Preserving Order of Data When Validating Defect Prediction Models

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Abstract. [Context] The use of defect prediction models, such as classifiers, can support testing resource allocations by using data of the previous releases of the same project for predicting which software components are likely to be defective. A validation technique, hereinafter “technique,” defines a specific way to split available data in training and test sets to measure a classifier’s accuracy. Time-series techniques have the unique ability to preserve the temporal order of data; i.e., preventing the testing set to have data antecedent to the training set. [Aim] The aim of this paper is twofold: first we check if there is a difference in the classifiers accuracy measured by time-series versus non-time-series techniques. Afterward, we check for a possible reason for this difference, i.e., if defect rates change across releases of a project. [Method] Our method consists of measuring the accuracy, i.e., AUC, of 10 classifiers on 13 open and two closed projects by using three validation techniques, namely cross validation, bootstrap, and walk-forward, where only the latter is a time-series technique. [Results] We find that the AUC of the same classifier used on the same project and measured by 10-fold varies compared to when measured by walk-forward in the range [-0.20, 0.22], and it is statistically different in 45% of the cases. Similarly, the AUC measured by bootstrap varies compared to when measured by walk-forward in the range [-0.17, 0.43], and it is statistically different in 56% of the cases. Moreover, our results show that the relative difference in defect rate between the second and first half of a project is, among projects, in the range [-75%, 218%], and it is statistically different in 13 out of 15 projects, thus suggesting non-time-series techniques provide results that are poorly realistic. [Conclusions] We recommend choosing the technique to be used by carefully considering the conclusions to draw, the property of the available datasets, and the level of realism with the classifier usage scenario.

Keywords: Defect prediction models, classifiers, model validation techniques.

1 Introduction

Prediction models can support test resource allocations by predicting the existence of defects\textsuperscript{1} in a software module (e.g., class). For this reason, the software engineering community has spent significant effort towards increasing the accuracy of prediction models in several ways including noise removal [1][2][3], tuning [4][5], feature selection [6], and many others. In this work, we focus on across releases prediction, i.e., a realistic context where data from previous releases are

\textsuperscript{1} As in Hall et al. [47] we use the term defect to indicate a fault or a bug. A failure is a possible result of a fault occurrence.
collected and used to estimate future releases of the same project. Among different types of prediction models, we focus on classifiers, i.e., the prediction models aiming at estimating a categorical variable, i.e., the existence or lack of at least one defect in a software module. Since different classifiers exist, it is important to use accurate ones. A validation technique, hereinafter “technique”, defines a specific way to split available data in train and test sets to measure a classifier’s accuracy. Specifically, a technique prescribes a specific way to construct one or multiple sets of data where the classifier is first trained and then tested. In a recent study Tantithamthavorn et al. [7] reports 12 techniques, each with its own computational cost, stability, and reliability. Hence, it is important to investigate validation techniques and the reason for when to use which.

One characteristic of a technique is its ability to preserve the temporal order of data; i.e., preventing the testing set to have data antecedent to the training set. These techniques are generally called time-series and must be used when the data is time-sensitive, i.e., when data shows a pattern related to time [8]. Suppose you have a dataset related to a project of five releases and suppose that the proportion of defective classes in releases four and five is significantly lower than in the previous three releases. In a realistic context, to predict release four, the model is trained on releases one to three; a technique that measures the accuracy of the model on release four would bias results if data of release five is used during training. Non-time-series techniques aim at estimating the classifier accuracy on a context similar to the data available [9]. Thus, in general, in case we have project data and a new technology aimed at improving the accuracy of a classifier, we can validate this technology using one of the following two main options: either we use a non-time-series technique to estimate the expected accuracy improvement if this technology will be used in a similar project or we use a time-series technique to measure the accuracy improvement that this technology would have had if used in early releases of that specific project.

As different types of techniques measure different types of accuracies; no technique can be claimed better or worse than another overall. Time-series techniques have both advantages and disadvantages when compared to non-time-series techniques. One of the main advantages is that they replicate a realistic usage scenario [10][11][12]. The rationale is that learning from the future is unrealistic [7][13]. Specifically, our experience in industrial context [10][11][12] shows that data of different releases are collected over time, and this data is used to predict defects of the next release of the same or different projects. However, the replicated scenario is not universal as the rate at which a prediction model is refreshed varies across contexts, i.e., not all past releases could be available to predict the next one. Another advantage is their ability to be relatively inexpensive and fast as the number of runs is equivalent to the number of ordered parts, which in the 101 datasets used by Tantithamthavorn et al. [7] is on average five (releases). Another important advantage is that they are not affected by any bias related to the randomness with which the training and test sets are generated [14][15]. An important disadvantage is that they require more than one set of (ordered) data; in software engineering terms this means multiple releases of the same project. Specifically, we have manually analyzed the 101 datasets used by Tantithamthavorn et al. [7], and we found that 91 projects are multi-release. For instance, the project Ant has five releases whereas the project Tomcat has only one release; thus, only non-time-series techniques can be used on Tomcat. We refer to Bergmeir and Benítez [8] for a detailed discussion of time-series techniques and Kim [16] on non-time-series techniques.

