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CRISTIANO SOUSA MELO

SUPPORTING CHANGE-PRONE CLASS PREDICTION

FORTALEZA

2020

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Dissertation submitted to the Post-Graduation Program in Computer Science of the Center of Science of the Federal University of Ceará, as a partial requirement for obtaining the title of Master in Computer Science. Concentration Area: Information Systems

Advisor: Prof. Dr. José Maria da Silva Monteiro Filho

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To my family, all my friends, and my advisor.

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ABSTRACT

During the development and maintenance of software, changes can occur due to new features, bug fixes, code refactoring, or technological advancements. In this context, change-prone class prediction can be very useful in guiding the maintenance team, since it is possible to focus efforts on improving the quality of these code snippets and make them more flexible for future changes. In this work, we have proposed a guideline to support the change-prone class prediction problem, which deals with a set of hardworking strategies to improve the quality of the predictive models. Besides, we have proposed two data structures that take the temporal dependencies between these changes into account, called Concatenated and Recurrent approaches. They are also called dynamic approaches, in contrast with the conventional state-of-art static approach. Our experimental results have shown that the proposed dynamic approaches have had a better Area Under the Curve (AUC) over the static approach.

Keywords: Guideline. Change-Prone Class Prediction. Time-Series. Recurrent Algorithms.

RESUMO

Durante o desenvolvimento e a manutenabilidade de um software, alterações podem ocorrer devido a novos recursos, correções de bugs, refatoração de código ou avanços tecnológicos. Nesse contexto, a predição de classe propensa a mudanças pode ser muito útil para orientar a equipe de manutenção, pois é possível concentrar esforços na melhoria da qualidade desses trechos de código e torná-los mais flexíveis para mudanças futuras. Neste trabalho, propusemos um *guideline* para o problema de predição de classe propensa a mudança, que lida com um conjunto de estratégias para melhorar a qualidade dos modelos preditivos. Além disso, propusemos duas estruturas de dados que levam em consideração as dependências temporais entre essas mudanças, chamadas abordagens concatenadas e recorrentes. Eles também são chamados de abordagens dinâmicas, em contraste com o conceito estático existente do estado da arte. Nossos resultados mostraram que as abordagens dinâmicas tiveram uma Área Sob a Curva (AUC) melhor do que a abordagem estática.

Palavras-chave: *Guideline*. Predição de Classe Propensa a Mudança. Séries Temporais. Algoritmos Recorrentes.

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1 INTRODUCTION

Software maintenance has been regarded as one of the most expensive and arduous tasks in the software lifecycle, according to Koru and Liu (2007). Software systems evolve in response to the world's changing needs and requirements. So, a change could occur due to the existence of bugs, new features, code refactoring, or technological advancements. As the systems evolve from a release to the next, Koru and Liu (2007) have observed they become larger and more complex. Besides, Elish and Al-Khiaty (2013) highlight that managing and controlling change in software maintenance is one of the most critical concerns of the software industry. As software systems evolve, focusing on all of their parts of the same way is hard and a waste of resources.

In this context, Elish *et al.* (2015) observe that a change-prone class is likely to change with a high probability after a new software release. Then, it can represent the weak part of a system. Therefore, change-prone class prediction can be beneficial and helpful in guiding the maintenance team, distributing resources more efficiently, and thus, enabling project managers to focus their effort and attention on these classes during the software evolution process. For instance, refactoring can emphasize change-prone classes to improve their quality and make them more flexible in order to better accommodate future changes and to localize the impact of changing them. Inspection and testing activities can stress such classes, and thus enable efficient allocation of precious resources.

In order to predict change-prone classes, different categories of software metrics have been proposed by different authors, such as Oriented Object metrics by Chidamber and Kemerer (1994), Code Smells by Khomh *et al.* (2009), Design Patterns by Posnett *et al.* (2011), and Evolution Metrics by Elish and Al-Khiaty (2013). Based on these metrics, some works which use machine learning techniques have been proposed for building change-prone class prediction models, such as Bayesian Networks by Koten and Gray (2006), Neural Networks by Amoui *et al.* (2009), and Ensemble methods by Elish *et al.* (2015). A typical prediction model based on machine learning is designed by learning from historical labeled data within a project in a supervised way.

However, despite the flexibility of emerging Machine Learning techniques, owing to its intrinsic mathematical and algorithmic complexity, they have often considered a "black magic" that requires a delicate balance of a large number of conflicting factors. This fact, together with the short description of data sources and modeling process, makes research results reported in many works hard to interpret. It is not rare to see potentially mistaken conclusions drawn from methodologically unsuitable studies. Most pitfalls of applying machine learning techniques to predict change-prone classes originate from a small number of common issues, including data leakage and overfitting.

Nevertheless, these traps can be avoided by adopting a suitable set of guidelines. The term guideline is defined as a recommendation that leads or directs a course of action to achieve a specific goal. Therefore, guidelines summarize expert knowledge as a collection of design judgments, rationales, and principles. Despite the several works that use Machine Learning techniques to predict change-prone classes, no significant work was done so far to assist a software engineer in selecting a suitable process for this particular problem.

Besides, in state-of-art, the change-prone class prediction is a problem in which its structure is a time-series since their releases are available in different period. However, this information is not part of the scenario when the predictive models are generated. Thus, to the best of the authors' knowledge, although many works are studying the change-prone class prediction problem, none of them take the temporal dependence between the instances in the datasets into account.

In this work, besides presenting a guideline in order to generate predictive models, we also present two approaches in order to build the datasets: (i) static and (ii) dynamic. The former means that each instance from the dataset is taken into account to generate predictive models individually, while the latter means there is a temporal dependence between the instances. To validate the proposed guideline and the novel dynamic approaches, we have performed two case studies. In the first case study, we have performed the guideline over an imbalanced dataset called Control of Merchandise (Coca) following the static approach. Coca has extracted from extensive commercial software, containing 8 static object-oriented metrics proposed by C&K and McCabe. In the second case study, we wanted to investigate the gain of the AUC using dynamic approaches over the static. For this, firstly, we have collected three Apache datasets (Ant, Beam, and Cassandra), and we have generated their baselines in the static approach, following some steps from the guideline. After that, we have built them in the Concatenated and Recurrent approaches for three different window sizes.

The main contributions of this work are:

1. A guideline to support change-prone class prediction problem to standardize a minimum list of activities and roadmaps for better generating of predictive models.

2. Four public datasets based on commercial software and open-source Apache projects.
3. Two novel structures involving time-series in the dataset in order to improve the quality of the generated models.
4. Two case studies, evaluating the proposed guideline and the novel time-series approaches in change-prone class prediction.

As a result of this work, we have had two main publications: the first one was related to the proposed guideline in the first case study in Melo *et al.* (2019), and the second publication is related to the second case study, which proposes two novel dynamic structures, in Melo *et al.* (2020). Besides, we have had the third publication in Martins *et al.* (2020) in which we applied the guideline in order to investigate code smells and static metrics as independent variables empirically.

2 RELATED WORKS

Elish and Al-Khiaty (2013) propose and validate a set of evolution-based metrics as potential indicators of change-proneness of the classes. Then, they have evaluated their proposed metrics empirically as independent variables of the change-proneness of an OO system when moving from its current release to next. The datasets used in their experiments are VSSPLUGIN and PeerSim, from the open-source software SourceForge. To evaluate these proposed metrics, release-by-release, these models were built in four different ways using multivariate logistic regression analysis: (1) using both the evolution-based and C&K metrics as independent variables, (2) using only the evolution-based metrics as independent variables, (3) using only C&K metrics as independent variables, and (4) using only the internal class probability of changes metrics as an independent variable. In their experiments, the authors have concluded that the inclusion of both the proposed evolution-based metrics and the C&K metrics in a prediction model for change-proneness do offer improved prediction accuracy compared with a model that only includes C&K metrics, evolution-based metrics, or internal class probability. However, the authors have not mentioned any cross-validation technique to validate their models. Besides, we do not know if their datasets are imbalanced.

Malhotra and Khanna (2014) examine the effectiveness of ten machine learning algorithms using C&K metrics in order to predict change-proneness classes. These algorithms are Support Vector Machine, Gene Expression Programming, Multilayer Perceptron with conjugate learning, Group Method Data Handling Network, K-means clustering, TreeBoost, Bagging, Naïve Bayes, J48 Decision Tree, and Random Forest. The main objective of this study was to evaluate several ML algorithms for their effectiveness in predicting software change. They have concluded that CBO, SLOC, and WMC are efficient predictors of change. Besides, in their experiments, SVM is the best ML algorithm that can be used for developing change prediction models. The authors have worked in three JAVA projects to generate their datasets, and during the statistical analysis for each one of them shows that there is one imbalanced dataset (26% changed classes). However, there was not any treatment as a resampling technique. Studies involving data normalization, outlier detection, and correlation were not performed. Although the authors of this research have explained the process to collect the independent and dependent variables, they did not provide the scripts containing the dataset with metrics generated.

Kaur *et al.* (2016) study a relationship between different types of object-oriented metrics, code smells, and change-prone classes. They argued that code smells are better predictors of change-proneness compared to OO metrics. For this, they have generated a dataset from a Java mobile application, called MOBAC. This dataset is imbalanced, then they have used resampling techniques such as SMOTE. They have concluded that code smells are more accurate predictors of change-proneness than static code metrics for all Machine Learning methods. Despite this conclusion, the authors did not provide the dataset used in their experiments.

Bansal (2017) compares the performance of search-based algorithms with machine learning algorithms constructing models related to both approaches. These metrics were collected from two open-source Apache projects, Rave and Commons Math. The generated datasets present imbalanced classes, 32.8% and 23.54%, respectively. The independent variables used were C&K. However, the author identifies some strong correlations between the independent variable, and he decided to apply Principal Component (PC) on them. In the end, the author concludes that search-based algorithms have proved to be capable of predicting change-prone class by showing high values of accuracy, although it is necessary a high CPU performance compared to ML techniques. For this work, the author uses two imbalanced datasets, but he does not use any resampling techniques. Besides, he uses accuracy to validate their result, and he does not provide the datasets to reproducibility.

Catolino *et al.* (2018) analyze 20 datasets exploiting the combination of developer-related factors (e.g., number of developers working on a class) and evolution-based metrics as independent variables to generate predictive models. All these datasets are imbalanced; however, the authors did not perform any resampling techniques in order to improve the performance metric. The authors achieved the following conclusions: developer-based change prediction models generally show good performance. The devised combined change prediction model has an overall F-measure of 79% and outperforms the standalone baselines by up to 22%.

