish the vulnerable code units from the non-vulnerable ones. The experimental process is divided in two phases, as shown in Fig. 1. The first phase, Preliminary Analysis, is focused on defining the configurations and settings to be used in the experiments. These configurations and settings are mainly related to the specification of the dataset (dimensions and class distribution), machine learning algorithms to be used for building the classification models, and definition of the scenarios under which the models will be evaluated. The second phase, Experimentation and Analysis, is focused on running the experiments based on the configurations defined in the previous phase, and analyzing the results obtained. In practice, these experiments involve building and evaluating classification models using different machine learning algorithms, different combinations of software metrics, and source code of different software projects within different
application scenarios. In addition to and integrated with the above principal phases, we validate the approach and methods used as well as the results obtained and demonstrate whether the results can be generalized. These Validation and Generalization (V&G) activities are shown in the Fig. 1 with green check marks. In short, our study considers:

i) Five representative software projects (Mozilla Firefox, Linux Kernel, Apache HTTPd, Xen and Glibc), used both individually and in combination;

ii) Five combinations of software metrics of different types (complexity, volume, coupling and cohesion) collected at different levels of code (file and function);

iii) Five widely-used machine learning algorithms (Random Forest, Extreme Boosting, Decision Tree, SVM Linear and SVM Radial), considering different configurations to achieve the best prediction results;

iv) Four application scenarios with diverse concerns regarding security (highly-critical, critical, low-critical, non-critical), which in practice are addressed by using different evaluation criteria (Recall, Informedness, F-Measure, Markedness).

The dataset used in this study, available at [61] and described in [12], contains detailed information about the whole source code, composing files, classes, and functions of several versions of five software projects implemented in C/C++: Mozilla Firefox (mozilla.org), Apache HTTPd (httpd.apache.org), Linux Kernel (kernel.org), Xen Hypervisor (xen.org), and Glibc (gnu.org/software/libc). This information was extracted by Alves et al. from the source code of several versions of the aforementioned projects using Understand [62], and represented through a long list of software metrics. Our analysis is performed on different architectural levels of these projects, namely file and function levels, each one having its own set of software metrics. It is worth noting that class-related metrics are not considered in this work as only one of the projects (Mozilla Firefox) is implemented in an object-oriented language, C++ in the case, and therefore contains classes.

As mentioned, we use a large set of software metrics of different types, including complexity (e.g., Cyclomatic Complexity), volume (e.g., Lines of Code), coupling (e.g., Coupling Between Objects), and cohesion (e.g., Lack of Cohesion) metrics. In practice, a total of 28 function-level metrics and 51 file-level metrics are considered (the complete list of metrics used in this work can be found in Table 3 and Table 4, and their description can be found in [62]). The dataset also includes detailed information about the known vulnerabilities, obtained by analyzing a large number of security patches gathered from various sources (CVEDetails, Mozilla Foundation Security Advisores (MFSA), and Xen Security Advisores (XSA)). Table 1 presents a summary of the projects and their vulnerabilities. It is worth mentioning that only source files (.c and .cpp files) are considered in our analysis, so the number of functions, files and lines of code presented in Table 1 do not include the information in C header files (.h files) that only contain function declaration and not implementation. As shown in the table, Linux Kernel and Mozilla Firefox are the biggest projects in terms of the number of files and functions and Apache HTTPd is the smallest one. In all projects, the percentage of vulnerable code is quite low, so that we need to somehow deal with highly imbalanced dataset when building the models. It becomes worse in the case of functions. Among all, project Glibc is extremely imbalanced. More details about the dataset can be found online [61].

We selected this dataset because it includes various versions of several important and representative projects from a security point of view: they are used by many worldwide users, they were already targeted by many security attacks, and they include several versions of the same file or function (including versions with and without vulnerabilities). This is important for building more effective prediction models.

FIGURE 1. Methodology used in this work.
for real cases, namely for contexts were the same project has many different versions and past knowledge should be used for preventing future vulnerabilities. Each project in the dataset is representative of a broader class of software in a particular category, in terms of functionality (e.g., the Apache HTTPd can be considered representative of HTTP servers). To the best of our knowledge, this is the most complete and extensive dataset available fitting our purposes.

### A. PRELIMINARY ANALYSIS

The first phase of our exploratory study is focused on the configuration and settings of the experiments. These configurations and settings are related to: i) reduction of the dataset dimension; ii) adjustment of the dataset class distribution; iii) selection of machine learning algorithms; and iv) definition of application scenarios and selection of appropriate evaluation criteria for the scenarios.

1) **DIMENSION REDUCTION**

Although some software metrics may contain useful information to detect vulnerable code units, others might be irrelevant or redundant. This way, in order to build a high performance classification model out of software metrics for vulnerable code detection, it may be important to search for the most informative and discriminative metrics and to discard the redundant or irrelevant ones, which may reduce the accuracy and the computational efficiency of the classifier [63]. In this step, we aim to find out whether the process of reducing the number of features under consideration can indeed help achieving better results.

There are several strategies to deal with the issue of identifying the less-informative software metrics [64]. The basic strategy is called *exponential search*, which is the most exhaustive search technique, guaranteeing that the optimal subset of software metrics is found. Nevertheless, this strategy is not promising or not feasible in practice when the number of features (software metrics in our work) is high (for a feature set of size n, the number of iterations would be $2^n$). Another strategy is *heuristic search*, which tries to guarantee the convergence to the (near) best subset of software metrics. This strategy is time consuming and its results depend on the classification model that is used as fitness function. Finally, *statistical-based filtering* can be used to find out which metrics may not be informative for the detection of vulnerable code units. In this work, we use this last strategy, since it is relatively fast and independent from the classification models.

Fig. 2 presents the process for dimension reduction. As shown, we conducted a detailed correlation and redundancy analysis on the software metrics at file and function levels for the five projects included in the dataset. These analyses allow identifying the least relevant or irrelevant metrics (i.e., not or lowly correlated with the class under study, which is the existence of vulnerability), and the redundant software metrics (with respect to other metrics).

To identify the irrelevant metrics, we calculate the correlation between metrics and the existence of vulnerabilities using two well-known techniques: *Pearson* [65] and *Spearman* [66] correlation coefficients. While the first evaluates the linear relationship between the software metrics and the existence of vulnerabilities, the second evaluates the monotonic relationship between them. Note that, in this work, we use both Pearson and Spearman correlation coefficient techniques to distinguish highly correlated features (i.e., when value of one feature increases then the value of other feature increases by a consistent amount) from the irrelevant ones.