In the earlier days of software defect prediction, we only had a handful of mono-release datasets, e.g., NASA MDP [17]. Thus, by following an in-vitro approach, researchers validated prediction
models by using non-time-series techniques by aiming at feasibility rather than realism. Afterwards, since replication is one of the main strengths of science, researchers continued, and few might still tend to use 1) mono-release datasets even if not realistic, and/or 2) non-time-series techniques on multi-release datasets; these multi-release datasets are now abundant due to the existence of community repositories and/or the ability to easily analyze GitHub repositories of large opensource projects. We claim it is now possible and recommendable to follow an in-vivo approach for technology transfer, i.e., using multi-release datasets and time series techniques as their results are more realistic to a real-world defect prediction usage scenario. However, if time-series and non-time-series results are the same, then non-time-series technique might be claimed preferable because they are applicable to a wider range of datasets. Thus, it is important to investigate if and why the accuracy of the same model on the same datasets differ when measured by a time-series versus a non-time-series technique.

In this paper we investigate the following two research questions:

- **RQ1**: Is there a difference between the classifier accuracy measured by a time-series versus a non-time series technique?
- **RQ2**: Does the defective rate of a project changes across time?

Our method consists of measuring the accuracy, i.e., AUC, of 10 classifiers on 13 open and two closed projects by using three validation techniques, two non-time-series, and one time-series technique. We find that the AUC of the same classifier applied to the same project varies according to the used techniques both practically and statistically. One possible reason for this difference is the difference in the defect rate among the training sets of the different techniques. As a matter of fact, our results show that the relative difference in defect rate between the first and second half of the projects hugely varies, again, both practically and statically. Thus, our results suggest non-time-series techniques make use of training sets with poorly realistic defect rates and hence provide accuracy results that are poorly realistic.

The reminder of the paper is structured as follows. Section 2 reports on related work. Section 3, 4 and 5 describe the design, results and conclusions. The threats to validity are discussed in Section 6. Section 7 concludes the paper.

## 2 Related work

In this section, we first provide an overall view of time-series vs. non-time-series validation techniques, then report the specific validation techniques used in defect prediction research during the last decade, and finally conclude with a discussion of other methodology papers that focused on the impact of different validation techniques to differentiate our work from earlier studies.

### 2.1 Validation Techniques: Time-series vs. Non-time-series

A technique prescribes a specific way to split available data in training and test sets to measure a classifier’s accuracy. Walk-forward is a widely used time-series technique. In walk-forward, the dataset is divided into parts, i.e., the smallest units that can be ordered, e.g., a release of a project. Then, parts are chronologically ordered, and in each run, all data available before the part to predict is used as the training set, and the part to predict is used as test-set. Afterward, the model accuracy is computed as the average among runs. The number of runs is equal to one less than the number
of parts. For instance, Figure 1 (a) describes the walk-forward technique; the parts used for training are in blue, the ones used for testing are in green, the ones not used are in white. Figure 1 (a) describes a dataset related to a (hypothetical) project of five releases, i.e., five parts, and four runs. In the first run the first part is used as a training, and the second as testing, in the second run the first two parts are used as a training and the second as testing, and so on. The accuracy is averaged among the four runs.

Non-time-series techniques vary in the way the dataset is split into the train and test sets as it could be due to random sampling, with or without replacement, etc. The v-fold (aka, k-fold) cross-validation is the most used non-time-series technique, and it makes use of random sampling strategies to construct several training and test sets on which the accuracy of the model is averaged [7][13]. In a k-fold cross-validation setting, the model accuracy is the average among runs and the number of runs equal to the number of folds, i.e., parts, in which the data is divided. Figure 1 (b) describes a five-fold cross-validation scenario. In Figure 1 (b) the dataset is randomly divided into five parts of equal size. Since the parts, i.e., folds, are randomly generated, to minimize effects related to random sampling, the procedure is usually repeated several times. Empirical studies suggest that k-fold cross-validation works well if “v” and repetitions are ten [9]. We note that when “v” equals to the number of observations, then the technique is called leave-one-out. As we can see in Figure 1 (b), in all runs other than the fifth, future data is used as a training set. An option of the v-fold cross validation is stratification, i.e., enforcing the parts to have the same defect ratio. The advantage of this stratified approach is to support model training as the model can analyze heterogeneous data during training. The disadvantage is that it reduces realism, and overestimates model accuracy, as it assumes the test set to have the same defect ratio of the training set (see RQ2).

The bootstrap method, proposed by Efron and Tibshirani [18], consists of creating the train set by randomly sampling data with replacement and using the original set as test set [19]. Several variants of bootstrap exist including the optimism reduced, where the effect of testing on the same data used as training is removed by subtracting to the measured accuracy the accuracy of the model tested on the training set. A further variant is called out-of-sample bootstrap where the model instead of being tested on the original dataset is tested on the data of the original dataset that is not used (sampled) in the training set. Tantithamthavorn et al. recently recommended the use of this out-of-sample bootstrap to measure the accuracy of defect prediction models [7]. Figure 1 (c) shows an example of out-of-sample bootstrap where in the first run the parts selected as training are the 2nd, 4th and 5th, and the remaining parts (i.e., first and third) are used as test-set.