Choudhary *et al.* (2018) have proposed the use of new metrics in order to avoid the *commonly used* independent variable to generate models in change-prone class prediction problems, like C&K or evolution-based metrics. These newly proposed metrics are execution time, frequency or method call, run time information of methods, popularity, and class dependency. They have evaluated their proposed metrics in two open-source software from Warehouse (SourceForge), called OpenClinic and OpenHospital datasets. For evaluating the performance of the prediction model, the authors used sensitivity, specificity, and ROC Curve. In OpenClinic dataset, the AUC improved from 0.750 to 0.925, and in the OpenHospital dataset, the AUC improved from 0.725 to 0.915.

Table 1 summarizes all aforementioned related works. It illustrates the (i) main author, (ii) the name of the dataset, (iii) the number of releases, (iv) the imbalanced rate, (v) if there was resampling technique, (vi) if there was statistical analysis of the dataset, (vii) if there was cross-validation, and (viii) if the dataset is available for download. In the paper written by Catolino, we provide the minimum and maximum releases and imbalanced rate from the 20 datasets. Some information has been omitted, as an example, the imbalanced rate of the VSSPlugin dataset, so we flagged it as unknown (unk). We highlight that almost all works do not provide their dataset or scripts for download. Even some papers specify some version of the software project used, their source codes are not available on the original website.

Table 1 – Overview of the Related Works

Paper	**Dataset**	**Releases**	**Imb. Rate**	**Res. Tech.**	**Stats**	**CV**	**Availab.**
2013	VSSPLUGIN	13	Unk	No	Yes	Unk	No
	PeerSim	9	Unk	No	Yes	Unk	No
2014	DrJava	2	49%	No	Yes	k-fold	No
	DSpace	2	60%	No	Yes	k-fold	No
	Robocode	2	26%	No	Yes	k-fold	No
2016	MOBAC	4	Unk	Yes	No	k-fold	No
2017	Rave	2	32.8%	No	Yes	k-fold	No
	Commons Math	2	23.5%	No	Yes	k-fold	No
2018	+20	9-44	19%-35%	No	No	k-fold	Yes
2018	OpenClinic	4	75.8%	No	Yes	k-fold	No
	OpenHospital	2	5.9%	No	Yes	k-fold	No

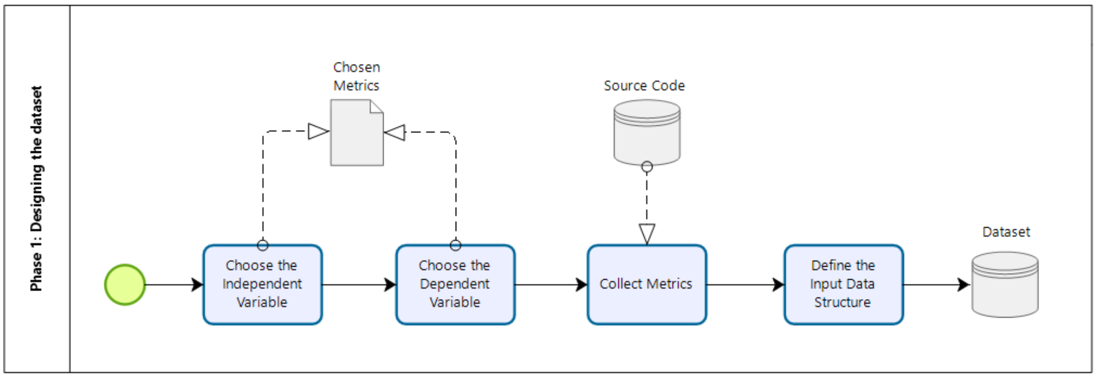
3 A GUIDELINE TO SUPPORT CHANGE-PRONE CLASS PREDICTION PROBLEM

This chapter describes the proposed guide to support the change-prone class prediction problem, published in Melo *et al.* (2019). It is organized into two phases: (i) designing the dataset from software project and (ii) generating predictive models. Each one of these phases will be detailed next.

3.1 Phase 1: Designing the Dataset

The first phase in the proposed guide aims to design and build the dataset that will be used by the machine learning algorithms to generate predictive models for change-prone classes. This phase, illustrated in Figure 1, encompasses the following activities: choose the dependent variables, choose the independent variable, collect the selected metrics, and define the data structure into static or dynamic.

Figure 1 – Phase 1: Designing the Dataset



Source: Author.

3.1.1 Choose the Independent Variables

In order to predict change-prone classes, different categories of software metrics can be used, such as Object-Oriented (OO), McCabe's metrics, Code Smells, Design Patterns, and Evolution metrics. Then, the first step to design a proper dataset consists of answering the following question "which set of metrics (features) should be chosen as input to the prediction model?". In other words, which independent variables to choose? The independent variables, also known in a statistical context as regressors, represent inputs or causes, i.e., potential reasons for a variation on the target feature (called dependent variable). So, they are used to predict the target feature. It is essential to highlight that the choice of a suitable set of metrics impacts directly in the prediction model performance. So, different metrics have been proposed in the literature.

Chidamber and Kemerer (1994) have proposed a metric set specifically for software systems that are developed using the object-oriented programming paradigm. These metrics are WMC (Weighted Methods per Class), DIT (Depth of Inheritance Tree), CBO (Class Between Object), Response for a Class (RFC), NOC (Number of Children) and LCOM (Lack of Cohesion in Methods).

McCabe (1976) have proposed Cyclomatic Complexity (CC), and there are extended versions of these metrics as MAX_CC (maximum values of methods in the same class), and AVG_CC (mean values of methods in the same class) also are used.

Halstead (1977) states that software modules that are hard to read tend to be more defect prone. He calculates the software complexity of a module by defining four critical attributes like the Number of Operators, the Number of Operands, the Number of Unique Operators, and the Number of Unique Operands, then derives his metrics that provide insight about the source code complexity.

Bansiya and Davis (2002) have observed that there are metrics to model design properties like abstraction, messaging, and inheritance, but no object-oriented design metrics exist for several other design properties like encapsulation and composition. Furthermore, they state that some existing metrics to measure complexity, coupling, and cohesion require almost a full implementation, and that is why they are difficult to generate during design. So, they define five new metrics (known as QMOOD metrics suite), which can be calculated from the design information only. These metrics are DAM (Data Access Metric), NPM (Number of Public Methods), MFA (Measure of Functional Abstraction), CAM (Cohesion Among Methods), and MOA (Measure Of Aggregation).

Besides, they have proposed new additional OO metrics like FanIn (Number of other classes that reference the class), FanOut (Number of other classes referenced by the class), NOA (Number of Attributes), NOPA (Number of Public Attributes), NOPRA (Number of Private Attributes), NOAI (Number of Attributes Inherited), NOM (Number of Methods), NOPM (Number of public methods), NOPRM (Number of Private Methods), NOMI (Number of Methods Inherited) and LOC (Lines of Code). Gyimothy *et al.* (2005) have shown that Lines of Code (LOC) is one of the best metrics for fault prediction.

All these aforementioned metrics measure the source code related attributes of a software product. On the other hand, process-based metrics that measure the changing nature of the software and that are collected over a certain period can be related to developers, revisions, and source code changes.

3.1.2 Choose the Dependent Variable

The next step consists in defining the dependent variable, which is the variable to be predicted. Change-prone class prediction studies the alterations of a class analyzing the difference between an old version and a more recent new version. Lu *et al.* (2012) define a change of a class when there is an alteration in the number of Lines of Code (LOC). The domain of change-prone prediction can be either labeled 0-1 to indicate whether there was some alteration or not. Thus, following its definition, an instance from the dataset, i.e., an object-oriented class, will be labeled as 1 if in the next release occurs alteration in its LOC independent variable, and 0 otherwise.

Besides, the dependent variable can be a probability computed by

$$P_i = \frac{|(L_1)_i|}{|(L_0 + L_1)_i|} \tag{3.1}$$

where P_i is a change probability of a i-th class, $|(L_1)_i|$ and $|(L_0 + L_1)_i|$ being the amount of labels 1 and total labels of a i-th class, respectively.

3.1.3 Collect Metrics

This step in this phase consists of collecting the metrics chosen previously (independent and dependent variables) from a given software project. Singh *et al.* (2013) cite a list of tools to collect the most common metrics according to a used Object-Oriented programming language (JAVA, C++, or C#). As example, we can have Scitools Understand for collect independent variables from JAVA projects or NDepends plugin in Visual Studio to collect independent variables from C# projects.

3.1.4 Define the Input Data Structure

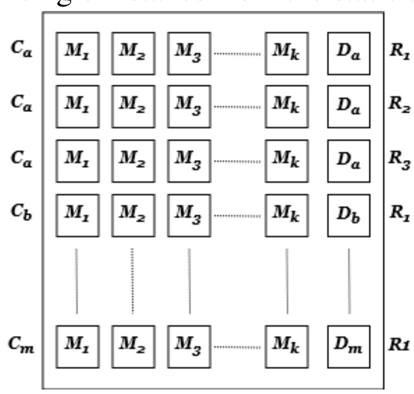
After choosing the independent and dependent variable, it is necessary to define the data structure according to the predictive model that will be generated. In this case, we can have two approaches: (i) static and (ii) dynamic. The former means that each instance from the dataset is taken into account to generate predictive models individually, while the latter means there is a temporal dependence between the instances.

The static structure is the *traditional way* from the used dataset to generate predictive models in change-prone class prediction problems mentioned in Related Works, Section 2. However, we are going to define two dynamic structures since they can improve the performance metrics of the models over the static structure. These results can be seen in the second Case Study, section 5.

3.1.4.1 Static Approach

In the static approach, each instance from the dataset will be taken into account individually, i.e., each instance contains the metric values for a particular class in a specific release as independent variables. Figure 2 illustrates an example of this structure. Note that each line, i.e., instance, represents a class from the software project in a particular release, and its columns contain *k* metrics *M*, i.e., independent variables, and one last column representing the dependent variable *D*. Observe that in this example, the C_a class has three instances, one for each release in which it appears. In practice, the Machine Learning algorithms use the *k* columns *M* and the dependent variable *D* to generate their models, ignoring the class identifier *C* and the release number *R*. It means this usual approach is just engaging in learn a pattern to predict which class will suffer modification in the next release, ignoring their history, i.e., the temporal dependence between the instances.

Figure 2 – A single instance from the static approach.



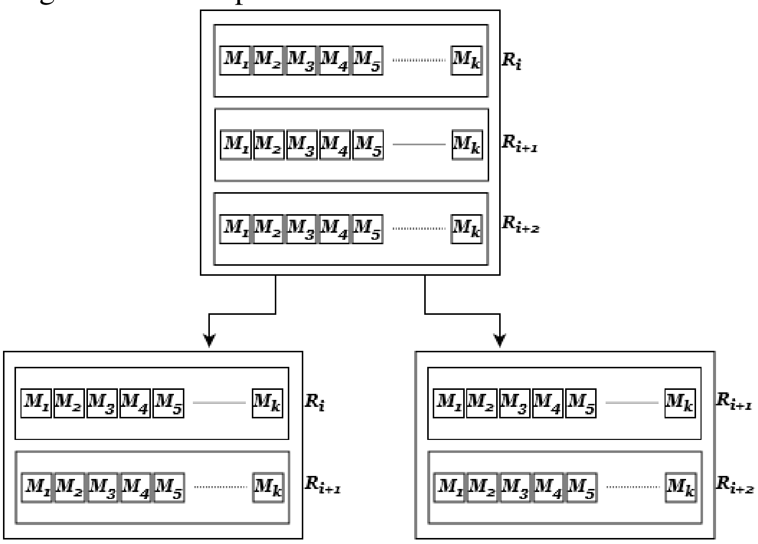
Source: Author.