Once the calculations are done, the software metrics are ranked by correlation value (from the highly correlated metrics to the least correlated ones). To select the irrelevant software metrics from this ordered list, a threshold should be defined. In this work, we consider the median as a threshold, as it is commonly used in the literature [67]. Thus, the software metrics with both Pearson and Spearman correlation values below the median are considered as irrelevant.

To identify the redundant metrics, the Markov Blanket Filtering [68], [69] is used. Based on this filtering technique, let $G$ be the current set of software metrics. If software metric (SM) $SM_j$ has a Markov Blanket $SM_j$ within $G$, it suggests that $SM_j$ contributes with no more information beyond $SM_i$ to the target class (i.e., existence of vulnerability in this work), and, therefore, $SM_j$ can be safely removed from $G$. Based on the Approximate Markov blanket definition from [68], given two predictive software metrics $SM_i$ and $SM_j$ and the target class $V$, $SM_j$ is redundant to $SM_i$, if both equations 1 and 2 are true:

$$C(SM_i, V) \geq C(SM_j, V) \quad (1)$$

$$C(SM_i, SM_j) > C(SM_j, V) \quad (2)$$
where, \( C(SM_i, V) \) is the correlation coefficient between \( SM_i \) and the target class \( V \), \( C(SM_j, V) \) is the correlation coefficient between \( SM_j \) and the target class \( V \), and \( C(SM_i, SM_j) \) is the correlation coefficient between the two predictive software metrics \( SM_i \) and \( SM_j \). For this analysis, we again use both Pearson and Spearman techniques to calculate the correlation coefficient. In practice, we consider software metrics as Redundant when they are identified as so (based on the Approximate Markov blanket), using both Pearson and Spearman techniques.

After identifying the irrelevant and redundant metrics, we generate 5 groups of software metrics to be analyzed in further experiments (the goal is to understand whether dimension reduction based on correlation and redundancy analyses can help to achieve better results):

i) **All**, which includes all software metrics present in the dataset;

ii) **All - Irrelevant** that includes all metrics minus the ones that are considered as irrelevant;

iii) **All - Redundant**, which includes all metrics minus the ones that are considered as redundant;

iv) **All - (Irrelevant AND Redundant)** that includes all metrics minus the ones that are listed as irrelevant and as redundant; and

V) **All - (Irrelevant OR Redundant)**, including all metrics minus the ones that are listed as irrelevant or as redundant.

2) **CLASS DISTRIBUTION IN THE DATASET**

As shown in Table 1, the dataset used in this work is quite imbalanced, as the vulnerable code units make a small fraction of the whole dataset (e.g., 2.27% in the case of Linux Kernel files). In such cases, research shows that machine learning algorithms tend to be overwhelmed by the large class and ignore the small ones [70]. On the other side, transforming a representative dataset into a balanced dataset (either by undersampling or by oversampling) may cause the loss of information about the frequency of each class and, thus, affecting the accuracy of the classification models [71]. For this reason, we performed an analysis to find out how balanced the dataset should be in order to build high performance classifiers for vulnerability detection (i.e., models with high true positive and low false positive rate). In practice, we apply one of the most effective (in terms of performance) and efficient (in term of time) strategies to deal with imbalanced data, which is to moderately undersample the majority class [72], to gradually balance the dataset (from a fully representative and imbalanced dataset to a 100% balanced dataset) and observe the impact on the performance. This allows to select a dataset with the near best class distribution that results in the near best performance compared to others.

✓ **V&G - Representativeness of Random Samples:** In some experiments, we do not use the whole dataset but a random sample of it (as a result of undersampling, which is done to balance the training sets helping to build more effective models, as explained in Section III-A2). For this reason, it is necessary to demonstrate that the randomly chosen samples are representative of the whole dataset and, thus, do not influence the overall results. To do so, we perform a correlation and redundancy analyses over 10 different random samples, including 10000 records each, from one project, namely Firefox. This is done in order to demonstrate that the randomly selected samples follow similar statistical patterns, thus, are able to build pretty much similar predictive models (to ensure that there is no sampling bias influencing the analysis).
3) MACHINE LEARNING ALGORITHMS

Our work is focused on the idea of using machine learning algorithms for detecting vulnerable code units based on software metrics. Thus, we selected several commonly used or recommended machine learning techniques to thoroughly explore this idea. By referring to [50], [58] that survey prediction models used for detecting vulnerabilities, the ones that seem to be the most commonly used in this area are: Decision Tree [73], Random Forest [74], Support Vector Machine [75], [76], and Logistic Regression (LR) [77]. Since, in practice, LR and SVM with linear kernel usually present similar results [78], we use linear SVM in addition to radial SVM and discard LR. In addition to these, we also include the Extreme Gradient Boosted [79], as its good performance has been shown in many cases [80]. In short, the machine learning algorithms used in this study are:

- **Decision Tree (DT):** commonly and most used supervised learning technique to support decision making. Given a dataset composed of several features and target classes, by using the Decision Tree technique, a sequence of classification rules are generated to make decisions in diverse cases. To generate these rules, it uses a tree-like model to break up a complex decision into several simpler decisions [73].

- **Random forest (RF):** is one of the most popular ensemble learning algorithm. This algorithm consists of a combination of several DT-based classifiers, each one fitted on a random sample of a dataset, making it more accurate and robust to outliers and noise than a single DT-based classifier [74].

- **Extreme Gradient Boost (EGB):** a specific implementation of the Gradient Boosting method that uses more accurate approximations to find the best tree models. Its main difference compared with random forest is that it builds one tree at a time. Each new tree helps to correct errors made by the previously trained tree. EGB models are becoming popular due to their effectiveness at classifying complex data [79], [81].

- **Linear Support Vector Machine (SVM):** SVM is another widely used supervised machine learning algorithm, which is usually used for solving classification problems with two classes. Linear SVM performs classifications by finding a line that best differentiates the target classes by maximizing the margin between them [75].

- **Radial Support Vector Machine (SVM):** a nonlinear or radial SVM applies the kernel trick to find a hyperplane (decision surface), instead of a line, to best separate two classes, when there are non-linear interactions in the data. It does a non-linear transformation on the features and converts them to a higher dimensional space to add non-linearities to the learning process [76].