![Figure 1](image-url)

Figure 1: Different validation techniques; the parts used for training are in blue, the ones used for testing are in green, the ones not used are in white.
2.2 Which Validation Techniques Are Used in Defect Prediction?

To have an overall view about which techniques have been used, why they have been used, and whether they preserved temporal order of data, we performed a non-committal literature review [20]. Please note that our aim here is not to provide a systematic literature review of related literature, which is out of the scope of this paper, but rather to get insight regarding the use of time-series validation techniques in defect prediction research during the last decade.

To identify relevant studies, we performed a search on Google scholar using the following search string in the title: bug* OR defect* OR fault*) AND (predict* OR estimate*). This string allowed us to find studies related to defect prediction, using different synonyms and declinations such as bug or defects and prediction or estimations. As in a previous study [21], we chose Google Scholar because it provides the complete coverage of scientific literature; moreover, it does not suffer from the idiosyncrasies reported earlier for such collections of scientific papers as IEEE Xplore and ACM DL [22].

The search resulted in identifying 9,763 studies. We filtered out studies older than ten years and published in venues other than peer-reviewed journals, leading to 106 studies. Then, we removed studies not applying any validation technique (e.g., secondary studies) and where the variable predicted by the model is of the numeric type (i.e., regression studies to predict the number of defects). This led to a final set of 51 studies. To ensure reliability and to reduce researcher bias, the gathering and filtering procedure was performed by the second and the third author independently. Later, the first author resolved inconsistencies among the second and third author and cross-checked a random sample of ten studies for correctness.

To identify which technique has been used in each study, we analyzed the section of the studies discussing the evaluation procedure. We started from an empty list of techniques and we added techniques as we found them in identified studies. To identify the criteria used for choosing techniques, we checked the reported rationale. Similarly, we started with an empty list of criteria and we added them as we found them in the studies. Finally, we proceeded by checking the types of datasets, i.e. mono-release vs. multi-released, used in the studies and hence the proportion of times whether time-series techniques were feasible and/or not used.

Table 1 reports the proportion of techniques used in past studies. The most notable result is that only one time-series technique is used, i.e., the walk-forward cross-validation, and this technique is used by only 6 (9%) studies. The most used technique is by far k-fold cross-validation with 31 (61%) studies. Additional analysis of data shows that 10-fold cross-validation is used by 26 (51%) studies and hence it is the most used type of k-fold technique and the most used technique in general. This result is in line with Tantithamthavorn et al. [7].

The fact that only 9% of studies used a time-series technique (see Table 1) means that the great majority of past studies aimed at estimating the performance of a classifier on temporally random data rather than measuring it on future data. However, our experience in talking with practitioners during technology transfer of classifiers [23] shows that it makes more sense to find evidence on a statement like “This technology would have helped us if we had used in the past” (i.e., measuring on data to have come) than evidence for a statement like “This technology can help us if we use it in the future” (i.e. estimating on temporally random data). In this context, it is especially important, considering we have no better way to make assumptions about future data than past data. To make an analogy with human-based experiments for validating software engineering technologies via controlled experiments, we look at past performances of the subjects using different treatments to
generalize into future performance of the sampling population [24]. The rationale is to allow the potential technology user for interpreting the results and deciding how much the future is different from the past and hence how the experimental results are generalizable to the specific usage context.

Table 1: Number of studies using a technique.

|                      | k-fold cross validation | Holdout | Bootstrap | Different projects | Time-series cross-validation |
|----------------------|-------------------------|---------|-----------|--------------------|-----------------------------|
| Number of studies    | 31                      | 5       | 9         | 2                  | 6                           |

As for the rationale for using specific validation techniques, the most used criterion (37%) is being “specific to the research context”. For instance, a past study aimed at validating a technology related to cross-company prediction used a specific sample of projects as training set and other projects as a testing set. The second most used criterion (29%) is “not reported”, specifically, it was impossible for us to retrieve why the technique was used. To ensure that this result was not biased by individual members of our research team, all three researchers independently analyzed the studies with the unknown criterion and unanimously concluded that the criterion was not reported. The third most used criterion (26%) is being “widely used” in the past. The last used criterion is being “used by specific studies” (8%).

2.3 Studies on validation techniques

Similar to what we report above, Tantithamthavorn et al. [7] recently found that the most used technique is 10-fold cross-validation and, by comparing 12 different techniques, they recommend the use of out-of-sample bootstrap technique [13]. We share with them the need to better investigate the intrinsic and practical differences among validation techniques. However, in our view, no technique can be recommended without considering the conclusions to draw, the property of the available dataset, and the level of realism with the classifier usage scenario. To the best of our knowledge, no study other than Tantithamthavorn et al. [7] explicitly compared validation techniques, but there are studies that are related to model selection criteria which we discuss below.

Hall et al. [25] performed a systematic literature review to investigate if the context of models, the independent variables used, and the modeling techniques applied, impact the accuracy of prediction models. Their results show that “the methodology used to build models seems to be influential to predictive performance” [25]. Their results motivate our work (RQ1) in investigating if the same classifier has different accuracy across different validation methodologies, i.e., the techniques.