3.1.4.2 Dynamic Approach

In the dynamic approach, we have proposed two time-series structures, called Concatenated and Recurrent, in order to exploit the temporal dependence between the instances to improve the quality of the performance metrics of the predictive models. The Concatenated structure has its temporal dimension incorporated from the presentation of versions of the input at different times (releases, to be more specific). The Recurrent structure contains an internal memory that is modified according to the presentation of the available patterns.

In these new time-series structures, depending on window size, each instance will contain the total - or partial - history of the metrics values of a class, following its release order. Thus, initially, to design a dataset according to those novel proposed approaches is necessary to define a window size. The value of the window size parameter will be fixed and will define the number of releases that will compose each instance. So, the window size value must be chosen carefully. During the dataset building, if the number of releases that a certain class *C* appears is less than the window size, the data about this class *C* will be dropped. However, the opposite is not true. If the number of releases that a certain class *C* appears is greater than the window size, the data about class *C* will be split, as shown in Figure 3. Note that, in Figure 3, there is a class *C* that appears in three different releases. Now, suppose that the window size was set as two. In this scenario, the data about class *C* will be split into two instances, i.e., from release *i* to release $i+1$ and from release $i+1$ to release $i+2$.

Figure 3 – The Split Process for Window Size two.



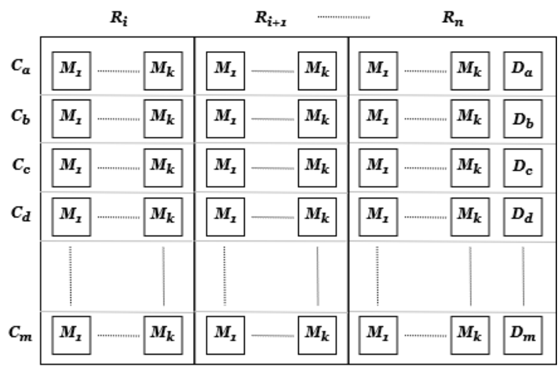
Source: Author.

Concatenated Approach (CA)

To generate a dataset according to the Concatenated Approach is necessary, initially, to compute the values of the k metrics for each release R in which a specific class C appears. So, this process will produce R instances, each one with k columns. After that, for each class C, it needs to concatenate its n sequential instances, where n is the window size, according to the split process. Note that in this step, the produced instances will contain $n * k$ columns, as the independent variable. For example, if a class C appears in $R = 4$ releases and the window size $n = 3$, two instances, each one with $k * 3$ columns will be generated.

Figure 4 illustrates a dataset built according to the Concatenated Approach. Note that M represents the chosen metrics (they can be Oriented Object, Evolution, or Code Smells). Thus, an instance in this dataset contains $n * k$ columns, i.e., independent variables, respecting the releases order $i, i+1, ..., n$ to ensure the use of time-series information.

Figure 4 – Concatenated Structure.



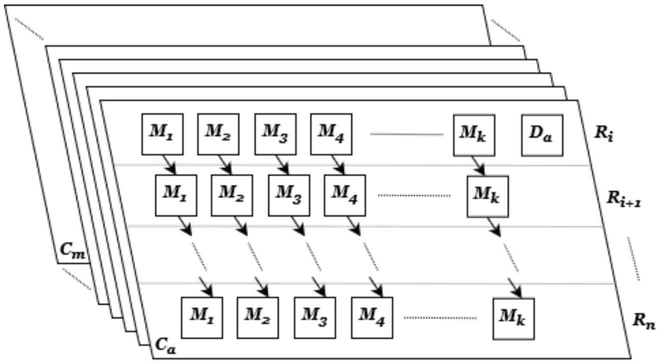
Source: Author.

Recurrent Approach (RA)

The Recurrent Approach consists of storage the partial or total history into a single instance of a class, forming a three-dimensional matrix (m, k, n), where m means the number of classes, k means the number of metrics, and n means the window size.

Figure 5 depicts an example of the data structure used in the recurrent approach. R represents the releases of a certain class C, and it will follow the release order $i, i+1, ..., n$. Each one of these releases contains k metrics M. In short, this dataset contains m classes C, i.e, there are m instances of window size n, where each release has k metrics. Note that if the window size is less than the number of the release of a class C, this last one will be split, generating more instances into the dataset.

Figure 5 – Recurrent Structure.

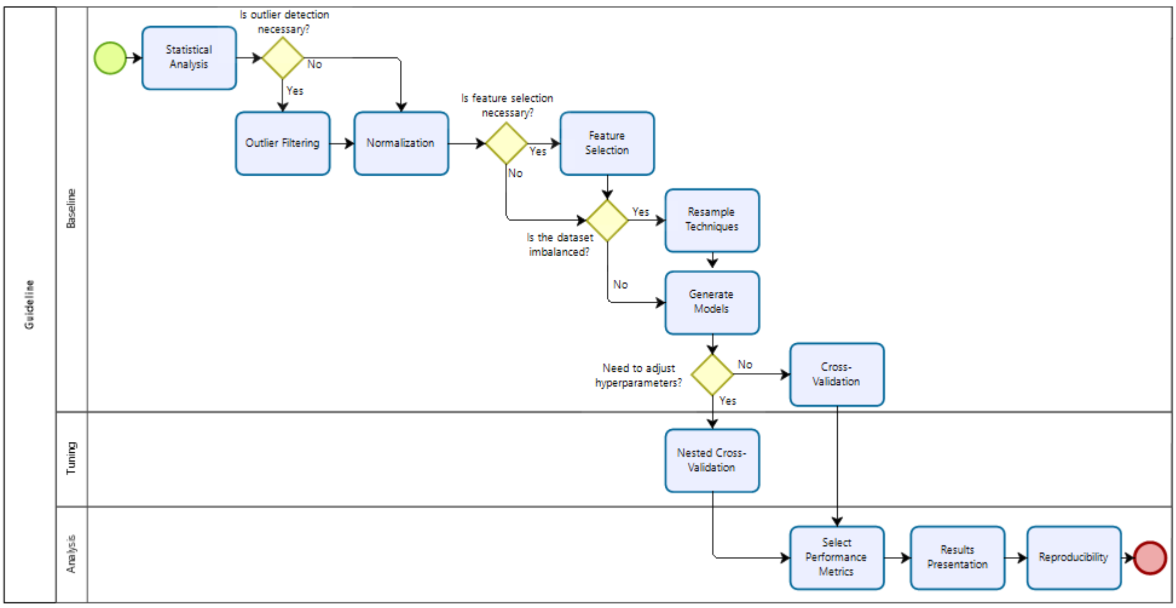


Source: Author.

3.2 Phase 2: Applying Change-Proneness Prediction

The second phase of this proposed guide aims to build change-prone class predictive models. A prediction model is designed by learning from historical labeled data within a project in a supervised way. Besides, this phase encompasses the activities related to the analysis of the prediction model, performance metrics, the presentation of the results, and the ensure of the experiments' reproducibility. Figure 6 illustrates the activities that compose the second phase of the proposed guide.

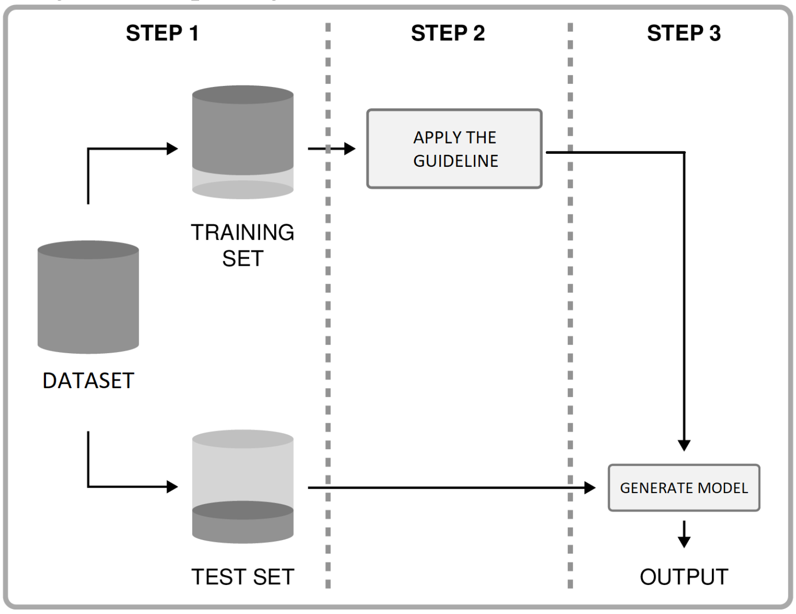
Figure 6 – Phase 2: Applying Change-Proneness Prediction.



Source: Author.

It is important to highlight that before starting to execute the guideline is essential to split the dataset into train and test sets, according to Figure 7. The former will be performed whole the guideline, while the latter serves to simulate the real-world data. In the case of an imbalanced dataset, it is necessary to split the labels proportionally in order to avoid the bias during the model generation. For this scenario, we recommend *train_test_split* function from scikit-learn. During the cross-validation step from the guideline, the train set will be split into train and validation sets, in order to use the test set to check the overfitting.

Figure 7 – Splitting Dataset into Train and Test.



Source: Author.

3.2.1 Statistical Analyses

Initially, a general analysis of the dataset is strongly recommended. Thus, generate a table containing for each feature a set of valuable information, such as minimum, maximum, mean, median (med), and standard deviation (SD) values.

After that, it is important to check the correlation between the features. Pearson's correlation checks the linearity between the data. It is related to the fact that the generated prediction model may be highly biased by correlated features, then it is essential to identify those correlations. Bishara and Hittner (2012) recommend Spearman's correlation for nonnormally distributed data.

3.2.2 Outlier Filtering

Outliers are extreme values that deviate from other observations on data, i.e., an observation that diverges from an overall pattern on a sample. According to Liu *et al.* (2004), detected outliers are candidates for aberrant data that may otherwise adversely lead to model mispecification, biased parameter estimation, and incorrect result. It is, therefore, interesting to identify them before create the prediction model.