All of the above algorithms are used to perform supervised machine learning. Supervised classification requires that the data is totally labeled, as is the case in our work. The algorithms are tuned to achieve the best prediction result at the cost of having longer training time. In the case of Xboost, Linear and Radial SVM, a list of values (based on literature) are given to the algorithms for each parameter to try different combinations and the best result is selected in each case. In the case of Random Forest and Decision Tree, the recommended default values from the literature are used for each parameter.

4) APPLICATION SCENARIOS AND DECISION CRITERIA

To improve the effectiveness of machine learning algorithms, it is important to adequately evaluate the scenarios according to their characteristics. We consider four distinct scenarios where security assurance has different levels of relevance, depending on the criticality level of the applications being developed and also on the availability of resources to deal with security problems. The four scenarios analyzed were adapted from [82], where the authors define different real-world scenarios of applications to benchmark static analysis tools. We analyzed the specific characteristics of each scenario and selected an appropriate criterion associated to each one in order to evaluate the classifiers built on top of the selected software metrics. The scenarios and associated criteria are:

- **Highly-Critical:** this scenario represents highly business or safety critical systems with demanding security requirements (e.g., e-banking and e-health), in which the detection and elimination of security vulnerabilities is of high priority (because a successful security attack may cause serious damages to the system, to business, or to people’s life). Thus, the classifier models should be able to detect the highest number of vulnerable code units, even if some false positives are reported. For this scenario, we choose **Recall** as criterion to evaluate the classifiers, as it measures the ratio of vulnerable code units that are correctly classified independently from false positives.

- **Critical:** this scenario represents not highly but still critical systems (e.g., e-commerce web applications and large scale social networks) in which an exploited vulnerability usually reflects sensitive data breaches or considerable financial losses. In such scenario, classifiers should detect the highest number of vulnerabilities while avoiding reporting too many false positives as the resources available to fix and remove vulnerabilities need to be used appropriately. For this reason, we chose **Bookmaker Informedness** as criterion, as it still gives a high importance to true positive rate while moderately penalizing classification models with high false positive rates.

- **Low-Critical:** this scenario includes systems that are less critical and less exposed to attacks. Projects developing these systems usually have limited budget to be allocated for finding and fixing vulnerabilities. Thus, both detecting and eliminating the highest number of vulnerabilities and spending less resources for analysing false positives have equal priority. In this scenario,
**TABLE 2.** Summary of the application scenarios and their corresponding criteria [83].

| Scenario  | Criterion         | Formula                                      | Definition                                                                 |
|-----------|-------------------|----------------------------------------------|-----------------------------------------------------------------------------|
| Highly-Critical | Recall            | $\frac{TP}{P} = \frac{TP}{TP + FN}$        | Represents the ratio of vulnerable code units that are correctly classified as vulnerable. |
| Critical   | Bookmaker Informedness | $\frac{TP}{P} - \frac{FP}{N} = \frac{TP}{TP + FN} - \frac{FP}{TN + FP}$ | Combines TP and FP rates but still gives a high importance to the number of vulnerable code units that are correctly classified and moderately penalizes classification models with high number of FP. |
| Low-Critical | F-Measure        | $\frac{2 \times \text{precision} \times \text{recall}}{\text{precision} + \text{recall}} = \frac{2 \times TP}{2 \times TP + FN + FP}$ | Represents the harmonic mean of Recall and Precision, thus evenly combines TP and FP rates. |
| Non-Critical | Markedness       | $\frac{Precision + \text{Inverse Precision} - 1}{\frac{TP}{TP + FP} + \frac{TN}{FN + TN} - 1}$ | Quantifies how consistently the outcome has the classifier as a marker. It does consider both true and false positives, but in practice, it rewards the low false positive rate. |

**F-Measure** that evenly combines precision and recall, is an appropriate criterion.

- **Non-Critical**: this scenario includes non-critical systems from a security perspective (i.e., systems that are not usually exposed to attackers). Thus, we are more concerned with the number of false alarms due to tight budget and resource restrictions, although we still want to detect vulnerable code and eliminate vulnerabilities. **Markedness** is an appropriate criterion in this context, as it rewards low false alarms and at the same time does not ignore true positives.

More details about the selected criteria are presented in Table 2. In the formulas, True Positive (TP) represents the number of vulnerable code that are correctly classified, True Negative (TN) represents the number of non-vulnerable code that are correctly classified, False Positive (FP) represents the number of non-vulnerable code units that are misclassified as vulnerable and False Negative (FN) represents the number of vulnerable code that are misclassified as non-vulnerable.

**B. EXPERIMENTATION AND ANALYSIS**

The second phase of the study consists of running the experiments. As shown in Fig. 3, the data (balanced training sets and representative test sets belonging to all projects at both file and function levels) are prepared according to the configurations determined in the previous phase and then passed to the selected machine learning algorithms. The classification models are built over the dataset of the five different projects at file and function levels by considering the several combinations of software metrics and the different application scenarios. It is worth noting that the machine learning algorithms are trained using balanced training sets and tested using a representative test set in order to build more accurate vulnerable code detectors and have more realistic performance estimations. Internal and external cross-validation (CV) is performed in all cases, as discussed next.

- **V&G - Internal Cross Validation**: In order to avoid any overfitting that might be caused by unrepresentative training sets, internal cross validation is necessary. Cross-validation
is a statistical resampling technique used to estimate the performance of machine learning models [84]. Using this technique, data is split into \( k \) subsets or folds of equal size. Each time, one fold is used as test set and the remaining \( k-1 \) folds are used to train and fit the model. In this work, we use an internal 10 fold cross validation for building the models, helping to achieve a fair estimation of the performance for each individual model.

\( \checkmark \) V\&G - External Cross Validation: Internal cross validation might not be enough to ensure fair comparison between distinct models due to the fact that the initial training and test sets might not be representative of the whole dataset. For this reason, in this work, we use an external 4-fold cross validation to validate the classification models built. In practice, we divide the whole dataset into 4 folds. Each machine learning algorithm is executed four times; each time, it uses one fold for testing and 3 folds for training (which internally uses a 10 folds cross validation). The final performance estimation of each classification model is an average of the four estimations.