Myrtveit et al. [15] demonstrated that the selection of the most accurate prediction model is highly impacted by specific choices made during the experimental design such as accuracy metrics. We share with them the need to better investigate how experimental choices impact results. However, they investigated models predicting a numeric variable (i.e., effort) whereas our variable is binary (i.e., class defectiveness). Another major difference is that they focus on evaluating the impact of the accuracy metric on the decision of which prediction model is best whereas in our RQ1 we evaluate the impact of the validation technique on the prediction model accuracy measurement. We do not investigate the impact of accuracy metrics because previous studies suggest AUC to be a reliable metric, not sensitive to defect ratios, in the context of class defectiveness prediction [26].
In our view, no validation technique or metric is better or worse than another; everything is context dependent. Specifically, the issue is to understand the extent to which current techniques and metrics replicate specific classifier usage scenarios.

Kocaguneli and Menzies [27] suggest the use of leave-one-out technique (i.e., k-fold with k equal to the size of number of observations) for validating models on effort estimation. Their results show that 10-fold cross validation produce similar results and similar time than leave-one-out; however, leave-one-out is perfectly replicable and hence should be preferred. We share their concerns and we note that non-time-series techniques are perfectly replicable as well since there are no random splits required.

3 Design

3.1 RQ1: Is there a difference between the classifier accuracy measured by a time-series versus a non-time series technique?

Thus, our null hypothesis is:

H01: There is no difference in the classifiers’ accuracy when measured by the most used non-time-series technique (i.e., 10-fold cross validation) versus the only time-series technique (i.e., walk-forward cross validation).

H02: There is no difference in the classifiers’ accuracy when measured by the only recommended non-time-series technique (i.e., out-of-sample bootstrap) versus the only time-series technique (i.e., walk-forward cross validation).

3.1.1 Dependent variable

Our dependent variable is the accuracy of the classifier as measured by the standard and suggested metric called area under the receiver operating characteristic curve, i.e., AUC [9]. The receiver operating characteristic curve is created by plotting the true positive rate (i.e., the ratio of classes classified as defective and actually defective over the number of classifications), against the false positive rate (i.e., the ratio of classes classified as defective and actually not defective over the number of classifications) at various threshold settings. AUC is preferable over other metrics such as F1 because it is threshold independent [26]. We compute AUC for each specific technique, classifier, and dataset.

3.1.2 Independent variable

Our independent variable is the technique used to validate a classifier accuracy. As time-series technique we use the time-series cross-validation because resulting from our literature review, it is the only time-series technique used in previous studies. As a non-time-series technique, we used 10*10-fold cross-validation and out-of-sample bootstrap because resulting from our literature review, they are the most used and only recommended validation techniques, respectively.

3.1.3 Classifiers

As classifiers we use the following classifiers since they are widely used in software engineering studies [30]:
- Random Forest: It generates some separate, randomized decision trees and provides as classification the mode of the classifications. It has proven to be highly accurate and robust against noise [31]. However, it can be highly computationally expensive as it requires the building of several trees.

- Logistic Regression: It estimates the probabilities of the different possible outcomes of a categorically distributed dependent variable, given a set of independent variables. The estimation is performed through the logistic distribution function [32].

- Naïve Bayes: It uses the Bayes theorem, i.e., it assumes that the contribution of an individual feature towards deciding the probability of a particular class is independent of other features in that project instance [33].

- HyperPipes: It simply constructs a hyper-rectangle for each label that records the bounds for each numeric attribute and what values occur for nominal attributes. During the classifier application, the label is chosen whose hyper-rectangle most contains the instance (i.e., that which has the highest number of attribute values of the test instance fall within the corresponding bounds of the hyper-rectangle)².

- IBK: also known as k-nearest neighbors algorithm (k-NN) is a non-parametric method. The classification is based on the majority vote of its neighbors, with the object being assigned to the class most common among its k nearest neighbors [34].

- IB1: it is a special case of IBK with K = 1, i.e., it uses the closest neighbor [34].

- J48: builds decision trees from a set of training data [35]. It extends the Iterative Dichotomiser 3 classifier [36] by accounting for missing values, decision trees pruning, continuous attribute value ranges and the derivation of rules.

- VFI: also known as voting feature intervals [37]. A set of feature intervals represents a concept on each feature dimension separately. Afterward, each feature is used by distributing votes among classes. The predicted class is the class receiving the highest vote [37].

- Voted Perceptron: it uses a new perceptron every time an example is wrongly classified, initializing the weights vector with the final weights of the last perceptron. Each perceptron will also be given another weight corresponding to how many examples do they correctly classify before wrongly classifying one, and at the end, the output will be a weighted vote on all perceptron [38].

- ZeroR (aka, Dummy): provides as a prediction the most frequent category. For instance, in a training set where the most common category is defective, all classes in the testing set are predicted as defective. A dummy classifier is used as a baseline for accuracy interpretation [39].

3.1.4 Analysis procedure

The analysis procedure consists of two main phases: simulation and analysis. Regarding the simulation, we implement the three different techniques in JAVA by using the WEKA API 3.6.15³.