We are going to cite a usual strategy to check outlier: Interquartile Range (IQR). It is a measure of statistical dispersion, often used to detect outliers. The IQR is the length of the box in the boxplot, i.e., Q3 - Q1. Here, outliers are defined as instances that are below $Q1 - 1.5 * IQR$ or above $Q3 + 1.5 * IQR$. For non-normal distribution of the dataset, Hubert and Vandervieren (2008) suggest an IQR adaptative, since when the data are skewed, usually many points exceed the whiskers and are often erroneously declared as outliers.

Outliers are one of the main problems when building a predictive model. Indeed, they cause data scientists to achieve more unsatisfactory results than they could. To solve that, we need practical methods to deal with that spurious points and remove them. If it is evident the outlier is due to incorrectly entered or measured data, it should drop it. If the outlier does not change the results but does affect assumptions, it also may drop the outlier. More commonly, the outlier affects both results and assumptions. In this situation, it is not legitimate to drop it. It just may run the analysis both with and without it. Besides, it should state how the results changed.

3.2.3 Normalization

It is essential to check if the features are on the same scale. For example, two features A and B may have two different ranges: the first one into a range between zero and one, meanwhile the second one is into a range in the integers domain. In this case, it is necessary to normalize all features in the dataset. There are different strategies to normalize data. However, it is essential to emphasize that the normalization approach must be chosen according to the nature of the investigated problem and the used prediction algorithm. For example, Basheer and Hajmeer (2000) have observed that for activation function in a neural network is recommended that the data be normalized between 0.1 and 0.9 rather than 0 and 1 to avoid saturation of the sigmoid function. Hereafter, the leading data normalization techniques are presented.

In **min-max normalization** features are normalized using the following equation:

$$x' = \lambda_1 + (\lambda_2 - \lambda_1)\Big(\frac{x - min_A}{max_A - min_A}\Big) \tag{3.2}$$

In the equation 3.2, λ_1 and λ_2 are values to adjust the data domain to a desired range. For example, to normalize the values from a dataset to [-0.3, 0.8], λ_1 and λ_2 must be -0.3 and 0.8, respectively. The min_A and max_A are the minimum and the maximum values of the feature A. The original and the normalized value of the attribute are represented by x and x', respectively. The standard range is [0,1].

The **z-score normalization** can be computed using the following equation:

$$z = \frac{x - \mu_A}{\sigma_A} \tag{3.3}$$

In the equation 3.3, μ_A and σ_A are the mean and the standard deviation of the feature A. The original and the normalized feature are represented by x and z, respectively. After normalization, the mean and the standard deviation of all the features values become 0 and 1, respectively.

3.2.4 Feature Selection

According to Janecek *et al.* (2008), high dimensionality data is problematic for classification algorithms due to high computational cost and memory usage. So, it is essential to check if all features in the dataset are indeed necessary. In addition, Ladha and Deepa (2011) say that the main benefits from feature selection techniques reduce the dimensionality space, remove redundant, irrelevant, or noisy data and performance improvement to gain in predictive accuracy.

Table 2 – Taxonomy of some Feature Selection Algorithms.

Model Search		**Techniques**
Filter	**Univariate**	Chi-square, One-R, Information Gain
	Multivariate	Correlation-based Feature (CFS), Markov Blanket Filter (MBF)
Wrapper	**Deterministic**	Sequential Forward Selection (SFS), Sequential Backward Elimination (SBE)
	Randomized	Simulated Annealing, Genetic Algorithms
Embedded		Feature Selection using the weights vectors of SVM, Decision Trees

Source: the author.

Table 2 shows the feature selection methods in three categories: filters, wrappers, and embedded/hybrid method. The following definitions have been presented by Veerabhadrappa and Rangarajan (2010): Wrapper methods are brute-force feature selection, which exhaustively evaluates all possible combinations of the input features and then find the best subset. Filter methods have low computational cost but inefficient reliability in classification compared to wrapper methods. Hybrid/ embedded methods are developed to utilize the advantages of both filters and wrappers approaches. This strategy uses both an independent test and performance evaluation function of the feature subset.

3.2.5 Resample Techniques for Imbalanced Data

Machine Learning techniques require an efficient training dataset, which has an amount instances of the classes; however, as observed by Prati *et al.* (2009), in real-world problems, some datasets can be imbalanced, i.e., a majority class containing most samples meanwhile the other class contains few samples, this one generally of our interest. Using imbalanced datasets to train models leads to higher misclassifications for the minority class. It occurs because there is a lack of information about it.

The class imbalance problem has been encountered in multiple areas such as telecommunication management, bioinformatics, fraud detection, and medical diagnosis. Yang and Wu (2006) have considered the imbalance problem as one of the top 10 problems in data mining and pattern recognition.

In order to compute the balancing ratio (r_χ), we can use:

$$r_\chi = \frac{|\chi_{min}|}{|\chi_{maj}|} \tag{3.4}$$

where χ is the dataset, $|\cdot|$ denotes the cardinality of a set with χ_{min} and χ_{maj} being the subset of samples belonging to the minority and majority class, respectively.

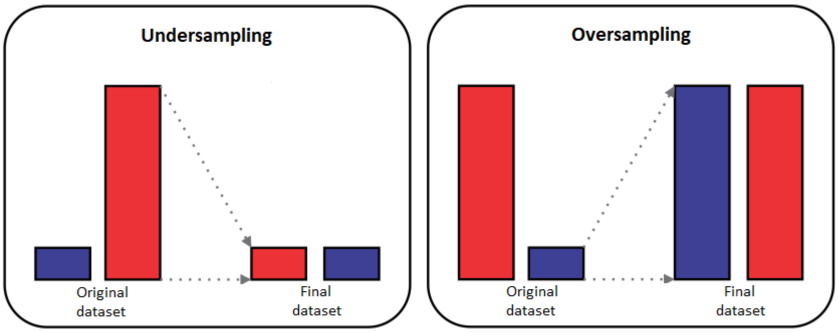
The state-of-the-art methods which deal with imbalanced data for classification problems can be categorized into four groups:

Undersampling (US): it refers to the process of reducing the number of samples in χ_{maj}. Three US known techniques are: Random Under-Sampler (RUS) proposed by Batista *et al.* (2004), which consists in randomly choose an instance from the majority class and remove it; Tomek's Link, proposed by Tomek (1976), which consists in finding two instance, one from the majority class and the other from the minority class, that are the nearest neighbour of each other and then remove one of the instances; Edited Nearest Neighbours, proposed by Wilson (1972), which consists in remove the nearest instances that do not belong to the class of the instance.

Oversampling (OS): It consists of generating synthetic data in χ_{min} in order to balance the proportion of data. Three OS known techniques are: Random Over-Sampler (ROS), proposed by Batista *et al.* (2004), which consists in randomly choose an instance from the minority class and repeat it; Synthetic Minority Oversampling Technique (SMOTE), proposed by Chawla *et al.* (2002), which consists in generates new synthetic instances obtained by combining the features of an instance and its k-nearest neighbours; Adaptive Synthetic (ADASYN), proposed by He *et al.* (2008), which consists in creating synthetic instances of the minority class considering the difficult to classify this instance with a KNN algorithm, then it will focus on the harder instances.

The basic idea of the techniques aforementioned can be viewed in Figure 8.

Figure 8 – Undersampling and Oversampling Techniques.



Source: Author.

Combination of over and undersampling: According to Prati *et al.* (2009), over-sampling can lead to overfitting, which can be avoided by applying cleaning undersampling methods.

Ensemble learning methods: Undersampling methods imply that samples of the majority class are lost during the balancing procedure. Ensemble methods offer an alternative to use most of the samples. In fact, an ensemble of balanced sets is created and used to train any classifier later.

For imbalanced multiple class classification problems, the authors Fernández *et al.* (2013) have done an experimental analysis to determine the behavior of the different approaches proposed in the specialized literature. Vluymans *et al.* (2017) also have proposed an extension to multi-class data using one-vs-one decomposition.

It is essential to mention that it is necessary to separate the imbalanced dataset into two subsets: training and test sets. After that, any of the techniques aforementioned should only be applied in the training set because the predictive model cannot be trained with synthetic instances.

3.2.6 Generating Models

When all the previous steps have been performed, it is time to generate predictive models. In this case, a range of *libraries* and API software have been developed to support this step. *Scikit-learn* is a free software machine learning library for the Python programming language, proposed by Pedregosa *et al.* (2011), commonly used in academic research. In addition, TensorFlow is a free and open-source software library for dataflow and differentiable programming across a range of tasks. It is a symbolic math library and is also used for machine learning applications such as neural networks. For API, we recommend WEKA, Waikato Environment for Knowledge Analysis, presented by Witten *et al.* (1999). It is free software licensed under the GNU General Public License.

3.2.7 Cross-Validation

Training an algorithm and evaluating its statistical performance on the same data yields an overoptimistic result. Cross-Validation (CV) was raised to fix this issue, starting from the remark that testing the output of the algorithm on new data would yield a reasonable estimate of its performance. In most real applications, only a limited amount of data is available, which leads to the idea of splitting the data: Part of data (the training sample) is used for training the algorithm, and the remaining data (the validation sample) are used for evaluating the performance of the algorithm. The validation sample can play the role of "new data". As observed by Arlot and Celisse (2010), a single data split yields a validation estimate of the risk and averaging over several splits yields a cross-validation estimate. The significant interest of CV lies in the universality of the data splitting heuristics.

A technique widely used to generalize the model in classification problems is ***k*-Fold Cross Validation**. This approach divides the set in k subsets, or *folds*, of approximately equal size. One fold is treated as test set meanwhile the others $k-1$ folds work as training set. This process occurs k times. According to James *et al.* (2013), a suitable k value is $k = 5$ or $k = 10$.

3.2.8 Tuning the Predictive Model

All the steps presented in this paper so far have served to show good practicals on how to obtain baseline according to a Machine Learning algorithm selected. Tuning it consists of finding the best possible configuration of this algorithm at hand, wherewith best configuration.

It means the one that is deemed to yield the best results on the instances that the algorithm will be eventually faced. Tuning machine learning algorithms consist of finding the best set of hyperparameters, which yields the best results.

Hyperparameters are tuned by hand at *trial-and-error* procedure guided by some rules of thumb. However, some papers analyze a set of hyperparameters for specifics algorithms in machine learning for tuning them. For Support Vector Machine algorithm using RBF kernel, Hsu *et al.* (2016) recommend a grid-search setting $C = \{2^{-5}, 2^{-3}, ..., 2^{15}\}$ and $\gamma = \{2^{-15}, 2^{-13}, ..., 2^{3}\}$. After defining a grid-search in a specific region, a **nested cross validation** must be used to estimate the generalization error of the underlying model and its hyperparameter search. Thus, Cawley and Talbot (2010) highlight that it makes sense to take advantage of this structure and fit the model iteratively using a pair of nested loops, with the hyperparameters adjusted to optimize a model selection criterion in the outer loop (model selection) and the parameters set to optimize a training criterion in the inner loop (model fitting/training).