\( \checkmark \) V\&G - Generalization Assessment: We perform two sets of tests to understand to which extent we can generalize the obtained results. The first set of tests is focused on inter-project cross assessment. In these tests, the machine learning algorithms are trained using the dataset of one project (e.g., Linux Kernel) and are tested using the dataset of the other projects. This helps to understand how machine learning algorithms perform in new situation. In the second set of tests, the machine learning algorithms are trained using a combined dataset including all projects and tested using the dataset of each project individually. This helps to understand whether it is helpful to combine all existing information from source code of different software projects to achieve a better result.

IV. PRELIMINARY ANALYSIS PHASE
We used the R Project [85] and several R libraries, including CARET [86], RandomForest [87], e1071 [88], and dplyr [89] to perform the experiments. All the experiments were executed on virtual machines with Ubuntu 16.04.6 LTS, a 2.0 GHz Intel Xeon E312xx (Sandy Bridge) processor, 8GB RAM and 16MB cache. In this section, we present and analyze the results obtained during the preliminary analysis phase.

A. DIMENSION REDUCTION
Correlation and redundancy analysis were performed for all projects at both file and function levels. Tables 3 and 4 present the results obtained for both levels. Although the list of irrelevant or redundant metrics identified are not the same in all projects, we can see a high level of similarity between them. For instance, as shown in Table 3, from the 27 file-level metrics (out of a total of 51 metrics) that are considered as irrelevant in all five projects, 25 appear at least in 3 projects (e.g., AvgCyclomatic, AltAvgLineBlank, AvgCyclomaticModified, AvgCyclomaticStrict). Similarly, from the 38 file-level metrics considered as redundant in all projects, 26 appear at least in 3 projects (e.g., AvgCyclomatic, CountLineBlank, CountLineCodeExe, CountSemicolon). Despite these similarities, in order to be more precise, we run our experiments over the 5 groups of software metrics (i.e., All, All - Irrelevant, All - Redundant, All - [Irrelevant AND Redundant], and All - [Irrelevant OR Redundant]) that were created separately for each individual project at both file and function levels, which are used as input features for the machine learning algorithms.

B. CLASS DISTRIBUTION IN THE DATASET
One important factor to build high performance classifiers (i.e., classifiers with high true positive and low false positive rate) is related to the distribution of the classes (i.e., vulnerable and non-vulnerable code units in this work) in the dataset. As explained before, we used undersampling to gradually balance the dataset (from fully imbalanced dataset to 100% balanced) and observed the impact on performance. Table 5 presents the characteristics of those resampled datasets. This study is performed at file level for the Linux Kernel project by using various machine learning algorithms. Linux Kernel was chosen for this analysis due to the fact that it has a higher number of reported vulnerabilities than other projects, so a low number of vulnerable records would not be a threat to the validity of the results.

In all experiments, 75% of the resampled dataset was used to train the machine learning algorithms and 25% of it (disjoint from the training sets) was used to test them (TS1). In addition, to guarantee a fair and representative evaluation of the classification models, we (randomly) created an additional test set composed of 25% of the whole dataset (TS2), which is fully imbalanced and is ensured to be disjoint from the training sets. By doing this, we aim to understand how the estimation made by a balanced test set differs from the estimation made by an imbalanced, but representative test set.

Fig. 4 (x-axis: % of vulnerable records in the dataset (from 2.27% to 50%), y-axis: true positive rate (left) and false positive rate (right)) shows how performance, in terms of true positive rate and false positive rate estimated using resampled test set (TS1), changes when the training set becomes more balanced. For all machine learning algorithms, we observe that the true positive rate increases (e.g., from 0.54 to 0.92 in the case of Random Forest and from 0.08 to 0.73 in the case of Decision Tree). This means that more vulnerable code units are detected and less vulnerable code units are misclassified as non-vulnerable. Thus, for highly critical systems where one wants to detect as many vulnerabilities as possible (regardless of the false alarms), it is quite effective to balance the dataset when the number of vulnerable records is lower than the number of non-vulnerable ones.

Another observation is that the false positive rate increases for all algorithms (e.g., from 0.003 to 0.08 in the case of Random Forest and from 0.0007 to 0.31 in the case of Decision Tree), which means that a higher number of non-vulnerable
code units are misclassified as vulnerable. Thus, for scenarios in which there are limited resources for fixing or removing vulnerabilities, undersampling the non-vulnerable class to balance the dataset does not seem to be a good approach. Similar results are obtained for true positive rate and false positive rate, using the imbalanced test set (TS2). This way, since we are more concerned about detecting vulnerable code units and aim to improve the tools and techniques in this regard, we have decided to use the totally balanced (50% vulnerable code units) datasets for training the machine learning algorithms.

We also conducted a more detailed comparison between the classifiers using balanced and imbalanced test sets. For this comparison, we used all machine learning algorithms, trained using a totally balanced training set and tested using both balanced (TS1) and imbalanced (TS2) test sets, and evaluated the classification models by using the four criteria representing the four scenarios under study. As shown
TABLE 4. Irrelevant and redundant function-level software metrics.

| # | Software Metrics      | MOZILLA | KERNEL | XEN | APACHE | GLIBC |
|---|-----------------------|---------|--------|-----|--------|-------|
| 1 | MinEssentialKnots     | I / R   | I / R  | I / R| I / R  | R     |
| 2 | MaxEssentialKnots     | I / R   | I / R  | I / R| I / R  | R     |
| 3 | CyclomaticStrict      | R       | R      | R   | I / R  | R     |
| 4 | AltCountLineBlank     | R       | R      | I   | / R    | R     |
| 5 | CountStmtExe          | R       | R      | R   | R      | R     |
| 6 | Cyclomatic            | R       | R      | R   | R      | R     |
| 7 | CountLineCodeExe      | R       | R      | R   | R      | R     |
| 8 | CountLineinactive     | I       | I      | I   | I      | I     |
| 9 | CountLinePreprocessor | I       | I      | I   | I      | I     |
| 10| CountStmtEmpty        | I       | I      | I   | I      | I     |
| 11| AltCountLineComment   | R       | R      | R   | R      | R     |
| 12| CyclomaticModified    | R       | R      | R   | R      | R     |
| 13| CountSemicolon        | R       | R      | R   | R      | R     |
| 14| CountStmt             | R       | R      | R   | R      | R     |
| 15| AltCountLineComment   | R       | R      | I   | I      | R     |
| 16| RatioCommentToCode    | I       | I      | I   | I      | I     |
| 17| CountLine             | R       | R      | R   | R      | R     |
| 18| CountLineCode         | R       | R      | R   | R      | R     |
| 19| Knots                 | I       | I      | I   | I      | I     |
| 20| Essential             | I       | I      | R   | I      | I     |
| 21| CountLineBlank        | R       | I / R  | R   | I      | I     |
| 22| CountLineCodeDecl     | I       | I / R  | I   | R      | R     |
| 23| CountLineComment      | I       | I / R  | I   | R      | R     |
| 24| CountStmtDecl         | I       | R      | R   | R      | R     |
| 25| CountInput            | I       | R      | I   | R      | R     |
| 26| MaxNesting            | I       | R      | I   | R      | R     |
| 27| CountOutput           | I       | R      | I   | R      | R     |
| 28| CountPath             | I       | R      | I   | R      | R     |