² https://ils.unc.edu/bmh/neoref/nrproduction/tmp/weka-3-4/doc/weka/classifiers/misc/HyperPipes.html
³ https://sourceforge.net/projects/weka/files/weka-3-6/3.6.15/
We use the nine classifiers and the dummy one in the WEKA API. We tune the classifiers, i.e., an automated classifiers parameter optimization, [4] [5] [12] by using the CVParameterSelection\(^4\) [40] supported by the WEKA API. Tuning is performed for each classifier and dataset and each training set. For instance, a 10*10-fold cross-validation technique requires each classifier to be tuned 100 times for each dataset. The entire simulation took about three weeks on a Linux VM, on top of a Cisco UCS C240 M3 Rack Server running VMWare ESXi 5.5 featuring four cores and 16GB of RAM, hosted at CalPoly.

Regarding the analysis, after the simulation, we compare the extent to which the accuracy of the same classifier varies across different technique. Specifically, we performed the Kruskal-Wallis [41] test which does not have any assumptions about the distribution of the data. Moreover, this test is recommended when the distributions are not independent. In our case, the distributions are computed over the same 15 projects and hence are not independent.

## 3.2 RQ2: Does the defective rate of a project changes across time?

One of the possible reasons why the results of non-time series differ from the one of time-series can be the difference in defect rate of their training sets. In this research question we want to investigate if defect rate in late releases are different from the ones in early releases; if this is true, then it is important to ensure that train set data is prior to the test set data, otherwise validation results would not be realistic. Our null hypothesis is:

H03: There is no difference, in defective rate, between the first and second half of a project.

### 3.2.1 Dependent variable

Our dependent variable is class defectiveness, i.e., if a class has at least one defect or not. We chose this variable because it is exactly what classifiers predict. We note that this variable is measured for a specific class of a release and it is of the binary type (i.e., True or False).

### 3.2.2 Independent variable

Our independent variable is time as measured by release order. We chose this measurement because current datasets contain classes related to specific releases of a project and releases are ordered (e.g., Ant 1.1 is antecedent Ant 1.2). We note that classes of the same release are not ordered.

### 3.2.3 Analysis procedure

We modified the datasets used in RQ1 by adding a further column called “Order” which value is binary: “first” or “second”. Specifically, given a project with \(n\) releases, all classes of release \(m\), where \(m > n/2\), are tagged as “second”, “first” otherwise. For instance, all classes of releases Ant 1.3, Ant 1.4, and Ant 1.5 are tagged “first”, all classes of releases Ant 1.6 and Ant 1.7 are tagged “second”.

Afterward, for each dataset, we compare the defective rate of “first” versus “second” distributions of defective rates by performing the Fisher exact test [42]. We chose this test since it is non-parametric and highly recommended when the data is small, i.e., less than 1000 observations, or

\(^4\) [http://weka.sourceforge.net/doc.dev/weka/classifiers/meta/CVParameterSelection.html](http://weka.sourceforge.net/doc.dev/weka/classifiers/meta/CVParameterSelection.html)
can be unequally distributed [43]. In this and the following research question, we use a confidence level, i.e., alpha, of 5% as standard in software engineering studies.

3.3 Datasets

To select datasets, we replicate the dataset selection performed by Tantithamthavorn et al. [7], and we added two projects of our industrial partner Keymind as they were already successfully used in the past [11]. All the 101 datasets available online\(^5\) used in Tantithamthavorn et al. [7] relates to a single release of a project. Thus, we merge in one dataset the data related to different releases of the same project by keeping the information about the related release. For instance, we create the dataset Ant by merging datasets Ant 1.3, Ant 1.4, Ant 1.5, Ant 1.6 and Ant 1.7 and by adding a column called “Release ID” reporting the release number of a class. Afterward, we removed single release datasets; this led to 16 datasets. We removed datasets Eclipse, Forrest and Prop since each of them took more than two weeks to complete the simulation.

Table 2 reports the details about the used projects regarding the number of releases, number of observations, number of features available for prediction, average defective rate, and standard deviation of defective rate. According to Table 2, the number of features changes across datasets, however, the number of events per variable (i.e., the number of observations divided by the number of features) is higher than three in all datasets, other than PBeans. Thus, according to Tantithamthavorn et al. [7], random effects, due to sampling, should not impact our results.

The specific features available in specific datasets are described in the original papers using those datasets [11] [28] [29].

4 Results

4.1 RQ1: Are validation results different among techniques?

Figure 2 reports the AUC of different classifiers (vertical axis) on different projects (horizontal axis) as computed by specific techniques (color). Figure 3 reports the distribution across different datasets of differences in AUC of the same classifiers (horizontal axis) as measured by different techniques (color). Moreover, to better analyze the differences in AUC measured by different techniques we report in Figure 3 the distribution across different datasets of differences in AUC of the same classifiers (horizontal axis) as measured by different techniques (color) when compared to walk-forward.

Table 3, respectively Table 4, reports the p-value (Kruskal-Wallis test) of the difference in AUC between 10-fold, respectively bootstrap, and walk-forward techniques of different classifiers (columns) on different projects (rows). According to Table 5, we can reject H10 in 45 (30%) out of 150 cases, i.e., 15 datasets and ten classifiers. According to Table 6, we can reject H20 in 84 (56%) out of 150 cases.