3.2.9 Selection of Performance Metrics

To evaluate the Machine Learning model for the classification problem is necessary to select the appropriate performance metrics according to two possible scenarios: for a balanced or imbalanced dataset.

A **confusion matrix** gives an overview of output that was sorted correctly and incorrectly, classifying them as True Positive (TP), True Negative (TN), False Positive (FP), or False Negative (FN).

The following metrics are widely used to validate performance results:

$$accuracy = \frac{TP + TN}{TP + TN + FP + FN} \tag{3.5}$$

$$precision = \frac{TP}{TP + FP} \tag{3.6}$$

$$recall\ or\ sensitivity = \frac{TP}{TP + FN} \tag{3.7}$$

$$specificity = \frac{TN}{TN + FP} \tag{3.8}$$

In the case of balanced datasets, such metrics (accuracy, precision, recall, and specificity) can be used without more concerns. However, in the case of imbalanced data, these metrics are not suitable, since they can lead to dubious results. For example, Akosa (2017) has observed that the accuracy metric is not suitable because it tends to give a high score due to a correct prediction of the majority class.

The **Receiver Operating Characteristic** (ROC) curve is a graphical plot that illustrates the diagnostic ability of a binary classifier system as its discrimination threshold is varied. It is a comparison of two operating characteristics: True Positive Rate (Equation 3.7) and False Positive Rate (Equation 3.8) as the criterion changes. The **Area Under the ROC Curve** (AUC) measures the entire two-dimensional area underneath the entire ROC curve from (0,0) to (1,1).

F-score (Equation 3.9), also known as *F-measure*, is the harmonic average of the *precision* (Equation 3.6) and *recall* (Equation 3.7) and its domain is [0,1]. F-score is also known as F_1-score when β value is 1.

$$F_\beta = (1+\beta) \cdot \frac{precision \cdot recall}{\beta^2 \cdot precision + recall} \tag{3.9}$$

It is essential to highlight that in the case of imbalanced data, the more suitable metrics are AUC and **F-score**. These performance metrics are suitable for imbalanced data because they take the minority classes correctly classified into account, unlike the accuracy.

3.2.10 Ensure the Reproducibility

The last step consists in to ensure the experiments reproducibility in order to verify the credibility of the proposed study. Olorisade *et al.* (2017) have evaluated 30 studies in order to highlight the difficulty of reproducing most of the works in state-of-art. While the studies provide useful reports of their results, they lack information on access to the dataset in the form and order as used in the original study, the software environment used, randomization control, and the implementation of proposed techniques.

Some authors have proposed basic rules for reproducible computational research, as Sandve *et al.* (2013) which list ten rules:

1. *For every result, keep track of how it was produced.* Whenever a result may be of potential interest, keep track of how it was produced. When doing this, one will frequently find that getting from raw data to the final result involves many interrelated steps (single commands, scripts, programs).

2. *Avoid manual data manipulation steps*. Whenever possible, rely on the execution of programs instead of manual procedures to modify data. Such manual procedures are not only inefficient and error-prone, they are also difficult to reproduce.
3. *Keep in a note the exact version of all external programs used*. In order to exactly reproduce a given result, it may be necessary to use programs in the exact versions used originally. Also, as both input and output formats may change between versions, a newer version of a program may not even run without modifying its inputs. Even having noted which version was used of a given program, it is not always trivial to get hold of a program in anything but the current version. Archiving the exact versions of programs actually used may thus save a lot of hassle at later stages.
4. *Version control all custom scripts*. Even the slightest change to a computer program can have large intended or unintended consequences. When a continually developed piece of code (typically a small script) has been used to generate a certain result, only that exact state of the script may be able to produce that exact output, even given the same input data and parameters.
5. *Record all intermediate results, when possible in standardized formats*. In principle, as long as the full process used to produce a given result is tracked, all intermediate data can also be regenerated. In practice, having easily accessible intermediate results may be of great value. Quickly browsing through intermediate results can reveal discrepancies toward what is assumed, and can in this way uncover bugs or faulty interpretations that are not apparent in the final results.
6. *For Analysis that includes randomness, note underlying random seed*. Many analyses and predictions include some element of randomness, meaning the same program will typically give slightly different results every time it is executed (even when receiving identical inputs and parameters). However, given the same initial seed, all random numbers used in an analysis will be equal, thus giving identical results every time it is run.
7. *Always store raw data behind plots*. From the time a figure is first generated to it being part of a published article, it is often modified several times. In some cases, such modifications are merely visual adjustments to improve readability, or to ensure visual consistency between figures. If raw data behind figures are stored in a systematic manner, so as to allow raw data for a given figure to be easily retrieved, one can simply modify the plotting procedure, instead of having to redo the whole analysis.

8. *Generate hierarchical analysis output, allowing layers of increasing detail to be inspected*. The final results that make it to an article, be it plots or tables, often represent highly summarized data. For instance, each value along a curve may in turn represent averages from an underlying distribution. In order to validate and fully understand the main result, it is often useful to inspect the detailed values underlying the summaries. A common but impractical way of doing this is to incorporate various debug outputs in the source code of scripts and programs.
9. *Connect textual statement to the underlying result*. Throughout a typical research project, a range of different analyses are tried and interpretation of the results made. Although the results of analyses and their corresponding textual interpretations are clearly interconnected at the conceptual level, they tend to live quite separate lives in their representations: results usually live on a data area on a server or personal computer, while interpretations live in text documents in the form of personal notes or emails to collaborators.
10. *Provide public access to scripts, runs, and results*. Last, but not least, all input data, scripts, versions, parameters, and intermediate results should be made publicly and easily accessible.

These rules are not the *definitive guide* of reproducibility. In some cases, such Machine Learning for Health Care requires some particular attention in extra details, since there are more resources to retrieve information, as an example, ECG signals and its preprocessor to deal with this kind of data, as observed by McDermott *et al.* (2019).

4 CASE STUDY I: USING THE STATIC APPROACH

In order to evaluate the proposed guideline in Chapter 3, we have performed an exploratory case study using 10 Machine Learning algorithms in a change-prone class dataset called **Co**ntrol of Mer**c**h**a**ndise (Coca). This dataset has been extracted from extensive commercial software, containing the values of 8 static OO metrics. In this chapter, we are going to focus it on the dataset, which follows the static approach presented in phase 1 of the guideline, defined in subsection 3.1.4.1.

4.1 Phase 1: Designing the Dataset with Static Approach

This section will describe all the necessary steps to generate the dataset following the static approach in order to apply it in the proposed guideline.

4.1.1 Independent Variables

In order to build the datasets, we have used OO metrics proposed by Chidamber and Kemerer (1994), also known as C&K metrics, Cyclomatic Complexity proposed by McCabe (1976), and Lines of Code. The definition of each chosen metric follows:

- **Class Between Object (CBO)**: It is a count of the number of non-inheritance related couples with other classes. Excessive coupling between objects outside of the inheritance hierarchy is detrimental to modular design and prevents reuse. The more independent an object is, the easier it is to reuse it in another application;
- **Cyclomatic Complexity (CC)**: It has been used to indicate the complexity of a program. It is a quantitative measure of the number of linearly independent paths through a program's source code;
- **Depth of Inheritance Tree (DIT)**: It is the length of the longest path from a given class to the root class in the inheritance hierarchy. The deeper a class is in the hierarchy, the higher the number of methods it is likely to inherit making it more complex;
- **Lack of Cohesion in Methods (LCOM)**: It is the methods of the class are cohesive if they use the same attributes within that class, where 0 is strongly cohesive, and 1 is lacking cohesive. The cohesiveness of methods within a class is desirable since it promotes encapsulation of object, meanwhile, lack of cohesion implies classes should probably be split into two or more sub-classes;

- **Line of Code (LOC)**: It is the number of line of code, except blank lines, imports or comments;
- **Number of Child (NOC)**: It is the number of immediate sub-classes subordinated to a class in the class hierarchy. It gives an idea of the potential influence a class has on the design. If a class has a large number of children, it may require more testing of the methods in that class;
- **Response for a Class (RFC)**: It is the number of methods that an object of a given class can execute in response to a received message; if a large number of methods can be invoked in response to a message, the testing and debugging of the object becomes more complicated;
- **Weighted Methods per Class (WMC)**: The number of methods implemented in a given class where each one can have different weights. In this dataset, each method has the same weight (value equal to one), except *getters*, *setters* and constructors, which have weight equal to zero. This variable points that a larger number of methods in an object implies in the greater the potential impact on children since they will inherit all the methods defined in the object.

4.1.2 Dependent Variable

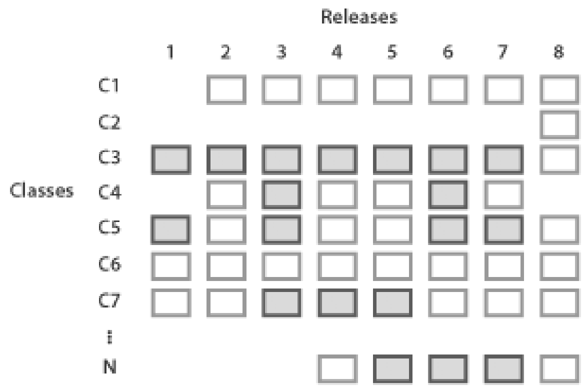
In this work, the binary label was adopted as the dependent variable in order to investigate its relationship with the independent variables presented in the previous subsection, following the definition proposed by Lu *et al.* (2012). The authors define that a class will be labeled as 1 if in the next release occurs alteration in the LOC independent variable, and 0 otherwise.

4.1.3 Collect Metrics

The dataset of this section called **Co**ntrol of Mer**cha**ndise (Coca) has been generated from the back-end source code of a WEB application started in 2013, and until 2018 were collected 8 releases to analyze change-prone classes. This application has involved the development of modules that manages the needs of multinationals related to different processes, such as return control of merchandise and product quality.

As an example, Figure 9 shows the system evolution; *n* represents the number of classes for each release (which increases over the years). Each box represents a class. The

Figure 9 – Evolution of Classes through Releases.



Source: Author.

boxes in the same row represent the same class at different releases, while the absence of a box indicates the opposite. Shaded boxes indicate that the class has changed from the previous release. A change is characterized by altering one of the attributes. The back-end system has been implemented in C#; all its features were collected through the Visual Studio NDepends. *Ndepends* is a static analysis tool for .NET managed code. Also, the tool has a feature called CQLinq, which allows the user to get features, accurate metrics, and estimate technical debts. The following code shows an example of a query that retrieves WMC metric:

```
//WMC Weighted Methods per Class


warnif count > 0
from t in Application.Types
let methods = t.Methods
    .Where(m => !m.IsPropertyGetter &&
                !m.IsPropertyGetter &&
                !m.IsConstructor)
where methods.Count() >= 0
orderby methods.Count() descending
select new { t, methods }
```

For further technical details of how the other metrics were obtained, the Ndepends documentation details how queries were used.