TABLE 5. Resampled datasets (Linux Kernel files).

| # Vulnerable Files | # Non-vulnerable Files | Total | Training Set | Test Set 1 (TS1) | Test Set 2 (TS2) |
|--------------------|------------------------|-------|--------------|------------------|------------------|
| Imbalanced         |                        |       |              |                  |                  |
| 8712 (2.27%)        | 374910 (97.73%)        | 383622| 287717       | 95905            | 95905            |
| 8712 (10%)          | 78408 (90%)            | 87120 | 65340        | 21780            | 95905            |
| 8712 (20%)          | 34848 (80%)            | 43560 | 32670        | 10890            | 95905            |
| 8712 (30%)          | 20328 (70%)            | 29040 | 21780        | 7260             | 95905            |
| 8712 (40%)          | 13068 (60%)            | 21780 | 16335        | 5445             | 95905            |
| 8712 (50%)          | 8712 (50%)             | 17424 | 13068        | 4356             | 95905            |

Balanced

| # Vulnerable Files | # Non-vulnerable Files | Total | Training Set | Test Set 1 (TS1) | Test Set 2 (TS2) |
|--------------------|------------------------|-------|--------------|------------------|------------------|
| 8712 (2.27%)        | 374910 (97.73%)        | 383622| 287717       | 95905            | 95905            |
| 8712 (10%)          | 78408 (90%)            | 87120 | 65340        | 21780            | 95905            |
| 8712 (20%)          | 34848 (80%)            | 43560 | 32670        | 10890            | 95905            |
| 8712 (30%)          | 20328 (70%)            | 29040 | 21780        | 7260             | 95905            |
| 8712 (40%)          | 13068 (60%)            | 21780 | 16335        | 5445             | 95905            |
| 8712 (50%)          | 8712 (50%)             | 17424 | 13068        | 4356             | 95905            |

FIGURE 4. Impact of undersampling on performance.

In Fig. 5, the Recall and Informedness obtained using TS1 are in par with the results obtained using TS2. This means that using either a balanced or an imbalanced test set does not influence the classification results when highly-critical and
critical scenarios are the target of the analysis. But we observe lower values for F-measure and Markedness in TS2 across all machine learning algorithms. This is caused by the high number of false positives compared to true positives, which comes naturally from the TS2 that has a much higher percentage of non-vulnerable records. Thus, we have decided to use imbalanced but representative test sets in the following experiments, in order to have realistic performance estimation for all scenarios.

It is worth noting that, since this analysis is done only at file level, our decision regarding how to train and test the models may not perfectly fit in function-based experiments, but we believe that the implications are negligible, due to the fact that the nature and context of the problem is quite similar.

In order to demonstrate that the samples generated for training or testing are representative, we performed the V&G - Representativeness of Random Samples validation analysis. To do so, we repeated the correlation and redundancy analyses (presented in Section IV-A) ten times over 10 random samples (with 10000 records each) of file level data from the Mozilla Firefox project. Results show that in all cases, 30 software metrics (out of a total of 51 file level metrics) are identified as irrelevant and 28 software metrics are identified as redundant. In addition to that, there is a large group of metrics that appear repeatedly across different sample sets as irrelevant and redundant. For example, as shown in the last two columns of Table 3, 26 out of 30 irrelevant metrics are identified in at least 7 samples (e.g., FanOut in 10 samples, AvgCyclomatic in 9 samples). We obtained similar results regarding redundant metrics: out of a total of 28 redundant metrics, 23 are identified as such in at least 6 samples (e.g., AvgCyclomatic in 10 samples, AltAvgLineBlank in 7 samples). These results show that the random samples have quite similar characteristics and patterns in terms of correlation between the software metrics, and between the software metrics and the existence of vulnerabilities, which are important factors in building predictive models out of software metrics. One of these samples is randomly chosen for further experiments and analysis to re-ensure the avoidance of any sampling bias that may exist.

V. EXPERIMENTATION AND ANALYSIS PHASE

In this section, we present and analyze the results obtained during the experimentation and analysis phase, including the performance of the machine learning algorithms, importance of software metrics, and generalization of the approach.

A. PERFORMANCE OF THE MACHINE LEARNING ALGORITHMS

We first focus on the results obtained for each project individually and then make a comparison. Fig. 6 and Fig. 7 present the results obtained respectively for file and function level software metrics of the Linux Kernel project. Both figures include the results obtained by all machine learning algorithms for different scenarios over five combinations of software metrics. It is worth reminding that all 5 software projects are analyzed by using four criteria representing four different scenarios. In fact, the assumptions regarding the criticality level of the projects are made based on scenarios.

File level results show that the best performance is always achieved by Random Forest and Xboost algorithms. As expected from the non-linear nature of the dataset, radial SVM always achieve a better performance than linear SVM, which is almost in par with Decision Tree. Among different combinations of software metrics, the combination from which the irrelevant metrics are eliminated slightly shows a better result than other combinations in most cases. In Fig. 6, we can also see that the combination in which the redundant
metrics are eliminated shows (slightly) worse results than the combination with all metrics. In contrast, function level results show no significant difference between these combinations. This happens because the function-level dataset is not considered as a high-dimensional dataset (it only has 28 features), and in such cases it is hard to achieve a better result with dimension reduction. However, this is not always the same for other projects (see Fig. 8 and Fig. 9).

After analysing the results of all projects and all algorithms, we can state that, dimension reduction, does not always help to achieve a better performance. In fact, dimension reduction has to be done carefully and several techniques should be tried depending on the classification model in use and the characteristics of the dataset in order to achieve a better performance.