4.2 RQ2: Does the defective rate of a project change across time?

Table 5 reports the defective rates of the first and second half of a dataset. According to Table 5, the difference of means in the defective rate ranges from [-0.57, 0.63] among the datasets. Since

\(^5\) https://github.com/software-analytics/DefectData/tree/master/inst/extdata
the distributions of defective rates between the first and the second half are statistically different in 13 out of 15 datasets, we can reject H01 in 78% of the projects.

| Dataset           | Number of Releases | Number of Observations | Number of Features Available for Prediction | Average Defective Rate | Standard Deviation of Defective Rate |
|-------------------|--------------------|------------------------|--------------------------------------------|------------------------|--------------------------------------|
| Ant               | 5                  | 1692                   | 21                                         | 0.207                  | 0.405                                |
| Ar                | 5                  | 428                    | 30                                         | 0.140                  | 0.348                                |
| Camel             | 4                  | 2784                   | 21                                         | 0.202                  | 0.402                                |
| Ivy               | 3                  | 704                    | 21                                         | 0.169                  | 0.375                                |
| JEdit             | 5                  | 1749                   | 21                                         | 0.173                  | 0.379                                |
| Keymind - B       | 5                  | 702                    | 24                                         | -                      | 0.425                                |
| Keymind - A       | 5                  | 475                    | 24                                         | -                      | 0.337                                |
| Log4J             | 3                  | 449                    | 21                                         | 0.579                  | 0.493                                |
| Lucene            | 3                  | 782                    | 21                                         | 0.560                  | 0.497                                |
| PBeans            | 2                  | 77                     | 21                                         | 0.390                  | 0.491                                |
| Poi               | 4                  | 1378                   | 21                                         | 0.513                  | 0.500                                |
| Synapse           | 3                  | 635                    | 21                                         | 0.255                  | 0.436                                |
| Velocity          | 3                  | 639                    | 21                                         | 0.574                  | 0.495                                |
| Xalan             | 4                  | 3320                   | 21                                         | 0.544                  | 0.498                                |
| Xerces            | 4                  | 1643                   | 21                                         | 0.398                  | 0.490                                |

Table 2: Characteristics of the used 15 datasets. The average defective rate of the two Keymind projects is not reported due to a non-disclosure agreement.
Figure 2: AUC of different classifiers (vertical axis) on different projects (horizontal axis) as computed by specific techniques (color).
Figure 3: Distribution across different datasets of differences in AUC of the same classifiers (horizontal axis) as measured by different techniques (color).

Table 3: P-value (Kruskal-Wallis test) of the difference in AUC between 10-fold and walk-forward techniques of different classifiers (columns) on different projects (rows).
Table 4: P-value (Kruskal-Wallis test) of the difference in AUC between bootstrap and walk-forward techniques of different classifiers (columns) AUC on different projects (rows).

| Project Name | Hyper Pipes | IB1 | IBk | J48 | Logistic | Naive Bayes | Random Forest | VFI | Voted Perception | ZeroR |
|--------------|-------------|-----|-----|-----|----------|-------------|--------------|-----|----------------|-------|
| ant          | 0.092       | 0.001 | 0.001 | 0.001 | 0.151    | <0.001      | 0.672        | 0.966 | <0.001          |
| ar           | 0.093       | 0.000 | 0.148 | 0.093 | 0.089    | 0.886       | <0.001       | 0.184 | 0.092           | <0.001 |
| camel        | 0.328       | 0.003 | 0.003 | 0.003 | 0.005    | 0.498       | 0.002        | 0.331 | 0.331           | <0.001 |
| ivy          | 0.016       | 0.010 | 0.016 | 0.433 | 0.016    | 0.180       | <0.001       | 0.283 | 0.942           | <0.001 |
| jedit        | 0.001       | 0.001 | 0.068 | 0.806 | 0.352    | <0.001      | 0.294        | 0.079 | <0.001          |
| Keymind-A     | 0.660       | 0.001 | 0.872 | 0.002 | 0.001    | 0.642       | 0.001        | 0.092 | 0.003           | <0.001 |
| Keymind-D     | 0.310       | 0.144 | 0.357 | 0.001 | 0.019    | 0.092       | <0.001       | 0.993 | 0.001           | <0.001 |
| log4j         | 0.056       | 0.016 | 0.990 | 0.082 | 0.990    | 0.990       | 0.016        | 0.952 | 0.014           | <0.001 |
| lucene        | 0.116       | 0.016 | 0.016 | 0.016 | 0.138    | 0.015       | 0.030        | 0.990 | <0.001          |
| pbeans        | 0.089       | 0.000 | 0.000 | 0.089 | 0.089    | 0.096       | 0.089        | 0.631 | 0.119           | <0.001 |
| poi           | 0.003       | 0.003 | 0.003 | 0.003 | 0.331    | 0.003       | 0.331        | 0.251 | <0.001          |
| synapse       | 0.990       | 0.016 | 0.016 | 0.016 | 0.016    | 0.058       | 0.012        | 0.022 | 0.990           | <0.001 |
| velocity      | 0.933       | 0.016 | 0.016 | 0.016 | 0.016    | 0.019       | 0.990        | 0.016 | 0.016           | <0.001 |
| xalan         | 0.003       | 0.003 | 0.331 | 0.331 | 0.331    | 0.331       | 0.331        | 0.331 | <0.001          |
| xerces        | 0.004       | 0.003 | 0.003 | 0.003 | 0.331    | 0.003       | 0.331        | 0.356 | <0.001          |