4.1.4 *Defining the Input Data Structure*

In this chapter, we are going to investigate the gain of the proposed guideline in order to retrieve a better performance for the dataset, which follows the static approach described in subsection 3.1.4.1, i.e., each independent variable will not contain any temporal dependency from each other.

4.2 Phase 2: Applying Change-Proneness Prediction using Static Approach

4.2.1 *Statistical Analysis*

As the first step of this phase, we performed a general statistic analysis of the Coca dataset. Table 3 shows the descriptive statistics of this dataset, including minimum, maximum, mean, median (med), and standard deviation (SD) values for each feature (metric).

Table 3 – Descriptive Statistics.

Metric	Min	Max	Mean	Med	SD
LOC	0	1369	36.814	12	91.211
CBO	0	162	7.107	3	12.305
DIT	0	7	0.785	0	1.764
LCOM	0	1	0.179	0	0.289
NOC	0	189	0.612	0	6.545
RFC	0	413	9.966	1	25.694
WMC	0	56	1.558	0	4.244
CC	0	488.0	15.918	8	30.343

Source: The author.

Also, we generate the Spearman's correlation presented in Table 4. We want to highlight the correlation between CBO and RFC, scoring 0.89, the highest correlation. This information will be used in the Feature Selection step.

4.2.2 *Outlier Filtering*

The next step was to investigate the existence of outliers in the Coca dataset. In order to do this, we used the IQR method for each feature. However, since the proposed dataset contains 8 features, we used a multivariate strategy to remove outliers, which is described as follows. If an instance contains at least 4 features with outliers, it will be dropped. Table 5 shows the number of instances with labels 0 and 1, before and after outliers removal. According

Table 4 – Spearman's Correlation of the Independent Variables

	CBO	**CC**	**DIT**	**LCOM**	**LOC**	**NOC**	**RFC**	**WMC**
CBO	1	0.67	0.48	0.19	0.62	-0.02	**0.89**	0.53
CC	0.67	1	0.24	0.25	0.75	0.04	0.73	0.69
DIT	0.48	0.24	1	0.15	0.29	0.04	0.35	0.24
LCOM	0.19	0.25	0.15	1	0.21	0	0.22	0.28
LOC	0.62	0.75	0.29	0.21	1	0.04	0.69	0.62
NOC	-0.02	0.04	0.04	0	0.04	1	-0.02	0.12
RFC	**0.89**	0.73	0.35	0.22	0.69	-0.02	1	0.6
WMC	0.53	0.69	0.24	0.28	0.62	0.12	0.6	1

to this table, 259 instances were removed from the original dataset. Another observation is the imbalanced dataset, containing 3637 instances with label 0 and 287 instances with label 1. According to Equation 3.4, the imbalanced ratio after outlier removal is 7,89%.

Table 5 – Overview of the Dataset Before and After Outliers Removal.

	0	**1**	**Total**
Before outliers removal	3871	312	4183
After outliers removal	3637	287	3924

Source: The author.

4.2.3 Normalization

Since there are features with different scale, the dataset was normalized using min-max normalization (Equation 3.2) into [0,1] range. For example, LCOM and LOC have different ranges: [0,1] and [0,1369], respectively. Moreover, the use of min-max normalization with range into [0,1] in all features does not affect the original values of LCOM.

4.2.4 Feature Selection

The Coca dataset has 8 features. So, not all features may be necessary or even useful to generate good predictive models. Therefore, it is necessary to investigate some feature selection methods. Thus, in this step, it has explored four (three univariate and one multivariate) feature selection methods and compared their results in order to choose the best set of features. More precisely, we have used Chi-square (CS), One-R (OR) proposed by Holte (1993), Information Gain (IG), and Symmetrical Uncertainty (SU) proposed by Kannan and Ramaraj (2010).

Table 6 shows the results obtained of each feature selection techniques for each

Table 6 – Feature Selection Results.

	CS	IG	OR	SU	∑
CBO	8	7	7	6	28
RFC	7	6	6	5	24
WMC	6	5	6	4	21
CC	4	4	5	3	16
LCOM	3	4	3	3	14
LOC	5	3	4	2	13
DIT	2	2	2	2	8
NOC	1	1	1	1	4

Source: The author.

metric, i.e., the relevance of the metric in a specific method. Another criteria to determine the number of features to keep is: getting the value of the highest sum and establish a threshold of half of its value. 5 features contain their sum into [28,14]. However, according to Pearson's correlation CBO and RFC have value 0.89, i.e., they are strongly correlated. Since RFC has a sum less than CBO, RFC is dropped. Therefore, the features selected were CBO, WMC, CC, and LCOM.

4.2.5 Resample Techniques

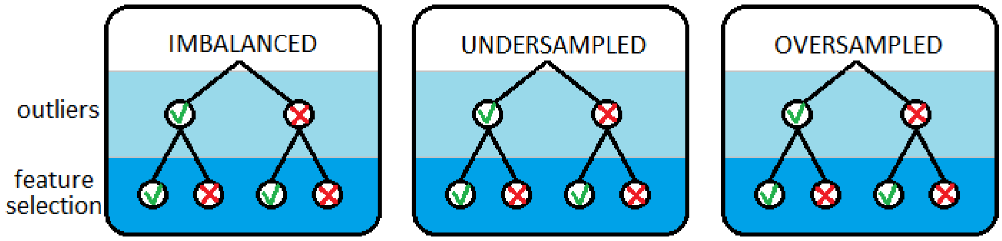
However, since the Coca dataset is imbalanced, we also run all the previous experiments using three undersample and three oversample techniques: Random Under-Sampler, Tomek's Link, Edited Nearest Neighbours, Random Over-Sampler, SMOTE and ADASYN, respectively.

4.2.6 Generate Models and Cross-Validation

In order to generate models, 10 classification algorithms have been used to run the experiments, with the default values for its hyperparameters, implemented in Python using *Scikit-Learn's libraries*. The 10 classifiers explored in this step were: Logistic Regression, LightGBM, XGBoost, Decision Tree, Random Forest, KNN, Adaboost, Gradient Boost, SVM with Linear Kernel, and SVM with RBF kernel. Each classifier was performed in four different scenarios: with and without outliers and with and without feature selection. Methods like XgBoost and LightGBM have used random state = 42, and the KNN method has set the number of neighbors as 5. Then, *k*-fold cross-validation was used, with k = 10, and the scoring function has been set to "roc_auc" instead of accuracy (default of Scikit-Learn).

Figure 10 shows the summarize of all experimental scenarios that we have tested. We perform outlier filtering and feature selection in the imbalanced, undersampled, and oversampled scenarios. In the end, we have 12 results.

Figure 10 – Execution Tree of all Experimental Scenarios.

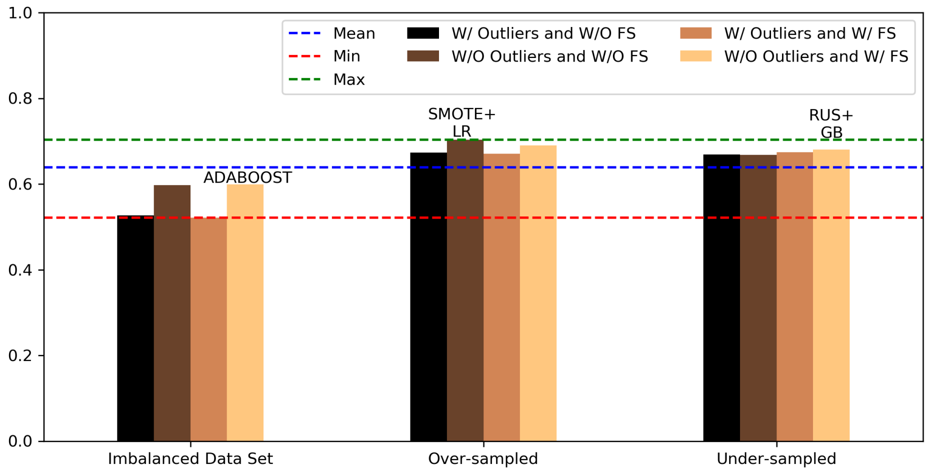


Source: Author.

4.2.7 Selecting Performance Metrics

Since Coca dataset is imbalanced, we have used the Area Under the Curve (AUC) to measure our performance and analyze our results. Figure 11 shows the results of these experiments in different scenarios, such as with (W/) or without (W/O) outliers, and with or without feature selection. The x-axis shows the AUC metric and y-axis the different scenarios. The best evaluation founded was using the oversampled technique: SMOTE + Logistic Regression, without outliers, and no feature selection, with AUC 0.703 and SD ±0.056.

Figure 11 – Performance Evaluation in Different Baselines Scenarios.



Source: Author.

4.2.8 Tuning the Prediction Model

This step aims to explore a region of hyperparameters in order to improve the results. The grid search function was used for performing hyperparameters optimization. The nested cross-validation, i.e., the outer cross-validation used to generalize the model and the inner cross-validation used to validate the hyperparameters during the training phase, have been set k = 10 for both of them.

In general, the AUC obtained by tuning the models outperforms the AUC obtained from baseline experiments. Besides, the best result from this tuning outperforms even the best AUC from any of the scenarios baselines. It occurs using Random Under Sampler + SVM Linear got an AUC 0,710. For this result, the grid search was set as C: [0.002, 1, 512, 1024, 2048] and Class Weight: [1:1, 1:10, 1:15, 1:20].

However, it is always important to warn that tuning is not a silver bullet. For instance, we performed the tuning over the model with the best result from baseline experiments and achieved a worse model where AUC has decreased from 0.703 to 0.699.

4.2.9 Ensure the Reproducibility

The results of all experiments run in this first exploratory case study are available in public Github repository[1]. This repository consists of two main folders: a dataset and a case study. The former contains all the raw data used to perform the experiments, while the latter contains all executed scripts in Jupyter Notebook.

4.3 Discussion of Results

One of the goals of this first study case is experimentally to evaluate how a set of steps proposed in our guideline tends to improve the Area Under the Curve (AUC) of a dataset which follows the static approach, i.e., a structure that has no dependence between the instances of the dataset.

Our experimental results have shown that some steps can harshly improve the AUC, as an example, the resampling technique, since imbalanced dataset presents AUC around 50% while a resampled dataset presents 70%. Only feature selection did not improve the AUC. It may have occurred since we have only 8 independent variables in the dataset.

[1] <https://github.com/cristmelo/PracticalGuide.git>

Besides, we highlight the importance of tuning, since in some cases, it can improve the results. However, it can decrease it too. Tuning is a process that is necessary to try a range of hyperparameters and valuated them using, as an example, nested cross-validation, and it implies it will be necessary more time to execute them. In the Coca dataset, we have had a scenario that we improved from 70% to 71% of AUC.