Regarding the effectiveness of using software metrics and machine learning algorithms to detect vulnerable code, we can conclude that, although the machine learning algorithms could achieve a reasonable performance in terms of Recall and Informedness (highly critical and critical scenarios), the results for F-measure and Markedness (low-critical and non-critical scenarios), which are highly dependent on
the number of false positives compared to true positives (refer to Table 2), are not convincing at all. Despite having high true positive (TPR = TP/P) and low false positive rates (FPR = FP/N), having a very imbalanced test set leads to a high number of false positive cases when compared to the number of true positive cases.

Similar observations can be pointed for the function level results presented in Fig. 7, with the difference that the performance of the algorithms using file level metrics is usually higher than when using function level metrics. Also, the difference between machine learning algorithms is more visible in file level results. For example, we cannot see any difference between the algorithms in terms of F-Measure and Markedness in Fig. 7. These are happening due to the fact that the function-level data is even more imbalanced than the file-level data (refer to Table 1).

To make a comparison between different projects, we present in Fig. 10 the results obtained for all projects over
the data sets with all file level metrics. In general, the results for the different projects are quite different mainly due to the fact that the characteristics of the datasets (i.e., size and distribution of classes) are different for each project. In most cases, the best performance is achieved for the Linux Kernel dataset, which is the biggest project and has more vulnerable code units. This means that the machine learning algorithms had more evidences and more balanced information to avoid overfitting and learn (of course not equally) about both classes involved in the dataset. We also have high Recall and Informedness for Glibc, but, by looking to the very low F-measure and Markedness values, we can conclude that the high true positive rate in this case is achieved thanks to highly overfitted models.

Interestingly, the results achieved by both ensemble algorithms, Random Forest and Xboost, are quite similar in the case of all projects, for both file and function level metrics (see Fig. 10 and Fig. 11). Random Forest and Xboost are both tree-based algorithms. In both cases, the performance of the model depends on two distinct sources of error: bias and variance. Gradient boosting models deal with these sources of error by boosting for many rounds at a low learning rate. In contrast, Random Forest models deal with them via the number of trees and tree depth. Achieving very similar results by these algorithms in almost all cases may imply that both models were able to achieve their best model with our dataset and no bias or variant could be reduced by neither methods due to the limitations that exist in the dataset (e.g., being imbalanced with imperfect labeling).

We also observe similar patterns between Linear SVM and DT. However, showing a comparable performance does not imply that the code is classified or misclassified similarly by these classifiers. For this reason, we decided to analyse their behaviour in more detail. Fig. 12 presents Venn diagrams showing all possible intersections between the subset of vulnerable code units (respectively, files and functions of the Linux kernel project) that are classified as non-vulnerable by the different machine learning algorithms. The diagram shows that 76 vulnerable files and 102 vulnerable functions are misclassified by all classifiers. Interestingly, 136 out of 146 vulnerable files and 137 out of 163 vulnerable functions that are classified as non-vulnerable by XBoost, are also misclassified by Random Forest. This led us to analyze the characteristics of the vulnerable/non-vulnerable files and functions that are misclassified by all classifiers to find the missing information that the machine learning algorithms could use to improve their performance.

In our analysis we observed that most of the vulnerable code units that are classified as non-vulnerable are small and simple in terms of structure. In contrast, most of the files and functions that are incorrectly classified as vulnerable are huge or complex. An example of a misclassified vulnerable file from Linux Kernel source code is presented below.

```c
/* File Path: fs/ramfs/file-mmu.c
 * Software Metrics values:
 * CountLineCode: 15
 * SumCyclomatic: 0
 * SumCyclomaticMod: 0
 * SumCyclomaticStrict: 0
 * SumEssential: 0
 * CountPath: 0
 * FanIn: 0
 * FanOut: 0
 */

#include <linux/fs.h>
#include <linux/mm.h>
#include <linux/ramfs.h>
#include "internal.h"

const struct file_operations ramfs_file_operations = {
  .read = new_sync_read,
  .read_iter = generic_file_read_iter,
  .write = new_sync_write,
  .write_iter = generic_file_write_iter,
  .mmap = generic_file_mmap,
  .fsync = noop_fsync,
  .splice_read = generic_file_splice_read,
  .splice_write = generic_file_splice_write,
  .llseek = generic_file_llseek,
};

const struct inode_operations ramfs_file_inode_operations = {
  .setattr = simple_setattr,
  .getattr = simple_getattr,
};
```

We added the first 13 lines just to provide some information about the file. File path is added in line 2 and the values of several representative software metrics are added in lines 4 to 12. The values of the metrics show how simple the file is. Indeed, it is impossible to indicate this file as vulnerable file by using software metrics, but we are aware of one exploitable vulnerability that has been reported for this file (i.e., CWE-264 - Permissions, Privileges, and Access Controls). The vulnerability consists of a Wrong Assignment Value (according to the ODC classification [90]) in line 29, which allows local users to cause a denial of service (system crash). To fix this vulnerability the line should be simply replaced by `splice_write = iter_file_splice_write;`. Given this example, the analysis of the misclassified vulnerable but simple files and functions, may allow finding other evidences that help to improve the performance of vulnerability detection tools. This will be explored in future work.

Fig. 13 and Fig. 14 present the average value of several software metrics respectively for misclassified files and functions. As we can see, there is a huge difference between these two groups of misclassified code units (i.e., false positives and false negatives). Note that the standard deviation is high too, which means that the average variation around the mean is quite large. Regarding the false positive cases, as mentioned before, the source of information regarding the vulnerabilities is limited to security reports. Consequently, the functions
and files without reported vulnerabilities are not necessarily flawless. For this reason, given the above results regarding misclassified non-vulnerable files and functions, it is quite probable that some of the considered false positives are indeed vulnerable (although no vulnerability has yet been disclosed). A few lines of an example of a misclassified non-vulnerable file (i.e., no attack related to this file is reported so far) from Linux Kernel source code is presented below (the whole file is not presented due to the lack of space).