Table 5: Defective rate in the first and second halves of a dataset.

| Dataset     | Defective Rate First Half | Defective Rate Second Half | Difference of Means of Defective Rate | Relative Difference | P-Value |
|-------------|---------------------------|---------------------------|---------------------------------------|---------------------|---------|
| Ant         | 0.154                      | 0.235                     | 0.081                                 | 52%                 | <0.001  |
| Ar          | 0.127                      | 0.168                     | 0.041                                 | 32%                 | 0.300   |
| Camel       | 0.242                      | 0.181                     | -0.061                                | -25%                | 0.002   |
| Ivy         | 0.224                      | 0.114                     | -0.111                                | -49%                | <0.001  |
| JEdit       | 0.274                      | 0.069                     | -0.206                                | -75%                | <0.001  |
| Keymind - B | -                          | -                         | -                                     | -                   | <0.001  |
| Keymind - A | -                          | -                         | -                                     | -                   | 0.020   |
| Log4J       | 0.291                      | 0.922                     | 0.631                                 | 217%                | <0.001  |
| Lucene      | 0.532                      | 0.597                     | 0.065                                 | 12%                 | 0.070   |
| PBeans      | 0.769                      | 0.196                     | -0.573                                | -75%                | <0.001  |
| Poi         | 0.323                      | 0.640                     | 0.317                                 | 98%                 | <0.001  |
| Synapse     | 0.201                      | 0.336                     | 0.135                                 | 68%                 | <0.001  |
| Velocity    | 0.705                      | 0.341                     | -0.364                                | -52%                | <0.001  |
| Xalan       | 0.326                      | 0.730                     | 0.404                                 | 124%                | <0.001  |
| Xerces      | 0.246                      | 0.486                     | 0.240                                 | 98%                 | <0.001  |
5 Discussion

5.1 RQ1: Are validation results different among techniques?

According to Figure 3 the difference in AUC between 10-fold and walk-forward is in the range \([-0.20, 0.22]\), and between bootstrap and walk-forward is in the range \([-0.17, 0.43]\). Thus, we cannot claim walk-forward provides a lower or a higher AUC compared to either 10-fold or bootstrap. However, since the blue plots in Figure 3 of IB1 and Random Forest are positive, then we can claim that, for such two classifiers, the AUC measured by bootstrap is higher than the one measured by walk-forward in each of the 15 datasets. This means bootstrap significantly overestimates the accuracy of IB1 and Random Forest. In other words, a research improvement on IB1 or Random Forest classifiers is harder to validate via bootstrap than other techniques. This is because the accuracy of both the improved and non-improved versions of the classifiers will likely remain optimistic and since AUC has an upper bound (1.0), their difference will likely be less visible [39].

Moreover, according to Figure 3, the difference between bootstrap and walk-forward is higher than the difference between 10-fold and walk-forward in all classifiers other than HyperPipes. This difference is particularly higher in the case of RandomForest, one of the most accurate and widely used classifier in software engineering. Thus, we can conclude bootstrap is more different to walk-forward than 10-fold.

According to Figure 2, the green plots are wider than red and blue plots; this means walk-forward has a higher variance among runs than 10-fold and bootstrap. One reason for this high variance is that in walk-forward the training set increases in size over different runs whereas in the other two techniques the training set is constant in size over different runs. Another reason is that since the two non-time-series techniques are subject to random sampling, their training and test sets are likely less different among themselves than sets created by following a temporal order. The variance among runs has been discussed in many studies [14] [15] [44] as a potential source of bias and threats to study replication. However, the variance referred to in these papers is a source of instability caused by the random sampling procedure which is \textit{de facto} used in all non-time-series techniques such as bootstrap and ten-fold. Non-time-series technique is perfectly replicable as the variance relates to how data is temporally grouped in the dataset(s) and not in the way it is sampled which can vary among contexts. Thus, the variance in a time-series technique is very informative; it describes how much the AUC varies among the different releases and hence possible realistic usages of the classifier.

According to Table 3 and Table 4, the AUC measured by walk-forward is statistically different from the one measured by 10-fold in 30\% of the cases and by bootstrap in 56\% of the cases. Such a result must be interpreted by considering that the number of observations of the walk-forward distribution varies between one and four across datasets (i.e., number of releases less one, see Table 2). Statistical tests are prone to type II error, i.e., not rejecting a false null hypothesis, if used on distributions of small observations. For instance, PBeans has two only releases, and hence its walking-forward distribution is represented by one observation only. In PBeans we were able to reject H10 only in only one classifier and H20 in only three classifiers out of the ten classifiers. Thus, the rejections in PBeans is less than the half of the average rejections among datasets.
Both statistical and descriptive statistics suggest that ten-fold is closer to walk-forward than bootstrap. This result suggests estimating accuracy via ten-fold is closer than via bootstrap in measuring accuracy.

We did not observe any significant difference between open and closed datasets.

**RQ1 summary:** The AUC measured by walk-forward is statistically different from the one measured by 10-fold in 30% of the cases and by bootstrap in 56% of the cases. The difference varies in sign across datasets and classifiers.