4.4 Threats to Validity

In this chapter, we have present a guideline to support the change-prone class prediction problem in the static approach. This approach is the state-of-art of this field of study since there are no datasets in the literature that deal with time-series. So, following the guideline, we have made an exploratory case in different scenarios in order to explore higher performance metrics. In the end, we have seen that imbalanced scenario tends to have the worst result, and tuning the baselines can improve some results. After that, we share all this information in Jupyter Notebook scripts to ensure the reproducibility of the experiments. However, we identify some threats to validity in this experimental analysis:

1. *Outlier Filtering*. Although removing outlier have presented good results, there are a lot of algorithms and strategies to identify outliers in the dataset. However, we have used only one strategy, the IQR. So probably this result can be better even more, or in some cases, there may be no improvements.
2. *Feature Selection*. We did not have good results in removing some features. It probably happened because we have a little amount of the independent variables, so removing them can not be useful.

5 CASE STUDY II: USING THE DYNAMIC APPROACHES

This second case study refers to the datasets which follow the dynamic approaches, published in Melo *et al.* (2020), and mentioned in subsection 3.1.4.2. In this evaluation performance, we have used three Apache dataset: Ant, Beam, and Cassandra. Then, we have generated them into the static approach in order to collect their baselines to compare with dynamic approaches baselines. We also generate dynamic approaches to the Coca dataset.

For dynamic approaches, we have generated the two proposed structures presented in subsection 3.1.4.2: Concatenated and Recurrent. In the former, we have not executed feature selection since in the previous chapter, it did not improve the results. In the latter, we did not perform feature selection, outlier filtering, nor resample technique. These steps in the Recurrent approach will be discussed in Future Works. In the end of this chapter, we are going to discuss these comparative performances in Discussion section to highlight the advantages and limitations of dynamic approaches.

5.1 Generating Baseline in Apache Dataset using Static Approach

5.1.1 Phase 1: Designing the Dataset with Static Approach

To evaluate the proposed dynamic approaches proposed in this work, we have chosen four software projects. The first one was mentioned in the previous chapter, the Coca dataset, and we used their results presented in Chapter 4 to compare their performance against dynamic structures. The remaining datasets were built from three JAVA open-source projects: Apache Ant, Apache Beam, and Apache Cassandra, respectively. Each one of these datasets was modeled following both approaches: static and dynamic (both Concatenated and Recurrent structures) in order to compare their performances. An overview of these Apache software projects can be seen in Table 7. It shows (i) the project names, (ii) the period in which these projects were developed, (iii) the average percentage of change-prone classes, (iv) the number of releases, and (v) the number of object-oriented classes present in the first and in last releases. The ratio of the imbalanced dataset is calculated by the cardinality of minority class over the majority class. In this problem, the minority class tends to be that we want to predict. According to Table 7, Apache Ant is the only balanced dataset, while the other datasets are imbalanced.

Table 7 – Characteristics of the Apache Software Projects Used to Generate the Datasets.

Software Project	Period	Imb. Rate	Releases	Classes
Apache Ant	Jan 2016 - May 2019	70.1%	10	1020-19611
Apache Beam	Oct 2017 - Jun 2019	22.4%	15	36595-73923
Apache Cassandra	Mar 2010 - Feb 2019	30.3%	49	4244-30308

5.1.2 Phase 2: Applying Change-Proneness Prediction using Static Approach

In this section, we will summarize the decisions taken to generate predictive models in the static approach and collect their baseline results.

5.1.2.1 Overview of Baseline

Tables 8, 9, and 10 show the descriptive statistics of the Apache Ant, Apache Beam, and Apache Cassandra datasets, respectively. All these tables show the minimum, maximum, mean, median, and standard deviation for each chosen independent variable.

Table 8 – Descriptive Statistics for Apache Ant.

Metric	Min	Max	Mean	Med	SD
LOC	0	1586	79.39	37	127.17
CBO	0	40	3.21	2	4.26
DIT	0	7	2.16	2	1.14
LCOM	0	100	32.55	19	35.27
NOC	0	166	0.52	0	4.99
RFC	0	210	23.46	12	27.67
WMC	0	125	7.79	4	10.07
CC	0	99	36.22	33	29.73

Table 9 – Descriptive Statistics for Apache Beam.

Metric	Min	Max	Mean	Med	SD
LOC	0	2749	57.74	22	117.08
CBO	0	106	5.33	5.33	7.23
DIT	0	6	1.62	1	0.75
LCOM	0	100	17.53	0	28.56
NOC	0	901	0.44	0	11.27
RFC	0	100	8.67	6	8.96
WMC	0	100	4.28	2	5.61
CC	0	179	5.89	3	9.42

In order to generate predictive models using the static approach in selected datasets, we have set the following steps to phase 2 in the guideline:

1. **Outlier Filtering:** IQR.

Table 10 – Descriptive Statistics for Apache Cassandra.

Metric	Min	Max	Mean	Med	SD
LOC	0	45517	103.10	32	754.57
CBO	0	145	5.74	3	8.65
DIT	0	6	1.65	2	0.74
LCOM	0	100	20.57	0	30.62
NOC	0	116	0.27	0	2.30
RFC	0	294	10.98	4	17.91
WMC	0	294	6.51	3	12.08
CC	0	843	13.78	5	31.16

2. **Normalization:** Min-Max Normalization.
3. **Resample Techniques:** Undersampling: RUS, ENN, and TL. Oversampling: ROS, SMOTE, and ADASYN.
4. **Cross-validation:** k-fold, k = 5 or k = 10.
5. **Performance Metrics:** AUC and F1-Score.

5.1.2.2 Baseline Results

Table 11 shows the best results found for each dataset using the static approach. So, Table 11 illustrates the (i) resample technique used, (ii) the algorithm performed, (iii) if outlier removal (OR) was used, (iv) the spent time for the execution, and (v) the values of performance metrics. Note that, for each dataset was necessary to run some resample technique since an imbalanced dataset tends to provides the worst results. Besides, another interesting result was that no dataset presented the best result using outlier removal. In addition, we register into this table, on the first row, the best result of the static approach in the Coca dataset, according to Figure 11.

Table 11 – Best Results for each Dataset Using the Static Approach.

Dataset	Sample	Alg.	OR	Time	Performance Metrics				
					Acc	Spec	Sens	F1	AUC
Coca	SMO	LR	Y	-	-	-	-	-	0.703
Ant	ROS	MLP	N	37.7 s	0.6725	0.6636	0.6886	0.6789	0.6761
Beam	ROS	RF	N	45.4 s	0.7229	0.7599	0.5370	0.7493	0.6484
Cassandra	SMO	MLP	N	37min	0.7214	0.7096	0.7767	0.7525	0.7432

5.2 Generating Baseline in Apache Dataset using Dynamic Approaches

5.2.1 Phase 1: Designing the Dataset with Dynamic Approaches

This section will discuss all necessary processes to build the dataset using the dynamic approaches in concatenated and recurrent structures for all software projects previously mentioned. Then, all baselines for these generated dynamic structures will be necessary to compare them to the results of the static approach presented in Table 11.

5.2.1.1 Defining the Input Data Structure

In this subsection, we are going to detail the process performed to obtain our best results in the Concatenated and Recurrent approaches.

For the concatenated approach, we have evaluated three different values for the window size: 2, 3, and 4. Thus, for each previously selected dataset, we have generated three distinct versions, according to the window size. In this scenario, we have followed the proposed guideline. However, we neither perform the outlier filtering nor the feature selection steps. We have decided to keep the outliers and independent variables since this structure aims to learn through their history.

For the recurrent approach, we have evaluated three different values for the window size: 2, 3, and 4. Thus, for each previously selected dataset, we have generated three distinct versions, according to the window size. However, unlike the concatenated approach, we did not use our proposed guideline. We have just built the data structure into a Tensor using Keras and uses it with the Gated Recurrent Unit (GRU) algorithm. So, we have used imbalanced datasets.

The GRU structure used in recurrent approach is presented in Algorithm 1.

Algoritmo 1: GRU Layers

```
Result: model
model = Sequential()
model.add(GRU(256, input_shape=input_shape, return_sequences=True))
model.add(Dropout(0.3))
model.add(GRU(128, return_sequences=True))
model.add(Dropout(0.3))
model.add(GRU(64))
model.add(Dropout(0.3))
model.add(Dense(output_dim, activation='softmax'))
model.summary()
```

In this approach, we have used three layers of GRU, from 256 entry to 1, and its activation function is *softmax*. We also added three Dropout layers (set as 0.3) in order to avoid overfitting. The number of epochs was set by 20, the number of batches was set by 512, and the number of *k*, in stratified *k*-fold, was set by 5.

5.2.2 Phase 2: Applying Change-Proneness Prediction using Dynamic Approaches

After defining the window sizes and generating models, we execute for concatenated structure the following algorithms in this step: Logistic Regression, Decision Tree, Random Forest, and MLP. We discard some algorithms used in the first case study, such as XgBoost or SVM, because they hardly ever presented a good result. Besides, our tree execution was extensive, since we have a dataset for each window size to evaluate.

Table 12 shows the best results found for each dataset using the Concatenated Approach. It is important to note that for the Coca dataset, the window size 4 was not used due to the small number of C# classes present in 4 or more releases.

Table 13 depicts the best predictive model found for each dataset and each window size using the Recurrent Approach (RA). We want to remember that outlier filtering, feature selection or resample techniques were not performed here.

Table 12 – Best Results for Different Window Size (WS) Using the Concatenated Approach.

Dataset	**Sample**	**Alg.**	**WS**	**Time**	**Performance Metrics**				
					Acc	**Spec**	**Sens**	**F1**	**AUC**
Coca	ADA	LR	2	0.27 s	0.7562	0.7593	0.6914	0.8256	0.7254
	SMO	LR	3	0.20 s	0.7807	0.7846	0.7066	0.8404	**0.7456**
	-	-	4	-	-	-	-	-	-
Ant	ROS	MLP	2	45.8 s	0.8092	0.8160	0.8007	0.8094	**0.8083**
	ROS	MLP	3	14.8 s	0.7985	0.8000	0.7967	0.7989	0.7983
	-	MLP	4	8.84 s	0.7899	0.7537	0.8269	0.7897	0.7903
Beam	ROS	MLP	2	39.0 s	0.7112	0.7584	0.5260	0.7296	0.6422
	ROS	DT	3	4.61 s	0.7522	0.8237	0.4872	0.7579	**0.6554**
	ADA	MLP	4	9.5min	0.6841	0.7230	0.5505	0.7034	0.6368
Cassandra	ROS	RF	2	33.0 s	0.9106	0.9323	0.8157	0.9124	**0.8740**
	ROS	RF	3	1min	0.9060	0.9347	0.7806	0.9071	0.8576
	SMO	RF	4	2min	0.8858	0.8970	0.8377	0.8909	0.8673

Table 13 – Best Results for Different Window Size (WS) Using the Recurrent Approach.