As the values of software metrics show (lines 4 to 12), the file is quite complex. Using our models, this file is classified as vulnerable. To find out whether this file is vulnerable or a real false alarm, we applied several static code analyser tools including FlawFinder, CppCheck, and Rats [91] over the file. These tools found several issues in the file, of which two vulnerabilities were confirmed by a security expert. One of these vulnerabilities is found in line 18 of the code below (i.e., CWE-134 - Use of Externally-Controlled Format String) where `sprintf` operation is used without checking the input.
value (Missing Checking Input Value bug according to ODC classification).

```c
1 /*
2 * File Path: drivers/pcmcia/ds.c
3 *
4 * Software Metrics Values:
5 * CountLineCode: 772
6 * SumCyclomatic: 208
7 * SumCyclomaticMod: 206
8 * SumCyclomaticStrict: 226
9 * SumEssential: 115
10 * CountPath: 2122
11 * FanIn: 399
12 * FanOut: 159
13 */
14 static ssize_t field__show (struct device __dev,
15   struct device_attribute __attr, char __buf)
16 { 
17   struct pcmcia_device __p_dev = to_pcmcia_dev(dev)
18   return p_dev->test ? snprintf (buf, format, p_dev
19     ->field) : -ENODEV;
20 }
```

B. IMPORTANCE OF SOFTWARE METRICS

In all the experiments above, we collected information regarding the importance of the software metrics calculated by each machine learning algorithm for the five projects. In general, the rankings given by the algorithms are different from each other, as the algorithms build the models differently and the datasets of the projects have different characteristics (in terms of size, distribution of classes, and structure of the code).

To better understanding the results, we compared the ranking of the software metrics given by the two classifiers that performed higher (Xboost and Random Forest) in the two projects with the best results (Linux Kernel and Mozilla Firefox). We compared the most important (importance of software metrics refers to the score assigned to them by each machine learning algorithm for the five projects, thus achieving a reasonable performance level).

Interestingly, for Low Critical and Non-Critical scenarios, Xen achieves a better result than the other project. This happens due to the fact that this small project has a more balanced test set compared to other projects (Refer to Table 1). The same observations are seen when data of Mozilla Firefox is used as training set in both file and function levels, but in other cases, when the data of the small projects are used for training, we observed that the performance of the classifiers is way lower and all classifiers perform similarly in both file and function level. This happens because the training set is small and there is not enough variation in training set.

The results of the experiments in which the machine learning algorithms are run over the combined dataset, are presented in Fig. 17 and Fig. 18 for files and functions, respectively. We can observe that the performance of the classifiers is slightly degraded when we use a dataset composed of all 5 projects for building the classification models. This potentially means that classifiers are able to find similar characteristics and patterns in the code of five different projects, thus achieving a reasonable performance level. The results are similar for function level metrics. This is a promising observation as it may mean that we can build of software metrics, it seems that the correlation between software metrics and also their correlation with security issues in the code is sufficiently complex to be identified by our simple correlation and redundancy analysis. Even the machine learning algorithms did not rank them equally (or even with a high level of similarity). Thus, giving privilege to a group of metrics for building vulnerability prediction models does not seem to be a promising idea.

C. GENERALIZATION ASSESSMENT

To understand to which extent we can generalize the results and how the machine learning algorithms perform in new (previously unseen) situations, we first performed a inter-project cross assessment, where data of a specific project are used for training and data of the other projects are used for testing. At the file level and using data of Linux Kernel as training set, we observe that the performance decreases in all projects, except in the case of the Linux Kernel itself, whose data is used for training the machine learning algorithms (see Fig. 15). An interesting observation is that Linear SVM and DT seem to make better classifications than other machine learning algorithms when the test set is completely unknown to the classifiers. This means that these machine learning algorithms build more generalizable models than other algorithms, thus being more suitable for unseen code. This is simply because, they build simpler models, which is more appropriate when the data is more non-parametric in nature (i.e., when we cannot make assumptions about the distribution of data).

At function level and using data of Linux Kernel as training set (see Fig. 16), all classifiers seem to perform similarly. Interestingly, for Low Critical and Non-Critical scenarios, Xen achieves a better result than the other project. This happens to a group of metrics for building vulnerability prediction models does not seem to be a promising idea.
a dataset with higher diversity (including different types of software project), which is quite helpful for vulnerability prediction of unseen code but still have a reasonable level of performance.
VI. DISCUSSION AND THREATS TO VALIDITY

The main objective of this work was to perform a comprehensive experiment to demonstrate how effective software metrics combined with machine learning techniques can be to distinguish vulnerable from non-vulnerable code units in different application scenarios. Thus, we used several machine learning algorithms, several software project at both file and function levels, several application scenarios with different security concerns and several subset of software metrics to explore this idea. The main insights from the results are as follows:

- Machine learning algorithms using software metrics data can detect vulnerable code with a relatively high level of confidence for security-critical software systems (e.g., Recall and Informedness more than 0.8). However, a high number of false alarms makes the software metrics almost useless for low-critical or non-critical systems (i.e., response to RQ1 defined in Section I).
- The larger and more complex a unit of code is, the more likely it is to have security issues. Thus, models built over software metrics that provide information regarding the structure and complexity of code can help to
predict vulnerabilities. Nevertheless, the high number of false alarms implies that software metrics are not sufficient to distinguish vulnerable and non-vulnerable code with high level of confidence and low cost (as false positives require resources to be verified). Moreover, software metrics are not able to indicate the exact place of the existing vulnerabilities. These limitations of software metrics imply that more evidences of low quality code (e.g., code smells or absence of security best practices) and deeper static (and dynamic) code analyses are required for building a high performance vulnerability detection/prediction tool.

- Undersampling the larger class of a dataset, in which a low percentage of data belongs to vulnerable code, helps to detect more vulnerable code, but with a higher false positive rate. Thus, the class distribution in the dataset to be used to train the classifiers is influenced by the application scenario.
Random Forest and Xboost were able to build more precise models than other algorithms to detect vulnerable code in a software project when data from the same project is used for training. In contrast, Decision Tree and Linear SVM seem to build more generalizable models, thus, give a better estimation when the data from another project is used to evaluate the model (i.e., response to RQ3).

Considering particular application scenarios when building or choosing vulnerability detection tools is an important factor. We balanced the training set to build the classification models, which was helpful for detecting more vulnerable code at the cost of more false positive alarms, (suitable for highly critical systems where one prefers to detect more vulnerabilities, no matter how many false alarms are reported). In spite of that, balancing the training set for building the model was harmful for low or non-critical applications, making the models almost useless for these scenarios.

In general, we cannot conclude that dimension reduction is or is not helpful to achieve better results in terms of performance. Indeed, the combination of metrics that leads to the best performance strongly depends on the machine learning algorithm. For example, Xboost achieves the best result when all metrics are used, while Decision Tree shows a better performance when the redundant file-level metrics are eliminated (i.e., response to RQ2).