### 5.2 RQ2: Does the defective rate of a project change across time?

According to Table 5, the relative difference between the second and first half is in the range [-75%, 218%]. It is interesting to note that the relation between time and class defectiveness is not monotone, i.e., classes do not constantly tend to have a higher or a lower defective rate over time. Specifically, in 9 cases (out of 15 projects) the rate is higher in the second half, and in the remaining 6 cases, it is higher in the first half. This result also applies to the two industrial datasets; in Keymind-A, the higher defective rate is in the first half, in Keymind-B is in the second half.

Anyway, regardless of the sign, the average relative difference, among datasets, is very high: 82%. This high difference is not considered by the sampling procedure adopted in non-time-series techniques which makes validation results poorly realistic.

As intuitive, according to Table 2 and Table 5, a high p-value was the combination of a low relative difference among halves and a small number of observations in the dataset. For instance, if we compare datasets Ar with Camel, Ar has a has a much higher p-value (0.300 > 0.002) since it has a slightly higher absolute relative difference (32% > 25%) and a major lower dataset size (428 < 2784).

**RQ2 summary:** The defective rate of classes in the first and second half varies in sign and it is practically (82% average relative difference) and statistically different (in 78% of datasets).

### 6 Threats to validity

In this section, we discuss possible threats to validity related to our study. The threats are organized by type (i.e., Conclusion, Internal, Construct, and External).

Conclusion validity regards issues that affect the ability to draw accurate conclusions about relations between the treatments and the outcome of an experiment [24]. In both research questions we used non-parametric tests; thus, we are more prone to type I error (i.e., rejecting a true null hypothesis) than to type II error (i.e., non-rejecting a false null hypothesis). This is particularly relevant for RQ1 where the ability to reject the hypotheses has also been inhibited by the very low number of data points (one to four) for one of the factors (walk-forward). Thus, we recommend care in judging as low the number of times we have been able to find a statistically significant difference in classifier accuracy between a time-series and a non-time-series technique. Another important threat to construct validity in RQ1 is measuring a classifier accuracy by using a single
dependent variable, i.e., AUC. This choice was driven by previous researchers suggesting to avoid threshold-dependent metrics such as Precision and Recall and to use AUC [26]. We did not use additional threshold-independent metrics such as the Brier score [45] mainly because they are practically irrelevant for a classification task.

Internal validity regards the influences that can affect the independent variables concerning causality [24]. The only threat to the validity of this type that is relevant in this study is the use of halves as the measure of temporal order (RQ2). An alternative approach could have been using the release ID as a metric of temporal order. However, this alternative approach would have reduced the number of observations per treatment. This reduction would have increased the risk of Type II error, which is already high due to the use of non-parametric-tests (see above discussion), without reducing the risk of Type I error.

Construct validity regards the ability to generalize the results of an experiment to the theory behind the experiment [24]. This threat to validity is low as the used datasets have been already successfully used and published by other researchers. We did not add any information to the datasets.

External validity regards the extent to which the research elements (e.g., subjects and artifacts) are representative of actual elements [24]. In other to mitigate this threat we used all multi-release datasets we knew are publicly available. Moreover, we report the datasets characteristics in Table 2.

7 Conclusions

As testing remains one of the most important activities in software engineering, prioritizing test cases by predicting components likely to be defective is vital to prioritize effort allocation. The software engineering community has provided significant advances in prediction models, and more advances are probably on their way.

This paper reflects on the importance of preserving order when validating prediction models, i.e., in the use of the time-series technique. We compared the performance of the most used time-series technique (i.e., walk-forward) with the performances of the most used (10-fold) and the suggested (out-of-sample bootstrap) validation techniques, both of which are non-time-series. Our results show that the accuracy measured by bootstrap is different statistically and practically from the ones measured by the other two non-time-series techniques. We checked one of the possible reasons for this difference, i.e., the defect rate used in the training sets. Our results show that the relative difference in defect rate between the second and first half of a project is, among projects, in the range [-75%, 218%], and it is statistically different in 13 out of 15 projects. Since non-time-series techniques randomly sample the datasets to create test and training sets, they do not preserve such difference which exists in practice. Therefore, the accuracy measured by non-time-series techniques is poorly realistic of any prediction models’ practical adoptions.

If on the one side, we recommend in general validating prediction models by using time-series techniques, on the other side we need to keep in mind there is no silver bullet in software engineering [46]. Similarly, our take is that when choosing the technique to use we must carefully consider the prediction model usage scenario, the type of research question, the conclusions to draw, and, when possible, validating the techniques empirically (i.e., meta-validation).
Validation techniques that do not consider the temporal order of data might be appropriate for testing the feasibility of prediction models in in-vitro settings. However, when it comes to technology transfer and in-vivo applications, they tend to have a misleading positive bias towards applied models. Hence, we recommend the use of validation techniques that reserve the temporal order of data for the evaluation of defect prediction models in industry settings. Non-time-series techniques might be preferable over time-series-technique in contexts different than accuracy validation. For instance, the non-time-series technique might be preferable to use inside tuning techniques for estimating the best sets of parameters to use; this because they maximize data usage. However, we note that to achieve realism in the validation, tuning techniques, made with or without non-time-series techniques, shall be validated via time-series techniques.

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