Dataset	**WS**	**Performance Metrics**					**Time**
		Acc	**Spec**	**Sens**	**F1**	**AUC**	
Coca	2	0.7737	0.7942	0.7390	0.7656	**0.7737**	29.54 s
	3	0.7318	0.6874	0.8503	0.7602	0.7318	38.33 s
	4	-	-	-	-	-	-
Ant	2	0.7753	0.7580	0.8090	0.7827	**0.7753**	28.81 s
	3	0.7586	0.7558	0.7640	0.7599	0.7586	35.42 s
	4	0.7371	0.7374	0.7363	0.7369	0.7371	39.78 s
Beam	2	0.6714	0.6430	0.7706	0.7011	0.6714	3min56s
	3	0.7003	0.6514	0.8617	0.7419	**0.7003**	4min48s
	4	0.6549	0.6670	0.6186	0.6419	0.6549	5min
Cassandra	2	0.8687	0.8848	0.8478	0.8659	0.8687	5min15s
	3	0.9188	0.9287	0.9073	0.9179	**0.9188**	6min8s
	4	0.9152	0.9308	0.8972	0.9137	0.9152	8min4s

5.2.2.1 Ensure the Reproducibility

The results of all experiments run in this second exploratory case study are available in public Github repository[1]. This repository consists of folders containing their static and dynamic approaches applied in their datasets, executed in Jupyter Notebook. Besides, there is a folder called DownloadApacheRepositories, which downloads all raw data used in our experiments. All information about program versions can be read in the README file.

[1] <https://github.com/cristmelo/PracticalGuide_DynamicApproaches>

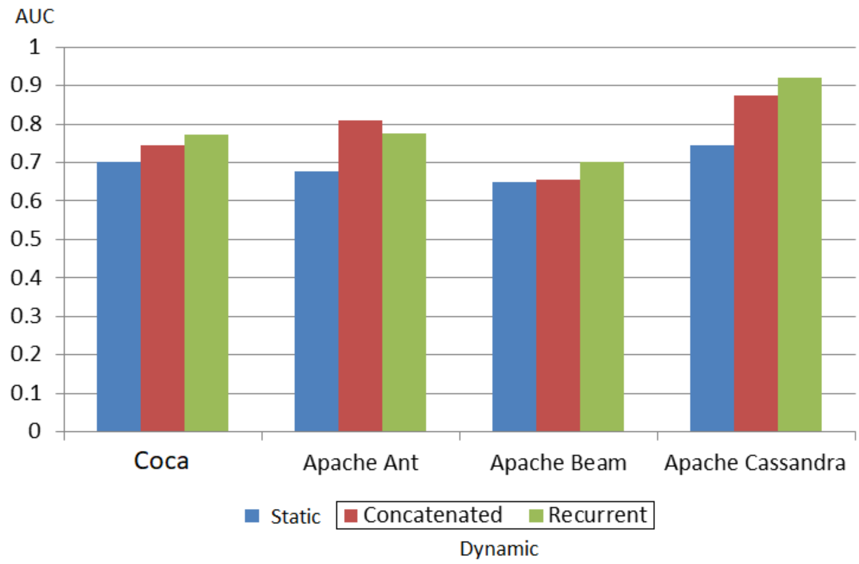
5.2.3 Discussion of Results

One of the goals of this second study case is experimentally to evaluate how time-series approaches tend to improve the performance metrics of predictive models used to solve the change-prone class prediction problem in imbalanced datasets compared to static approach.

Given the results discussed in the last subsection, we have decided to get the best AUC metric obtained from each dataset and compare them according to different approaches. Figure 12 shows the results of this comparison, which x-axis means the AUC and y-axis means the static and dynamic approaches.

For all evaluated datasets, the proposed dynamic approaches outperformed the static approach. Note that, in Apache Cassandra, we had the best performance in the static approach with the AUC 0.7432 using SMOTE resample with MLP while the Recurrent Approach provided the AUC 0.9188, up to 23.6% more effective than the standard approach in literature. Besides this improvement, we highlight the reduction of execution time in this dataset. For the static approach, the execution time was 37 minutes while in the Concatenated we spent nearly 34 minutes, and the Recurrent only took 8 minutes.

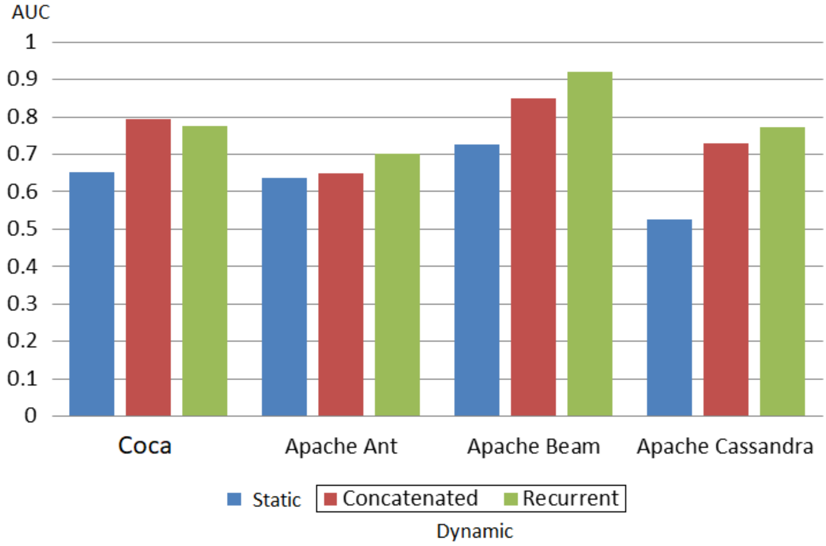
Figure 12 – Comparison of the Best Results between Different Approaches.



Source: Author.

We want to highlight the difference of AUC between the baselines in all approaches, i.e., neither in static nor in Concatenated we perform outlier filtering or resample technique. According to Figure 13, dynamic approaches have the best result over the static approach in all scenarios. In this figure, the x-axis means the AUC and y-axis means the best scenario from each dataset in different approaches. The results in the static approach have been the worst since no treatment was performed. It shows that dynamic approaches, specially Recurrent ones, deal with imbalanced scenarios.

Figure 13 – Baselines Comparison between Different Approaches.



Source: Author.

To conclude this section, Table 14 shows the overview of datasets presented in Related Work; however, we have included our generated datasets and their general information, compared to the other authors.

Table 14 – Overview of the Related Works

Paper	**Dataset**	**Releases**	**Imb. Rate**	**Res. Tech.**	**Stats**	**CV**	**Availab.**
Elish	VSSPLUGIN	13	Unk	No	Yes	Unk	No
	PeerSim	9	Unk	No	Yes	Unk	No
Malhotra	DrJava	2	49%	No	Yes	k-fold	No
	DSpace	2	60%	No	Yes	k-fold	No
	Robocode	2	26%	No	Yes	k-fold	No
Kaur	MOBAC	4	Unk	Yes	No	k-fold	No
Bansal	Rave	2	32.8%	No	Yes	k-fold	No
	Commons Math	2	23.5%	No	Yes	k-fold	No
Catolino	+20	9-44	19%-35%	No	No	k-fold	Yes
Choudhary	OpenClinic	4	75.8%	No	Yes	k-fold	No
	OpenHospital	2	5.9%	No	Yes	k-fold	No
Melo	Coca	8	8.05%	Yes	Yes	k-fold	Yes
	Apache Ant	10	70.1%	Yes	Yes	k-fold	Yes
	Apache Beam	15	22.4%	Yes	Yes	k-fold	Yes
	Apache Cassandra	49	30.3%	Yes	Yes	k-fold	Yes

5.2.4 Threats to Validity

In this section, we have presented a novel dynamic approach in order to have the temporal dependence between the instances from the dataset. However, we identify some threats to validity in this experimental analysis:

1. *Amount of releases*. All datasets described in Table 7 contain a reasonable amount of releases. It allowed us to test different window sizes. When we have decided to use dynamic approaches, it is interesting to check more than one window size to investigate different values.
2. *Dropped releases*. It is necessary to keep in mind that when we have a large window size, all classes that contain less release that window size is dropped. Even that the result can be harshly improved, the large window size can drop a considerable amount of releases, and it can compromise the history of the project.
3. *Amount of datasets*. In our experiment, we have tested our novel approaches in four datasets. We cannot generalize the results of using these four datasets to ensure that time-series is always going to retrieve the best results. Also, we have used only one different dataset besides our generated by Apache repositories. It has happened mainly due to the lack of dataset available, or some dataset did not have enough information about the class to generate the dynamic structures.

6 CONCLUSION AND FUTURE WORKS

In this work, we have provided a practical guideline to support the change-prone class prediction problem in order to standardize a set of steps for generating predictive models. Besides, we highlighted that state-of-art datasets do not have temporal dependence between their instances. Thus, we have proposed two data structures in order to take this dependence into account, called Concatenated and Recurrent. These structures we have called dynamic approaches, and we have investigated if there is some gain in the performance metrics over the state-of-art structure, that we have called the static approach. To validate the proposed guideline and the novel dynamic approaches, we have performed two case studies.

In the first case study, we have performed the guideline over an imbalanced dataset called Control of Merchandise (Coca) following the static approach. Coca has extracted from extensive commercial software, containing 8 static object-oriented metrics proposed by C&K and McCabe. We have run different scenarios in order to compare the gain if performing outlier filtering, feature selection, resampling techniques, and tuning. In our experiments, only feature selection did not improve the Area Under the Curve (AUC), and it can have occurred since the dataset has only 8 independent variables. Despite this, applying the guideline in an imbalanced reached 71% of the AUC, while not applying it reached nearly 50% in most cases.

In the second case study, we wanted to investigate the gain of the AUC using dynamic approaches over the static. For this, firstly, we have collected three Apache datasets (Ant, Beam, and Cassandra), and we have generated their baselines in the static approach, following some steps from the guideline. After that, we have built them in the Concatenated and Recurrent approaches for three different window sizes. Since the Coca dataset had its static baseline computed in the first case study, we needed to build only the dynamic structure in this case. Our experimental results show that dynamic approaches outperform the static one. Moreover, the Recurrent approach had the best AUC, and we highlight that, in this case, it was not necessary to use resampling techniques. As an example, the Cassandra dataset has the AUC 0.74% in the static approach using SMOTE + MLP, while using the Recurrent approach has 0.9188% in the original imbalanced dataset.

As future works, we plan to apply all the steps of the proposed guideline in the dynamic approaches in order to investigate the gain of performance metrics, such as outlier filtering. Besides, in the Recurrent approach, we want to try another recurrent algorithm, such as Long Short-Term Memory (LSTM), in order to check if there is a better result. In addition, we want to investigate the use of a convolutional neural network to generate predictive models with dynamic structures. We also want to investigate other kinds of independent variables different from static OO metrics.

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