Misclassified vulnerable files seem to have different characteristics from misclassified non-vulnerable files in terms of structure and complexity. The same is true in the case of misclassified functions. Performing a deeper analysis of the source code in these files and functions can help to find new evidences or features that enable improving the performance of classifiers. To give an example, looking at Fig. 13 and Fig. 14, the average value of CountPath for misclassified vulnerable functions is 5.67, way lower than the average value for misclassified non-vulnerable functions. It means that, most of the misclassified vulnerable functions are quite small and simple. By looking at their source code, we may find that only a single line of code with a sensitive operation (e.g., memcpy) made the code exploitable against attackers that could be simply avoided by adding a check before the operation. We intend to explore this deep analysis of the misclassified code in future.

Our analysis of misclassified code shows that, although there is a group of code units that are misclassified by all the models, a bigger group of code units are misclassified by only one or two models. Thus, it might be helpful to build a hybrid prediction model using several machine learning algorithms to lower the number of false alarms.

The complex correlation between software metrics and between metrics and the existence of a vulnerability in the code makes it very difficult, if not impossible, to find a meaningful universal ranking of software metrics based on their importance in the prediction of vulnerable code (i.e., response to RQ2).

The generalization assessment showed that the performance of classifiers is not degraded significantly when a dataset with diverse projects is used for training the
models. This can generally imply that the idea of using software metrics for the indication of vulnerable code can be generalized (i.e., response to RQ4).

We are aware that this experimental work has limitations that need to be taken into account when considering the insights above. Most of these threats to validity are related to the dataset used (selected due to the reasons mentioned in Section III). First, all the selected projects in the dataset are implemented in C/C++, and each programming language has its own characteristics in terms of security [92]. Consequently, some of the outcomes obtained from our analysis may not be representative for software implemented in other languages (e.g., Java).

The source of information regarding the vulnerabilities in the projects is limited to security reports. Consequently, the functions and files without reported vulnerabilities are not necessarily flawless. To build the classifier model, we followed a supervised approach, which considers that our dataset is completely labeled. However, although the records with vulnerabilities are (reliable) labeled, but the rest can be seen as being unlabeled. This way, semi-supervised approaches should be studied as alternative choices for such cases, where it is not trivial to verify the label of all records due to the size of the dataset and complexity of the code.

Although we used the well-known, commonly used, recommended, and representative machine learning algorithms, the number and diversity are still limited for a comprehensive analysis. Furthermore, the analysis for demonstrating the representativeness of random samples as well as the analysis performed for the understanding the impact of class distribution are done over the source code of a single project. This may have some implications on the results obtained with the other projects.

We believe that main limitation and thread to the validity of this work and to the other similar works in the literature, comes from the fact that it is extremely difficult to build a dataset that is relatively balanced (i.e., having enough number of vulnerable code to prevent over-fitting), precisely labeled (i.e., all existing vulnerabilities identified for code labeled as vulnerable, and for code labeled as non-vulnerable assure that it is free of any vulnerability), and highly representative (i.e., covering a vast range of software projects implemented in different languages). Without such dataset, we will not be able to fully understand how effective software metrics can be to detect/predict vulnerable code for different application scenarios. Even if we imagine that such dataset already exists or can be built, it will be still a big challenge to build models that can guarantee a good performance with a low number of false alarms for previously unseen patterns of code.

**VII. CONCLUSION AND FUTURE WORK**

This paper presented a comprehensive study on the use of software metrics and machine learning algorithms for the detection/prediction of vulnerable code. The most important observation is that using machine learning algorithms on top of software metrics helps identifying vulnerable code units with relatively high level of confidence for security-critical software systems (where the focus is on detecting the maximum number of vulnerabilities, even if false positives are reported), but they are not helpful for low-critical or non-critical systems due to the relatively high number of false positive alarms reported when compared to the number of true positive cases (that bring an additional development cost frequently not affordable), which is mainly caused by the imbalanced nature of our dataset (and similar datasets used in other works).

According to our observations, insights and threats to the validity of the work, we can conclude that software metrics are not sufficient evidence of security issues to be used solely for building detection/prediction models that are able to distinguish vulnerable code from non-vulnerable code with good performance and low vulnerability removal cost. Moreover, due to the natural limitations of existing datasets for training and testing these models, it becomes even more difficult to precisely understand how effective software metrics can be to detect vulnerable code in different application scenarios. Based on this strong conclusion, we have two directions in front of us for future works.

The first direction will be focused on using other evidences rather than software metrics, like code smells [93], lack of security best practices in the code, alerts given by static code analysers, among others, to improve the detection/prediction models to produce less false alarms and try to find the location and type of vulnerabilities to provide some suggestions to developers for removing the detected or predicted vulnerabilities and improving the code. This requires a deep understanding of all (known) types of security issues and vulnerabilities as well as possible solutions for fixing them. In this scenario, we will still face the aforementioned limitations of models in new unknown situations. To address this issue, we can let the models to continuously adjust themselves by receiving feedback from developers of the code under development. After analysing the situation, and in the case of false alarms, the developers will send feedback to the analyser platform to readjust the prediction model. Otherwise, the suggestion is applied in the code either by writing new code or by changing (or removing) existing code. In practice, the prediction model will be continuously improved by new data generated from the code under development and feedback provided by developers. Here, the main challenge is to ensure that i) the software functionality remains after applying the changes; and ii) the changes do not introduce a new bug or vulnerability in the system.

The second direction will be focused on using software metrics not for predicting or detecting vulnerabilities but for assessing the trustworthiness of the code and warn the developers about their untrustworthy (insecure) code units. In a previous work [94], we proposed a trustworthiness model directly by using a group of software metrics that were weighted based on the scores given by a classification model. Despite the merit of that work, the results of the current work show that such model cannot be generalized, since it is
almost impossible to find a meaningful universal ranking of software metrics, based on their importance in the prediction of vulnerable code, to be used for any kind of software. For this reason, we suggest to build a trustworthiness model, not directly based on software metrics, but based on the classification results of several machine learning algorithms that are trained using software metrics. This solution does not find vulnerable code, but may be able to warn developers about the units of code that seem to be more untrustworthy.

By assigning a trustworthiness score to each unit of code, it is up to the developers to decide what part of the code needs more attention (depending on the criticality of the application and the available resources), thus being suitable for any application scenarios.

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